



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:55 PM UTC

PDB ID : 7YL6 / pdb_00007yl6
Title : Cell surface protein YwfG protein complexed with alpha-1,2-mannobiose
Authors : Tsuchiya, W.; Fujimoto, Z.; Suzuki, C.
Deposited on : 2022-07-25
Resolution : 2.95 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

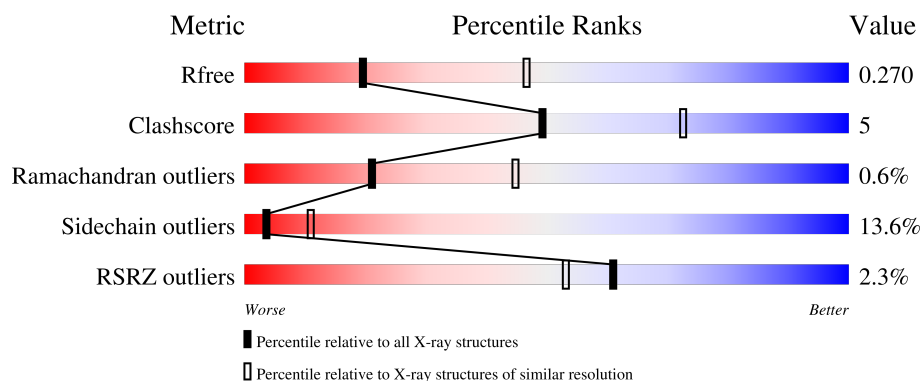
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	505	 62% 27% • 7%
1	B	505	 59% 18% • 21%
2	C	2	 100%
2	D	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6673 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 GRAM_POS_ANCHORING domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3552	2207	590	750	5			
1	B	398	Total	C	N	O	S	0	0	0
			2982	1853	495	629	5			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	initiating methionine	UNP S6FKX6
A	8	GLY	-	expression tag	UNP S6FKX6
A	9	SER	-	expression tag	UNP S6FKX6
A	10	SER	-	expression tag	UNP S6FKX6
A	11	HIS	-	expression tag	UNP S6FKX6
A	12	HIS	-	expression tag	UNP S6FKX6
A	13	HIS	-	expression tag	UNP S6FKX6
A	14	HIS	-	expression tag	UNP S6FKX6
A	15	HIS	-	expression tag	UNP S6FKX6
A	16	HIS	-	expression tag	UNP S6FKX6
A	17	SER	-	expression tag	UNP S6FKX6
A	18	SER	-	expression tag	UNP S6FKX6
A	19	GLY	-	expression tag	UNP S6FKX6
A	20	LEU	-	expression tag	UNP S6FKX6
A	21	VAL	-	expression tag	UNP S6FKX6
A	22	PRO	-	expression tag	UNP S6FKX6
A	23	ARG	-	expression tag	UNP S6FKX6
A	24	GLY	-	expression tag	UNP S6FKX6
A	25	SER	-	expression tag	UNP S6FKX6
A	26	HIS	-	expression tag	UNP S6FKX6
A	27	MET	-	expression tag	UNP S6FKX6
B	7	MET	-	initiating methionine	UNP S6FKX6
B	8	GLY	-	expression tag	UNP S6FKX6
B	9	SER	-	expression tag	UNP S6FKX6
B	10	SER	-	expression tag	UNP S6FKX6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	11	HIS	-	expression tag	UNP S6FKX6
B	12	HIS	-	expression tag	UNP S6FKX6
B	13	HIS	-	expression tag	UNP S6FKX6
B	14	HIS	-	expression tag	UNP S6FKX6
B	15	HIS	-	expression tag	UNP S6FKX6
B	16	HIS	-	expression tag	UNP S6FKX6
B	17	SER	-	expression tag	UNP S6FKX6
B	18	SER	-	expression tag	UNP S6FKX6
B	19	GLY	-	expression tag	UNP S6FKX6
B	20	LEU	-	expression tag	UNP S6FKX6
B	21	VAL	-	expression tag	UNP S6FKX6
B	22	PRO	-	expression tag	UNP S6FKX6
B	23	ARG	-	expression tag	UNP S6FKX6
B	24	GLY	-	expression tag	UNP S6FKX6
B	25	SER	-	expression tag	UNP S6FKX6
B	26	HIS	-	expression tag	UNP S6FKX6
B	27	MET	-	expression tag	UNP S6FKX6

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose.



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

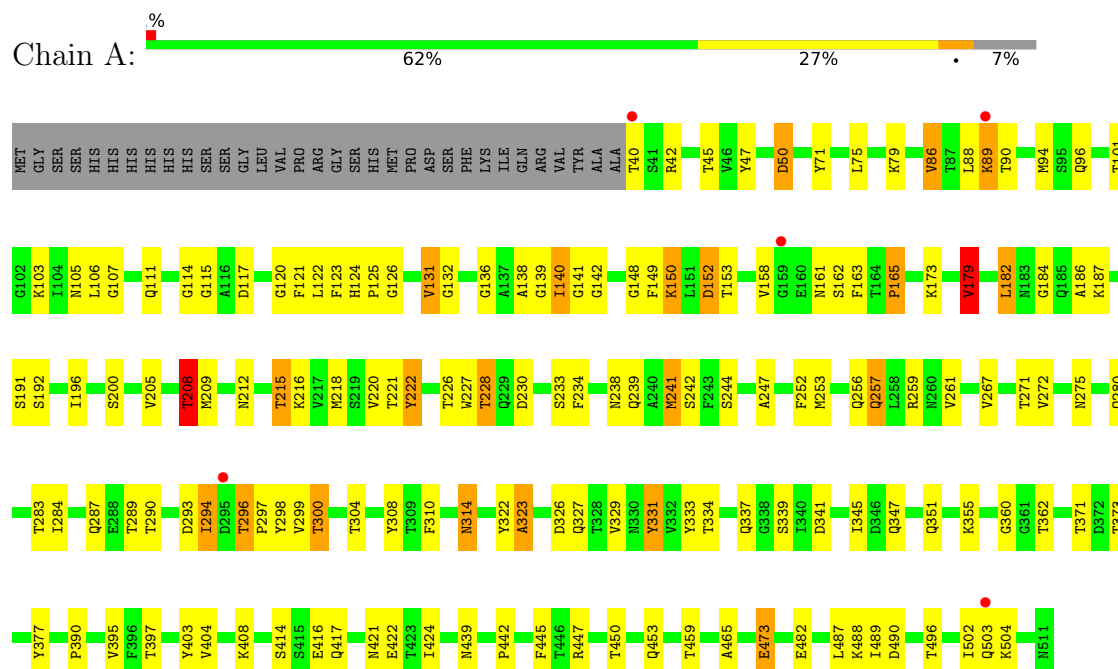
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	14	Total	O	0	0
			14	14		
5	B	27	Total	O	0	0
			27	27		

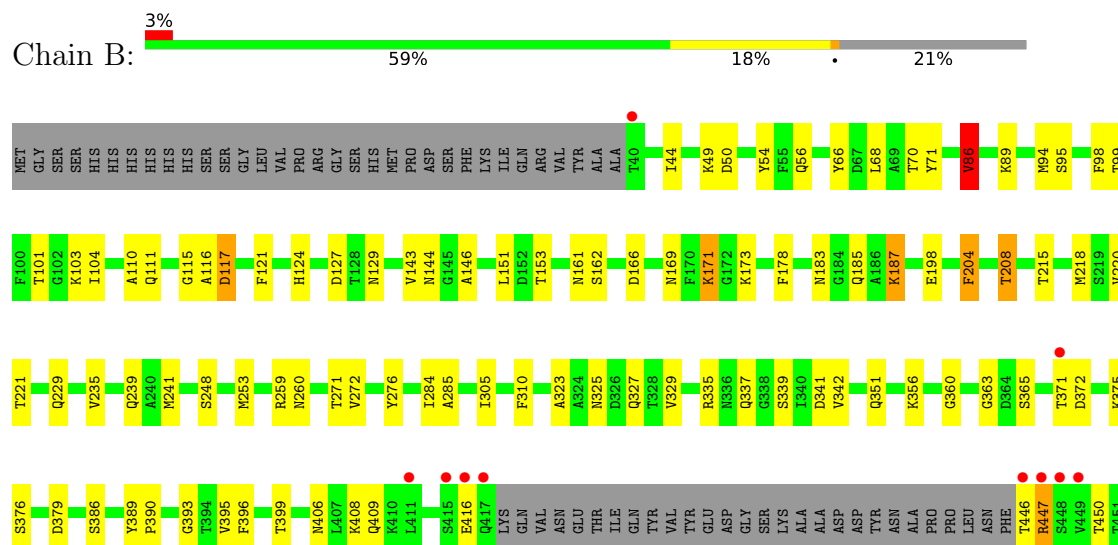
3 Residue-property plots [i](#)

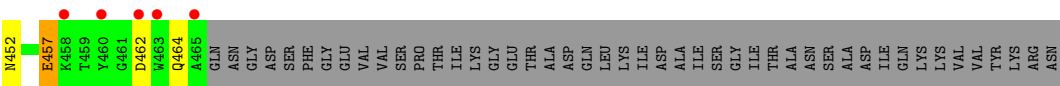
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: GRAM_POS_ANCHORING domain-containing protein





● Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain C: 100%



● Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain D: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	43.45Å 276.63Å 321.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.51 – 2.95 41.51 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.51-2.95) 99.9 (41.51-2.95)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.211 , 0.268 0.217 , 0.270	Depositor DCC
R_{free} test set	2151 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6673	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: CA, MAN, 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	1.30	12/3620 (0.3%)	1.65	36/4924 (0.7%)
1	B	1.29	8/3040 (0.3%)	1.58	22/4137 (0.5%)
All	All	1.29	20/6660 (0.3%)	1.62	58/9061 (0.6%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	LYS	C-O	-8.95	1.12	1.24
1	B	204	PHE	C-O	-8.58	1.13	1.23
1	A	106	LEU	C-O	7.03	1.33	1.24
1	A	331	TYR	C-O	6.93	1.32	1.24
1	B	151	LEU	C-O	6.43	1.31	1.23
1	B	416	GLU	CD-OE1	6.02	1.36	1.25
1	A	88	LEU	C-O	5.95	1.31	1.24
1	B	323	ALA	C-O	5.79	1.30	1.23
1	B	104	ILE	C-O	5.68	1.30	1.24
1	A	162	SER	C-O	5.62	1.31	1.24
1	A	196	ILE	C-O	5.55	1.29	1.23
1	A	297	PRO	C-O	-5.49	1.17	1.23
1	A	123	PHE	C-O	5.33	1.30	1.24
1	A	395	VAL	C-O	-5.27	1.18	1.24
1	A	179	VAL	C-O	5.25	1.29	1.24
1	B	86	VAL	C-O	5.20	1.29	1.24
1	A	222	TYR	C-O	5.20	1.30	1.24
1	A	323	ALA	C-O	5.15	1.30	1.23
1	A	351	GLN	C-O	5.12	1.29	1.23
1	B	124	HIS	CE1-NE2	5.04	1.37	1.32

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	THR	CA-CB-OG1	-9.38	95.54	109.60
1	A	208	THR	CA-CB-OG1	-8.30	97.15	109.60
1	A	230	ASP	CA-CB-CG	7.88	120.48	112.60
1	B	208	THR	CA-CB-OG1	-7.82	97.86	109.60
1	A	310	PHE	CA-C-O	-7.58	113.37	120.95
1	A	271	THR	CA-CB-OG1	-7.07	99.00	109.60
1	A	153	THR	CA-CB-OG1	6.74	119.71	109.60
1	B	95	SER	N-CA-C	-6.62	105.02	113.23
1	B	271	THR	CA-CB-OG1	-6.58	99.73	109.60
1	A	221	THR	CA-CB-OG1	-6.53	99.80	109.60
1	A	377	TYR	CA-C-O	-6.16	113.89	120.42
1	B	121	PHE	CA-C-O	-6.12	113.91	120.46
1	A	139	GLY	O-C-N	6.01	129.53	122.38
1	A	107	GLY	N-CA-C	5.92	117.54	111.56
1	A	101	THR	CA-CB-OG1	-5.89	100.77	109.60
1	A	117	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	355	LYS	CA-C-O	-5.80	114.09	120.24
1	B	70	THR	CA-CB-OG1	-5.74	100.99	109.60
1	B	399	THR	CA-CB-OG1	-5.72	101.02	109.60
1	A	283	THR	CA-C-O	-5.70	114.19	120.69
1	B	99	THR	CA-CB-OG1	-5.67	101.09	109.60
1	A	215	THR	CA-CB-OG1	-5.66	101.11	109.60
1	B	393	GLY	CA-C-O	-5.65	117.37	122.57
1	B	117	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	182	LEU	CA-C-O	-5.62	114.92	120.82
1	A	496	THR	CA-CB-OG1	-5.62	101.18	109.60
1	A	294	ILE	CA-C-O	-5.61	114.43	121.11
1	B	98	PHE	CA-CB-CG	5.58	119.38	113.80
1	A	304	THR	CA-CB-OG1	-5.49	101.36	109.60
1	A	473	GLU	CB-CA-C	5.45	118.97	109.65
1	B	379	ASP	CA-C-O	-5.44	115.11	120.82
1	A	482	GLU	CB-CG-CD	5.38	121.75	112.60
1	B	457	GLU	CB-CA-C	5.38	116.42	109.80
1	B	372	ASP	N-CA-C	-5.38	105.50	111.36
1	A	50	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	275	ASN	CA-CB-CG	-5.32	107.28	112.60
1	A	289	THR	CA-CB-OG1	-5.30	101.66	109.60
1	B	235	VAL	N-CA-C	-5.30	107.01	111.56
1	A	228	THR	CA-CB-OG1	-5.28	101.68	109.60
1	A	152	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	226	THR	CA-CB-OG1	-5.27	101.70	109.60
1	B	221	THR	CA-CB-OG1	-5.25	101.72	109.60
1	A	323	ALA	CA-C-N	5.25	128.09	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	ALA	C-N-CA	5.25	128.09	120.79
1	A	261	VAL	CA-C-N	5.24	130.50	122.95
1	A	261	VAL	C-N-CA	5.24	130.50	122.95
1	B	166	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	47	TYR	CB-CA-C	5.19	117.62	109.37
1	B	363	GLY	N-CA-C	-5.18	107.85	114.37
1	A	89	LYS	CA-C-O	-5.17	115.39	120.82
1	B	66	TYR	CA-C-O	-5.16	114.59	120.58
1	A	86	VAL	CA-C-O	-5.09	115.04	120.39
1	B	218	MET	CA-C-O	-5.09	115.27	121.28
1	A	215	THR	O-C-N	5.07	128.51	122.27
1	B	153	THR	CA-CB-OG1	5.07	117.20	109.60
1	A	296	THR	N-CA-C	-5.06	102.50	110.14
1	B	310	PHE	CA-C-O	-5.04	115.17	120.92
1	B	215	THR	N-CA-C	-5.00	107.21	113.72

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	3552	0	3355	41	0
1	B	2982	0	2802	28	0
2	C	23	0	21	0	0
2	D	23	0	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	25	0	0	0	0
4	B	25	0	0	1	0
5	A	14	0	0	1	0
5	B	27	0	0	0	0
All	All	6673	0	6199	69	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 (69) 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:326:ASP:HB2	5:A:702:HOH:O	1.34	1.23
1:A:205:VAL:HB	1:A:222:TYR:CE1	2.24	0.72
1:A:209:MET:HG3	1:A:220:VAL:HG22	1.82	0.61
1:A:142:GLY:N	1:A:184:GLY:O	2.35	0.59
1:A:390:PRO:HD3	1:A:403:TYR:CE1	2.38	0.58
1:B:284:ILE:HG13	1:B:305:ILE:HD13	1.84	0.58
1:A:421:ASN:ND2	1:A:442:PRO:HB3	2.23	0.54
1:A:120:GLY:HA3	1:A:138:ALA:O	2.08	0.54
1:A:300:THR:HB	1:A:331:TYR:OH	2.07	0.54
1:B:178:PHE:CD2	1:B:229:GLN:HB2	2.45	0.52
1:A:40:THR:HG21	1:A:42:ARG:HH21	1.75	0.52
1:B:110:ALA:HB1	1:B:198:GLU:OE1	2.10	0.52
1:A:314:ASN:OD1	1:A:314:ASN:C	2.53	0.51
1:A:141:GLY:CA	1:A:186:ALA:HB2	2.40	0.51
1:A:42:ARG:HD3	1:A:293:ASP:OD1	2.11	0.50
1:B:409:GLN:HB3	1:B:452:ASN:HD21	1.76	0.49
1:A:422:GLU:HA	1:A:502:ILE:O	2.13	0.49
1:A:182:LEU:HD11	1:A:234:PHE:HD1	1.79	0.48
1:B:94:MET:HG3	1:B:241:MET:HG3	1.96	0.48
1:A:115:GLY:HA2	1:A:253:MET:O	2.14	0.48
1:A:192:SER:O	1:A:227:TRP:CD1	2.68	0.47
1:A:293:ASP:O	1:A:322:TYR:HB2	2.13	0.47
1:B:208:THR:O	1:B:220:VAL:HA	2.15	0.47
1:A:445:PHE:CE2	1:A:465:ALA:HB2	2.49	0.47
1:A:424:ILE:HG12	1:A:489:ILE:HG13	1.97	0.46
1:B:161:ASN:O	1:B:185:GLN:HG3	2.16	0.46
1:A:272:VAL:HG21	1:A:298:TYR:CG	2.51	0.46
1:A:284:ILE:HD11	1:A:333:TYR:HB2	1.97	0.46
1:B:117:ASP:HB2	1:B:248:SER:O	2.16	0.46
1:B:183:ASN:HD21	1:B:187:LYS:NZ	2.14	0.46
1:A:208:THR:O	1:A:220:VAL:HA	2.16	0.45
1:A:140:ILE:HG21	1:A:179:VAL:HB	1.97	0.45
1:B:127:ASP:HA	1:B:325:ASN:OD1	2.17	0.45
1:A:75:LEU:HB3	1:A:247:ALA:HB3	1.98	0.45
1:A:122:LEU:HD13	1:A:140:ILE:HA	1.98	0.45
1:A:131:VAL:HG12	1:A:132:GLY:H	1.82	0.45
1:B:335:ARG:O	1:B:337:GLN:HG2	2.17	0.45
1:A:71:TYR:O	1:A:259:ARG:HA	2.16	0.45
1:B:171:LYS:HE3	1:B:171:LYS:HB2	1.64	0.45
1:B:56:GLN:O	1:B:86:VAL:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:VAL:HA	1:B:327:GLN:O	2.17	0.44
1:B:341:ASP:HA	1:B:356:LYS:O	2.17	0.44
1:B:386:SER:OG	1:B:406:ASN:HB2	2.17	0.44
1:B:115:GLY:HA2	1:B:253:MET:O	2.18	0.44
1:B:276:TYR:O	1:B:284:ILE:HG12	2.18	0.44
1:A:161:ASN:HD22	1:A:161:ASN:HA	1.63	0.44
1:A:337:GLN:HA	1:A:360:GLY:O	2.18	0.43
1:B:44:ILE:HD13	1:B:54:TYR:CE2	2.53	0.43
1:A:136:GLY:C	1:A:163:PHE:CD2	2.96	0.43
1:A:294:ILE:HG23	1:A:323:ALA:HA	2.01	0.43
1:B:71:TYR:O	1:B:259:ARG:HA	2.19	0.43
1:A:308:TYR:HB3	1:A:333:TYR:HB3	2.01	0.43
1:A:94:MET:HG3	1:A:241:MET:HG3	2.00	0.42
1:A:105:ASN:HD22	1:A:257:GLN:HG3	1.84	0.42
1:A:149:PHE:CE2	1:A:220:VAL:HG11	2.54	0.42
1:B:360:GLY:HA3	1:B:396:PHE:CE2	2.55	0.42
1:A:121:PHE:O	1:A:148:GLY:HA3	2.19	0.42
1:B:276:TYR:HB2	1:B:285:ALA:HB3	2.01	0.42
1:B:183:ASN:HD21	1:B:187:LYS:HZ1	1.67	0.42
1:A:114:GLY:HA2	1:A:252:PHE:CD2	2.55	0.41
1:A:124:HIS:HB2	1:A:125:PRO:HD2	2.01	0.41
1:A:114:GLY:HA2	1:A:252:PHE:CG	2.56	0.41
1:B:56:GLN:HA	4:B:603:SO4:O3	2.20	0.41
1:B:103:LYS:HB3	1:B:204:PHE:HB3	2.03	0.41
1:B:389:TYR:HA	1:B:390:PRO:HD3	1.92	0.41
1:B:116:ALA:HB1	1:B:117:ASP:HA	2.04	0.40
1:B:143:VAL:HB	1:B:146:ALA:HB2	2.02	0.40
1:A:150:LYS:HD2	1:A:152:ASP:HB2	2.02	0.40
1:A:205:VAL:HB	1:A:222:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	470/505 (93%)	437 (93%)	29 (6%)	4 (1%)	14	34
1	B	394/505 (78%)	374 (95%)	19 (5%)	1 (0%)	36	59
All	All	864/1010 (86%)	811 (94%)	48 (6%)	5 (1%)	21	45

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	447	ARG
1	A	165	PRO
1	A	371	THR
1	A	362	THR
1	A	126	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	383/411 (93%)	318 (83%)	65 (17%)	2	5
1	B	321/411 (78%)	290 (90%)	31 (10%)	8	21
All	All	704/822 (86%)	608 (86%)	96 (14%)	3	11

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	50	ASP
1	A	79	LYS
1	A	86	VAL
1	A	89	LYS
1	A	90	THR
1	A	96	GLN
1	A	103	LYS
1	A	111	GLN
1	A	131	VAL
1	A	140	ILE

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Mol	Chain	Res	Type
1	A	150	LYS
1	A	158	VAL
1	A	165	PRO
1	A	173	LYS
1	A	179	VAL
1	A	187	LYS
1	A	191	SER
1	A	200	SER
1	A	208	THR
1	A	212	ASN
1	A	215	THR
1	A	216	LYS
1	A	218	MET
1	A	228	THR
1	A	233	SER
1	A	238	ASN
1	A	239	GLN
1	A	241	MET
1	A	242	SER
1	A	244	SER
1	A	256	GLN
1	A	257	GLN
1	A	267	VAL
1	A	280	GLN
1	A	287	GLN
1	A	290	THR
1	A	296	THR
1	A	299	VAL
1	A	300	THR
1	A	314	ASN
1	A	327	GLN
1	A	329	VAL
1	A	334	THR
1	A	339	SER
1	A	341	ASP
1	A	345	ILE
1	A	347	GLN
1	A	373	THR
1	A	404	VAL
1	A	408	LYS
1	A	414	SER
1	A	416	GLU

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Mol	Chain	Res	Type
1	A	417	GLN
1	A	439	ASN
1	A	447	ARG
1	A	450	THR
1	A	453	GLN
1	A	459	THR
1	A	473	GLU
1	A	487	LEU
1	A	488	LYS
1	A	490	ASP
1	A	503	GLN
1	A	504	LYS
1	B	49	LYS
1	B	50	ASP
1	B	68	LEU
1	B	86	VAL
1	B	101	THR
1	B	111	GLN
1	B	129	ASN
1	B	144	ASN
1	B	162	SER
1	B	169	ASN
1	B	171	LYS
1	B	173	LYS
1	B	187	LYS
1	B	239	GLN
1	B	260	ASN
1	B	329	VAL
1	B	339	SER
1	B	342	VAL
1	B	351	GLN
1	B	365	SER
1	B	371	THR
1	B	375	LYS
1	B	376	SER
1	B	395	VAL
1	B	408	LYS
1	B	446	THR
1	B	447	ARG
1	B	450	THR
1	B	457	GLU
1	B	462	ASP

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Mol	Chain	Res	Type
1	B	464	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	112	ASN
1	A	161	ASN
1	A	238	ASN
1	A	257	GLN
1	A	269	GLN
1	A	275	ASN
1	A	280	GLN
1	A	282	ASN
1	A	287	GLN
1	A	302	GLN
1	A	321	ASN
1	A	401	GLN
1	A	406	ASN
1	A	419	GLN
1	A	421	ASN
1	A	498	ASN
1	A	503	GLN
1	B	201	ASN
1	B	262	ASN
1	B	275	ASN
1	B	287	GLN
1	B	452	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
2	MAN	C	1	2	12,12,12	1.39	4 (33%)	17,17,17	1.59	2 (11%)
2	MAN	C	2	2	11,11,12	0.87	0	15,15,17	2.07	4 (26%)
2	MAN	D	1	2	12,12,12	1.09	2 (16%)	17,17,17	1.80	6 (35%)
2	MAN	D	2	2	11,11,12	1.33	3 (27%)	15,15,17	3.11	10 (66%)

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	MAN	C	1	2	-	0/2/22/22	0/1/1/1
2	MAN	C	2	2	-	2/2/19/22	0/1/1/1
2	MAN	D	1	2	-	0/2/22/22	0/1/1/1
2	MAN	D	2	2	-	0/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	MAN	C1-C2	2.32	1.57	1.52
2	D	1	MAN	O1-C1	2.32	1.46	1.39
2	D	1	MAN	C1-C2	2.21	1.57	1.52
2	C	1	MAN	O1-C1	2.18	1.46	1.39
2	D	2	MAN	C4-C3	2.17	1.58	1.52
2	C	1	MAN	O3-C3	2.17	1.48	1.43
2	C	1	MAN	C1-C2	2.08	1.57	1.52
2	D	2	MAN	O5-C1	2.05	1.47	1.43
2	C	1	MAN	C4-C5	2.02	1.57	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	MAN	O4-C4-C5	-5.49	95.81	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	MAN	O3-C3-C4	4.89	121.90	110.38
2	D	2	MAN	O3-C3-C2	-4.76	100.34	110.05
2	D	1	MAN	O2-C2-C3	-4.27	100.32	110.38
2	D	2	MAN	O4-C4-C3	4.13	120.11	110.38
2	C	2	MAN	O3-C3-C2	4.08	118.38	110.05
2	D	2	MAN	O5-C1-C2	3.99	120.31	110.79
2	C	1	MAN	C4-C3-C2	-3.80	104.16	110.83
2	C	2	MAN	O2-C2-C1	-3.56	101.08	109.22
2	C	2	MAN	C2-C3-C4	-3.51	104.68	110.86
2	D	2	MAN	O5-C5-C4	-3.36	102.66	110.83
2	D	1	MAN	C1-C2-C3	3.21	116.90	110.36
2	C	1	MAN	O3-C3-C4	2.79	116.95	110.38
2	D	2	MAN	C1-C2-C3	2.58	113.40	109.64
2	D	1	MAN	O1-C1-C2	2.50	116.24	108.98
2	D	1	MAN	C3-C4-C5	2.41	114.61	110.23
2	D	2	MAN	O2-C2-C1	2.24	114.36	109.22
2	D	1	MAN	O3-C3-C4	-2.21	105.18	110.38
2	D	2	MAN	O6-C6-C5	-2.19	103.86	111.33
2	C	2	MAN	O5-C5-C6	2.11	111.77	107.66
2	D	2	MAN	O5-C5-C6	2.08	111.72	107.66
2	D	1	MAN	O5-C5-C4	2.03	113.35	109.70

There are no chirality outliers.

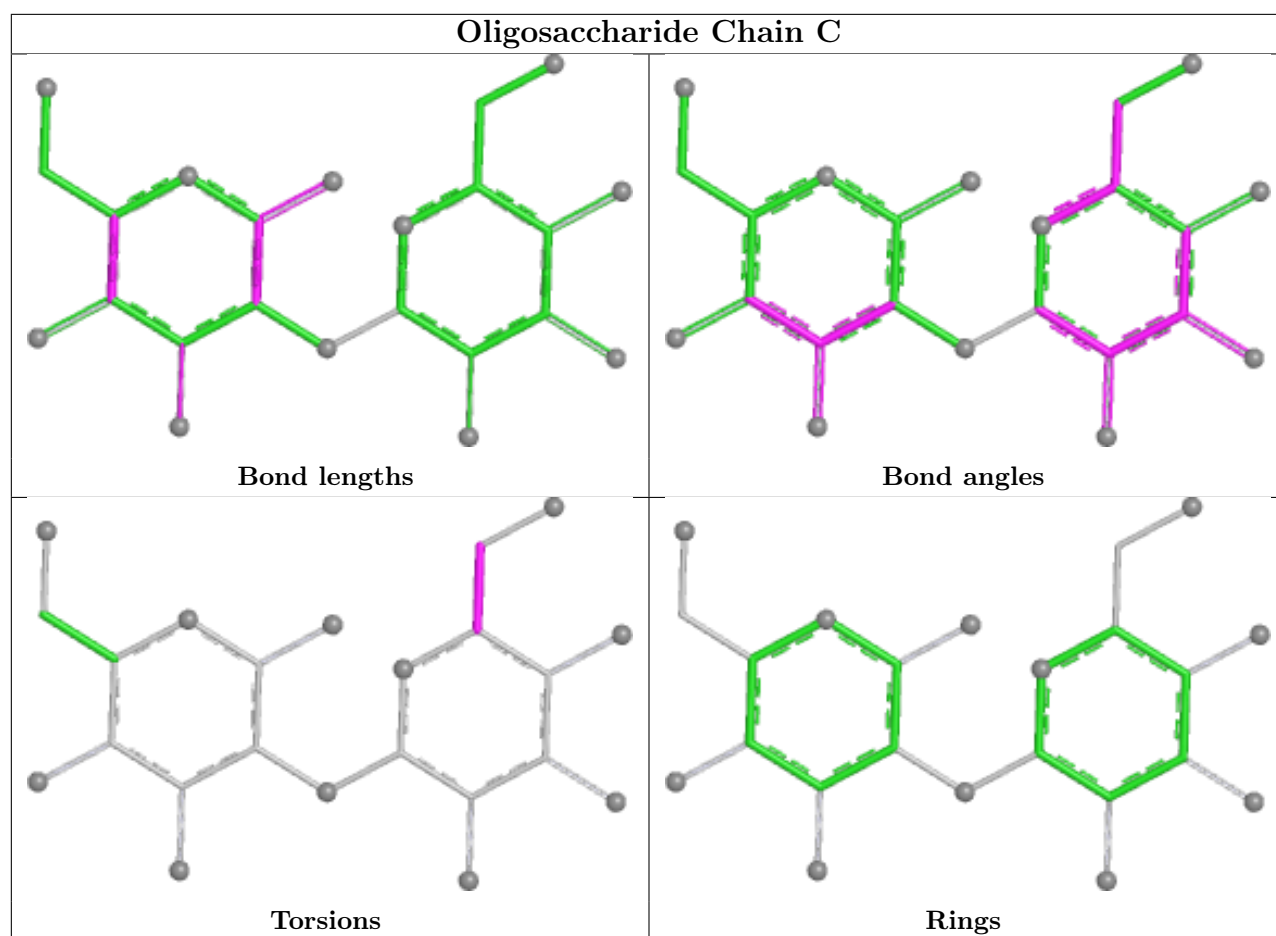
All (2) torsion outliers are listed below:

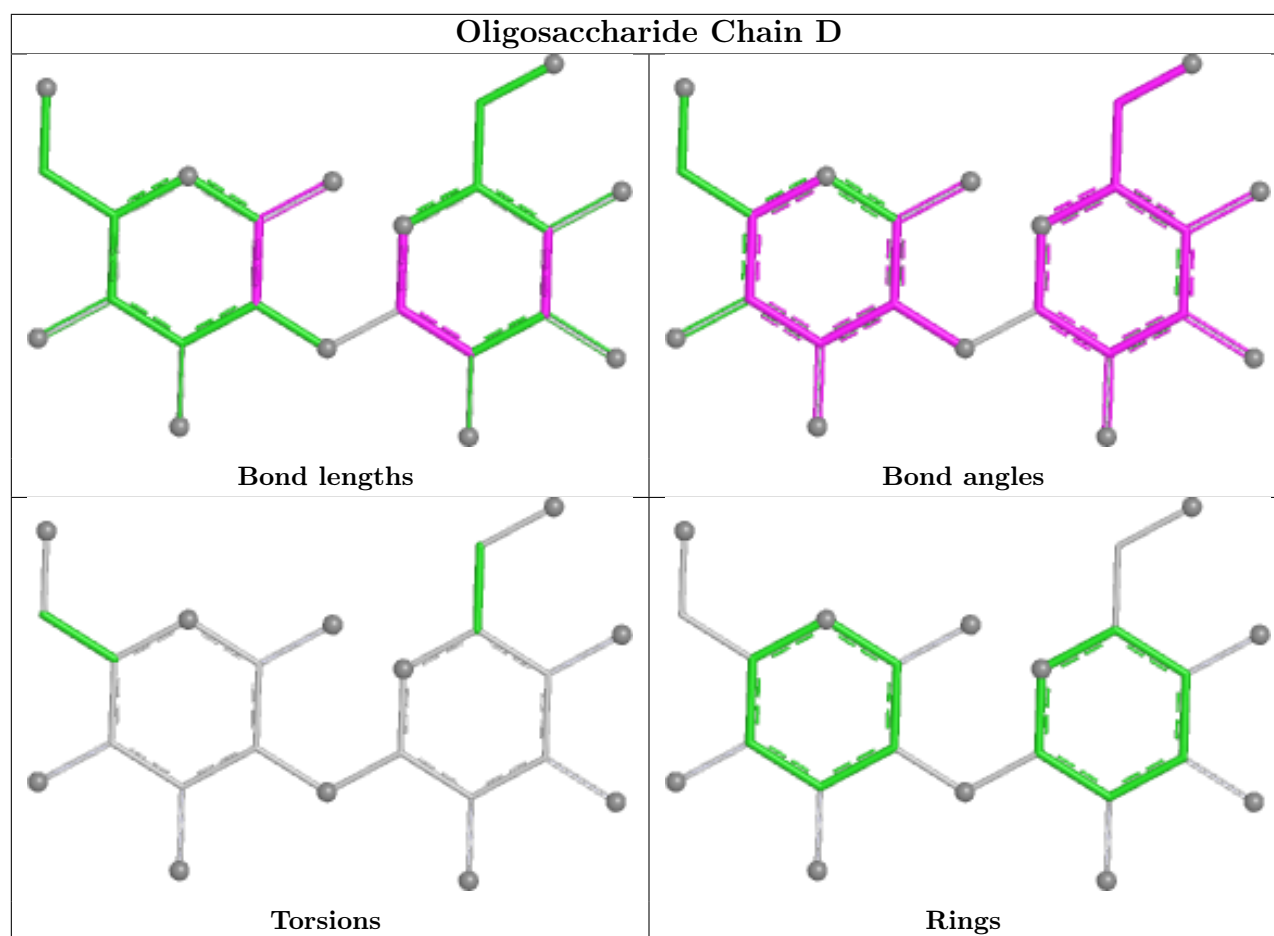
Mol	Chain	Res	Type	Atoms
2	C	2	MAN	C4-C5-C6-O6
2	C	2	MAN	O5-C5-C6-O6

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 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z > 2$
4	SO4	B	603	-	4,4,4	0.23	0	6,6,6	0.39	0
4	SO4	A	605	-	4,4,4	0.28	0	6,6,6	0.11	0
4	SO4	B	601	-	4,4,4	0.36	0	6,6,6	0.17	0
4	SO4	B	604	-	4,4,4	0.28	0	6,6,6	0.30	0
4	SO4	A	606	-	4,4,4	0.33	0	6,6,6	0.14	0
4	SO4	A	603	-	4,4,4	0.35	0	6,6,6	0.46	0
4	SO4	A	602	-	4,4,4	0.41	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	604	-	4,4,4	0.26	0	6,6,6	0.24	0
4	SO4	B	606	-	4,4,4	0.27	0	6,6,6	0.24	0
4	SO4	B	605	-	4,4,4	0.31	0	6,6,6	0.24	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
4	B	603	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	472/505 (93%)	0.24	5 (1%) 78 73	46, 74, 105, 125	0
1	B	398/505 (78%)	-0.13	15 (3%) 44 36	35, 56, 110, 169	0
All	All	870/1010 (86%)	0.07	20 (2%) 61 53	35, 66, 106, 169	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	465	ALA	4.2
1	B	460	TYR	4.1
1	B	40	THR	3.7
1	B	463	TRP	3.2
1	B	448	SER	3.1
1	B	458	LYS	3.1
1	B	446	THR	2.8
1	A	89	LYS	2.6
1	A	40	THR	2.6
1	B	417	GLN	2.5
1	B	462	ASP	2.3
1	B	371	THR	2.2
1	B	447	ARG	2.2
1	A	295	ASP	2.2
1	B	415	SER	2.1
1	B	449	VAL	2.1
1	B	416	GLU	2.1
1	B	411	LEU	2.0
1	A	159	GLY	2.0
1	A	503	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

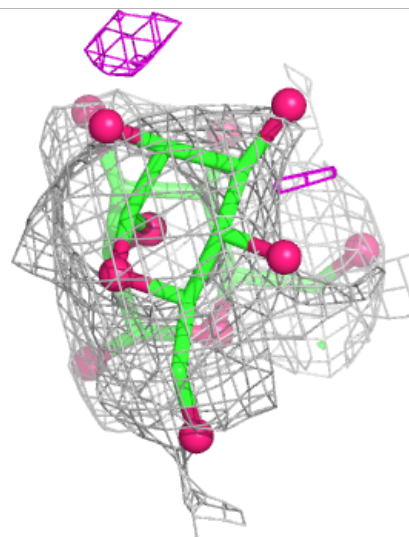
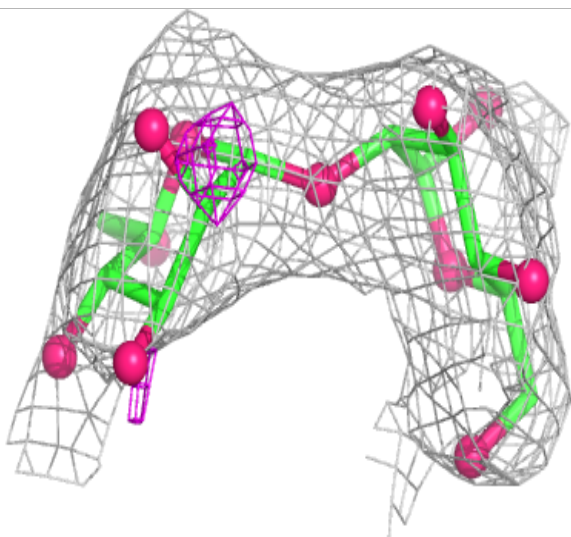
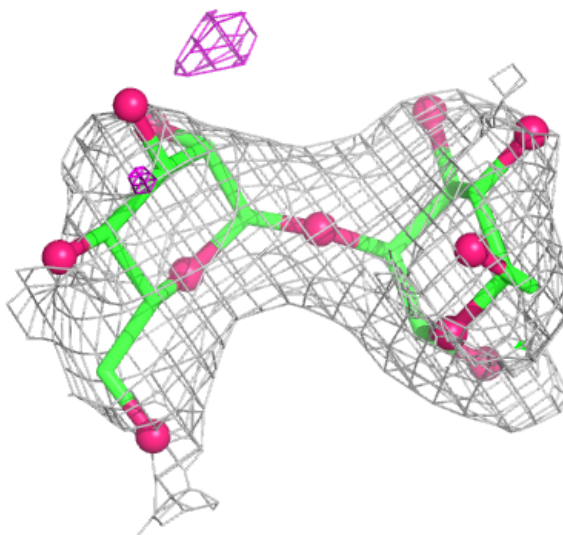
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

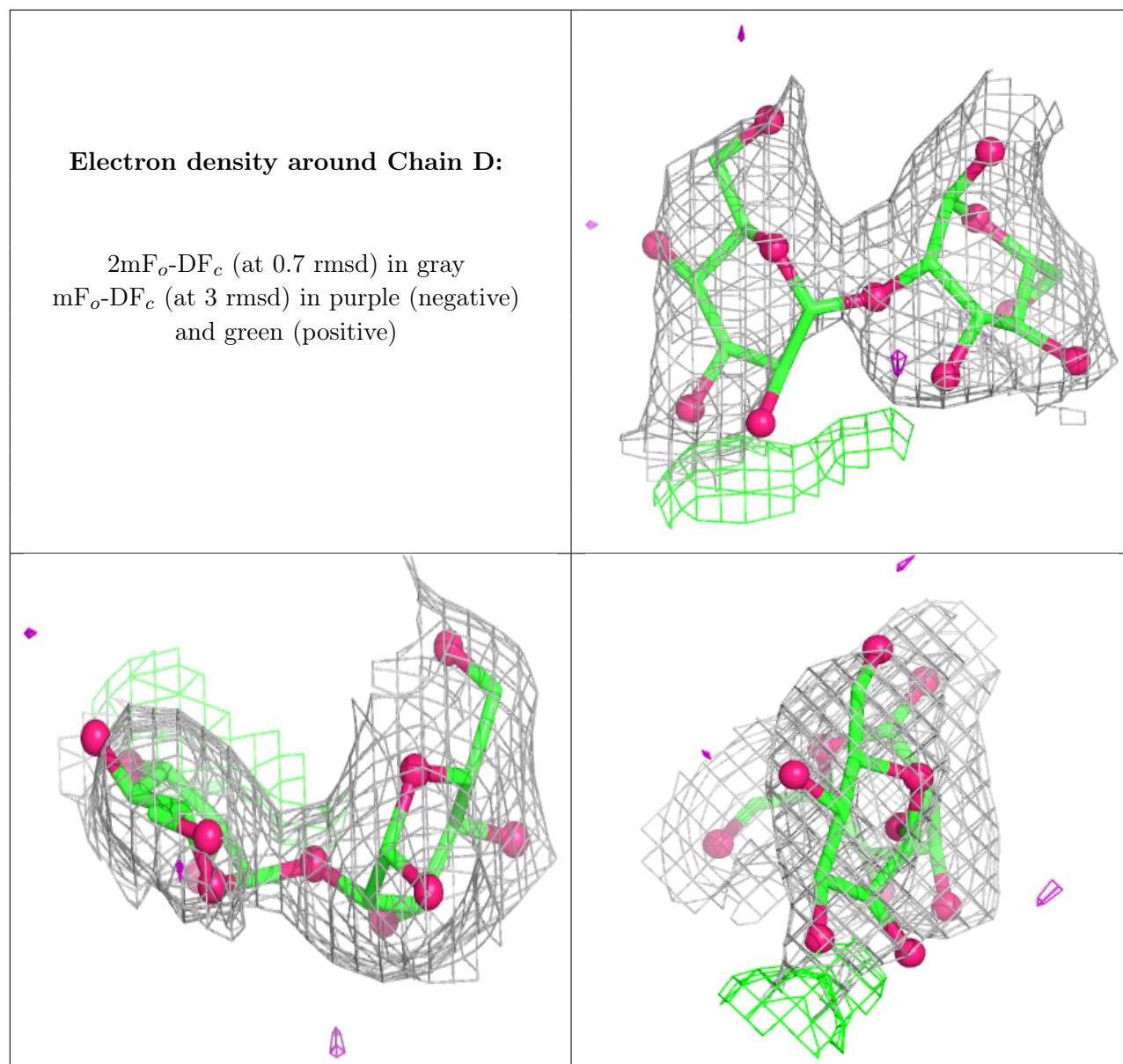
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	D	2	11/12	0.81	0.19	94,113,160,170	0
2	MAN	C	1	12/12	0.91	0.13	76,100,104,105	0
2	MAN	C	2	11/12	0.93	0.12	88,104,113,129	0
2	MAN	D	1	12/12	0.96	0.08	65,75,86,139	0

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

Electron density around Chain C:

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





6.4 Ligands ⓘ

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
4	SO4	B	601	5/5	0.79	0.20	107,108,119,128	0
4	SO4	B	605	5/5	0.79	0.15	123,123,141,185	0
4	SO4	A	604	5/5	0.82	0.13	126,142,161,166	0
4	SO4	B	604	5/5	0.86	0.16	78,81,121,140	0
4	SO4	A	605	5/5	0.87	0.12	95,115,135,140	0

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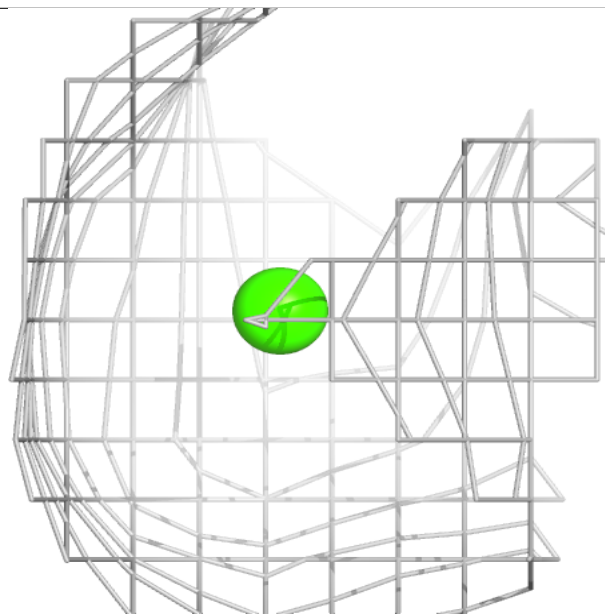
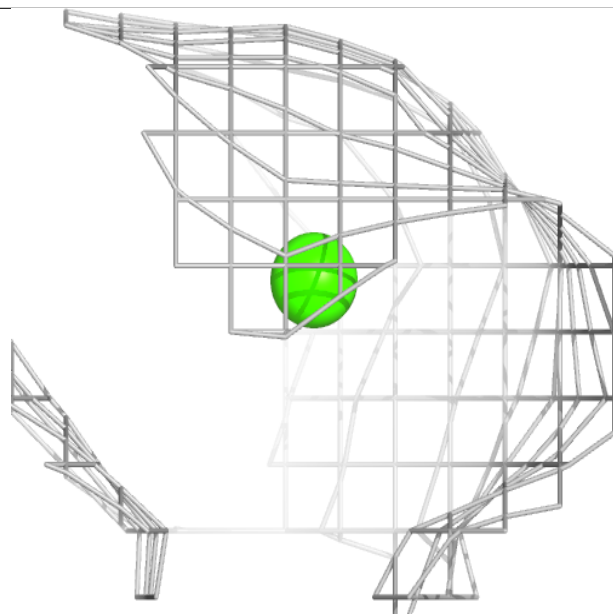
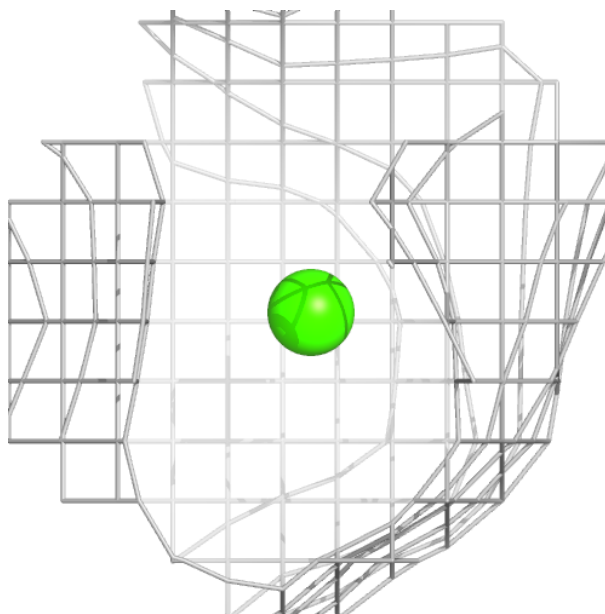
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	606	5/5	0.89	0.21	106,114,149,157	0
4	SO4	B	606	5/5	0.90	0.15	85,110,126,141	0
4	SO4	B	603	5/5	0.93	0.13	74,84,87,93	0
4	SO4	A	603	5/5	0.94	0.12	65,72,85,112	0
4	SO4	A	602	5/5	0.96	0.09	78,84,114,134	0
3	CA	A	601	1/1	0.99	0.04	64,64,64,64	0
3	CA	B	602	1/1	0.99	0.04	54,54,54,54	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

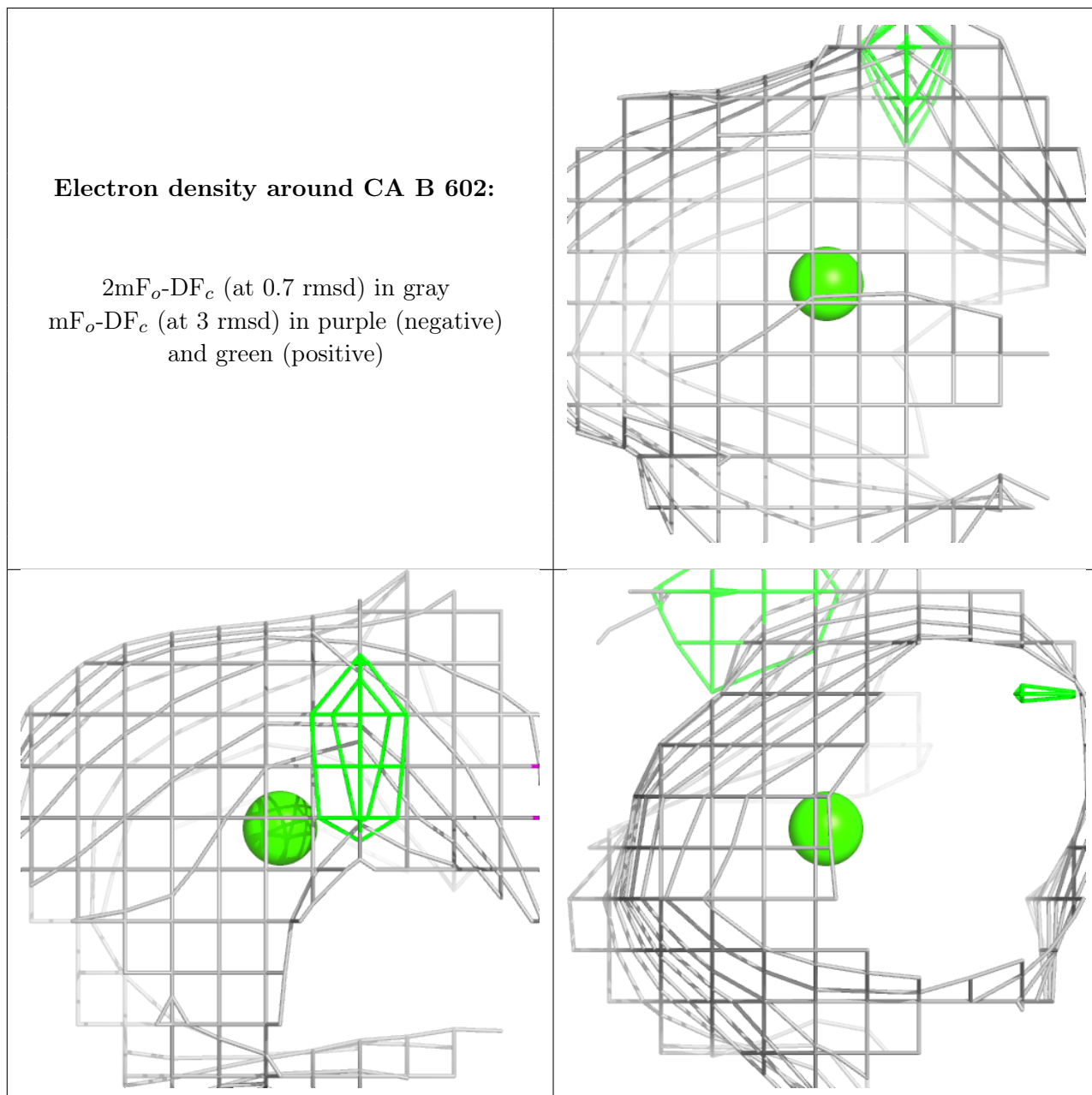
Electron density around CA A 601:

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



Electron density around CA B 602:

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

**6.5 Other polymers** [i](#)

There are no such residues in this entry.