



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:05 PM UTC

PDB ID : 9VDZ / pdb_00009vdz
Title : hA5-6(W30B/E45) Fab bound to SFTSV glycoprotein Gn
Authors : Deng, Z.; Kuang, W.; Zhao, H.
Deposited on : 2025-06-09
Resolution : 2.43 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

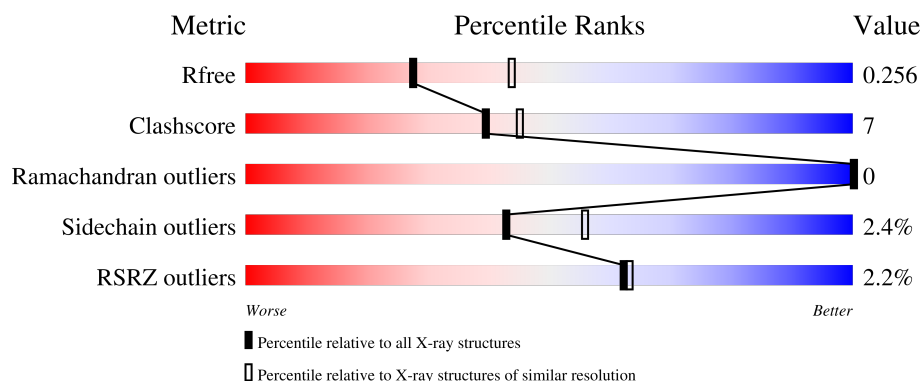
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	232	 4% 75% 18% 7%
1	H	232	 4% 77% 14% 8%
2	B	218	 2% 84% 15% .
2	L	218	 82% 16% ..
3	C	338	 2% 79% 14% 7%

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Mol	Chain	Length	Quality of chain
3	D	338	% 78%13%8%
4	G	3	33%67%
4	J	3	33%67%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11704 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 hA5-6(W30B/E45) Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1624	1027	268	322	7			
1	H	214	Total	C	N	O	S	0	0	0
			1615	1021	266	321	7			

- Molecule 2 is a protein called hA5-6(W30B/E45) Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1653	1034	274	340	5			
2	L	215	Total	C	N	O	S	0	0	0
			1649	1032	273	339	5			

- Molecule 3 is a protein called Envelopment polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	314	Total	C	N	O	S	0	0	0
			2401	1506	417	452	26			
3	D	312	Total	C	N	O	S	0	0	0
			2399	1504	415	454	26			

There are 34 discrepancies between the modelled and reference sequences:

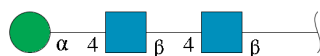
Chain	Residue	Modelled	Actual	Comment	Reference
C	341	GLY	-	expression tag	UNP W5VWE0
C	342	SER	-	expression tag	UNP W5VWE0
C	343	THR	-	expression tag	UNP W5VWE0
C	344	LEU	-	expression tag	UNP W5VWE0
C	345	GLU	-	expression tag	UNP W5VWE0
C	346	VAL	-	expression tag	UNP W5VWE0
C	347	LEU	-	expression tag	UNP W5VWE0
C	348	PHE	-	expression tag	UNP W5VWE0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	349	GLN	-	expression tag	UNP W5VWE0
C	350	GLY	-	expression tag	UNP W5VWE0
C	351	PRO	-	expression tag	UNP W5VWE0
C	352	HIS	-	expression tag	UNP W5VWE0
C	353	HIS	-	expression tag	UNP W5VWE0
C	354	HIS	-	expression tag	UNP W5VWE0
C	355	HIS	-	expression tag	UNP W5VWE0
C	356	HIS	-	expression tag	UNP W5VWE0
C	357	HIS	-	expression tag	UNP W5VWE0
D	341	GLY	-	expression tag	UNP W5VWE0
D	342	SER	-	expression tag	UNP W5VWE0
D	343	THR	-	expression tag	UNP W5VWE0
D	344	LEU	-	expression tag	UNP W5VWE0
D	345	GLU	-	expression tag	UNP W5VWE0
D	346	VAL	-	expression tag	UNP W5VWE0
D	347	LEU	-	expression tag	UNP W5VWE0
D	348	PHE	-	expression tag	UNP W5VWE0
D	349	GLN	-	expression tag	UNP W5VWE0
D	350	GLY	-	expression tag	UNP W5VWE0
D	351	PRO	-	expression tag	UNP W5VWE0
D	352	HIS	-	expression tag	UNP W5VWE0
D	353	HIS	-	expression tag	UNP W5VWE0
D	354	HIS	-	expression tag	UNP W5VWE0
D	355	HIS	-	expression tag	UNP W5VWE0
D	356	HIS	-	expression tag	UNP W5VWE0
D	357	HIS	-	expression tag	UNP W5VWE0

- Molecule 4 is an oligosaccharide called alpha-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
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

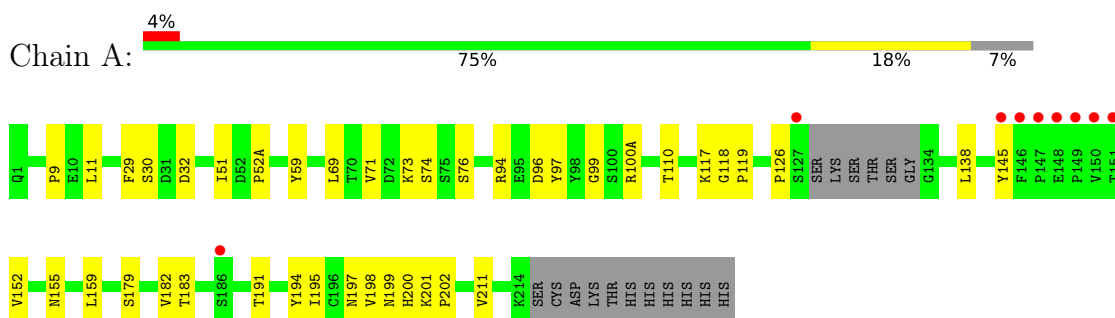
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total 27	O 27	0	0
5	B	29	Total 29	O 29	0	0
5	C	90	Total 90	O 90	0	0
5	D	74	Total 74	O 74	0	0
5	H	33	Total 33	O 33	0	0
5	L	32	Total 32	O 32	0	0

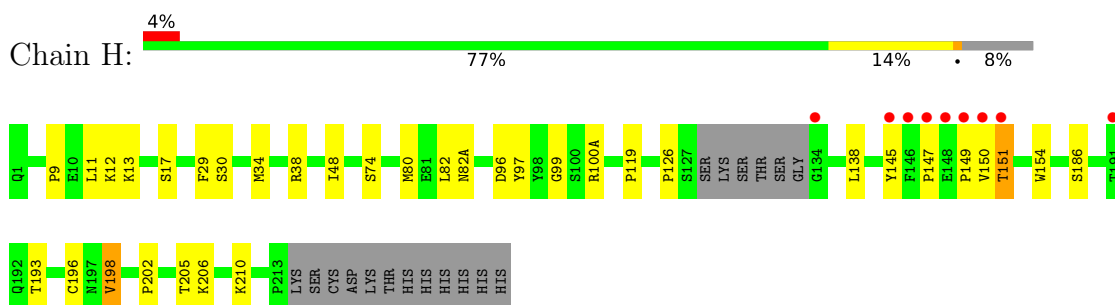
3 Residue-property plots

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.

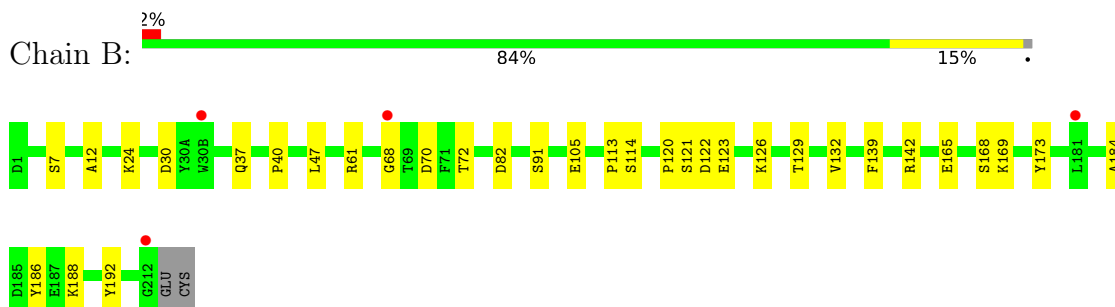
- Molecule 1: hA5-6(W30B/E45) Fab heavy chain



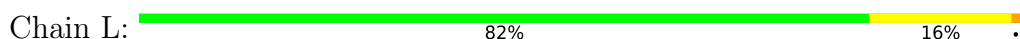
- Molecule 1: hA5-6(W30B/E45) Fab heavy chain

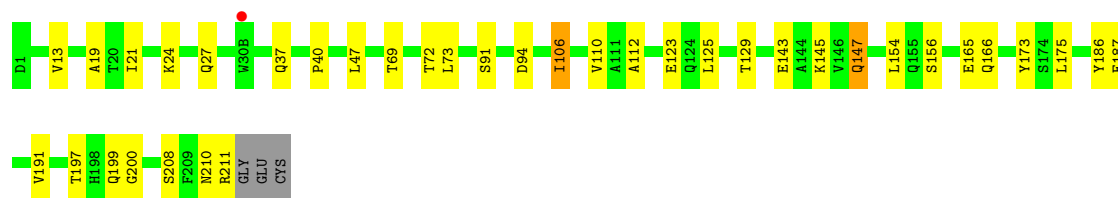


- Molecule 2: hA5-6(W30B/E45) Fab light chain

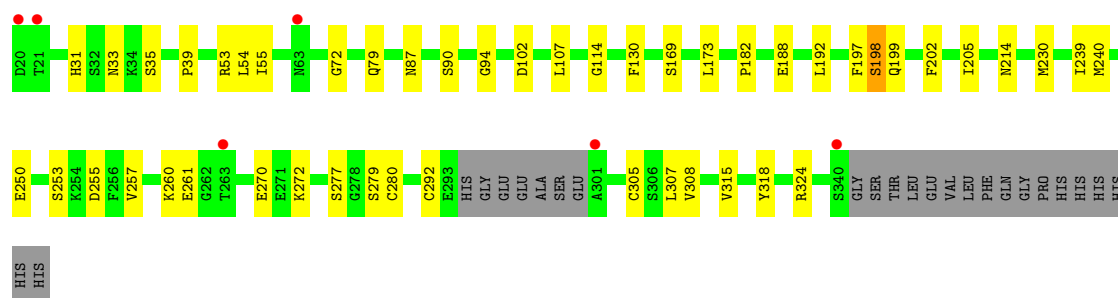
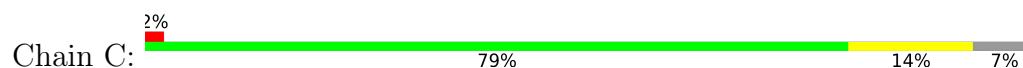


- Molecule 2: hA5-6(W30B/E45) Fab light chain

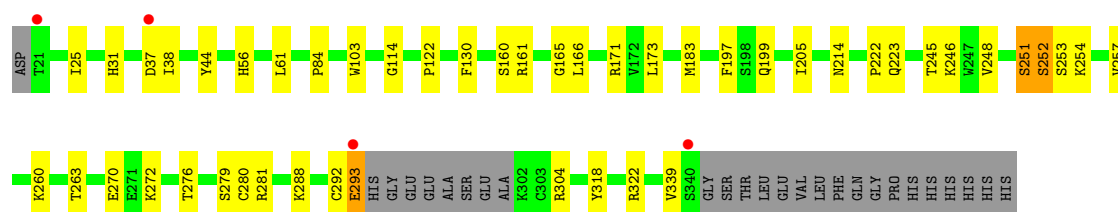
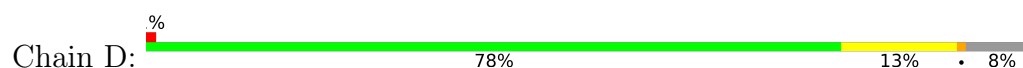




• Molecule 3: Envelopment polyprotein



• Molecule 3: Envelopment polyprotein



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.20Å 91.36Å 309.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.43 29.88 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.88-2.43) 99.2 (29.88-2.43)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.202 , 0.256 0.204 , 0.256	Depositor DCC
R_{free} test set	3522 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11704	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.44	0/1664	0.69	0/2264
1	H	0.40	0/1655	0.63	1/2253 (0.0%)
2	B	0.45	0/1689	0.64	0/2297
2	L	0.46	0/1685	0.69	0/2292
3	C	0.43	0/2461	0.63	0/3320
3	D	0.45	0/2459	0.65	0/3316
All	All	0.44	0/11613	0.65	1/15742 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	149	PRO	N-CA-CB	-5.01	97.08	102.60

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	1624	0	1586	24	0
1	H	1615	0	1573	18	0
2	B	1653	0	1586	19	0
2	L	1649	0	1583	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2401	0	2299	38	0
3	D	2399	0	2300	33	0
4	G	39	0	34	0	0
4	J	39	0	34	0	0
5	A	27	0	0	0	0
5	B	29	0	0	2	0
5	C	90	0	0	7	0
5	D	74	0	0	2	0
5	H	33	0	0	2	0
5	L	32	0	0	1	0
All	All	11704	0	10995	151	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (151) 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:C:250:GLU:OE2	3:C:324:ARG:NH2	1.75	1.20
2:L:123:GLU:OE1	2:L:123:GLU:N	2.00	0.93
1:H:126:PRO:HG3	1:H:138:LEU:HB3	1.52	0.90
3:C:260:LYS:NZ	5:C:401:HOH:O	2.05	0.89
3:C:315:VAL:HG22	3:C:324:ARG:HG3	1.56	0.88
2:B:24:LYS:HE3	5:B:320:HOH:O	1.75	0.86
2:B:122:ASP:O	2:B:126:LYS:HG2	1.82	0.78
3:C:188:GLU:O	3:C:192:LEU:HD23	1.83	0.78
2:B:121:SER:OG	2:B:123:GLU:OE1	2.02	0.76
2:B:123:GLU:OE1	2:B:123:GLU:N	2.16	0.70
1:H:206:LYS:NZ	5:H:301:HOH:O	2.20	0.70
1:A:152:VAL:HG22	1:A:198:VAL:HG22	1.73	0.69
3:D:245:THR:OG1	5:D:401:HOH:O	2.13	0.67
3:C:250:GLU:CD	3:C:324:ARG:HH22	1.96	0.67
1:A:100(A):ARG:HG2	2:B:91:SER:HB2	1.78	0.66
1:A:51:ILE:HD13	1:A:71:VAL:HG13	1.77	0.66
2:L:110:VAL:HG21	2:L:199:GLN:HE21	1.60	0.66
1:A:155:ASN:ND2	1:A:195:ILE:H	1.95	0.65
1:H:13:LYS:NZ	5:H:303:HOH:O	2.29	0.65
2:B:165:GLU:H	2:B:165:GLU:CD	2.05	0.64
2:L:166:GLN:HG3	2:L:173:TYR:CZ	2.34	0.63
3:C:199:GLN:HG2	3:C:214:ASN:OD1	1.99	0.62
2:L:147:GLN:HG3	2:L:154:LEU:CD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:193:THR:HB	1:H:210:LYS:HE2	1.82	0.62
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.82	0.61
3:C:202:PHE:HB3	3:C:205:ILE:HD12	1.83	0.61
3:D:339:VAL:O	3:D:339:VAL:HG23	2.02	0.60
3:D:25:ILE:HD11	3:D:257:VAL:HB	1.84	0.59
2:L:143:GLU:H	2:L:143:GLU:CD	2.11	0.59
1:A:117:LYS:HE3	1:A:118:GLY:O	2.03	0.58
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.85	0.58
1:A:155:ASN:HD21	1:A:194:TYR:HA	1.68	0.58
3:D:272:LYS:O	3:D:276:THR:HG23	2.04	0.58
1:A:9:PRO:HG2	1:A:202:PRO:HD3	1.86	0.58
3:D:31:HIS:HB2	3:D:166:LEU:HD12	1.85	0.57
1:H:100(A):ARG:HG2	2:L:91:SER:HB2	1.88	0.56
1:H:119:PRO:HD2	1:H:205:THR:HG21	1.87	0.56
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.88	0.56
3:C:39:PRO:HB2	5:C:405:HOH:O	2.06	0.56
1:H:38:ARG:HB3	1:H:48:ILE:HD11	1.88	0.55
3:D:272:LYS:HE2	3:D:276:THR:HG21	1.88	0.55
1:A:159:LEU:HD21	1:A:182:VAL:HG21	1.88	0.55
3:C:205:ILE:O	3:C:214:ASN:HB2	2.07	0.54
1:H:29:PHE:HE1	1:H:34:MET:HE2	1.73	0.53
3:D:288:LYS:O	3:D:288:LYS:HD3	2.09	0.53
3:D:161:ARG:HH21	3:D:171:ARG:HH12	1.55	0.53
1:H:11:LEU:O	1:H:12:LYS:HD2	2.09	0.53
3:C:182:PRO:HA	5:C:472:HOH:O	2.09	0.52
3:C:250:GLU:HG3	3:C:324:ARG:HH12	1.74	0.52
3:D:246:LYS:HD2	3:D:248:VAL:CG2	2.40	0.52
2:L:40:PRO:HG2	2:L:165:GLU:HG3	1.91	0.51
2:B:12:ALA:HA	2:B:105:GLU:O	2.10	0.51
3:D:37:ASP:OD1	3:D:38:ILE:N	2.44	0.51
3:D:280:CYS:O	3:D:292:CYS:HB2	2.11	0.51
3:D:281:ARG:NH2	3:D:304:ARG:HD2	2.26	0.51
2:B:70:ASP:HB3	5:B:320:HOH:O	2.11	0.51
2:L:211:ARG:HG2	2:L:211:ARG:HH11	1.76	0.50
3:C:261:GLU:HA	3:C:261:GLU:OE1	2.11	0.50
2:L:21:ILE:HD12	2:L:73:LEU:HD23	1.94	0.49
3:C:87:ASN:HD22	3:C:90:SER:H	1.60	0.49
1:A:155:ASN:HD21	1:A:195:ILE:H	1.60	0.49
3:C:324:ARG:HB3	5:C:433:HOH:O	2.12	0.49
3:D:222:PRO:C	3:D:223:GLN:HG2	2.36	0.49
1:A:29:PHE:CD2	1:A:76:SER:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:13:VAL:HG21	2:L:19:ALA:HB2	1.94	0.48
2:B:40:PRO:HG2	2:B:165:GLU:HG3	1.95	0.48
3:D:279:SER:HA	3:D:293:GLU:HB2	1.94	0.48
1:H:9:PRO:HG2	1:H:202:PRO:HD3	1.95	0.48
3:D:84:PRO:HD2	5:D:418:HOH:O	2.12	0.48
2:L:145:LYS:HB3	2:L:197:THR:HB	1.95	0.48
1:A:59:TYR:HE1	1:A:69:LEU:HG	1.79	0.48
3:C:33:ASN:ND2	3:C:35:SER:H	2.12	0.47
2:L:147:GLN:HG3	2:L:154:LEU:HD11	1.96	0.47
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.95	0.47
3:C:54:LEU:HD12	3:C:72:GLY:HA3	1.96	0.47
3:C:280:CYS:O	3:C:292:CYS:HB2	2.13	0.47
3:D:122:PRO:HB3	3:D:173:LEU:HD21	1.97	0.47
2:B:113:PRO:HB3	2:B:139:PHE:HB3	1.97	0.47
3:D:114:GLY:HA2	1:H:97:TYR:CD2	2.49	0.47
2:L:211:ARG:HG2	2:L:211:ARG:NH1	2.30	0.47
3:C:31:HIS:HE1	5:C:426:HOH:O	1.98	0.47
3:C:188:GLU:OE2	3:C:192:LEU:HD21	2.14	0.46
3:D:246:LYS:HD3	3:D:248:VAL:HG22	1.96	0.46
2:L:106:ILE:HB	2:L:166:GLN:HE22	1.81	0.46
3:C:130:PHE:HA	3:C:173:LEU:O	2.16	0.46
1:A:126:PRO:HG3	1:A:138:LEU:HB3	1.97	0.46
3:C:324:ARG:HD3	5:C:433:HOH:O	2.15	0.46
3:C:94:GLY:HA3	3:C:308:VAL:CG1	2.45	0.46
1:A:11:LEU:HD12	1:A:110:THR:O	2.16	0.46
2:B:30:ASP:CG	2:B:68:GLY:H	2.24	0.46
3:C:188:GLU:O	3:C:192:LEU:CD2	2.60	0.46
2:L:24:LYS:O	5:L:301:HOH:O	2.20	0.45
1:H:96:ASP:OD2	1:H:99:GLY:HA3	2.17	0.45
2:L:187:GLU:HA	2:L:211:ARG:NE	2.31	0.45
1:H:11:LEU:HB2	1:H:147:PRO:HG3	1.99	0.45
2:L:125:LEU:HD21	2:L:186:TYR:CD2	2.52	0.45
3:C:192:LEU:HD22	3:C:192:LEU:N	2.32	0.45
1:H:80:MET:HE3	1:H:82:LEU:HB2	1.98	0.45
2:L:191:VAL:HG22	2:L:210:ASN:OD1	2.16	0.45
1:A:199:ASN:HD22	1:A:200:HIS:N	2.14	0.45
3:C:102:ASP:HA	3:C:107:LEU:O	2.16	0.45
3:D:246:LYS:CD	3:D:248:VAL:CG2	2.95	0.45
1:A:52(A):PRO:O	1:A:73:LYS:HD2	2.17	0.44
3:C:79:GLN:HB2	3:C:169:SER:HB2	1.99	0.44
3:D:322:ARG:HH11	3:D:322:ARG:HG3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:161:ARG:NE	3:D:171:ARG:HH22	2.15	0.44
3:D:197:PHE:HD2	3:D:318:TYR:CZ	2.36	0.44
1:H:151:THR:O	1:H:198:VAL:HA	2.18	0.44
1:A:96:ASP:OD2	1:A:99:GLY:HA3	2.17	0.44
2:B:61:ARG:HH21	2:B:82:ASP:CG	2.25	0.43
3:C:94:GLY:HA3	3:C:308:VAL:HG13	1.99	0.43
3:D:205:ILE:O	3:D:214:ASN:HB2	2.18	0.43
1:H:17:SER:OG	1:H:82(A):ASN:HB3	2.18	0.43
2:L:165:GLU:H	2:L:165:GLU:CD	2.27	0.43
3:C:53:ARG:HB2	3:C:55:ILE:HD13	2.00	0.43
2:B:142:ARG:HB2	2:B:173:TYR:CE2	2.52	0.43
2:B:168:SER:C	2:B:169:LYS:HE2	2.44	0.43
3:D:251:SER:O	3:D:251:SER:OG	2.28	0.43
3:C:255:ASP:O	3:C:307:LEU:HD12	2.18	0.43
3:D:56:HIS:HB3	3:D:103:TRP:CD2	2.54	0.43
3:D:183:MET:HE3	3:D:183:MET:HB3	1.90	0.42
3:C:270:GLU:OE1	5:C:401:HOH:O	2.20	0.42
2:B:24:LYS:HB3	2:B:24:LYS:HE2	1.79	0.42
3:D:260:LYS:NZ	3:D:270:GLU:OE2	2.49	0.42
1:A:152:VAL:HA	1:A:197:ASN:O	2.19	0.42
1:A:201:LYS:N	1:A:202:PRO:HD2	2.34	0.42
3:C:198:SER:OG	3:C:239:ILE:O	2.35	0.42
3:D:130:PHE:HA	3:D:173:LEU:O	2.19	0.42
1:A:138:LEU:HD12	1:A:211:VAL:CG2	2.49	0.42
2:B:186:TYR:O	2:B:192:TYR:OH	2.36	0.42
2:L:27:GLN:O	2:L:69:THR:HG22	2.19	0.42
2:L:112:ALA:HB2	2:L:200:GLY:O	2.20	0.42
1:A:32:ASP:OD2	1:A:94:ARG:HD2	2.20	0.41
3:D:252:SER:OG	3:D:253:SER:N	2.53	0.41
3:D:44:TYR:CZ	3:D:254:LYS:HG3	2.55	0.41
3:D:56:HIS:HB3	3:D:103:TRP:CG	2.56	0.41
1:A:97:TYR:CD1	3:C:114:GLY:HA2	2.56	0.41
1:A:119:PRO:HB3	1:A:145:TYR:HB3	2.02	0.41
1:A:155:ASN:N	1:A:155:ASN:HD22	2.18	0.41
3:C:54:LEU:HD23	3:C:54:LEU:HA	1.93	0.41
3:C:277:SER:OG	3:C:279:SER:OG	2.21	0.41
3:C:315:VAL:HG22	3:C:324:ARG:CG	2.37	0.41
3:D:199:GLN:HG2	3:D:214:ASN:OD1	2.21	0.41
1:H:154:TRP:CZ3	1:H:196:CYS:HB3	2.56	0.41
1:A:73:LYS:HE3	1:A:73:LYS:HB3	1.89	0.40
3:C:197:PHE:HD1	3:C:318:TYR:CZ	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:257:VAL:O	3:C:305:CYS:HA	2.21	0.40
3:D:165:GLY:C	3:D:166:LEU:HD22	2.46	0.40
2:L:175:LEU:HD23	2:L:175:LEU:C	2.46	0.40
3:C:230:MET:HE2	3:C:240:MET:SD	2.61	0.40
2:B:184:ALA:O	2:B:188:LYS:HG2	2.21	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	211/232 (91%)	203 (96%)	8 (4%)	0	100	100
1	H	210/232 (90%)	204 (97%)	6 (3%)	0	100	100
2	B	214/218 (98%)	210 (98%)	4 (2%)	0	100	100
2	L	213/218 (98%)	208 (98%)	5 (2%)	0	100	100
3	C	310/338 (92%)	300 (97%)	10 (3%)	0	100	100
3	D	308/338 (91%)	298 (97%)	10 (3%)	0	100	100
All	All	1466/1576 (93%)	1423 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	183/199 (92%)	178 (97%)	5 (3%)	39	52
1	H	182/199 (92%)	176 (97%)	6 (3%)	33	45
2	B	186/189 (98%)	182 (98%)	4 (2%)	45	59
2	L	186/189 (98%)	179 (96%)	7 (4%)	29	41
3	C	266/292 (91%)	263 (99%)	3 (1%)	65	75
3	D	268/292 (92%)	262 (98%)	6 (2%)	45	59
All	All	1271/1360 (94%)	1240 (98%)	31 (2%)	43	56

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	SER
1	A	74	SER
1	A	179	SER
1	A	183	THR
1	A	191	THR
2	B	7	SER
2	B	72	THR
2	B	114	SER
2	B	129	THR
3	C	198	SER
3	C	253	SER
3	C	272	LYS
3	D	61	LEU
3	D	160	SER
3	D	251	SER
3	D	252	SER
3	D	263	THR
3	D	293	GLU
1	H	30	SER
1	H	74	SER
1	H	150	VAL
1	H	151	THR
1	H	186	SER
1	H	198	VAL
2	L	72	THR
2	L	94	ASP
2	L	106	ILE
2	L	129	THR
2	L	147	GLN
2	L	156	SER

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Mol	Chain	Res	Type
2	L	208	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	39	GLN
1	A	155	ASN
1	A	199	ASN
2	B	38	GLN
2	B	137	ASN
3	C	31	HIS
3	C	33	ASN
3	C	40	HIS
3	C	66	GLN
3	C	87	ASN
3	C	223	GLN
3	C	285	GLN
3	D	33	ASN
3	D	249	GLN
2	L	137	ASN
2	L	199	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

6 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	G	1	3,4	14,14,15	0.92	1 (7%)	17,19,21	1.14	1 (5%)
4	NAG	G	2	4	14,14,15	0.71	0	17,19,21	0.62	0
4	MAN	G	3	4	11,11,12	1.74	3 (27%)	15,15,17	1.49	2 (13%)
4	NAG	J	1	3,4	14,14,15	1.07	2 (14%)	17,19,21	0.94	1 (5%)
4	NAG	J	2	4	14,14,15	0.57	0	17,19,21	0.76	0
4	MAN	J	3	4	11,11,12	1.84	3 (27%)	15,15,17	1.42	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	G	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	MAN	G	3	4	-	1/2/19/22	1/1/1/1
4	NAG	J	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	MAN	J	3	4	-	1/2/19/22	1/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	3	MAN	C1-C2	4.00	1.61	1.52
4	G	3	MAN	C1-C2	3.88	1.61	1.52
4	G	1	NAG	C1-C2	3.33	1.56	1.52
4	J	1	NAG	C1-C2	3.01	1.56	1.52
4	J	3	MAN	C4-C5	2.82	1.59	1.53
4	J	3	MAN	O3-C3	2.50	1.49	1.43
4	G	3	MAN	O3-C3	2.45	1.49	1.43
4	J	1	NAG	O5-C1	-2.39	1.39	1.43
4	G	3	MAN	C4-C5	2.34	1.58	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	C1-O5-C5	3.91	117.43	112.19
4	G	3	MAN	C1-O5-C5	3.39	116.72	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	3	MAN	C1-O5-C5	3.31	116.62	112.19
4	J	3	MAN	O2-C2-C3	-2.75	104.45	110.15
4	J	1	NAG	C1-O5-C5	2.53	115.58	112.19
4	G	3	MAN	O3-C3-C2	2.48	115.11	110.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

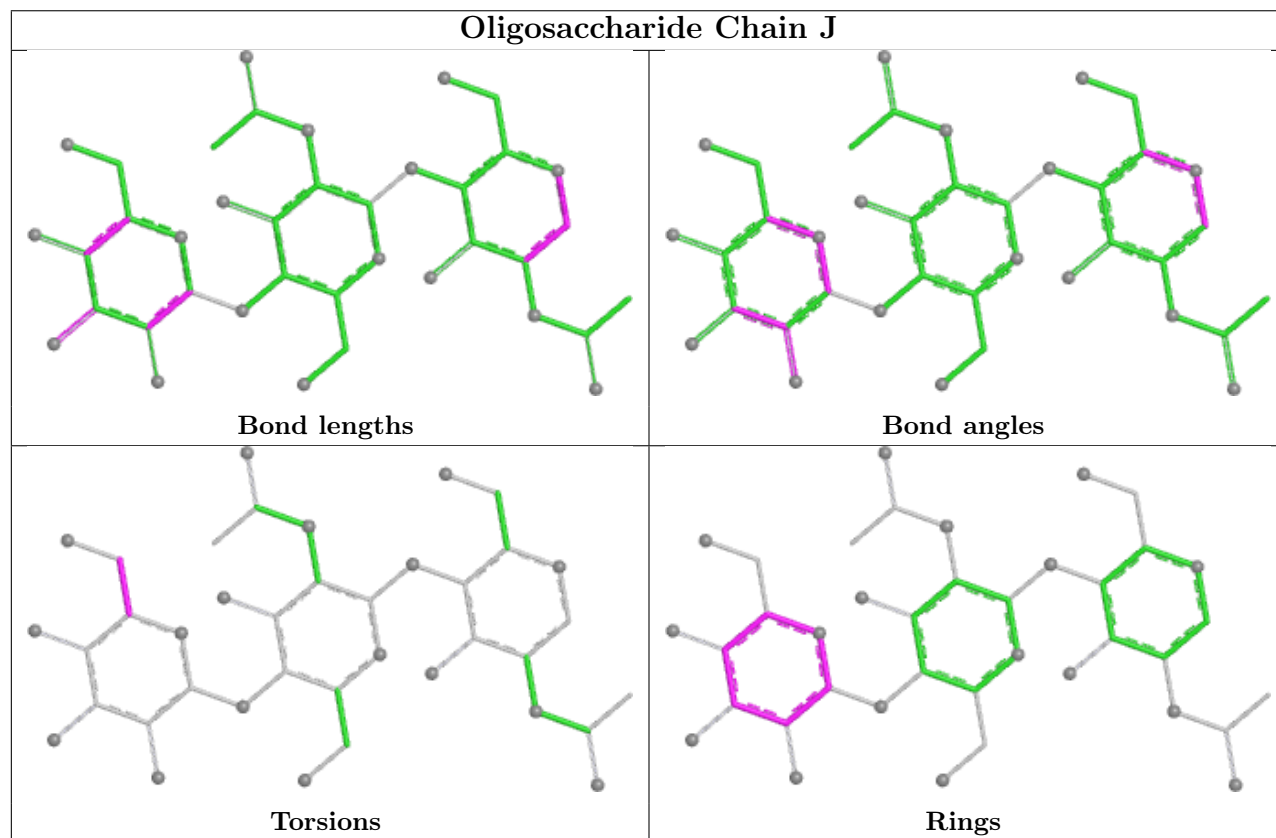
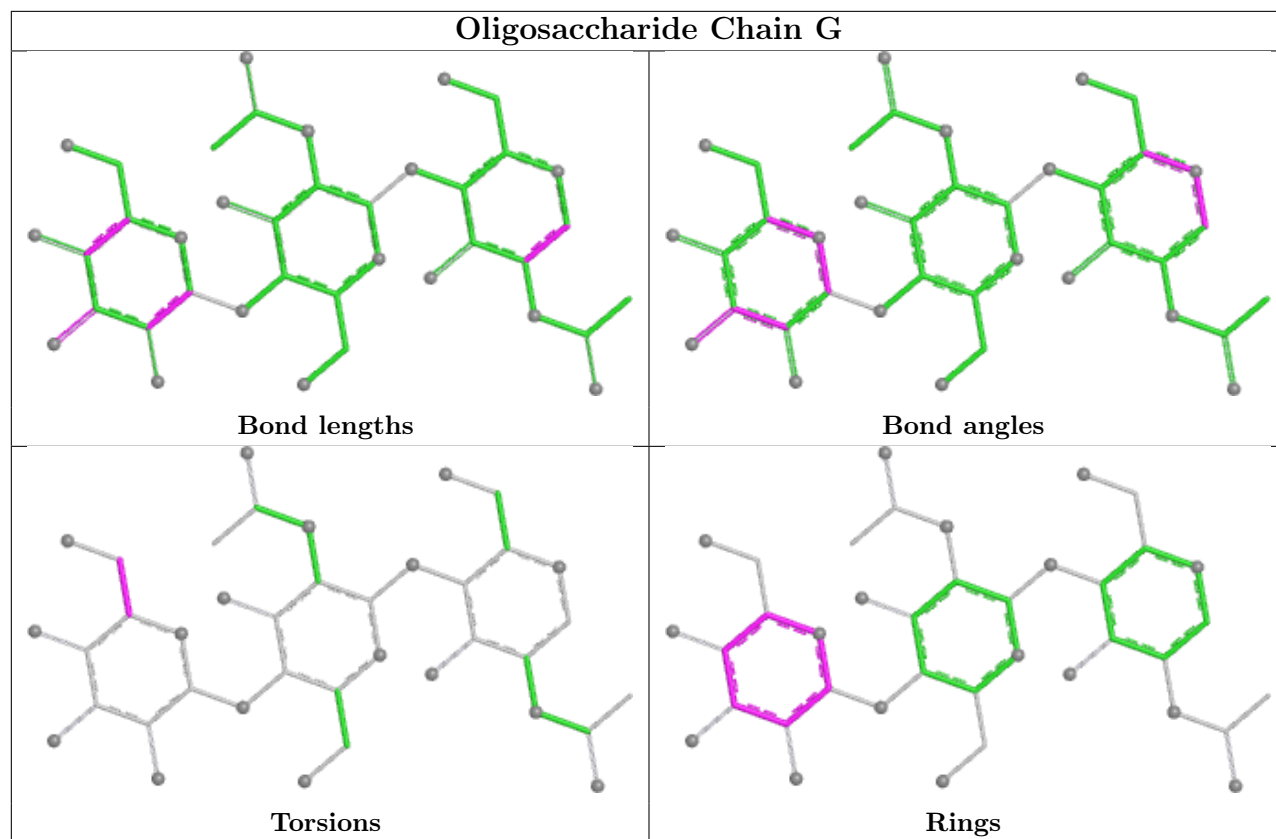
Mol	Chain	Res	Type	Atoms
4	J	3	MAN	C4-C5-C6-O6
4	G	3	MAN	C4-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	3	MAN	C1-C2-C3-C4-C5-O5
4	G	3	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

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



5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	215/232 (92%)	0.22	9 (4%)	40 38	37, 53, 76, 99	0
1	H	214/232 (92%)	0.11	9 (4%)	40 38	35, 49, 75, 99	0
2	B	216/218 (99%)	0.17	4 (1%)	66 67	30, 55, 67, 80	0
2	L	215/218 (98%)	0.03	1 (0%)	87 89	30, 52, 65, 73	0
3	C	314/338 (92%)	-0.07	6 (1%)	66 67	30, 43, 64, 79	0
3	D	312/338 (92%)	-0.12	4 (1%)	75 77	29, 43, 59, 76	0
All	All	1486/1576 (94%)	0.04	33 (2%)	62 63	29, 49, 67, 99	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	145	TYR	5.9
1	A	146	PHE	5.6
1	H	149	PRO	5.6
1	H	146	PHE	5.6
1	H	150	VAL	5.4
1	A	150	VAL	5.2
1	A	145	TYR	5.0
1	H	151	THR	4.6
1	A	149	PRO	4.5
1	A	151	THR	4.4
1	H	148	GLU	4.4
1	H	147	PRO	4.3
3	C	301	ALA	3.9
1	A	147	PRO	3.6
1	A	148	GLU	3.4
3	D	340	SER	3.3
2	L	30(B)	TRP	3.0
3	C	20	ASP	2.9
3	C	63	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	212	GLY	2.7
3	C	340	SER	2.6
1	H	134	GLY	2.5
2	B	30(B)	TRP	2.5
3	D	293	GLU	2.5
3	D	37	ASP	2.4
1	H	191	THR	2.3
3	C	21	THR	2.2
1	A	127	SER	2.1
3	D	21	THR	2.1
2	B	181	LEU	2.0
2	B	68	GLY	2.0
3	C	263	THR	2.0
1	A	186	SER	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](#)

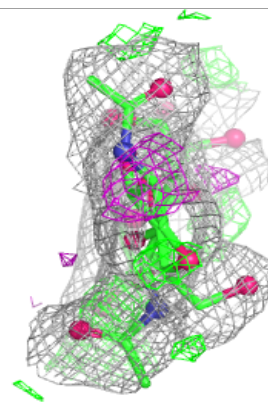
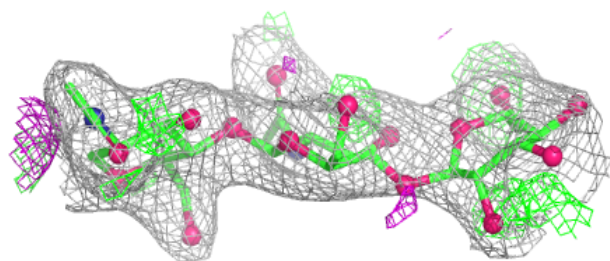
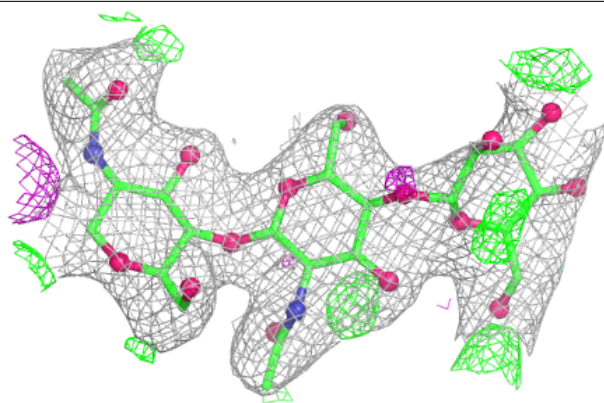
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MAN	G	3	11/12	0.74	0.14	56,65,76,84	0
4	NAG	G	2	14/15	0.88	0.12	47,54,61,71	0
4	NAG	G	1	14/15	0.91	0.08	36,45,49,51	0
4	NAG	J	1	14/15	-	-	38,46,50,51	0
4	NAG	J	2	14/15	-	-	46,54,56,71	0
4	MAN	J	3	11/12	-	-	51,64,68,77	0

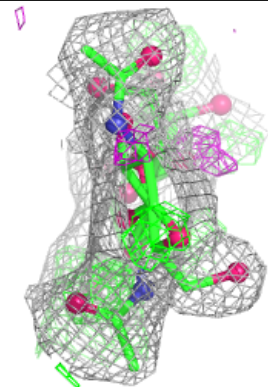
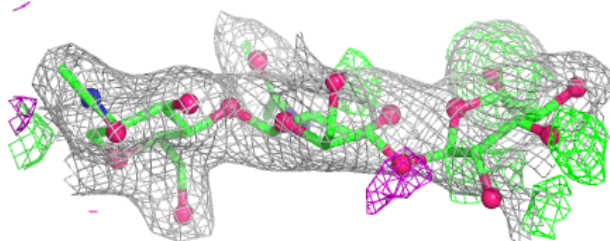
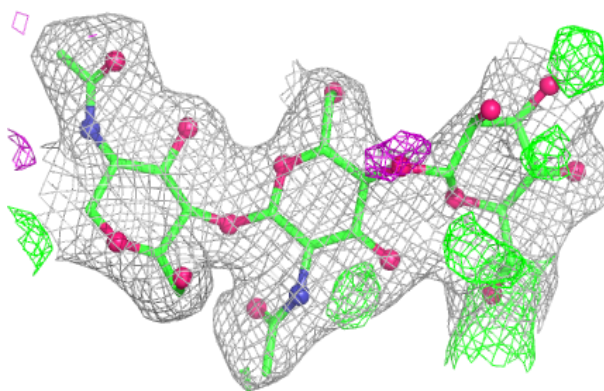
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

**Electron density around Chain J:**

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.