



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2020 – 09:07 PM BST

PDB ID : 6WOQ
Title : Structure of Hepatitis C Virus Envelope Glycoprotein E2 core from genotype 1a bound to neutralizing antibody HC1AM and non neutralizing antibody E1
Authors : Tzarum, N.; Wilson, I.A.; Law, M.
Deposited on : 2020-04-25
Resolution : 3.67 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 : 2.14.6
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) : 2.14.6

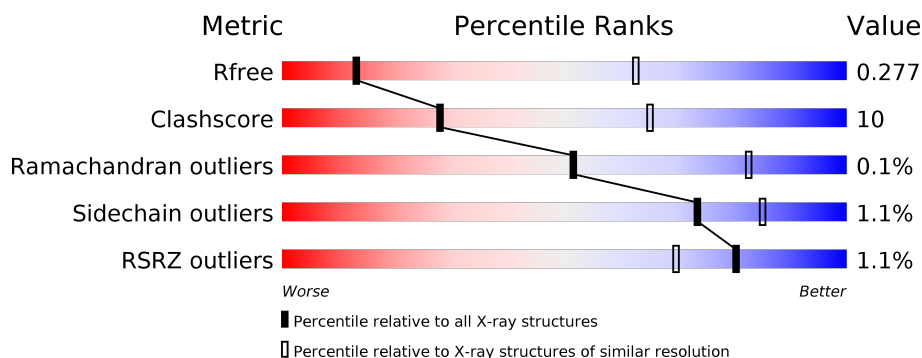
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.67 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	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)

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 $\leq 5\%$. 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	227	<div> <div>78%</div> <div>16%</div> <div>5%</div> </div>
1	C	227	<div> <div>68%</div> <div>16%</div> <div>16%</div> </div>
2	B	221	<div> <div>78%</div> <div>20%</div> <div>•</div> </div>
2	D	221	<div> <div>75%</div> <div>23%</div> <div>••</div> </div>
3	E	191	<div> <div>48%</div> <div>24%</div> <div>28%</div> </div>
3	F	191	<div> <div>46%</div> <div>19%</div> <div>35%</div> </div>

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Mol	Chain	Length	Quality of chain
4	G	229	
4	J	229	
5	H	215	
5	K	215	
6	I	2	
6	L	2	
6	M	2	
6	N	2	
6	O	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	N	2	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14990 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 Fab E1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1597	1011	264	314	8			
1	C	191	Total	C	N	O	S	0	0	0
			1436	916	236	276	8			

- Molecule 2 is a protein called Fab E1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1676	1049	290	332	5			
2	D	217	Total	C	N	O	S	0	0	0
			1676	1049	290	332	5			

- Molecule 3 is a protein called Envelope glycoprotein E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	137	Total	C	N	O	S	0	0	0
			1065	681	183	189	12			
3	F	125	Total	C	N	O	S	0	0	0
			982	630	167	175	10			

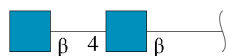
- Molecule 4 is a protein called Fab HC1AM heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	218	Total	C	N	O	S	0	0	0
			1627	1031	275	315	6			
4	G	213	Total	C	N	O	S	0	0	0
			1597	1015	267	309	6			

- Molecule 5 is a protein called Fab HC1AM light chain.

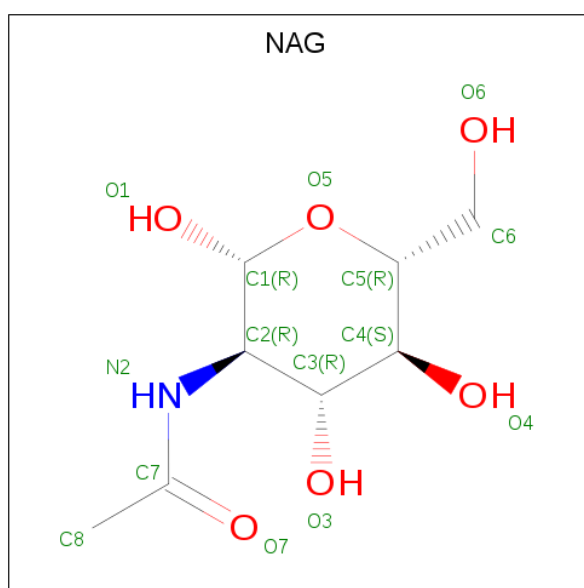
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	212	Total	C	N	O	S	0	0	0
			1631	1020	285	322	4			
5	H	195	Total	C	N	O	S	0	0	0
			1521	960	259	298	4			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	O	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

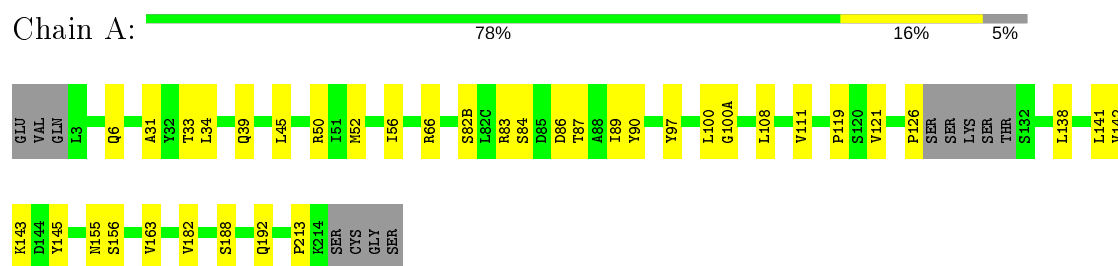


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		

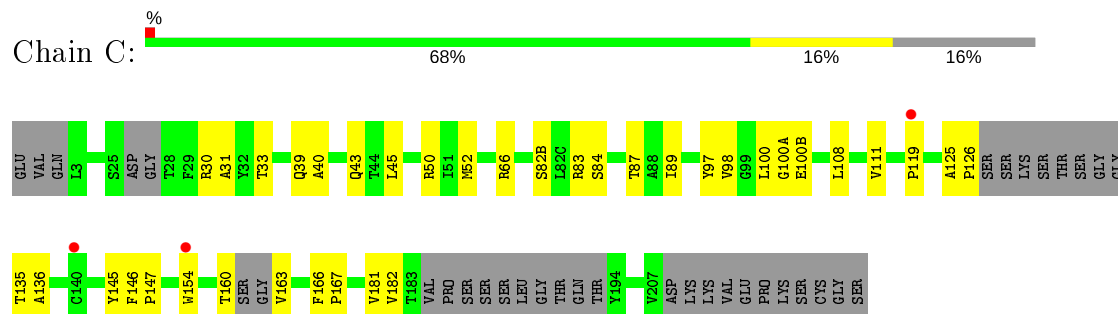
3 Residue-property plots

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.

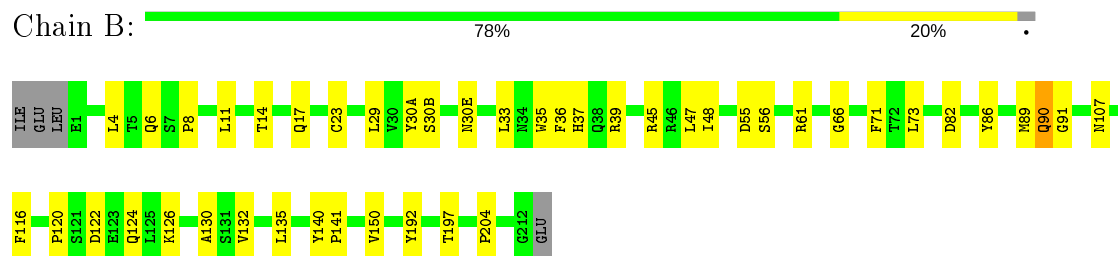
- Molecule 1: Fab E1 heavy chain



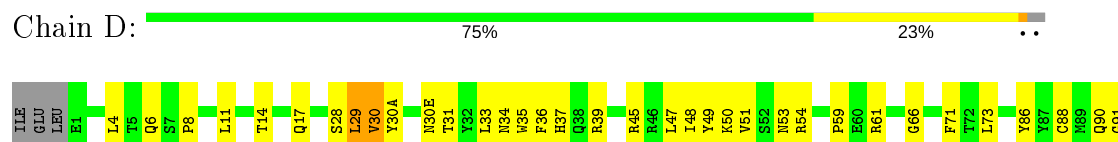
- Molecule 1: Fab E1 heavy chain

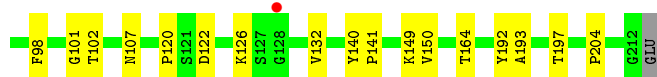


- Molecule 2: Fab E1 light chain

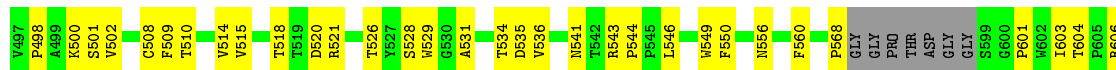
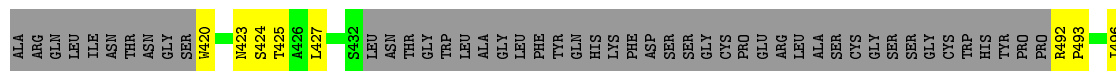


- Molecule 2: Fab E1 light chain

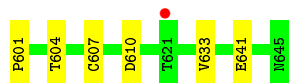
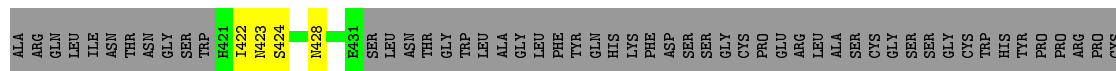




• Molecule 3: Envelope glycoprotein E2



• Molecule 3: Envelope glycoprotein E2



• Molecule 4: Fab HC1AM heavy chain



• Molecule 4: Fab HC1AM heavy chain





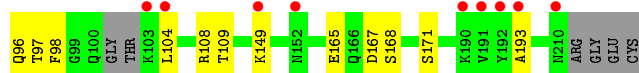
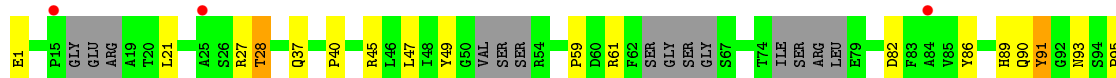
- Molecule 5: Fab HC1AM light chain

Chain K: 82% 16%



- Molecule 5: Fab HC1AM light chain

Chain H: 6% 77% 13% 9%



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

Chain I: 50% 50%



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

Chain L: 50% 50%



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

Chain M: 50% 50%

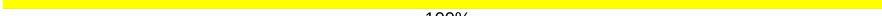


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 50%

HA01
HA02

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

Chain O:  100%

HA01
HA02

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	200.74Å 103.72Å 196.15Å 90.00° 113.65° 90.00°	Depositor
Resolution (Å)	34.66 – 3.67 34.66 – 3.67	Depositor EDS
% Data completeness (in resolution range)	82.2 (34.66-3.67) 82.2 (34.66-3.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.66Å)	Xtriage
Refinement program	PHENIX 1.12 _2829	Depositor
R, R_{free}	0.227 , 0.277 0.228 , 0.277	Depositor DCC
R_{free} test set	1589 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	110.9	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14990	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/1634	0.46	0/2224
1	C	0.25	0/1468	0.46	0/1996
2	B	0.25	0/1715	0.45	0/2331
2	D	0.28	0/1715	0.47	0/2331
3	E	0.28	0/1103	0.50	1/1514 (0.1%)
3	F	0.30	0/1015	0.50	1/1392 (0.1%)
4	G	0.25	0/1630	0.46	0/2218
4	J	0.25	0/1662	0.47	0/2264
5	H	0.25	0/1552	0.44	0/2102
5	K	0.28	0/1665	0.46	0/2257
All	All	0.26	0/15159	0.46	2/20629 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	510	THR	C-N-CD	-5.03	109.53	120.60
3	E	510	THR	C-N-CD	-5.03	109.54	120.60

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	1597	0	1582	22	0
1	C	1436	0	1421	22	0
2	B	1676	0	1629	25	0
2	D	1676	0	1629	43	0
3	E	1065	0	993	42	0
3	F	982	0	926	32	0
4	G	1597	0	1609	31	0
4	J	1627	0	1637	52	0
5	H	1521	0	1485	24	0
5	K	1631	0	1603	27	0
6	I	28	0	25	1	0
6	L	28	0	25	6	0
6	M	28	0	25	2	0
6	N	28	0	25	5	0
6	O	28	0	25	2	0
7	E	14	0	13	0	0
7	F	14	0	12	0	0
7	G	14	0	13	0	0
All	All	14990	0	14677	295	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 10.

All (295) 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:E:531:ALA:HB2	4:J:100(D):VAL:HG21	1.42	0.98
3:F:424:SER:O	3:F:518:THR:HG23	1.63	0.97
3:F:423:ASN:HB3	3:F:527:TYR:HB3	1.53	0.87
5:K:29:ILE:HG22	5:K:29:ILE:O	1.78	0.81
3:E:534:THR:CG2	6:L:1:NAG:HN2	1.96	0.79
1:A:100(A):GLY:HA2	2:B:91:GLY:HA3	1.65	0.76
3:E:534:THR:HG22	6:L:1:NAG:HN2	1.51	0.74
2:D:29:LEU:HD22	2:D:71:PHE:HE2	1.51	0.74
4:G:48:LEU:HA	4:G:63:PHE:HZ	1.51	0.74
1:C:119:PRO:HB3	1:C:145:TYR:HB3	1.70	0.73
1:C:100(B):GLU:C	2:D:34:ASN:HD21	1.92	0.72
6:M:1:NAG:O3	6:M:1:NAG:O7	2.05	0.72
4:J:99:GLY:H	4:J:100(E):ARG:HG2	1.55	0.71
3:E:568:PRO:HB2	3:E:603:ILE:HG22	1.72	0.70
3:E:604:THR:HB	3:E:607:CYS:HB2	1.74	0.70
1:C:87:THR:HB	1:C:111:VAL:HG22	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:90:GLN:HE21	5:K:97:THR:HG22	1.59	0.68
2:D:34:ASN:OD1	2:D:49:TYR:HA	1.92	0.68
3:F:604:THR:HB	3:F:607:CYS:HB2	1.76	0.68
2:D:29:LEU:HD22	2:D:71:PHE:CE2	2.29	0.67
3:E:518:THR:HG23	3:E:526:THR:HG23	1.77	0.67
1:A:87:THR:HB	1:A:111:VAL:HG22	1.76	0.67
3:F:610:ASP:HB3	3:F:641:GLU:HB3	1.77	0.66
5:H:28:THR:OG1	6:N:1:NAG:H4	1.95	0.66
5:K:149:LYS:HB2	5:K:193:ALA:HB3	1.78	0.66
3:F:424:SER:HB2	3:F:518:THR:OG1	1.96	0.66
4:G:96:LEU:C	4:G:96:LEU:HD23	2.15	0.65
3:F:428:ASN:ND2	3:F:499:ALA:O	2.29	0.65
1:A:100:LEU:HD11	3:E:546:LEU:HB2	1.79	0.65
4:J:100(F):PRO:HG3	5:K:49:TYR:HB2	1.80	0.64
1:A:33:THR:HG22	1:A:52:MET:HG2	1.81	0.63
1:C:33:THR:HG22	1:C:52:MET:HG2	1.81	0.62
1:C:163:VAL:HA	1:C:182:VAL:HG12	1.82	0.61
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.82	0.61
3:F:498:PRO:HA	3:F:536:VAL:HG12	1.82	0.61
5:H:90:GLN:HE21	5:H:97:THR:HG22	1.66	0.61
4:J:73:ARG:HH11	4:J:74:THR:H	1.49	0.60
3:E:518:THR:OG1	3:E:535:ASP:HB3	2.01	0.60
2:B:36:PHE:HE2	2:B:89:MET:HB3	1.65	0.60
4:J:52:ILE:HD13	4:J:100(B):LEU:HD23	1.82	0.60
5:K:28:THR:HG1	6:L:1:NAG:HO6	1.48	0.60
3:F:528:SER:HA	5:H:93:ASN:HA	1.83	0.60
4:G:73:ARG:HH11	4:G:74:THR:H	1.50	0.60
4:G:48:LEU:HD23	4:G:63:PHE:CZ	2.37	0.60
1:A:163:VAL:HA	1:A:182:VAL:HG12	1.82	0.59
3:E:534:THR:N	6:L:1:NAG:H82	2.17	0.59
1:A:66:ARG:NH2	1:A:82(B):SER:O	2.36	0.59
5:K:33:LEU:HB3	5:K:51:VAL:HG22	1.84	0.59
3:E:496:ILE:HD11	3:E:536:VAL:HG21	1.85	0.59
4:J:33:VAL:HB	4:J:95:VAL:HB	1.84	0.59
3:E:544:PRO:HG3	3:E:550:PHE:CE1	2.38	0.58
3:F:508:CYS:O	3:F:514:VAL:HG22	2.02	0.58
4:J:70:SER:HB3	4:J:79:TYR:HB2	1.84	0.58
3:E:550:PHE:CD1	3:E:568:PRO:HA	2.38	0.58
4:J:100(D):VAL:CG1	5:K:32:HIS:CD2	2.87	0.58
5:K:37:GLN:HB3	5:K:47:LEU:HD11	1.86	0.57
1:C:100(B):GLU:C	2:D:34:ASN:ND2	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:95:VAL:HG13	4:G:100(E):ARG:HB2	1.87	0.57
4:J:61:GLN:HE21	6:I:1:NAG:C8	2.18	0.56
5:H:91:TYR:HA	5:H:96:GLN:HG3	1.87	0.56
4:G:95:VAL:CG1	4:G:100(E):ARG:HB2	2.35	0.56
4:J:123:PRO:HD3	4:J:209:LYS:HE2	1.88	0.56
4:J:52:ILE:HG22	4:J:54:PHE:H	1.71	0.56
3:E:610:ASP:HB3	3:E:641:GLU:HB3	1.86	0.56
1:A:39:GLN:HB2	1:A:45:LEU:HD23	1.88	0.55
5:H:37:GLN:HB3	5:H:47:LEU:HD11	1.89	0.55
4:J:100(D):VAL:HG11	5:K:32:HIS:CD2	2.42	0.55
1:A:56:ILE:HD11	3:E:514:VAL:HG11	1.88	0.55
5:K:29:ILE:CG2	5:K:29:ILE:O	2.50	0.55
4:J:87:THR:HG23	4:J:110:THR:HA	1.88	0.54
1:C:39:GLN:HB2	1:C:45:LEU:HD23	1.88	0.54
3:F:545:PRO:HG3	3:F:633:VAL:HG22	1.89	0.54
4:G:96:LEU:O	4:G:96:LEU:HD23	2.06	0.54
5:K:10:ILE:HG12	5:K:103:LYS:HB3	1.90	0.54
3:F:528:SER:OG	3:F:535:ASP:OD2	2.25	0.54
5:H:59:PRO:HB2	5:H:61:ARG:HG2	1.90	0.53
3:F:423:ASN:HB2	3:F:527:TYR:CD1	2.43	0.53
4:J:6:GLN:H	4:J:105:GLN:HE22	1.54	0.53
2:B:61:ARG:NH1	2:B:82:ASP:OD2	2.36	0.53
3:E:502:VAL:HA	3:E:556:ASN:HA	1.89	0.53
1:C:30:ARG:HD3	3:F:523:GLY:HA2	1.91	0.53
1:C:66:ARG:NH2	1:C:82(B):SER:O	2.39	0.53
3:E:424:SER:CA	3:E:518:THR:HG22	2.38	0.53
3:E:534:THR:H	6:L:1:NAG:H82	1.74	0.52
2:B:14:THR:HG22	2:B:107:ASN:HB3	1.91	0.52
4:G:6:GLN:HE21	4:G:20:VAL:HG11	1.75	0.52
5:K:167:ASP:OD1	5:K:168:SER:N	2.42	0.52
3:E:528:SER:OG	3:E:535:ASP:OD2	2.27	0.52
4:J:7:SER:HB2	4:J:21:SER:H	1.74	0.52
4:G:100(F):PRO:HG3	5:H:49:TYR:HB2	1.92	0.51
3:E:531:ALA:CB	4:J:100(D):VAL:HG21	2.29	0.51
1:C:100(A):GLY:HA2	2:D:91:GLY:HA3	1.92	0.51
3:F:496:ILE:HD11	3:F:536:VAL:HG21	1.91	0.51
5:K:89:HIS:CG	5:K:98:PHE:HE1	2.29	0.51
2:D:29:LEU:N	2:D:29:LEU:CD1	2.73	0.51
1:A:126:PRO:HG3	1:A:138:LEU:HD12	1.92	0.51
1:C:50:ARG:HD3	1:C:100:LEU:HD23	1.92	0.51
2:D:34:ASN:OD1	2:D:49:TYR:O	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:126:PRO:HB3	4:J:138:LEU:HB3	1.92	0.51
4:J:35:SER:HB3	4:J:100(G):LEU:HD23	1.92	0.51
4:J:32:GLU:HB3	4:J:33:VAL:HG23	1.91	0.51
1:A:89:ILE:HG13	1:A:108:LEU:HD13	1.93	0.51
4:J:6:GLN:HE21	4:J:20:VAL:HG11	1.76	0.50
4:J:96:LEU:HG	4:J:97:GLN:HG3	1.94	0.50
2:D:66:GLY:HA3	2:D:71:PHE:HA	1.93	0.50
3:E:424:SER:O	3:E:518:THR:HG22	2.11	0.50
3:E:534:THR:HG22	6:L:1:NAG:N2	2.24	0.50
2:B:35:TRP:CE2	2:B:73:LEU:HB2	2.46	0.50
2:D:35:TRP:CE2	2:D:73:LEU:HB2	2.47	0.49
4:G:87:THR:HG23	4:G:110:THR:HA	1.92	0.49
3:E:541:ASN:ND2	3:E:550:PHE:O	2.45	0.49
3:E:427:LEU:HD13	4:J:52:ILE:HD11	1.94	0.49
4:J:95:VAL:HA	4:J:100(G):LEU:HA	1.93	0.49
2:D:150:VAL:HG22	2:D:192:TYR:CD1	2.48	0.49
2:D:6:GLN:NE2	2:D:86:TYR:O	2.40	0.49
3:F:424:SER:HB2	3:F:518:THR:N	2.28	0.49
5:H:89:HIS:CD2	5:H:98:PHE:HE1	2.31	0.48
4:G:126:PRO:HB3	4:G:138:LEU:HB3	1.94	0.48
5:H:167:ASP:OD1	5:H:168:SER:N	2.46	0.48
4:G:70:SER:HB3	4:G:79:TYR:HB2	1.94	0.48
4:G:32:GLU:HA	4:G:52(A):PRO:HG2	1.96	0.48
4:J:23:LYS:NZ	4:J:77:THR:OG1	2.46	0.48
4:J:35:SER:HB2	4:J:50:VAL:HG12	1.95	0.48
2:D:39:ARG:HH21	2:D:45:ARG:HH21	1.62	0.48
3:E:544:PRO:HG3	3:E:550:PHE:CZ	2.48	0.48
1:A:126:PRO:HD2	1:A:213:PRO:HA	1.96	0.48
2:B:35:TRP:HB2	2:B:48:ILE:HB	1.96	0.48
4:J:40:ALA:HB3	4:J:43:GLU:HB3	1.94	0.48
5:K:2:ILE:HD12	5:K:27:ARG:HB2	1.96	0.48
2:B:8:PRO:HG2	2:B:11:LEU:HB2	1.96	0.48
3:E:550:PHE:CE1	3:E:568:PRO:HA	2.49	0.48
4:J:6:GLN:H	4:J:105:GLN:NE2	2.12	0.48
4:J:23:LYS:HG2	4:J:77:THR:HG23	1.96	0.48
3:F:520:ASP:OD1	3:F:521:ARG:N	2.47	0.47
5:K:82:ASP:O	5:K:86:TYR:OH	2.21	0.47
1:A:50:ARG:HD3	1:A:100:LEU:HD23	1.95	0.47
2:D:48:ILE:HD13	2:D:54:ARG:HA	1.96	0.47
4:G:108:LEU:HD21	4:G:148:GLU:HB3	1.96	0.47
5:H:89:HIS:CG	5:H:98:PHE:HE1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:423:ASN:OD1	4:J:58:ASP:OD2	2.33	0.47
5:K:30(A):ARG:O	5:K:30(A):ARG:HG3	2.13	0.47
2:B:124:GLN:HG2	2:B:130:ALA:HA	1.97	0.47
2:D:36:PHE:CD2	2:D:98:PHE:HE2	2.32	0.47
3:F:428:ASN:HA	4:G:100(A):ASN:HA	1.97	0.47
3:E:604:THR:HG22	3:E:606:ARG:H	1.80	0.47
4:G:23:LYS:HG2	4:G:77:THR:HG23	1.96	0.47
5:K:86:TYR:HE1	5:K:104:LEU:HD22	1.80	0.47
5:K:59:PRO:HB2	5:K:61:ARG:HG2	1.96	0.47
3:F:424:SER:HB3	3:F:526:THR:O	2.15	0.47
3:E:501:SER:O	3:E:556:ASN:HB2	2.15	0.46
5:K:18:ARG:HG3	5:K:75:ILE:O	2.14	0.46
2:D:150:VAL:HG22	2:D:192:TYR:HD1	1.80	0.46
4:J:23:LYS:HA	4:J:76:SER:O	2.16	0.46
5:K:40:PRO:HG3	5:K:165:GLU:HG2	1.98	0.46
4:G:58:ASP:OD1	4:G:59:TYR:N	2.49	0.46
4:J:83:ARG:HG2	4:J:86:ASP:OD1	2.16	0.46
2:D:14:THR:OG1	2:D:17:GLN:HG3	2.16	0.46
1:C:100:LEU:HD11	3:F:546:LEU:HB2	1.97	0.46
3:F:502:VAL:HG12	3:F:554:TRP:CD1	2.51	0.46
2:D:33:LEU:HD11	2:D:88:CYS:HB2	1.97	0.46
2:B:39:ARG:HH21	2:B:45:ARG:HH21	1.64	0.46
1:C:167:PRO:HD3	2:D:164:THR:HG22	1.97	0.46
2:D:122:ASP:O	2:D:126:LYS:HG2	2.17	0.45
2:D:28:SER:HB3	2:D:30:VAL:HG22	1.97	0.45
2:D:86:TYR:O	2:D:101:GLY:HA2	2.16	0.45
3:E:498:PRO:HA	3:E:536:VAL:HG12	1.98	0.45
2:D:149:LYS:HB2	2:D:193:ALA:HB3	1.98	0.45
4:J:96:LEU:HD22	4:J:101:ASP:OD2	2.16	0.45
2:B:29:LEU:HD21	2:B:90:GLN:HB2	1.98	0.45
2:D:6:GLN:NE2	2:D:102:THR:HG23	2.31	0.45
3:E:492:ARG:N	3:E:493:PRO:HD2	2.31	0.45
1:A:188:SER:HG	1:A:192:GLN:HB2	1.80	0.45
2:B:140:TYR:CD2	2:B:141:PRO:HA	2.51	0.45
2:B:4:LEU:HD23	2:B:23:CYS:SG	2.57	0.45
2:D:120:PRO:HD3	2:D:132:VAL:HG22	1.99	0.45
2:D:37:HIS:HB2	2:D:47:LEU:HD11	1.99	0.45
2:D:30:VAL:HA	2:D:31:THR:HG22	1.97	0.45
2:D:4:LEU:HD21	2:D:90:GLN:HB3	1.98	0.45
3:F:423:ASN:HB2	3:F:527:TYR:HD1	1.80	0.45
3:F:424:SER:HB2	3:F:518:THR:HG1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:VAL:HG22	2:B:192:TYR:CD1	2.52	0.45
2:D:140:TYR:CD2	2:D:141:PRO:HA	2.52	0.45
4:G:40:ALA:HB3	4:G:43:GLU:HB3	1.98	0.45
5:K:108:ARG:HG2	5:K:109:THR:N	2.32	0.45
3:F:560:PHE:CD2	6:O:1:NAG:H5	2.52	0.45
1:C:31:ALA:C	1:C:97:TYR:HB2	2.37	0.45
4:G:7:SER:HB2	4:G:21:SER:H	1.81	0.45
5:H:149:LYS:HB2	5:H:193:ALA:HB3	1.98	0.45
3:F:424:SER:HB2	3:F:518:THR:H	1.82	0.44
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.98	0.44
3:E:508:CYS:HB3	3:E:549:TRP:CG	2.53	0.44
5:H:28:THR:N	6:N:1:NAG:O6	2.50	0.44
2:D:28:SER:HB3	2:D:30:VAL:CG2	2.48	0.44
2:D:8:PRO:HG2	2:D:11:LEU:HB2	1.99	0.44
3:E:520:ASP:OD1	3:E:521:ARG:N	2.50	0.44
3:E:544:PRO:HG3	3:E:550:PHE:CD1	2.52	0.44
3:F:424:SER:C	3:F:518:THR:HG23	2.33	0.44
4:J:74:THR:OG1	4:J:75:THR:N	2.51	0.44
2:B:122:ASP:O	2:B:126:LYS:HG2	2.18	0.44
1:C:89:ILE:HG13	1:C:108:LEU:HD13	2.00	0.44
5:H:21:LEU:HD21	5:H:104:LEU:HD11	1.99	0.44
4:J:100(D):VAL:HG12	5:K:32:HIS:CD2	2.53	0.44
3:F:509:PHE:CZ	3:F:601:PRO:HG3	2.53	0.44
4:G:51:PHE:HB2	4:G:69:ILE:HG21	2.00	0.44
2:B:33:LEU:HD13	2:B:71:PHE:CD2	2.53	0.44
5:K:89:HIS:CD2	5:K:98:PHE:HE1	2.35	0.44
5:H:27:ARG:HB3	6:N:1:NAG:O6	2.17	0.44
4:G:6:GLN:O	4:G:105:GLN:NE2	2.42	0.43
4:J:4:LEU:HA	4:J:24:ALA:HA	2.00	0.43
4:G:193:THR:HG23	4:G:210:LYS:HE2	2.00	0.43
5:H:82:ASP:O	5:H:86:TYR:OH	2.24	0.43
5:H:37:GLN:HE21	5:H:45:ARG:HD3	1.83	0.43
1:A:155:ASN:O	1:A:156:SER:HB2	2.19	0.43
2:D:14:THR:HG22	2:D:107:ASN:HB3	2.00	0.43
2:D:59:PRO:HG2	2:D:61:ARG:HH21	1.82	0.43
4:G:93:ALA:HA	4:G:102:LEU:O	2.18	0.43
4:G:23:LYS:HA	4:G:76:SER:O	2.19	0.43
5:H:108:ARG:HG2	5:H:109:THR:N	2.33	0.43
4:J:35:SER:OG	4:J:36:TRP:N	2.51	0.43
4:G:83:ARG:HG2	4:G:86:ASP:OD1	2.18	0.43
5:K:56:ILE:H	5:K:56:ILE:HD12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:95:VAL:HG22	4:G:100(G):LEU:HD23	2.00	0.43
5:H:108:ARG:HG2	5:H:109:THR:H	1.82	0.43
5:K:148:TRP:CE2	5:K:179:LEU:HB2	2.54	0.43
2:D:50:LYS:O	2:D:53:ASN:N	2.48	0.43
5:H:40:PRO:HG3	5:H:165:GLU:HG2	2.00	0.43
4:J:63:PHE:O	4:J:67:VAL:HG12	2.18	0.43
3:E:424:SER:HA	3:E:518:THR:HG22	2.01	0.43
1:A:86:ASP:O	1:A:90:TYR:OH	2.26	0.42
2:D:35:TRP:CZ3	2:D:88:CYS:HB3	2.54	0.42
4:J:51:PHE:HB2	4:J:69:ILE:HG21	2.00	0.42
3:F:532:ASN:OD1	6:N:1:NAG:C7	2.67	0.42
1:A:121:VAL:HG12	1:A:142:VAL:HG22	2.00	0.42
4:J:32:GLU:H	4:J:94:LYS:HZ3	1.67	0.42
1:C:166:PHE:HE2	1:C:181:VAL:HG22	1.84	0.42
3:E:630:ARG:NH1	3:E:639:ARG:HH21	2.17	0.42
4:J:58:ASP:OD1	4:J:59:TYR:N	2.50	0.42
4:J:97:GLN:NE2	5:K:56:ILE:HD11	2.34	0.42
2:B:6:GLN:NE2	2:B:86:TYR:O	2.39	0.42
1:C:40:ALA:HB3	1:C:43:GLN:HB2	2.02	0.42
4:J:193:THR:HG23	4:J:210:LYS:HE2	2.01	0.42
1:A:34:LEU:HD12	1:A:34:LEU:HA	1.90	0.42
1:C:83:ARG:HD2	1:C:84:SER:H	1.84	0.42
2:D:197:THR:HG22	2:D:204:PRO:HB3	2.02	0.42
5:H:28:THR:N	6:N:1:NAG:HO6	2.17	0.42
1:A:6:GLN:NE2	1:A:90:TYR:O	2.52	0.42
3:E:509:PHE:CZ	3:E:601:PRO:HG3	2.55	0.42
2:B:30(B):SER:HB2	3:E:543:ARG:HG3	2.02	0.42
4:G:4:LEU:HA	4:G:24:ALA:HA	2.01	0.42
4:J:100(E):ARG:HD2	4:J:100(E):ARG:HA	1.75	0.42
2:D:34:ASN:OD1	2:D:49:TYR:CA	2.63	0.42
4:J:59:TYR:HE1	4:J:69:ILE:HG13	1.85	0.42
1:C:146:PHE:HA	1:C:147:PRO:HA	1.85	0.42
2:D:33:LEU:HD22	2:D:71:PHE:CG	2.55	0.42
1:C:154:TRP:HD1	1:C:163:VAL:HG13	1.84	0.42
2:D:36:PHE:CE2	2:D:98:PHE:HE2	2.38	0.42
4:J:47:TRP:CZ2	4:J:50:VAL:HG13	2.55	0.42
1:A:83:ARG:HD2	1:A:84:SER:H	1.85	0.41
2:B:116:PHE:HB2	2:B:135:LEU:HB3	2.01	0.41
3:F:560:PHE:CE1	6:O:2:NAG:H82	2.55	0.41
4:G:100(D):VAL:HG13	5:H:91:TYR:O	2.20	0.41
3:E:500:LYS:HE2	3:E:531:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:19:LYS:HA	4:J:80:MET:O	2.20	0.41
3:F:508:CYS:HB3	3:F:549:TRP:CG	2.55	0.41
4:G:74:THR:OG1	4:G:75:THR:N	2.52	0.41
1:A:31:ALA:C	1:A:97:TYR:HB2	2.41	0.41
4:G:100(F):PRO:HG3	5:H:49:TYR:CB	2.50	0.41
5:H:108:ARG:HD2	5:H:171:SER:HG	1.85	0.41
2:B:14:THR:OG1	2:B:17:GLN:HG3	2.20	0.41
3:E:420:TRP:HE3	3:E:515:VAL:HG11	1.84	0.41
2:B:55:ASP:OD1	2:B:56:SER:N	2.53	0.41
2:B:66:GLY:HA3	2:B:71:PHE:HA	2.03	0.41
4:J:100(G):LEU:H	4:J:100(G):LEU:HD12	1.85	0.41
4:J:35:SER:CB	4:J:50:VAL:HG12	2.51	0.41
1:C:125:ALA:HA	1:C:126:PRO:HD3	1.95	0.41
3:F:503:CYS:N	3:F:555:MET:O	2.43	0.41
5:K:123:GLU:OE1	5:K:123:GLU:N	2.50	0.41
3:E:427:LEU:HD13	4:J:52:ILE:CD1	2.51	0.41
2:B:37:HIS:HB2	2:B:47:LEU:HD11	2.03	0.41
2:D:30(A):TYR:HE2	3:F:543:ARG:HB2	1.86	0.41
5:H:1:GLU:HA	5:H:95:PRO:HG2	2.03	0.41
1:C:135:THR:OG1	1:C:136:ALA:N	2.55	0.40
2:D:14:THR:HA	2:D:107:ASN:HB3	2.03	0.40
2:D:34:ASN:OD1	2:D:49:TYR:C	2.59	0.40
4:G:85:GLU:OE1	4:G:85:GLU:N	2.53	0.40
4:J:100(A):ASN:ND2	4:J:100(A):ASN:H	2.17	0.40
2:D:33:LEU:HB3	2:D:51:VAL:HG12	2.03	0.40
3:E:425:THR:O	3:E:529:TRP:HA	2.21	0.40
1:A:141:LEU:HD21	1:A:143:LYS:HB2	2.03	0.40
2:B:150:VAL:HG22	2:B:192:TYR:HD1	1.87	0.40
3:F:509:PHE:CE1	3:F:601:PRO:HG3	2.57	0.40
4:J:184:VAL:HG11	4:J:194:TYR:CE1	2.57	0.40
3:E:560:PHE:CD2	6:M:1:NAG:H5	2.57	0.40
2:B:197:THR:HG22	2:B:204:PRO:HB3	2.04	0.40
4:J:48:LEU:HD21	4:J:80:MET:HE1	2.02	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	211/227 (93%)	204 (97%)	7 (3%)	0	100	100
1	C	181/227 (80%)	174 (96%)	7 (4%)	0	100	100
2	B	215/221 (97%)	208 (97%)	7 (3%)	0	100	100
2	D	215/221 (97%)	212 (99%)	3 (1%)	0	100	100
3	E	131/191 (69%)	120 (92%)	11 (8%)	0	100	100
3	F	119/191 (62%)	109 (92%)	10 (8%)	0	100	100
4	G	205/229 (90%)	195 (95%)	10 (5%)	0	100	100
4	J	214/229 (93%)	204 (95%)	10 (5%)	0	100	100
5	H	183/215 (85%)	177 (97%)	6 (3%)	0	100	100
5	K	208/215 (97%)	200 (96%)	7 (3%)	1 (0%)	29	66
All	All	1882/2166 (87%)	1803 (96%)	78 (4%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	K	51	VAL

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	179/190 (94%)	179 (100%)	0	100	100
1	C	160/190 (84%)	158 (99%)	2 (1%)	69	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	190/194 (98%)	187 (98%)	3 (2%)	62	79
2	D	190/194 (98%)	187 (98%)	3 (2%)	62	79
3	E	118/159 (74%)	118 (100%)	0	100	100
3	F	109/159 (69%)	107 (98%)	2 (2%)	59	77
4	G	183/193 (95%)	182 (100%)	1 (0%)	88	94
4	J	185/193 (96%)	180 (97%)	5 (3%)	44	68
5	H	171/186 (92%)	169 (99%)	2 (1%)	71	84
5	K	183/186 (98%)	183 (100%)	0	100	100
All	All	1668/1844 (90%)	1650 (99%)	18 (1%)	73	85

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	30(A)	TYR
2	B	30(E)	ASN
2	B	90	GLN
4	J	63	PHE
4	J	100	ARG
4	J	100(A)	ASN
4	J	100(E)	ARG
4	J	100(G)	LEU
1	C	98	VAL
1	C	160	THR
2	D	29	LEU
2	D	30	VAL
2	D	30(E)	ASN
3	F	422	ILE
3	F	534	THR
4	G	96	LEU
5	H	28	THR
5	H	91	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
4	J	61	GLN
5	K	32	HIS
5	K	89	HIS

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Mol	Chain	Res	Type
5	K	90	GLN
2	D	34	ASN
5	H	37	GLN
5	H	90	GLN

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 ⓘ

10 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	$\# Z > 2$
6	NAG	I	1	6	14,14,15	0.55	0	17,19,21	0.59	0
6	NAG	I	2	6	14,14,15	0.35	0	17,19,21	0.45	0
6	NAG	L	1	3,6	14,14,15	0.33	0	17,19,21	0.71	0
6	NAG	L	2	6	14,14,15	0.38	0	17,19,21	0.38	0
6	NAG	M	1	3,6	14,14,15	0.37	0	17,19,21	0.90	1 (5%)
6	NAG	M	2	6	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	N	1	6	14,14,15	0.37	0	17,19,21	0.55	0
6	NAG	N	2	6	14,14,15	0.40	0	17,19,21	0.41	0
6	NAG	O	1	3,6	14,14,15	0.41	0	17,19,21	0.49	0
6	NAG	O	2	6	14,14,15	0.36	0	17,19,21	0.55	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	I	1	6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	NAG	L	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	NAG	M	1	3,6	-	4/6/23/26	0/1/1/1
6	NAG	M	2	6	-	1/6/23/26	0/1/1/1
6	NAG	N	1	6	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	NAG	O	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	O	2	6	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1	NAG	C2-N2-C7	-2.59	119.22	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

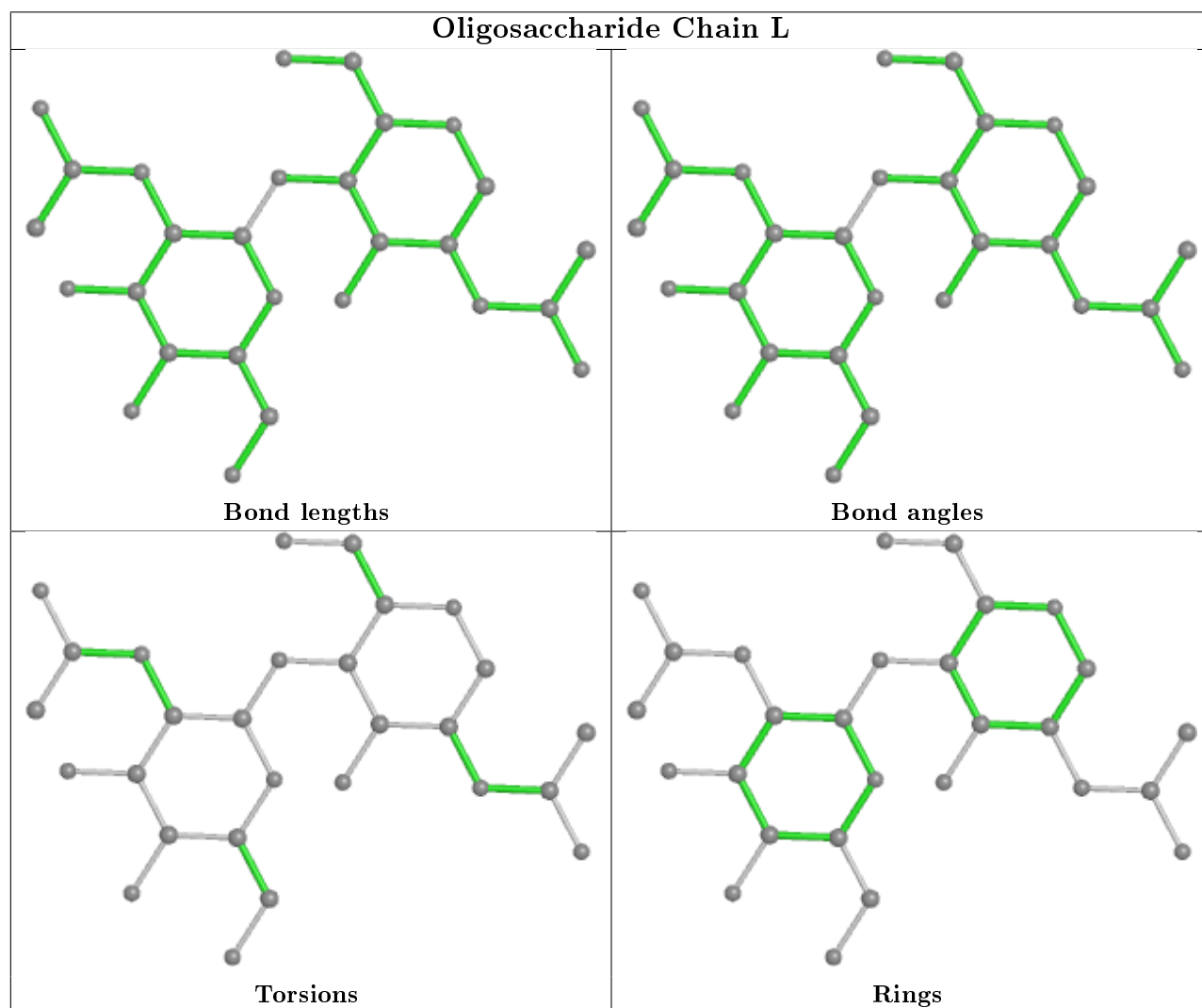
Mol	Chain	Res	Type	Atoms
6	O	2	NAG	O5-C5-C6-O6
6	M	1	NAG	C1-C2-N2-C7
6	M	2	NAG	O5-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
6	M	1	NAG	C8-C7-N2-C2
6	N	1	NAG	O5-C5-C6-O6
6	M	1	NAG	O7-C7-N2-C2
6	M	1	NAG	C3-C2-N2-C7

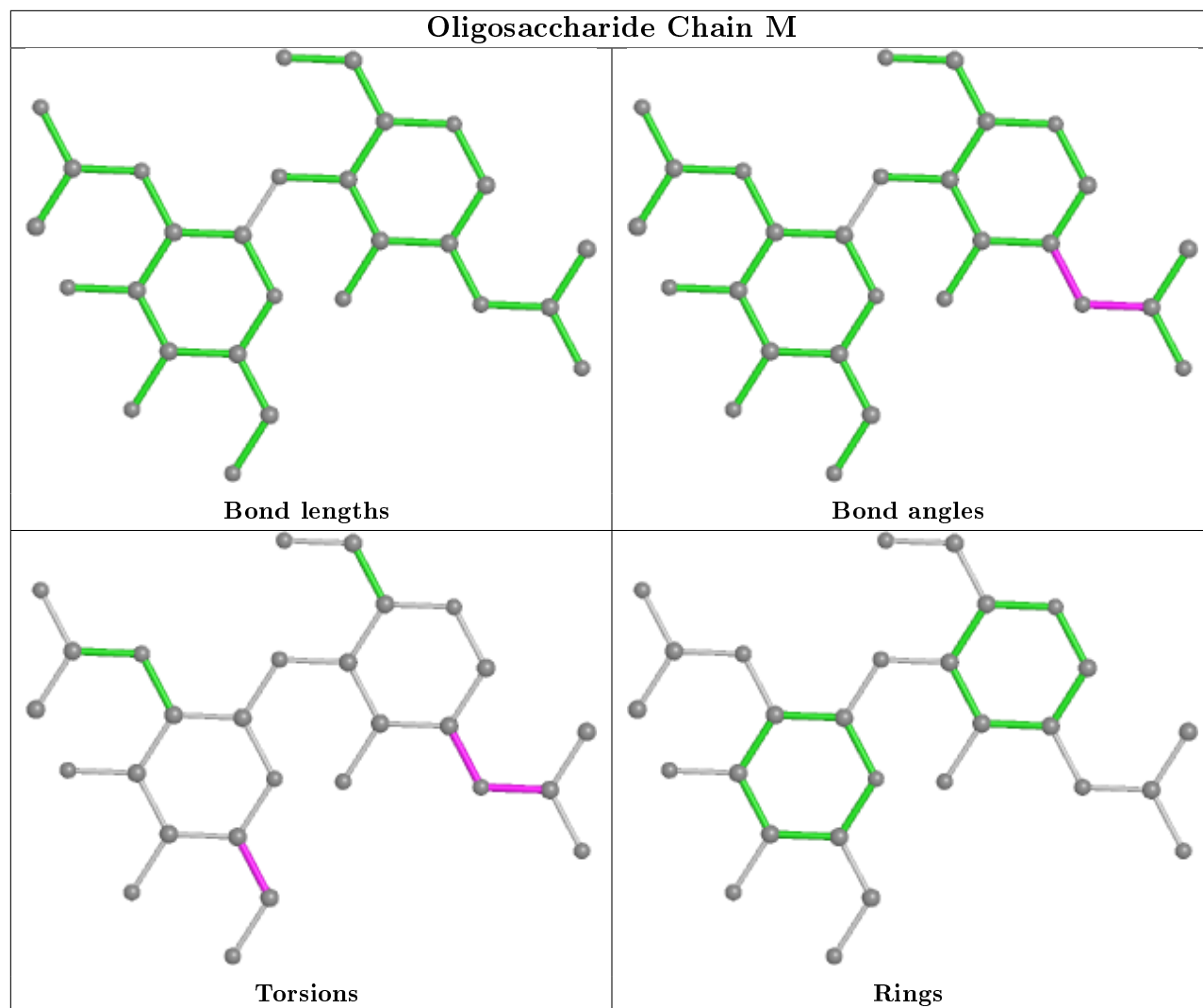
There are no ring outliers.

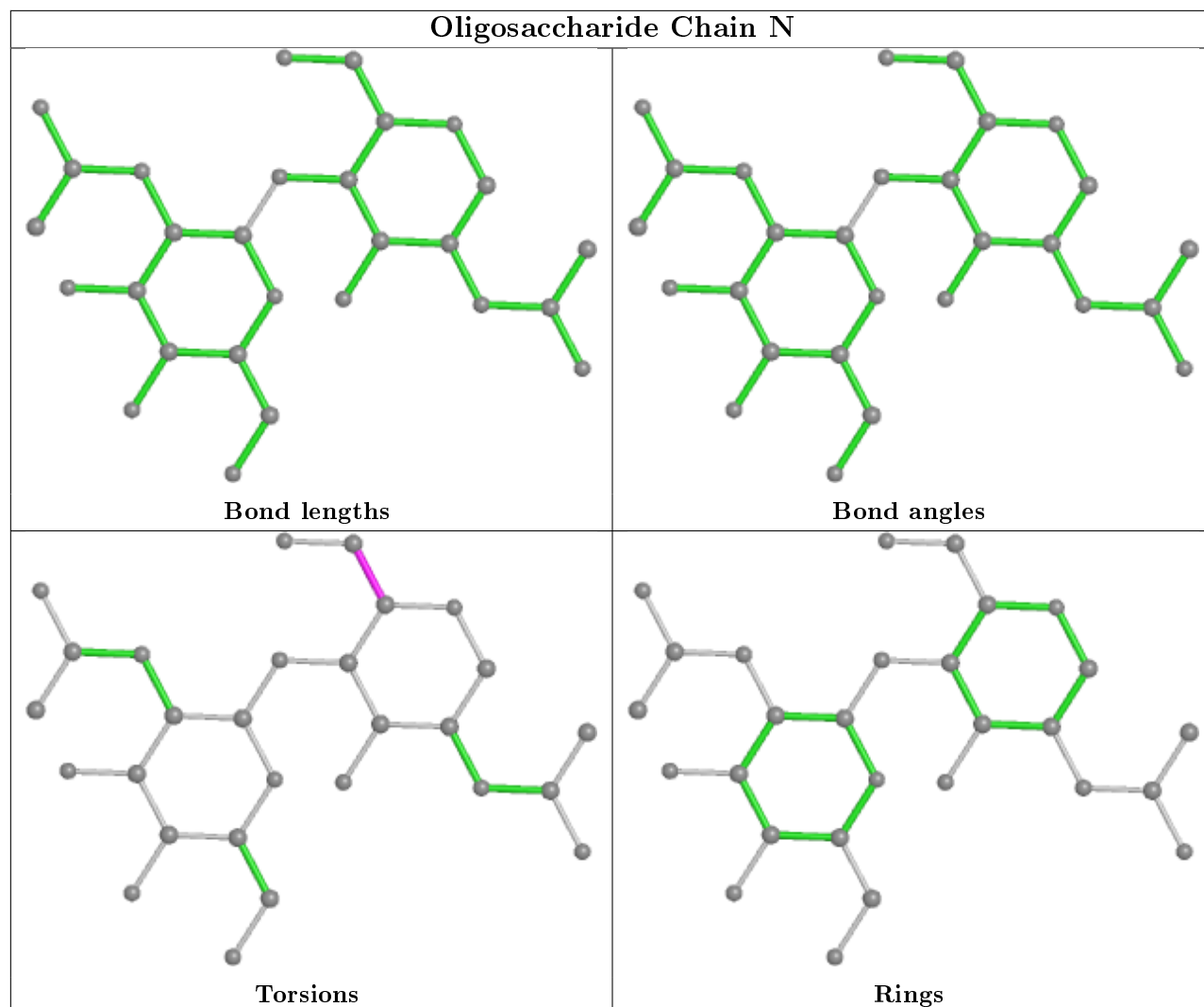
6 monomers are involved in 16 short contacts:

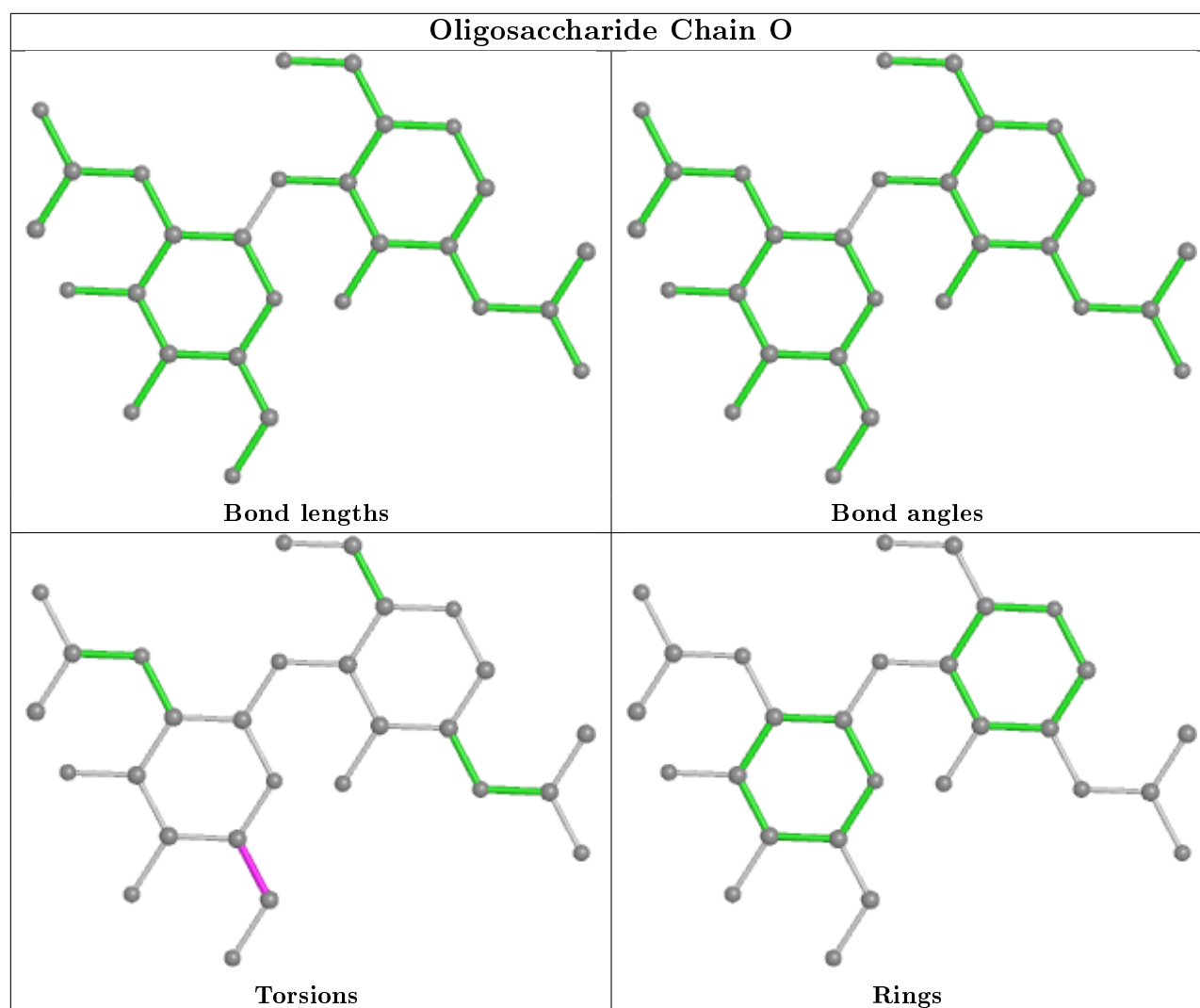
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	O	1	NAG	1	0
6	L	1	NAG	6	0
6	I	1	NAG	1	0
6	N	1	NAG	5	0
6	O	2	NAG	1	0
6	M	1	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
7	NAG	E	705	3	14,14,15	0.28	0	17,19,21	0.44	0
7	NAG	G	301	-	14,14,15	0.34	0	17,19,21	0.37	0
7	NAG	F	901	3	14,14,15	0.86	1 (7%)	17,19,21	0.97	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	E	705	3	-	0/6/23/26	0/1/1/1
7	NAG	G	301	-	-	2/6/23/26	0/1/1/1
7	NAG	F	901	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	901	NAG	O5-C1	-3.13	1.38	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	901	NAG	C1-O5-C5	-3.06	108.04	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	901	NAG	C4-C5-C6-O6
7	F	901	NAG	O5-C5-C6-O6
7	G	301	NAG	C4-C5-C6-O6
7	G	301	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	215/227 (94%)	-0.22	0 100 100	52, 102, 137, 158	0
1	C	191/227 (84%)	0.06	3 (1%) 72 59	97, 144, 178, 205	0
2	B	217/221 (98%)	-0.33	0 100 100	40, 95, 134, 156	0
2	D	217/221 (98%)	0.15	1 (0%) 91 85	65, 153, 183, 218	0
3	E	137/191 (71%)	-0.01	1 (0%) 87 80	71, 120, 152, 170	0
3	F	125/191 (65%)	0.27	4 (3%) 47 34	83, 147, 170, 178	0
4	G	213/229 (93%)	-0.13	1 (0%) 91 85	89, 129, 162, 181	0
4	J	218/229 (95%)	-0.35	0 100 100	60, 101, 138, 185	0
5	H	195/215 (90%)	0.38	12 (6%) 20 13	99, 150, 189, 212	0
5	K	212/215 (98%)	-0.32	0 100 100	60, 99, 133, 158	0
All	All	1940/2166 (89%)	-0.07	22 (1%) 80 70	40, 122, 171, 218	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	119	PRO	3.6
5	H	25	ALA	3.5
5	H	191	VAL	3.4
5	H	103	LYS	3.4
5	H	192	TYR	3.3
5	H	193	ALA	3.0
5	H	210	ASN	2.9
3	F	561	THR	2.7
2	D	128	GLY	2.7
3	E	608	MET	2.6
5	H	190	LYS	2.5
1	C	140	CYS	2.5
3	F	621	THR	2.3

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Mol	Chain	Res	Type	RSRZ
4	G	194	TYR	2.3
3	F	562	LYS	2.3
5	H	149	LYS	2.2
1	C	154	TRP	2.2
5	H	152	ASN	2.2
5	H	15	PRO	2.2
3	F	563	VAL	2.1
5	H	84	ALA	2.1
5	H	104	LEU	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](#)

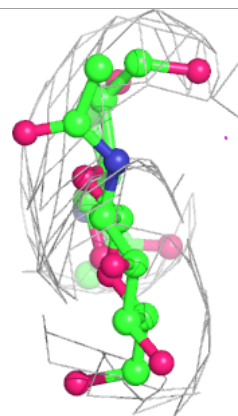
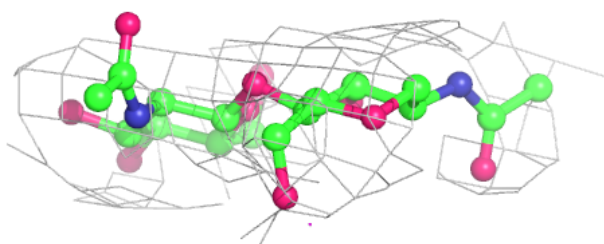
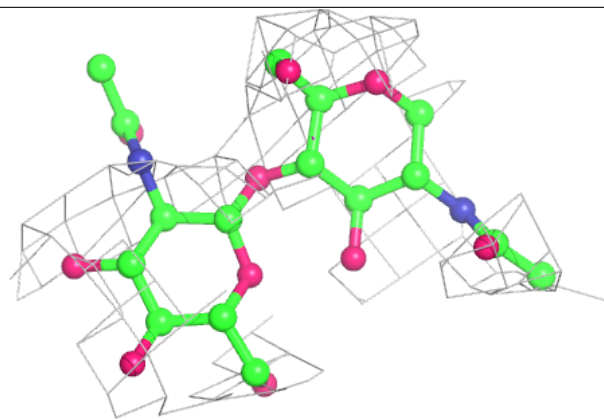
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	N	2	14/15	0.77	0.44	154,182,204,208	0
6	NAG	I	2	14/15	0.77	0.26	143,182,210,216	0
6	NAG	N	1	14/15	0.79	0.25	144,167,199,205	0
6	NAG	L	2	14/15	0.79	0.37	159,172,216,232	0
6	NAG	I	1	14/15	0.83	0.23	93,141,170,172	0
6	NAG	L	1	14/15	0.87	0.18	124,142,173,199	0
6	NAG	O	2	14/15	0.88	0.28	155,163,179,199	0
6	NAG	M	2	14/15	0.90	0.28	132,153,185,189	0
6	NAG	O	1	14/15	0.92	0.26	155,175,188,192	0
6	NAG	M	1	14/15	0.93	0.21	101,130,163,163	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.

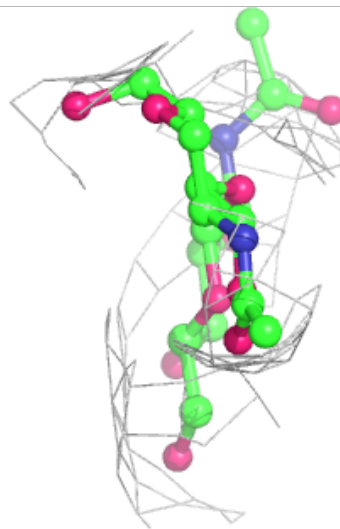
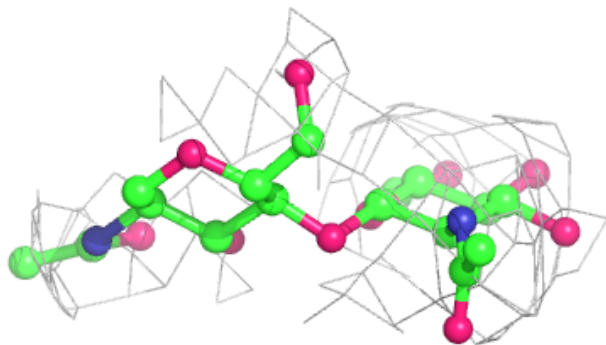
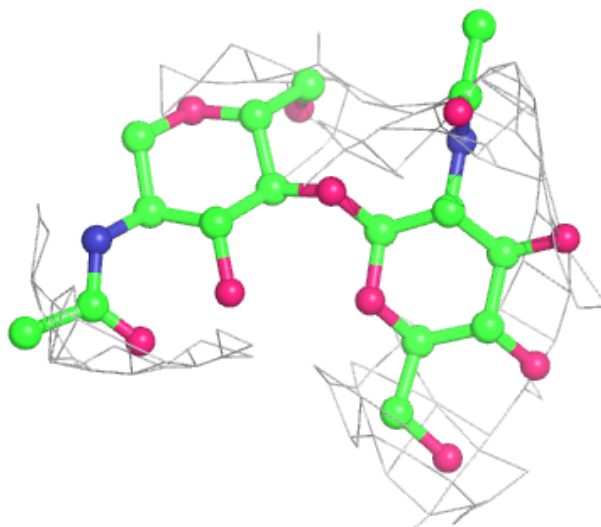
Electron density around Chain L:

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



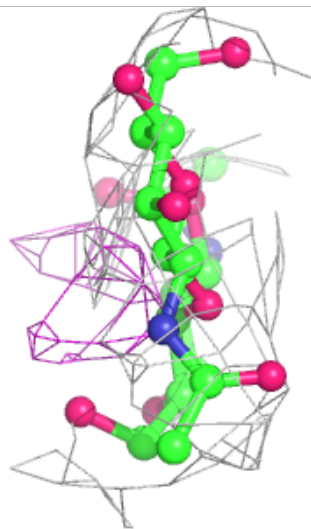
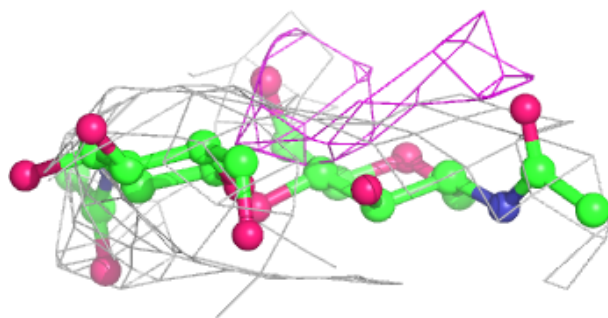
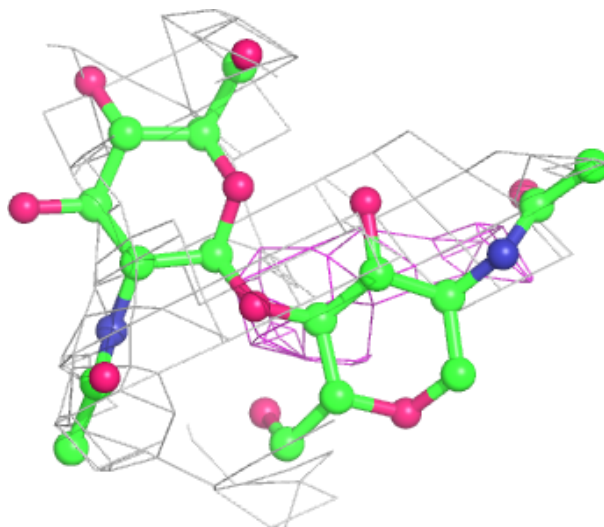
Electron density around Chain M:

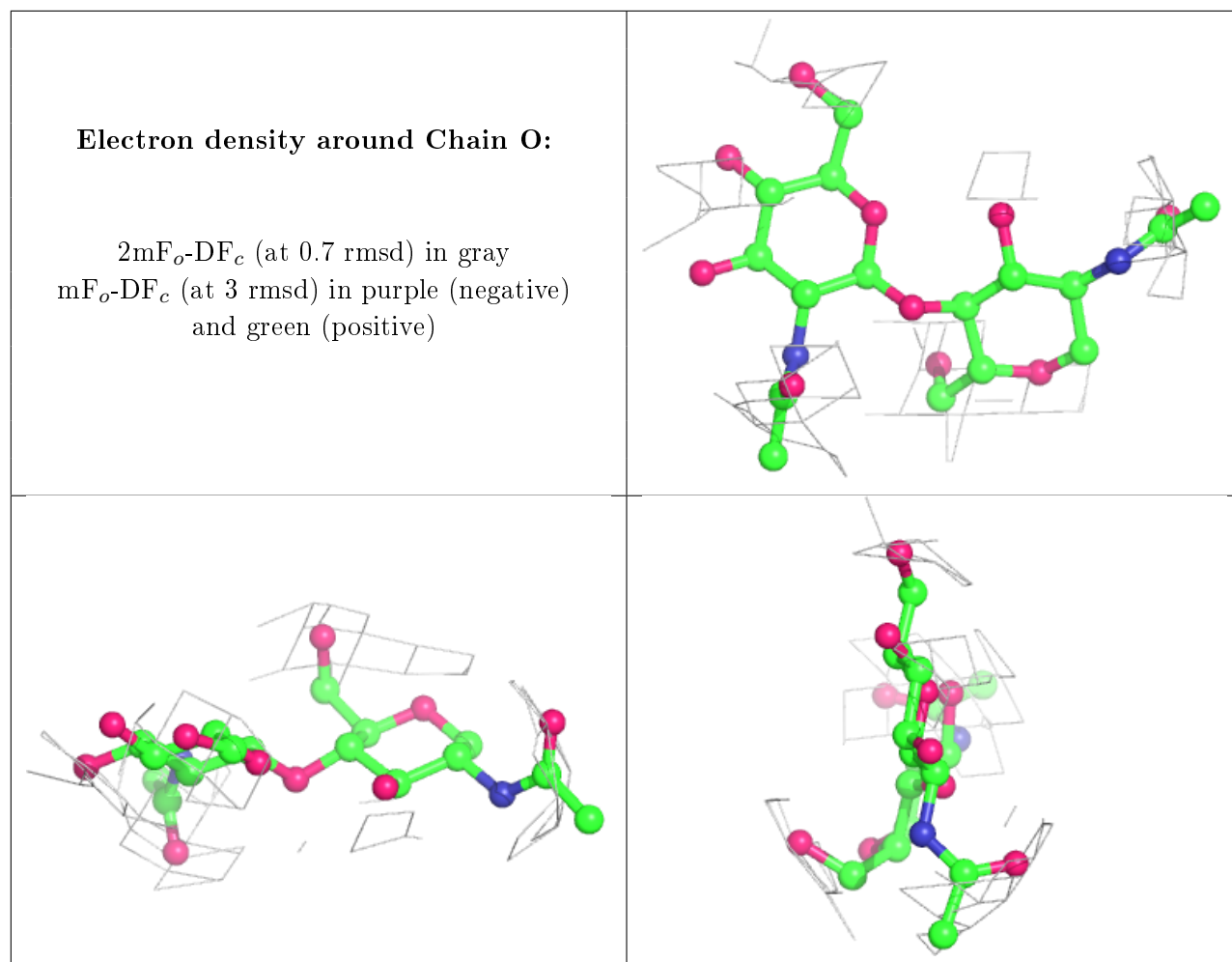
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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](#)

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
7	NAG	G	301	14/15	0.80	0.32	160,174,207,210	0
7	NAG	F	901	14/15	0.86	0.24	138,169,186,188	0
7	NAG	E	705	14/15	0.87	0.28	106,126,143,163	0

6.5 Other polymers [i](#)

There are no such residues in this entry.