



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:47 PM GMT

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 X-ray Structure 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/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

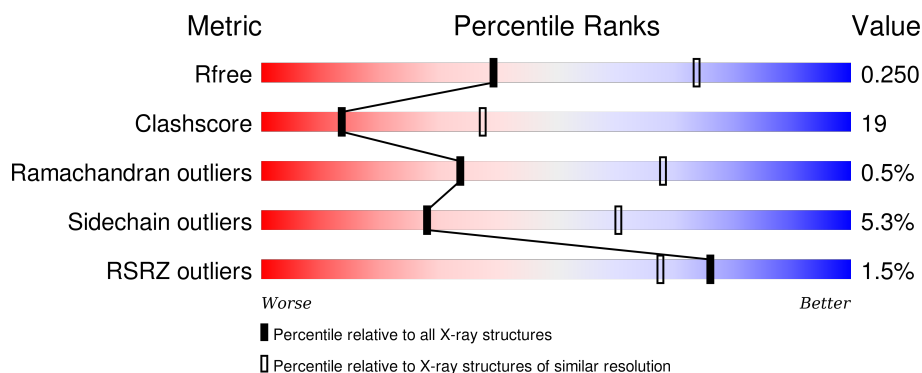
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.82 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))
$R_{free}$	91344	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (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. 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	84	<div> <div>2%</div> <div>54%</div> <div>31%</div> <div>•</div> <div>13%</div> </div>
1	C	84	<div> <div>61%</div> <div>24%</div> <div>•</div> <div>14%</div> </div>
1	E	84	<div> <div>%</div> <div>64%</div> <div>21%</div> <div>•</div> <div>13%</div> </div>
1	G	84	<div> <div>%</div> <div>52%</div> <div>33%</div> <div>14%</div> </div>
1	I	84	<div> <div>64%</div> <div>19%</div> <div>•</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
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, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	F	800	X	-	-	-
3	NAG	H	800	X	-	-	-
3	NAG	I	770	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 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	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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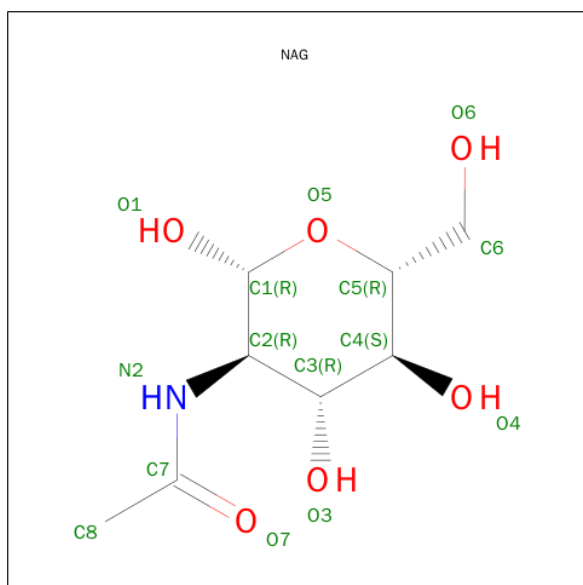
Chain	Residue	Modelled	Actual	Comment	Reference
B	514	GLY	-	EXPRESSION TAG	UNP Q84850
B	515	LEU	-	EXPRESSION TAG	UNP Q84850
B	516	GLU	-	EXPRESSION TAG	UNP Q84850
B	517	VAL	-	EXPRESSION TAG	UNP Q84850
B	518	LEU	-	EXPRESSION TAG	UNP Q84850
B	519	PHE	-	EXPRESSION TAG	UNP Q84850
B	520	GLN	-	EXPRESSION TAG	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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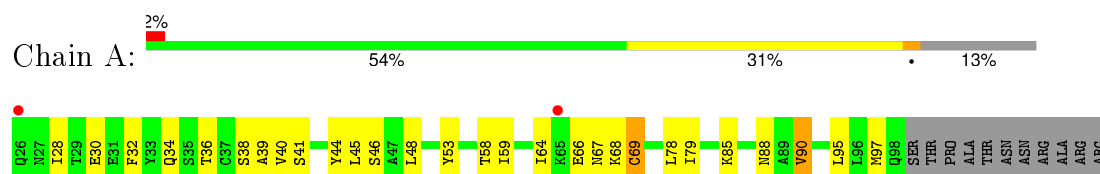
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		
3	M	1	Total	C	N	O	0	0
			14	8	1	5		
3	N	1	Total	C	N	O	0	0
			14	8	1	5		

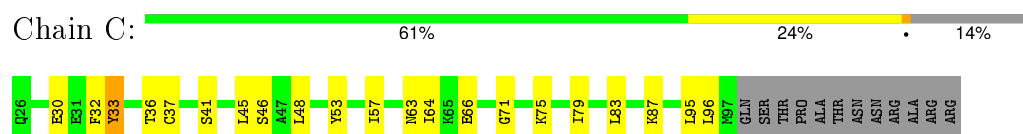
### 3 Residue-property plots [i](#)

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.

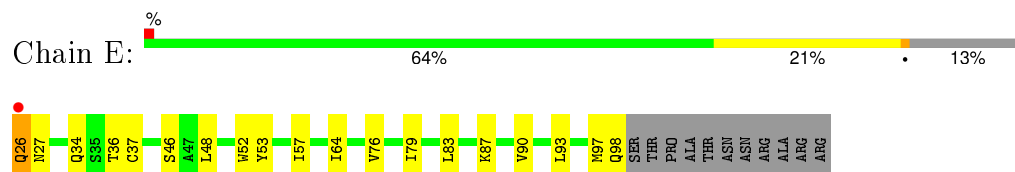
- Molecule 1: Fusion glycoprotein F0



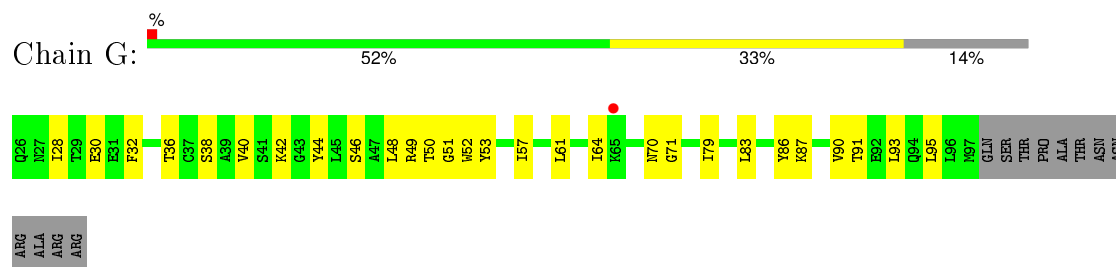
- Molecule 1: Fusion glycoprotein F0



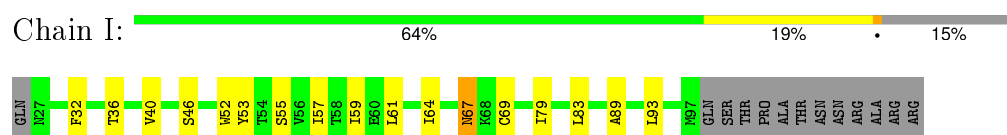
- Molecule 1: Fusion glycoprotein F0



- Molecule 1: Fusion glycoprotein F0

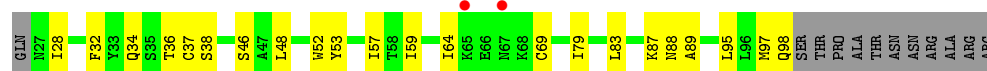


- Molecule 1: Fusion glycoprotein F0

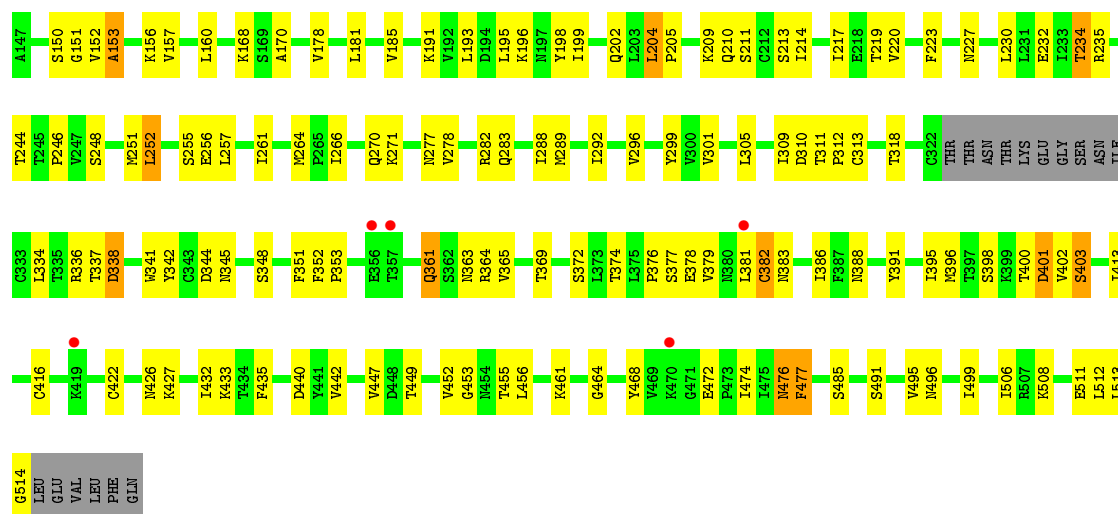


- Molecule 1: Fusion glycoprotein F0

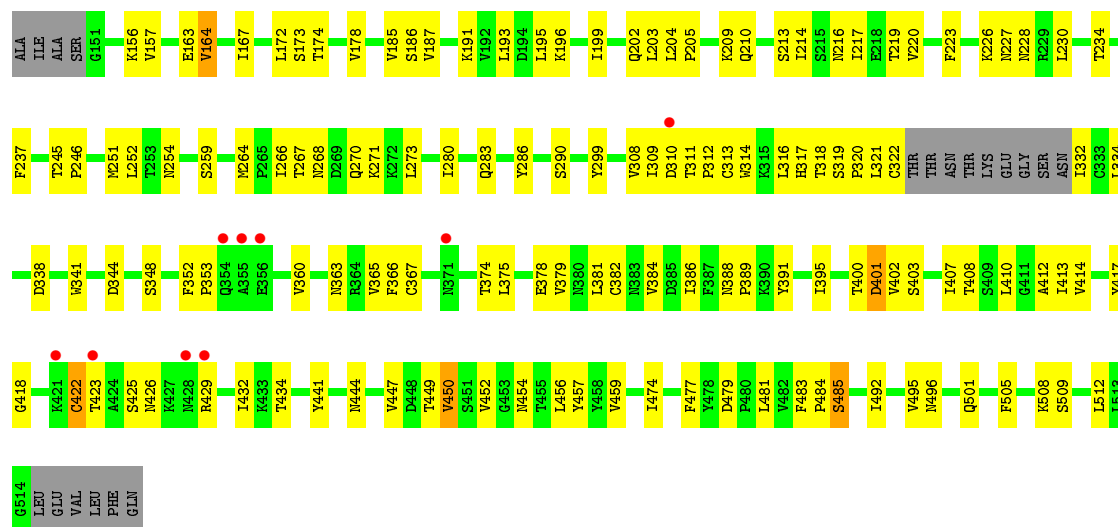




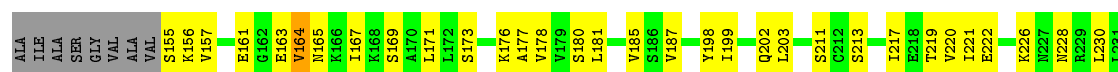
• Molecule 2: Fusion glycoprotein F0



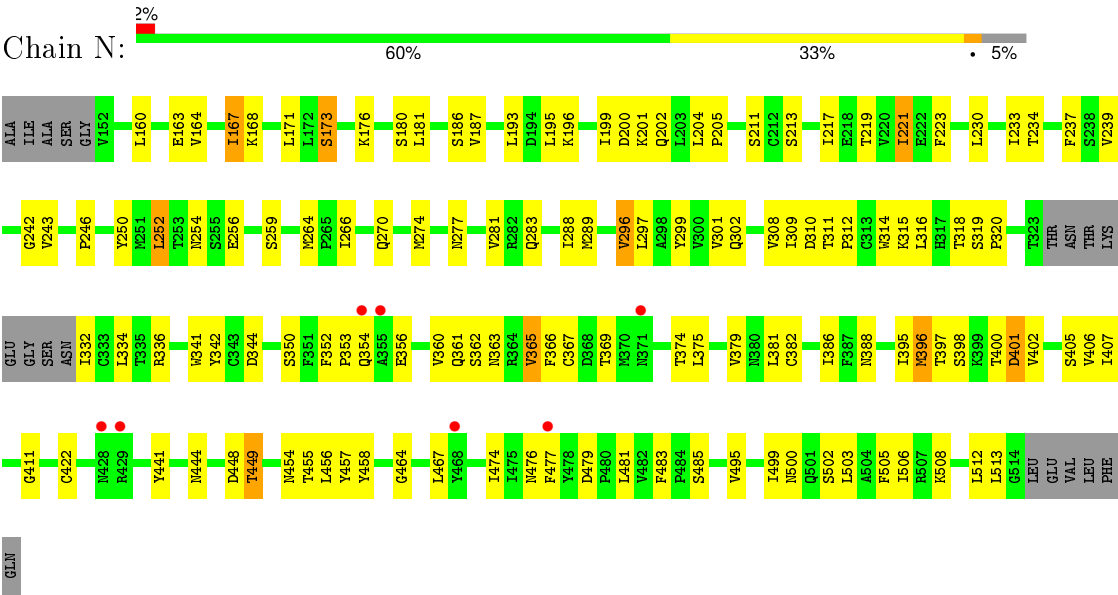
• Molecule 2: Fusion glycoprotein F0



• Molecule 2: Fusion glycoprotein F0







## 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 0.209 , 0.250	Depositor DCC
$R_{free}$ test set	3585 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> )	0.34 , 28.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	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.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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

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 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	580	587	588	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	571	579	579	36	0
1	E	580	587	588	25	0
1	G	571	579	580	33	0
1	I	562	571	572	28	0
1	M	571	579	580	33	0
2	B	2765	2798	2797	128	0
2	D	2749	2783	2782	146	0
2	F	2726	2757	2756	134	0
2	H	2773	2809	2808	145	0
2	L	2747	2780	2779	134	0
2	N	2752	2787	2786	139	0
3	A	14	0	13	0	0
3	B	14	0	13	3	0
3	C	14	0	13	1	0
3	D	14	0	13	0	0
3	E	14	0	13	0	0
3	F	14	0	13	1	0
3	G	14	0	13	1	0
3	H	14	0	13	1	0
3	I	14	0	13	1	0
3	L	14	0	13	0	0
3	M	14	0	13	4	0
3	N	14	0	13	2	0
All	All	20115	20196	20351	753	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 19.

The worst 5 of 753 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)
2:B:496:ASN:HB3	3:B:800:NAG:H81	1.40	1.01
2:H:308:VAL:HB	2:N:455:THR:HG22	1.60	0.84
2:N:449:THR:HB	2:N:456:LEU:HD11	1.62	0.81
2:N:334:LEU:HB3	2:N:395:ILE:HD11	1.64	0.79
2:H:280:ILE:HD11	2:H:361:GLN:HB2	1.63	0.79

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	71/84 (84%)	65 (92%)	5 (7%)	1 (1%)	14	40
1	C	70/84 (83%)	68 (97%)	2 (3%)	0	100	100
1	E	71/84 (84%)	65 (92%)	5 (7%)	1 (1%)	14	40
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%)	46	78
2	D	351/374 (94%)	326 (93%)	23 (7%)	2 (1%)	30	63
2	F	347/374 (93%)	320 (92%)	23 (7%)	4 (1%)	16	45
2	H	355/374 (95%)	327 (92%)	28 (8%)	0	100	100
2	L	350/374 (94%)	331 (95%)	17 (5%)	2 (1%)	30	63
2	N	351/374 (94%)	328 (93%)	22 (6%)	1 (0%)	46	78
All	All	2529/2748 (92%)	2360 (93%)	157 (6%)	12 (0%)	34	68

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 [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	66/75 (88%)	62 (94%)	4 (6%)	23	54
1	C	65/75 (87%)	64 (98%)	1 (2%)	72	93
1	E	66/75 (88%)	64 (97%)	2 (3%)	48	81
1	G	65/75 (87%)	65 (100%)	0	100	100
1	I	64/75 (85%)	63 (98%)	1 (2%)	70	92
1	M	65/75 (87%)	64 (98%)	1 (2%)	72	93
2	B	329/344 (96%)	304 (92%)	25 (8%)	16	41
2	D	328/344 (95%)	315 (96%)	13 (4%)	38	72
2	F	326/344 (95%)	304 (93%)	22 (7%)	20	49
2	H	330/344 (96%)	310 (94%)	20 (6%)	23	54
2	L	329/344 (96%)	310 (94%)	19 (6%)	25	56
2	N	329/344 (96%)	311 (94%)	18 (6%)	27	58
All	All	2362/2514 (94%)	2236 (95%)	126 (5%)	28	60

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 59 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	345	ASN
2	H	270	GLN
2	N	380	ASN
2	F	383	ASN
2	F	454	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	14,14,15	0.44	0	15,19,21	0.73	1 (6%)
3	NAG	B	800	2	14,14,15	0.39	0	15,19,21	1.49	1 (6%)
3	NAG	C	770	1	14,14,15	0.52	0	15,19,21	0.92	1 (6%)
3	NAG	D	800	2	14,14,15	0.46	0	15,19,21	0.86	1 (6%)
3	NAG	E	770	1	14,14,15	0.35	0	15,19,21	1.83	2 (13%)
3	NAG	F	800	2	14,14,15	0.41	0	15,19,21	1.40	1 (6%)
3	NAG	G	770	1	14,14,15	0.59	0	15,19,21	1.44	1 (6%)
3	NAG	H	800	2	14,14,15	0.45	0	15,19,21	1.30	1 (6%)
3	NAG	I	770	1	14,14,15	0.47	0	15,19,21	0.64	0
3	NAG	L	800	2	14,14,15	0.48	0	15,19,21	1.25	1 (6%)
3	NAG	M	770	1	14,14,15	0.43	0	15,19,21	1.67	1 (6%)
3	NAG	N	800	2	14,14,15	0.47	0	15,19,21	0.73	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

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

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	770	NAG	C4-C3-C2	-2.26	107.71	111.23
3	A	770	NAG	C1-O5-C5	2.14	114.97	112.25
3	C	770	NAG	C1-O5-C5	2.19	115.03	112.25
3	D	800	NAG	C1-O5-C5	2.44	115.35	112.25
3	L	800	NAG	C1-O5-C5	4.13	117.49	112.25

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.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	800	NAG	3	0
3	C	770	NAG	1	0
3	F	800	NAG	1	0
3	G	770	NAG	1	0
3	H	800	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	770	NAG	1	0
3	M	770	NAG	4	0
3	N	800	NAG	2	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	73/84 (86%)	-0.19	2 (2%) 58 46	25, 44, 85, 125	0
1	C	72/84 (85%)	-0.37	0 100 100	17, 35, 83, 157	0
1	E	73/84 (86%)	-0.20	1 (1%) 78 69	16, 40, 87, 121	0
1	G	72/84 (85%)	-0.10	1 (1%) 78 69	21, 50, 104, 169	0
1	I	71/84 (84%)	-0.30	0 100 100	12, 39, 88, 116	0
1	M	72/84 (85%)	-0.16	2 (2%) 56 44	15, 41, 86, 143	0
2	B	358/374 (95%)	-0.19	5 (1%) 78 69	14, 43, 82, 130	0
2	D	355/374 (94%)	-0.04	9 (2%) 61 48	15, 48, 95, 178	0
2	F	351/374 (93%)	-0.16	4 (1%) 82 75	14, 39, 87, 139	0
2	H	359/374 (95%)	-0.14	6 (1%) 73 63	15, 44, 84, 127	0
2	L	354/374 (94%)	-0.22	2 (0%) 90 86	13, 39, 82, 141	0
2	N	355/374 (94%)	-0.05	7 (1%) 68 58	17, 50, 94, 201	0
All	All	2565/2748 (93%)	-0.15	39 (1%) 76 68	12, 44, 91, 201	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	429	ARG	6.9
2	D	429	ARG	4.7
1	G	65	LYS	4.2
2	D	355	ALA	3.8
2	N	428	ASN	3.7

### 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 [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	N	800	14/15	0.85	0.25	-	62,80,85,86	0
3	NAG	H	800	14/15	0.79	0.33	-	88,106,112,113	0
3	NAG	I	770	14/15	0.69	0.39	-	128,147,151,151	0
3	NAG	D	800	14/15	0.79	0.22	-	58,76,82,82	0
3	NAG	F	800	14/15	0.87	0.22	-	71,89,94,95	0
3	NAG	B	800	14/15	0.82	0.21	-	57,74,81,82	0
3	NAG	E	770	14/15	0.76	0.43	-	99,117,122,124	0
3	NAG	C	770	14/15	0.78	0.24	-	82,100,106,107	0
3	NAG	G	770	14/15	0.79	0.24	-	95,113,119,120	0
3	NAG	M	770	14/15	0.82	0.26	-	91,110,114,115	0
3	NAG	A	770	14/15	0.77	0.18	-	62,81,84,86	0
3	NAG	L	800	14/15	0.90	0.18	-	64,82,87,87	0

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

There are no such residues in this entry.