



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 20, 2024 – 08:52 AM EDT

PDB ID : 4OJC
Title : Crystal structure of the wild-type full-length trimeric ectodomain of the C. elegans fusion protein EFF-1
Authors : Krey, T.; Rey, F.A.
Deposited on : 2014-01-21
Resolution : 2.93 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

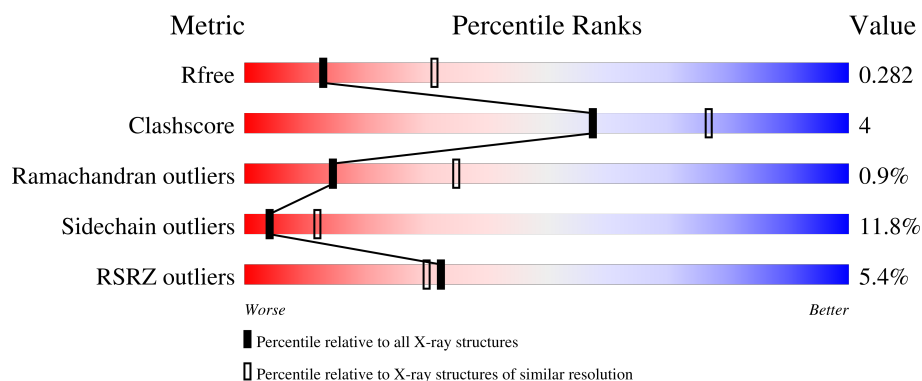
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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}	164625	1067 (2.96-2.92)
Clashscore	180529	1122 (2.96-2.92)
Ramachandran outliers	177936	1075 (2.96-2.92)
Sidechain outliers	177891	1075 (2.96-2.92)
RSRZ outliers	164620	1067 (2.96-2.92)

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	580	
2	B	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3773 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 EFF-1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3639	2277	645	690	27			

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ARG	-	expression tag	UNP G5ECA1
A	22	SER	-	expression tag	UNP G5ECA1
A	562	GLY	-	expression tag	UNP G5ECA1
A	563	PRO	-	expression tag	UNP G5ECA1
A	564	PHE	-	expression tag	UNP G5ECA1
A	565	GLU	-	expression tag	UNP G5ECA1
A	566	ASP	-	expression tag	UNP G5ECA1
A	567	ASP	-	expression tag	UNP G5ECA1
A	568	ASP	-	expression tag	UNP G5ECA1
A	569	ASP	-	expression tag	UNP G5ECA1
A	570	LYS	-	expression tag	UNP G5ECA1
A	571	ALA	-	expression tag	UNP G5ECA1
A	572	GLY	-	expression tag	UNP G5ECA1
A	573	TRP	-	expression tag	UNP G5ECA1
A	574	SER	-	expression tag	UNP G5ECA1
A	575	HIS	-	expression tag	UNP G5ECA1
A	576	PRO	-	expression tag	UNP G5ECA1
A	577	GLN	-	expression tag	UNP G5ECA1
A	578	PHE	-	expression tag	UNP G5ECA1
A	579	GLU	-	expression tag	UNP G5ECA1
A	580	LYS	-	expression tag	UNP G5ECA1
A	581	GLY	-	expression tag	UNP G5ECA1
A	582	GLY	-	expression tag	UNP G5ECA1
A	583	GLY	-	expression tag	UNP G5ECA1
A	584	SER	-	expression tag	UNP G5ECA1
A	585	GLY	-	expression tag	UNP G5ECA1
A	586	GLY	-	expression tag	UNP G5ECA1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	587	GLY	-	expression tag	UNP G5ECA1
A	588	SER	-	expression tag	UNP G5ECA1
A	589	GLY	-	expression tag	UNP G5ECA1
A	590	GLY	-	expression tag	UNP G5ECA1
A	591	GLY	-	expression tag	UNP G5ECA1
A	592	SER	-	expression tag	UNP G5ECA1
A	593	TRP	-	expression tag	UNP G5ECA1
A	594	SER	-	expression tag	UNP G5ECA1
A	595	HIS	-	expression tag	UNP G5ECA1
A	596	PRO	-	expression tag	UNP G5ECA1
A	597	GLN	-	expression tag	UNP G5ECA1
A	598	PHE	-	expression tag	UNP G5ECA1
A	599	GLU	-	expression tag	UNP G5ECA1
A	600	LYS	-	expression tag	UNP G5ECA1

- 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	B	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	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

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

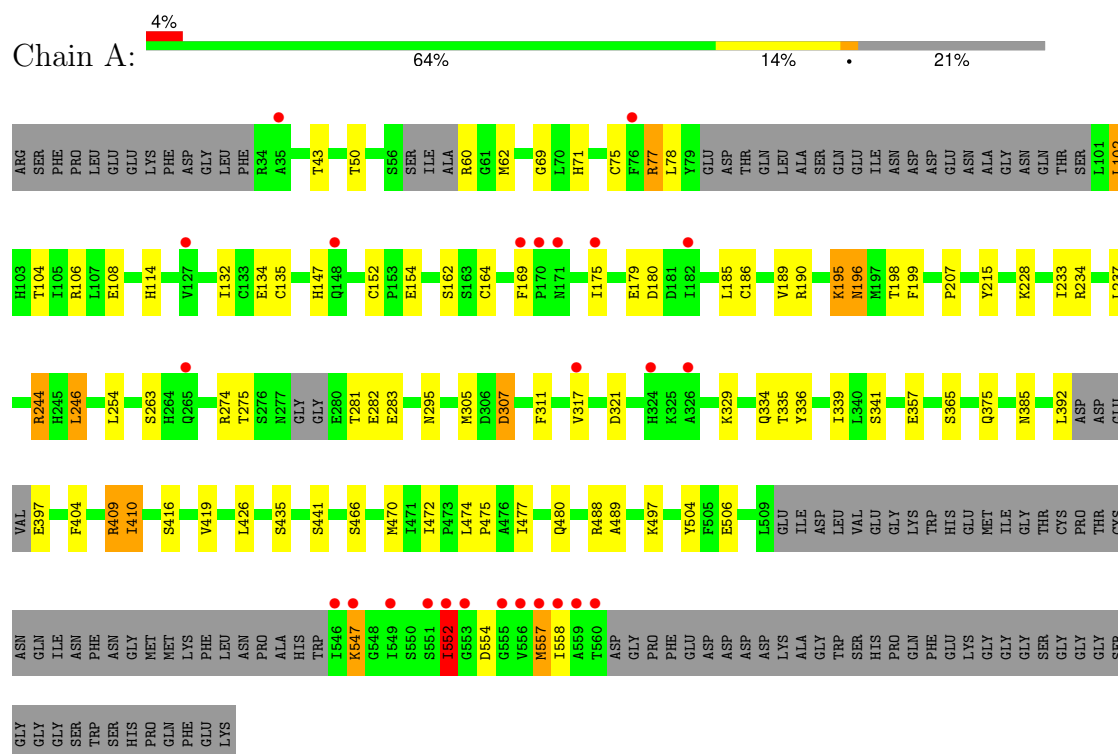
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total	O	0	0
			19	19		

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: EFF-1A



• 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	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	173.70Å 173.70Å 173.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.42 – 2.93 46.42 – 2.93	Depositor EDS
% Data completeness (in resolution range)	92.9 (46.42-2.93) 92.8 (46.42-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.220 , 0.278 0.228 , 0.282	Depositor DCC
R_{free} test set	991 reflections (5.65%)	wwPDB-VP
Wilson B-factor (Å ²)	89.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3773	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: NAG, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/3715	0.79	1/5017 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	LEU	CA-CB-CG	5.03	126.88	115.30

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	3639	0	3529	32	0
2	B	28	0	25	1	0
3	A	42	0	39	1	0
4	A	45	0	0	1	0
5	A	19	0	0	0	0
All	All	3773	0	3593	32	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.

The worst 5 of 32 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:409:ARG:HD3	1:A:435:SER:HB3	1.76	0.68
1:A:282:GLU:HG2	1:A:283:GLU:H	1.66	0.59
1:A:196:ASN:ND2	3:A:1105:NAG:O7	2.39	0.56
1:A:75:CYS:SG	1:A:104:THR:HG22	2.49	0.53
1:A:336:TYR:HE2	1:A:552:ILE:HG22	1.73	0.53

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	449/580 (77%)	407 (91%)	38 (8%)	4 (1%)	14 35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	552	ILE
1	A	179	GLU
1	A	307	ASP
1	A	317	VAL

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	406/502 (81%)	358 (88%)	48 (12%)	4 12

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307	ASP
1	A	409	ARG
1	A	321	ASP
1	A	375	GLN
1	A	416	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

2 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	B	1	2,1	14,14,15	2.04	6 (42%)	17,19,21	2.44	7 (41%)
2	NAG	B	2	2	14,14,15	2.95	8 (57%)	17,19,21	2.71	8 (47%)

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	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	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)
2	B	2	NAG	C1-C2	6.52	1.61	1.52
2	B	2	NAG	C4-C3	3.94	1.62	1.52
2	B	2	NAG	C3-C2	3.83	1.60	1.52
2	B	1	NAG	C2-N2	3.42	1.51	1.46
2	B	2	NAG	C2-N2	3.36	1.51	1.46

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C2-N2-C7	6.70	131.88	122.90
2	B	2	NAG	C2-N2-C7	6.04	131.00	122.90
2	B	1	NAG	C4-C3-C2	4.35	117.39	111.02
2	B	2	NAG	C1-C2-N2	4.32	117.24	110.43
2	B	2	NAG	C8-C7-N2	-3.45	110.40	116.12

There are no chirality outliers.

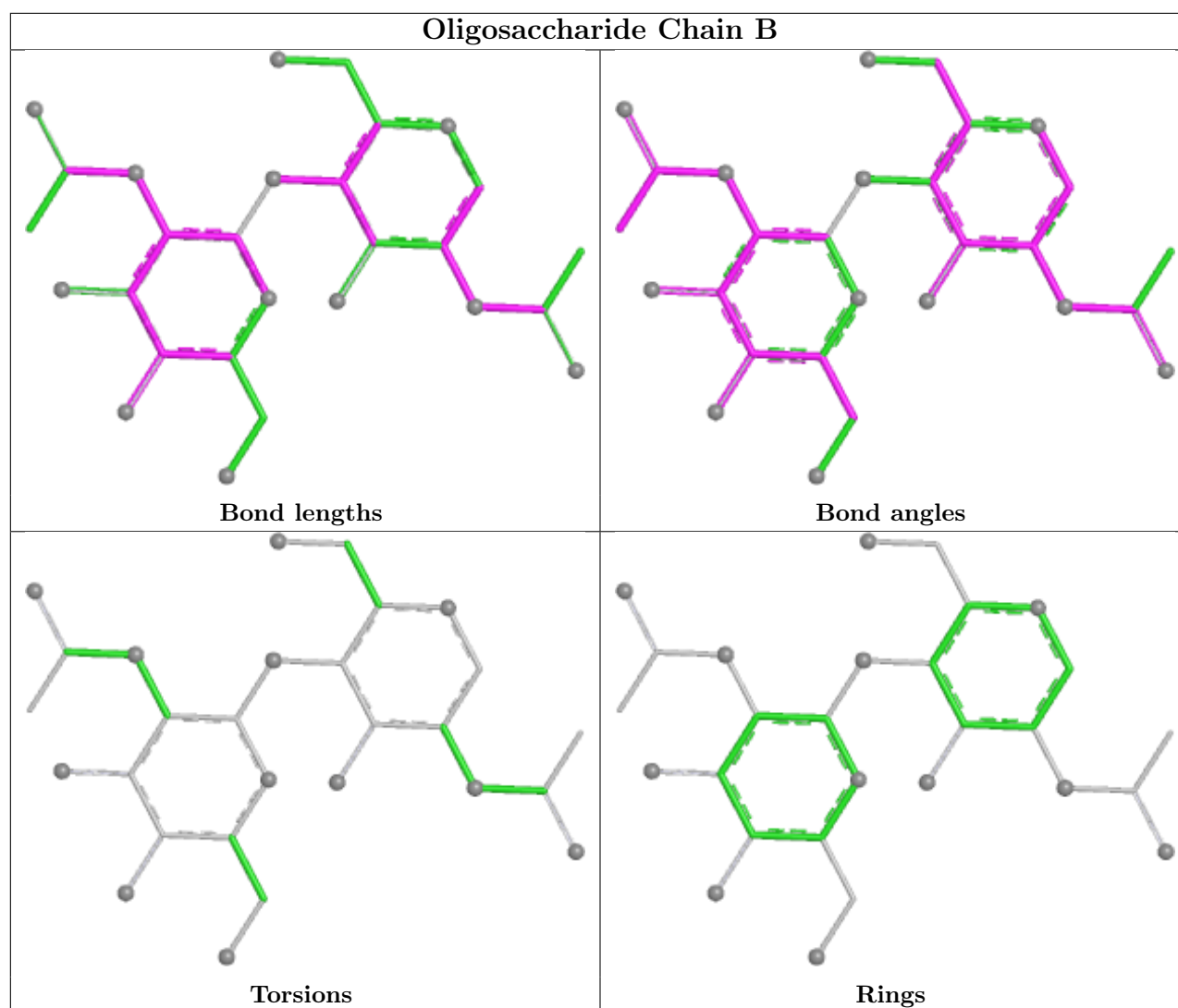
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	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](#)

12 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	$\# Z > 2$
4	SO4	A	1108	-	4,4,4	0.34	0	6,6,6	0.21	0
4	SO4	A	1107	-	4,4,4	0.53	0	6,6,6	0.32	0
4	SO4	A	1109	-	4,4,4	0.16	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	1105	1	14,14,15	2.33	5 (35%)	17,19,21	4.01	6 (35%)
3	NAG	A	1103	1	14,14,15	1.27	1 (7%)	17,19,21	2.56	8 (47%)
4	SO4	A	1111	-	4,4,4	0.36	0	6,6,6	0.22	0
4	SO4	A	1112	-	4,4,4	0.38	0	6,6,6	0.24	0
4	SO4	A	1113	-	4,4,4	0.45	0	6,6,6	0.08	0
4	SO4	A	1114	-	4,4,4	0.28	0	6,6,6	0.11	0
4	SO4	A	1110	-	4,4,4	0.32	0	6,6,6	0.37	0
3	NAG	A	1104	1	14,14,15	1.81	3 (21%)	17,19,21	1.89	6 (35%)
4	SO4	A	1106	-	4,4,4	0.28	0	6,6,6	0.04	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	NAG	A	1104	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1103	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1105	1	-	1/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1105	NAG	C3-C2	4.39	1.61	1.52
3	A	1105	NAG	C4-C3	3.96	1.62	1.52
3	A	1104	NAG	C4-C3	3.64	1.61	1.52
3	A	1105	NAG	C2-N2	3.52	1.52	1.46
3	A	1104	NAG	C4-C5	3.36	1.60	1.53

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1105	NAG	C1-O5-C5	-10.06	98.71	112.19
3	A	1105	NAG	C2-N2-C7	7.71	133.23	122.90
3	A	1105	NAG	C1-C2-N2	6.74	121.05	110.43
3	A	1103	NAG	C1-C2-N2	5.08	118.43	110.43
3	A	1105	NAG	C6-C5-C4	4.98	125.24	113.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1104	NAG	C3-C2-N2-C7
3	A	1105	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1108	SO4	1	0
3	A	1105	NAG	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	461/580 (79%)	0.49	25 (5%) 32 30	57, 86, 134, 177	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	560	THR	4.1
1	A	546	ILE	3.3
1	A	559	ALA	3.3
1	A	558	ILE	3.2
1	A	326	ALA	3.2

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

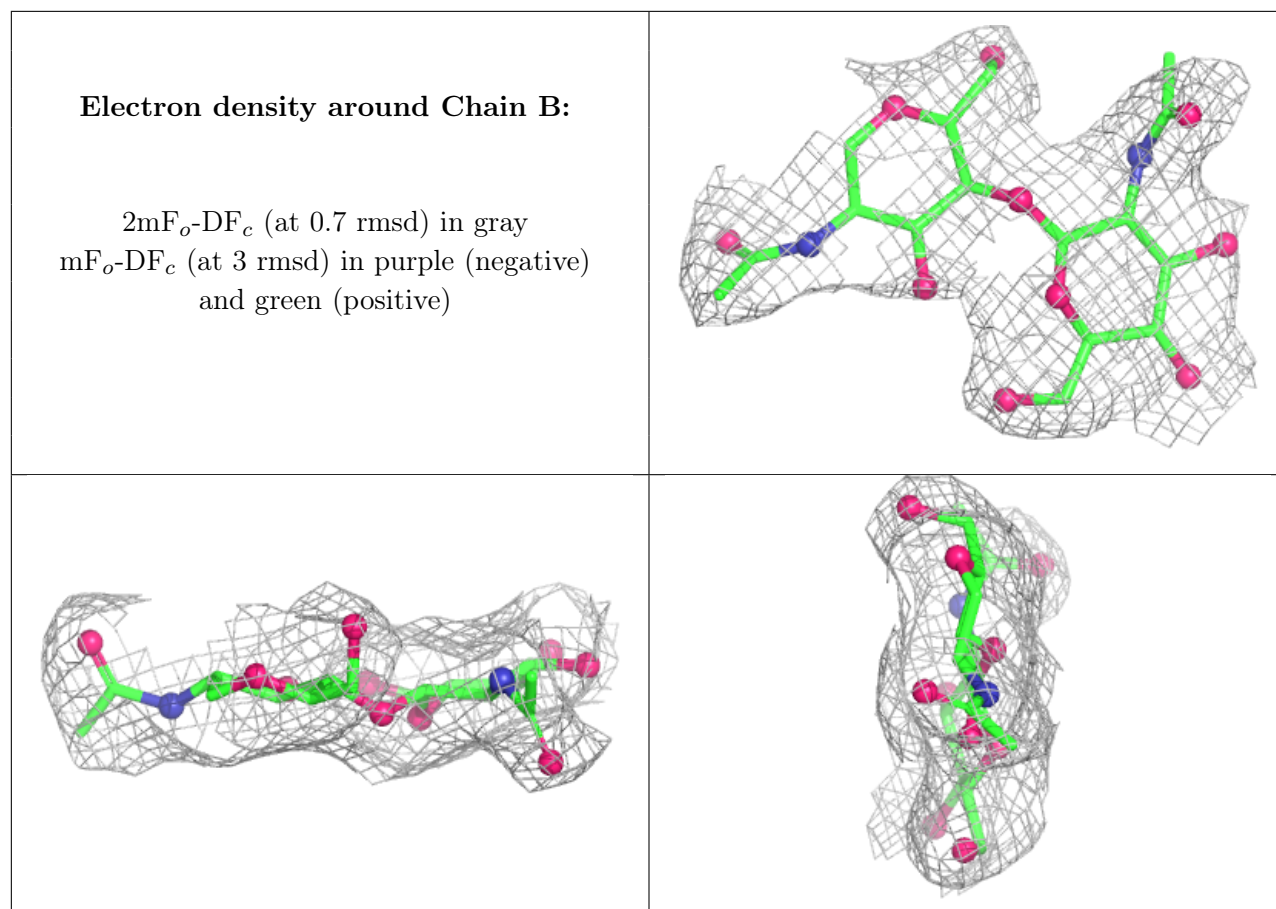
There are no non-standard protein/DNA/RNA residues in this entry.

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	B	2	14/15	0.75	0.14	107,111,113,113	0
2	NAG	B	1	14/15	0.85	0.12	101,105,107,107	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	1105	14/15	0.41	0.16	143,146,149,149	0
4	SO4	A	1112	5/5	0.63	0.12	162,167,168,168	0
4	SO4	A	1114	5/5	0.66	0.16	207,212,213,213	0
3	NAG	A	1104	14/15	0.67	0.13	128,132,135,135	0
4	SO4	A	1113	5/5	0.76	0.17	150,155,155,156	0
4	SO4	A	1108	5/5	0.77	0.13	140,144,145,145	0
4	SO4	A	1110	5/5	0.83	0.12	120,124,125,125	0
4	SO4	A	1109	5/5	0.88	0.14	112,116,117,117	0
4	SO4	A	1111	5/5	0.89	0.09	99,103,104,107	0
3	NAG	A	1103	14/15	0.91	0.11	84,88,90,90	0
4	SO4	A	1107	5/5	0.96	0.10	49,53,54,55	5
4	SO4	A	1106	5/5	0.96	0.12	84,89,90,91	5

6.5 Other polymers [i](#)

There are no such residues in this entry.