



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2026 – 10:08 PM UTC

PDB ID : 7PR9 / pdb_00007pr9
Title : Crystal structure of Burkholderia pseudomallei heparanase in complex with covalent inhibitor VL166
Authors : Wu, L.; Armstrong, Z.; Davies, G.J.
Deposited on : 2021-09-21
Resolution : 1.34 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

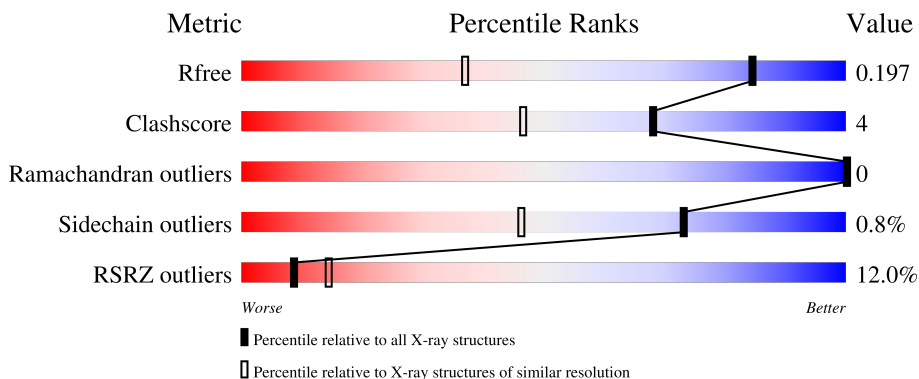
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.34 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	2194 (1.36-1.32)
Clashscore	190562	2222 (1.36-1.32)
Ramachandran outliers	187476	2197 (1.36-1.32)
Sidechain outliers	187428	2197 (1.36-1.32)
RSRZ outliers	180081	2193 (1.36-1.32)

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	438	 3% 93% 7%
1	B	438	 21% 94% 6%
2	C	2	 100%
2	D	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	502	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13984 atoms, of which 6419 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.

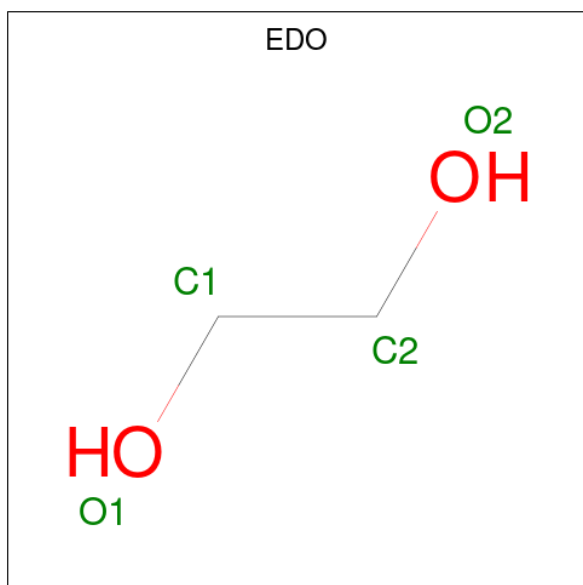
- Molecule 1 is a protein called Glyco_hydro_44 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	437	Total 6498	C 2057	H 3209	N 590	O 633	S 9	93	18	0
1	B	437	Total 6334	C 2015	H 3128	N 567	O 616	S 8	90	7	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-(2R,3S,5R,6R)-2,3,4,5,6-pentakis(oxidanyl)cyclohexane-1-carboxylic acid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	C	2	Total 50	C 15	H 23	N 1	O 11	6	0	0
2	D	2	Total 50	C 15	H 23	N 1	O 11	6	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	1	0
			10	2	6	2		
3	A	1	Total	C	H	O	1	0
			10	2	6	2		
3	B	1	Total	C	H	O	1	0
			10	2	6	2		
3	B	1	Total	C	H	O	1	0
			10	2	6	2		
3	B	1	Total	C	H	O	1	0
			10	2	6	2		

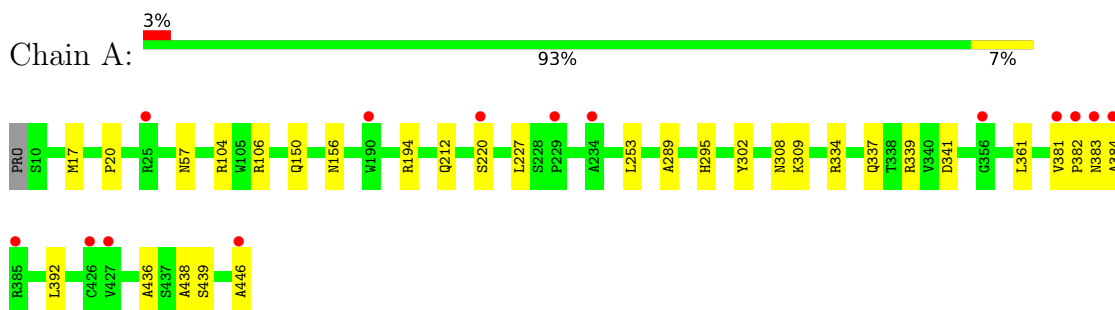
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	597	Total	O	0	0
			597	597		
4	B	395	Total	O	0	0
			395	395		

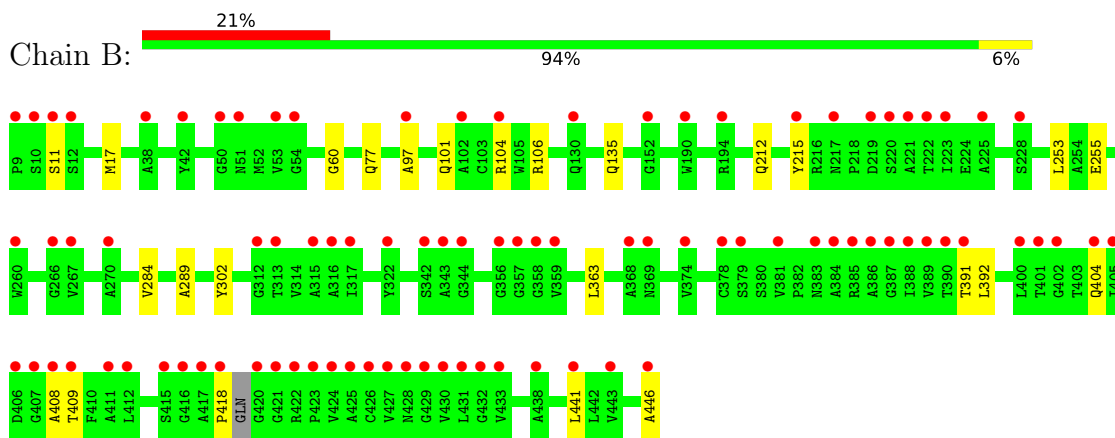
3 Residue-property plots [i](#)

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.

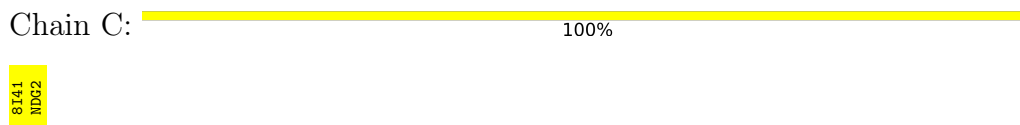
- Molecule 1: Glyco_hydro_44 domain-containing protein



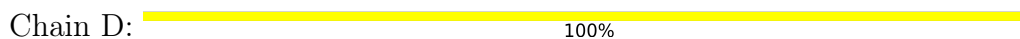
- Molecule 1: Glyco_hydro_44 domain-containing protein



- Molecule 2: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-(2R,3S,5R,6R)-2,3,4,5,6-pentakis (oxidanyl)cyclohexane-1-carboxylic acid



- Molecule 2: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-(2R,3S,5R,6R)-2,3,4,5,6-pentakis (oxidanyl)cyclohexane-1-carboxylic acid



8141
MDC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.87Å 104.14Å 113.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.00 – 1.34 76.88 – 1.34	Depositor EDS
% Data completeness (in resolution range)	98.7 (77.00-1.34) 98.2 (76.88-1.34)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.34Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.176 , 0.199 0.175 , 0.197	Depositor DCC
R_{free} test set	10583 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtrriage
Anisotropy	0.407	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13984	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 8I4, NDG, EDO

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	1.11	2/3360 (0.1%)	1.14	1/4585 (0.0%)
1	B	1.12	2/3277 (0.1%)	1.17	2/4475 (0.0%)
All	All	1.12	4/6637 (0.1%)	1.15	3/9060 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	HIS	CE1-NE2	6.23	1.38	1.32
1	B	255	GLU	CD-OE2	6.09	1.36	1.25
1	B	77	GLN	C-O	5.13	1.29	1.23
1	A	289	ALA	C-O	5.03	1.30	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	GLN	CB-CG-CD	-6.29	101.90	112.60
1	B	391	THR	CA-CB-OG1	-5.62	101.17	109.60
1	B	60	GLY	CA-C-O	-5.42	117.58	122.57

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	3289	3209	3186	39	0
1	B	3206	3128	3113	17	0
2	C	27	23	12	0	0
2	D	27	23	12	0	0
3	A	8	12	12	5	0
3	B	16	24	23	0	0
4	A	597	0	0	12	1
4	B	395	0	0	0	0
All	All	7565	6419	6358	47	1

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.

The worst 5 of 47 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:384:ALA:O	4:A:601:HOH:O	1.78	1.01
1:A:339[B]:ARG:HH22	1:A:341:ASP:HB2	1.30	0.97
1:A:156:ASN:OD1	3:A:502:EDO:H11	1.75	0.87
1:A:156:ASN:OD1	3:A:502:EDO:C1	2.26	0.82
1:A:57:ASN:HB3	3:A:501:EDO:H12	1.65	0.78

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:782:HOH:O	4:A:978:HOH:O[2_455]	2.13	0.07

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	452/438 (103%)	445 (98%)	7 (2%)	0	100	100
1	B	440/438 (100%)	433 (98%)	7 (2%)	0	100	100
All	All	892/876 (102%)	878 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	326/310 (105%)	325 (100%)	1 (0%)	86	70
1	B	316/310 (102%)	311 (98%)	5 (2%)	55	20
All	All	642/620 (104%)	636 (99%)	6 (1%)	73	41

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	215[A]	TYR
1	B	215[B]	TYR
1	B	302	TYR
1	B	11	SER
1	A	302	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	308	ASN
1	B	404	GLN
1	B	428	ASN
1	A	286	GLN
1	A	101	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	8I4	C	1	2,1	13,13,14	1.20	1 (7%)	18,19,21	1.44	2 (11%)
2	NDG	C	2	2	14,14,15	0.78	0	17,19,21	1.76	4 (23%)
2	8I4	D	1	2,1	13,13,14	1.41	3 (23%)	18,19,21	1.44	3 (16%)
2	NDG	D	2	2	14,14,15	0.86	0	17,19,21	1.91	2 (11%)

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	8I4	C	1	2,1	-	0/4/24/28	0/1/1/1
2	NDG	C	2	2	-	0/6/23/26	0/1/1/1
2	8I4	D	1	2,1	-	0/4/24/28	0/1/1/1
2	NDG	D	2	2	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	8I4	O6A-C6	2.50	1.29	1.22
2	D	1	8I4	C5-C7	-2.26	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	8I4	C1-C7	-2.16	1.48	1.52
2	D	1	8I4	C5-C4	-2.14	1.50	1.53

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NDG	C1-O5-C5	6.06	120.31	112.19
2	C	2	NDG	C1-O5-C5	3.66	117.10	112.19
2	C	1	8I4	O4-C4-C5	-3.25	102.43	109.80
2	C	2	NDG	O7-C7-C8	3.01	127.41	122.05
2	C	2	NDG	C8-C7-N2	-2.81	111.45	116.12

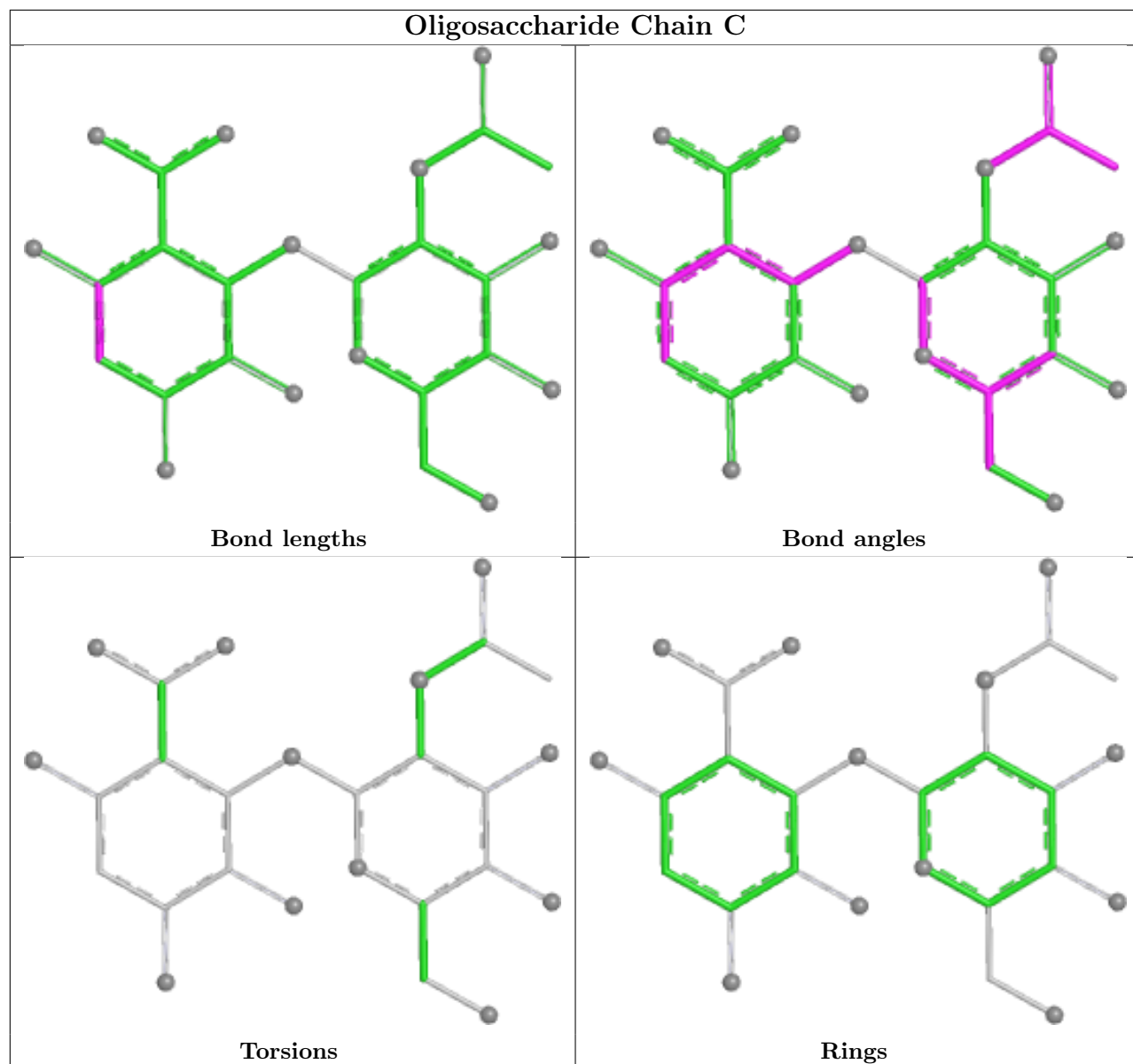
There are no chirality outliers.

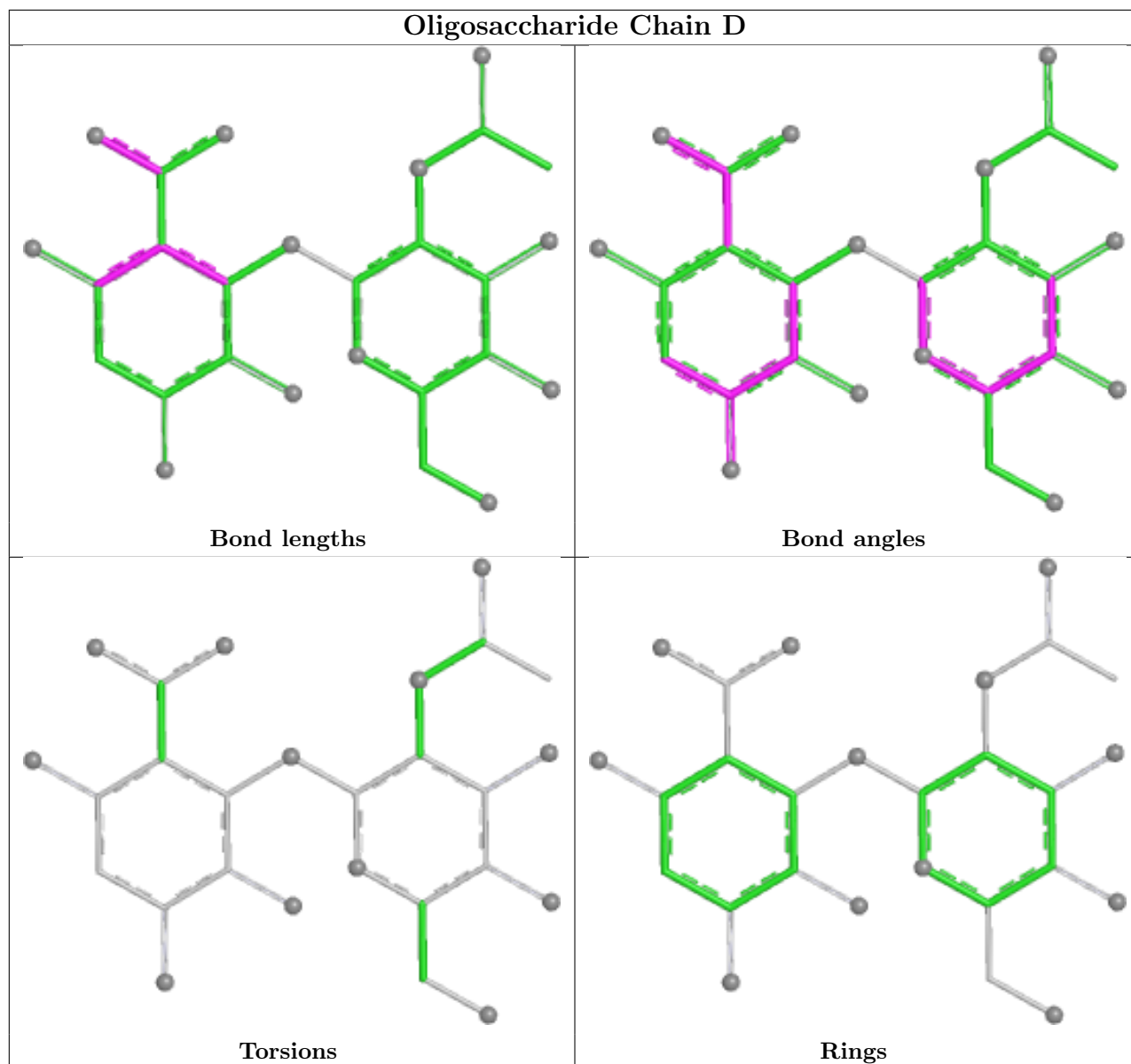
There are no torsion outliers.

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](#)

6 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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	502	-	3,3,3	0.24	0	2,2,2	0.14	0
3	EDO	B	503	-	3,3,3	0.58	0	2,2,2	0.11	0
3	EDO	A	502	-	3,3,3	0.05	0	2,2,2	0.49	0
3	EDO	B	504	-	3,3,3	0.47	0	2,2,2	0.31	0
3	EDO	A	501	-	3,3,3	0.12	0	2,2,2	0.61	0
3	EDO	B	501	-	3,3,3	0.92	0	2,2,2	0.01	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	502	-	-	1/1/1/1	-
3	EDO	B	503	-	-	0/1/1/1	-
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	B	504	-	-	0/1/1/1	-
3	EDO	A	501	-	-	1/1/1/1	-
3	EDO	B	501	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	EDO	O1-C1-C2-O2
3	B	502	EDO	O1-C1-C2-O2
3	A	502	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	EDO	4	0
3	A	501	EDO	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 [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	437/438 (99%)	0.06	14 (3%) 50 61	7, 16, 28, 53	18 (4%)
1	B	437/438 (99%)	1.09	91 (20%) 2 4	8, 24, 47, 87	7 (1%)
All	All	874/876 (99%)	0.57	105 (12%) 9 14	7, 19, 40, 87	25 (2%)

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	418	PRO	7.0
1	B	417	ALA	7.0
1	B	426	CYS	6.4
1	B	9	PRO	5.6
1	B	446	ALA	5.5

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

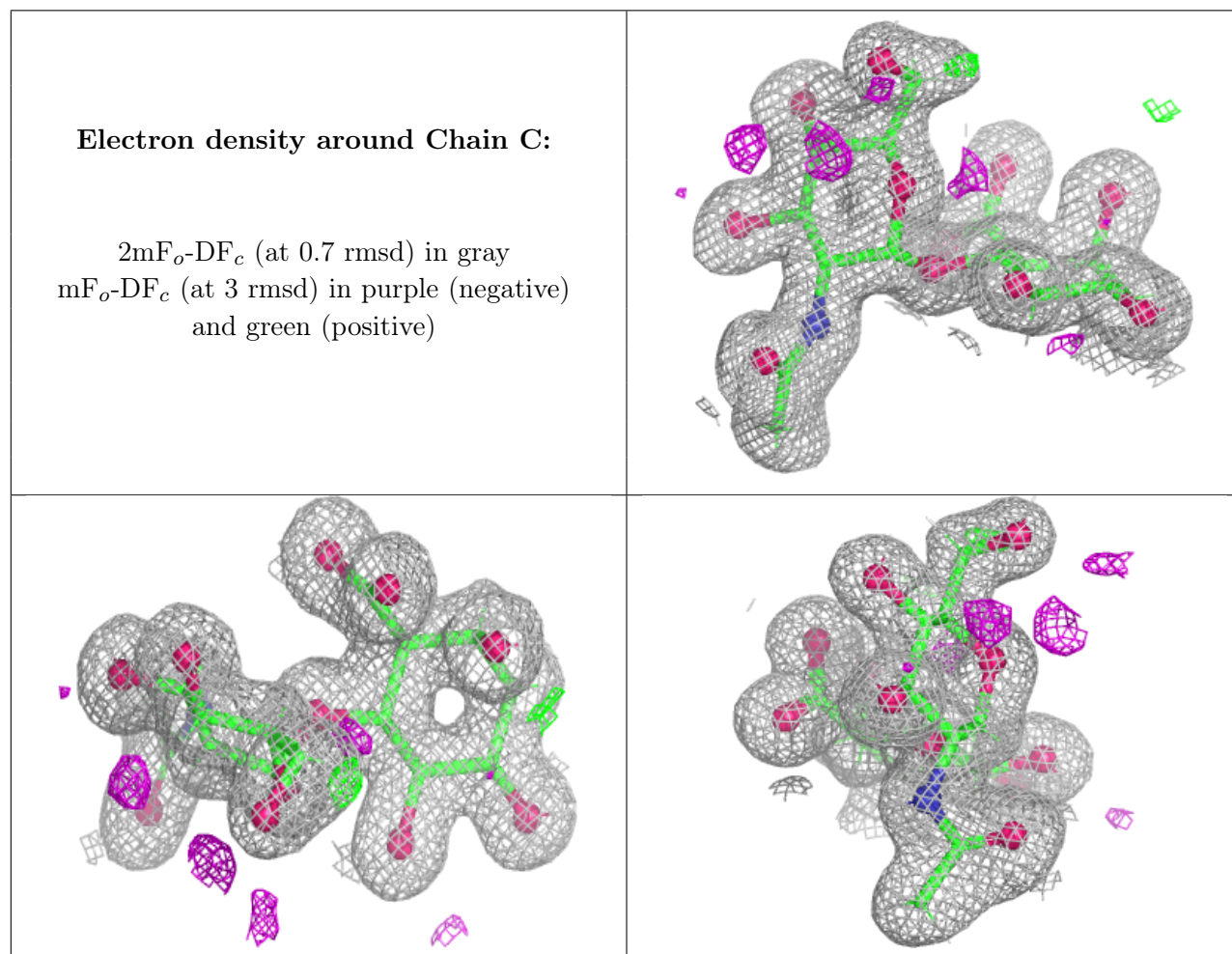
There are no non-standard protein/DNA/RNA residues in this entry.

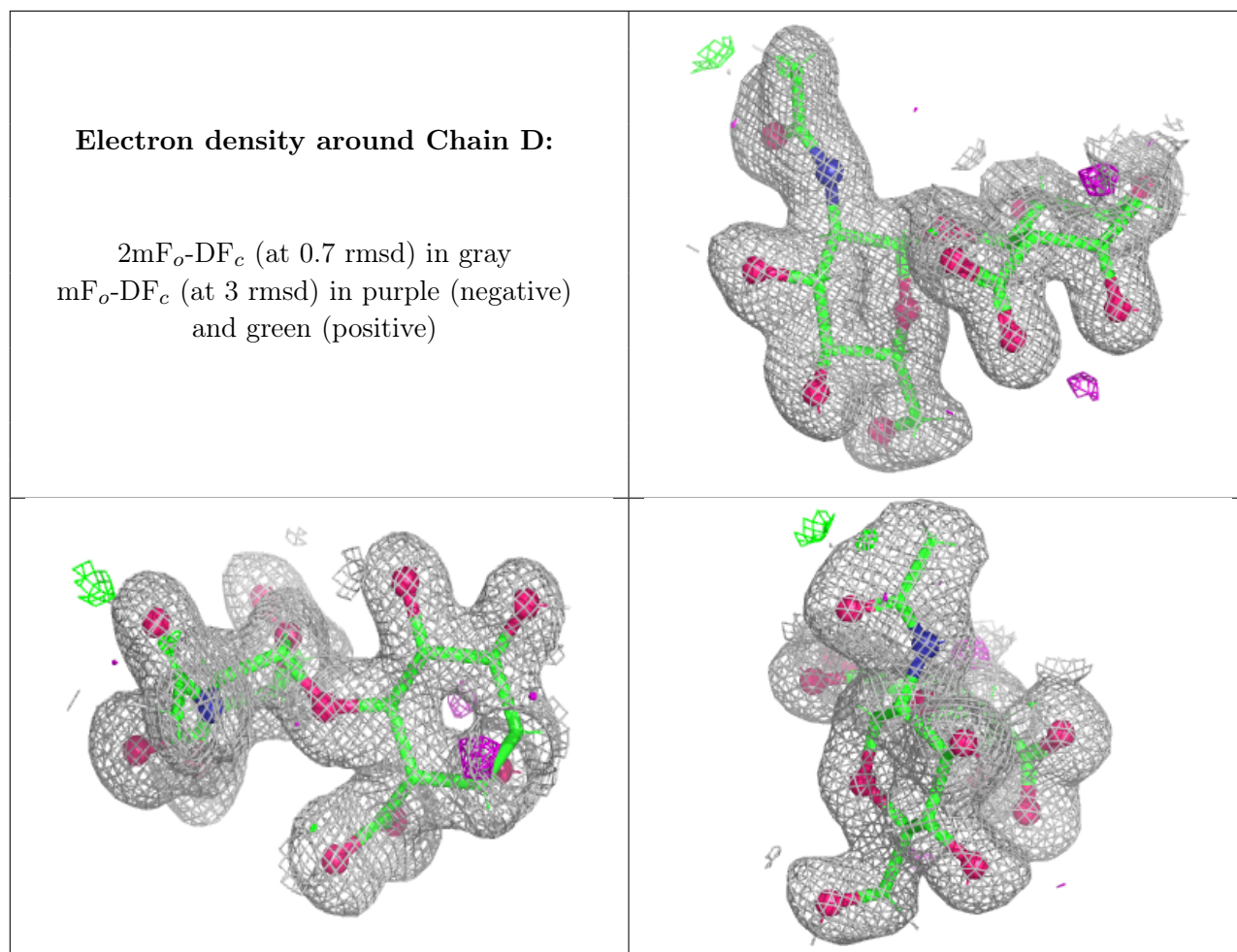
6.3 Carbohydrates [i](#)

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	NDG	D	2	14/15	0.95	0.08	21,25,28,33	3
2	8I4	D	1	13/14	0.97	0.06	18,19,20,22	3
2	NDG	C	2	14/15	0.97	0.06	16,20,25,29	3
2	8I4	C	1	13/14	0.98	0.04	14,15,16,16	3

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
3	EDO	A	501	4/4	0.79	0.16	40,40,41,42	1
3	EDO	B	502	4/4	0.79	0.14	37,48,51,52	1
3	EDO	B	504	4/4	0.88	0.12	31,32,35,37	1
3	EDO	A	502	4/4	0.89	0.12	28,30,33,33	1
3	EDO	B	503	4/4	0.94	0.09	25,30,35,37	1
3	EDO	B	501	4/4	0.97	0.06	20,22,22,22	1

6.5 Other polymers [i](#)

There are no such residues in this entry.