



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:45 PM UTC

PDB ID : 6XPX / pdb_00006xpx
Title : Human antibody S1V2-51 in complex with the influenza hemagglutinin head domain of A/Aichi/2/1968 (X-31)(H3N2)
Authors : McCarthy, K.R.; Harrison, S.C.
Deposited on : 2020-07-09
Resolution : 2.60 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

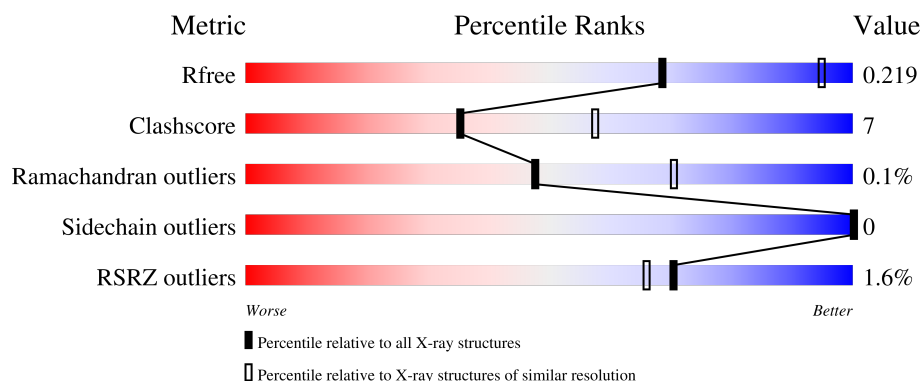
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

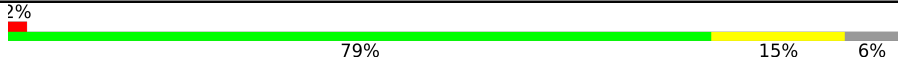
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	289	 2% 79% 15% 6%
2	C	220	 % 83% 16% .
3	B	227	 % 82% 12% 6%
4	D	3	 67% 33%

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
7	GOL	C	302	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5535 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2109	1326	368	404	11			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	ASP	ASN	conflict	UNP P03437
A	320	LEU	-	expression tag	UNP P03437
A	321	GLU	-	expression tag	UNP P03437
A	322	VAL	-	expression tag	UNP P03437
A	323	LEU	-	expression tag	UNP P03437
A	324	PHE	-	expression tag	UNP P03437
A	325	GLN	-	expression tag	UNP P03437

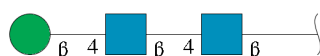
- Molecule 2 is a protein called S1V2-51 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	218	Total	C	N	O	S	0	0	0
			1686	1055	284	342	5			

- Molecule 3 is a protein called S1V2-51 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	213	Total	C	N	O	S	0	0	0
			1577	985	275	311	6			

- Molecule 4 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.



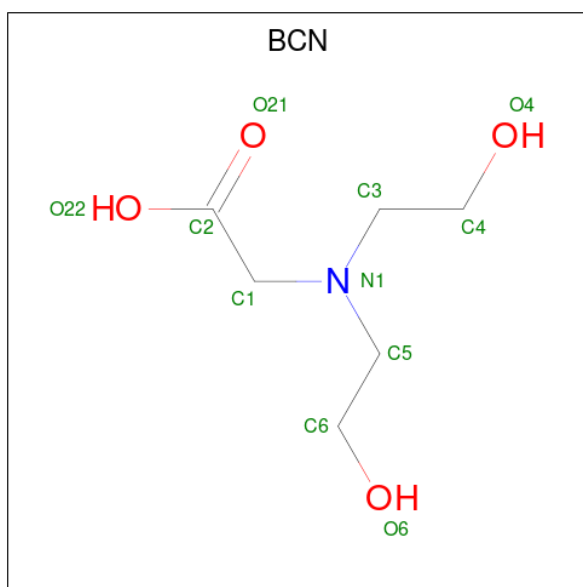
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is BICINE (CCD ID: BCN) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			11	6	1	4		
6	A	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



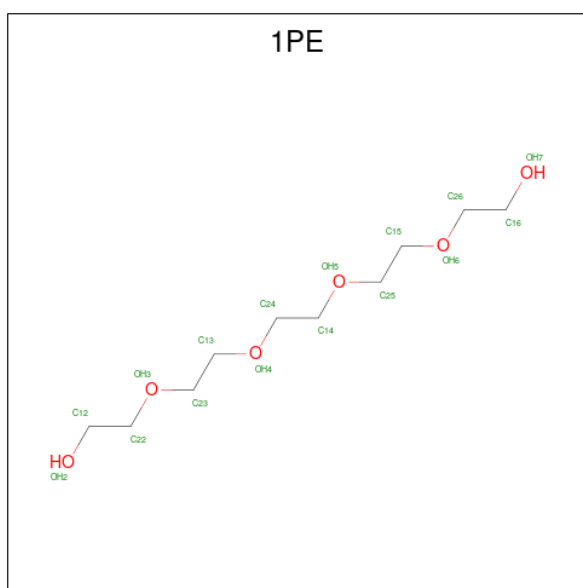
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			16	10	6		

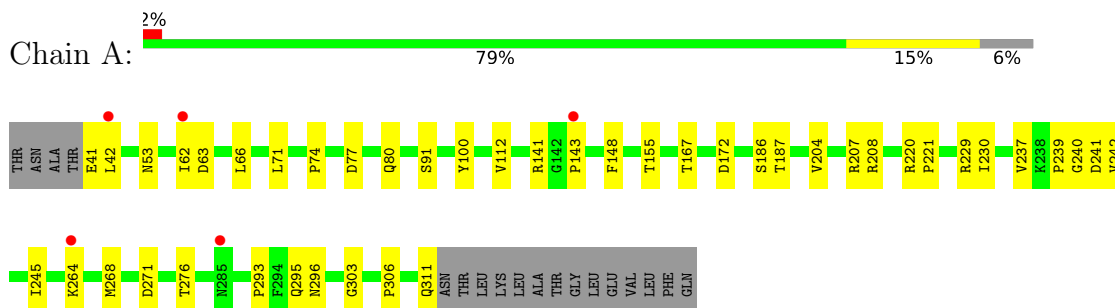
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	7	Total	O	0	0
			7	7		
9	C	7	Total	O	0	0
			7	7		
9	B	2	Total	O	0	0
			2	2		

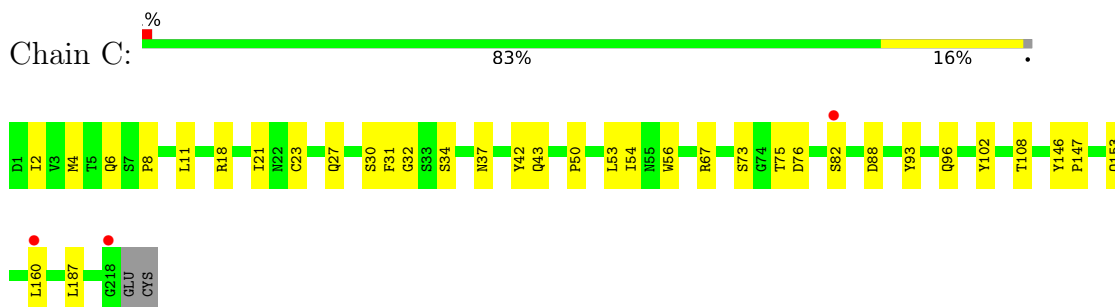
3 Residue-property plots [i](#)

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.

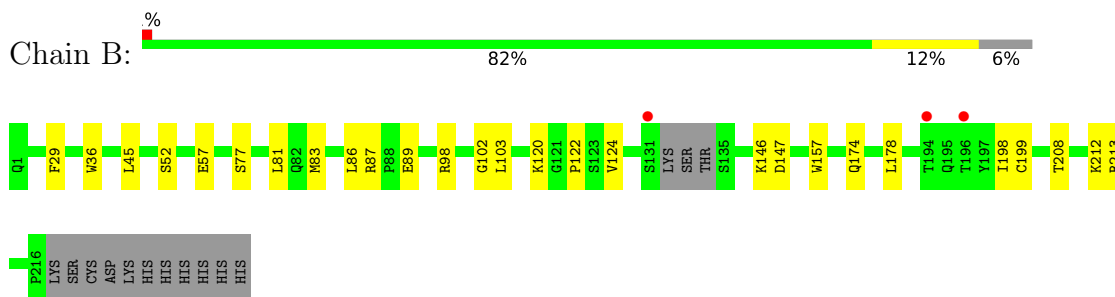
- Molecule 1: Hemagglutinin



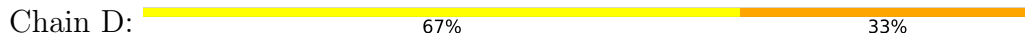
- Molecule 2: S1V2-51 Fab light chain



- Molecule 3: S1V2-51 Fab heavy chain



- Molecule 4: beta-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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.42Å 101.56Å 77.41Å 90.00° 108.01° 90.00°	Depositor
Resolution (Å)	42.65 – 2.60 42.65 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (42.65-2.60) 98.8 (42.65-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.185 , 0.215 0.193 , 0.219	Depositor DCC
R_{free} test set	1579 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	72.1	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5535	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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: BMA, NAG, 1PE, GOL, BCN

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	0.60	0/2161	0.75	0/2942
2	C	0.61	0/1724	0.78	0/2340
3	B	0.59	0/1611	0.77	0/2192
All	All	0.60	0/5496	0.77	0/7474

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	32	GLY	Peptide

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	2109	0	2050	31	0
2	C	1686	0	1626	27	0
3	B	1577	0	1547	22	0
4	D	39	0	34	3	0
5	A	28	0	26	0	0
6	A	22	0	24	1	0
7	A	18	0	23	1	0
7	B	6	0	8	0	0
7	C	18	0	23	5	0
8	C	16	0	20	1	0
9	A	7	0	0	1	0
9	B	2	0	0	0	0
9	C	7	0	0	1	0
All	All	5535	0	5381	81	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 (81) 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:B:120:LYS:NZ	3:B:147:ASP:O	1.80	1.12
3:B:120:LYS:HZ2	3:B:147:ASP:HB3	1.19	1.06
1:A:77:ASP:OD2	1:A:141:ARG:NH1	2.09	0.84
3:B:120:LYS:NZ	3:B:147:ASP:HB3	1.95	0.81
1:A:155:THR:OG1	9:A:501:HOH:O	1.98	0.80
2:C:153:GLN:NE2	2:C:160:LEU:HD23	1.97	0.80
3:B:120:LYS:HZ2	3:B:147:ASP:CB	1.94	0.77
3:B:147:ASP:OD1	3:B:174:GLN:NE2	2.22	0.72
1:A:42:LEU:HB2	1:A:293:PRO:HD2	1.70	0.71
3:B:174:GLN:HG2	3:B:178:LEU:O	1.97	0.64
7:C:303:GOL:O2	9:C:401:HOH:O	2.14	0.64
3:B:120:LYS:NZ	3:B:147:ASP:CB	2.56	0.64
2:C:30:SER:OG	2:C:37:ASN:OD1	2.17	0.61
1:A:167:THR:HG23	1:A:242:VAL:CG2	2.34	0.58
2:C:43:GLN:HB2	2:C:53:LEU:HD11	1.84	0.58
2:C:42:TYR:OH	3:B:102:GLY:O	2.17	0.57
2:C:73:SER:O	7:C:302:GOL:H2	2.04	0.56
1:A:186:SER:OG	1:A:187:THR:HG23	2.05	0.56
1:A:74:PRO:HA	1:A:77:ASP:OD2	2.06	0.56
3:B:146:LYS:HE3	3:B:147:ASP:OD2	2.06	0.55
3:B:29:PHE:CD2	3:B:77:SER:HA	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:LYS:HZ1	1:A:303:GLY:HA2	1.73	0.53
2:C:67:ARG:NH1	2:C:88:ASP:OD2	2.41	0.53
1:A:167:THR:HG23	1:A:242:VAL:HG21	1.90	0.53
2:C:8:PRO:HG3	2:C:11:LEU:HD13	1.91	0.53
2:C:96:GLN:NE2	2:C:102:TYR:HA	2.24	0.53
2:C:6:GLN:HE22	2:C:93:TYR:HA	1.74	0.53
1:A:221:PRO:HD3	3:B:52:SER:HB3	1.90	0.53
2:C:153:GLN:NE2	2:C:160:LEU:HB3	2.24	0.53
2:C:75:THR:N	7:C:302:GOL:O2	2.39	0.53
1:A:91:SER:OG	1:A:271:ASP:OD2	2.27	0.52
2:C:2:ILE:HG12	2:C:27:GLN:HB2	1.91	0.51
2:C:153:GLN:HE21	2:C:160:LEU:HB3	1.76	0.51
1:A:264:LYS:NZ	1:A:303:GLY:HA2	2.26	0.50
1:A:66:LEU:HD21	1:A:112:VAL:HG12	1.94	0.48
2:C:76:ASP:N	7:C:302:GOL:O2	2.35	0.47
1:A:62:ILE:HG13	1:A:62:ILE:O	2.15	0.47
1:A:237:VAL:HG13	1:A:241:ASP:HB3	1.96	0.47
1:A:295:GLN:HG2	1:A:306:PRO:HG2	1.97	0.47
1:A:268:MET:HE2	1:A:268:MET:HB3	1.75	0.47
1:A:53:ASN:OD1	1:A:276:THR:HA	2.15	0.46
1:A:100:TYR:HA	1:A:230:ILE:O	2.15	0.46
2:C:50:PRO:HG3	3:B:45:LEU:HD21	1.97	0.46
3:B:98:ARG:O	3:B:103:LEU:HA	2.16	0.46
1:A:220:ARG:HH21	7:A:407:GOL:H11	1.80	0.46
2:C:21:ILE:HG12	2:C:108:THR:HG21	1.96	0.46
2:C:76:ASP:OD2	7:C:302:GOL:H12	2.16	0.45
1:A:62:ILE:O	1:A:63:ASP:HB2	2.17	0.45
1:A:71:LEU:O	1:A:148:PHE:HB3	2.17	0.45
2:C:4:MET:HE3	2:C:23:CYS:SG	2.57	0.45
1:A:204:VAL:HG22	1:A:245:ILE:HG12	1.98	0.45
1:A:229:ARG:NE	3:B:57:GLU:OE2	2.50	0.44
3:B:124:VAL:O	3:B:212:LYS:HE3	2.17	0.44
4:D:1:NAG:C3	4:D:1:NAG:C8	2.95	0.44
2:C:18:ARG:HG3	2:C:82:SER:HA	1.97	0.44
2:C:56:TRP:CG	8:C:301:1PE:H152	2.53	0.44
4:D:1:NAG:C8	4:D:1:NAG:H3	2.48	0.44
2:C:37:ASN:OD1	2:C:73:SER:HA	2.18	0.44
1:A:42:LEU:HD12	1:A:293:PRO:HG2	2.00	0.44
1:A:207:ARG:NH2	1:A:240:GLY:O	2.51	0.44
2:C:146:TYR:CD2	2:C:147:PRO:HA	2.53	0.43
1:A:172:ASP:O	1:A:239:PRO:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLU:HB3	1:A:42:LEU:H	1.66	0.43
6:A:406:BCN:H61	6:A:406:BCN:H32	1.57	0.43
3:B:83:MET:HE2	3:B:86:LEU:HD21	2.01	0.42
1:A:296:ASN:HD21	1:A:311:GLN:HB2	1.84	0.42
1:A:77:ASP:O	1:A:80:GLN:HG3	2.20	0.42
2:C:6:GLN:NE2	2:C:93:TYR:HA	2.34	0.42
2:C:31:PHE:HB3	2:C:34:SER:OG	2.20	0.42
3:B:36:TRP:CE2	3:B:81:LEU:HB2	2.55	0.42
3:B:87:ARG:HG3	3:B:89:GLU:HG2	2.00	0.42
1:A:208:ARG:O	1:A:208:ARG:HG3	2.18	0.42
2:C:153:GLN:CD	2:C:160:LEU:HD23	2.45	0.42
2:C:187:LEU:HD12	2:C:187:LEU:N	2.35	0.42
3:B:198:ILE:HD13	3:B:213:ARG:HA	2.01	0.41
2:C:53:LEU:O	2:C:54:ILE:HD13	2.20	0.41
1:A:264:LYS:HG2	1:A:264:LYS:O	2.20	0.41
3:B:122:PRO:HD2	3:B:208:THR:HG21	2.03	0.41
4:D:1:NAG:O3	4:D:1:NAG:H83	2.21	0.41
3:B:157:TRP:CZ3	3:B:199:CYS:HB3	2.56	0.41
3:B:36:TRP:CD1	3:B:81:LEU:HD13	2.57	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	269/289 (93%)	255 (95%)	13 (5%)	1 (0%)	30	51
2	C	216/220 (98%)	204 (94%)	12 (6%)	0	100	100
3	B	209/227 (92%)	198 (95%)	11 (5%)	0	100	100
All	All	694/736 (94%)	657 (95%)	36 (5%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	PRO

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	240/255 (94%)	240 (100%)	0	100	100
2	C	191/193 (99%)	191 (100%)	0	100	100
3	B	178/192 (93%)	178 (100%)	0	100	100
All	All	609/640 (95%)	609 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	171	ASN
1	A	189	GLN
1	A	211	GLN
2	C	153	GLN
3	B	195	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](#)

3 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	D	1	4,1	14,14,15	0.75	0	17,19,21	2.78	4 (23%)
4	NAG	D	2	4	14,14,15	0.89	1 (7%)	17,19,21	0.96	1 (5%)
4	BMA	D	3	4	11,11,12	1.25	2 (18%)	15,15,17	1.17	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
4	NAG	D	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	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)
4	D	3	BMA	C1-C2	2.25	1.57	1.52
4	D	3	BMA	C4-C3	2.06	1.57	1.52
4	D	2	NAG	C3-C2	2.00	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C2-N2-C7	9.76	135.98	122.90
4	D	1	NAG	C3-C4-C5	3.94	117.37	110.23
4	D	3	BMA	C1-O5-C5	2.54	115.59	112.19
4	D	1	NAG	C1-C2-N2	2.21	113.92	110.43
4	D	2	NAG	O4-C4-C5	-2.12	104.11	109.32
4	D	1	NAG	C8-C7-N2	2.01	119.45	116.12

There are no chirality outliers.

All (5) torsion outliers are listed below:

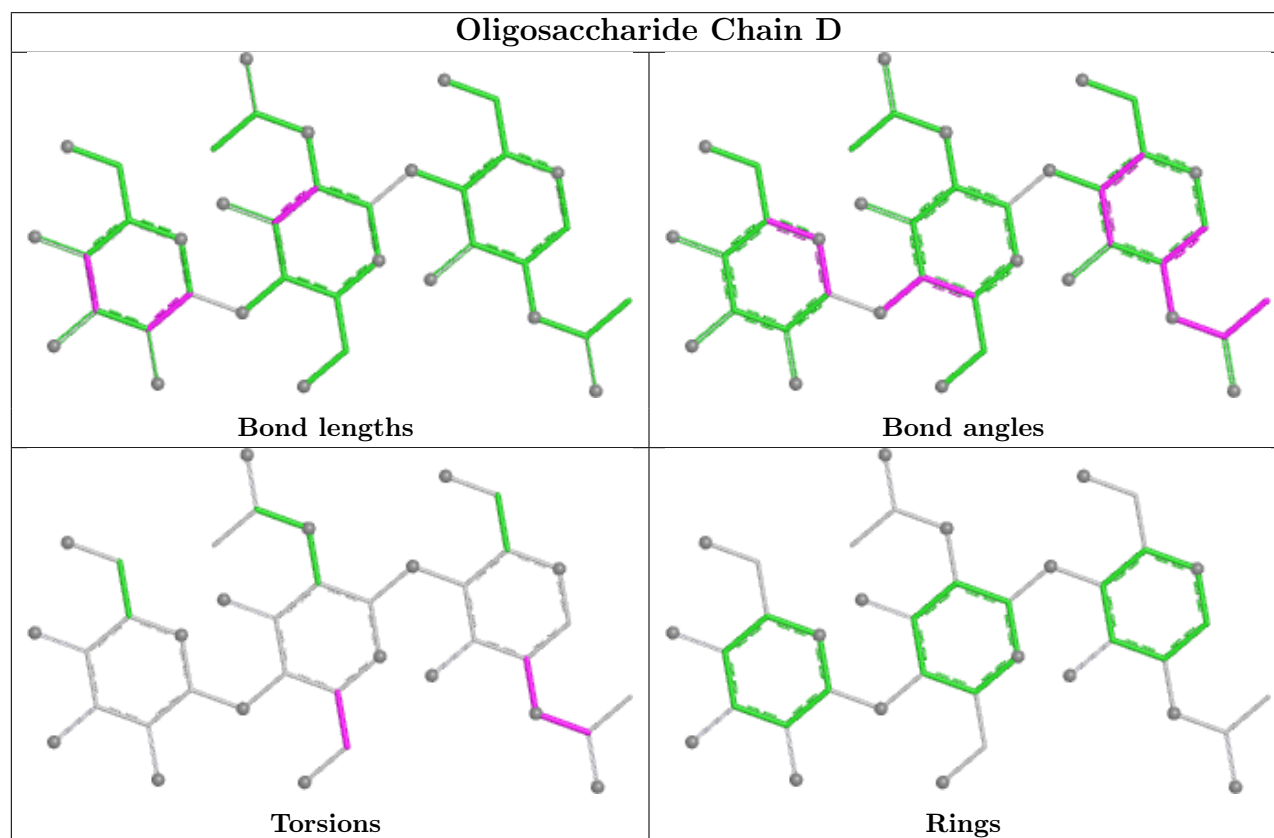
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C3-C2-N2-C7
4	D	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	3	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](#)

12 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	GOL	A	404	-	5,5,5	0.74	0	5,5,5	1.21	0
7	GOL	A	407	-	5,5,5	1.19	1 (20%)	5,5,5	1.04	0
6	BCN	A	403	-	10,10,10	1.65	2 (20%)	11,11,11	1.00	1 (9%)
7	GOL	C	303	-	5,5,5	1.51	2 (40%)	5,5,5	0.98	0
5	NAG	A	401	1	14,14,15	1.34	2 (14%)	17,19,21	0.90	1 (5%)
7	GOL	B	501	-	5,5,5	0.83	0	5,5,5	0.99	0
7	GOL	C	302	-	5,5,5	1.03	0	5,5,5	1.16	0
5	NAG	A	402	1	14,14,15	0.83	1 (7%)	17,19,21	0.89	1 (5%)
8	1PE	C	301	-	15,15,15	0.74	0	14,14,14	0.94	0
6	BCN	A	406	-	10,10,10	1.95	3 (30%)	11,11,11	1.04	1 (9%)
7	GOL	C	304	-	5,5,5	1.41	1 (20%)	5,5,5	1.28	0
7	GOL	A	405	-	5,5,5	1.26	1 (20%)	5,5,5	1.34	1 (20%)

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	GOL	A	404	-	-	0/4/4/4	-
7	GOL	A	407	-	-	0/4/4/4	-
6	BCN	A	403	-	-	5/10/10/10	-
7	GOL	C	303	-	-	2/4/4/4	-
5	NAG	A	401	1	-	2/6/23/26	0/1/1/1
7	GOL	B	501	-	-	2/4/4/4	-
7	GOL	C	302	-	-	1/4/4/4	-
5	NAG	A	402	1	-	1/6/23/26	0/1/1/1
8	1PE	C	301	-	-	7/13/13/13	-
6	BCN	A	406	-	-	4/10/10/10	-
7	GOL	C	304	-	-	3/4/4/4	-
7	GOL	A	405	-	-	0/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401	NAG	O5-C1	4.13	1.50	1.43
6	A	406	BCN	C1-C2	3.72	1.58	1.51
6	A	403	BCN	C1-C2	2.93	1.57	1.51
5	A	402	NAG	O5-C1	2.67	1.48	1.43
5	A	401	NAG	C1-C2	2.65	1.56	1.52
7	A	407	GOL	O2-C2	-2.44	1.36	1.43
6	A	406	BCN	C1-N1	2.36	1.52	1.47
6	A	406	BCN	C3-N1	2.35	1.52	1.47
7	C	303	GOL	C3-C2	2.33	1.60	1.51
7	A	405	GOL	C3-C2	2.32	1.60	1.51
7	C	303	GOL	C1-C2	2.23	1.60	1.51
6	A	403	BCN	C3-N1	2.22	1.52	1.47
7	C	304	GOL	O2-C2	-2.16	1.37	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	402	NAG	C1-O5-C5	2.69	115.79	112.19
5	A	401	NAG	C1-O5-C5	2.61	115.68	112.19
6	A	406	BCN	O22-C2-O21	-2.60	116.65	123.33
6	A	403	BCN	O22-C2-O21	-2.08	117.97	123.33
7	A	405	GOL	C3-C2-C1	-2.04	104.33	111.80

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	403	BCN	N1-C1-C2-O22
6	A	406	BCN	N1-C1-C2-O21
7	C	303	GOL	C1-C2-C3-O3
7	C	304	GOL	C1-C2-C3-O3
6	A	403	BCN	C2-C1-N1-C5
6	A	403	BCN	N1-C1-C2-O21
6	A	406	BCN	N1-C1-C2-O22
5	A	401	NAG	O5-C5-C6-O6
8	C	301	1PE	OH4-C13-C23-OH3
6	A	406	BCN	C6-C5-N1-C3
8	C	301	1PE	OH5-C14-C24-OH4
7	C	303	GOL	O2-C2-C3-O3
6	A	406	BCN	N1-C3-C4-O4
7	B	501	GOL	O1-C1-C2-C3
6	A	403	BCN	N1-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
5	A	401	NAG	C4-C5-C6-O6
8	C	301	1PE	OH6-C15-C25-OH5
7	C	304	GOL	O2-C2-C3-O3
7	B	501	GOL	O1-C1-C2-O2
8	C	301	1PE	OH7-C16-C26-OH6
8	C	301	1PE	C15-C25-OH5-C14
8	C	301	1PE	OH2-C12-C22-OH3
8	C	301	1PE	C14-C24-OH4-C13
5	A	402	NAG	C1-C2-N2-C7
7	C	304	GOL	O1-C1-C2-O2
7	C	302	GOL	O2-C2-C3-O3
6	A	403	BCN	C4-C3-N1-C5

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	407	GOL	1	0
7	C	303	GOL	1	0
7	C	302	GOL	4	0
8	C	301	1PE	1	0
6	A	406	BCN	1	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 [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	271/289 (93%)	0.12	5 (1%) 67 63	58, 79, 111, 137	0
2	C	218/220 (99%)	0.03	3 (1%) 73 69	56, 77, 102, 117	0
3	B	213/227 (93%)	0.01	3 (1%) 73 69	56, 75, 106, 129	0
All	All	702/736 (95%)	0.06	11 (1%) 70 66	56, 77, 106, 137	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	218	GLY	3.0
3	B	194	THR	2.9
1	A	42	LEU	2.8
2	C	82	SER	2.7
2	C	160	LEU	2.5
3	B	131	SER	2.3
1	A	143	PRO	2.2
1	A	62	ILE	2.2
1	A	285	ASN	2.1
1	A	264	LYS	2.1
3	B	196	THR	2.0

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

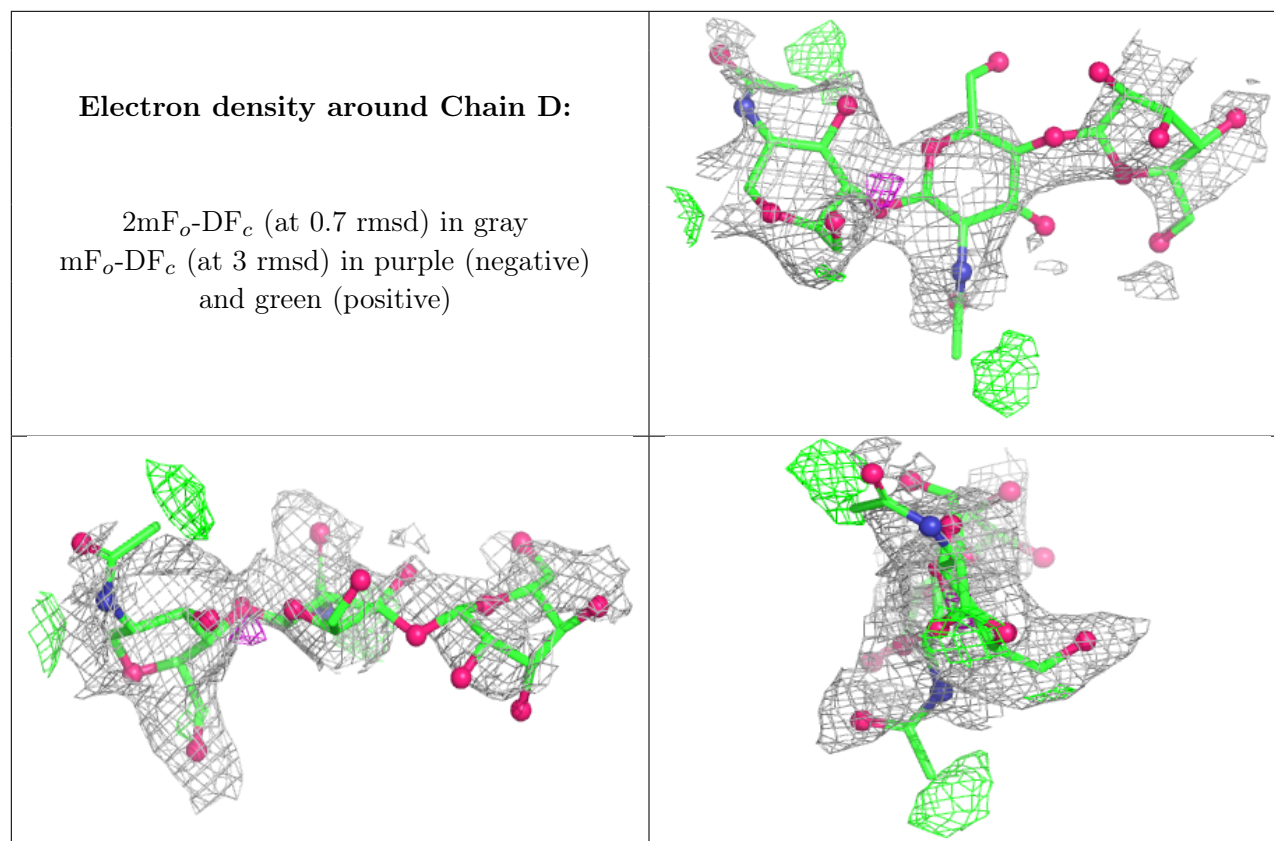
There are no non-standard protein/DNA/RNA residues in this entry.

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	BMA	D	3	11/12	0.29	0.14	158,162,164,165	0
4	NAG	D	2	14/15	0.43	0.15	150,157,161,164	0
4	NAG	D	1	14/15	0.49	0.17	118,127,138,148	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.



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, 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
5	NAG	A	401	14/15	0.65	0.14	92,104,111,113	0
6	BCN	A	406	11/11	0.67	0.18	107,112,114,114	0
5	NAG	A	402	14/15	0.72	0.15	100,113,119,121	0
7	GOL	A	405	6/6	0.80	0.16	97,102,103,104	0
7	GOL	A	404	6/6	0.82	0.21	94,108,112,112	0
7	GOL	C	302	6/6	0.83	0.28	133,139,140,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BCN	A	403	11/11	0.84	0.20	96,104,109,109	0
7	GOL	C	303	6/6	0.86	0.18	83,87,89,89	0
8	1PE	C	301	16/16	0.86	0.18	88,96,104,105	0
7	GOL	A	407	6/6	0.87	0.18	99,100,101,103	0
7	GOL	B	501	6/6	0.88	0.14	91,93,97,100	0
7	GOL	C	304	6/6	0.92	0.15	102,103,103,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.