



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:51 PM UTC

PDB ID : 6KI0 / pdb_00006ki0
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

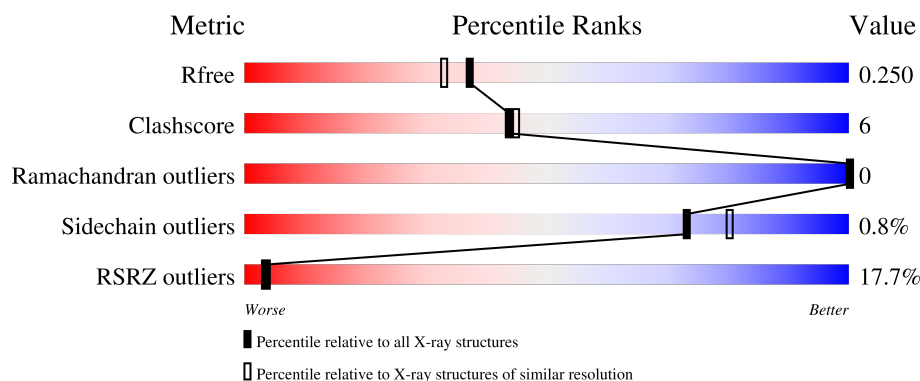
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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	6% 89% 9% ..
1	B	466	29% 81% 17% ..
2	C	3	33% 67%
2	D	3	100%

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

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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 (CCD ID: 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		

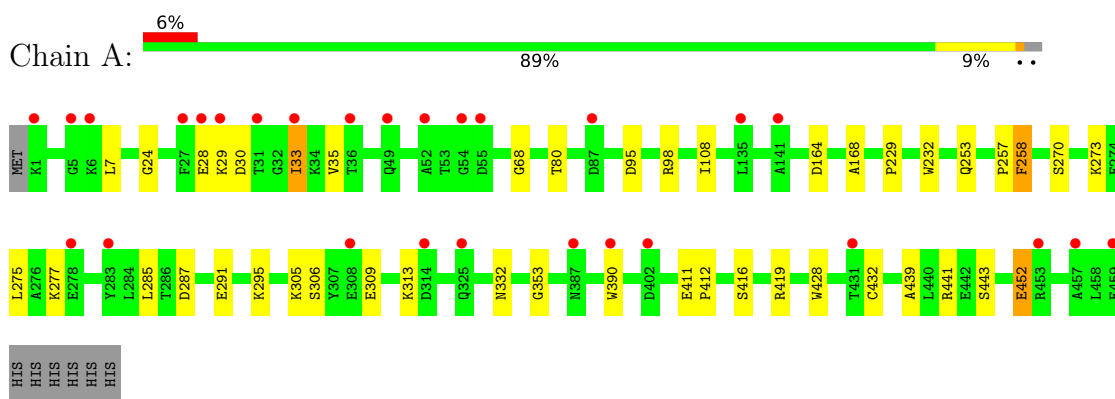
- Molecule 4 is water.

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

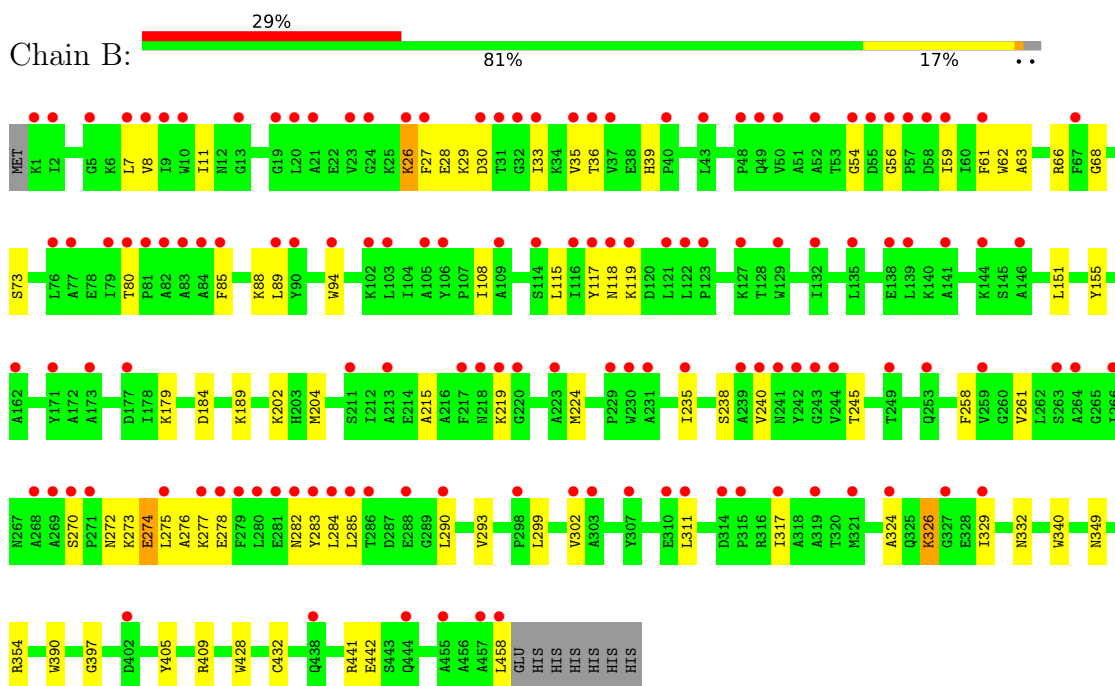
3 Residue-property plots

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 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 C:  33% 67%

GLC1
GLC2
GLC3

- 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) 99.0 (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 0.224 , 0.250	Depositor DCC
R_{free} test set	4625 reflections (4.96%)	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 , 41.7	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: SO4, GLC

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	0.47	5/3654 (0.1%)	0.50	1/4970 (0.0%)
1	B	0.46	1/3645 (0.0%)	0.62	6/4958 (0.1%)
All	All	0.46	6/7299 (0.1%)	0.57	7/9928 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	ALA	C-O	-7.55	1.17	1.23
1	A	257	PRO	C-O	-6.07	1.16	1.23
1	A	313	LYS	N-CA	-5.56	1.38	1.46
1	B	324	ALA	C-N	-5.41	1.25	1.33
1	A	452	GLU	C-O	-5.10	1.18	1.24
1	A	258	PHE	C-O	-5.06	1.17	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	GLU	N-CA-C	-11.95	99.18	113.88
1	B	26	LYS	N-CA-C	-7.28	104.42	112.72
1	B	326	LYS	N-CA-C	-6.76	103.72	112.23
1	B	324	ALA	CA-C-O	6.74	127.56	119.61
1	A	33	ILE	CB-CA-C	-5.64	103.92	110.91
1	B	56	GLY	N-CA-C	-5.36	101.40	112.34
1	B	54	GLY	N-CA-C	5.27	119.51	112.77

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:115:LEU:HD11	1:B:224:MET:HE2	1.69	0.73
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:73:SER:HB3	1:B:458:LEU:HD13	1.80	0.64
1:B:108:ILE:HG13	1:B:285:LEU:HD21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:2:GLC:H4	2:D:3:GLC:HO6	1.66	0.60
1:A:7:LEU:HB2	1:A:35:VAL:HG12	1.84	0.60
1:B:80:THR:H	1:B:277:LYS:HZ1	1.51	0.58
1:B:59:ILE:HD11	1:B:276:ALA:HB1	1.85	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:HG23	1:B:35:VAL:O	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
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: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:85:PHE:HA	1:B:88:LYS:HE3	1.94	0.49
1:B:235:ILE:HA	1:B:238:SER:HB3	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
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:390:TRP:HH2	1:B:442:GLU:OE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LYS:HD3	1:A:30:ASP:OD1	2.16	0.46
1:B:68:GLY:HA3	1:B:332:ASN:O	2.17	0.45
1:B:118:ASN:ND2	1:B:240:VAL:HG13	2.32	0.45
1:B:215:ALA:O	1:B:219:LYS:HD3	2.16	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:O	1:B:39:HIS:ND1	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:80:THR:H	1:B:277:LYS:NZ	2.15	0.42
1:B:151:LEU:HD11	1:B:204:MET:HG2	2.02	0.42
1:B:274:GLU:OE1	1:B:274:GLU:CA	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
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
1:B:80:THR:O	1:B:80:THR:OG1	2.39	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	65/466 (14%)	63 (97%)	2 (3%)	0	100	100
1	B	412/466 (88%)	401 (97%)	11 (3%)	0	100	100
All	All	477/932 (51%)	464 (97%)	13 (3%)	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	365/372 (98%)	363 (100%)	2 (0%)	81	87
1	B	364/372 (98%)	360 (99%)	4 (1%)	65	73
All	All	729/744 (98%)	723 (99%)	6 (1%)	73	80

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	258	PHE
1	B	258	PHE
1	B	274	GLU
1	B	326	LYS
1	B	441	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	234	ASN

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	1.16	0	17,17,17	1.09	0
2	GLC	C	2	2	11,11,12	1.62	3 (27%)	15,15,17	0.98	1 (6%)
2	GLC	C	3	2	11,11,12	1.44	1 (9%)	15,15,17	1.20	2 (13%)
2	GLC	D	1	2	12,12,12	1.08	0	17,17,17	3.59	14 (82%)
2	GLC	D	2	2	11,11,12	1.79	2 (18%)	15,15,17	4.08	9 (60%)
2	GLC	D	3	2	11,11,12	1.74	3 (27%)	15,15,17	2.93	7 (46%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	GLC	O5-C1	-4.58	1.36	1.43
2	D	3	GLC	O5-C1	-4.08	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GLC	O5-C1	-2.73	1.39	1.43
2	D	2	GLC	O3-C3	-2.61	1.36	1.43
2	D	3	GLC	O5-C5	-2.54	1.38	1.43
2	C	3	GLC	O5-C5	-2.48	1.38	1.43
2	D	3	GLC	C4-C5	-2.44	1.47	1.53
2	C	2	GLC	O5-C5	-2.43	1.38	1.43
2	C	2	GLC	O3-C3	-2.37	1.37	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLC	O3-C3-C2	-8.04	93.66	110.05
2	D	2	GLC	O3-C3-C4	-6.26	95.61	110.38
2	D	2	GLC	O2-C2-C1	6.18	123.36	109.22
2	D	1	GLC	O5-C5-C4	6.04	120.59	109.70
2	D	2	GLC	C2-C3-C4	5.64	120.79	110.86
2	D	1	GLC	C4-C3-C2	5.39	120.29	110.83
2	D	1	GLC	C6-C5-C4	-5.32	99.95	113.02
2	D	1	GLC	O3-C3-C4	-5.24	98.02	110.38
2	D	3	GLC	C3-C4-C5	-4.99	101.19	110.23
2	D	3	GLC	C6-C5-C4	4.98	125.24	113.02
2	D	2	GLC	C1-C2-C3	4.54	116.25	109.64
2	D	3	GLC	O5-C5-C4	-4.53	99.81	110.83
2	D	3	GLC	O5-C5-C6	-4.48	98.94	107.66
2	D	3	GLC	O2-C2-C3	4.13	118.71	110.15
2	D	1	GLC	O2-C2-C3	-3.98	101.00	110.38
2	D	2	GLC	O4-C4-C3	-3.76	101.51	110.38
2	D	2	GLC	O5-C1-C2	-3.76	101.83	110.79
2	D	2	GLC	O5-C5-C6	-3.63	100.59	107.66
2	D	1	GLC	O4-C4-C3	-3.60	101.89	110.38
2	D	1	GLC	O2-C2-C1	3.44	117.18	109.25
2	D	1	GLC	O3-C3-C2	-3.16	102.92	110.38
2	C	2	GLC	C1-O5-C5	3.13	116.38	112.19
2	D	1	GLC	C3-C4-C5	3.08	115.82	110.23
2	D	3	GLC	O5-C1-C2	-3.08	103.44	110.79
2	D	1	GLC	O6-C6-C5	-3.08	100.84	111.33
2	D	1	GLC	C1-O5-C5	2.80	119.07	113.65
2	D	1	GLC	C1-C2-C3	2.68	115.81	110.36
2	D	2	GLC	O4-C4-C5	2.53	115.54	109.32
2	C	3	GLC	C2-C3-C4	-2.44	106.57	110.86
2	C	3	GLC	C1-O5-C5	2.41	115.42	112.19
2	D	1	GLC	O4-C4-C5	2.41	115.25	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	GLC	O6-C6-C5	-2.15	104.00	111.33
2	D	1	GLC	O5-C1-C2	2.10	113.99	110.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

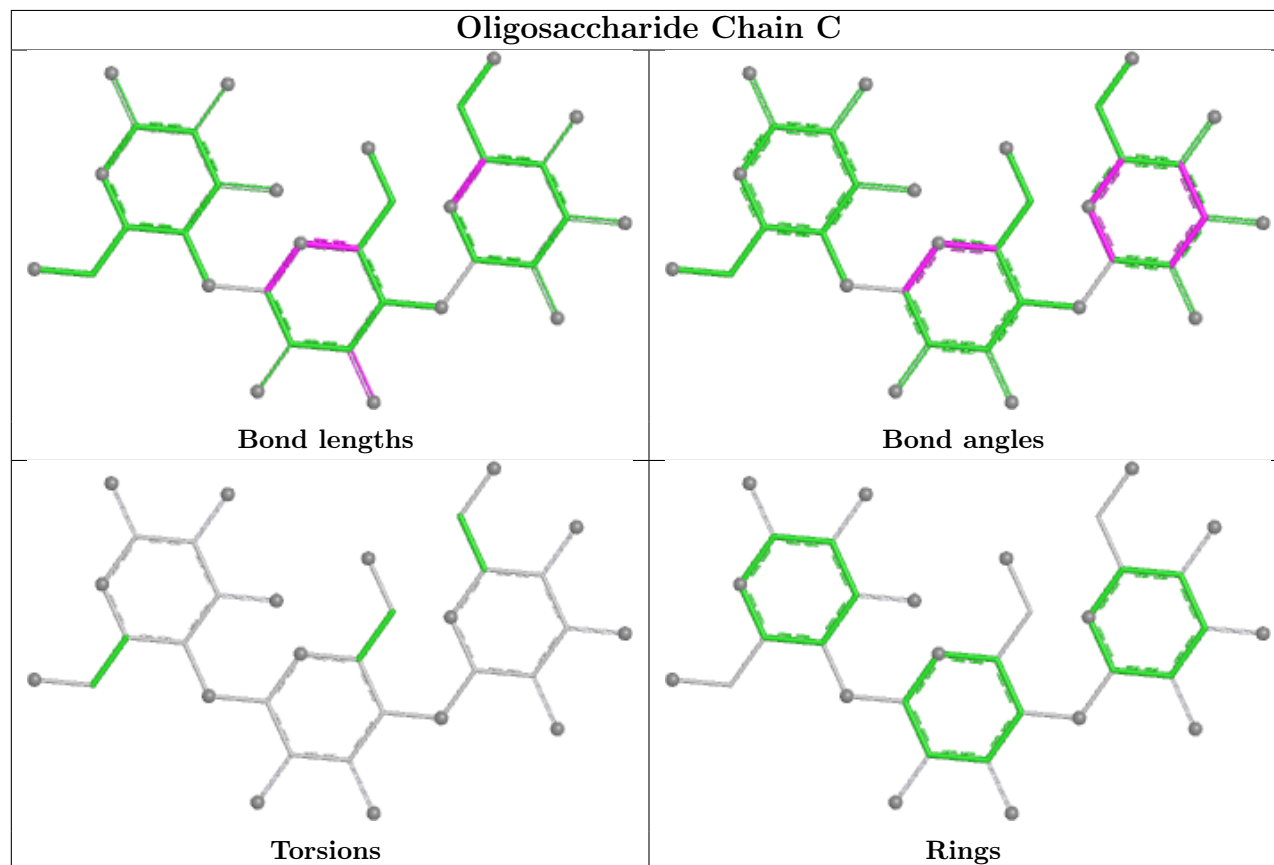
Mol	Chain	Res	Type	Atoms
2	D	1	GLC	O5-C5-C6-O6

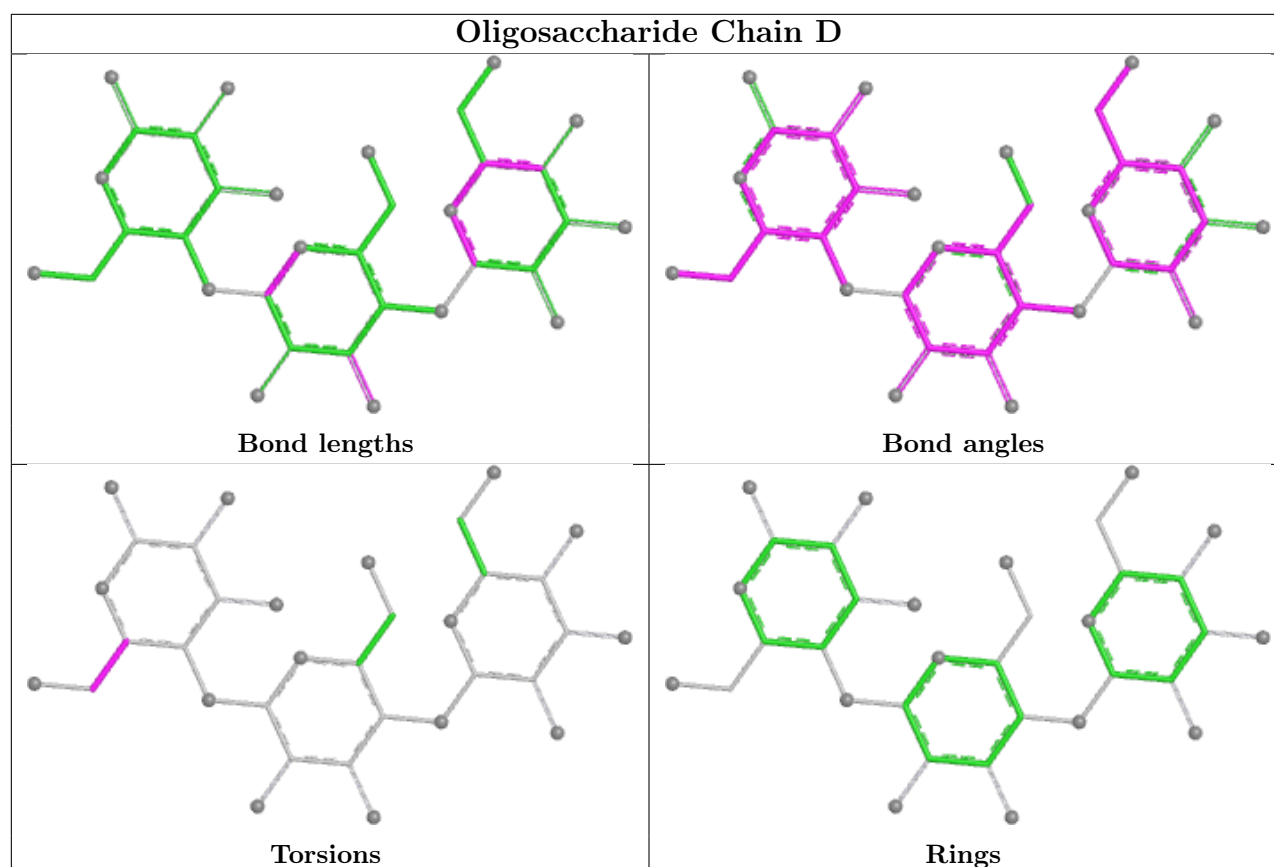
There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	GLC	4	0
2	D	1	GLC	5	0
2	D	3	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	B	501	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	A	502	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	A	501	-	4,4,4	0.23	0	6,6,6	0.15	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%)	0.55	28 (6%) 27 26	27, 42, 69, 90	0
1	B	458/466 (98%)	1.52	134 (29%) 1 1	37, 64, 115, 139	0
All	All	917/932 (98%)	1.03	162 (17%) 4 3	27, 51, 106, 139	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ILE	6.2
1	B	458	LEU	5.0
1	B	317	ILE	5.0
1	B	324	ALA	4.8
1	B	82	ALA	4.5
1	B	280	LEU	4.5
1	B	8	VAL	4.4
1	B	275	LEU	4.4
1	B	271	PRO	4.2
1	B	122	LEU	4.1
1	B	314	ASP	4.1
1	B	33	ILE	4.1
1	B	220	GLY	4.1
1	B	23	VAL	4.1
1	B	36	THR	4.0
1	B	242	TYR	3.9
1	B	279	PHE	3.9
1	B	284	LEU	3.9
1	A	31	THR	3.8
1	B	27	PHE	3.8
1	B	283	TYR	3.7
1	B	239	ALA	3.7
1	B	311	LEU	3.6
1	B	1	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	33	ILE	3.5
1	B	123	PRO	3.5
1	A	5	GLY	3.4
1	B	35	VAL	3.4
1	A	54	GLY	3.4
1	B	457	ALA	3.4
1	B	7	LEU	3.4
1	B	59	ILE	3.3
1	B	31	THR	3.3
1	B	19	GLY	3.3
1	B	90	TYR	3.2
1	B	109	ALA	3.2
1	B	329	ILE	3.2
1	B	121	LEU	3.2
1	B	85	PHE	3.2
1	B	20	LEU	3.1
1	B	37	VAL	3.1
1	B	288	GLU	3.1
1	A	52	ALA	3.1
1	B	94	TRP	3.1
1	B	102	LYS	3.0
1	A	141	ALA	3.0
1	B	21	ALA	3.0
1	B	80	THR	3.0
1	B	106	TYR	3.0
1	B	117	TYR	3.0
1	A	27	PHE	3.0
1	B	26	LYS	3.0
1	B	243	GLY	3.0
1	B	58	ASP	3.0
1	B	231	ALA	3.0
1	B	171	TYR	3.0
1	B	218	ASN	2.9
1	B	290	LEU	2.9
1	B	235	ILE	2.9
1	B	141	ALA	2.9
1	B	32	GLY	2.9
1	A	325	GLN	2.9
1	B	438	GLN	2.9
1	B	83	ALA	2.9
1	B	146	ALA	2.8
1	B	43	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	285	LEU	2.8
1	B	298	PRO	2.8
1	B	49	GLN	2.8
1	B	327	GLY	2.8
1	B	259	VAL	2.8
1	B	302	VAL	2.8
1	A	453	ARG	2.7
1	B	249	THR	2.7
1	B	57	PRO	2.7
1	B	402	ASP	2.7
1	A	29	LYS	2.7
1	A	135	LEU	2.7
1	B	266	ILE	2.7
1	A	55	ASP	2.7
1	A	457	ALA	2.7
1	A	390	TRP	2.7
1	B	84	ALA	2.6
1	B	281	GLU	2.6
1	B	89	LEU	2.6
1	B	103	LEU	2.6
1	B	263	SER	2.6
1	B	241	ASN	2.6
1	A	6	LYS	2.6
1	A	459	GLU	2.6
1	B	286	THR	2.6
1	B	270	SER	2.6
1	B	268	ALA	2.6
1	B	217	PHE	2.5
1	B	229	PRO	2.5
1	B	79	ILE	2.5
1	B	240	VAL	2.5
1	B	30	ASP	2.5
1	B	52	ALA	2.5
1	B	162	ALA	2.5
1	A	49	GLN	2.5
1	B	211	SER	2.5
1	B	81	PRO	2.5
1	B	10	TRP	2.5
1	B	315	PRO	2.4
1	B	223	ALA	2.4
1	B	5	GLY	2.4
1	B	9	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	40	PRO	2.4
1	B	321	MET	2.4
1	B	24	GLY	2.4
1	B	278	GLU	2.4
1	B	132	ILE	2.4
1	B	127	LYS	2.4
1	B	269	ALA	2.4
1	B	303	ALA	2.4
1	B	48	PRO	2.4
1	B	173	ALA	2.3
1	B	54	GLY	2.3
1	B	105	ALA	2.3
1	B	282	ASN	2.3
1	B	50	VAL	2.3
1	B	144	LYS	2.3
1	B	219	LYS	2.3
1	A	28	GLU	2.3
1	B	244	VAL	2.3
1	A	387	ASN	2.3
1	B	76	LEU	2.3
1	A	308	GLU	2.2
1	B	118	ASN	2.2
1	B	119	LYS	2.2
1	B	55	ASP	2.2
1	A	314	ASP	2.2
1	B	310	GLU	2.2
1	B	307	TYR	2.2
1	B	114	SER	2.2
1	A	1	LYS	2.2
1	B	177	ASP	2.2
1	B	138	GLU	2.2
1	B	455	ALA	2.2
1	B	230	TRP	2.2
1	B	116	ILE	2.1
1	B	56	GLY	2.1
1	B	277	LYS	2.1
1	A	87	ASP	2.1
1	A	278	GLU	2.1
1	A	431	THR	2.1
1	B	129	TRP	2.1
1	B	253	GLN	2.1
1	A	402	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	283	TYR	2.1
1	B	67	PHE	2.1
1	B	135	LEU	2.1
1	B	61	PHE	2.1
1	B	77	ALA	2.1
1	B	213	ALA	2.1
1	B	264	ALA	2.1
1	B	319	ALA	2.1
1	B	139	LEU	2.0
1	B	13	GLY	2.0
1	B	444	GLN	2.0
1	A	36	THR	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](#)

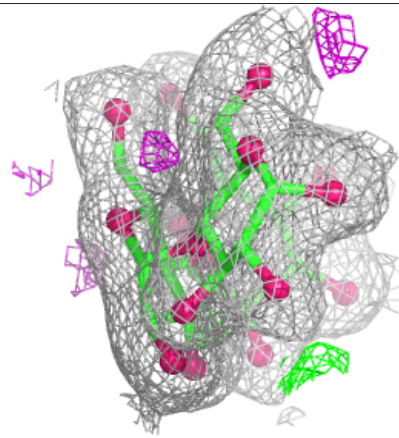
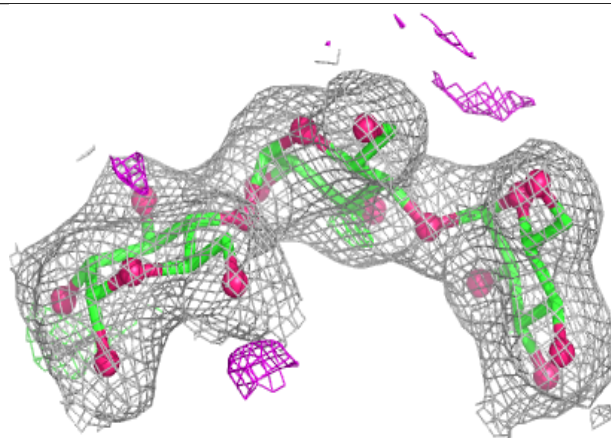
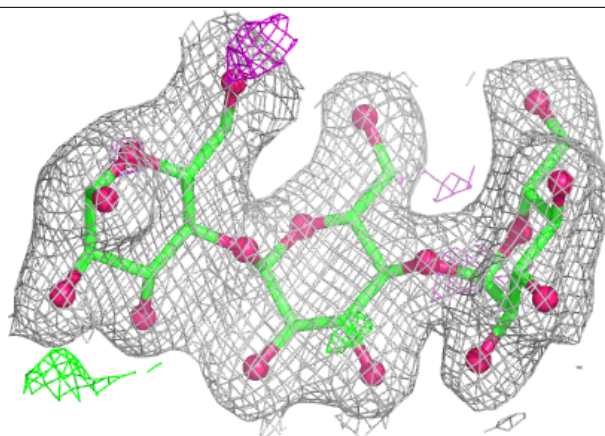
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

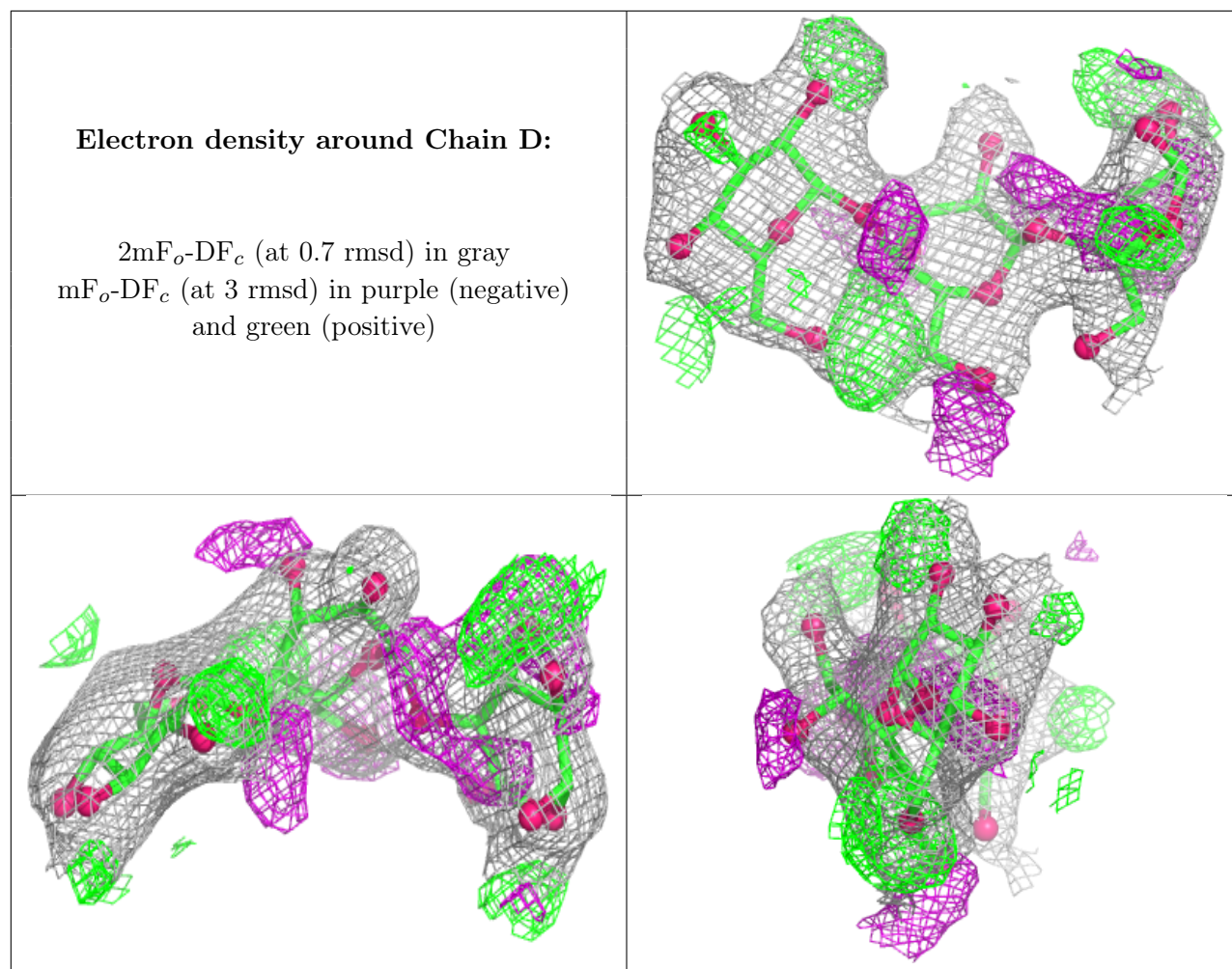
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	D	2	11/12	0.73	0.18	50,56,72,75	0
2	GLC	D	1	12/12	0.74	0.21	54,61,77,78	0
2	GLC	D	3	11/12	0.77	0.17	57,69,82,86	0
2	GLC	C	1	12/12	0.96	0.06	29,35,39,41	0
2	GLC	C	3	11/12	0.97	0.07	34,36,39,43	0
2	GLC	C	2	11/12	0.97	0.07	24,29,31,32	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	0.72	0.11	68,73,97,99	0
3	SO4	B	501	5/5	0.86	0.10	58,80,92,93	0
3	SO4	A	501	5/5	0.94	0.09	49,54,58,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.