



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5V2S / pdb_00005v2s
Title : Crystal structure of glycoprotein B from Herpes Simplex Virus type I
Authors : Cooper, R.S.; Heldwein, E.E.
Deposited on : 2017-03-06
Resolution : 3.60 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

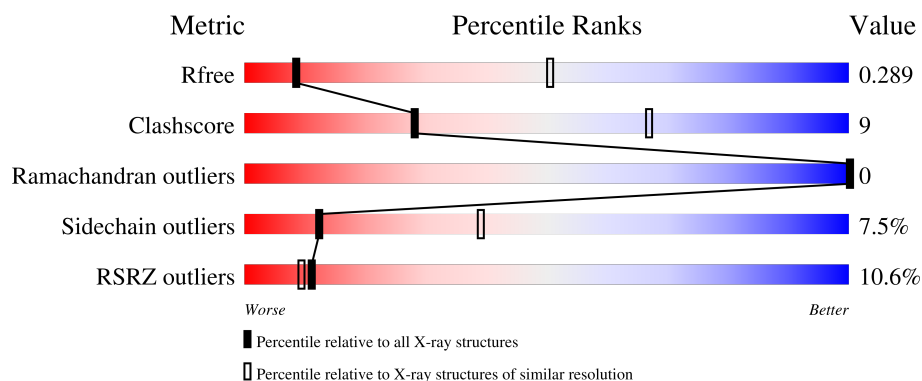
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	841	9% 65% 16% • 16%
2	B	2	50% 50%
2	C	2	50% 50%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5716 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 Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	705	Total	C	N	O	S	0	0	0
			5646	3570	991	1057	28			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	905	GLY	-	expression tag	UNP A1Z0P7
A	906	SER	-	expression tag	UNP A1Z0P7
A	907	HIS	-	expression tag	UNP A1Z0P7
A	908	HIS	-	expression tag	UNP A1Z0P7
A	909	HIS	-	expression tag	UNP A1Z0P7
A	910	HIS	-	expression tag	UNP A1Z0P7
A	911	HIS	-	expression tag	UNP A1Z0P7
A	912	HIS	-	expression tag	UNP A1Z0P7

- Molecule 2 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
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

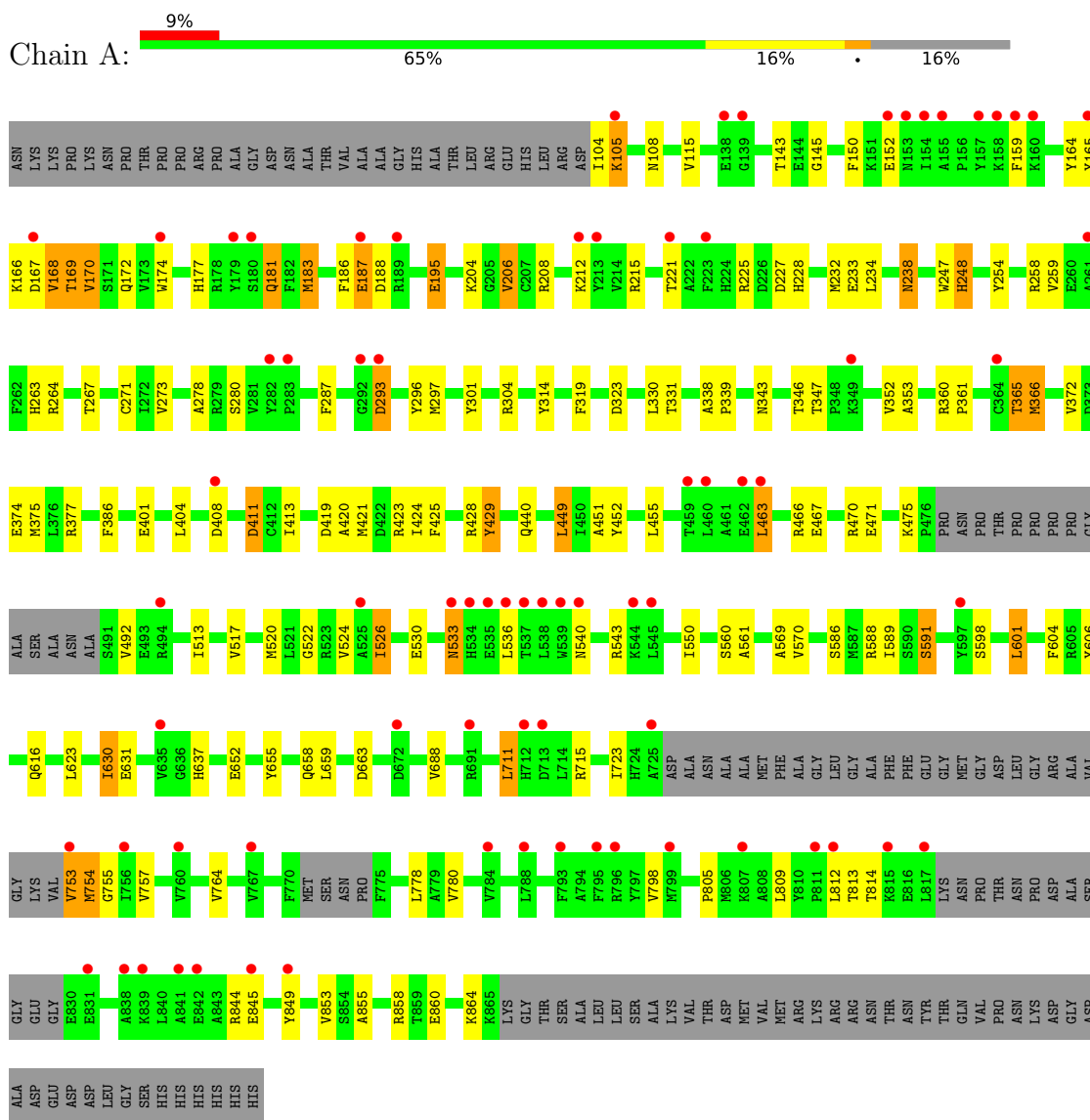


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: Envelope glycoprotein B



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





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

Chain C:
50% 50%

A horizontal progress bar for Chain C. The bar is divided into two equal halves. The left half is green and the right half is yellow. Below the bar, the text '50%' is centered under each half.



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.66Å 118.66Å 216.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	108.23 – 3.60 108.23 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (108.23-3.60) 91.6 (108.23-3.60)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.68 (at 3.41Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.244 , 0.273 0.248 , 0.289	Depositor DCC
R_{free} test set	1994 reflections (8.00%)	wwPDB-VP
Wilson B-factor (Å ²)	82.9	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 95.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.056 for -h,-k,l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	5716	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: 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	0.15	0/5776	0.37	0/7830

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 [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	5646	0	5485	97	1
2	B	28	0	25	3	0
2	C	28	0	25	0	0
3	A	14	0	13	0	0
All	All	5716	0	5548	100	1

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:ALA:HA	1:A:569:ALA:O	1.86	0.76
2:B:1:NAG:O3	2:B:1:NAG:O7	2.03	0.76
1:A:365:THR:OG1	1:A:408:ASP:O	2.03	0.73
1:A:366:MET:HG3	1:A:413:ILE:HD11	1.72	0.71
1:A:754:MET:N	1:A:754:MET:SD	2.64	0.70
1:A:280:SER:HB2	1:A:287:PHE:HB3	1.74	0.70
1:A:560:SER:O	1:A:570:VAL:HA	1.91	0.69
1:A:166:LYS:HG2	1:A:271:CYS:HA	1.72	0.69
1:A:543:ARG:HB3	1:A:550:ILE:HG21	1.76	0.67
1:A:540:ASN:O	1:A:543:ARG:HG3	1.96	0.65
1:A:159:PHE:O	1:A:278:ALA:HB3	1.97	0.65
1:A:304:ARG:NH1	1:A:323:ASP:OD1	2.31	0.64
1:A:601:LEU:HA	1:A:616:GLN:HA	1.81	0.62
1:A:860:GLU:HG2	1:A:864:LYS:HE3	1.82	0.60
1:A:206:VAL:HG12	1:A:233:GLU:HA	1.84	0.59
1:A:411:ASP:N	1:A:411:ASP:OD1	2.34	0.59
1:A:247:TRP:HE1	1:A:331:THR:HG1	1.51	0.59
1:A:296:TYR:HB2	1:A:314:TYR:HE2	1.67	0.58
1:A:533:ASN:N	1:A:533:ASN:OD1	2.38	0.56
1:A:561:ALA:HB2	1:A:570:VAL:HG12	1.86	0.56
1:A:177:HIS:O	1:A:258:ARG:NH2	2.38	0.56
1:A:225:ARG:HG2	1:A:254:TYR:HB2	1.88	0.55
1:A:152:GLU:HA	1:A:366:MET:HE2	1.88	0.55
1:A:145:GLY:HA2	1:A:455:LEU:HD12	1.88	0.54
1:A:169:THR:HA	1:A:186:PHE:O	2.07	0.54
1:A:170:VAL:HG13	1:A:186:PHE:HB3	1.90	0.53
1:A:247:TRP:NE1	1:A:331:THR:OG1	2.31	0.53
1:A:425:PHE:HD2	1:A:429:TYR:HB2	1.73	0.53
1:A:425:PHE:CD2	1:A:429:TYR:HB2	2.44	0.53
2:B:1:NAG:HO3	2:B:1:NAG:C7	2.13	0.53
1:A:513:ILE:O	1:A:517:VAL:HG12	2.08	0.53
1:A:421:MET:HE1	1:A:452:TYR:N	2.24	0.53
1:A:805:PRO:O	1:A:809:LEU:N	2.38	0.52
1:A:169:THR:HG23	1:A:187:GLU:HB3	1.91	0.52
1:A:212:LYS:NZ	1:A:221:THR:OG1	2.34	0.52
1:A:105:LYS:O	1:A:658:GLN:NE2	2.37	0.52
1:A:440:GLN:HE22	1:A:471:GLU:HB3	1.74	0.52
1:A:314:TYR:HE1	1:A:347:THR:HG22	1.74	0.52
1:A:754:MET:SD	1:A:755:GLY:N	2.83	0.51
1:A:374:GLU:OE2	1:A:428:ARG:NH2	2.44	0.51
1:A:227:ASP:OD1	1:A:228:HIS:N	2.42	0.49
1:A:238:ASN:OD1	1:A:238:ASN:N	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ASP:N	1:A:293:ASP:OD1	2.45	0.49
1:A:177:HIS:C	1:A:258:ARG:HH22	2.19	0.48
1:A:377:ARG:HD3	1:A:386:PHE:CZ	2.49	0.48
1:A:440:GLN:NE2	1:A:471:GLU:HB3	2.28	0.48
1:A:338:ALA:HB1	1:A:339:PRO:HD2	1.96	0.47
1:A:234:LEU:HD13	1:A:330:LEU:HD21	1.95	0.47
1:A:204:LYS:HB3	1:A:206:VAL:HG22	1.96	0.47
1:A:377:ARG:HH22	1:A:471:GLU:CD	2.23	0.47
1:A:115:VAL:HG22	1:A:623:LEU:HB2	1.97	0.46
1:A:463:LEU:HD22	1:A:466:ARG:HH11	1.80	0.46
1:A:659:LEU:HD21	1:A:663:ASP:HB2	1.96	0.46
1:A:520:MET:O	1:A:524:VAL:HG23	2.16	0.46
1:A:247:TRP:NE1	1:A:331:THR:HG1	2.11	0.46
1:A:637:HIS:N	1:A:652:GLU:OE2	2.49	0.46
1:A:248:HIS:HA	1:A:271:CYS:O	2.16	0.45
1:A:377:ARG:NH2	1:A:471:GLU:OE1	2.48	0.45
1:A:711:LEU:O	1:A:715:ARG:HB2	2.17	0.45
1:A:232:MET:HE2	1:A:232:MET:HB3	1.90	0.45
1:A:420:ALA:O	1:A:424:ILE:HG12	2.16	0.45
1:A:172:GLN:HG2	1:A:183:MET:HB2	1.97	0.45
1:A:589:ILE:HD11	1:A:591:SER:HB3	1.98	0.45
1:A:343:ASN:O	1:A:353:ALA:HA	2.17	0.45
1:A:360:ARG:HB2	1:A:361:PRO:HD3	1.99	0.44
1:A:164:TYR:CD2	1:A:273:VAL:HG22	2.53	0.44
1:A:195:GLU:OE1	1:A:208:ARG:NH2	2.51	0.44
1:A:526:ILE:O	1:A:530:GLU:HG3	2.18	0.44
1:A:753:VAL:HB	1:A:754:MET:H	1.67	0.44
1:A:429:TYR:CD2	1:A:455:LEU:HD13	2.53	0.44
1:A:401:GLU:CD	1:A:440:GLN:HB3	2.43	0.44
1:A:174:TRP:HD1	1:A:263:HIS:ND1	2.15	0.43
1:A:543:ARG:HA	1:A:550:ILE:HG13	2.00	0.43
1:A:104:ILE:HG21	1:A:655:TYR:CE1	2.53	0.43
1:A:181:GLN:HB3	1:A:183:MET:HE3	2.01	0.43
1:A:604:PHE:HE1	1:A:606:TYR:CZ	2.36	0.43
1:A:812:LEU:HD13	1:A:812:LEU:HA	1.74	0.43
1:A:849:TYR:O	1:A:853:VAL:HG23	2.19	0.43
1:A:188:ASP:CG	1:A:215:ARG:HH21	2.26	0.43
1:A:166:LYS:HE2	1:A:271:CYS:HB2	2.00	0.43
1:A:421:MET:HE1	1:A:451:ALA:C	2.43	0.43
1:A:150:PHE:HB2	1:A:449:LEU:HB3	2.00	0.42
1:A:297:MET:HE1	1:A:319:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASP:HB3	1:A:423:ARG:HH12	1.84	0.42
1:A:401:GLU:OE2	1:A:475:LYS:HD2	2.18	0.42
1:A:598:SER:HB3	1:A:631:GLU:HB3	2.02	0.42
1:A:586:SER:OG	1:A:588:ARG:HG2	2.20	0.42
1:A:297:MET:HE3	1:A:301:TYR:HD2	1.85	0.42
1:A:855:ALA:HA	1:A:858:ARG:HD2	2.01	0.42
1:A:168:VAL:O	1:A:187:GLU:HA	2.20	0.42
1:A:467:GLU:O	1:A:471:GLU:HG2	2.20	0.42
1:A:372:VAL:HG11	1:A:375:MET:HE2	2.02	0.41
1:A:522:GLY:O	1:A:526:ILE:HD12	2.20	0.41
1:A:259:VAL:HG12	1:A:264:ARG:HD2	2.01	0.41
2:B:1:NAG:O3	2:B:2:NAG:C1	2.68	0.41
1:A:297:MET:HE3	1:A:301:TYR:HB3	2.01	0.41
1:A:164:TYR:HD2	1:A:273:VAL:HG22	1.86	0.41
1:A:143:THR:HG21	1:A:377:ARG:NH2	2.36	0.41
1:A:860:GLU:O	1:A:864:LYS:HG3	2.21	0.41
1:A:169:THR:O	1:A:267:THR:HA	2.21	0.40

All (1) 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)
1:A:630:ILE:O	1:A:844:ARG:NH2[3_654]	2.17	0.03

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	695/841 (83%)	663 (95%)	32 (5%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/707 (85%)	558 (92%)	45 (8%)	12	39

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LYS
1	A	108	ASN
1	A	165	TYR
1	A	167	ASP
1	A	168	VAL
1	A	169	THR
1	A	170	VAL
1	A	181	GLN
1	A	183	MET
1	A	187	GLU
1	A	195	GLU
1	A	206	VAL
1	A	238	ASN
1	A	248	HIS
1	A	293	ASP
1	A	346	THR
1	A	352	VAL
1	A	365	THR
1	A	366	MET
1	A	404	LEU
1	A	411	ASP
1	A	429	TYR
1	A	449	LEU
1	A	463	LEU
1	A	470	ARG
1	A	492	VAL
1	A	526	ILE
1	A	533	ASN
1	A	536	LEU
1	A	591	SER

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Mol	Chain	Res	Type
1	A	601	LEU
1	A	630	ILE
1	A	688	VAL
1	A	711	LEU
1	A	723	ILE
1	A	753	VAL
1	A	754	MET
1	A	757	VAL
1	A	764	VAL
1	A	778	LEU
1	A	780	VAL
1	A	798	VAL
1	A	813	THR
1	A	814	THR
1	A	845	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	224	HIS
1	A	861	HIS

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](#)

4 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	B	1	2,1	14,14,15	0.63	0	17,19,21	1.05	1 (5%)
2	NAG	B	2	2	14,14,15	0.70	0	17,19,21	0.80	0
2	NAG	C	1	2,1	14,14,15	0.72	1 (7%)	17,19,21	1.69	1 (5%)
2	NAG	C	2	2	14,14,15	0.48	0	17,19,21	0.63	0

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	O5-C1	2.56	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-O5-C5	6.36	120.71	112.19
2	B	1	NAG	C2-N2-C7	2.48	126.23	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

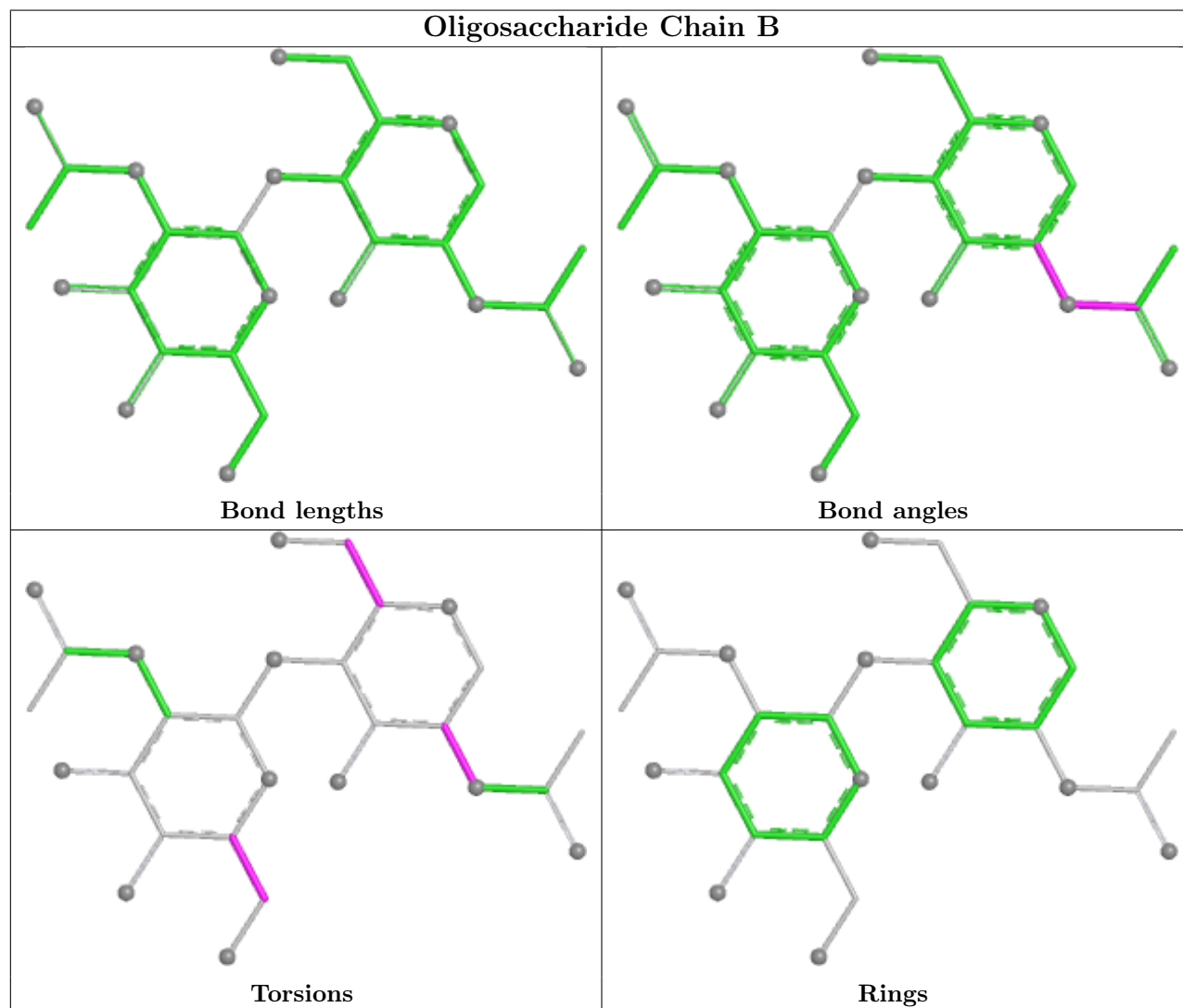
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C3-C2-N2-C7
2	C	2	NAG	C1-C2-N2-C7
2	C	2	NAG	C3-C2-N2-C7

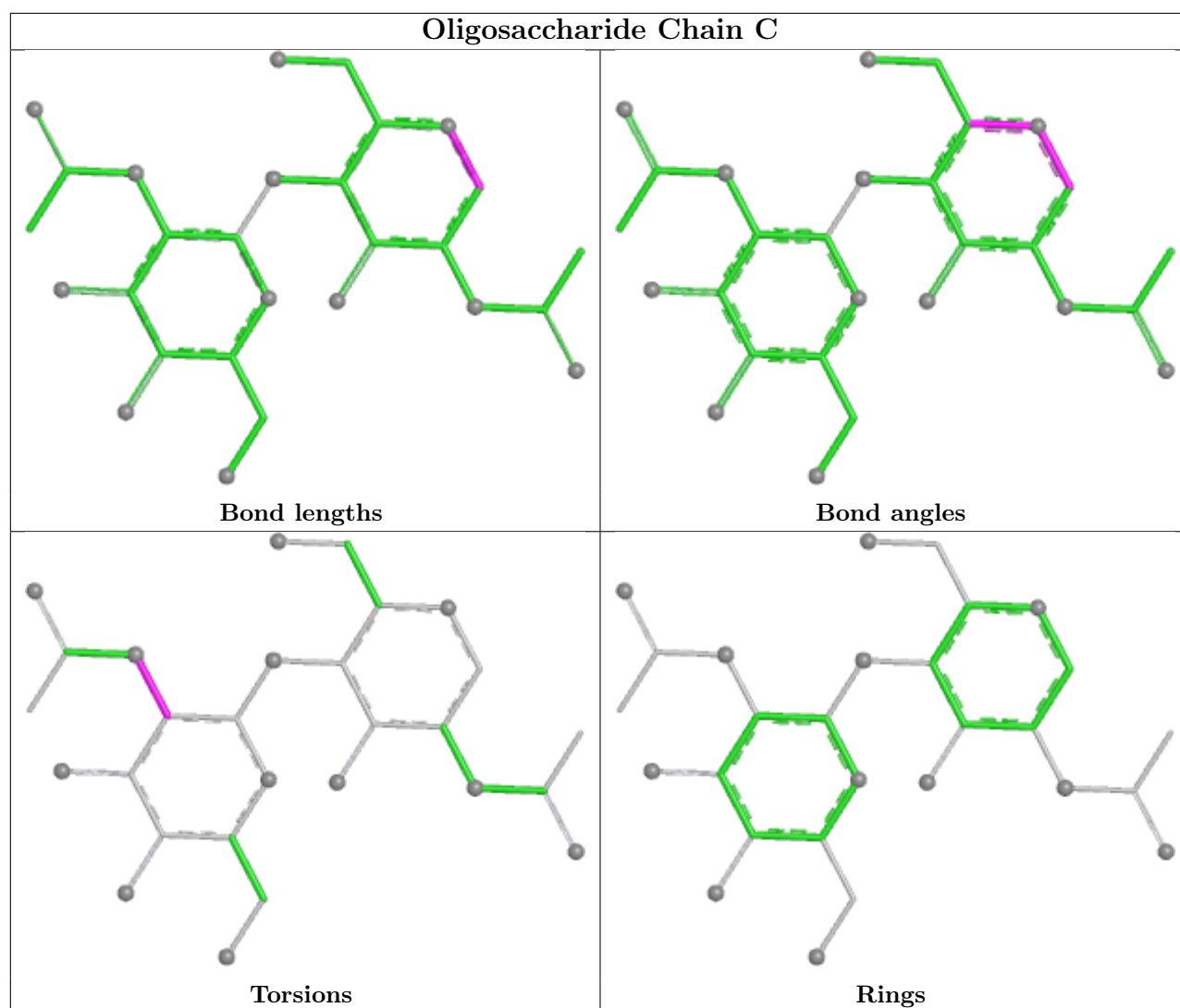
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	3	0
2	B	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](#)

1 ligand is 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	1003	1	14,14,15	0.27	0	17,19,21	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1003	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	NAG	C8-C7-N2-C2
3	A	1003	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	705/841 (83%)	0.69	75 (10%) 11 9	53, 121, 162, 213	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	ARG	9.7
1	A	845	GLU	8.5
1	A	842	GLU	8.4
1	A	462	GLU	5.5
1	A	460	LEU	5.5
1	A	138	GLU	5.2
1	A	293	ASP	5.2
1	A	539	TRP	4.7
1	A	187	GLU	4.5
1	A	535	GLU	4.3
1	A	839	LYS	4.3
1	A	713	ASP	4.2
1	A	213	TYR	4.1
1	A	179	TYR	4.0
1	A	838	ALA	3.9
1	A	154	ILE	3.9
1	A	817	LEU	3.7
1	A	597	TYR	3.5
1	A	212	LYS	3.4
1	A	282	TYR	3.4
1	A	788	LEU	3.3
1	A	221	THR	3.3
1	A	459	THR	3.3
1	A	538	LEU	3.2
1	A	223	PHE	3.2
1	A	283	PRO	3.1
1	A	795	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	463	LEU	3.0
1	A	545	LEU	2.9
1	A	167	ASP	2.9
1	A	672	ASP	2.9
1	A	153	ASN	2.9
1	A	544	LYS	2.9
1	A	349	LYS	2.8
1	A	408	ASP	2.8
1	A	494	ARG	2.8
1	A	292	GLY	2.7
1	A	155	ALA	2.7
1	A	139	GLY	2.7
1	A	756	ILE	2.7
1	A	537	THR	2.6
1	A	533	ASN	2.6
1	A	831	GLU	2.6
1	A	760	VAL	2.5
1	A	364	CYS	2.5
1	A	725	ALA	2.5
1	A	767	VAL	2.5
1	A	160	LYS	2.5
1	A	812	LEU	2.5
1	A	807	LYS	2.5
1	A	261	ALA	2.4
1	A	799	MET	2.4
1	A	174	TRP	2.4
1	A	691	ARG	2.4
1	A	159	PHE	2.3
1	A	796	ARG	2.3
1	A	157	TYR	2.3
1	A	525	ALA	2.3
1	A	165	TYR	2.3
1	A	105	LYS	2.3
1	A	540	ASN	2.2
1	A	815	LYS	2.2
1	A	784	VAL	2.2
1	A	536	LEU	2.2
1	A	534	HIS	2.1
1	A	158	LYS	2.1
1	A	849	TYR	2.1
1	A	841	ALA	2.1
1	A	180	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	152	GLU	2.1
1	A	753	VAL	2.1
1	A	712	HIS	2.0
1	A	811	PRO	2.0
1	A	793	PHE	2.0
1	A	635	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

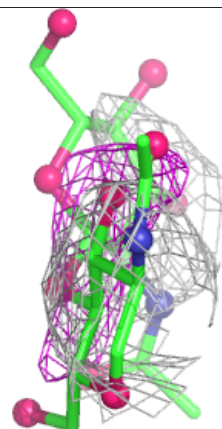
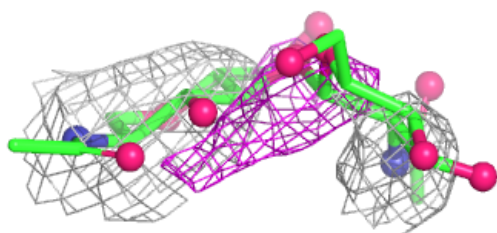
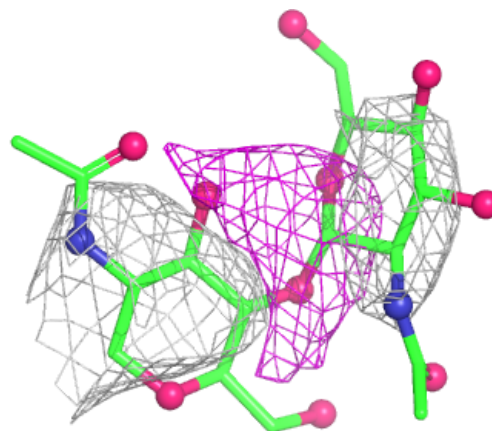
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	B	2	14/15	0.52	0.12	121,164,184,194	0
2	NAG	B	1	14/15	0.57	0.12	158,165,183,201	0
2	NAG	C	2	14/15	0.66	0.12	113,164,185,186	0
2	NAG	C	1	14/15	0.77	0.10	93,128,150,154	0

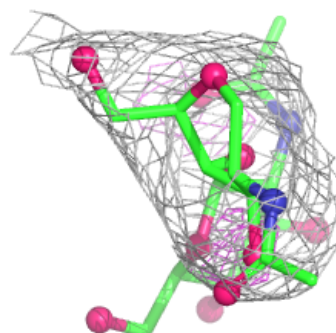
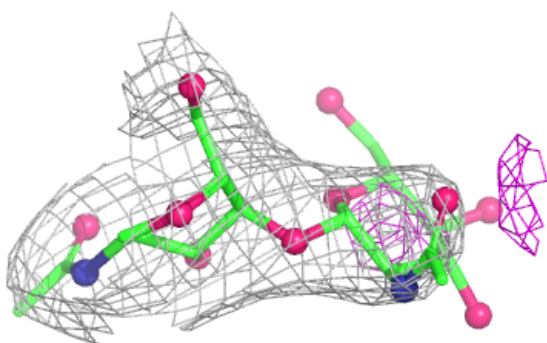
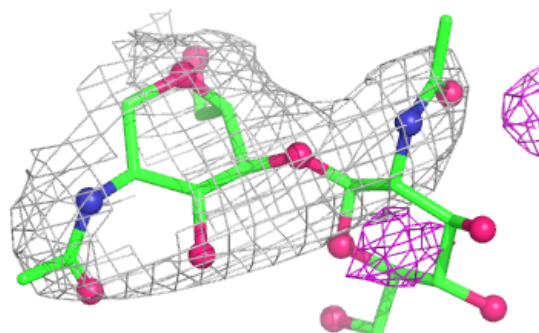
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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

**Electron density around Chain C:**

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
3	NAG	A	1003	14/15	0.81	0.11	90,126,154,156	0

6.5 Other polymers [i](#)

There are no such residues in this entry.