



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:41 PM UTC

PDB ID : 5GZV / pdb_00005gzv
Title : Crystal Structure of Chitinase ChiW from Paenibacillus sp. str. FPU-7 Reveals a Novel Type of Bacterial Cell-Surface-Expressed Multi-Modular Enzyme Machinery
Authors : Itoh, T.; Hibi, T.; Suzuki, F.; Sugimoto, I.; Fujiwara, A.; Inaka, K.; Tanaka, H.; Ohta, K.; Fujii, Y.; Taketo, A.; Kimoto, H.
Deposited on : 2016-10-01
Resolution : 2.61 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

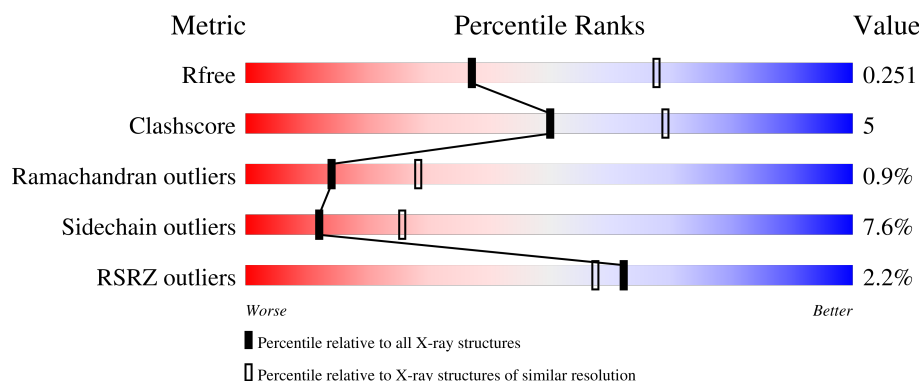
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	885	% 80% 15% ..
1	B	885	3% 77% 17% ..
2	C	2	100%
2	D	2	100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13773 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 Chitinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	860	Total	C	N	O	S	0	3	0
			6762	4324	1112	1314	12			
1	B	859	Total	C	N	O	S	0	1	0
			6741	4310	1108	1311	12			

There are 46 discrepancies between the modelled and reference sequences:

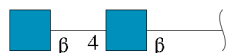
Chain	Residue	Modelled	Actual	Comment	Reference
A	534	MET	-	initiating methionine	UNP K7ZLW6
A	535	ASN	-	expression tag	UNP K7ZLW6
A	536	HIS	-	expression tag	UNP K7ZLW6
A	537	LYS	-	expression tag	UNP K7ZLW6
A	538	VAL	-	expression tag	UNP K7ZLW6
A	539	HIS	-	expression tag	UNP K7ZLW6
A	540	HIS	-	expression tag	UNP K7ZLW6
A	541	HIS	-	expression tag	UNP K7ZLW6
A	542	HIS	-	expression tag	UNP K7ZLW6
A	543	HIS	-	expression tag	UNP K7ZLW6
A	544	HIS	-	expression tag	UNP K7ZLW6
A	545	ILE	-	expression tag	UNP K7ZLW6
A	546	GLU	-	expression tag	UNP K7ZLW6
A	547	GLY	-	expression tag	UNP K7ZLW6
A	548	ARG	-	expression tag	UNP K7ZLW6
A	549	HIS	-	expression tag	UNP K7ZLW6
A	550	MET	-	expression tag	UNP K7ZLW6
A	551	GLU	-	expression tag	UNP K7ZLW6
A	552	LEU	-	expression tag	UNP K7ZLW6
A	553	GLY	-	expression tag	UNP K7ZLW6
A	554	THR	-	expression tag	UNP K7ZLW6
A	555	LEU	-	expression tag	UNP K7ZLW6
A	556	GLU	-	expression tag	UNP K7ZLW6
B	534	MET	-	initiating methionine	UNP K7ZLW6
B	535	ASN	-	expression tag	UNP K7ZLW6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	536	HIS	-	expression tag	UNP K7ZLW6
B	537	LYS	-	expression tag	UNP K7ZLW6
B	538	VAL	-	expression tag	UNP K7ZLW6
B	539	HIS	-	expression tag	UNP K7ZLW6
B	540	HIS	-	expression tag	UNP K7ZLW6
B	541	HIS	-	expression tag	UNP K7ZLW6
B	542	HIS	-	expression tag	UNP K7ZLW6
B	543	HIS	-	expression tag	UNP K7ZLW6
B	544	HIS	-	expression tag	UNP K7ZLW6
B	545	ILE	-	expression tag	UNP K7ZLW6
B	546	GLU	-	expression tag	UNP K7ZLW6
B	547	GLY	-	expression tag	UNP K7ZLW6
B	548	ARG	-	expression tag	UNP K7ZLW6
B	549	HIS	-	expression tag	UNP K7ZLW6
B	550	MET	-	expression tag	UNP K7ZLW6
B	551	GLU	-	expression tag	UNP K7ZLW6
B	552	LEU	-	expression tag	UNP K7ZLW6
B	553	GLY	-	expression tag	UNP K7ZLW6
B	554	THR	-	expression tag	UNP K7ZLW6
B	555	LEU	-	expression tag	UNP K7ZLW6
B	556	GLU	-	expression tag	UNP K7ZLW6

- 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	C	2	Total	C	N	O	0	0	0
			29	16	2	11			
2	D	2	Total	C	N	O	0	0	0
			29	16	2	11			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

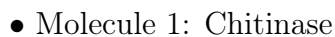


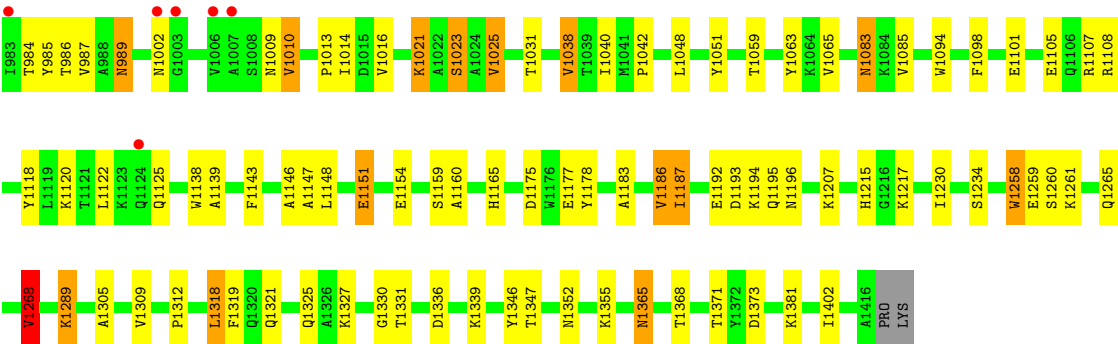
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

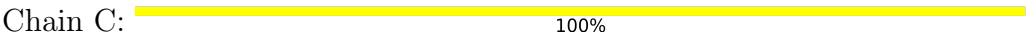
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		
4	B	85	Total	O	0	0
			85	85		

- Molecule 1: Chitinase





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



• 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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.99Å 127.23Å 161.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.61 50.01 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.01-2.61) 99.0 (50.01-2.61)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.20 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.203 , 0.253 0.206 , 0.251	Depositor DCC
R_{free} test set	3459 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13773	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8065e-03.*

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: NAG, PO4

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	1.00	2/6945 (0.0%)	1.11	12/9463 (0.1%)
1	B	1.06	4/6918 (0.1%)	1.15	19/9427 (0.2%)
All	All	1.03	6/13863 (0.0%)	1.13	31/18890 (0.2%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1025	VAL	CA-C	7.40	1.59	1.52
1	B	1051	TYR	C-O	-6.57	1.16	1.23
1	A	693	PRO	C-O	-5.33	1.17	1.23
1	B	1336	ASP	CA-C	-5.19	1.46	1.52
1	A	558	GLN	N-CA	5.11	1.52	1.46

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1330	GLY	N-CA-C	-8.93	103.45	111.67
1	A	979	ILE	N-CA-C	-8.80	100.32	108.95
1	B	1234	SER	N-CA-C	7.34	121.68	112.87
1	B	989	ASN	N-CA-C	-7.21	97.84	109.96
1	A	1330	GLY	N-CA-C	-6.25	105.92	111.67

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	6762	0	6539	71	0
1	B	6741	0	6511	71	0
2	C	29	0	27	0	0
2	D	29	0	27	6	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	117	0	0	0	0
4	B	85	0	0	1	0
All	All	13773	0	13104	141	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.

The worst 5 of 141 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:906:GLU:OE2	1:B:908:SER:OG	2.07	0.70
1:A:1094:TRP:CZ3	1:A:1107:ARG:HG3	2.26	0.70
1:B:1010:VAL:HG11	1:B:1014:ILE:HD11	1.75	0.69
1:B:909:GLN:HE22	2:D:2:NAG:H81	1.57	0.68
1:A:1310:ASN:HA	1:A:1366:GLY:HA3	1.74	0.68

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	861/885 (97%)	805 (94%)	53 (6%)	3 (0%)	36 56
1	B	858/885 (97%)	763 (89%)	83 (10%)	12 (1%)	9 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1719/1770 (97%)	1568 (91%)	136 (8%)	15 (1%)	14	28

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1180	VAL
1	B	595	ASN
1	B	614	THR
1	B	694	VAL
1	B	1023	SER

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	710/730 (97%)	662 (93%)	48 (7%)	14	30
1	B	707/730 (97%)	647 (92%)	60 (8%)	10	21
All	All	1417/1460 (97%)	1309 (92%)	108 (8%)	12	26

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	646	LEU
1	B	949	THR
1	B	1265	GLN
1	B	678	MET
1	B	896	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1093	ASN
1	B	1325	GLN
1	B	1124	GLN

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Mol	Chain	Res	Type
1	B	1215	HIS
1	B	1335	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	NAG	C	1	2	15,15,15	0.75	0	21,21,21	2.74	5 (23%)
2	NAG	C	2	2	14,14,15	0.89	0	17,19,21	1.59	3 (17%)
2	NAG	D	1	2	15,15,15	0.89	0	21,21,21	2.52	7 (33%)
2	NAG	D	2	2	14,14,15	0.60	0	17,19,21	2.34	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	C	1	2	-	1/6/26/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2	-	6/6/26/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C1-C2	10.42	119.98	109.52
2	D	2	NAG	C1-O5-C5	7.41	122.11	112.19
2	D	1	NAG	O5-C1-C2	5.84	115.38	109.52
2	D	1	NAG	C1-O5-C5	5.32	123.94	113.65
2	D	1	NAG	C1-C2-C3	4.19	116.26	110.54

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

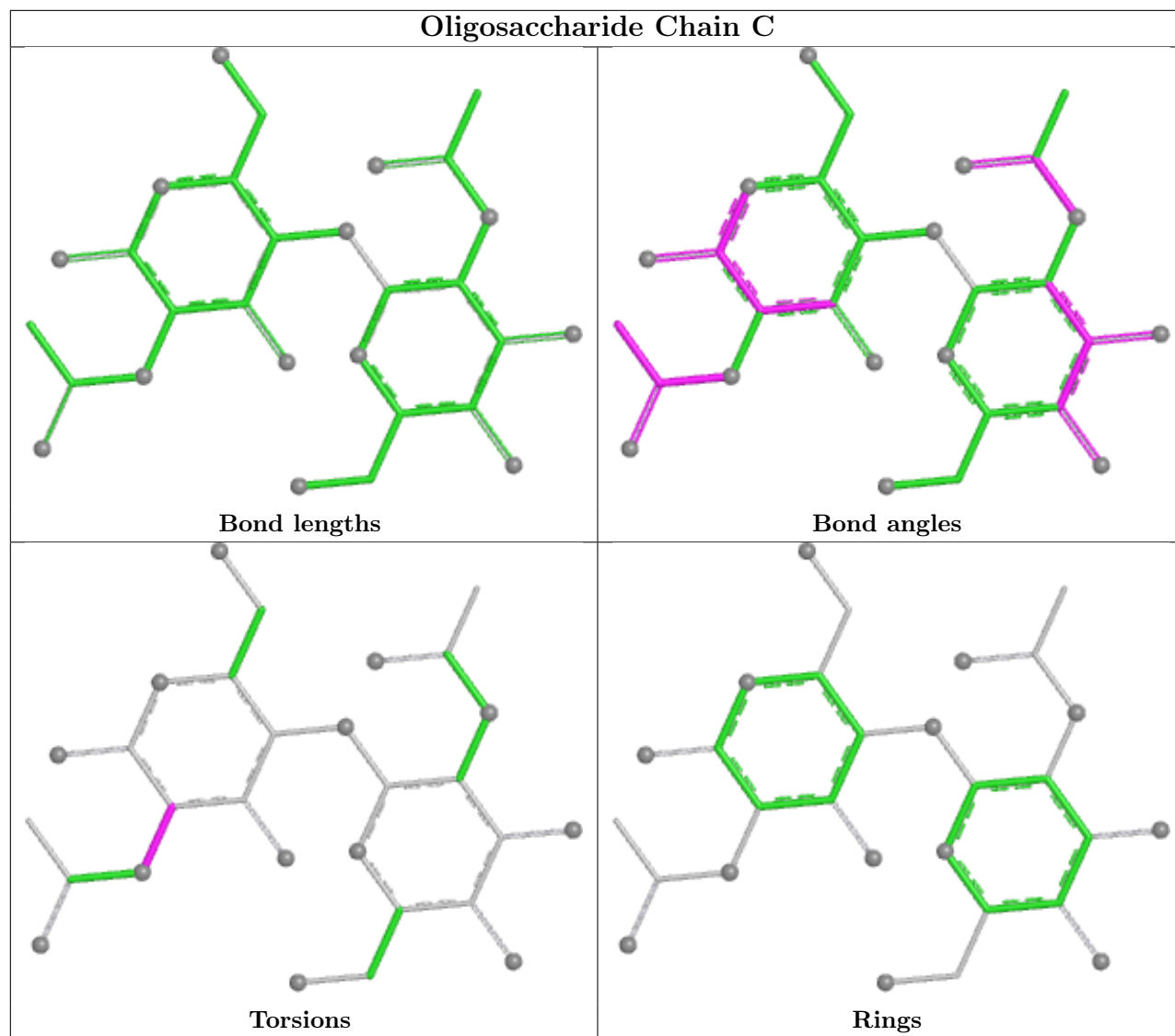
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C1-C2-N2-C7
2	D	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2

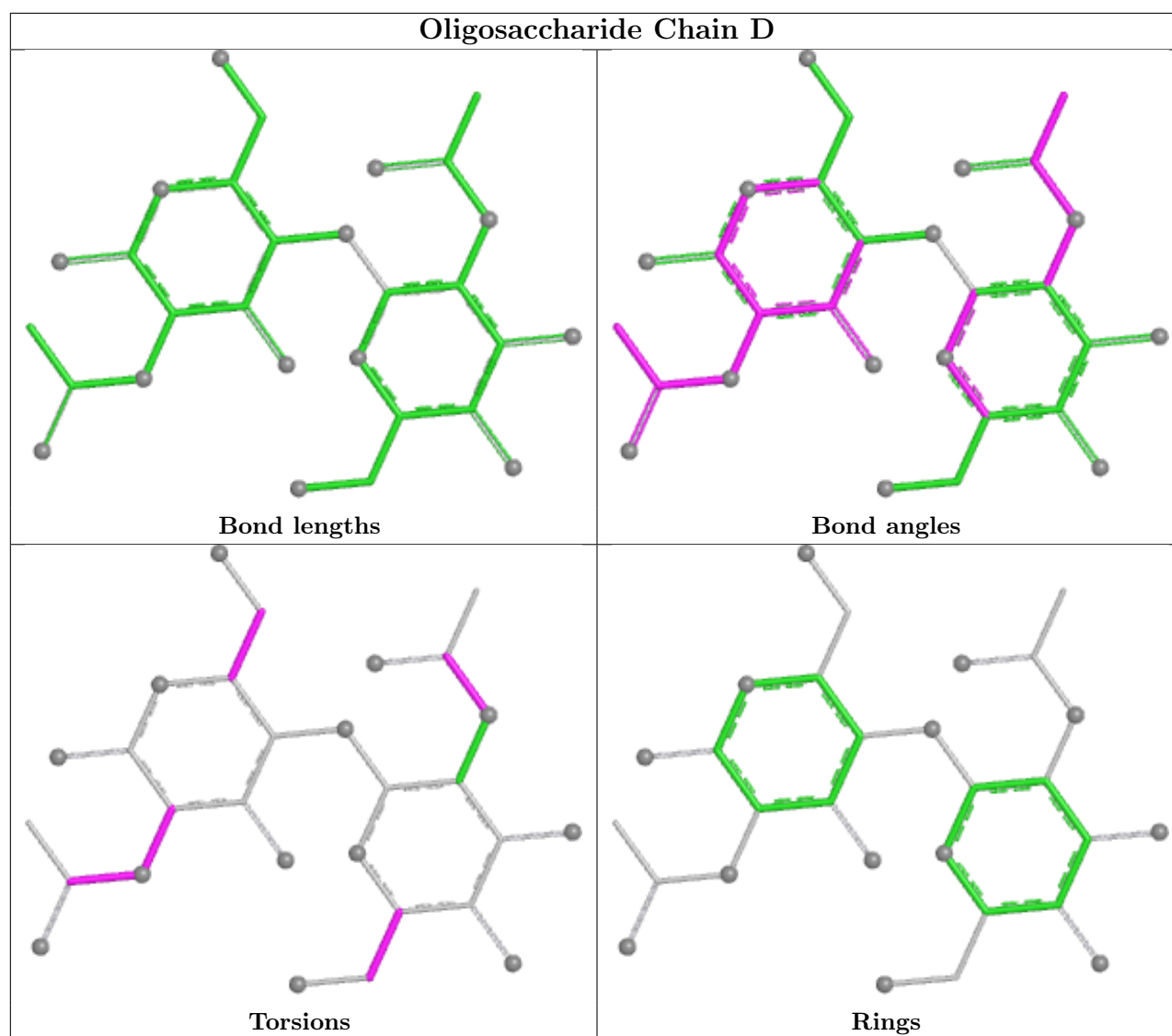
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	3	0
2	D	2	NAG	3	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](#)

2 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	PO4	A	3003	-	4,4,4	1.71	1 (25%)	6,6,6	1.31	1 (16%)
3	PO4	B	1503	-	4,4,4	0.89	0	6,6,6	1.61	1 (16%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3003	PO4	P-O2	-2.09	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1503	PO4	O4-P-O3	-2.64	99.71	107.91
3	A	3003	PO4	O4-P-O1	-2.34	102.69	110.95

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	860/885 (97%)	-0.11	12 (1%) 73 70	17, 40, 76, 104	3 (0%)
1	B	859/885 (97%)	0.09	26 (3%) 52 47	16, 41, 81, 109	1 (0%)
All	All	1719/1770 (97%)	-0.01	38 (2%) 62 57	16, 41, 79, 109	4 (0%)

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	613	ILE	5.6
1	A	557	VAL	5.1
1	A	613	ILE	3.9
1	B	1003	GLY	3.2
1	B	983	ILE	3.0

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

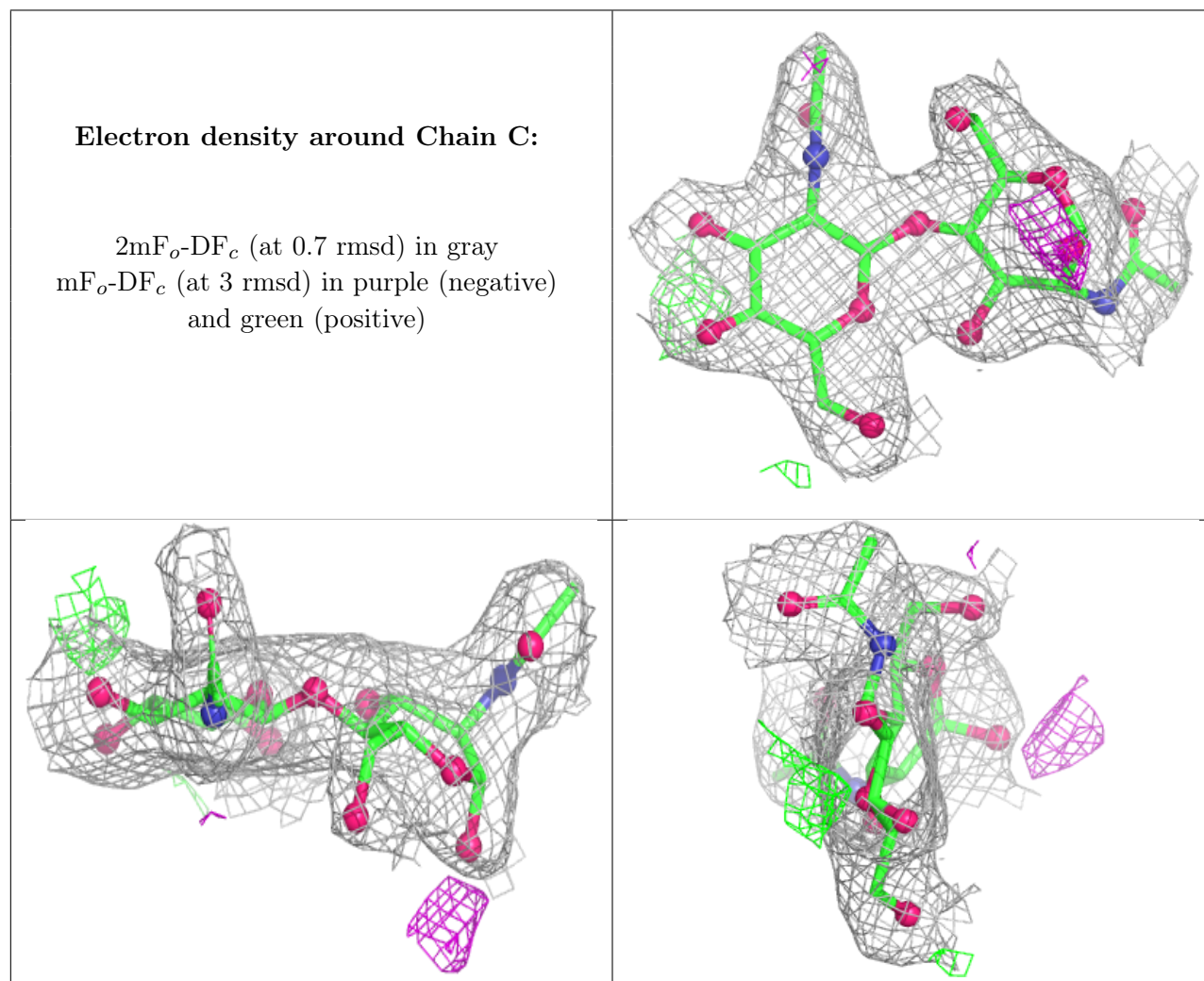
There are no non-standard protein/DNA/RNA residues in this entry.

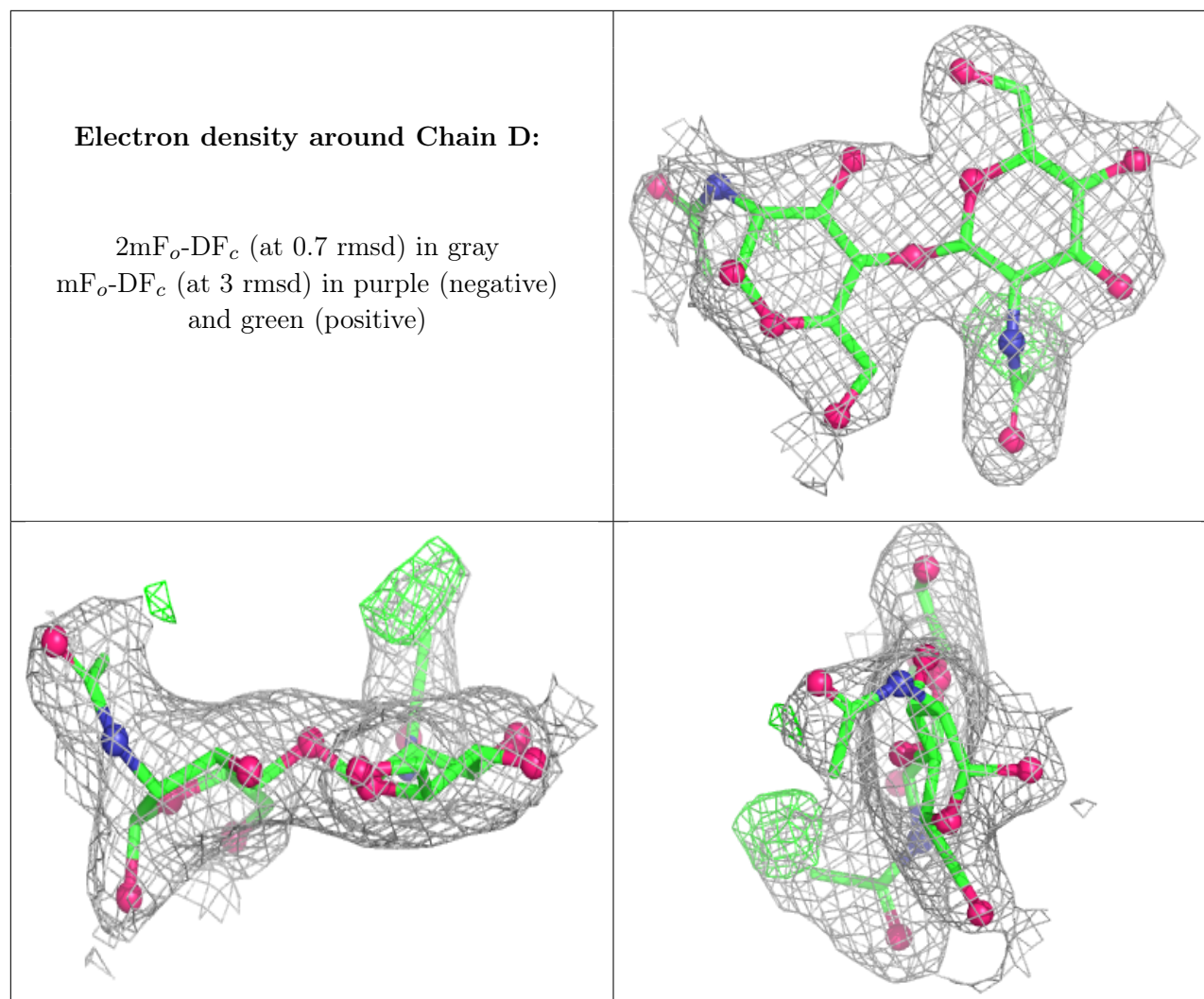
6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	1	15/15	0.93	0.10	33,37,52,62	0
2	NAG	D	2	14/15	0.93	0.07	28,36,38,41	0
2	NAG	C	2	14/15	0.94	0.08	26,31,35,38	0
2	NAG	C	1	15/15	0.95	0.08	33,35,39,40	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	PO4	B	1503	5/5	0.95	0.09	41,43,48,54	0
3	PO4	A	3003	5/5	0.99	0.05	30,31,40,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.