



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 09:49 AM EDT

PDB ID : 6EAI  
Title : CRYSTAL STRUCTURE OF HUMAN RESPIRATORY SYNCYTIAL VIRUS FUSION GLYCOPROTEIN INHIBITOR ESCAPE VARIANT S398L STABILIZED IN THE PREFUSION STATE  
Authors : Battles, M.B.; McLellan, J.S.  
Deposited on : 2018-08-03  
Resolution : 2.80 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](mailto: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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

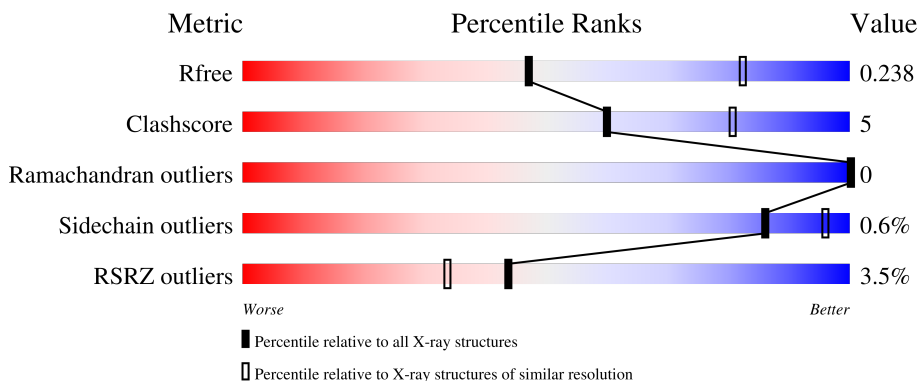
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	 3% 65% 10% 24%
1	B	568	 2% 67% 9% 24%
1	C	568	 4% 66% 11% 23%

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
2	NAG	A	601	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10249 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
			Total	C	N	O	S			
1	A	429	3331	2115	545	650	21	0	0	0
1	B	429	3331	2115	545	650	21	0	0	0
1	C	435	3374	2140	553	660	21	0	0	0

There are 183 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	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
A	530	TYR	-	expression tag	UNP W8RJF9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
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
B	207	LEU	VAL	engineered mutation	UNP W8RJF9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	290	CYS	SER	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
B	552	SER	-	expression tag	UNP W8RJF9
B	553	HIS	-	expression tag	UNP W8RJF9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
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	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
C	532	ARG	-	expression tag	UNP W8RJF9
C	533	LYS	-	expression tag	UNP W8RJF9
C	534	ASP	-	expression tag	UNP W8RJF9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
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

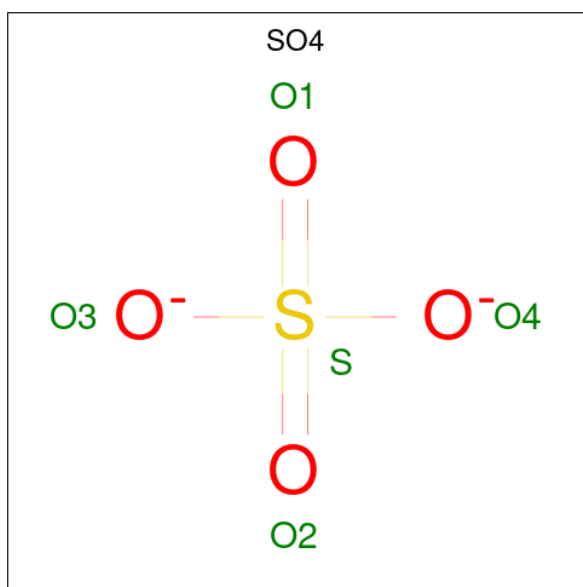
- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).





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

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



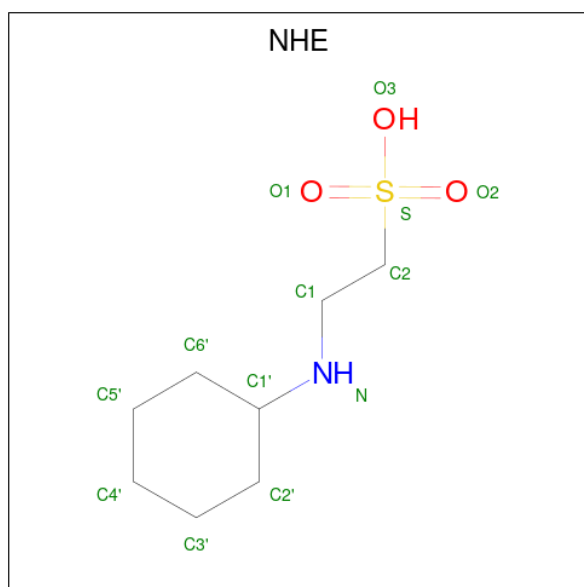
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0

*Continued on next page...*

Continued from previous page...

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	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			

- Molecule 4 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: C<sub>8</sub>H<sub>17</sub>NO<sub>3</sub>S).



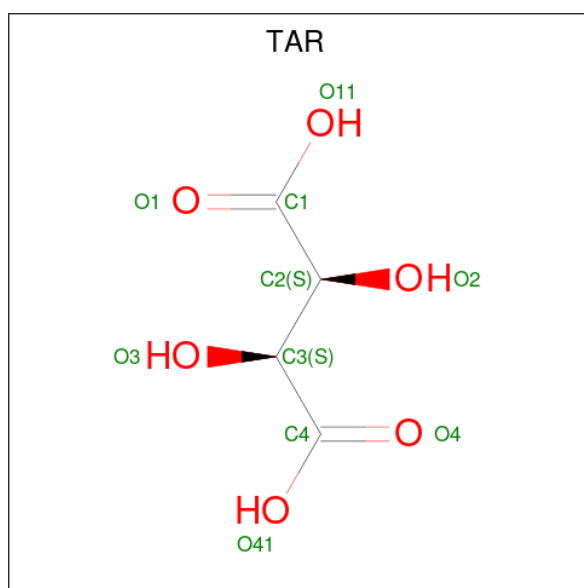
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

Continued on next page...

Continued from previous page...

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

- Molecule 5 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	C O	0	0
			10	4 6		
5	C	1	Total	C O	0	0
			10	4 6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	O	0	0
			5	5		
6	B	9	Total	O	0	0
			9	9		

Continued on next page...

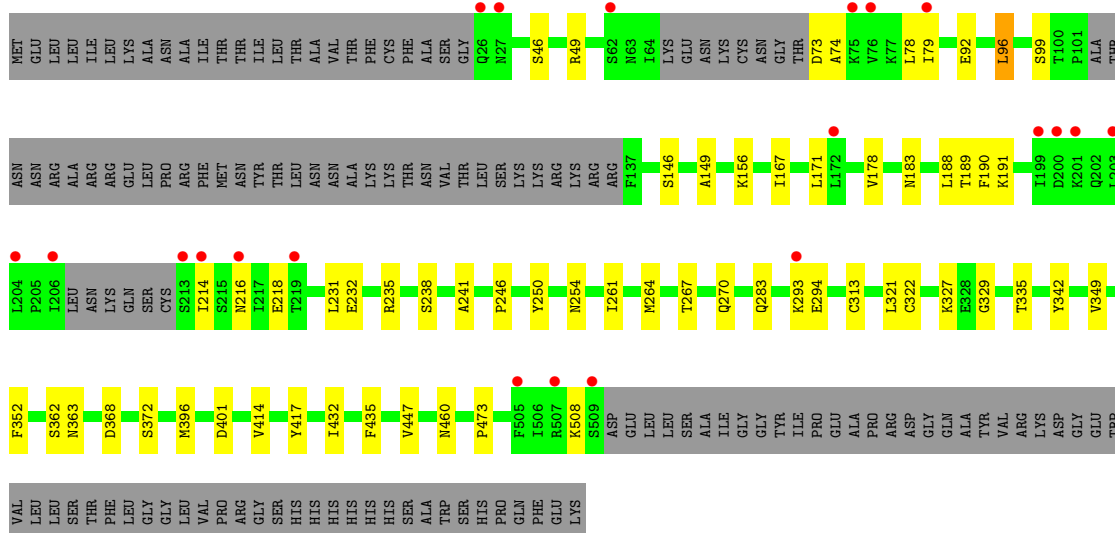
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	4	Total	O	0	0
			4	4		



GLN  
PHE  
GLU  
LYS

● Molecule 1: Fusion glycoprotein F0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.32Å 167.32Å 174.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.61 – 2.80 43.61 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (43.61-2.80) 99.1 (43.61-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.210 , 0.239 0.210 , 0.238	Depositor DCC
$R_{free}$ test set	3080 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.6	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k 0.011 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10249	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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, NHE, SO4, TAR

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	0.27	0/3380	0.46	0/4581
1	B	0.26	0/3380	0.46	0/4581
1	C	0.26	0/3423	0.46	0/4638
All	All	0.26	0/10183	0.46	0/13800

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	3331	0	3374	40	0
1	B	3331	0	3374	28	0
1	C	3374	0	3419	35	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
3	A	15	0	0	1	0
3	B	20	0	0	0	0
3	C	20	0	0	0	0
4	A	26	0	34	1	0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	26	0	34	0	0
4	C	26	0	34	1	0
5	B	10	0	4	0	0
5	C	10	0	4	1	0
6	A	5	0	0	0	0
6	B	9	0	0	1	0
6	C	4	0	0	0	0
All	All	10249	0	10316	94	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.

All (94) 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:246:PRO:HB3	1:B:283:GLN:HA	1.64	0.79
1:C:246:PRO:HB3	1:C:283:GLN:HA	1.66	0.76
1:A:246:PRO:HB3	1:A:283:GLN:HA	1.69	0.73
1:A:92:GLU:OE1	1:B:254:ASN:ND2	2.24	0.67
1:B:432:ILE:HD11	1:B:447:VAL:HG22	1.80	0.64
1:C:146:SER:HB2	1:C:149:ALA:HB2	1.80	0.63
1:C:432:ILE:HD11	1:C:447:VAL:HG22	1.79	0.63
1:A:361:GLN:HE22	1:C:99:SER:HA	1.64	0.62
1:B:261:ILE:HA	1:B:264:MET:HE3	1.82	0.62
1:B:321:LEU:HD11	1:B:473:PRO:HB3	1.82	0.62
1:A:283:GLN:OE1	1:C:241:ALA:HB2	2.01	0.60
1:A:327:LYS:HE3	1:A:329:GLY:H	1.67	0.60
1:A:427:LYS:HB3	1:A:448:ASP:OD2	2.02	0.60
1:A:426:ASN:OD1	1:A:427:LYS:HG2	2.04	0.58
1:A:250:TYR:OH	1:C:235:ARG:NE	2.38	0.57
1:A:426:ASN:ND2	1:A:446:GLY:O	2.37	0.57
1:A:62:SER:HB2	1:A:196:LYS:HA	1.87	0.56
1:B:350:SER:OG	6:B:703:HOH:O	2.18	0.56
1:B:267:THR:HG23	1:B:270:GLN:H	1.70	0.56
1:C:321:LEU:HD11	1:C:473:PRO:HB3	1.88	0.56
1:A:167:ILE:HG23	1:A:189:THR:HG21	1.89	0.55
1:C:327:LYS:HE3	1:C:329:GLY:H	1.72	0.55
5:C:608:TAR:O1	5:C:608:TAR:O3	2.24	0.54
1:A:178:VAL:HG22	1:A:188:LEU:HD13	1.89	0.54
1:A:267:THR:HG23	1:A:270:GLN:H	1.73	0.54
1:A:291:ILE:HD11	1:A:293:LYS:HD2	1.90	0.54

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ILE:HG23	1:B:189:THR:HG21	1.90	0.54
1:B:291:ILE:HD11	1:B:293:LYS:HD2	1.90	0.53
1:A:198:TYR:OH	1:A:222:GLU:HG3	2.10	0.52
1:A:277:ASN:ND2	3:A:604:SO4:O2	2.41	0.51
1:C:401:ASP:OD1	1:C:401:ASP:N	2.40	0.51
1:A:279:GLN:NE2	1:C:238:SER:O	2.38	0.50
1:A:361:GLN:NE2	1:C:99:SER:HA	2.25	0.50
1:C:167:ILE:HG23	1:C:189:THR:HG21	1.93	0.50
1:C:293:LYS:HG2	1:C:294:GLU:HG3	1.92	0.50
1:C:216:ASN:HB3	1:C:218:GLU:OE2	2.12	0.50
1:A:321:LEU:HD11	1:A:473:PRO:HB3	1.92	0.50
1:A:279:GLN:HG2	1:C:96:LEU:HD13	1.93	0.50
1:C:261:ILE:HA	1:C:264:MET:HE3	1.94	0.50
1:B:335:THR:HB	1:B:396:MET:HG2	1.93	0.50
1:B:178:VAL:HG22	1:B:188:LEU:HD13	1.94	0.49
1:B:427:LYS:HB2	1:B:448:ASP:OD2	2.11	0.49
1:B:92:GLU:OE1	1:C:254:ASN:ND2	2.30	0.49
1:C:335:THR:HB	1:C:396:MET:HG2	1.94	0.49
1:A:284:GLN:HE22	1:A:366:PHE:HB3	1.77	0.49
1:C:73:ASP:OD1	1:C:74:ALA:N	2.44	0.49
1:B:62:SER:HB2	1:B:196:LYS:HA	1.94	0.49
1:C:171:LEU:HD13	1:C:191:LYS:HB2	1.95	0.48
1:C:362:SER:OG	1:C:363:ASN:N	2.46	0.48
1:A:338:ASP:HB2	1:A:342:TYR:OH	2.14	0.48
1:B:61:LEU:O	1:B:295:GLU:HB3	2.14	0.47
1:B:96:LEU:HD22	1:B:289:MET:HG2	1.96	0.47
1:A:254:ASN:OD1	1:C:92:GLU:HG2	2.15	0.47
1:A:231:LEU:HB3	1:A:235:ARG:HH12	1.80	0.47
1:B:90:VAL:HG13	1:B:292:ILE:HD11	1.96	0.47
1:A:90:VAL:HG13	1:A:292:ILE:HD11	1.97	0.46
1:C:352:PHE:CE1	1:C:372:SER:HB3	2.50	0.45
1:C:267:THR:HG23	1:C:270:GLN:H	1.81	0.45
1:A:310:ASP:OD1	1:A:364:ARG:NH1	2.40	0.45
1:A:352:PHE:CE1	1:A:372:SER:HB3	2.52	0.45
1:A:461:LYS:HA	1:A:461:LYS:HD2	1.74	0.45
1:C:46:SER:HB3	1:C:313:CYS:SG	2.56	0.45
1:B:461:LYS:HA	1:B:461:LYS:HD2	1.81	0.45
1:B:352:PHE:CE1	1:B:372:SER:HB3	2.51	0.45
1:C:178:VAL:HG22	1:C:188:LEU:HD13	1.99	0.44
1:B:198:TYR:HE2	1:B:223:PHE:HD1	1.63	0.44
1:C:322:CYS:HB2	1:C:417:TYR:CE1	2.52	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HD13	1:A:191:LYS:HB2	1.99	0.44
1:C:232:GLU:HG3	1:C:250:TYR:CZ	2.53	0.44
1:B:101:PRO:HB2	1:B:152:VAL:HG22	1.99	0.44
1:C:49:ARG:NH2	1:C:368:ASP:OD1	2.51	0.44
4:A:605:NHE:HC12	4:A:605:NHE:H2'1	1.81	0.43
1:B:264:MET:HE3	1:B:264:MET:HB2	1.92	0.43
1:A:461:LYS:O	1:C:156:LYS:NZ	2.48	0.43
1:B:362:SER:OG	1:B:363:ASN:N	2.52	0.42
1:A:335:THR:HB	1:A:396:MET:HG2	2.00	0.42
1:A:505:PHE:HE1	1:B:505:PHE:HB3	1.84	0.42
1:C:231:LEU:O	1:C:235:ARG:HG3	2.18	0.42
1:B:197:ASN:OD1	1:B:201:LYS:HE2	2.20	0.42
1:A:222:GLU:HB3	1:C:78:LEU:HD21	2.01	0.42
1:C:79:ILE:HG13	1:C:214:ILE:HD13	2.01	0.42
1:A:96:LEU:HD22	1:A:289:MET:HG2	2.01	0.41
1:A:231:LEU:HB3	1:A:235:ARG:NH1	2.34	0.41
1:B:199:ILE:O	1:B:203:LEU:HB2	2.20	0.41
1:A:362:SER:OG	1:A:363:ASN:N	2.48	0.41
1:C:414:VAL:HG21	1:C:435:PHE:CE2	2.56	0.41
1:B:79:ILE:O	1:B:83:LEU:N	2.51	0.41
1:A:188:LEU:HD21	1:A:263:ASP:HB2	2.02	0.41
1:A:199:ILE:O	1:A:203:LEU:HB2	2.21	0.41
1:A:28:ILE:HG22	1:A:410:LEU:HD11	2.03	0.40
1:B:423:THR:HG21	1:B:431:ILE:HD13	2.03	0.40
4:C:607:NHE:H2'2	4:C:607:NHE:HC11	1.82	0.40
1:C:342:TYR:HD2	1:C:349:VAL:HG11	1.86	0.40
1:A:46:SER:HB3	1:A:313:CYS:SG	2.62	0.40

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	421/568 (74%)	406 (96%)	15 (4%)	0	100	100
1	B	421/568 (74%)	408 (97%)	13 (3%)	0	100	100
1	C	427/568 (75%)	413 (97%)	14 (3%)	0	100	100
All	All	1269/1704 (74%)	1227 (97%)	42 (3%)	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	391/510 (77%)	391 (100%)	0	100	100
1	B	391/510 (77%)	389 (100%)	2 (0%)	88	96
1	C	397/510 (78%)	392 (99%)	5 (1%)	69	91
All	All	1179/1530 (77%)	1172 (99%)	7 (1%)	86	96

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

Mol	Chain	Res	Type
1	B	76	VAL
1	B	195	LEU
1	C	96	LEU
1	C	183	ASN
1	C	190	PHE
1	C	460	ASN
1	C	508	LYS

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

22 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	NHE	C	606	-	13,13,13	1.42	3 (23%)	16,17,17	1.86	5 (31%)
3	SO4	B	603	-	4,4,4	0.13	0	6,6,6	0.05	0
5	TAR	B	608	1	9,9,9	1.00	0	12,12,12	1.32	2 (16%)
3	SO4	A	602	-	4,4,4	0.15	0	6,6,6	0.06	0
5	TAR	C	608	-	9,9,9	0.99	0	12,12,12	1.33	2 (16%)
4	NHE	A	605	-	13,13,13	1.45	3 (23%)	16,17,17	1.89	4 (25%)
4	NHE	B	607	-	13,13,13	1.33	2 (15%)	16,17,17	1.89	4 (25%)
3	SO4	C	604	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	C	603	-	4,4,4	0.14	0	6,6,6	0.07	0
2	NAG	B	601	1	14,14,15	0.18	0	17,19,21	0.41	0
4	NHE	C	607	-	13,13,13	1.43	3 (23%)	16,17,17	1.88	5 (31%)
3	SO4	A	604	-	4,4,4	0.13	0	6,6,6	0.06	0
3	SO4	A	603	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	B	604	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	605	-	4,4,4	0.13	0	6,6,6	0.06	0
2	NAG	C	601	1	14,14,15	0.18	0	17,19,21	0.45	0
3	SO4	C	605	-	4,4,4	0.13	0	6,6,6	0.05	0
4	NHE	A	606	-	13,13,13	1.41	3 (23%)	16,17,17	1.81	4 (25%)
3	SO4	B	602	-	4,4,4	0.15	0	6,6,6	0.07	0
2	NAG	A	601	1	14,14,15	0.18	0	17,19,21	0.44	0
4	NHE	B	606	-	13,13,13	1.35	2 (15%)	16,17,17	1.81	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	C	602	-	4,4,4	0.15	0	6,6,6	0.08	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	B	607	-	-	0/7/15/15	0/1/1/1
2	NAG	C	601	1	-	2/6/23/26	0/1/1/1
4	NHE	C	606	-	-	5/7/15/15	0/1/1/1
2	NAG	B	601	1	-	2/6/23/26	0/1/1/1
4	NHE	C	607	-	-	0/7/15/15	0/1/1/1
4	NHE	A	606	-	-	0/7/15/15	0/1/1/1
5	TAR	B	608	1	-	8/12/12/12	-
4	NHE	B	606	-	-	1/7/15/15	0/1/1/1
2	NAG	A	601	1	-	1/6/23/26	0/1/1/1
5	TAR	C	608	-	-	10/12/12/12	-
4	NHE	A	605	-	-	1/7/15/15	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	NHE	C2-S	2.96	1.81	1.77
4	B	606	NHE	C2-S	2.84	1.81	1.77
4	C	607	NHE	C2-S	2.83	1.81	1.77
4	B	607	NHE	C2-S	2.72	1.81	1.77
4	C	606	NHE	C2-S	2.69	1.81	1.77
4	A	606	NHE	C2-S	2.65	1.81	1.77
4	C	607	NHE	O1-S	2.48	1.52	1.45
4	A	605	NHE	O1-S	2.46	1.52	1.45
4	A	606	NHE	O1-S	2.45	1.52	1.45
4	C	606	NHE	O1-S	2.43	1.52	1.45
4	B	606	NHE	O2-S	2.14	1.51	1.45
4	A	605	NHE	O2-S	2.13	1.51	1.45
4	A	606	NHE	O2-S	2.12	1.51	1.45
4	C	606	NHE	O2-S	2.10	1.51	1.45
4	B	607	NHE	O2-S	2.09	1.51	1.45
4	C	607	NHE	O2-S	2.09	1.51	1.45

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	607	NHE	O2-S-C2	4.13	111.89	106.92
4	A	605	NHE	O3-S-O2	-4.09	101.28	111.27
4	C	606	NHE	O3-S-O2	-4.04	101.41	111.27
4	C	607	NHE	O3-S-O2	-4.02	101.46	111.27
4	A	605	NHE	O2-S-C2	3.94	111.67	106.92
4	B	607	NHE	O1-S-C2	3.83	111.53	106.92
4	A	606	NHE	O3-S-O2	-3.82	101.93	111.27
4	B	606	NHE	O2-S-C2	3.75	111.43	106.92
4	B	607	NHE	O2-S-O1	-3.75	100.99	113.95
4	B	606	NHE	O2-S-O1	-3.64	101.36	113.95
4	B	606	NHE	O1-S-C2	3.62	111.27	106.92
4	C	607	NHE	O2-S-C2	3.52	111.15	106.92
4	C	607	NHE	O3-S-C2	3.43	111.32	105.77
4	C	606	NHE	O2-S-C2	3.29	110.88	106.92
4	A	606	NHE	O1-S-C2	3.28	110.87	106.92
4	A	606	NHE	O2-S-C2	3.23	110.81	106.92
4	A	605	NHE	O3-S-C2	3.23	110.99	105.77
4	C	606	NHE	O3-S-C2	3.21	110.96	105.77
4	A	606	NHE	O3-S-C2	3.18	110.91	105.77
4	C	607	NHE	O1-S-C2	2.99	110.52	106.92
4	C	606	NHE	O1-S-C2	2.97	110.49	106.92
4	B	606	NHE	O3-S-C2	2.74	110.20	105.77
4	A	605	NHE	O1-S-C2	2.74	110.21	106.92
5	C	608	TAR	O41-C4-C3	2.59	120.27	113.27
4	B	607	NHE	O3-S-C2	2.59	109.95	105.77
5	B	608	TAR	O11-C1-C2	2.56	120.19	113.27
5	C	608	TAR	O11-C1-C2	2.46	119.93	113.27
5	B	608	TAR	O41-C4-C3	2.40	119.75	113.27
4	C	607	NHE	C1-N-C1'	-2.37	109.49	114.14
4	C	606	NHE	C1-N-C1'	-2.27	109.68	114.14

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	606	NHE	N-C1-C2-S
4	C	606	NHE	N-C1-C2-S
4	C	606	NHE	C1-C2-S-O3
5	C	608	TAR	C1-C2-C3-C4
5	C	608	TAR	O2-C2-C3-O3
5	C	608	TAR	O3-C3-C4-O4
5	C	608	TAR	O3-C3-C4-O41
5	B	608	TAR	O3-C3-C4-O4

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	608	TAR	O3-C3-C4-O41
5	B	608	TAR	C2-C3-C4-O4
5	B	608	TAR	C2-C3-C4-O41
5	C	608	TAR	C1-C2-C3-O3
5	C	608	TAR	O2-C2-C3-C4
2	C	601	NAG	C8-C7-N2-C2
2	C	601	NAG	O7-C7-N2-C2
2	B	601	NAG	C4-C5-C6-O6
5	B	608	TAR	O1-C1-C2-C3
2	B	601	NAG	O5-C5-C6-O6
5	B	608	TAR	O11-C1-C2-C3
2	A	601	NAG	O5-C5-C6-O6
4	C	606	NHE	C2-C1-N-C1'
5	C	608	TAR	O1-C1-C2-C3
5	C	608	TAR	O11-C1-C2-C3
5	B	608	TAR	O1-C1-C2-O2
4	C	606	NHE	C1-C2-S-O1
4	C	606	NHE	C1-C2-S-O2
5	C	608	TAR	C2-C3-C4-O41
5	B	608	TAR	O11-C1-C2-O2
5	C	608	TAR	C2-C3-C4-O4
4	A	605	NHE	N-C1-C2-S

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	608	TAR	1	0
4	A	605	NHE	1	0
4	C	607	NHE	1	0
3	A	604	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	429/568 (75%)	-0.01	15 (3%) 44 34	44, 72, 132, 166	0
1	B	429/568 (75%)	-0.12	9 (2%) 63 54	38, 69, 128, 172	0
1	C	435/568 (76%)	0.04	21 (4%) 30 21	41, 74, 146, 203	0
All	All	1293/1704 (75%)	-0.03	45 (3%) 44 34	38, 72, 141, 203	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	26	GLN	6.9
1	C	204	LEU	5.5
1	A	26	GLN	5.0
1	C	219	THR	4.6
1	A	505	PHE	4.4
1	A	506	ILE	4.1
1	C	509	SER	4.0
1	C	76	VAL	4.0
1	A	206	ILE	4.0
1	A	204	LEU	4.0
1	B	204	LEU	3.8
1	B	507	ARG	3.7
1	C	200	ASP	3.5
1	B	62	SER	3.3
1	C	203	LEU	3.2
1	B	26	GLN	3.1
1	A	201	LYS	3.0
1	C	214	ILE	3.0
1	A	62	SER	2.8
1	A	79	ILE	2.8
1	C	199	ILE	2.8
1	C	507	ARG	2.6
1	B	78	LEU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	201	LYS	2.5
1	A	63	ASN	2.5
1	C	62	SER	2.5
1	A	64	ILE	2.4
1	A	203	LEU	2.4
1	A	429	ARG	2.4
1	C	293	LYS	2.4
1	A	296	VAL	2.3
1	B	206	ILE	2.3
1	C	27	ASN	2.2
1	C	79	ILE	2.2
1	A	76	VAL	2.2
1	B	219	THR	2.1
1	B	200	ASP	2.1
1	B	505	PHE	2.1
1	C	206	ILE	2.1
1	C	213	SER	2.1
1	C	75	LYS	2.1
1	A	197	ASN	2.1
1	C	172	LEU	2.1
1	C	216	ASN	2.0
1	C	505	PHE	2.0

## 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 [\(i\)](#)

There are no monosaccharides in this entry.

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	601	14/15	0.70	0.39	91,129,138,140	0

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	601	14/15	0.75	0.41	113,137,154,161	0
2	NAG	B	601	14/15	0.80	0.37	116,129,138,139	0
3	SO4	C	605	5/5	0.84	0.23	142,144,155,155	0
3	SO4	B	605	5/5	0.85	0.38	146,146,154,158	0
3	SO4	B	604	5/5	0.87	0.53	144,146,148,152	0
3	SO4	A	604	5/5	0.88	0.30	122,127,131,147	0
5	TAR	C	608	10/10	0.88	0.25	93,105,113,115	0
5	TAR	B	608	10/10	0.90	0.18	100,106,121,122	0
3	SO4	C	604	5/5	0.91	0.38	140,145,148,148	0
3	SO4	A	603	5/5	0.94	0.30	123,125,129,131	0
3	SO4	B	603	5/5	0.94	0.22	91,92,107,115	0
3	SO4	C	603	5/5	0.95	0.15	90,96,101,107	0
4	NHE	C	606	13/13	0.96	0.17	75,85,96,98	0
4	NHE	A	605	13/13	0.96	0.14	76,86,92,107	0
4	NHE	B	606	13/13	0.96	0.14	78,86,99,103	0
3	SO4	A	602	5/5	0.97	0.12	74,88,92,93	0
4	NHE	B	607	13/13	0.98	0.28	60,65,83,84	0
3	SO4	C	602	5/5	0.98	0.10	58,69,72,77	0
4	NHE	C	607	13/13	0.98	0.24	60,70,76,82	0
4	NHE	A	606	13/13	0.98	0.22	54,65,75,80	0
3	SO4	B	602	5/5	0.98	0.11	64,68,81,88	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.