



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 07:01 AM EDT

PDB ID : 5W1M
Title : MACV GP1 CR1-07 Fab complex
Authors : Raymond, D.D.; Clark, L.E.; Abraham, J.
Deposited on : 2017-06-03
Resolution : 3.91 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)
Xtrriage (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

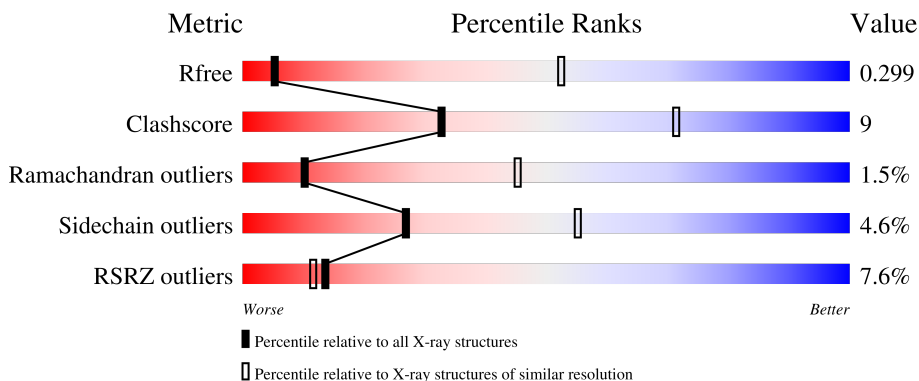
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.91 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.



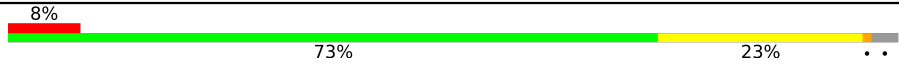

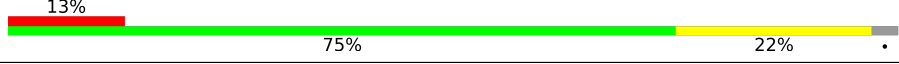
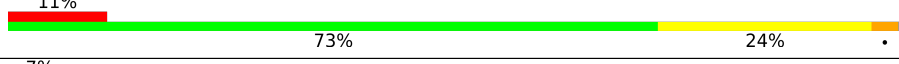

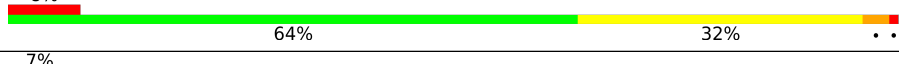
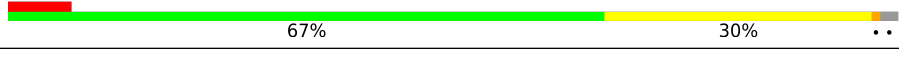

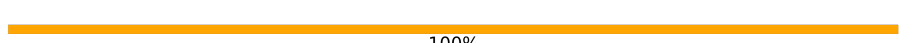
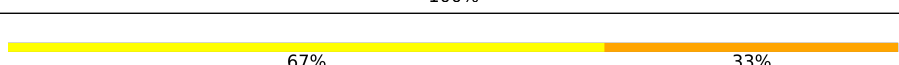
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

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	221	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2% 81% 16% •</p>
1	C	221	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">8% 78% 21% •</p>
1	E	221	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">3% 79% 20% •</p>
1	G	221	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">7% 81% 18% ••</p>
2	B	226	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">9% 73% 23% •</p>

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Mol	Chain	Length	Quality of chain
2	D	226	
2	F	226	
2	H	226	
3	Q	152	
3	R	152	
3	S	152	
3	T	152	
4	I	2	
4	J	2	
5	K	3	

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
4	NAG	I	1	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 18425 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 CR1-07 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	221	Total 1708	C 1068	N 284	O 351	S 5	0	0	0
1	C	221	Total 1711	C 1070	N 284	O 352	S 5	0	1	0
1	E	221	Total 1708	C 1068	N 284	O 351	S 5	0	0	0
1	G	219	Total 1695	C 1061	N 282	O 347	S 5	0	0	0

- Molecule 2 is a protein called CR1-07 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	218	Total 1658	C 1053	N 282	O 316	S 7	0	0	0
2	D	220	Total 1670	C 1059	N 284	O 319	S 8	0	0	0
2	F	218	Total 1658	C 1053	N 282	O 316	S 7	0	0	0
2	H	219	Total 1667	C 1058	N 283	O 319	S 7	0	1	0

- Molecule 3 is a protein called Pre-glycoprotein polyprotein GP complex.

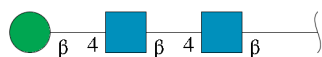
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	Q	151	Total 1209	C 761	N 209	O 225	S 14	0	0	0
3	R	152	Total 1218	C 766	N 211	O 227	S 14	0	0	0
3	S	151	Total 1209	C 761	N 209	O 225	S 14	0	0	0
3	T	149	Total 1194	C 752	N 206	O 223	S 13	0	0	0

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



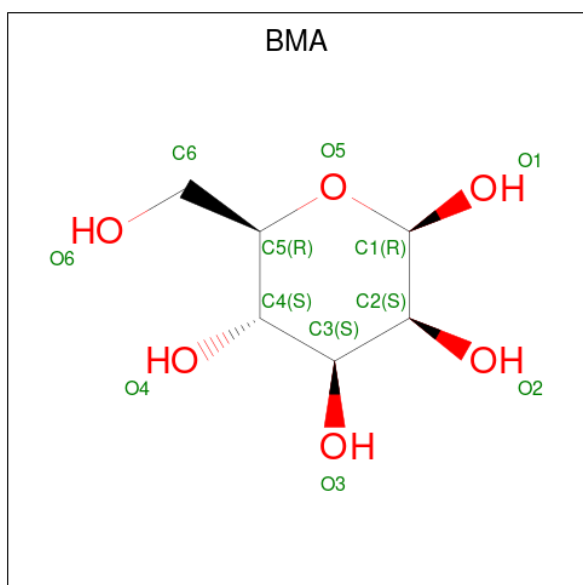
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	I	2	28	16	2	10	0	0	0
4	J	2	28	16	2	10	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



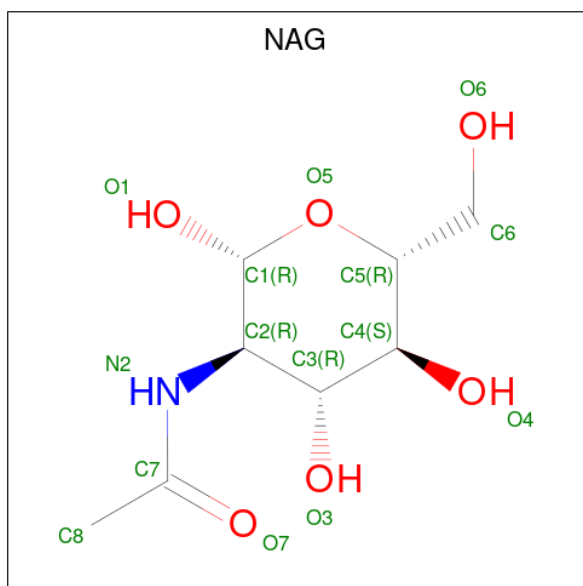
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	K	3	39	22	2	15	0	0	0

- Molecule 6 is beta-D-mannopyranose (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	Q	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

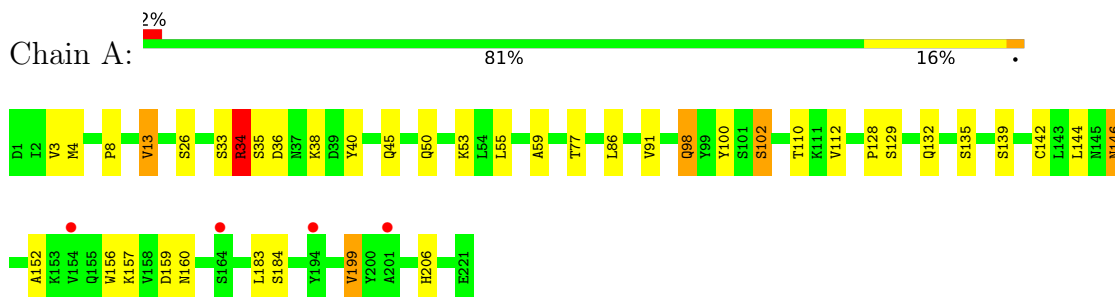


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	T	1	Total	C	N	O	0	0
			14	8	1	5		

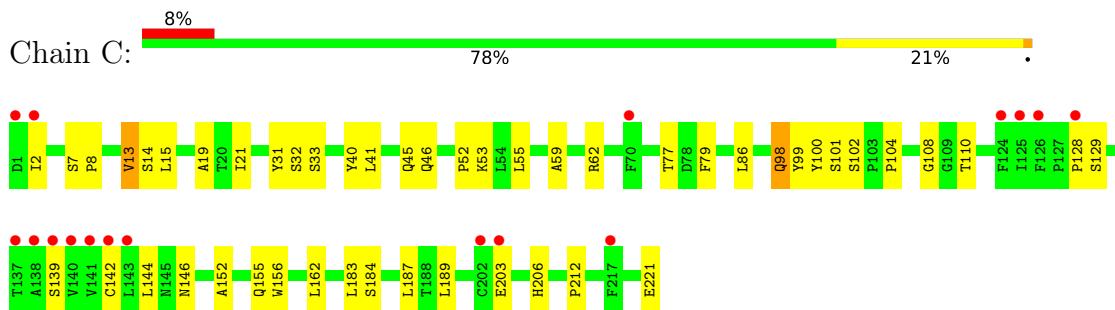
3 Residue-property plots [i](#)

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.

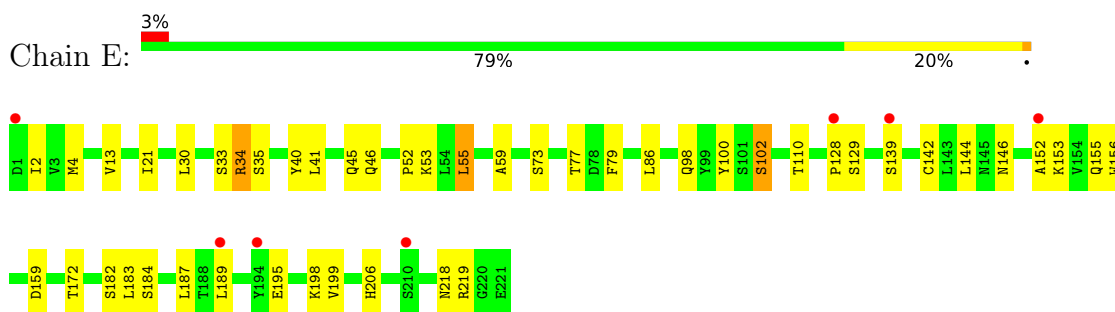
- Molecule 1: CR1-07 Fab light chain



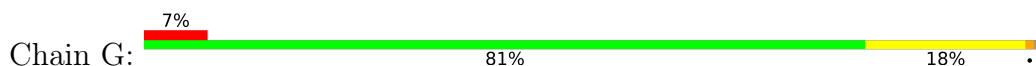
- Molecule 1: CR1-07 Fab light chain

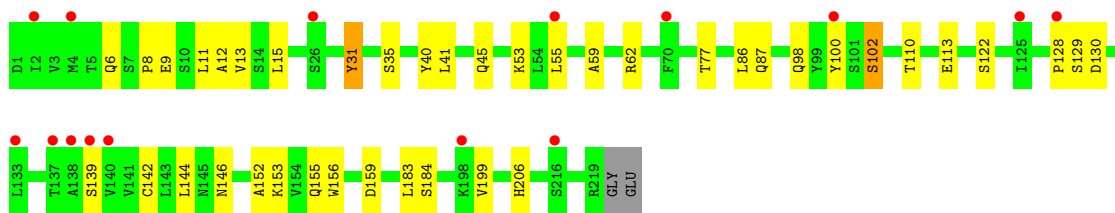


- Molecule 1: CR1-07 Fab light chain

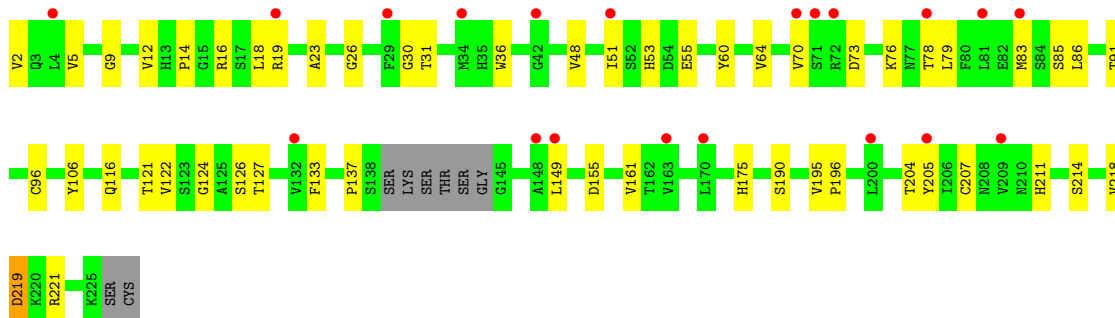
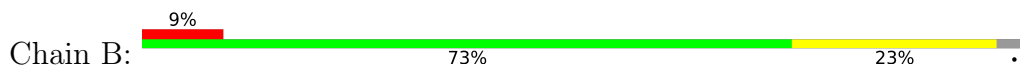


- Molecule 1: CR1-07 Fab light chain

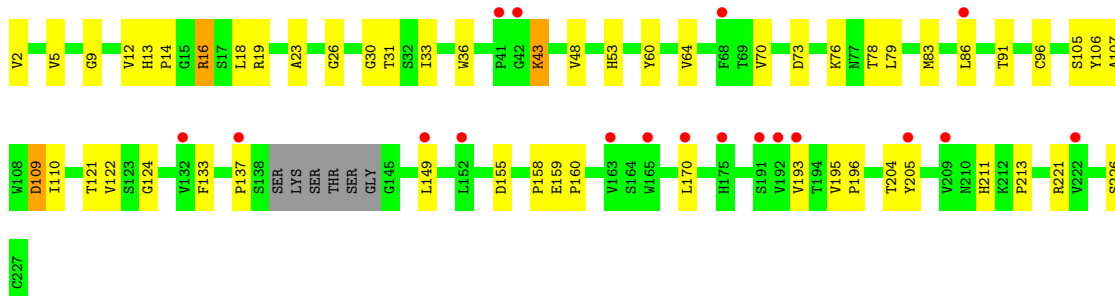
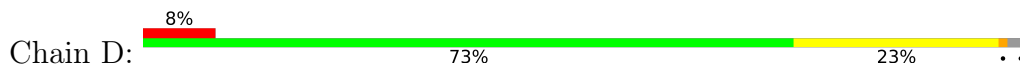




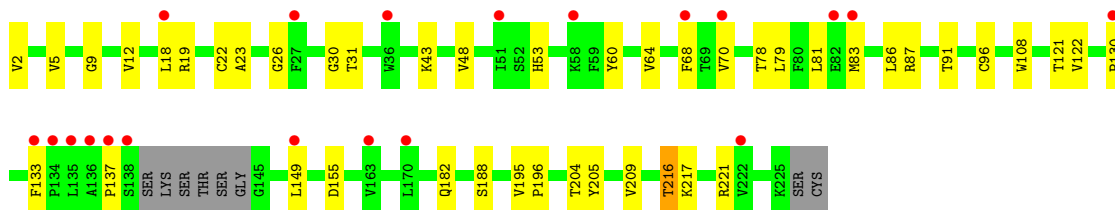
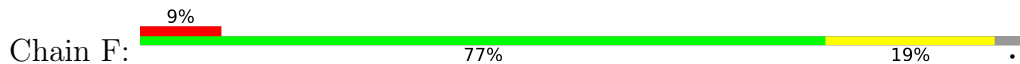
- Molecule 2: CR1-07 Fab heavy chain



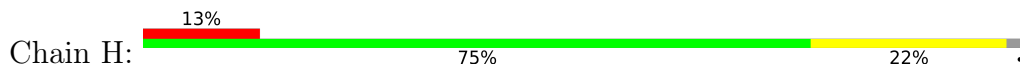
- Molecule 2: CR1-07 Fab heavy chain

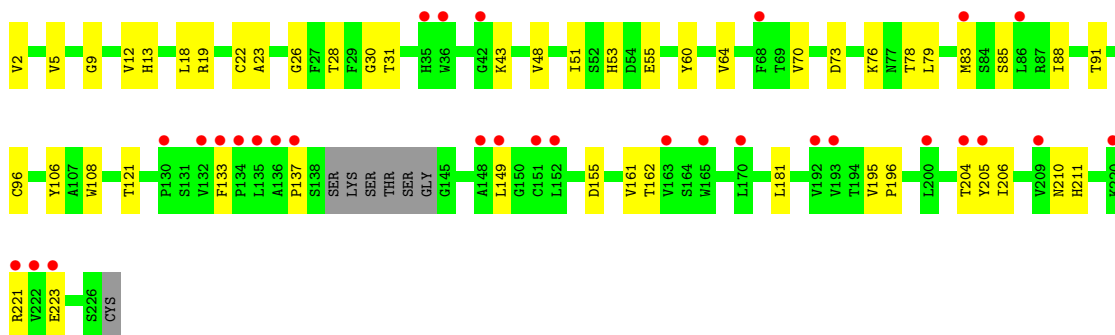


- Molecule 2: CR1-07 Fab heavy chain

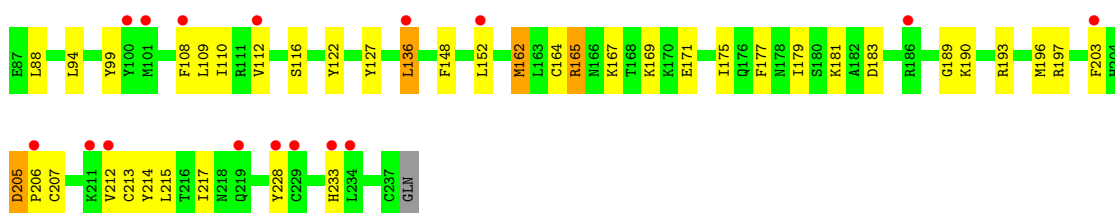
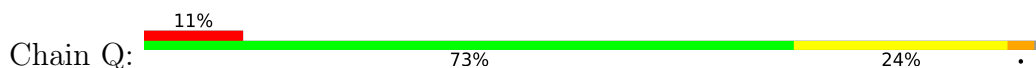


- Molecule 2: CR1-07 Fab heavy chain

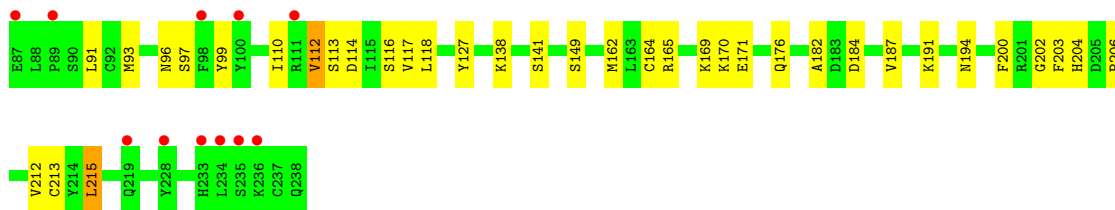
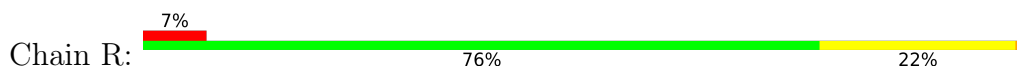




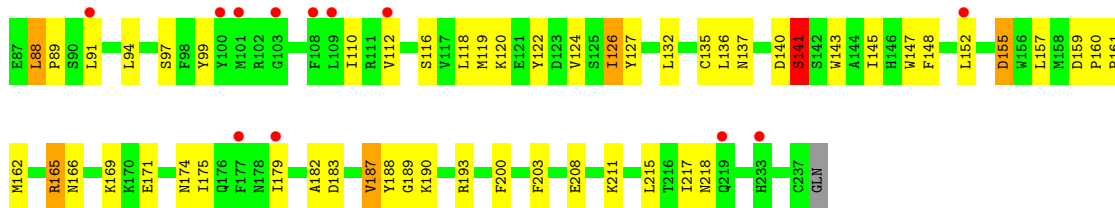
- Molecule 3: Pre-glycoprotein polyprotein GP complex



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- Molecule 3: Pre-glycoprotein polyprotein GP complex





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

Chain I: 100%

MAG1
MAG2

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

Chain J: 100%

MAG1
MAG2

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 67% 33%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	206.97Å 206.97Å 238.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 3.91 49.12 – 3.91	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.12-3.91) 98.6 (49.12-3.91)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 3.88Å)	Xtrriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.248 , 0.264 0.276 , 0.299	Depositor DCC
R_{free} test set	2332 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	183.6	Xtrriage
Anisotropy	0.321	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18425	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.51	0/1745	0.78	2/2369 (0.1%)
1	C	0.50	0/1751	0.74	0/2377
1	E	0.51	0/1745	0.74	0/2369
1	G	0.48	0/1732	0.72	0/2352
2	B	0.49	0/1702	0.75	0/2316
2	D	0.54	0/1714	0.78	0/2332
2	F	0.58	0/1702	0.77	0/2316
2	H	0.52	0/1714	0.75	0/2332
3	Q	0.67	0/1239	0.85	0/1670
3	R	0.77	0/1248	0.89	0/1682
3	S	0.81	0/1239	0.95	1/1670 (0.1%)
3	T	0.84	0/1224	0.99	2/1651 (0.1%)
All	All	0.59	0/18755	0.80	5/25436 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	174	ASN	C-N-CA	5.81	136.23	121.70
1	A	34	ARG	N-CA-C	-5.47	96.24	111.00
3	S	141	SER	N-CA-C	-5.43	96.33	111.00
1	A	34	ARG	C-N-CA	5.11	134.47	121.70
3	T	214	TYR	C-N-CA	5.09	134.41	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1708	0	1650	25	0
1	C	1711	0	1655	27	0
1	E	1708	0	1650	22	0
1	G	1695	0	1641	19	0
2	B	1658	0	1619	31	0
2	D	1670	0	1629	35	0
2	F	1658	0	1619	35	0
2	H	1667	0	1629	25	0
3	Q	1209	0	1150	38	0
3	R	1218	0	1158	21	0
3	S	1209	0	1150	42	0
3	T	1194	0	1134	31	0
4	I	28	0	24	4	0
4	J	28	0	25	4	0
5	K	39	0	34	4	0
6	Q	11	0	10	1	0
7	T	14	0	13	0	0
All	All	18425	0	17790	316	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 (316) 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:Q:175:ILE:HG23	3:Q:217:ILE:HG23	1.39	1.04
3:Q:162:MET:HG2	3:Q:177:PHE:CE1	1.99	0.98
1:A:8:PRO:O	1:A:110:THR:HG22	1.62	0.97
3:R:99:TYR:HH	3:R:203:PHE:HD1	0.99	0.96
3:S:99:TYR:HH	3:S:203:PHE:HD1	0.99	0.95
1:C:13:VAL:HG23	1:C:86:LEU:HD22	1.50	0.92
2:F:64:VAL:CG2	2:F:68:PHE:CG	2.52	0.91
1:C:8:PRO:O	1:C:110:THR:HG22	1.71	0.89
2:F:60:TYR:HE2	2:F:70:VAL:HG22	1.37	0.88
2:F:64:VAL:HG23	2:F:68:PHE:CG	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:99:TYR:HH	3:T:203:PHE:HD1	0.89	0.85
2:F:64:VAL:HG23	2:F:68:PHE:CD1	2.13	0.84
2:D:91:THR:HG22	2:D:122:VAL:H	1.44	0.83
3:S:110:ILE:CG2	3:S:215:LEU:HD11	2.09	0.81
3:Q:162:MET:HG2	3:Q:177:PHE:HE1	1.47	0.80
3:Q:175:ILE:CG2	3:Q:217:ILE:HG23	2.11	0.80
3:T:99:TYR:OH	3:T:203:PHE:HD1	1.65	0.78
3:Q:175:ILE:HG23	3:Q:217:ILE:CG2	2.13	0.78
3:S:120:LYS:HD3	5:K:1:NAG:H83	1.66	0.78
2:F:83:MET:HB3	2:F:86:LEU:HD21	1.66	0.77
1:A:13:VAL:HG23	1:A:86:LEU:HD22	1.67	0.75
1:E:13:VAL:HG23	1:E:86:LEU:HD22	1.67	0.74
1:G:13:VAL:HG23	1:G:86:LEU:HD22	1.70	0.74
2:F:81:LEU:HD12	2:F:83:MET:HG3	1.69	0.73
2:D:91:THR:CG2	2:D:122:VAL:H	2.00	0.73
1:G:8:PRO:O	1:G:110:THR:HG22	1.87	0.73
2:F:64:VAL:HG21	2:F:68:PHE:CD2	2.24	0.73
3:S:110:ILE:HG22	3:S:215:LEU:HD11	1.71	0.72
2:D:105:SER:HB2	3:T:119:MET:HE3	1.72	0.72
2:F:60:TYR:CE2	2:F:70:VAL:HG22	2.24	0.72
2:B:91:THR:HG22	2:B:122:VAL:H	1.53	0.70
3:Q:179:ILE:HG12	3:Q:215:LEU:HG	1.71	0.70
3:T:172:GLY:HA3	3:T:224:SER:HB3	1.74	0.70
2:D:105:SER:HB2	3:T:119:MET:CE	2.22	0.69
2:H:106:TYR:HD2	3:S:165:ARG:HE	1.40	0.69
2:F:91:THR:HG22	2:F:122:VAL:H	1.55	0.69
2:F:64:VAL:CG2	2:F:68:PHE:HB2	2.23	0.69
2:F:81:LEU:CD1	2:F:83:MET:HG3	2.22	0.69
3:Q:197:ARG:NH2	3:Q:205:ASP:H	1.90	0.69
3:S:126:ILE:HD11	3:S:135:CYS:SG	2.34	0.68
2:B:91:THR:CG2	2:B:122:VAL:H	2.07	0.68
1:C:187:LEU:HG	1:C:189:LEU:CD1	2.23	0.68
1:C:187:LEU:HG	1:C:189:LEU:HD11	1.76	0.68
3:Q:197:ARG:HH22	3:Q:205:ASP:H	1.40	0.67
3:S:126:ILE:HD13	3:S:132:LEU:HD23	1.76	0.67
2:F:64:VAL:HG22	2:F:68:PHE:HB2	1.77	0.66
1:E:187:LEU:HG	1:E:189:LEU:CD1	2.26	0.65
2:F:64:VAL:HG21	2:F:68:PHE:CG	2.29	0.65
1:E:129:SER:OG	2:F:133:PHE:HB3	1.97	0.65
2:B:127:THR:HB	3:S:88:LEU:HD11	1.79	0.64
3:Q:99:TYR:HB2	3:Q:110:ILE:HB	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:TYR:HE1	3:R:117:VAL:HB	1.62	0.64
1:E:21:ILE:HG12	1:E:110:THR:HG21	1.80	0.63
1:C:129:SER:OG	2:D:133:PHE:HB3	1.97	0.63
2:F:91:THR:CG2	2:F:122:VAL:H	2.11	0.63
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.81	0.63
1:E:187:LEU:HG	1:E:189:LEU:HD11	1.80	0.63
2:H:181:LEU:HG	2:H:181:LEU:O	1.99	0.62
3:Q:165:ARG:HH11	3:Q:165:ARG:CG	2.14	0.60
3:S:155:ASP:HB3	3:S:159:ASP:H	1.67	0.60
3:T:148:PHE:HD2	3:T:148:PHE:O	1.83	0.60
2:D:83:MET:HB3	2:D:86:LEU:HD21	1.84	0.60
2:D:106:TYR:CE1	3:T:117:VAL:HB	2.38	0.59
1:E:172:THR:HG22	1:E:182:SER:H	1.66	0.59
3:T:136:LEU:HD13	3:T:141:SER:HB3	1.85	0.59
1:C:41:LEU:HD22	1:C:79:PHE:CG	2.37	0.58
3:T:165:ARG:NH2	3:T:171:GLU:HB2	2.18	0.58
3:S:126:ILE:HG21	3:S:132:LEU:CD2	2.34	0.58
2:F:64:VAL:CG2	2:F:68:PHE:CB	2.81	0.58
3:Q:212:VAL:HG12	4:I:1:NAG:H82	1.86	0.58
2:F:64:VAL:CG2	2:F:68:PHE:CD2	2.86	0.57
3:T:126:ILE:HD13	3:T:132:LEU:HD23	1.85	0.57
2:B:207:CYS:O	2:B:219:ASP:HA	2.04	0.57
1:G:129:SER:OG	2:H:133:PHE:HB3	2.04	0.57
3:Q:190:LYS:HD2	3:Q:193:ARG:NH1	2.20	0.57
1:E:195:GLU:HA	1:E:219:ARG:HD3	1.86	0.57
1:A:34:ARG:HG3	3:R:127:TYR:OH	2.05	0.57
3:T:126:ILE:HD11	3:T:135:CYS:SG	2.45	0.57
3:S:91:LEU:HB3	3:S:200:PHE:CE1	2.40	0.56
3:R:93:MET:HE1	3:R:202:GLY:O	2.05	0.56
2:D:159:GLU:HG2	2:D:160:PRO:HA	1.88	0.56
1:C:101:SER:HB2	3:T:168:THR:HB	1.88	0.55
2:H:12:VAL:HG12	2:H:13:HIS:O	2.06	0.55
1:A:102:SER:HB2	3:R:170:LYS:H	1.72	0.55
3:Q:228:TYR:HA	3:Q:233:HIS:CD2	2.42	0.55
3:T:172:GLY:HA2	3:T:223:PRO:HD2	1.87	0.55
2:H:2:VAL:HA	2:H:26:GLY:HA3	1.89	0.55
3:S:136:LEU:HD13	3:S:141:SER:HB2	1.87	0.55
2:B:36:TRP:NE1	2:B:79:LEU:CD1	2.70	0.54
1:E:34:ARG:HA	3:Q:127:TYR:CE2	2.41	0.54
1:C:45:GLN:HB2	1:C:55:LEU:HD11	1.89	0.54
2:D:12:VAL:HG13	2:D:16:ARG:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:116:SER:HB3	3:Q:214:TYR:CE2	2.43	0.54
3:Q:190:LYS:HD2	3:Q:193:ARG:HH12	1.72	0.54
3:T:179:ILE:HG21	3:T:192:ILE:HB	1.89	0.54
2:B:2:VAL:HA	2:B:26:GLY:HA3	1.90	0.54
3:T:172:GLY:HA3	3:T:224:SER:CB	2.37	0.54
2:H:5:VAL:HG13	2:H:23:ALA:HB3	1.89	0.54
3:R:96:ASN:HB3	3:R:204:HIS:CE1	2.43	0.54
3:Q:165:ARG:HH11	3:Q:165:ARG:HG3	1.71	0.54
3:S:126:ILE:HG21	3:S:132:LEU:HD21	1.90	0.54
2:B:106:TYR:CE1	3:R:117:VAL:HB	2.43	0.53
2:F:5:VAL:HG13	2:F:23:ALA:HB3	1.90	0.53
2:F:48:VAL:HG13	2:F:64:VAL:HG11	1.89	0.53
1:G:45:GLN:HB2	1:G:55:LEU:HD11	1.91	0.53
3:S:118:LEU:HD21	3:S:165:ARG:HB2	1.90	0.53
3:T:177:PHE:HB2	3:T:215:LEU:HB2	1.91	0.53
3:T:181:LYS:HE3	3:T:207:CYS:HB2	1.90	0.53
1:A:129:SER:OG	2:B:133:PHE:HB3	2.09	0.52
3:R:182:ALA:HB2	4:J:2:NAG:H83	1.90	0.52
1:A:157:LYS:HE2	2:D:43:LYS:NZ	2.25	0.52
2:B:60:TYR:HE2	2:B:70:VAL:HG12	1.74	0.52
2:D:12:VAL:HG12	2:D:13:HIS:O	2.08	0.52
1:A:8:PRO:HB3	1:C:212:PRO:HB2	1.89	0.52
1:C:31:TYR:CE2	1:C:33:SER:HB3	2.45	0.52
1:A:45:GLN:HB2	1:A:55:LEU:HD11	1.90	0.52
3:R:184:ASP:HB2	4:J:1:NAG:O6	2.09	0.52
2:H:30:GLY:O	2:H:53:HIS:HB2	2.10	0.52
3:R:118:LEU:HD21	3:R:165:ARG:HB2	1.92	0.52
2:F:81:LEU:HD12	2:F:83:MET:CG	2.38	0.52
3:T:165:ARG:HH22	3:T:171:GLU:HB2	1.73	0.52
3:R:91:LEU:HB3	3:R:200:PHE:CE1	2.45	0.51
2:F:2:VAL:HA	2:F:26:GLY:HA3	1.93	0.51
1:C:21:ILE:HG23	1:C:110:THR:HG21	1.91	0.51
2:D:36:TRP:NE1	2:D:79:LEU:CD1	2.74	0.51
2:F:30:GLY:O	2:F:53:HIS:HB2	2.10	0.51
2:F:108:TRP:HA	3:Q:122:TYR:CZ	2.46	0.51
2:F:130:PRO:HD2	2:F:216:THR:HG21	1.93	0.51
2:D:2:VAL:HA	2:D:26:GLY:HA3	1.92	0.51
2:F:209:VAL:O	2:F:217:LYS:HA	2.11	0.51
2:D:5:VAL:HG13	2:D:23:ALA:HB3	1.92	0.51
3:Q:165:ARG:HD3	3:Q:171:GLU:HB2	1.93	0.50
3:Q:228:TYR:HA	3:Q:233:HIS:HD2	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:175:ILE:HD12	3:S:217:ILE:HB	1.92	0.50
2:B:126:SER:HB3	3:S:88:LEU:HG	1.93	0.50
2:F:91:THR:HG22	2:F:121:THR:HA	1.93	0.50
1:G:12:ALA:HA	1:G:113:GLU:O	2.11	0.50
1:G:31:TYR:HE2	3:S:166:ASN:ND2	2.09	0.50
2:F:87:ARG:O	2:F:122:VAL:HG11	2.12	0.50
1:E:41:LEU:HD22	1:E:79:PHE:CG	2.47	0.49
2:B:91:THR:HG22	2:B:121:THR:HA	1.94	0.49
3:T:148:PHE:O	3:T:148:PHE:CD2	2.66	0.49
2:D:195:VAL:HG11	2:D:205:TYR:CZ	2.48	0.49
3:R:138:LYS:HB2	3:R:141:SER:OG	2.12	0.49
2:D:30:GLY:O	2:D:53:HIS:HB2	2.12	0.49
1:G:152:ALA:HB2	1:G:206:HIS:HD2	1.77	0.49
1:E:2:ILE:HG22	1:E:4:MET:CE	2.43	0.49
2:H:195:VAL:HG11	2:H:205:TYR:CZ	2.48	0.49
2:B:30:GLY:O	2:B:53:HIS:HB2	2.12	0.49
1:C:155:GLN:HG2	1:C:162:LEU:HD11	1.94	0.49
3:Q:181:LYS:HE3	3:Q:207:CYS:HB2	1.94	0.49
3:T:91:LEU:HB3	3:T:200:PHE:CE1	2.48	0.48
2:B:195:VAL:HG11	2:B:205:TYR:CZ	2.48	0.48
2:D:14:PRO:HD3	2:D:124:GLY:N	2.27	0.48
3:S:148:PHE:CE2	3:S:152:LEU:HD11	2.47	0.48
2:D:204:THR:HG22	2:D:221:ARG:HH21	1.78	0.48
2:H:221:ARG:NH1	2:H:223:GLU:HG3	2.28	0.48
2:B:5:VAL:HG13	2:B:23:ALA:HB3	1.95	0.48
1:E:102:SER:HB2	3:Q:169:LYS:HA	1.95	0.48
2:H:60:TYR:HE2	2:H:70:VAL:HG12	1.78	0.48
3:S:155:ASP:OD1	3:S:157:LEU:HB2	2.13	0.48
1:A:36:ASP:OD2	3:Q:88:LEU:HD11	2.14	0.48
2:H:22:CYS:HB3	2:H:79:LEU:HB3	1.96	0.48
3:R:169:LYS:HB3	3:R:171:GLU:OE1	2.14	0.48
2:H:195:VAL:HG13	2:H:196:PRO:HD2	1.96	0.47
2:B:204:THR:HG22	2:B:221:ARG:HH21	1.79	0.47
3:T:120:LYS:HG3	3:T:163:LEU:HD11	1.96	0.47
1:E:152:ALA:HB2	1:E:206:HIS:HD2	1.77	0.47
2:D:137:PRO:HD3	2:D:149:LEU:HD23	1.97	0.47
2:D:91:THR:HG22	2:D:121:THR:HA	1.97	0.47
2:D:105:SER:HB2	3:T:119:MET:HE2	1.97	0.47
2:F:195:VAL:HG11	2:F:205:TYR:CZ	2.50	0.47
2:H:137:PRO:HD3	2:H:149:LEU:HD23	1.95	0.47
3:S:124:VAL:CG2	3:S:166:ASN:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:118:LEU:HD12	3:T:176:GLN:HB2	1.97	0.47
1:A:128:PRO:HB3	1:A:139:SER:H	1.80	0.47
3:S:120:LYS:CD	5:K:1:NAG:H83	2.42	0.47
1:G:102:SER:HB2	3:S:169:LYS:HA	1.96	0.46
1:G:153:LYS:HE2	1:G:155:GLN:HE21	1.80	0.46
2:H:204:THR:HG22	2:H:221:ARG:HH21	1.80	0.46
3:S:126:ILE:O	3:S:161:PRO:HB3	2.15	0.46
1:G:40:TYR:HB2	1:G:100:TYR:HB2	1.98	0.46
3:Q:148:PHE:CE2	3:Q:152:LEU:HD11	2.51	0.46
1:C:40:TYR:HB2	1:C:100:TYR:HB2	1.97	0.46
2:D:33:ILE:HG21	2:D:107:ALA:HB2	1.96	0.46
1:E:40:TYR:HB2	1:E:100:TYR:HB2	1.97	0.46
1:E:153:LYS:HE2	1:E:155:GLN:HE21	1.80	0.46
2:D:60:TYR:HE2	2:D:70:VAL:HG12	1.80	0.46
3:Q:197:ARG:HH22	3:Q:205:ASP:HB2	1.80	0.46
3:R:112:VAL:HG11	3:R:206:PRO:HG2	1.98	0.46
3:S:155:ASP:C	3:S:157:LEU:H	2.19	0.46
1:E:41:LEU:HD22	1:E:79:PHE:CD1	2.51	0.46
3:S:174:ASN:ND2	3:S:218:ASN:HD21	2.14	0.46
3:T:98:PHE:HE2	3:T:228:TYR:HB3	1.81	0.46
1:G:6:GLN:HE21	1:G:110:THR:HG23	1.79	0.45
2:D:91:THR:HG22	2:D:122:VAL:N	2.23	0.45
2:D:211:HIS:CD2	2:D:213:PRO:HD2	2.51	0.45
1:G:11:LEU:HD11	1:G:13:VAL:HG13	1.97	0.45
3:Q:196:MET:HB3	3:Q:203:PHE:CE1	2.51	0.45
2:B:137:PRO:HD3	2:B:149:LEU:HD23	1.99	0.45
1:C:99:TYR:CZ	2:D:110:ILE:HD11	2.51	0.45
2:D:73:ASP:OD2	2:D:76:LYS:HD3	2.16	0.45
2:F:182:GLN:OE1	2:F:188:SER:HB2	2.15	0.45
2:F:68:PHE:CD2	2:F:81:LEU:HD11	2.52	0.45
1:C:152:ALA:HB2	1:C:206:HIS:HD2	1.81	0.45
1:G:9:GLU:HG3	2:H:43:LYS:NZ	2.32	0.45
2:F:204:THR:HG22	2:F:221:ARG:HH21	1.81	0.44
2:H:108:TRP:HA	3:S:122:TYR:CZ	2.51	0.44
3:Q:177:PHE:HB2	3:Q:215:LEU:HB2	1.98	0.44
3:Q:179:ILE:HG22	3:Q:189:GLY:HA2	1.98	0.44
3:S:182:ALA:HB3	5:K:1:NAG:H62	2.00	0.44
1:A:40:TYR:HB2	1:A:100:TYR:HB2	1.99	0.44
2:B:48:VAL:HG13	2:B:64:VAL:HG21	1.99	0.44
2:B:218:VAL:HG12	2:B:219:ASP:N	2.33	0.44
1:C:41:LEU:HD22	1:C:79:PHE:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:214:TYR:CZ	4:I:1:NAG:H83	2.52	0.44
1:A:142:CYS:HB2	1:A:156:TRP:CZ2	2.53	0.44
2:D:48:VAL:HG13	2:D:64:VAL:HG21	1.98	0.44
1:G:128:PRO:HB3	1:G:139:SER:H	1.83	0.44
3:Q:165:ARG:HH11	3:Q:165:ARG:CB	2.30	0.44
3:S:174:ASN:HD22	3:S:218:ASN:HD21	1.65	0.44
3:Q:109:LEU:O	3:Q:217:ILE:HA	2.16	0.44
1:C:13:VAL:HG21	1:C:19:ALA:HB2	2.00	0.44
3:Q:108:PHE:HB3	3:Q:217:ILE:HD11	2.00	0.44
1:A:152:ALA:HB2	1:A:206:HIS:HD2	1.82	0.44
3:S:165:ARG:HD2	3:S:171:GLU:HB2	1.98	0.44
3:Q:212:VAL:HG12	4:I:1:NAG:C8	2.47	0.43
2:B:195:VAL:HG13	2:B:196:PRO:HD2	1.99	0.43
2:D:195:VAL:HG13	2:D:196:PRO:HD2	2.00	0.43
2:D:170:LEU:HD21	2:D:193:VAL:HG11	2.01	0.43
2:F:195:VAL:HG13	2:F:196:PRO:HD2	2.00	0.43
3:T:152:LEU:HD21	3:T:196:MET:HG2	1.99	0.43
3:T:136:LEU:HD13	3:T:141:SER:CB	2.47	0.43
1:C:142:CYS:HB2	1:C:156:TRP:CZ2	2.53	0.43
1:E:128:PRO:HB3	1:E:139:SER:H	1.83	0.43
2:H:48:VAL:HG13	2:H:64:VAL:HG21	2.01	0.43
1:A:146:ASN:HD21	2:B:175:HIS:CE1	2.37	0.43
1:A:34:ARG:NH1	1:A:38:LYS:HZ1	2.16	0.43
2:D:158:PRO:HD2	2:D:213:PRO:CB	2.48	0.43
2:H:206:ILE:HG13	2:H:221:ARG:HG3	2.01	0.43
1:E:159:ASP:HA	1:E:199:VAL:HG12	2.01	0.43
3:S:89:PRO:HG2	3:S:147:TRP:CE3	2.53	0.43
1:A:33:SER:O	1:A:34:ARG:HB2	2.18	0.42
1:A:159:ASP:HA	1:A:199:VAL:HG12	2.01	0.42
1:C:155:GLN:HB2	1:C:203:GLU:HG2	2.00	0.42
1:E:45:GLN:HB3	1:E:55:LEU:HD21	2.01	0.42
1:G:6:GLN:NE2	1:G:110:THR:HG23	2.34	0.42
3:S:160:PRO:HA	3:S:161:PRO:HD3	1.97	0.42
3:T:110:ILE:HG13	3:T:217:ILE:HG23	2.00	0.42
2:B:14:PRO:O	3:S:140:ASP:HB2	2.19	0.42
1:G:142:CYS:HB2	1:G:156:TRP:CZ2	2.55	0.42
1:G:159:ASP:HA	1:G:199:VAL:HG12	2.01	0.42
2:H:18:LEU:HD23	2:H:19:ARG:N	2.33	0.42
3:Q:177:PHE:HD2	3:Q:215:LEU:HB2	1.84	0.42
3:S:124:VAL:HG21	3:S:166:ASN:HB3	2.01	0.42
1:E:144:LEU:HB2	1:E:183:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:182:ALA:HB3	4:J:1:NAG:C6	2.49	0.42
3:S:119:MET:CE	5:K:1:NAG:H81	2.50	0.42
1:A:144:LEU:HB2	1:A:183:LEU:HB3	2.01	0.42
2:H:73:ASP:OD2	2:H:76:LYS:HD2	2.20	0.42
3:R:165:ARG:HD3	3:R:171:GLU:OE1	2.19	0.42
2:B:18:LEU:HD23	2:B:19:ARG:N	2.35	0.42
1:E:142:CYS:HB2	1:E:156:TRP:CZ2	2.54	0.42
3:S:110:ILE:HG23	3:S:215:LEU:HD11	1.92	0.42
2:H:51:ILE:HD11	2:H:55:GLU:HG2	2.01	0.42
2:H:91:THR:HG23	2:H:121:THR:HA	2.02	0.42
2:B:211:HIS:ND1	2:B:214:SER:HB3	2.35	0.42
1:G:9:GLU:HG3	2:H:43:LYS:HZ2	1.85	0.42
1:C:128:PRO:HB3	1:C:139:SER:H	1.85	0.42
1:C:142:CYS:HB2	1:C:156:TRP:CH2	2.55	0.42
3:S:208:GLU:HB2	3:S:211:LYS:HB2	2.02	0.42
1:E:198:LYS:HE3	1:E:218:ASN:HB3	2.02	0.41
1:A:50:GLN:HA	2:B:116:GLN:NE2	2.36	0.41
2:B:73:ASP:OD2	2:B:76:LYS:HD2	2.21	0.41
1:A:4:MET:SD	1:A:98:GLN:HB2	2.61	0.41
2:B:51:ILE:HD11	2:B:55:GLU:HG2	2.01	0.41
3:S:145:ILE:HD12	3:S:217:ILE:HG21	2.01	0.41
1:A:157:LYS:HE2	2:D:43:LYS:HZ3	1.85	0.41
1:C:2:ILE:HB	1:C:98:GLN:NE2	2.35	0.41
3:Q:136:LEU:O	3:Q:167:LYS:HD2	2.21	0.41
1:A:3:VAL:HG22	1:A:26:SER:HB3	2.02	0.41
2:B:12:VAL:HG13	2:B:16:ARG:HB2	2.03	0.41
2:F:137:PRO:HD3	2:F:149:LEU:HD23	2.03	0.41
3:Q:99:TYR:OH	3:Q:203:PHE:HD2	2.03	0.41
3:R:99:TYR:HB2	3:R:110:ILE:HB	2.01	0.41
2:B:124:GLY:O	3:S:143:TRP:HB2	2.20	0.41
3:R:182:ALA:HB3	4:J:1:NAG:H62	2.02	0.41
3:T:132:LEU:HD23	3:T:132:LEU:HA	1.95	0.41
3:Q:112:VAL:HG11	3:Q:206:PRO:HG2	2.02	0.41
3:R:204:HIS:O	3:R:206:PRO:HD3	2.21	0.41
1:A:160:ASN:OD1	1:C:108:GLY:N	2.54	0.41
1:C:102:SER:HB2	3:T:169:LYS:HA	2.03	0.41
2:F:22:CYS:HB3	2:F:79:LEU:HB3	2.03	0.41
3:Q:165:ARG:HG3	3:Q:165:ARG:NH1	2.35	0.41
3:S:136:LEU:HD13	3:S:141:SER:CB	2.51	0.41
3:S:187:VAL:HG23	3:S:188:TYR:H	1.84	0.41
3:T:165:ARG:CZ	3:T:171:GLU:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:GLN:HG3	1:C:52:PRO:HG3	2.03	0.41
2:D:18:LEU:HD23	2:D:19:ARG:N	2.36	0.41
2:H:161:VAL:HG23	2:H:211:HIS:HB2	2.03	0.41
3:R:176:GLN:HA	3:R:215:LEU:O	2.21	0.41
1:A:91:VAL:HG13	1:A:112:VAL:O	2.22	0.40
1:C:144:LEU:HB2	1:C:183:LEU:HB3	2.02	0.40
6:Q:303:BMA:H2	4:I:2:NAG:O3	2.21	0.40
2:D:36:TRP:NE1	2:D:79:LEU:HD11	2.37	0.40
1:E:46:GLN:HG3	1:E:52:PRO:HG3	2.03	0.40
2:F:18:LEU:HD23	2:F:19:ARG:N	2.36	0.40
3:S:179:ILE:HA	3:S:189:GLY:HA2	2.03	0.40
3:S:190:LYS:HD2	3:S:193:ARG:HH21	1.87	0.40
3:T:126:ILE:HG23	3:T:131:ASP:HB2	2.03	0.40
1:A:132:GLN:O	1:A:135:SER:HB3	2.21	0.40
2:B:161:VAL:HG23	2:B:211:HIS:HB2	2.03	0.40
1:G:144:LEU:HB2	1:G:183:LEU:HB3	2.02	0.40
2:H:162:THR:OG1	2:H:210:ASN:HB3	2.21	0.40
1:C:104:PRO:HD3	2:D:109:ASP:OD2	2.21	0.40
3:R:114:ASP:O	3:R:212:VAL:HG23	2.22	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	219/221 (99%)	203 (93%)	12 (6%)	4 (2%)	8	41
1	C	220/221 (100%)	206 (94%)	11 (5%)	3 (1%)	11	46
1	E	219/221 (99%)	205 (94%)	9 (4%)	5 (2%)	6	37
1	G	217/221 (98%)	206 (95%)	8 (4%)	3 (1%)	11	46
2	B	214/226 (95%)	201 (94%)	11 (5%)	2 (1%)	17	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	216/226 (96%)	204 (94%)	8 (4%)	4 (2%)	8	40
2	F	214/226 (95%)	201 (94%)	9 (4%)	4 (2%)	8	40
2	H	216/226 (96%)	202 (94%)	12 (6%)	2 (1%)	17	54
3	Q	149/152 (98%)	132 (89%)	15 (10%)	2 (1%)	12	48
3	R	150/152 (99%)	132 (88%)	17 (11%)	1 (1%)	22	60
3	S	149/152 (98%)	128 (86%)	16 (11%)	5 (3%)	3	30
3	T	147/152 (97%)	131 (89%)	15 (10%)	1 (1%)	22	60
All	All	2330/2396 (97%)	2151 (92%)	143 (6%)	36 (2%)	10	45

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	C	32	SER
3	S	183	ASP
1	A	35	SER
1	A	146	ASN
1	C	146	ASN
1	E	146	ASN
2	F	216	THR
1	G	146	ASN
3	Q	183	ASP
3	S	141	SER
1	A	59	ALA
1	E	33	SER
1	E	35	SER
1	G	59	ALA
3	R	191	LYS
2	B	155	ASP
1	C	59	ALA
2	D	155	ASP
1	E	59	ALA
2	F	9	GLY
2	F	155	ASP
1	G	35	SER
2	H	155	ASP
3	S	137	ASN
2	D	9	GLY
2	D	16	ARG
1	E	34	ARG

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Mol	Chain	Res	Type
2	F	43	LYS
2	H	9	GLY
2	D	43	LYS
3	Q	205	ASP
3	T	205	ASP
2	B	9	GLY
3	S	187	VAL
3	S	126	ILE

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	A	195/195 (100%)	188 (96%)	7 (4%)	35	61
1	C	196/195 (100%)	186 (95%)	10 (5%)	24	53
1	E	195/195 (100%)	187 (96%)	8 (4%)	30	57
1	G	194/195 (100%)	182 (94%)	12 (6%)	18	47
2	B	186/193 (96%)	180 (97%)	6 (3%)	39	63
2	D	188/193 (97%)	183 (97%)	5 (3%)	44	67
2	F	186/193 (96%)	182 (98%)	4 (2%)	52	71
2	H	188/193 (97%)	181 (96%)	7 (4%)	34	60
3	Q	136/137 (99%)	130 (96%)	6 (4%)	28	56
3	R	137/137 (100%)	126 (92%)	11 (8%)	12	41
3	S	136/137 (99%)	127 (93%)	9 (7%)	16	46
3	T	134/137 (98%)	124 (92%)	10 (8%)	13	42
All	All	2071/2100 (99%)	1976 (95%)	95 (5%)	27	55

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	53	LYS

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Mol	Chain	Res	Type
1	A	77	THR
1	A	98	GLN
1	A	102	SER
1	A	184	SER
1	A	199	VAL
2	B	31	THR
2	B	78	THR
2	B	85	SER
2	B	96	CYS
2	B	190	SER
2	B	219	ASP
1	C	7	SER
1	C	13	VAL
1	C	14	SER
1	C	15	LEU
1	C	53	LYS
1	C	62	ARG
1	C	77	THR
1	C	98	GLN
1	C	184	SER
1	C	221	GLU
2	D	31	THR
2	D	78	THR
2	D	96	CYS
2	D	109	ASP
2	D	226	SER
1	E	30	LEU
1	E	53	LYS
1	E	55	LEU
1	E	73	SER
1	E	77	THR
1	E	98	GLN
1	E	102	SER
1	E	184	SER
2	F	12	VAL
2	F	31	THR
2	F	78	THR
2	F	96	CYS
1	G	15	LEU
1	G	31	TYR
1	G	41	LEU
1	G	53	LYS

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Mol	Chain	Res	Type
1	G	62	ARG
1	G	77	THR
1	G	87	GLN
1	G	98	GLN
1	G	102	SER
1	G	122	SER
1	G	130	ASP
1	G	184	SER
2	H	28	THR
2	H	31	THR
2	H	78	THR
2	H	83	MET
2	H	85	SER
2	H	88	ILE
2	H	96	CYS
3	Q	94	LEU
3	Q	136	LEU
3	Q	162	MET
3	Q	164	CYS
3	Q	165	ARG
3	Q	213	CYS
3	R	97	SER
3	R	112	VAL
3	R	113	SER
3	R	116	SER
3	R	149	SER
3	R	162	MET
3	R	164	CYS
3	R	187	VAL
3	R	194	ASN
3	R	213	CYS
3	R	215	LEU
3	S	88	LEU
3	S	94	LEU
3	S	97	SER
3	S	112	VAL
3	S	116	SER
3	S	127	TYR
3	S	155	ASP
3	S	162	MET
3	S	165	ARG
3	T	92	CYS

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Mol	Chain	Res	Type
3	T	94	LEU
3	T	116	SER
3	T	148	PHE
3	T	162	MET
3	T	164	CYS
3	T	165	ARG
3	T	201	ARG
3	T	204	HIS
3	T	213	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	146	ASN
1	A	155	GLN
1	C	197	HIS
1	E	37	ASN
1	E	46	GLN
1	E	145	ASN
1	E	146	ASN
1	E	155	GLN
2	F	39	GLN
2	F	175	HIS
1	G	46	GLN
1	G	146	ASN
1	G	155	GLN
2	H	39	GLN
2	H	175	HIS
3	Q	233	HIS
3	R	174	ASN
3	R	219	GLN
3	R	238	GLN
3	S	174	ASN
3	T	95	ASN
3	T	96	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](#)

7 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	4,3	14,14,15	0.68	0	17,19,21	1.40	3 (17%)
4	NAG	I	2	4	14,14,15	1.12	1 (7%)	17,19,21	2.82	7 (41%)
4	NAG	J	1	4,3	14,14,15	0.57	0	17,19,21	1.37	2 (11%)
4	NAG	J	2	4	14,14,15	0.62	0	17,19,21	1.24	2 (11%)
5	NAG	K	1	5,3	14,14,15	0.44	0	17,19,21	1.69	3 (17%)
5	NAG	K	2	5	14,14,15	0.54	0	17,19,21	0.99	1 (5%)
5	BMA	K	3	5	11,11,12	0.62	0	15,15,17	1.13	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
4	NAG	I	1	4,3	-	4/6/23/26	0/1/1/1
4	NAG	I	2	4	-	3/6/23/26	0/1/1/1
4	NAG	J	1	4,3	-	3/6/23/26	0/1/1/1
4	NAG	J	2	4	-	4/6/23/26	0/1/1/1
5	NAG	K	1	5,3	-	3/6/23/26	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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	2	NAG	O5-C1	2.10	1.47	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2	NAG	O5-C1-C2	7.96	123.85	111.29
5	K	1	NAG	C2-N2-C7	4.83	129.79	122.90
4	I	2	NAG	O4-C4-C3	3.99	119.58	110.35
4	I	2	NAG	C1-C2-N2	3.65	116.73	110.49
4	I	2	NAG	O3-C3-C4	3.41	118.24	110.35
4	I	2	NAG	C1-O5-C5	3.32	116.70	112.19
4	J	1	NAG	C1-C2-N2	3.27	116.07	110.49
4	J	1	NAG	O5-C1-C2	3.14	116.25	111.29
4	J	2	NAG	C1-C2-N2	-3.09	105.21	110.49
4	I	2	NAG	C2-N2-C7	2.79	126.88	122.90
5	K	1	NAG	C1-O5-C5	2.72	115.88	112.19
4	I	1	NAG	O5-C1-C2	2.58	115.35	111.29
5	K	3	BMA	O2-C2-C3	2.50	115.15	110.14
4	I	1	NAG	C2-N2-C7	2.48	126.44	122.90
4	I	2	NAG	O5-C5-C4	-2.48	104.79	110.83
5	K	1	NAG	O3-C3-C4	-2.37	104.87	110.35
4	J	2	NAG	C1-O5-C5	2.36	115.39	112.19
4	I	1	NAG	O4-C4-C5	-2.32	103.55	109.30
5	K	3	BMA	O3-C3-C4	2.31	115.70	110.35
5	K	2	NAG	O3-C3-C4	-2.15	105.37	110.35

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C3-C2-N2-C7
5	K	1	NAG	C3-C2-N2-C7
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
4	J	1	NAG	C1-C2-N2-C7
4	I	1	NAG	O7-C7-N2-C2

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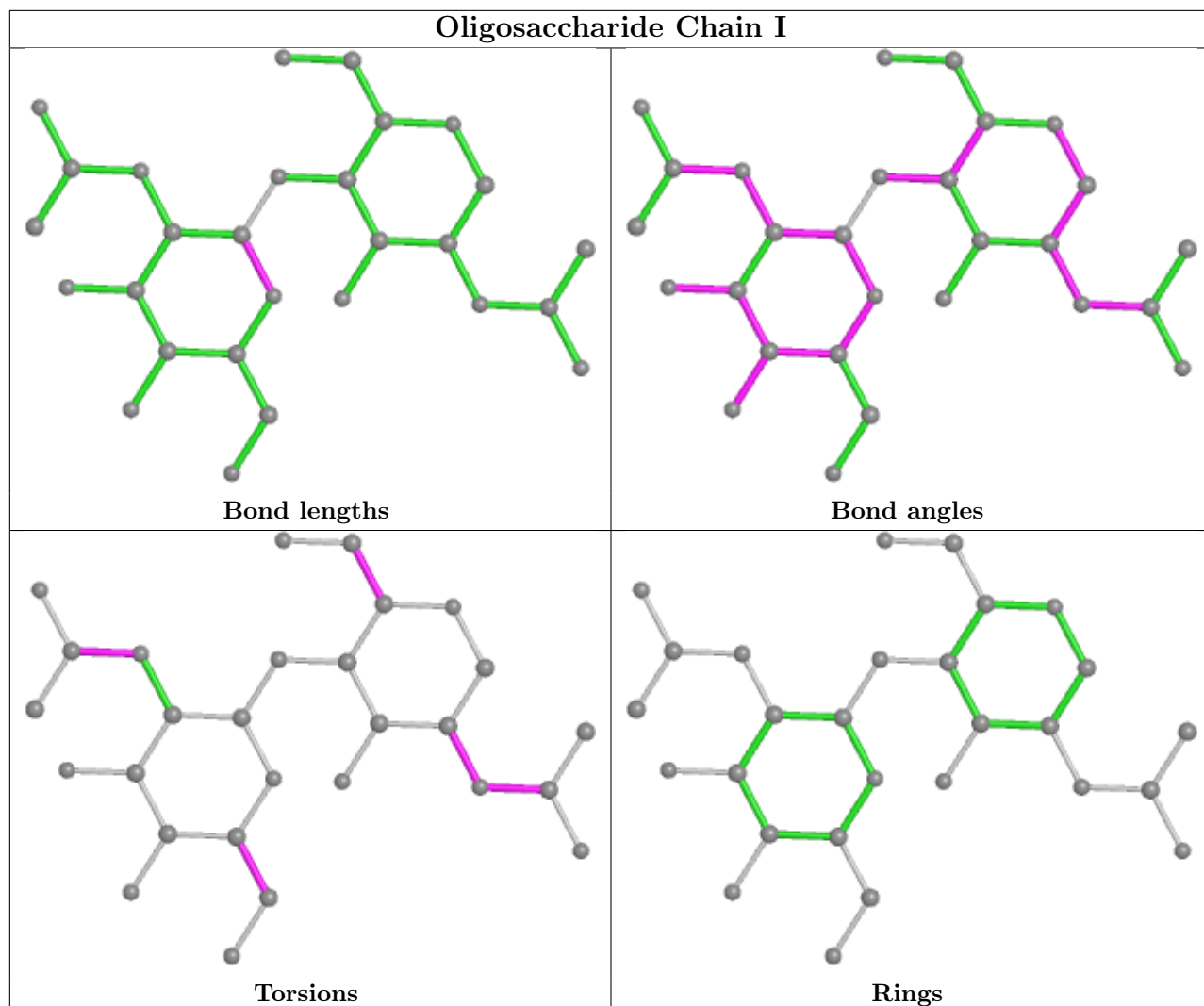
Mol	Chain	Res	Type	Atoms
4	J	2	NAG	C4-C5-C6-O6
4	I	1	NAG	C8-C7-N2-C2
4	J	2	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	I	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C4-C5-C6-O6

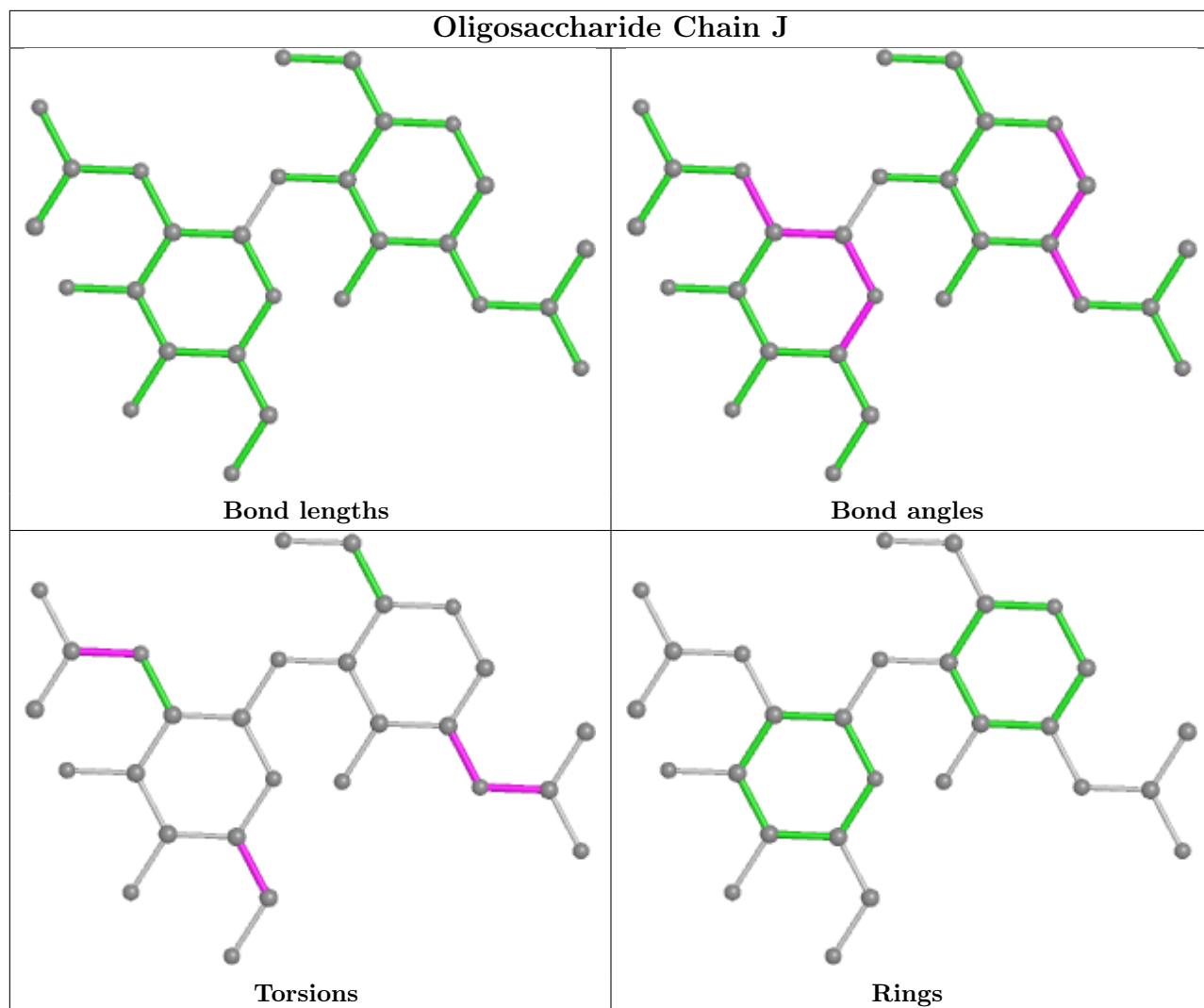
There are no ring outliers.

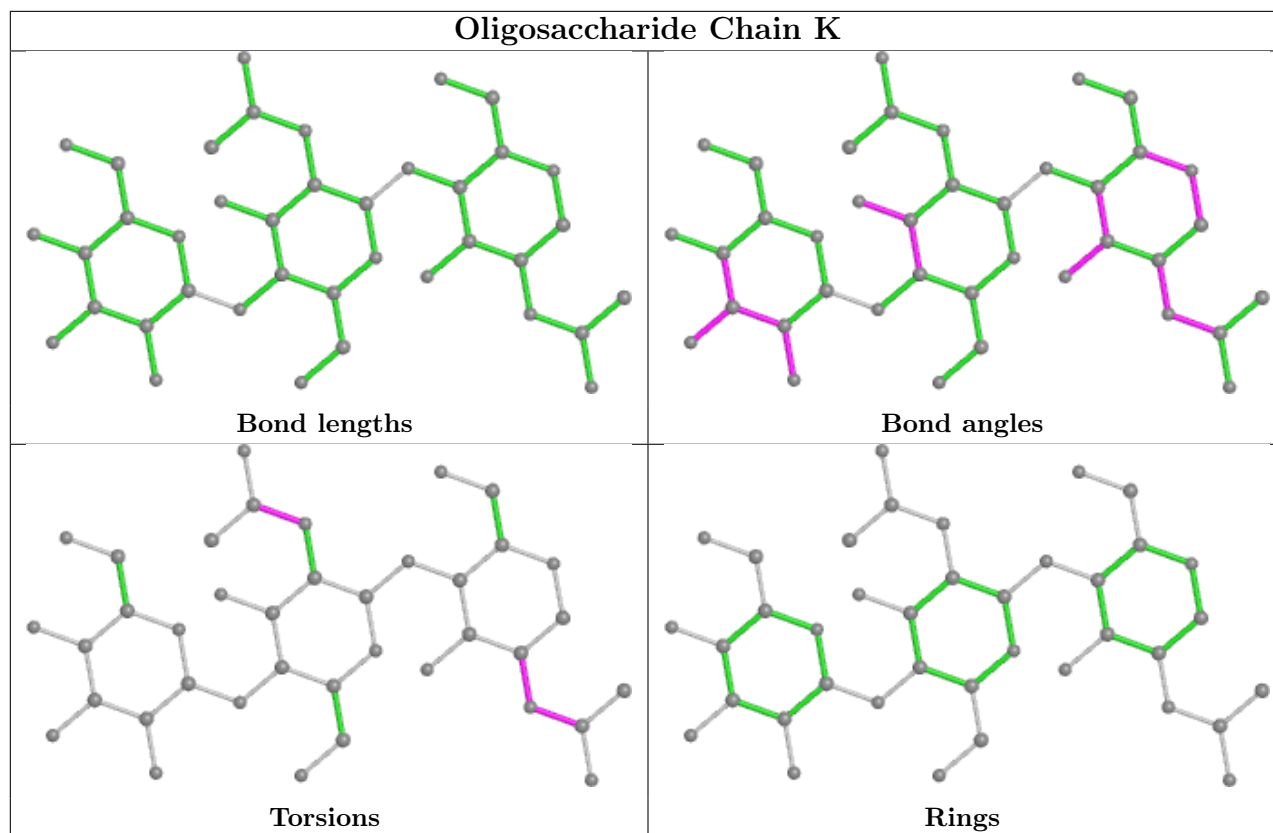
5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	3	0
4	J	1	NAG	3	0
4	I	2	NAG	1	0
5	K	1	NAG	4	0
4	J	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 [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	T	301	3	14,14,15	0.55	0	17,19,21	1.47	3 (17%)
6	BMA	Q	303	-	11,11,12	1.62	3 (27%)	15,15,17	2.56	6 (40%)

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	T	301	3	-	4/6/23/26	0/1/1/1
6	BMA	Q	303	-	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	303	BMA	C1-C2	-4.07	1.42	1.52
6	Q	303	BMA	O5-C5	2.35	1.48	1.43
6	Q	303	BMA	O5-C1	-2.07	1.40	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	303	BMA	O2-C2-C3	5.71	121.57	110.14
6	Q	303	BMA	O5-C1-C2	-4.23	104.24	110.77
7	T	301	NAG	C2-N2-C7	3.44	127.81	122.90
6	Q	303	BMA	C1-O5-C5	3.14	116.44	112.19
6	Q	303	BMA	O3-C3-C4	3.06	117.42	110.35
6	Q	303	BMA	C2-C3-C4	2.84	115.80	110.89
6	Q	303	BMA	C6-C5-C4	2.76	119.48	113.00
7	T	301	NAG	C1-O5-C5	2.63	115.75	112.19
7	T	301	NAG	C1-C2-N2	2.40	114.58	110.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	T	301	NAG	C3-C2-N2-C7
7	T	301	NAG	C8-C7-N2-C2
7	T	301	NAG	O7-C7-N2-C2
7	T	301	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Q	303	BMA	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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	221/221 (100%)	0.30	4 (1%) 68 60	21, 34, 49, 60	0
1	C	221/221 (100%)	0.41	17 (7%) 13 11	21, 33, 49, 60	0
1	E	221/221 (100%)	0.34	7 (3%) 47 37	21, 33, 49, 60	0
1	G	219/221 (99%)	0.47	15 (6%) 17 14	21, 33, 49, 60	0
2	B	218/226 (96%)	0.58	20 (9%) 9 8	20, 34, 49, 76	0
2	D	220/226 (97%)	0.53	18 (8%) 11 10	20, 34, 49, 80	0
2	F	218/226 (96%)	0.58	20 (9%) 9 8	20, 34, 49, 76	0
2	H	219/226 (96%)	0.66	30 (13%) 3 3	20, 34, 49, 76	0
3	Q	151/152 (99%)	0.65	16 (10%) 6 6	38, 50, 60, 76	0
3	R	152/152 (100%)	0.40	11 (7%) 15 12	18, 24, 35, 49	0
3	S	151/152 (99%)	0.63	12 (7%) 12 11	12, 18, 30, 43	0
3	T	149/152 (98%)	0.45	10 (6%) 17 14	12, 18, 28, 43	0
All	All	2360/2396 (98%)	0.50	180 (7%) 13 11	12, 33, 52, 80	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	S	100	TYR	6.5
2	H	222	VAL	5.9
3	Q	100	TYR	5.9
3	Q	108	PHE	4.6
2	F	137	PRO	4.5
2	H	170	LEU	4.4
1	C	125	ILE	4.4
3	S	108	PHE	4.2
2	H	137	PRO	4.2
3	R	87	GLU	4.1
2	H	205	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
2	H	149	LEU	3.9
2	F	134	PRO	3.8
2	F	138	SER	3.7
2	D	42	GLY	3.7
3	Q	186	ARG	3.7
3	Q	203	PHE	3.6
1	C	2	ILE	3.5
3	T	100	TYR	3.5
3	S	101	MET	3.5
2	D	132	VAL	3.5
2	H	134	PRO	3.4
2	H	200	LEU	3.4
3	R	233	HIS	3.4
3	R	234	LEU	3.4
3	Q	219	GLN	3.4
2	F	222	VAL	3.4
2	H	132	VAL	3.4
3	S	91	LEU	3.4
1	C	139	SER	3.4
2	B	51	ILE	3.3
2	B	71	SER	3.3
2	H	36	TRP	3.3
2	D	192	VAL	3.3
1	E	128	PRO	3.2
3	R	228	TYR	3.2
2	F	27	PHE	3.2
2	H	220	LYS	3.2
2	H	42	GLY	3.2
2	F	70	VAL	3.2
2	H	148	ALA	3.1
1	G	125	ILE	3.1
1	G	4	MET	3.1
2	B	42	GLY	3.1
2	F	133	PHE	3.1
2	H	221	ARG	3.0
2	F	82	GLU	3.0
1	G	137	THR	3.0
2	B	34	MET	3.0
2	B	149	LEU	3.0
3	Q	101	MET	3.0
3	S	179	ILE	3.0
1	G	2	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	83	MET	2.9
2	B	72	ARG	2.9
3	Q	152	LEU	2.9
2	B	19	ARG	2.9
2	D	191	SER	2.9
3	S	177	PHE	2.9
3	T	211	LYS	2.9
1	G	70	PHE	2.9
2	F	58	LYS	2.8
1	E	194	TYR	2.8
2	B	170	LEU	2.8
2	D	205	TYR	2.8
2	B	29	PHE	2.8
3	T	234	LEU	2.8
3	S	103	GLY	2.8
3	Q	212	VAL	2.7
3	S	152	LEU	2.7
3	T	97	SER	2.7
3	R	89	PRO	2.7
2	D	149	LEU	2.7
3	Q	234	LEU	2.7
1	G	139	SER	2.7
2	B	70	VAL	2.7
2	F	51	ILE	2.7
2	H	83	MET	2.7
1	A	201	ALA	2.7
2	B	148	ALA	2.6
1	C	128	PRO	2.6
3	S	219	GLN	2.6
2	F	18	LEU	2.6
2	H	133	PHE	2.6
3	Q	206	PRO	2.6
2	F	68	PHE	2.6
3	T	87	GLU	2.6
2	B	163	VAL	2.6
2	D	193	VAL	2.6
2	F	163	VAL	2.6
1	G	100	TYR	2.5
2	B	83	MET	2.5
1	C	138	ALA	2.5
1	C	143	LEU	2.5
2	D	86	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	152	LEU	2.5
3	Q	228	TYR	2.5
1	E	210	SER	2.5
2	H	35	HIS	2.5
2	B	209	VAL	2.5
3	T	219	GLN	2.5
2	H	204	THR	2.5
1	C	124	PHE	2.5
2	B	132	VAL	2.5
2	H	152	LEU	2.5
3	R	111	ARG	2.5
2	F	36	TRP	2.5
2	F	130	PRO	2.5
3	Q	211	LYS	2.5
1	G	133	LEU	2.4
2	B	81	LEU	2.4
2	H	209	VAL	2.4
3	R	236	LYS	2.4
2	D	175	HIS	2.4
1	G	128	PRO	2.4
2	H	68	PHE	2.4
1	C	137	THR	2.4
2	H	135	LEU	2.4
2	H	151	CYS	2.4
2	D	222	VAL	2.4
2	F	149	LEU	2.4
2	H	193	VAL	2.4
3	T	103	GLY	2.3
1	A	164	SER	2.3
2	H	223	GLU	2.3
3	R	100	TYR	2.3
2	D	165	TRP	2.3
1	E	1	ASP	2.3
2	F	135	LEU	2.3
2	D	41	PRO	2.3
3	R	219	GLN	2.3
1	G	138	ALA	2.3
2	H	192	VAL	2.2
2	F	136	ALA	2.2
3	Q	229	CYS	2.2
3	T	233	HIS	2.2
2	H	130	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	136	ALA	2.2
1	C	140	VAL	2.2
2	H	165	TRP	2.2
1	A	154	VAL	2.2
1	E	189	LEU	2.2
3	T	121	GLU	2.2
1	E	139	SER	2.1
2	F	170	LEU	2.1
1	C	70	PHE	2.1
2	D	170	LEU	2.1
3	Q	136	LEU	2.1
2	B	4	LEU	2.1
2	H	163	VAL	2.1
1	C	126	PHE	2.1
2	H	86	LEU	2.1
3	S	112	VAL	2.1
2	B	200	LEU	2.1
2	D	68	PHE	2.1
1	E	152	ALA	2.1
1	G	198	LYS	2.1
2	D	137	PRO	2.1
1	G	140	VAL	2.1
1	G	55	LEU	2.1
1	G	216	SER	2.1
1	C	1	ASP	2.1
2	B	205	TYR	2.1
2	D	209	VAL	2.1
3	S	109	LEU	2.1
1	C	142	CYS	2.0
1	C	141	VAL	2.0
1	C	203	GLU	2.0
1	C	217	PHE	2.0
3	R	235	SER	2.0
1	C	202	CYS	2.0
3	T	101	MET	2.0
1	G	26	SER	2.0
3	R	98	PHE	2.0
1	A	194	TYR	2.0
2	D	163	VAL	2.0
2	B	78	THR	2.0
3	Q	112	VAL	2.0
3	Q	233	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
3	S	233	HIS	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](#)

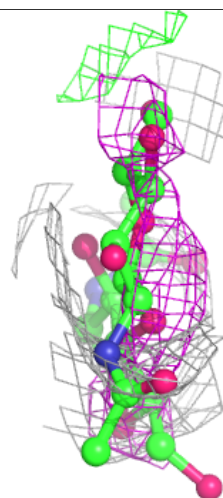
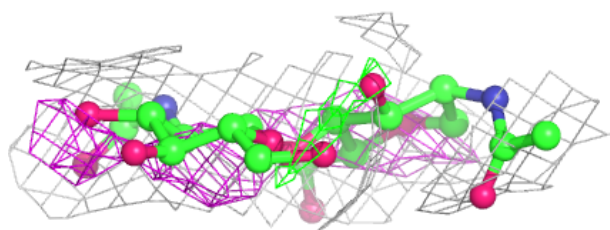
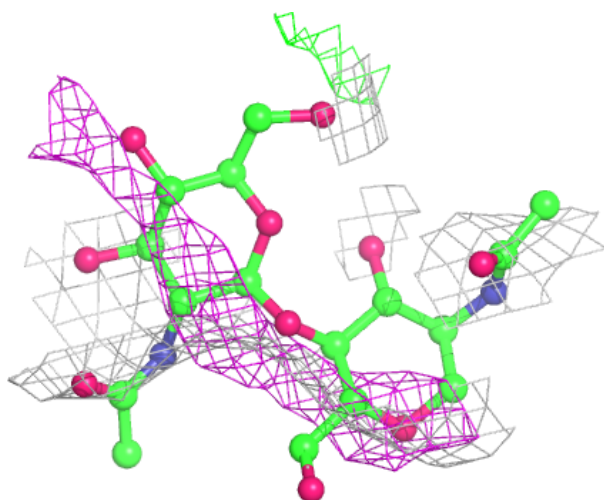
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	I	1	14/15	0.64	0.46	30,30,30,30	0
4	NAG	I	2	14/15	0.70	0.37	30,30,30,30	0
4	NAG	J	2	14/15	0.75	0.25	30,30,30,30	0
4	NAG	J	1	14/15	0.88	0.24	30,30,30,30	0
5	BMA	K	3	11/12	0.88	0.12	30,30,30,30	0
5	NAG	K	2	14/15	0.89	0.21	30,30,30,30	0
5	NAG	K	1	14/15	0.90	0.27	30,30,30,30	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.

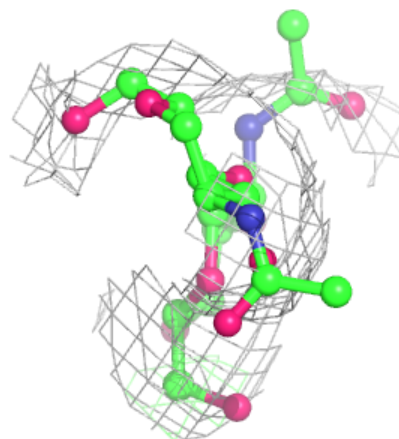
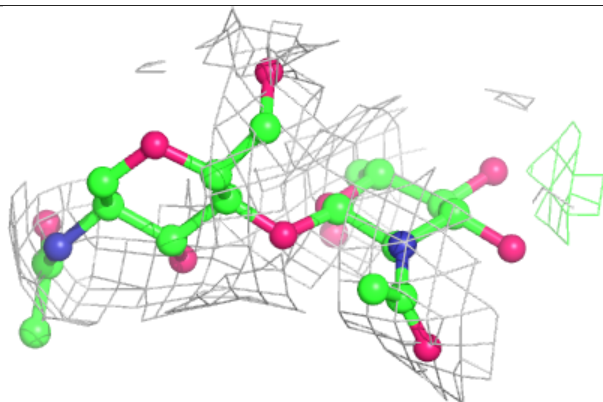
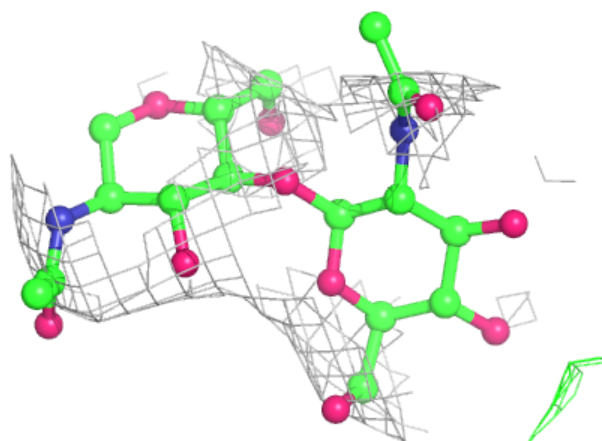
Electron density around Chain I:

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

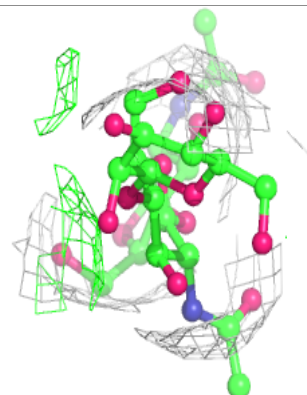
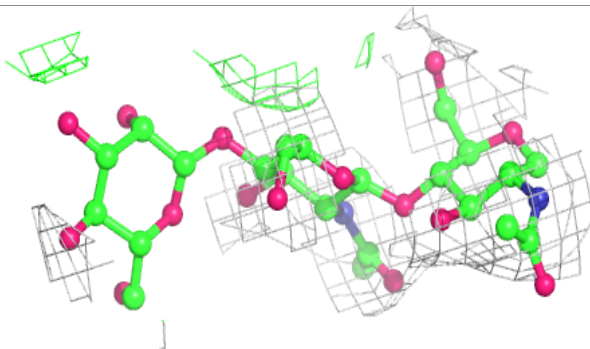
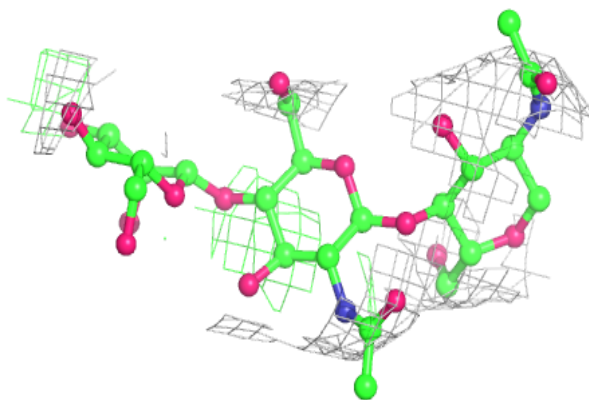


Electron density around Chain J:

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

**Electron density around Chain K:**

$2mF_o-DF_c$ (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	T	301	14/15	0.79	0.33	30,30,30,30	0
6	BMA	Q	303	11/12	0.87	0.29	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.