



# wwPDB X-ray Structure Validation Summary Report i

Mar 27, 2014 – 04:25 PM EDT

PDB ID : 3RRR  
Title : Structure of the RSV F protein in the post-fusion conformation  
Authors : McLellan, J.S.; Yongping, Y.; Graham, B.S.; Kwong, P.D.  
Deposited on : 2011-04-30  
Resolution : 2.82 Å(reported)

This is a wwPDB validation summary 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 <http://wwpdb.org/ValidationPDFNotes.html>

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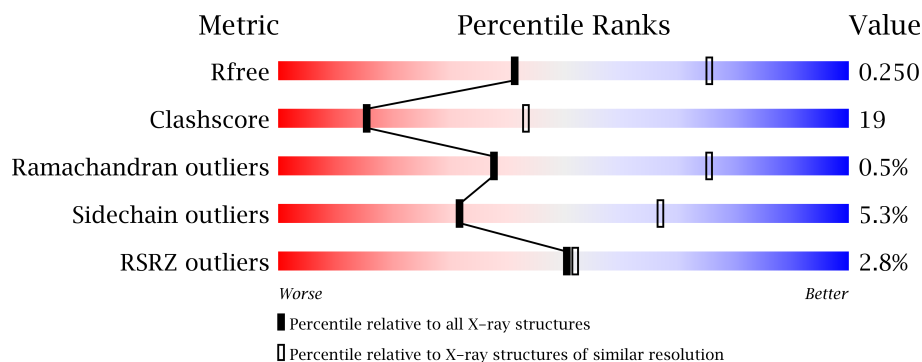
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable22978
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 2.82 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))
$R_{free}$	66092	1963 (2.84-2.80)
Clashscore	79885	2478 (2.84-2.80)
Ramachandran outliers	78287	2429 (2.84-2.80)
Sidechain outliers	78261	2431 (2.84-2.80)
RSRZ outliers	66119	1966 (2.84-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	84	
1	C	84	
1	E	84	
1	G	84	
1	I	84	
1	M	84	
2	B	374	
2	D	374	
2	F	374	
2	H	374	
2	L	374	
2	N	374	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	D	800	-	X
3	NAG	E	770	-	X
3	NAG	H	800	-	X
3	NAG	I	770	-	X
3	NAG	L	800	-	X
3	NAG	N	800	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 40311 atoms, of which 20196 are hydrogens and 0 are deuterium.

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	73	Total	C	H	N	O	S	0	0	0
			1167	366	587	95	116	3			
1	C	72	Total	C	H	N	O	S	0	0	0
			1150	361	579	93	114	3			
1	E	73	Total	C	H	N	O	S	0	0	0
			1167	366	587	95	116	3			
1	G	72	Total	C	H	N	O	S	0	0	0
			1150	361	579	93	114	3			
1	I	71	Total	C	H	N	O	S	0	0	0
			1133	356	571	91	112	3			
1	M	72	Total	C	H	N	O	S	0	0	0
			1150	361	579	93	114	3			

- Molecule 2 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	358	Total	C	H	N	O	S	0	0	0
			5563	1744	2798	458	545	18			
2	D	355	Total	C	H	N	O	S	0	0	0
			5532	1735	2783	455	541	18			
2	F	351	Total	C	H	N	O	S	0	0	0
			5483	1720	2757	451	537	18			
2	H	359	Total	C	H	N	O	S	0	0	0
			5582	1750	2809	459	546	18			
2	L	354	Total	C	H	N	O	S	0	0	0
			5527	1733	2780	454	542	18			
2	N	355	Total	C	H	N	O	S	0	0	0
			5539	1737	2787	455	542	18			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	342	TYR	PHE	SEE REMARK 999	UNP Q84850

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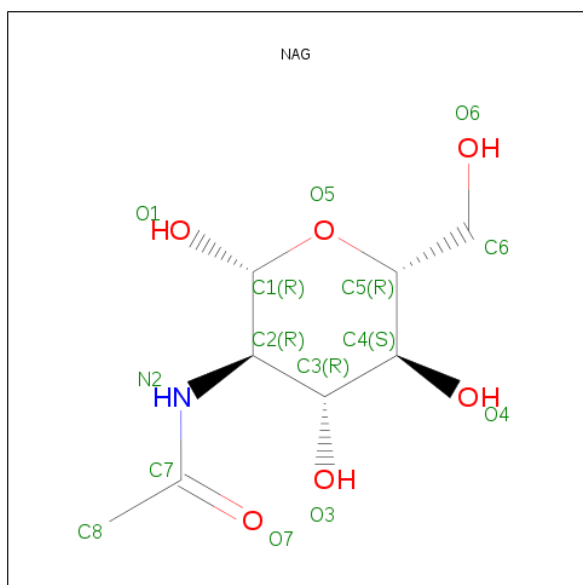
Chain	Residue	Modelled	Actual	Comment	Reference
B	514	GLY	-	EXPRESSION TAG	UNP Q84850
B	515	LEU	-	EXPRESSION TAG	UNP Q84850
B	516	GLU	-	EXPRESSION TAG	UNP Q84850
B	517	VAL	-	EXPRESSION TAG	UNP Q84850
B	518	LEU	-	EXPRESSION TAG	UNP Q84850
B	519	PHE	-	EXPRESSION TAG	UNP Q84850
B	520	GLN	-	EXPRESSION TAG	UNP Q84850
D	342	TYR	PHE	SEE REMARK 999	UNP Q84850
D	514	GLY	-	EXPRESSION TAG	UNP Q84850
D	515	LEU	-	EXPRESSION TAG	UNP Q84850
D	516	GLU	-	EXPRESSION TAG	UNP Q84850
D	517	VAL	-	EXPRESSION TAG	UNP Q84850
D	518	LEU	-	EXPRESSION TAG	UNP Q84850
D	519	PHE	-	EXPRESSION TAG	UNP Q84850
D	520	GLN	-	EXPRESSION TAG	UNP Q84850
F	342	TYR	PHE	SEE REMARK 999	UNP Q84850
F	514	GLY	-	EXPRESSION TAG	UNP Q84850
F	515	LEU	-	EXPRESSION TAG	UNP Q84850
F	516	GLU	-	EXPRESSION TAG	UNP Q84850
F	517	VAL	-	EXPRESSION TAG	UNP Q84850
F	518	LEU	-	EXPRESSION TAG	UNP Q84850
F	519	PHE	-	EXPRESSION TAG	UNP Q84850
F	520	GLN	-	EXPRESSION TAG	UNP Q84850
H	342	TYR	PHE	SEE REMARK 999	UNP Q84850
H	514	GLY	-	EXPRESSION TAG	UNP Q84850
H	515	LEU	-	EXPRESSION TAG	UNP Q84850
H	516	GLU	-	EXPRESSION TAG	UNP Q84850
H	517	VAL	-	EXPRESSION TAG	UNP Q84850
H	518	LEU	-	EXPRESSION TAG	UNP Q84850
H	519	PHE	-	EXPRESSION TAG	UNP Q84850
H	520	GLN	-	EXPRESSION TAG	UNP Q84850
L	342	TYR	PHE	SEE REMARK 999	UNP Q84850
L	514	GLY	-	EXPRESSION TAG	UNP Q84850
L	515	LEU	-	EXPRESSION TAG	UNP Q84850
L	516	GLU	-	EXPRESSION TAG	UNP Q84850
L	517	VAL	-	EXPRESSION TAG	UNP Q84850
L	518	LEU	-	EXPRESSION TAG	UNP Q84850
L	519	PHE	-	EXPRESSION TAG	UNP Q84850
L	520	GLN	-	EXPRESSION TAG	UNP Q84850
N	342	TYR	PHE	SEE REMARK 999	UNP Q84850
N	514	GLY	-	EXPRESSION TAG	UNP Q84850
N	515	LEU	-	EXPRESSION TAG	UNP Q84850

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Chain	Residue	Modelled	Actual	Comment	Reference
N	516	GLU	-	EXPRESSION TAG	UNP Q84850
N	517	VAL	-	EXPRESSION TAG	UNP Q84850
N	518	LEU	-	EXPRESSION TAG	UNP Q84850
N	519	PHE	-	EXPRESSION TAG	UNP Q84850
N	520	GLN	-	EXPRESSION TAG	UNP Q84850

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		

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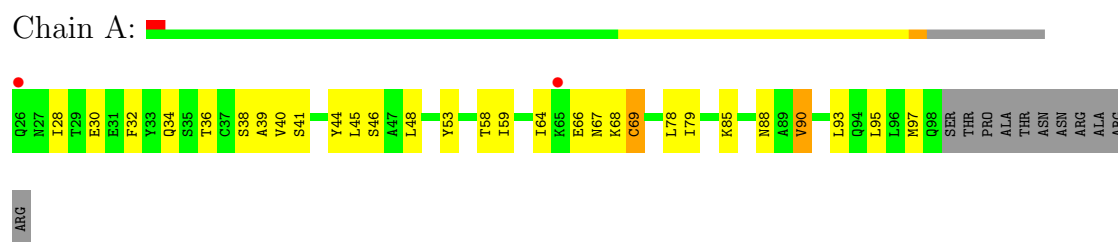
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		
3	M	1	Total	C	N	O	0	0
			14	8	1	5		
3	N	1	Total	C	N	O	0	0
			14	8	1	5		

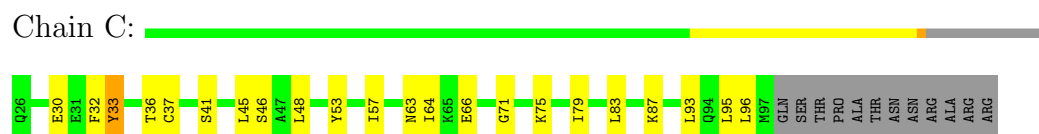
### 3 Residue-property plots i

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

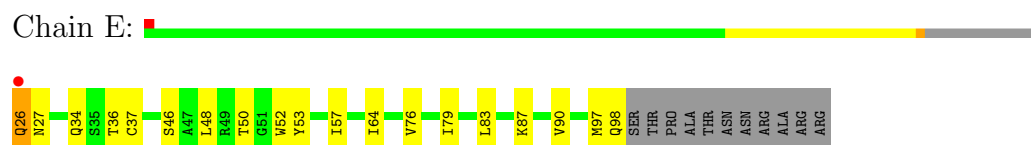
- Molecule 1: Fusion glycoprotein F0



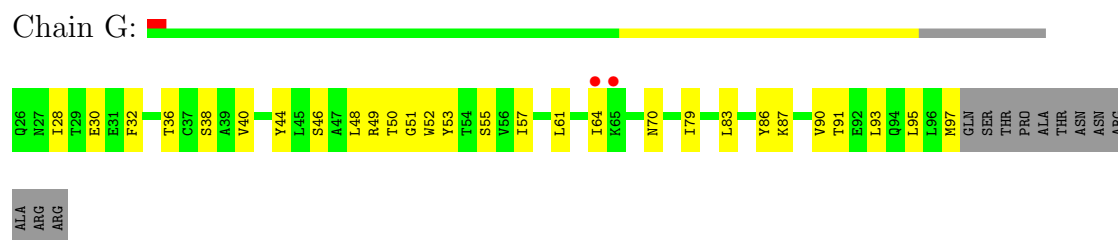
- Molecule 1: Fusion glycoprotein F0



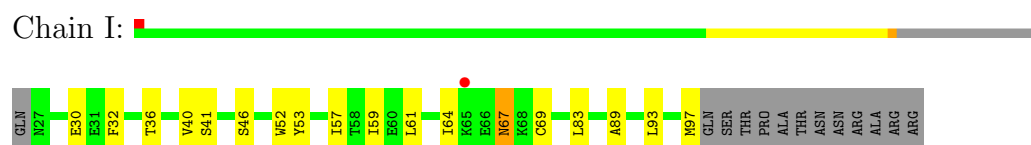
- Molecule 1: Fusion glycoprotein F0



- Molecule 1: Fusion glycoprotein F0



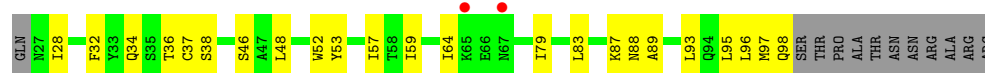
- Molecule 1: Fusion glycoprotein F0



- Molecule 1: Fusion glycoprotein F0

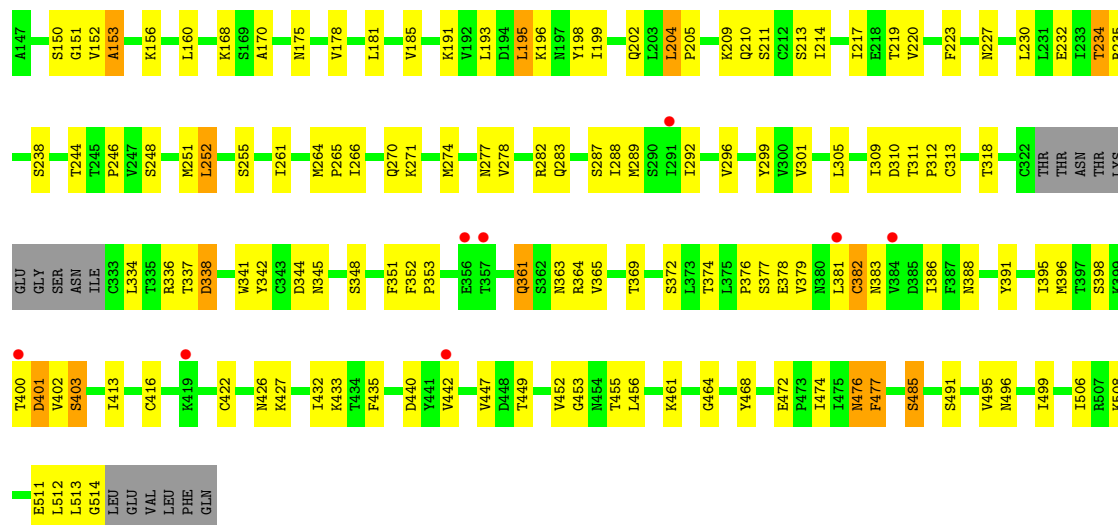


Chain M:



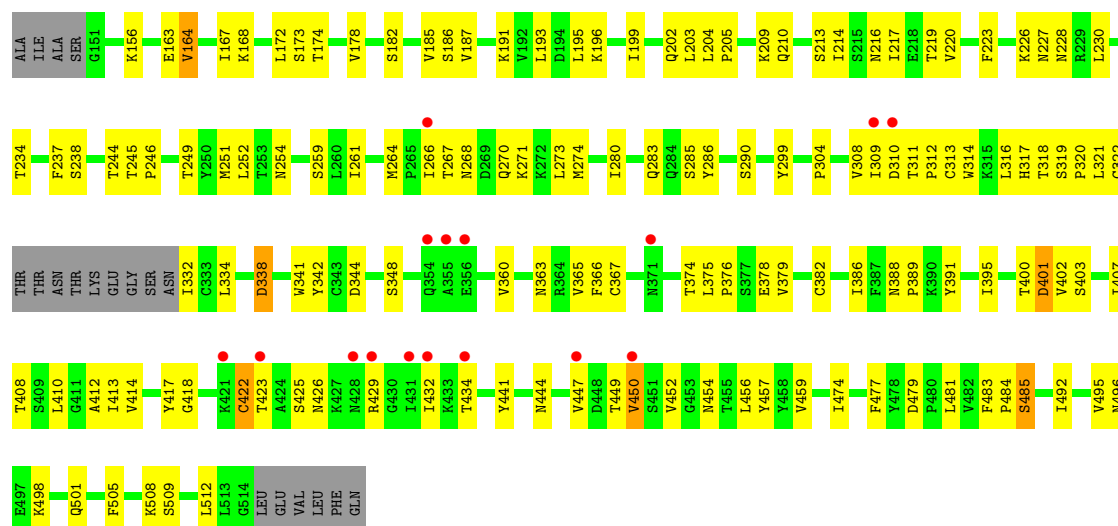
• Molecule 2: Fusion glycoprotein F0

Chain B:



• Molecule 2: Fusion glycoprotein F0

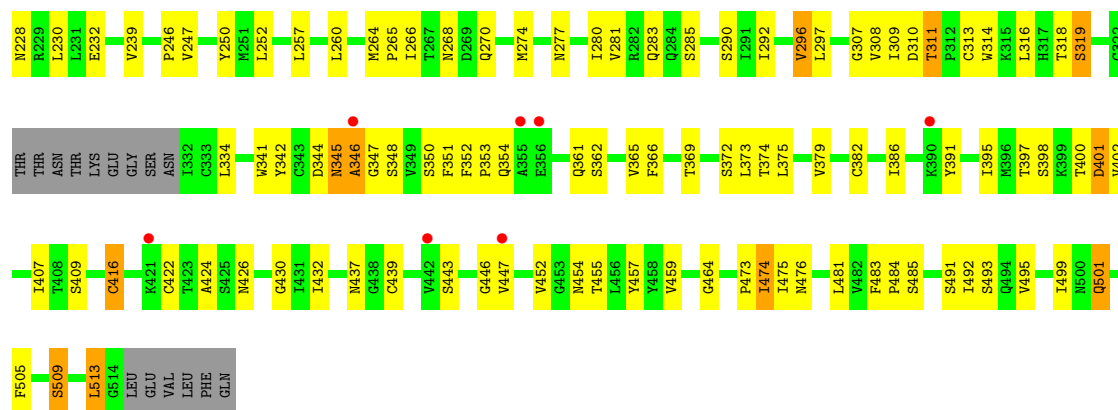
Chain D:



• Molecule 2: Fusion glycoprotein F0

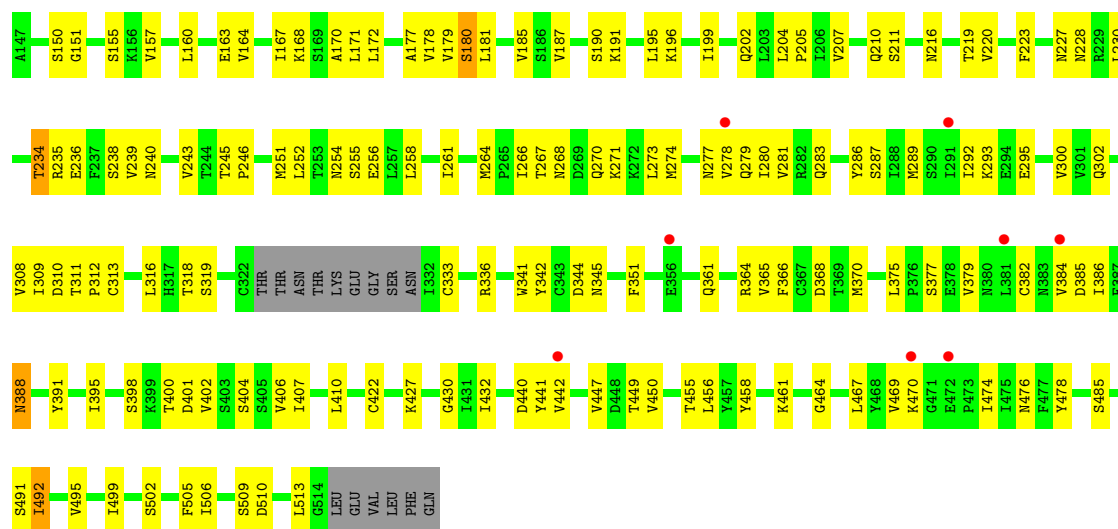
Chain F:





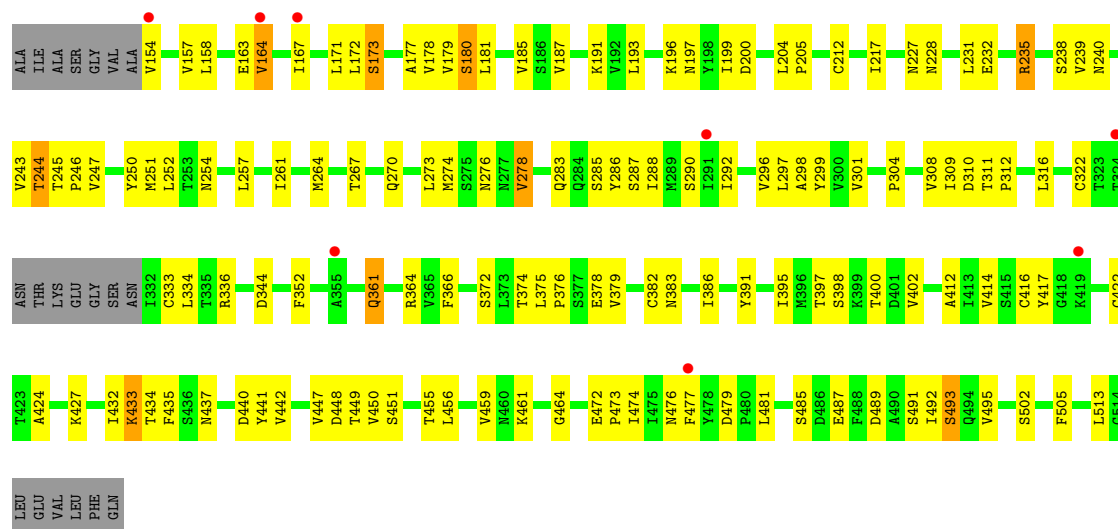
### • Molecule 2: Fusion glycoprotein F0

Chain H:



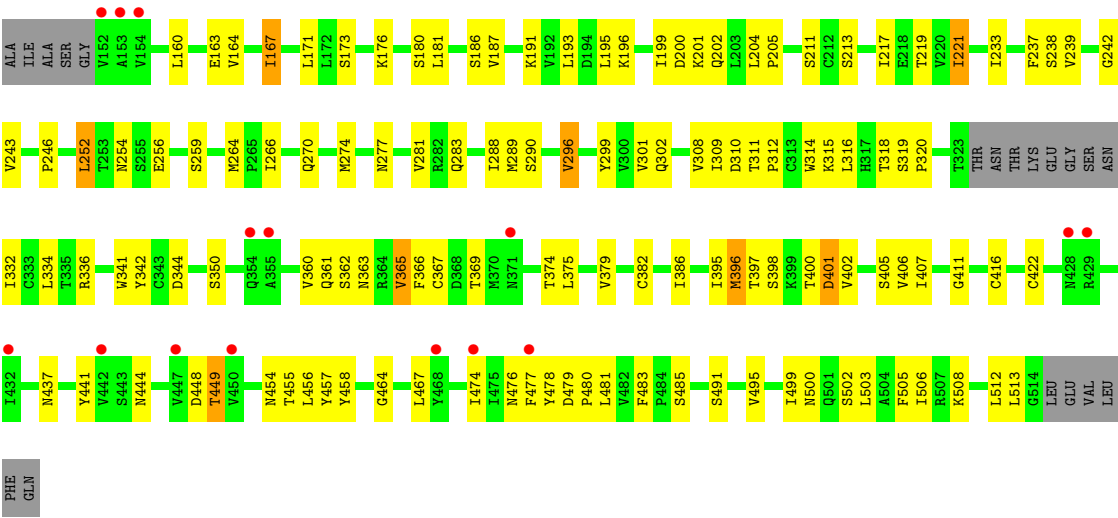
### • Molecule 2: Fusion glycoprotein F0

Chain L:



● Molecule 2: Fusion glycoprotein F0

Chain N: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.17Å 131.50Å 164.28Å 90.00° 103.17° 90.00°	Depositor
Resolution (Å)	44.21 – 2.82 44.21 – 2.82	Depositor EDS
% Data completeness (in resolution range)	63.7 (44.21-2.82) 63.7 (44.21-2.82)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.221 , 0.262 0.207 , 0.250	Depositor DCC
$R_{free}$ test set	3581 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 3.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 71909 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	40311	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.27	0/586	0.50	0/789
1	C	0.28	0/577	0.47	0/777
1	E	0.31	0/586	0.45	0/789
1	G	0.27	0/577	0.45	0/777
1	I	0.29	0/568	0.45	0/765
1	M	0.27	0/577	0.46	0/777
2	B	0.29	0/2805	0.47	0/3803
2	D	0.28	0/2789	0.46	0/3781
2	F	0.28	0/2766	0.47	0/3749
2	H	0.28	0/2813	0.47	0/3814
2	L	0.29	0/2787	0.47	0/3779
2	N	0.27	0/2792	0.46	0/3786
All	All	0.28	0/20223	0.46	0/27386

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	580	587	0	34	0
1	C	571	579	0	36	0
1	E	580	587	0	24	0
1	G	571	579	0	36	0
1	I	562	571	0	27	0
1	M	571	579	0	35	0
2	B	2765	2798	0	129	0
2	D	2749	2783	0	151	0
2	F	2726	2757	0	137	0
2	H	2773	2809	0	150	0
2	L	2747	2780	0	139	0
2	N	2752	2787	0	134	0
3	A	14	0	0	0	0
3	B	14	0	0	1	0
3	C	14	0	0	0	0
3	D	14	0	0	0	0
3	E	14	0	0	0	0
3	F	14	0	0	0	0
3	G	14	0	0	1	0
3	H	14	0	0	0	0
3	I	14	0	0	0	0
3	L	14	0	0	0	0
3	M	14	0	0	1	0
3	N	14	0	0	1	0
All	All	20115	20196	0	754	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

The worst 5 of 754 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:308:VAL:HB	2:N:455:THR:HG22	1.59	0.84
2:L:261:ILE:HA	2:L:264:MET:HE2	1.62	0.81
2:N:449:THR:HB	2:N:456:LEU:HD11	1.62	0.81
2:N:334:LEU:HB3	2:N:395:ILE:HD11	1.63	0.79
2:F:264:MET:HE3	2:F:274:MET:SD	2.24	0.77

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	71/84 (84%)	65 (92%)	5 (7%)	1 (1%)	16	48
1	C	70/84 (83%)	68 (97%)	2 (3%)	0	100	100
1	E	71/84 (84%)	65 (92%)	5 (7%)	1 (1%)	16	48
1	G	70/84 (83%)	65 (93%)	5 (7%)	0	100	100
1	I	69/84 (82%)	65 (94%)	4 (6%)	0	100	100
1	M	70/84 (83%)	64 (91%)	6 (9%)	0	100	100
2	B	354/374 (95%)	336 (95%)	17 (5%)	1 (0%)	50	83
2	D	351/374 (94%)	326 (93%)	23 (7%)	2 (1%)	33	71
2	F	347/374 (93%)	320 (92%)	23 (7%)	4 (1%)	19	53
2	H	355/374 (95%)	327 (92%)	28 (8%)	0	100	100
2	L	350/374 (94%)	331 (95%)	17 (5%)	2 (1%)	33	71
2	N	351/374 (94%)	328 (93%)	22 (6%)	1 (0%)	50	83
All	All	2529/2748 (92%)	2360 (93%)	157 (6%)	12 (0%)	38	75

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	CYS
2	B	153	ALA
2	F	164	VAL
2	F	346	ALA
2	F	353	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	66/75 (88%)	62 (94%)	4 (6%)	26	60
1	C	65/75 (87%)	64 (98%)	1 (2%)	76	96
1	E	66/75 (88%)	64 (97%)	2 (3%)	53	86
1	G	65/75 (87%)	65 (100%)	0	100	100
1	I	64/75 (85%)	63 (98%)	1 (2%)	75	96
1	M	65/75 (87%)	64 (98%)	1 (2%)	76	96
2	B	329/344 (96%)	304 (92%)	25 (8%)	19	46
2	D	328/344 (95%)	315 (96%)	13 (4%)	42	78
2	F	326/344 (95%)	304 (93%)	22 (7%)	23	55
2	H	330/344 (96%)	310 (94%)	20 (6%)	26	60
2	L	329/344 (96%)	310 (94%)	19 (6%)	28	62
2	N	329/344 (96%)	311 (94%)	18 (6%)	30	65
All	All	2362/2514 (94%)	2236 (95%)	126 (5%)	32	67

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	401	ASP
2	H	190	SER
2	N	350	SER
2	F	416	CYS
2	F	493	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	345	ASN
2	H	202	GLN
2	N	345	ASN
2	F	383	ASN
2	F	476	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	770	1	12,14,15	0.62	0	15,19,21	0.72	1 (6%)
3	NAG	B	800	2	12,14,15	0.51	0	15,19,21	1.31	2 (13%)
3	NAG	C	770	1	12,14,15	0.65	0	15,19,21	0.80	0
3	NAG	D	800	2	12,14,15	0.59	0	15,19,21	0.63	0
3	NAG	E	770	1	12,14,15	0.50	0	15,19,21	1.15	1 (6%)
3	NAG	F	800	2	12,14,15	0.58	0	15,19,21	0.79	0
3	NAG	G	770	1	12,14,15	0.68	1 (8%)	15,19,21	0.85	1 (6%)
3	NAG	H	800	2	12,14,15	0.59	0	15,19,21	0.65	0
3	NAG	I	770	1	12,14,15	0.63	0	15,19,21	0.73	0
3	NAG	L	800	2	12,14,15	0.64	0	15,19,21	0.59	0
3	NAG	M	770	1	12,14,15	0.57	0	15,19,21	0.90	1 (6%)
3	NAG	N	800	2	12,14,15	0.61	0	15,19,21	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	770	1	-	0/6/23/26	0/1/1/1
3	NAG	B	800	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	770	1	-	0/6/23/26	0/1/1/1
3	NAG	D	800	2	-	0/6/23/26	0/1/1/1
3	NAG	E	770	1	-	0/6/23/26	0/1/1/1
3	NAG	F	800	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	G	770	1	-	0/6/23/26	0/1/1/1
3	NAG	H	800	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	I	770	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	L	800	2	-	0/6/23/26	0/1/1/1
3	NAG	M	770	1	-	0/6/23/26	0/1/1/1
3	NAG	N	800	2	1/1/5/7	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	770	NAG	O5-C5	-2.14	1.41	1.45

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	800	NAG	O5-C5-C4	3.77	115.43	110.65
3	E	770	NAG	O5-C5-C4	2.74	114.13	110.65
3	M	770	NAG	O5-C5-C6	2.18	109.27	106.98
3	A	770	NAG	O5-C5-C6	2.13	109.21	106.98
3	G	770	NAG	C3-C2-N2	-2.10	108.56	111.76

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	N	800	NAG	C1
3	H	800	NAG	C1
3	I	770	NAG	C1
3	F	800	NAG	C1

There are no torsion outliers.

There are no ring outliers.

## 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, 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	73/84 (86%)	-0.02	2 (2%) 52 53	25, 44, 85, 125	0
1	C	72/84 (85%)	-0.27	0 100 100	17, 37, 83, 157	0
1	E	73/84 (86%)	-0.05	1 (1%) 72 72	16, 40, 87, 121	0
1	G	72/84 (85%)	0.06	2 (2%) 50 52	21, 50, 104, 169	0
1	I	71/84 (84%)	-0.13	1 (1%) 72 72	12, 40, 88, 116	0
1	M	72/84 (85%)	0.03	2 (2%) 50 52	17, 42, 86, 143	0
2	B	358/374 (95%)	-0.03	8 (2%) 59 60	14, 44, 82, 130	0
2	D	355/374 (94%)	0.16	16 (4%) 32 32	15, 48, 95, 178	0
2	F	351/374 (93%)	0.01	9 (2%) 53 54	14, 40, 87, 139	0
2	H	359/374 (95%)	-0.00	8 (2%) 59 60	15, 45, 85, 127	0
2	L	354/374 (94%)	-0.09	8 (2%) 57 58	13, 40, 82, 141	0
2	N	355/374 (94%)	0.14	15 (4%) 35 35	17, 50, 94, 201	0
All	All	2565/2748 (93%)	0.01	72 (2%) 50 52	12, 44, 91, 201	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	429	ARG	7.8
2	D	429	ARG	5.9
2	D	447	VAL	4.5
2	N	442	VAL	4.4
2	D	355	ALA	4.0

### 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 ⓘ

There are no carbohydrates in this entry.

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	D	800	14/15	0.23	10.78	58,76,82,82	0
3	NAG	N	800	14/15	0.25	3.47	62,80,85,86	0
3	NAG	I	770	14/15	0.41	3.29	128,147,151,151	0
3	NAG	H	800	14/15	0.36	3.10	88,106,112,113	0
3	NAG	E	770	14/15	0.42	2.56	99,117,122,124	0
3	NAG	L	800	14/15	0.19	2.37	64,82,87,87	0
3	NAG	F	800	14/15	0.25	1.95	71,89,94,95	0
3	NAG	G	770	14/15	0.27	1.62	95,113,119,120	0
3	NAG	C	770	14/15	0.23	0.65	82,100,106,107	0
3	NAG	M	770	14/15	0.28	0.64	91,110,114,115	0
3	NAG	B	800	14/15	0.19	0.16	57,74,81,82	0
3	NAG	A	770	14/15	0.19	-0.14	62,81,84,86	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.