



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2021 – 02:10 PM JST

PDB ID : 6KI0
Title : Crystal Structure of Human ASC-CARD
Authors : Xu, Z.H.; Jin, T.C.
Deposited on : 2019-07-16
Resolution : 2.00 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

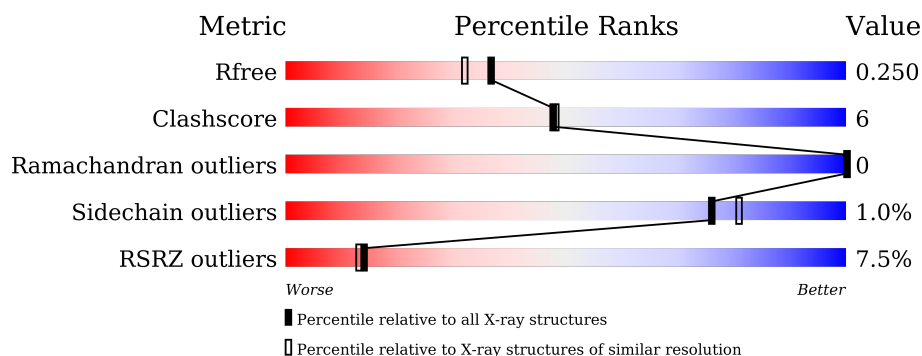
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	466	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 90%; height: 10px; background-color: green;"></div> <div style="width: 9%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> <div style="width: 14%; height: 10px; background-color: red;"></div> <div style="width: 81%; height: 10px; background-color: green;"></div> <div style="width: 17%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>
1	B	466	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 81%; height: 10px; background-color: green;"></div> <div style="width: 17%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>
2	C	3	<div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> </div>
2	D	3	<div> <div style="width: 100%; height: 10px; background-color: orange;"></div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7479 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 Maltose/maltodextrin-binding periplasmic protein, Apoptosis-associated speck-like protein containing a CARD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3568	2296	588	676	8			
1	B	458	Total	C	N	O	S	0	0	0
			3559	2291	587	673	8			

There are 58 discrepancies between the modelled and reference sequences:

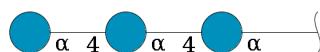
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP P0AEX9
A	82	ALA	ASP	engineered mutation	UNP P0AEX9
A	83	ALA	LYS	engineered mutation	UNP P0AEX9
A	172	ALA	GLU	engineered mutation	UNP P0AEX9
A	173	ALA	ASN	engineered mutation	UNP P0AEX9
A	239	ALA	LYS	engineered mutation	UNP P0AEX9
A	359	ALA	-	linker	UNP P0AEX9
A	360	ALA	-	linker	UNP P0AEX9
A	361	LEU	-	linker	UNP P0AEX9
A	362	ALA	-	linker	UNP P0AEX9
A	363	ALA	-	linker	UNP P0AEX9
A	364	ALA	-	linker	UNP P0AEX9
A	365	GLN	-	linker	UNP P0AEX9
A	366	THR	-	linker	UNP P0AEX9
A	367	ASN	-	linker	UNP P0AEX9
A	368	ALA	-	linker	UNP P0AEX9
A	369	VAL	-	linker	UNP P0AEX9
A	370	ASP	-	linker	UNP P0AEX9
A	455	ALA	-	expression tag	UNP Q9ULZ3
A	456	ALA	-	expression tag	UNP Q9ULZ3
A	457	ALA	-	expression tag	UNP Q9ULZ3
A	458	LEU	-	expression tag	UNP Q9ULZ3
A	459	GLU	-	expression tag	UNP Q9ULZ3
A	460	HIS	-	expression tag	UNP Q9ULZ3

Continued on next page...

Continued from previous page...

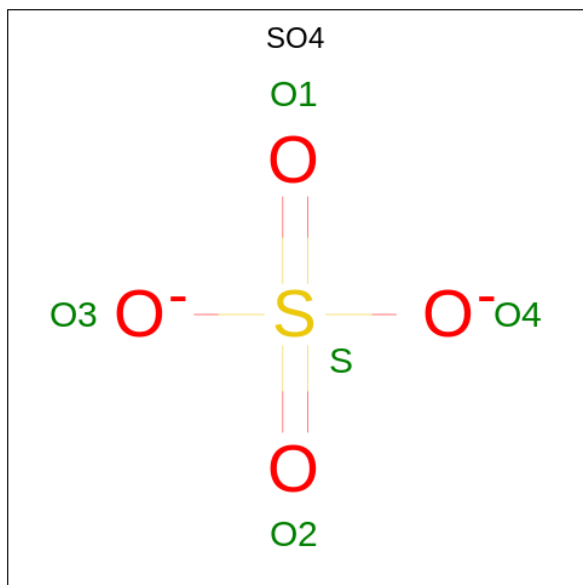
Chain	Residue	Modelled	Actual	Comment	Reference
A	461	HIS	-	expression tag	UNP Q9ULZ3
A	462	HIS	-	expression tag	UNP Q9ULZ3
A	463	HIS	-	expression tag	UNP Q9ULZ3
A	464	HIS	-	expression tag	UNP Q9ULZ3
A	465	HIS	-	expression tag	UNP Q9ULZ3
B	0	MET	-	expression tag	UNP P0AEX9
B	82	ALA	ASP	engineered mutation	UNP P0AEX9
B	83	ALA	LYS	engineered mutation	UNP P0AEX9
B	172	ALA	GLU	engineered mutation	UNP P0AEX9
B	173	ALA	ASN	engineered mutation	UNP P0AEX9
B	239	ALA	LYS	engineered mutation	UNP P0AEX9
B	359	ALA	-	linker	UNP P0AEX9
B	360	ALA	-	linker	UNP P0AEX9
B	361	LEU	-	linker	UNP P0AEX9
B	362	ALA	-	linker	UNP P0AEX9
B	363	ALA	-	linker	UNP P0AEX9
B	364	ALA	-	linker	UNP P0AEX9
B	365	GLN	-	linker	UNP P0AEX9
B	366	THR	-	linker	UNP P0AEX9
B	367	ASN	-	linker	UNP P0AEX9
B	368	ALA	-	linker	UNP P0AEX9
B	369	VAL	-	linker	UNP P0AEX9
B	370	ASP	-	linker	UNP P0AEX9
B	455	ALA	-	expression tag	UNP Q9ULZ3
B	456	ALA	-	expression tag	UNP Q9ULZ3
B	457	ALA	-	expression tag	UNP Q9ULZ3
B	458	LEU	-	expression tag	UNP Q9ULZ3
B	459	GLU	-	expression tag	UNP Q9ULZ3
B	460	HIS	-	expression tag	UNP Q9ULZ3
B	461	HIS	-	expression tag	UNP Q9ULZ3
B	462	HIS	-	expression tag	UNP Q9ULZ3
B	463	HIS	-	expression tag	UNP Q9ULZ3
B	464	HIS	-	expression tag	UNP Q9ULZ3
B	465	HIS	-	expression tag	UNP Q9ULZ3

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	0	0
			34	18	16			
2	D	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

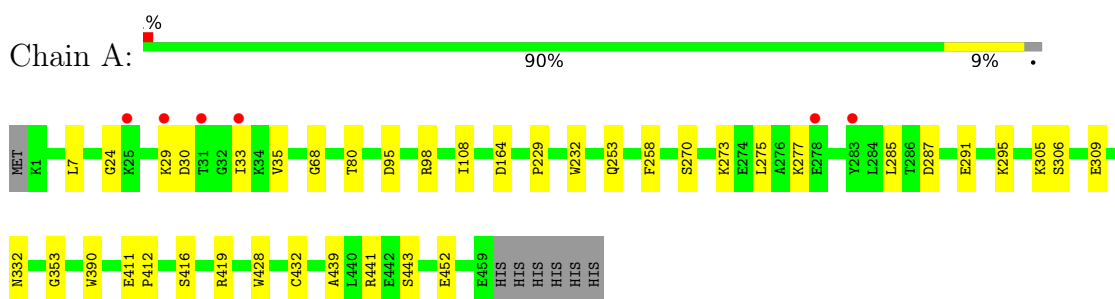
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	208	Total	O	0	0
			208	208		
4	B	61	Total	O	0	0
			61	61		

3 Residue-property plots

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: Maltose/maltodextrin-binding periplasmic protein, Apoptosis-associated speck-like protein containing a CARD



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:  100%

GLC1
GLC2
GLC3

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.76Å 56.02Å 146.93Å 90.00° 106.58° 90.00°	Depositor
Resolution (Å)	47.12 – 2.00 47.12 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.12-2.00) 99.1 (47.12-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.220 , 0.252 0.222 , 0.250	Depositor DCC
R_{free} test set	4616 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7479	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

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

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	0.43	0/3654	0.53	0/4970
1	B	0.41	0/3645	0.57	0/4958
All	All	0.42	0/7299	0.55	0/9928

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	3568	0	3536	28	0
1	B	3559	0	3530	58	0
2	C	34	0	30	0	0
2	D	34	0	29	10	0
3	A	10	0	0	1	0
3	B	5	0	0	0	0
4	A	208	0	0	2	0
4	B	61	0	0	2	0
All	All	7479	0	7125	88	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 6.

All (88) 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:27:PHE:CE1	1:B:283:TYR:HD2	1.70	1.09
1:B:27:PHE:HE1	1:B:283:TYR:CD2	1.71	1.07
1:B:272:ASN:HA	1:B:275:LEU:HD13	1.40	1.01
1:B:340:TRP:HB3	2:D:1:GLC:O3	1.67	0.95
1:A:275:LEU:HD12	4:A:782:HOH:O	1.74	0.87
1:B:27:PHE:HE1	1:B:283:TYR:HD2	0.89	0.86
1:B:27:PHE:CE1	1:B:283:TYR:CD2	2.55	0.85
1:B:66:ARG:NH1	2:D:1:GLC:H61	1.93	0.84
1:A:33:ILE:HD13	1:A:275:LEU:HD23	1.58	0.83
1:B:7:LEU:HB2	1:B:35:VAL:HG12	1.70	0.74
1:B:340:TRP:CB	2:D:1:GLC:O3	2.36	0.73
1:B:349:ASN:OD1	1:B:354:ARG:NH1	2.22	0.72
1:B:290:LEU:HD13	1:B:302:VAL:HG11	1.73	0.71
1:B:204:MET:HG3	4:B:640:HOH:O	1.91	0.70
2:D:2:GLC:H4	2:D:3:GLC:O6	1.93	0.69
1:A:33:ILE:CD1	1:A:275:LEU:HD23	2.24	0.68
1:B:108:ILE:HG13	1:B:285:LEU:HD21	1.80	0.64
1:B:73:SER:HB3	1:B:458:LEU:HD13	1.80	0.64
1:A:390:TRP:CE3	1:A:443:SER:HB3	2.34	0.62
1:A:95:ASP:OD1	1:A:98:ARG:NH1	2.33	0.62
1:B:7:LEU:CB	1:B:35:VAL:HG12	2.30	0.60
1:A:7:LEU:HB2	1:A:35:VAL:HG12	1.84	0.60
1:B:59:ILE:HD11	1:B:276:ALA:HB1	1.85	0.57
1:B:80:THR:H	1:B:277:LYS:HZ1	1.51	0.57
1:B:27:PHE:O	1:B:33:ILE:O	2.23	0.57
1:A:287:ASP:OD1	1:A:306:SER:OG	2.22	0.56
1:A:275:LEU:CD1	4:A:782:HOH:O	2.39	0.55
1:B:66:ARG:HD2	2:D:1:GLC:O6	2.05	0.55
1:B:63:ALA:HB2	2:D:3:GLC:H62	1.87	0.55
1:B:35:VAL:O	1:B:35:VAL:HG23	2.07	0.54
1:A:108:ILE:HD12	1:A:285:LEU:HD21	1.89	0.54
1:B:261:VAL:HG23	1:B:329:ILE:HD11	1.90	0.54
1:B:66:ARG:HH11	2:D:1:GLC:H61	1.73	0.54
1:B:8:VAL:HG22	1:B:36:THR:HB	1.91	0.53
1:B:274:GLU:HA	1:B:274:GLU:OE1	2.09	0.53
1:A:305:LYS:O	1:A:309:GLU:HG3	2.09	0.53
1:B:7:LEU:O	1:B:35:VAL:HA	2.09	0.53
1:B:29:LYS:HD3	1:B:30:ASP:OD1	2.09	0.52
1:A:390:TRP:HZ3	1:A:439:ALA:O	1.92	0.52
2:D:2:GLC:H62	2:D:3:GLC:O6	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ASP:OD1	1:A:253:GLN:NE2	2.43	0.51
1:B:155:TYR:HB2	2:D:2:GLC:C3	2.41	0.51
1:A:24:GLY:HA3	1:A:35:VAL:HG21	1.92	0.50
1:B:115:LEU:HD11	1:B:224:MET:HE2	1.93	0.50
1:B:293:VAL:HG12	1:B:299:LEU:HD21	1.94	0.50
1:B:272:ASN:HB3	1:B:275:LEU:HB2	1.94	0.49
1:B:235:ILE:HA	1:B:238:SER:HB3	1.94	0.49
1:B:85:PHE:HA	1:B:88:LYS:HE3	1.94	0.49
1:B:117:TYR:CE2	1:B:119:LYS:HG2	2.48	0.48
1:B:179:LYS:HE2	4:B:659:HOH:O	2.13	0.48
1:A:24:GLY:HA3	1:A:35:VAL:CG2	2.44	0.48
1:A:68:GLY:HA3	1:A:332:ASN:O	2.13	0.48
1:A:80:THR:O	1:A:277:LYS:NZ	2.47	0.47
2:D:2:GLC:H4	2:D:3:GLC:HO6	1.78	0.47
1:B:62:TRP:CD1	1:B:66:ARG:HG3	2.49	0.47
1:A:428:TRP:HB3	1:A:432:CYS:HB2	1.96	0.47
1:B:284:LEU:HG	1:B:285:LEU:HD23	1.96	0.47
1:B:117:TYR:HE1	1:B:245:THR:HG23	1.78	0.47
1:A:419:ARG:NH2	3:A:502:SO4:O1	2.48	0.47
1:B:126:PRO:HD2	1:B:224:MET:HE1	1.98	0.46
1:B:390:TRP:HH2	1:B:442:GLU:OE1	1.98	0.46
1:A:29:LYS:HD3	1:A:30:ASP:OD1	2.16	0.46
1:B:80:THR:H	1:B:277:LYS:NZ	2.15	0.45
1:B:68:GLY:HA3	1:B:332:ASN:O	2.17	0.45
1:B:215:ALA:O	1:B:219:LYS:HD3	2.16	0.45
1:B:118:ASN:ND2	1:B:240:VAL:HG13	2.32	0.45
1:A:270:SER:O	1:A:273:LYS:NZ	2.51	0.44
1:B:202:LYS:HB2	1:B:202:LYS:HE3	1.85	0.44
1:B:270:SER:O	1:B:273:LYS:NZ	2.51	0.43
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.53	0.43
1:B:428:TRP:HB3	1:B:432:CYS:HB2	2.00	0.43
1:A:411:GLU:HG3	1:A:412:PRO:HD2	2.00	0.43
1:B:26:LYS:HA	1:B:29:LYS:HB3	2.01	0.43
1:B:39:HIS:ND1	1:B:39:HIS:O	2.52	0.42
1:B:278:GLU:HG3	1:B:282:ASN:OD1	2.20	0.42
1:B:405:TYR:CZ	1:B:409:ARG:HD3	2.54	0.42
1:A:108:ILE:CD1	1:A:285:LEU:HD21	2.50	0.42
1:B:151:LEU:HD11	1:B:204:MET:HG2	2.02	0.42
1:B:274:GLU:CA	1:B:274:GLU:OE1	2.68	0.42
1:B:184:ASP:O	1:B:189:LYS:HE3	2.20	0.41
1:A:353:GLY:O	1:B:397:GLY:HA2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:LEU:HB3	1:B:317:ILE:HD12	2.02	0.41
1:A:291:GLU:O	1:A:295:LYS:HB2	2.21	0.41
1:B:89:LEU:HD12	1:B:94:TRP:CZ2	2.56	0.41
1:A:441:ARG:NH2	1:A:452:GLU:OE2	2.50	0.41
1:A:411:GLU:HG2	1:A:416:SER:O	2.21	0.40
1:B:11:ILE:HA	1:B:61:PHE:HB2	2.03	0.40
1:A:7:LEU:O	1:A:35:VAL:HA	2.22	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 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	457/466 (98%)	447 (98%)	10 (2%)	0	100	100
1	B	456/466 (98%)	445 (98%)	11 (2%)	0	100	100
All	All	913/932 (98%)	892 (98%)	21 (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 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	365/372 (98%)	364 (100%)	1 (0%)	92	95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	364/372 (98%)	358 (98%)	6 (2%)	62	67
All	All	729/744 (98%)	722 (99%)	7 (1%)	76	81

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

Mol	Chain	Res	Type
1	A	258	PHE
1	B	100	ASN
1	B	127	LYS
1	B	238	SER
1	B	258	PHE
1	B	326	LYS
1	B	441	ARG

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 ⓘ

6 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	GLC	C	1	2	12,12,12	1.19	1 (8%)	17,17,17	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	C	2	2	11,11,12	1.66	3 (27%)	15,15,17	1.02	1 (6%)
2	GLC	C	3	2	11,11,12	1.46	1 (9%)	15,15,17	1.31	3 (20%)
2	GLC	D	1	2	12,12,12	1.10	0	17,17,17	3.63	14 (82%)
2	GLC	D	2	2	11,11,12	1.87	2 (18%)	15,15,17	4.50	9 (60%)
2	GLC	D	3	2	11,11,12	1.79	3 (27%)	15,15,17	3.23	8 (53%)

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	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2	-	1/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	3	2	-	0/2/19/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	GLC	O5-C1	-4.83	1.36	1.43
2	D	3	GLC	O5-C1	-4.30	1.36	1.43
2	C	2	GLC	O5-C1	-2.88	1.39	1.43
2	D	2	GLC	O3-C3	-2.76	1.36	1.43
2	C	2	GLC	O3-C3	-2.50	1.37	1.43
2	D	3	GLC	C4-C5	-2.48	1.47	1.53
2	D	3	GLC	O5-C5	-2.45	1.38	1.43
2	C	3	GLC	O5-C5	-2.39	1.38	1.43
2	C	2	GLC	O5-C5	-2.34	1.38	1.43
2	C	1	GLC	O3-C3	-2.01	1.38	1.43

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLC	O3-C3-C2	-8.53	93.66	109.99
2	D	2	GLC	O2-C2-C1	6.95	123.36	109.15
2	D	2	GLC	O3-C3-C4	-6.37	95.61	110.35
2	D	1	GLC	O5-C5-C4	6.00	120.59	109.69
2	D	2	GLC	O5-C1-C2	-5.79	101.83	110.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLC	C2-C3-C4	5.72	120.79	110.89
2	D	1	GLC	C6-C5-C4	-5.57	99.95	113.00
2	D	1	GLC	C4-C3-C2	5.42	120.29	110.82
2	D	2	GLC	C1-C2-C3	5.36	116.25	109.67
2	D	1	GLC	O3-C3-C4	-5.33	98.02	110.35
2	D	3	GLC	O5-C5-C6	-5.27	98.94	107.20
2	D	3	GLC	C6-C5-C4	5.23	125.24	113.00
2	D	3	GLC	C3-C4-C5	-5.08	101.19	110.24
2	D	3	GLC	O5-C1-C2	-4.75	103.44	110.77
2	D	3	GLC	O5-C5-C4	-4.53	99.81	110.83
2	D	3	GLC	O2-C2-C3	4.28	118.71	110.14
2	D	2	GLC	O5-C5-C6	-4.22	100.59	107.20
2	D	1	GLC	O2-C2-C3	-4.04	101.00	110.35
2	D	2	GLC	O4-C4-C3	-3.82	101.51	110.35
2	D	1	GLC	O4-C4-C3	-3.66	101.89	110.35
2	D	1	GLC	O2-C2-C1	3.46	117.18	109.16
2	D	1	GLC	O3-C3-C2	-3.21	102.92	110.35
2	D	1	GLC	C3-C4-C5	3.13	115.82	110.24
2	C	2	GLC	C1-O5-C5	3.09	116.38	112.19
2	D	1	GLC	O6-C6-C5	-3.05	100.84	111.29
2	D	1	GLC	C1-O5-C5	2.86	119.07	113.66
2	D	1	GLC	C1-C2-C3	2.65	115.81	110.31
2	D	2	GLC	O4-C4-C5	2.52	115.54	109.30
2	C	3	GLC	C2-C3-C4	-2.50	106.57	110.89
2	D	1	GLC	O4-C4-C5	2.40	115.25	109.30
2	C	3	GLC	C1-O5-C5	2.38	115.42	112.19
2	D	3	GLC	C1-C2-C3	2.28	112.47	109.67
2	D	3	GLC	O6-C6-C5	-2.13	104.00	111.29
2	C	3	GLC	O5-C1-C2	-2.09	107.54	110.77
2	D	1	GLC	O5-C1-C2	2.08	113.99	110.28

There are no chirality outliers.

All (1) torsion outliers are listed below:

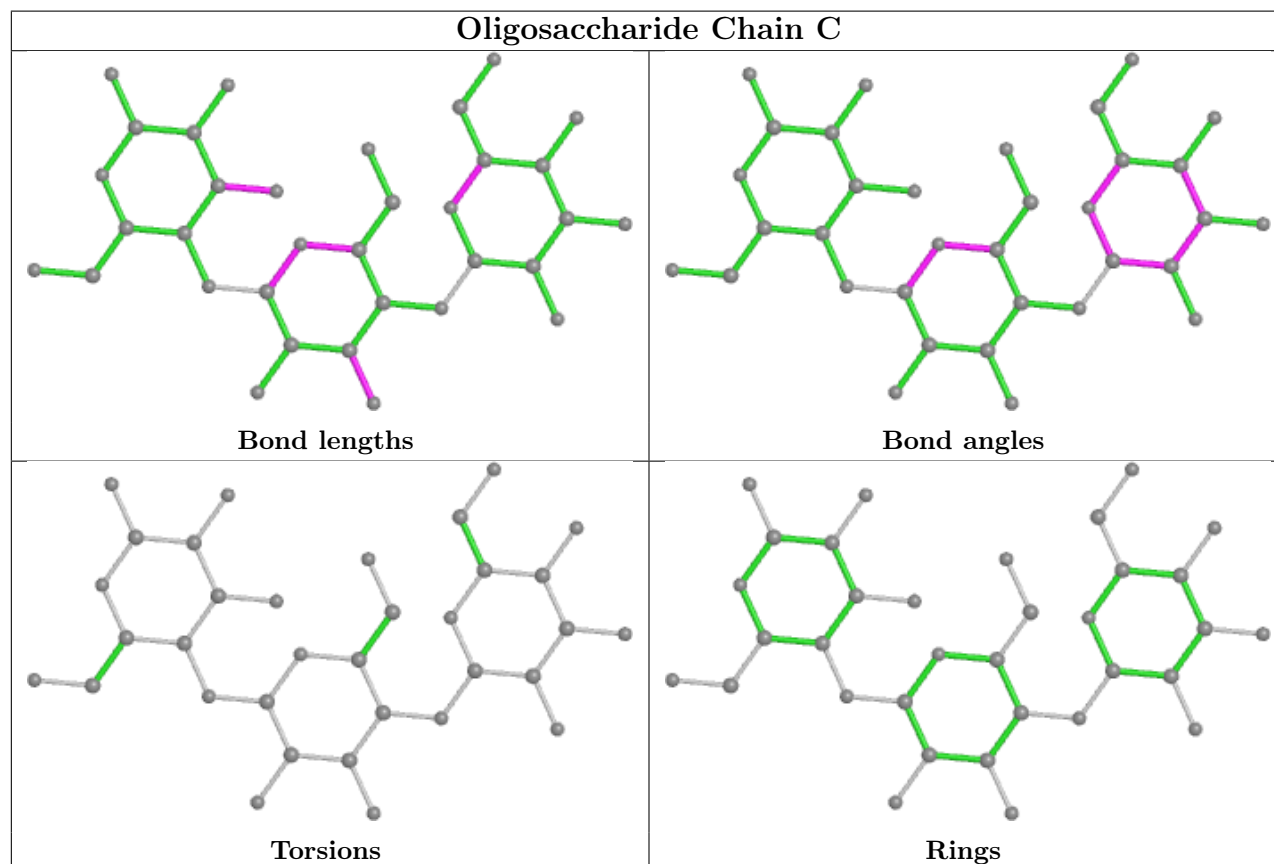
Mol	Chain	Res	Type	Atoms
2	D	1	GLC	O5-C5-C6-O6

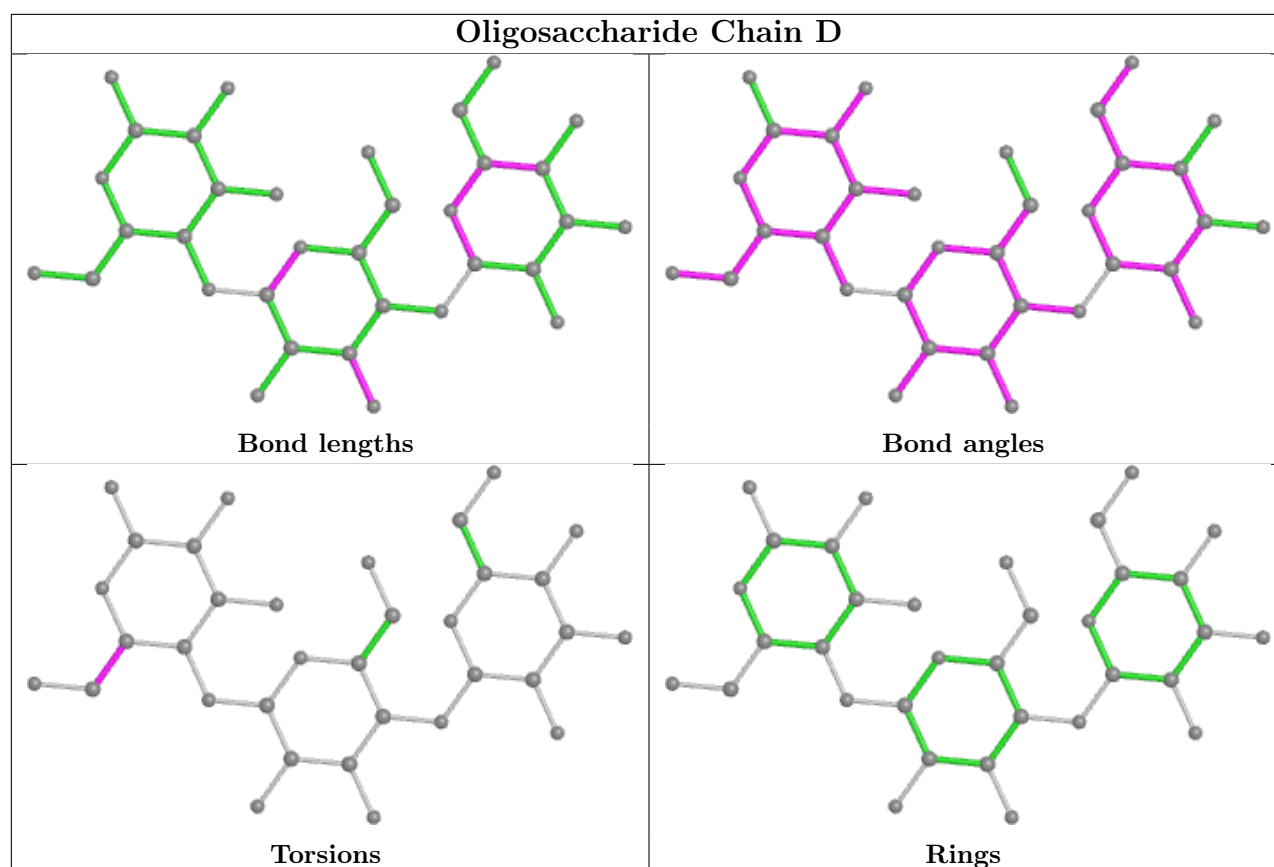
There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	GLC	5	0
2	D	3	GLC	4	0
2	D	2	GLC	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
3	SO4	A	502	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.13	0
3	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.06	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	SO4	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	459/466 (98%)	0.16	6 (1%) 77 76	27, 42, 69, 90	0
1	B	458/466 (98%)	0.66	63 (13%) 2 2	37, 64, 115, 139	0
All	All	917/932 (98%)	0.41	69 (7%) 14 13	27, 51, 106, 139	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	ILE	8.8
1	B	31	THR	7.9
1	B	283	TYR	7.7
1	B	276	ALA	6.2
1	B	32	GLY	6.2
1	B	36	THR	5.5
1	B	1	LYS	5.4
1	B	27	PHE	5.3
1	B	7	LEU	5.1
1	A	33	ILE	5.0
1	B	282	ASN	4.9
1	B	239	ALA	4.8
1	B	29	LYS	4.7
1	B	288	GLU	4.7
1	B	82	ALA	4.6
1	B	34	LYS	4.5
1	B	284	LEU	4.4
1	B	28	GLU	4.3
1	B	85	PHE	4.3
1	B	275	LEU	4.2
1	B	8	VAL	4.1
1	B	21	ALA	4.0
1	B	141	ALA	3.9
1	B	37	VAL	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	84	ALA	3.9
1	B	25	LYS	3.7
1	B	122	LEU	3.7
1	B	279	PHE	3.6
1	B	289	GLY	3.5
1	B	313	LYS	3.5
1	B	6	LYS	3.5
1	B	278	GLU	3.4
1	B	4	GLU	3.3
1	B	3	GLU	3.1
1	B	121	LEU	3.1
1	B	140	LYS	3.1
1	B	144	LYS	3.0
1	B	271	PRO	3.0
1	B	120	ASP	3.0
1	B	22	GLU	2.9
1	B	220	GLY	2.9
1	B	307	TYR	2.9
1	A	31	THR	2.7
1	B	26	LYS	2.7
1	B	58	ASP	2.7
1	B	216	ALA	2.6
1	B	106	TYR	2.6
1	B	30	ASP	2.6
1	B	274	GLU	2.6
1	B	310	GLU	2.6
1	B	143	GLY	2.5
1	B	118	ASN	2.5
1	B	242	TYR	2.5
1	B	123	PRO	2.4
1	B	139	LEU	2.4
1	A	29	LYS	2.4
1	B	88	LYS	2.4
1	A	25	LYS	2.3
1	B	270	SER	2.3
1	A	283	TYR	2.2
1	B	311	LEU	2.2
1	B	55	ASP	2.2
1	B	243	GLY	2.1
1	B	5	GLY	2.1
1	B	223	ALA	2.1
1	B	304	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	241	ASN	2.0
1	B	235	ILE	2.0
1	A	278	GLU	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](#)

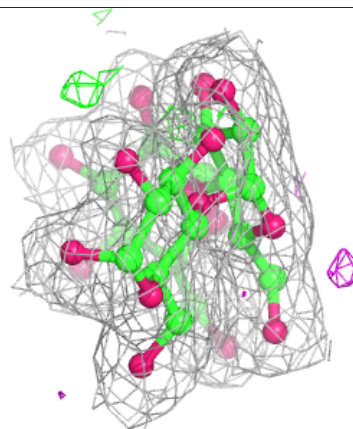
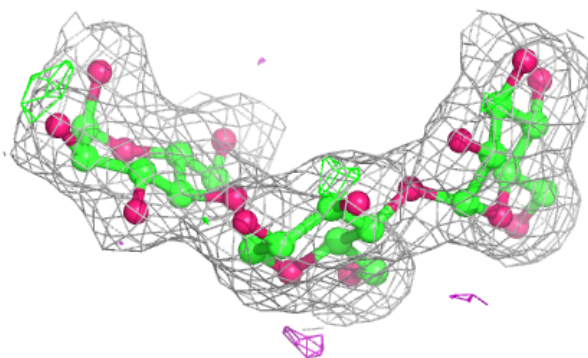
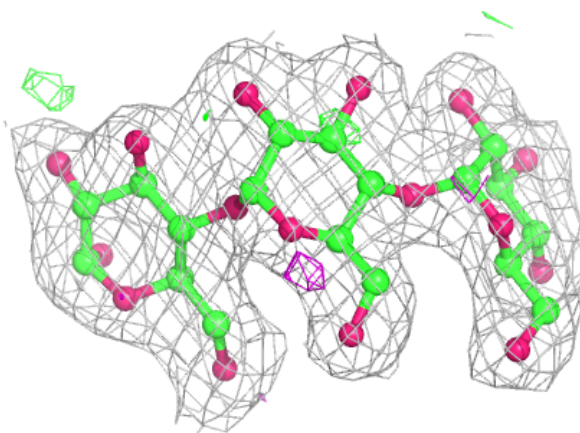
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

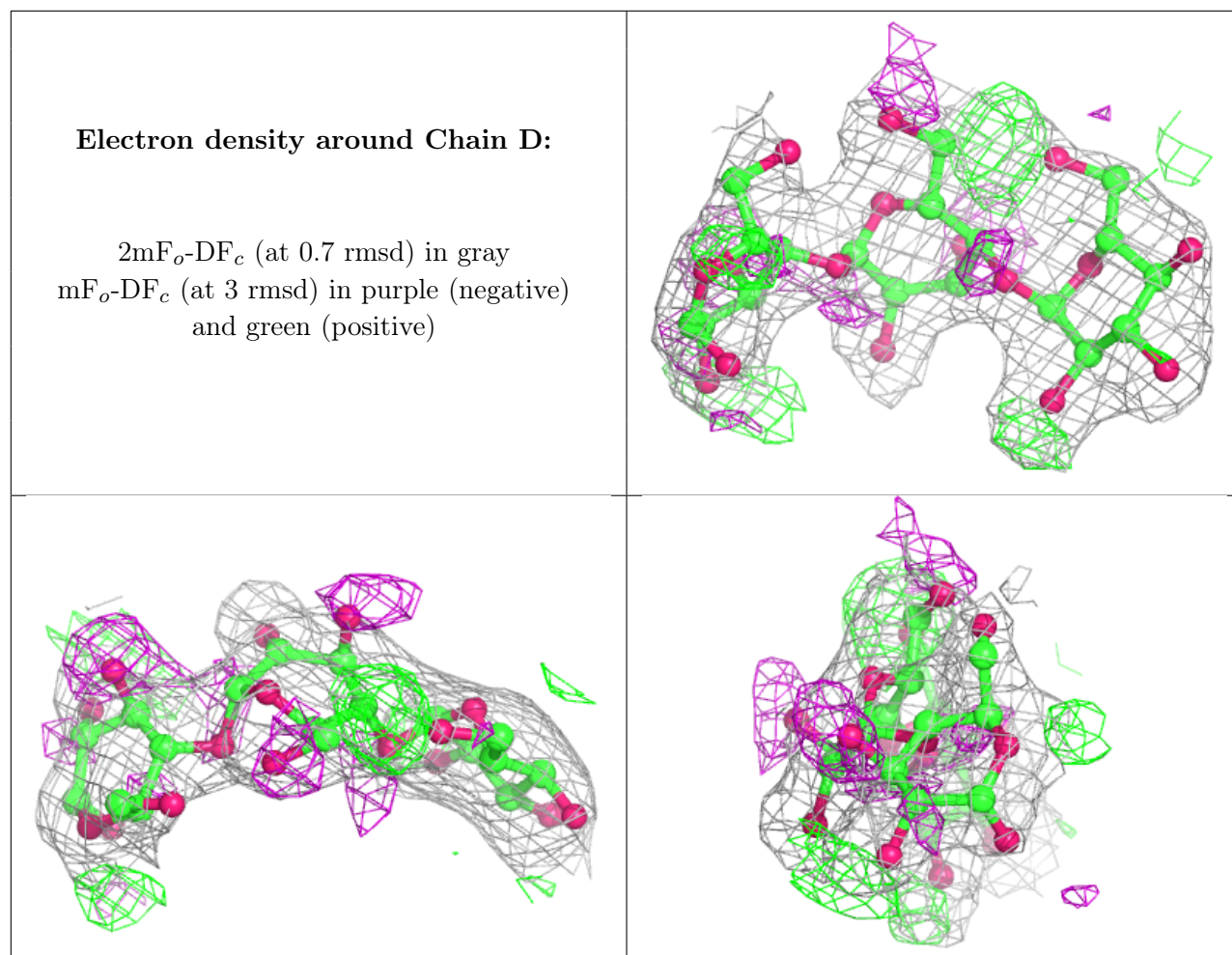
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	D	2	11/12	0.77	0.18	50,56,72,75	0
2	GLC	D	1	12/12	0.83	0.19	54,61,77,78	0
2	GLC	D	3	11/12	0.86	0.22	57,69,82,86	0
2	GLC	C	3	11/12	0.96	0.08	34,36,39,43	0
2	GLC	C	1	12/12	0.96	0.12	29,35,39,41	0
2	GLC	C	2	11/12	0.97	0.15	24,29,31,32	0

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.

Electron density around Chain C:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





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	SO4	A	502	5/5	0.90	0.17	68,73,97,99	0
3	SO4	B	501	5/5	0.96	0.09	58,80,92,93	0
3	SO4	A	501	5/5	0.98	0.11	49,54,58,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.