

wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 10:18 PM EDT

PDB ID : 6XPZ

Title: Human antibody S1V2-83 in complex with the influenza hemagglutinin head

domain of A/Moscow/10/1999(H3N2)

Authors : McCarthy, K.R.; Harrison, S.C.

Deposited on : 2020-07-09

Resolution : 3.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.35.1

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

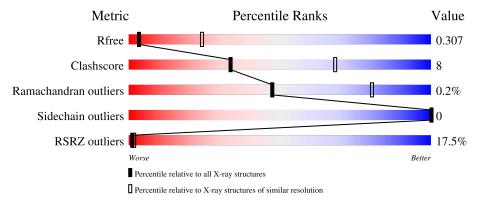
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(\mathring{A}))$
R_{free}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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		
			19%		
1	A	290	73%	19%	8%
	_		9%		
1	D	290	72%	20%	7%
	_		23%		
2	В	243	74%	22%	•
			16%		
2	E	243	73%	23%	•
			16%		_
3	С	214	81%	17%	•



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Mol	Chain	Length		Quality of chain		
	Б	21.4	18%			
3	F	214		84%	15%	•
4	G	2		100%		
5	Н	3	33%	33%	33%	
	т	9				
5	J	3	33%	33%	33%	
6	I	3	6	7%	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
4	NAG	G	2	-	-	=	X
5	NAG	J	1	-	-	=	X
5	BMA	J	3	-	-	=	X
6	BMA	I	3	-	-	-	X



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11182 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.

\mathbf{Mol}	Chain	Residues		Atoms					AltConf	Trace
1	A	268	Total 2107	C 1319	N 377	O 401	S 10	0	0	0
1	D	269	Total 2116	C 1323	N 381	O 402	S 10	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	ALA	-	expression tag	UNP Q1NZ37
A	321	LEU	-	expression tag	UNP Q1NZ37
A	322	GLU	_	expression tag	UNP Q1NZ37
A	323	VAL	-	expression tag	UNP Q1NZ37
A	324	LEU	-	expression tag	UNP Q1NZ37
A	325	PHE	-	expression tag	UNP Q1NZ37
A	326	GLN	-	expression tag	UNP Q1NZ37
D	320	ALA	-	expression tag	UNP Q1NZ37
D	321	LEU	-	expression tag	UNP Q1NZ37
D	322	GLU	-	expression tag	UNP Q1NZ37
D	323	VAL	-	expression tag	UNP Q1NZ37
D	324	LEU	-	expression tag	UNP Q1NZ37
D	325	PHE	-	expression tag	UNP Q1NZ37
D	326	GLN	-	expression tag	UNP Q1NZ37

• Molecule 2 is a protein called antibody S1V2-83 heavy chain.

Mol	Chain	Residues		Atoms					AltConf	Trace
2	В	233	Total 1761	C 1114	N 298	O 342	S 7	0	0	0
2	E	233	Total 1761	C 1114	N 298	O 342	S 7	0	0	0

• Molecule 3 is a protein called antibody S1V2-83 light chain.



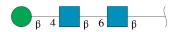
Mol	Chain	Residues		Atoms					AltConf	Trace
3	С	211	Total 1632	C 1021	11	O 335	S 5	0	0	0
3	F	211	Total 1632	C 1021		O 335	S 5	0	0	0

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



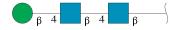
Mol	Chain	Residues	At	toms		ZeroOcc	AltConf	Trace
4	G	2	Total 0	C N 16 2	O 10	0	0	0

• Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atom	ıs	ZeroOcc	AltConf	Trace
5	Н	3	Total C 39 22	N O 2 15	0	0	0
5	J	3	Total C 39 22	N O 2 15	0	0	0

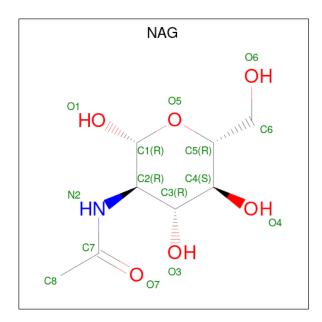
• Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	F	Aton	ns		ZeroOcc	AltConf	Trace
6	I	3	Total 39	C 22	N 2	O 15	0	0	0

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





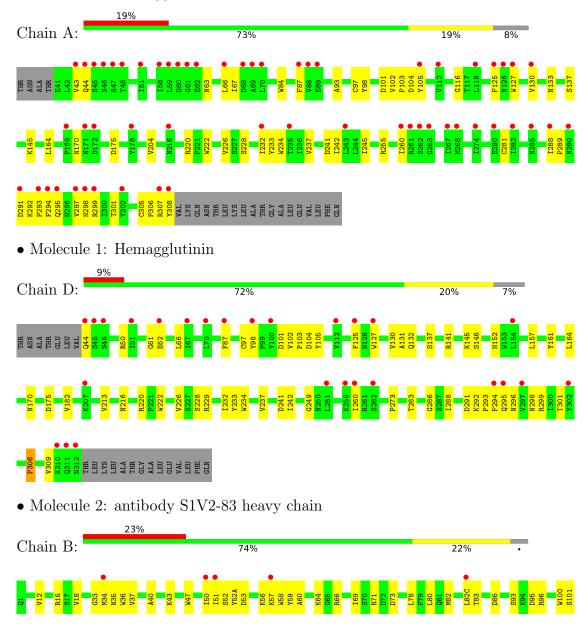
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	Λ	1	Total	С	N	О	0	0	
'	(A	1	14	8	1	5	0	U	
7	D	1	Total	С	N	О	0	0	
'	ש	1	14	8	1	5	U	U	



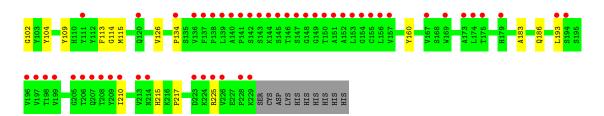
3 Residue-property plots (i)

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.

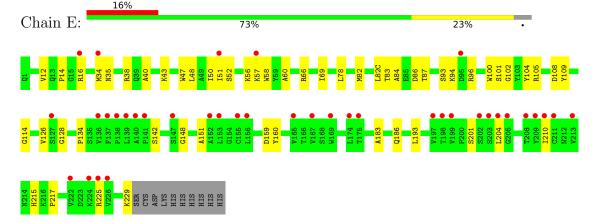
• Molecule 1: Hemagglutinin



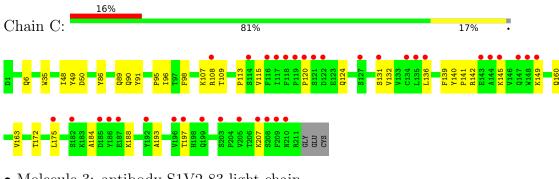




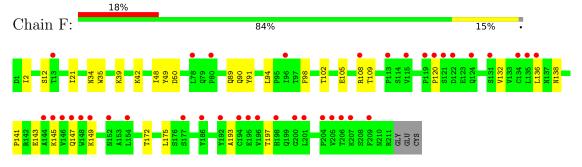
 \bullet Molecule 2: antibody S1V2-83 heavy chain



 \bullet Molecule 3: antibody S1V2-83 light chain



 \bullet Molecule 3: antibody S1V2-83 light chain



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

Chain G: 100%





	beta-D-mannop oxy-beta-D-gluco	yranose-(1-4)-2-acetami pyranose	do-2-deoxy-beta-D-gl	ucopyranose-(1-6)-2-a
Chain H:	33%	33%	33%	
MAG1 NAG2 BMA3				
	beta-D-mannop oxy-beta-D-gluco	yranose-(1-4)-2-acetami pyranose	do-2-deoxy-beta-D-gl	ucopyranose-(1-6)-2-a
Chain J:	33%	33%	33%	
NAG2 NAG2 BMA3				
	beta-D-mannop oxy-beta-D-gluco	yranose-(1-4)-2-acetami pyranose	do-2-deoxy-beta-D-gl	ucopyranose-(1-4)-2-a
Chain I:	6	7%	33%	





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants	85.79Å 103.71Å 220.00Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.10 - 3.45	Depositor
resolution (A)	49.10 - 3.45	EDS
% Data completeness	99.5 (49.10-3.45)	Depositor
(in resolution range)	85.4 (49.10-3.45)	EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.05 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
D.D.	0.251 , 0.307	Depositor
R, R_{free}	0.251 , 0.307	DCC
R_{free} test set	1327 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	83.6	Xtriage
Anisotropy	1.020	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33, 81.5	EDS
L-test for twinning ²	$ < L >=0.45, < L^2>=0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11182	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond	lengths	Bond	angles
IVIOI	Moi Chain		# Z > 5	RMSZ	# Z > 5
1	A	0.24	0/2159	0.43	0/2935
1	D	0.24	0/2168	0.44	0/2946
2	В	0.25	0/1807	0.46	0/2457
2	Е	0.26	0/1807	0.46	0/2457
3	С	0.25	0/1667	0.46	0/2265
3	F	0.25	0/1667	0.45	0/2265
All	All	0.25	0/11275	0.45	0/15325

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	2107	0	2042	37	0
1	D	2116	0	2052	42	0
2	В	1761	0	1703	43	0
2	Е	1761	0	1703	41	0
3	С	1632	0	1574	23	0
3	F	1632	0	1574	20	0
4	G	28	0	25	0	0



Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
5	Н	39	0	34	1	0
5	J	39	0	34	1	0
6	I	39	0	34	0	0
7	A	14	0	13	0	0
7	D	14	0	13	0	0
All	All	11182	0	10801	186	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 8.

The worst 5 of 186 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:44:GLN:HE22	1:A:289:PRO:HD2	1.43	0.84
1:A:295:GLN:HE21	1:A:297:VAL:HB	1.45	0.82
1:D:137:SER:HB3	1:D:145:LYS:HE2	1.66	0.75
1:A:104:ASP:HB3	1:A:234:TRP:HH2	1.52	0.75
2:E:66:ARG:NH2	2:E:86:ASP:OD2	2.21	0.74

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	266/290~(92%)	254 (96%)	12 (4%)	0	100 100
1	D	$267/290\ (92\%)$	254 (95%)	12 (4%)	1 (0%)	34 70
2	В	$231/243\ (95\%)$	218 (94%)	13 (6%)	0	100 100
2	E	$231/243\ (95\%)$	211 (91%)	18 (8%)	2 (1%)	17 54
3	C	$209/214\ (98\%)$	198 (95%)	11 (5%)	0	100 100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
3	F	209/214 (98%)	197 (94%)	12 (6%)	0	100	100
All	All	1413/1494 (95%)	1332 (94%)	78 (6%)	3 (0%)	47	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	306	PRO
2	Е	109	TYR
2	Е	148	GLY

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	Perce	ntiles
1	A	239/257~(93%)	239 (100%)	0	100	100
1	D	240/257 (93%)	240 (100%)	0	100	100
2	В	193/203 (95%)	193 (100%)	0	100	100
2	E	193/203 (95%)	193 (100%)	0	100	100
3	С	188/190 (99%)	188 (100%)	0	100	100
3	F	188/190 (99%)	188 (100%)	0	100	100
All	All	1241/1300 (96%)	1241 (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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	295	GLN
1	D	170	ASN
2	В	35	ASN



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

11 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	Trino	Chain	Res	Link	Bo	Bond lengths			ond ang	eles
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	G	1	4,1	14,14,15	0.28	0	17,19,21	0.41	0
4	NAG	G	2	4	14,14,15	0.34	0	17,19,21	0.54	0
5	NAG	Н	1	5,1	14,14,15	0.19	0	17,19,21	0.41	0
5	NAG	Н	2	5	14,14,15	0.42	0	17,19,21	1.40	2 (11%)
5	BMA	Н	3	5	11,11,12	0.57	0	15,15,17	0.82	1 (6%)
6	NAG	I	1	6,1	14,14,15	0.31	0	17,19,21	0.59	0
6	NAG	I	2	6	14,14,15	0.29	0	17,19,21	0.49	0
6	BMA	I	3	6	11,11,12	1.00	1 (9%)	15,15,17	0.94	1 (6%)
5	NAG	J	1	5,1	14,14,15	1.14	1 (7%)	17,19,21	1.21	1 (5%)
5	NAG	J	2	5	14,14,15	0.88	1 (7%)	17,19,21	0.92	1 (5%)
5	BMA	J	3	5	11,11,12	0.69	0	15,15,17	0.70	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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	Н	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	Н	2	5	-	4/6/23/26	0/1/1/1
5	BMA	Н	3	5	-	0/2/19/22	0/1/1/1
6	NAG	I	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	BMA	I	3	6	-	0/2/19/22	0/1/1/1
5	NAG	J	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	BMA	J	3	5	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$oxed{Ideal(A)}$
5	J	1	NAG	C1-C2	3.90	1.58	1.52
5	J	2	NAG	O5-C1	-3.09	1.38	1.43
6	I	3	BMA	C1-C2	2.70	1.58	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
5	Н	2	NAG	C2-N2-C7	4.42	129.20	122.90
5	J	1	NAG	C2-N2-C7	3.71	128.19	122.90
5	Н	2	NAG	C1-C2-N2	2.21	114.27	110.49
6	I	3	BMA	O2-C2-C3	-2.15	105.82	110.14
5	Н	3	BMA	C1-O5-C5	2.06	114.99	112.19

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

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

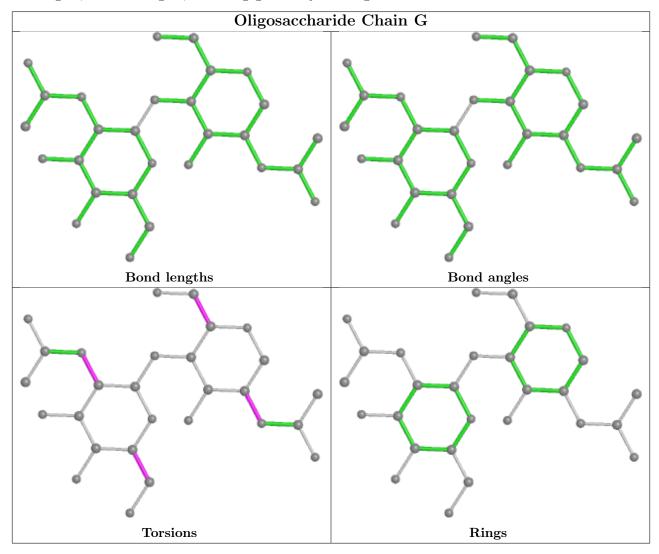
There are no ring outliers.

2 monomers are involved in 2 short contacts:

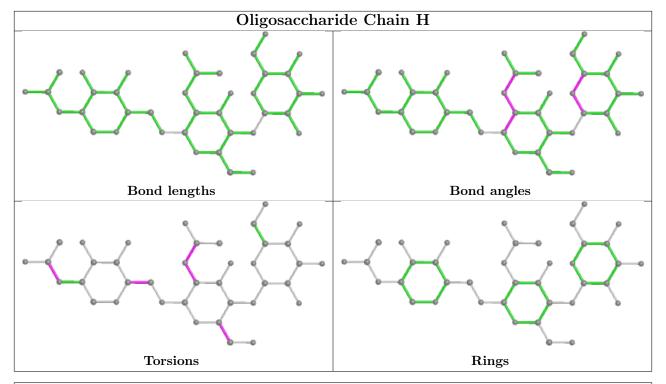


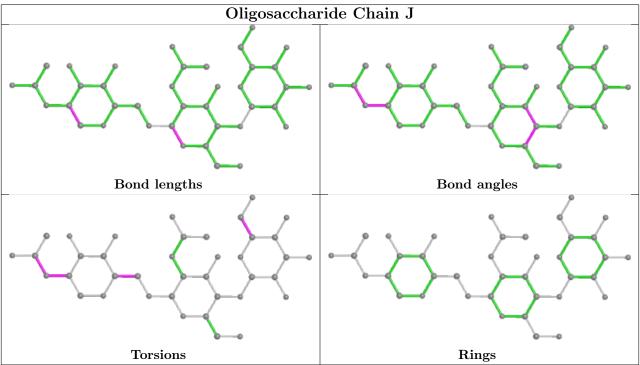
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Н	2	NAG	1	0
5	J	1	NAG	1	0

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

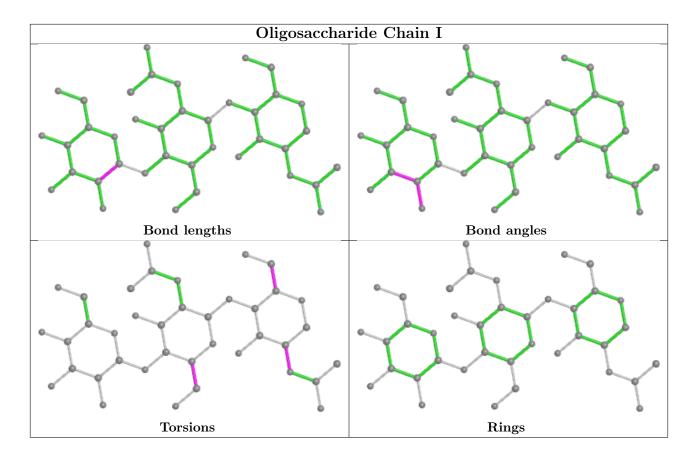












5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bo	Bond lengths		В	ond ang	les
MIOI	туре	Chain	rtes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	401	1	14,14,15	0.24	0	17,19,21	0.54	0
7	NAG	D	401	1	14,14,15	0.17	0	17,19,21	0.43	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
7	NAG	A	401	1	-	3/6/23/26	0/1/1/1
7	NAG	D	401	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	401	NAG	O5-C5-C6-O6
7	A	401	NAG	C4-C5-C6-O6
7	D	401	NAG	C8-C7-N2-C2
7	D	401	NAG	O7-C7-N2-C2
7	D	401	NAG	O5-C5-C6-O6

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 (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, 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>	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	A	$268/290 \ (92\%)$	1.12	56 (20%) 1 1	95, 139, 186, 226	0
1	D	269/290~(92%)	0.82	26 (9%) 7 10	75, 113, 171, 240	0
2	В	233/243 (95%)	1.49	56 (24%) 0 0	89, 128, 253, 442	0
2	E	233/243 (95%)	1.07	38 (16%) 1 2	79, 124, 271, 333	0
3	С	211/214 (98%)	1.11	35 (16%) 1 2	81, 135, 229, 282	0
3	F	211/214 (98%)	1.04	38 (18%) 1 2	70, 146, 214, 261	0
All	All	1425/1494 (95%)	1.10	249 (17%) 1 2	70, 129, 232, 442	0

The worst 5 of 249 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	145	SER	13.5
2	В	152	ALA	13.5
2	В	153	LEU	12.6
2	В	136	VAL	8.6
2	В	141	PRO	8.2

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

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

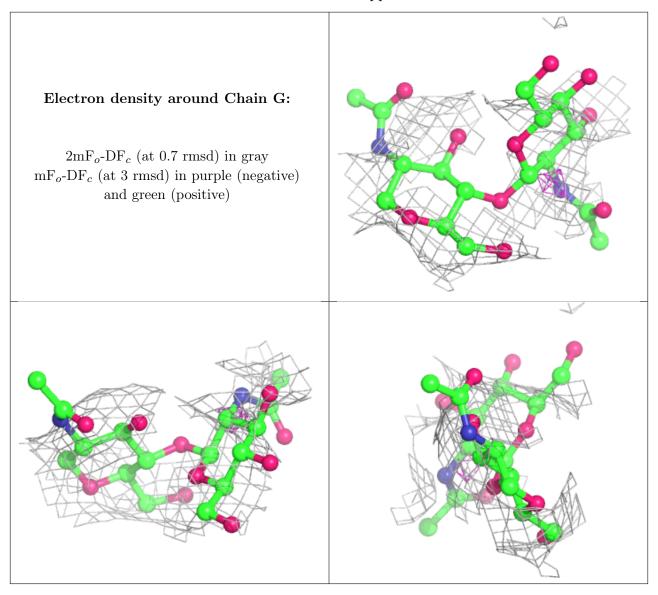
6.3 Carbohydrates (i)

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, 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
4	NAG	G	2	14/15	0.53	0.46	162,185,194,196	0
6	BMA	I	3	11/12	0.54	0.41	165,175,180,183	0
5	NAG	J	1	14/15	0.63	0.44	113,137,147,147	0
5	BMA	J	3	11/12	0.66	0.45	160,167,179,182	0
5	NAG	J	2	14/15	0.71	0.40	141,157,174,178	0
5	NAG	Н	2	14/15	0.73	0.22	134,153,164,169	0
4	NAG	G	1	14/15	0.74	0.37	153,172,183,186	0
5	NAG	Н	1	14/15	0.76	0.39	138,159,167,168	0
6	NAG	I	2	14/15	0.78	0.35	126,157,172,176	0
5	BMA	Н	3	11/12	0.78	0.37	155,160,164,164	0
6	NAG	I	1	14/15	0.83	0.26	105,125,143,154	0

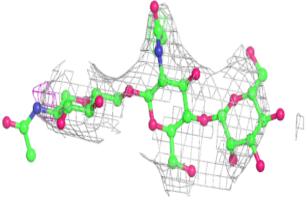
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

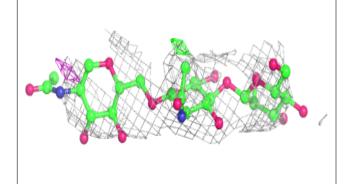


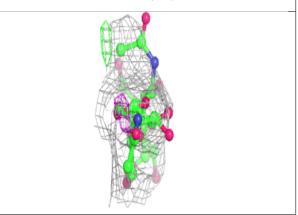


Electron density around Chain H:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

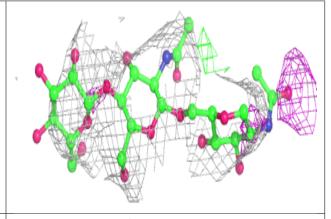


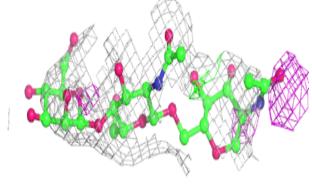


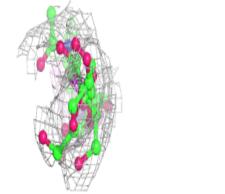


Electron density around Chain J:

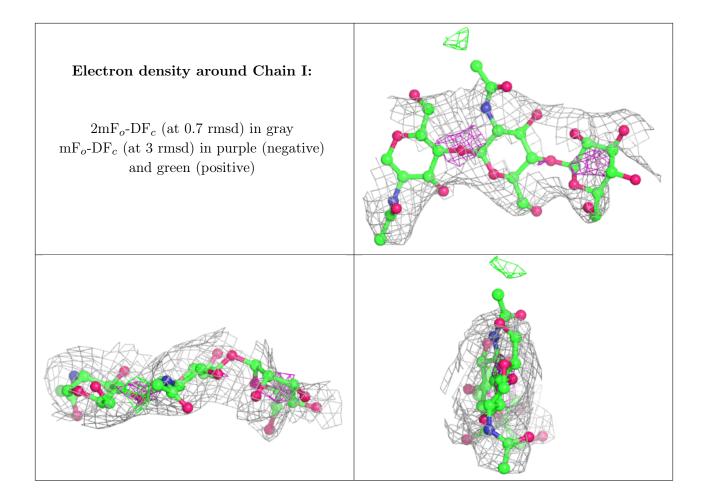
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











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, 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	$\operatorname{B-factors}({ m \AA}^2)$	Q < 0.9
7	NAG	D	401	14/15	0.63	0.34	140,148,158,159	0
7	NAG	A	401	14/15	0.83	0.21	123,135,140,142	0

6.5 Other polymers (i)

There are no such residues in this entry.

