



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2023 – 10:41 PM EDT

PDB ID : 5KZC
Title : Crystal structure of an HIV-1 gp120 engineered outer domain with a Man9 glycan at position N276, in complex with broadly neutralizing antibody VRC01
Authors : Julien, J.-P.; Jardine, J.G.; Diwanji, D.; Schief, W.R.; Wilson, I.A.
Deposited on : 2016-07-24
Resolution : 3.25 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

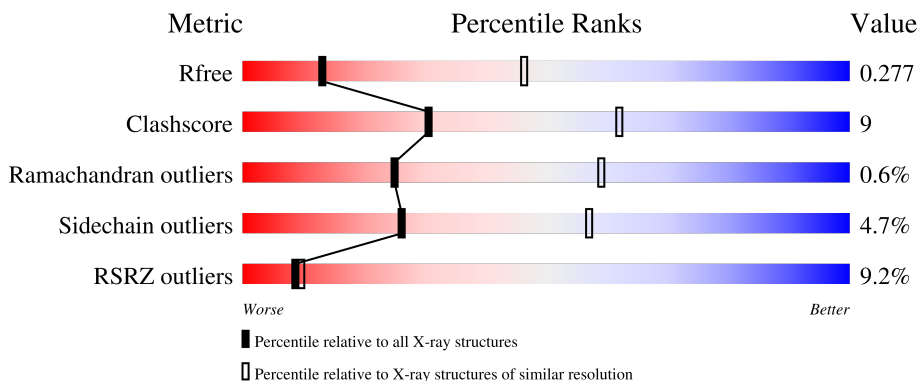
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	B	224	
1	E	224	
1	H	224	
2	A	182	
2	C	182	

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Mol	Chain	Length	Quality of chain
2	F	182	<p>10% 59% 24% 14%</p>
3	D	210	<p>24% 75% 24%</p>
3	G	210	<p>3% 75% 22%</p>
3	L	210	<p>5% 76% 21%</p>
4	I	9	<p>33% 67%</p>
4	J	9	<p>22% 78%</p>
5	K	7	<p>43% 57%</p>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13849 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 VRC01 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	214	1644	1041	285	308	10	0	0	0
1	B	214	1644	1041	285	308	10	0	0	0
1	E	214	1644	1041	285	308	10	0	0	0

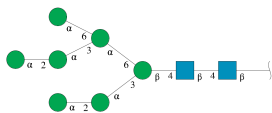
- Molecule 2 is a protein called Engineered outer domain of gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	170	1277	799	225	244	9	0	0	0
2	C	170	1277	799	224	245	9	0	0	0
2	F	156	1185	747	205	225	8	0	0	0

- Molecule 3 is a protein called VRC01 Fab light chain.

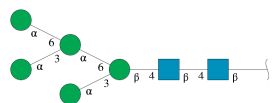
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	206	1603	1007	275	317	4	0	0	0
3	D	209	1623	1017	278	323	5	0	0	0
3	G	206	1603	1007	275	317	4	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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.



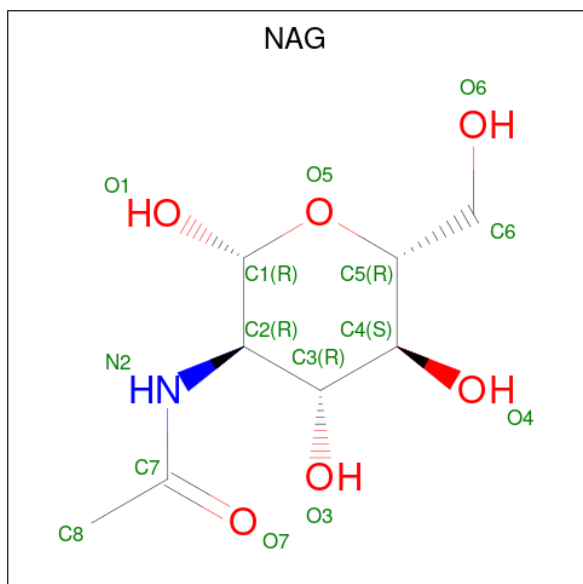
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	I	9	105	58	2	45	0	0	0
4	J	9	105	58	2	45	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	K	7	83	46	2	35	0	0	0

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

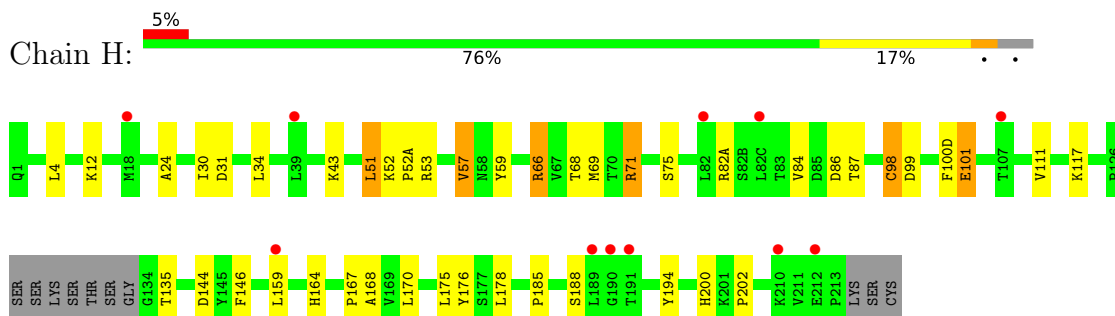


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 14	C 8	N 1	O 5	0	0
6	A	1	Total 14	C 8	N 1	O 5	0	0
6	C	1	Total 14	C 8	N 1	O 5	0	0
6	C	1	Total 14	C 8	N 1	O 5	0	0

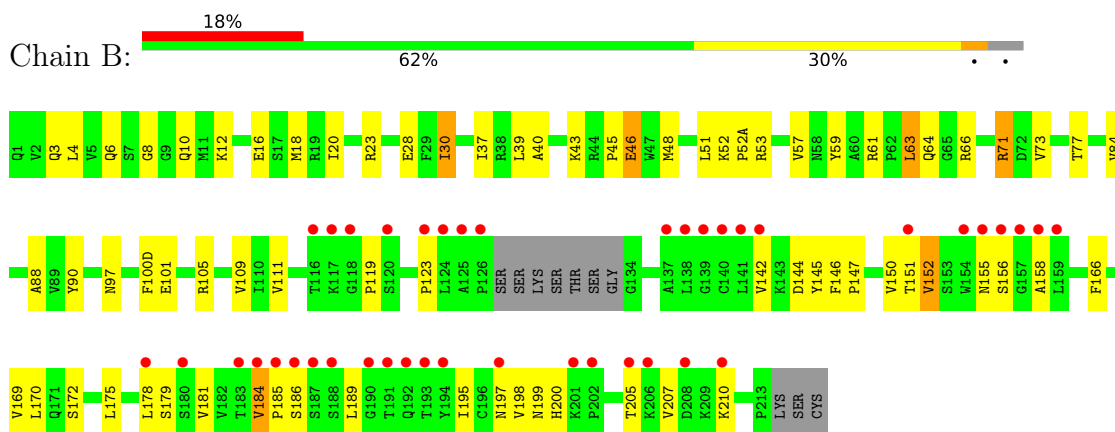
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

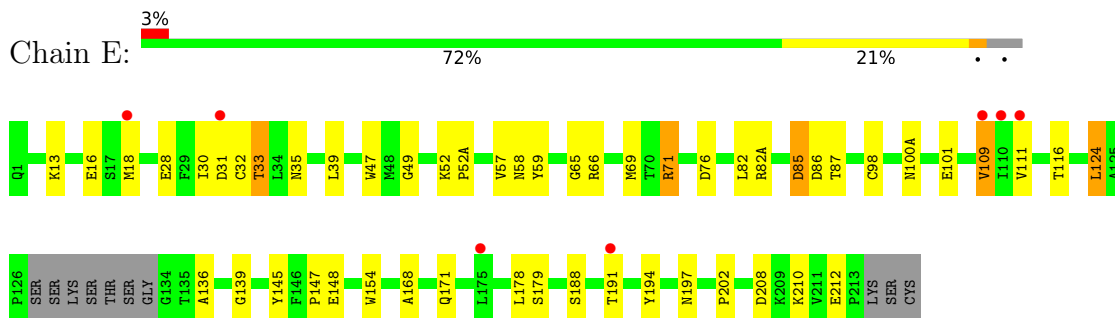
- Molecule 1: VRC01 Fab heavy chain



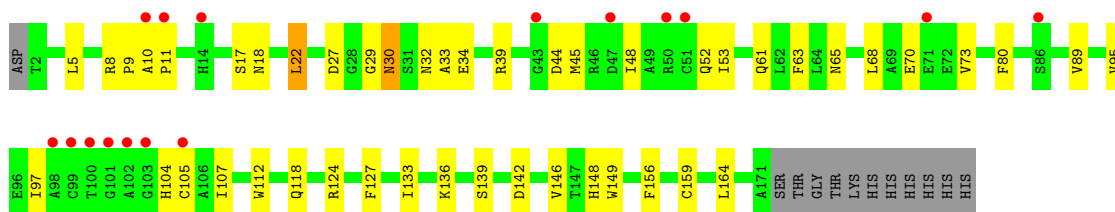
- Molecule 1: VRC01 Fab heavy chain



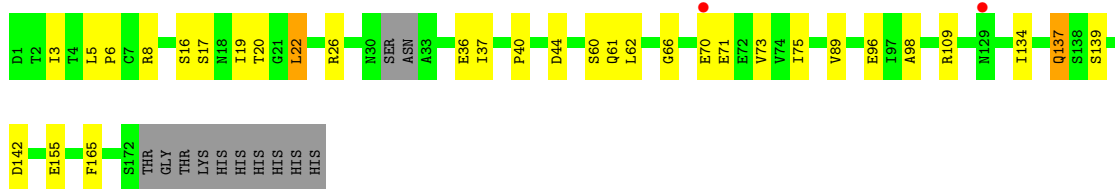
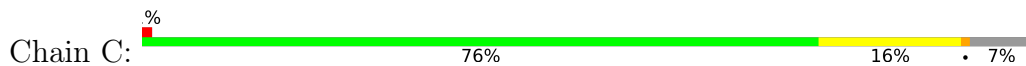
- Molecule 1: VRC01 Fab heavy chain



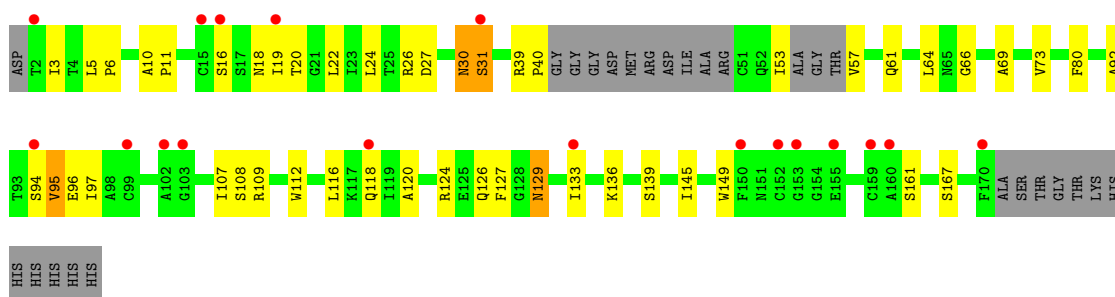
- Molecule 2: Engineered outer domain of gp120



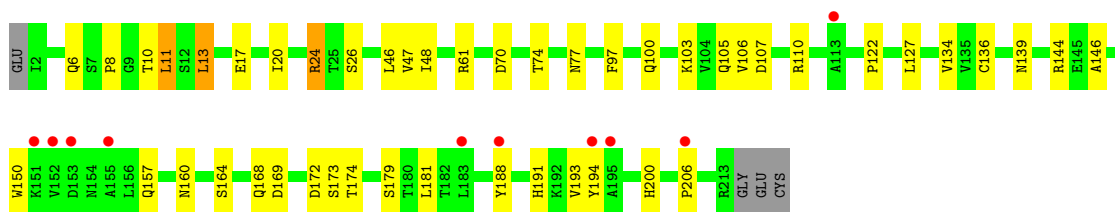
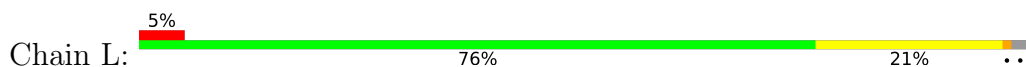
- Molecule 2: Engineered outer domain of gp120



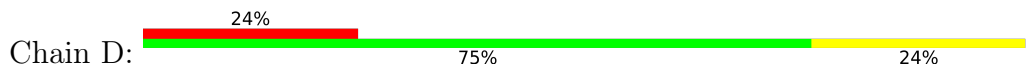
- Molecule 2: Engineered outer domain of gp120

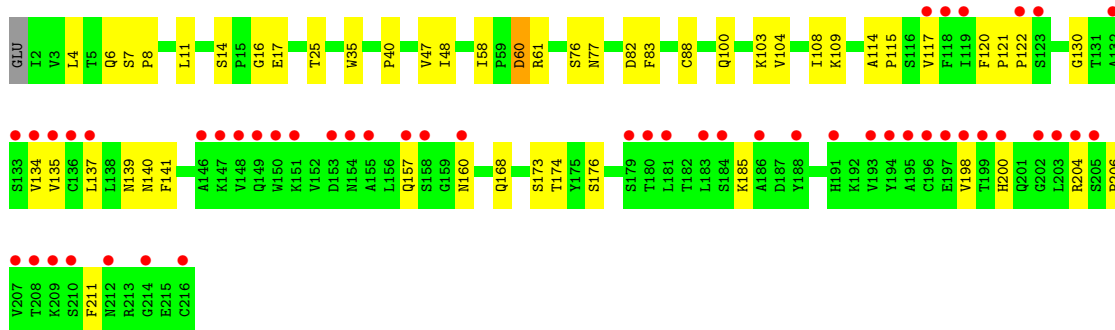


- Molecule 3: VRC01 Fab light chain

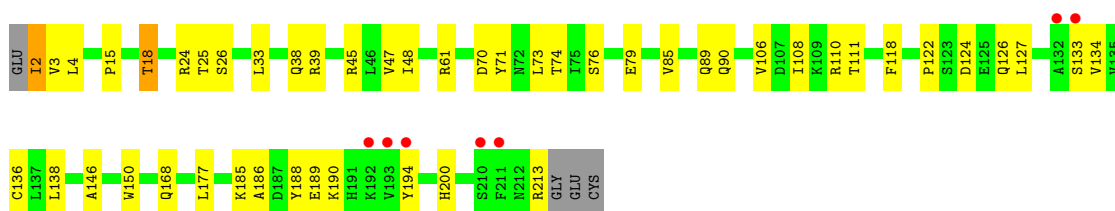
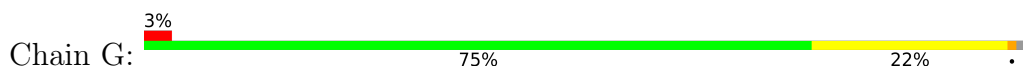


- Molecule 3: VRC01 Fab light chain

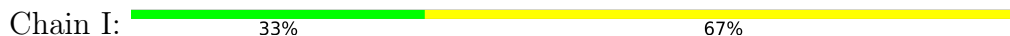




- Molecule 3: VRC01 Fab light chain



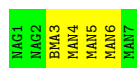
- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	113.51Å 113.51Å 412.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.94 – 3.25 39.94 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.94-3.25) 100.0 (39.94-3.25)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.25Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.223 , 0.274 0.224 , 0.277	Depositor DCC
R_{free} test set	2181 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	99.7	Xtrriage
Anisotropy	0.054	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 79.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13849	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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, MAN, 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	B	0.29	0/1688	0.51	0/2299
1	E	0.28	0/1688	0.48	0/2299
1	H	0.26	0/1688	0.48	0/2299
2	A	0.26	0/1303	0.43	0/1767
2	C	0.28	0/1302	0.46	0/1764
2	F	0.25	0/1209	0.45	0/1639
3	D	0.28	0/1660	0.45	0/2253
3	G	0.27	0/1640	0.42	0/2228
3	L	0.27	0/1640	0.46	0/2228
All	All	0.27	0/13818	0.46	0/18776

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	99	ASP	Peptide

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	B	1644	0	1611	45	0
1	E	1644	0	1611	34	0
1	H	1644	0	1611	34	0
2	A	1277	0	1239	29	0
2	C	1277	0	1239	15	0
2	F	1185	0	1151	27	0
3	D	1623	0	1566	32	0
3	G	1603	0	1552	23	0
3	L	1603	0	1552	27	0
4	I	105	0	88	0	0
4	J	105	0	88	0	0
5	K	83	0	70	0	0
6	A	28	0	26	1	0
6	C	28	0	26	1	0
All	All	13849	0	13430	252	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 9.

All (252) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52(A):PRO:O	1:E:71:ARG:NH2	2.04	0.90
3:L:110:ARG:HD2	3:L:173:SER:HB2	1.56	0.87
3:L:188:TYR:O	3:L:194:TYR:OH	1.96	0.83
3:D:47:VAL:HG12	3:D:48:ILE:HG12	1.63	0.81
1:E:32:CYS:HB3	1:E:98:CYS:HB3	1.68	0.75
1:E:87:THR:HG22	1:E:111:VAL:H	1.53	0.73
3:D:157:GLN:HB3	3:D:160:ASN:HD21	1.56	0.70
1:B:181:VAL:HG21	3:D:137:LEU:HD11	1.71	0.70
3:G:47:VAL:HG12	3:G:48:ILE:HG12	1.75	0.69
3:L:47:VAL:HG12	3:L:48:ILE:HG12	1.74	0.69
1:B:12:LYS:HZ3	1:B:18:MET:HA	1.57	0.69
3:D:120:PHE:HB2	3:D:135:VAL:HG22	1.76	0.68
1:H:51:LEU:HD23	1:H:57:VAL:HG23	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:22:LEU:HD12	2:A:89:VAL:HB	1.74	0.68
2:A:95:VAL:HG12	2:A:107:ILE:HD11	1.76	0.68
2:A:52:GLN:HE22	2:C:137:GLN:H	1.40	0.68
2:F:20:THR:HG21	2:F:66:GLY:H	1.59	0.68
3:L:24:ARG:NH1	3:L:70:ASP:OD1	2.27	0.67
2:F:107:ILE:HD12	2:F:108:SER:H	1.59	0.67
1:H:59:TYR:HE1	1:H:69:MET:HG2	1.60	0.67
1:H:68:THR:OG1	1:H:82(A):ARG:NH2	2.29	0.66
1:H:66:ARG:NH2	1:H:86:ASP:OD2	2.28	0.66
3:G:188:TYR:O	3:G:194:TYR:OH	2.14	0.66
2:C:20:THR:HG21	2:C:66:GLY:H	1.60	0.65
1:B:144:ASP:HB3	1:B:175:LEU:HD13	1.77	0.65
1:B:51:LEU:HD23	1:B:57:VAL:HG22	1.77	0.65
3:L:6:GLN:O	3:L:100:GLN:NE2	2.30	0.64
2:F:19:ILE:HB	2:F:95:VAL:HG23	1.79	0.64
1:H:101:GLU:HG2	3:L:46:LEU:HD23	1.78	0.64
3:G:18:THR:HB	3:G:76:SER:HA	1.80	0.63
1:H:52(A):PRO:O	1:H:71:ARG:NH1	2.32	0.62
1:E:145:TYR:OH	1:E:148:GLU:OE1	2.16	0.62
1:E:30:ILE:HA	1:E:52(A):PRO:HB2	1.82	0.62
1:B:61:ARG:HA	1:B:64:GLN:HG2	1.82	0.61
3:G:122:PRO:HD3	3:G:134:VAL:HG22	1.81	0.61
1:B:142:VAL:HB	1:B:178:LEU:HG	1.82	0.61
3:D:61:ARG:NH1	3:D:82:ASP:OD2	2.35	0.60
1:H:51:LEU:HD11	1:H:71:ARG:HB3	1.84	0.60
2:A:80:PHE:HB3	2:A:127:PHE:HE1	1.67	0.60
3:D:4:LEU:HD22	3:D:25:THR:HG22	1.84	0.59
2:A:97:ILE:HA	2:A:107:ILE:HD13	1.85	0.59
3:D:122:PRO:HD3	3:D:134:VAL:HG22	1.83	0.59
3:D:168:GLN:HE21	3:D:173:SER:HB3	1.68	0.59
2:C:3:ILE:HG13	2:C:109:ARG:HB2	1.85	0.59
1:E:85:ASP:OD1	1:E:85:ASP:N	2.27	0.58
1:H:87:THR:HG22	1:H:111:VAL:H	1.68	0.58
2:A:22:LEU:CD1	2:A:89:VAL:HB	2.33	0.58
1:B:48:MET:HG2	1:B:63:LEU:HD21	1.85	0.58
1:B:90:TYR:HE1	1:B:109:VAL:HG22	1.69	0.58
1:B:51:LEU:HD11	1:B:71:ARG:HG2	1.86	0.57
3:D:60:ASP:OD1	3:D:60:ASP:N	2.31	0.57
3:L:103:LYS:NZ	3:L:105:GLN:OE1	2.36	0.57
3:L:107:ASP:OD1	3:L:168:GLN:NE2	2.37	0.57
3:D:139:ASN:O	3:D:176:SER:OG	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:61:ARG:NH1	3:L:77:ASN:O	2.38	0.57
1:B:166:PHE:HD2	1:B:179:SER:HB2	1.69	0.56
1:B:57:VAL:HG11	1:B:59:TYR:CZ	2.40	0.56
2:F:3:ILE:HG13	2:F:109:ARG:HB2	1.86	0.56
2:F:112:TRP:CZ3	2:F:116:LEU:HD22	2.40	0.56
3:L:122:PRO:HD3	3:L:134:VAL:HG22	1.87	0.56
1:B:152:VAL:HG12	1:B:198:VAL:HG22	1.88	0.56
2:A:80:PHE:HB3	2:A:127:PHE:CE1	2.40	0.56
1:E:28:GLU:HB3	1:E:31:ASP:HB2	1.88	0.56
1:B:186:SER:HA	1:B:189:LEU:HD13	1.88	0.55
1:H:168:ALA:HA	1:H:178:LEU:HB3	1.88	0.55
1:H:71:ARG:NH2	2:A:142:ASP:OD1	2.40	0.55
3:D:83:PHE:HA	3:D:104:VAL:HG23	1.88	0.55
3:D:141:PHE:HB2	3:D:200:HIS:CE1	2.40	0.55
3:G:108:ILE:HB	3:G:168:GLN:HE22	1.71	0.55
2:A:148:HIS:HD2	2:A:159:CYS:HB2	1.72	0.55
1:H:164:HIS:HD2	3:L:139:ASN:HD21	1.55	0.54
1:H:12:LYS:O	1:H:111:VAL:HA	2.07	0.54
2:F:129:ASN:OD1	2:F:129:ASN:N	2.40	0.54
1:B:155:ASN:HB2	1:B:158:ALA:HB3	1.89	0.54
3:D:17:GLU:OE1	3:D:109:LYS:NZ	2.39	0.54
1:H:4:LEU:HD23	1:H:24:ALA:HB2	1.90	0.53
1:H:51:LEU:HD22	1:H:52:LYS:N	2.23	0.53
1:B:12:LYS:O	1:B:111:VAL:HA	2.08	0.53
3:G:38:GLN:HB3	3:G:85:VAL:HG13	1.91	0.53
3:G:110:ARG:NH1	3:G:111:THR:O	2.41	0.53
2:A:149:TRP:HE1	2:A:156:PHE:HB3	1.74	0.53
2:F:18:ASN:HB3	2:F:94:SER:HB3	1.91	0.53
3:L:191:HIS:O	3:L:193:VAL:N	2.40	0.52
1:H:164:HIS:CD2	3:L:139:ASN:HD21	2.27	0.52
2:C:75:ILE:HG22	2:C:89:VAL:HG22	1.90	0.52
2:A:112:TRP:CZ2	2:A:164:LEU:HG	2.43	0.52
1:B:145:TYR:CZ	1:B:150:VAL:HG23	2.45	0.52
3:D:8:PRO:HD2	3:D:11:LEU:HD11	1.92	0.52
1:H:167:PRO:HG2	3:L:164:SER:HB2	1.92	0.51
2:F:61:GLN:NE2	2:F:145:ILE:O	2.33	0.51
2:A:61:GLN:NE2	2:A:146:VAL:O	2.41	0.51
2:F:26:ARG:HD3	2:F:127:PHE:HE2	1.76	0.51
1:B:151:THR:HB	1:B:199:ASN:HB2	1.93	0.51
2:C:70:GLU:H	2:C:70:GLU:CD	2.13	0.51
1:E:18:MET:SD	1:E:109:VAL:HG11	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:4:LEU:HD22	3:G:25:THR:HG22	1.93	0.51
1:B:119:PRO:HD2	1:B:205:THR:HB	1.93	0.51
3:D:130:GLY:O	3:D:185:LYS:N	2.44	0.51
1:B:84:VAL:HA	1:B:111:VAL:HG22	1.93	0.50
3:G:189:GLU:HA	3:G:213:ARG:HD3	1.92	0.50
1:E:59:TYR:HE1	1:E:69:MET:HG2	1.77	0.50
2:A:5:LEU:HB2	2:A:105:CYS:HB2	1.94	0.50
2:F:97:ILE:HG22	2:F:107:ILE:HB	1.94	0.50
2:C:22:LEU:HD12	2:C:89:VAL:HB	1.93	0.49
2:A:73:VAL:HG11	2:A:118:GLN:HB3	1.94	0.49
3:L:146:ALA:HB2	3:L:200:HIS:HD2	1.76	0.49
1:H:188:SER:OG	1:H:194:TYR:OH	2.16	0.49
1:E:124:LEU:HB2	1:E:139:GLY:C	2.32	0.49
1:B:52(A):PRO:O	1:B:71:ARG:NH2	2.45	0.49
1:B:150:VAL:HG11	1:B:152:VAL:HG13	1.95	0.49
1:E:71:ARG:HG3	1:E:71:ARG:HH21	1.77	0.49
3:G:2:ILE:HB	3:G:26:SER:HB2	1.95	0.49
3:D:204:ARG:O	3:D:204:ARG:NH1	2.46	0.48
2:F:69:ALA:HB3	2:F:92:ALA:HB2	1.95	0.48
1:H:185:PRO:HG2	1:H:188:SER:HB2	1.94	0.48
3:G:33:LEU:HD13	3:G:71:TYR:CD1	2.48	0.48
1:H:84:VAL:HA	1:H:111:VAL:HG23	1.95	0.48
2:A:30:ASN:HB3	3:L:97:PHE:CZ	2.48	0.48
2:C:37:ILE:HD13	2:C:134:ILE:HB	1.96	0.48
2:A:17:SER:OG	2:A:65:ASN:OD1	2.32	0.48
3:D:108:ILE:HB	3:D:168:GLN:HE22	1.79	0.48
1:B:184:VAL:HG22	1:B:185:PRO:HD2	1.95	0.47
1:E:59:TYR:CE1	1:E:69:MET:HG2	2.49	0.47
1:E:116:THR:HG22	1:E:147:PRO:HD3	1.96	0.47
1:E:66:ARG:HD2	1:E:82:LEU:HD11	1.97	0.47
1:B:30:ILE:HA	1:B:52(A):PRO:HB2	1.97	0.47
1:B:195:ILE:HG22	1:B:210:LYS:HA	1.97	0.47
1:E:58:ASN:ND2	2:F:26:ARG:O	2.40	0.47
2:A:32:ASN:O	2:A:34:GLU:N	2.40	0.47
2:A:124:ARG:HG3	2:A:133:ILE:HD11	1.97	0.47
2:C:40:PRO:HG3	2:C:165:PHE:CD2	2.50	0.46
1:B:23:ARG:HA	1:B:77:THR:HA	1.97	0.46
3:D:61:ARG:HH12	3:D:82:ASP:CG	2.19	0.46
3:D:35:TRP:CZ3	3:D:88:CYS:HB3	2.51	0.46
1:B:39:LEU:HD22	1:B:45:PRO:HB3	1.98	0.46
2:A:29:GLY:HA3	2:A:30:ASN:HA	1.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:GLN:NE2	1:B:20:ILE:HG22	2.30	0.46
1:E:47:TRP:CZ2	1:E:49:GLY:HA2	2.50	0.46
3:G:136:CYS:HB2	3:G:150:TRP:CH2	2.50	0.46
1:E:35:ASN:ND2	1:E:100(A):ASN:OD1	2.45	0.46
1:E:66:ARG:NH1	1:E:86:ASP:OD2	2.48	0.46
2:F:120:ALA:HA	2:F:133:ILE:HD12	1.97	0.46
1:H:51:LEU:HD22	1:H:51:LEU:C	2.36	0.46
2:A:30:ASN:HD22	2:A:30:ASN:H	1.62	0.46
3:L:150:TRP:CE2	3:L:181:LEU:HB2	2.51	0.46
2:A:17:SER:HA	6:A:210:NAG:H83	1.97	0.46
1:E:168:ALA:HA	1:E:178:LEU:HB3	1.97	0.46
2:F:57:VAL:HG11	2:F:64:LEU:HB2	1.98	0.46
1:E:139:GLY:HA2	1:E:154:TRP:CH2	2.51	0.45
1:E:194:TYR:H	1:E:210:LYS:HZ3	1.64	0.45
2:F:73:VAL:HG11	2:F:118:GLN:HB3	1.97	0.45
1:B:40:ALA:HB2	1:B:88:ALA:HB2	1.99	0.45
3:G:39:ARG:HH12	3:G:45:ARG:HH11	1.64	0.45
2:A:48:ILE:HG23	2:A:63:PHE:HE1	1.82	0.45
3:D:6:GLN:O	3:D:100:GLN:NE2	2.50	0.45
3:D:141:PHE:HB2	3:D:200:HIS:HE1	1.82	0.45
3:L:136:CYS:HB2	3:L:150:TRP:CZ2	2.52	0.45
1:B:205:THR:HG22	1:B:207:VAL:HG23	1.98	0.45
2:F:39:ARG:NH2	2:F:136:LYS:HD3	2.31	0.45
3:G:24:ARG:NE	3:G:70:ASP:OD1	2.49	0.45
3:G:89:GLN:HG2	3:G:90:GLN:N	2.31	0.45
1:B:146:PHE:HA	1:B:147:PRO:HA	1.72	0.45
2:C:17:SER:OG	6:C:211:NAG:O7	2.28	0.45
3:D:121:PRO:HB3	3:D:211:PHE:CE2	2.52	0.45
1:E:197:ASN:ND2	1:E:208:ASP:OD1	2.48	0.45
3:L:10:THR:OG1	3:L:144:ARG:NH1	2.50	0.44
2:F:126:GLN:HG3	2:F:127:PHE:CD1	2.53	0.44
3:G:146:ALA:HB2	3:G:200:HIS:HD2	1.82	0.44
2:A:39:ARG:NH2	2:A:136:LYS:HD3	2.33	0.44
1:B:40:ALA:HB3	1:B:43:LYS:HE3	1.99	0.44
1:E:33:THR:HG23	1:E:52:LYS:HG2	2.00	0.44
1:H:30:ILE:HA	1:H:52(A):PRO:HB2	1.97	0.44
3:L:169:ASP:O	3:L:173:SER:N	2.40	0.44
1:E:171:GLN:H	1:E:171:GLN:HG2	1.62	0.44
2:F:120:ALA:O	2:F:124:ARG:HB2	2.17	0.44
3:G:126:GLN:HE22	3:G:133:SER:HB2	1.82	0.44
3:G:138:LEU:HB2	3:G:177:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:16:SER:OG	2:C:98:ALA:HA	2.17	0.44
2:A:17:SER:OG	2:A:18:ASN:N	2.50	0.44
1:E:147:PRO:HD2	1:E:202:PRO:HB2	2.00	0.44
1:H:146:PHE:HB2	1:H:175:LEU:HD22	2.00	0.44
3:D:11:LEU:HB2	3:D:104:VAL:HG12	2.00	0.44
1:E:57:VAL:O	2:F:139:SER:OG	2.28	0.44
2:F:24:LEU:HD23	2:F:40:PRO:HA	2.00	0.43
3:G:61:ARG:HH12	3:G:79:GLU:HB2	1.83	0.43
3:G:127:LEU:O	3:G:185:LYS:HD2	2.17	0.43
3:D:117:VAL:HG21	3:D:198:VAL:HG21	2.01	0.43
3:D:168:GLN:HE21	3:D:173:SER:CB	2.31	0.43
3:G:186:ALA:O	3:G:190:LYS:HG3	2.18	0.43
3:L:20:ILE:HG12	3:L:74:THR:HG22	2.00	0.43
3:L:157:GLN:HB3	3:L:160:ASN:HD21	1.84	0.43
1:B:3:GLN:O	1:B:4:LEU:HD23	2.18	0.43
1:H:30:ILE:HD12	1:H:53:ARG:HE	1.84	0.43
1:E:87:THR:CG2	1:E:111:VAL:H	2.28	0.43
1:E:188:SER:HB2	1:E:191:THR:HB	1.99	0.43
2:F:18:ASN:HA	2:F:96:GLU:HA	2.00	0.43
1:H:200:HIS:CD2	1:H:202:PRO:HD2	2.53	0.43
3:D:115:PRO:HA	3:D:140:ASN:O	2.19	0.43
1:E:13:LYS:O	1:E:16:GLU:HG2	2.19	0.43
1:E:136:ALA:HA	3:G:118:PHE:HE2	1.83	0.43
3:G:15:PRO:HD3	3:G:106:VAL:HG23	2.01	0.43
3:L:20:ILE:HG23	3:L:74:THR:HG22	2.01	0.43
3:L:136:CYS:HB3	3:L:179:SER:HB3	2.00	0.43
1:B:30:ILE:HG22	1:B:73:VAL:HG13	2.00	0.43
1:B:119:PRO:HD3	1:B:200:HIS:CD2	2.53	0.43
1:H:75:SER:HB3	1:E:76:ASP:OD2	2.19	0.42
1:H:117:LYS:HD2	1:H:144:ASP:O	2.18	0.42
2:F:5:LEU:HA	2:F:6:PRO:HD2	1.85	0.42
2:F:10:ALA:HA	2:F:11:PRO:HD3	1.72	0.42
2:A:5:LEU:O	2:A:104:HIS:HA	2.19	0.42
1:B:156:SER:N	1:B:197:ASN:OD1	2.52	0.42
1:H:170:LEU:HD13	1:H:176:TYR:CE1	2.54	0.42
1:B:71:ARG:NH1	2:C:142:ASP:OD1	2.53	0.42
1:H:57:VAL:HG11	1:H:59:TYR:CZ	2.54	0.42
2:F:96:GLU:O	2:F:107:ILE:HD13	2.18	0.42
1:H:57:VAL:HG12	2:A:139:SER:HB2	2.01	0.42
1:H:52:LYS:HA	1:H:52(A):PRO:HD3	1.84	0.42
1:B:8:GLY:HA2	1:B:105:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:7:SER:HA	3:D:8:PRO:HA	1.79	0.42
3:D:16:GLY:O	3:D:77:ASN:HA	2.19	0.42
3:D:114:ALA:HA	3:D:115:PRO:HD3	1.88	0.42
3:D:140:ASN:ND2	3:D:174:THR:OG1	2.34	0.42
2:F:30:ASN:O	2:F:31:SER:HB2	2.19	0.42
1:E:210:LYS:HE3	1:E:212:GLU:HG3	2.02	0.41
2:C:60:SER:O	2:C:62:LEU:N	2.46	0.41
2:F:16:SER:HB3	2:F:97:ILE:O	2.19	0.41
1:B:37:ILE:HG23	1:B:46:GLU:O	2.20	0.41
2:A:8:ARG:HA	2:A:9:PRO:HA	1.83	0.41
2:A:44:ASP:OD1	2:A:45:MET:N	2.49	0.41
1:B:52:LYS:HA	1:B:52(A):PRO:HD3	1.73	0.41
1:B:123:PRO:HB3	1:B:210:LYS:O	2.21	0.41
1:B:150:VAL:HG12	1:B:151:THR:N	2.36	0.41
2:C:19:ILE:HD13	2:C:62:LEU:HD13	2.02	0.41
3:L:8:PRO:HG2	3:L:11:LEU:HB2	2.03	0.41
3:L:13:LEU:HB2	3:L:17:GLU:OE2	2.20	0.41
1:B:146:PHE:HB2	1:B:175:LEU:CD2	2.51	0.41
3:D:58:ILE:HD13	3:D:58:ILE:HA	1.91	0.41
3:D:204:ARG:HA	3:D:204:ARG:HD2	1.95	0.41
2:F:80:PHE:HB3	2:F:127:PHE:CE1	2.56	0.41
1:H:43:LYS:HE3	1:H:43:LYS:HB2	1.93	0.41
1:E:65:GLY:O	1:E:82(A):ARG:NH2	2.54	0.41
1:H:87:THR:HG22	1:H:111:VAL:N	2.35	0.40
1:H:12:LYS:HB2	1:H:111:VAL:HG12	2.02	0.40
1:H:31:ASP:HB3	1:H:98:CYS:SG	2.61	0.40
1:B:6:GLN:NE2	1:B:90:TYR:O	2.49	0.40
1:B:12:LYS:NZ	1:B:18:MET:HA	2.30	0.40
2:C:5:LEU:HA	2:C:6:PRO:HD3	1.90	0.40
2:A:10:ALA:HA	2:A:11:PRO:HD3	1.83	0.40
1:B:57:VAL:HG11	1:B:59:TYR:CE1	2.55	0.40
3:L:127:LEU:HA	3:L:127:LEU:HD23	1.84	0.40
2:C:26:ARG:HD2	2:C:36:GLU:OE1	2.22	0.40
1:E:194:TYR:H	1:E:210:LYS:NZ	2.18	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	B	210/224 (94%)	195 (93%)	13 (6%)	2 (1%)	15	47
1	E	210/224 (94%)	199 (95%)	11 (5%)	0	100	100
1	H	210/224 (94%)	199 (95%)	10 (5%)	1 (0%)	29	62
2	A	168/182 (92%)	154 (92%)	12 (7%)	2 (1%)	13	43
2	C	166/182 (91%)	158 (95%)	7 (4%)	1 (1%)	25	59
2	F	150/182 (82%)	137 (91%)	11 (7%)	2 (1%)	12	41
3	D	207/210 (99%)	197 (95%)	8 (4%)	2 (1%)	15	47
3	G	204/210 (97%)	194 (95%)	10 (5%)	0	100	100
3	L	204/210 (97%)	193 (95%)	10 (5%)	1 (0%)	29	62
All	All	1729/1848 (94%)	1626 (94%)	92 (5%)	11 (1%)	25	59

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	SER
2	F	30	ASN
2	A	70	GLU
1	B	100(D)	PHE
2	A	33	ALA
1	H	100(D)	PHE
2	C	61	GLN
3	D	40	PRO
2	F	31	SER
3	L	206	PRO
3	D	206	PRO

5.3.2 Protein sidechains [i](#)

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	B	183/193 (95%)	169 (92%)	14 (8%)	13	38
1	E	183/193 (95%)	175 (96%)	8 (4%)	28	58
1	H	183/193 (95%)	174 (95%)	9 (5%)	25	55
2	A	138/149 (93%)	133 (96%)	5 (4%)	35	63
2	C	138/149 (93%)	129 (94%)	9 (6%)	17	46
2	F	131/149 (88%)	123 (94%)	8 (6%)	18	49
3	D	181/182 (100%)	177 (98%)	4 (2%)	52	74
3	G	179/182 (98%)	173 (97%)	6 (3%)	37	64
3	L	179/182 (98%)	172 (96%)	7 (4%)	32	61
All	All	1495/1572 (95%)	1425 (95%)	70 (5%)	26	57

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	34	LEU
1	H	51	LEU
1	H	57	VAL
1	H	66	ARG
1	H	71	ARG
1	H	98	CYS
1	H	101	GLU
1	H	135	THR
1	H	159	LEU
2	A	22	LEU
2	A	27	ASP
2	A	30	ASN
2	A	53	ILE
2	A	68	LEU
3	L	11	LEU
3	L	13	LEU
3	L	24	ARG
3	L	26	SER

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Mol	Chain	Res	Type
3	L	106	VAL
3	L	172	ASP
3	L	174	THR
1	B	16	GLU
1	B	28	GLU
1	B	30	ILE
1	B	46	GLU
1	B	53	ARG
1	B	63	LEU
1	B	66	ARG
1	B	71	ARG
1	B	97	ASN
1	B	101	GLU
1	B	152	VAL
1	B	169	VAL
1	B	170	LEU
1	B	184	VAL
2	C	8	ARG
2	C	22	LEU
2	C	44	ASP
2	C	71	GLU
2	C	73	VAL
2	C	96	GLU
2	C	137	GLN
2	C	139	SER
2	C	155	GLU
3	D	14	SER
3	D	60	ASP
3	D	76	SER
3	D	103	LYS
1	E	33	THR
1	E	39	LEU
1	E	71	ARG
1	E	85	ASP
1	E	101	GLU
1	E	109	VAL
1	E	124	LEU
1	E	179	SER
2	F	22	LEU
2	F	27	ASP
2	F	53	ILE
2	F	95	VAL

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Mol	Chain	Res	Type
2	F	129	ASN
2	F	149	TRP
2	F	161	SER
2	F	167	SER
3	G	2	ILE
3	G	3	VAL
3	G	18	THR
3	G	73	LEU
3	G	74	THR
3	G	124	ASP

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

Mol	Chain	Res	Type
1	H	102	HIS
1	H	164	HIS
2	A	30	ASN
2	A	52	GLN
2	A	83	ASN
2	A	148	HIS
3	D	157	GLN
3	D	160	ASN
2	F	90	GLN
2	F	163	GLN
3	G	126	GLN

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](#)

25 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
4	NAG	I	1	2,4	14,14,15	0.43	0	17,19,21	0.48	0
4	NAG	I	2	4	14,14,15	0.49	0	17,19,21	0.48	0
4	BMA	I	3	4	11,11,12	0.84	1 (9%)	15,15,17	1.16	1 (6%)
4	MAN	I	4	4	11,11,12	0.71	0	15,15,17	1.14	2 (13%)
4	MAN	I	5	4	11,11,12	0.77	1 (9%)	15,15,17	1.11	1 (6%)
4	MAN	I	6	4	11,11,12	0.92	0	15,15,17	0.97	0
4	MAN	I	7	4	11,11,12	1.14	1 (9%)	15,15,17	1.02	1 (6%)
4	MAN	I	8	4	11,11,12	0.69	0	15,15,17	1.09	2 (13%)
4	MAN	I	9	4	11,11,12	1.02	1 (9%)	15,15,17	0.88	1 (6%)
4	NAG	J	1	2,4	14,14,15	0.16	0	17,19,21	0.56	0
4	NAG	J	2	4	14,14,15	0.50	0	17,19,21	0.40	0
4	BMA	J	3	4	11,11,12	0.72	1 (9%)	15,15,17	1.07	1 (6%)
4	MAN	J	4	4	11,11,12	1.03	1 (9%)	15,15,17	1.22	1 (6%)
4	MAN	J	5	4	11,11,12	0.91	1 (9%)	15,15,17	0.99	2 (13%)
4	MAN	J	6	4	11,11,12	0.98	1 (9%)	15,15,17	0.97	1 (6%)
4	MAN	J	7	4	11,11,12	0.63	0	15,15,17	1.21	2 (13%)
4	MAN	J	8	4	11,11,12	1.01	1 (9%)	15,15,17	1.09	1 (6%)
4	MAN	J	9	4	11,11,12	0.96	1 (9%)	15,15,17	1.21	3 (20%)
5	NAG	K	1	5,2	14,14,15	0.23	0	17,19,21	0.51	0
5	NAG	K	2	5	14,14,15	0.25	0	17,19,21	0.50	0
5	BMA	K	3	5	11,11,12	0.93	1 (9%)	15,15,17	1.01	0
5	MAN	K	4	5	11,11,12	0.66	0	15,15,17	1.23	2 (13%)
5	MAN	K	5	5	11,11,12	0.71	0	15,15,17	1.01	2 (13%)
5	MAN	K	6	5	11,11,12	0.89	0	15,15,17	1.12	1 (6%)
5	MAN	K	7	5	11,11,12	0.90	0	15,15,17	0.88	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	1	2,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1
4	MAN	I	4	4	-	1/2/19/22	0/1/1/1
4	MAN	I	5	4	-	2/2/19/22	0/1/1/1
4	MAN	I	6	4	-	0/2/19/22	0/1/1/1
4	MAN	I	7	4	-	2/2/19/22	0/1/1/1
4	MAN	I	8	4	-	0/2/19/22	0/1/1/1
4	MAN	I	9	4	-	2/2/19/22	0/1/1/1
4	NAG	J	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	MAN	J	4	4	-	0/2/19/22	0/1/1/1
4	MAN	J	5	4	-	1/2/19/22	0/1/1/1
4	MAN	J	6	4	-	1/2/19/22	0/1/1/1
4	MAN	J	7	4	-	2/2/19/22	0/1/1/1
4	MAN	J	8	4	-	0/2/19/22	0/1/1/1
4	MAN	J	9	4	-	2/2/19/22	0/1/1/1
5	NAG	K	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	MAN	K	4	5	-	2/2/19/22	0/1/1/1
5	MAN	K	5	5	-	2/2/19/22	0/1/1/1
5	MAN	K	6	5	-	2/2/19/22	0/1/1/1
5	MAN	K	7	5	-	0/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	7	MAN	O5-C1	-3.01	1.38	1.43
4	J	4	MAN	O5-C1	-2.87	1.39	1.43
4	I	9	MAN	O5-C1	-2.57	1.39	1.43
4	J	5	MAN	O5-C1	-2.48	1.39	1.43
4	J	6	MAN	O5-C1	-2.41	1.39	1.43
4	I	3	BMA	O5-C1	-2.39	1.39	1.43
5	K	3	BMA	O5-C1	-2.34	1.40	1.43
4	J	9	MAN	O5-C1	-2.09	1.40	1.43
4	J	8	MAN	O5-C1	-2.06	1.40	1.43
4	I	5	MAN	O5-C1	-2.04	1.40	1.43
4	J	3	BMA	O5-C1	-2.00	1.40	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	4	MAN	C1-O5-C5	2.95	116.19	112.19
4	I	4	MAN	C1-O5-C5	2.86	116.07	112.19
4	J	7	MAN	C1-O5-C5	2.85	116.05	112.19
4	J	8	MAN	C1-O5-C5	2.78	115.95	112.19
4	J	4	MAN	O2-C2-C3	-2.75	104.62	110.14
4	J	9	MAN	C1-O5-C5	2.75	115.91	112.19
4	I	4	MAN	O2-C2-C3	-2.65	104.82	110.14
4	I	8	MAN	C1-O5-C5	2.61	115.72	112.19
4	J	5	MAN	O2-C2-C3	-2.59	104.95	110.14
5	K	4	MAN	O2-C2-C3	-2.57	104.99	110.14
4	I	3	BMA	C1-O5-C5	2.43	115.49	112.19
4	I	5	MAN	O2-C2-C3	-2.43	105.27	110.14
4	J	9	MAN	C1-C2-C3	-2.30	106.84	109.67
4	J	7	MAN	O2-C2-C3	-2.30	105.54	110.14
5	K	6	MAN	C1-O5-C5	2.29	115.30	112.19
4	J	9	MAN	O2-C2-C3	-2.23	105.67	110.14
5	K	5	MAN	O2-C2-C3	-2.20	105.73	110.14
4	J	6	MAN	O2-C2-C3	-2.16	105.81	110.14
4	J	3	BMA	C1-O5-C5	2.16	115.12	112.19
5	K	5	MAN	C1-O5-C5	2.15	115.11	112.19
4	I	7	MAN	C1-C2-C3	-2.08	107.10	109.67
4	I	9	MAN	O2-C2-C3	-2.07	105.99	110.14
4	I	8	MAN	O2-C2-C3	-2.07	106.00	110.14
4	J	5	MAN	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O5-C5-C6-O6
5	K	6	MAN	O5-C5-C6-O6
4	I	7	MAN	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	K	5	MAN	O5-C5-C6-O6
4	I	7	MAN	C4-C5-C6-O6
5	K	6	MAN	C4-C5-C6-O6
4	I	5	MAN	O5-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
4	I	5	MAN	C4-C5-C6-O6
4	J	7	MAN	O5-C5-C6-O6

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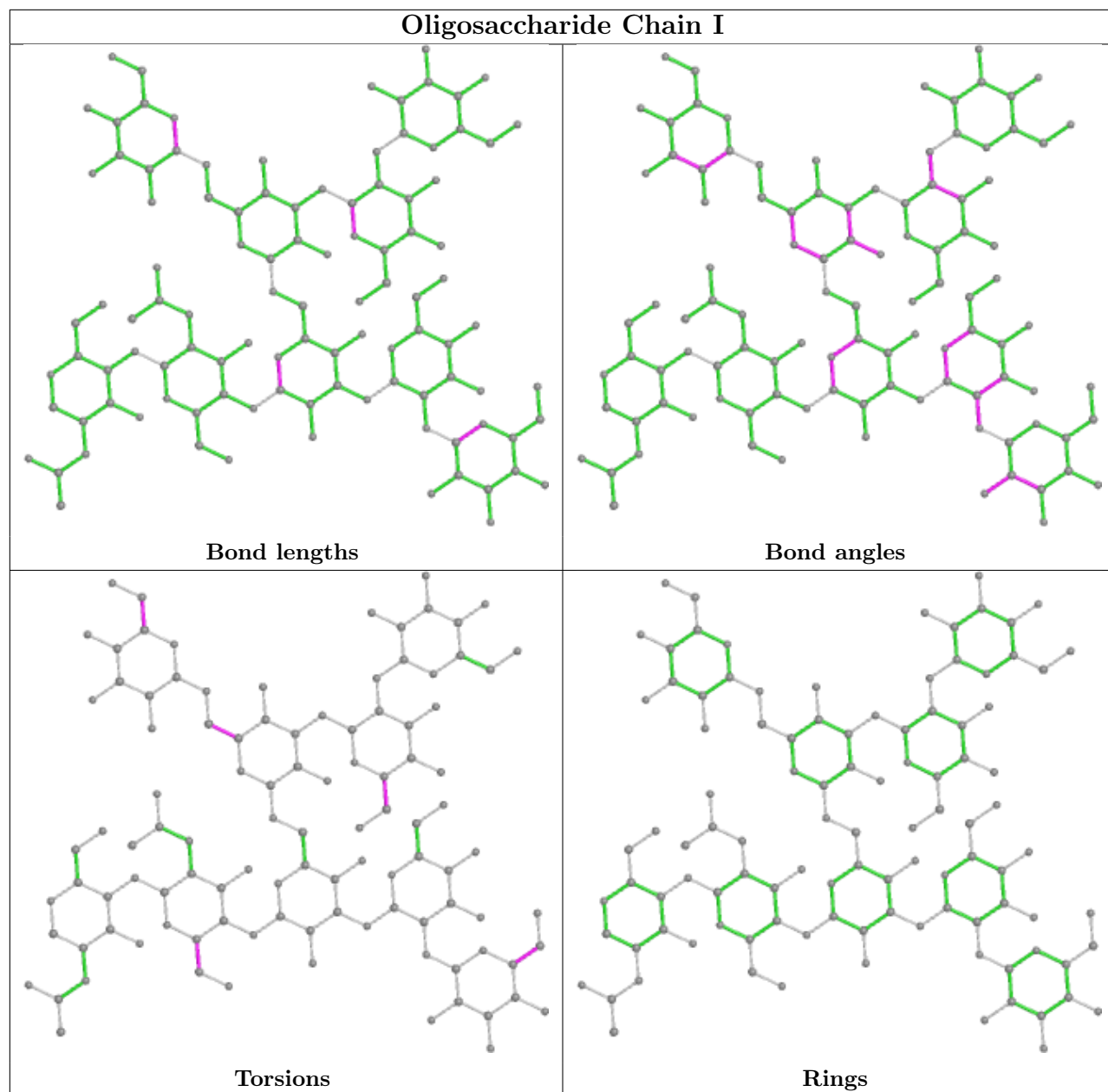
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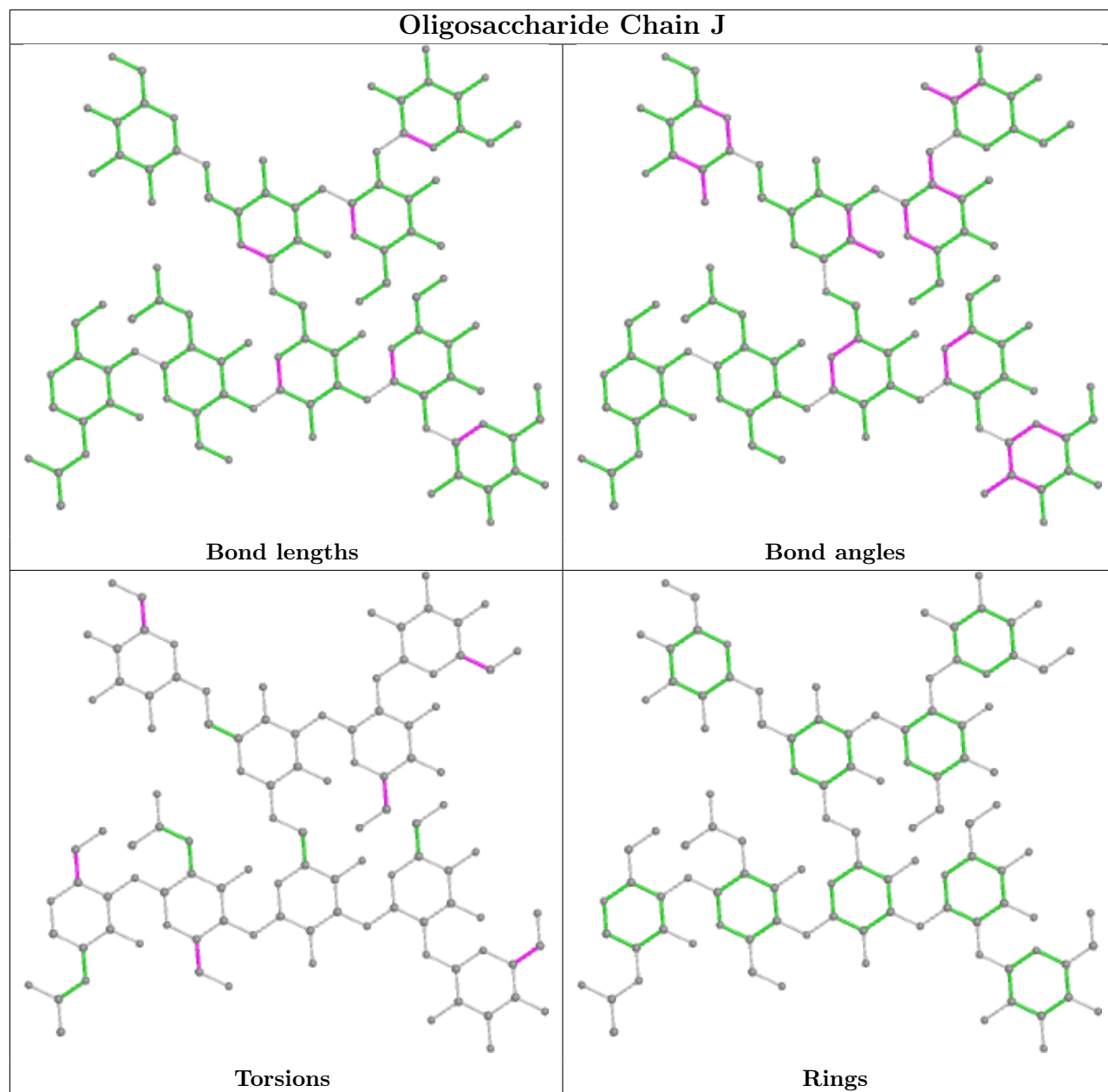
Mol	Chain	Res	Type	Atoms
5	K	4	MAN	O5-C5-C6-O6
4	I	9	MAN	O5-C5-C6-O6
5	K	5	MAN	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	J	5	MAN	O5-C5-C6-O6
4	J	9	MAN	O5-C5-C6-O6
4	J	7	MAN	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
5	K	4	MAN	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	I	9	MAN	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
4	J	9	MAN	C4-C5-C6-O6
4	J	6	MAN	C4-C5-C6-O6
4	I	4	MAN	O5-C5-C6-O6

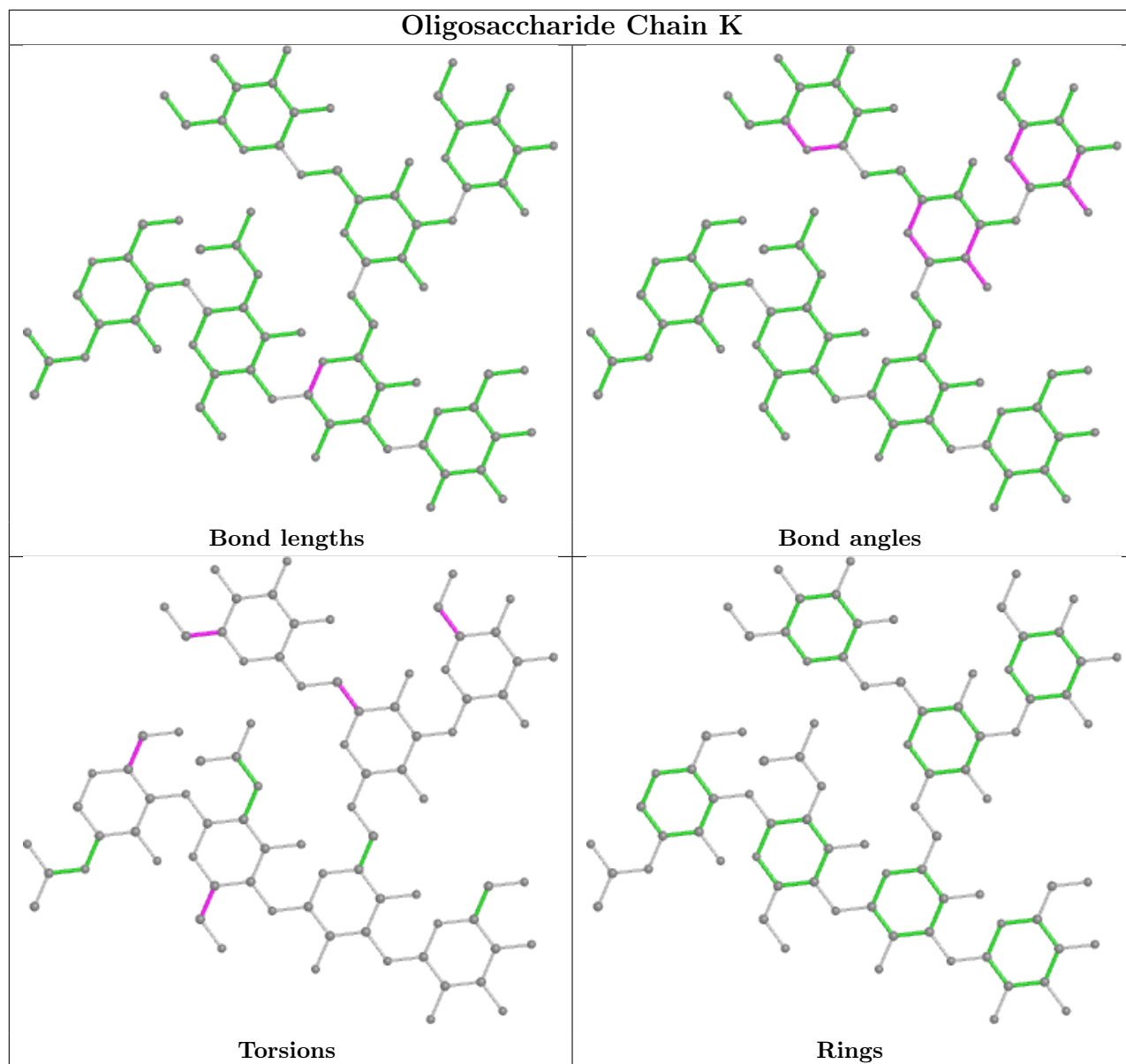
There are no ring outliers.

No monomer is involved in short contacts.

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](#)

4 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	NAG	C	211	2	14,14,15	0.25	0	17,19,21	0.68	0
6	NAG	C	201	2	14,14,15	0.48	0	17,19,21	0.57	0
6	NAG	A	211	2	14,14,15	0.33	0	17,19,21	0.61	0
6	NAG	A	210	2	14,14,15	0.23	0	17,19,21	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	211	2	-	3/6/23/26	0/1/1/1
6	NAG	C	201	2	-	3/6/23/26	0/1/1/1
6	NAG	A	211	2	-	3/6/23/26	0/1/1/1
6	NAG	A	210	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	211	NAG	O5-C5-C6-O6
6	A	211	NAG	C4-C5-C6-O6
6	A	210	NAG	O5-C5-C6-O6
6	C	211	NAG	O5-C5-C6-O6
6	A	210	NAG	C4-C5-C6-O6
6	C	211	NAG	C4-C5-C6-O6
6	C	201	NAG	O5-C5-C6-O6
6	C	201	NAG	C4-C5-C6-O6
6	A	211	NAG	C3-C2-N2-C7
6	C	201	NAG	C3-C2-N2-C7
6	A	210	NAG	C3-C2-N2-C7
6	C	211	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	211	NAG	1	0
6	A	210	NAG	1	0

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 [i](#)

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

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	B	214/224 (95%)	1.03	41 (19%) 1 1	51, 99, 238, 258	0
1	E	214/224 (95%)	0.32	7 (3%) 46 43	73, 116, 153, 166	0
1	H	214/224 (95%)	0.34	11 (5%) 28 26	69, 116, 155, 168	0
2	A	170/182 (93%)	0.65	16 (9%) 8 9	76, 131, 172, 213	0
2	C	170/182 (93%)	0.21	2 (1%) 79 77	54, 91, 135, 186	0
2	F	156/182 (85%)	0.81	18 (11%) 4 4	109, 162, 198, 207	0
3	D	209/210 (99%)	1.00	50 (23%) 0 0	46, 110, 243, 263	0
3	G	206/210 (98%)	0.17	7 (3%) 45 42	55, 95, 157, 188	0
3	L	206/210 (98%)	0.29	10 (4%) 29 27	58, 103, 167, 185	0
All	All	1759/1848 (95%)	0.53	162 (9%) 9 10	46, 115, 207, 263	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	138	LEU	13.4
1	B	126	PRO	11.6
3	D	195	ALA	11.4
1	B	159	LEU	9.0
1	B	158	ALA	8.0
1	B	193	THR	7.5
1	B	125	ALA	7.1
3	D	135	VAL	6.4
1	B	194	TYR	6.3
3	D	134	VAL	6.0
3	D	196	CYS	5.9
3	D	148	VAL	5.8
1	B	157	GLY	5.7
3	D	147	LYS	5.6
3	D	136	CYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	180	SER	5.2
3	D	153	ASP	5.2
3	D	157	GLN	5.1
1	B	192	GLN	4.9
3	D	146	ALA	4.7
1	B	191	THR	4.7
1	B	202	PRO	4.6
3	D	183	LEU	4.4
3	D	207	VAL	4.4
3	D	154	ASN	4.4
3	L	194	TYR	4.3
3	D	133	SER	4.3
1	B	187	SER	4.3
1	B	185	PRO	4.2
3	D	181	LEU	4.1
2	A	99	CYS	4.1
3	D	203	LEU	4.0
2	F	159	CYS	3.9
3	D	208	THR	3.8
2	F	19	ILE	3.8
3	D	214	GLY	3.8
3	D	198	VAL	3.8
2	A	102	ALA	3.7
3	D	186	ALA	3.7
1	E	18	MET	3.7
1	B	141	LEU	3.6
3	D	216	CYS	3.6
3	D	194	TYR	3.6
1	B	208	ASP	3.6
1	B	186	SER	3.6
3	D	205	SER	3.6
2	F	160	ALA	3.6
1	B	137	ALA	3.5
3	L	195	ALA	3.5
3	D	180	THR	3.5
1	B	178	LEU	3.4
1	H	212	GLU	3.4
3	D	150	TRP	3.4
1	B	188	SER	3.3
2	F	152	CYS	3.3
3	G	210	SER	3.2
3	L	113	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	189	LEU	3.2
3	D	188	TYR	3.2
1	H	18	MET	3.1
1	B	117	LYS	3.1
2	A	43	GLY	3.1
1	B	183	THR	3.0
3	D	117	VAL	3.0
2	A	47	ASP	3.0
1	B	120	SER	3.0
3	D	160	ASN	3.0
2	A	100	THR	3.0
1	B	206	LYS	3.0
1	E	191	THR	3.0
3	G	194	TYR	2.9
3	L	151	LYS	2.9
1	H	82(C)	LEU	2.9
3	D	200	HIS	2.9
3	G	211	PHE	2.9
3	D	210	SER	2.9
1	B	124	LEU	2.9
1	B	210	LYS	2.9
2	F	15	CYS	2.9
1	B	155	ASN	2.9
2	F	118	GLN	2.8
3	L	152	VAL	2.8
1	E	175	LEU	2.8
1	B	156	SER	2.8
3	D	179	SER	2.8
3	D	151	LYS	2.8
1	B	197	ASN	2.8
3	L	155	ALA	2.8
1	B	184	VAL	2.7
3	L	188	TYR	2.7
2	A	86	SER	2.7
2	F	150	PHE	2.7
1	B	123	PRO	2.7
1	B	139	GLY	2.7
3	D	149	GLN	2.7
2	A	50	ARG	2.7
3	G	133	SER	2.7
2	A	71	GLU	2.7
3	D	209	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	118	PHE	2.6
1	B	140	CYS	2.6
1	B	154	TRP	2.6
3	D	184	SER	2.6
2	F	133	ILE	2.6
2	F	31	SER	2.5
1	H	159	LEU	2.5
1	B	116	THR	2.5
3	D	155	ALA	2.5
1	E	110	ILE	2.5
2	F	170	PHE	2.5
3	G	132	ALA	2.5
3	D	197	GLU	2.5
2	A	98	ALA	2.4
2	A	11	PRO	2.4
1	B	118	GLY	2.4
1	H	82	LEU	2.4
3	D	119	ILE	2.4
3	G	192	LYS	2.4
3	D	193	VAL	2.4
2	A	101	GLY	2.4
2	F	2	THR	2.4
3	D	122	PRO	2.3
2	F	155	GLU	2.3
1	B	201	LYS	2.3
3	D	199	THR	2.3
3	D	212	ASN	2.3
1	E	111	VAL	2.3
2	F	102	ALA	2.3
2	F	103	GLY	2.2
2	F	153	GLY	2.2
2	A	103	GLY	2.2
3	D	158	SER	2.2
3	D	191	HIS	2.2
2	F	99	CYS	2.2
3	G	193	VAL	2.2
1	H	210	LYS	2.2
3	D	132	ALA	2.1
1	B	205	THR	2.1
2	F	16	SER	2.1
2	F	94	SER	2.1
1	B	190	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
3	L	153	ASP	2.1
2	A	51	CYS	2.1
2	A	14	HIS	2.1
3	L	206	PRO	2.1
1	E	31	ASP	2.1
2	C	129	ASN	2.1
3	D	137	LEU	2.1
3	D	123	SER	2.1
1	H	191	THR	2.1
2	A	105	CYS	2.1
2	A	10	ALA	2.1
2	C	70	GLU	2.1
1	H	190	GLY	2.1
3	L	183	LEU	2.1
1	B	142	VAL	2.1
1	B	151	THR	2.0
1	H	39	LEU	2.0
1	H	107	THR	2.0
3	D	202	GLY	2.0
3	D	204	ARG	2.0
1	E	109	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MAN	K	7	11/12	0.76	0.28	125,131,136,139	0
4	MAN	I	9	11/12	0.81	0.17	102,132,137,138	0
5	MAN	K	6	11/12	0.81	0.23	117,121,142,147	0
4	MAN	I	6	11/12	0.81	0.30	126,136,147,151	0
4	MAN	J	9	11/12	0.84	0.27	141,147,160,161	0
5	BMA	K	3	11/12	0.88	0.20	110,116,126,133	0
4	MAN	I	8	11/12	0.89	0.27	97,108,121,128	0

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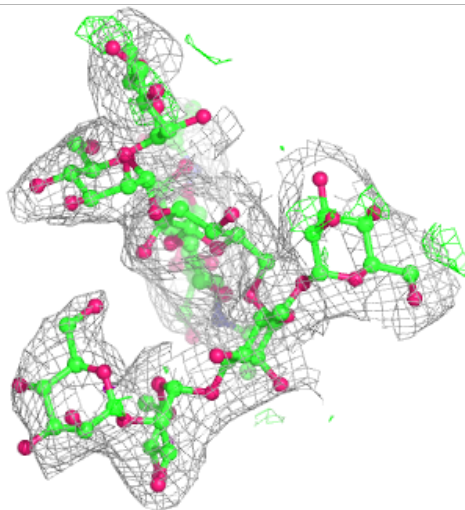
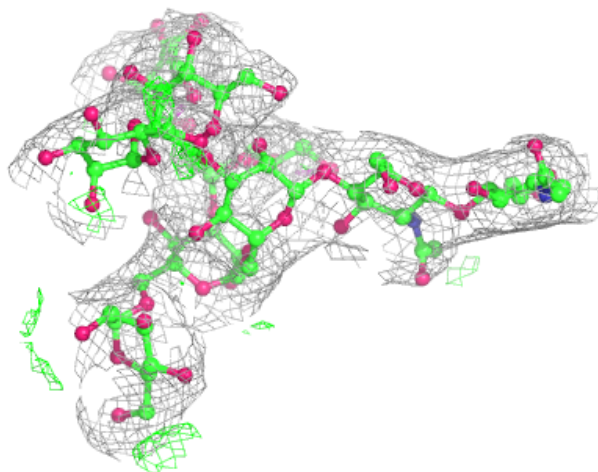
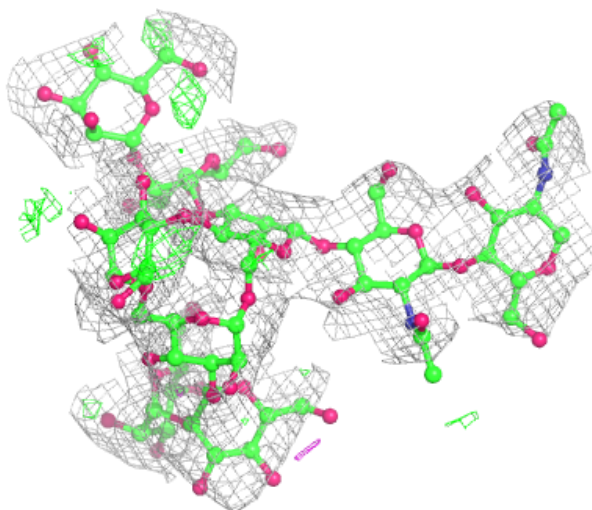
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MAN	I	5	11/12	0.90	0.20	109,122,127,138	0
5	MAN	K	5	11/12	0.91	0.13	121,127,139,143	0
4	MAN	J	7	11/12	0.91	0.20	65,69,88,91	0
4	MAN	J	8	11/12	0.91	0.18	94,119,127,128	0
4	MAN	J	6	11/12	0.92	0.18	83,111,119,120	0
4	MAN	I	7	11/12	0.93	0.15	82,97,107,109	0
4	NAG	J	1	14/15	0.93	0.20	59,67,108,108	0
4	BMA	I	3	11/12	0.93	0.17	74,89,102,110	0
5	NAG	K	1	14/15	0.93	0.16	90,100,134,138	0
5	MAN	K	4	11/12	0.94	0.12	96,104,110,111	0
4	BMA	J	3	11/12	0.94	0.16	73,88,95,113	0
5	NAG	K	2	14/15	0.95	0.21	93,109,116,117	0
4	MAN	J	5	11/12	0.95	0.15	75,86,105,110	0
4	NAG	I	1	14/15	0.95	0.17	50,68,88,99	0
4	MAN	I	4	11/12	0.96	0.18	77,93,104,106	0
4	NAG	J	2	14/15	0.96	0.17	69,75,88,93	0
4	NAG	I	2	14/15	0.96	0.17	78,83,86,90	0
4	MAN	J	4	11/12	0.96	0.14	58,60,68,71	0

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

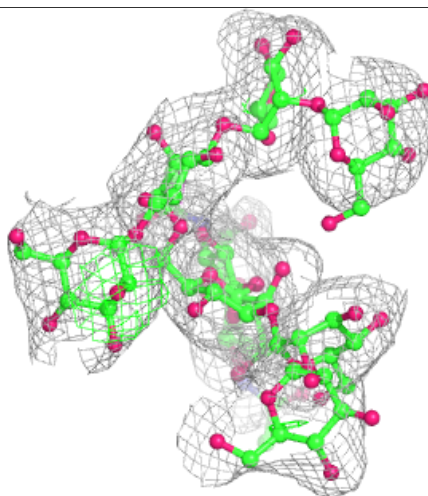
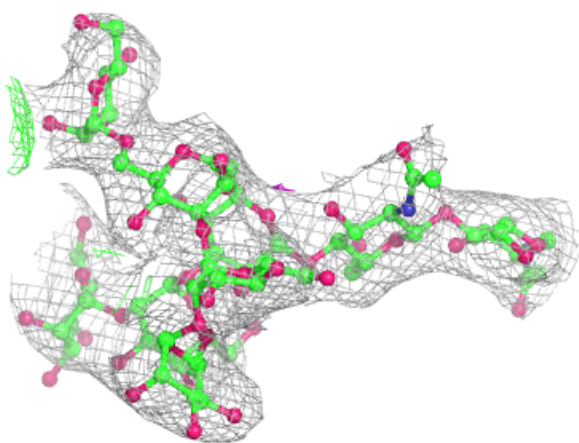
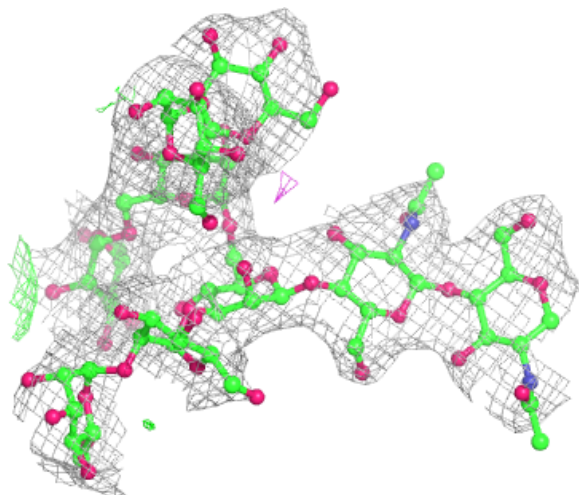
Electron density around Chain I:

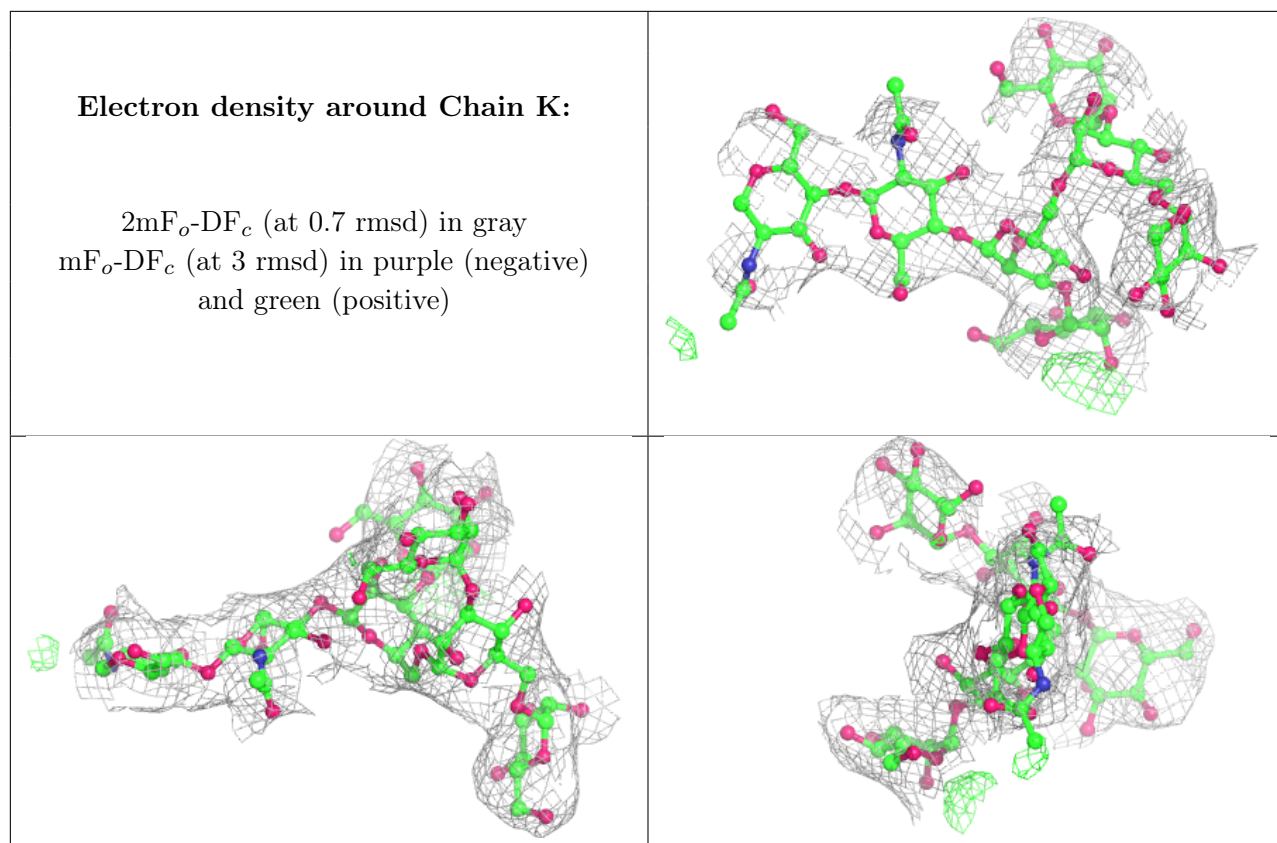
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain J:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	C	201	14/15	0.67	0.25	102,113,121,121	0
6	NAG	A	211	14/15	0.79	0.22	113,124,128,132	0
6	NAG	A	210	14/15	0.81	0.39	122,143,163,167	0
6	NAG	C	211	14/15	0.84	0.27	86,115,119,125	0

6.5 Other polymers [i](#)

There are no such residues in this entry.