Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2024 – 02:47 am GMT

PDB ID	:	8OPX
Title	:	Structure of Mycobacterium tuberculosis beta-oxidation trifunctional enzyme in complex with Trehalose (Fragment-B-TRE)
Authors	:	Dalwani, S.; Wierenga, R.K.; Venkatesan, R.
Deposited on	:	2023-04-10
Resolution	:	2.90 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:

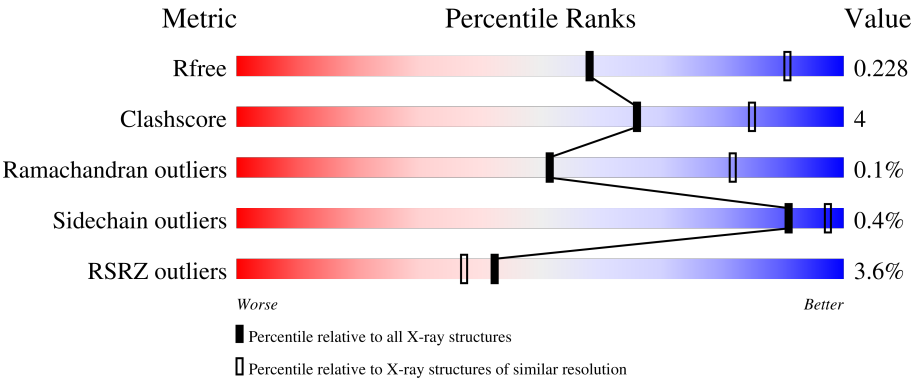
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	A	736	8% 88% 10%
1	B	736	3% 89% 10%
2	C	403	89% 10%
2	D	403	91% 8%
3	G	2	100%

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Mol	Chain	Length	Quality of chain
4	H	2	50% 50%

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
4	GLC	H	1	-	-	-	X
4	GLC	H	2	-	-	-	X
5	SO4	C	506	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16868 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 3-hydroxyacyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	726	Total	C	N	O	S	0	6	0
			5387	3411	923	1031	22			
1	A	726	Total	C	N	O	S	0	4	0
			5368	3396	921	1030	21			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP O53872
B	-14	GLY	-	expression tag	UNP O53872
B	-13	SER	-	expression tag	UNP O53872
B	-12	SER	-	expression tag	UNP O53872
B	-11	HIS	-	expression tag	UNP O53872
B	-10	HIS	-	expression tag	UNP O53872
B	-9	HIS	-	expression tag	UNP O53872
B	-8	HIS	-	expression tag	UNP O53872
B	-7	HIS	-	expression tag	UNP O53872
B	-6	HIS	-	expression tag	UNP O53872
B	-5	SER	-	expression tag	UNP O53872
B	-4	GLN	-	expression tag	UNP O53872
B	-3	ASP	-	expression tag	UNP O53872
B	-2	PRO	-	expression tag	UNP O53872
B	-1	ASN	-	expression tag	UNP O53872
B	0	SER	-	expression tag	UNP O53872
A	-15	MET	-	initiating methionine	UNP O53872
A	-14	GLY	-	expression tag	UNP O53872
A	-13	SER	-	expression tag	UNP O53872
A	-12	SER	-	expression tag	UNP O53872
A	-11	HIS	-	expression tag	UNP O53872
A	-10	HIS	-	expression tag	UNP O53872
A	-9	HIS	-	expression tag	UNP O53872
A	-8	HIS	-	expression tag	UNP O53872
A	-7	HIS	-	expression tag	UNP O53872

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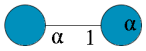
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	HIS	-	expression tag	UNP O53872
A	-5	SER	-	expression tag	UNP O53872
A	-4	GLN	-	expression tag	UNP O53872
A	-3	ASP	-	expression tag	UNP O53872
A	-2	PRO	-	expression tag	UNP O53872
A	-1	ASN	-	expression tag	UNP O53872
A	0	SER	-	expression tag	UNP O53872

- Molecule 2 is a protein called Putative acyltransferase Rv0859.

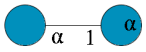
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	398	Total	C	N	O	S	0	3	0
			2945	1840	521	569	15			
2	D	399	Total	C	N	O	S	0	4	0
			2955	1846	522	572	15			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose.



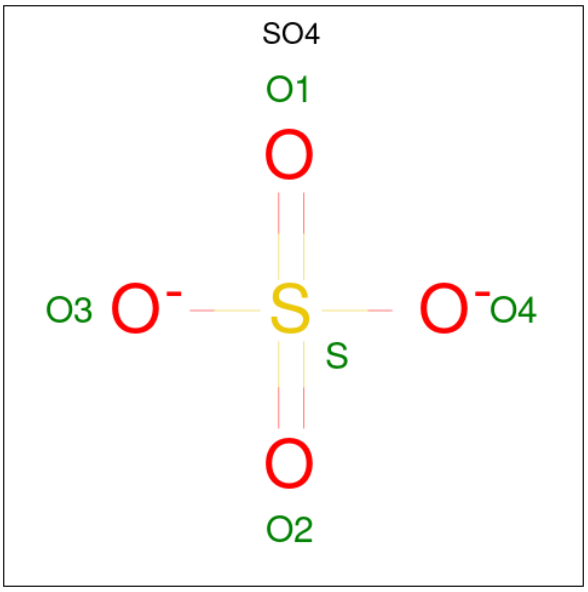
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	O		0	0	0
			23	12	11				

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	2	Total	C	O		0	0	0
			23	12	11				

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 6 is water.

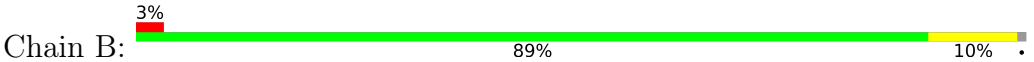
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	14	Total O 14 14	0	0
6	C	10	Total O 10 10	0	0
6	A	13	Total O 13 13	0	0
6	D	10	Total O 10 10	0	0

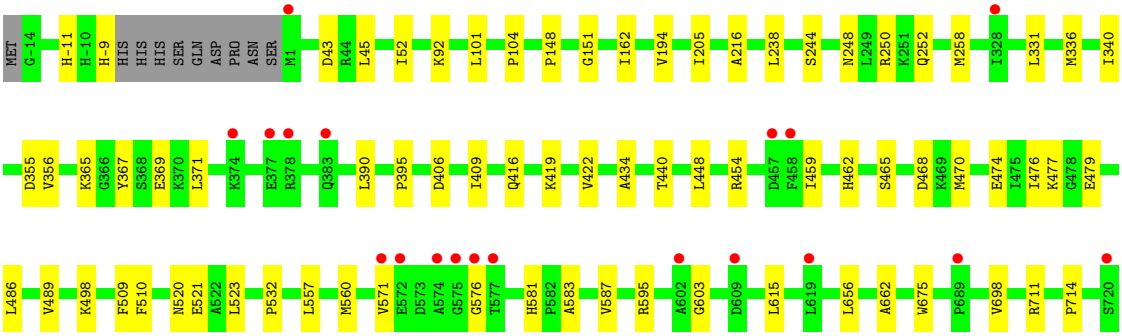
3 Residue-property plots (i)

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: 3-hydroxyacyl-CoA dehydrogenase

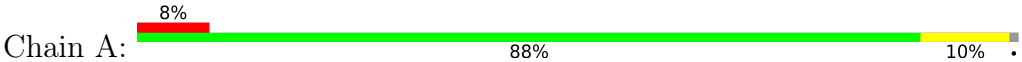
Chain B:

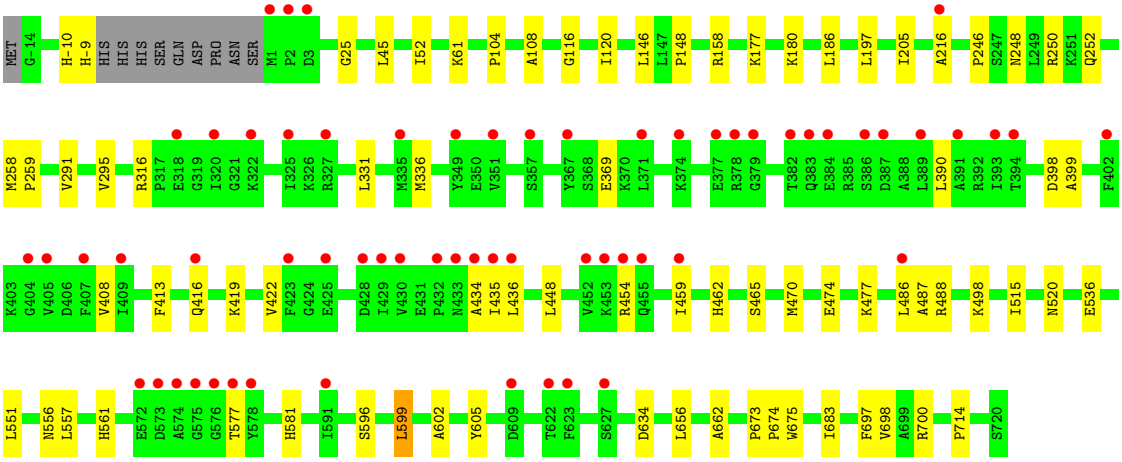




• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

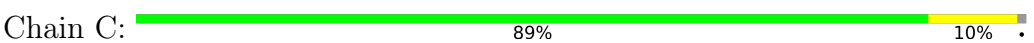
Chain A:

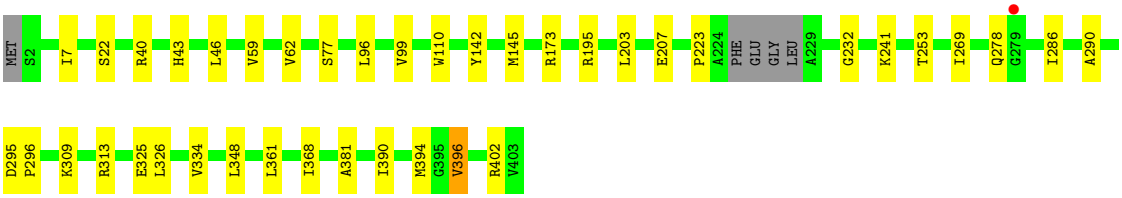




• Molecule 2: Putative acyltransferase Rv0859

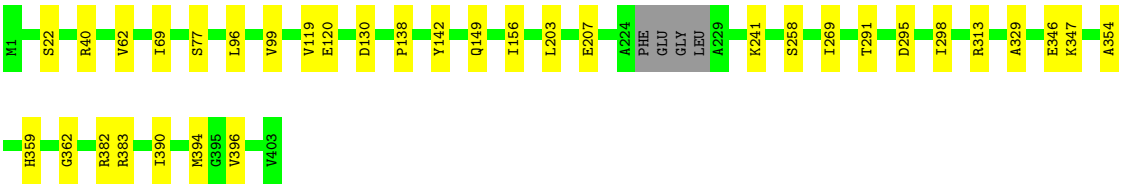
Chain C:





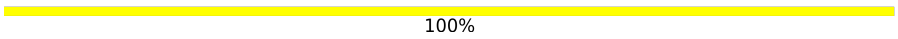
• Molecule 2: Putative acyltransferase Rv0859

Chain D:



• Molecule 3: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain G:



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

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	248.41Å 135.16Å 119.16Å 90.00° 110.56° 90.00°	Depositor
Resolution (Å)	48.37 – 2.90 48.37 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (48.37-2.90) 97.9 (48.37-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.199 , 0.229 0.198 , 0.228	Depositor DCC
R_{free} test set	3904 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	59.4	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16868	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.25	0/5479	0.47	0/7422
1	B	0.25	0/5504	0.46	0/7452
2	C	0.24	0/2997	0.50	0/4058
2	D	0.25	0/3010	0.50	0/4076
All	All	0.25	0/16990	0.48	0/23008

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	5368	0	5385	42	0
1	B	5387	0	5427	46	0
2	C	2945	0	2971	28	0
2	D	2955	0	2980	27	0
3	G	23	0	21	3	0
4	H	23	0	21	1	0
5	A	25	0	0	1	0
5	B	30	0	0	1	0
5	C	35	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	30	0	0	1	0
6	A	13	0	0	1	0
6	B	14	0	0	0	0
6	C	10	0	0	0	0
6	D	10	0	0	0	0
All	All	16868	0	16805	135	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 4.

All (135) 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:250:ARG:NH1	2:C:142:TYR:O	2.27	0.68
2:C:241:LYS:NZ	3:G:1:GLC:O2	2.29	0.66
1:B:-9:HIS:NE2	5:B:803:SO4:O1	2.28	0.66
2:D:291:THR:HG22	2:D:396[A]:VAL:HG23	1.77	0.66
1:A:158:ARG:NH1	6:A:901:HOH:O	2.31	0.64
1:A:556:ASN:HD21	1:A:599:LEU:HD22	1.64	0.62
1:A:557:LEU:HD12	1:A:596:SER:HA	1.82	0.62
2:C:195:ARG:NH2	5:C:502:SO4:O3	2.25	0.61
1:A:369:GLU:HG2	1:A:390:LEU:HD13	1.82	0.61
1:B:244:SER:HB2	2:C:232:GLY:HA3	1.83	0.61
2:D:291:THR:HG22	2:D:396[B]:VAL:HG22	1.83	0.60
1:A:250:ARG:NH1	2:D:142:TYR:O	2.35	0.58
1:A:470:MET:O	1:A:498:LYS:NZ	2.34	0.57
1:A:413:PHE:O	1:A:419:LYS:NZ	2.38	0.56
1:B:367:TYR:OH	1:B:468:ASP:OD1	2.24	0.55
2:C:22:SER:OG	2:C:207:GLU:OE2	2.24	0.55
1:B:520:ASN:HB3	1:B:581:HIS:CE1	2.42	0.55
1:B:369:GLU:HG2	1:B:390:LEU:HD13	1.89	0.54
1:A:698:VAL:HG13	1:A:714:PRO:HG3	1.89	0.54
1:B:477:LYS:HB2	1:B:486:LEU:HD21	1.90	0.54
1:A:177:LYS:HB2	1:A:180:LYS:HD3	1.89	0.54
1:A:25:GLY:O	1:A:61:LYS:NZ	2.35	0.53
1:A:331:LEU:HD13	1:A:422:VAL:HG12	1.90	0.53
2:C:62:VAL:HG12	2:D:62:VAL:HG12	1.91	0.53
1:B:459:ILE:HD11	1:B:486:LEU:HD23	1.90	0.52
2:D:346:GLU:HG2	2:D:347:LYS:HG3	1.91	0.52
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.91	0.52
1:A:104:PRO:HG2	1:A:205:ILE:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:LEU:HA	1:B:560:MET:HG3	1.91	0.52
2:C:110:TRP:O	2:D:313:ARG:NH1	2.43	0.52
1:B:419:LYS:HE2	1:B:440:THR:HB	1.92	0.51
1:B:355:ASP:OD1	1:B:356:VAL:N	2.36	0.51
1:B:459:ILE:HG21	1:B:489:VAL:HG21	1.91	0.51
1:B:595:ARG:HB3	1:B:603:GLY:HA2	1.92	0.51
1:B:250:ARG:HH22	3:G:1:GLC:H62	1.74	0.50
1:B:532:PRO:HB2	1:B:615:LEU:HD13	1.93	0.50
2:D:99:VAL:HG13	2:D:269:ILE:HD11	1.92	0.50
1:B:258:MET:HG2	1:B:675:TRP:HB3	1.93	0.50
1:A:435:ILE:HD11	1:A:488:ARG:HB3	1.94	0.50
2:D:313:ARG:NE	5:D:506:SO4:O3	2.40	0.50
1:B:162:ILE:HD12	1:B:238:LEU:HD21	1.92	0.50
2:D:96:LEU:HD23	2:D:396[A]:VAL:HG13	1.94	0.50
1:B:521:GLU:OE2	1:B:711:ARG:NE	2.34	0.50
1:B:331:LEU:HD13	1:B:422:VAL:HG12	1.93	0.49
1:B:510:PHE:CG	1:B:656[A]:LEU:HD21	2.48	0.49
1:B:523:LEU:HD11	1:B:560:MET:HE1	1.94	0.49
1:B:571:VAL:HA	1:B:576:GLY:O	2.12	0.49
1:B:470:MET:O	1:B:498:LYS:NZ	2.40	0.49
1:A:398:ASP:OD1	1:A:399:ALA:N	2.45	0.48
2:C:59:VAL:HG21	2:C:361:LEU:HB3	1.96	0.48
2:C:390:ILE:HB	2:C:394:MET:HB2	1.95	0.48
2:C:96:LEU:HD23	2:C:396[A]:VAL:HG13	1.95	0.47
2:C:173:ARG:NH2	2:C:348:LEU:O	2.37	0.47
1:A:515:ILE:HD11	1:A:551:LEU:HD21	1.97	0.47
1:B:434:ALA:O	1:B:454:ARG:NH2	2.40	0.47
1:B:104:PRO:HD3	1:B:216:ALA:HB1	1.97	0.47
2:C:309:LYS:HE2	2:C:313:ARG:HH22	1.80	0.47
1:A:108:ALA:HB1	1:A:197:LEU:HB3	1.97	0.47
2:D:156:ILE:HG12	2:D:298:ILE:HD11	1.98	0.46
1:B:416:GLN:HG3	1:B:448:LEU:HD23	1.97	0.46
1:A:259:PRO:HD2	1:A:295:VAL:HG11	1.96	0.46
2:D:203:LEU:HD11	2:D:207:GLU:HG3	1.98	0.45
2:C:110:TRP:CD1	2:D:313:ARG:HD3	2.51	0.45
1:A:258:MET:HG2	1:A:675:TRP:HB3	1.98	0.45
1:B:459:ILE:HD13	1:B:489:VAL:HG21	1.98	0.45
2:C:223:PRO:HA	2:C:253:THR:HG22	1.98	0.45
1:A:336:MET:SD	1:A:465:SER:HB3	2.57	0.45
1:A:408:VAL:HG11	1:A:436:LEU:HD23	1.99	0.45
2:D:258:SER:HB3	2:D:329:ALA:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ASN:HB3	1:A:581:HIS:CE1	2.52	0.45
1:A:248:ASN:O	1:A:252:GLN:HG2	2.17	0.44
2:D:22:SER:OG	2:D:207:GLU:OE2	2.24	0.44
1:B:340:ILE:HG21	1:B:409:ILE:HG21	1.99	0.44
2:C:43:HIS:HA	5:C:506:SO4:O4	2.17	0.44
1:A:104:PRO:HD3	1:A:216:ALA:HB1	1.98	0.44
2:D:69:ILE:HD13	2:D:119:VAL:HG11	1.99	0.44
1:A:336:MET:HB3	1:A:336:MET:HE3	1.92	0.44
1:A:634:ASP:OD1	1:A:700:ARG:NH2	2.37	0.44
2:C:381:ALA:O	2:C:402:ARG:NE	2.30	0.44
2:C:46:LEU:HD22	2:C:278:GLN:HB3	2.00	0.44
2:D:40:ARG:NH1	2:D:77:SER:O	2.36	0.44
1:B:45:LEU:HD23	1:B:52:ILE:HD13	1.99	0.44
1:B:248:ASN:O	1:B:252:GLN:HG2	2.18	0.43
1:A:146:LEU:HD22	1:A:291:VAL:HG22	1.99	0.43
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.90	0.43
1:A:683:ILE:HG12	1:A:697:PHE:CZ	2.53	0.43
2:D:382:ARG:HG3	2:D:383:ARG:HG3	1.99	0.43
2:C:99:VAL:HG13	2:C:269:ILE:HD11	2.01	0.43
1:A:673:PRO:HA	1:A:674:PRO:HD3	1.93	0.43
2:D:120:GLU:HB2	2:D:362:GLY:H	1.82	0.43
1:A:116:GLY:O	1:A:120:ILE:HG12	2.18	0.43
1:A:434:ALA:O	1:A:454:ARG:NH2	2.42	0.43
1:B:92:LYS:HD3	1:B:151:GLY:N	2.34	0.43
1:B:476:ILE:HG21	1:B:509:PHE:CE1	2.54	0.43
2:C:296:PRO:HG3	3:G:2:GLC:H61	2.01	0.43
1:A:416:GLN:HG3	1:A:448:LEU:HD23	2.00	0.43
2:C:325:GLU:HG2	2:C:368:ILE:HB	2.01	0.43
1:A:596:SER:N	1:A:602:ALA:O	2.51	0.43
1:A:462:HIS:HB3	1:A:474:GLU:HB3	2.01	0.42
2:D:96:LEU:HD23	2:D:396[B]:VAL:HG12	2.01	0.42
1:B:104:PRO:HG2	1:B:205:ILE:HG23	2.02	0.42
1:B:656[B]:LEU:HD13	1:B:662:ALA:HB2	2.00	0.42
2:C:326:LEU:HD23	2:C:334:VAL:HA	2.01	0.42
2:D:354:ALA:HB1	2:D:359:HIS:HB2	2.01	0.42
1:B:-11:HIS:ND1	1:B:43:ASP:OD1	2.49	0.42
1:B:406:ASP:N	1:B:406:ASP:OD1	2.51	0.42
2:D:62:VAL:HG11	2:D:130:ASP:HA	2.02	0.42
2:D:241:LYS:NZ	4:H:2:GLC:H61	2.35	0.42
2:D:390:ILE:HB	2:D:394:MET:HB2	2.02	0.42
2:D:390:ILE:HD11	2:D:396[B]:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:40:ARG:NH1	2:C:77:SER:O	2.48	0.41
1:A:-10:HIS:ND1	5:A:804:SO4:O3	2.53	0.41
1:B:583:ALA:O	1:B:587:VAL:HG23	2.20	0.41
2:D:149:GLN:H	2:D:149:GLN:HG2	1.66	0.41
2:C:203:LEU:HD11	2:C:207:GLU:HG3	2.01	0.41
1:A:459:ILE:HD11	1:A:486:LEU:HD12	2.01	0.41
1:A:246:PRO:HG3	2:D:138:PRO:HB3	2.02	0.41
1:B:101:LEU:HD12	1:B:101:LEU:HA	1.92	0.41
1:B:477:LYS:HD2	1:B:486:LEU:HD11	2.03	0.41
2:C:390:ILE:HD11	2:C:396[B]:VAL:HG23	2.02	0.41
1:B:336:MET:SD	1:B:465:SER:HB3	2.61	0.41
1:B:371:LEU:HD12	1:B:371:LEU:HA	1.96	0.41
2:C:7:ILE:HD11	2:C:286:ILE:HD11	2.01	0.41
2:C:290:ALA:HB1	2:C:309:LYS:HD3	2.02	0.41
2:D:295:ASP:OD2	2:D:298:ILE:HG22	2.21	0.41
1:B:250:ARG:NH1	2:C:145:MET:HG2	2.36	0.41
1:B:365:LYS:HD2	1:B:395:PRO:HD3	2.03	0.41
2:C:241:LYS:HE2	2:C:295:ASP:OD1	2.19	0.41
1:A:316:ARG:CZ	1:A:487:ALA:HB1	2.51	0.41
1:A:656[B]:LEU:HD13	1:A:662:ALA:HB2	2.02	0.41
1:B:698:VAL:HG13	1:B:714:PRO:HG3	2.03	0.41
1:A:45:LEU:HD23	1:A:52:ILE:HD13	2.02	0.41
1:A:477:LYS:HB2	1:A:486:LEU:HD11	2.03	0.40
1:A:536:GLU:OE2	1:A:605:TYR:OH	2.28	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	726/736 (99%)	697 (96%)	28 (4%)	1 (0%)	51 82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	728/736 (99%)	702 (96%)	25 (3%)	1 (0%)	51 82
2	C	397/403 (98%)	385 (97%)	12 (3%)	0	100 100
2	D	399/403 (99%)	387 (97%)	12 (3%)	0	100 100
All	All	2250/2278 (99%)	2171 (96%)	77 (3%)	2 (0%)	51 82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	148	PRO
1	A	148	PRO

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	549/566 (97%)	545 (99%)	4 (1%)	84 95
1	B	554/566 (98%)	552 (100%)	2 (0%)	91 97
2	C	308/310 (99%)	306 (99%)	2 (1%)	86 96
2	D	309/310 (100%)	309 (100%)	0	100 100
All	All	1720/1752 (98%)	1712 (100%)	8 (0%)	91 96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	194	VAL
1	B	479	GLU
2	C	396[A]	VAL
2	C	396[B]	VAL
1	A	-9	HIS
1	A	561	HIS
1	A	577	THR
1	A	599	LEU

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

Mol	Chain	Res	Type
1	A	556	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

4 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	$\#\|Z\| > 2$
3	GLC	G	1	3	11,11,12	0.32	0	15,15,17	0.60	0
3	GLC	G	2	3	12,12,12	0.26	0	17,17,17	0.71	0
4	GLC	H	1	4	12,12,12	0.19	0	17,17,17	0.33	0
4	GLC	H	2	4	11,11,12	0.38	0	15,15,17	0.32	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	GLC	G	1	3	-	2/2/19/22	0/1/1/1
3	GLC	G	2	3	-	2/2/22/22	0/1/1/1
4	GLC	H	1	4	-	0/2/22/22	0/1/1/1
4	GLC	H	2	4	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	GLC	C4-C5-C6-O6
3	G	1	GLC	C4-C5-C6-O6
3	G	2	GLC	O5-C5-C6-O6
3	G	1	GLC	O5-C5-C6-O6
4	H	2	GLC	O5-C5-C6-O6

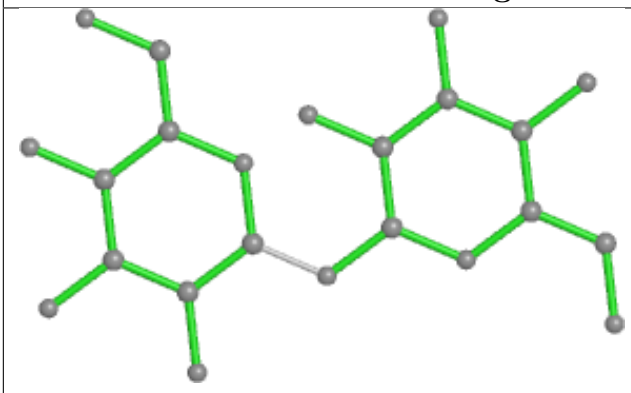
There are no ring outliers.

3 monomers are involved in 4 short contacts:

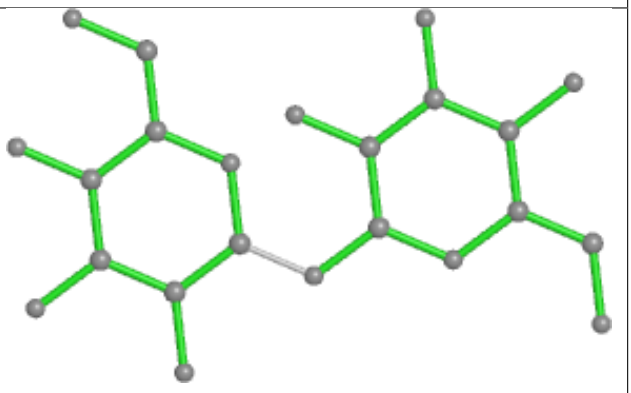
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	GLC	2	0
3	G	2	GLC	1	0
4	H	2	GLC	1	0

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

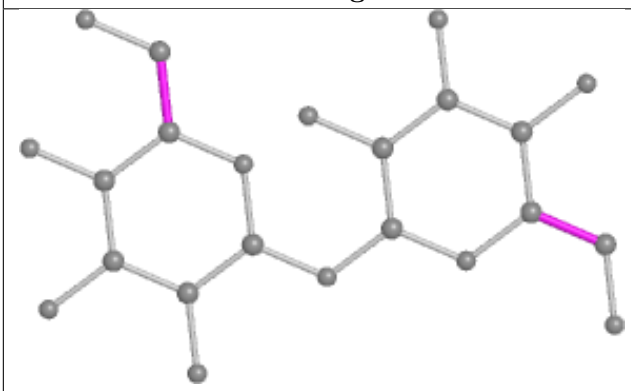
Oligosaccharide Chain G



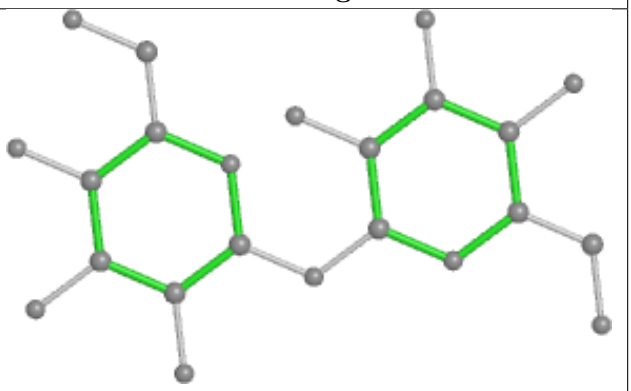
Bond lengths



Bond angles

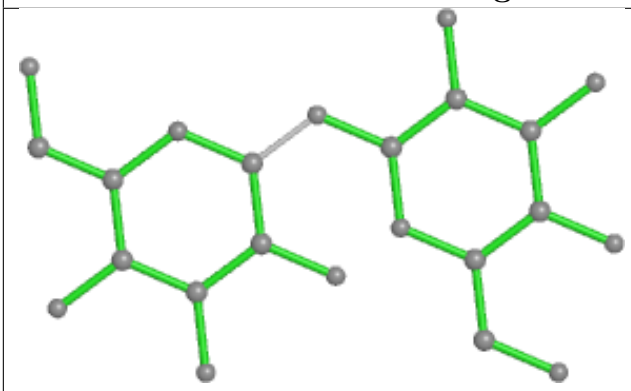


Torsions

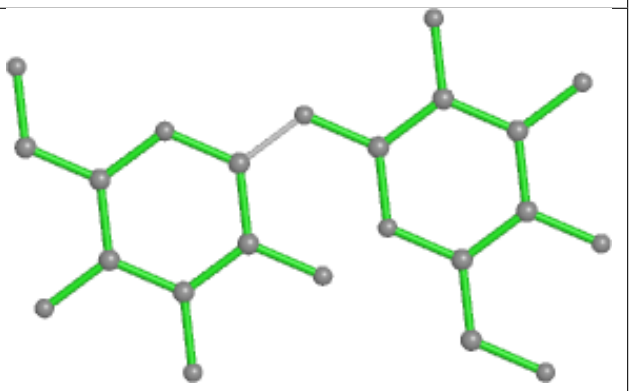


Rings

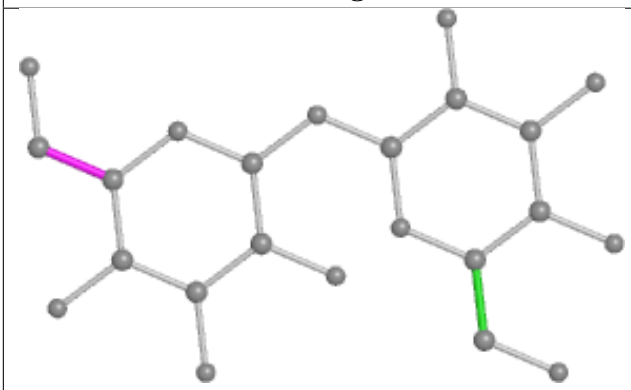
Oligosaccharide Chain H



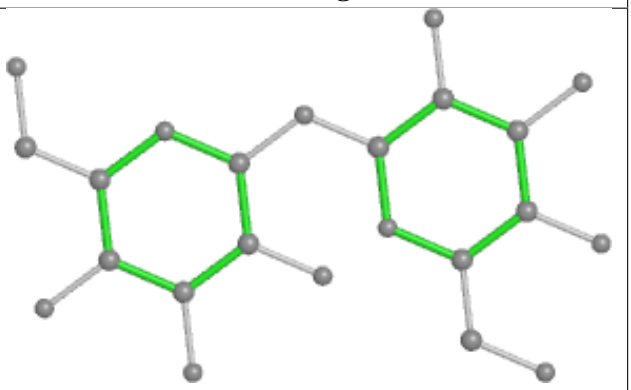
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

24 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	$\#\|Z\| > 2$
5	SO4	D	501	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	C	504	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	B	803	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	A	802	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	C	503	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	D	502	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	D	506	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	B	805	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	A	804	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	B	806	-	4,4,4	0.15	0	6,6,6	0.04	0
5	SO4	C	501	-	4,4,4	0.13	0	6,6,6	0.08	0
5	SO4	B	802	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	C	505	-	4,4,4	0.15	0	6,6,6	0.07	0
5	SO4	C	507	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	D	505	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	B	801	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	A	803	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	A	805	-	4,4,4	0.15	0	6,6,6	0.16	0
5	SO4	C	506	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	B	804	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	D	504	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	A	801	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	D	503	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	C	502	-	4,4,4	0.15	0	6,6,6	0.04	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.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	803	SO4	1	0
5	D	506	SO4	1	0
5	A	804	SO4	1	0
5	C	506	SO4	1	0
5	C	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, 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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	726/736 (98%)	0.38	62 (8%) 10 8	39, 73, 147, 241	0
1	B	726/736 (98%)	-0.02	19 (2%) 56 52	37, 64, 114, 196	0
2	C	398/403 (98%)	-0.17	1 (0%) 94 94	34, 50, 74, 109	0
2	D	399/403 (99%)	-0.15	0 100 100	36, 54, 80, 129	0
All	All	2249/2278 (98%)	0.06	82 (3%) 42 37	34, 60, 129, 241	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	576	GLY	33.1
1	A	575	GLY	22.7
1	A	577	THR	13.7
1	A	574	ALA	11.7
1	A	573	ASP	6.7
1	B	574	ALA	6.6
1	B	576	GLY	6.0
1	A	434	ALA	5.5
1	A	383	GLN	5.4
1	B	377	GLU	5.0
1	A	382	THR	5.0
1	A	572	GLU	4.7
1	A	387	ASP	4.6
1	B	575	GLY	4.4
1	A	1	MET	4.3
1	A	404	GLY	4.1
1	A	322	LYS	4.1
1	A	377	GLU	4.0
1	A	351	VAL	3.9
1	A	423	PHE	3.9
1	A	325	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	391	ALA	3.5
1	A	393	ILE	3.5
1	A	453	LYS	3.5
1	A	454	ARG	3.5
1	A	433	ASN	3.3
1	A	402	PHE	3.3
1	A	609	ASP	3.3
1	B	378	ARG	3.3
1	A	386	SER	3.3
1	A	389	LEU	3.2
1	A	622	THR	3.2
1	A	578	TYR	3.2
1	A	379	GLY	3.1
1	B	577	THR	3.1
1	A	452	VAL	3.1
1	A	3	ASP	3.0
1	A	357	SER	3.0
1	A	371	LEU	3.0
1	B	619	LEU	2.9
1	A	432	PRO	2.9
1	A	430	VAL	2.9
1	B	720	SER	2.8
1	A	384	GLU	2.8
1	A	428	ASP	2.8
1	B	1	MET	2.8
1	A	378	ARG	2.8
1	B	602	ALA	2.8
1	B	609	ASP	2.7
1	A	416	GLN	2.6
1	A	318	GLU	2.6
1	B	383	GLN	2.6
1	A	394	THR	2.6
1	A	435	ILE	2.5
1	A	216	ALA	2.5
1	A	436	LEU	2.5
1	A	455	GLN	2.5
1	B	571	VAL	2.5
1	B	572	GLU	2.5
1	A	486	LEU	2.4
1	A	374	LYS	2.4
1	A	2	PRO	2.4
1	B	374	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	327	ARG	2.3
1	A	425	GLU	2.3
1	A	429	ILE	2.3
1	B	328	ILE	2.3
1	A	407	PHE	2.3
1	A	320	ILE	2.2
1	A	459	ILE	2.1
1	A	405	VAL	2.1
2	C	279	GLY	2.1
1	B	457	ASP	2.1
1	A	367	TYR	2.1
1	A	409	ILE	2.1
1	A	335	MET	2.1
1	B	458	PHE	2.1
1	A	627	SER	2.1
1	A	349	TYR	2.1
1	B	689	PRO	2.1
1	A	623	PHE	2.0
1	A	591	ILE	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)

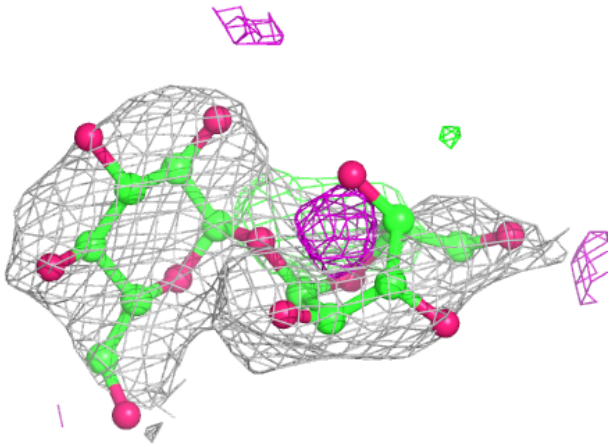
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

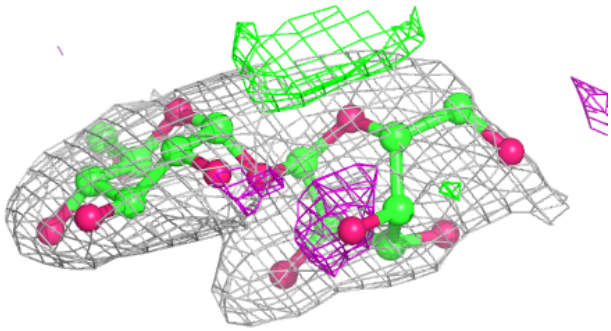
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GLC	H	2	11/12	0.77	0.45	80,83,88,92	11
3	GLC	G	2	12/12	0.78	0.30	72,84,106,108	12
4	GLC	H	1	12/12	0.79	0.42	64,70,79,80	12
3	GLC	G	1	11/12	0.86	0.24	78,86,90,100	11

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 G:

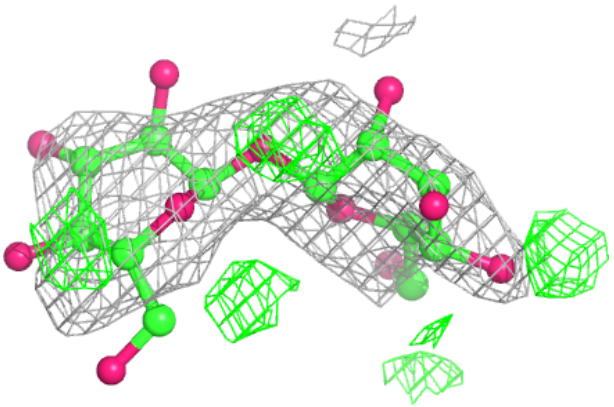
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

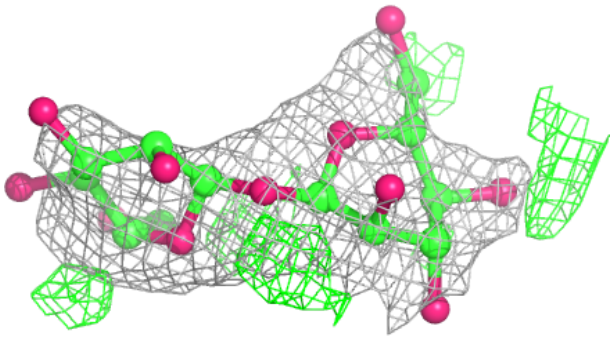


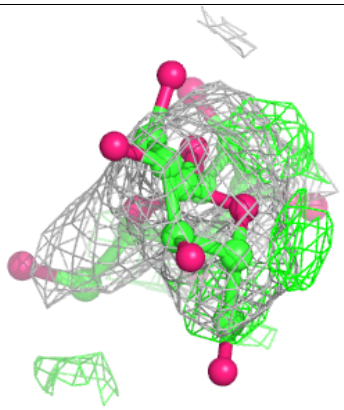


Electron density around Chain H:

$2mF_o$-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, 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(Å^2)	Q<0.9
5	SO4	C	506	5/5	0.76	0.41	102,151,167,190	0
5	SO4	D	506	5/5	0.79	0.18	115,135,142,172	0
5	SO4	A	804	5/5	0.81	0.27	98,107,127,150	0
5	SO4	B	806	5/5	0.85	0.62	120,130,156,186	0
5	SO4	B	805	5/5	0.85	0.36	116,119,154,170	0
5	SO4	C	507	5/5	0.88	0.33	111,131,139,164	0
5	SO4	D	505	5/5	0.89	0.34	103,110,131,162	0
5	SO4	B	803	5/5	0.89	0.18	91,123,131,151	0
5	SO4	A	805	5/5	0.90	0.13	99,120,125,129	0
5	SO4	D	504	5/5	0.91	0.12	127,129,133,143	5
5	SO4	C	504	5/5	0.91	0.34	100,101,116,141	0
5	SO4	C	505	5/5	0.91	0.15	88,92,94,115	0
5	SO4	C	502	5/5	0.93	0.15	80,84,107,118	0
5	SO4	B	804	5/5	0.93	0.26	70,91,107,130	0
5	SO4	D	503	5/5	0.94	0.12	102,104,110,115	0
5	SO4	C	503	5/5	0.95	0.18	95,99,106,122	0
5	SO4	D	502	5/5	0.95	0.29	78,88,105,109	0
5	SO4	B	802	5/5	0.95	0.14	69,85,96,101	0
5	SO4	D	501	5/5	0.96	0.22	79,83,99,101	0
5	SO4	A	802	5/5	0.96	0.14	63,70,101,101	0
5	SO4	A	803	5/5	0.97	0.08	79,80,108,112	0
5	SO4	A	801	5/5	0.97	0.12	70,76,108,117	0
5	SO4	C	501	5/5	0.97	0.23	84,85,92,97	0
5	SO4	B	801	5/5	0.98	0.09	76,81,86,90	0

6.5 Other polymers (i)

There are no such residues in this entry.