



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:07 AM UTC

PDB ID : 7ZM6 / pdb_00007zm6
Title : Nariva virus receptor binding protein
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Deposited on : 2022-04-19
Resolution : 2.07 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

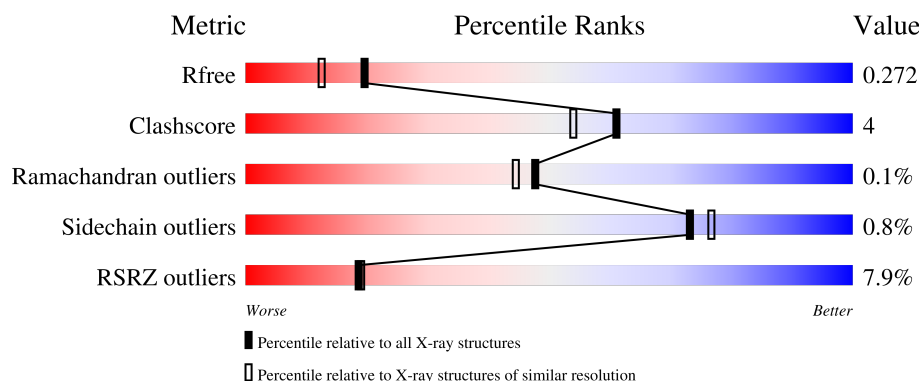
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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 $\leq 5\%$. 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	657	5% 58% 7% 35%
1	B	657	6% 58% 7% 34%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7423 atoms, of which 0 are hydrogens and 0 are deuteriums.

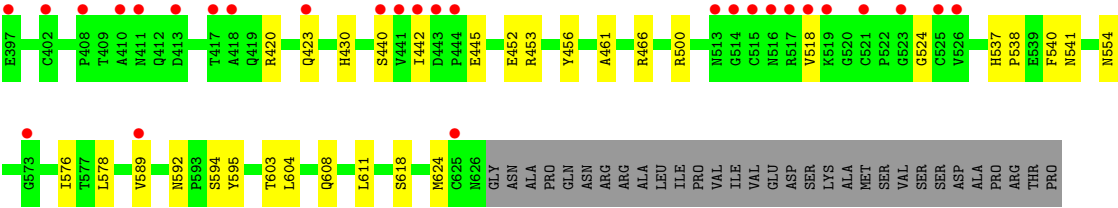
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Attachment protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3335	2112	583	616	24			
1	B	433	Total	C	N	O	S	0	0	0
			3367	2133	588	622	24			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	381	Total	O	0	0
			381	381		
2	B	340	Total	O	0	0
			340	340		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.38Å 82.96Å 92.99Å 90.00° 90.86° 90.00°	Depositor
Resolution (Å)	61.93 – 2.07 61.93 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.0 (61.93-2.07) 99.3 (61.93-2.07)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.07Å)	Xtriage
Refinement program	PHENIX dev_3488	Depositor
R, R_{free}	0.230 , 0.270 0.232 , 0.272	Depositor DCC
R_{free} test set	2623 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.656	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7423	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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

5.1 Standard geometry

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	0.13	0/3425	0.37	0/4671
1	B	0.13	0/3459	0.37	0/4719
All	All	0.13	0/6884	0.37	0/9390

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

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	3335	0	3243	29	0
1	B	3367	0	3270	29	0
2	A	381	0	0	8	0
2	B	340	0	0	7	0
All	All	7423	0	6513	56	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 4.

All (56) 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:301:ALA:HB3	2:A:722:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ARG:NH2	2:B:703:HOH:O	2.31	0.63
1:B:608:GLN:NE2	2:B:705:HOH:O	2.33	0.62
1:A:521:CYS:O	2:A:701:HOH:O	2.16	0.61
1:B:198:ALA:HB1	1:B:315:HIS:CE1	2.35	0.60
1:A:335:LYS:NZ	2:A:710:HOH:O	2.34	0.60
1:A:398:TYR:N	2:A:703:HOH:O	2.26	0.59
1:B:197:ASN:HA	1:B:294:LEU:HD21	1.85	0.59
1:B:362:LEU:HD12	1:B:445:GLU:HG3	1.89	0.54
1:A:315:HIS:ND1	2:A:709:HOH:O	2.33	0.54
1:A:420:ARG:HD3	1:A:423:GLN:HA	1.90	0.54
1:A:575:ASN:ND2	2:A:708:HOH:O	2.30	0.54
1:A:319:ALA:HB3	1:A:343:PHE:HB2	1.91	0.52
1:B:392:ARG:NH2	1:B:452:GLU:OE1	2.42	0.52
1:B:453:ARG:HA	1:B:456:TYR:CZ	2.46	0.51
1:B:541:ASN:ND2	2:B:716:HOH:O	2.40	0.51
1:B:420:ARG:HD3	1:B:423:GLN:HA	1.93	0.50
1:A:592:ASN:HB3	1:A:595:TYR:O	2.13	0.49
1:B:466:ARG:NH1	2:B:707:HOH:O	2.36	0.48
1:B:227:ILE:HG13	1:B:618:SER:HB2	1.95	0.48
1:A:482:TRP:CG	1:A:522:PRO:HA	2.49	0.48
1:A:246:PRO:HG3	1:A:603:THR:HG23	1.96	0.47
1:A:578:LEU:HA	1:A:604:LEU:HD23	1.96	0.47
1:B:592:ASN:HB3	1:B:595:TYR:O	2.15	0.47
1:B:500:ARG:NH2	2:B:710:HOH:O	2.38	0.46
1:B:218:GLN:HB3	1:B:624:MET:HG2	1.96	0.46
1:B:242:CYS:HB2	1:B:611:LEU:HD13	1.99	0.45
1:A:320:LEU:HB2	1:A:384:PHE:CE2	2.52	0.45
1:A:329:LEU:HD23	1:A:332:ARG:NH2	2.32	0.45
1:A:585:CYS:HA	1:A:598:CYS:HA	1.98	0.44
1:A:218:GLN:HA	1:A:626:ASN:HB2	1.98	0.44
1:A:508:ARG:NE	2:A:727:HOH:O	2.49	0.44
1:A:200:TYR:O	1:A:282:THR:OG1	2.30	0.44
1:A:286:PHE:CE1	1:B:263:ARG:HD3	2.53	0.44
1:A:624:MET:HE2	1:A:624:MET:HB3	1.89	0.43
1:A:233:THR:HA	1:B:233:THR:HA	2.01	0.43
1:A:594:SER:HB3	1:A:624:MET:HE2	2.00	0.43
1:B:246:PRO:HG3	1:B:603:THR:HG23	2.01	0.43
1:B:395:GLN:O	2:B:701:HOH:O	2.21	0.43
1:B:240:ARG:NH2	2:B:714:HOH:O	2.39	0.43
1:A:289:PRO:HD2	1:A:597:LEU:HD21	1.99	0.42
1:B:518:VAL:HG12	1:B:524:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LEU:HD23	1:A:332:ARG:HH22	1.84	0.42
1:A:403:ARG:HD2	1:A:408:PRO:O	2.20	0.42
1:B:373:VAL:HB	1:B:461:ALA:HA	2.02	0.42
1:B:390:VAL:HG23	1:B:430:HIS:HB2	2.01	0.42
1:B:624:MET:HE3	1:B:624:MET:HB3	1.95	0.42
1:B:578:LEU:HA	1:B:604:LEU:HD23	2.02	0.41
1:B:440:SER:OG	1:B:442:ILE:O	2.38	0.41
1:A:235:THR:HG21	1:A:243:VAL:HG21	2.02	0.41
1:B:554:ASN:ND2	1:B:576:ILE:O	2.49	0.41
1:B:594:SER:HB3	1:B:624:MET:HE3	2.02	0.41
1:A:537:HIS:CG	1:A:538:PRO:HD2	2.56	0.41
1:A:536:MET:HG3	1:A:544:VAL:HG23	2.03	0.41
1:B:537:HIS:CG	1:B:538:PRO:HD2	2.56	0.41
1:A:395:GLN:HB2	2:A:703:HOH:O	2.21	0.40

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	427/657 (65%)	415 (97%)	12 (3%)	0	100	100
1	B	431/657 (66%)	418 (97%)	12 (3%)	1 (0%)	43	38
All	All	858/1314 (65%)	833 (97%)	24 (3%)	1 (0%)	48	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	589	VAL

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	367/564 (65%)	363 (99%)	4 (1%)	65	68
1	B	370/564 (66%)	368 (100%)	2 (0%)	81	85
All	All	737/1128 (65%)	731 (99%)	6 (1%)	73	77

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	387	PHE
1	A	540	PHE
1	A	617	LEU
1	A	624	MET
1	B	387	PHE
1	B	540	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	ASN
1	A	381	HIS
1	A	399	GLN
1	A	426	ASN
1	A	503	GLN
1	A	513	ASN
1	B	423	GLN
1	B	503	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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

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	429/657 (65%)	0.56	30 (6%)	22 22	12, 20, 36, 79	0
1	B	433/657 (65%)	0.71	38 (8%)	15 16	11, 21, 44, 66	0
All	All	862/1314 (65%)	0.63	68 (7%)	18 19	11, 21, 41, 79	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	ALA	7.2
1	A	199	LEU	7.1
1	A	514	GLY	6.4
1	B	514	GLY	5.4
1	A	200	TYR	5.1
1	A	384	PHE	5.1
1	B	441	VAL	5.1
1	B	442	ILE	4.9
1	B	200	TYR	4.4
1	B	198	ALA	4.1
1	A	523	GLY	4.1
1	B	518	VAL	3.9
1	B	515	CYS	3.9
1	A	513	ASN	3.9
1	B	513	ASN	3.7
1	A	515	CYS	3.4
1	B	194	ALA	3.4
1	B	418	ALA	3.3
1	B	195	TYR	3.1
1	B	516	ASN	3.0
1	B	397	GLU	3.0
1	B	440	SER	2.9
1	B	238	LEU	2.8
1	B	199	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	349	GLY	2.8
1	B	221	GLN	2.7
1	A	380	TYR	2.6
1	B	525	CYS	2.6
1	B	625	CYS	2.6
1	A	367	PHE	2.6
1	B	517	ARG	2.6
1	A	267	GLN	2.5
1	B	526	VAL	2.5
1	A	516	ASN	2.5
1	B	410	ALA	2.5
1	B	423	GLN	2.4
1	A	525	CYS	2.4
1	B	411	ASN	2.4
1	B	523	GLY	2.4
1	A	203	ARG	2.4
1	B	589	VAL	2.3
1	B	196	PRO	2.3
1	A	364	GLY	2.3
1	A	573	GLY	2.3
1	A	363	SER	2.3
1	A	439	ASP	2.3
1	A	551	GLN	2.2
1	A	576	ILE	2.2
1	A	512	PRO	2.2
1	B	417	THR	2.2
1	A	405	THR	2.2
1	A	524	GLY	2.2
1	B	521	CYS	2.2
1	A	624	MET	2.2
1	A	424	GLU	2.1
1	A	349	GLY	2.1
1	B	402	CYS	2.1
1	B	408	PRO	2.1
1	A	202	ILE	2.1
1	B	393	VAL	2.1
1	B	443	ASP	2.1
1	A	315	HIS	2.1
1	B	444	PRO	2.1
1	A	314	GLY	2.1
1	B	519	LYS	2.0
1	B	413	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	215	CYS	2.0
1	B	573	GLY	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 oligosaccharides 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.