



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 01:59 AM BST

PDB ID : 1PU4
Title : Crystal structure of human vascular adhesion protein-1
Authors : Salminen, T.A.; Airenne, T.T.
Deposited on : 2003-06-24
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

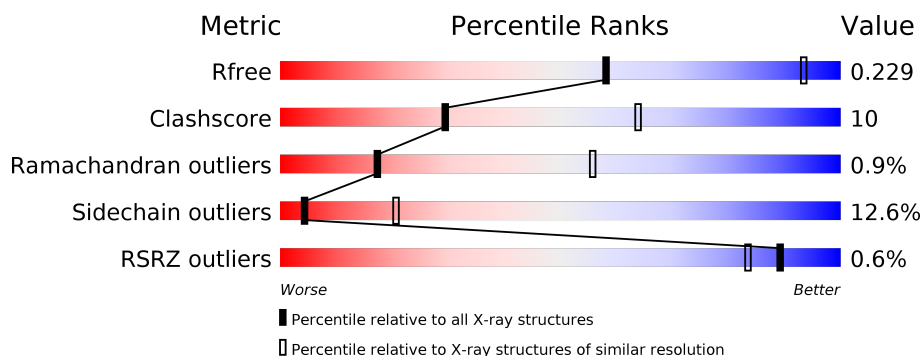
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 on 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	763	<div> <div>66%</div> <div>23%</div> <div>• • 8%</div> </div>
1	B	763	<div> <div>%</div> <div>67%</div> <div>21%</div> <div>• 8%</div> </div>
2	C	2	<div> <div>100%</div> </div>
2	D	2	<div> <div>100%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11153 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 Membrane copper amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	704	Total	C	N	O	S	0	0	0
			5545	3560	953	1012	20			
1	B	699	Total	C	N	O	S	0	0	0
			5518	3543	950	1005	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	471	TPQ	TYR	modified residue	UNP Q16853
B	471	TPQ	TYR	modified residue	UNP Q16853

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

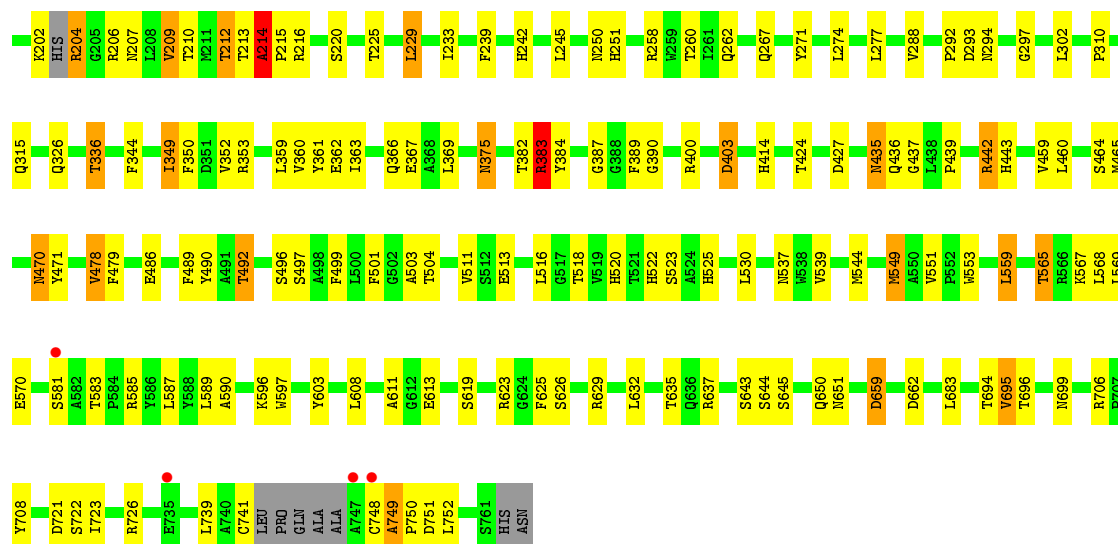
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cu	0	0
			1	1		
4	A	1	Total	Cu	0	0
			1	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Ca	0	0
			2	2		
5	A	2	Total	Ca	0	0
			2	2		

- Molecule 1: Membrane copper amine oxidase





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

Chain C:  100%

HA61
HA62

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

Chain D:  100%

HA61
HA62

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	225.92Å 225.92Å 218.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.20 19.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-3.20) 96.4 (19.99-3.20)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.75 (at 3.22Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.217 , 0.254 0.193 , 0.229	Depositor DCC
R_{free} test set	2619 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 19.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11153	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: CA, TPQ, NAG, CU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.81	0/5705	0.96	16/7779 (0.2%)
1	B	0.80	1/5676 (0.0%)	0.93	6/7735 (0.1%)
All	All	0.80	1/11381 (0.0%)	0.95	22/15514 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	7
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	549	MET	SD-CE	5.04	2.06	1.77

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ASP	CB-CG-OD1	-10.10	109.21	118.30
1	A	62	ASP	CB-CG-OD2	9.03	126.43	118.30
1	B	403	ASP	CB-CG-OD2	7.92	125.43	118.30
1	A	216	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	A	180	ASP	CB-CG-OD2	7.75	125.27	118.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	THR	Peptide
1	A	214	ALA	Peptide
1	A	292	PRO	Peptide
1	A	750	PRO	Peptide
1	B	57	SER	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	5545	0	5293	118	0
1	B	5518	0	5271	119	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
All	All	11153	0	10640	208	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 10.

The worst 5 of 208 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:549:MET:SD	1:B:549:MET:CE	2.06	1.44
1:A:571:MET:SD	1:A:571:MET:CE	2.04	1.43
1:A:441:ARG:HA	1:B:492:THR:HG21	1.56	0.87
1:A:495:ILE:HD12	1:A:495:ILE:H	1.41	0.85
1:A:216:ARG:HD2	1:A:651:ASN:OD1	1.76	0.83

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	699/763 (92%)	646 (92%)	46 (7%)	7 (1%)	15	54
1	B	692/763 (91%)	634 (92%)	53 (8%)	5 (1%)	22	61
All	All	1391/1526 (91%)	1280 (92%)	99 (7%)	12 (1%)	17	56

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ALA
1	A	746	ALA
1	A	748	CYS
1	B	214	ALA
1	B	749	ALA

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	583/634 (92%)	502 (86%)	81 (14%)	3	16
1	B	581/634 (92%)	515 (89%)	66 (11%)	5	24
All	All	1164/1268 (92%)	1017 (87%)	147 (13%)	4	21

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	608	LEU

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Mol	Chain	Res	Type
1	B	95	CYS
1	B	619	SER
1	A	618	ASN
1	A	650	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	650	GLN
1	B	94	ASN
1	B	636	GLN
1	A	687	HIS
1	B	250	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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$
1	TPQ	B	471	1,4	13,14,15	3.41	7 (53%)	15,19,21	2.53	7 (46%)
1	TPQ	A	471	1,4	13,14,15	3.31	7 (53%)	15,19,21	2.70	4 (26%)

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
1	TPQ	B	471	1,4	-	4/5/22/24	0/1/1/1
1	TPQ	A	471	1,4	-	4/5/22/24	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	471	TPQ	C3-C4	6.47	1.45	1.35
1	A	471	TPQ	C1-C2	-5.99	1.40	1.49
1	A	471	TPQ	C3-C4	5.70	1.44	1.35
1	B	471	TPQ	O5-C5	5.24	1.38	1.24
1	A	471	TPQ	O2-C2	5.11	1.38	1.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	TPQ	C3-C4-C5	-6.72	114.31	121.26
1	A	471	TPQ	C4-C3-C2	5.45	126.34	120.30
1	B	471	TPQ	C3-C4-C5	-5.22	115.86	121.26
1	B	471	TPQ	C4-C3-C2	4.63	125.43	120.30
1	B	471	TPQ	CB-C1-C2	4.16	126.02	118.57

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	471	TPQ	C-CA-CB-C1
1	B	471	TPQ	C2-C1-CB-CA
1	A	471	TPQ	C-CA-CB-C1
1	A	471	TPQ	C2-C1-CB-CA
1	A	471	TPQ	C6-C1-CB-CA

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	471	TPQ	2	0

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	1,2	14,14,15	0.60	0	17,19,21	1.94	5 (29%)
2	NAG	C	2	2	14,14,15	0.91	0	17,19,21	2.00	5 (29%)
2	NAG	D	1	1,2	14,14,15	0.64	0	17,19,21	1.84	7 (41%)
2	NAG	D	2	2	14,14,15	0.96	1 (7%)	17,19,21	2.35	6 (35%)

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	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C3-C2	2.62	1.58	1.52

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-O5-C5	5.28	119.35	112.19
2	C	1	NAG	C1-O5-C5	4.84	118.75	112.19
2	D	2	NAG	O3-C3-C2	4.62	119.02	109.47
2	C	2	NAG	C3-C4-C5	-4.02	103.06	110.24
2	D	2	NAG	O5-C1-C2	-3.64	105.54	111.29

There are no chirality outliers.

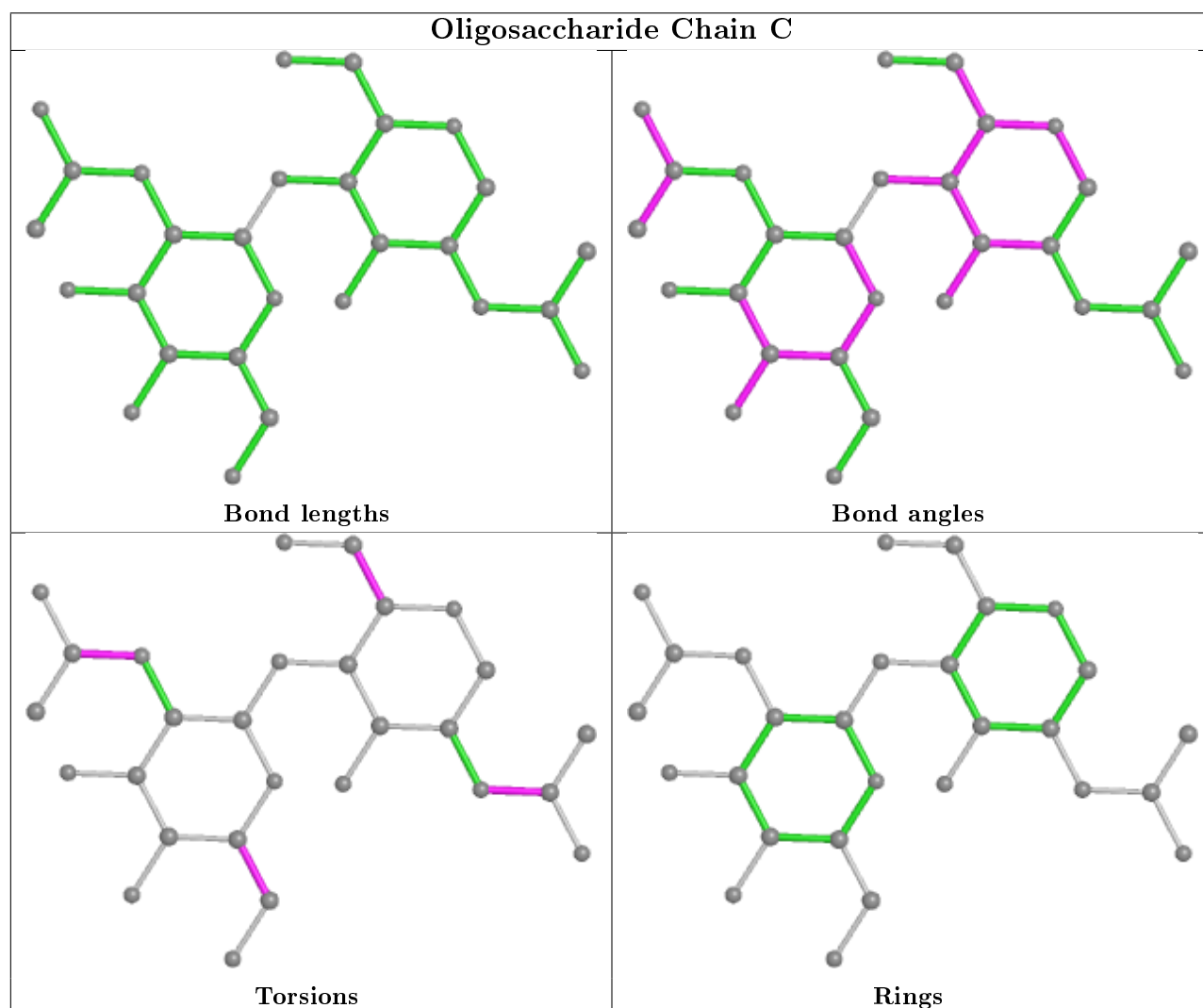
5 of 14 torsion outliers are listed below:

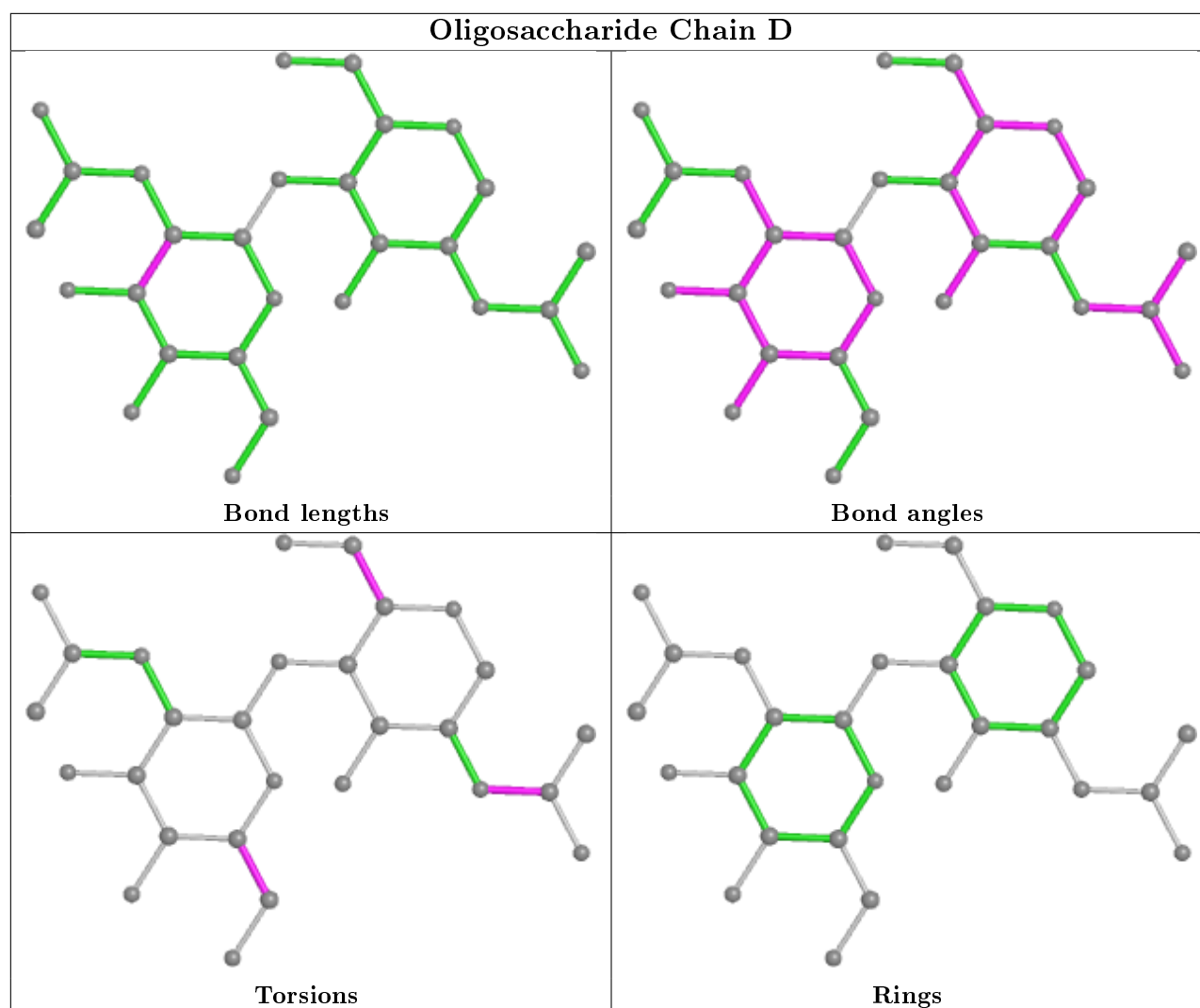
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
2	D	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\# Z > 2$
3	NAG	B	2781	1	14,14,15	0.98	1 (7%)	17,19,21	1.68	5 (29%)
3	NAG	A	2781	1	14,14,15	0.80	0	17,19,21	1.56	4 (23%)

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	NAG	B	2781	1	-	5/6/23/26	0/1/1/1
3	NAG	A	2781	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2781	NAG	C1-C2	2.11	1.55	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2781	NAG	O5-C5-C6	3.74	113.06	107.20
3	A	2781	NAG	C1-C2-N2	3.09	115.77	110.49
3	A	2781	NAG	C1-O5-C5	2.98	116.23	112.19
3	B	2781	NAG	C2-N2-C7	2.44	126.38	122.90
3	B	2781	NAG	C1-C2-N2	2.41	114.60	110.49

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2781	NAG	O5-C5-C6-O6
3	B	2781	NAG	C8-C7-N2-C2
3	B	2781	NAG	O7-C7-N2-C2
3	A	2781	NAG	C4-C5-C6-O6
3	B	2781	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	703/763 (92%)	-0.63	3 (0%) 92 89	15, 28, 45, 69	0
1	B	698/763 (91%)	-0.64	5 (0%) 87 81	16, 28, 45, 65	0
All	All	1401/1526 (91%)	-0.64	8 (0%) 89 83	15, 28, 45, 69	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	747	ALA	4.0
1	B	81	PRO	2.5
1	A	81	PRO	2.4
1	A	744	GLN	2.4
1	B	735	GLU	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [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.

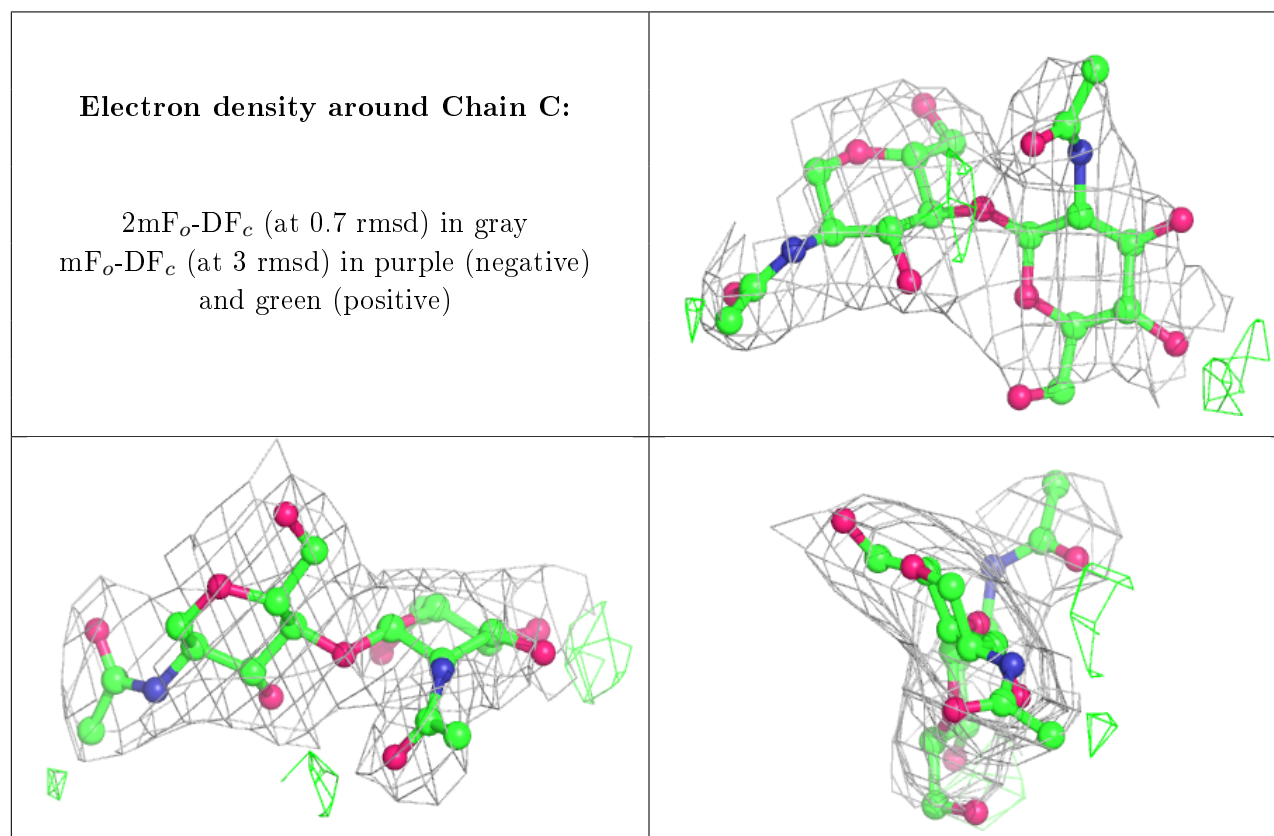
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPQ	B	471	14/15	0.96	0.14	21,26,31,32	0
1	TPQ	A	471	14/15	0.96	0.14	21,25,30,32	0

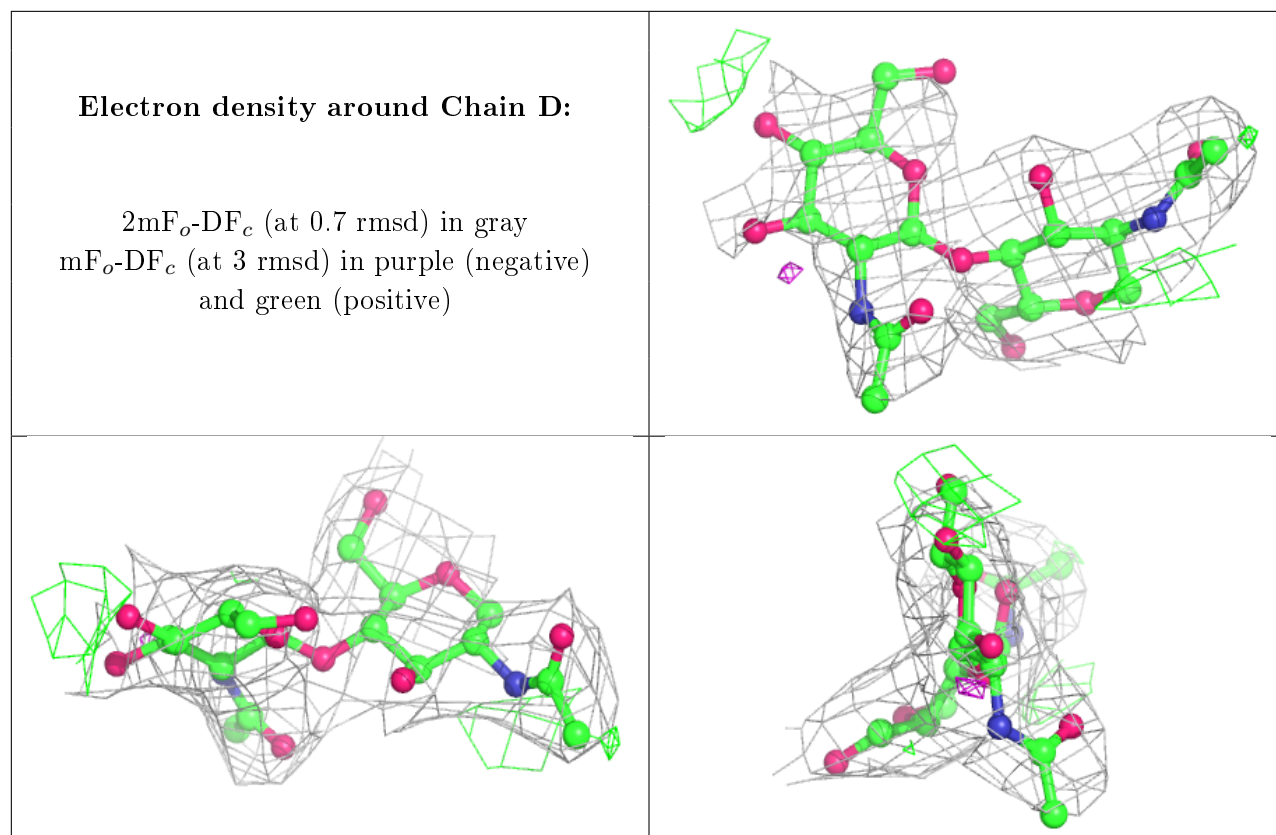
6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
2	NAG	D	2	14/15	0.80	0.31	43,47,50,52	0
2	NAG	C	2	14/15	0.84	0.32	42,45,51,53	0
2	NAG	D	1	14/15	0.94	0.13	30,34,37,42	0
2	NAG	C	1	14/15	0.95	0.16	31,33,38,40	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(\AA^2)	Q<0.9
3	NAG	A	2781	14/15	0.85	0.31	49,51,52,53	0
5	CA	A	802	1/1	0.89	0.09	24,24,24,24	0
3	NAG	B	2781	14/15	0.90	0.27	47,51,53,53	0
5	CA	B	802	1/1	0.95	0.11	23,23,23,23	0
5	CA	A	803	1/1	0.96	0.08	37,37,37,37	0
5	CA	B	803	1/1	0.97	0.09	37,37,37,37	0
4	CU	A	801	1/1	0.99	0.06	22,22,22,22	0
4	CU	B	801	1/1	0.99	0.07	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.