WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2023 – 06:00 PM EDT

PDB ID	:	7UJ3
Title	:	Crystal structure of Human respiratory syncytial virus F variant (construct pXCS847A)
Authors	:	Han, S.; Ammirati, M.
Deposited on	:	2022-03-30
Resolution	:	3.50 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.36
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)	:	2.36

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 3.50 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.
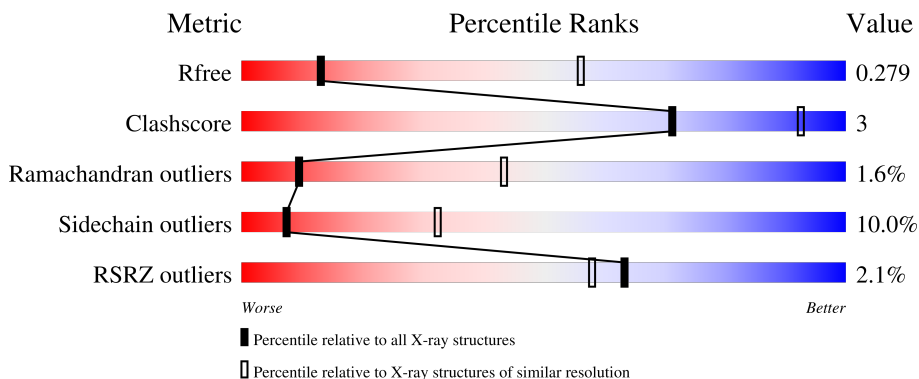
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	109	6% / 50% 17% · 31%
2	B	410	73% 14% · 11%

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	SO4	B	601	-	-	-	X
3	SO4	B	603	-	-	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 3421 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 RSV variant (construct pXCS847A) F2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	75	588	370	97	118	3	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A7D5GVC1
A	2	GLU	-	expression tag	UNP A0A7D5GVC1
A	3	LEU	-	expression tag	UNP A0A7D5GVC1
A	103	CYS	ALA	variant	UNP A0A7D5GVC1

- Molecule 2 is a protein called RSV variant (construct pXCS847A) F1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	364	2804	1776	462	548	18	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	148	CYS	ILE	variant	UNP A0A7D5GVC1
B	190	ILE	SER	variant	UNP A0A7D5GVC1
B	486	SER	ASP	variant	UNP A0A7D5GVC1
B	514	SER	-	expression tag	UNP A0A7D5GVC1
B	515	ALA	-	expression tag	UNP A0A7D5GVC1
B	516	ILE	-	expression tag	UNP A0A7D5GVC1
B	517	GLY	-	expression tag	UNP A0A7D5GVC1
B	518	GLY	-	expression tag	UNP A0A7D5GVC1
B	519	TYR	-	expression tag	UNP A0A7D5GVC1
B	520	ILE	-	expression tag	UNP A0A7D5GVC1
B	521	PRO	-	expression tag	UNP A0A7D5GVC1
B	522	GLU	-	expression tag	UNP A0A7D5GVC1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	523	ALA	-	expression tag	UNP A0A7D5GVC1
B	524	PRO	-	expression tag	UNP A0A7D5GVC1
B	525	ARG	-	expression tag	UNP A0A7D5GVC1
B	526	ASP	-	expression tag	UNP A0A7D5GVC1
B	527	GLY	-	expression tag	UNP A0A7D5GVC1
B	528	GLN	-	expression tag	UNP A0A7D5GVC1
B	529	ALA	-	expression tag	UNP A0A7D5GVC1
B	530	TYR	-	expression tag	UNP A0A7D5GVC1
B	531	VAL	-	expression tag	UNP A0A7D5GVC1
B	532	ARG	-	expression tag	UNP A0A7D5GVC1
B	533	LYS	-	expression tag	UNP A0A7D5GVC1
B	534	ASP	-	expression tag	UNP A0A7D5GVC1
B	535	GLY	-	expression tag	UNP A0A7D5GVC1
B	536	GLU	-	expression tag	UNP A0A7D5GVC1
B	537	TRP	-	expression tag	UNP A0A7D5GVC1
B	538	VAL	-	expression tag	UNP A0A7D5GVC1
B	539	LEU	-	expression tag	UNP A0A7D5GVC1
B	540	LEU	-	expression tag	UNP A0A7D5GVC1
B	541	SER	-	expression tag	UNP A0A7D5GVC1
B	542	THR	-	expression tag	UNP A0A7D5GVC1
B	543	PHE	-	expression tag	UNP A0A7D5GVC1
B	544	LEU	-	expression tag	UNP A0A7D5GVC1
B	545	GLY	-	expression tag	UNP A0A7D5GVC1
B	546	GLY	-	expression tag	UNP A0A7D5GVC1

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
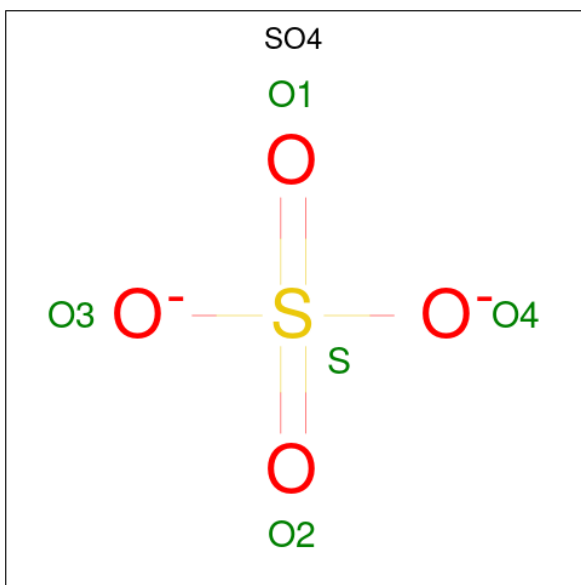
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
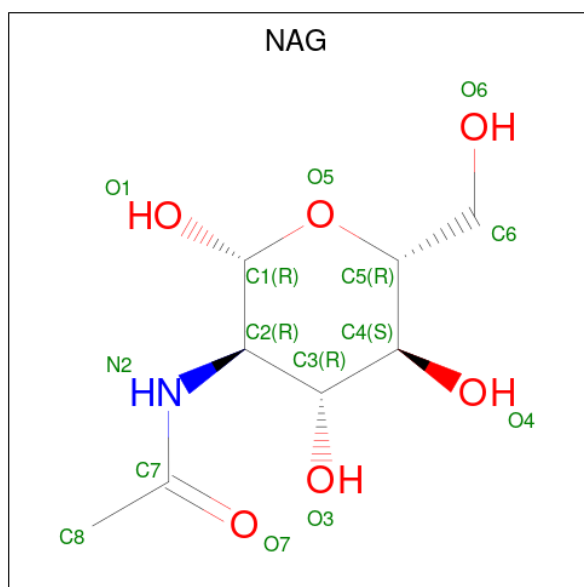
| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 14	C 8	N 1	O 5	0	0

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: RSV variant (construct pXCS847A) F2
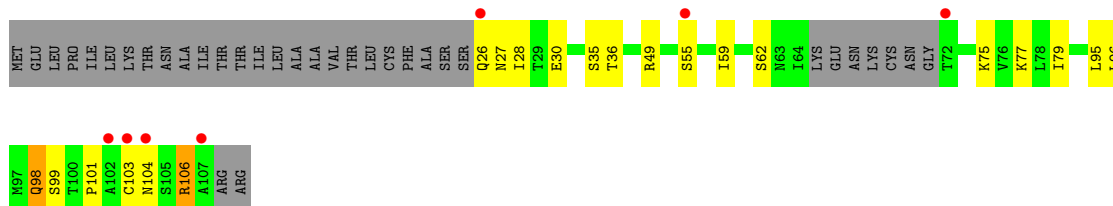
• Molecule 2: RSV variant (construct pXCS847A) F1
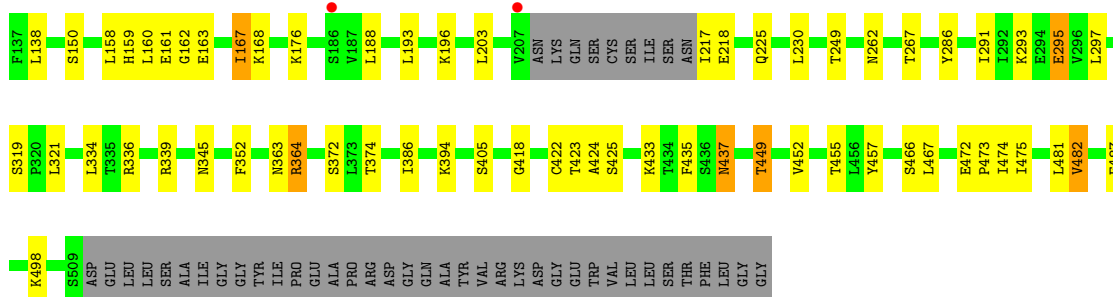
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	170.02Å 170.02Å 170.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 3.50 47.16 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.08-3.50) 100.0 (47.16-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.236 , 0.264 0.245 , 0.279	Depositor DCC
R_{free} test set	558 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	132.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 100.4	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3421	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.45	0/594	0.68	0/802
2	B	0.40	0/2846	0.65	1/3858 (0.0%)
All	All	0.41	0/3440	0.66	1/4660 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	159	HIS	CB-CA-C	-6.12	98.17	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-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 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	588	0	594	10	2
2	B	2804	0	2847	23	2
3	B	15	0	0	0	0
4	B	14	0	13	0	0
All	All	3421	0	3454	24	2

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 3.

The worst 5 of 24 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:CYS:SG	2:B:286:TYR:CE1	2.91	0.64
2:B:334:LEU:HB2	2:B:475:ILE:HD13	1.82	0.61
2:B:418:GLY:H	2:B:437:ASN:HD21	1.51	0.58
2:B:321:LEU:HD11	2:B:473:PRO:HB3	1.85	0.56
1:A:79:ILE:HD11	2:B:203:LEU:HD22	1.92	0.52

All (2) 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:A:106:ARG:NH2	2:B:339:ARG:NE[5_555]	1.16	1.04
1:A:106:ARG:NH2	2:B:339:ARG:CD[5_555]	1.75	0.45

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	71/109 (65%)	67 (94%)	2 (3%)	2 (3%)	5	32
2	B	360/410 (88%)	325 (90%)	30 (8%)	5 (1%)	11	46
All	All	431/519 (83%)	392 (91%)	32 (7%)	7 (2%)	9	43

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
2	B	293	LYS
2	B	482	VAL
1	A	106	ARG
2	B	295	GLU

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	67/96 (70%)	57 (85%)	10 (15%)	3	17
2	B	332/369 (90%)	302 (91%)	30 (9%)	9	37
All	All	399/465 (86%)	359 (90%)	40 (10%)	7	32

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	374	THR
2	B	467	LEU
2	B	386	ILE
2	B	437	ASN
2	B	481	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	345	ASN
2	B	361	GLN
2	B	437	ASN
2	B	363	ASN
2	B	331	ASN

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	0.17	0	6,6,6	0.05	0
3	SO4	B	604	-	4,4,4	0.15	0	6,6,6	0.06	0
4	NAG	B	602	2	14,14,15	0.33	0	17,19,21	0.42	0
3	SO4	B	603	-	4,4,4	0.19	0	6,6,6	0.10	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	NAG	B	602	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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	75/109 (68%)	0.31	7 (9%)	8	9	17, 94, 156, 250	0
2	B	364/410 (88%)	-0.19	2 (0%)	91	88	10, 63, 166, 254	0
All	All	439/519 (84%)	-0.10	9 (2%)	63	58	10, 67, 167, 254	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	ALA	3.4
2	B	186	SER	2.8
1	A	107	ALA	2.7
1	A	26	GLN	2.5
1	A	55	SER	2.3

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 monosaccharides 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. 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(Å²)	Q<0.9
3	SO4	B	601	5/5	0.14	1.68	233,233,234,234	0
3	SO4	B	603	5/5	0.55	0.55	121,123,124,126	0
4	NAG	B	602	14/15	0.55	0.34	151,157,160,161	0
3	SO4	B	604	5/5	0.85	0.23	179,180,181,183	0

6.5 Other polymers ⓘ

There are no such residues in this entry.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK