



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:13 AM UTC

PDB ID : 4R9T / pdb_00004r9t
Title : L-ficolin complexed to sulphates
Authors : Laffly, E.; Lacroix, M.; Martin, L.; Vassal-Stermann, E.; Thielens, N.; Gaboriaud, C.
Deposited on : 2014-09-08
Resolution : 2.25 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

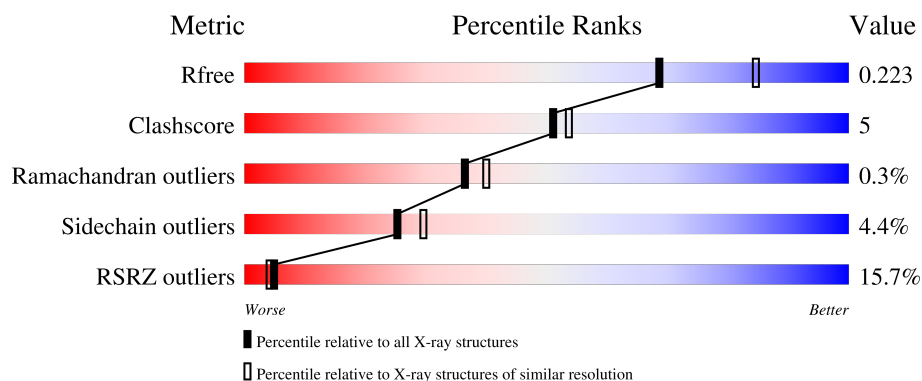
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	218	44% 81%14% . .
1	B	218	% 90%9% .
1	C	218	2% 89%8% ..
2	D	2	100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5330 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.

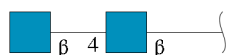
- Molecule 1 is a protein called Ficolin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	218	Total	C	N	O	S	3	0	0
			1744	1098	307	330	9			
1	A	217	Total	C	N	O	S	1	1	0
			1745	1099	307	330	9			
1	C	214	Total	C	N	O	S	5	1	0
			1721	1084	302	327	8			

There are 3 discrepancies between the modelled and reference sequences:

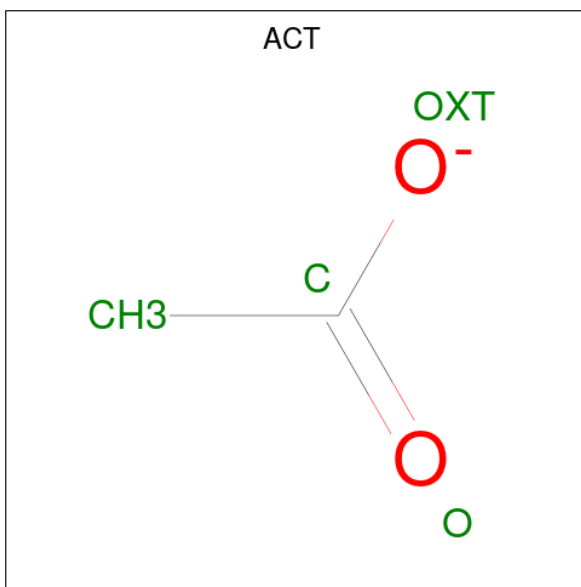
Chain	Residue	Modelled	Actual	Comment	Reference
B	71	ASN	-	expression tag	UNP Q15485
A	71	ASN	-	expression tag	UNP Q15485
C	71	ASN	-	expression tag	UNP Q15485

- 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	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

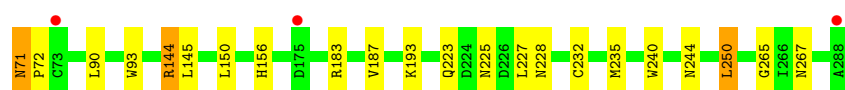
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	33	Total	O	0	0
			33	33		
6	A	7	Total	O	0	0
			7	7		
6	C	21	Total	O	0	0
			21	21		

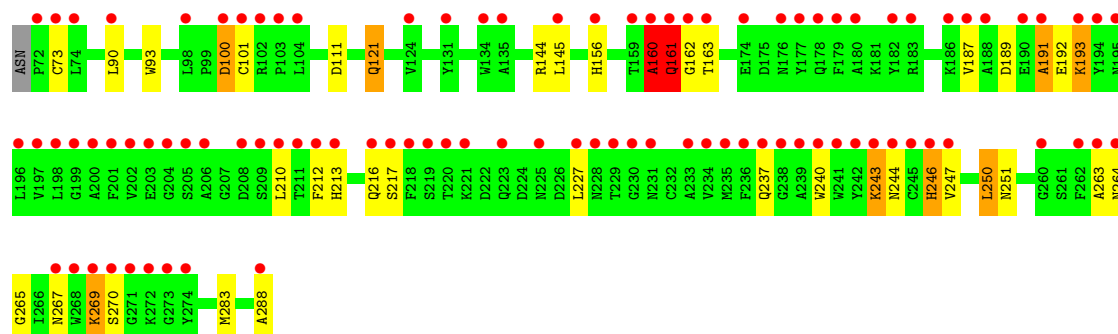
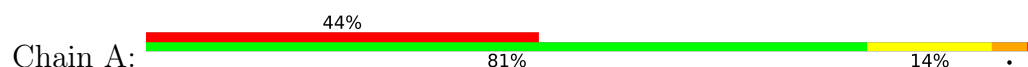
3 Residue-property plots [i](#)

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.

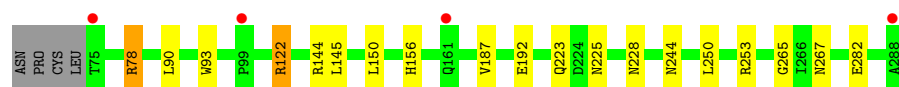
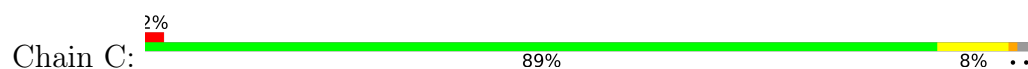
• Molecule 1: Ficolin-2



• Molecule 1: Ficolin-2



• Molecule 1: Ficolin-2



• 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	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	96.11Å 96.11Å 141.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.05 – 2.25 48.05 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.05-2.25) 100.0 (48.05-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.97 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.188 , 0.218 0.194 , 0.223	Depositor DCC
R_{free} test set	1821 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5330	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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, ACT, NAG, CA

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	0.92	0/1793	0.98	4/2425 (0.2%)
1	B	1.17	2/1792 (0.1%)	0.98	1/2425 (0.0%)
1	C	1.12	1/1771 (0.1%)	0.95	1/2395 (0.0%)
All	All	1.08	3/5356 (0.1%)	0.97	6/7245 (0.1%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	144	ARG	CD-NE	-6.52	1.37	1.46
1	C	253	ARG	CD-NE	-5.42	1.38	1.46
1	B	227	LEU	N-CA	5.38	1.52	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	ASN	N-CA-C	-7.52	100.98	111.81
1	A	191	ALA	N-CA-C	-6.82	98.91	109.76
1	C	78	ARG	CG-CD-NE	6.52	126.35	112.00
1	A	246	HIS	N-CA-C	6.44	118.64	108.79
1	A	160	ALA	N-CA-C	-6.19	101.11	110.28
1	B	193	LYS	CG-CD-CE	5.43	123.79	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	ALA	Peptide

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	1745	0	1620	39	0
1	B	1744	0	1615	8	0
1	C	1721	0	1595	6	0
2	D	28	0	25	0	0
3	B	4	0	3	0	0
3	C	4	0	3	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	5	0	0	0	0
5	B	10	0	0	0	0
5	C	5	0	0	0	0
6	A	7	0	0	0	0
6	B	33	0	0	0	0
6	C	21	0	0	0	0
All	All	5330	0	4861	53	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 5.

All (53) 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:247:VAL:CG2	1:A:269:LYS:HG2	1.60	1.29
1:A:161:GLN:HB3	1:A:162:GLY:HA3	1.36	1.05
1:A:247:VAL:HG23	1:A:269:LYS:HG2	1.44	0.96
1:A:247:VAL:CG2	1:A:269:LYS:CG	2.51	0.88
1:A:247:VAL:HG23	1:A:269:LYS:CG	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:VAL:HG22	1:A:269:LYS:HG2	1.64	0.79
1:A:189:ASP:OD1	1:A:191:ALA:O	2.02	0.78
1:A:160:ALA:O	1:A:161:GLN:HB2	1.84	0.77
1:A:247:VAL:HG21	1:A:269:LYS:HG2	1.65	0.77
1:A:216:GLN:HB3	1:A:243:LYS:HD3	1.67	0.77
1:A:269:LYS:HG3	1:A:270:SER:N	2.03	0.72
1:A:161:GLN:HB3	1:A:162:GLY:CA	2.18	0.72
1:A:161:GLN:CB	1:A:162:GLY:HA3	2.16	0.71
1:A:121[A]:GLN:HG2	1:A:283:MET:HG3	1.78	0.66
1:A:191:ALA:O	1:A:192:GLU:HB2	1.98	0.64
1:A:247:VAL:HG23	1:A:269:LYS:CB	2.33	0.58
1:A:163:THR:HG22	1:A:288:ALA:HB3	1.87	0.56
1:B:156:HIS:HD2	1:B:187:VAL:O	1.89	0.55
1:A:192:GLU:O	1:A:193:LYS:HG2	2.07	0.54
1:A:237:GLN:HE21	1:A:264:ASN:HD22	1.56	0.54
1:A:213:HIS:HA	1:A:216:GLN:CD	2.33	0.53
1:A:247:VAL:HG23	1:A:269:LYS:HB3	1.90	0.53
1:B:223:GLN:HE21	1:B:225:ASN:HD21	1.56	0.52
1:A:216:GLN:CD	1:A:243:LYS:HG2	2.35	0.52
1:A:216:GLN:CB	1:A:243:LYS:HD3	2.39	0.52
1:A:237:GLN:NE2	1:A:264:ASN:HD22	2.08	0.52
1:B:228:ASN:ND2	1:B:244:ASN:OD1	2.42	0.52
1:C:223:GLN:HE21	1:C:225:ASN:HD21	1.59	0.49
1:C:265:GLY:H	1:C:267:ASN:HD21	1.60	0.49
1:C:156:HIS:HD2	1:C:187:VAL:O	1.95	0.49
1:A:156:HIS:HD2	1:A:187:VAL:O	1.96	0.49
1:C:93:TRP:CZ2	1:C:144:ARG:HA	2.48	0.49
1:A:121[A]:GLN:OE1	1:A:251:ASN:OD1	2.30	0.49
1:A:193:LYS:HG3	1:A:217:SER:OG	2.14	0.47
1:A:73:CYS:SG	1:A:101:CYS:SG	3.04	0.47
1:B:265:GLY:H	1:B:267:ASN:HD21	1.62	0.47
1:A:216:GLN:NE2	1:A:243:LYS:HG2	2.31	0.45
1:A:121[A]:GLN:HG2	1:A:283:MET:CG	2.47	0.44
1:A:227:LEU:HG	1:A:243:LYS:HE2	2.00	0.42
1:A:265:GLY:H	1:A:267:ASN:HD21	1.67	0.42
1:C:122:ARG:HD2	1:C:282:GLU:OE2	2.19	0.42
1:B:240:TRP:CH2	1:B:250:LEU:HB2	2.55	0.42
1:A:243:LYS:HD2	1:A:243:LYS:HA	1.61	0.42
1:C:228:ASN:ND2	1:C:244:ASN:OD1	2.41	0.42
1:A:246:HIS:CD2	1:A:246:HIS:C	2.98	0.42
1:B:71:ASN:N	1:B:72:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:PHE:O	1:A:216:GLN:NE2	2.53	0.41
1:A:213:HIS:HA	1:A:216:GLN:NE2	2.35	0.41
1:A:246:HIS:HE1	1:A:263:ALA:O	2.04	0.41
1:B:93:TRP:CZ2	1:B:144:ARG:HA	2.56	0.40
1:A:93:TRP:CZ2	1:A:144:ARG:HA	2.55	0.40
1:A:240:TRP:CH2	1:A:250:LEU:HB2	2.56	0.40
1:B:232:CYS:HA	1:B:235:MET:HE3	2.04	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	216/218 (99%)	198 (92%)	16 (7%)	2 (1%)	14	12
1	B	216/218 (99%)	205 (95%)	11 (5%)	0	100	100
1	C	213/218 (98%)	201 (94%)	12 (6%)	0	100	100
All	All	645/654 (99%)	604 (94%)	39 (6%)	2 (0%)	36	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	100	ASP

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	183/183 (100%)	171 (93%)	12 (7%)	15	14
1	B	183/183 (100%)	177 (97%)	6 (3%)	33	42
1	C	180/183 (98%)	172 (96%)	8 (4%)	25	29
All	All	546/549 (100%)	520 (95%)	26 (5%)	25	25

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	71	ASN
1	B	90	LEU
1	B	145	LEU
1	B	150	LEU
1	B	183	ARG
1	B	250	LEU
1	A	90	LEU
1	A	100	ASP
1	A	111	ASP
1	A	121[A]	GLN
1	A	121[B]	GLN
1	A	145	LEU
1	A	161	GLN
1	A	193	LYS
1	A	210	LEU
1	A	243	LYS
1	A	250	LEU
1	A	269	LYS
1	C	78	ARG
1	C	90	LEU
1	C	122	ARG
1	C	145	LEU
1	C	150	LEU
1	C	192[A]	GLU
1	C	192[B]	GLU
1	C	250	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	88	HIS

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Mol	Chain	Res	Type
1	B	94	HIS
1	B	156	HIS
1	B	223	GLN
1	B	246	HIS
1	B	267	ASN
1	A	88	HIS
1	A	94	HIS
1	A	156	HIS
1	A	161	GLN
1	A	214	ASN
1	A	216	GLN
1	A	223	GLN
1	A	237	GLN
1	A	246	HIS
1	A	267	ASN
1	C	88	HIS
1	C	156	HIS
1	C	161	GLN
1	C	225	ASN
1	C	267	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 ⓘ

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	D	1	1,2	14,14,15	1.29	1 (7%)	17,19,21	1.96	6 (35%)
2	NAG	D	2	2	14,14,15	0.57	0	17,19,21	1.40	3 (17%)

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	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	O5-C1	-3.28	1.38	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	O5-C5-C6	-4.32	99.25	107.66
2	D	1	NAG	C1-C2-N2	-3.11	105.54	110.43
2	D	2	NAG	O4-C4-C5	3.01	116.74	109.32
2	D	1	NAG	C6-C5-C4	2.84	119.99	113.02
2	D	1	NAG	O3-C3-C2	2.32	114.22	109.40
2	D	1	NAG	O3-C3-C4	2.24	115.65	110.38
2	D	1	NAG	C3-C4-C5	-2.17	106.30	110.23
2	D	2	NAG	C2-N2-C7	2.09	125.70	122.90
2	D	2	NAG	O7-C7-C8	-2.01	118.47	122.05

There are no chirality outliers.

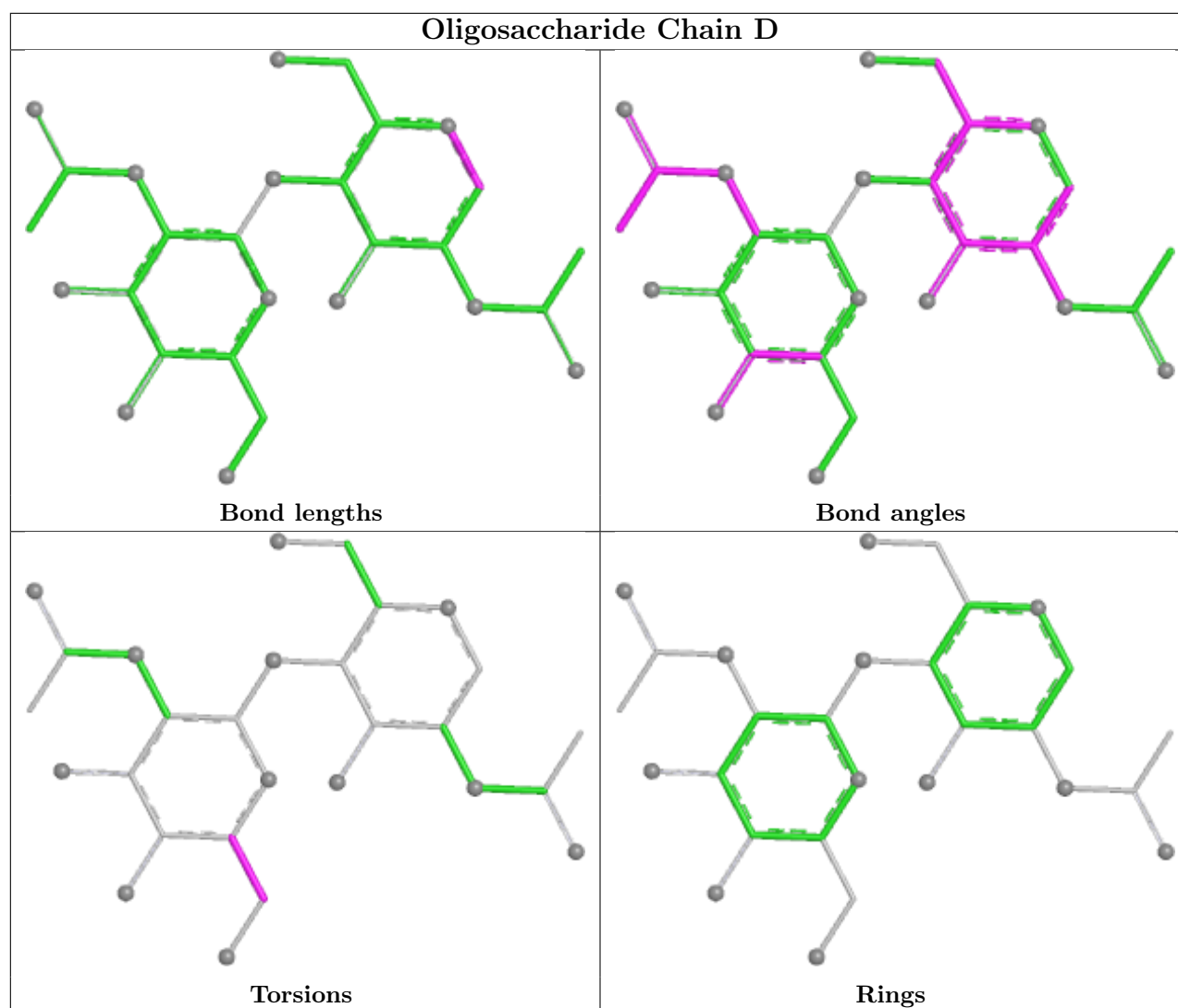
All (1) torsion outliers are listed below:

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

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.



5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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	C	303	-	4,4,4	0.43	0	6,6,6	0.35	0
3	ACT	C	301	-	3,3,3	0.85	0	3,3,3	0.74	0
3	ACT	B	303	-	3,3,3	0.85	0	3,3,3	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	B	306	-	4,4,4	0.35	0	6,6,6	0.51	0
5	SO4	A	302	-	4,4,4	0.40	0	6,6,6	0.39	0
5	SO4	B	305	-	4,4,4	0.51	0	6,6,6	1.10	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	305	SO4	O3-S-O1	2.20	121.07	109.56

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 [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	217/218 (99%)	1.95	95 (43%) 0 0	20, 79, 141, 220	1 (0%)
1	B	218/218 (100%)	-0.22	3 (1%) 73 74	18, 29, 51, 78	2 (0%)
1	C	214/218 (98%)	-0.11	4 (1%) 66 67	20, 32, 57, 101	2 (0%)
All	All	649/654 (99%)	0.54	102 (15%) 5 4	18, 38, 116, 220	5 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	PHE	8.0
1	A	202	VAL	6.1
1	A	204	GLY	6.1
1	A	227	LEU	5.2
1	A	229	THR	5.2
1	A	269	LYS	4.9
1	A	218	PHE	4.9
1	A	177	TYR	4.7
1	C	75	THR	4.7
1	A	216	GLN	4.6
1	A	245	CYS	4.3
1	A	205	SER	4.3
1	A	201	PHE	4.3
1	A	100	ASP	4.2
1	A	264	ASN	4.2
1	A	163	THR	4.1
1	A	271	GLY	4.0
1	A	193	LYS	4.0
1	A	134	TRP	4.0
1	A	197	VAL	3.9
1	A	203	GLU	3.9
1	A	217	SER	3.8
1	A	211	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	242	TYR	3.7
1	A	180	ALA	3.5
1	C	288	ALA	3.5
1	A	262	PHE	3.5
1	A	235	MET	3.5
1	A	288	ALA	3.5
1	A	198	LEU	3.4
1	A	188	ALA	3.4
1	A	241	TRP	3.4
1	A	260	GLY	3.4
1	A	219	SER	3.3
1	A	243	LYS	3.3
1	A	191	ALA	3.2
1	A	234	VAL	3.3
1	A	74	LEU	3.2
1	A	236	PHE	3.2
1	A	160	ALA	3.2
1	A	72	PRO	3.2
1	A	131	TYR	3.1
1	A	194	TYR	3.1
1	A	270	SER	3.1
1	A	225	ASN	3.1
1	A	228	ASN	3.1
1	A	179	PHE	3.0
1	A	244	ASN	3.0
1	A	103	PRO	3.0
1	A	223	GLN	3.0
1	A	230	GLY	3.0
1	A	220	THR	2.8
1	A	246	HIS	2.8
1	A	101	CYS	2.8
1	A	239	ALA	2.8
1	A	102	ARG	2.7
1	A	268	TRP	2.7
1	A	233	ALA	2.7
1	A	210	LEU	2.7
1	A	196	LEU	2.6
1	A	161	GLN	2.6
1	A	195	ASN	2.6
1	A	272	LYS	2.6
1	A	183	ARG	2.6
1	A	240	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	199	GLY	2.5
1	A	156	HIS	2.5
1	A	213	HIS	2.5
1	A	182	TYR	2.5
1	B	288	ALA	2.5
1	A	73	CYS	2.4
1	A	238	GLY	2.4
1	A	124	VAL	2.4
1	A	162	GLY	2.4
1	A	90	LEU	2.4
1	A	98	LEU	2.4
1	C	161	GLN	2.4
1	A	159	THR	2.3
1	A	237	GLN	2.3
1	A	274	TYR	2.3
1	A	208	ASP	2.3
1	A	174	GLU	2.3
1	A	178	GLN	2.3
1	B	73	CYS	2.2
1	A	273	GLY	2.2
1	A	221	LYS	2.2
1	A	231	ASN	2.2
1	A	190	GLU	2.2
1	A	135	ALA	2.2
1	A	263	ALA	2.2
1	B	175	ASP	2.2
1	A	247	VAL	2.2
1	A	104	LEU	2.1
1	A	187	VAL	2.1
1	C	99	PRO	2.1
1	A	206	ALA	2.1
1	A	145	LEU	2.1
1	A	267	ASN	2.1
1	A	200	ALA	2.0
1	A	186	LYS	2.0
1	A	209	SER	2.0
1	A	176	ASN	2.0

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

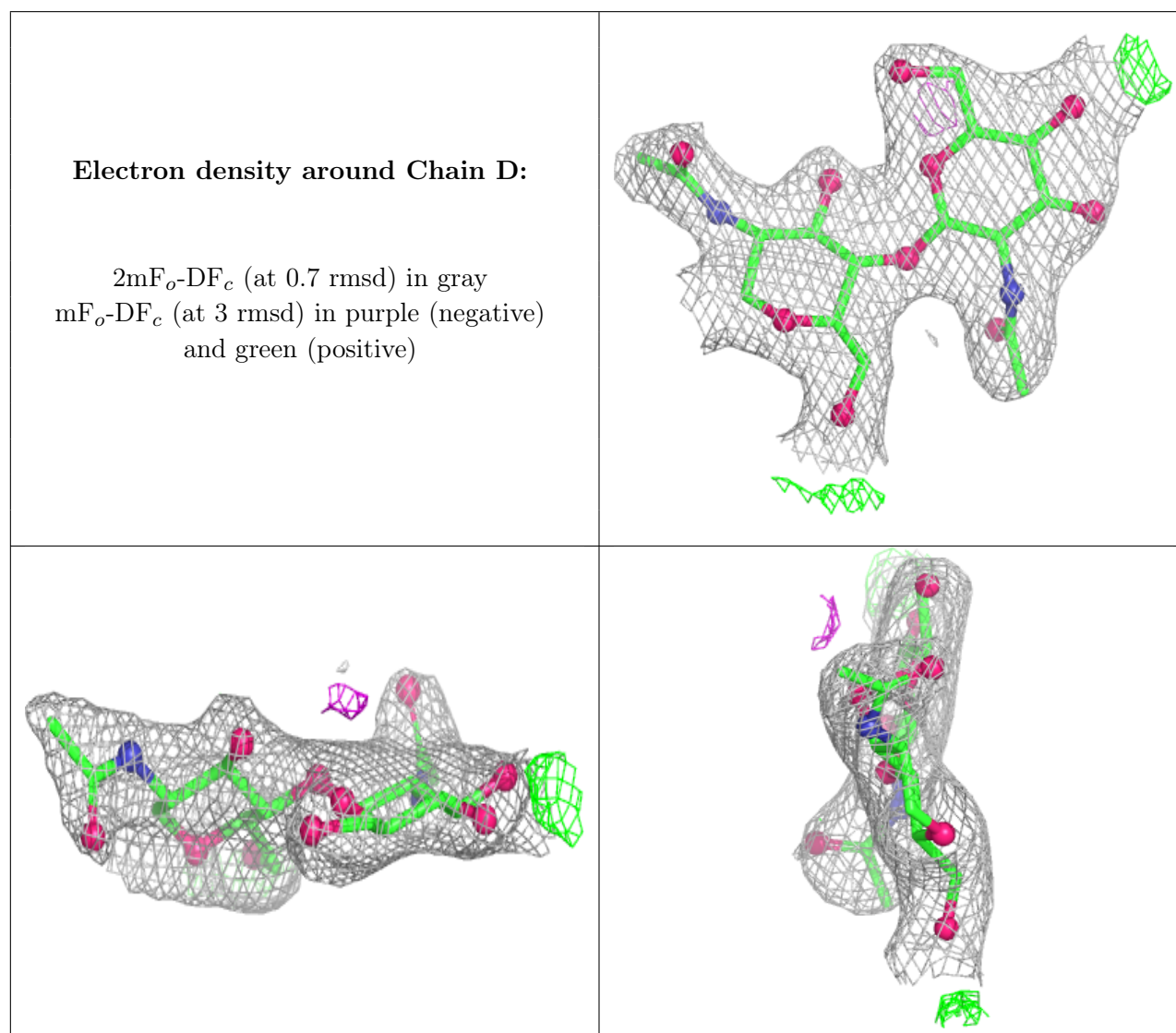
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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	NAG	D	2	14/15	0.91	0.10	43,52,58,59	0
2	NAG	D	1	14/15	0.92	0.09	35,42,47,53	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(Å ²)	Q<0.9
5	SO4	A	302	5/5	0.64	0.29	59,60,63,64	5
4	CA	A	301	1/1	0.79	0.10	71,71,71,71	1
5	SO4	B	305	5/5	0.81	0.20	27,36,44,47	5
5	SO4	B	306	5/5	0.88	0.16	42,43,47,47	5
3	ACT	B	303	4/4	0.91	0.14	33,35,38,38	0
3	ACT	C	301	4/4	0.93	0.23	26,26,27,29	4
5	SO4	C	303	5/5	0.97	0.07	38,39,44,45	5
4	CA	C	302	1/1	0.98	0.07	42,42,42,42	0
4	CA	B	304	1/1	0.99	0.02	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.