Full wwPDB X-ray Structure Validation Report ⓘ

Mar 11, 2025 – 08:09 PM EDT

PDB ID	:	8VF1
Title	:	Crystal Structure of the Hendra Virus Attachment G glycoprotein (HeV-G)
Authors	:	Ve, T.; von Itzstein, M.S.; Winger, M.; Malde, A.K.; Holt, S.; McAtamney, S.; Hartley-Tassell, L.; Maggioni, A.; von Itzstein, M.
Deposited on	:	2023-12-21
Resolution	:	3.00 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:

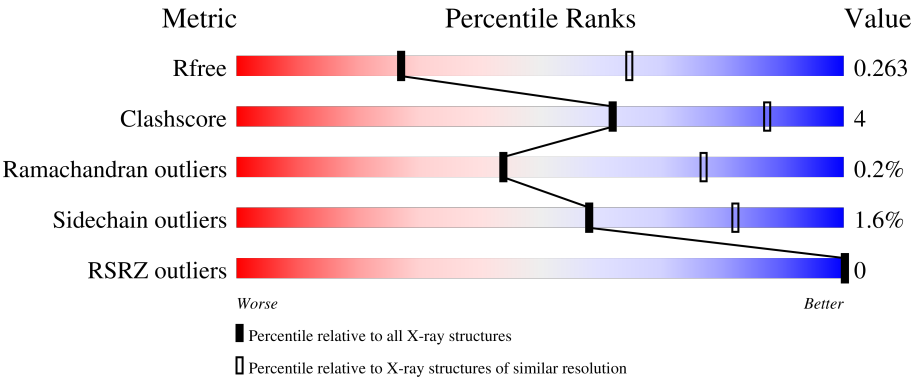
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 3.00 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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 <=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	453	84% 8% 8%
1	B	453	82% 10% 8%
2	C	5	80% 20%
2	D	5	20% 20% 60%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13404 atoms, of which 6634 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 Glycoprotein G.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	418	Total	C	H	N	O	S	0	0	0
			6549	2104	3245	555	626	19			
1	B	418	Total	C	H	N	O	S	0	0	0
			6549	2104	3247	555	624	19			

There are 38 discrepancies between the modelled and reference sequences:

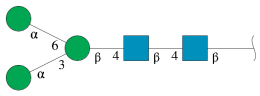
Chain	Residue	Modelled	Actual	Comment	Reference
A	152	ASP	-	expression tag	UNP O89343
A	153	ARG	-	expression tag	UNP O89343
A	154	SER	-	expression tag	UNP O89343
A	155	LEU	-	expression tag	UNP O89343
A	156	HIS	-	expression tag	UNP O89343
A	157	HIS	-	expression tag	UNP O89343
A	158	HIS	-	expression tag	UNP O89343
A	159	HIS	-	expression tag	UNP O89343
A	160	HIS	-	expression tag	UNP O89343
A	161	HIS	-	expression tag	UNP O89343
A	162	GLY	-	expression tag	UNP O89343
A	163	GLY	-	expression tag	UNP O89343
A	164	GLU	-	expression tag	UNP O89343
A	165	ASN	-	expression tag	UNP O89343
A	166	LEU	-	expression tag	UNP O89343
A	167	TYR	-	expression tag	UNP O89343
A	168	PHE	-	expression tag	UNP O89343
A	169	GLN	-	expression tag	UNP O89343
A	170	GLY	-	expression tag	UNP O89343
B	152	ASP	-	expression tag	UNP O89343
B	153	ARG	-	expression tag	UNP O89343
B	154	SER	-	expression tag	UNP O89343
B	155	LEU	-	expression tag	UNP O89343
B	156	HIS	-	expression tag	UNP O89343
B	157	HIS	-	expression tag	UNP O89343

Continued on next page...

Continued from previous page...

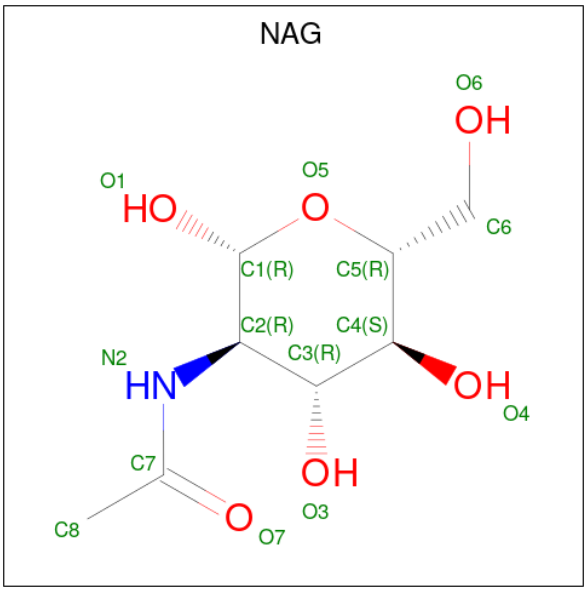
Chain	Residue	Modelled	Actual	Comment	Reference
B	158	HIS	-	expression tag	UNP O89343
B	159	HIS	-	expression tag	UNP O89343
B	160	HIS	-	expression tag	UNP O89343
B	161	HIS	-	expression tag	UNP O89343
B	162	GLY	-	expression tag	UNP O89343
B	163	GLY	-	expression tag	UNP O89343
B	164	GLU	-	expression tag	UNP O89343
B	165	ASN	-	expression tag	UNP O89343
B	166	LEU	-	expression tag	UNP O89343
B	167	TYR	-	expression tag	UNP O89343
B	168	PHE	-	expression tag	UNP O89343
B	169	GLN	-	expression tag	UNP O89343
B	170	GLY	-	expression tag	UNP O89343

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	5	Total	C	H	N	O	0	0	0
			113	34	52	2	25			
2	D	5	Total	C	H	N	O	0	0	0
			112	34	51	2	25			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



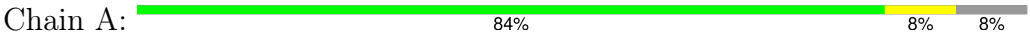
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

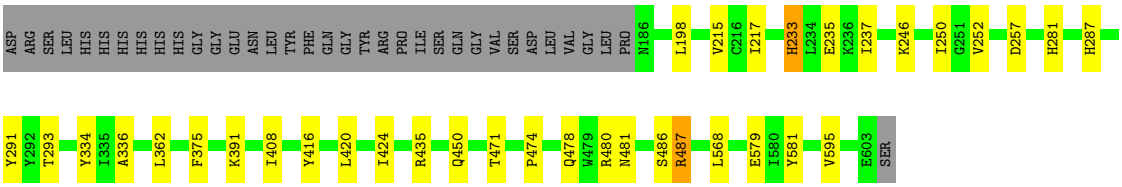
3 Residue-property plots (i)

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: Glycoprotein G

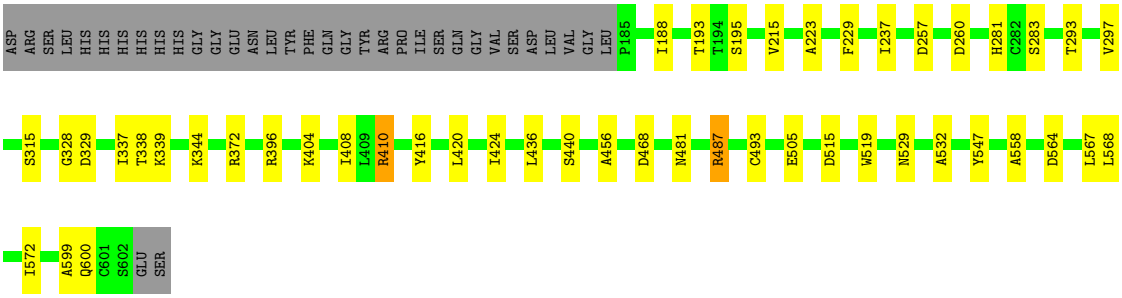
Chain A:





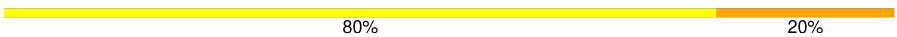
• Molecule 1: Glycoprotein G

Chain B:



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

Chain C:



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

Chain D:


NAG1
NAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.82Å 80.16Å 95.14Å 90.00° 106.48° 90.00°	Depositor
Resolution (Å)	45.61 – 3.00 45.61 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.61-3.00) 98.9 (45.61-3.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.215 , 0.266 0.216 , 0.263	Depositor DCC
R_{free} test set	856 reflections (5.29%)	wwPDB-VP
Wilson B-factor (Å^2)	55.5	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13404	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, BMA, MAN

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	0/3384	0.50	0/4608
1	B	0.25	0/3383	0.51	0/4607
All	All	0.26	0/6767	0.51	0/9215

There are no bond length outliers.

There are no bond angle outliers.

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	3304	3245	3242	21	1
1	B	3302	3247	3246	27	1
2	C	61	52	52	3	2
2	D	61	51	52	8	2
3	A	28	26	26	0	0
3	B	14	13	13	2	0
All	All	6770	6634	6631	54	3

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 4.

All (54) 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)
2:D:2:NAG:H83	2:D:2:NAG:H3	1.63	0.80
2:D:1:NAG:H61	2:D:2:NAG:H82	1.74	0.69
1:A:579:GLU:OE2	1:A:581:TYR:OH	2.14	0.62
2:D:2:NAG:H3	2:D:2:NAG:C8	2.29	0.61
1:A:287:HIS:HB2	1:A:362:LEU:HD21	1.85	0.57
1:A:471:THR:OG1	1:A:474:PRO:O	2.18	0.57
1:A:257:ASP:HB2	1:A:568:LEU:HD11	1.88	0.55
1:B:193:THR:HG22	1:B:195:SER:H	1.72	0.54
2:D:1:NAG:H83	2:D:1:NAG:H3	1.89	0.54
1:B:532:ALA:HB1	1:B:558:ALA:O	2.10	0.52
1:B:529:ASN:OD1	3:B:701:NAG:C2	2.59	0.51
1:B:410:ARG:HD2	1:B:436:LEU:HD11	1.93	0.51
1:A:375:PHE:CD1	1:A:408:ILE:HD13	2.46	0.51
1:B:416:TYR:CE1	1:B:424:ILE:HG13	2.46	0.51
1:A:420:LEU:HD23	1:A:420:LEU:O	2.11	0.51
1:A:480:ARG:CZ	2:C:1:NAG:H81	2.41	0.51
1:B:215:VAL:HG12	1:B:237:ILE:HD13	1.92	0.50
1:B:338:THR:HG22	1:B:339:LYS:HG2	1.94	0.50
1:B:215:VAL:CG1	1:B:237:ILE:HD13	2.41	0.50
1:B:487:ARG:NH2	1:B:505:GLU:O	2.47	0.48
1:A:250:ILE:HG21	1:A:293:THR:HG21	1.96	0.47
1:B:567:LEU:HD21	1:B:572:ILE:HG13	1.96	0.47
1:A:416:TYR:CE1	1:A:424:ILE:HG23	2.49	0.47
2:D:1:NAG:C1	2:D:1:NAG:H82	2.43	0.47
1:A:215:VAL:HG13	1:A:235:GLU:HG3	1.97	0.47
1:B:260:ASP:OD1	1:B:260:ASP:N	2.48	0.46
1:B:372:ARG:HG2	1:B:408:ILE:HG23	1.98	0.46
1:B:404:LYS:O	1:B:404:LYS:HG2	2.17	0.45
1:A:237:ILE:HD11	1:A:246:LYS:HD3	1.99	0.45
1:B:440:SER:HB2	1:B:456:ALA:HB3	1.98	0.45
2:D:2:NAG:H83	2:D:2:NAG:C3	2.41	0.45
1:A:375:PHE:CG	1:A:408:ILE:HD13	2.52	0.45
1:B:257:ASP:HB2	1:B:568:LEU:HD21	1.99	0.44
1:B:529:ASN:OD1	3:B:701:NAG:H2	2.17	0.44
1:B:337:ILE:O	1:B:339:LYS:N	2.50	0.44
1:B:188:ILE:HA	1:B:599:ALA:HA	1.99	0.44
1:B:600:GLN:N	1:B:600:GLN:OE1	2.51	0.43
1:A:486:SER:OG	1:A:487:ARG:N	2.51	0.43
1:A:391:LYS:HD2	1:A:391:LYS:H	1.83	0.43
1:B:328:GLY:O	1:B:329:ASP:HB2	2.19	0.43
1:B:420:LEU:HD12	1:B:420:LEU:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ASN:OD1	2:C:1:NAG:H2	2.18	0.43
2:D:2:NAG:C8	2:D:2:NAG:C3	2.95	0.43
1:A:233:HIS:CD2	1:A:233:HIS:C	2.92	0.43
1:B:223:ALA:O	1:B:229:PHE:HA	2.19	0.42
1:A:217:ILE:HG23	1:A:233:HIS:CG	2.54	0.42
1:B:481:ASN:OD1	2:D:1:NAG:C1	2.67	0.42
1:A:336:ALA:HB2	1:B:297:VAL:HG11	2.00	0.42
1:A:252:VAL:HG11	1:A:291:TYR:HB2	2.02	0.42
1:A:480:ARG:NH1	2:C:1:NAG:H81	2.34	0.41
1:A:198:LEU:HD22	1:A:595:VAL:CG1	2.50	0.41
1:B:515:ASP:O	1:B:519:TRP:HA	2.20	0.41
1:B:283:SER:O	1:B:293:THR:HA	2.21	0.41
1:B:493:CYS:N	1:B:505:GLU:OE2	2.42	0.41

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2:NAG:O6	2:D:1:NAG:O3[1_656]	2.08	0.12
1:A:478:GLN:OE1	2:D:4:MAN:O4[1_656]	2.11	0.09
1:B:468:ASP:OD2	2:C:4:MAN:O3[1_454]	2.11	0.09

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	416/453 (92%)	387 (93%)	28 (7%)	1 (0%)	44	77
1	B	416/453 (92%)	375 (90%)	40 (10%)	1 (0%)	44	77
All	All	832/906 (92%)	762 (92%)	68 (8%)	2 (0%)	44	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	281	HIS
1	A	281	HIS

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	375/405 (93%)	370 (99%)	5 (1%)	65 85
1	B	375/405 (93%)	368 (98%)	7 (2%)	52 79
All	All	750/810 (93%)	738 (98%)	12 (2%)	58 82

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	HIS
1	A	334	TYR
1	A	435	ARG
1	A	450	GLN
1	A	487	ARG
1	B	315	SER
1	B	344	LYS
1	B	396	ARG
1	B	410	ARG
1	B	487	ARG
1	B	547	TYR
1	B	564	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	0.55	0	17,19,21	0.54	0
2	NAG	C	2	2	14,14,15	0.21	0	17,19,21	0.54	0
2	BMA	C	3	2	11,11,12	0.58	0	15,15,17	0.90	1 (6%)
2	MAN	C	4	2	11,11,12	0.82	1 (9%)	15,15,17	0.83	1 (6%)
2	MAN	C	5	2	11,11,12	0.67	0	15,15,17	1.04	2 (13%)
2	NAG	D	1	2	14,14,15	0.59	0	17,19,21	1.23	2 (11%)
2	NAG	D	2	2	14,14,15	0.24	0	17,19,21	1.18	1 (5%)
2	BMA	D	3	2	11,11,12	0.78	0	15,15,17	0.72	0
2	MAN	D	4	2	11,11,12	0.72	0	15,15,17	0.90	1 (6%)
2	MAN	D	5	2	11,11,12	0.89	1 (9%)	15,15,17	0.94	1 (6%)

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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	1/2/19/22	1/1/1/1
2	NAG	D	1	2	-	6/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	MAN	D	5	2	-	2/2/19/22	1/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	MAN	O5-C1	-2.40	1.39	1.43
2	D	5	MAN	O5-C5	2.04	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	NAG	C2-N2-C7	3.69	127.84	122.90
2	D	1	NAG	C2-N2-C7	3.04	126.98	122.90
2	C	5	MAN	C1-O5-C5	2.98	116.18	112.19
2	D	5	MAN	C1-O5-C5	2.48	115.51	112.19
2	D	1	NAG	C1-O5-C5	2.41	115.42	112.19
2	C	4	MAN	O2-C2-C3	-2.16	105.67	110.15
2	D	4	MAN	O2-C2-C3	-2.06	105.89	110.15
2	C	3	BMA	C1-O5-C5	2.04	114.92	112.19
2	C	5	MAN	O2-C2-C3	-2.01	105.99	110.15

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C1-C2-N2-C7
2	D	5	MAN	O5-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	D	5	MAN	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	D	2	NAG	C3-C2-N2-C7
2	C	5	MAN	O5-C5-C6-O6
2	D	1	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6

All (2) ring outliers are listed below:

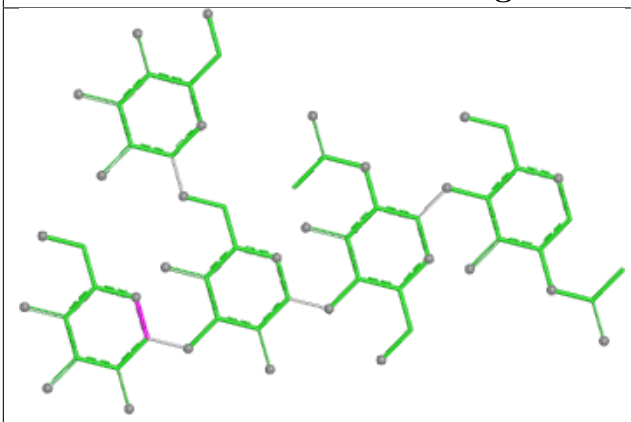
Mol	Chain	Res	Type	Atoms
2	D	5	MAN	C1-C2-C3-C4-C5-O5
2	C	5	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 14 short contacts:

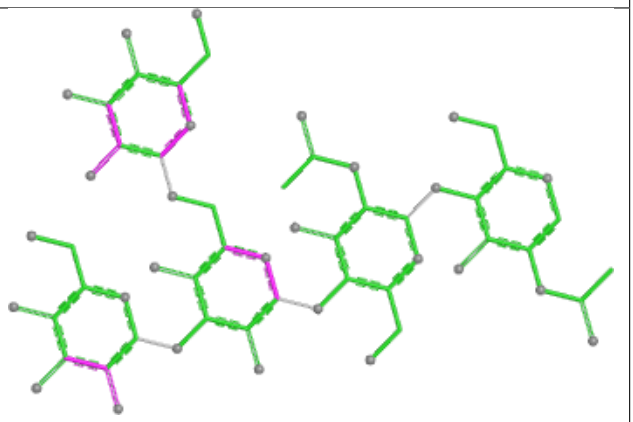
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4	MAN	0	1
2	C	4	MAN	0	1
2	D	1	NAG	4	1
2	D	2	NAG	5	0
2	C	1	NAG	3	0
2	C	2	NAG	0	1

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

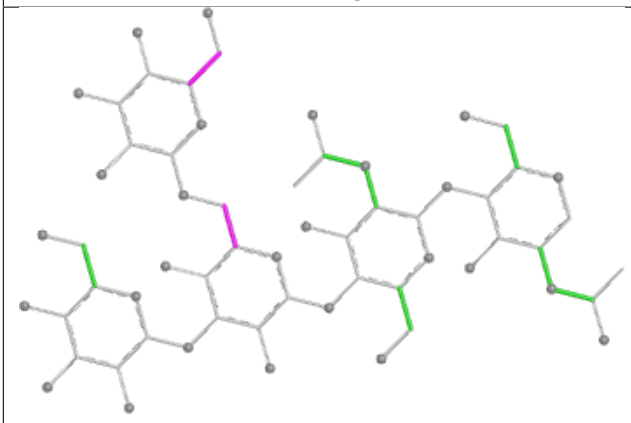
Oligosaccharide Chain C



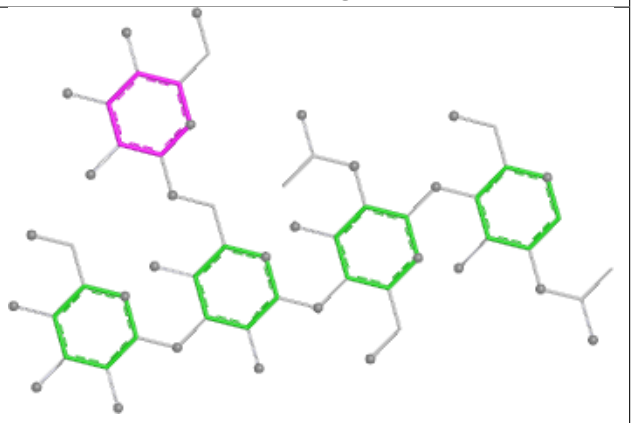
Bond lengths



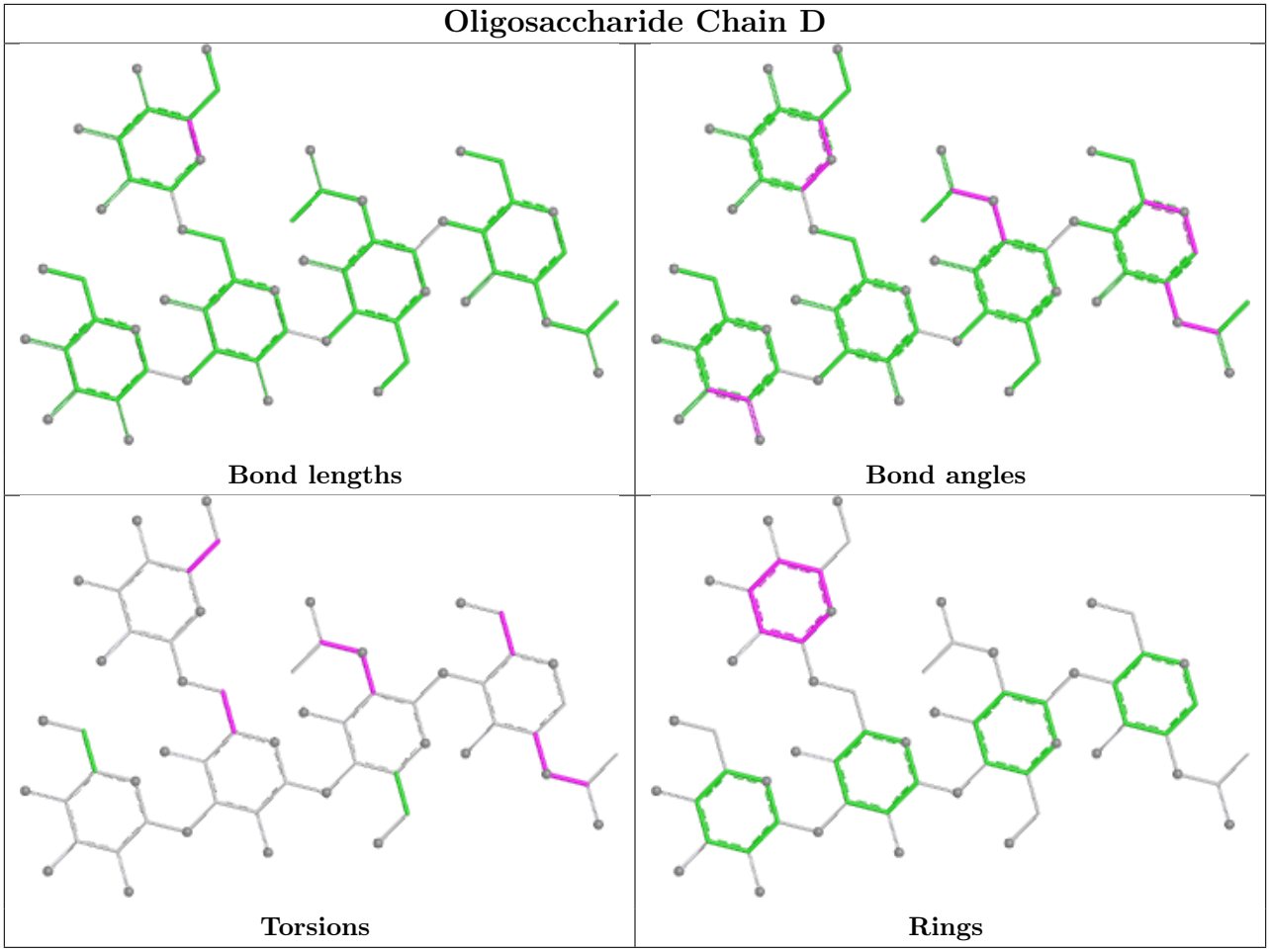
Bond angles



Torsions



Rings



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	$\#\|Z\| > 2$
3	NAG	A	702	1	14,14,15	0.36	0	17,19,21	0.73	1 (5%)
3	NAG	A	701	1	14,14,15	0.28	0	17,19,21	0.70	1 (5%)
3	NAG	B	701	1	14,14,15	1.05	2 (14%)	17,19,21	1.02	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
3	NAG	A	702	1	-	2/6/23/26	0/1/1/1
3	NAG	A	701	1	-	2/6/23/26	0/1/1/1
3	NAG	B	701	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	NAG	O5-C1	2.93	1.48	1.43
3	B	701	NAG	C1-C2	2.48	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	701	NAG	C1-O5-C5	3.39	116.73	112.19
3	A	701	NAG	C1-O5-C5	2.55	115.60	112.19
3	A	702	NAG	C1-O5-C5	2.26	115.22	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	NAG	C8-C7-N2-C2
3	A	702	NAG	O7-C7-N2-C2
3	A	701	NAG	O5-C5-C6-O6
3	A	701	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	701	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	418/453 (92%)	-0.21	0	100	100	33, 55, 95, 136	0
1	B	418/453 (92%)	-0.18	0	100	100	36, 62, 110, 147	0
All	All	836/906 (92%)	-0.19	0	100	100	33, 58, 104, 147	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

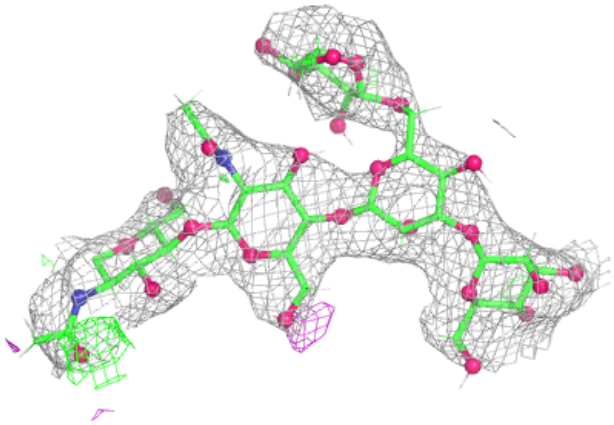
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	D	2	14/15	0.58	0.14	59,79,93,103	0
2	MAN	D	5	11/12	0.65	0.16	37,76,95,100	0
2	MAN	C	5	11/12	0.71	0.13	65,84,102,104	0
2	NAG	C	1	14/15	0.71	0.14	48,61,82,84	0
2	NAG	C	2	14/15	0.71	0.12	53,70,83,91	0
2	NAG	D	1	14/15	0.76	0.16	54,71,80,86	0
2	BMA	C	3	11/12	0.84	0.12	59,69,84,96	0
2	BMA	D	3	11/12	0.85	0.11	46,63,77,79	0
2	MAN	C	4	11/12	0.85	0.08	53,66,82,99	0
2	MAN	D	4	11/12	0.88	0.09	45,56,66,80	0

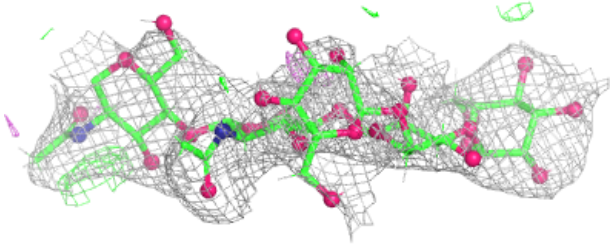
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

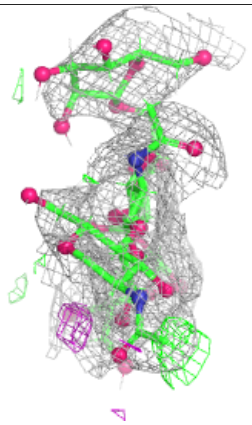
charide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

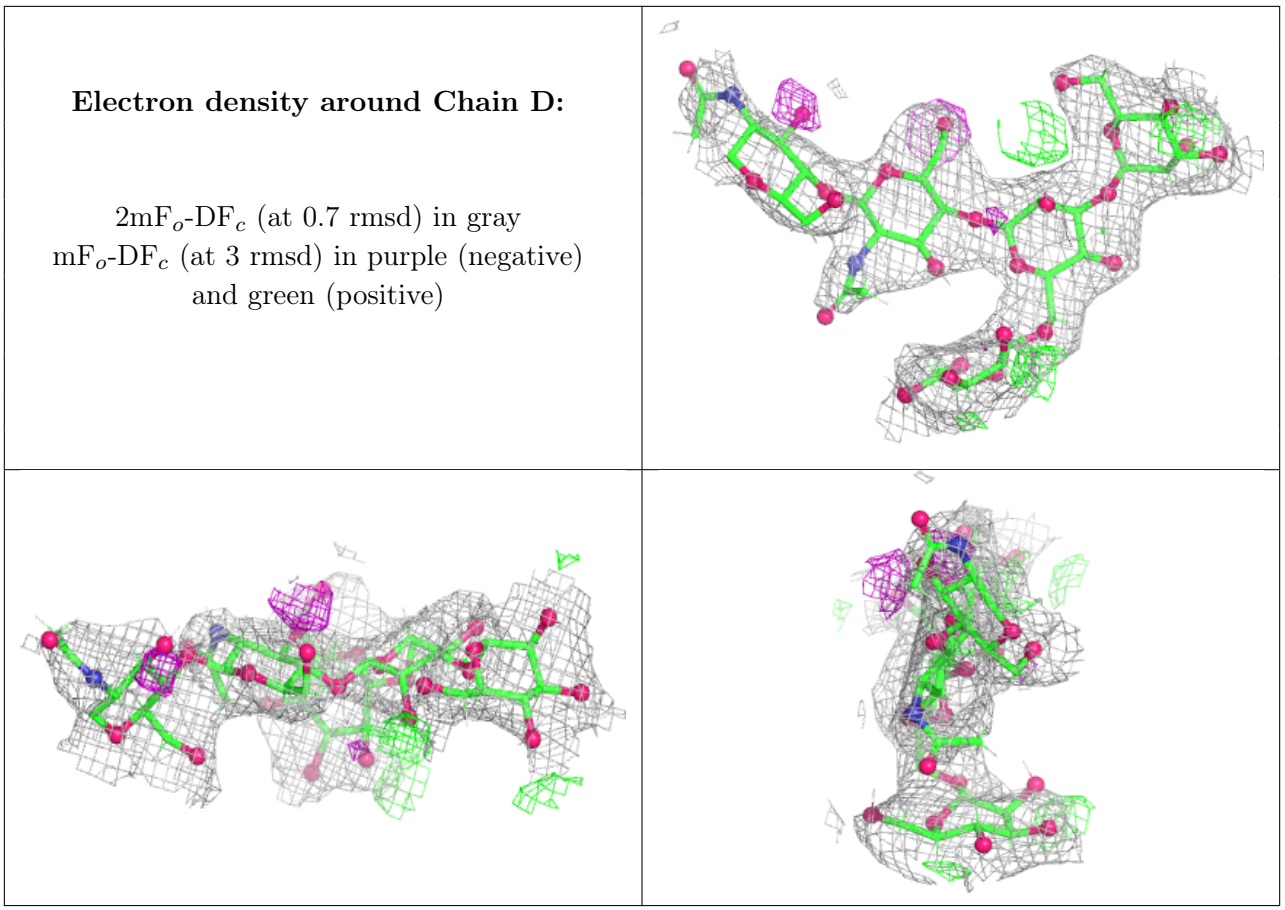






Electron density around Chain D:

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



6.4 Ligands

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, 95^{th} 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
3	NAG	A	701	14/15	0.62	0.15	35,61,80,83	0
3	NAG	A	702	14/15	0.76	0.10	34,66,90,109	0
3	NAG	B	701	14/15	0.78	0.14	54,75,115,121	0

6.5 Other polymers

There are no such residues in this entry.