Full wwPDB X-ray Structure Validation Report (i)

Dec 9, 2023 – 12:57 pm GMT

PDB ID	:	1OJO
Title	:	SPECIFICITY AND MECHANISM OF STREPTOCOCCUS PNEUMONIAE HYALURONATE LYASE: COMPLEX OF THE TYR408PHE MUTANT WITH 4-SULPHATED CHONDROITIN DISACCHARIDE
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Deposited on	:	2003-07-11
Resolution	:	1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

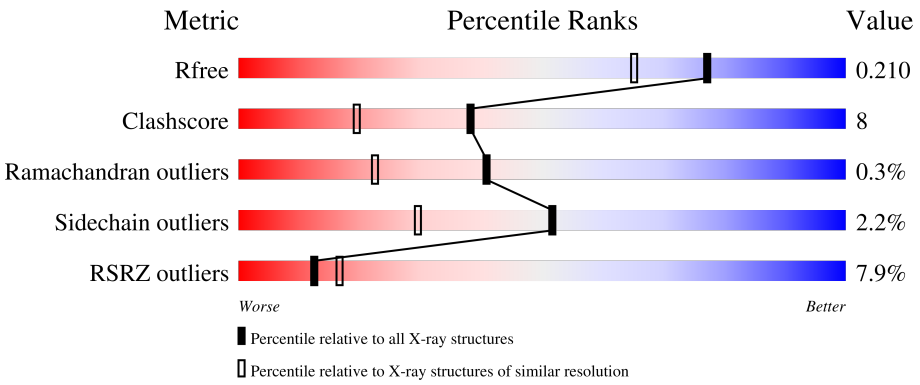
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	731	8% 84% 13% • •
2	B	2	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6581 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.

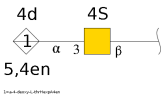
- Molecule 1 is a protein called HYALURONATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	722	5995	3770	1006	1196	23	0	23	0

There are 8 discrepancies between the modelled and reference sequences:

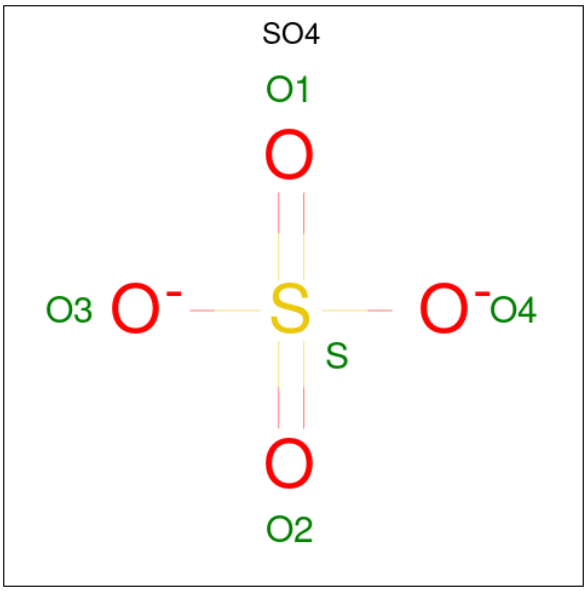
Chain	Residue	Modelled	Actual	Comment	Reference
A	173	THR	ALA	conflict	UNP Q54873
A	196	ASP	GLU	SEE REMARK 999	UNP Q54873
A	223	ILE	THR	conflict	UNP Q54873
A	408	PHE	TYR	engineered mutation	UNP Q54873
A	496	ARG	CYS	conflict	UNP Q54873
A	541	THR	PRO	conflict	UNP Q54873
A	704	SER	GLY	conflict	UNP Q54873
A	736	SER	PHE	conflict	UNP Q54873

- Molecule 2 is an oligosaccharide called 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-4-O-sulfo-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	2	30	14	1	14	1	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

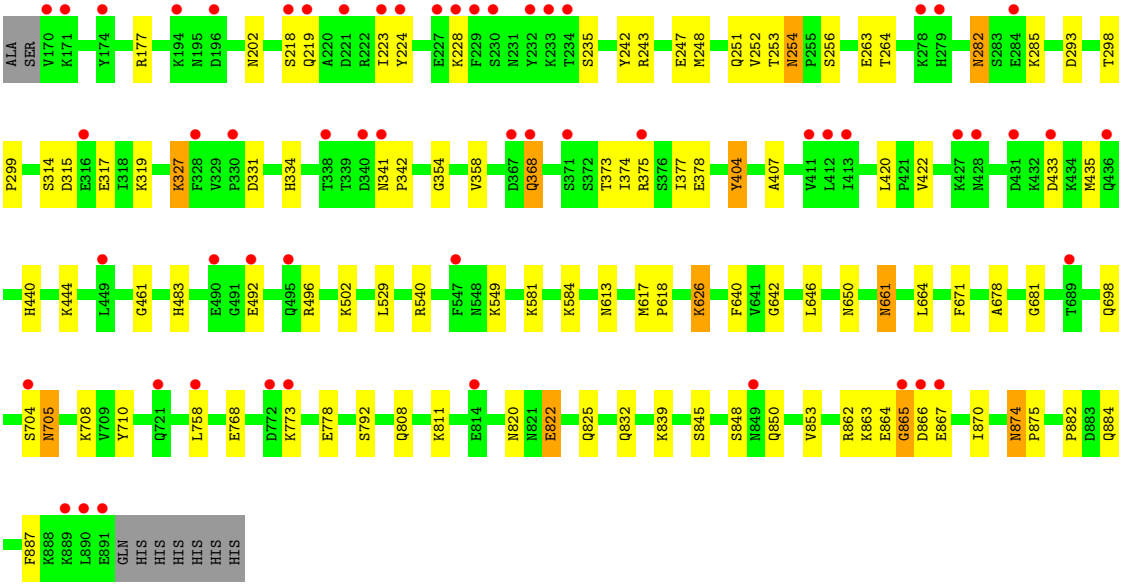
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	536	Total O 536 536	0	0

3 Residue-property plots (i)

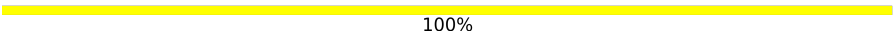
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: HYALURONATE LYASE

Chain A:



• Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-4-O-sulfo-beta-D-galactopyranose

Chain B: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.74Å 103.78Å 101.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.96 – 1.75 40.43 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.96-1.75) 86.9 (40.43-1.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 1.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.202 , 0.219 0.193 , 0.210	Depositor DCC
R_{free} test set	5959 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6581	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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 (i)

5.1 Standard geometry (i)

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

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	0.31	0/6116	0.60	0/8251

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5995	0	5803	90	0
2	B	30	0	14	0	0
3	A	20	0	0	1	0
4	A	536	0	0	9	0
All	All	6581	0	5817	90	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 8.

All (90) 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:A:613:ASN:H	1:A:698:GLN:HE22	1.03	0.97
1:A:315:ASP:O	1:A:319[B]:LYS:HG3	1.87	0.75
1:A:248:MET:O	1:A:252[A]:VAL:HG23	1.91	0.70
1:A:708:LYS:HE3	1:A:710:TYR:OH	1.95	0.67
1:A:223:ILE:HG13	1:A:224:TYR:CD2	2.31	0.66
1:A:529:LEU:C	1:A:529:LEU:HD23	2.17	0.65
1:A:282:ASN:ND2	1:A:285:LYS:HG2	2.13	0.64
1:A:581:LYS:HB3	1:A:768:GLU:HB2	1.81	0.62
1:A:704[A]:SER:C	1:A:705:ASN:HD22	2.03	0.62
1:A:874:ASN:C	1:A:874:ASN:HD22	2.03	0.62
1:A:839:LYS:HD2	1:A:853:VAL:HG23	1.83	0.59
1:A:863:LYS:HE2	1:A:865[A]:GLY:O	2.01	0.59
1:A:422:VAL:HA	4:A:2007:HOH:O	2.03	0.58
1:A:626:LYS:CD	1:A:626:LYS:H	2.16	0.58
1:A:282:ASN:C	1:A:282:ASN:HD22	2.07	0.58
1:A:704[B]:SER:C	1:A:705:ASN:HD22	2.05	0.58
1:A:865[B]:GLY:C	1:A:867:GLU:H	2.06	0.58
1:A:254:ASN:C	1:A:254:ASN:HD22	2.06	0.57
1:A:492:GLU:OE2	1:A:496:ARG:HD3	2.06	0.55
1:A:502:LYS:HB2	1:A:529:LEU:HD21	1.87	0.55
1:A:440:HIS:CE1	1:A:444[B]:LYS:HD2	2.42	0.55
1:A:254:ASN:ND2	1:A:256:SER:H	2.05	0.55
1:A:626:LYS:H	1:A:626:LYS:HD3	1.72	0.54
1:A:243:ARG:O	1:A:247:GLU:HG3	2.07	0.54
1:A:864:GLU:O	1:A:865[B]:GLY:C	2.46	0.54
1:A:373:THR:O	1:A:377:ILE:HG12	2.08	0.54
1:A:650:ASN:HD21	1:A:832:GLN:HE22	1.55	0.54
1:A:613:ASN:N	1:A:698:GLN:HE22	1.88	0.53
1:A:646:LEU:HD21	1:A:862[A]:ARG:HB2	1.91	0.53
1:A:502:LYS:CB	1:A:529:LEU:HD21	2.39	0.52
1:A:248:MET:O	1:A:252[B]:VAL:HG13	2.08	0.52
1:A:440:HIS:NE2	1:A:444[B]:LYS:HD2	2.25	0.52
1:A:264:THR:HG22	4:A:2075:HOH:O	2.09	0.51
1:A:626:LYS:HD3	1:A:626:LYS:N	2.27	0.50
1:A:252[B]:VAL:HG23	1:A:253:THR:HG23	1.93	0.49
1:A:327:LYS:HD3	1:A:327:LYS:C	2.32	0.49
1:A:331:ASP:OD2	1:A:334:HIS:ND1	2.43	0.49
1:A:822:GLU:H	1:A:822:GLU:CD	2.16	0.49
1:A:584:LYS:HE2	3:A:1200:SO4:O1	2.12	0.49
1:A:848:SER:O	1:A:850:GLN:HG3	2.12	0.49
1:A:864:GLU:O	1:A:867:GLU:HB2	2.12	0.48
1:A:298:THR:HB	1:A:299:PRO:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LEU:HD13	1:A:435:MET:CE	2.44	0.48
1:A:374:ILE:O	1:A:378:GLU:HG3	2.14	0.48
1:A:314:SER:OG	1:A:317:GLU:HG3	2.14	0.47
1:A:808[B]:GLN:HG2	4:A:2479:HOH:O	2.14	0.47
1:A:820:ASN:HD22	1:A:825:GLN:HG2	1.78	0.47
1:A:650:ASN:ND2	1:A:862[B]:ARG:HH21	2.13	0.47
1:A:808[B]:GLN:HG3	4:A:2484:HOH:O	2.14	0.47
1:A:811:LYS:HE3	4:A:2481:HOH:O	2.14	0.47
1:A:845:SER:HB2	1:A:853:VAL:HG23	1.97	0.46
1:A:228[B]:LYS:HG2	1:A:228[B]:LYS:O	2.15	0.46
1:A:540[B]:ARG:HH11	1:A:540[B]:ARG:HG2	1.80	0.46
1:A:584:LYS:NZ	1:A:768:GLU:HG2	2.31	0.46
1:A:242:TYR:CD2	1:A:298:THR:HG23	2.52	0.45
1:A:671:PHE:HB2	1:A:678:ALA:HB3	1.99	0.45
1:A:642:GLY:HA2	4:A:2300:HOH:O	2.17	0.45
1:A:705:ASN:HD22	1:A:705:ASN:N	2.12	0.44
1:A:864:GLU:O	1:A:865[B]:GLY:O	2.36	0.44
1:A:626:LYS:H	1:A:626:LYS:HZ3	1.65	0.44
1:A:404:TYR:CE1	1:A:461:GLY:HA3	2.53	0.43
1:A:549[A]:LYS:HE3	4:A:2515:HOH:O	2.19	0.43
1:A:254:ASN:C	1:A:254:ASN:ND2	2.68	0.43
1:A:882:PRO:HB2	1:A:884:GLN:NE2	2.33	0.43
1:A:758[B]:LEU:HD23	1:A:778:GLU:HB2	1.99	0.43
1:A:354:GLY:O	1:A:358:VAL:HB	2.20	0.42
1:A:661:ASN:C	1:A:661:ASN:HD22	2.23	0.42
1:A:870:ILE:HD11	1:A:887:PHE:CD2	2.55	0.42
1:A:341:ASN:N	1:A:342:PRO:HD3	2.34	0.42
1:A:483:HIS:NE2	1:A:529:LEU:HD12	2.35	0.42
1:A:671:PHE:CD1	1:A:671:PHE:N	2.87	0.42
1:A:420:LEU:HD13	1:A:435:MET:HE3	2.00	0.42
1:A:617:MET:HA	1:A:618[B]:PRO:HD3	1.95	0.42
1:A:862[A]:ARG:HD3	1:A:864:GLU:OE1	2.20	0.41
1:A:865[B]:GLY:O	1:A:867:GLU:N	2.53	0.41
1:A:235:SER:HB2	1:A:293:ASP:HB2	2.02	0.41
1:A:202:ASN:ND2	1:A:251:GLN:HE22	2.16	0.41
1:A:882:PRO:HB2	1:A:884:GLN:HE22	1.86	0.41
1:A:177:ARG:HA	1:A:177:ARG:NE	2.36	0.41
1:A:650:ASN:ND2	1:A:862[B]:ARG:NH2	2.69	0.41
1:A:529:LEU:C	1:A:529:LEU:CD2	2.87	0.41
1:A:368:GLN:HE21	1:A:368:GLN:HB3	1.71	0.40
1:A:664:LEU:HD23	1:A:664:LEU:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808[A]:GLN:HG3	4:A:2485:HOH:O	2.20	0.40
1:A:865[B]:GLY:C	1:A:867:GLU:N	2.73	0.40
1:A:263[A]:GLU:H	1:A:263[A]:GLU:HG3	1.72	0.40
1:A:640:PHE:CD1	1:A:875:PRO:HG2	2.56	0.40
1:A:375:ARG:HD3	4:A:2166:HOH:O	2.21	0.40
1:A:404:TYR:CD1	1:A:407:ALA:HB3	2.57	0.40
1:A:681:GLY:O	1:A:792:SER:HB2	2.21	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	743/731 (102%)	714 (96%)	26 (4%)	3 (0%)	34 17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	866	ASP
1	A	865[A]	GLY
1	A	865[B]	GLY

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	663/650 (102%)	648 (98%)	15 (2%)	50 28

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	SER
1	A	219	GLN
1	A	254	ASN
1	A	282	ASN
1	A	327	LYS
1	A	368	GLN
1	A	404	TYR
1	A	433[A]	ASP
1	A	433[B]	ASP
1	A	626	LYS
1	A	661	ASN
1	A	705	ASN
1	A	773	LYS
1	A	822	GLU
1	A	874	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	231	ASN
1	A	237	ASN
1	A	254	ASN
1	A	261	GLN
1	A	277	HIS
1	A	282	ASN
1	A	341	ASN
1	A	368	GLN
1	A	386	GLN
1	A	392	GLN
1	A	418	GLN
1	A	650	ASN
1	A	661	ASN
1	A	667	HIS
1	A	683	ASN
1	A	698	GLN
1	A	759	GLN

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Mol	Chain	Res	Type
1	A	788	GLN
1	A	820	ASN
1	A	825	GLN
1	A	874	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

2 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	ASG	B	1	2	19,19,19	2.12	7 (36%)	23,28,28	1.17	1 (4%)
2	GCD	B	2	2	10,11,12	4.72	4 (40%)	13,15,17	3.73	9 (69%)

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	ASG	B	1	2	-	0/11/31/31	0/1/1/1
2	GCD	B	2	2	-	0/4/17/20	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	GCD	O5-C5	11.82	1.54	1.37
2	B	2	GCD	O5-C1	6.78	1.55	1.45
2	B	1	ASG	O5-C5	4.23	1.54	1.44
2	B	2	GCD	C3-C4	4.07	1.55	1.50
2	B	1	ASG	O5-C1	3.87	1.52	1.42
2	B	1	ASG	C2-N2	3.86	1.52	1.45
2	B	1	ASG	O4-C4	-3.24	1.39	1.46
2	B	2	GCD	C4-C5	3.13	1.38	1.33
2	B	1	ASG	C3-C4	2.75	1.59	1.52
2	B	1	ASG	O4-S	-2.53	1.49	1.57
2	B	1	ASG	C7-N2	2.50	1.42	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	GCD	O5-C5-C4	-7.46	118.51	124.81
2	B	2	GCD	C2-C3-C4	5.55	119.91	112.32
2	B	2	GCD	O3-C3-C4	4.88	120.28	109.31
2	B	2	GCD	O3-C3-C2	-4.66	101.33	109.42
2	B	2	GCD	O6A-C6-C5	-3.56	111.04	120.48
2	B	2	GCD	O6B-C6-O6A	3.36	131.29	123.61
2	B	2	GCD	O5-C5-C6	3.07	116.12	111.52
2	B	1	ASG	C8-C7-N2	-2.62	111.66	116.10
2	B	2	GCD	C3-C4-C5	-2.51	117.35	121.60
2	B	2	GCD	C1-C2-C3	-2.51	106.58	109.67

There are no chirality outliers.

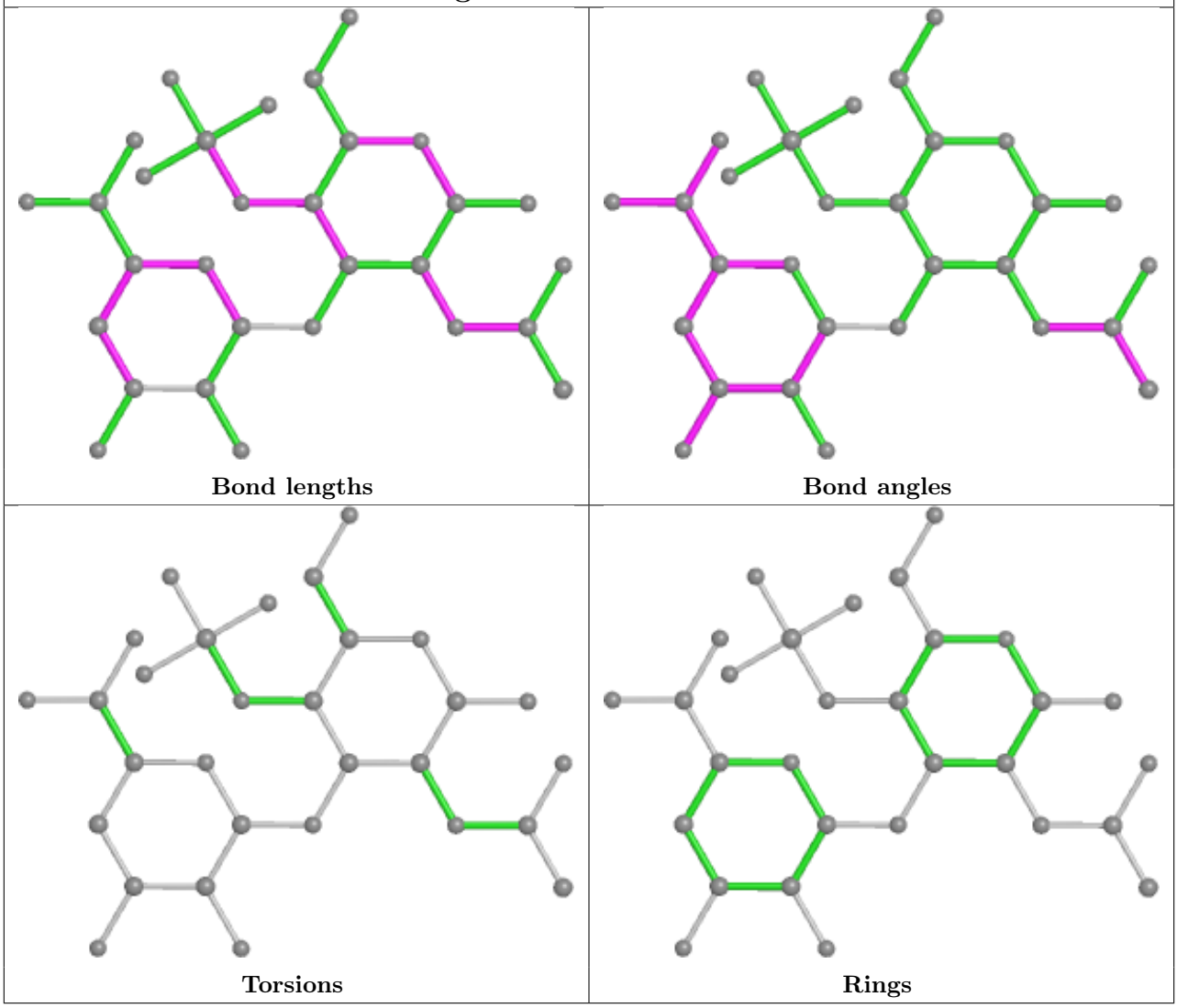
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain B



5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	1203	-	4,4,4	0.19	0	6,6,6	0.05	0
3	SO4	A	1201	-	4,4,4	0.15	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	1202	-	4,4,4	0.19	0	6,6,6	0.06	0
3	SO4	A	1200	-	4,4,4	0.15	0	6,6,6	0.05	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	1200	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	722/731 (98%)	0.45	57 (7%) 12 16	12, 23, 41, 58	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	VAL	11.9
1	A	224	TYR	7.5
1	A	221	ASP	7.3
1	A	223	ILE	6.1
1	A	233	LYS	5.3
1	A	427	LYS	5.3
1	A	171	LYS	5.1
1	A	891	GLU	4.9
1	A	340[A]	ASP	4.5
1	A	232	TYR	4.4
1	A	279	HIS	4.3
1	A	230	SER	4.1
1	A	316[A]	GLU	4.0
1	A	375	ARG	4.0
1	A	865[A]	GLY	4.0
1	A	341	ASN	4.0
1	A	866	ASP	3.7
1	A	495	GLN	3.4
1	A	433[A]	ASP	3.4
1	A	890	LEU	3.1
1	A	368	GLN	3.1
1	A	428	ASN	3.0
1	A	449	LEU	3.0
1	A	689	THR	3.0
1	A	174	TYR	2.9
1	A	704[A]	SER	2.8
1	A	867	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	284	GLU	2.7
1	A	218	SER	2.7
1	A	849	ASN	2.7
1	A	431	ASP	2.7
1	A	278	LYS	2.6
1	A	758[A]	LEU	2.6
1	A	773	LYS	2.5
1	A	228[A]	LYS	2.5
1	A	492	GLU	2.5
1	A	194	LYS	2.5
1	A	889	LYS	2.4
1	A	547	PHE	2.4
1	A	227	GLU	2.4
1	A	411	VAL	2.4
1	A	234	THR	2.4
1	A	338	THR	2.4
1	A	413	ILE	2.3
1	A	219	GLN	2.3
1	A	772	ASP	2.3
1	A	436	GLN	2.2
1	A	196	ASP	2.2
1	A	490	GLU	2.2
1	A	721	GLN	2.1
1	A	814	GLU	2.1
1	A	330	PRO	2.1
1	A	367	ASP	2.1
1	A	328	PHE	2.1
1	A	412	LEU	2.1
1	A	371	SER	2.1
1	A	229	PHE	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)

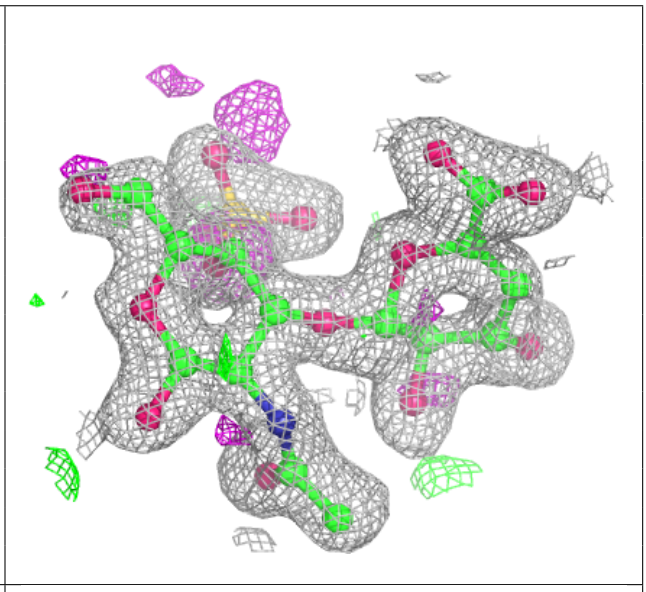
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

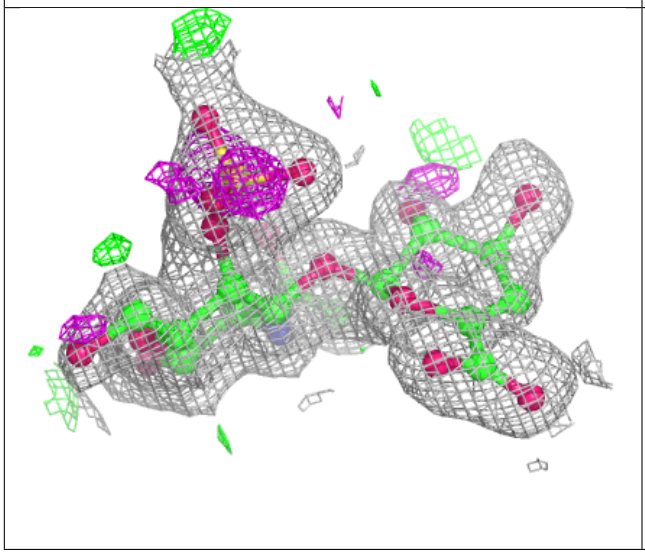
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GCD	B	2	11/12	0.88	0.11	24,30,33,33	0
2	ASG	B	1	19/19	0.90	0.11	21,27,41,43	0

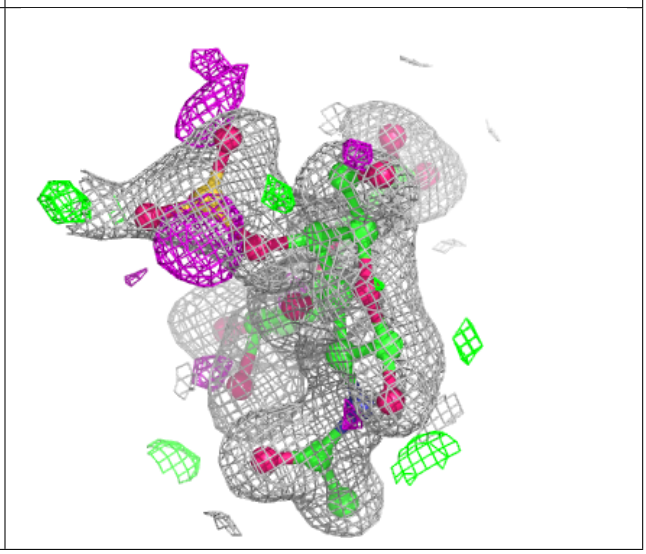
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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	1200	5/5	0.92	0.18	34,39,45,48	0
3	SO4	A	1201	5/5	0.93	0.14	34,34,44,45	0
3	SO4	A	1202	5/5	0.94	0.15	53,54,55,55	0
3	SO4	A	1203	5/5	0.96	0.25	58,60,62,63	0

6.5 Other polymers (i)

There are no such residues in this entry.