

May 14, 2024 - 10:25 am BST

PDB ID	:	8R54
EMDB ID	:	EMD-18891
Title	:	Mouse teneurin-3 non-compact subunit - A0B0 isoform
Authors	:	Gogou, C.; Meijer, D.H.
Deposited on	:	2023-11-15
Resolution	:	3.50 Å(reported)

This is a Full wwPDB EM 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/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.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
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)	:	2.36.2

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 3.50 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
INIEUTIC	$(\# {\rm Entries})$	$(\# { m Entries})$
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	2391	64%	18%	·	17%			
2	В	2	50%	50%					
2	Е	2	100%						
2	F	2	100%						
2	G	2	100%						
2	Н	2	100%						
2	Ι	2	100%						
2	J	2	100%						
3	С	3	67%		33%				



Mol	Chain	Length	Quality of chain
3	D	3	100%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15900 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	Teneurin-3.
•	monecure	Τ.	no a	protoni	canca	remeanin 0.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	А	1982	Total 15570	C 9813	N 2683	O 2994	S 80	1	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	312	MET	-	initiating methionine	UNP Q9WTS6
А	313	ALA	-	expression tag	UNP Q9WTS6
А	314	ARG	-	expression tag	UNP Q9WTS6
А	315	PRO	-	expression tag	UNP Q9WTS6
А	316	LEU	-	expression tag	UNP Q9WTS6
А	317	CYS	-	expression tag	UNP Q9WTS6
А	318	THR	-	expression tag	UNP Q9WTS6
А	319	LEU	-	expression tag	UNP Q9WTS6
А	320	LEU	-	expression tag	UNP Q9WTS6
А	321	LEU	-	expression tag	UNP Q9WTS6
А	322	LEU	-	expression tag	UNP Q9WTS6
А	323	MET	-	expression tag	UNP Q9WTS6
А	324	ALA	-	expression tag	UNP Q9WTS6
А	325	THR	-	expression tag	UNP Q9WTS6
А	326	LEU	-	expression tag	UNP Q9WTS6
А	327	ALA	-	expression tag	UNP Q9WTS6
А	328	GLY	-	expression tag	UNP Q9WTS6
А	329	ALA	-	expression tag	UNP Q9WTS6
А	330	LEU	-	expression tag	UNP Q9WTS6
А	331	ALA	-	expression tag	UNP Q9WTS6
А	332	GLY	-	expression tag	UNP Q9WTS6
А	333	SER	-	expression tag	UNP Q9WTS6
А	334	HIS	-	expression tag	UNP Q9WTS6
А	335	HIS	-	expression tag	UNP Q9WTS6
А	336	HIS	-	expression tag	UNP Q9WTS6
А	337	HIS	-	expression tag	UNP Q9WTS6
А	338	HIS	-	expression tag	UNP Q9WTS6
А	339	HIS	-	expression tag	UNP Q9WTS6



Chain	Residue	Modelled	Actual	Comment	Reference
А	340	GLY	-	expression tag	UNP Q9WTS6
А	341	SER	-	expression tag	UNP Q9WTS6
А	2316	ILE	THR	conflict	UNP Q9WTS6
А	2700	ALA	-	expression tag	UNP Q9WTS6
А	2701	ALA	-	expression tag	UNP Q9WTS6
А	2702	ALA	-	expression tag	UNP Q9WTS6

• 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	AltConf	Trace	
2	В	2	Total C N O	0	0	
_	2	-	28 16 2 10		Ŭ	
2	E	9	Total C N O	0	0	
	Ľ		28 16 2 10	0	0	
2	F	9	Total C N O	0	0	
		2	28 16 2 10	0		
0	2 G	C 2	2	Total C N O	0	0
		2	28 16 2 10	0	0	
0	Ц	2	Total C N O	0	0	
	11	2	28 16 2 10	0	0	
0	Т	0	Total C N O	0	0	
	1	2	28 16 2 10	0	0	
0	Т	2	Total C N O	0	0	
2	J	J 2	28 16 2 10	0	U	

• Molecule 3 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			
3	С	3	Total	С	Ν	0	0	0		
	5	39	22	2	15	0	0			
2	D	р	Л	2	Total	С	Ν	0	0	0
3 D	5	39	22	2	15	0	U			



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



Mol	Chain	Residues	Atoms	AltConf	
4	Δ	1	Total C N O	0	
4	Л	1	14 8 1 5	0	
4	Δ	1	Total C N O	0	
-1	Л	I	14 8 1 5	0	
4	Δ	٨	1	Total C N O	0
-1	Л	I	14 8 1 5	0	
4	Δ	1	Total C N O	0	
4	А	1	14 8 1 5	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. 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: Teneurin-3



GLU	TYR	VAL	GLY	LYS H1396		L1402 F1403	S1404	A 1 4 07		V1410	51411 V1412		L1416	T1419	E1420	T1421	D1422	E1423 K1424		R1428	11429 1420	01431	V1432	TAAAA	11444 P1445	S1446	K1451	-	q1460	K1470		P14/4	N1506	E1512	-	Q1519	T1523		Y1532	11533 V1534	V1 F A1		S1548
N1549		V1556 T1557	D1558	S1559	L1564	R1565 T1566		R1572 M1573	P1574		V1578 V1578	S1579		01583 V1584	I1585		L1595	K1620		E1623	T1624	07015	L1 <mark>638</mark>	H CAO	74011	V1648	D1656		E1670 D1671	V1672	S1673	116/4	L1678	S16/9 S1680	I1681	D1682	V1688		L1692	K1693	<mark>գ1697</mark>	Y1700	D1701
	R1705	11/06 F1707		S1714	T1718	H1791		P1729 T1730		M1736	11/3/ 1.1738		N1742	G1743 D1744	N1745	L1746	V1747	E1/48 W1749	R1750		L1767	D1790	D1791		70017	S1814	K1815 L1816		N1820 V1821	17OT A	S1824	01828		E1839 K1840	V1841	D1842	R1852		D1856	G1857	K1867	L1873	H1874
S1875		11880	D1884	M1885 W1886	D1887	R1888 1.1889		11892 T1803	00011	M1902	R1912	N1913	I1914	Y1915 N1916		S1923	11924	T1926	D1927		Q1936	R1944	R1945	р1061	R1952	Q1953	T1954 R1955	L1956	S1957	V1966		K1978 T1979		F1982	C1989		R1992	Y2019		N2023	T2037	D2048	_
V2061		12000	12 <mark>070</mark>	S2071 T2072	A2073	V2074 M2075		A2083	12090		12094 F2095		L2098	W2101	12102		12117	K2118 T2119		A2123	10107	Y2128	A2129	Y2130		D2135	V2141	Y2142	L2143 N2144	E2145	K2146	R2150		U2154 L2155		N2158	L2159 H2160	L2161	L2162	P2164	10100	A2168	_
L2173			D2194	T 01 97		E2203	E2206	Y2207	00770	R2215	S2218	K2219		<mark>02244</mark>	A2251		T2260	19774	S2267	S2268	E2269	T2271		M2284	12286	S2287	S2288	N2298		E0074	K2314	42315 12316		1.2319	E2323		L2334 V2335	12336		K2303	E2370	R2374	
P2381		12401 Y2402	12403	T2404 D2405	V2406	N2407 S2408	W2409	L2410	F2424		K2428	W2444	E2445	D2446 V2447	P2448		G2452	V2473		F2489	A2490	T C T C T C	S2494	00704	N2430	N2512	V2513	F2532	EOE40	I2550		P2000	L2559	32566		V2579	T2583	T2584	VAL	ASN	GLY	THR	R2591
R2592		F7005	G2610	M2611 T2612	L2613	R9697		E2636	L2649		K2656	Y2667		S2684	F2690	L2691	R2692	F.2695	ILE	GLY	LYS	ALA	ALA	ALA																			

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

Chain B:

50%

NAG1 NAG2

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

Chain E:

100%

50%

NAG1 NAG2

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

Chain F:

100%

NAG1 NAG2



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

Chain G:

100%

NAG1 NAG2

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

Chain H:

100%

NAG1 NAG2

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

Chain I:	100%	
NAG1 NAG2		
• Molecule 2: opyranose	2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido	o-2-deoxy-beta-D-gluc
Chain J:	100%	
NAG1 NAG2		

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

Chain C:

33%

NAG1 NAG2 BMA3

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

Chain D:

100%

67%





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66637	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 $(6k \ge 4k)$	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: NAG, BMA

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			
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	А	0.34	0/15910	0.53	0/21597		

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	15570	0	15032	266	0
2	В	28	0	25	1	0
2	Е	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	Н	28	0	25	4	0
2	Ι	28	0	25	0	0
2	J	28	0	25	2	0
3	С	39	0	34	0	0
3	D	39	0	34	0	0
4	А	56	0	52	0	0
All	All	15900	0	15327	271	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 9.

All (271) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	$\begin{array}{c c c c c c c c c c c c c c c c c c c $			
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:2447:VAL:HG13	1:A:2448:PRO:HD3	1.69	0.74		
1:A:2119:ILE:HD11	1:A:2304:ALA:HB2	1.70	0.72		
1:A:1880:ILE:HB	1:A:1893:THR:HB	1.71	0.71		
1:A:2123:ALA:HB1	2:H:1:NAG:H61	1.73	0.70		
1:A:1506:ASN:ND2	1:A:1512:GLU:OE2	2.25	0.70		
1:A:706:ALA:H	1:A:709:GLN:HE22	1.39	0.68		
1:A:1234:ASN:O	1:A:1236:ARG:NH1	2.27	0.67		
1:A:1558:ASP:OD1	1:A:1559:SER:N	2.28	0.67		
1:A:1297:ILE:HG23	1:A:1308:VAL:HB	1.77	0.67		
1:A:2164:PRO:HG2	1:A:2167:SER:HB3	1.76	0.67		
1:A:2160:HIS:HA	1:A:2173:LEU:HB2	1.78	0.66		
1:A:1043:ARG:NH2	1:A:1065:ASP:O	2.27	0.65		
1:A:715:ARG:NH2	1:A:738:CYS:O	2.29	0.65		
1:A:769:ARG:HG2	1:A:777:MET:HE2	1.76	0.65		
1:A:1351:ASN:HB3	1:A:1410:VAL:HG11	1.80	0.64		
1:A:1143:PRO:HG3	1:A:1700:TYR:HD2	1.62	0.64		
1:A:2286:ILE:HG22	1:A:2288:SER:H	1.63	0.64		
1:A:1790:ASP:OD1	1:A:1791:ASP:N	2.31	0.64		
1:A:1335:MET:O	1:A:1373:GLN:NE2	2.32	0.63		
1:A:729:CYS:SG	1:A:738:CYS:N	2.72	0.63		
1:A:2583:THR:OG1	1:A:2592:ARG:NH1	2.32	0.63		
1:A:1190:ASP:OD2	1:A:1195:ARG:NH2	2.32	0.62		
1:A:777:MET:SD	1:A:777:MET:N	2.71	0.62		
1:A:1815:LYS:HE3	1:A:2066:ILE:HD11	1.81	0.62		
1:A:1411:SER:OG	1:A:1412:TYR:N	2.32	0.62		
1:A:1548:SER:OG	1:A:1549:ASN:N	2.34	0.61		
1:A:2191:LEU:HD23	1:A:2197:LEU:HA	1.83	0.61		
1:A:1191:PHE:HD1	1:A:1214:ALA:HB2	1.65	0.61		
1:A:1363:ASN:ND2	1:A:1402:LEU:O	2.31	0.61		
1:A:735:GLY:HA2	1:A:740:ILE:HB	1.82	0.61		
1:A:2072:THR:HG22	1:A:2073:ALA:H	1.66	0.60		
1:A:1236:ARG:HB3	1:A:1283:LEU:HD21	1.82	0.60		
2:J:1:NAG:H61	2:J:2:NAG:HN2	1.66	0.60		
1:A:987:GLU:OE2	1:A:2452:GLY:N	2.35	0.60		
1:A:1884:ASP:OD1	1:A:1888:ARG:N	2.28	0.59		
1:A:1701:ASP:N	1:A:1701:ASP:OD1	2.33	0.59		
1:A:2591:ARG:NH2	1:A:2610:GLY:O	2.35	0.59		
1:A:1416:LEU:HB3	1:A:1432:VAL:HB	1.84	0.59		



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1292:ASP:OD1	1:A:1293:LYS:N	2.28	0.58
1:A:2194:ASP:OD1	1:A:2194:ASP:N	2.33	0.58
1:A:702:TRP:HE1	1:A:707:CYS:HA	1.68	0.58
1:A:2167:SER:OG	1:A:2168:ALA:N	2.37	0.58
1:A:709:GLN:N	1:A:709:GLN:OE1	2.36	0.57
1:A:2549:PHE:HE2	1:A:2605:LEU:HD23	1.67	0.57
1:A:2584:THR:O	1:A:2591:ARG:N	2.37	0.57
1:A:1820:ASN:OD1	1:A:1821:VAL:N	2.38	0.57
1:A:1873:LEU:HD11	1:A:2381:PRO:HG3	1.87	0.57
1:A:873:THR:OG1	1:A:875:ASP:OD1	2.23	0.56
1:A:2405:ASP:OD2	1:A:2408:SER:N	2.38	0.56
1:A:1936:GLN:OE1	1:A:1945:ARG:NH1	2.38	0.56
1:A:2260:THR:HG1	1:A:2261:HIS:CE1	2.23	0.56
1:A:2284:MET:HE1	1:A:2334:LEU:HD21	1.85	0.56
1:A:723:LYS:N	1:A:726:LYS:O	2.39	0.56
1:A:2061:VAL:HG22	1:A:2070:ILE:HG12	1.87	0.56
1:A:2636:GLU:HG3	1:A:2690:PHE:HE2	1.71	0.56
1:A:778:GLU:HA	1:A:787:ASN:HB2	1.86	0.56
1:A:853:LEU:HD23	1:A:854:PRO:HD2	1.87	0.56
1:A:1216:ARG:NH2	1:A:1218:TYR:OH	2.35	0.55
1:A:898:ARG:NH2	1:A:904:ASP:OD1	2.39	0.55
1:A:1743:GLY:O	1:A:1744:GLN:NE2	2.40	0.55
1:A:1682:ASP:OD2	1:A:1697:GLN:NE2	2.40	0.55
1:A:1167:ALA:HB1	1:A:1170:ASN:HB2	1.88	0.55
1:A:1718:THR:HG21	1:A:1729:PRO:HB2	1.89	0.55
1:A:2206:GLU:OE2	1:A:2215:ARG:NH1	2.35	0.54
1:A:687:SER:OG	1:A:1671:ASP:OD2	2.18	0.54
1:A:2401:ASP:O	1:A:2403:ILE:HG13	2.06	0.54
1:A:769:ARG:H	1:A:777:MET:HE1	1.72	0.54
1:A:831:GLN:OE1	1:A:1572:ARG:NH2	2.40	0.54
1:A:1824:SER:OG	1:A:1828:GLN:O	2.23	0.54
1:A:1333:THR:OG1	1:A:1334:SER:N	2.40	0.54
1:A:1289:MET:HB3	1:A:1299:PHE:HA	1.90	0.54
1:A:1688:VAL:HG22	1:A:1693:ARG:HG2	1.90	0.54
1:A:1289:MET:HA	1:A:1348:LEU:HD12	1.90	0.54
1:A:817:ASP:OD2	1:A:898:ARG:NH1	2.42	0.53
1:A:1742:ASN:ND2	1:A:2023:ASN:H	2.06	0.53
1:A:1889:LEU:HD21	1:A:1892:ILE:HD11	1.89	0.53
1:A:1018:LEU:HD12	1:A:1101:LEU:HD21	1.90	0.53
1:A:1363:ASN:HD21	1:A:1404:SER:H	1.56	0.53
1:A:1875:SER:OG	1:A:2135:ASP:OD1	2.25	0.53



	has page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1978:LYS:HG3	1:A:1979:THR:HG23	1.90	0.53
2:H:1:NAG:H62	2:H:2:NAG:C7	2.39	0.53
1:A:1523:ILE:HD11	1:A:1532:TYR:HD2	1.72	0.53
1:A:860:ASN:HB3	1:A:863:LEU:HB2	1.91	0.53
1:A:966:ILE:HD11	1:A:1079:VAL:HG21	1.90	0.53
1:A:1166:GLN:NE2	1:A:1168:ASP:OD1	2.42	0.53
1:A:1839:GLU:OE2	1:A:1852:ARG:NH1	2.38	0.53
1:A:2158:ASN:OD1	1:A:2363:ARG:NH2	2.42	0.53
1:A:2532:PHE:HB2	1:A:2550:ILE:HG23	1.91	0.52
1:A:1842:ASP:OD1	1:A:1842:ASP:N	2.42	0.52
1:A:1856:ASP:OD1	1:A:1857:GLY:N	2.42	0.52
1:A:2566:SER:HA	1:A:2579:VAL:HG13	1.91	0.52
1:A:1026:VAL:HG12	1:A:1026:VAL:O	2.10	0.52
1:A:1293:LYS:HE3	1:A:1352:PRO:HA	1.91	0.52
1:A:2403:ILE:HG22	1:A:2404:THR:H	1.75	0.52
1:A:1131:LYS:HE2	1:A:1135:GLU:HB3	1.92	0.51
1:A:1697:GLN:HB2	1:A:1705:ARG:HB3	1.92	0.51
1:A:1041:VAL:HG23	1:A:1041:VAL:O	2.11	0.51
1:A:1095:GLU:OE2	1:A:1097:ARG:NH2	2.44	0.51
1:A:1342:LEU:HG	1:A:1345:PRO:HG3	1.92	0.51
1:A:815:LEU:HG	1:A:896:ILE:HG22	1.93	0.51
1:A:930:TRP:HH2	1:A:1182:ILE:HG22	1.76	0.51
1:A:1566:ILE:HD11	1:A:1574:PRO:HB3	1.92	0.51
1:A:2037:THR:O	1:A:2037:THR:OG1	2.28	0.51
1:A:2691:LEU:HD11	1:A:2695:GLU:HB2	1.93	0.51
1:A:1264:CYS:N	1:A:1283:LEU:O	2.42	0.51
1:A:2319:THR:HG22	1:A:2323:GLU:H	1.75	0.51
1:A:2298:ASN:N	1:A:2298:ASN:OD1	2.44	0.50
1:A:750:ASN:ND2	1:A:773:CYS:O	2.44	0.50
1:A:1154:ARG:HG3	1:A:1171:LYS:HD3	1.92	0.50
1:A:774:ASP:OD1	1:A:774:ASP:N	2.42	0.50
1:A:1642:THR:HG22	1:A:1648:VAL:HG12	1.93	0.50
1:A:1916:ASN:OD1	1:A:1923:SER:OG	2.27	0.50
1:A:2335:VAL:HG23	1:A:2336:ILE:HG12	1.93	0.50
1:A:768:TRP:HZ3	1:A:776:ALA:HA	1.77	0.50
1:A:1027:ILE:HD12	1:A:1027:ILE:H	1.76	0.50
1:A:1444:ILE:HG13	1:A:1445:PRO:HD2	1.94	0.50
1:A:850:THR:O	1:A:895:THR:OG1	2.19	0.49
1:A:859:PHE:HE2	1:A:906:VAL:HG13	1.78	0.49
1:A:719:HIS:HB3	1:A:733:TRP:CE2	2.47	0.49
1:A:2512:ASN:OD1	1:A:2513:VAL:N	2.45	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:1337:ILE:HG13	1:A:1372:ARG:HB2	1.95	0.49
1:A:1367:GLN:OE1	1:A:1375:ARG:NH1	2.44	0.49
1:A:984:ILE:HG23	1:A:1638:LEU:HD23	1.94	0.49
1:A:2129:ALA:HB3	1:A:2142:TYR:HB2	1.95	0.48
1:A:1625:GLY:HA2	1:A:2498:LYS:HD2	1.94	0.48
1:A:988:THR:OG1	1:A:990:VAL:HG23	2.13	0.48
1:A:1372:ARG:O	1:A:1372:ARG:HG3	2.13	0.48
1:A:1407:ALA:O	1:A:1419:THR:OG1	2.29	0.48
1:A:2409:TRP:O	1:A:2410:LEU:HB2	2.14	0.48
1:A:1167:ALA:HB3	1:A:1203:VAL:HB	1.96	0.48
1:A:1262:GLU:OE2	1:A:1263:GLN:N	2.46	0.48
1:A:1334:SER:HB3	1:A:1373:GLN:OE1	2.13	0.48
1:A:1332:ASP:OD1	1:A:1332:ASP:N	2.44	0.48
1:A:884:VAL:HG22	1:A:917:PHE:CD1	2.49	0.48
1:A:755:LEU:HD22	1:A:760:TRP:CZ2	2.49	0.48
1:A:932:PRO:HG2	1:A:935:VAL:HG21	1.95	0.47
1:A:927:HIS:NE2	1:A:942:LEU:HD11	2.28	0.47
1:A:1623:GLU:CD	1:A:1886:TRP:HE1	2.17	0.47
1:A:2409:TRP:HB2	1:A:2410:LEU:HD12	1.97	0.47
1:A:1579:SER:OG	1:A:1583:GLN:O	2.27	0.47
1:A:2612:THR:OG1	1:A:2613:LEU:N	2.46	0.47
1:A:1222:ASP:HB3	1:A:1225:THR:O	2.14	0.47
1:A:2143:LEU:HA	1:A:2143:LEU:HD12	1.76	0.47
1:A:844:LEU:HD22	1:A:850:THR:HG22	1.97	0.47
1:A:1249:ASP:OD2	1:A:1251:THR:OG1	2.31	0.47
1:A:2159:LEU:HD21	1:A:2162:LEU:HD13	1.96	0.47
1:A:2444:TRP:NE1	1:A:2445:GLU:OE2	2.48	0.47
1:A:2656:ARG:O	1:A:2656:ARG:NE	2.36	0.47
1:A:1342:LEU:HD12	1:A:1343:GLU:H	1.79	0.47
1:A:1361:ASP:O	1:A:1364:VAL:HG22	2.15	0.47
1:A:1419:THR:HG22	1:A:1429:ILE:HG12	1.96	0.47
1:A:1673:SER:O	1:A:1674:ILE:HD13	2.15	0.47
1:A:1721:HIS:ND1	1:A:1730:THR:HG21	2.30	0.47
1:A:967:VAL:HG21	1:A:1656:ASP:O	2.16	0.46
1:A:1681:ILE:HA	1:A:1700:TYR:CE1	2.51	0.46
1:A:1705:ARG:HG2	1:A:1707:PHE:CZ	2.50	0.46
1:A:2102:ILE:HG22	1:A:2117:ILE:HG12	1.96	0.46
1:A:1670:GLU:O	1:A:1672:VAL:HG13	2.15	0.46
1:A:1912:ARG:NH1	1:A:1925:ILE:HD12	2.30	0.46
1:A:696:CYS:HB3	1:A:707:CYS:SG	2.56	0.46
1:A:2405:ASP:O	1:A:2407[B]:ASN:N	2.46	0.46



		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:1446:SER:HB3	1:A:1470:LYS:HD2	1.98	0.46		
1:A:2143:LEU:HG	1:A:2144:ASN:H	1.81	0.46		
1:A:1951:ARG:HB2	1:A:1957:SER:HB3	1.98	0.46		
1:A:2667:TYR:CE1	1:A:2692:ARG:HG2	2.51	0.46		
1:A:1249:ASP:H	1:A:1252:LYS:NZ	2.14	0.45		
1:A:1305:ILE:HD11	1:A:1342:LEU:HD23	1.98	0.45		
1:A:1927:ASP:OD2	1:A:1936:GLN:NE2	2.49	0.45		
2:H:1:NAG:H4	2:H:2:NAG:HN2	1.80	0.45		
1:A:2019:TYR:OH	1:A:2251:ALA:O	2.32	0.45		
1:A:743:CYS:HA	1:A:762:CYS:SG	2.57	0.45		
1:A:1678:LEU:HD12	1:A:1679:SER:N	2.31	0.45		
1:A:795:CYS:HA	1:A:800:CYS:SG	2.57	0.45		
1:A:1424:LYS:HD3	1:A:1424:LYS:N	2.31	0.45		
2:H:1:NAG:H4	2:H:2:NAG:N2	2.32	0.45		
1:A:1027:ILE:HD11	1:A:1053:PRO:HA	1.97	0.45		
1:A:1358:TYR:CE2	1:A:1367:GLN:HG3	2.52	0.45		
1:A:1642:THR:O	1:A:1642:THR:OG1	2.34	0.45		
1:A:1966:VAL:HG22	1:A:1982:LEU:HD12	1.99	0.45		
1:A:2549:PHE:CE2	1:A:2605:LEU:HD23	2.49	0.45		
1:A:1816:LEU:HD13	1:A:2083:ALA:O	2.17	0.44		
1:A:1889:LEU:HD12	1:A:1889:LEU:HA	1.73	0.44		
1:A:1090:ASP:OD1	1:A:1090:ASP:N	2.50	0.44		
1:A:2555:PRO:O	1:A:2559:LEU:HD12	2.17	0.44		
1:A:1263:GLN:HG2	1:A:1264:CYS:O	2.18	0.44		
1:A:1428:ARG:HE	1:A:1430:ARG:HD3	1.82	0.44		
1:A:1523:ILE:HD11	1:A:1532:TYR:CD2	2.51	0.44		
1:A:2072:THR:HG22	1:A:2073:ALA:N	2.31	0.44		
1:A:1335:MET:SD	1:A:1335:MET:N	2.91	0.44		
1:A:2203:GLU:HG3	1:A:2218:SER:HB2	1.99	0.44		
1:A:795:CYS:SG	1:A:801:CYS:HB3	2.58	0.44		
1:A:1902:MET:HB3	1:A:2489:PHE:CG	2.53	0.44		
1:A:2219:LYS:H	1:A:2219:LYS:HG2	1.53	0.44		
1:A:1259:GLY:HA2	1:A:1283:LEU:HD22	1.99	0.44		
1:A:703:THR:O	1:A:710:ARG:HA	2.18	0.43		
1:A:2267:SER:OG	1:A:2269:GLU:OE2	2.25	0.43		
1:A:1746:LEU:HB3	1:A:1748:GLU:OE2	2.18	0.43		
1:A:2550:ILE:HD11	1:A:2611:MET:O	2.19	0.43		
1:A:1688:VAL:HA	1:A:1692:LEU:O	2.18	0.43		
1:A:1296:LEU:HD11	1:A:1307:LYS:HD3	2.00	0.43		
1:A:1914:ILE:HD13	1:A:1925:ILE:HG22	2.00	0.43		
1:A:2154:ASP:OD1	1:A:2155:LEU:N	2.43	0.43		



	juo puge	Interatomic	Clash		
Atom-1	Atom-2	distance $(Å)$	overlap (Å)		
1:A:1189:GLY:HA2	1:A:1194:VAL:HG12	2.01	0.43		
1:A:1156:ARG:HB2	1:A:1171:LYS:HB2	2.01	0.43		
1:A:797:ASP:OD2	1:A:799:ASP:HB2	2.19	0.43		
1:A:1034:VAL:HG23	1:A:1049:PHE:HB2	2.01	0.43		
1:A:1380:ARG:HE	1:A:1381:PRO:HD2	1.82	0.43		
1:A:2260:THR:OG1	1:A:2261:HIS:ND1	2.50	0.43		
1:A:1292:ASP:N	1:A:1296:LEU:O	2.38	0.43		
1:A:923:LEU:H	1:A:923:LEU:HD23	1.83	0.42		
1:A:1242:LYS:N	1:A:1253:ASN:OD1	2.51	0.42		
1:A:1301:ASP:OD2	1:A:1306:ARG:NH1	2.52	0.42		
1:A:932:PRO:HB3	1:A:1412:TYR:HD2	1.84	0.42		
1:A:1292:ASP:OD2	1:A:1298:TYR:OH	2.37	0.42		
1:A:2267:SER:HB2	2:B:1:NAG:O6	2.19	0.42		
1:A:865:SER:HB2	1:A:935:VAL:H	1.84	0.42		
1:A:930:TRP:HE1	1:A:1412:TYR:HH	1.65	0.42		
1:A:1271:ARG:HG2	1:A:1273:GLY:H	1.84	0.42		
1:A:2649:LEU:HD12	1:A:2649:LEU:O	2.19	0.42		
1:A:905:LEU:HD23	1:A:905:LEU:HA	1.83	0.42		
1:A:1885:MET:HG2	1:A:1886:TRP:CD2	2.54	0.42		
1:A:2090:ILE:O	1:A:2101:TRP:HA	2.20	0.42		
1:A:2314:LYS:HE2	1:A:2316:ILE:HD11	2.02	0.42		
2:J:1:NAG:H61	2:J:2:NAG:N2	2.33	0.42		
1:A:995:THR:HG23	1:A:1004:LEU:HB2	2.01	0.42		
1:A:1814:SER:O	1:A:1815:LYS:HG3	2.20	0.42		
1:A:2146:LYS:HE2	1:A:2146:LYS:HB3	1.74	0.42		
1:A:2260:THR:HG1	1:A:2261:HIS:CG	2.37	0.42		
1:A:871:VAL:HG12	1:A:942:LEU:HB2	2.02	0.42		
1:A:913:LEU:O	1:A:928:THR:HA	2.20	0.42		
1:A:1027:ILE:HG21	1:A:1031:LEU:HD22	2.01	0.42		
1:A:1156:ARG:HG2	1:A:1157:SER:O	2.20	0.42		
1:A:1303:THR:HG23	1:A:1342:LEU:O	2.19	0.42		
1:A:715:ARG:HG3	1:A:716:CYS:N	2.35	0.42		
1:A:1714:SER:HA	1:A:1736:MET:HA	2.01	0.42		
1:A:2144:ASN:OD1	1:A:2145:GLU:N	2.53	0.42		
1:A:2428:LYS:HE3	1:A:2428:LYS:HB2	1.73	0.42		
1:A:1534:VAL:HG12	1:A:1541:TYR:CD1	2.55	0.41		
1:A:2370:GLU:OE2	1:A:2374:ARG:NH2	2.34	0.41		
1:A:1287:LYS:HZ1	1:A:1344:TRP:HZ3	1.67	0.41		
1:A:1143:PRO:HG3	1:A:1700:TYR:CD2	2.50	0.41		
1:A:1577:VAL:HG23	1:A:1585:ILE:HB	2.02	0.41		
1:A:1299:PHE:CZ	1:A:1306:ARG:HB2	2.56	0.41		



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1359:VAL:HG12	1:A:1366:LEU:HB2	2.02	0.41
1:A:1595:LEU:HD12	1:A:1595:LEU:HA	1.87	0.41
1:A:1841:VAL:HG12	1:A:1852:ARG:HG3	2.01	0.41
1:A:710:ARG:HE	1:A:710:ARG:HB2	1.70	0.41
1:A:1556:VAL:HG22	1:A:1564:LEU:HB3	2.02	0.41
1:A:1953:GLN:HB3	1:A:1955:ARG:HD2	2.03	0.41
1:A:2271:THR:HG23	1:A:2286:ILE:HG12	2.03	0.41
1:A:841:ILE:HD13	1:A:866:VAL:HG23	2.02	0.41
1:A:1421:THR:HB	1:A:1474:PRO:HD2	2.03	0.41
1:A:2094:ILE:HG22	1:A:2095:PHE:CD2	2.56	0.41
1:A:1309:ASP:OD1	1:A:1313:ILE:HB	2.22	0.40
1:A:1423:GLU:C	1:A:1424:LYS:HD3	2.41	0.40
1:A:768:TRP:HB3	1:A:773:CYS:HB2	2.04	0.40
1:A:865:SER:OG	1:A:931:ILE:HD12	2.21	0.40
1:A:1624:THR:HG21	1:A:2491:THR:OG1	2.20	0.40
1:A:2127:LYS:HG3	1:A:2144:ASN:HA	2.04	0.40
1:A:2130:TYR:HD1	1:A:2141:VAL:HG22	1.85	0.40
1:A:1249:ASP:HB3	1:A:1252:LYS:HZ2	1.87	0.40
1:A:1304:MET:H	1:A:1304:MET:HG2	1.74	0.40
1:A:1460:GLN:HE22	1:A:1470:LYS:NZ	2.19	0.40
1:A:2098:LEU:HD12	1:A:2098:LEU:HA	1.80	0.40
1:A:919:ARG:HA	1:A:919:ARG:HD2	1.88	0.40
1:A:1742:ASN:OD1	1:A:2023:ASN:ND2	2.54	0.40
1:A:788:GLU:HG2	1:A:790:ASP:CG	2.41	0.40
1:A:997:ILE:HG22	1:A:1585:ILE:HD13	2.03	0.40
1:A:1357:ILE:HB	1:A:1368:ILE:HB	2.02	0.40
1:A:1373:GLN:OE1	1:A:1374:VAL:N	2.55	0.40
1:A:2405:ASP:O	1:A:2407[A]:ASN:N	2.46	0.40

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	Percen	tiles
1	А	1969/2391~(82%)	1794 (91%)	174 (9%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	2473	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 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	Analysed Rotameric Outliers		Percentiles	
1	А	1695/2060~(82%)	1640~(97%)	55 (3%)	39	69

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	691	CYS
1	А	692	MET
1	А	724	ASP
1	А	777	MET
1	А	889	TYR
1	А	926	TYR
1	А	939	MET
1	А	940	ASP
1	А	982	SER
1	А	1048	TRP
1	А	1074	LEU
1	А	1086	GLU
1	А	1090	ASP
1	А	1091	LEU
1	А	1097	ARG
1	А	1142	GLN
1	A	1168	ASP
1	А	1227	ASP
1	A	1234	ASN
1	А	1264	CYS



Mol	Chain	Res	Type
1	А	1271	ARG
1	А	1289	MET
1	А	1298	TYR
1	А	1311	ASN
1	А	1321	ASN
1	А	1335	MET
1	А	1354	ASP
1	А	1451	LYS
1	А	1519	GLN
1	А	1572	ARG
1	А	1620	LYS
1	А	1671	ASP
1	А	1738	LEU
1	А	1750	ARG
1	А	1767	LEU
1	А	1802	ASP
1	А	1815	LYS
1	А	1816	LEU
1	А	1867	LYS
1	А	1888	ARG
1	А	1944	ARG
1	А	1989	CYS
1	А	1992	ARG
1	А	2048	ASP
1	А	2075	MET
1	А	2131	GLU
1	А	2150	ARG
1	А	2194	ASP
1	А	2208	SER
1	А	2244	GLN
1	А	2424	PHE
1	А	2494	SER
1	A	2498	LYS
1	А	2627	ARG
1	А	2684	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	1742	ASN
1	А	2023	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)

20 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	Tuno	Chain	Dog	Link	Bo	ond leng	ths	B	ond ang	les
	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	В	1	2,1	14,14,15	0.24	0	17,19,21	0.54	0
2	NAG	В	2	2	14,14,15	0.18	0	17,19,21	0.36	0
3	NAG	С	1	1,3	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	С	2	3	14,14,15	0.17	0	17,19,21	0.43	0
3	BMA	С	3	3	11,11,12	0.59	0	15,15,17	0.89	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.45	0	17,19,21	0.51	0
3	NAG	D	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	BMA	D	3	3	11,11,12	0.60	0	15,15,17	0.72	0
2	NAG	Е	1	2,1	14,14,15	0.29	0	17,19,21	0.43	0
2	NAG	Е	2	2	14,14,15	0.28	0	17,19,21	0.38	0
2	NAG	F	1	2,1	14,14,15	0.47	0	17,19,21	0.38	0
2	NAG	F	2	2	14,14,15	0.23	0	17,19,21	0.49	0
2	NAG	G	1	2,1	14,14,15	0.17	0	17,19,21	0.57	0
2	NAG	G	2	2	14,14,15	0.25	0	17,19,21	0.40	0
2	NAG	Н	1	2,1	14,14,15	0.33	0	17,19,21	0.52	0
2	NAG	Н	2	2	14,14,15	0.50	0	17,19,21	0.58	0
2	NAG	Ι	1	2,1	14,14,15	0.38	0	17,19,21	0.47	0
2	NAG	Ι	2	2	14,14,15	0.23	0	17,19,21	0.46	0
2	NAG	J	1	2,1	14,14,15	0.20	0	17,19,21	0.60	0
2	NAG	J	2	2	14,14,15	0.24	0	17,19,21	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	В	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	В	2	2	-	2/6/23/26	0/1/1/1
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
3	BMA	С	3	3	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	_	0/2/19/22	0/1/1/1
2	NAG	Е	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Е	2	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Н	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Н	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Ι	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	Ι	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1

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.

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	С	3	BMA	O2-C2-C3	-2.06	106.01	110.14

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	В	2	NAG	C4-C5-C6-O6
2	Н	1	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6



Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	Е	1	NAG	C4-C5-C6-O6
3	С	2	NAG	O5-C5-C6-O6
2	Е	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	Ι	2	NAG	C8-C7-N2-C2
2	Ι	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	С	2	NAG	C4-C5-C6-O6
2	Н	2	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	В	2	NAG	O5-C5-C6-O6
2	Н	1	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	Ι	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	J	1	NAG	C3-C2-N2-C7
3	С	3	BMA	O5-C5-C6-O6
2	Е	2	NAG	C4-C5-C6-O6
2	Н	2	NAG	C4-C5-C6-O6
2	В	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C3-C2-N2-C7
2	F	2	NAG	C1-C2-N2-C7

Continued from previous page...

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	2	NAG	2	0
2	В	1	NAG	1	0
2	Н	1	NAG	4	0
2	Н	2	NAG	3	0
2	J	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)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	А	2804	1	14,14,15	0.27	0	17,19,21	0.35	0
4	NAG	А	2803	1	14,14,15	0.49	0	17,19,21	0.39	0
4	NAG	А	2801	1	14,14,15	0.29	0	17,19,21	0.40	0
4	NAG	А	2802	1	14,14,15	0.20	0	17,19,21	0.50	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
4	NAG	А	2804	1	-	3/6/23/26	0/1/1/1
4	NAG	А	2803	1	-	2/6/23/26	0/1/1/1
4	NAG	А	2801	1	-	1/6/23/26	0/1/1/1
4	NAG	А	2802	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	2803	NAG	O5-C5-C6-O6
4	А	2803	NAG	C4-C5-C6-O6
4	А	2804	NAG	C8-C7-N2-C2
4	А	2804	NAG	O7-C7-N2-C2
4	А	2801	NAG	O5-C5-C6-O6
4	А	2804	NAG	O5-C5-C6-O6
4	А	2802	NAG	O5-C5-C6-O6



There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-18891. 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 standard-deviation projections (False-color) (i)

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

6.6 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.

