



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:17 AM UTC

PDB ID : 1AUK / pdb_00001auk
Title : HUMAN ARYLSULFATASE A
Authors : Lukatela, G.; Krauss, N.; Theis, K.; Gieselmann, V.; Von Figura, K.; Saenger, W.
Deposited on : 1997-08-29
Resolution : 2.10 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

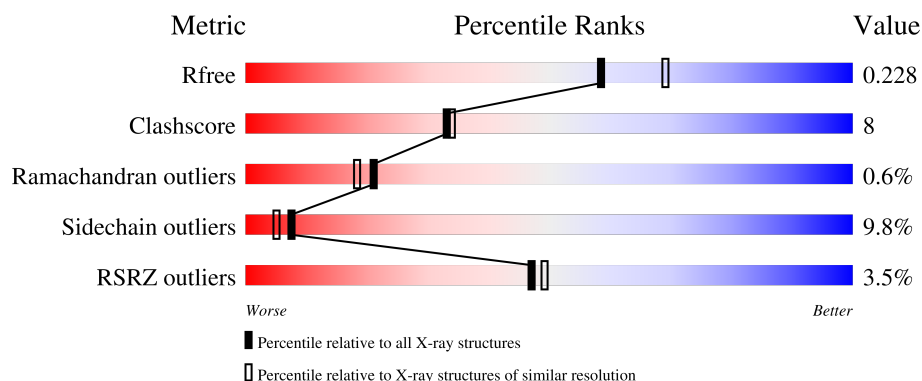
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	489	
2	B	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	1	X	-	-	-
2	NAG	B	2	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3785 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 ARYLSULFATASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3580	2281	611	665	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	FGL	CYS	modified residue	UNP P15289

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

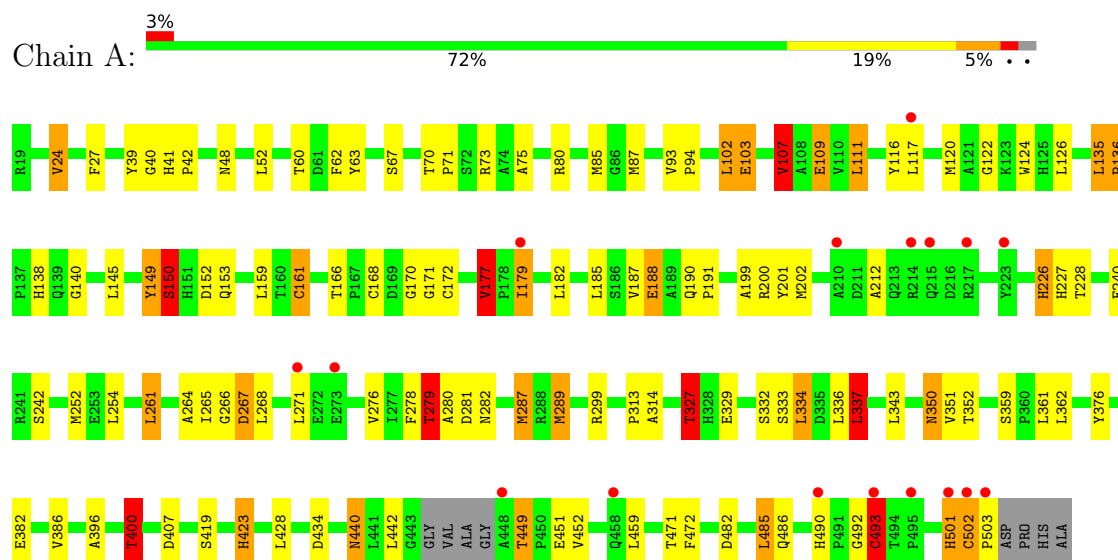
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	176	Total	O	0	0
			176	176		

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: ARYLSULFATASE A



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	132.63Å 132.63Å 192.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-2.10) 98.3 (30.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.13 (at 2.10Å)	Xtriage
Refinement program	REFMAC, X-PLOR	Depositor
R, R_{free}	0.232 , 0.273 0.197 , 0.228	Depositor DCC
R_{free} test set	2463 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.008 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3785	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FGL, NAG, MG

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	0.82	2/3682 (0.1%)	1.65	62/5031 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	503	PRO	N-CD	5.80	1.55	1.47
1	A	41	HIS	CA-C	-5.19	1.47	1.53

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	CYS	N-CA-CB	-8.94	95.39	110.49
1	A	179	ILE	CA-CB-CG2	8.93	125.67	110.50
1	A	327	THR	CB-CA-C	-8.11	94.53	109.37
1	A	27	PHE	CA-CB-CG	7.97	121.77	113.80
1	A	136	PRO	N-CA-C	7.96	120.41	110.70
1	A	177	VAL	N-CA-CB	-7.74	100.37	111.21
1	A	400	THR	N-CA-CB	-7.63	97.48	111.37
1	A	407	ASP	CA-CB-CG	7.33	119.93	112.60
1	A	73	ARG	CD-NE-CZ	7.32	134.65	124.40
1	A	502	CYS	CA-C-O	7.22	130.05	120.16
1	A	179	ILE	N-CA-C	6.72	115.53	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ILE	N-CA-CB	-6.66	103.89	110.08
1	A	150	SER	N-CA-CB	6.62	119.71	110.17
1	A	107	VAL	N-CA-CB	6.51	120.35	110.58
1	A	170	GLY	N-CA-C	6.45	124.11	115.59
1	A	281	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	171	GLY	N-CA-C	6.40	123.85	115.40
1	A	80	ARG	NE-CZ-NH2	6.25	124.82	119.20
1	A	107	VAL	CB-CA-C	-6.17	103.70	112.22
1	A	279	THR	CB-CA-C	-6.10	99.06	113.02
1	A	299	ARG	NH1-CZ-NH2	6.04	127.15	119.30
1	A	39	TYR	N-CA-C	-5.93	104.57	112.94
1	A	109	GLU	CA-CB-CG	-5.90	102.30	114.10
1	A	503	PRO	CA-N-CD	-5.88	103.76	112.00
1	A	279	THR	N-CA-CB	5.84	121.16	110.76
1	A	440	ASN	CA-CB-CG	5.83	118.43	112.60
1	A	350	ASN	CA-CB-CG	-5.82	106.78	112.60
1	A	333	SER	CA-C-N	5.72	129.76	120.60
1	A	333	SER	C-N-CA	5.72	129.76	120.60
1	A	492	GLY	CA-C-O	5.66	125.87	119.59
1	A	179	ILE	CB-CG1-CD1	-5.62	101.99	113.80
1	A	152	ASP	N-CA-C	-5.60	105.79	113.30
1	A	40	GLY	N-CA-C	5.57	122.17	114.92
1	A	472	PHE	CA-CB-CG	5.57	119.37	113.80
1	A	42	PRO	CA-C-N	-5.55	113.49	121.98
1	A	42	PRO	C-N-CA	-5.55	113.49	121.98
1	A	60	THR	CA-C-O	5.55	125.24	119.14
1	A	226	HIS	N-CA-C	-5.53	106.38	113.23
1	A	376	TYR	CA-C-O	5.52	127.33	120.54
1	A	149	TYR	CA-C-O	-5.50	115.28	121.05
1	A	287	MET	O-C-N	-5.46	115.98	122.20
1	A	289	MET	CB-CA-C	-5.39	110.37	116.63
1	A	337	LEU	CA-CB-CG	5.39	135.18	116.30
1	A	187	VAL	CB-CA-C	-5.39	105.48	111.35
1	A	166	THR	CA-C-O	5.37	123.60	119.46
1	A	63	TYR	N-CA-C	5.29	117.73	109.52
1	A	327	THR	N-CA-CB	5.27	119.28	110.85
1	A	226	HIS	CA-CB-CG	-5.24	108.56	113.80
1	A	102	LEU	CA-C-O	-5.23	113.96	119.97
1	A	299	ARG	N-CA-CB	-5.19	101.82	110.23
1	A	122	GLY	CA-C-N	5.18	128.21	120.95
1	A	122	GLY	C-N-CA	5.18	128.21	120.95
1	A	501	HIS	CA-CB-CG	5.12	118.92	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	LEU	CA-C-N	5.12	125.66	120.38
1	A	135	LEU	C-N-CA	5.12	125.66	120.38
1	A	279	THR	CA-CB-OG1	5.12	117.28	109.60
1	A	138	HIS	CA-CB-CG	-5.07	108.73	113.80
1	A	48	ASN	CA-CB-CG	-5.05	107.55	112.60
1	A	423	HIS	CA-CB-CG	-5.05	108.75	113.80
1	A	87	MET	CA-C-N	5.04	130.32	122.26
1	A	87	MET	C-N-CA	5.04	130.32	122.26
1	A	434	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	327	THR	Mainchain

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	3580	0	3451	54	0
2	B	28	0	25	1	0
3	A	1	0	0	0	0
4	A	176	0	0	7	0
All	All	3785	0	3476	55	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 (55) 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:102:LEU:O	4:A:605:HOH:O	2.00	0.76
1:A:117:LEU:HD23	1:A:212:ALA:HB2	1.73	0.71
1:A:67:SER:OG	4:A:714:HOH:O	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:THR:HG22	1:A:452:VAL:H	1.61	0.66
1:A:423:HIS:HD2	4:A:667:HOH:O	1.77	0.66
1:A:482:ASP:HB3	1:A:485:LEU:HD22	1.83	0.60
1:A:150:SER:H	1:A:153:GLN:HE21	1.50	0.59
1:A:109:GLU:OE2	4:A:715:HOH:O	2.17	0.58
1:A:265:ILE:HG22	1:A:271:LEU:HD23	1.84	0.58
1:A:242:SER:HB3	1:A:252:MET:HE2	1.86	0.58
1:A:490:HIS:O	1:A:493:CYS:HB2	2.02	0.58
1:A:62:PHE:CE1	1:A:279:THR:HG21	2.40	0.57
1:A:400:THR:CG2	1:A:423:HIS:HE1	2.18	0.56
1:A:279:THR:HG22	1:A:280:ALA:H	1.71	0.55
1:A:107:VAL:HG13	1:A:337:LEU:HB2	1.89	0.55
1:A:75:ALA:HB1	1:A:334:LEU:HD13	1.89	0.54
1:A:202:MET:SD	1:A:261:LEU:HD13	2.48	0.53
1:A:400:THR:HG21	1:A:423:HIS:HE1	1.72	0.53
1:A:24:VAL:CG1	1:A:276:VAL:HG22	2.40	0.52
1:A:201:TYR:OH	1:A:226:HIS:HE1	1.92	0.52
1:A:501:HIS:O	1:A:502:CYS:HB3	2.10	0.52
1:A:188:GLU:O	1:A:188:GLU:HG3	2.09	0.51
1:A:327:THR:HG22	1:A:329:GLU:H	1.75	0.51
1:A:177:VAL:HB	1:A:486:GLN:OE1	2.11	0.51
1:A:111:LEU:O	1:A:116:TYR:HB2	2.12	0.48
1:A:109:GLU:CD	4:A:715:HOH:O	2.56	0.47
1:A:428:LEU:H	1:A:440:ASN:ND2	2.12	0.47
1:A:135:LEU:HB3	1:A:136:PRO:HD2	1.96	0.47
1:A:124:TRP:CE2	1:A:126:LEU:HB2	2.51	0.46
1:A:149:TYR:HB2	1:A:153:GLN:NE2	2.32	0.45
1:A:400:THR:HG23	4:A:724:HOH:O	2.17	0.45
1:A:289:MET:HE2	4:A:703:HOH:O	2.16	0.45
1:A:190:GLN:HA	1:A:191:PRO:HA	1.70	0.44
1:A:266:GLY:O	1:A:267:ASP:C	2.60	0.44
1:A:120:MET:HE1	1:A:124:TRP:HA	2.01	0.43
1:A:264:ALA:O	1:A:268:LEU:HG	2.19	0.43
1:A:327:THR:HG21	1:A:361:LEU:HD11	2.01	0.43
1:A:242:SER:N	1:A:252:MET:HE1	2.33	0.43
1:A:199:ALA:O	1:A:200:ARG:C	2.63	0.42
1:A:161:CYS:HB2	1:A:168:CYS:HA	2.02	0.42
1:A:396:ALA:HB2	1:A:459:LEU:HD13	2.01	0.42
1:A:332:SER:OG	1:A:334:LEU:HB2	2.20	0.41
1:A:70:THR:N	1:A:71:PRO:HD2	2.35	0.41
1:A:93:VAL:HB	1:A:94:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:HD12	1:A:182:LEU:O	2.20	0.41
1:A:159:LEU:HD21	1:A:191:PRO:HG3	2.02	0.41
1:A:227:HIS:HA	1:A:228:THR:HA	1.82	0.41
1:A:279:THR:HG23	1:A:314:ALA:HB2	2.02	0.41
1:A:327:THR:HG22	1:A:329:GLU:HG3	2.03	0.41
1:A:150:SER:H	1:A:153:GLN:NE2	2.15	0.41
1:A:103:GLU:H	1:A:103:GLU:HG3	1.57	0.41
1:A:278:PHE:O	1:A:314:ALA:HA	2.21	0.41
2:B:1:NAG:H3	2:B:1:NAG:H83	2.02	0.41
1:A:279:THR:HG23	1:A:313:PRO:O	2.20	0.41
1:A:109:GLU:HG3	1:A:140:GLY:HA3	2.02	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	476/489 (97%)	451 (95%)	22 (5%)	3 (1%)	21 18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	493	CYS
1	A	267	ASP
1	A	172	CYS

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	376/384 (98%)	339 (90%)	37 (10%)	7 5

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	52	LEU
1	A	85	MET
1	A	103	GLU
1	A	107	VAL
1	A	111	LEU
1	A	150	SER
1	A	161	CYS
1	A	177	VAL
1	A	179	ILE
1	A	185	LEU
1	A	188	GLU
1	A	240	GLU
1	A	254	LEU
1	A	261	LEU
1	A	279	THR
1	A	282	ASN
1	A	287	MET
1	A	327	THR
1	A	334	LEU
1	A	336	LEU
1	A	337	LEU
1	A	343	LEU
1	A	350	ASN
1	A	351	VAL
1	A	352	THR
1	A	359	SER
1	A	362	LEU
1	A	382	GLU
1	A	386	VAL
1	A	400	THR
1	A	419	SER
1	A	442	LEU
1	A	449	THR
1	A	451	GLU

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Mol	Chain	Res	Type
1	A	471	THR
1	A	485	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	153	GLN
1	A	226	HIS
1	A	282	ASN
1	A	328	HIS
1	A	423	HIS
1	A	440	ASN
1	A	458	GLN
1	A	465	GLN
1	A	501	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	FGL	A	69	1	3,3,7	0.77	0	1,2,9	0.10	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
1	FGL	A	69	1	-	0/0/1/8	-

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.

No monomer is involved in short contacts.

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	NAG	B	1	2,1	14,14,15	1.48	2 (14%)	17,19,21	2.32	5 (29%)
2	NAG	B	2	2	14,14,15	1.30	1 (7%)	17,19,21	1.64	4 (23%)

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	NAG	B	1	2,1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	B	2	2	1/1/5/7	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O7-C7	-3.65	1.15	1.23
2	B	1	NAG	O7-C7	-3.56	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C2-N2	3.42	1.51	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	O7-C7-N2	-4.75	113.59	121.98
2	B	1	NAG	C1-O5-C5	4.62	118.38	112.19
2	B	1	NAG	C2-N2-C7	-4.13	117.36	122.90
2	B	1	NAG	O5-C1-C2	3.44	116.61	111.29
2	B	2	NAG	C4-C3-C2	-3.08	106.51	111.02
2	B	2	NAG	C1-O5-C5	2.98	116.18	112.19
2	B	1	NAG	C8-C7-N2	2.90	120.94	116.12
2	B	2	NAG	O5-C1-C2	-2.79	106.97	111.29
2	B	2	NAG	C2-N2-C7	-2.11	120.08	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	NAG	C1
2	B	2	NAG	C1

All (6) torsion outliers are listed below:

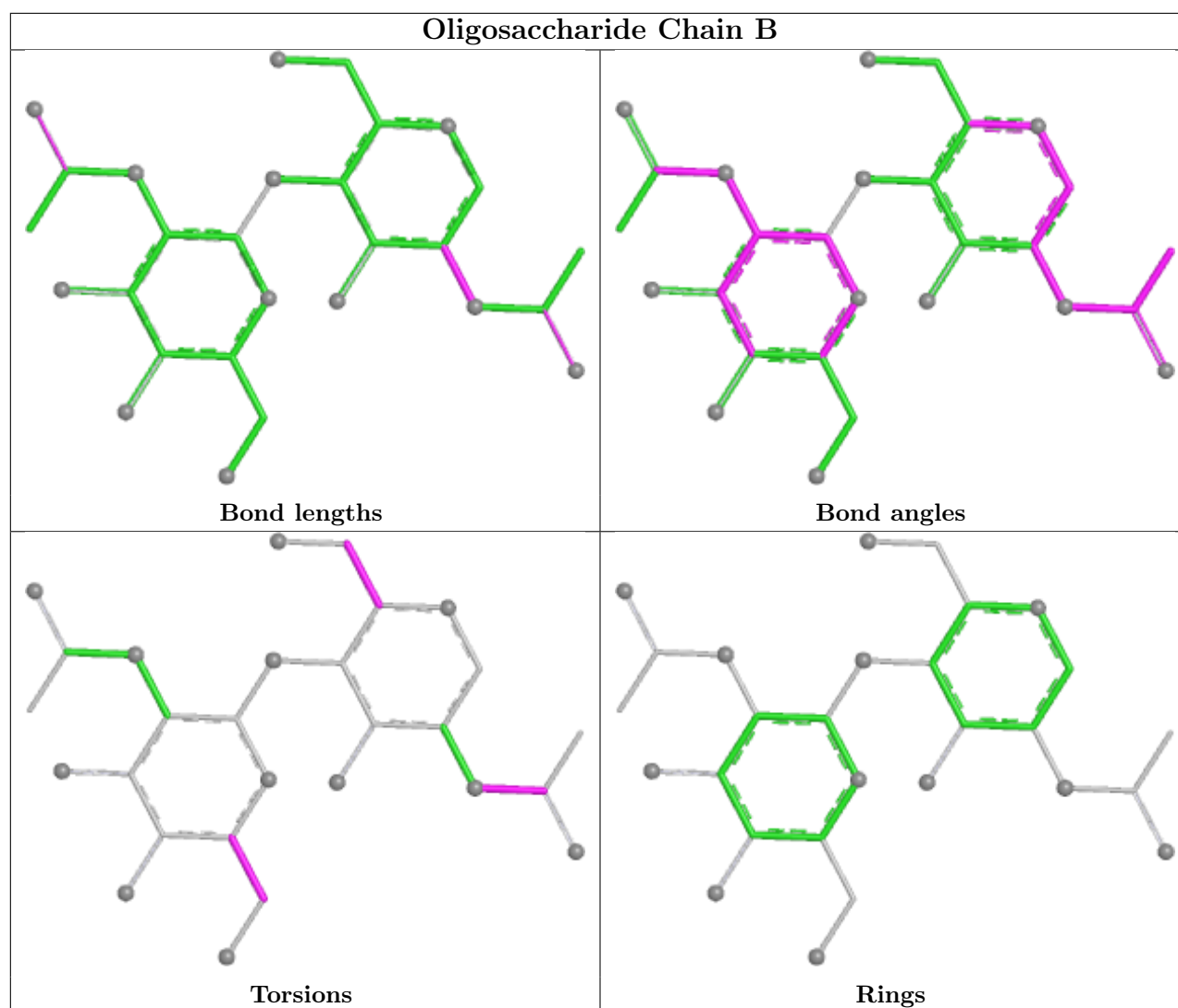
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0

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



5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	480/489 (98%)	0.32	17 (3%) 47 49	22, 41, 65, 85	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	490	HIS	4.3
1	A	448	ALA	3.9
1	A	503	PRO	3.0
1	A	117	LEU	2.9
1	A	458	GLN	2.8
1	A	179	ILE	2.7
1	A	501	HIS	2.5
1	A	214	ARG	2.5
1	A	502	CYS	2.4
1	A	495	PRO	2.4
1	A	493	CYS	2.3
1	A	217	ARG	2.3
1	A	273	GLU	2.2
1	A	210	ALA	2.1
1	A	215	GLN	2.1
1	A	223	TYR	2.1
1	A	271	LEU	2.0

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

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.

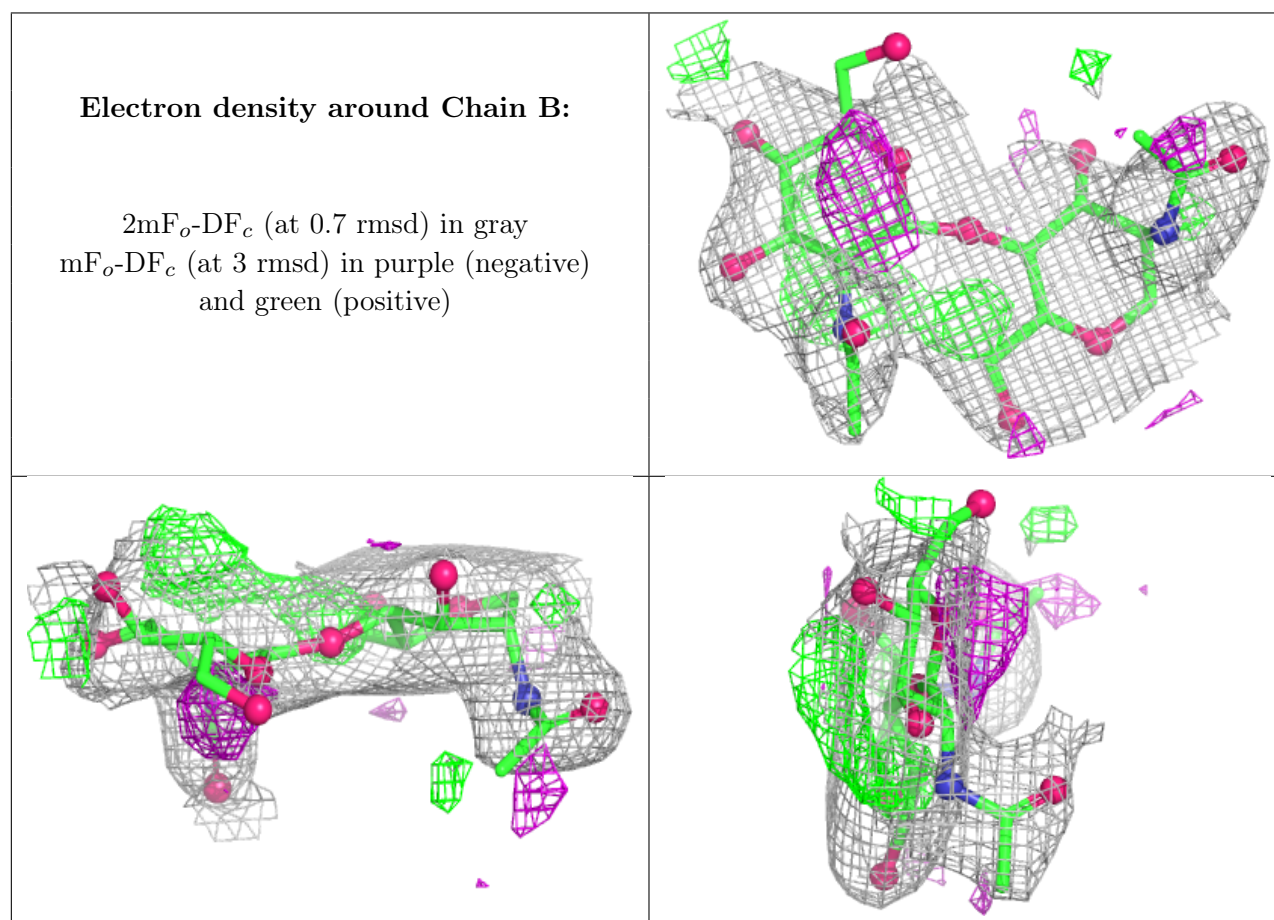
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	FGL	A	69	4/8	0.54	0.16	30,32,34,35	0

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	NAG	B	2	14/15	0.60	0.20	94,99,101,102	0
2	NAG	B	1	14/15	0.84	0.15	62,66,68,72	0

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	603	1/1	0.98	0.03	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.