



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:43 PM UTC

PDB ID : 5BXP / pdb_00005bxp
Title : LNBase in complex with LNB-LOGNAc
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Deposited on : 2015-06-09
Resolution : 1.70 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

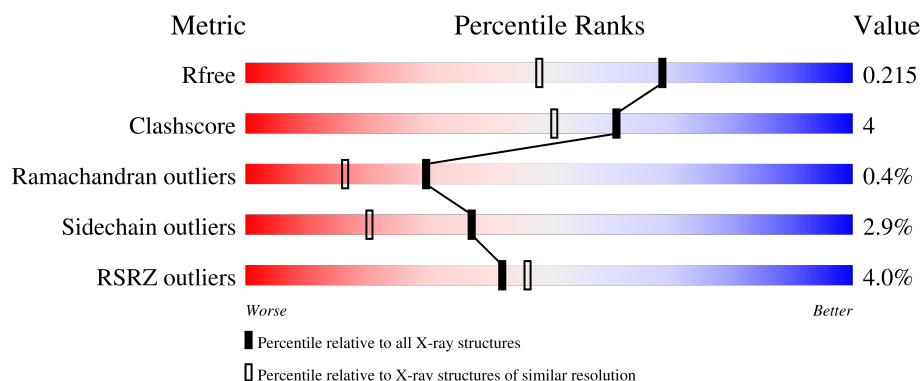
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	644	3% 85% 11% ..
1	B	644	5% 84% 12% ...
2	C	2	50% 50%
2	D	2	100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11012 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 Lacto-N-biosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	636	Total	C	N	O	S	0	0	0
			4997	3148	853	979	17			
1	B	636	Total	C	N	O	S	0	0	0
			4997	3148	853	979	17			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP B3TLD6
A	21	GLY	-	expression tag	UNP B3TLD6
A	22	SER	-	expression tag	UNP B3TLD6
A	23	SER	-	expression tag	UNP B3TLD6
A	24	HIS	-	expression tag	UNP B3TLD6
A	25	HIS	-	expression tag	UNP B3TLD6
A	26	HIS	-	expression tag	UNP B3TLD6
A	27	HIS	-	expression tag	UNP B3TLD6
A	28	HIS	-	expression tag	UNP B3TLD6
A	29	HIS	-	expression tag	UNP B3TLD6
A	30	SER	-	expression tag	UNP B3TLD6
A	31	SER	-	expression tag	UNP B3TLD6
A	32	GLY	-	expression tag	UNP B3TLD6
A	33	LEU	-	expression tag	UNP B3TLD6
A	34	VAL	-	expression tag	UNP B3TLD6
A	35	PRO	-	expression tag	UNP B3TLD6
A	36	ARG	-	expression tag	UNP B3TLD6
A	37	GLY	-	expression tag	UNP B3TLD6
A	38	SER	-	expression tag	UNP B3TLD6
A	39	HIS	-	expression tag	UNP B3TLD6
A	40	MET	-	expression tag	UNP B3TLD6
B	20	MET	-	initiating methionine	UNP B3TLD6
B	21	GLY	-	expression tag	UNP B3TLD6
B	22	SER	-	expression tag	UNP B3TLD6
B	23	SER	-	expression tag	UNP B3TLD6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	24	HIS	-	expression tag	UNP B3TLD6
B	25	HIS	-	expression tag	UNP B3TLD6
B	26	HIS	-	expression tag	UNP B3TLD6
B	27	HIS	-	expression tag	UNP B3TLD6
B	28	HIS	-	expression tag	UNP B3TLD6
B	29	HIS	-	expression tag	UNP B3TLD6
B	30	SER	-	expression tag	UNP B3TLD6
B	31	SER	-	expression tag	UNP B3TLD6
B	32	GLY	-	expression tag	UNP B3TLD6
B	33	LEU	-	expression tag	UNP B3TLD6
B	34	VAL	-	expression tag	UNP B3TLD6
B	35	PRO	-	expression tag	UNP B3TLD6
B	36	ARG	-	expression tag	UNP B3TLD6
B	37	GLY	-	expression tag	UNP B3TLD6
B	38	SER	-	expression tag	UNP B3TLD6
B	39	HIS	-	expression tag	UNP B3TLD6
B	40	MET	-	expression tag	UNP B3TLD6

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-3)-N-acetylglucosaminon o-1,5-lactone (Z)-oxime.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			27	14	2	11			
2	D	2	Total	C	N	O	0	0	0
			27	14	2	11			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

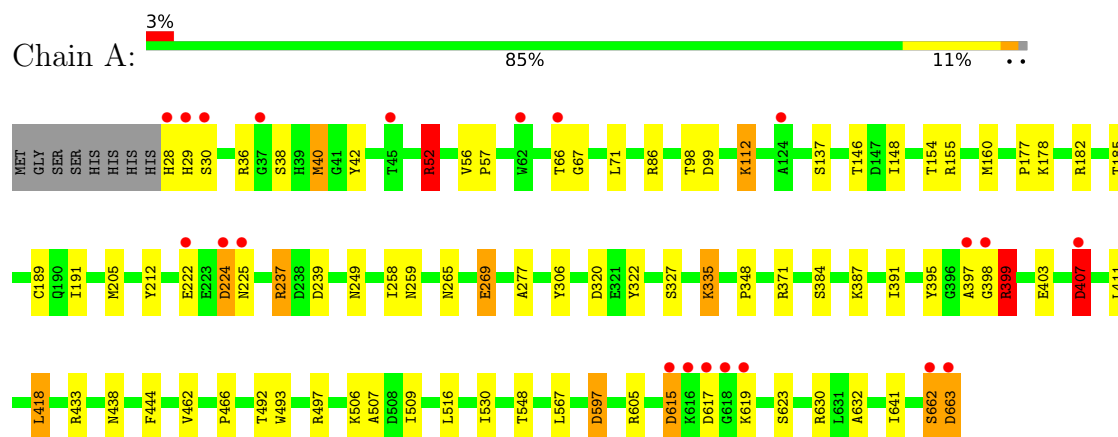
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	460	Total	O	0	0
			460	460		
4	B	479	Total	O	0	0
			479	479		

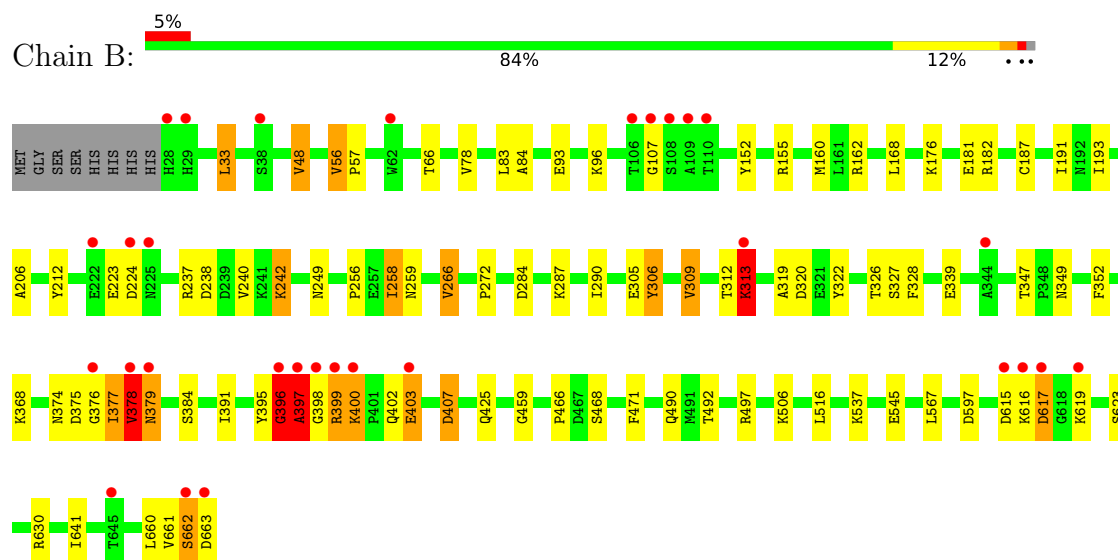
3 Residue-property plots

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: Lacto-N-biosidase



• Molecule 1: Lacto-N-biosidase



• Molecule 2: beta-D-galactopyranose-(1-3)-N-acetylglucosaminono-1,5-lactone (Z)-oxime



- Molecule 2: beta-D-galactopyranose-(1-3)-N-acetylglucosaminono-1,5-lactone (Z)-oxime

Chain D:

100%

LOG1
GAL2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	116.76Å 131.62Å 104.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 1.70 29.94 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.94-1.70) 99.6 (29.94-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.175 , 0.206 0.186 , 0.215	Depositor DCC
R_{free} test set	8805 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11012	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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, GAL, LOG

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	1.55	26/5108 (0.5%)	1.30	20/6932 (0.3%)
1	B	1.61	39/5108 (0.8%)	1.36	28/6932 (0.4%)
All	All	1.58	65/10216 (0.6%)	1.33	48/13864 (0.3%)

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
1	B	0	4
All	All	0	5

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	376	GLY	N-CA	11.15	1.63	1.45
1	B	400	LYS	CA-C	8.14	1.64	1.53
1	A	237	ARG	CD-NE	-8.00	1.35	1.46
1	B	309	VAL	N-CA	-7.79	1.37	1.46
1	A	632	ALA	CA-C	-7.54	1.43	1.52
1	B	397	ALA	CA-C	7.32	1.62	1.52
1	B	374	ASN	CA-C	7.12	1.62	1.52
1	A	597	ASP	CB-CG	6.89	1.69	1.52
1	B	497	ARG	CZ-NH2	6.89	1.42	1.33
1	A	398	GLY	C-O	6.70	1.29	1.23
1	B	56	VAL	CA-CB	6.63	1.59	1.54
1	B	258	ILE	C-O	6.49	1.31	1.24
1	B	83	LEU	N-CA	6.48	1.54	1.46
1	B	309	VAL	CA-C	6.42	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	256	PRO	CA-C	-6.33	1.44	1.52
1	A	205	MET	CA-C	6.22	1.60	1.52
1	B	240	VAL	CA-CB	-6.22	1.47	1.54
1	A	155	ARG	N-CA	6.20	1.53	1.46
1	B	545	GLU	CA-CB	-6.17	1.45	1.53
1	B	376	GLY	CA-C	6.14	1.63	1.52
1	B	206	ALA	N-CA	6.07	1.53	1.46
1	A	148	ILE	N-CA	5.95	1.54	1.46
1	A	418	LEU	N-CA	-5.90	1.39	1.46
1	B	319	ALA	C-O	-5.89	1.12	1.24
1	B	223	GLU	CA-CB	-5.84	1.44	1.53
1	A	507	ALA	N-CA	-5.83	1.39	1.46
1	A	178	LYS	N-CA	-5.75	1.39	1.46
1	B	224	ASP	CA-C	-5.62	1.45	1.52
1	B	328	PHE	N-CA	5.58	1.53	1.46
1	B	399	ARG	CA-C	5.54	1.59	1.52
1	B	290	ILE	CA-C	5.53	1.59	1.52
1	A	322	TYR	N-CA	5.52	1.53	1.46
1	B	306	TYR	CA-CB	-5.51	1.44	1.53
1	A	146	THR	N-CA	-5.48	1.38	1.45
1	A	548	THR	N-CA	5.48	1.52	1.45
1	B	193	ILE	C-O	5.48	1.30	1.24
1	B	272	PRO	C-O	-5.48	1.17	1.24
1	B	425	GLN	CA-C	5.46	1.62	1.52
1	B	56	VAL	N-CA	-5.43	1.41	1.45
1	A	52	ARG	N-CA	5.43	1.52	1.46
1	B	400	LYS	C-N	5.41	1.41	1.34
1	A	239	ASP	CG-OD2	-5.35	1.15	1.25
1	B	155	ARG	N-CA	5.33	1.52	1.46
1	A	371	ARG	CZ-NH1	5.32	1.40	1.32
1	A	224	ASP	C-O	-5.32	1.17	1.24
1	B	187	CYS	CA-CB	-5.31	1.46	1.52
1	A	185	THR	C-O	5.29	1.30	1.24
1	B	352	PHE	C-O	-5.28	1.18	1.24
1	B	377	ILE	CA-C	5.27	1.59	1.52
1	B	266	VAL	N-CA	-5.21	1.38	1.46
1	B	319	ALA	N-CA	-5.19	1.38	1.46
1	A	444	PHE	CA-CB	-5.18	1.44	1.53
1	A	66	THR	CA-CB	5.17	1.61	1.53
1	A	399	ARG	C-O	5.16	1.30	1.24
1	A	86	ARG	CZ-NH2	-5.15	1.26	1.33
1	A	277	ALA	N-CA	5.13	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	605	ARG	N-CA	-5.12	1.40	1.46
1	A	433	ARG	CD-NE	-5.12	1.39	1.46
1	B	490	GLN	CA-C	-5.09	1.46	1.52
1	B	322	TYR	C-O	5.08	1.30	1.24
1	B	152	TYR	CA-CB	-5.07	1.45	1.53
1	B	497	ARG	CD-NE	-5.05	1.39	1.46
1	A	225	ASN	CA-C	5.04	1.59	1.52
1	B	313	LYS	N-CA	-5.04	1.39	1.46
1	B	162	ARG	N-CA	5.01	1.51	1.46

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ARG	NE-CZ-NH2	-14.00	106.60	119.20
1	B	375	ASP	N-CA-C	13.40	129.09	113.01
1	A	237	ARG	CD-NE-CZ	12.29	141.60	124.40
1	B	662	SER	N-CA-C	9.82	122.06	111.36
1	A	52	ARG	NE-CZ-NH2	7.96	126.36	119.20
1	B	378	VAL	N-CA-CB	7.65	123.85	111.23
1	B	266	VAL	CG1-CB-CG2	7.49	127.28	110.80
1	B	309	VAL	N-CA-CB	-7.34	101.85	111.90
1	A	438	ASN	N-CA-C	6.33	120.30	112.58
1	B	312	THR	N-CA-C	6.13	118.68	110.35
1	A	52	ARG	CA-C-O	-5.96	115.41	119.29
1	A	269	GLU	CG-CD-OE2	-5.96	104.70	118.40
1	B	223	GLU	N-CA-C	5.86	119.44	110.36
1	B	56	VAL	CA-C-O	-5.83	116.91	119.94
1	A	112	LYS	N-CA-C	-5.78	106.19	113.18
1	A	52	ARG	CD-NE-CZ	5.77	132.47	124.40
1	A	67	GLY	O-C-N	5.77	128.38	122.90
1	B	242	LYS	N-CA-C	5.73	117.20	111.07
1	B	641	ILE	N-CA-C	5.71	117.13	110.62
1	A	154	THR	N-CA-CB	5.70	118.99	110.22
1	A	497	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	B	326	THR	CA-C-O	5.69	124.28	120.19
1	A	407	ASP	N-CA-C	5.61	119.96	113.18
1	B	506	LYS	N-CA-C	5.54	118.04	111.33
1	B	379	ASN	N-CA-C	5.51	118.52	109.76
1	B	347	THR	N-CA-C	5.49	119.14	110.58
1	B	403	GLU	CB-CG-CD	5.48	121.92	112.60
1	B	237	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	A	38	SER	N-CA-C	5.47	117.79	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	537	LYS	N-CA-C	5.45	117.97	111.71
1	B	84	ALA	N-CA-C	5.34	117.10	111.28
1	A	615	ASP	N-CA-C	5.31	117.39	110.43
1	A	52	ARG	CG-CD-NE	5.29	123.64	112.00
1	B	379	ASN	CA-C-O	5.28	126.71	120.69
1	B	379	ASN	CB-CA-C	5.20	118.31	109.84
1	A	615	ASP	CB-CA-C	-5.17	98.95	109.65
1	B	176	LYS	CA-C-N	-5.14	114.66	119.85
1	B	176	LYS	C-N-CA	-5.14	114.66	119.85
1	B	400	LYS	CA-C-N	-5.13	113.64	118.97
1	B	400	LYS	C-N-CA	-5.13	113.64	118.97
1	A	399	ARG	CB-CA-C	-5.10	100.27	110.42
1	B	375	ASP	CA-C-N	5.09	130.86	121.70
1	B	375	ASP	C-N-CA	5.09	130.86	121.70
1	A	516	LEU	N-CA-C	5.05	117.44	111.33
1	B	471	PHE	N-CA-C	5.05	118.70	112.54
1	B	377	ILE	CB-CA-C	-5.03	104.87	110.96
1	A	641	ILE	N-CA-C	5.03	116.35	110.62
1	A	237	ARG	NE-CZ-NH1	5.02	126.52	121.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	ARG	Sidechain
1	B	396	GLY	Peptide
1	B	397	ALA	Peptide
1	B	468	SER	Peptide
1	B	615	ASP	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	4997	0	4861	34	0
1	B	4997	0	4861	50	0
2	C	27	0	23	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	27	0	23	0	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
4	A	460	0	0	6	0
4	B	479	0	0	10	0
All	All	11012	0	9768	83	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (83) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ILE:HD11	1:B:391:ILE:HD13	1.34	1.04
1:B:378:VAL:HG23	1:B:379:ASN:N	1.71	1.01
1:B:378:VAL:HG23	1:B:379:ASN:H	1.32	0.93
1:A:160:MET:HE3	4:A:806:HOH:O	1.70	0.91
1:B:399:ARG:NH2	1:B:407:ASP:OD2	2.04	0.90
1:B:378:VAL:CG2	1:B:379:ASN:N	2.42	0.79
1:B:33:LEU:C	1:B:33:LEU:HD23	2.09	0.78
1:B:661:VAL:C	1:B:663:ASP:HB3	2.09	0.78
1:B:597:ASP:HB3	4:B:1205:HOH:O	1.85	0.77
1:B:238:ASP:HB3	4:B:1057:HOH:O	1.86	0.74
1:B:377:ILE:HD11	1:B:391:ILE:CD1	2.17	0.72
1:B:78:VAL:CG1	1:B:107:GLY:C	2.63	0.71
1:B:313:LYS:O	1:B:313:LYS:HG2	1.92	0.67
1:B:305:GLU:CD	4:B:898:HOH:O	2.38	0.67
1:B:377:ILE:CG2	1:B:399:ARG:HD3	2.26	0.65
1:A:662:SER:O	1:A:663:ASP:C	2.39	0.65
1:A:265:ASN:O	1:A:269:GLU:HG3	1.96	0.64
1:A:615:ASP:O	1:A:617:ASP:HA	1.99	0.63
1:B:662:SER:N	1:B:663:ASP:HB3	2.14	0.63
1:B:377:ILE:HG22	1:B:399:ARG:HG3	1.81	0.61
1:B:399:ARG:HH22	1:B:407:ASP:CG	2.09	0.59
1:A:335:LYS:HG2	1:A:348:PRO:HD3	1.83	0.59
1:A:399:ARG:NH1	1:A:403:GLU:OE1	2.36	0.58
1:B:48:VAL:HG12	4:B:1077:HOH:O	2.04	0.57
1:B:78:VAL:HG12	1:B:107:GLY:O	2.06	0.56
1:B:378:VAL:CG2	1:B:379:ASN:H	2.04	0.54
1:A:623:SER:OG	1:A:630:ARG:HD3	2.09	0.53
1:B:33:LEU:C	1:B:33:LEU:CD2	2.80	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:TYR:O	1:B:397:ALA:N	2.42	0.51
1:A:42:TYR:CG	1:A:137:SER:HA	2.46	0.51
1:B:597:ASP:CB	4:B:1205:HOH:O	2.52	0.51
1:A:40:MET:HG2	1:A:112:LYS:HE2	1.94	0.50
1:B:377:ILE:HG22	1:B:399:ARG:CG	2.42	0.49
1:A:506:LYS:HA	1:A:509:ILE:HG12	1.95	0.49
1:A:56:VAL:HA	1:A:57:PRO:C	2.37	0.49
1:A:182:ARG:HG2	1:A:492:THR:HB	1.95	0.49
1:B:258:ILE:HD11	1:B:306:TYR:CE1	2.48	0.48
1:A:40:MET:CG	1:A:112:LYS:HE2	2.43	0.48
1:A:28:HIS:HB2	1:B:663:ASP:OD2	2.13	0.48
1:B:284:ASP:OD2	1:B:287:LYS:NZ	2.42	0.48
1:B:33:LEU:HD23	1:B:33:LEU:O	2.14	0.48
1:B:616:LYS:O	1:B:617:ASP:CB	2.61	0.48
1:B:160:MET:HE3	1:B:168:LEU:HD13	1.96	0.47
1:B:398:GLY:HA3	4:B:804:HOH:O	2.13	0.47
1:B:78:VAL:HG12	1:B:107:GLY:C	2.37	0.47
1:A:191:ILE:C	1:A:191:ILE:HD12	2.40	0.46
1:A:249:ASN:HB3	4:A:825:HOH:O	2.15	0.46
1:B:349:ASN:ND2	1:B:378:VAL:CG2	2.79	0.46
1:A:615:ASP:HB2	1:A:619:LYS:H	1.79	0.46
1:B:259:ASN:ND2	1:B:320:ASP:OD1	2.38	0.46
1:B:242:LYS:HE3	4:B:1057:HOH:O	2.16	0.46
1:A:395:TYR:CZ	1:A:397:ALA:HB3	2.50	0.46
1:A:530:ILE:HD11	4:A:1139:HOH:O	2.16	0.46
1:A:615:ASP:OD2	1:A:619:LYS:HB2	2.16	0.45
1:A:399:ARG:HB2	4:A:1099:HOH:O	2.16	0.45
1:A:259:ASN:ND2	1:A:320:ASP:OD1	2.45	0.45
1:B:396:GLY:O	1:B:397:ALA:CB	2.64	0.45
1:A:30:SER:CB	1:B:619:LYS:HB3	2.47	0.45
1:A:177:PRO:HD3	1:A:493:TRP:CH2	2.52	0.45
1:B:212:TYR:CD1	1:B:212:TYR:C	2.95	0.45
1:B:56:VAL:HA	1:B:57:PRO:C	2.43	0.44
1:B:398:GLY:O	1:B:399:ARG:C	2.60	0.44
1:A:387:LYS:HE3	1:A:407:ASP:O	2.18	0.44
1:B:182:ARG:HG2	1:B:492:THR:HB	1.99	0.44
1:B:339:GLU:CD	4:B:819:HOH:O	2.60	0.44
1:B:402:GLN:NE2	1:B:402:GLN:HA	2.33	0.44
1:B:96:LYS:HD2	1:B:516:LEU:HD21	1.98	0.44
1:B:191:ILE:C	1:B:191:ILE:HD12	2.43	0.43
1:A:615:ASP:C	1:A:617:ASP:HA	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LYS:HE3	4:B:903:HOH:O	2.19	0.43
1:B:623:SER:OG	1:B:630:ARG:HD3	2.18	0.43
1:B:249:ASN:HB3	4:B:1037:HOH:O	2.18	0.43
1:A:418:LEU:HB3	1:A:462:VAL:HA	2.00	0.42
1:A:212:TYR:CD1	1:A:212:TYR:C	2.97	0.42
1:A:391:ILE:HB	1:A:411:LEU:HD23	2.02	0.41
2:C:1:LOG:O7	2:C:1:LOG:C1	2.67	0.41
1:A:52:ARG:CZ	4:A:850:HOH:O	2.67	0.41
1:B:313:LYS:O	1:B:313:LYS:CG	2.66	0.41
1:A:98:THR:O	1:A:99:ASP:HB2	2.20	0.41
1:A:189:CYS:HB2	4:A:1132:HOH:O	2.21	0.41
1:A:258:ILE:HD11	1:A:306:TYR:CE1	2.56	0.41
1:B:181:GLU:O	1:B:459:GLY:HA3	2.21	0.41
1:A:71:LEU:HD23	1:A:71:LEU:C	2.47	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	634/644 (98%)	619 (98%)	14 (2%)	1 (0%)	43	28
1	B	634/644 (98%)	615 (97%)	15 (2%)	4 (1%)	21	9
All	All	1268/1288 (98%)	1234 (97%)	29 (2%)	5 (0%)	30	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	396	GLY
1	B	397	ALA
1	B	617	ASP
1	A	466	PRO

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Mol	Chain	Res	Type
1	B	466	PRO

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	533/540 (99%)	518 (97%)	15 (3%)	38	21
1	B	533/540 (99%)	517 (97%)	16 (3%)	36	19
All	All	1066/1080 (99%)	1035 (97%)	31 (3%)	37	20

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	36	ARG
1	A	40	MET
1	A	52	ARG
1	A	222	GLU
1	A	224	ASP
1	A	327	SER
1	A	335	LYS
1	A	384	SER
1	A	399	ARG
1	A	407	ASP
1	A	567	LEU
1	A	597	ASP
1	A	662	SER
1	A	663	ASP
1	B	33	LEU
1	B	48	VAL
1	B	66	THR
1	B	93	GLU
1	B	266	VAL
1	B	309	VAL
1	B	313	LYS

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Mol	Chain	Res	Type
1	B	327	SER
1	B	368	LYS
1	B	378	VAL
1	B	384	SER
1	B	400	LYS
1	B	403	GLU
1	B	407	ASP
1	B	567	LEU
1	B	660	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	402	GLN
1	B	341	GLN
1	B	349	ASN
1	B	369	GLN
1	B	555	GLN

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	LOG	C	1	2	13,16,16	1.72	3 (23%)	14,22,22	2.09	5 (35%)
2	GAL	C	2	2	11,11,12	1.29	2 (18%)	15,15,17	1.88	2 (13%)
2	LOG	D	1	2	13,16,16	1.35	2 (15%)	14,22,22	1.65	3 (21%)
2	GAL	D	2	2	11,11,12	1.20	0	15,15,17	1.30	2 (13%)

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	LOG	C	1	2	-	1/6/28/28	0/1/1/1
2	GAL	C	2	2	-	0/2/19/22	0/1/1/1
2	LOG	D	1	2	-	2/6/28/28	0/1/1/1
2	GAL	D	2	2	-	0/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	LOG	O1-N1	3.90	1.52	1.40
2	C	1	LOG	C3-C2	3.37	1.57	1.52
2	C	2	GAL	C2-C3	-2.86	1.48	1.52
2	D	1	LOG	O1-N1	2.66	1.48	1.40
2	C	1	LOG	O7-C7	2.20	1.28	1.23
2	C	2	GAL	C4-C5	2.17	1.57	1.53
2	D	1	LOG	C8-C7	2.06	1.54	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	GAL	O3-C3-C2	-5.39	99.06	110.05
2	D	1	LOG	C3-C4-C5	-3.84	103.26	110.23
2	C	1	LOG	C2-N2-C7	-3.76	115.37	121.82
2	C	1	LOG	C3-C4-C5	-3.68	103.56	110.23
2	C	2	GAL	O3-C3-C4	3.11	117.70	110.38
2	D	2	GAL	O2-C2-C3	-3.08	103.77	110.15
2	C	1	LOG	C3-C2-N2	-3.07	107.33	112.26
2	C	1	LOG	O4-C4-C3	2.82	117.03	110.38
2	D	1	LOG	O3-C3-C2	-2.46	103.99	108.98
2	C	1	LOG	O3-C3-C2	-2.28	104.38	108.98
2	D	1	LOG	O5-C5-C6	-2.06	103.98	106.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GAL	C1-O5-C5	-2.02	109.48	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

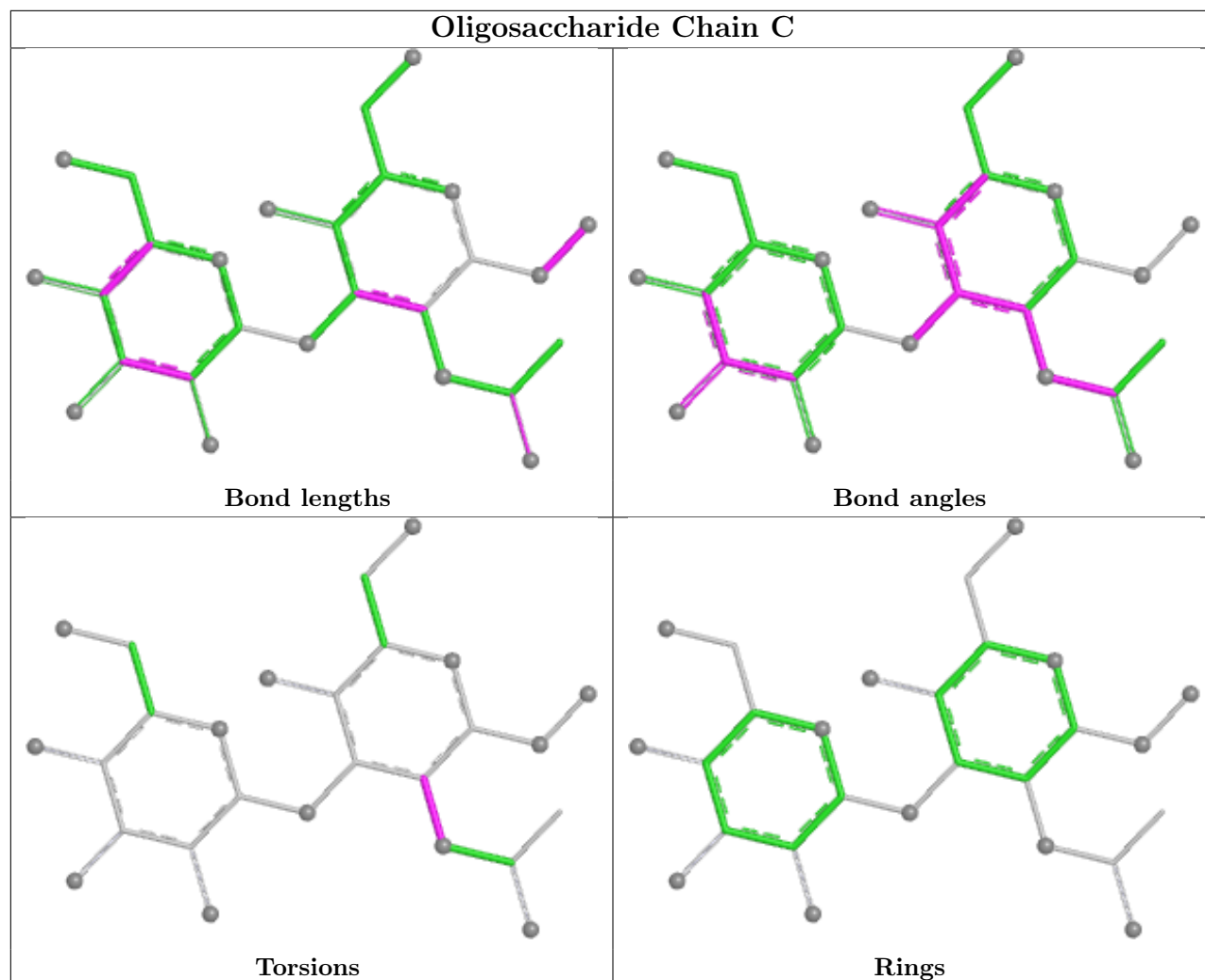
Mol	Chain	Res	Type	Atoms
2	C	1	LOG	C1-C2-N2-C7
2	D	1	LOG	C1-C2-N2-C7
2	D	1	LOG	O7-C7-N2-C2

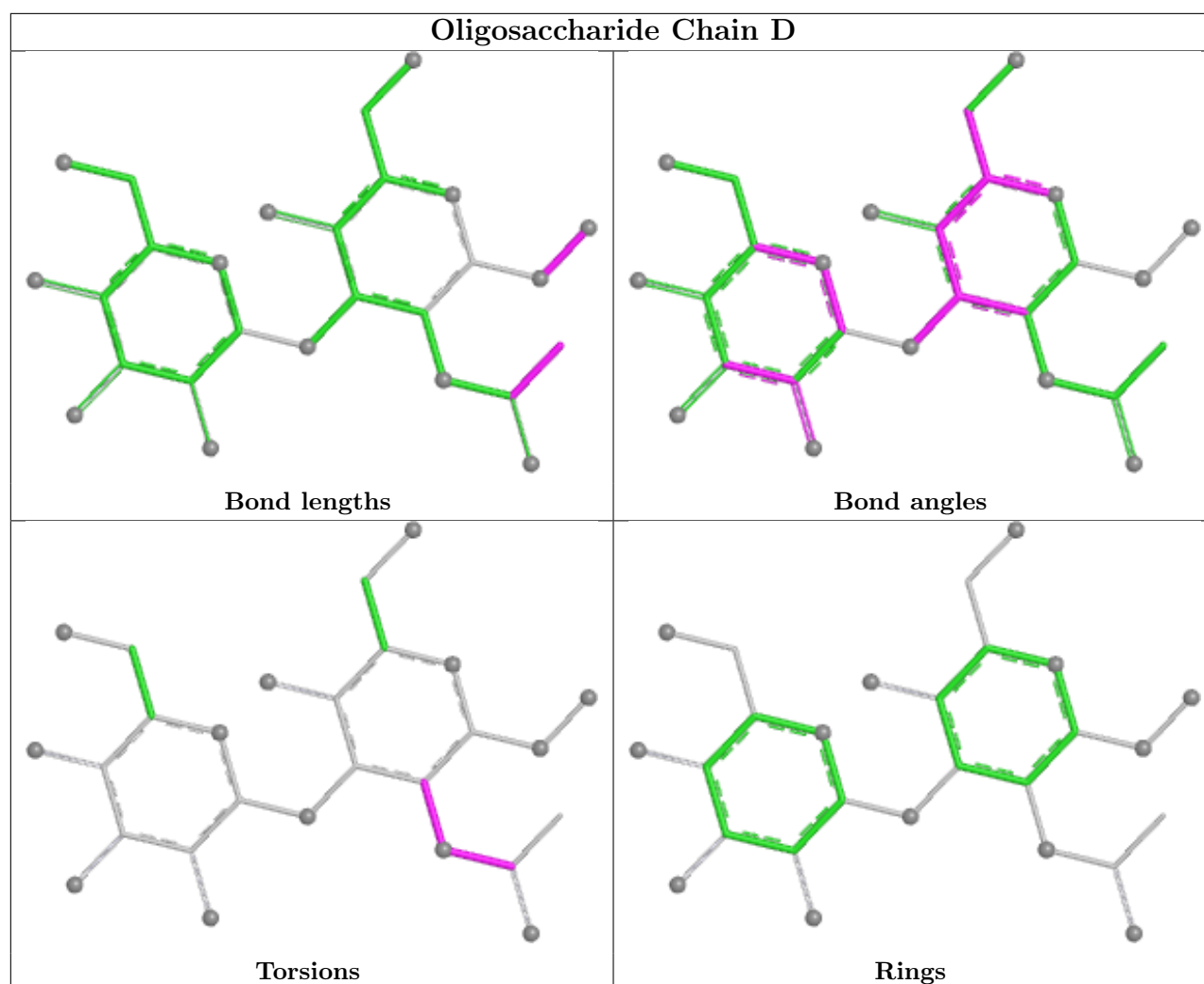
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	LOG	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](#)

5 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	705	-	4,4,4	0.81	0	6,6,6	0.20	0
3	SO4	B	703	-	4,4,4	1.28	0	6,6,6	0.98	0
3	SO4	B	704	-	4,4,4	0.57	0	6,6,6	0.31	0
3	SO4	A	703	-	4,4,4	0.70	0	6,6,6	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	704	-	4,4,4	1.17	0	6,6,6	0.88	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.

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	636/644 (98%)	0.01	21 (3%) 49 53	11, 18, 35, 76	0
1	B	636/644 (98%)	0.06	30 (4%) 36 40	10, 18, 36, 68	0
All	All	1272/1288 (98%)	0.03	51 (4%) 42 46	10, 18, 36, 76	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	398	GLY	7.1
1	A	29	HIS	6.6
1	B	397	ALA	6.6
1	B	378	VAL	5.7
1	A	616	LYS	5.6
1	B	663	ASP	5.1
1	B	379	ASN	5.0
1	B	110	THR	5.0
1	B	29	HIS	4.8
1	B	399	ARG	4.5
1	B	109	ALA	4.4
1	B	107	GLY	4.4
1	B	400	LYS	4.2
1	A	398	GLY	4.0
1	B	662	SER	4.0
1	A	617	ASP	4.0
1	A	224	ASP	3.9
1	A	62	TRP	3.7
1	B	616	LYS	3.6
1	B	645	THR	3.5
1	A	28	HIS	3.4
1	B	376	GLY	3.4
1	A	66	THR	3.3
1	A	618	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	28	HIS	3.2
1	A	615	ASP	3.1
1	A	663	ASP	3.1
1	B	106	THR	2.9
1	A	222	GLU	2.8
1	B	38	SER	2.8
1	B	396	GLY	2.8
1	A	397	ALA	2.7
1	A	619	LYS	2.7
1	B	615	ASP	2.7
1	A	37	GLY	2.7
1	A	30	SER	2.6
1	A	662	SER	2.6
1	A	407	ASP	2.6
1	B	619	LYS	2.5
1	B	108	SER	2.5
1	B	62	TRP	2.4
1	A	124	ALA	2.4
1	A	45	THR	2.4
1	A	225	ASN	2.3
1	B	617	ASP	2.3
1	B	313	LYS	2.3
1	B	224	ASP	2.3
1	B	403	GLU	2.2
1	B	222	GLU	2.1
1	B	225	ASN	2.1
1	B	344	ALA	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.

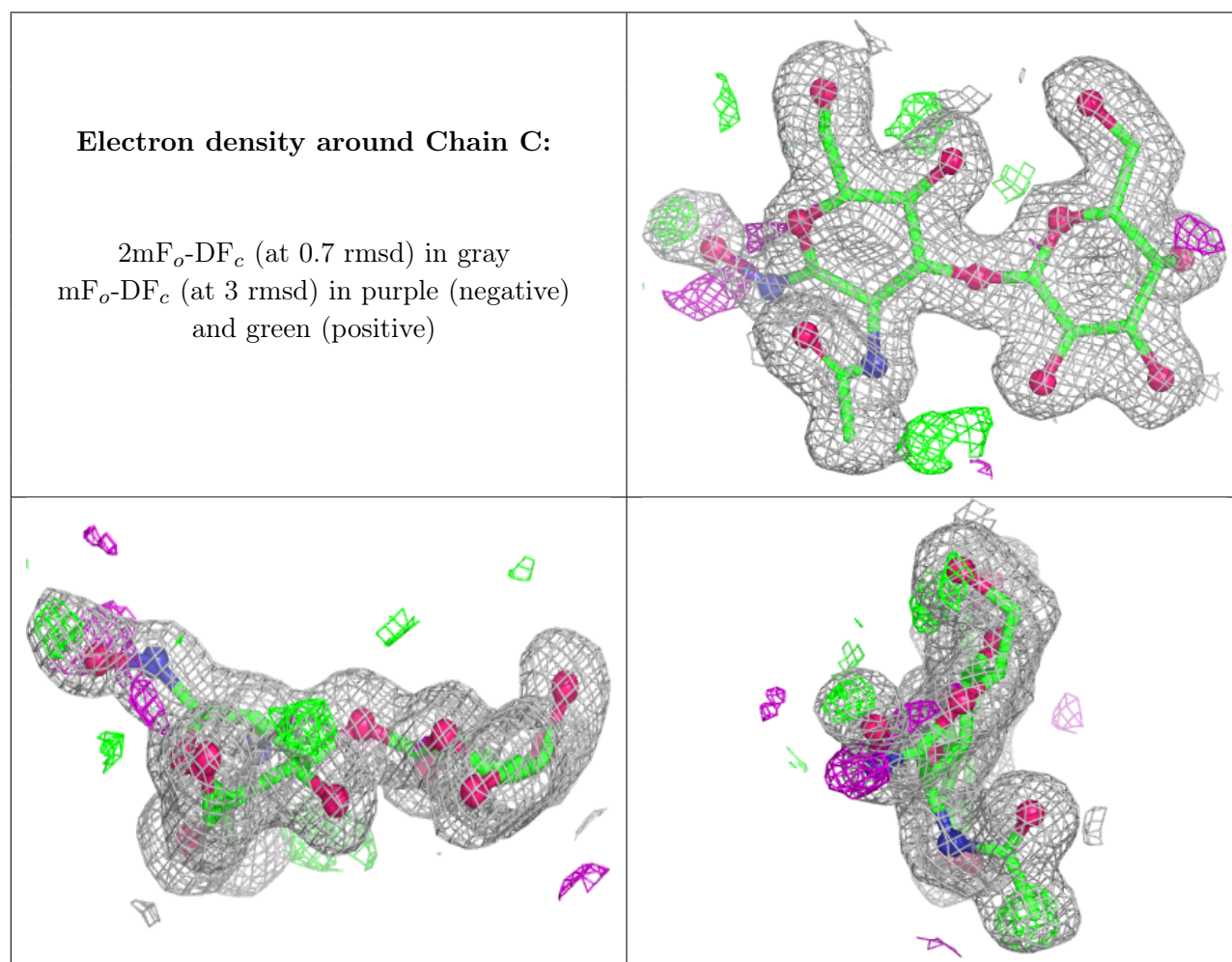
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LOG	D	1	16/16	0.92	0.09	16,19,21,28	0

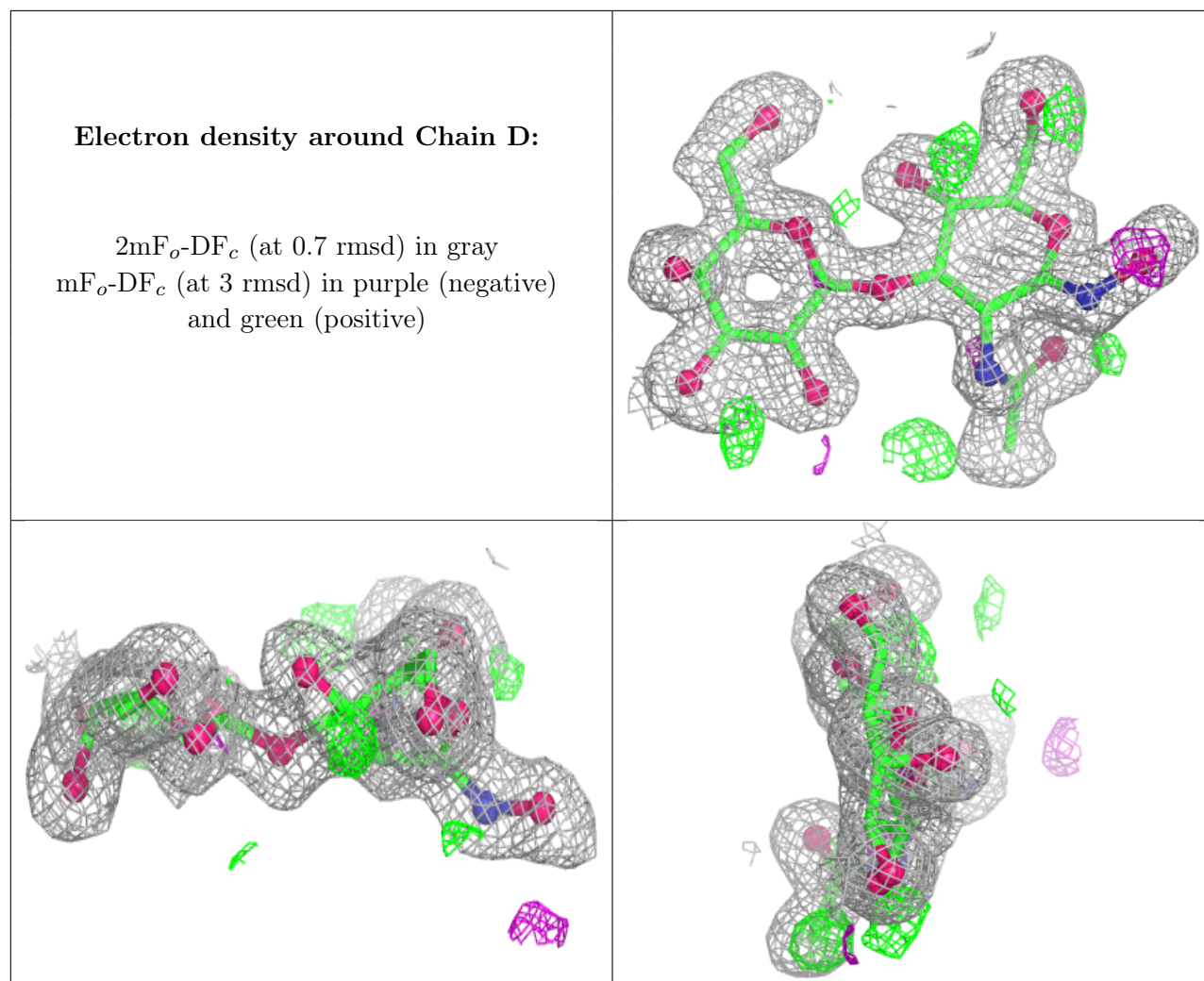
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LOG	C	1	16/16	0.93	0.08	17,21,23,34	0
2	GAL	C	2	11/12	0.94	0.08	18,21,23,24	0
2	GAL	D	2	11/12	0.94	0.07	17,18,22,22	0

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	SO4	B	703	5/5	0.90	0.18	26,30,36,41	0
3	SO4	A	704	5/5	0.93	0.22	28,30,35,43	0
3	SO4	A	703	5/5	0.97	0.12	26,32,35,37	0
3	SO4	A	705	5/5	0.99	0.04	17,18,19,22	0
3	SO4	B	704	5/5	0.99	0.05	16,17,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.