



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2025 – 04:06 pm BST

PDB ID : 8S6T / pdb_00008s6t
Title : Crystal structure of Fab-3F1 complexed to a bis-STn glycopeptide
Authors : Hurtado-Guerrero, R.; Gines, I.
Deposited on : 2024-02-28
Resolution : 1.85 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
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) : 2.44

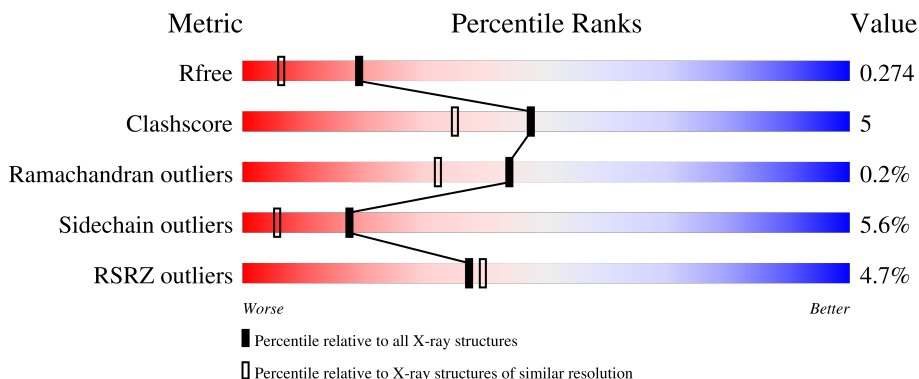
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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 $\leq 5\%$. 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	215	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>10% ..</div> </div> </div>
2	B	211	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>13% .</div> </div> </div>
3	C	13	<div> <div>15%</div> <div> <div>8%</div> <div>8%</div> <div>85%</div> </div> </div>
4	D	2	<div> <div>100%</div> </div>
4	E	2	<div> <div>100%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3517 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 3F1 (VH-VH1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1618	1026	263	323	6			

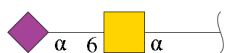
- Molecule 2 is a protein called 3F1 (VL-CL).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1640	1021	277	335	7			

- Molecule 3 is a protein called Mucin-1 subunit beta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			11	6	2	3			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-2-acetamido-2-deoxy-alpha-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			34	19	2	13			
4	E	2	Total	C	N	O	0	0	0
			34	19	2	13			

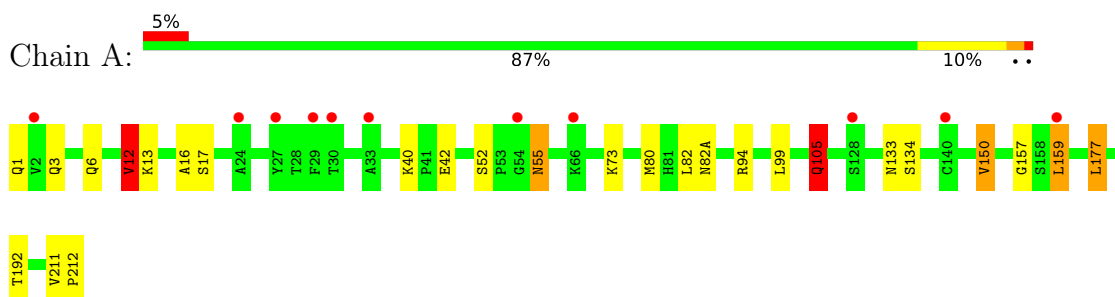
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	95	Total 95	O 95	0	0
5	B	83	Total 83	O 83	0	0
5	C	2	Total 2	O 2	0	0

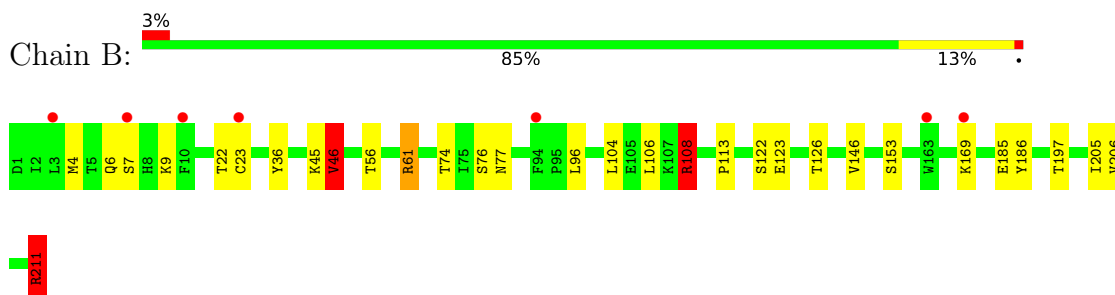
3 Residue-property plots [i](#)

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: 3F1 (VH-VH1)



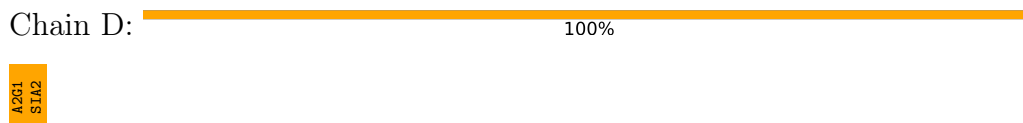
- Molecule 2: 3F1 (VL-CL)



- Molecule 3: Mucin-1 subunit beta



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-2-acetamido-2-deoxy-alpha-D-galactopyranos e



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-2-acetamido-2-deoxy-alpha-D-galactopyranos e

Chain E:

100%

A261
S1A2

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	74.78Å 74.78Å 392.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.77 – 1.85 19.77 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.77-1.85) 99.9 (19.77-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.230 , 0.267 0.237 , 0.274	Depositor DCC
R_{free} test set	2305 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3517	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A2G, SIA

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	0.61	0/1658	1.11	7/2263 (0.3%)
2	B	0.59	0/1676	1.15	9/2272 (0.4%)
3	C	0.71	0/10	2.68	1/12 (8.3%)
All	All	0.60	0/3344	1.14	17/4547 (0.4%)

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	1
2	B	0	3
All	All	0	4

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	108	ARG	N-CA-CB	-9.09	97.47	111.46
1	A	40	LYS	CB-CA-C	8.51	120.42	108.76
2	B	123	GLU	CG-CD-OE1	-7.12	102.02	118.40
3	C	6	THR	N-CA-CB	-6.94	99.71	111.50
1	A	150	VAL	N-CA-CB	-6.89	99.18	111.93

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	ARG	Sidechain
2	B	108	ARG	Sidechain
2	B	211	ARG	Sidechain
2	B	61	ARG	Sidechain

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	1618	0	1603	21	0
2	B	1640	0	1578	14	0
3	C	11	0	8	0	0
4	D	34	0	28	4	0
4	E	34	0	28	0	0
5	A	95	0	0	0	0
5	B	83	0	0	2	0
5	C	2	0	0	0	0
All	All	3517	0	3245	34	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 34 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:105:GLN:HE21	1:A:105:GLN:H	1.17	0.87
2:B:186:TYR:CE2	2:B:211:ARG:HD3	2.21	0.75
1:A:6:GLN:H	1:A:105:GLN:HE22	1.34	0.74
2:B:7:SER:HB2	2:B:22:THR:OG1	1.87	0.74
1:A:55:ASN:HD22	4:D:1:A2G:H2	1.58	0.69

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	213/215 (99%)	204 (96%)	8 (4%)	1 (0%)	25	13
2	B	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
All	All	422/426 (99%)	406 (96%)	15 (4%)	1 (0%)	44	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASN

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	186/187 (100%)	178 (96%)	8 (4%)	25	10
2	B	190/190 (100%)	179 (94%)	11 (6%)	17	5
3	C	2/8 (25%)	0	2 (100%)	0	0
All	All	378/385 (98%)	357 (94%)	21 (6%)	17	6

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	108	ARG
2	B	169	LYS
3	C	6	THR
2	B	185	GLU

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Mol	Chain	Res	Type
2	B	153	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	210	ASN
2	B	8	HIS
1	A	131	GLN
1	A	105	GLN
1	A	133	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
4	A2G	D	1	4,3	14,14,15	1.38	1 (7%)	17,19,21	1.68	3 (17%)
4	SIA	D	2	4	20,20,21	1.57	4 (20%)	24,28,31	1.21	1 (4%)
4	A2G	E	1	4,3	14,14,15	1.12	2 (14%)	17,19,21	1.43	3 (17%)
4	SIA	E	2	4	20,20,21	1.00	1 (5%)	24,28,31	1.36	3 (12%)

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
4	A2G	D	1	4,3	-	2/6/23/26	0/1/1/1
4	SIA	D	2	4	-	3/18/34/38	0/1/1/1
4	A2G	E	1	4,3	-	0/6/23/26	0/1/1/1
4	SIA	E	2	4	-	1/18/34/38	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	SIA	O6-C6	3.82	1.49	1.44
4	D	1	A2G	O4-C4	3.69	1.51	1.43
4	D	2	SIA	C4-C5	3.10	1.55	1.53
4	E	1	A2G	O5-C5	2.57	1.48	1.43
4	E	2	SIA	C2-C1	2.52	1.54	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	A2G	C1-O5-C5	4.96	118.91	112.19
4	E	2	SIA	C3-C4-C5	-3.71	106.97	111.46
4	D	2	SIA	O6-C2-C3	-3.18	106.08	110.46
4	E	1	A2G	C1-O5-C5	-3.09	108.01	112.19
4	E	2	SIA	O1A-C1-C2	-2.58	116.47	122.57

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	SIA	C5-C6-C7-O7
4	D	2	SIA	O6-C6-C7-O7
4	D	1	A2G	O5-C5-C6-O6
4	D	1	A2G	C4-C5-C6-O6
4	E	2	SIA	O1A-C1-C2-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

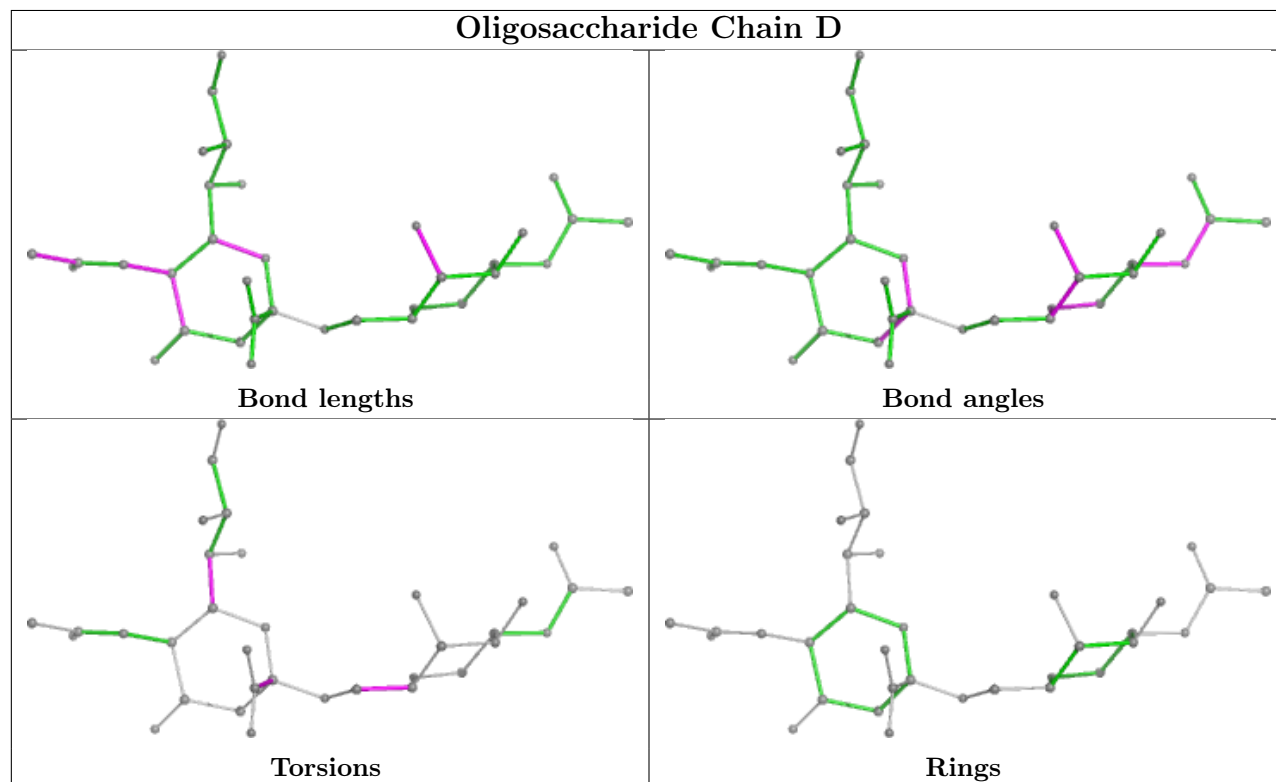
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	A2G	3	0

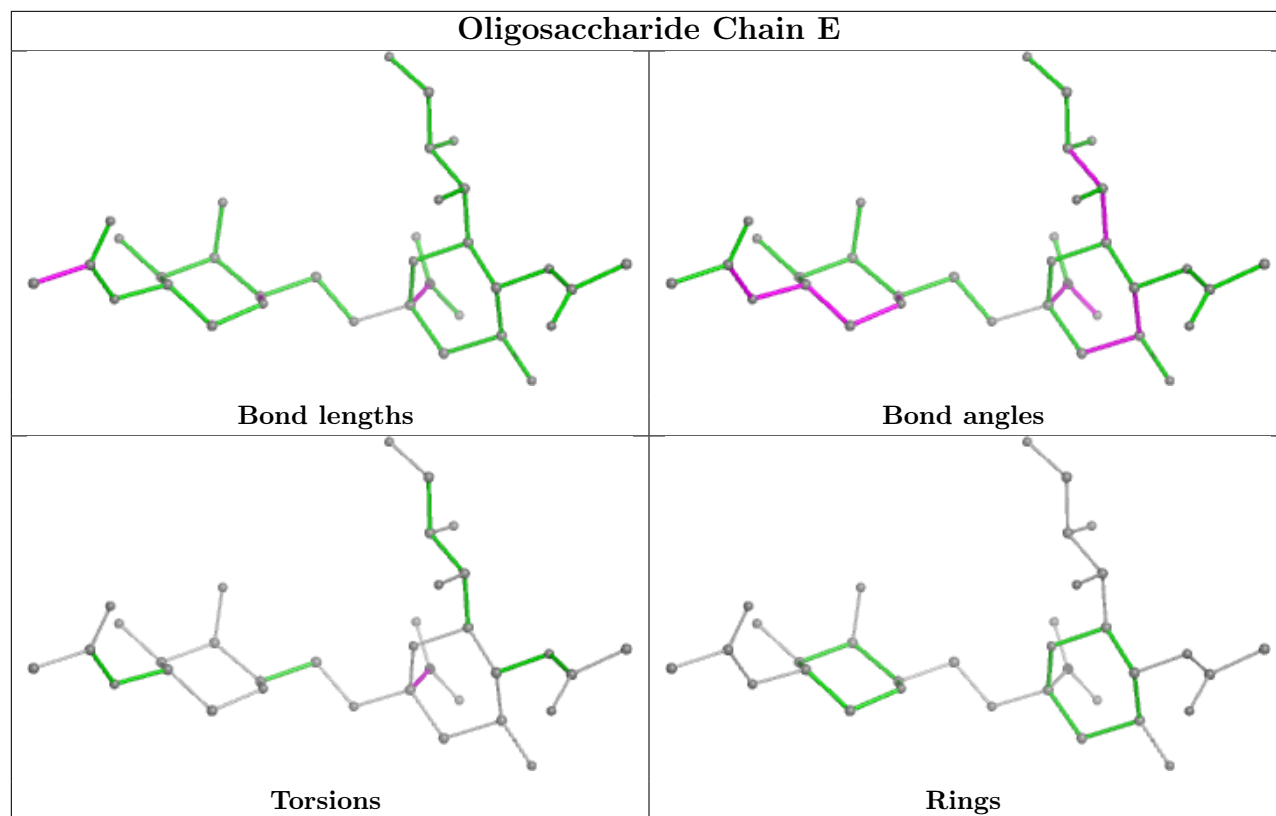
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	SIA	1	0

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](#)

There are no ligands in this entry.

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	215/215 (100%)	0.39	11 (5%) 34 36	33, 54, 89, 107	0
2	B	211/211 (100%)	0.39	7 (3%) 49 53	35, 57, 85, 118	0
3	C	2/13 (15%)	2.74	2 (100%) 0 0	101, 101, 101, 102	0
All	All	428/439 (97%)	0.40	20 (4%) 37 39	33, 56, 87, 118	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	5	SER	3.4
1	A	54	GLY	3.3
2	B	7	SER	3.2
2	B	3	LEU	3.0
1	A	27	TYR	2.9

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.

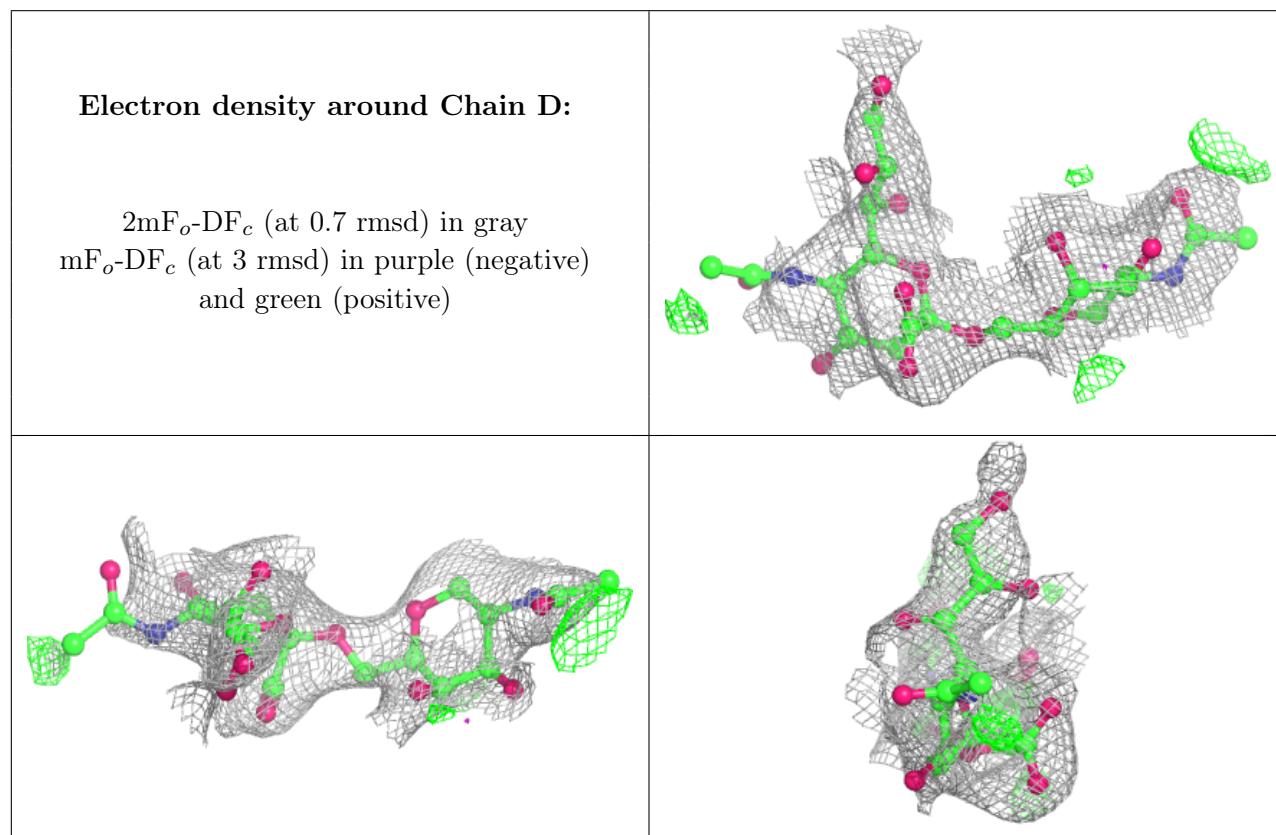
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SIA	D	2	20/21	0.56	0.14	82,109,117,117	0
4	A2G	D	1	14/15	0.81	0.14	73,91,99,105	0
4	SIA	E	2	20/21	0.86	0.10	66,73,81,94	0

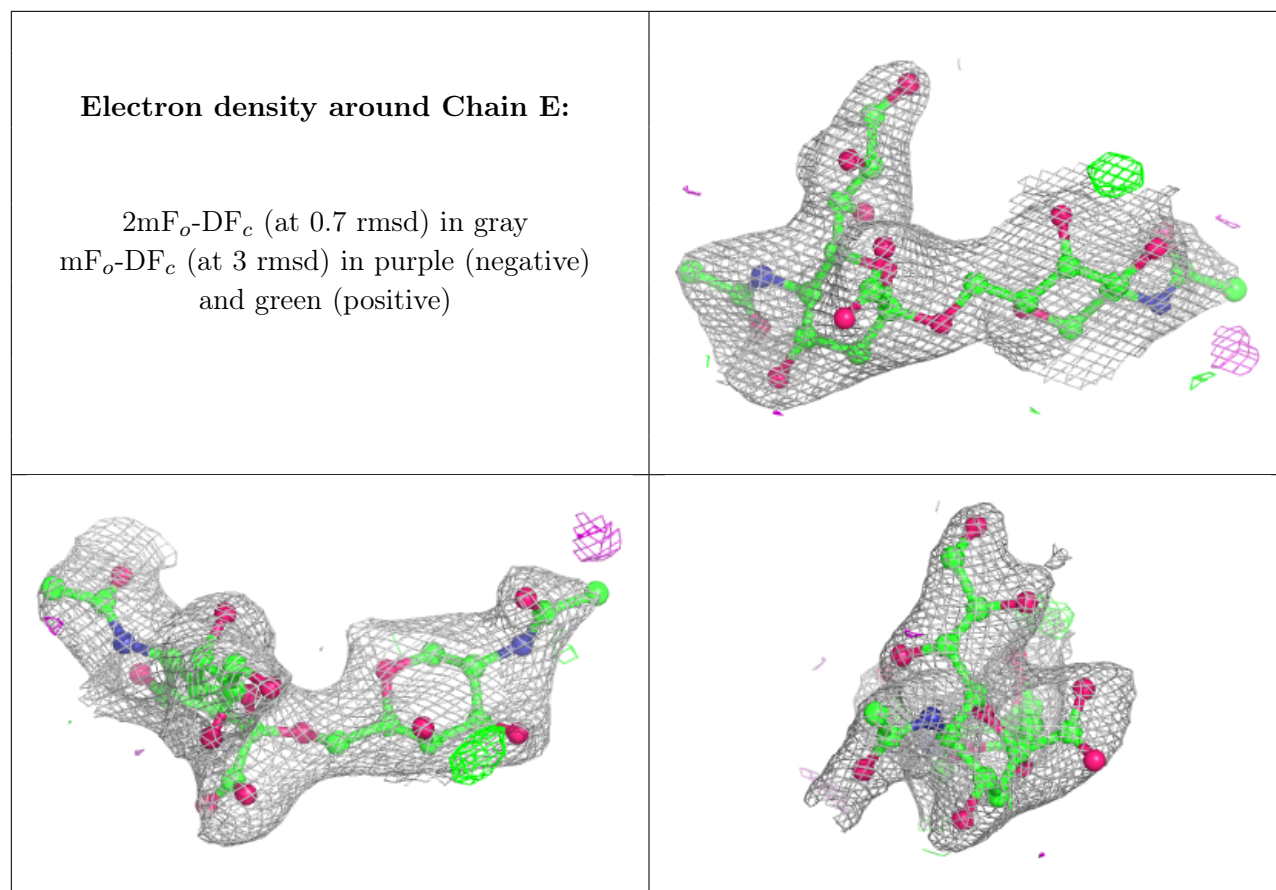
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	A2G	E	1	14/15	0.88	0.11	70,75,83,91	0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.