



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:02 AM BST

PDB ID : 6MAM
Title : Cleaved Ebola GP in complex with a broadly neutralizing human antibody, ADI-15946
Authors : West, B.R.; Moyer, C.L.; Fusco, M.L.; Saphire, E.O.
Deposited on : 2018-08-28
Resolution : 4.10 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 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
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

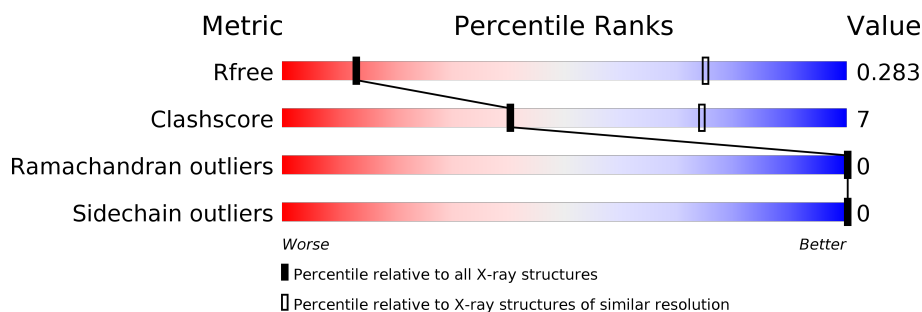
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	242	74% 20% 7%
1	C	242	75% 21% .
1	E	242	74% 23% .
2	B	216	88% 12%
2	D	216	79% 21%
2	F	216	77% 23%
3	G	234	57% 10% 33%

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Mol	Chain	Length	Quality of chain
3	I	234	
3	K	234	
4	H	110	
4	J	110	
4	L	110	
5	M	5	
5	O	5	
6	N	4	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16530 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 ADI-15946 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1706	1083	282	334	7			
1	C	233	Total	C	N	O	S	0	0	0
			1763	1117	290	348	8			
1	E	235	Total	C	N	O	S	0	0	0
			1774	1121	291	354	8			

- Molecule 2 is a protein called ADI-15946 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1668	1045	286	333	4			
2	D	215	Total	C	N	O	S	0	0	0
			1668	1045	286	333	4			
2	F	216	Total	C	N	O	S	0	0	0
			1675	1048	287	335	5			

- Molecule 3 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	157	Total	C	N	O	S	0	0	0
			1199	761	210	223	5			
3	I	156	Total	C	N	O	S	0	0	0
			1190	756	208	221	5			
3	K	156	Total	C	N	O	S	0	0	0
			1190	756	208	221	5			

- Molecule 4 is a protein called Envelope glycoprotein.

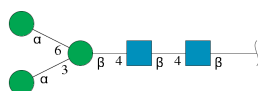
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	108	Total	C	N	O	S	0	0	0
			846	540	147	153	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	109	Total	C	N	O	S	0	0	0
			851	543	148	154	6			
4	L	105	Total	C	N	O	S	0	0	0
			828	530	144	148	6			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	M	5	Total	C	N	O		0	0	0
			61	34	2	25				
5	O	5	Total	C	N	O		0	0	0
			61	34	2	25				

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



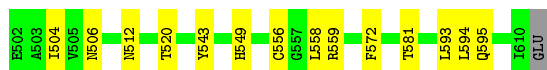
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	N	4	Total	C	N	O		0	0	0
			50	28	2	20				





- Molecule 4: Envelope glycoprotein

Chain J: 86% 13%



- Molecule 4: Envelope glycoprotein

Chain L: 85% 11% 5%



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 40% 60%



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 20% 80%



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

Chain N: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	182.27Å 182.27Å 262.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.54 – 4.10 48.54 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.54-4.10) 99.6 (48.54-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.262 , 0.281 0.268 , 0.283	Depositor DCC
R_{free} test set	1796 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	157.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 78.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	16530	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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: BMA, NAG, 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	0.25	0/1748	0.47	0/2380
1	C	0.25	0/1805	0.47	0/2457
1	E	0.25	0/1815	0.49	0/2470
2	B	0.25	0/1706	0.45	0/2315
2	D	0.24	0/1706	0.44	0/2315
2	F	0.26	0/1713	0.47	0/2323
3	G	0.26	0/1228	0.49	0/1668
3	I	0.25	0/1219	0.47	0/1656
3	K	0.26	0/1219	0.48	0/1656
4	H	0.25	0/866	0.40	0/1179
4	J	0.24	0/871	0.41	0/1186
4	L	0.24	0/847	0.39	0/1152
All	All	0.25	0/16743	0.46	0/22757

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1706	0	1669	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1763	0	1723	31	0
1	E	1774	0	1719	39	0
2	B	1668	0	1622	20	0
2	D	1668	0	1622	32	0
2	F	1675	0	1626	32	0
3	G	1199	0	1177	17	0
3	I	1190	0	1169	16	0
3	K	1190	0	1169	13	0
4	H	846	0	825	13	0
4	J	851	0	830	14	0
4	L	828	0	810	10	0
5	M	61	0	52	0	0
5	O	61	0	52	1	0
6	N	50	0	43	0	0
All	All	16530	0	16108	234	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 7.

All (234) 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)
3:I:38:ILE:HA	3:I:42:THR:O	1.76	0.84
1:E:99:THR:HG21	1:E:118:PHE:HB3	1.60	0.81
1:E:138:SER:O	1:E:160:VAL:HA	1.82	0.78
1:E:65:PRO:O	1:E:69:ARG:NH1	2.21	0.74
4:J:506:ASN:HD22	4:J:556:CYS:HB3	1.52	0.74
1:C:90:THR:HA	1:C:129:VAL:HG11	1.69	0.74
1:E:93:THR:HG23	1:E:128:THR:HA	1.71	0.73
2:F:122:PRO:HD3	2:F:134:VAL:HG22	1.71	0.73
3:G:130:ARG:HH21	3:G:164:ARG:HH21	1.34	0.72
1:E:50:ARG:NH2	1:E:61:ASP:OD2	2.22	0.71
1:A:56:ASP:OD2	1:A:106:ARG:NH2	2.24	0.71
2:D:45:LYS:NZ	2:D:47:LEU:HD21	2.06	0.71
2:D:110:ARG:HH12	2:D:113:ALA:HB2	1.56	0.69
2:B:122:PRO:HD3	2:B:134:VAL:HG22	1.75	0.68
1:A:88:LEU:HD22	1:A:129:VAL:HG21	1.75	0.68
3:I:130:ARG:HH21	3:I:164:ARG:NH1	1.91	0.68
1:A:93:THR:HG22	1:A:129:VAL:H	1.59	0.67
1:E:111:LEU:HD21	3:G:106:GLU:HG3	1.74	0.67
1:A:88:LEU:HD21	1:A:92:ASP:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:TRP:HB2	2:D:48:ILE:HB	1.77	0.66
1:A:40:ALA:HB3	1:A:43:LYS:HB2	1.78	0.66
2:D:47:LEU:HD22	2:D:58:VAL:HG22	1.77	0.65
1:E:40:ALA:HB3	1:E:43:LYS:HB2	1.79	0.65
1:E:33:TRP:HB2	1:E:101:TYR:HB3	1.79	0.65
3:K:130:ARG:HH21	3:K:164:ARG:NH1	1.93	0.65
1:A:53:SER:HA	1:A:74:ARG:NH1	2.12	0.64
1:C:53:SER:HA	1:C:74:ARG:NH1	2.13	0.64
4:J:506:ASN:ND2	4:J:556:CYS:HB3	2.13	0.64
1:C:17:SER:HA	1:C:85:MET:O	1.97	0.64
3:G:103:GLU:OE1	4:H:559:ARG:NH1	2.24	0.64
2:D:122:PRO:HD3	2:D:134:VAL:HG22	1.79	0.63
1:E:101:TYR:CE2	1:E:106:ARG:HD2	2.33	0.63
1:E:17:SER:HA	1:E:85:MET:O	1.99	0.63
1:E:88:LEU:HD22	1:E:129:VAL:HG21	1.81	0.62
2:D:45:LYS:HZ2	2:D:47:LEU:HD21	1.65	0.62
1:A:17:SER:HA	1:A:85:MET:O	2.00	0.62
2:D:212:ASN:HB2	2:D:215:GLU:HB2	1.82	0.62
2:F:90:GLN:HG3	2:F:99:THR:HG23	1.82	0.61
2:D:191:HIS:O	2:D:213:ARG:NH2	2.26	0.61
2:F:35:TRP:HB2	2:F:48:ILE:HB	1.83	0.61
3:K:39:HIS:HB2	3:K:42:THR:HB	1.82	0.60
3:G:38:ILE:HA	3:G:42:THR:O	2.01	0.60
1:A:101:TYR:CE2	1:A:106:ARG:HG2	2.37	0.60
3:I:132:PHE:HE1	3:I:161:LEU:HD23	1.66	0.60
1:E:53:SER:HA	1:E:74:ARG:NH1	2.16	0.59
3:G:37:VAL:O	3:G:43:LEU:HA	2.01	0.59
3:K:51:LEU:HD23	4:L:607:ASP:HA	1.85	0.59
1:C:189:GLN:HA	2:D:162:GLN:HE22	1.67	0.59
2:D:138:LEU:HD21	2:D:198:VAL:HG21	1.82	0.59
1:A:126:LEU:HD12	1:A:167:PRO:HG3	1.84	0.58
2:F:199:THR:HG23	2:F:206:PRO:HG3	1.86	0.58
1:C:161:LYS:HE2	1:C:189:GLN:HE22	1.68	0.58
1:C:33:TRP:HB2	1:C:101:TYR:HB3	1.84	0.58
3:K:50:LYS:O	4:L:595:GLN:NE2	2.37	0.58
1:E:51:ILE:HD13	1:E:60:ILE:HG12	1.84	0.58
1:E:144:PRO:HD3	1:E:156:LEU:HD21	1.86	0.57
2:B:144:ARG:HE	2:B:165:VAL:HG11	1.69	0.57
2:D:188:TYR:O	2:D:194:TYR:OH	2.21	0.57
2:D:110:ARG:HG2	2:D:111:THR:H	1.69	0.57
2:D:34:ASN:HB2	2:D:48:ILE:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:572:PHE:HE2	4:J:581:THR:HG21	1.70	0.56
1:E:236:LEU:HB2	1:E:238:VAL:HG13	1.87	0.56
3:I:71:GLU:OE2	3:I:107:ASN:N	2.39	0.56
2:F:188:TYR:O	2:F:194:TYR:OH	2.23	0.55
1:A:102:THR:O	1:A:106:ARG:HG3	2.07	0.55
4:L:572:PHE:HE2	4:L:581:THR:HG21	1.72	0.55
1:C:40:ALA:HB3	1:C:43:LYS:HB2	1.87	0.54
1:E:142:LEU:HB2	1:E:157:GLY:O	2.07	0.54
2:F:20:THR:HA	2:F:73:LEU:O	2.08	0.54
2:F:169:ASP:OD1	2:F:170:SER:N	2.39	0.54
1:A:53:SER:HA	1:A:74:ARG:HH12	1.73	0.54
2:F:133:SER:HA	2:F:181:LEU:O	2.08	0.53
2:B:95:PRO:HA	2:B:99:THR:HG21	1.89	0.53
3:I:103:GLU:OE1	4:J:559:ARG:NH1	2.28	0.53
2:F:138:LEU:HD21	2:F:198:VAL:HG11	1.90	0.52
3:I:47:ASP:HB3	3:I:50:LYS:HB2	1.91	0.52
1:C:101:TYR:CE1	1:C:116:GLU:HB2	2.44	0.52
1:A:12:VAL:HG13	1:A:129:VAL:HG22	1.92	0.52
2:B:90:GLN:OE1	2:B:92:TYR:N	2.40	0.52
3:I:163:ASP:OD1	4:J:543:TYR:OH	2.23	0.52
1:A:52:LYS:HB2	1:A:58:GLY:HA2	1.91	0.51
1:E:187:VAL:HG21	2:F:162:GLN:HB2	1.93	0.51
1:A:89:LYS:HE3	1:A:91:GLU:HB2	1.92	0.51
2:B:188:TYR:O	2:B:194:TYR:OH	2.27	0.51
2:B:49:TYR:CZ	2:B:53:ASN:HB3	2.46	0.51
1:C:99:THR:OG1	1:C:118:PHE:HB3	2.10	0.51
2:D:19:VAL:O	2:D:74:THR:HA	2.11	0.51
2:D:29:ILE:HG13	2:D:92:TYR:HB2	1.92	0.51
1:E:207:LEU:HD13	1:E:231:PRO:HG3	1.90	0.51
2:F:204:ARG:NH2	2:F:204:ARG:O	2.40	0.51
3:G:164:ARG:NH1	4:H:543:TYR:CE1	2.79	0.51
1:A:169:THR:HG23	1:A:217:ASN:HB3	1.92	0.51
1:C:49:GLY:HA3	1:C:72:ILE:HD11	1.92	0.51
3:G:163:ASP:OD2	3:G:164:ARG:NH2	2.44	0.51
1:A:34:MET:HG3	1:A:81:VAL:HG21	1.93	0.51
2:F:49:TYR:O	2:F:53:ASN:HB2	2.10	0.51
2:D:33:LEU:HA	2:D:89:GLN:O	2.11	0.50
2:D:95:PRO:HB3	2:D:99:THR:HG21	1.93	0.50
1:C:22:CYS:HB3	1:C:81:VAL:HG13	1.93	0.50
2:D:110:ARG:NH1	2:D:113:ALA:HB2	2.26	0.50
1:C:109:ASP:OD1	2:D:32:TYR:OH	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:89:GLN:NE2	2:D:90:GLN:O	2.44	0.50
2:F:19:VAL:O	2:F:74:THR:HA	2.12	0.50
1:A:50:ARG:HD2	1:A:116:GLU:OE2	2.11	0.50
2:F:116:SER:HB2	2:F:139:ASN:OD1	2.12	0.50
1:A:102:THR:HG23	1:A:105:MET:H	1.75	0.49
2:B:49:TYR:O	2:B:53:ASN:HB2	2.12	0.49
2:D:199:THR:HG23	2:D:206:PRO:HG3	1.95	0.49
1:E:88:LEU:CD2	1:E:129:VAL:HG21	2.43	0.48
1:E:22:CYS:HB3	1:E:81:VAL:HG13	1.95	0.48
1:A:107:TYR:OH	4:J:506:ASN:ND2	2.46	0.48
3:K:162:TYR:CE1	3:K:176:PHE:HB3	2.48	0.48
3:G:34:PRO:HD2	4:H:565:THR:HG23	1.95	0.48
3:K:35:LEU:HD21	3:K:185:ILE:HD11	1.94	0.48
3:G:45:VAL:HG23	4:H:504:ILE:HD11	1.96	0.48
1:C:130:SER:HB2	1:C:164:PHE:HZ	1.78	0.48
2:F:13:ALA:O	2:F:109:LYS:N	2.46	0.48
4:J:594:LEU:HD23	4:L:593:LEU:HD21	1.95	0.48
1:C:56:ASP:OD2	1:C:106:ARG:NH2	2.46	0.48
1:C:50:ARG:HH22	1:C:52:LYS:HG2	1.79	0.48
1:E:88:LEU:HD21	1:E:92:ASP:HB2	1.96	0.48
2:F:96:GLY:N	2:F:99:THR:OG1	2.47	0.48
1:A:111:LEU:HD23	2:B:32:TYR:CE1	2.49	0.47
4:H:593:LEU:HD21	4:L:594:LEU:HD23	1.95	0.47
3:I:37:VAL:O	3:I:43:LEU:HA	2.13	0.47
3:K:156:GLU:HG2	5:O:2:NAG:H61	1.96	0.47
4:H:512:ASN:HD22	4:H:559:ARG:NH1	2.13	0.47
3:G:51:LEU:HD23	4:H:607:ASP:HA	1.96	0.47
1:E:150:SER:HB3	2:F:118:PHE:HE1	1.79	0.47
4:H:597:TRP:CE2	4:L:597:TRP:HB3	2.49	0.47
2:F:215:GLU:HG2	2:F:216:CYS:H	1.80	0.47
4:J:512:ASN:HB3	4:J:559:ARG:NH1	2.29	0.47
2:F:110:ARG:NH1	2:F:113:ALA:HB2	2.30	0.47
1:A:7:SER:OG	1:A:21:SER:OG	2.30	0.47
1:C:63:ALA:O	1:C:67:LYS:HG3	2.14	0.47
2:D:45:LYS:HZ3	2:D:47:LEU:HD21	1.79	0.47
3:G:164:ARG:HD3	4:H:520:THR:HG21	1.98	0.46
2:B:152:VAL:O	2:B:155:ALA:HB3	2.16	0.46
4:H:512:ASN:HB3	4:H:559:ARG:NH1	2.30	0.46
2:D:138:LEU:HD21	2:D:198:VAL:CG2	2.45	0.46
2:F:144:ARG:HE	2:F:165:VAL:HG11	1.81	0.46
1:E:199:VAL:HG11	2:F:137:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:594:LEU:HD23	4:J:593:LEU:HD21	1.97	0.46
1:A:123:GLN:HA	2:B:43:ALA:HB2	1.98	0.46
1:E:66:VAL:HG13	1:E:70:PHE:CD1	2.50	0.46
3:I:164:ARG:HD3	4:J:520:THR:HG21	1.98	0.46
1:E:111:LEU:HB2	2:F:32:TYR:OH	2.16	0.46
1:A:152:GLY:H	1:A:204:SER:HB3	1.81	0.46
2:F:33:LEU:HD22	2:F:71:PHE:CG	2.50	0.45
1:A:6:GLU:OE2	1:A:122:GLY:HA3	2.16	0.45
2:D:34:ASN:O	2:D:88:CYS:HA	2.16	0.45
3:I:126:PRO:HD2	3:I:129:ILE:HD12	1.97	0.45
1:E:50:ARG:HH12	1:E:52:LYS:CG	2.29	0.45
1:C:162:ASP:HA	1:C:193:LEU:HB3	1.97	0.45
2:D:133:SER:HA	2:D:181:LEU:O	2.16	0.45
3:I:45:VAL:HG23	4:J:504:ILE:HD11	1.99	0.45
3:I:50:LYS:O	4:J:595:GLN:NE2	2.49	0.45
3:G:71:GLU:OE2	3:G:107:ASN:N	2.49	0.45
3:G:52:VAL:O	4:H:596:ARG:NH2	2.48	0.45
3:I:129:ILE:HG12	3:I:165:LEU:HD13	1.97	0.45
2:F:169:ASP:HB3	2:F:172:ASP:O	2.17	0.45
1:E:64:ALA:HB3	1:E:65:PRO:HD3	1.99	0.45
1:C:112:LEU:HD13	4:L:510:LYS:HE2	1.99	0.45
1:A:33:TRP:HB2	1:A:101:TYR:HB3	1.98	0.44
1:C:102:THR:HG23	1:C:105:MET:H	1.82	0.44
2:F:161:SER:HB3	2:F:181:LEU:HD13	1.99	0.44
3:I:184:LEU:HD21	4:J:558:LEU:HD13	1.97	0.44
1:C:62:TYR:HB2	1:C:67:LYS:HG2	1.99	0.44
1:E:137:PRO:HD3	1:E:218:HIS:CD2	2.53	0.44
4:H:572:PHE:HE2	4:H:581:THR:HG21	1.82	0.44
1:A:228:LYS:NZ	1:A:230:GLU:OE2	2.50	0.44
1:E:156:LEU:HD23	1:E:156:LEU:HA	1.84	0.44
1:A:64:ALA:HB3	1:A:65:PRO:HD3	2.00	0.44
3:I:71:GLU:OE2	3:I:107:ASN:ND2	2.51	0.44
2:F:49:TYR:CZ	2:F:53:ASN:HB3	2.53	0.44
1:C:172:TRP:CZ3	1:C:214:CYS:HB3	2.53	0.43
1:E:34:MET:HB2	1:E:51:ILE:HG23	2.00	0.43
3:K:63:LEU:HD23	3:K:185:ILE:HG12	2.00	0.43
1:C:64:ALA:HB3	1:C:65:PRO:HD3	2.00	0.43
3:K:37:VAL:HG23	3:K:46:SER:HB2	2.00	0.43
2:B:35:TRP:HB2	2:B:48:ILE:HB	1.98	0.43
2:B:90:GLN:HE21	2:B:99:THR:HG22	1.84	0.43
1:C:72:ILE:HG12	1:C:83:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:GLN:H	2:F:102:GLN:HE22	1.66	0.43
3:I:155:LYS:HE2	4:L:534:TYR:CZ	2.54	0.43
1:C:91:GLU:N	1:C:91:GLU:OE1	2.52	0.43
2:B:53:ASN:OD1	4:J:549:HIS:HB2	2.19	0.43
1:A:137:PRO:HB3	1:A:163:TYR:HB3	2.01	0.42
1:C:1:GLU:HG3	1:C:2:VAL:HG23	2.00	0.42
3:G:86:TRP:CZ3	3:G:111:LEU:HD11	2.54	0.42
3:K:130:ARG:NH2	3:K:164:ARG:NH1	2.65	0.42
4:L:558:LEU:O	4:L:561:LEU:HB3	2.20	0.42
2:B:108:ILE:HB	2:B:168:GLN:OE1	2.19	0.42
2:D:48:ILE:HG12	2:D:54:LEU:HD23	2.01	0.42
1:E:101:TYR:CG	1:E:116:GLU:HB2	2.54	0.42
3:G:126:PRO:HD2	3:G:129:ILE:HD12	2.01	0.42
3:K:164:ARG:HD3	4:L:520:THR:HG21	2.02	0.42
1:C:101:TYR:CZ	1:C:116:GLU:HB2	2.55	0.42
1:E:22:CYS:HB3	1:E:81:VAL:CG1	2.50	0.42
3:G:47:ASP:HB3	3:G:50:LYS:HB2	2.02	0.42
2:B:96:GLY:H	2:B:99:THR:CG2	2.33	0.42
1:A:118:PHE:N	2:B:36:TYR:OH	2.53	0.41
1:C:169:THR:HG23	1:C:217:ASN:HB3	2.02	0.41
2:D:18:ARG:HH11	2:D:74:THR:HG21	1.85	0.41
2:F:142:TYR:CG	2:F:143:PRO:HA	2.55	0.41
2:F:18:ARG:NH1	2:F:74:THR:HG21	2.35	0.41
2:D:169:ASP:OD1	2:D:170:SER:N	2.53	0.41
2:D:20:THR:HA	2:D:73:LEU:O	2.21	0.41
3:G:64:ARG:HA	3:G:100:GLU:OE2	2.20	0.41
2:D:187:ASP:HA	2:D:190:LYS:HD3	2.03	0.41
1:A:111:LEU:HD23	2:B:32:TYR:HE1	1.84	0.41
1:C:144:PRO:HG2	1:C:231:PRO:HB3	2.02	0.41
1:C:134:THR:HG23	1:C:165:PRO:HD3	2.02	0.41
1:E:161:LYS:HG3	1:E:162:ASP:OD1	2.21	0.41
1:E:177:LEU:HA	1:E:177:LEU:HD13	1.96	0.41
2:D:142:TYR:CG	2:D:143:PRO:HA	2.56	0.41
2:F:121:PRO:HB3	2:F:211:PHE:CE2	2.56	0.41
1:A:33:TRP:CZ2	1:A:52:LYS:HE3	2.55	0.41
2:B:169:ASP:O	2:B:173:SER:HA	2.21	0.41
1:E:167:PRO:O	1:E:218:HIS:ND1	2.47	0.41
1:C:89:LYS:HG2	1:C:90:THR:H	1.86	0.41
2:D:33:LEU:HA	2:D:90:GLN:HA	2.02	0.41
1:E:188:LEU:HD12	1:E:194:TYR:CZ	2.56	0.41
1:E:224:LYS:HE2	1:E:224:LYS:HB3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:90:GLN:OE1	2:F:92:TYR:N	2.48	0.40
1:E:172:TRP:CZ3	1:E:214:CYS:HB3	2.56	0.40
3:K:37:VAL:CG2	3:K:46:SER:HB2	2.51	0.40
1:A:66:VAL:HG13	1:A:70:PHE:CD1	2.57	0.40
1:A:113:ARG:HB3	2:B:92:TYR:O	2.21	0.40
2:B:192:LYS:HE2	2:B:192:LYS:HB3	1.91	0.40
1:E:227:LYS:HA	1:E:227:LYS:HD3	1.94	0.40
3:K:99:TYR:OH	3:K:162:TYR:O	2.35	0.40
1:C:218:HIS:CE1	1:C:221:SER:H	2.40	0.40
2:F:35:TRP:CE2	2:F:73:LEU:HB2	2.57	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	222/242 (92%)	220 (99%)	2 (1%)	0	100	100
1	C	229/242 (95%)	228 (100%)	1 (0%)	0	100	100
1	E	229/242 (95%)	225 (98%)	4 (2%)	0	100	100
2	B	213/216 (99%)	210 (99%)	3 (1%)	0	100	100
2	D	213/216 (99%)	211 (99%)	2 (1%)	0	100	100
2	F	214/216 (99%)	211 (99%)	3 (1%)	0	100	100
3	G	155/234 (66%)	151 (97%)	4 (3%)	0	100	100
3	I	154/234 (66%)	150 (97%)	4 (3%)	0	100	100
3	K	154/234 (66%)	149 (97%)	5 (3%)	0	100	100
4	H	106/110 (96%)	103 (97%)	3 (3%)	0	100	100
4	J	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
4	L	101/110 (92%)	98 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2097/2406 (87%)	2060 (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	189/205 (92%)	189 (100%)	0	100	100
1	C	197/205 (96%)	197 (100%)	0	100	100
1	E	198/205 (97%)	198 (100%)	0	100	100
2	B	189/190 (100%)	189 (100%)	0	100	100
2	D	189/190 (100%)	189 (100%)	0	100	100
2	F	190/190 (100%)	190 (100%)	0	100	100
3	G	129/190 (68%)	129 (100%)	0	100	100
3	I	128/190 (67%)	128 (100%)	0	100	100
3	K	128/190 (67%)	128 (100%)	0	100	100
4	H	88/89 (99%)	88 (100%)	0	100	100
4	J	88/89 (99%)	88 (100%)	0	100	100
4	L	87/89 (98%)	87 (100%)	0	100	100
All	All	1800/2022 (89%)	1800 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

14 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	M	1	5,4	14,14,15	0.25	0	17,19,21	0.43	0
5	NAG	M	2	5	14,14,15	0.22	0	17,19,21	0.42	0
5	BMA	M	3	5	11,11,12	1.10	1 (9%)	15,15,17	1.49	3 (20%)
5	MAN	M	4	5	11,11,12	0.88	1 (9%)	15,15,17	1.44	2 (13%)
5	MAN	M	5	5	11,11,12	0.72	1 (9%)	15,15,17	1.16	2 (13%)
6	NAG	N	1	4,6	14,14,15	0.36	0	17,19,21	0.47	0
6	NAG	N	2	6	14,14,15	0.21	0	17,19,21	0.44	0
6	BMA	N	3	6	11,11,12	1.12	1 (9%)	15,15,17	1.26	2 (13%)
6	MAN	N	4	6	11,11,12	0.87	1 (9%)	15,15,17	0.90	1 (6%)
5	NAG	O	1	5,4	14,14,15	0.25	0	17,19,21	0.46	0
5	NAG	O	2	5	14,14,15	0.18	0	17,19,21	0.52	0
5	BMA	O	3	5	11,11,12	0.96	0	15,15,17	1.24	3 (20%)
5	MAN	O	4	5	11,11,12	0.83	0	15,15,17	0.89	1 (6%)
5	MAN	O	5	5	11,11,12	0.98	1 (9%)	15,15,17	1.52	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	M	1	5,4	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	MAN	M	4	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	M	5	5	-	0/2/19/22	0/1/1/1
6	NAG	N	1	4,6	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	4/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1
6	MAN	N	4	6	-	0/2/19/22	0/1/1/1
5	NAG	O	1	5,4	-	1/6/23/26	0/1/1/1
5	NAG	O	2	5	-	3/6/23/26	0/1/1/1
5	BMA	O	3	5	-	1/2/19/22	0/1/1/1
5	MAN	O	4	5	-	2/2/19/22	0/1/1/1
5	MAN	O	5	5	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	3	BMA	C2-C3	2.68	1.56	1.52
5	O	5	MAN	C1-C2	2.53	1.58	1.52
5	M	4	MAN	C1-C2	2.45	1.57	1.52
5	M	3	BMA	O3-C3	2.24	1.48	1.43
6	N	4	MAN	O5-C1	-2.14	1.40	1.43
5	M	5	MAN	C1-C2	2.07	1.56	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	5	MAN	C1-O5-C5	4.76	118.65	112.19
5	M	4	MAN	C1-O5-C5	4.19	117.87	112.19
5	M	3	BMA	O3-C3-C2	3.99	117.64	109.99
5	M	3	BMA	C1-O5-C5	3.19	116.52	112.19
5	M	5	MAN	C1-O5-C5	2.91	116.13	112.19
6	N	3	BMA	O3-C3-C2	2.84	115.43	109.99
6	N	4	MAN	O2-C2-C3	-2.36	105.42	110.14
5	O	5	MAN	O2-C2-C3	-2.29	105.55	110.14
5	O	3	BMA	O3-C3-C2	2.24	114.29	109.99
5	O	4	MAN	O2-C2-C3	-2.22	105.70	110.14
5	M	4	MAN	O2-C2-C3	-2.20	105.73	110.14
5	O	3	BMA	O3-C3-C4	2.20	115.44	110.35
5	M	5	MAN	O2-C2-C3	-2.18	105.77	110.14
6	N	3	BMA	C1-O5-C5	2.17	115.13	112.19
5	O	3	BMA	O5-C5-C6	2.13	110.55	107.20
5	M	3	BMA	C1-C2-C3	-2.03	107.17	109.67

There are no chirality outliers.

All (15) torsion outliers are listed below:

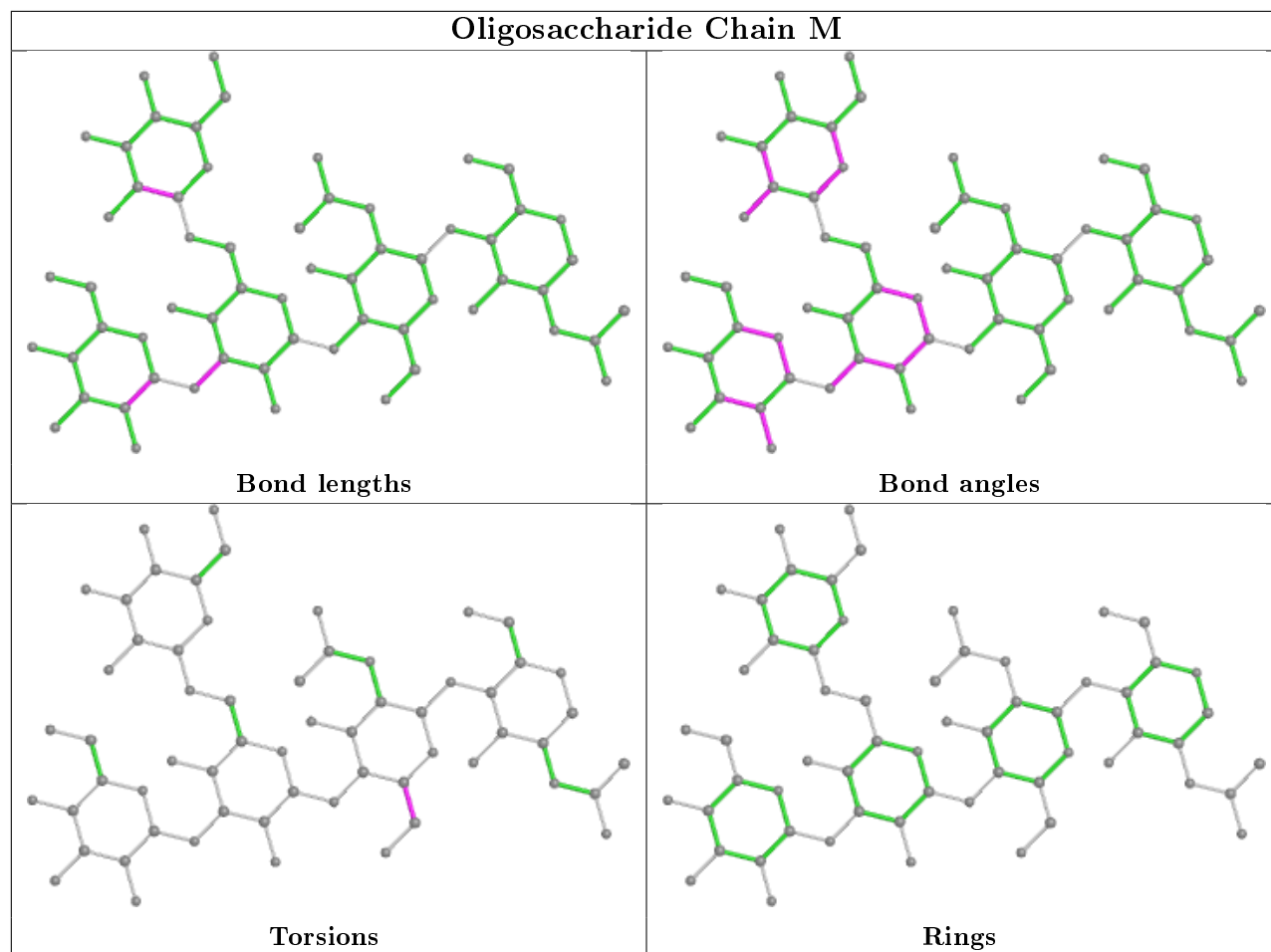
Mol	Chain	Res	Type	Atoms
5	M	2	NAG	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
5	O	2	NAG	C8-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
6	N	2	NAG	C8-C7-N2-C2
6	N	2	NAG	O7-C7-N2-C2
6	N	1	NAG	C4-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	O	4	MAN	C4-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	O	4	MAN	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
5	O	3	BMA	C4-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6

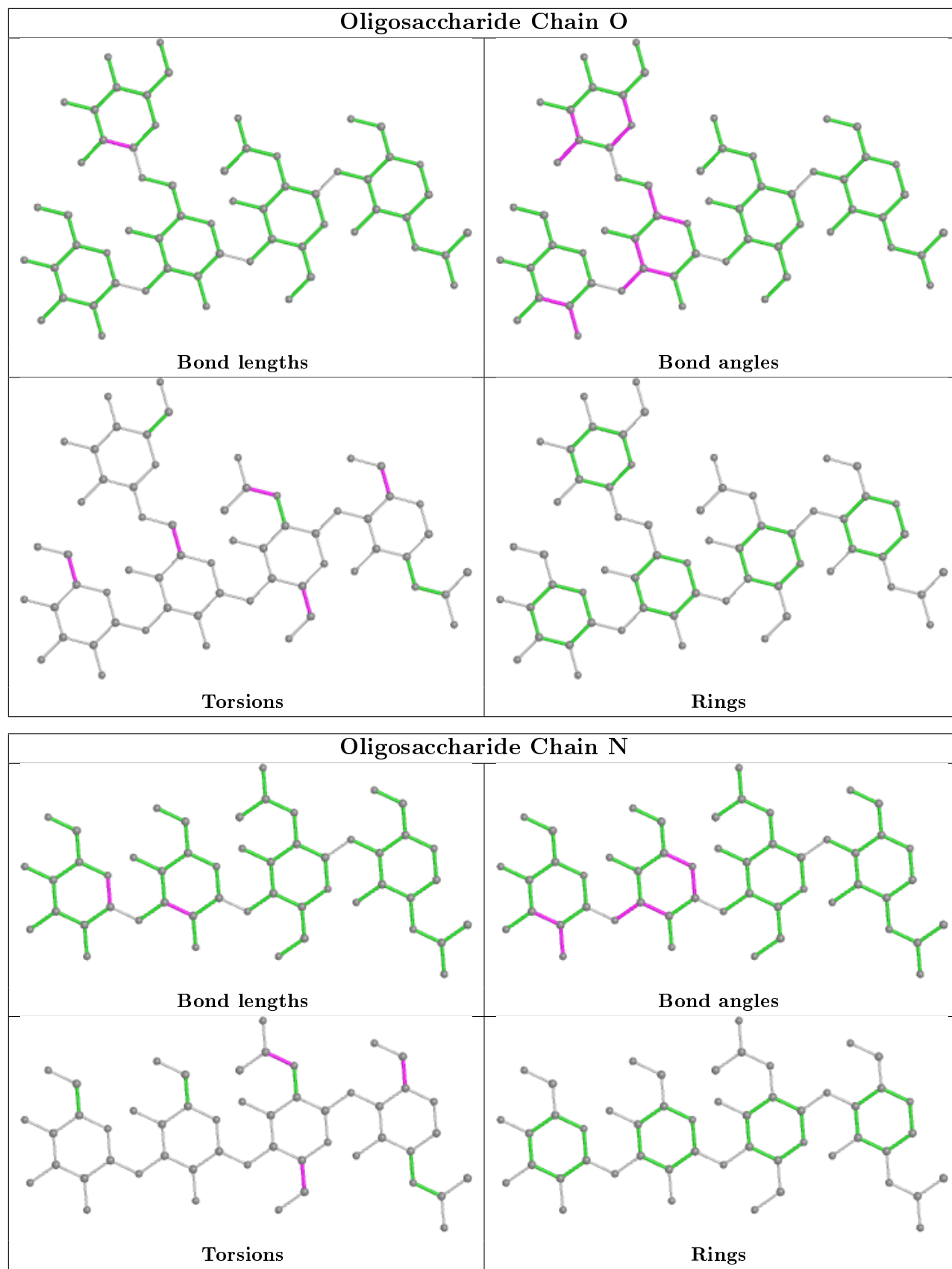
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

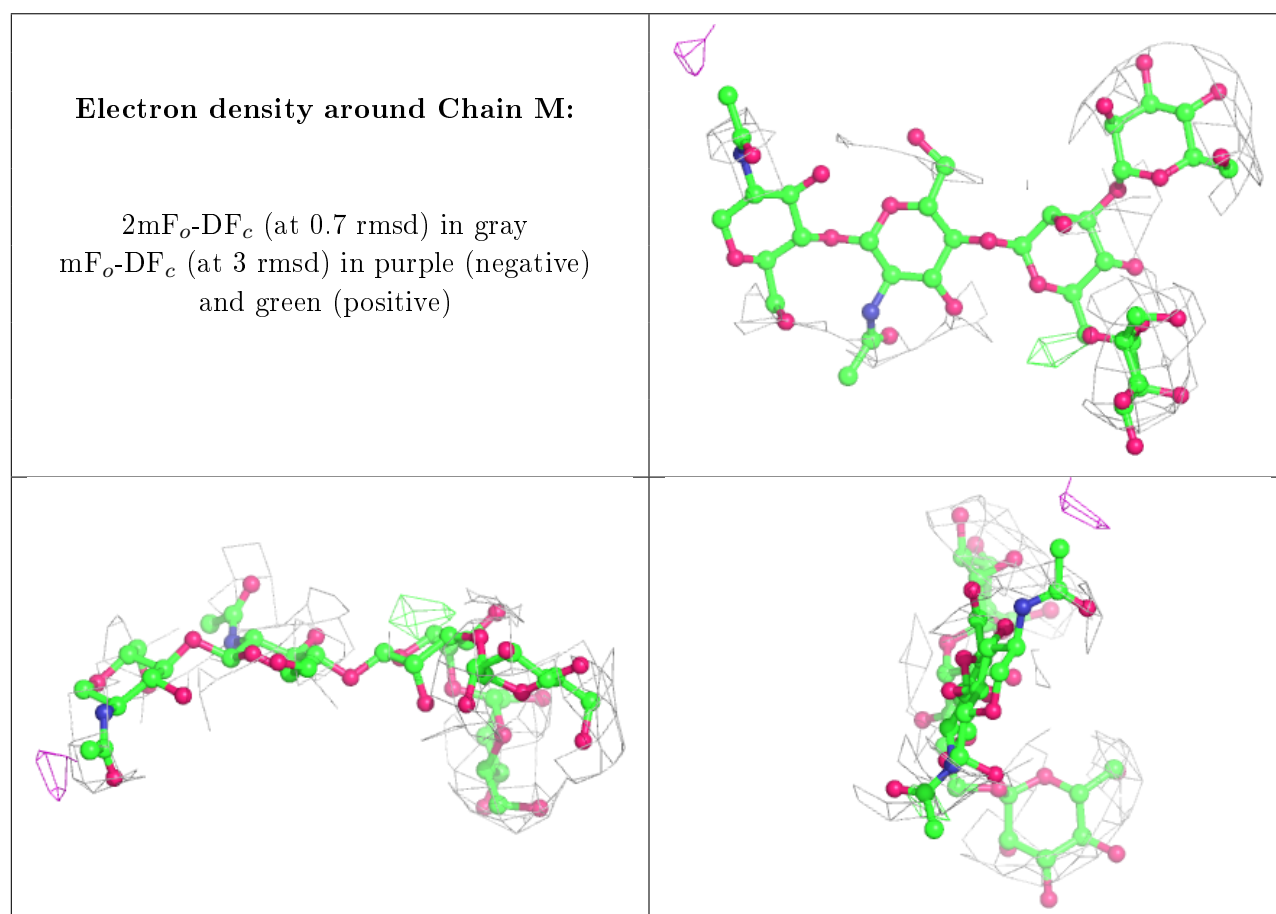
6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

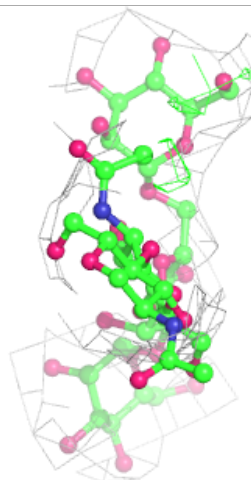
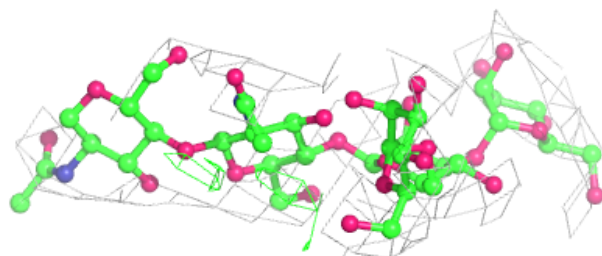
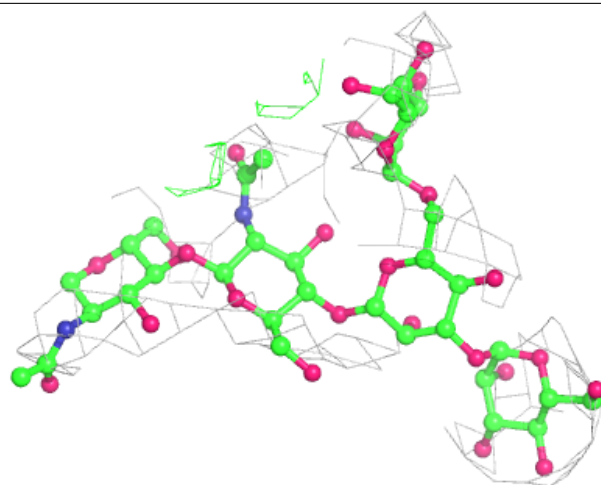
Unable to reproduce the depositors R factor - this section is therefore empty.

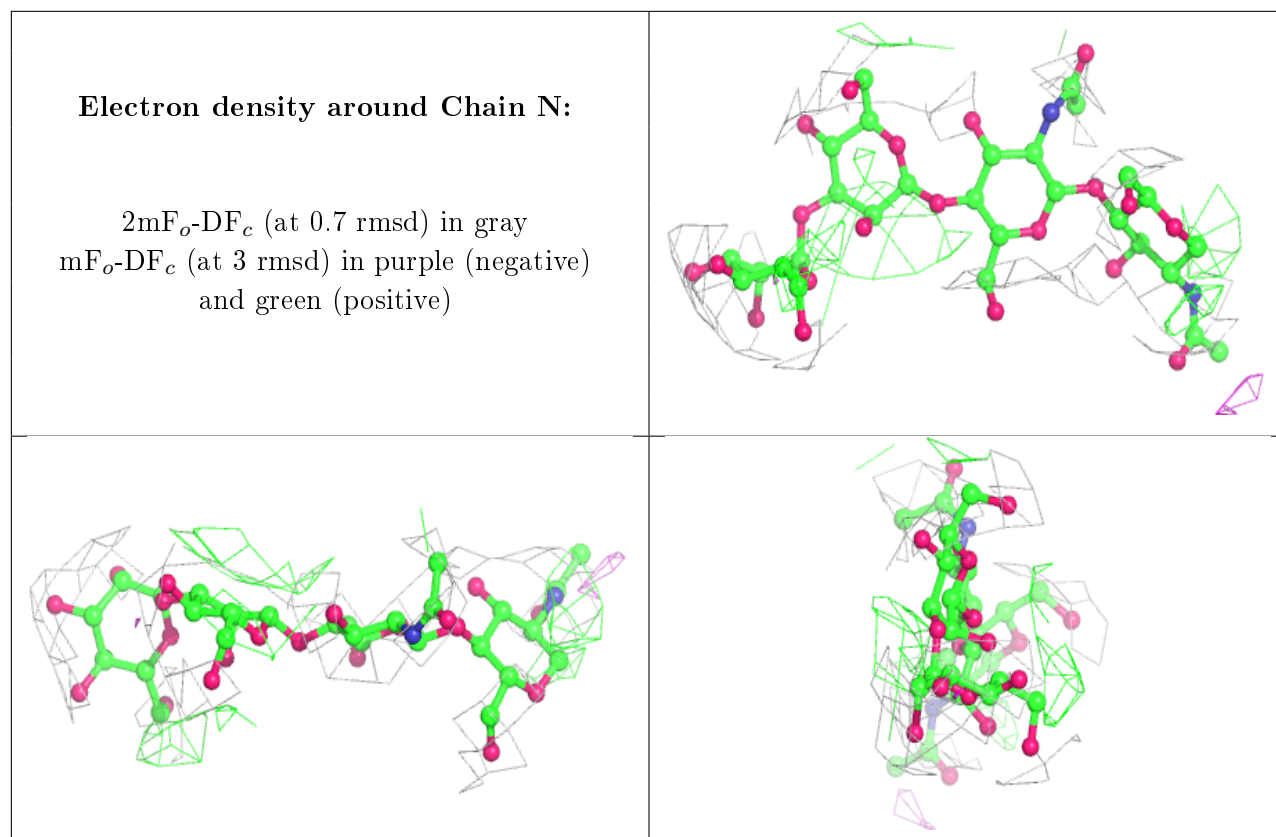
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain O:

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





6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.