



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 11:10 AM GMT

PDB ID : 1ZTM
Title : Structure of the Uncleaved Paramyxovirus (hPIV3) Fusion Protein
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Deposited on : 2005-05-27
Resolution : 3.05 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

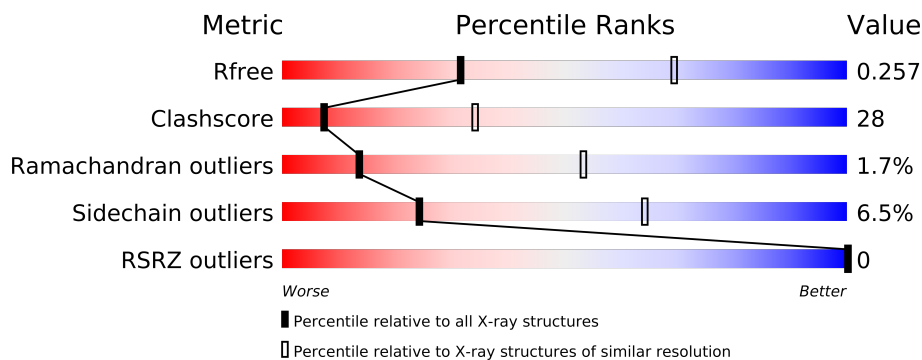
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
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) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.05 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	2079 (3.12-3.00)
Clashscore	79885	2629 (3.12-3.00)
Ramachandran outliers	78287	2536 (3.12-3.00)
Sidechain outliers	78261	2539 (3.12-3.00)
RSRZ outliers	66119	2081 (3.12-3.00)

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 ≥ 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	490	
1	B	490	
1	C	490	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9432 atoms, of which 0 are hydrogen 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3137	1983	522	618	14			
1	B	418	Total	C	N	O	S	0	0	0
			3117	1970	516	617	14			
1	C	424	Total	C	N	O	S	0	0	0
			3149	1986	526	623	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	SER	ARG	ENGINEERED	UNP P06828
A	494	GLY	-	CLONING ARTIFACT	UNP P06828
A	495	GLY	-	CLONING ARTIFACT	UNP P06828
A	496	PRO	-	CLONING ARTIFACT	UNP P06828
A	497	LEU	-	CLONING ARTIFACT	UNP P06828
A	498	VAL	-	CLONING ARTIFACT	UNP P06828
A	499	PRO	-	CLONING ARTIFACT	UNP P06828
A	500	ARG	-	CLONING ARTIFACT	UNP P06828
A	501	GLY	-	CLONING ARTIFACT	UNP P06828
A	502	SER	-	CLONING ARTIFACT	UNP P06828
A	503	HIS	-	EXPRESSION TAG	UNP P06828
A	504	HIS	-	EXPRESSION TAG	UNP P06828
A	505	HIS	-	EXPRESSION TAG	UNP P06828
A	506	HIS	-	EXPRESSION TAG	UNP P06828
A	507	HIS	-	EXPRESSION TAG	UNP P06828
A	508	HIS	-	EXPRESSION TAG	UNP P06828
B	106	SER	ARG	ENGINEERED	UNP P06828
B	494	GLY	-	CLONING ARTIFACT	UNP P06828
B	495	GLY	-	CLONING ARTIFACT	UNP P06828
B	496	PRO	-	CLONING ARTIFACT	UNP P06828
B	497	LEU	-	CLONING ARTIFACT	UNP P06828
B	498	VAL	-	CLONING ARTIFACT	UNP P06828
B	499	PRO	-	CLONING ARTIFACT	UNP P06828

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Chain	Residue	Modelled	Actual	Comment	Reference
B	500	ARG	-	CLONING ARTIFACT	UNP P06828
B	501	GLY	-	CLONING ARTIFACT	UNP P06828
B	502	SER	-	CLONING ARTIFACT	UNP P06828
B	503	HIS	-	EXPRESSION TAG	UNP P06828
B	504	HIS	-	EXPRESSION TAG	UNP P06828
B	505	HIS	-	EXPRESSION TAG	UNP P06828
B	506	HIS	-	EXPRESSION TAG	UNP P06828
B	507	HIS	-	EXPRESSION TAG	UNP P06828
B	508	HIS	-	EXPRESSION TAG	UNP P06828
C	106	SER	ARG	ENGINEERED	UNP P06828
C	494	GLY	-	CLONING ARTIFACT	UNP P06828
C	495	GLY	-	CLONING ARTIFACT	UNP P06828
C	496	PRO	-	CLONING ARTIFACT	UNP P06828
C	497	LEU	-	CLONING ARTIFACT	UNP P06828
C	498	VAL	-	CLONING ARTIFACT	UNP P06828
C	499	PRO	-	CLONING ARTIFACT	UNP P06828
C	500	ARG	-	CLONING ARTIFACT	UNP P06828
C	501	GLY	-	CLONING ARTIFACT	UNP P06828
C	502	SER	-	CLONING ARTIFACT	UNP P06828
C	503	HIS	-	EXPRESSION TAG	UNP P06828
C	504	HIS	-	EXPRESSION TAG	UNP P06828
C	505	HIS	-	EXPRESSION TAG	UNP P06828
C	506	HIS	-	EXPRESSION TAG	UNP P06828
C	507	HIS	-	EXPRESSION TAG	UNP P06828
C	508	HIS	-	EXPRESSION TAG	UNP P06828

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	O	0	0
			1	1		

L445	L446	N447	S448	V449	I458	N473	S477	N478	L481	D482	S483	I484	G485	ASN	TRP	HIS	GLN	SER	SER	THR	THR	GLY	GLY	PRO	LEU	VAL	PRO	ARG	GLY	SER	HIS	HIS	HIS	HIS
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● Molecule 1: Fusion glycoprotein

Chain C:

N430	S336	T259	A171	GLU	SER	I20
T434	S337	I262	I172	ASN	ASN	
F437	I339	K263	V175	GLU	GLU	K24
	C340	V264	Q176	ASN	ASN	L25
P440	G345	R265	D177	THR	THR	V28
M441	F346	V266	Y178	ASP	PRO	G29
		I267	V179	SER	SER	V30
T444	M352	D268	N180	THR	THR	L31
		V269	K181	LYS	ARG	V32
N447	G358	D270	E182	THR	THR	N33
	I360	L271	I183	PHE	PHE	
L451	R359	I276	V184	GLY	GLY	K36
D452	I360		P185	GLY	GLY	G37
F453	C363	Q279	S186	VAL	VAL	K38
		V280	R189	ILE	ILE	I40
I454	T366	R281	L190	GLY	GLY	
L460	V367	L282	G191	THR	THR	E45
	V368			ILE	ILE	
A463	R369	T286	Q198	ALA	ALA	Y48
K464	S370	R287	L199	LEU	LEU	
S465	D371	L288	L203	GLY	GLY	L53
E472	I372			VAL	VAL	I54
	V373	T291	H206	ALA	ALA	P55
R475	A377	V296		THR	THR	K56
R476	F378		E209	SER	SER	I57
	V379	T299	L210	ALA	ALA	E58
Q479	N380	S300	T211	GLN	GLN	D59
		Y301		ILE	ILE	S60
I484	V383	N302	G215	THR	THR	N61
ASN	V384	I303	D216	ALA	ALA	S62
TRP	I388	Q304		ALA	ALA	C63
HIS	T389		I226	VAL	VAL	G64
GLN	T390	E307	K227	ALA	ALA	D65
SER	T391	I310	L228	LEU	LEU	Q66
SER	C392		Q229	VAL	VAL	D67
THR	T393	P313	E136			I68
THR	C394		Y235			
GLY	N395	I316	R236	S142	S142	Y71
PRO	G396	K317	T237	E145	E145	L75
LEU	I397	T318	I239	K146	K146	D76
VAL	G398	K319	T240	L147	L147	
PRO	N399	G320	E241	K148	K148	I79
ARG		A321	I242			I80
GLY	Q403	F322		I151	I151	P81
SER	V409	L323	T245	T154	T154	L82
HIS		G324	S246			Y83
HIS	T413	G325	T247	Q159	Q159	
HIS	H414	V328	V248			L86
HIS	K415	K329	D249	Q162	Q162	R87
HIS		E330	D252			L88
HIS	I420	C331	I253	I165	I165	I93
	G421	I332	Y254	L168	L168	V94
	I422	E333		I169	I169	SER
	N423	A334	L257	V170	V170	ASN
		F335	F258			GLN

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.56Å 122.17Å 195.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.02 – 3.05 30.02 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.02-3.05) 99.6 (30.02-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.40 (at 3.06Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.264 0.211 , 0.257	Depositor DCC
R_{free} test set	2365 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.772	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 31.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 48676 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9432	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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	0.37	0/3183	0.69	1/4337 (0.0%)
1	B	0.37	0/3163	0.68	0/4318
1	C	0.37	0/3193	0.67	1/4356 (0.0%)
All	All	0.37	0/9539	0.68	2/13011 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	LYS	N-CA-C	-5.71	95.59	111.00
1	A	35	PRO	N-CA-CB	5.26	109.61	103.30

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	3137	0	3062	185	0
1	B	3117	0	3006	206	0
1	C	3149	0	3034	205	0
2	A	14	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	14	0	13	0	0
3	B	1	0	0	0	0
All	All	9432	0	9128	516	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 28.

The worst 5 of 516 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:413:THR:HG22	1:C:415:LYS:H	1.13	1.11
1:C:259:THR:HG23	1:C:332:ILE:HG21	1.46	0.96
1:C:264:VAL:HG12	1:C:280:VAL:HA	1.49	0.94
1:B:168:LEU:HD21	1:C:169:ILE:HG22	1.50	0.94
1:A:417:CYS:HB2	1:A:420:ILE:HG22	1.52	0.92

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	412/490 (84%)	364 (88%)	41 (10%)	7 (2%)	14	53
1	B	414/490 (84%)	371 (90%)	36 (9%)	7 (2%)	14	53
1	C	420/490 (86%)	367 (87%)	46 (11%)	7 (2%)	14	53
All	All	1246/1470 (85%)	1102 (88%)	123 (10%)	21 (2%)	14	53

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	447	ASN
1	A	448	SER
1	B	359	ASN
1	B	380	ASN
1	B	447	ASN

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	346/433 (80%)	324 (94%)	22 (6%)	25	65
1	B	340/433 (78%)	323 (95%)	17 (5%)	34	76
1	C	339/433 (78%)	311 (92%)	28 (8%)	16	52
All	All	1025/1299 (79%)	958 (94%)	67 (6%)	24	64

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	253	ILE
1	B	434	THR
1	C	393	THR
1	B	299	ILE
1	B	318	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	229	GLN
1	B	302	ASN
1	C	380	ASN
1	B	279	GLN
1	B	315	HIS

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 ⓘ

2 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	$\# Z > 2$
2	NAG	A	1359	1	12,14,15	0.55	0	15,19,21	0.88	0
2	NAG	B	1359	1	12,14,15	0.90	0	15,19,21	1.04	1 (6%)

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
2	NAG	A	1359	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1359	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1359	NAG	C3-C2-N2	-2.05	108.64	111.76

There are no chirality outliers.

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, 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	416/490 (84%)	-0.46	0 100 100	26, 53, 89, 123	0
1	B	418/490 (85%)	-0.49	0 100 100	23, 52, 87, 116	0
1	C	424/490 (86%)	-0.47	0 100 100	24, 56, 91, 117	0
All	All	1258/1470 (85%)	-0.47	0 100 100	23, 54, 90, 123	0

There are no RSRZ outliers to report.

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	B	1359	14/15	0.20	0.08	49,99,105,105	0
2	NAG	A	1359	14/15	0.17	-5.49	65,84,97,98	0

6.5 Other polymers ⓘ

There are no such residues in this entry.