



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2021 – 04:10 PM GMT

PDB ID : 7B8I
Title : Tetragonal structure of human protein kinase CK2 catalytic subunit in complex with a heparin oligo saccharide
Authors : Niefind, K.; Schnitzler, A.
Deposited on : 2020-12-12
Resolution : 2.55 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.16
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) : 2.16

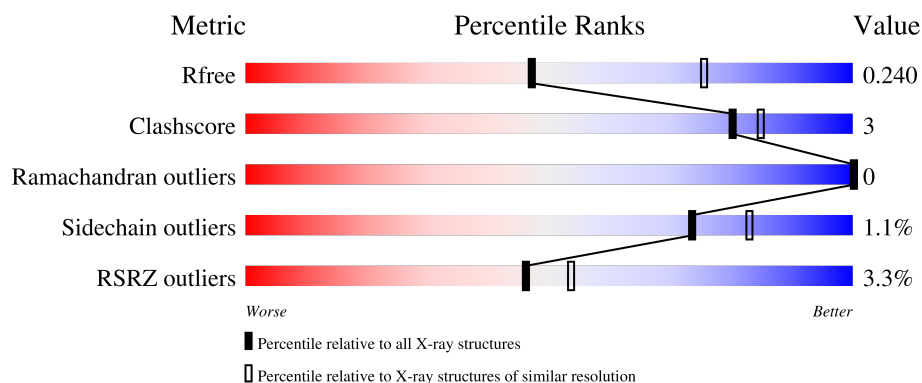
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

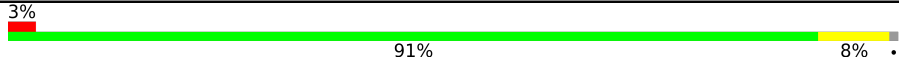
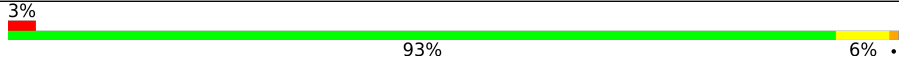

The reported resolution of this entry is 2.55 Å.

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 $\leq 5\%$. 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	335	
1	B	335	
2	C	8	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IDS	C	1	-	-	-	X
2	SGN	C	8	-	-	-	X
3	GOL	A	401	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5924 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.

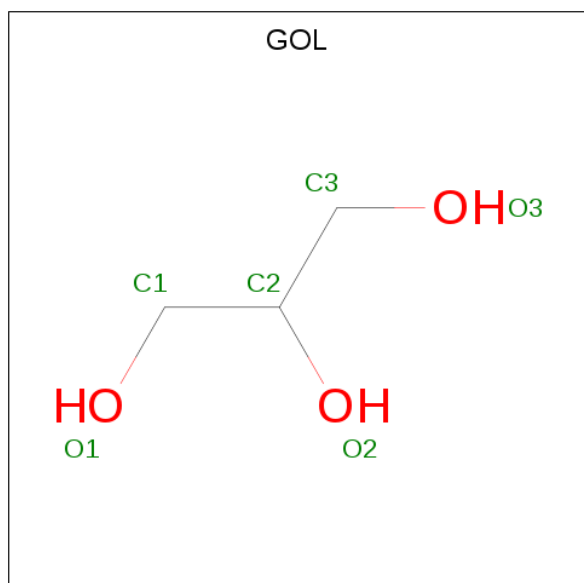
- Molecule 1 is a protein called Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2804	1795	495	503	11			
1	B	332	Total	C	N	O	S	0	1	0
			2815	1801	499	504	11			

- Molecule 2 is an oligosaccharide called 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	S	0	0	0
			141	48	4	77	12			

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



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

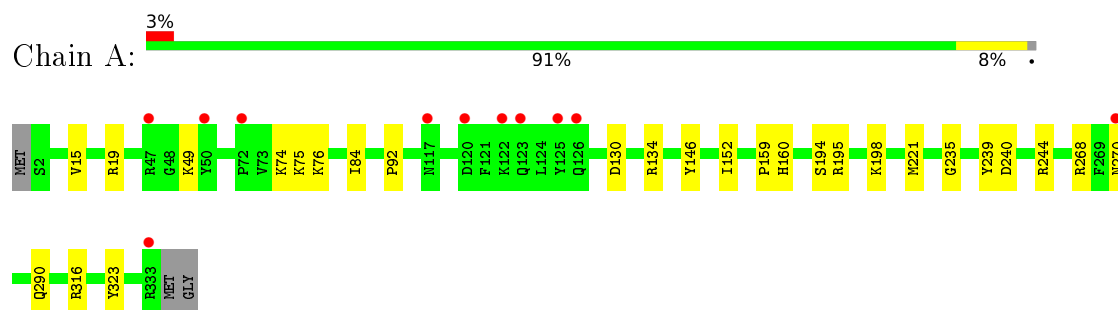
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	71	Total	O	0	0
			71	71		
5	B	72	Total	O	0	0
			72	72		

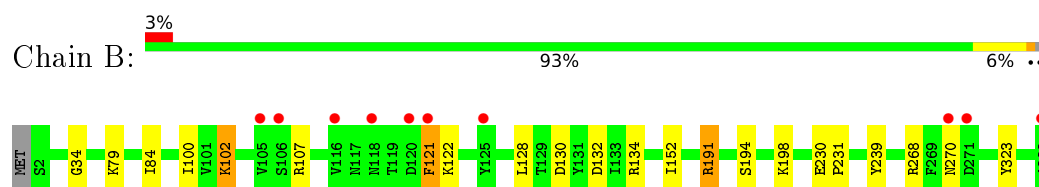
3 Residue-property plots [i](#)

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: Casein kinase II subunit alpha



- Molecule 1: Casein kinase II subunit alpha



- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.40Å 128.40Å 124.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.40 – 2.55 45.40 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.40-2.55) 98.5 (45.40-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.204 , 0.240 0.204 , 0.240	Depositor DCC
R_{free} test set	1696 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5924	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4783e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, IDS, SGN

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	A	0.24	0/2879	0.40	0/3893
1	B	0.24	0/2890	0.40	0/3907
All	All	0.24	0/5769	0.40	0/7800

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

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	2804	0	2748	17	0
1	B	2815	0	2760	13	0
2	C	141	0	50	3	0
3	A	6	0	8	1	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
5	A	71	0	0	1	0
5	B	72	0	0	0	0
All	All	5924	0	5566	31	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 3.

All (31) 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:121:PHE:HE1	1:B:128:LEU:HD11	1.66	0.61
1:A:75:LYS:HG2	2:C:4:SGN:H61	1.87	0.56
1:B:84:ILE:HG23	1:B:152:ILE:HD13	1.88	0.55
1:A:49:LYS:HD2	1:A:49:LYS:H	1.71	0.55
1:B:134:ARG:HG2	1:B:323:TYR:CZ	2.43	0.54
1:A:134:ARG:HG2	1:A:323:TYR:CZ	2.43	0.53
1:A:84:ILE:HG23	1:A:152:ILE:HD13	1.89	0.52
1:A:146:TYR:HD1	3:A:401:GOL:H2	1.74	0.52
1:B:128:LEU:HD22	1:B:132:ASP:HB3	1.93	0.51
1:A:316:ARG:NH2	5:A:503:HOH:O	2.43	0.51
1:A:74:LYS:HD3	1:A:76:LYS:HE2	1.93	0.50
1:B:194:SER:O	1:B:198:LYS:HG3	2.13	0.48
1:B:130:ASP:O	1:B:134:ARG:HG3	2.14	0.48
2:C:7:IDS:H4	2:C:8:SGN:H3	1.97	0.47
1:A:130:ASP:O	1:A:134:ARG:HG3	2.15	0.46
1:A:159:PRO:HD3	1:A:221:MET:HG2	1.96	0.45
1:B:79:LYS:NZ	2:C:6:SGN:H61	2.31	0.45
1:B:34:GLY:N	1:B:100:ILE:O	2.44	0.45
1:A:134:ARG:HD3	1:A:323:TYR:O	2.17	0.45
1:A:194:SER:O	1:A:198:LYS:HG3	2.16	0.45
1:B:102:LYS:HE2	1:B:107:ARG:CZ	2.49	0.42
1:B:230:GLU:HA	1:B:231:PRO:HA	1.91	0.42
1:A:49:LYS:N	1:A:49:LYS:HD2	2.34	0.42
1:A:240:ASP:O	1:A:244:ARG:HG2	2.19	0.42
1:A:239:TYR:CZ	1:A:268:ARG:HD3	2.55	0.42
1:A:92:PRO:HD2	1:A:146:TYR:CG	2.54	0.42
1:A:195:ARG:NH1	1:A:235:GLY:O	2.53	0.41
1:B:191:ARG:HA	1:B:191:ARG:HD2	1.52	0.41
1:B:239:TYR:CZ	1:B:268:ARG:HD3	2.55	0.41
1:B:122:LYS:HE2	1:B:122:LYS:HB3	1.75	0.40
1:A:15:VAL:O	1:A:19:ARG:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	330/335 (98%)	319 (97%)	11 (3%)	0	100	100
1	B	331/335 (99%)	319 (96%)	12 (4%)	0	100	100
All	All	661/670 (99%)	638 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/307 (99%)	302 (99%)	3 (1%)	76	84
1	B	306/307 (100%)	302 (99%)	4 (1%)	69	80
All	All	611/614 (100%)	604 (99%)	7 (1%)	73	83

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

Mol	Chain	Res	Type
1	A	160	HIS
1	A	270	ASN
1	A	290	GLN
1	B	102	LYS
1	B	121	PHE
1	B	191	ARG
1	B	270	ASN

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

8 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	IDS	C	1	2	14,17,17	1.41	1 (7%)	17,26,26	0.76	0
2	SGN	C	2	2	18,19,20	4.59	2 (11%)	22,29,31	1.61	4 (18%)
2	IDS	C	3	2	13,16,17	1.54	2 (15%)	15,24,26	0.73	0
2	SGN	C	4	2	18,19,20	4.70	2 (11%)	22,29,31	1.34	2 (9%)
2	IDS	C	5	2	13,16,17	1.09	2 (15%)	15,24,26	0.82	1 (6%)
2	SGN	C	6	2	18,19,20	1.33	1 (5%)	22,29,31	1.25	2 (9%)
2	IDS	C	7	2	13,16,17	1.55	2 (15%)	15,24,26	0.73	0
2	SGN	C	8	2	18,19,20	4.58	4 (22%)	22,29,31	1.93	2 (9%)

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	IDS	C	1	2	-	0/5/29/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SGN	C	2	2	-	6/11/28/31	0/1/1/1
2	IDS	C	3	2	-	0/5/26/29	0/1/1/1
2	SGN	C	4	2	-	3/11/28/31	0/1/1/1
2	IDS	C	5	2	-	0/5/26/29	0/1/1/1
2	SGN	C	6	2	-	3/11/28/31	0/1/1/1
2	IDS	C	7	2	-	0/5/26/29	0/1/1/1
2	SGN	C	8	2	-	3/11/28/31	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	SGN	O1S-S1	19.19	1.64	1.42
2	C	2	SGN	O1S-S1	19.15	1.63	1.42
2	C	8	SGN	O2S-S1	18.80	1.63	1.42
2	C	1	IDS	O1S-S	4.38	1.64	1.45
2	C	7	IDS	O2S-S	4.38	1.64	1.45
2	C	6	SGN	O5S-S2	4.37	1.64	1.45
2	C	4	SGN	O5S-S2	4.37	1.63	1.45
2	C	3	IDS	O2S-S	4.36	1.63	1.45
2	C	3	IDS	O2-C2	-2.85	1.42	1.47
2	C	5	IDS	O2-C2	-2.84	1.42	1.47
2	C	7	IDS	O2-C2	-2.83	1.43	1.47
2	C	8	SGN	C1-C2	2.67	1.56	1.52
2	C	8	SGN	O6S-S2	2.21	1.64	1.50
2	C	5	IDS	O3S-S	2.21	1.64	1.50
2	C	2	SGN	O6S-S2	2.20	1.63	1.50
2	C	8	SGN	O5-C1	2.10	1.47	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	8	SGN	C1-O5-C5	7.49	122.34	112.19
2	C	4	SGN	O2S-S1-O1S	-4.55	109.40	120.16
2	C	6	SGN	O2S-S1-O1S	-4.54	109.42	120.16
2	C	2	SGN	O2S-S1-O1S	-4.33	109.92	120.16
2	C	8	SGN	O2S-S1-O1S	-4.30	110.00	120.16
2	C	2	SGN	C1-O5-C5	3.40	116.79	112.19
2	C	4	SGN	O5-C1-C2	-3.15	106.32	111.29
2	C	2	SGN	O5-C1-C2	-3.01	106.54	111.29
2	C	5	IDS	O2-C2-C3	2.34	110.22	106.95
2	C	2	SGN	O4-C4-C3	-2.28	105.09	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	SGN	C1-O5-C5	2.11	115.05	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

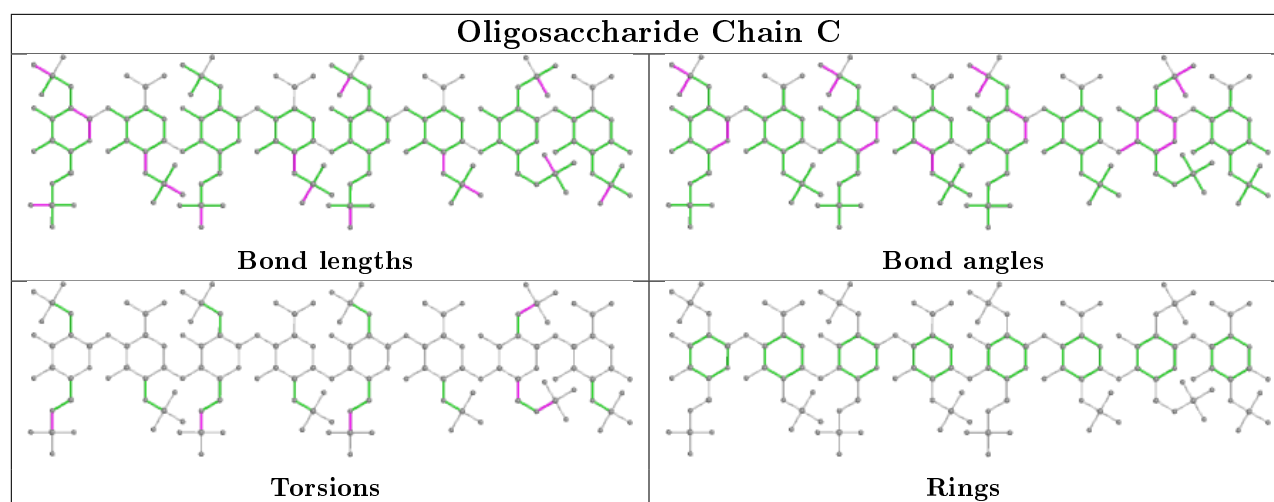
Mol	Chain	Res	Type	Atoms
2	C	2	SGN	C4-C5-C6-O6
2	C	2	SGN	C2-N2-S1-O2S
2	C	4	SGN	C6-O6-S2-O5S
2	C	6	SGN	C6-O6-S2-O5S
2	C	8	SGN	C6-O6-S2-O5S
2	C	2	SGN	C6-O6-S2-O4S
2	C	2	SGN	C6-O6-S2-O5S
2	C	2	SGN	O5-C5-C6-O6
2	C	4	SGN	C6-O6-S2-O6S
2	C	6	SGN	C6-O6-S2-O6S
2	C	2	SGN	C6-O6-S2-O6S
2	C	8	SGN	C6-O6-S2-O4S
2	C	4	SGN	C6-O6-S2-O4S
2	C	6	SGN	C6-O6-S2-O4S
2	C	8	SGN	C6-O6-S2-O6S

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	8	SGN	1	0
2	C	4	SGN	1	0
2	C	7	IDS	1	0
2	C	6	SGN	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 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	SO4	A	402	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	401	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	A	403	-	4,4,4	0.14	0	6,6,6	0.05	0
3	GOL	A	401	-	5,5,5	0.90	0	5,5,5	0.96	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	GOL	C1-C2-C3-O3
3	A	401	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	GOL	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

6.1 Protein, DNA and RNA chains

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, 95th 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>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	332/335 (99%)	0.01	11 (3%) 46 53	34, 50, 99, 143	0
1	B	332/335 (99%)	0.02	11 (3%) 46 53	33, 50, 100, 161	0
All	All	664/670 (99%)	0.02	22 (3%) 46 53	33, 50, 100, 161	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	121	PHE	5.0
1	A	117	ASN	4.4
1	A	50	TYR	3.9
1	B	125	TYR	3.9
1	A	122	LYS	3.6
1	A	125	TYR	3.4
1	B	120	ASP	3.3
1	A	123	GLN	3.1
1	B	333	ARG	3.1
1	B	270	ASN	3.0
1	B	106	SER	2.9
1	A	120	ASP	2.9
1	A	333	ARG	2.8
1	B	116	VAL	2.7
1	A	72	PRO	2.6
1	B	332	ALA	2.6
1	B	271	ASP	2.6
1	B	105	VAL	2.4
1	A	126	GLN	2.3
1	A	270	ASN	2.2
1	A	47	ARG	2.1
1	B	118	ASN	2.0

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

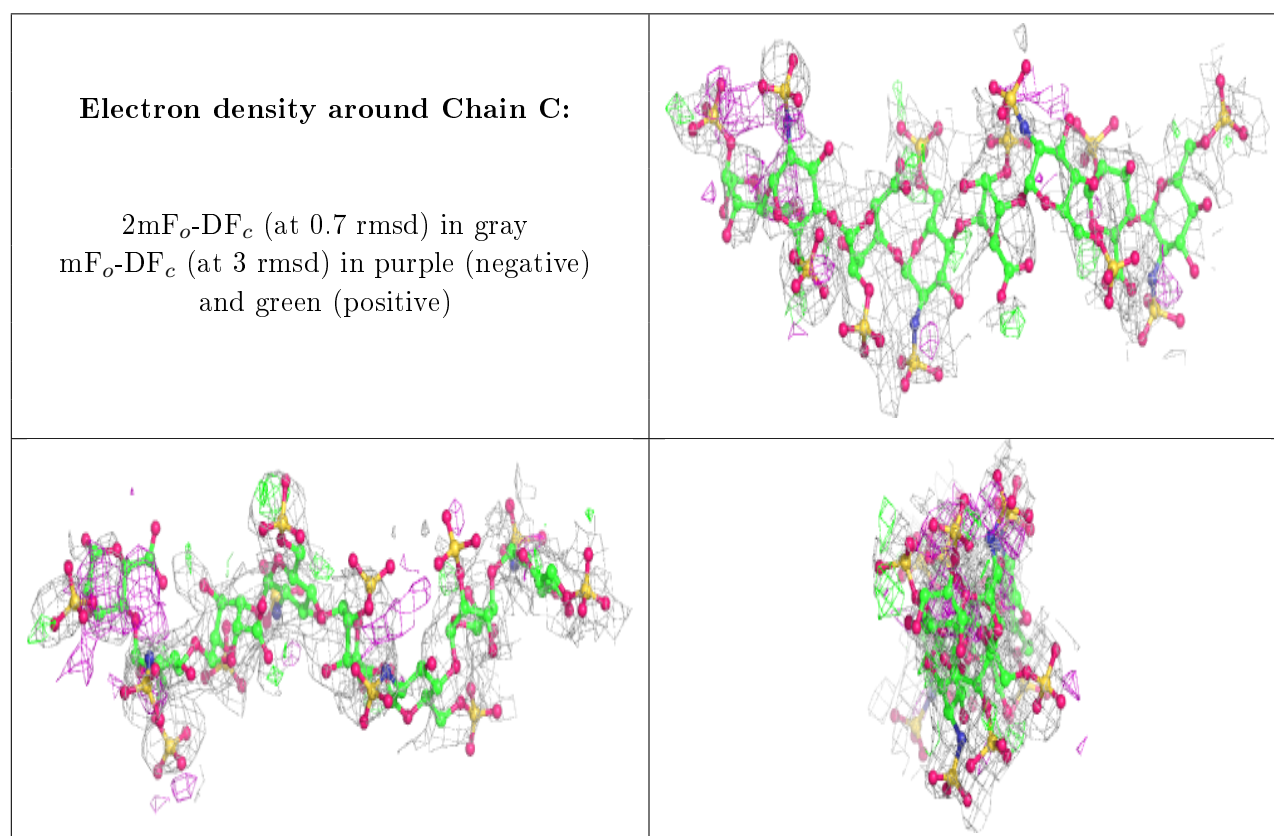
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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, 95th 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(Å ²)	Q<0.9
2	SGN	C	8	19/20	0.08	0.46	194,205,214,215	0
2	IDS	C	1	17/17	0.56	0.49	134,143,153,153	0
2	IDS	C	7	16/17	0.57	0.29	199,203,216,216	0
2	SGN	C	6	19/20	0.58	0.35	202,205,209,209	0
2	IDS	C	5	16/17	0.63	0.30	189,195,203,204	0
2	SGN	C	4	19/20	0.68	0.27	157,167,172,180	0
2	IDS	C	3	16/17	0.77	0.19	157,160,170,170	0
2	SGN	C	2	19/20	0.77	0.24	127,134,145,152	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, 95th 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(Å ²)	Q<0.9
3	GOL	A	401	6/6	0.76	0.49	65,66,67,67	0
4	SO4	A	403	5/5	0.87	0.23	110,112,112,114	0
4	SO4	A	402	5/5	0.96	0.16	63,70,73,76	0
4	SO4	B	401	5/5	0.97	0.15	60,65,68,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.