

wwPDB EM Validation Summary Report (i)

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PDB ID	:	6X3S
EMDB ID	:	EMD-22031
Title	:	Human GABAA receptor alpha1-beta2-gamma2 subtype in complex with bicu-
		culline methbromide
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Deposited on	:	2020-05-21
Resolution	:	3.12 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp 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:

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 3.12 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.



Motria	Whole archive	EM structures		
Metric	$(\# {\rm Entries})$	$(\# {\rm Entries})$		
Clashscore	158937	4297		
Ramachandran outliers	154571	4023		
Sidechain outliers	154315	3826		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length		Quality of chain							
1	А	364		73%					8%		
1	С	364		72%							
2	В	358			75%			19%	6%		
2	D	358	73%				21%	6%			
3	Е	417	59% 21%			21%	20	%			
4	Ι	213		39%	10%		51%				
4	L	213		42%	8%		50%				
5	J	454	19%	7%		74%					
5	K	454	19%	7%		74%					

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Mol	Chain	Length	Quality of chain						
6	F	3		100%					
6	Н	3	33%	67%					
7	G	9	33%	67%					
8	М	2		100%					



2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 17407 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Gamma-aminobutyric acid receptor subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	А	334	Total 2732	C 1791	N 440	0 485	S 16	0	0
1	С	334	Total 2732	C 1791	N 440	0 485	S 16	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	308	SER	-	linker	UNP P47870
А	309	GLN	-	linker	UNP P47870
А	310	PRO	-	linker	UNP P47870
А	311	ALA	-	linker	UNP P47870
А	312	ARG	-	linker	UNP P47870
А	313	ALA	-	linker	UNP P47870
А	314	ALA	-	linker	UNP P47870
А	315	ALA	-	linker	UNP P47870
С	308	SER	-	linker	UNP P47870
С	309	GLN	-	linker	UNP P47870
С	310	PRO	-	linker	UNP P47870
С	311	ALA	-	linker	UNP P47870
С	312	ARG	-	linker	UNP P47870
С	313	ALA	-	linker	UNP P47870
С	314	ALA	-	linker	UNP P47870
С	315	ALA	-	linker	UNP P47870

There are 16 discrepancies between the modelled and reference sequences:

• Molecule 2 is a protein called Gamma-aminobutyric acid receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	В	338	Total	С	Ν	0	\mathbf{S}	0	0
	550	2730	1763	461	490	16	0	0	
9	Л	338	Total	С	Ν	0	S	0	0
		550	2730	1763	461	490	16	0	U



Chain	Residue	Modelled	Actual	Comment	Reference
В	313	SER	-	linker	UNP P14867
В	314	GLN	-	linker	UNP P14867
В	315	PRO	-	linker	UNP P14867
В	316	ALA	-	linker	UNP P14867
В	317	ARG	-	linker	UNP P14867
В	318	ALA	-	linker	UNP P14867
В	319	ALA	-	linker	UNP P14867
D	313	SER	-	linker	UNP P14867
D	314	GLN	-	linker	UNP P14867
D	315	PRO	-	linker	UNP P14867
D	316	ALA	-	linker	UNP P14867
D	317	ARG	-	linker	UNP P14867
D	318	ALA	-	linker	UNP P14867
D	319	ALA	-	linker	UNP P14867

There are 14 discrepancies between the modelled and reference sequences:

• Molecule 3 is a protein called Gamma-aminobutyric acid type A receptor subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Е	333	Total 2729	C 1781	N 448	0 485	S 15	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Е	323	SER	-	linker	UNP P18507
Е	324	GLN	-	linker	UNP P18507
Е	325	PRO	-	linker	UNP P18507
Е	326	ALA	-	linker	UNP P18507
Е	327	ARG	-	linker	UNP P18507
Е	328	ALA	-	linker	UNP P18507
Е	329	ALA	-	linker	UNP P18507

• Molecule 4 is a protein called Kappa Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	т	105	Total	С	Ν	Ο	S	0	0
4	4 1		802	504	130	163	5	0	U
4	т	106	Total	С	Ν	Ο	S	0	0
4 L	100	811	510	132	164	5	0	U	

• Molecule 5 is a protein called IgG2b Fab Heavy Chain.



Mol	Chain	Residues	Atoms				AltConf	Trace	
5	Т	116	Total	С	Ν	Ο	\mathbf{S}	0	0
5 5	0	110	907	574	151	178	4	0	0
5	V	K 117	Total	С	Ν	Ο	\mathbf{S}	0	0
D K	Γ		914	578	152	180	4	0	0

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



Mol	Chain	Residues	Atoms			AltConf	Trace
6	F	3	Total C 39 22	N 2	O 15	0	0
6	Н	3	Total C 39 22	N 2	O 15	0	0

• Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran ose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy -beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace	
7	G	9	Total 105	C 58	N 2	0 45	0	0

• Molecule 8 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			AltConf	Trace	
8	М	2	Total 28	C 16	N 2	O 10	0	0



• Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
9	А	1	Total C N O 14 8 1 5	0
9	С	1	Total C N O 14 8 1 5	0
9	D	1	Total C N O 14 8 1 5	0

• Molecule 10 is (5S)-6,6-dimethyl-5-[(6R)-8-oxo-6,8-dihydrofuro[3,4-e][1,3]benzodioxol-6-y l]-5,6,7,8-tetrahydro[1,3]dioxolo[4,5-g]isoquinolin-6-ium (three-letter code: J94) (formula: $C_{21}H_{20}NO_6$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				AltConf
10	Δ	1	Total	С	Ν	0	0
10	А	1	28	21	1	6	0
10	C	1	Total	С	Ν	0	0
10	U		28	21	1	6	0

• Molecule 11 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	AltConf
11	Е	1	Total C O 11 6 5	0



3 Residue-property plots (i)

PRO GILN CEU CEU PRO PRO PRO FIR

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. 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. 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: Gamma-aminobutyric acid receptor subunit beta-2

• Molecule 2. Gal	mna-ammoo	atyric acid rec	eptor subunit a	ipna-1	
Chain D:		73%		21%	6%
GLIN PRO SER SER CLU CLU CLU CLU DIO DIO DIO DIO DIO DIO DIO DIO DIO DIO	L23 Y26 L30 L30 R31 P32 G33	K42 T43 D44 145 F50 F50 M57 F50	Υ 60 869 869 869 172 184 188 186 186 186 186	N8/ 194 199 K105	M112 T113 L119 L127
A137 E138 C139 D145 M148 M148 P154 P154 S159	Y169 E170 B171 D184 C185 C185 S186 R187	q204 T207 C208 E209 H216 1223	V227 1228 0229 0229 1237 1237 1237 1238 1238 1238	P253 A254 V257 C258 G259	N203 1265 1265 1265 1266 1266 1275 1275
P278 K279 V280 A281 T284 T284 T284 C293 C293	L301 V307 T311 K320 L324	R347 GLU PRO GLN GLN LEU LEU LVS ALA PRO THR	NJD		
• Molecule 3: Gar	nma-aminob	utyric acid typ	be A receptor su	bunit gan	ıma-2
Chain E:	59%		21%	20%	
TRP SER HIS PHE GLN CLU CLY GLY GLY SER CLY SER	GLY GLY GLY GLY GLY GLY SER SER ALA TRP	HIS PRO GLN PHE CLU CVS CLU CVS CLU CVS CLU CVS CLU	PHE GLN GLY GLY GLN CLYS SER ASP ASP ASP ASP ASP	GLU ASP ALA ALA SER ASN LYS	TRP TRP VAL LEU LEU PRO LYS VAL
CLU 255 225 226 226 226 226 234 24 24 24 24 24 24 24 24 24 24 24 24 24	155 758 758 764 765 867 866	173 173 173 174 174 174 174 174 174 175 174 177 177 177 177 177 177 177 177 177	8100 6104 K105 T111 T111 S116 K117 K117 K118	L131 R132 1133 G137	1140 A149 E150 C151 L155
C165 R176 7181 7181 7181 7183 7183 8183 8188 8188	E189 R197 Q200 F203 L206 L206	2217 2217 0218 0219 0219 N223 N223 N223 N223 N223	2251 2243 2244 2245 1246 1246 1246 1248 1248 1250 1250	2554 2554 N258 K259 K259	4209 1272 1277 1277 1279
1281 8284 8285 8286 8286 1287 91 9291 9291 9291 9291	F308 L311 V312 T316 L317 L317	4327 K330 K330 F343 L357 SER	GLY GLY SER GLY ALA ALA ASN ASN ASN ERR SER LEU LEU LEU	GLN ALA GLY ASP VAL GLU GLU	AND PRO GLY
• Molecule 4: Kap	opa Fab Ligh	t Chain			
Chain I:	39%	10%	51%		
N1 S7 87 822 822 733 731 731 733	Q37 A51 R54 Y55 V58	F62 66 867 867 A68 T69 F71 F71	E81 E81 F86 F92 F105 LYS ARG ARG	ASP ALA ALA PRO THR VAL SER	HLE PRO PRO SER SER GLU GLU
THR SER GLY GLY GLY ALA SER VAL VAL CYS PHE LEU ASN	PHE TYR PRO LYS ASP ILE ASP VAL LYS TRP	LYS LYS ASP ASP GLY SER ASP ASP ASV ASV	VAL VAL LEU ASN SER TRP TRP ASP ASP ASP SER LYS	ASP SER TYR SER MET SER SER	THR THR LEU THR LEU LYS ASP
TYR GLU ARG HIS ASN SER TYR TYR CYS GLU ALA ALA HIS	LYS THR SER THR SER PRO ILE LYS CVAL	PHE ASN ARG ASN CVS			
• Molecule 4: Kap	opa Fab Ligh	t Chain			
Chain L:	42%	8%	50%		_
N 1 V 29 V 33 Q 37 A 3 F 40 F 40 F 46 L 47 L 47	148 148 N53 N53 Y55 V58 V58 N58 N58	F71 B82 L83 A84 Y92 T106	ARG ARG ALA ALA ALA ALA PRO PRO SER SER SER SER	PHE PRO SER SER GLU GLU	LHEU SEER GLY GLY ALA ALA VAL
CYS PHE LEU ASN ASN PHE TYR PRO LYS ASP ASP ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	LYS TRP LYS LYS LLS ASP GLY GLY GLU ARG	ASN GLY VAL VAL LEU ASN SER THR ASP ASP	ASP SER LYS ASP ASP SER THR TTR SER SER SER	THR LLEU LLEU LEU LFYS ASP	TYR GLU ARG ASN SER TYR

• Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-1



CYS GLU HHIS LHRIS LHRIS THR THR THR SER PHC PRO PRO PRO PRO PRO PRO PRO GLU CYS CYS CYS CYS CYS CUL

• Molecule 5: IgG2b Fab Heavy Chain



 \bullet Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

100%



NAG1 NAG2 BMA3

• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:	33%	67%

NAG1 NAG2 BMA3

 $\label{eq:constraint} \bullet \mbox{Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannop$

Chain G:	33%	67%
NAG1 NAG2 BMA3 MAN4 MAN5 MAN5 MAN7 MAN8 MAN9		

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:	100%

NAG1 NAG2



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80103	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	85.05	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor



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, MAN, J94

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	$\mathbf{lengths}$	Bond	angles
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.31	0/2804	0.43	0/3818
1	С	0.30	0/2804	0.44	0/3818
2	В	0.33	0/2799	0.45	0/3805
2	D	0.31	0/2799	0.46	0/3805
3	Е	0.31	0/2805	0.45	0/3822
4	Ι	0.32	0/820	0.47	0/1112
4	L	0.31	0/829	0.46	0/1123
5	J	0.28	0/928	0.46	0/1260
5	Κ	0.27	0/935	0.46	0/1270
All	All	0.31	0/17523	0.45	0/23833

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	А	2732	0	2741	57	0
1	С	2732	0	2741	49	0
2	В	2730	0	2724	59	0
2	D	2730	0	2724	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Е	2729	0	2714	68	0
4	Ι	802	0	771	12	0
4	L	811	0	784	10	0
5	J	907	0	877	19	0
5	K	914	0	884	18	0
6	F	39	0	34	2	0
6	Н	39	0	34	1	0
7	G	105	0	88	10	0
8	М	28	0	25	4	0
9	А	14	0	13	0	0
9	С	14	0	13	0	0
9	D	14	0	13	1	0
10	А	28	0	20	0	0
10	С	28	0	20	1	0
11	Е	11	0	10	1	0
All	All	17407	0	17230	309	0

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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 9.

The worst 5 of 309 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)
2:D:301:LEU:HD23	3:E:250:LEU:HD11	1.57	0.87
1:C:107:HIS:HE2	1:C:131:THR:HG1	1.30	0.79
2:B:238:VAL:HG12	2:B:242:GLN:HE22	1.47	0.79
2:B:156:LYS:HG2	2:B:214:THR:HG23	1.66	0.78
1:A:130:ILE:CG2	2:B:112:MET:HE1	2.14	0.77

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 PDB entries followed by that with respect to all EM entries.

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	Perce	entiles
1	А	332/364~(91%)	321~(97%)	11 (3%)	0	100	100
1	\mathbf{C}	332/364~(91%)	321~(97%)	11 (3%)	0	100	100
2	В	336/358~(94%)	326~(97%)	10 (3%)	0	100	100
2	D	336/358~(94%)	321~(96%)	15~(4%)	0	100	100
3	Ε	331/417~(79%)	314 (95%)	17 (5%)	0	100	100
4	Ι	103/213~(48%)	96~(93%)	7 (7%)	0	100	100
4	L	104/213~(49%)	97~(93%)	7 (7%)	0	100	100
5	J	114/454~(25%)	105~(92%)	9~(8%)	0	100	100
5	Κ	115/454 (25%)	112 (97%)	3 (3%)	0	100	100
All	All	2103/3195~(66%)	2013 (96%)	90 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	А	302/326~(93%)	301 (100%)	1 (0%)	92	96
1	С	302/326~(93%)	301 (100%)	1 (0%)	92	96
2	В	300/319~(94%)	300 (100%)	0	100	100
2	D	300/319~(94%)	299 (100%)	1 (0%)	92	96
3	Ε	305/372~(82%)	305 (100%)	0	100	100
4	Ι	89/188~(47%)	89 (100%)	0	100	100
4	L	90/188~(48%)	90 (100%)	0	100	100
5	J	97/407~(24%)	97~(100%)	0	100	100
5	Κ	98/407~(24%)	98 (100%)	0	100	100
All	All	1883/2852~(66%)	1880 (100%)	3 (0%)	93	97

All (3) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	26	ARG
1	С	26	ARG
2	D	81	MET

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such side chains are listed below:

Mol	Chain	Res	Type
4	L	37	GLN
4	L	38	GLN
5	Κ	39	GLN
1	С	309	GLN
1	С	41	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)

17 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	Mol Type Chair	Chain	\mathbf{Res}	Tink	Bo	ond leng	$_{\rm ths}$	В	ond ang	les		
1VIOI	туре	Unam		nes	ries	nes		Counts	RMSZ	# Z >2	Counts	RMSZ
6	NAG	F	1	1,6	14,14,15	0.23	0	$17,\!19,\!21$	0.68	0		
6	NAG	F	2	6	14,14,15	0.32	0	$17,\!19,\!21$	0.80	0		
6	BMA	F	3	6	11,11,12	0.29	0	$15,\!15,\!17$	0.89	1 (6%)		
7	NAG	G	1	2,7	14,14,15	0.30	0	17,19,21	0.72	0		
7	NAG	G	2	7	14,14,15	0.37	0	$17,\!19,\!21$	0.77	0		
7	BMA	G	3	7	11,11,12	0.28	0	$15,\!15,\!17$	1.25	1 (6%)		



Mal	Type Chain Bes Lin		Tink	Bond lengths			Bond angles			
INIOI	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	G	4	7	11,11,12	0.27	0	$15,\!15,\!17$	0.94	0
7	MAN	G	5	7	11,11,12	0.19	0	$15,\!15,\!17$	0.93	0
7	MAN	G	6	7	11,11,12	0.26	0	$15,\!15,\!17$	0.71	0
7	MAN	G	7	7	11,11,12	0.18	0	$15,\!15,\!17$	0.81	0
7	MAN	G	8	7	11,11,12	0.27	0	$15,\!15,\!17$	1.27	3 (20%)
7	MAN	G	9	7	11,11,12	0.26	0	$15,\!15,\!17$	0.74	0
6	NAG	Н	1	1,6	14,14,15	0.24	0	17,19,21	0.63	0
6	NAG	Н	2	6	14,14,15	0.80	0	17,19,21	1.61	2 (11%)
6	BMA	Н	3	6	11,11,12	0.31	0	$15,\!15,\!17$	0.69	0
8	NAG	М	1	3,8	14,14,15	0.29	0	17,19,21	0.60	0
8	NAG	М	2	8	14,14,15	0.27	0	17,19,21	0.71	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
6	NAG	F	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	BMA	F	3	6	-	2/2/19/22	0/1/1/1
7	NAG	G	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	G	2	7	-	4/6/23/26	0/1/1/1
7	BMA	G	3	7	-	0/2/19/22	0/1/1/1
7	MAN	G	4	7	-	2/2/19/22	0/1/1/1
7	MAN	G	5	7	-	1/2/19/22	0/1/1/1
7	MAN	G	6	7	-	2/2/19/22	0/1/1/1
7	MAN	G	7	7	-	0/2/19/22	0/1/1/1
7	MAN	G	8	7	-	0/2/19/22	0/1/1/1
7	MAN	G	9	7	-	0/2/19/22	0/1/1/1
6	NAG	Н	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	Н	2	6	-	2/6/23/26	0/1/1/1
6	BMA	Н	3	6	-	2/2/19/22	0/1/1/1
8	NAG	М	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	М	2	8	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
6	Н	2	NAG	C4-C3-C2	4.60	117.76	111.02
7	G	3	BMA	O5-C5-C6	3.63	112.89	107.20
7	G	8	MAN	O2-C2-C3	-2.94	104.25	110.14
7	G	8	MAN	C2-C3-C4	-2.36	106.81	110.89
6	Н	2	NAG	C2-N2-C7	-2.28	119.65	122.90

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	3	BMA	O5-C5-C6-O6
6	Н	3	BMA	O5-C5-C6-O6
7	G	6	MAN	O5-C5-C6-O6
6	F	3	BMA	C4-C5-C6-O6
6	Н	3	BMA	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1	NAG	2	0
6	F	2	NAG	1	0
8	М	2	NAG	2	0
7	G	5	MAN	4	0
7	G	2	NAG	1	0
7	G	6	MAN	4	0
6	Н	1	NAG	1	0
7	G	9	MAN	1	0
8	М	1	NAG	2	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)

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).

Mal	Turne	Chain	Dog	Link	B	Bond lengths			Bond angles		
INIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
10	J94	С	405	-	33,33,33	4.19	18 (54%)	48,52,52	1.88	8 (16%)	
9	NAG	D	401	2	14,14,15	0.19	0	17,19,21	0.52	0	
10	J94	А	405	-	33,33,33	4.22	18 (54%)	48,52,52	1.90	8 (16%)	



Mal	Mal Trupa Chain Da		Dec	Tiple	Bond lengths			Bond angles		
WIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	А	404	1	14,14,15	0.27	0	17,19,21	0.48	0
11	MAN	Е	401	-	11,11,12	0.24	0	15,15,17	0.91	0
9	NAG	С	404	1	14,14,15	0.28	0	17,19,21	0.40	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
10	J94	С	405	-	-	3/4/44/44	0/6/6/6
9	NAG	D	401	2	-	1/6/23/26	0/1/1/1
10	J94	А	405	-	-	3/4/44/44	0/6/6/6
9	NAG	А	404	1	-	0/6/23/26	0/1/1/1
11	MAN	Е	401	-	-	1/2/19/22	0/1/1/1
9	NAG	С	404	1	-	2/6/23/26	0/1/1/1

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	А	405	J94	O22-C21	-10.73	1.22	1.38
10	С	405	J94	O22-C21	-10.69	1.23	1.38
10	А	405	J94	O10-C09	-10.11	1.22	1.38
10	А	405	J94	O24-C25	-10.07	1.22	1.38
10	С	405	J94	O10-C09	-10.07	1.22	1.38

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
10	А	405	J94	C16-O17-C18	-7.42	106.67	111.03
10	С	405	J94	C16-O17-C18	-7.23	106.78	111.03
10	С	405	J94	O17-C18-C20	5.58	112.70	108.26
10	А	405	J94	O17-C18-C20	5.52	112.65	108.26
10	А	405	J94	O12-C11-O10	-3.68	102.21	108.08

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	С	404	NAG	O5-C5-C6-O6
9	С	404	NAG	C4-C5-C6-O6

Continued on next page...



Mol	Chain	Res	Type	Atoms
9	D	401	NAG	O5-C5-C6-O6
11	Е	401	MAN	O5-C5-C6-O6
10	А	405	J94	C07-C15-C16-O17

Continued from previous page...

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	С	405	J94	1	0
9	D	401	NAG	1	0
11	Е	401	MAN	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22031. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal surface views (i)

This section was not generated.

6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section was not generated.

