WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 7, 2024 – 10:22 pm GMT

PDB ID	:	6G1E
Title	:	BEAT Fc with improved heterodimerization (Q3A-D84.4Q)
Authors	:	Stutz, C.; Blein, S.
Deposited on	:	2018-03-21
Resolution	:	1.88 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 (i) 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 (i)) were used in the production of this report:

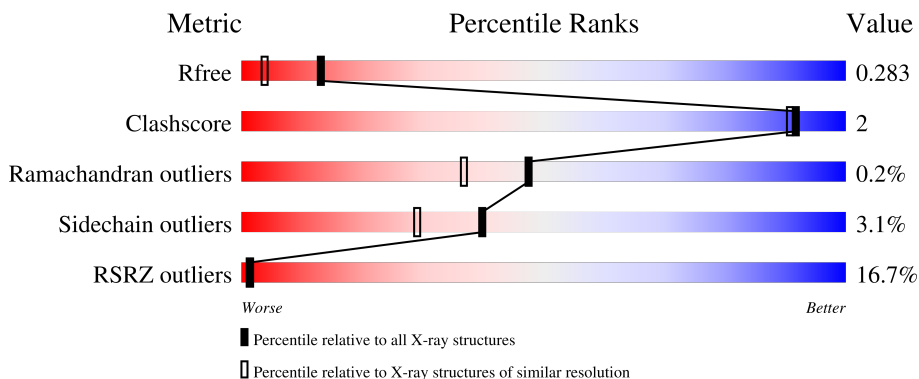|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.88 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	Percentile Ranks	Value
Rfree		0.283
Clashscore		2
Ramachandran outliers		0.2%
Sidechain outliers		3.1%
RSRZ outliers		16.7%

Worse   Better

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 <=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	233	9%; 84%, 5%, 11%
2	B	227	21%; 84%, 7%, 9%
3	C	9	44%, 56%
3	D	9	56%, 44%

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	FUL	D	9	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3893 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 Immunoglobulin heavy constant gamma 1,Immunoglobulin heavy constant gamma 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total 1679	C 1073	N 279	O 318	S 9	0	2	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	ALA	LEU	engineered mutation	UNP P01860
A	235	ALA	LEU	engineered mutation	UNP P01860
A	347	ALA	GLN	engineered mutation	UNP P01860
A	364	LYS	SER	engineered mutation	UNP P01860
A	366	VAL	THR	engineered mutation	UNP P01860
A	370	THR	LYS	engineered mutation	UNP P01860
A	392	TYR	ASN	engineered mutation	UNP P01860
A	405	SER	PHE	engineered mutation	UNP P01860
A	407	VAL	TYR	engineered mutation	UNP P01860
A	409	TRP	LYS	engineered mutation	UNP P01860
A	411	ASN	THR	engineered mutation	UNP P01860
A	448	HIS	-	expression tag	UNP P01860
A	449	HIS	-	expression tag	UNP P01860
A	450	HIS	-	expression tag	UNP P01860
A	451	HIS	-	expression tag	UNP P01860
A	452	HIS	-	expression tag	UNP P01860
A	453	HIS	-	expression tag	UNP P01860

- Molecule 2 is a protein called Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	207	Total 1675	C 1065	N 286	O 317	S 7	0	3	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	234	ALA	LEU	engineered mutation	UNP P0DOX5
B	235	ALA	LEU	engineered mutation	UNP P0DOX5
B	347	GLU	GLN	engineered mutation	UNP P0DOX5
B	349	ALA	TYR	engineered mutation	UNP P0DOX5
B	351	PHE	LEU	engineered mutation	UNP P0DOX5
B	364	THR	SER	engineered mutation	UNP P0DOX5
B	366	VAL	THR	engineered mutation	UNP P0DOX5
B	370	THR	LYS	engineered mutation	UNP P0DOX5
B	394	ASP	THR	engineered mutation	UNP P0DOX5
B	397	LEU	VAL	engineered mutation	UNP P0DOX5
B	399	GLU	ASP	engineered mutation	UNP P0DOX5
B	401	GLN	ASP	engineered mutation	UNP P0DOX5
B	405	ALA	PHE	engineered mutation	UNP P0DOX5
B	407	SER	TYR	engineered mutation	UNP P0DOX5
B	409	ARG	LYS	engineered mutation	UNP P0DOX5
B	411	ARG	THR	engineered mutation	UNP P0DOX5

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.
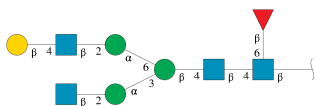
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total 110	C 62	N 4	O 44	0	0	0
3	D	9	Total 110	C 62	N 4	O 44	0	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	175	Total 175	O 175	0	0
4	B	144	Total 144	O 144	0	0

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: Immunoglobulin heavy constant gamma 1,Immunoglobulin heavy constant gamma 3
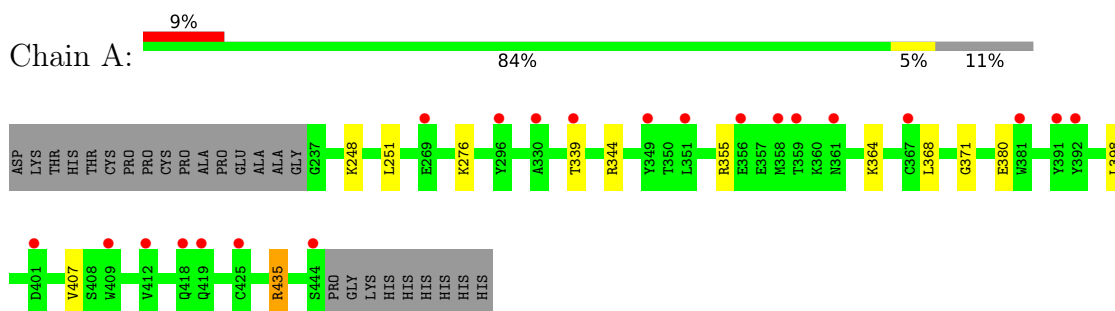
• Molecule 2: Immunoglobulin gamma-1 heavy chain
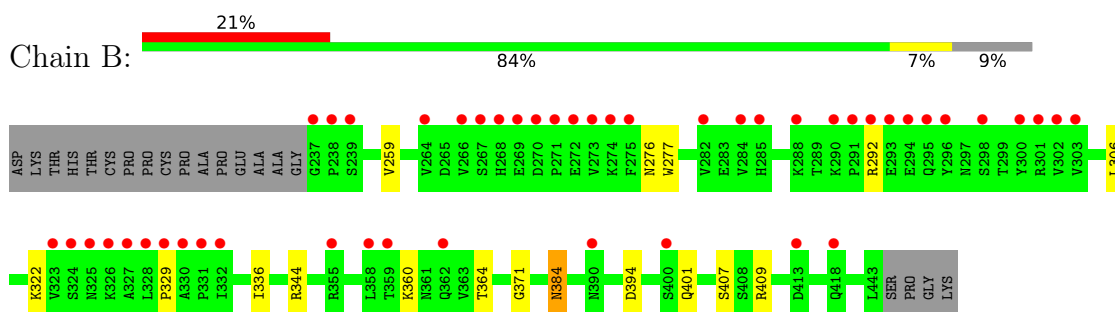
• Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose
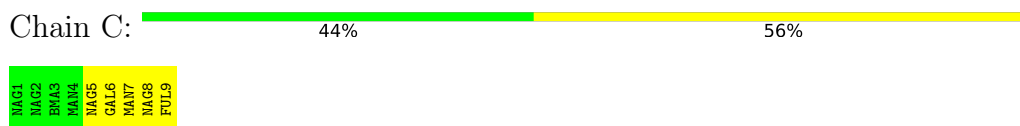
• Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

56%   44%

NAG1 NAG2 BMA3 MAN4 NAG5 GAL6 MAN7 NAG8 FUL9

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.65Å 73.02Å 140.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.88 29.41 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-1.88) 99.4 (29.41-1.88)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.231 , 0.272 0.243 , 0.283	Depositor DCC
R_{free} test set	1976 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.5	EDS
L-test for twinning[2]	$< |L| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3893	wwPDB-VP
Average B, all atoms (Å^2)	57.0	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 42.03 % 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 2.1644e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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:
MAN, FUL, NAG, BMA, GAL, MLY

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	0.37	0/1721	0.61	0/2346
2	B	0.36	0/1718	0.59	0/2341
All	All	0.37	0/3439	0.60	0/4687

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1679	0	1650	6	0
2	B	1675	0	1651	7	0
3	C	110	0	93	0	0
3	D	110	0	93	0	0
4	A	175	0	0	0	0
4	B	144	0	0	0	0
All	All	3893	0	3487	11	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 2.

The worst 5 of 11 close contacts within the same asymmetric unit are listed below, sorted by their

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clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LEU:HB3	1:A:435:ARG:HG2	1.91	0.52
1:A:368:LEU:HD21	2:B:364:THR:HG21	1.91	0.52
2:B:277:TRP:CE3	2:B:306:LEU:HD22	2.47	0.49
1:A:251:LEU:HD22	1:A:435:ARG:CG	2.42	0.49
2:B:259:VAL:HG13	2:B:336:ILE:HD11	1.93	0.49

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	207/233 (89%)	205 (99%)	2 (1%)	0	100	100
2	B	207/227 (91%)	204 (99%)	2 (1%)	1 (0%)	29	17
All	All	414/460 (90%)	409 (99%)	4 (1%)	1 (0%)	47	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	329	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	195/213 (92%)	189 (97%)	6 (3%)	40	29
2	B	193/205 (94%)	187 (97%)	6 (3%)	40	29
All	All	388/418 (93%)	376 (97%)	12 (3%)	40	29

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	360	LYS
2	B	384	ASN
2	B	409	ARG
2	B	394	ASP
1	A	364	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	389	ASN
2	B	295	GLN
2	B	384	ASN
2	B	401	GLN

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	$\#|Z| > 2$
2	MLY	B	248	2	9,10,11	0.67	0	6,11,13	0.59	0
1	MLY	A	248	1	9,10,11	0.47	0	6,11,13	0.45	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
2	MLY	B	248	2	-	0/8/9/11	-
1	MLY	A	248	1	-	0/8/9/11	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	248	MLY	1	0

5.5 Carbohydrates (i)

18 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	$\#|Z| > 2$
3	NAG	C	1	3,1	14,14,15	0.28	0	17,19,21	0.81	0
3	NAG	C	2	3	14,14,15	0.29	0	17,19,21	0.69	0
3	BMA	C	3	3	11,11,12	0.36	0	15,15,17	0.74	0
3	MAN	C	4	3	11,11,12	0.32	0	15,15,17	0.86	0
3	NAG	C	5	3	14,14,15	0.40	0	17,19,21	1.31	3 (17%)
3	GAL	C	6	3	11,11,12	0.67	0	15,15,17	1.50	3 (20%)
3	MAN	C	7	3	11,11,12	0.40	0	15,15,17	0.99	1 (6%)
3	NAG	C	8	3	14,14,15	0.32	0	17,19,21	1.25	2 (11%)
3	FUL	C	9	3	10,10,11	0.39	0	14,14,16	1.50	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z|$ > 2	Counts	RMSZ	#$|Z|$ > 2
3	NAG	D	1	2,3	14,14,15	0.35	0	17,19,21	0.83	0
3	NAG	D	2	3	14,14,15	0.33	0	17,19,21	0.74	0
3	BMA	D	3	3	11,11,12	0.33	0	15,15,17	0.77	0
3	MAN	D	4	3	11,11,12	0.32	0	15,15,17	0.79	0
3	NAG	D	5	3	14,14,15	0.34	0	17,19,21	1.23	2 (11%)
3	GAL	D	6	3	11,11,12	0.54	0	15,15,17	1.41	2 (13%)
3	MAN	D	7	3	11,11,12	0.32	0	15,15,17	0.73	0
3	NAG	D	8	3	14,14,15	0.28	0	17,19,21	1.18	2 (11%)
3	FUL	D	9	3	10,10,11	0.45	0	14,14,16	1.82	2 (14%)

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	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	NAG	C	5	3	-	2/6/23/26	0/1/1/1
3	GAL	C	6	3	-	0/2/19/22	0/1/1/1
3	MAN	C	7	3	-	1/2/19/22	0/1/1/1
3	NAG	C	8	3	-	2/6/23/26	0/1/1/1
3	FUL	C	9	3	-	-	0/1/1/1
3	NAG	D	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	NAG	D	5	3	-	2/6/23/26	0/1/1/1
3	GAL	D	6	3	-	0/2/19/22	0/1/1/1
3	MAN	D	7	3	-	0/2/19/22	0/1/1/1
3	NAG	D	8	3	-	2/6/23/26	0/1/1/1
3	FUL	D	9	3	-	-	0/1/1/1

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	9	FUL	C1-C2-C3	5.54	116.48	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	9	FUL	C1-C2-C3	3.93	114.50	109.67
3	D	6	GAL	C1-C2-C3	3.90	114.45	109.67
3	C	6	GAL	C1-C2-C3	3.22	113.62	109.67
3	D	5	NAG	C2-N2-C7	2.84	126.95	122.90

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	5	NAG	C8-C7-N2-C2
3	C	5	NAG	O7-C7-N2-C2
3	C	8	NAG	C8-C7-N2-C2
3	C	8	NAG	O7-C7-N2-C2
3	D	5	NAG	C8-C7-N2-C2

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.

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D	
 Bond lengths	 Bond angles
 Torsions	 Rings
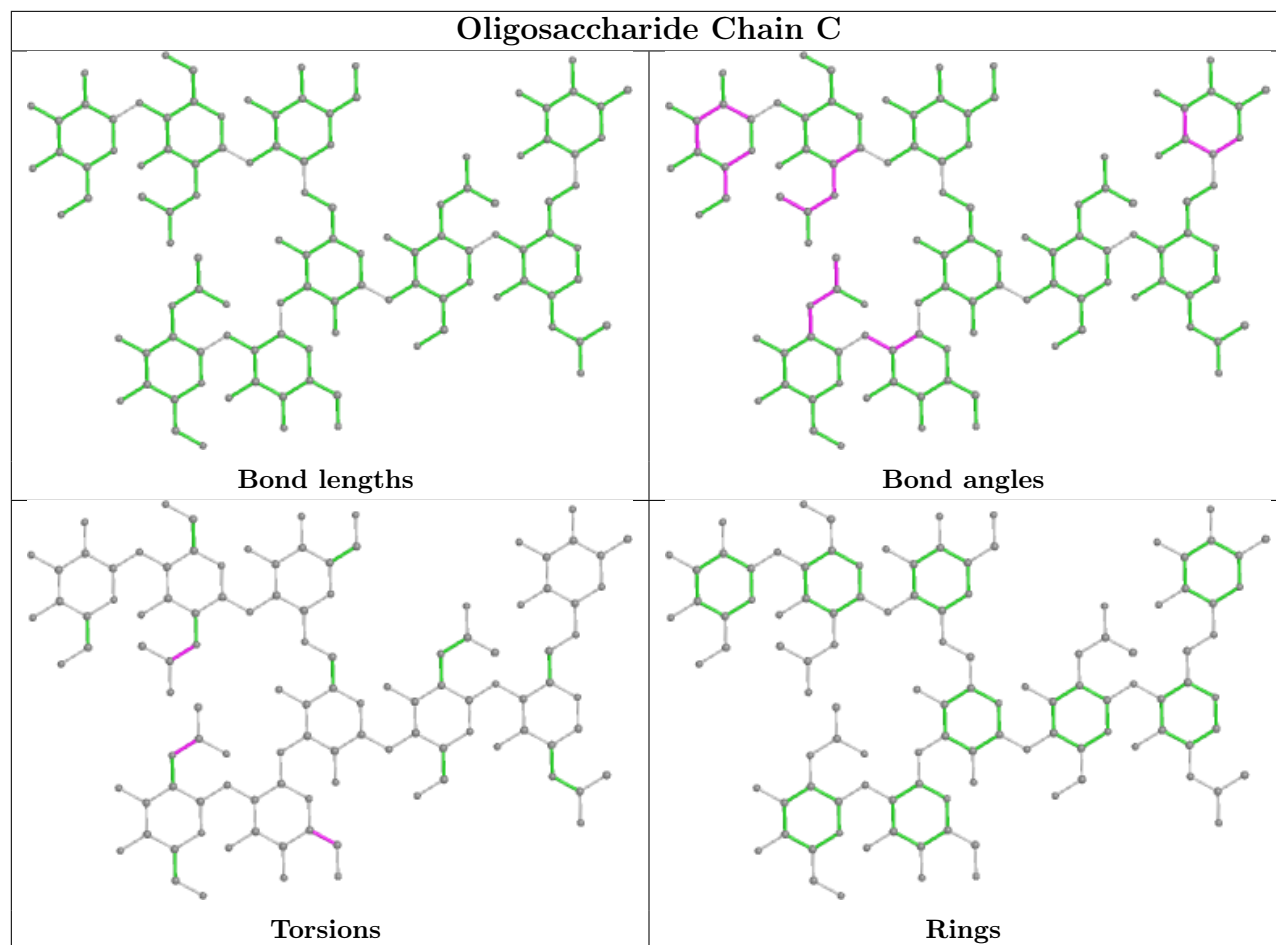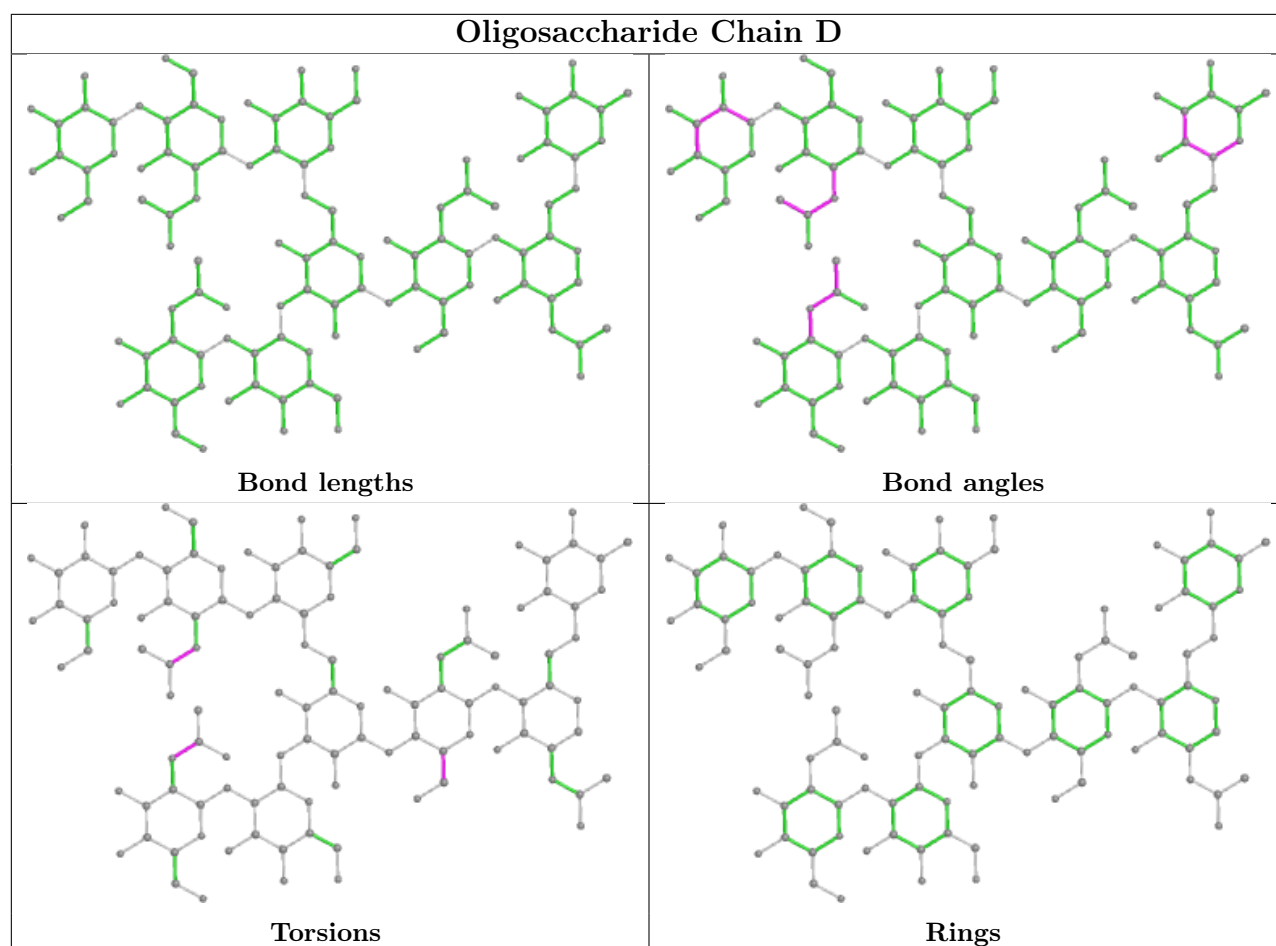
5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

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	207/233 (88%)	0.77	21 (10%)	7	7	23, 45, 89, 103	0
2	B	206/227 (90%)	1.15	48 (23%)	0	0	20, 51, 145, 182	0
All	All	413/460 (89%)	0.96	69 (16%)	1	1	20, 47, 127, 182	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	296	TYR	8.5
1	A	359	THR	8.2
2	B	300	TYR	6.5
1	A	358	MET	6.0
2	B	324	SER	6.0

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

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	MLY	A	248	11/12	0.94	0.17	25,30,35,37	0
2	MLY	B	248	11/12	0.95	0.17	29,31,36,38	0

6.3   Carbohydrates ⓘ

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	NAG	D	8	14/15	0.50	0.39	97,103,107,108	0
3	NAG	D	1	14/15	0.55	0.27	140,143,158,161	0
3	NAG	C	8	14/15	0.64	0.38	86,90,103,103	0
3	FUL	D	9	10/11	0.67	0.51	146,154,158,165	0
3	BMA	D	3	11/12	0.68	0.23	65,74,76,82	0
3	MAN	D	7	11/12	0.70	0.34	87,91,93,96	0
3	GAL	C	6	11/12	0.73	0.15	41,46,49,50	0
3	FUL	C	9	10/11	0.75	0.21	93,98,103,106	0
3	MAN	D	4	11/12	0.78	0.20	93,101,103,108	0
3	GAL	D	6	11/12	0.82	0.14	48,49,52,54	0
3	BMA	C	3	11/12	0.82	0.13	60,63,68,73	0
3	NAG	C	1	14/15	0.83	0.14	71,80,87,87	0
3	NAG	C	5	14/15	0.85	0.12	46,48,56,58	0
3	MAN	C	4	11/12	0.85	0.23	55,62,65,67	0
3	MAN	C	7	11/12	0.85	0.32	79,86,90,92	0
3	NAG	D	2	14/15	0.86	0.24	72,76,79,82	0
3	NAG	D	5	14/15	0.86	0.13	51,54,66,70	0
3	NAG	C	2	14/15	0.91	0.11	60,66,70,73	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.

Electron density around Chain C:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain D:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
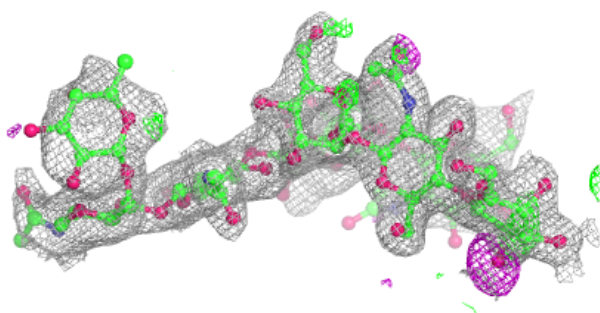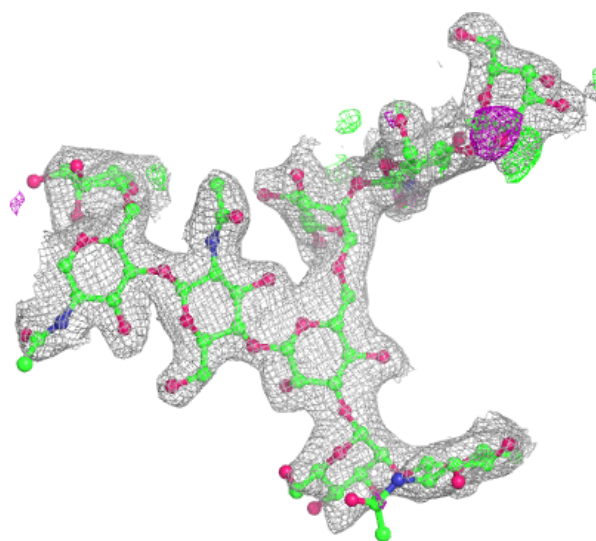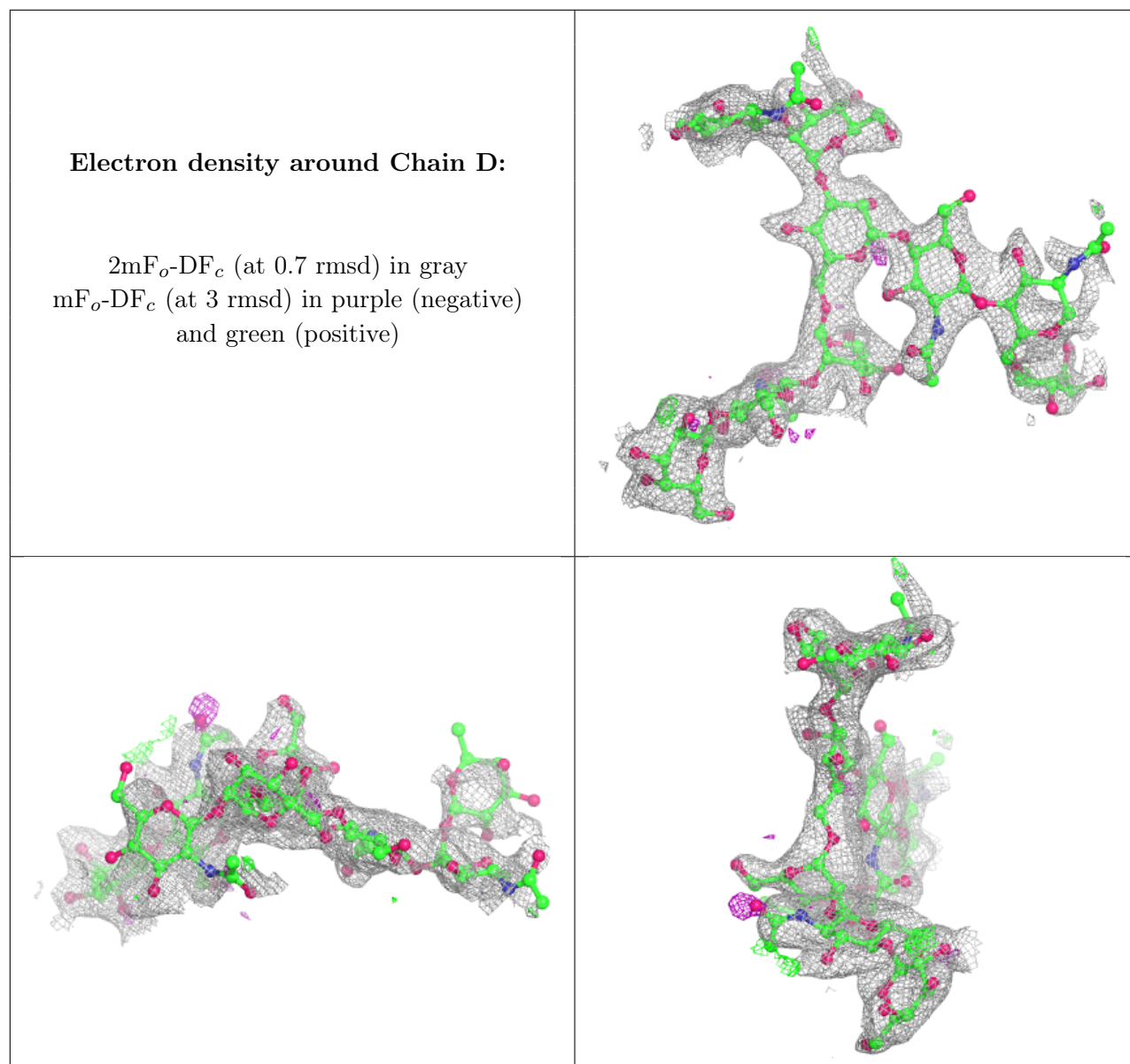
6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.