



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 2, 2021 – 11:11 am GMT

PDB ID : 7A3P
Title : Crystal structure of dengue 3 virus envelope glycoprotein in complex with the scFv fragment of the broadly neutralizing human antibody EDE1 C10
Authors : Sharma, A.; Vaney, M.C.; Guardado-Calvo, P.; Duquerroy, S.; Rouvinski, A.; Rey, F.A.
Deposited on : 2020-08-18
Resolution : 3.19 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
Mogul : 1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

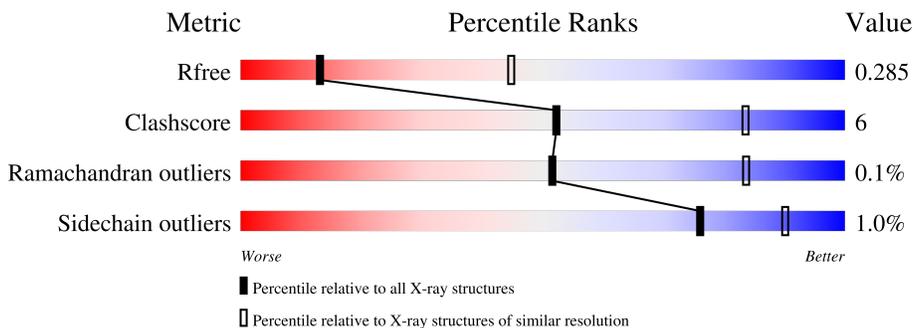
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	428	
1	B	428	
2	H	144	
2	I	144	
3	L	154	
3	M	154	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9173 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 Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	351	2721	1725	456	519	21	0	0	0
1	B	361	2799	1774	473	531	21	0	0	0

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	394	LEU	-	expression tag	UNP Q07019
A	395	VAL	-	expression tag	UNP Q07019
A	396	PRO	-	expression tag	UNP Q07019
A	397	ARG	-	expression tag	UNP Q07019
A	398	GLY	-	expression tag	UNP Q07019
A	399	SER	-	expression tag	UNP Q07019
A	400	SER	-	expression tag	UNP Q07019
A	401	ALA	-	expression tag	UNP Q07019
A	402	TRP	-	expression tag	UNP Q07019
A	403	SER	-	expression tag	UNP Q07019
A	404	HIS	-	expression tag	UNP Q07019
A	405	PRO	-	expression tag	UNP Q07019
A	406	GLN	-	expression tag	UNP Q07019
A	407	PHE	-	expression tag	UNP Q07019
A	408	GLU	-	expression tag	UNP Q07019
A	409	LYS	-	expression tag	UNP Q07019
A	410	GLY	-	expression tag	UNP Q07019
A	411	GLY	-	expression tag	UNP Q07019
A	412	SER	-	expression tag	UNP Q07019
A	413	GLY	-	expression tag	UNP Q07019
A	414	GLY	-	expression tag	UNP Q07019
A	415	GLY	-	expression tag	UNP Q07019
A	416	SER	-	expression tag	UNP Q07019
A	417	GLY	-	expression tag	UNP Q07019
A	418	GLY	-	expression tag	UNP Q07019

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	SER	-	expression tag	UNP Q07019
A	420	ALA	-	expression tag	UNP Q07019
A	421	TRP	-	expression tag	UNP Q07019
A	422	SER	-	expression tag	UNP Q07019
A	423	HIS	-	expression tag	UNP Q07019
A	424	PRO	-	expression tag	UNP Q07019
A	425	GLN	-	expression tag	UNP Q07019
A	426	PHE	-	expression tag	UNP Q07019
A	427	GLU	-	expression tag	UNP Q07019
A	428	LYS	-	expression tag	UNP Q07019
B	394	LEU	-	expression tag	UNP Q07019
B	395	VAL	-	expression tag	UNP Q07019
B	396	PRO	-	expression tag	UNP Q07019
B	397	ARG	-	expression tag	UNP Q07019
B	398	GLY	-	expression tag	UNP Q07019
B	399	SER	-	expression tag	UNP Q07019
B	400	SER	-	expression tag	UNP Q07019
B	401	ALA	-	expression tag	UNP Q07019
B	402	TRP	-	expression tag	UNP Q07019
B	403	SER	-	expression tag	UNP Q07019
B	404	HIS	-	expression tag	UNP Q07019
B	405	PRO	-	expression tag	UNP Q07019
B	406	GLN	-	expression tag	UNP Q07019
B	407	PHE	-	expression tag	UNP Q07019
B	408	GLU	-	expression tag	UNP Q07019
B	409	LYS	-	expression tag	UNP Q07019
B	410	GLY	-	expression tag	UNP Q07019
B	411	GLY	-	expression tag	UNP Q07019
B	412	SER	-	expression tag	UNP Q07019
B	413	GLY	-	expression tag	UNP Q07019
B	414	GLY	-	expression tag	UNP Q07019
B	415	GLY	-	expression tag	UNP Q07019
B	416	SER	-	expression tag	UNP Q07019
B	417	GLY	-	expression tag	UNP Q07019
B	418	GLY	-	expression tag	UNP Q07019
B	419	SER	-	expression tag	UNP Q07019
B	420	ALA	-	expression tag	UNP Q07019
B	421	TRP	-	expression tag	UNP Q07019
B	422	SER	-	expression tag	UNP Q07019
B	423	HIS	-	expression tag	UNP Q07019
B	424	PRO	-	expression tag	UNP Q07019
B	425	GLN	-	expression tag	UNP Q07019

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	426	PHE	-	expression tag	UNP Q07019
B	427	GLU	-	expression tag	UNP Q07019
B	428	LYS	-	expression tag	UNP Q07019

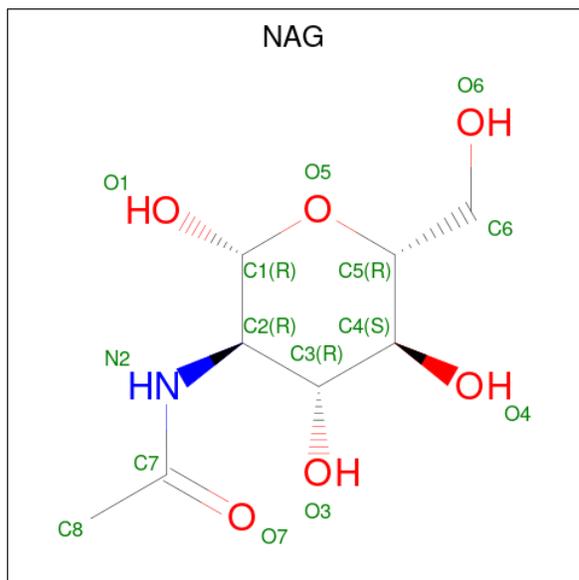
- Molecule 2 is a protein called Single Chain Variable Fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	125	Total 1006	C 642	N 167	O 192	S 5	0	0	0
2	I	126	Total 1015	C 647	N 168	O 195	S 5	0	0	0

- Molecule 3 is a protein called Single Chain Variable Fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	109	Total 793	C 491	N 135	O 164	S 3	0	0	0
3	M	111	Total 808	C 499	N 138	O 168	S 3	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is water.

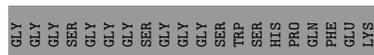
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	6	Total O 6 6	0	0
5	B	2	Total O 2 2	0	0
5	H	1	Total O 1 1	0	0
5	L	1	Total O 1 1	0	0
5	I	3	Total O 3 3	0	0
5	M	4	Total O 4 4	0	0



● Molecule 3: Single Chain Variable Fragment



● Molecule 3: Single Chain Variable Fragment



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.74Å 101.41Å 249.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 3.19 19.95 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.95-3.19) 97.4 (19.95-3.19)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 3.22Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.240 , 0.284 0.240 , 0.285	Depositor DCC
R_{free} test set	1220 reflections (5.35%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtrriage
Anisotropy	0.909	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	9173	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.7289e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

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	0.29	0/2766	0.53	0/3740
1	B	0.28	0/2847	0.52	1/3850 (0.0%)
2	H	0.26	0/1035	0.47	0/1407
2	I	0.30	0/1044	0.53	0/1419
3	L	0.33	0/811	0.51	0/1101
3	M	0.35	0/826	0.52	0/1121
All	All	0.29	0/9329	0.52	1/12638 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	LEU	CB-CG-CD2	-5.90	100.98	111.00

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	2721	0	2723	27	0
1	B	2799	0	2804	42	0
2	H	1006	0	946	9	0
2	I	1015	0	955	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	793	0	755	6	0
3	M	808	0	771	14	0
4	B	14	0	13	0	0
5	A	6	0	0	0	0
5	B	2	0	0	1	0
5	H	1	0	0	0	0
5	I	3	0	0	0	0
5	L	1	0	0	0	0
5	M	4	0	0	1	0
All	All	9173	0	8967	100	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 6.

The worst 5 of 100 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)
3:M:92:THR:HG1	3:M:95(A):THR:HG1	1.18	0.87
1:B:375:ASN:HA	1:B:386:LYS:HZ3	1.44	0.82
1:B:370:PRO:HG3	1:B:376:ILE:HD11	1.66	0.77
3:M:33:VAL:HB	3:M:51:VAL:HG22	1.69	0.72
1:A:196:LEU:HD11	1:A:268:ILE:HD11	1.73	0.71

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	333/428 (78%)	321 (96%)	12 (4%)	0	100	100
1	B	345/428 (81%)	326 (94%)	19 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	123/144 (85%)	119 (97%)	4 (3%)	0	100	100
2	I	124/144 (86%)	120 (97%)	4 (3%)	0	100	100
3	L	107/154 (70%)	105 (98%)	1 (1%)	1 (1%)	17	56
3	M	109/154 (71%)	105 (96%)	4 (4%)	0	100	100
All	All	1141/1452 (79%)	1096 (96%)	44 (4%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	51	VAL

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	304/357 (85%)	302 (99%)	2 (1%)	84	94
1	B	311/357 (87%)	308 (99%)	3 (1%)	76	90
2	H	105/112 (94%)	105 (100%)	0	100	100
2	I	106/112 (95%)	104 (98%)	2 (2%)	57	81
3	L	89/116 (77%)	87 (98%)	2 (2%)	52	79
3	M	91/116 (78%)	90 (99%)	1 (1%)	73	88
All	All	1006/1170 (86%)	996 (99%)	10 (1%)	76	90

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	7	SER
2	I	64	GLN
3	M	27(B)	ASP
1	B	277	PHE
1	B	375	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	375	ASN

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](#)

1 ligand is modelled in this entry.

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 [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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.