



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 10:51 AM BST

PDB ID : 6EAH
Title : CRYSTAL STRUCTURE OF HUMAN RESPIRATORY SYNCYTIAL VIRUS FUSION GLYCOPROTEIN INHIBITOR ESCAPE VARIANT K394R-S398L STABILIZED IN THE PREFUSION STATE
Authors : Battles, M.B.; McLellan, J.S.
Deposited on : 2018-08-03
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

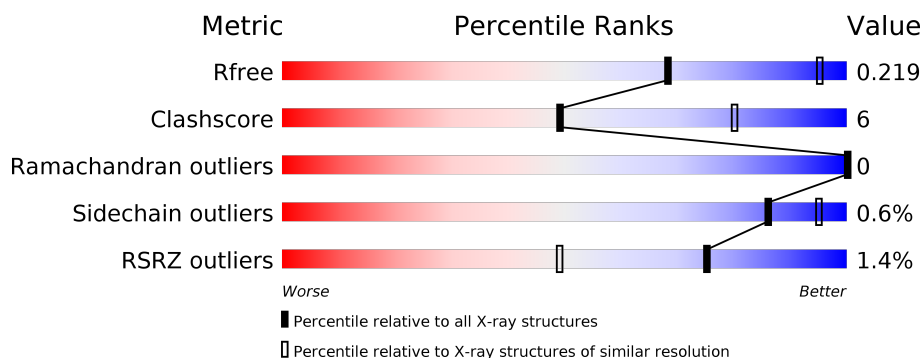
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	568	<div> <div></div> <div> <div></div> <div>66%</div> <div>13%</div> <div>21%</div> </div> </div>
1	B	568	<div> <div></div> <div> <div></div> <div>67%</div> <div>10%</div> <div>23%</div> </div> </div>
1	C	568	<div> <div></div> <div> <div></div> <div>65%</div> <div>13%</div> <div>23%</div> </div> </div>
2	D	3	<div> <div></div> <div> <div></div> <div>33%</div> <div>67%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	1	-	-	-	X
2	NAG	D	2	-	-	-	X
3	SO4	A	609	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10405 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3448	2180	569	676	23			
1	B	440	Total	C	N	O	S	0	0	0
			3404	2157	558	667	22			
1	C	439	Total	C	N	O	S	0	0	0
			3402	2155	560	666	21			

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	GLU	LYS	conflict	UNP W8RJF9
A	155	CYS	SER	engineered mutation	UNP W8RJF9
A	190	PHE	SER	engineered mutation	UNP W8RJF9
A	207	LEU	VAL	engineered mutation	UNP W8RJF9
A	290	CYS	SER	engineered mutation	UNP W8RJF9
A	394	ARG	LYS	engineered mutation	UNP W8RJF9
A	398	LEU	SER	engineered mutation	UNP W8RJF9
A	514	SER	-	expression tag	UNP W8RJF9
A	515	ALA	-	expression tag	UNP W8RJF9
A	516	ILE	-	expression tag	UNP W8RJF9
A	517	GLY	-	expression tag	UNP W8RJF9
A	518	GLY	-	expression tag	UNP W8RJF9
A	519	TYR	-	expression tag	UNP W8RJF9
A	520	ILE	-	expression tag	UNP W8RJF9
A	521	PRO	-	expression tag	UNP W8RJF9
A	522	GLU	-	expression tag	UNP W8RJF9
A	523	ALA	-	expression tag	UNP W8RJF9
A	524	PRO	-	expression tag	UNP W8RJF9
A	525	ARG	-	expression tag	UNP W8RJF9
A	526	ASP	-	expression tag	UNP W8RJF9
A	527	GLY	-	expression tag	UNP W8RJF9
A	528	GLN	-	expression tag	UNP W8RJF9
A	529	ALA	-	expression tag	UNP W8RJF9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	530	TYR	-	expression tag	UNP W8RJF9
A	531	VAL	-	expression tag	UNP W8RJF9
A	532	ARG	-	expression tag	UNP W8RJF9
A	533	LYS	-	expression tag	UNP W8RJF9
A	534	ASP	-	expression tag	UNP W8RJF9
A	535	GLY	-	expression tag	UNP W8RJF9
A	536	GLU	-	expression tag	UNP W8RJF9
A	537	TRP	-	expression tag	UNP W8RJF9
A	538	VAL	-	expression tag	UNP W8RJF9
A	539	LEU	-	expression tag	UNP W8RJF9
A	540	LEU	-	expression tag	UNP W8RJF9
A	541	SER	-	expression tag	UNP W8RJF9
A	542	THR	-	expression tag	UNP W8RJF9
A	543	PHE	-	expression tag	UNP W8RJF9
A	544	LEU	-	expression tag	UNP W8RJF9
A	545	GLY	-	expression tag	UNP W8RJF9
A	546	GLY	-	expression tag	UNP W8RJF9
A	547	LEU	-	expression tag	UNP W8RJF9
A	548	VAL	-	expression tag	UNP W8RJF9
A	549	PRO	-	expression tag	UNP W8RJF9
A	550	ARG	-	expression tag	UNP W8RJF9
A	551	GLY	-	expression tag	UNP W8RJF9
A	552	SER	-	expression tag	UNP W8RJF9
A	553	HIS	-	expression tag	UNP W8RJF9
A	554	HIS	-	expression tag	UNP W8RJF9
A	555	HIS	-	expression tag	UNP W8RJF9
A	556	HIS	-	expression tag	UNP W8RJF9
A	557	HIS	-	expression tag	UNP W8RJF9
A	558	HIS	-	expression tag	UNP W8RJF9
A	559	SER	-	expression tag	UNP W8RJF9
A	560	ALA	-	expression tag	UNP W8RJF9
A	561	TRP	-	expression tag	UNP W8RJF9
A	562	SER	-	expression tag	UNP W8RJF9
A	563	HIS	-	expression tag	UNP W8RJF9
A	564	PRO	-	expression tag	UNP W8RJF9
A	565	GLN	-	expression tag	UNP W8RJF9
A	566	PHE	-	expression tag	UNP W8RJF9
A	567	GLU	-	expression tag	UNP W8RJF9
A	568	LYS	-	expression tag	UNP W8RJF9
B	66	GLU	LYS	conflict	UNP W8RJF9
B	155	CYS	SER	engineered mutation	UNP W8RJF9
B	190	PHE	SER	engineered mutation	UNP W8RJF9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	207	LEU	VAL	engineered mutation	UNP W8RJF9
B	290	CYS	SER	engineered mutation	UNP W8RJF9
B	394	ARG	LYS	engineered mutation	UNP W8RJF9
B	398	LEU	SER	engineered mutation	UNP W8RJF9
B	514	SER	-	expression tag	UNP W8RJF9
B	515	ALA	-	expression tag	UNP W8RJF9
B	516	ILE	-	expression tag	UNP W8RJF9
B	517	GLY	-	expression tag	UNP W8RJF9
B	518	GLY	-	expression tag	UNP W8RJF9
B	519	TYR	-	expression tag	UNP W8RJF9
B	520	ILE	-	expression tag	UNP W8RJF9
B	521	PRO	-	expression tag	UNP W8RJF9
B	522	GLU	-	expression tag	UNP W8RJF9
B	523	ALA	-	expression tag	UNP W8RJF9
B	524	PRO	-	expression tag	UNP W8RJF9
B	525	ARG	-	expression tag	UNP W8RJF9
B	526	ASP	-	expression tag	UNP W8RJF9
B	527	GLY	-	expression tag	UNP W8RJF9
B	528	GLN	-	expression tag	UNP W8RJF9
B	529	ALA	-	expression tag	UNP W8RJF9
B	530	TYR	-	expression tag	UNP W8RJF9
B	531	VAL	-	expression tag	UNP W8RJF9
B	532	ARG	-	expression tag	UNP W8RJF9
B	533	LYS	-	expression tag	UNP W8RJF9
B	534	ASP	-	expression tag	UNP W8RJF9
B	535	GLY	-	expression tag	UNP W8RJF9
B	536	GLU	-	expression tag	UNP W8RJF9
B	537	TRP	-	expression tag	UNP W8RJF9
B	538	VAL	-	expression tag	UNP W8RJF9
B	539	LEU	-	expression tag	UNP W8RJF9
B	540	LEU	-	expression tag	UNP W8RJF9
B	541	SER	-	expression tag	UNP W8RJF9
B	542	THR	-	expression tag	UNP W8RJF9
B	543	PHE	-	expression tag	UNP W8RJF9
B	544	LEU	-	expression tag	UNP W8RJF9
B	545	GLY	-	expression tag	UNP W8RJF9
B	546	GLY	-	expression tag	UNP W8RJF9
B	547	LEU	-	expression tag	UNP W8RJF9
B	548	VAL	-	expression tag	UNP W8RJF9
B	549	PRO	-	expression tag	UNP W8RJF9
B	550	ARG	-	expression tag	UNP W8RJF9
B	551	GLY	-	expression tag	UNP W8RJF9

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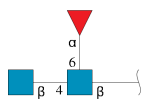
Chain	Residue	Modelled	Actual	Comment	Reference
B	552	SER	-	expression tag	UNP W8RJF9
B	553	HIS	-	expression tag	UNP W8RJF9
B	554	HIS	-	expression tag	UNP W8RJF9
B	555	HIS	-	expression tag	UNP W8RJF9
B	556	HIS	-	expression tag	UNP W8RJF9
B	557	HIS	-	expression tag	UNP W8RJF9
B	558	HIS	-	expression tag	UNP W8RJF9
B	559	SER	-	expression tag	UNP W8RJF9
B	560	ALA	-	expression tag	UNP W8RJF9
B	561	TRP	-	expression tag	UNP W8RJF9
B	562	SER	-	expression tag	UNP W8RJF9
B	563	HIS	-	expression tag	UNP W8RJF9
B	564	PRO	-	expression tag	UNP W8RJF9
B	565	GLN	-	expression tag	UNP W8RJF9
B	566	PHE	-	expression tag	UNP W8RJF9
B	567	GLU	-	expression tag	UNP W8RJF9
B	568	LYS	-	expression tag	UNP W8RJF9
C	66	GLU	LYS	conflict	UNP W8RJF9
C	155	CYS	SER	engineered mutation	UNP W8RJF9
C	190	PHE	SER	engineered mutation	UNP W8RJF9
C	207	LEU	VAL	engineered mutation	UNP W8RJF9
C	290	CYS	SER	engineered mutation	UNP W8RJF9
C	394	ARG	LYS	engineered mutation	UNP W8RJF9
C	398	LEU	SER	engineered mutation	UNP W8RJF9
C	514	SER	-	expression tag	UNP W8RJF9
C	515	ALA	-	expression tag	UNP W8RJF9
C	516	ILE	-	expression tag	UNP W8RJF9
C	517	GLY	-	expression tag	UNP W8RJF9
C	518	GLY	-	expression tag	UNP W8RJF9
C	519	TYR	-	expression tag	UNP W8RJF9
C	520	ILE	-	expression tag	UNP W8RJF9
C	521	PRO	-	expression tag	UNP W8RJF9
C	522	GLU	-	expression tag	UNP W8RJF9
C	523	ALA	-	expression tag	UNP W8RJF9
C	524	PRO	-	expression tag	UNP W8RJF9
C	525	ARG	-	expression tag	UNP W8RJF9
C	526	ASP	-	expression tag	UNP W8RJF9
C	527	GLY	-	expression tag	UNP W8RJF9
C	528	GLN	-	expression tag	UNP W8RJF9
C	529	ALA	-	expression tag	UNP W8RJF9
C	530	TYR	-	expression tag	UNP W8RJF9
C	531	VAL	-	expression tag	UNP W8RJF9

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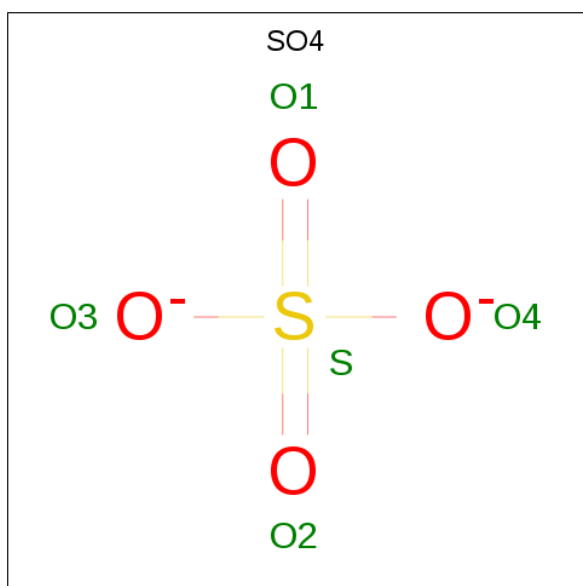
Chain	Residue	Modelled	Actual	Comment	Reference
C	532	ARG	-	expression tag	UNP W8RJF9
C	533	LYS	-	expression tag	UNP W8RJF9
C	534	ASP	-	expression tag	UNP W8RJF9
C	535	GLY	-	expression tag	UNP W8RJF9
C	536	GLU	-	expression tag	UNP W8RJF9
C	537	TRP	-	expression tag	UNP W8RJF9
C	538	VAL	-	expression tag	UNP W8RJF9
C	539	LEU	-	expression tag	UNP W8RJF9
C	540	LEU	-	expression tag	UNP W8RJF9
C	541	SER	-	expression tag	UNP W8RJF9
C	542	THR	-	expression tag	UNP W8RJF9
C	543	PHE	-	expression tag	UNP W8RJF9
C	544	LEU	-	expression tag	UNP W8RJF9
C	545	GLY	-	expression tag	UNP W8RJF9
C	546	GLY	-	expression tag	UNP W8RJF9
C	547	LEU	-	expression tag	UNP W8RJF9
C	548	VAL	-	expression tag	UNP W8RJF9
C	549	PRO	-	expression tag	UNP W8RJF9
C	550	ARG	-	expression tag	UNP W8RJF9
C	551	GLY	-	expression tag	UNP W8RJF9
C	552	SER	-	expression tag	UNP W8RJF9
C	553	HIS	-	expression tag	UNP W8RJF9
C	554	HIS	-	expression tag	UNP W8RJF9
C	555	HIS	-	expression tag	UNP W8RJF9
C	556	HIS	-	expression tag	UNP W8RJF9
C	557	HIS	-	expression tag	UNP W8RJF9
C	558	HIS	-	expression tag	UNP W8RJF9
C	559	SER	-	expression tag	UNP W8RJF9
C	560	ALA	-	expression tag	UNP W8RJF9
C	561	TRP	-	expression tag	UNP W8RJF9
C	562	SER	-	expression tag	UNP W8RJF9
C	563	HIS	-	expression tag	UNP W8RJF9
C	564	PRO	-	expression tag	UNP W8RJF9
C	565	GLN	-	expression tag	UNP W8RJF9
C	566	PHE	-	expression tag	UNP W8RJF9
C	567	GLU	-	expression tag	UNP W8RJF9
C	568	LYS	-	expression tag	UNP W8RJF9

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



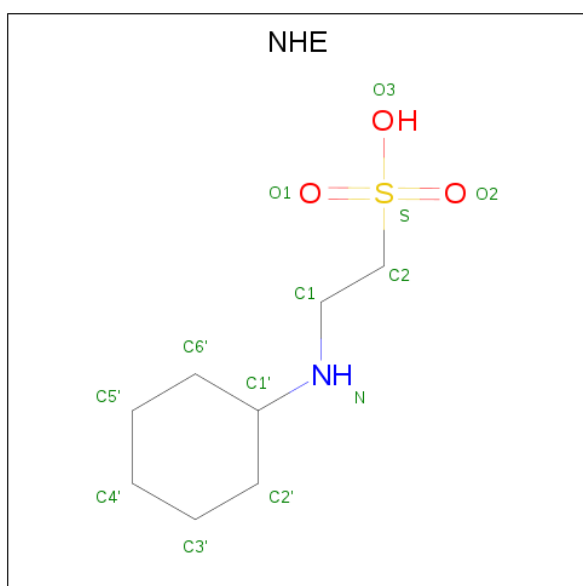
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: C₈H₁₇NO₃S).

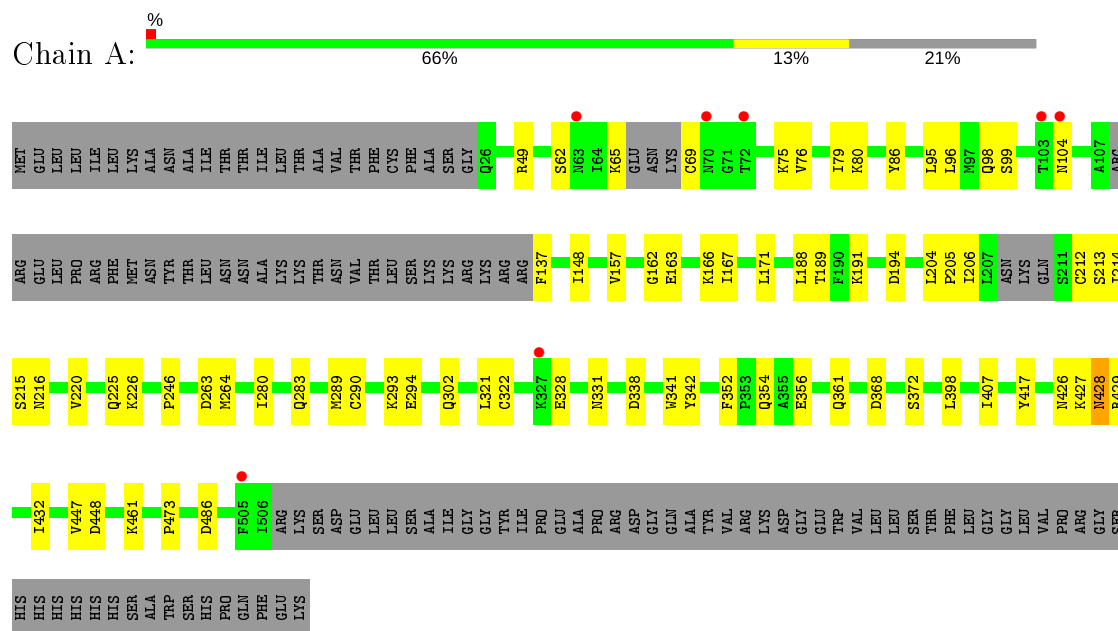


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

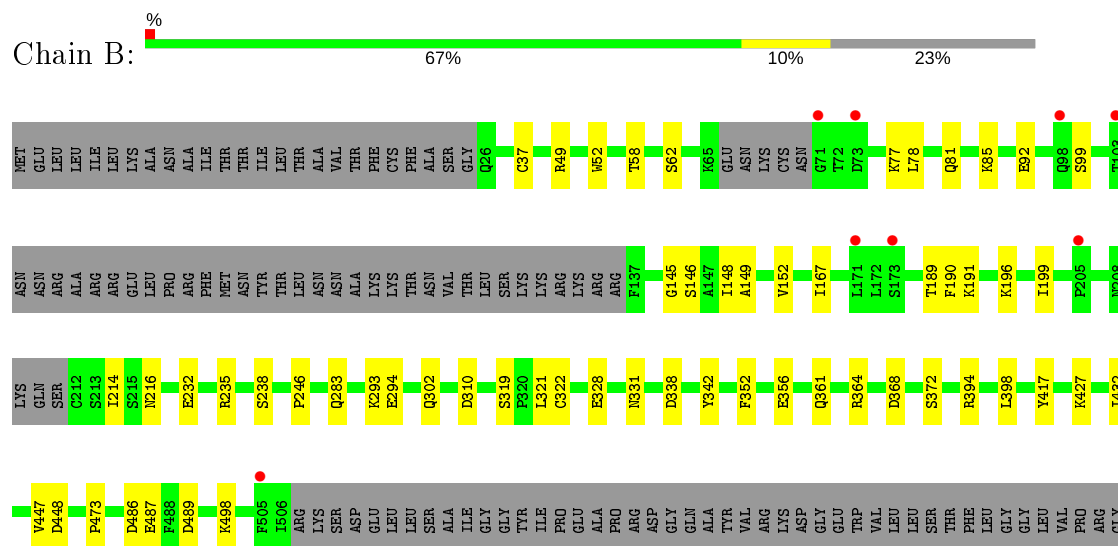
3 Residue-property plots

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: Fusion glycoprotein F0

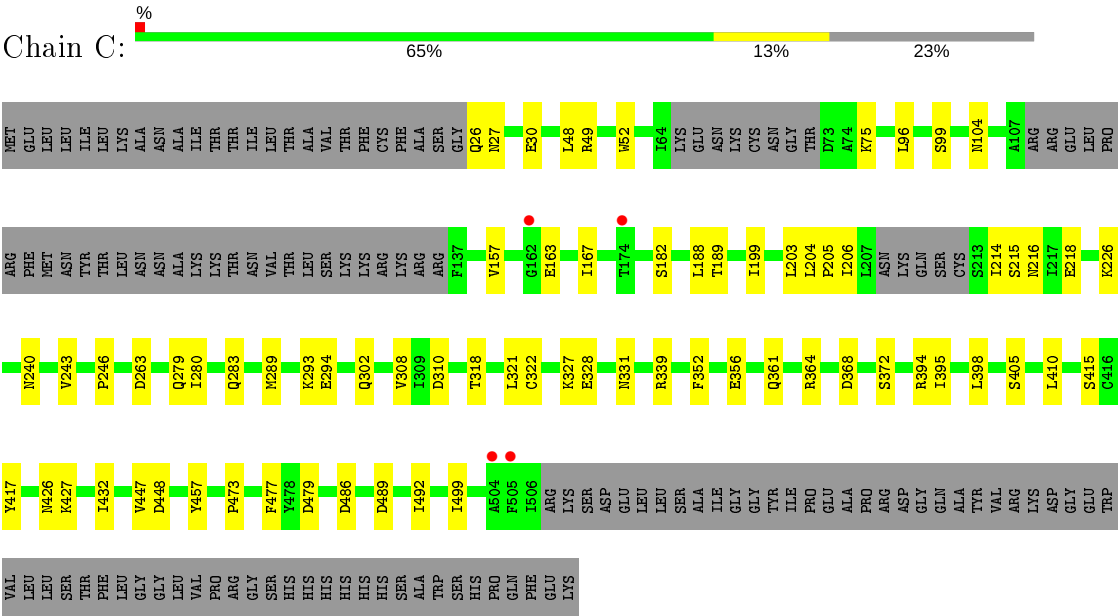


• Molecule 1: Fusion glycoprotein F0



SER
HIS
HIS
HIS
HIS
HIS
HIS
HIS
SER
SER
ALA
TRP
SER
HIS
HIS
PRO
PHE
GLN
PHE
GLU
LYS

● Molecule 1: Fusion glycoprotein F0



● Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	166.64Å 166.64Å 174.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.92 – 3.00 58.92 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (58.92-3.00) 99.9 (58.92-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.193 , 0.219 0.193 , 0.219	Depositor DCC
R_{free} test set	2439 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	71.9	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.029 for -h,l,k 0.024 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10405	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: NHE, FUC, SO4, NAG

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	0.39	0/3497	0.52	0/4740
1	B	0.38	0/3453	0.52	0/4681
1	C	0.39	0/3451	0.53	0/4679
All	All	0.39	0/10401	0.52	0/14100

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 [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	3448	0	3484	48	0
1	B	3404	0	3446	34	0
1	C	3402	0	3441	45	1
2	D	38	0	34	4	0
3	A	45	0	0	2	0
3	B	30	0	0	0	0
3	C	25	0	0	1	0
4	A	13	0	17	1	0
All	All	10405	0	10422	122	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 6.

All (122) 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:432:ILE:HD11	1:B:447:VAL:HG22	1.55	0.88
1:A:280:ILE:HD11	1:A:361:GLN:HE21	1.42	0.85
1:C:432:ILE:HD11	1:C:447:VAL:HG22	1.59	0.83
1:C:246:PRO:HB3	1:C:283:GLN:HA	1.61	0.82
1:B:246:PRO:HB3	1:B:283:GLN:HA	1.60	0.81
2:D:2:NAG:N2	2:D:3:FUC:O2	2.12	0.80
1:A:246:PRO:HB3	1:A:283:GLN:HA	1.66	0.76
1:C:398:LEU:HD23	1:C:486:ASP:HA	1.69	0.75
1:C:394:ARG:NH1	1:C:489:ASP:OD2	2.23	0.70
1:A:428:ASN:OD1	1:A:429:ARG:NH2	2.26	0.69
1:B:398:LEU:HD23	1:B:486:ASP:HA	1.75	0.69
1:A:398:LEU:HD23	1:A:486:ASP:HA	1.74	0.68
1:A:69:CYS:O	1:A:80:LYS:NZ	2.25	0.68
1:A:214:ILE:HG12	1:A:216:ASN:H	1.60	0.67
1:A:354:GLN:NE2	3:A:609:SO4:O2	2.31	0.64
1:B:394:ARG:NH2	1:B:489:ASP:OD2	2.31	0.63
1:C:328:GLU:HA	1:C:331:ASN:HD22	1.63	0.62
1:A:194:ASP:N	3:A:606:SO4:O3	2.32	0.61
1:B:328:GLU:HA	1:B:331:ASN:HD22	1.64	0.61
1:A:361:GLN:OE1	1:B:99:SER:HB2	2.01	0.61
1:A:206:ILE:O	1:A:212:CYS:HB2	2.00	0.60
1:C:214:ILE:HG12	1:C:216:ASN:H	1.65	0.60
1:B:49:ARG:NH2	1:B:368:ASP:OD1	2.34	0.59
1:B:62:SER:HB2	1:B:196:LYS:HA	1.86	0.58
1:C:321:LEU:HD11	1:C:473:PRO:HB3	1.86	0.57
1:A:75:LYS:HE2	1:C:218:GLU:OE2	2.05	0.57
1:C:96:LEU:HD22	1:C:289:MET:HG2	1.88	0.56
1:A:79:ILE:HG13	1:A:220:VAL:HG22	1.87	0.56
1:A:321:LEU:HD11	1:A:473:PRO:HB3	1.88	0.55
1:B:427:LYS:HB2	1:B:448:ASP:OD2	2.07	0.55
1:A:426:ASN:OD1	1:A:427:LYS:HG2	2.06	0.55
1:A:352:PHE:CE2	1:A:372:SER:HB3	2.42	0.54
1:A:96:LEU:HD22	1:A:289:MET:HG2	1.90	0.54
1:A:293:LYS:HG2	1:A:294:GLU:HG3	1.89	0.54
1:A:99:SER:OG	1:C:279:GLN:NE2	2.40	0.54
1:B:146:SER:HB3	1:B:149:ALA:HB2	1.89	0.54
1:A:157:VAL:HG12	1:A:163:GLU:HG2	1.89	0.53
1:B:310:ASP:OD1	1:B:364:ARG:NH2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:LEU:HD21	1:C:263:ASP:HB2	1.91	0.53
1:A:427:LYS:HG3	1:A:428:ASN:ND2	2.24	0.53
1:A:171:LEU:O	1:A:191:LYS:NZ	2.28	0.53
1:A:356:GLU:CD	1:A:356:GLU:H	2.13	0.53
1:A:171:LEU:HD13	1:A:191:LYS:HB2	1.91	0.52
1:C:293:LYS:HG2	1:C:294:GLU:HG3	1.90	0.52
1:B:293:LYS:HG2	1:B:294:GLU:HG3	1.90	0.52
1:C:477:PHE:O	2:D:3:FUC:O3	2.17	0.52
1:B:58:THR:HG22	1:B:191:LYS:HA	1.91	0.52
1:B:92:GLU:OE2	1:B:238:SER:OG	2.22	0.51
1:C:167:ILE:HG23	1:C:189:THR:HG21	1.91	0.51
1:C:499:ILE:HG21	2:D:3:FUC:O5	2.10	0.51
1:C:294:GLU:N	3:C:607:SO4:O4	2.41	0.51
1:C:479:ASP:N	2:D:3:FUC:O4	2.43	0.51
1:A:280:ILE:HD11	1:A:361:GLN:NE2	2.21	0.50
1:B:78:LEU:HD23	1:B:81:GLN:OE1	2.12	0.50
1:B:214:ILE:HG13	1:B:216:ASN:H	1.76	0.49
1:C:49:ARG:NH2	1:C:368:ASP:OD1	2.45	0.49
1:B:361:GLN:OE1	1:C:99:SER:HB2	2.11	0.49
1:C:427:LYS:HB2	1:C:448:ASP:OD2	2.12	0.49
1:A:148:ILE:HA	1:A:302:GLN:HE22	1.77	0.49
1:A:432:ILE:HD11	1:A:447:VAL:HG22	1.94	0.49
1:B:356:GLU:O	1:C:104:ASN:HB3	2.11	0.49
1:C:356:GLU:H	1:C:356:GLU:CD	2.17	0.49
1:C:206:ILE:HG21	1:C:214:ILE:HG22	1.95	0.48
1:C:352:PHE:CE2	1:C:372:SER:HB3	2.47	0.48
1:B:352:PHE:CE2	1:B:372:SER:HB3	2.48	0.48
1:C:52:TRP:CE3	1:C:302:GLN:HG2	2.48	0.48
1:A:95:LEU:O	1:A:98:GLN:HB2	2.15	0.47
1:B:62:SER:HB3	1:B:199:ILE:HD12	1.97	0.47
1:A:426:ASN:OD1	1:A:427:LYS:N	2.44	0.47
1:A:76:VAL:HG21	1:A:213:SER:HA	1.96	0.46
1:B:58:THR:HG22	1:B:190:PHE:O	2.16	0.46
1:C:328:GLU:HA	1:C:331:ASN:ND2	2.30	0.46
1:C:322:CYS:HB2	1:C:417:TYR:CE1	2.51	0.46
1:A:95:LEU:HD12	1:A:95:LEU:HA	1.82	0.46
1:C:75:LYS:HD3	1:C:215:SER:HB2	1.98	0.46
1:B:167:ILE:HG23	1:B:189:THR:HG21	1.97	0.45
1:B:338:ASP:HB2	1:B:342:TYR:OH	2.16	0.45
1:C:204:LEU:N	1:C:205:PRO:HD2	2.31	0.45
1:B:321:LEU:HD11	1:B:473:PRO:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ARG:NH2	1:A:368:ASP:OD1	2.50	0.44
1:C:157:VAL:HG12	1:C:163:GLU:HG2	1.97	0.44
1:A:188:LEU:HD21	1:A:263:ASP:HB2	2.00	0.44
1:A:427:LYS:HB3	1:A:448:ASP:OD2	2.17	0.44
1:C:206:ILE:HD12	1:C:214:ILE:HB	1.99	0.44
1:C:395:ILE:HD13	1:C:492:ILE:HD13	1.99	0.44
1:C:318:THR:HG23	1:C:339:ARG:HB3	2.00	0.43
1:A:225:GLN:OE1	1:B:85:LYS:NZ	2.49	0.43
1:B:322:CYS:HB2	1:B:417:TYR:CE1	2.53	0.43
1:A:75:LYS:NZ	1:A:215:SER:O	2.47	0.43
1:A:407:ILE:HB	1:B:145:GLY:HA2	1.99	0.43
1:A:341:TRP:HB2	1:A:352:PHE:HB2	2.01	0.43
1:B:37:CYS:SG	1:B:319:SER:HB3	2.59	0.43
1:C:415:SER:HB3	1:C:417:TYR:CE2	2.54	0.43
1:A:461:LYS:HD2	1:A:461:LYS:HA	1.85	0.43
1:A:264:MET:HB2	1:A:264:MET:HE3	1.87	0.43
4:A:610:NHE:H2'2	4:A:610:NHE:HC12	1.78	0.43
1:B:487:GLU:OE2	1:B:498:LYS:NZ	2.40	0.43
1:B:77:LYS:O	1:B:81:GLN:HG3	2.19	0.42
1:A:75:LYS:HD2	1:A:215:SER:HA	1.99	0.42
1:C:327:LYS:HA	1:C:327:LYS:HD2	1.79	0.42
1:C:405:SER:HB3	1:C:457:TYR:CE2	2.54	0.42
1:C:199:ILE:HG12	1:C:203:LEU:HD12	2.01	0.42
1:A:338:ASP:HB2	1:A:342:TYR:OH	2.18	0.42
1:C:26:GLN:HB3	1:C:27:ASN:H	1.54	0.42
1:C:48:LEU:HB2	1:C:308:VAL:HB	2.02	0.42
1:A:204:LEU:N	1:A:205:PRO:HD2	2.35	0.42
1:A:322:CYS:HB2	1:A:417:TYR:CE1	2.55	0.41
1:C:240:ASN:HB3	1:C:243:VAL:O	2.20	0.41
1:B:232:GLU:OE2	1:B:235:ARG:NH1	2.53	0.41
1:C:310:ASP:OD1	1:C:364:ARG:NH2	2.45	0.41
1:B:52:TRP:CE3	1:B:302:GLN:HG2	2.56	0.41
1:A:62:SER:N	1:A:86:TYR:OH	2.45	0.41
1:A:167:ILE:HG23	1:A:189:THR:HG21	2.01	0.41
1:B:148:ILE:O	1:B:152:VAL:HG23	2.21	0.41
1:A:171:LEU:HD11	1:A:189:THR:HG22	2.03	0.41
1:A:162:GLY:O	1:A:166:LYS:HG3	2.21	0.40
1:C:30:GLU:HB2	1:C:410:LEU:HD12	2.01	0.40
1:C:163:GLU:OE2	1:C:182:SER:N	2.51	0.40
1:C:280:ILE:HD11	1:C:361:GLN:HE21	1.85	0.40
1:C:426:ASN:OD1	1:C:427:LYS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:LYS:HE3	1:B:448:ASP:OD2	2.21	0.40
1:A:328:GLU:HA	1:A:331:ASN:HD22	1.85	0.40

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)
1:C:215:SER:OG	1:C:215:SER:OG[8_554]	2.08	0.12

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	438/568 (77%)	421 (96%)	17 (4%)	0	100	100
1	B	432/568 (76%)	414 (96%)	18 (4%)	0	100	100
1	C	431/568 (76%)	418 (97%)	13 (3%)	0	100	100
All	All	1301/1704 (76%)	1253 (96%)	48 (4%)	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	405/510 (79%)	399 (98%)	6 (2%)	65	87
1	B	400/510 (78%)	400 (100%)	0	100	100
1	C	399/510 (78%)	398 (100%)	1 (0%)	92	97
All	All	1204/1530 (79%)	1197 (99%)	7 (1%)	86	95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LYS
1	A	104	ASN
1	A	137	PHE
1	A	226	LYS
1	A	290	CYS
1	A	428	ASN
1	C	226	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	81	GLN
1	C	354	GLN

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 ⓘ

3 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	D	1	1,2	14,14,15	0.43	0	17,19,21	0.64	0
2	NAG	D	2	2	14,14,15	0.26	0	17,19,21	0.43	0
2	FUC	D	3	2	10,10,11	0.29	0	14,14,16	0.62	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	NAG	D	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	FUC	D	3	2	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

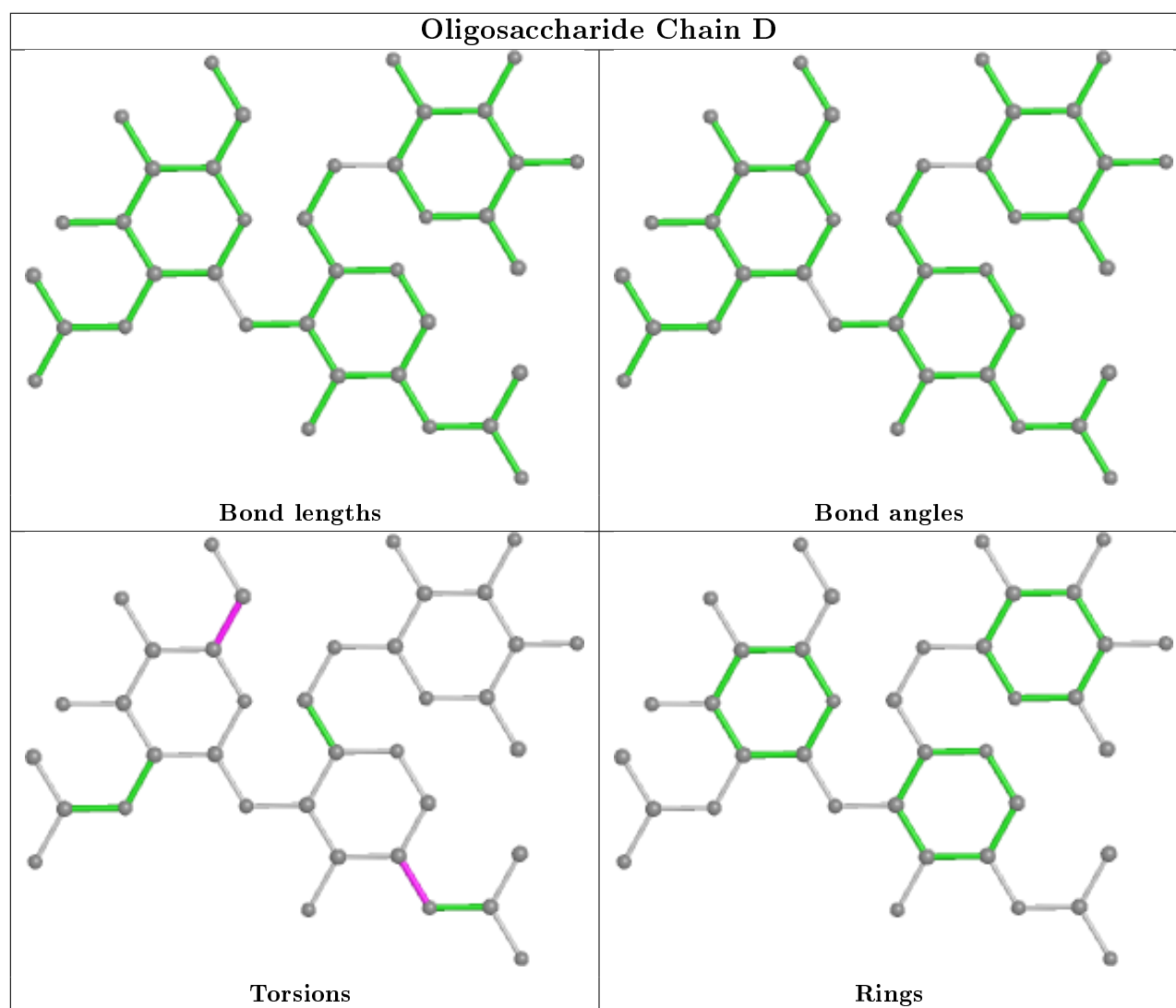
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	FUC	4	0
2	D	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](#)

21 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	$\# Z > 2$
3	SO4	B	601	-	4,4,4	0.18	0	6,6,6	0.21	0
3	SO4	A	601	-	4,4,4	0.18	0	6,6,6	0.14	0
3	SO4	B	605	-	4,4,4	0.13	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	605	-	4,4,4	0.13	0	6,6,6	0.18	0
3	SO4	B	604	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	A	602	-	4,4,4	0.14	0	6,6,6	0.14	0
3	SO4	C	606	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	B	603	-	4,4,4	0.14	0	6,6,6	0.14	0
3	SO4	A	606	-	4,4,4	0.17	0	6,6,6	0.11	0
3	SO4	A	608	-	4,4,4	0.16	0	6,6,6	0.08	0
3	SO4	A	607	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	C	608	-	4,4,4	0.17	0	6,6,6	0.11	0
4	NHE	A	610	-	13,13,13	1.46	2 (15%)	16,17,17	1.77	4 (25%)
3	SO4	C	607	-	4,4,4	0.15	0	6,6,6	0.11	0
3	SO4	B	602	-	4,4,4	0.14	0	6,6,6	0.16	0
3	SO4	A	609	-	4,4,4	0.12	0	6,6,6	0.13	0
3	SO4	A	604	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	A	603	-	4,4,4	0.15	0	6,6,6	0.16	0
3	SO4	C	604	-	4,4,4	0.15	0	6,6,6	0.20	0
3	SO4	B	606	-	4,4,4	0.17	0	6,6,6	0.15	0
3	SO4	C	605	-	4,4,4	0.15	0	6,6,6	0.23	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
4	NHE	A	610	-	-	5/7/15/15	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	610	NHE	C2-S	3.14	1.82	1.77
4	A	610	NHE	O2-S	2.69	1.53	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	610	NHE	O3-S-O1	-4.02	101.44	111.27
4	A	610	NHE	O2-S-C2	3.47	111.10	106.92
4	A	610	NHE	O3-S-C2	3.13	110.83	105.77
4	A	610	NHE	O1-S-C2	2.65	110.11	106.92

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	610	NHE	C2'-C1'-N-C1
4	A	610	NHE	C1-C2-S-O2
4	A	610	NHE	C1-C2-S-O3
4	A	610	NHE	C2-C1-N-C1'
4	A	610	NHE	C1-C2-S-O1

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	606	SO4	1	0
4	A	610	NHE	1	0
3	C	607	SO4	1	0
3	A	609	SO4	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

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	446/568 (78%)	-0.08	7 (1%)	72 44	36, 78, 158, 194	0
1	B	440/568 (77%)	-0.10	8 (1%)	68 40	35, 77, 153, 184	0
1	C	439/568 (77%)	-0.16	4 (0%)	84 63	36, 74, 142, 183	0
All	All	1325/1704 (77%)	-0.11	19 (1%)	75 49	35, 76, 149, 194	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	ASN	4.7
1	B	103	THR	4.1
1	C	505	PHE	3.9
1	B	505	PHE	3.8
1	A	505	PHE	3.8
1	C	504	ALA	3.4
1	A	103	THR	3.4
1	B	173	SER	2.8
1	B	98	GLN	2.8
1	B	205	PRO	2.8
1	A	327	LYS	2.5
1	C	174	THR	2.4
1	B	71	GLY	2.4
1	A	63	ASN	2.3
1	A	72	THR	2.3
1	B	73	ASP	2.3
1	A	104	ASN	2.2
1	B	171	LEU	2.0
1	C	162	GLY	2.0

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

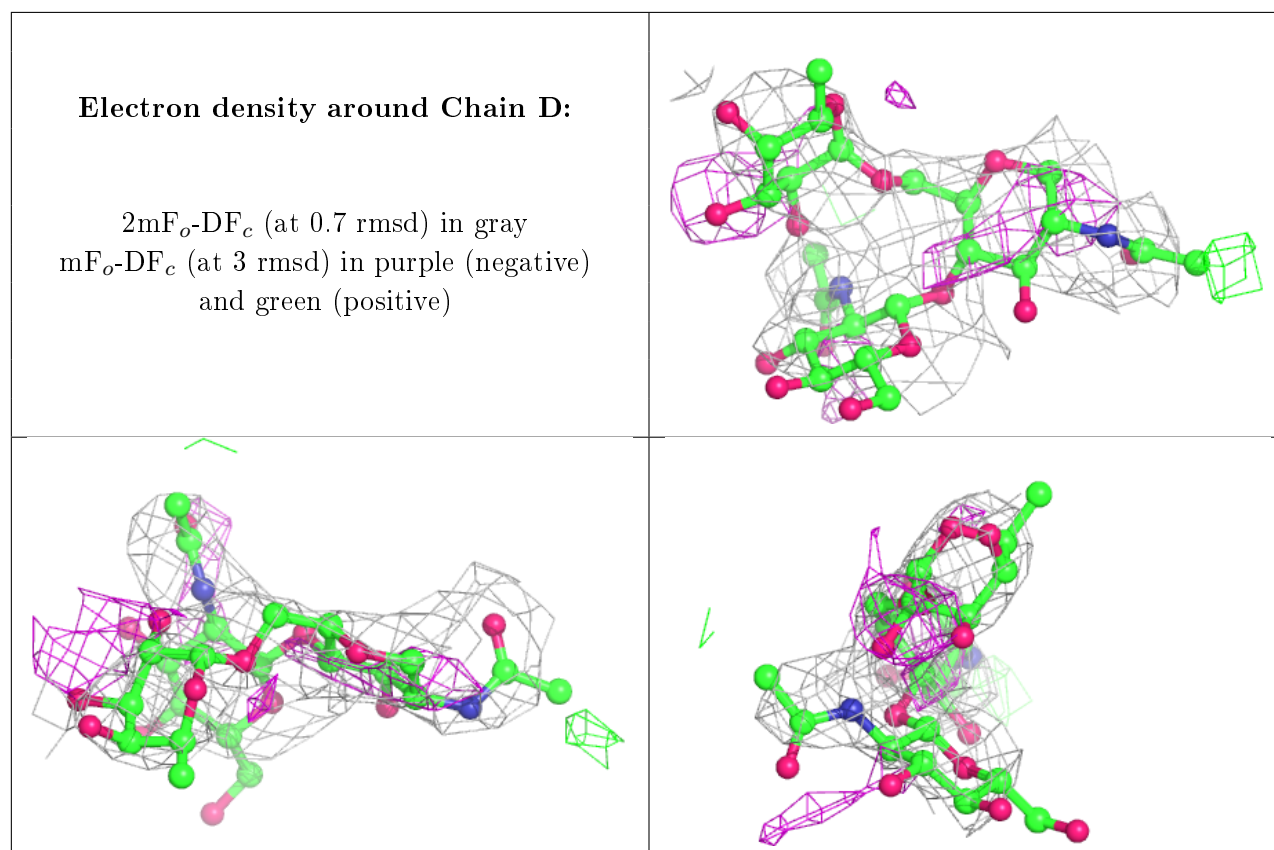
There are no non-standard protein/DNA/RNA residues in this entry.

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
2	NAG	D	1	14/15	0.68	0.48	119,128,132,138	0
2	NAG	D	2	14/15	0.79	0.53	142,145,148,148	0
2	FUC	D	3	10/11	0.87	0.58	127,128,132,132	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 ⓘ

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	SO4	A	609	5/5	0.77	0.50	158,158,160,160	0
3	SO4	C	605	5/5	0.77	0.22	134,136,136,137	0
3	SO4	C	608	5/5	0.80	0.41	141,141,142,142	0
3	SO4	A	607	5/5	0.82	0.30	153,153,154,154	0
3	SO4	B	604	5/5	0.82	0.55	150,150,150,151	0
3	SO4	C	606	5/5	0.83	0.40	157,158,158,159	0
3	SO4	B	605	5/5	0.85	0.41	151,151,152,153	0
3	SO4	B	603	5/5	0.85	0.24	143,143,144,144	0
3	SO4	B	606	5/5	0.86	0.51	135,136,137,137	0
3	SO4	A	606	5/5	0.87	0.20	151,152,152,153	0
3	SO4	A	603	5/5	0.88	0.22	118,121,121,122	0
3	SO4	C	607	5/5	0.88	0.35	152,152,152,152	0
3	SO4	A	608	5/5	0.88	0.28	147,147,148,149	0
3	SO4	A	604	5/5	0.91	0.19	145,145,146,146	0
4	NHE	A	610	13/13	0.91	0.42	102,107,110,111	0
3	SO4	A	605	5/5	0.92	0.18	122,124,125,125	0
3	SO4	A	602	5/5	0.93	0.28	105,105,106,108	0
3	SO4	C	604	5/5	0.94	0.22	97,99,100,100	0
3	SO4	B	602	5/5	0.95	0.14	100,100,100,101	0
3	SO4	A	601	5/5	0.96	0.25	103,103,104,105	0
3	SO4	B	601	5/5	0.97	0.20	91,92,92,93	0

6.5 Other polymers ⓘ

There are no such residues in this entry.