

Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2020 – 02:19 PM BST

PDB ID : 5BRO

Title : Crystal structure of modified HexB (modB)

Authors : Kitakaze, K.; Maita, N.; Itoh, K.

Deposited on : 2015-06-01

Resolution : 2.40 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

 $\begin{array}{cccc} & CCP4 & : & 7.0.044 \; (Gargrove) \\ Ideal \; geometry \; (proteins) & : & Engh \; \& \; Huber \; (2001) \end{array}$

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

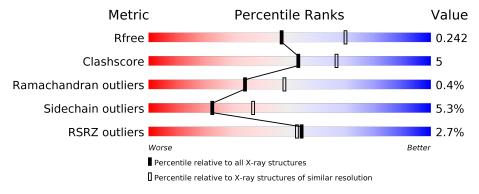
Validation Pipeline (wwPDB-VP) : 2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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	514	82%		11%	• 5%
2	В	2	50%	50%		
2	С	2	50%	50%		

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:



I	Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
	2	NAG	С	2	_	_	_	X



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4167 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 Beta-hexosaminidase subunit beta.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	490	Total	С	N	О	S	0	0	0
1	A	490	3952	2551	659	729	13	0	U	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	GLY	ARG	engineered mutation	UNP P07686
A	313	SER	GLN	engineered mutation	UNP P07686
A	314	GLU	ASN	engineered mutation	UNP P07686
A	315	PRO	LYS	engineered mutation	UNP P07686
A	452	ASN	ASP	engineered mutation	UNP P07686
A	453	ARG	LEU	engineered mutation	UNP P07686

• Molecule 2 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
2	В	2	Total 28		N 2	O 10	0	0	0
2	С	2	Total 28	C 16		O 10	0	0	0

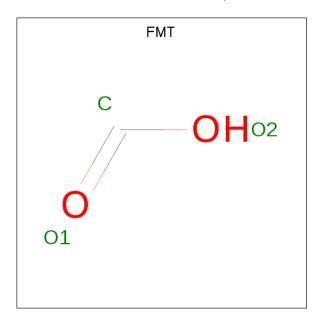
• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).





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

• Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



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

• Molecule 5 is water.



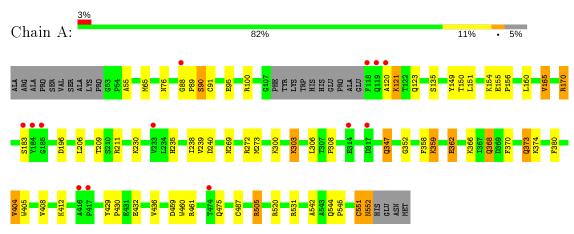
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	150	Total O 150 150	0	0



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

Chain B: 50% 50%

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

Chain C: 50% 50%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants	126.47Å 126.47Å 88.31Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 - 2.40	Depositor
Resolution (A)	36.43 - 2.40	EDS
% Data completeness	99.9 (40.00-2.40)	Depositor
(in resolution range)	100.0 (36.43-2.40)	EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.21 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
P. P.	0.187 , 0.240	Depositor
R, R_{free}	0.195 , 0.242	DCC
R_{free} test set	1428 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31, 25.5	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4167	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 3.75% 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: GOL, FMT, 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		
MIOI	Chain RMSZ		# Z >5	RMSZ	# Z > 5	
1	A	0.67	0/4066	0.79	$3/5529 \ (0.1\%)$	

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
1	A	505	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	A	505	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	A	170	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	551	CYS	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	A	3952	0	3856	43	1
2	В	28	0	25	1	0
2	С	28	0	25	4	0
3	A	6	0	8	3	0
4	A	3	0	1	0	0
5	A	150	0	0	5	0
All	All	4167	0	3915	43	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A	A	Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ ({\rm \AA})$	$overlap(\AA)$
1:A:459:ASP:OD1	3:A:601:GOL:O2	2.08	0.70
1:A:91:CYS:O	1:A:95:GLU:HG2	1.94	0.68
1:A:65:MET:HE2	2:B:1:NAG:H82	1.75	0.68
1:A:347:GLN:CG	2:C:1:NAG:H81	2.24	0.67
1:A:347:GLN:HG3	2:C:1:NAG:H81	1.76	0.67
1:A:238:ILE:HG23	1:A:239:VAL:HG13	1.78	0.66
1:A:89:PRO:HA	1:A:95:GLU:OE2	1.97	0.63
1:A:123:GLN:HG3	5:A:847:HOH:O	2.03	0.59
1:A:373:GLN:NE2	1:A:373:GLN:O	2.37	0.57
1:A:347:GLN:HG3	2:C:1:NAG:C8	2.35	0.56
1:A:303:LYS:HG3	5:A:814:HOH:O	2.05	0.56
1:A:362:GLU:HB2	1:A:380:PHE:CE2	2.41	0.55
1:A:303:LYS:HD3	1:A:303:LYS:O	2.08	0.54
1:A:88:GLY:HA2	5:A:821:HOH:O	2.11	0.50
1:A:89:PRO:O	1:A:95:GLU:OE2	2.30	0.49
1:A:206:LEU:HD12	1:A:235:HIS:CE1	2.49	0.48
1:A:155:GLU:HG2	1:A:156:PRO:HA	1.95	0.47
1:A:404:VAL:HG13	1:A:408:VAL:HB	1.96	0.47
1:A:206:LEU:C	1:A:206:LEU:HD23	2.35	0.47
1:A:370:PHE:CZ	1:A:374:LYS:HE3	2.49	0.47
1:A:429:TYR:N	1:A:430:PRO:CD	2.78	0.47
1:A:362:GLU:O	1:A:368:GLN:OE1	2.33	0.46
1:A:88:GLY:CA	5:A:821:HOH:O	2.62	0.46
1:A:120:ALA:O	1:A:121:LYS:HB2	2.16	0.45
1:A:170:ARG:HD2	1:A:230:LYS:HG2	1.98	0.45
1:A:347:GLN:HG2	2:C:1:NAG:H81	1.97	0.45

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Atom-1	Atom-2	Interatomic	Clash	
Atom-1	Atom-2	${f distance}\;({ m \AA})$	$overlap(ext{Å})$	
1:A:544:GLN:HB2	1:A:545:PRO:CD	2.47	0.45	
1:A:206:LEU:HB3	1:A:487:CYS:HA	2.00	0.43	
1:A:269:ASN:ND2	1:A:272:ARG:HH11	2.16	0.43	
1:A:432:GLU:O	1:A:436:VAL:HG23	2.18	0.43	
1:A:460:TRP:HD1	3:A:601:GOL:H2	1.84	0.42	
1:A:55:ALA:HB2	1:A:531:ARG:HB2	2.00	0.42	
1:A:135:SER:O	1:A:165:VAL:HB	2.19	0.42	
1:A:149:TYR:CE2	1:A:196:ASP:HB3	2.55	0.42	
1:A:461:ARG:HD3	5:A:806:HOH:O	2.19	0.41	
1:A:505:ARG:HG2	3:A:601:GOL:C1	2.50	0.41	
1:A:209:THR:OG1	1:A:238:ILE:HA	2.21	0.41	
1:A:306:LEU:O	1:A:308:PRO:HD3	2.21	0.41	
1:A:358:PHE:O	1:A:359:LYS:C	2.58	0.41	
1:A:362:GLU:HA	1:A:380:PHE:CZ	2.56	0.40	
1:A:151:LEU:HD13	1:A:160:LEU:HD13	2.03	0.40	
1:A:352:GLY:HA2	1:A:405:TRP:CD1	2.56	0.40	
1:A:551:CYS:O	1:A:552:ASN:HB2	2.22	0.40	

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	Clash overlap (Å)	
1:A:90:SER:O	1:A:90:SER:O[8_554]	1.25	0.95	

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	486/514 (95%)	463 (95%)	21 (4%)	2 (0%)	34 48	

All (2) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	240	ASP
1	A	542	ALA

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	Analysed Rotameric Outliers		Percentiles		
1	A	433/453 (96%)	410 (95%)	23 (5%)	22 37		

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	90	SER
1	A	100	ARG
1	A	121	LYS
1	A	150	THR
1	A	154	LYS
1	A	165	VAL
1	A	183	SER
1	A	211	ARG
1	A	273	MET
1	A	300	LYS
1	A	303	LYS
1	A	347	GLN
1	A	359	LYS
1	A	362	GLU
1	A	366	LYS
1	A	368	GLN
1	A	373	GLN
1	A	404	VAL
1	A	412	LYS
1	A	475	GLN
1	A	520	ARG
1	A	552	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such



sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	A	269	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)

4 monosaccharides are modelled in this entry.

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

Mol Type		Chain R	Res	Link	Bond lengths			Bond angles		
10101	Type	Chain	res	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	В	1	1,2	14,14,15	0.47	0	17,19,21	1.41	3 (17%)
2	NAG	В	2	2	14,14,15	0.63	0	17,19,21	1.48	3 (17%)
2	NAG	С	1	1,2	14,14,15	0.60	0	17,19,21	2.11	3 (17%)
2	NAG	С	2	2	14,14,15	0.83	0	17,19,21	1.99	7 (41%)

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

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

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\mathbf{Mol}	\mathbf{Type}	Chain	${f Res}$	Link	Chirals	Torsions	Rings
2	NAG	С	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	С	1	NAG	C1-O5-C5	7.04	121.74	112.19
2	С	2	NAG	C8-C7-N2	3.81	122.54	116.10
2	С	2	NAG	C2-N2-C7	3.19	127.44	122.90
2	В	2	NAG	O5-C1-C2	-3.13	106.35	111.29
2	С	2	NAG	O5-C5-C6	3.09	112.04	107.20
2	С	2	NAG	O7-C7-C8	-2.96	116.55	122.06
2	В	2	NAG	C4-C3-C2	-2.90	106.77	111.02
2	В	1	NAG	O5-C5-C6	2.65	111.36	107.20
2	В	2	NAG	C2-N2-C7	2.49	126.45	122.90
2	С	1	NAG	O5-C5-C4	2.43	116.74	110.83
2	В	1	NAG	C3-C4-C5	-2.43	105.91	110.24
2	С	1	NAG	O5-C5-C6	-2.36	103.51	107.20
2	С	2	NAG	C1-O5-C5	2.30	115.31	112.19
2	В	1	NAG	O5-C1-C2	-2.29	107.68	111.29
2	С	2	NAG	O3-C3-C2	2.28	114.19	109.47
2	С	2	NAG	C6-C5-C4	-2.20	107.85	113.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	С	2	NAG	C8-C7-N2-C2
2	С	2	NAG	O7-C7-N2-C2
2	В	2	NAG	C3-C2-N2-C7

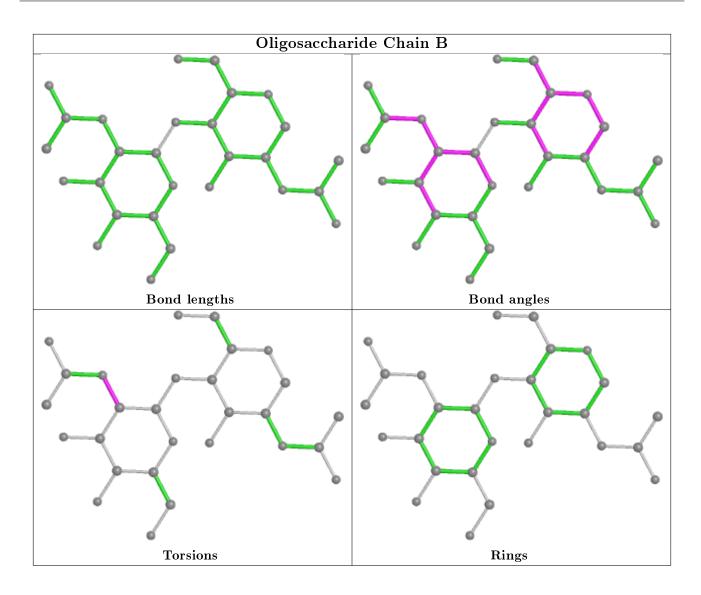
There are no ring outliers.

2 monomers are involved in 5 short contacts:

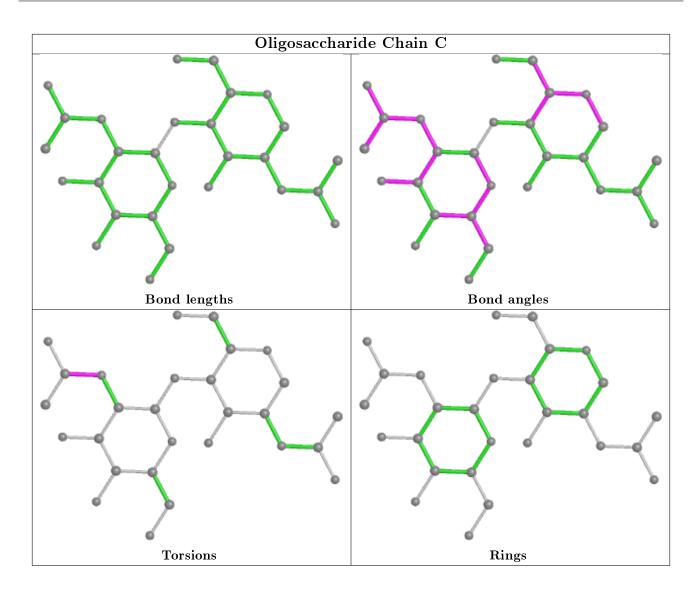
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	1	NAG	1	0
2	С	1	NAG	4	0

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	Mol Type Chain Res L		Link	В	Bond lengths			Bond angles		
MOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	601	-	5,5,5	0.47	0	5,5,5	0.52	0
4	FMT	A	602	-	0,2,2	0.00	-	0,1,1	0.00	-



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	${f Res}$	Link	Chirals	Torsions	Rings
3	GOL	A	601	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	GOL	O2-C2-C3-O3
3	A	601	GOL	C1-C2-C3-O3
3	A	601	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	GOL	3	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	490/514 (95%)	-0.12	13 (2%) 54 52	18, 32, 62, 122	0

All (13) RSRZ outliers are listed below:

Mol	Chain	${f Res}$	Type	RSRZ
1	A	118	PHE	6.4
1	A	184	TYR	5.2
1	A	183	SER	4.8
1	A	417	PRO	4.0
1	A	119	GLN	3.8
1	A	120	ALA	2.8
1	A	88	GLY	2.6
1	A	416	ALA	2.6
1	A	185	GLY	2.5
1	A	317	ASP	2.3
1	A	314	GLU	2.1
1	A	474	THR	2.1
1	A	233	VAL	2.1

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

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

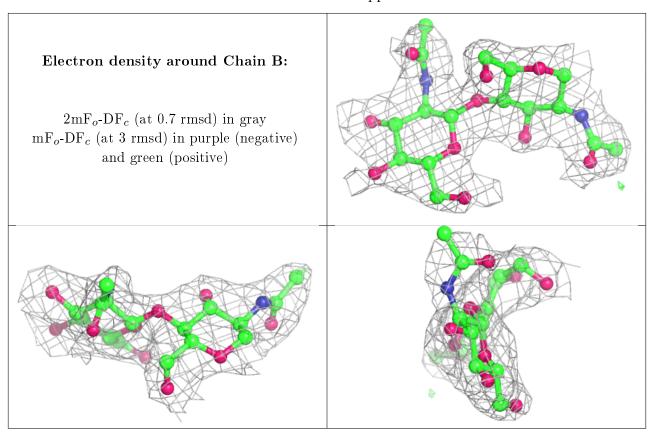
6.3 Carbohydrates (i)

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.

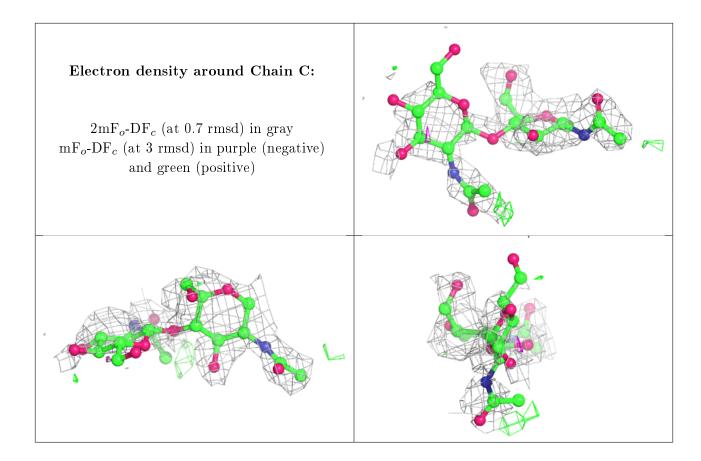


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	NAG	С	2	14/15	0.56	0.52	90,109,130,137	0
2	NAG	С	1	14/15	0.75	0.27	62,83,104,131	0
2	NAG	В	2	14/15	0.88	0.28	69,78,85,86	0
2	NAG	В	1	14/15	0.91	0.22	45,56,62,75	0

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	${f Res}$	Atoms	RSCC	RSR	${f B\text{-factors}}({f A}^2)$	Q<0.9
3	GOL	A	601	6/6	0.96	0.17	24,32,34,37	0
4	FMT	A	602	3/3	0.97	0.15	43,43,48,50	0

6.5 Other polymers (i)

There are no such residues in this entry.

