



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:34 AM UTC

PDB ID : 4X6D / pdb_00004x6d
Title : CD1a ternary complex with endogenous lipids and BK6 TCR
Authors : Birkinshaw, R.W.; Rossjohn, J.
Deposited on : 2014-12-08
Resolution : 2.98 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

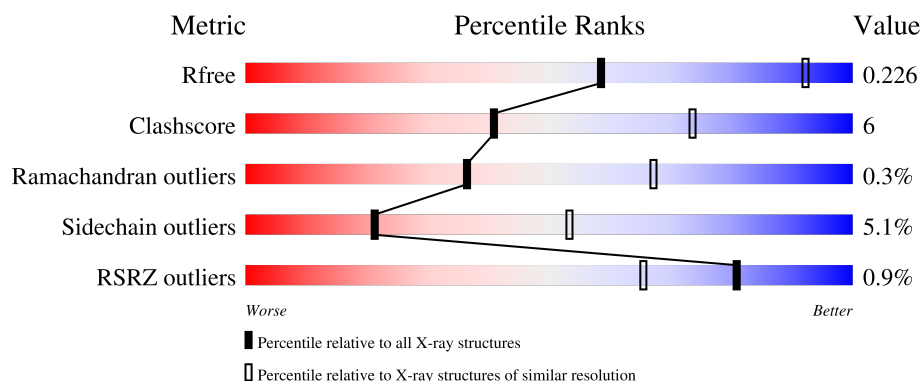
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	275	0% 72% 23% • •
1	C	275	2% 60% 18% • 21%
2	B	99	2% 69% 17% • 13%
2	D	99	59% 19% • 21%
3	E	207	81% 11% 9%

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Mol	Chain	Length	Quality of chain
3	G	207	% 80% 17%
4	F	245	% 82% 16%
4	H	245	86% 12%
5	I	3	33% 67%
5	J	3	33% 33% 33%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12304 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 CD1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2153	1379	375	391	8			
1	C	218	Total	C	N	O	S	0	0	0
			1787	1152	312	318	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ILE	THR	variant	UNP P06126
A	51	TRP	CYS	variant	UNP P06126
C	13	ILE	THR	variant	UNP P06126
C	51	TRP	CYS	variant	UNP P06126

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	86	Total	C	N	O	S	0	0	0
			719	463	119	135	2			
2	D	78	Total	C	N	O	S	0	0	0
			657	427	107	121	2			

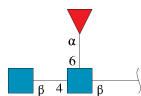
- Molecule 3 is a protein called TCR alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	189	Total	C	N	O	S	0	0	0
			1474	924	238	302	10			
3	G	200	Total	C	N	O	S	0	0	0
			1560	975	253	322	10			

- Molecule 4 is a protein called TCR beta.

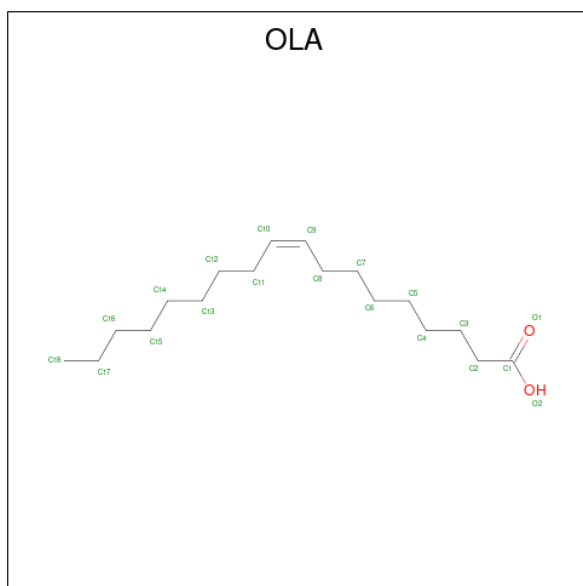
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	241	Total	C	N	O	S	0	0	0
			1917	1216	333	358	10			
4	H	242	Total	C	N	O	S	0	0	0
			1922	1219	334	359	10			

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



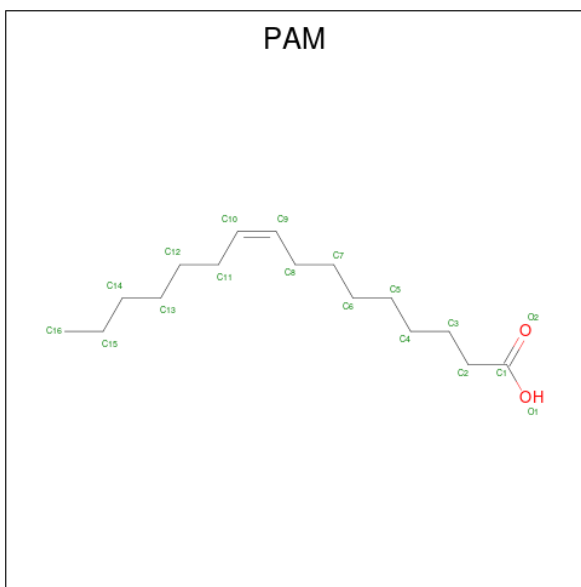
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	3	Total	C	N	O	0	0	0
			38	22	2	14			
5	J	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 6 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			20	18	2		

- Molecule 7 is PALMITOLEIC ACID (CCD ID: PAM) (formula: $C_{16}H_{30}O_2$).

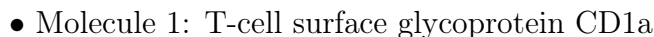


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			18	16	2		

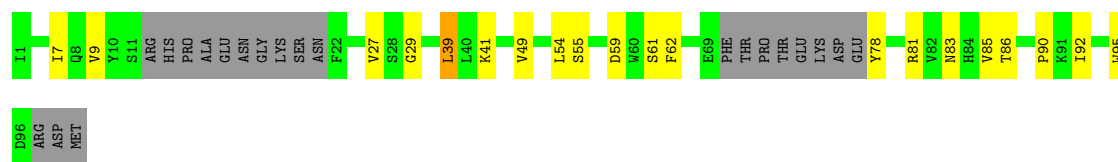
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	1	Total	O	0	0
			1	1		

- Molecule 1: T-cell surface glycoprotein CD1a

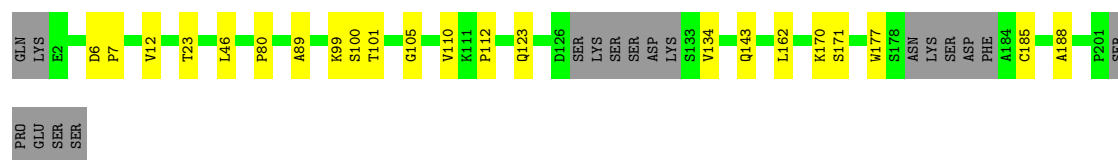


Chain D:  59% 19% 21%



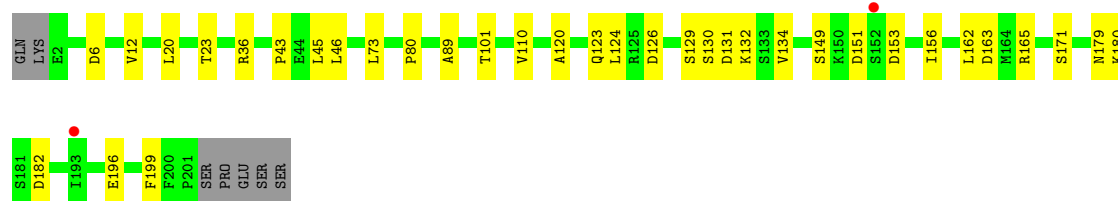
• Molecule 3: TCR alpha

Chain E:  81% 11% 9%



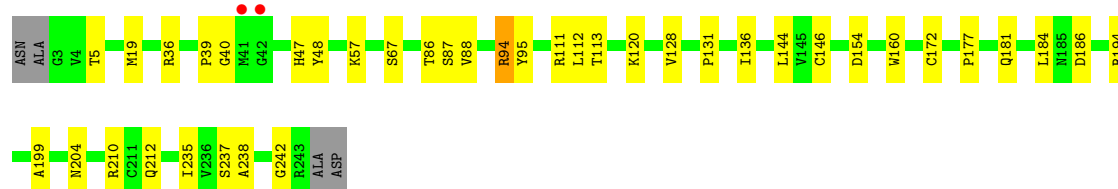
• Molecule 3: TCR alpha

Chain G:  80% 17%



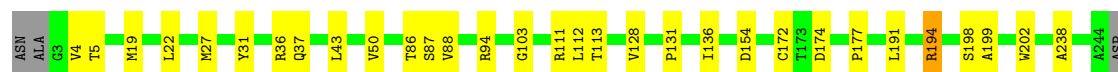
• Molecule 4: TCR beta

Chain F:  82% 16%



• Molecule 4: TCR beta

Chain H:  86% 12%



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 67%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 33% 33% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.13Å 126.32Å 226.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.98 48.00 – 2.98	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.00-2.98) 99.9 (48.00-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.96Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, R_{free}	0.177 , 0.229 0.181 , 0.226	Depositor DCC
R_{free} test set	2663 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	77.8	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 85.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12304	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: PAM, FUC, OLA, NAG

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	0.48	0/2221	0.88	5/3021 (0.2%)
1	C	0.40	0/1844	0.80	0/2503
2	B	0.40	0/741	0.75	0/1005
2	D	0.41	0/674	0.74	0/911
3	E	0.53	0/1507	0.89	2/2045 (0.1%)
3	G	0.55	0/1596	0.88	0/2165
4	F	0.53	0/1970	0.86	2/2678 (0.1%)
4	H	0.55	0/1975	0.88	0/2685
All	All	0.50	0/12528	0.85	9/17013 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	GLY	N-CA-C	6.21	122.56	111.02
4	F	181	GLN	CA-C-N	5.86	125.54	119.56
4	F	181	GLN	C-N-CA	5.86	125.54	119.56
1	A	33	SER	CB-CA-C	-5.66	109.53	117.23
3	E	188	ALA	N-CA-C	5.55	117.14	111.14
3	E	105	GLY	N-CA-C	5.43	119.71	112.65
1	A	128	ASN	CB-CA-C	-5.19	110.17	117.23
1	A	88	LEU	N-CA-C	-5.18	103.55	110.55
1	A	55	ARG	N-CA-C	5.15	118.72	112.23

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	2153	0	2038	52	0
1	C	1787	0	1693	25	0
2	B	719	0	683	10	0
2	D	657	0	636	8	0
3	E	1474	0	1383	8	0
3	G	1560	0	1467	18	0
4	F	1917	0	1840	21	0
4	H	1922	0	1845	20	0
5	I	38	0	34	4	0
5	J	38	0	31	2	0
6	A	20	0	33	0	0
7	C	18	0	29	3	0
8	H	1	0	0	0	0
All	All	12304	0	11712	156	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 6.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TYR:HD1	1:A:87:GLU:OE2	1.41	1.02
1:A:84:TYR:CD1	1:A:87:GLU:OE2	2.18	0.96
1:C:168:ARG:HD2	5:J:1:NAG:C8	2.06	0.84
1:A:51:TRP:O	1:A:54:SER:HB2	1.79	0.83
3:G:149:SER:HB2	3:G:156:ILE:HD12	1.60	0.83
1:A:84:TYR:HA	1:A:87:GLU:OE2	1.81	0.81
1:A:90:PHE:HD1	1:A:90:PHE:H	1.33	0.76
3:G:45:LEU:HD22	4:H:103:GLY:HA3	1.67	0.76
1:C:92:TYR:HB2	1:C:93:PRO:HD3	1.71	0.73
3:G:151:ASP:OD2	3:G:180:LYS:NZ	2.22	0.72
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.74	0.69
4:F:86:THR:HG23	4:F:113:THR:HA	1.77	0.67
4:F:120:LYS:NZ	4:F:186:ASP:OD2	2.29	0.65
4:F:19:MET:HE1	4:F:112:LEU:HD22	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:29:GLY:HA2	2:D:61:SER:HB3	1.80	0.64
1:A:89:GLN:HA	1:A:89:GLN:OE1	1.97	0.63
4:H:86:THR:HG23	4:H:113:THR:HA	1.80	0.63
1:A:53:TRP:H	1:A:53:TRP:CD1	2.17	0.62
1:A:219:MET:HG2	1:A:226:GLU:HG3	1.82	0.62
1:A:81:ILE:O	1:A:85:ALA:N	2.34	0.61
1:A:94:PHE:HD2	1:A:118:TYR:HE1	1.47	0.60
3:G:163:ASP:OD2	3:G:165:ARG:NH1	2.35	0.60
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.84	0.60
1:A:37:THR:O	1:A:54:SER:OG	2.21	0.57
1:C:84:TYR:HD1	1:C:87:GLU:HG3	1.69	0.57
1:A:217:TRP:HB3	1:A:264:LYS:HB2	1.85	0.57
1:C:24:LYS:HE3	1:C:82:ARG:HE	1.69	0.57
1:A:84:TYR:CD1	1:A:87:GLU:CD	2.82	0.57
2:D:54:LEU:HD11	2:D:62:PHE:HB3	1.87	0.56
1:A:217:TRP:HZ3	1:A:262:ARG:HG2	1.71	0.56
4:H:31:TYR:CE1	4:H:50:VAL:HG12	2.41	0.55
4:H:19:MET:HE1	4:H:112:LEU:HD22	1.89	0.54
3:E:134:VAL:HG22	3:E:177:TRP:HB3	1.89	0.54
1:A:237:PRO:HG2	2:B:65:LEU:HD13	1.89	0.54
1:A:90:PHE:CD2	1:A:94:PHE:HE2	2.26	0.54
1:A:237:PRO:O	2:B:10:TYR:OH	2.25	0.54
4:F:94:ARG:HD2	4:F:95:TYR:O	2.08	0.53
1:C:114:LEU:HB3	1:C:126:PHE:HB3	1.90	0.53
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.44	0.53
3:G:36:ARG:HB2	3:G:46:LEU:HD22	1.92	0.52
3:E:112:PRO:HB2	3:E:170:LYS:HD3	1.91	0.52
3:G:196:GLU:N	3:G:196:GLU:OE1	2.41	0.52
1:A:53:TRP:CE3	1:A:177:GLY:HA3	2.45	0.52
3:E:80:PRO:HA	3:E:110:VAL:HB	1.92	0.52
1:A:14:TRP:HB2	1:A:98:VAL:HB	1.92	0.52
1:C:168:ARG:CD	5:J:1:NAG:C8	2.78	0.51
5:I:1:NAG:O3	5:I:2:NAG:O6	2.26	0.51
1:A:90:PHE:CD1	1:A:90:PHE:N	2.72	0.51
4:F:210:ARG:NH1	4:F:212:GLN:HB2	2.25	0.51
4:H:111:ARG:NH2	4:H:154:ASP:OD2	2.44	0.50
1:A:37:THR:HG22	1:A:51:TRP:HD1	1.77	0.50
1:A:184:GLN:HB3	1:A:267:SER:HB3	1.92	0.50
3:G:129:SER:C	3:G:131:ASP:H	2.19	0.50
1:C:169:PHE:CD2	7:C:304:PAM:H10	2.47	0.50
2:D:83:ASN:HD22	2:D:90:PRO:HG3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PHE:HD2	1:A:94:PHE:HE2	1.60	0.49
4:F:204:ASN:O	4:F:242:GLY:HA3	2.12	0.49
1:C:55:ARG:NH2	1:C:60:ASN:OD1	2.44	0.49
1:A:89:GLN:O	1:A:90:PHE:C	2.54	0.49
4:F:87:SER:OG	4:F:88:VAL:N	2.46	0.49
4:H:36:ARG:HH21	4:H:87:SER:HB2	1.77	0.49
1:A:90:PHE:CD2	1:A:94:PHE:CE2	3.01	0.48
4:H:37:GLN:HB2	4:H:43:LEU:HD23	1.95	0.48
4:H:154:ASP:OD1	4:H:177:PRO:HG3	2.13	0.48
1:A:125:SER:HB2	1:A:134:TYR:CE1	2.49	0.48
4:H:128:VAL:HG23	4:H:238:ALA:HB3	1.96	0.47
3:E:6:ASP:OD1	3:E:7:PRO:HD2	2.14	0.47
4:F:212:GLN:HG3	4:F:235:ILE:HG23	1.96	0.47
1:A:90:PHE:HD1	1:A:90:PHE:N	2.03	0.47
4:F:39:PRO:HA	4:F:40:GLY:HA2	1.58	0.47
4:H:87:SER:OG	4:H:88:VAL:N	2.47	0.47
1:C:17:SER:HA	1:C:95:GLU:HG2	1.95	0.47
3:G:162:LEU:HB3	4:H:172:CYS:HB2	1.97	0.46
4:H:31:TYR:HE1	4:H:50:VAL:HG12	1.80	0.46
2:B:51:HIS:HB3	2:B:66:TYR:CE2	2.50	0.46
3:E:162:LEU:HB3	4:F:172:CYS:HB2	1.98	0.46
4:F:154:ASP:OD1	4:F:177:PRO:HG3	2.15	0.46
1:A:58:PHE:HE2	1:A:66:LEU:HD11	1.81	0.46
1:C:53:TRP:HB2	1:C:176:ALA:HB1	1.98	0.46
1:C:191:LEU:HA	1:C:206:CYS:N	2.31	0.46
1:C:14:TRP:CH2	7:C:304:PAM:H22	2.51	0.46
1:C:31:TRP:CZ2	2:D:55:SER:HB2	2.50	0.46
1:C:11:HIS:HB2	1:C:99:THR:HG22	1.98	0.46
2:D:39:LEU:HB2	2:D:49:VAL:HG21	1.97	0.45
1:A:90:PHE:HD2	1:A:94:PHE:CE2	2.35	0.45
3:G:126:ASP:HB2	3:G:132:LYS:HB2	1.98	0.45
1:A:26:ASN:HB2	1:A:78:PHE:CE2	2.52	0.45
1:A:58:PHE:N	1:A:58:PHE:CD1	2.82	0.45
3:G:123:GLN:C	3:G:124:LEU:HD12	2.41	0.45
1:A:264:LYS:NZ	1:A:272:ASP:OD2	2.45	0.45
4:H:131:PRO:HD2	4:H:202:TRP:CZ2	2.51	0.45
1:C:91:GLU:OE2	1:C:118:TYR:OH	2.34	0.45
1:A:58:PHE:CE2	1:A:66:LEU:HD11	2.52	0.45
3:E:123:GLN:HG3	3:E:185:CYS:SG	2.57	0.45
1:A:263:VAL:HB	1:A:273:ILE:HB	1.99	0.45
1:A:265:HIS:CE1	1:A:267:SER:HG	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ASN:HB3	1:C:129:ASN:H	1.62	0.45
2:B:17:ASN:OD1	2:B:73:THR:HA	2.17	0.44
1:C:166:CYS:HB3	1:C:167:PRO:HD3	1.98	0.44
7:C:304:PAM:H111	7:C:304:PAM:H81	1.72	0.44
1:A:166:CYS:HB3	1:A:167:PRO:HD3	1.99	0.44
4:H:174:ASP:HB2	4:H:191:LEU:HD12	1.99	0.44
4:H:194:ARG:N	4:H:194:ARG:HD3	2.32	0.44
4:F:184:LEU:HB3	3:G:153:ASP:OD2	2.18	0.44
4:F:131:PRO:HD3	4:F:144:LEU:HG	2.00	0.44
2:B:11:SER:HB2	2:B:21:ASN:HD21	1.82	0.44
1:C:191:LEU:N	1:C:207:HIS:HD2	2.16	0.44
3:G:120:ALA:HB2	3:G:199:PHE:HB3	1.99	0.44
1:A:174:LEU:HD13	1:A:174:LEU:HA	1.80	0.43
4:F:36:ARG:HH21	4:F:87:SER:HB2	1.83	0.43
3:G:43:PRO:HG2	4:H:43:LEU:HD11	1.99	0.43
1:A:128:ASN:HB3	1:A:129:ASN:H	1.46	0.43
1:C:104:LEU:HD12	1:C:109:VAL:HA	1.99	0.43
4:H:136:ILE:HG23	4:H:199:ALA:HB1	2.00	0.43
1:C:130:SER:HB2	1:C:149:ASN:ND2	2.34	0.43
4:H:4:VAL:HG23	4:H:27:MET:CE	2.49	0.43
1:A:36:GLN:OE1	2:B:53:ASP:HB2	2.18	0.43
1:C:13:ILE:HG22	1:C:99:THR:HG23	2.00	0.43
1:A:181:LEU:H	1:A:181:LEU:HG	1.46	0.43
1:A:189:ALA:HA	1:A:207:HIS:O	2.19	0.42
2:D:41:LYS:HD3	2:D:78:TYR:OH	2.18	0.42
1:A:214:LYS:HD2	1:A:243:TRP:CE2	2.54	0.42
1:C:40:TRP:CG	1:C:41:ASP:N	2.87	0.42
1:A:77:SER:O	1:A:81:ILE:HG13	2.19	0.42
4:F:128:VAL:HG23	4:F:238:ALA:HB3	2.00	0.42
3:G:20:LEU:HD12	3:G:73:LEU:HD23	2.01	0.42
3:G:129:SER:O	3:G:131:ASP:N	2.53	0.42
5:I:1:NAG:HO3	5:I:2:NAG:HO6	1.57	0.42
1:A:49:PHE:HD1	1:A:54:SER:HB3	1.85	0.42
3:G:89:ALA:HA	3:G:101:THR:O	2.20	0.42
1:A:31:TRP:CZ2	2:B:55:SER:HB2	2.55	0.41
4:H:37:GLN:HB2	4:H:43:LEU:CD2	2.50	0.41
1:C:66:LEU:HD23	1:C:66:LEU:HA	1.77	0.41
2:D:59:ASP:OD1	2:D:59:ASP:N	2.43	0.41
1:A:108:LYS:HE2	1:A:108:LYS:HB3	1.91	0.41
1:C:14:TRP:HB2	1:C:98:VAL:HB	2.02	0.41
1:C:132:LEU:HD13	1:C:132:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:1:NAG:O3	5:I:2:NAG:O5	2.38	0.41
1:A:151:ASN:ND2	1:A:154:GLU:HG2	2.35	0.41
3:G:80:PRO:HA	3:G:110:VAL:HB	2.03	0.41
4:F:111:ARG:NH2	4:F:154:ASP:HB3	2.36	0.41
1:A:51:TRP:HB3	1:A:53:TRP:NE1	2.36	0.41
5:I:1:NAG:O4	5:I:2:NAG:H83	2.19	0.41
4:F:136:ILE:HG23	4:F:199:ALA:HB1	2.03	0.41
4:F:146:CYS:HB2	4:F:160:TRP:CZ2	2.56	0.41
2:D:81:ARG:HG3	2:D:92:ILE:HG13	2.04	0.40
4:F:47:HIS:HD2	4:F:57:LYS:HA	1.86	0.40
4:H:19:MET:HB3	4:H:19:MET:HE2	1.68	0.40
1:A:26:ASN:HB2	1:A:78:PHE:HE2	1.85	0.40
1:A:45:SER:HB3	1:A:71:ARG:HD3	2.02	0.40
1:A:94:PHE:CD2	1:A:118:TYR:HE1	2.35	0.40
3:E:99:LYS:HE3	4:F:48:TYR:CE1	2.57	0.40
2:B:58:LYS:HB3	2:B:58:LYS:HE2	1.90	0.40
3:E:89:ALA:HA	3:E:101:THR:O	2.22	0.40
4:F:19:MET:HE2	4:F:19:MET:HB3	1.76	0.40
3:G:126:ASP:HB3	3:G:129:SER:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	263/275 (96%)	244 (93%)	17 (6%)	2 (1%)	16	47
1	C	208/275 (76%)	184 (88%)	23 (11%)	1 (0%)	24	58
2	B	82/99 (83%)	77 (94%)	5 (6%)	0	100	100
2	D	72/99 (73%)	68 (94%)	4 (6%)	0	100	100
3	E	183/207 (88%)	179 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	198/207 (96%)	192 (97%)	5 (2%)	1 (0%)	24	58
4	F	239/245 (98%)	232 (97%)	7 (3%)	0	100	100
4	H	240/245 (98%)	232 (97%)	8 (3%)	0	100	100
All	All	1485/1652 (90%)	1408 (95%)	73 (5%)	4 (0%)	36	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	PHE
1	A	90	PHE
3	G	130	SER
1	C	41	ASP

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	231/240 (96%)	213 (92%)	18 (8%)	11	37
1	C	195/240 (81%)	179 (92%)	16 (8%)	10	35
2	B	82/94 (87%)	77 (94%)	5 (6%)	17	47
2	D	75/94 (80%)	68 (91%)	7 (9%)	8	30
3	E	169/187 (90%)	163 (96%)	6 (4%)	31	63
3	G	180/187 (96%)	173 (96%)	7 (4%)	28	60
4	F	207/209 (99%)	202 (98%)	5 (2%)	43	72
4	H	207/209 (99%)	202 (98%)	5 (2%)	43	72
All	All	1346/1460 (92%)	1277 (95%)	69 (5%)	21	53

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	39	THR

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Mol	Chain	Res	Type
1	A	42	SER
1	A	54	SER
1	A	59	SER
1	A	73	ARG
1	A	83	ARG
1	A	90	PHE
1	A	91	GLU
1	A	94	PHE
1	A	121	SER
1	A	136	VAL
1	A	170	ILE
1	A	174	LEU
1	A	181	LEU
1	A	183	ARG
1	A	235	ILE
1	A	269	GLU
2	B	3	ARG
2	B	70	PHE
2	B	76	ASP
2	B	77	GLU
2	B	92	ILE
1	C	19	TYR
1	C	22	SER
1	C	23	TRP
1	C	27	LEU
1	C	45	SER
1	C	48	VAL
1	C	73	ARG
1	C	75	ILE
1	C	87	GLU
1	C	89	GLN
1	C	99	THR
1	C	102	CYS
1	C	106	SER
1	C	182	GLN
1	C	218	VAL
1	C	235	ILE
2	D	7	ILE
2	D	9	VAL
2	D	27	VAL
2	D	39	LEU
2	D	85	VAL

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Mol	Chain	Res	Type
2	D	86	THR
2	D	95	TRP
3	E	12	VAL
3	E	23	THR
3	E	46	LEU
3	E	100	SER
3	E	143	GLN
3	E	171	SER
4	F	5	THR
4	F	67	SER
4	F	94	ARG
4	F	194	ARG
4	F	237	SER
3	G	6	ASP
3	G	12	VAL
3	G	23	THR
3	G	134	VAL
3	G	171	SER
3	G	179	ASN
3	G	182	ASP
4	H	5	THR
4	H	22	LEU
4	H	94	ARG
4	H	194	ARG
4	H	198	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
2	B	2	GLN
1	C	105	HIS
1	C	153	HIS
2	D	42	ASN
3	E	21	ASN
3	E	79	GLN
4	F	17	GLN
4	F	176	GLN
4	H	17	GLN
4	H	73	ASN

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$
5	NAG	I	1	5,1	14,14,15	1.23	1 (7%)	17,19,21	2.35	6 (35%)
5	NAG	I	2	5	14,14,15	0.62	0	17,19,21	1.15	1 (5%)
5	FUC	I	3	5	10,10,11	0.46	0	14,14,16	1.72	2 (14%)
5	NAG	J	1	5,1	14,14,15	1.09	1 (7%)	17,19,21	1.27	1 (5%)
5	NAG	J	2	5	14,14,15	0.36	0	17,19,21	0.36	0
5	FUC	J	3	5	10,10,11	0.41	0	14,14,16	1.25	2 (14%)

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
5	NAG	I	1	5,1	-	5/6/23/26	0/1/1/1
5	NAG	I	2	5	-	4/6/23/26	0/1/1/1
5	FUC	I	3	5	-	-	0/1/1/1
5	NAG	J	1	5,1	-	6/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	FUC	J	3	5	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	1	NAG	C1-C2	3.72	1.57	1.52
5	I	1	NAG	C1-C2	3.52	1.57	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	NAG	C1-O5-C5	6.70	121.17	112.19
5	I	3	FUC	C1-C2-C3	4.30	115.91	109.64
5	I	1	NAG	C4-C3-C2	4.13	117.07	111.02
5	I	1	NAG	C6-C5-C4	-3.08	105.45	113.02
5	J	1	NAG	C4-C3-C2	2.79	115.11	111.02
5	I	1	NAG	O5-C5-C6	-2.77	102.27	107.66
5	J	3	FUC	C1-C2-C3	2.75	113.65	109.64
5	I	3	FUC	O5-C5-C4	2.61	114.25	109.55
5	I	1	NAG	O6-C6-C5	-2.44	103.03	111.33
5	I	2	NAG	O5-C1-C2	-2.43	107.54	111.29
5	J	3	FUC	O5-C5-C4	-2.37	105.28	109.55
5	I	1	NAG	O3-C3-C4	-2.04	105.56	110.38

There are no chirality outliers.

All (17) torsion outliers are listed below:

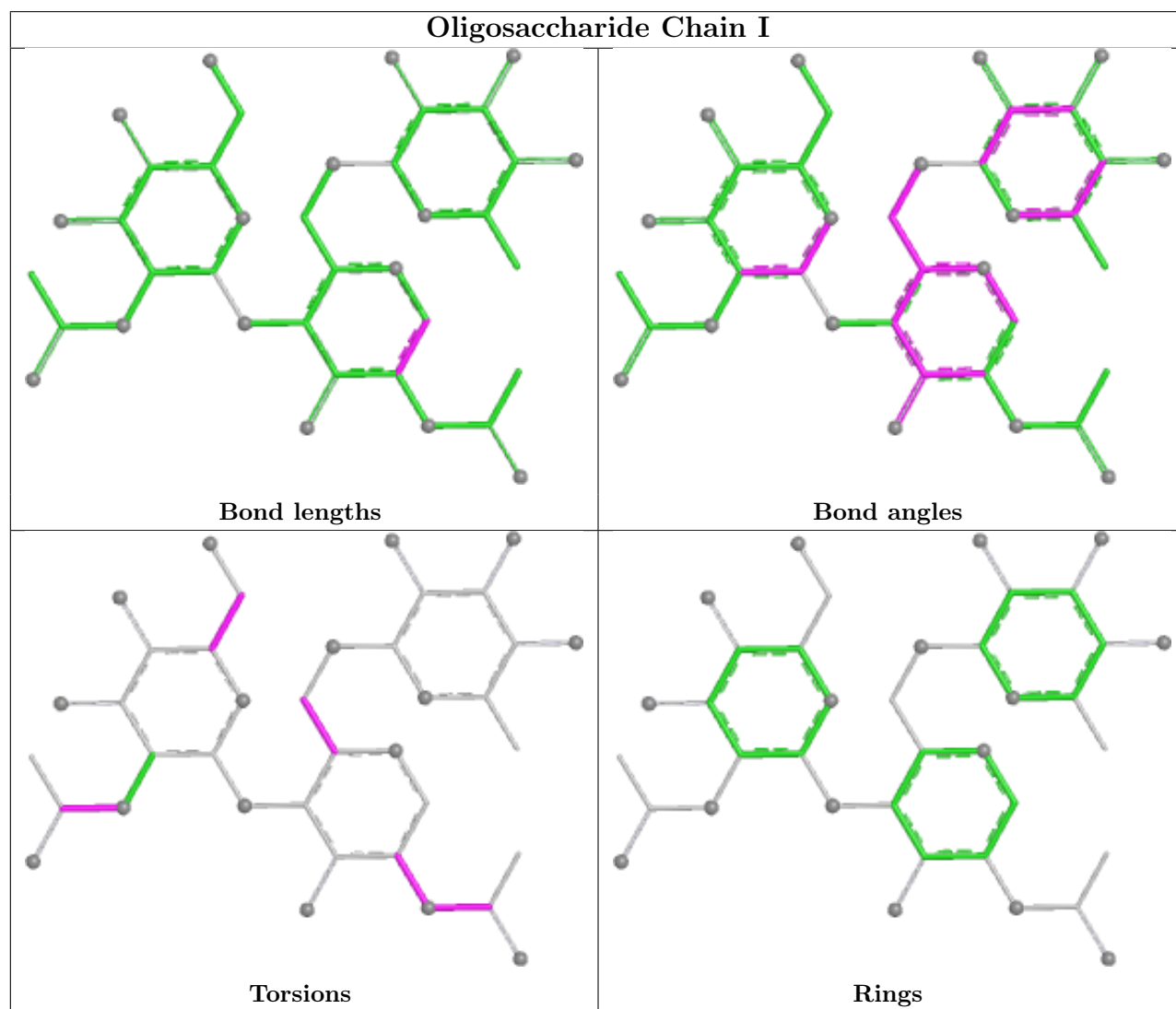
Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C1-C2-N2-C7
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
5	J	1	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	J	1	NAG	C3-C2-N2-C7
5	J	1	NAG	C1-C2-N2-C7

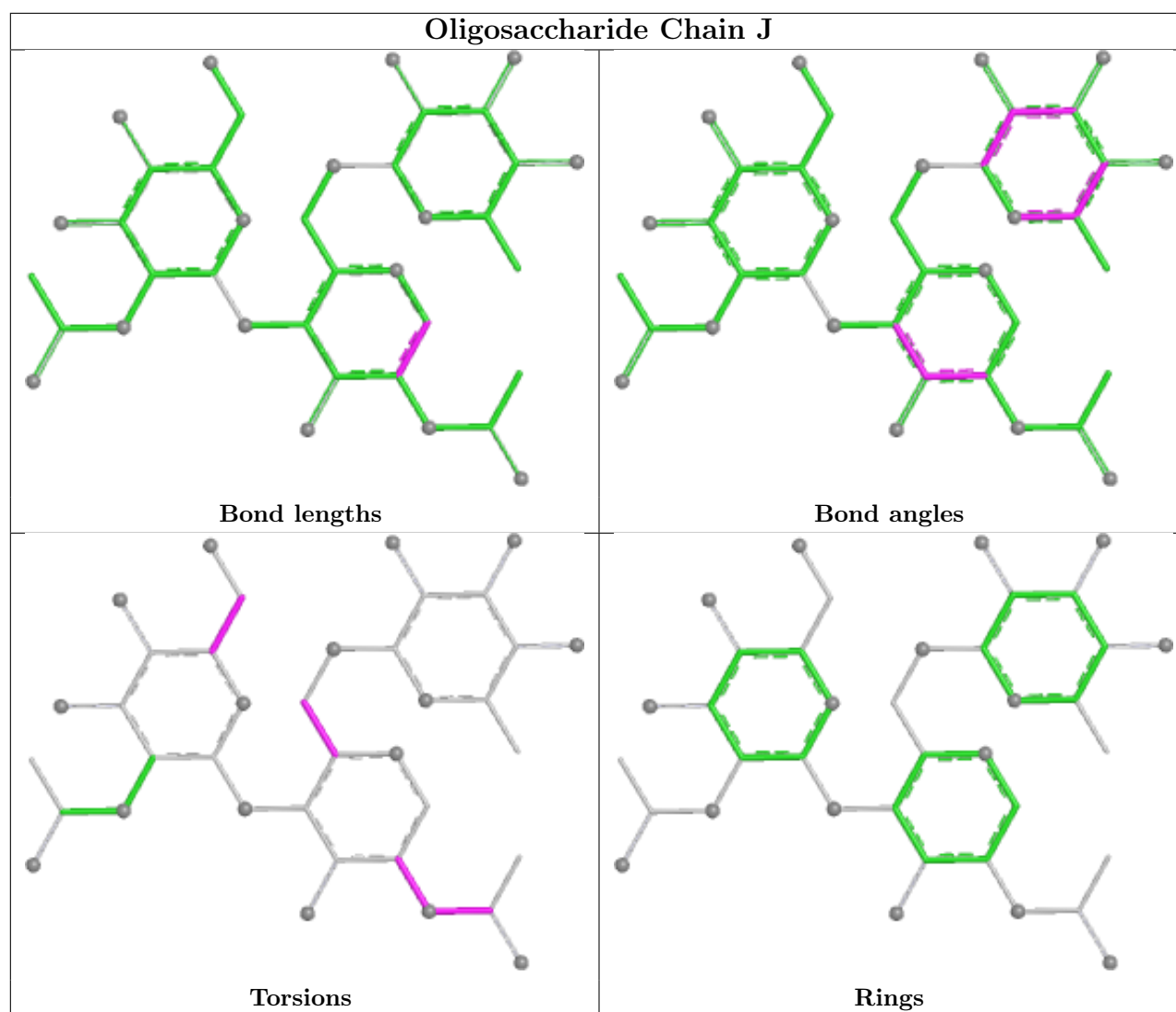
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	1	NAG	2	0
5	I	2	NAG	4	0
5	I	1	NAG	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 oligosaccharide.





5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
6	OLA	A	304	-	19,19,19	0.82	1 (5%)	19,19,19	0.89	1 (5%)
7	PAM	C	304	-	17,17,17	0.86	1 (5%)	17,17,17	1.02	1 (5%)

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
6	OLA	A	304	-	-	11/17/17/17	-
7	PAM	C	304	-	-	6/15/15/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	304	PAM	C10-C9	2.81	1.47	1.31
6	A	304	OLA	C10-C9	2.76	1.47	1.31

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	304	PAM	C3-C2-C1	-2.07	109.11	114.51
6	A	304	OLA	O2-C1-C2	2.02	120.38	114.00

There are no chirality outliers.

All (17) torsion outliers are listed below:

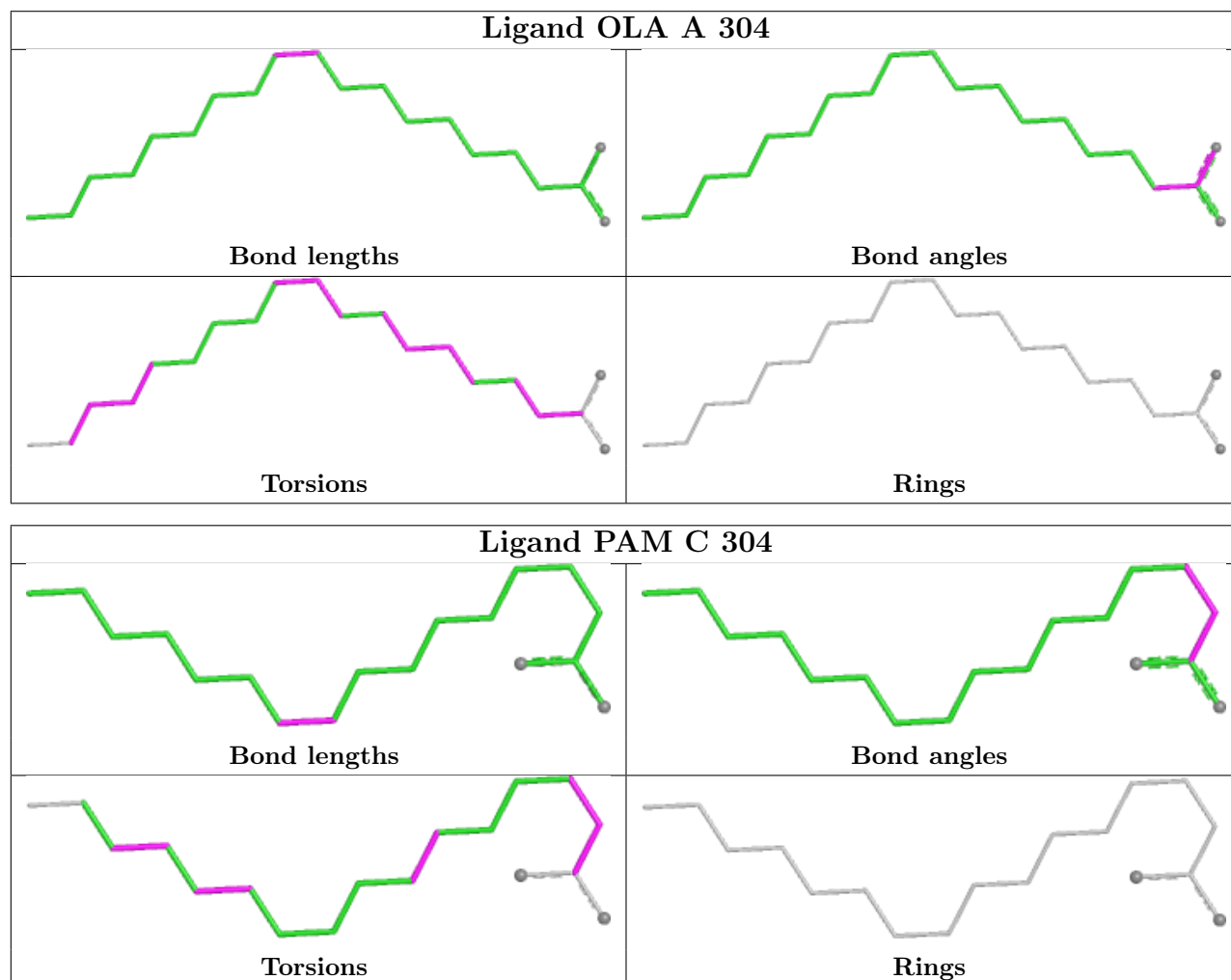
Mol	Chain	Res	Type	Atoms
6	A	304	OLA	C1-C2-C3-C4
7	C	304	PAM	C1-C2-C3-C4
6	A	304	OLA	C11-C10-C9-C8
6	A	304	OLA	C5-C6-C7-C8
6	A	304	OLA	C14-C15-C16-C17
6	A	304	OLA	C3-C4-C5-C6
6	A	304	OLA	C4-C5-C6-C7
7	C	304	PAM	C5-C6-C7-C8
6	A	304	OLA	C13-C14-C15-C16
7	C	304	PAM	C10-C11-C12-C13
6	A	304	OLA	O1-C1-C2-C3
6	A	304	OLA	O2-C1-C2-C3
7	C	304	PAM	O2-C1-C2-C3
7	C	304	PAM	C12-C13-C14-C15
7	C	304	PAM	O1-C1-C2-C3
6	A	304	OLA	C7-C8-C9-C10
6	A	304	OLA	C15-C16-C17-C18

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	304	PAM	3	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	267/275 (97%)	-0.27	3 (1%) 78 61	57, 100, 152, 204	0
1	C	218/275 (79%)	-0.02	5 (2%) 61 42	57, 121, 186, 222	0
2	B	86/99 (86%)	-0.03	2 (2%) 61 42	86, 136, 178, 200	0
2	D	78/99 (78%)	0.16	0 100 100	87, 140, 177, 198	0
3	E	189/207 (91%)	-0.45	0 100 100	43, 73, 137, 178	0
3	G	200/207 (96%)	-0.42	2 (1%) 79 63	46, 75, 141, 176	0
4	F	241/245 (98%)	-0.52	2 (0%) 82 67	44, 76, 123, 150	0
4	H	242/245 (98%)	-0.58	0 100 100	42, 74, 120, 154	0
All	All	1521/1652 (92%)	-0.33	14 (0%) 81 65	42, 91, 161, 222	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	267	SER	4.1
2	B	95	TRP	3.8
1	C	7	PRO	3.1
1	C	248	THR	3.0
1	C	244	TYR	2.6
1	A	129	ASN	2.6
1	C	268	LEU	2.4
1	A	56	GLY	2.4
1	A	278	GLU	2.4
3	G	193	ILE	2.2
3	G	152	SER	2.2
4	F	41	MET	2.2
2	B	79	ALA	2.1
4	F	42	GLY	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](#)

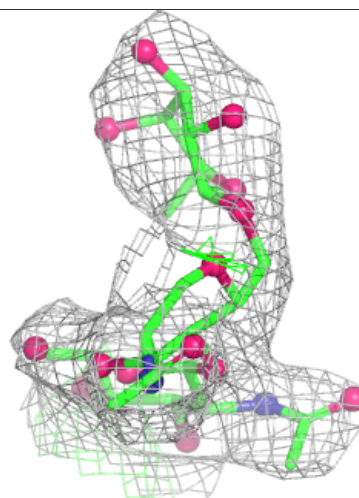
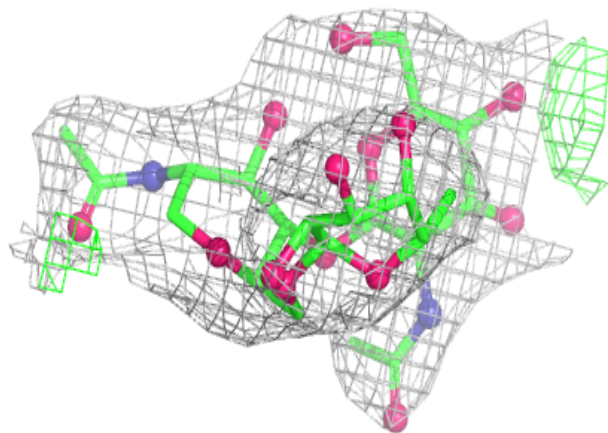
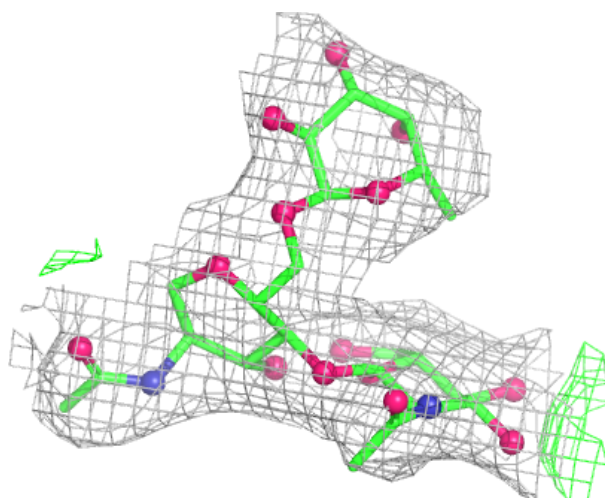
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

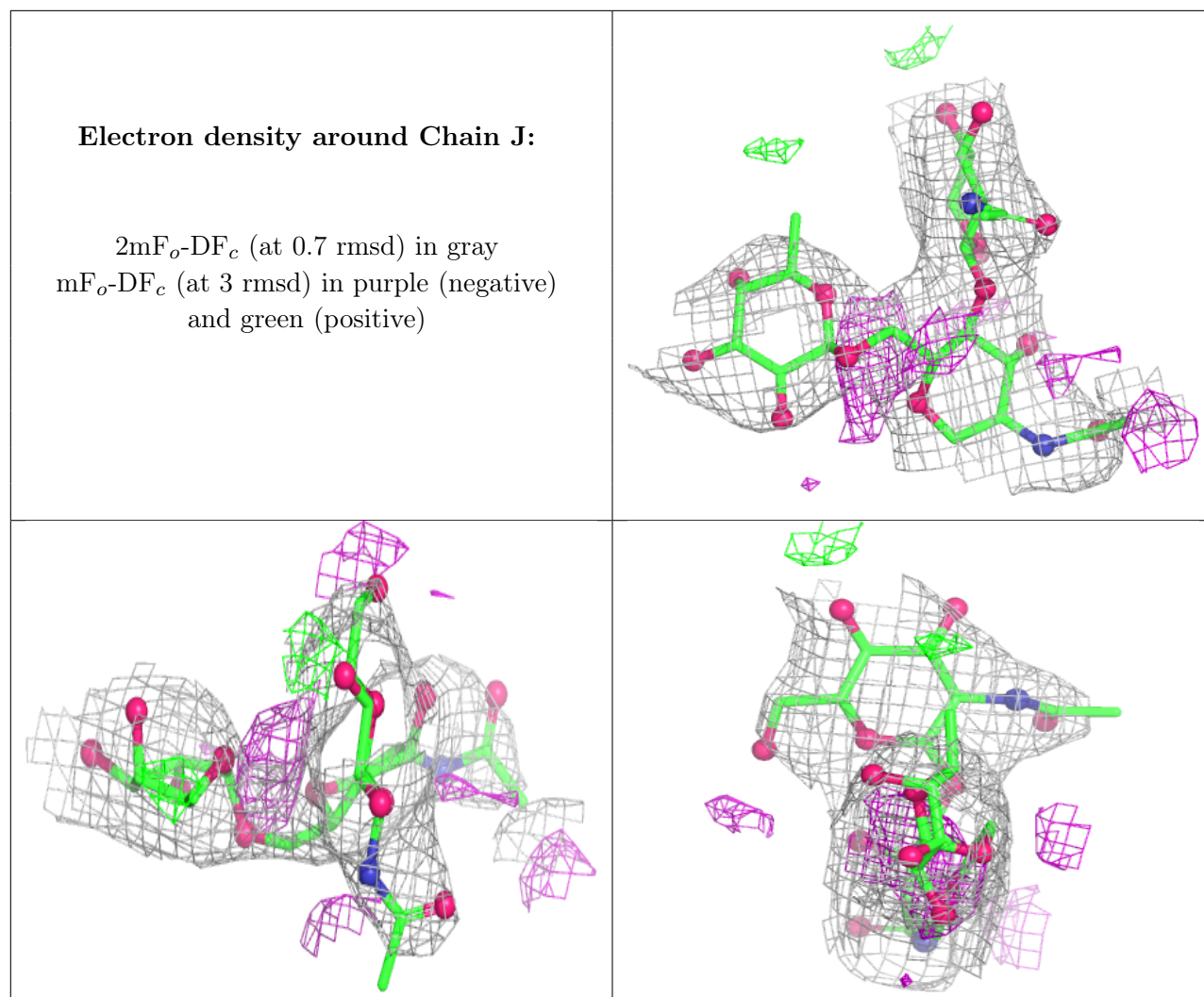
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FUC	J	3	10/11	0.58	0.14	118,142,149,153	0
5	NAG	I	2	14/15	0.73	0.12	121,129,135,135	0
5	FUC	I	3	10/11	0.75	0.11	134,143,160,165	0
5	NAG	J	2	14/15	0.80	0.12	125,129,137,140	0
5	NAG	J	1	14/15	0.87	0.10	104,125,140,141	0
5	NAG	I	1	14/15	0.91	0.08	96,107,124,133	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)





6.4 Ligands [i](#)

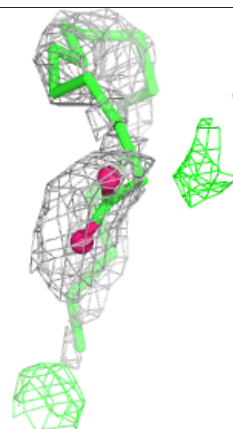
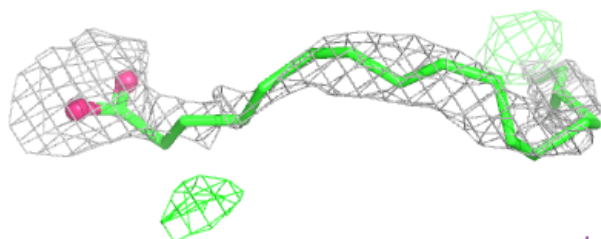
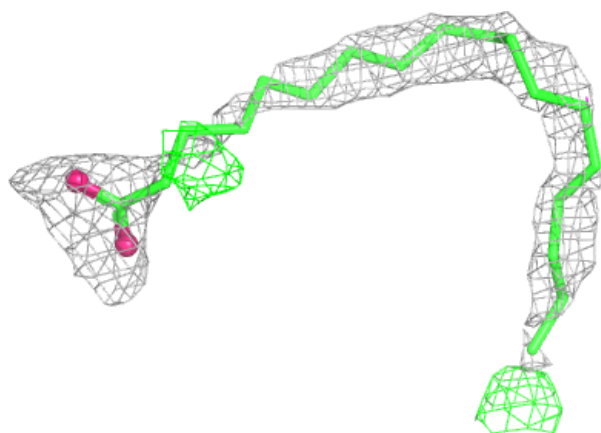
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	OLA	A	304	20/20	0.94	0.19	75,88,133,134	0
7	PAM	C	304	18/18	0.96	0.22	78,90,159,163	0

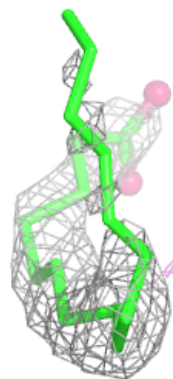
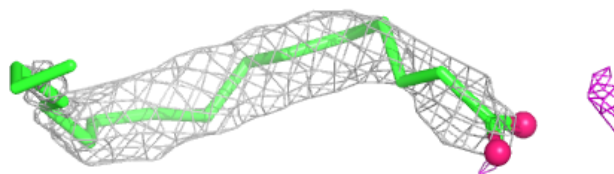
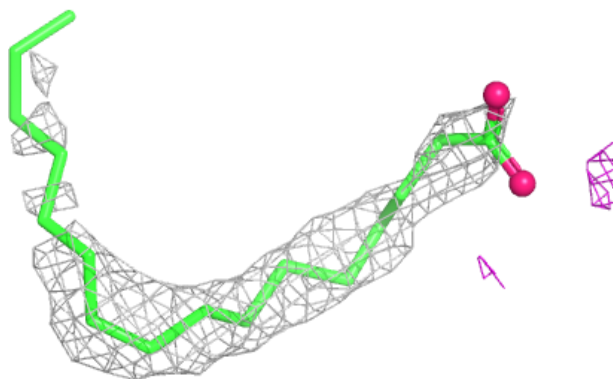
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 304:

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

**Electron density around PAM C 304:**

$2mF_o-DF_c$ (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.