

Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2020 – 10:04 AM BST

PDB ID : 6BLX

Title : Crystal structure of IAg7 in complex with insulin mimotope p8G9E

Authors : Wang, Y.; Dai, S.

Deposited on : 2017-11-11

Resolution : 2.32 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 (i) symbol.

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 : 2.13.1

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)

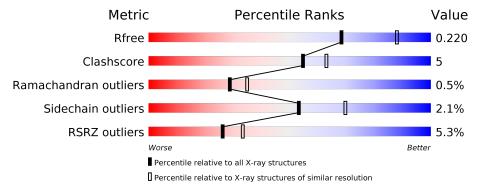
Validation Pipeline (wwPDB-VP) : 2.13.1

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 2.32 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	A	183	5% 87%	11%
2	В	221	79%	8% • 11%
3	С	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
3	NAG	С	2	_	_	_	X



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3397 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 H-2 class II histocompatibility antigen, A-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	182	Total	С	N	О	S	0	0	0
1	Α	102	1466	950	236	278	2	U	U	0

• Molecule 2 is a protein called H2-Ab1 protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	В	197	Total	C 1016	N	O 204	S	0	0	0
			1619	1016	292	304	1			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	-28	HIS	-	see remark 999	UNP Q31135
В	-27	LEU	-	see remark 999	UNP Q31135
В	-26	VAL	-	see remark 999	UNP Q31135
В	-25	GLU	_	see remark 999	UNP Q31135
В	-24	ARG	_	see remark 999	UNP Q31135
В	-23	LEU	_	see remark 999	UNP Q31135
В	-22	TYR	_	see remark 999	UNP Q31135
В	-21	LEU	-	see remark 999	UNP Q31135
В	-20	VAL	_	see remark 999	UNP Q31135
В	-19	CYS	_	see remark 999	UNP Q31135
В	-18	GLY	_	see remark 999	UNP Q31135
В	-17	GLY	_	see remark 999	UNP Q31135
В	-16	GLU	-	see remark 999	UNP Q31135
В	-15	GLY	_	linker	UNP Q31135
В	-14	ALA	_	linker	UNP Q31135
В	-8	GLY	_	linker	UNP Q31135
В	-7	GLY	_	linker	UNP Q31135
В	-6	GLY	-	linker	UNP Q31135
В	-5	SER	-	linker	UNP Q31135
В	-4	LEU	-	linker	UNP Q31135

Continued on next page...



Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
В	-3	VAL	-	linker	UNP Q31135
В	-2	GLY	-	linker	UNP Q31135
В	-1	GLY	-	linker	UNP Q31135
В	0	SER	-	linker	UNP Q31135
В	1	GLY	-	linker	UNP Q31135
В	2	GLY	-	linker	UNP Q31135
В	3	GLY	-	linker	UNP Q31135
В	192	GLY	-	expression tag	UNP Q31135
В	193	GLY	-	expression tag	UNP Q31135
В	194	LEU	-	expression tag	UNP Q31135
В	195	VAL	-	expression tag	UNP Q31135
В	196	PRO	-	expression tag	UNP Q31135
В	197	ARG	-	expression tag	UNP Q31135

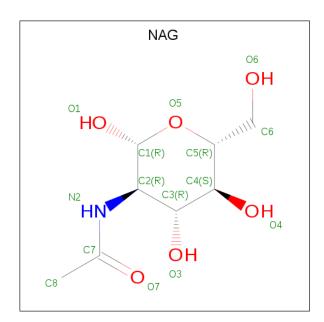
• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
3	С	2	Total 28	C 16	N 2	O 10	0	0	0

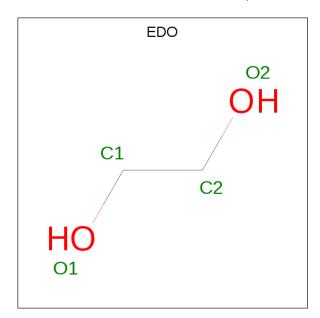
• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





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

 \bullet Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	В	1	Total C O 4 2 2	0	0

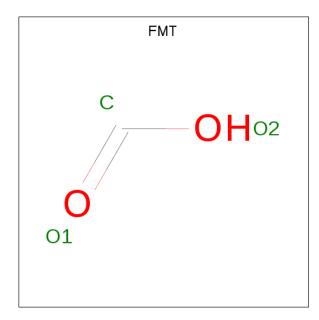
Continued on next page...



Continued from previous page...

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf
5	В	1	Total 4	C 2	O 2	0	0

 \bullet Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: $\mathrm{CH_2O_2}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 3 1 2	0	0

• Molecule 7 is water.

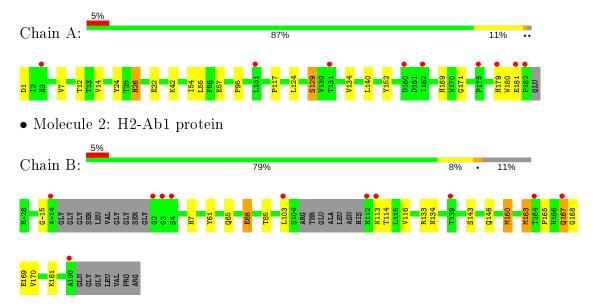
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	123	Total O 123 123	0	0
7	В	128	Total O 128 128	0	0



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: H-2 class II histocompatibility antigen, A-D alpha chain



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

aı · a	
Chain C:	100%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	$39.35 ext{Å}$ $112.63 ext{Å}$ $62.18 ext{Å}$	Depositor
a, b, c, α , β , γ	90.00° 107.36° 90.00°	Depositor
Resolution (Å)	40.85 - 2.32	Depositor
Resolution (A)	40.85 - 2.32	EDS
% Data completeness	96.2 (40.85-2.32)	Depositor
(in resolution range)	96.3 (40.85-2.32)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.81 (at 2.31Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
D D.	0.168 , 0.220	Depositor
R, R_{free}	0.168 , 0.220	DCC
R_{free} test set	1083 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	$0.35 \; , 46.4$	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3397	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.38% 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.



 $^{^{1}}$ Intensities 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: FMT, NAG, EDO

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	
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5
1	A	0.40	0/1512	0.57	0/2066
2	В	0.42	0/1656	0.58	0/2242
All	All	0.41	0/3168	0.57	0/4308

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	1466	0	1393	14	0
2	В	1619	0	1545	18	0
3	С	28	0	25	0	0
4	A	14	0	13	0	0
5	A	8	0	12	1	0
5	В	8	0	12	2	0
6	A	3	0	1	0	0
7	A	123	0	0	2	0
7	В	128	0	0	2	0
All	All	3397	0	3001	32	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 5.

All (32) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A + a rea 1	A 4 a res 2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({f \AA})$	overlap (Å)
1:A:169:HIS:HD2	1:A:171:GLY:H	1.18	0.89
1:A:169:HIS:CD2	1:A:171:GLY:H	1.97	0.83
1:A:7:VAL:HG23	5:A:205:EDO:H11	1.65	0.78
2:B:133:ARG:NH2	2:B:169:GLU:OE1	2.29	0.65
1:A:24:TYR:OH	1:A:26:HIS:HE1	1.85	0.58
2:B:134:ASN:ND2	2:B:170:VAL:H	2.03	0.57
2:B:116:VAL:HG22	2:B:160:MET:HG3	1.86	0.56
2:B:146:GLN:H	2:B:146:GLN:CD	2.10	0.55
2:B:134:ASN:HD21	2:B:169:GLU:HA	1.73	0.53
2:B:103:LEU:HD23	2:B:114:THR:O	2.10	0.51
1:A:55:LEU:HD21	1:A:57:GLU:OE1	2.11	0.51
2:B:61:TYR:HB2	5:B:201:EDO:H21	1.96	0.48
1:A:124:LEU:HD23	1:A:129:SER:HA	1.96	0.48
2:B:61:TYR:CZ	2:B:65:GLN:HG3	2.50	0.47
1:A:179:HIS:HE1	1:A:181:GLU:OE1	1.99	0.46
2:B:167:GLN:HB3	2:B:168:GLY:H	1.43	0.46
1:A:54:ILE:HD12	2:B:85:THR:HG22	1.96	0.46
1:A:42:LYS:NZ	7:A:307:HOH:O	2.48	0.46
1:A:14:VAL:HG21	1:A:117:PRO:HG3	1.98	0.45
2:B:103:LEU:HD21	2:B:163:MET:HE2	1.99	0.44
2:B:113:ASN:HB3	2:B:163:MET:CE	2.47	0.44
7:A:350:HOH:O	2:B:7:HIS:HD2	1.99	0.44
1:A:32:GLU:HB2	1:A:140:LEU:HD21	2.00	0.44
1:A:134:VAL:HA	1:A:152:TYR:O	2.18	0.43
2:B:163:MET:HE3	2:B:165:PRO:HD3	2.01	0.43
1:A:169:HIS:HD2	1:A:171:GLY:N	2.00	0.42
2:B:143:SER:O	2:B:160:MET:HE2	2.20	0.42
2:B:68:GLU:OE2	7:B:301:HOH:O	2.22	0.42
2:B:146:GLN:CD	2:B:146:GLN:N	2.73	0.42
1:A:95:PRO:HG3	1:A:180:TRP:CZ2	2.55	0.41
2:B:181:LYS:HD3	2:B:181:LYS:HA	1.81	0.41
5:B:202:EDO:H11	7:B:347:HOH:O	2.20	0.41

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	${f Analysed}$	Favoured	Allowed	Outliers	Perce	\mathbf{ntiles}
1	A	180/183 (98%)	176 (98%)	4 (2%)	0	100	100
2	В	191/221 (86%)	182 (95%)	7 (4%)	2 (1%)	15	17
All	All	371/404 (92%)	358 (96%)	11 (3%)	2 (0%)	29	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	167	GLN
2	В	-15	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	Percentiles
1	A	162/165 (98%)	158 (98%)	4 (2%)	47 64
2	В	175/191 (92%)	172 (98%)	3 (2%)	60 75
All	All	337/356 (95%)	330 (98%)	7 (2%)	53 70

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	12	THR
1	A	26	HIS
1	A	129	SER

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
2	В	68	GLU
2	В	160	MET
2	В	163	MET

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

Mol	Chain	Res	Type
1	A	26	HIS
1	A	169	HIS
1	A	179	HIS
2	В	7	HIS
2	В	134	ASN
2	В	167	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)

2 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	Т	Chain	Res	Link	Bo	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	NAG	С	1	1,3	14,14,15	0.39	0	17,19,21	0.76	1 (5%)	
3	NAG	С	2	3	14,14,15	0.97	1 (7%)	17,19,21	0.72	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	С	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	С	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	${ m Observed}({ m \AA})$	$\operatorname{Ideal}(ext{\AA})$
3	С	2	NAG	C1-C2	2.86	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
3	С	1	NAG	C1-O5-C5	2.63	115.75	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

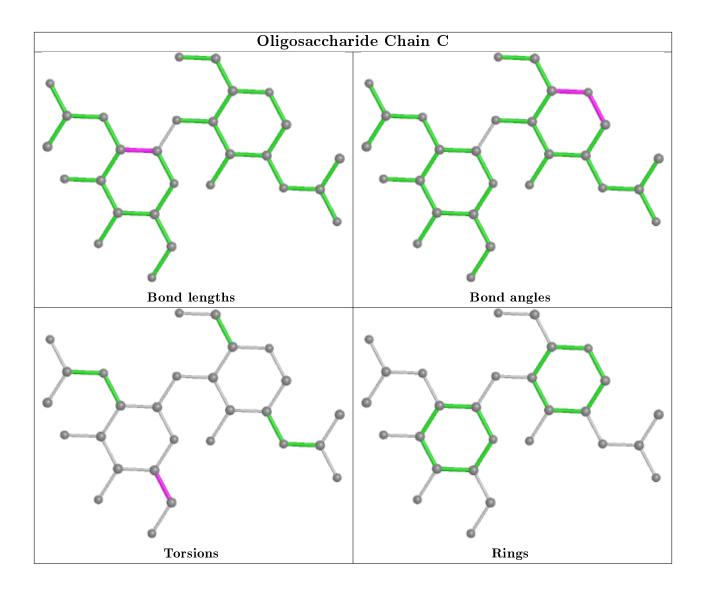
Mol	Chain	Res	Type	Atoms
3	С	2	NAG	C4-C5-C6-O6
3	С	2	NAG	O5-C5-C6-O6

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)

6 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	Trino	Chain	Res	Link	Bond lengths			В	ond ang	les
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	В	201	-	3,3,3	0.42	0	2,2,2	0.47	0
5	EDO	A	204	-	3,3,3	0.64	0	2,2,2	0.22	0
4	NAG	A	201	1	14,14,15	1.23	1 (7%)	17,19,21	0.98	1 (5%)



Mol	Tree	Chain	Res	Link	Bo	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
5	EDO	A	205	-	3,3,3	0.57	0	2,2,2	0.19	0	
6	FMT	A	206	-	0,2,2	0.00	-	0,1,1	0.00	ı	
5	EDO	В	202	-	3,3,3	0.80	0	2,2,2	0.93	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
5	EDO	A	205	-	-	0/1/1/1	=
5	EDO	В	201	_	-	0/1/1/1	-
4	NAG	A	201	1	-	1/6/23/26	0/1/1/1
5	EDO	A	204	_	-	0/1/1/1	-
5	EDO	В	202	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\mathbf{Ideal}(\mathbf{\AA})$
4	A	201	NAG	C1-C2	4.17	1.58	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	${f Res}$	Type	${f Atoms}$	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
4	A	201	NAG	C4-C3-C2	2.65	114.90	111.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	В	202	EDO	O1-C1-C2-O2
4	A	201	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	В	201	EDO	1	0
5	A	205	EDO	1	0
5	В	202	EDO	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, 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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	182/183 (99%)	0.22	9 (4%) 29 37	25, 32, 51, 70	0
2	В	197/221 (89%)	0.13	11 (5%) 24 31	23, 32, 58, 78	0
All	All	379/404 (93%)	0.17	20 (5%) 26 33	23, 32, 57, 78	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	PRO	4.4
2	В	190	ALA	3.5
2	В	167	GLN	3.5
2	В	-14	ALA	3.3
2	В	3	GLY	3.1
2	В	103	LEU	2.7
1	A	181	GLU	2.7
1	A	179	HIS	2.7
2	В	164	THR	2.6
1	A	101	LEU	2.5
1	A	131	THR	2.5
2	В	112	HIS	2.4
1	A	175	PRO	2.4
2	В	139	THR	2.4
1	A	3	GLU	2.3
2	В	4	SER	2.1
2	В	2	GLY	2.1
2	В	113	ASN	2.1
1	A	160	ASP	2.0
1	A	162	ILE	2.0



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

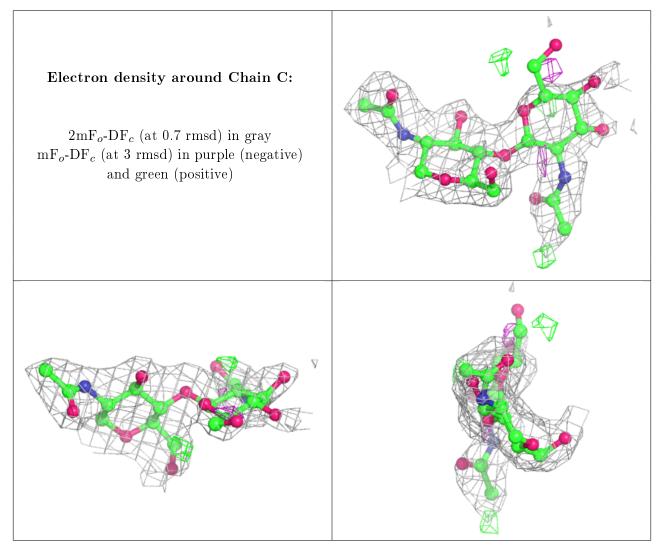
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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	${f B-factors}({f A}^2)$	Q<0.9
3	NAG	С	2	14/15	0.66	0.46	64,79,88,88	0
3	NAG	С	1	14/15	0.91	0.24	39,53,63,68	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 (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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	NAG	A	201	14/15	0.81	0.29	69,78,79,83	0
6	FMT	A	206	3/3	0.86	0.19	40,40,47,51	0
5	EDO	В	201	4/4	0.90	0.22	49,51,52,57	0
5	EDO	В	202	4/4	0.90	0.18	31,34,37,38	0
5	EDO	A	204	4/4	0.91	0.19	35,37,38,39	0
5	EDO	A	205	4/4	0.92	0.13	43,43,45,54	0

6.5 Other polymers (i)

There are no such residues in this entry.

