

wwPDB X-ray Structure Validation Summary Report (i)

Aug 27, 2023 – 11:27 AM EDT

PDB ID	:	3HS0
Title	:	Cobra Venom Factor (CVF) in complex with human factor B
Authors	:	Janssen, B.J.C.; Gomes, L.; Koning, R.I.; Svergun, D.I.; Koster, A.J.;
		Fritzinger, D.C.; Vogel, CW.; Gros, P.
Deposited on	:	2009-06-10
Resolution	:	3.00 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:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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	А	627	77%	20%	•
1	F	627	76%	21%	
2	В	252	75%	17%	• 8%
2	G	252	72%	18%	• 8%
3	С	379	.% 66%	26%	•• 5%

Continued on next page...



Continued from previous page...

Mol	Chain	Length	Quality of chain		
3	Н	379	78%	17%	
4	D	741	3% 68%	25%	•• 6%
4	Ι	741	3% 67%	25%	• 5%
5	Е	2	100%		
5	J	2	100%		

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
5	NAG	Е	2	-	-	-	Х
5	NAG	J	2	-	-	-	Х



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 30435 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 Cobra venom factor.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	613	Total 4794	C 3069	N 804	O 906	$\begin{array}{c} \mathrm{S} \\ 15 \end{array}$	0	0	0
1	F	617	Total 4826	C 3085	N 811	O 915	S 15	0	0	0

• Molecule 2 is a protein called Cobra venom factor.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	Р	022	Total	С	Ν	0	S	0	0	0
	D	200	1856	1194	311	346	5	0	0	0
0	C	022	Total	С	Ν	0	S	0	0	0
	G	233	1856	1194	311	346	5	U	0	0

• Molecule 3 is a protein called Cobra venom factor.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	С	359	Total 2900	C 1831	N 484	O 566	S 19	0	0	0
3	Н	366	Total 2957	C 1864	N 496	O 578	S 19	0	0	0

• Molecule 4 is a protein called Complement factor B.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
4	D	699	Total 5513	С 3474	N 954	O 1052	S 33	0	0	0
4	Ι	704	$\begin{array}{c} \text{Total} \\ 5567 \end{array}$	C 3506	N 972	O 1056	S 33	0	0	0

There are 8 discrepancies between the modelled and reference sequences:



3H50

Chain	Residue	Modelled	Actual	Comment	Reference
D	254	GLY	ASP	engineered mutation	UNP P00751
D	260	ASP	ASN	engineered mutation	UNP P00751
D	740	ALA	-	insertion	UNP P00751
D	741	ALA	-	insertion	UNP P00751
Ι	254	GLY	ASP	engineered mutation	UNP P00751
Ι	260	ASP	ASN	engineered mutation	UNP P00751
Ι	740	ALA	-	insertion	UNP P00751
Ι	741	ALA	-	insertion	UNP P00751

• Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Е	2	Total 28	C 16	N 2	O 10	0	0	0
5	J	2	Total 28	C 16	N 2	O 10	0	0	0

• Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





9 L	JCU
0	190

Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf	
6	Λ	1	Total	С	Ν	0	0	0	
0	A	1	14	8	1	5	0	0	
6	С	1	Total	С	Ν	Ο	0	0	
0	U	1	14	8	1	5	0	0	
6	Л	1	Total	С	Ν	Ο	0	0	
0	D	1	14	8	1	5	0	0	
6	Л	1	Total	С	Ν	Ο	0	0	
0	D		14	8	1	5	0	0	
6	F	1	Total	С	Ν	Ο	0	0	
0	1	I	14	8	1	5	0	0	
6	н	1	Total	С	Ν	Ο	0	0	
0	11	1	14	8	1	5	0	0	
6	Т	1	Total	С	Ν	Ο	0	0	
0			14	8	1	5		0	

• Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0
7	F	1	Total Mg 1 1	0	0
7	Ι	1	Total Mg 1 1	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	2	Total O 2 2	0	0
8	С	1	Total O 1 1	0	0
8	D	1	Total O 1 1	0	0
8	F	2	Total O 2 2	0	0
8	Н	1	Total O 1 1	0	0
8	Ι	1	Total O 1 1	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: Cobra venom factor

• Molecule 2: Cobra venom factor













• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

100%



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

100%

NAG1 NAG2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	134.03Å 136.97Å 283.74Å	Deneiten
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	34.88 - 3.00	Depositor
Resolution (A)	34.88 - 3.00	EDS
% Data completeness	99.8 (34.88-3.00)	Depositor
(in resolution range)	99.8 (34.88-3.00)	EDS
R _{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) > 1$	2.47 (at 3.00Å)	Xtriage
Refinement program	PHENIX	Depositor
P. P.	0.189 , 0.243	Depositor
n, n_{free}	0.179 , 0.236	DCC
R_{free} test set	2093 reflections $(2.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	72.0	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.25, 39.4	EDS
L-test for twinning ²	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	30435	wwPDB-VP
Average B, all atoms $(Å^2)$	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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: MG, 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).

Mal	Chain	Bond	lengths	Bond angles		
MIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.27	0/4902	0.46	0/6668	
1	F	0.27	0/4935	0.49	2/6715~(0.0%)	
2	В	0.27	0/1894	0.46	0/2570	
2	G	0.28	0/1894	0.51	1/2570~(0.0%)	
3	С	0.26	0/2950	0.51	1/3989~(0.0%)	
3	Н	0.26	0/3009	0.47	0/4071	
4	D	0.26	0/5636	0.48	2/7629~(0.0%)	
4	Ι	0.25	0/5691	0.46	0/7699	
All	All	0.26	0/30911	0.48	6/41911 (0.0%)	

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
1	F	1	0
3	С	0	1
All	All	1	1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
3	С	1553	LEU	N-CA-C	5.97	127.12	111.00
1	F	13	THR	C-N-CA	5.71	135.96	121.70
4	D	739	LEU	CA-CB-CG	5.49	127.93	115.30
2	G	917	GLY	N-CA-C	5.23	126.18	113.10
1	F	13	THR	CA-C-N	5.19	128.62	117.20



All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	13	THR	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	С	1551	LEU	Peptide

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	А	4794	0	4801	90	0
1	F	4826	0	4826	111	0
2	В	1856	0	1900	37	0
2	G	1856	0	1900	40	0
3	С	2900	0	2851	101	0
3	Н	2957	0	2900	62	0
4	D	5513	0	5376	153	0
4	Ι	5567	0	5446	160	0
5	Е	28	0	25	0	0
5	J	28	0	25	0	0
6	А	14	0	13	2	0
6	С	14	0	13	0	0
6	D	28	0	26	0	0
6	F	14	0	13	0	0
6	Н	14	0	13	0	0
6	Ι	14	0	13	0	0
7	А	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	Ι	1	0	0	0	0
8	А	2	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	2	0	0	0	0
8	Н	1	0	0	0	0
8	Ι	1	0	0	0	0

Continued on next page...



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	30435	0	30141	711	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 12.

The worst 5 of 711 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:H:1469:ARG:HG2	3:H:1469:ARG:HH11	1.10	1.12
4:D:714:ARG:HG2	4:D:714:ARG:HH11	1.17	1.07
4:I:705:ARG:HB3	4:I:707:LYS:HG2	1.37	1.04
4:D:699:VAL:HG23	4:D:707:LYS:HD2	1.42	1.01
1:F:13:THR:HG23	1:F:14:ASP:CB	1.89	1.01

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	Pe	erce	entiles
1	А	607/627~(97%)	577~(95%)	26 (4%)	4 (1%)		22	60
1	F	613/627~(98%)	571 (93%)	36 (6%)	6 (1%)		15	53
2	В	231/252~(92%)	218 (94%)	13 (6%)	0	1	.00	100
2	G	231/252~(92%)	218 (94%)	12 (5%)	1 (0%)		34	72
3	С	353/379~(93%)	318 (90%)	29 (8%)	6 (2%)		9	39
3	Н	362/379~(96%)	333~(92%)	24 (7%)	5 (1%)		11	43
4	D	687/741~(93%)	608 (88%)	63 (9%)	16 (2%)		6	30
4	Ι	694/741~(94%)	605 (87%)	65 (9%)	24 (4%)		3	20
All	All	3778/3998~(94%)	3448 (91%)	268 (7%)	62 (2%)		9	40



5 of 62 Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	247	ILE
4	D	44	TYR
4	D	46	VAL
4	D	344	PRO
4	D	505	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	535/548~(98%)	529~(99%)	6 (1%)	73	90
1	F	539/548~(98%)	528~(98%)	11 (2%)	55	83
2	В	210/227~(92%)	200~(95%)	10 (5%)	25	62
2	G	210/227~(92%)	202~(96%)	8 (4%)	33	69
3	С	329/345~(95%)	314~(95%)	15~(5%)	27	64
3	Н	335/345~(97%)	326~(97%)	9~(3%)	44	77
4	D	610/643~(95%)	596~(98%)	14 (2%)	50	80
4	Ι	615/643~(96%)	605 (98%)	10 (2%)	62	86
All	All	3383/3526~(96%)	3300 (98%)	83 (2%)	47	79

 $5~{\rm of}~83$ residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
2	G	851	LYS
3	Н	1478	LEU
2	G	918	THR
3	Н	1311	LEU
4	Ι	216	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:



Mol	Chain	Res	Type
1	А	593	GLN
4	D	47	GLN
4	D	601	GLN
1	F	473	GLN
4	Ι	468	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)

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).

Mal	Turne	Chain	Res Linl		Bond lengths				Bond angles			
IVIOI	туре	Unain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
5	NAG	E	1	4,5	14,14,15	0.52	0	17,19,21	1.84	5 (29%)		
5	NAG	Е	2	5	14,14,15	0.49	0	17,19,21	1.09	2 (11%)		
5	NAG	J	1	4,5	14,14,15	0.44	0	$17,\!19,\!21$	1.14	1 (5%)		
5	NAG	J	2	5	14,14,15	0.49	0	17,19,21	1.30	2 (11%)		

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
5	NAG	Е	1	4,5	-	3/6/23/26	0/1/1/1
5	NAG	Е	2	5	-	4/6/23/26	0/1/1/1

Continued on next page...



Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	J	1	4,5	-	4/6/23/26	0/1/1/1
5	NAG	J	2	5	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	Ε	1	NAG	C1-O5-C5	4.52	118.31	112.19
5	J	2	NAG	O5-C5-C6	4.28	113.92	107.20
5	J	1	NAG	C1-O5-C5	3.18	116.50	112.19
5	Е	1	NAG	C3-C4-C5	2.81	115.26	110.24
5	Е	1	NAG	C2-N2-C7	2.80	126.90	122.90

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Ε	1	NAG	C3-C2-N2-C7
5	Е	2	NAG	C8-C7-N2-C2
5	Е	2	NAG	O7-C7-N2-C2
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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











5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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	Tuno	SypeChainRes	Dog	Tipk	Bo	ond leng	$_{\rm ths}$	Bond angles		
MOI	Type			Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
6	NAG	А	9187	1	14,14,15	0.45	0	17,19,21	1.21	2 (11%)
6	NAG	D	9353	4	14,14,15	0.47	0	17,19,21	0.89	1 (5%)
6	NAG	С	9324	3	14,14,15	0.52	0	17,19,21	1.01	1 (5%)



Mol	Turne	Chain	Res	5 Link	Bo	ond leng	$_{\rm ths}$	Bond angles		
NIOI	Moi Type Chain	Chain			Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	Ι	9117	4	14,14,15	0.45	0	17,19,21	1.10	1 (5%)
6	NAG	D	9117	4	14,14,15	0.37	0	17,19,21	2.43	4 (23%)
6	NAG	Н	9324	3	14,14,15	0.46	0	17,19,21	0.82	0
6	NAG	F	9187	1	14,14,15	0.44	0	17,19,21	1.41	3 (17%)

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
6	NAG	А	9187	1	-	3/6/23/26	0/1/1/1
6	NAG	D	9353	4	-	2/6/23/26	0/1/1/1
6	NAG	С	9324	3	-	2/6/23/26	0/1/1/1
6	NAG	Ι	9117	4	-	4/6/23/26	0/1/1/1
6	NAG	D	9117	4	-	4/6/23/26	0/1/1/1
6	NAG	Н	9324	3	-	3/6/23/26	0/1/1/1
6	NAG	F	9187	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
6	D	9117	NAG	C1-O5-C5	8.51	123.73	112.19
6	F	9187	NAG	C1-O5-C5	3.79	117.33	112.19
6	А	9187	NAG	C1-O5-C5	3.39	116.79	112.19
6	Ι	9117	NAG	C1-O5-C5	3.37	116.76	112.19
6	С	9324	NAG	C1-O5-C5	3.20	116.52	112.19

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	А	9187	NAG	C8-C7-N2-C2
6	А	9187	NAG	O7-C7-N2-C2
6	С	9324	NAG	C8-C7-N2-C2
6	С	9324	NAG	O7-C7-N2-C2
6	D	9117	NAG	C8-C7-N2-C2



There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	А	9187	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 (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>2	$OWAB(Å^2)$	Q<0.9
1	А	613/627~(97%)	-0.67	1 (0%) 95 87	31, 68, 125, 182	0
1	F	617/627~(98%)	-0.61	3 (0%) 91 75	37, 75, 132, 187	0
2	В	233/252~(92%)	-0.73	0 100 100	34, 63, 111, 123	0
2	G	233/252~(92%)	-0.71	0 100 100	33, 66, 115, 151	0
3	С	359/379~(94%)	-0.42	3 (0%) 86 65	40, 94, 210, 291	0
3	Н	366/379~(96%)	-0.62	2 (0%) 91 75	33, 81, 135, 216	0
4	D	699/741~(94%)	-0.36	25 (3%) 42 17	35, 88, 189, 233	0
4	Ι	704/741~(95%)	-0.33	25 (3%) 42 17	37, 91, 191, 244	0
All	All	3824/3998~(95%)	-0.52	59 (1%) 73 46	31, 79, 168, 291	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Ι	16	GLY	8.8
4	Ι	30	GLY	6.8
4	Ι	51	CYS	6.4
4	Ι	50	THR	5.9
4	Ι	29	GLU	5.6

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,



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
5	NAG	Ε	2	14/15	0.64	0.49	161,168,182,183	0
5	NAG	J	2	14/15	0.66	0.63	173,184,194,201	0
5	NAG	J	1	14/15	0.80	0.26	126,139,157,173	0
5	NAG	Е	1	14/15	0.86	0.25	136,146,153,163	0

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.

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 (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	$B-factors(A^2)$	Q<0.9
6	NAG	Н	9324	14/15	0.76	0.36	129,140,144,146	0
6	NAG	С	9324	14/15	0.82	0.25	111,123,130,134	0
6	NAG	F	9187	14/15	0.87	0.30	106,116,125,127	0
6	NAG	D	9353	14/15	0.88	0.31	122,136,142,146	0
7	MG	А	628	1/1	0.89	0.07	105,105,105,105	0
6	NAG	Ι	9117	14/15	0.92	0.38	116,129,142,143	0
6	NAG	D	9117	14/15	0.93	0.22	98,117,131,132	0
6	NAG	А	9187	14/15	0.94	0.19	87,102,110,114	0
7	MG	F	628	1/1	0.97	0.04	73,73,73,73	0
7	MG	Ι	742	1/1	0.97	0.13	97,97,97,97	0
7	MG	D	742	1/1	0.98	0.10	107,107,107,107	0



6.5 Other polymers (i)

There are no such residues in this entry.

