Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 07:01 PM EST

PDB ID	:	6VAS
Title	:	Assembly of VIQKI I454(beta-L-homoisoleucine)with human parainfluenza virus type 3 (HPIV3) fusion glycoprotein N-terminal heptad repeat domain
Authors	:	Outlaw, V.K.; Gellman, S.H.
Deposited on	:	2019-12-17
Resolution	:	1.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

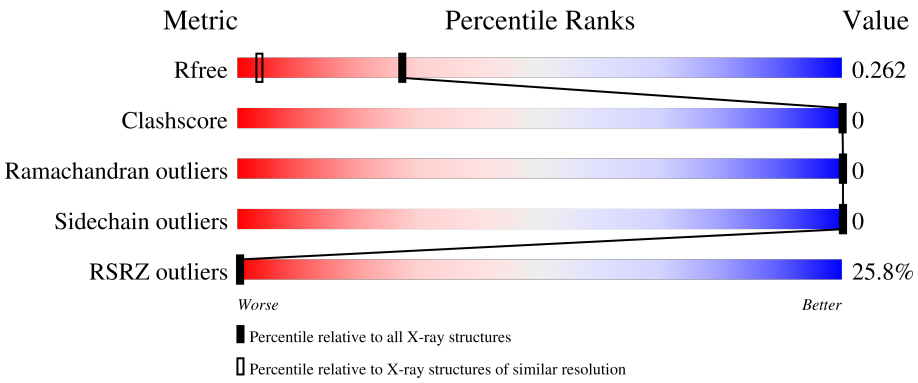
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.49 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	53	15% 83% 17%
1	C	53	19% 45% 55%
2	B	38	8% 82% 18%
2	D	38	26% 61% 39%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1954 atoms, of which 969 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	H	N	O			
1	A	44	665	203	335	60	67	0	0	0
1	C	24	372	111	190	33	38	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	ACE	-	acetylation	UNP P06828
A	190	NH2	-	amidation	UNP P06828
C	138	ACE	-	acetylation	UNP P06828
C	190	NH2	-	amidation	UNP P06828

- Molecule 2 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	B	31	519	157	269	45	48	0	0	1
2	D	23	355	111	175	34	35	0	0	1

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	448	ACE	-	acetylation	UNP P06828
B	454	BIL	ILE	engineered mutation	UNP P06828
B	459	VAL	GLU	engineered mutation	UNP P06828
B	463	ILE	ALA	engineered mutation	UNP P06828
B	466	GLN	ASP	engineered mutation	UNP P06828
B	479	LYS	GLN	engineered mutation	UNP P06828
B	480	ILE	LYS	engineered mutation	UNP P06828
B	485	NH2	-	amidation	UNP P06828

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Chain	Residue	Modelled	Actual	Comment	Reference
D	448	ACE	-	acetylation	UNP P06828
D	454	BIL	ILE	engineered mutation	UNP P06828
D	459	VAL	GLU	engineered mutation	UNP P06828
D	463	ILE	ALA	engineered mutation	UNP P06828
D	466	GLN	ASP	engineered mutation	UNP P06828
D	479	LYS	GLN	engineered mutation	UNP P06828
D	480	ILE	LYS	engineered mutation	UNP P06828
D	485	NH2	-	amidation	UNP P06828

- Molecule 3 is water.

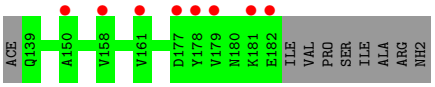
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	11	11	11	0	0
			Total	O		
3	B	20	20	20	0	0
			Total	O		
3	C	8	8	8	0	0
			Total	O		
3	D	4	4	4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

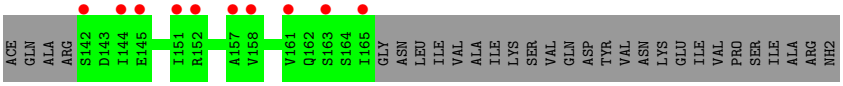
• Molecule 1: Fusion glycoprotein F0

Chain A:



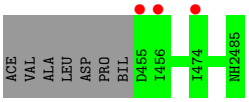
• Molecule 1: Fusion glycoprotein F0

Chain C:



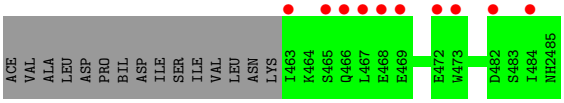
• Molecule 2: Fusion glycoprotein F0

Chain B:



• Molecule 2: Fusion glycoprotein F0

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	50.63Å 50.63Å 76.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.73 – 1.49 43.85 – 1.49	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.73-1.49) 95.3 (43.85-1.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 1.49Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.245 , 0.262 0.245 , 0.262	Depositor DCC
R_{free} test set	1886 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 67.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.059 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	1954	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.27% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NH2

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	0.24	0/330	0.34	0/444
1	C	0.32	0/181	0.42	0/241
2	B	0.23	0/250	0.35	0/333
2	D	0.22	0/180	0.32	0/240
All	All	0.25	0/941	0.36	0/1258

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	330	335	335	0	0
1	C	182	190	190	0	0
2	B	250	269	266	0	0
2	D	180	175	173	0	0
3	A	11	0	0	0	0
3	B	20	0	0	0	0
3	C	8	0	0	0	0
3	D	4	0	0	0	0
All	All	985	969	964	0	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 0.

There are no clashes within the asymmetric unit.

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	42/53 (79%)	42 (100%)	0	0	100	100
1	C	22/53 (42%)	22 (100%)	0	0	100	100
2	B	29/38 (76%)	29 (100%)	0	0	100	100
2	D	21/38 (55%)	21 (100%)	0	0	100	100
All	All	114/182 (63%)	114 (100%)	0	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	36/45 (80%)	36 (100%)	0	100	100
1	C	21/45 (47%)	21 (100%)	0	100	100
2	B	30/34 (88%)	30 (100%)	0	100	100
2	D	19/34 (56%)	19 (100%)	0	100	100
All	All	106/158 (67%)	106 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	44/53 (83%)	1.31	8 (18%)	1	1	16, 29, 65, 84	0
1	C	24/53 (45%)	1.87	10 (41%)	0	0	28, 45, 68, 78	0
2	B	30/38 (78%)	0.99	3 (10%)	7	7	19, 33, 50, 80	0
2	D	22/38 (57%)	2.35	10 (45%)	0	0	34, 52, 75, 77	0
All	All	120/182 (65%)	1.53	31 (25%)	0	0	16, 40, 72, 84	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	TYR	6.9
1	C	165	ILE	6.9
2	D	467	LEU	6.0
2	D	463	ILE	5.7
2	B	455	ASP	5.3
2	D	465	SER	4.9
1	C	161	VAL	4.6
1	A	179	VAL	4.1
2	B	456	ILE	3.8
1	A	177	ASP	3.6
1	A	181	LYS	3.5
2	D	482	ASP	3.3
2	D	466	GLN	3.3
2	D	468	GLU	3.3
2	D	472	GLU	3.0
1	C	163	SER	2.8
1	C	142	SER	2.7
2	D	469	GLU	2.6
1	C	144	ILE	2.6
1	A	158	VAL	2.6
2	D	473	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	182	GLU	2.5
2	D	484	ILE	2.4
1	C	157	ALA	2.3
1	C	145	GLU	2.2
1	A	161	VAL	2.1
2	B	474	ILE	2.1
1	C	152	ARG	2.1
1	C	151	ILE	2.0
1	C	158	VAL	2.0
1	A	150	ALA	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.