



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 09:20 am BST

PDB ID : 5U0U
Title : Crystal Structure of DH270.1 (unliganded, single-chain Fv) from the DH270 Broadly Neutralizing N332-glycan Dependent Lineage
Authors : Fera, D.; Harrison, S.C.
Deposited on : 2016-11-27
Resolution : 3.43 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

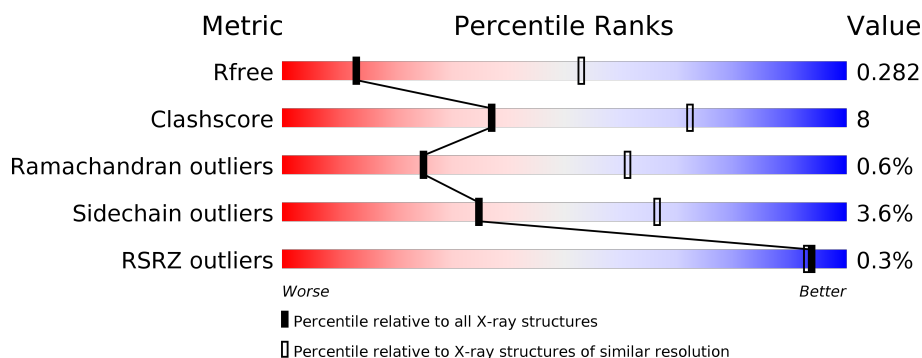
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.43 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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 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 $\leq 5\%$. 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	256	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>21%</div> <div>• 8%</div> </div> </div>
1	C	256	<div> <div>77%</div> <div>14%</div> <div>8%</div> </div>
1	E	256	<div> <div>72%</div> <div>20%</div> <div>8%</div> </div>
1	G	256	<div> <div>72%</div> <div>20%</div> <div>8%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7157 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.

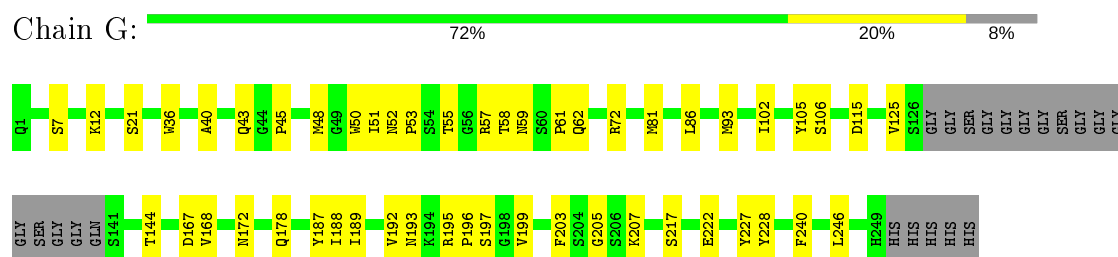
- Molecule 1 is a protein called DH270.1 single-chain variable fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	235	Total	C	N	O	S	0	0	0
			1791	1124	301	356	10			
1	A	235	Total	C	N	O	S	0	0	0
			1795	1127	302	356	10			
1	C	235	Total	C	N	O	S	0	0	0
			1791	1124	301	356	10			
1	E	235	Total	C	N	O	S	0	0	0
			1780	1116	299	356	9			

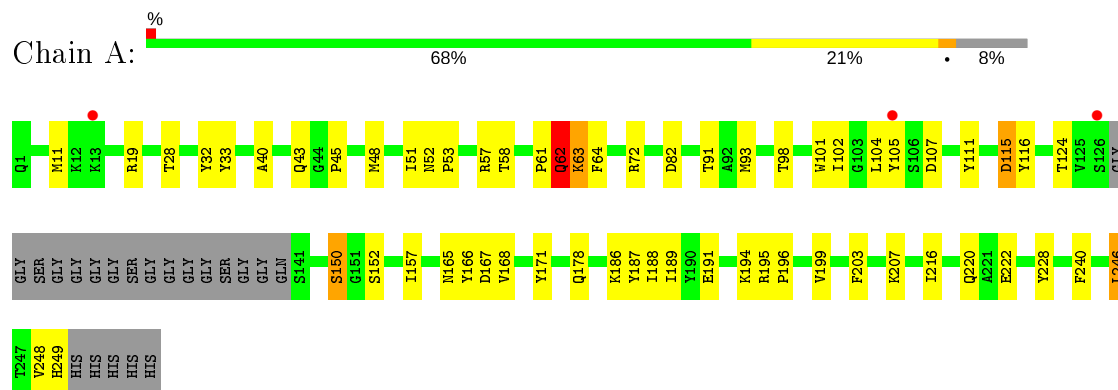
3 Residue-property plots [i](#)

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

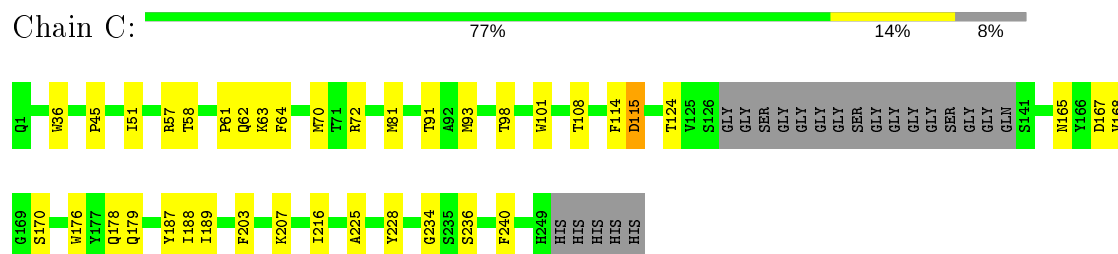
- Molecule 1: DH270.1 single-chain variable fragment



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Q1	T28	F29	Y32	W36	Q43	G44	W50	I51	M52	P53	S54	T55	T58	M59	S60	P61	Q62	K63	F64	M70	T71	R72	W81	T91	A92	M93	W101	T108	S109	G110	D115	Y116	T124	V125	S126	GLY	GLY	SER	SER	GLY	GLY	GLY	GLY	SER	SER	GLY	GLY	GLY	
GLY	SER	GLY	GLY	GLN	S141	Y166	D167	V168	Q178	Y187	I188	I189	V192	P196	V199	G205	S206	K207	L219	E222	T226	Y232	A233	G234	S235	S236	I237	I238	F239	L246	H249	HIS	HIS	HIS	HIS	HIS	GLY	GLY	SER	SER	GLY	GLY	GLY	GLY	SER	SER	GLY	GLY	GLY

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.87Å 111.28Å 89.13Å 90.00° 120.46° 90.00°	Depositor
Resolution (Å)	49.85 – 3.43 49.85 – 3.43	Depositor EDS
% Data completeness (in resolution range)	80.8 (49.85-3.43) 80.9 (49.85-3.43)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.254 , 0.282 0.254 , 0.282	Depositor DCC
R_{free} test set	726 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 9.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	7157	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

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	0.29	0/1842	0.48	0/2506
1	C	0.29	0/1838	0.48	0/2502
1	E	0.28	0/1827	0.50	0/2491
1	G	0.29	0/1838	0.50	0/2502
All	All	0.29	0/7345	0.49	0/10001

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	1795	0	1702	39	0
1	C	1791	0	1691	22	0
1	E	1780	0	1662	33	0
1	G	1791	0	1691	29	0
All	All	7157	0	6746	108	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 8.

The worst 5 of 108 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:178:GLN:HB2	1:A:188:ILE:HD11	1.46	0.97
1:A:62:GLN:O	1:A:64:PHE:N	1.96	0.97
1:E:178:GLN:HB2	1:E:188:ILE:HD11	1.49	0.95
1:G:178:GLN:HB2	1:G:188:ILE:HD11	1.48	0.93
1:C:178:GLN:HB2	1:C:188:ILE:HD11	1.56	0.86

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	231/256 (90%)	216 (94%)	13 (6%)	2 (1%)	17	53
1	C	231/256 (90%)	216 (94%)	13 (6%)	2 (1%)	17	53
1	E	231/256 (90%)	212 (92%)	17 (7%)	2 (1%)	17	53
1	G	231/256 (90%)	216 (94%)	15 (6%)	0	100	100
All	All	924/1024 (90%)	860 (93%)	58 (6%)	6 (1%)	25	61

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	C	63	LYS
1	E	63	LYS
1	A	62	GLN
1	C	61	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	196/205 (96%)	186 (95%)	10 (5%)	24	57
1	C	195/205 (95%)	190 (97%)	5 (3%)	46	74
1	E	192/205 (94%)	186 (97%)	6 (3%)	40	70
1	G	195/205 (95%)	188 (96%)	7 (4%)	35	66
All	All	778/820 (95%)	750 (96%)	28 (4%)	35	66

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	SER
1	A	187	TYR
1	E	187	TYR
1	A	152	SER
1	A	165	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	201	ASN
1	E	180	HIS

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 carbohydrates 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	235/256 (91%)	0.09	3 (1%) 77 75	54, 60, 68, 80	0
1	C	235/256 (91%)	0.09	0 100 100	50, 61, 70, 74	0
1	E	235/256 (91%)	0.10	0 100 100	55, 69, 83, 102	0
1	G	235/256 (91%)	0.03	0 100 100	40, 54, 62, 69	0
All	All	940/1024 (91%)	0.08	3 (0%) 94 93	40, 61, 76, 102	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	SER	2.6
1	A	105	TYR	2.3
1	A	13	LYS	2.2

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 carbohydrates 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.