



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2R7V / pdb_00002r7v
Title : Crystal Structure of Rotavirus SA11 VP1/RNA (GGCUUU) Complex
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Deposited on : 2007-09-10
Resolution : 2.80 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 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

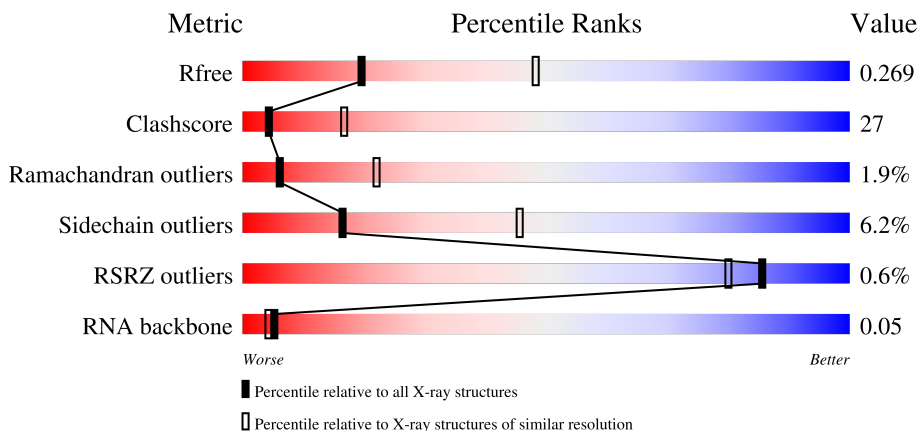
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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	X	6	
2	A	1095	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8799 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 RNA chain called RNA (5'-R(*G*GP*CP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	5	Total	C	N	O	P	0	0	0
			100	46	14	36	4			

- Molecule 2 is a protein called RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1073	Total	C	N	O	S	0	0	0
			8699	5579	1448	1634	38			

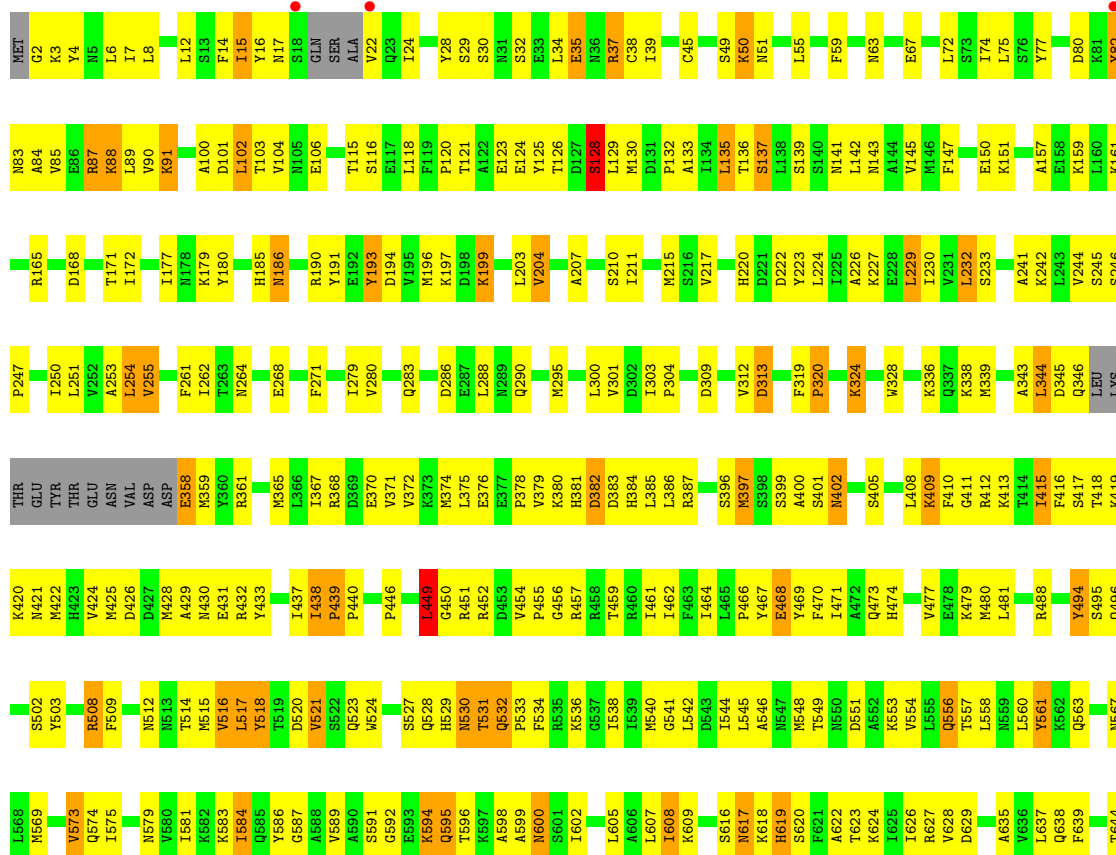
3 Residue-property plots

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: RNA (5'-R(*G*GP*CP*UP*UP*U)-3')



- Molecule 2: RNA-dependent RNA polymerase



K645	L733	T813	T886	S978	M1067
Q646	T734	S816	V887	D884	K1068
M647	K735	E817	S888	K985	K1069
I648	I736				M1070
Q649	M737		L892	I988	I1073
	Q738	L820	P893	L989	
D854	M739	F821	I894	E990	L1076
	T740	S822	Q895	S991	R1077
Y659		K823	Y896	Y992	S1078
A660	I744	N824	Q897	Y993	
R661	T745	N825	K898	Y994	F1086
		I826	F899		Q1087
K665	L748	V827	K900	S998	E1088
V666	R749	S828	P901	I999	PR0
K667	L750	R829	T902	N1000	HIS
	F751	G830	L903		HIS
V670	E754	I831	P904	G1002	HIS
S671		A832	D905	Y1004	HIS
T672	L757	L833		Q1005	HIS
V673	T758	T834	S916	L1006	
Q674		E835	R917	F1007	
I675	T762	K836	Y918		
		A837	Y919	D1008	
K679	F766	K838		F1009	
R680		L839	E922	P1012	
			D924		
I687	E769	A843	D924	L1012	
		P844		I1017	
R690	E774	I845	S928	I1018	
A691		S846	A929	A929	
	T777	L847	I930	R1019	
L895	T778		S931	I1020	
	V779	R850	R932	P1021	
E899	D780	R851	L933	F1022	
K700	E781		I934	K1023	
R701	V782	L858	S935	G1024	
		T859		K1025	
G702	V783	M860		I1026	
Q703	I784	L861	V893	P1027	
S704	Q785	Q862		A1028	
	R786	K863	T944	V1029	
T705	A787	P864	E945		
Q706	F788	V865	Y948	Y1036	
W707	M789	T866			
D708	S790	F867	Q959	K1047	
Q709		K868	L962	N1048	
	I712	S869			
L713			S963	S1053	
Y714	Y714	I872	S964	L1054	
		T873		F1055	
I718	I801	I874	I967	C1056	
V719	A803	N875	P968	N1057	
	A804		K969	Y1058	
R721	S805	R879	I970	P1059	
	S806	D880	D971	K1060	
L722	T807	T881	A972		
R723	F808	K882	D973	M1063	
		P883		I1064	
E726	K809	F884	V976	K1065	
	N810	F885	G977	L1066	
F731	V811				
I732	V812				

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.45Å 112.31Å 143.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	85.9 (50.00-2.80) 85.9 (50.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.279 0.221 , 0.269	Depositor DCC
R_{free} test set	2490 reflections (7.99%)	wwPDB-VP
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8799	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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	X	0.40	0/110	2.04	11/169 (6.5%)
2	A	0.59	0/8870	1.12	63/11989 (0.5%)
All	All	0.59	0/8980	1.14	74/12158 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	2	0

There are no bond length outliers.

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	824	ASN	N-CA-C	21.20	134.47	111.36
2	A	825	ASN	N-CA-C	14.62	127.21	111.28
2	A	196	MET	N-CA-C	11.99	124.43	111.36
1	X	1102	G	C4'-C3'-O3'	8.64	125.96	113.00
2	A	823	LYS	CA-C-N	8.53	132.40	120.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	X	1102	G	C3'
1	X	1105	U	C3'

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	X	100	0	54	7	0
2	A	8699	0	8793	473	0
All	All	8799	0	8847	475	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 27.

The worst 5 of 475 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)
2:A:520:ASP:HB3	2:A:667:LYS:HG2	1.26	1.08
2:A:865:VAL:HG22	2:A:866:THR:H	1.18	1.08
2:A:866:THR:HG22	2:A:867:PHE:H	1.24	1.02
2:A:385:LEU:HD23	2:A:479:LYS:HE2	1.41	1.01
2:A:556:GLN:HA	2:A:556:GLN:HE21	1.30	0.95

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	
2	A	1067/1095 (97%)	966 (90%)	81 (8%)	20 (2%)	6	22

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	382	ASP
2	A	431	GLU
2	A	822	SER
2	A	978	SER
2	A	1025	LYS

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
2	A	975/996 (98%)	915 (94%)	60 (6%)	16 45

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	532	GLN
2	A	1022	PHE
2	A	619	HIS
2	A	998	SER
2	A	1088	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	556	GLN
2	A	908	GLN
2	A	604	ASN
2	A	959	GLN
2	A	853	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	4/6 (66%)	3 (75%)	1 (25%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	1103	C
1	X	1104	U
1	X	1105	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1103	C

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 [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	X	5/6 (83%)	1.53	2 (40%) 1 0	113, 117, 155, 169	0
2	A	1073/1095 (97%)	-0.20	5 (0%) 87 82	17, 54, 89, 129	0
All	All	1078/1101 (97%)	-0.19	7 (0%) 85 80	17, 54, 90, 169	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	824	ASN	2.7
1	X	1106	U	2.6
2	A	82	TYR	2.4
1	X	1102	G	2.3
2	A	18	SER	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 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.