



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:02 AM UTC

PDB ID : 6MAM / pdb_00006mam
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 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:

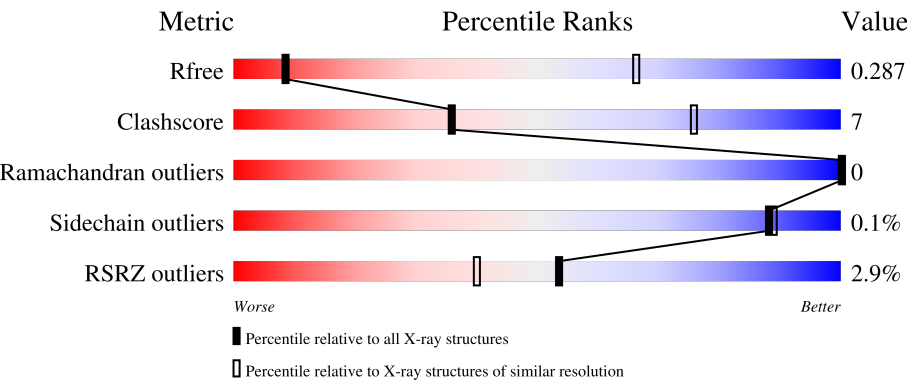
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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}	180053	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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	242	2% 74% 20% 7%
1	C	242	2% 74% 22%
1	E	242	% 74% 23%
2	B	216	7% 88% 12%
2	D	216	% 78% 21%

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Mol	Chain	Length	Quality of chain
2	F	216	
3	G	234	
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.

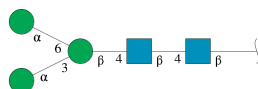
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	108	Total	C	N	O	S	0	0	0
			846	540	147	153	6			

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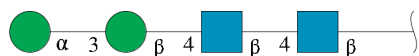
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	109	Total	C	N	O	S	0	0	0
			851	543	148	154	6			
4	L	105	Total	C	N	O	S	0	0	0
			828	530	144	148	6			

- 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.

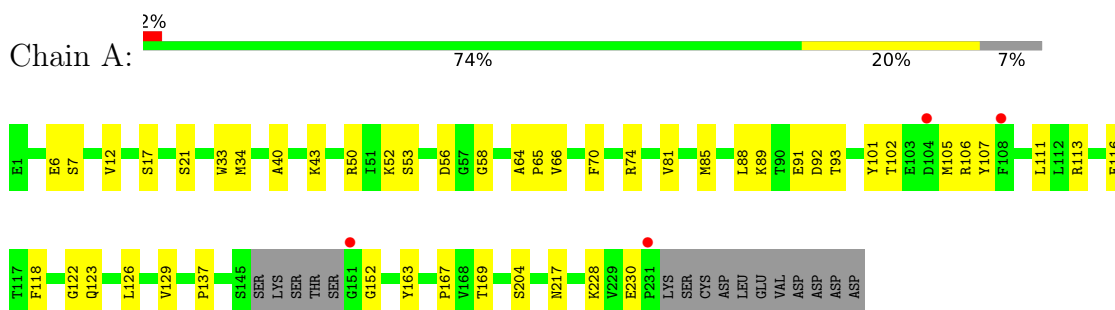


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	N	4	Total	C	N	O		0	0	0
			50	28	2	20				

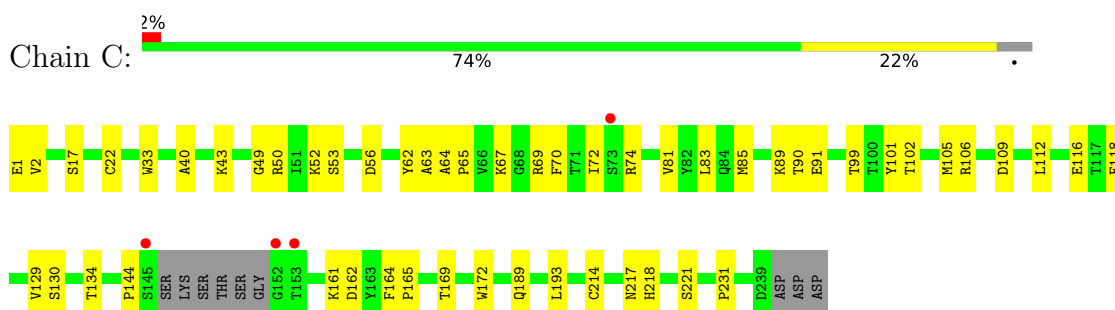
3 Residue-property plots [i](#)

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.

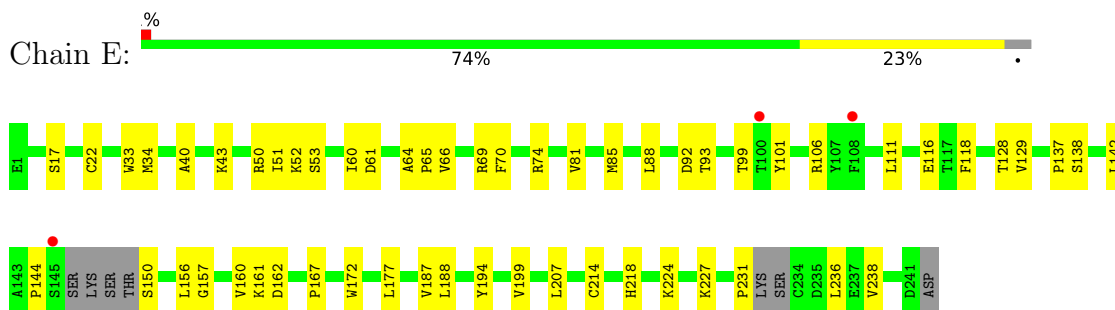
- Molecule 1: ADI-15946 Fab Heavy Chain



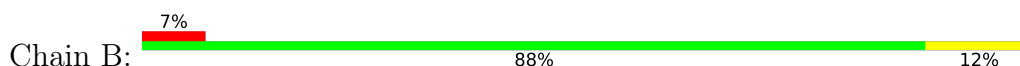
- Molecule 1: ADI-15946 Fab Heavy Chain

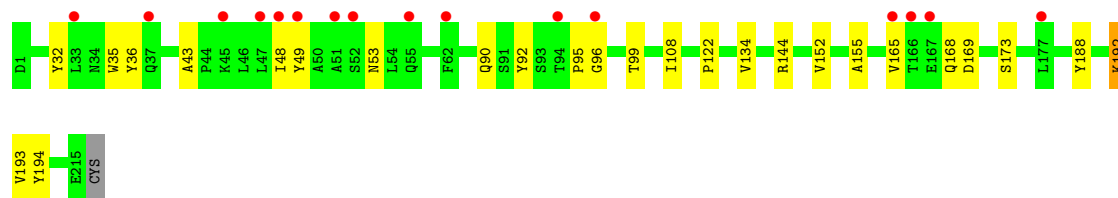


- Molecule 1: ADI-15946 Fab Heavy Chain

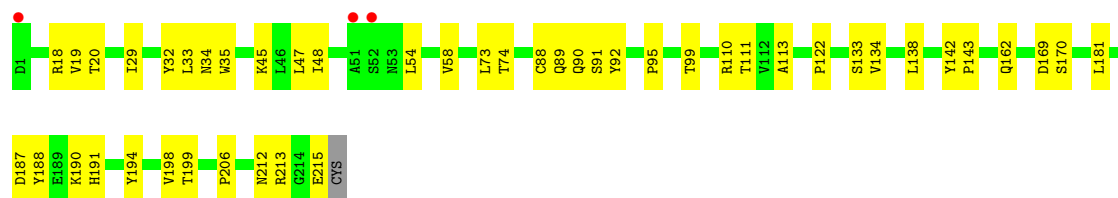
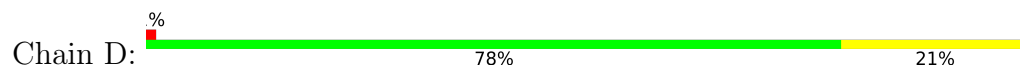


- Molecule 2: ADI-15946 Fab Light Chain

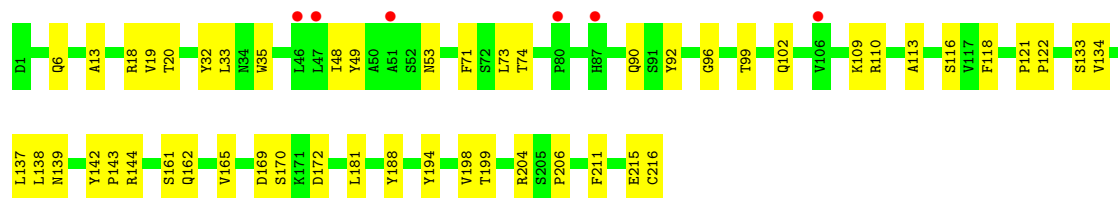
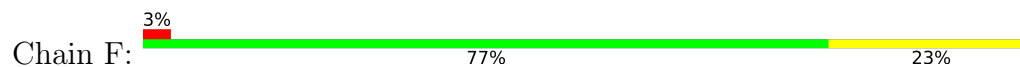




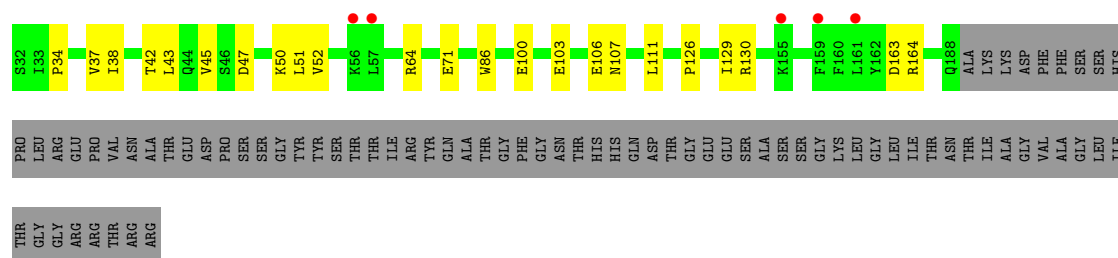
• Molecule 2: ADI-15946 Fab Light Chain



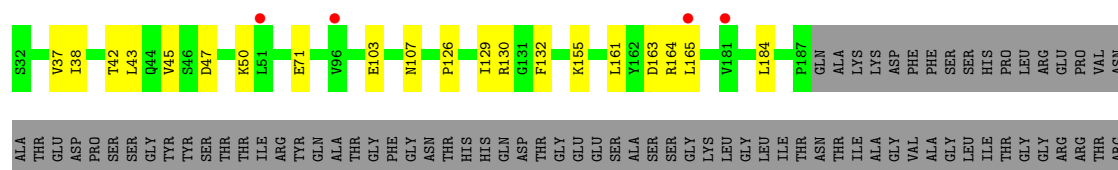
• Molecule 2: ADI-15946 Fab Light Chain



• Molecule 3: Envelope glycoprotein

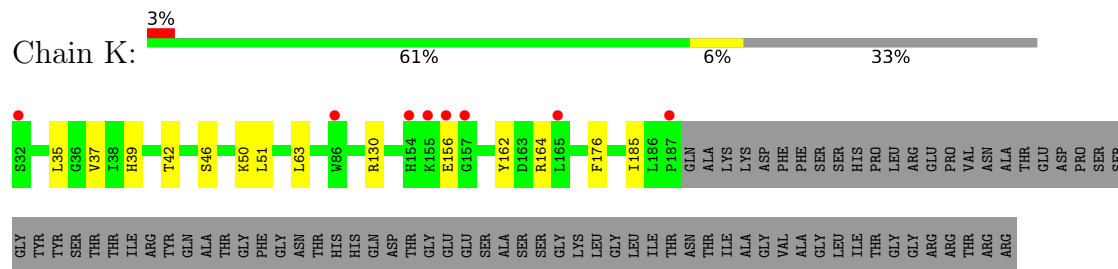


• Molecule 3: Envelope glycoprotein

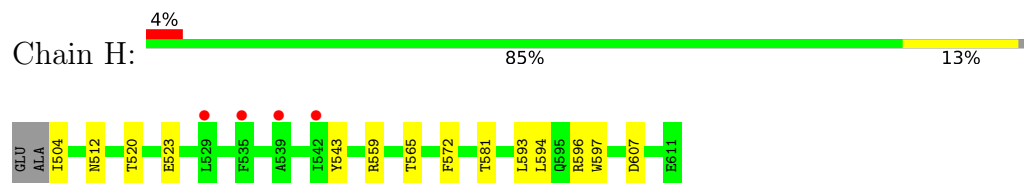


ARG

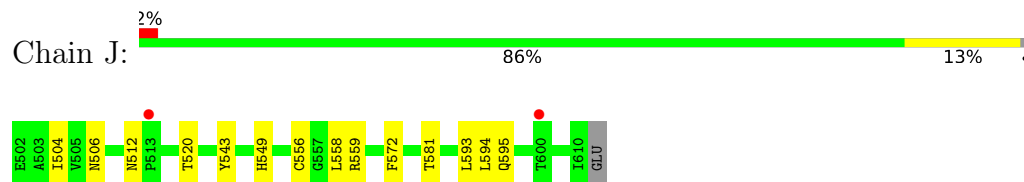
- Molecule 3: Envelope glycoprotein



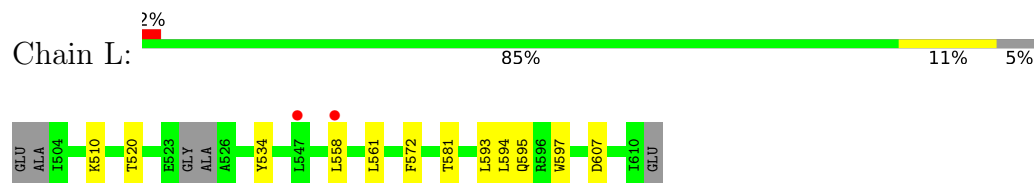
- Molecule 4: Envelope glycoprotein



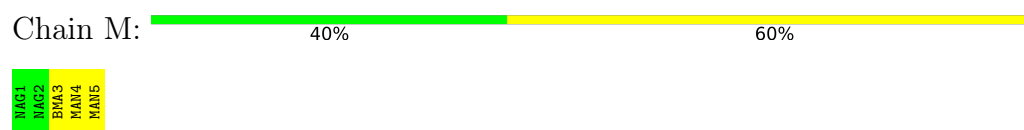
- Molecule 4: Envelope glycoprotein



- Molecule 4: Envelope glycoprotein



- 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



- 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





- 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) 99.5 (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 0.272 , 0.287	Depositor DCC
R_{free} test set	1796 reflections (5.08%)	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)	0.32 , 131.6	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	0.85	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, BMA

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	0.12	0/1748	0.33	0/2380
1	C	0.11	0/1805	0.31	0/2457
1	E	0.13	0/1815	0.35	0/2470
2	B	0.12	0/1706	0.36	1/2315 (0.0%)
2	D	0.09	0/1706	0.30	0/2315
2	F	0.12	0/1713	0.33	0/2323
3	G	0.13	0/1228	0.43	0/1668
3	I	0.12	0/1219	0.41	0/1656
3	K	0.12	0/1219	0.41	0/1656
4	H	0.10	0/866	0.29	0/1179
4	J	0.09	0/871	0.28	0/1186
4	L	0.09	0/847	0.29	0/1152
All	All	0.11	0/16743	0.34	1/22757 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	192	LYS	N-CA-C	6.09	118.00	111.36

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	1706	0	1669	33	0
1	C	1763	0	1723	33	0
1	E	1774	0	1719	39	0
2	B	1668	0	1622	20	0
2	D	1668	0	1622	33	0
2	F	1675	0	1626	32	0
3	G	1199	0	1177	18	0
3	I	1190	0	1169	16	0
3	K	1190	0	1169	12	0
4	H	846	0	825	15	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	238	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 (238) 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:34:ASN:HB2	2:D:48:ILE:O	2.05	0.57
2:D:110:ARG:HG2	2:D:111:THR:H	1.69	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:49:TYR:CZ	2:B:53:ASN:HB3	2.46	0.51
2:B:188:TYR:O	2:B:194:TYR:OH	2.27	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:O	2:F:204:ARG:NH2	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
1:C:33:TRP:CD1	1:C:106:ARG:HH12	2.29	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

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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:32:TYR:O	2:D:91:SER:OG	2.30	0.49
2:D:199:THR:HG23	2:D:206:PRO:HG3	1.95	0.49
1:E:22:CYS:HB3	1:E:81:VAL:HG13	1.95	0.48
1:E:88:LEU:CD2	1:E:129:VAL:HG21	2.43	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:A:7:SER:OG	1:A:21:SER:OG	2.30	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
3:G:51:LEU:HD23	4:H:607:ASP:HA	1.96	0.47
4:H:512:ASN:HD22	4:H:559:ARG:NH1	2.13	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: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
1:C:109:ASP:OD1	2:D:32:TYR:OH	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:144:ARG:HE	2:F:165:VAL:HG11	1.81	0.46
3:G:103:GLU:CD	4:H:559:ARG:HH12	2.18	0.46
1:E:199:VAL:HG11	2:F:137:LEU:HD22	1.98	0.46
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:52:VAL:O	4:H:596:ARG:NH2	2.48	0.45
3:G:71:GLU:OE2	3:G:107:ASN:N	2.49	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:C:112:LEU:HD13	4:L:510:LYS:HE2	1.99	0.45
1:E:64:ALA:HB3	1:E:65:PRO:HD3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:OE1	1:C:91:GLU:N	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
1:C:69:ARG:C	1:C:70:PHE:HD1	2.28	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
4:H:523:GLU:H	4:H:523:GLU:CD	2.28	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:18:ARG:NH1	2:F:74:THR:HG21	2.35	0.41
2:F:142:TYR:CG	2:F:143:PRO:HA	2.55	0.41
2:D:20:THR:HA	2:D:73:LEU:O	2.21	0.41
2:D:169:ASP:OD1	2:D:170:SER:N	2.53	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:HD13	1:E:177:LEU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:LYS:HG2	1:C:90:THR:H	1.86	0.41
1:E:167:PRO:O	1:E:218:HIS:ND1	2.47	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
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:HD3	1:E:227:LYS:HA	1.94	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/242 (92%)	220 (99%)	2 (1%)	0	100	100
1	C	62/242 (26%)	62 (100%)	0	0	100	100
1	E	229/242 (95%)	225 (98%)	4 (2%)	0	100	100
2	B	156/216 (72%)	154 (99%)	2 (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	44/234 (19%)	43 (98%)	1 (2%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	51/110 (46%)	49 (96%)	2 (4%)	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
All	All	1707/2406 (71%)	1676 (98%)	31 (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%)	188 (100%)	1 (0%)	81	82
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%)	1799 (100%)	1 (0%)	88	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	193	VAL

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

Mol	Chain	Res	Type
1	C	39	GLN
1	E	39	GLN
2	F	38	GLN
2	F	87	HIS
2	F	191	HIS
3	G	73	ASN
4	H	508	GLN
3	I	73	ASN
4	J	586	ASN
3	K	73	ASN
3	K	98	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

14 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	M	1	5,4	14,14,15	0.25	0	17,19,21	0.44	0
5	NAG	M	2	5	14,14,15	0.22	0	17,19,21	0.44	0
5	BMA	M	3	5	11,11,12	1.08	1 (9%)	15,15,17	1.41	2 (13%)
5	MAN	M	4	5	11,11,12	0.85	1 (9%)	15,15,17	1.39	2 (13%)
5	MAN	M	5	5	11,11,12	0.69	0	15,15,17	1.10	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	N	1	6,4	14,14,15	0.34	0	17,19,21	0.49	0
6	NAG	N	2	6	14,14,15	0.21	0	17,19,21	0.46	0
6	BMA	N	3	6	11,11,12	1.08	1 (9%)	15,15,17	1.23	2 (13%)
6	MAN	N	4	6	11,11,12	0.84	1 (9%)	15,15,17	0.86	1 (6%)
5	NAG	O	1	5,4	14,14,15	0.26	0	17,19,21	0.48	0
5	NAG	O	2	5	14,14,15	0.18	0	17,19,21	0.54	0
5	BMA	O	3	5	11,11,12	0.95	0	15,15,17	1.13	2 (13%)
5	MAN	O	4	5	11,11,12	0.81	0	15,15,17	0.86	1 (6%)
5	MAN	O	5	5	11,11,12	0.95	1 (9%)	15,15,17	1.49	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
5	MAN	M	5	5	-	0/2/19/22	0/1/1/1
6	NAG	N	1	6,4	-	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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	3	BMA	C2-C3	2.60	1.56	1.52
5	O	5	MAN	C1-C2	2.41	1.58	1.52
5	M	4	MAN	C1-C2	2.34	1.57	1.52
5	M	3	BMA	O3-C3	2.14	1.48	1.43
6	N	4	MAN	O5-C1	-2.02	1.40	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	5	MAN	C1-O5-C5	4.82	118.65	112.19
5	M	4	MAN	C1-O5-C5	4.24	117.87	112.19
5	M	3	BMA	O3-C3-C2	3.72	117.64	110.05
5	M	3	BMA	C1-O5-C5	3.23	116.52	112.19
5	M	5	MAN	C1-O5-C5	2.95	116.13	112.19
6	N	3	BMA	O3-C3-C2	2.63	115.43	110.05
6	N	4	MAN	O2-C2-C3	-2.29	105.42	110.15
5	O	5	MAN	O2-C2-C3	-2.22	105.55	110.15
6	N	3	BMA	C1-O5-C5	2.20	115.13	112.19
5	O	4	MAN	O2-C2-C3	-2.15	105.70	110.15
5	O	3	BMA	O3-C3-C4	2.15	115.44	110.38
5	M	4	MAN	O2-C2-C3	-2.14	105.73	110.15
5	M	5	MAN	O2-C2-C3	-2.11	105.77	110.15
5	O	3	BMA	O3-C3-C2	2.08	114.29	110.05

There are no chirality outliers.

All (15) torsion outliers are listed below:

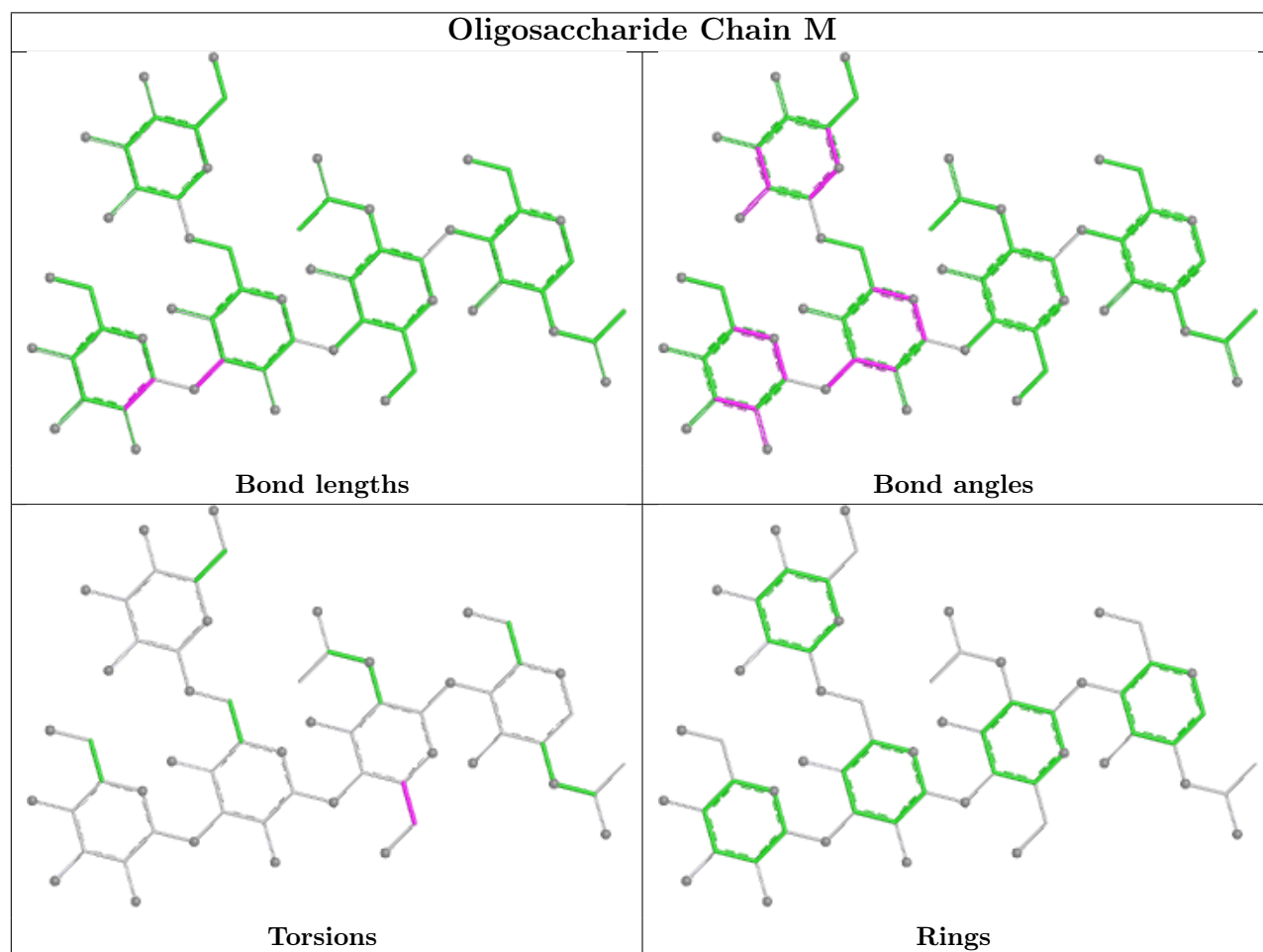
Mol	Chain	Res	Type	Atoms
5	M	2	NAG	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
5	O	2	NAG	C8-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
6	N	2	NAG	C8-C7-N2-C2
6	N	2	NAG	O7-C7-N2-C2
5	M	2	NAG	C4-C5-C6-O6
5	O	4	MAN	C4-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	O	4	MAN	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6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

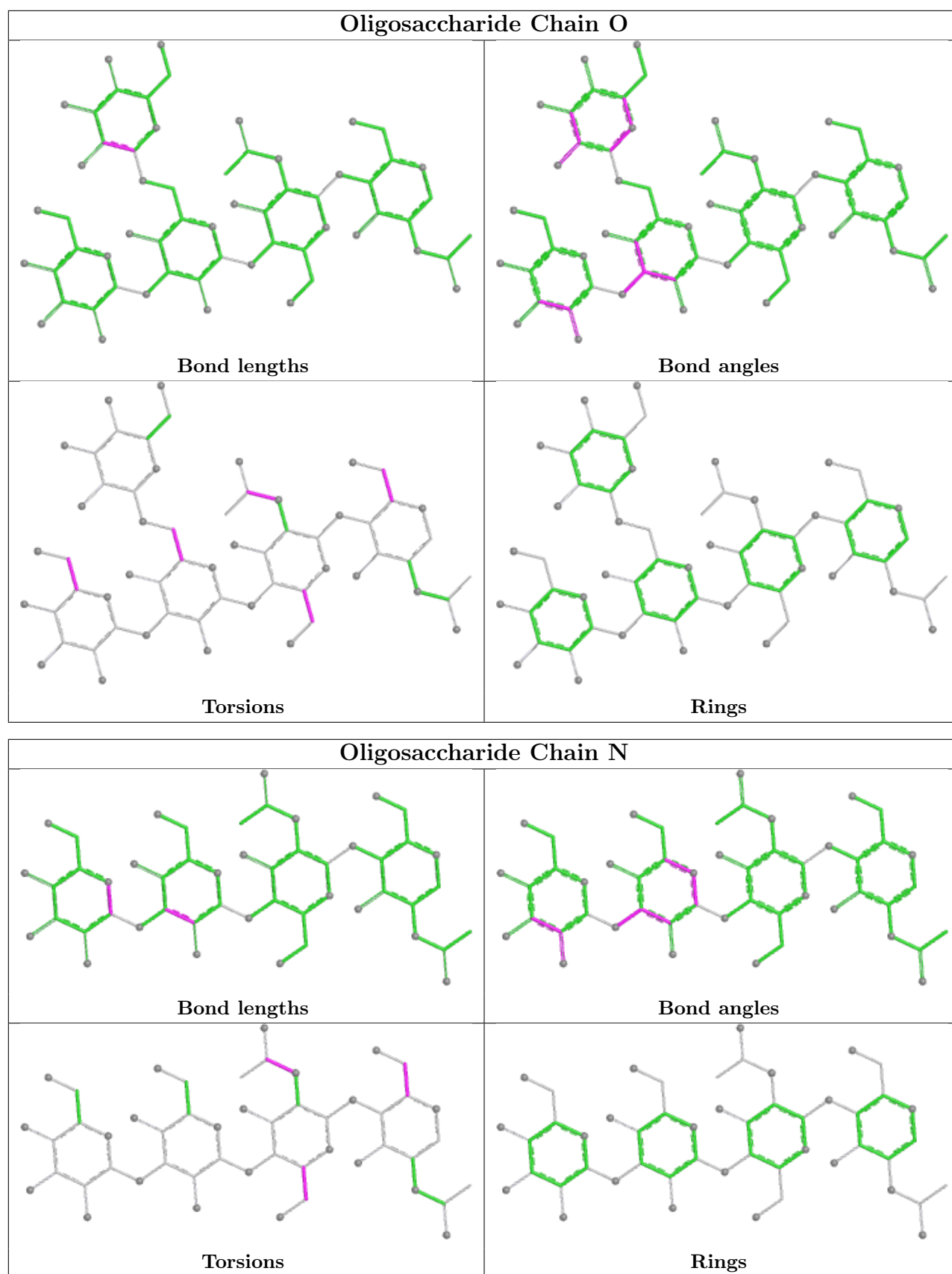
There are no ring outliers.

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 ⓘ

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	226/242 (93%)	0.39	4 (1%)	67 51	101, 124, 138, 139	0
1	C	233/242 (96%)	0.40	4 (1%)	69 52	109, 131, 136, 139	0
1	E	235/242 (97%)	0.40	3 (1%)	75 58	95, 115, 128, 131	0
2	B	215/216 (99%)	0.43	16 (7%)	20 20	30, 123, 148, 149	0
2	D	215/216 (99%)	0.36	3 (1%)	73 56	113, 123, 128, 131	0
2	F	216/216 (100%)	0.36	6 (2%)	55 41	98, 113, 123, 127	0
3	G	157/234 (67%)	0.49	5 (3%)	50 38	84, 89, 114, 121	0
3	I	156/234 (66%)	0.54	4 (2%)	57 42	88, 97, 116, 120	0
3	K	156/234 (66%)	0.51	8 (5%)	33 28	77, 103, 117, 119	0
4	H	108/110 (98%)	0.55	4 (3%)	45 35	86, 97, 125, 129	0
4	J	109/110 (99%)	0.60	2 (1%)	67 51	86, 99, 124, 126	0
4	L	105/110 (95%)	0.39	2 (1%)	66 50	92, 106, 122, 124	0
All	All	2131/2406 (88%)	0.44	61 (2%)	53 40	30, 114, 137, 149	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	145	SER	5.7
2	B	47	LEU	5.6
1	A	108	PHE	3.9
1	A	151	GLY	3.8
1	C	152	GLY	3.4
3	K	155	LYS	3.2
1	E	145	SER	3.1
2	B	62	PHE	3.1
4	H	535	PHE	3.1
3	I	96	VAL	2.9
3	K	187	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	153	THR	2.8
2	B	45	LYS	2.8
3	I	181	VAL	2.8
2	D	52	SER	2.7
2	F	106	VAL	2.7
2	B	96	GLY	2.7
3	K	157	GLY	2.6
1	A	104	ASP	2.6
2	F	51	ALA	2.6
3	I	165	LEU	2.6
2	B	52	SER	2.6
3	I	51	LEU	2.5
3	K	32	SER	2.5
2	B	48	ILE	2.5
2	F	46	LEU	2.5
2	B	165	VAL	2.5
4	J	600	THR	2.5
2	B	37	GLN	2.5
1	A	231	PRO	2.5
4	J	513	PRO	2.5
2	F	47	LEU	2.4
2	B	55	GLN	2.4
2	B	177	LEU	2.4
1	E	108	PHE	2.3
3	K	165	LEU	2.3
3	K	86	TRP	2.3
2	D	1	ASP	2.3
2	D	51	ALA	2.3
2	B	167	GLU	2.3
3	G	159	PHE	2.3
4	H	539	ALA	2.3
4	L	558	LEU	2.3
3	G	57	LEU	2.2
1	E	100	THR	2.2
3	G	56	LYS	2.2
2	B	33	LEU	2.2
3	K	156	GLU	2.2
2	B	166	THR	2.2
3	G	155	LYS	2.2
3	G	161	LEU	2.2
2	B	94	THR	2.2
4	L	547	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	73	SER	2.1
2	B	49	TYR	2.1
2	B	51	ALA	2.1
4	H	529	LEU	2.1
4	H	542	ILE	2.1
2	F	87	HIS	2.1
3	K	154	HIS	2.1
2	F	80	PRO	2.1

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

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

6.3 Carbohydrates ⓘ

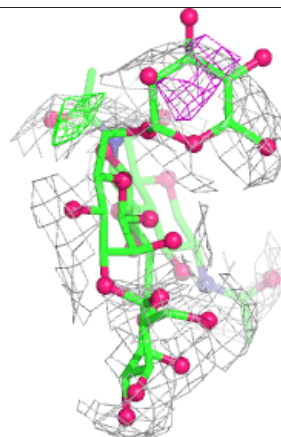
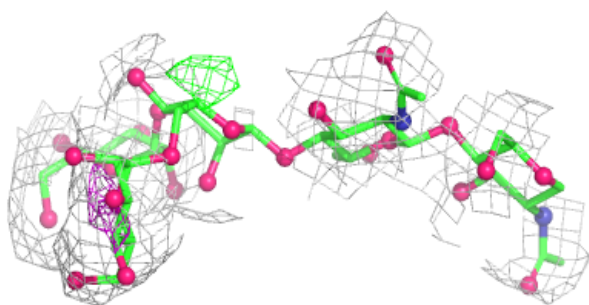
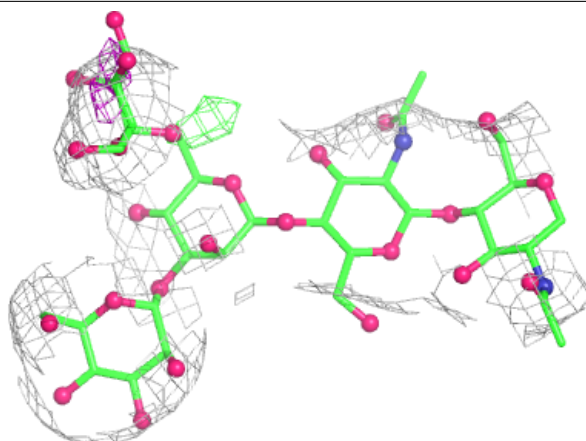
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MAN	O	5	11/12	0.26	0.15	117,117,117,117	0
6	MAN	N	4	11/12	0.49	0.15	112,112,112,112	0
6	BMA	N	3	11/12	0.54	0.14	111,111,111,111	0
5	MAN	M	5	11/12	0.60	0.18	106,106,106,106	0
5	BMA	M	3	11/12	0.60	0.10	102,102,102,102	0
5	MAN	O	4	11/12	0.64	0.12	119,119,119,119	0
5	BMA	O	3	11/12	0.66	0.10	117,117,117,117	0
5	NAG	O	2	14/15	0.71	0.12	111,111,111,111	0
6	NAG	N	2	14/15	0.79	0.12	107,107,107,107	0
5	MAN	M	4	11/12	0.81	0.11	104,104,104,104	0
5	NAG	M	1	14/15	0.86	0.15	91,91,91,91	0
6	NAG	N	1	14/15	0.88	0.14	102,102,102,102	0
5	NAG	M	2	14/15	0.90	0.11	95,95,95,95	0
5	NAG	O	1	14/15	0.92	0.12	106,106,106,106	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.

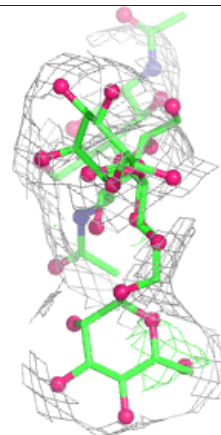
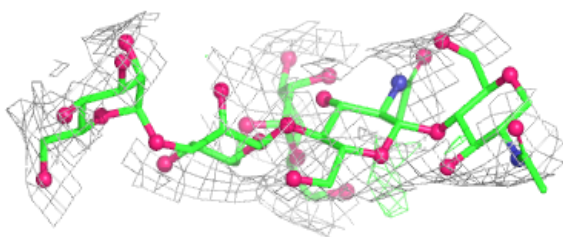
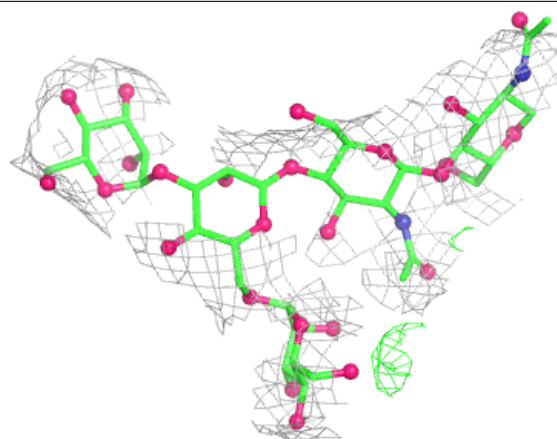
Electron density around Chain M:

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

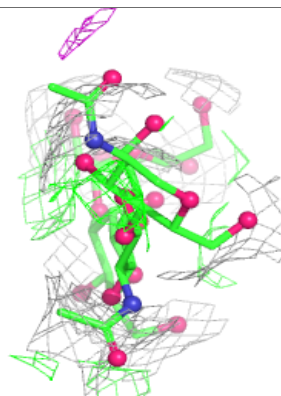
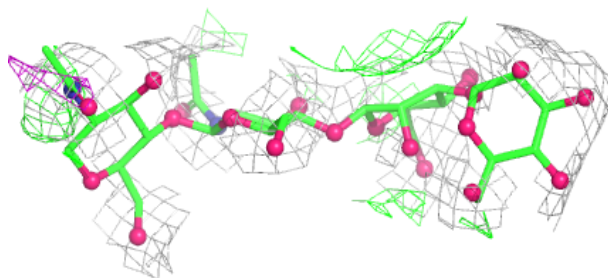
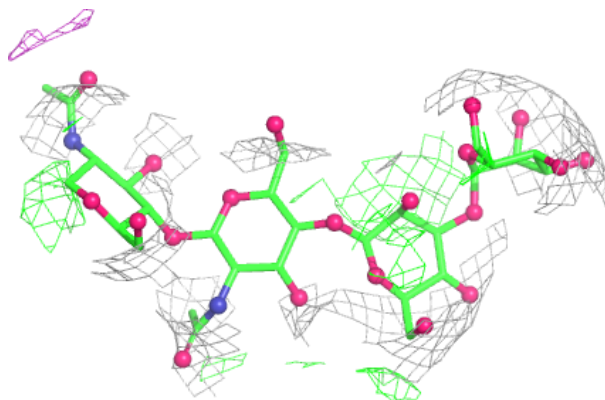


Electron density around Chain O:

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

**Electron density around Chain N:**

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.