

Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 08:15 AM EDT

PDB ID	:	5KN0
Title	:	Native bovine skeletal calsequestrin, low-Ca2+ form
Authors	:	Lewis, K.M.; Byrd, S.; Kang, C.
Deposited on	:	2016-06-27
Resolution	:	2.73 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

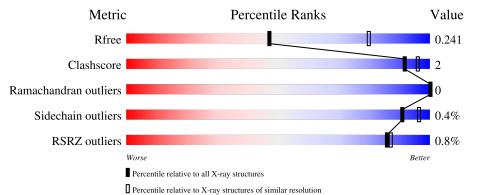
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.73 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3359(2.74-2.70)
Clashscore	141614	$3686\ (2.74-2.70)$
Ramachandran outliers	138981	3622(2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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

Mol	Chain	Length	Quality of chain					
1	А	361	.% 89% 6%	·				
1	В	361	89% 6%	•				
1	С	361	94% ·	•				
1	D	361	93% ·	•				
2	Е	2	100%					



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Mol	Chain	Length	Quality of chain
3	F	3	100%



5KN0

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 22000 atoms, of which 10601 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.

Mol	Chain	Residues		Atoms						AltConf	Trace
1	1 A 346	246	Total	С	Η	Ν	0	\mathbf{S}	0	0	0
	A	340	5362	1782	2575	416	583	6	0		
1	В	346	Total	С	Н	Ν	0	S	0	0	0
	D	340	5400	1790	2601	418	585	6			
1	С	345	Total	С	Н	Ν	0	S	0	0	0
		343	5370	1782	2587	417	578	6	0		0
1	П	346	Total	С	Н	Ν	0	S	0	0	0
	D	340	5416	1793	2613	419	585	6	0	0	0

• Molecule 1 is a protein called Calsequestrin.

• 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	Е	2	Total 53	C 16	Н 25	N 2	O 10	0	0	0

• 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.

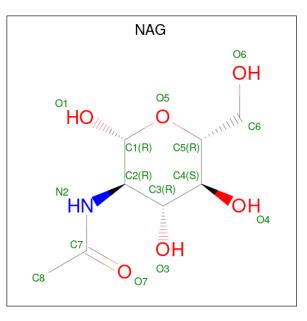


Mol	Chain	Residues		At	\mathbf{oms}			ZeroOcc	AltConf	Trace
3	F	3	Total 73	C 22	Н 34	N 2	0 15	0	0	0

• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:



 $C_8H_{15}NO_6$).



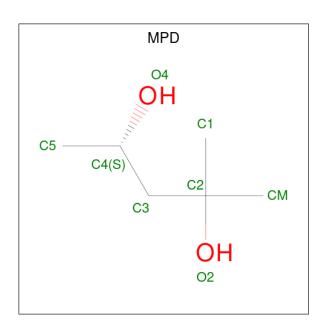
Mo	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	Δ	1	Total	С	Η	Ν	Ο	0	0
4	Л	L	27	8	13	1	5		0
4	C	1	Total	С	Η	Ν	Ο	0	0
4			27	8	13	1	5		0

• Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	5	Total Ca 5 5	0	0
5	В	5	Total Ca 5 5	0	0
5	С	5	Total Ca 5 5	0	0
5	D	4	Total Ca 4 4	0	0

• Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	Total C H O 22 6 14 2	0	0
6	А	1	Total C H O 22 6 14 2	0	0
6	В	1	Total C H O 22 6 14 2	0	0
6	В	1	Total C H O 22 6 14 2	0	0
6	В	1	Total C H O 22 6 14 2	0	0
6	С	1	Total C H O 22 6 14 2	0	0
6	С	1	Total C H O 22 6 14 2	0	0
6	С	1	Total C H O 22 6 14 2	0	0
6	D	1	Total C H O 22 6 14 2	0	0
6	D	1	Total C H O 22 6 14 2	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	6	Total O 6 6	0	0
7	В	10	Total O 10 10	0	0



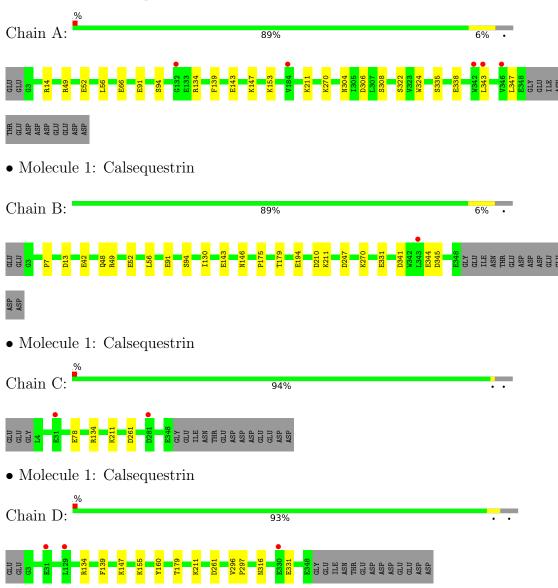
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	С	8	Total O 8 8	0	0
7	D	9	Total O 9 9	0	0



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: Calsequestrin

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





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 F:

100%

NAG1 NAG2 BMA3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	60.34Å 92.99Å 101.85Å	Depositor
a, b, c, α , β , γ	71.12° 84.57° 73.48°	Depositor
Resolution (Å)	49.66 - 2.73	Depositor
Resolution (A)	49.66 - 2.73	EDS
% Data completeness	98.3 (49.66-2.73)	Depositor
(in resolution range)	91.8(49.66-2.73)	EDS
R _{merge}	0.03	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.09 (at 2.73 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
D D.	0.196 , 0.240	Depositor
R, R_{free}	0.197 , 0.241	DCC
R_{free} test set	2000 reflections $(3.81%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	59.3	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36 , 38.2	EDS
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22000	wwPDB-VP
Average B, all atoms $(Å^2)$	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MPD, CA, 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).

Mol	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.31	0/2852	0.46	0/3881	
1	В	0.31	0/2864	0.45	0/3894	
1	С	0.31	0/2848	0.45	0/3874	
1	D	0.31	0/2868	0.46	0/3898	
All	All	0.31	0/11432	0.46	0/15547	

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	2787	2575	2582	12	1
1	В	2799	2601	2607	18	0
1	С	2783	2587	2593	4	0
1	D	2803	2613	2618	7	0
2	Е	28	25	25	0	0
3	F	39	34	34	0	0
4	А	14	13	13	0	0
4	С	14	13	13	0	0
5	А	5	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	В	5	0	0	0	0
5	С	5	0	0	0	0
5	D	4	0	0	0	0
6	А	16	28	28	0	0
6	В	24	42	42	1	0
6	С	24	42	42	1	0
6	D	16	28	28	1	0
7	А	6	0	0	0	0
7	В	10	0	0	6	0
7	С	8	0	0	1	0
7	D	9	0	0	0	0
All	All	11399	10601	10625	35	1

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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 2.

All (35) 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)
1:B:344:GLU:N	7:B:602:HOH:O	2.19	0.76
1:A:322:SER:OG	1:A:324:TRP:NE1	2.18	0.75
1:B:210:ASP:OD1	7:B:601:HOH:O	2.08	0.71
1:B:7:PRO:HB2	6:B:509:MPD:H53	1.78	0.66
1:C:134:ARG:NH2	1:D:261:ASP:OD2	2.30	0.65
1:D:316:ASN:HB2	6:D:509:MPD:HM2	1.79	0.65
1:B:247:ASP:N	7:B:603:HOH:O	2.22	0.60
1:C:261:ASP:CG	1:D:134:ARG:HH21	2.07	0.58
1:B:49:ARG:NH2	1:B:52:GLU:OE1	2.37	0.57
1:A:139:PHE:O	1:A:147:LYS:NZ	2.37	0.56
1:B:143:GLU:OE1	1:B:270:LYS:NZ	2.36	0.54
1:B:130:ILE:HB	1:B:179:THR:HG22	1.91	0.52
1:A:52:GLU:OE2	1:B:52:GLU:OE2	2.30	0.50
1:A:134:ARG:NH2	1:B:331:GLU:O	2.45	0.49
6:C:509:MPD:O4	6:C:509:MPD:H12	2.11	0.49
1:C:134:ARG:NH1	1:D:331:GLU:O	2.45	0.49
1:A:49:ARG:NH2	1:B:13:ASP:OD1	2.40	0.48
1:A:91:GLU:O	1:A:94:SER:OG	2.32	0.47
1:A:343:LEU:O	1:A:347:LEU:HD13	2.15	0.47
1:A:335:SER:OG	1:A:338:GLU:OE1	2.23	0.47
1:C:78:GLU:HB2	7:C:601:HOH:O	2.16	0.45
1:A:306:ASP:OD2	1:A:308:SER:OG	2.33	0.45



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:155:LYS:HG3	1:D:160:TYR:CE2	2.52	0.45
1:D:139:PHE:O	1:D:147:LYS:NZ	2.47	0.44
1:B:194:GLU:HG3	1:B:211:LYS:HD3	2.00	0.44
1:B:345:ASP:N	7:B:602:HOH:O	2.42	0.43
1:A:14:ARG:NE	1:A:66:GLU:OE1	2.47	0.43
1:B:344:GLU:HB2	7:B:602:HOH:O	2.19	0.42
1:B:42:GLU:O	1:B:48:GLN:NE2	2.52	0.42
1:B:341:ASP:C	7:B:602:HOH:O	2.58	0.41
1:A:143:GLU:OE1	1:A:270:LYS:NZ	2.40	0.41
1:A:56:LEU:HD12	1:B:56:LEU:HD12	2.03	0.41
1:B:91:GLU:O	1:B:94:SER:OG	2.39	0.41
1:B:146:ASN:O	1:B:175:PRO:HD2	2.21	0.40
1:D:296:VAL:HB	1:D:297:PRO:HD3	2.03	0.40

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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	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LYS:NZ	1:A:322:SER:O[1_455]	2.12	0.08

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	Percer	ntiles
1	А	344/361~(95%)	336~(98%)	8 (2%)	0	100	100
1	В	344/361~(95%)	337~(98%)	7(2%)	0	100	100
1	\mathbf{C}	343/361~(95%)	333~(97%)	10 (3%)	0	100	100
1	D	344/361~(95%)	338~(98%)	6(2%)	0	100	100
All	All	1375/1444~(95%)	1344 (98%)	31 (2%)	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 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 Outlier		Outliers	Percer		ntiles	
1	А	303/323~(94%)	301~(99%)	2(1%)		84	93	
1	В	306/323~(95%)	306 (100%)	0		100	100	
1	С	303/323~(94%)	302 (100%)	1 (0%)		92	97	
1	D	307/323~(95%)	305~(99%)	2(1%)		84	93	
All	All	1219/1292~(94%)	1214 (100%)	5~(0%)		91	96	

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	211	LYS
1	А	304	ASN
1	С	211	LYS
1	D	179	THR
1	D	211	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

5 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	ol Type Chain Res Link		Bo	Bond lengths			Bond angles			
Mol	Type	Chain	nes	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	NAG	Е	1	2,1	14,14,15	0.25	0	17,19,21	0.43	0
2	NAG	Е	2	2	14,14,15	0.18	0	17,19,21	0.54	0
3	NAG	F	1	3,1	14,14,15	0.36	0	17,19,21	0.47	0
3	NAG	F	2	3	14,14,15	0.27	0	17,19,21	0.45	0
3	BMA	F	3	3	11,11,12	0.65	0	$15,\!15,\!17$	0.68	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
2	NAG	Ε	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	Е	2	2	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

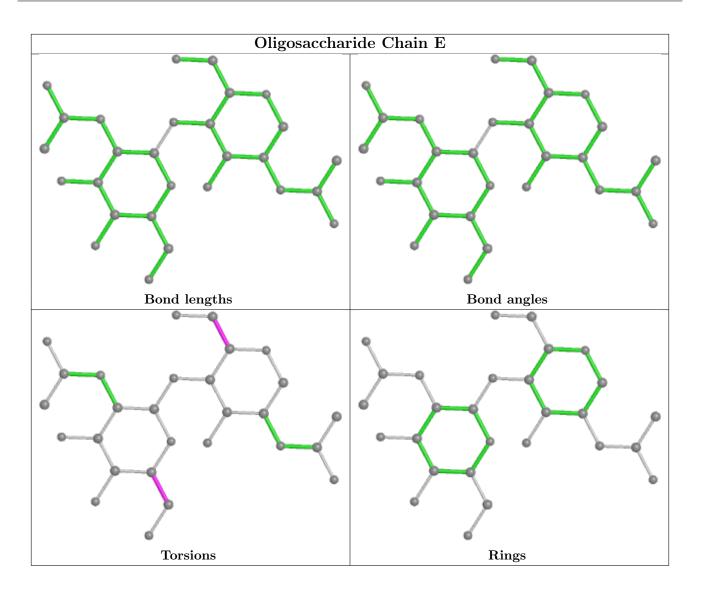
Mol	Chain	Res	Type	Atoms
2	Е	2	NAG	O5-C5-C6-O6
2	Е	2	NAG	C4-C5-C6-O6
2	Е	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6

There are no ring outliers.

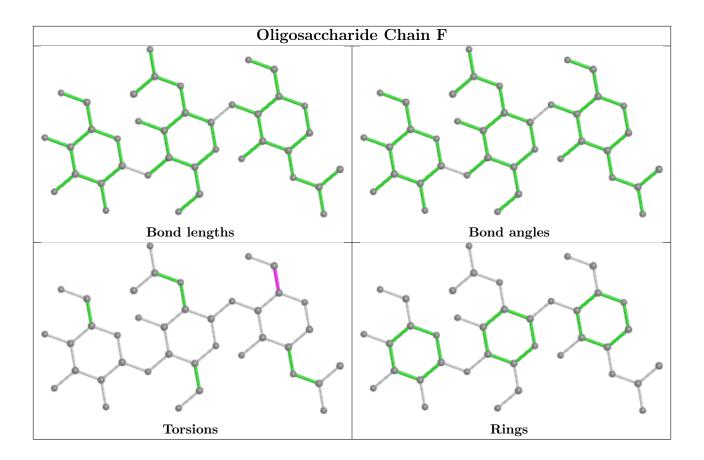
No monomer is involved in short contacts.

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)

Of 31 ligands modelled in this entry, 19 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Turne	Chain	Res	Link	Bo	ond leng	ths	Bond angles		
10101	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
4	NAG	С	501	1	$14,\!14,\!15$	0.32	0	17,19,21	0.45	0
6	MPD	В	508	-	7,7,7	0.28	0	9,10,10	0.28	0
6	MPD	В	509	-	7,7,7	0.63	0	9,10,10	0.77	0
6	MPD	С	508	-	7,7,7	0.44	0	9,10,10	0.41	0
6	MPD	С	507	-	7,7,7	0.35	0	9,10,10	0.25	0
6	MPD	В	510	-	7,7,7	0.44	0	9,10,10	0.44	0
4	NAG	А	501	1	14,14,15	0.46	0	17,19,21	0.46	0
6	MPD	D	508	-	7,7,7	0.38	0	9,10,10	0.36	0
6	MPD	С	509	-	7,7,7	0.45	0	9,10,10	0.20	0
6	MPD	А	508	-	7,7,7	0.33	0	9,10,10	0.31	0



Mol	Turne	Chain	Res	Link	Bo	ond leng	\mathbf{ths}	Bond angles		
IVIOI	ol Type Chain Res	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2		
6	MPD	А	507	-	7,7,7	0.46	0	$9,\!10,\!10$	0.69	0
6	MPD	D	509	-	7,7,7	0.30	0	$9,\!10,\!10$	0.39	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	С	501	1	-	0/6/23/26	0/1/1/1
6	MPD	В	508	-	-	0/5/5/5	-
6	MPD	В	509	-	-	2/5/5/5	-
6	MPD	С	508	-	-	0/5/5/5	-
6	MPD	С	507	-	-	2/5/5/5	-
6	MPD	В	510	-	-	2/5/5/5	-
4	NAG	А	501	1	-	0/6/23/26	0/1/1/1
6	MPD	D	508	-	-	2/5/5/5	-
6	MPD	С	509	-	-	2/5/5/5	-
6	MPD	А	508	-	-	1/5/5/5	-
6	MPD	А	507	-	-	1/5/5/5	-
6	MPD	D	509	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	В	509	MPD	C1-C2-C3-C4
6	В	509	MPD	O2-C2-C3-C4
6	D	508	MPD	C2-C3-C4-C5
6	С	507	MPD	C2-C3-C4-O4
6	А	507	MPD	CM-C2-C3-C4
6	В	510	MPD	C1-C2-C3-C4
6	В	510	MPD	O2-C2-C3-C4
6	С	507	MPD	C2-C3-C4-C5
6	С	509	MPD	C2-C3-C4-C5
6	А	508	MPD	C2-C3-C4-O4
6	С	509	MPD	C2-C3-C4-O4
6	D	508	MPD	C2-C3-C4-O4



There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	В	509	MPD	1	0
6	С	509	MPD	1	0
6	D	509	MPD	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	$\langle RSRZ \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	А	346/361~(95%)	-0.01	5 (1%) 75 77	47, 75, 120, 144	0
1	В	346/361~(95%)	-0.15	1 (0%) 94 95	45, 70, 106, 146	0
1	С	345/361~(95%)	-0.09	2 (0%) 89 90	47, 73, 108, 148	0
1	D	346/361~(95%)	-0.05	3 (0%) 84 85	47, 74, 107, 140	0
All	All	1383/1444~(95%)	-0.08	11 (0%) 86 87	45, 73, 110, 148	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	184	VAL	4.8
1	D	330	GLU	4.1
1	А	342	TRP	3.6
1	С	281	ASP	3.1
1	А	346	VAL	2.8
1	D	129	LEU	2.8
1	С	31	GLU	2.4
1	D	31	GLU	2.3
1	А	132	GLY	2.1
1	В	343	LEU	2.0
1	А	343	LEU	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)

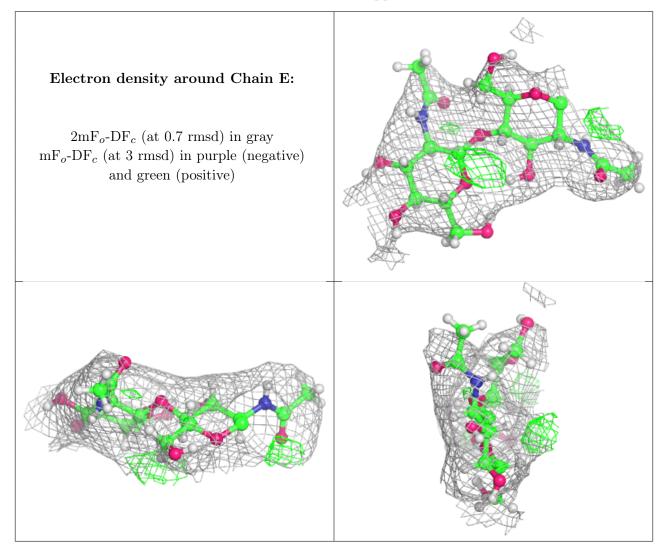
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



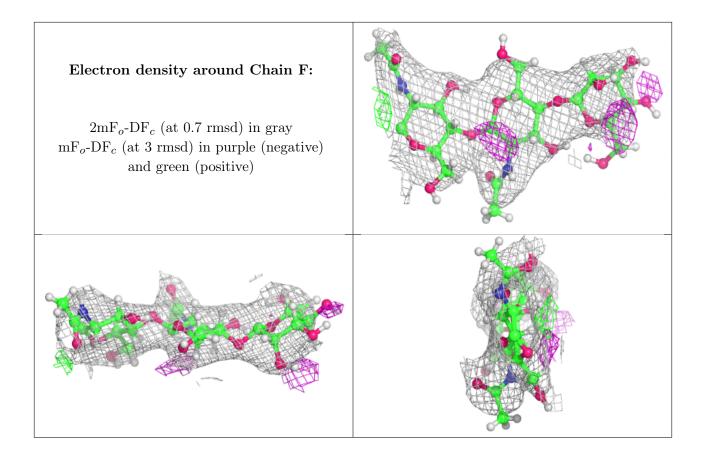
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q<0.9
3	BMA	F	3	11/12	0.81	0.31	$109,\!125,\!150,\!151$	0
3	NAG	F	1	14/15	0.88	0.14	100,131,158,160	0
2	NAG	Е	2	14/15	0.89	0.17	105,121,146,149	0
2	NAG	Е	1	14/15	0.90	0.13	74,107,137,141	0
3	NAG	F	2	14/15	0.91	0.18	108,135,162,176	0

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.







6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
5	CA	D	504	1/1	0.71	0.08	93,93,93,93	0
5	CA	В	503	1/1	0.77	0.14	89,89,89,89	0
5	CA	А	505	1/1	0.79	0.06	92,92,92,92	0
5	CA	С	504	1/1	0.80	0.17	92,92,92,92	0
5	CA	С	505	1/1	0.81	0.09	80,80,80,80	0
5	CA	С	502	1/1	0.81	0.07	$98,\!98,\!98,\!98$	0
5	CA	В	505	1/1	0.83	0.09	99,99,99,99	0
5	CA	D	505	1/1	0.84	0.10	88,88,88,88	0
5	CA	А	503	1/1	0.86	0.07	91,91,91,91	0
4	NAG	С	501	14/15	0.87	0.14	75,106,131,133	0
5	CA	А	504	1/1	0.87	0.35	117,117,117,117	0
6	MPD	D	509	8/8	0.88	0.35	141,185,196,196	0
4	NAG	А	501	14/15	0.89	0.13	78,92,108,111	0
5	CA	D	506	1/1	0.90	0.13	93,93,93,93	0



Continued from previous page								
Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	\mathbf{RSR}	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q < 0.9
6	MPD	С	507	8/8	0.90	0.24	76,91,103,109	0
5	CA	С	506	1/1	0.90	0.20	93,93,93,93	0
5	CA	А	506	1/1	0.91	0.12	90,90,90,90	0
6	MPD	А	508	8/8	0.91	0.24	146,182,197,197	0
6	MPD	В	509	8/8	0.92	0.25	58,82,99,99	0
5	CA	В	507	1/1	0.93	0.19	104,104,104,104	0
6	MPD	В	508	8/8	0.94	0.25	82,98,110,110	0
6	MPD	D	508	8/8	0.95	0.20	63,75,82,89	0
5	CA	А	502	1/1	0.95	0.07	91,91,91,91	0
6	MPD	В	510	8/8	0.96	0.26	66,81,93,93	0
6	MPD	С	509	8/8	0.96	0.24	62,76,92,92	0
6	MPD	А	507	8/8	0.97	0.28	81,97,106,106	0
5	CA	В	504	1/1	0.97	0.07	85,85,85,85	0
5	CA	В	506	1/1	0.97	0.18	80,80,80,80	0
5	CA	С	503	1/1	0.98	0.05	90,90,90,90	0
5	CA	D	507	1/1	0.98	0.12	86,86,86,86	0
6	MPD	С	508	8/8	0.98	0.23	50,64,77,80	0

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6.5 Other polymers (i)

There are no such residues in this entry.

