



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 02:01 AM UTC

PDB ID : 3AGQ / pdb_00003agq
Title : Structure of viral polymerase form II
Authors : Takeshita, D.; Tomita, K.
Deposited on : 2010-04-06
Resolution : 3.22 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

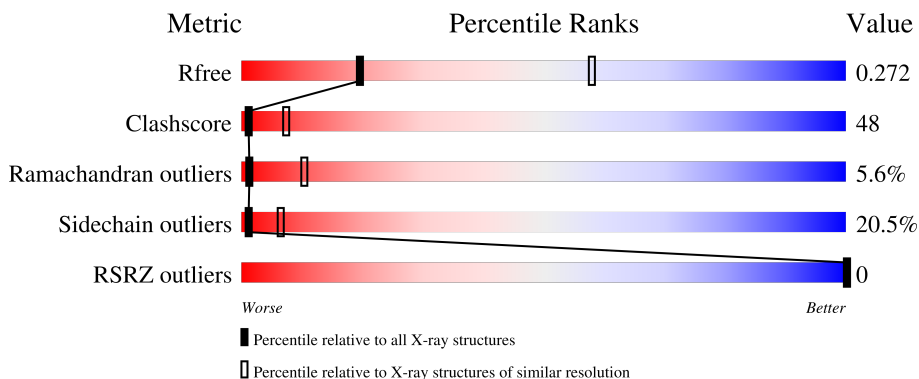
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 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	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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 $\leq 5\%$. 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	1289	28% 49% 15% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9257 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 Elongation factor Ts, Elongation factor Tu 1, LINKER, Q beta replicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1199	Total	C	N	O	S	0	0	0
			9252	5843	1600	1764	45			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	HIS	-	linker	UNP P0A6P3
A	1284	HIS	-	expression tag	UNP Q8LTE0
A	1285	HIS	-	expression tag	UNP Q8LTE0
A	1286	HIS	-	expression tag	UNP Q8LTE0
A	1287	HIS	-	expression tag	UNP Q8LTE0
A	1288	HIS	-	expression tag	UNP Q8LTE0
A	1289	HIS	-	expression tag	UNP Q8LTE0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

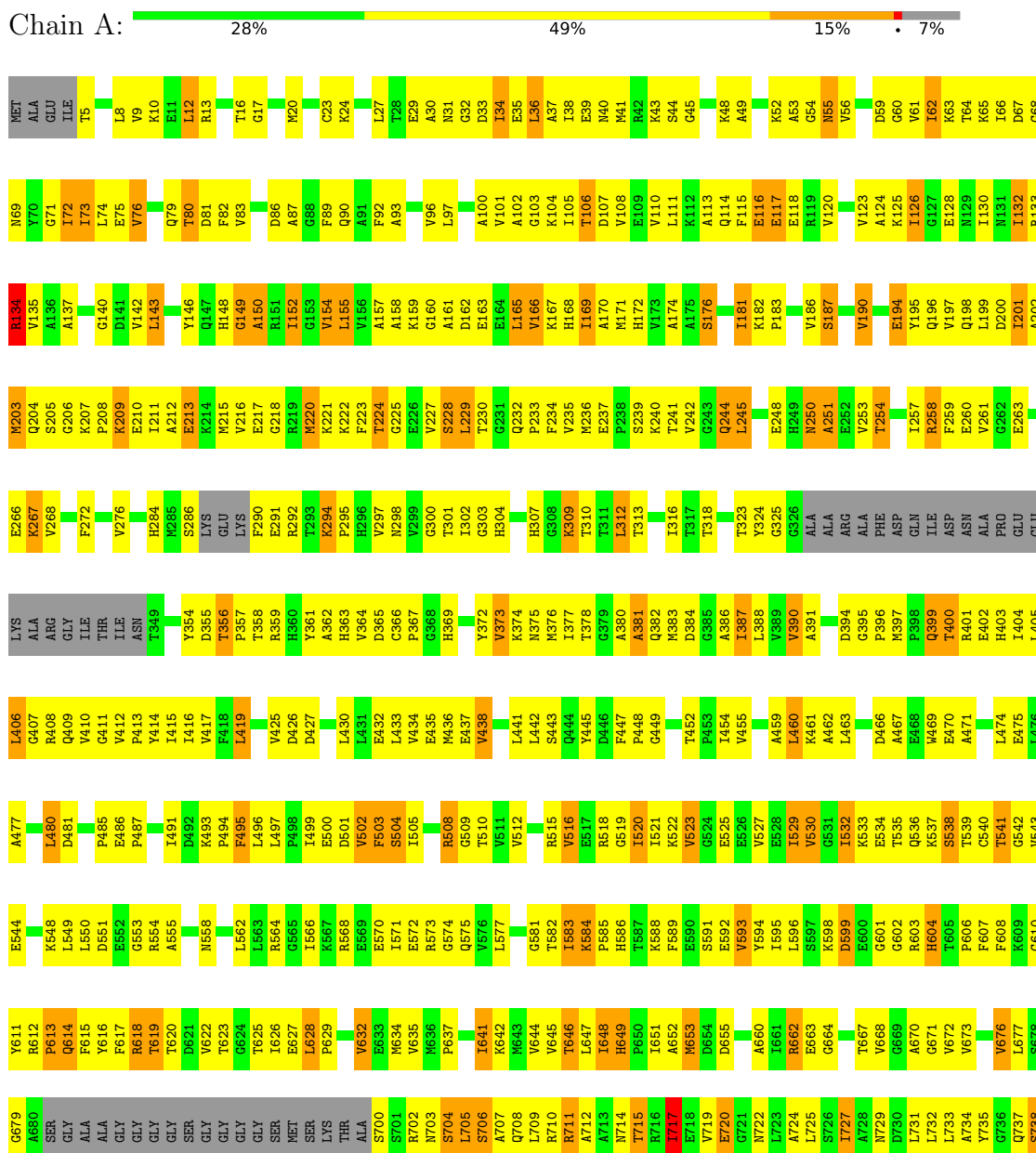
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		

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: Elongation factor Ts, Elongation factor Tu 1, LINKER, Q beta replicase



A1260	H1191	L1123	S1059	S998	L934	A868	R803	P739
C1261	T1192	R1125	C1060	P999	R937	R869	L804	F740
S1263	E1196	R1126	V1062	K1000	L938	P870	Y805	N741
R1264		A1127	P1063		R939	Q871	R806	S742
VAL	L1200	T1128	A1064	L1003	C940	C873	D808	A744
LEU	G1201	I1129	L1065	P1004	W941	T874	Y809	E743
ALA	S1202	D1130	R1066	D1005	G942	P875	S810	C746
PRO	Y1203	G1131	E1067	G1006	L943	R876	E811	I747
TYR	L1204	V1132	V1068	S1007	D944	A877	S748	S748
GLY	Y1205	W1133	F1069	V1009	L945	L878	N814	F749
VAL	D1206	D1134	K1070	T1010	Q948	K879	L817	S750
PHE	L1207	P1135	Y1071	Y1011	T949	Y880	G818	D754
GLN	F1208	R1136	V1072	E1012		V881	E819	G755
GLY	S1209	A1137	G1073	K1013			S820	T756
THR	L1210	R1138	F1074	I1014	Q952	L884	I822	
LYS	C1211	S1139	T1075	S1015	R953	R885	C821	
VAL	L1212	V1140	T1076	S1016	R954	A886	I822	D759
ALA	S1213		N1077	M1017	A955	S887	H823	F760
SER	E1214	K1143	T1078	G1018	H956	T888	M824	R761
LEU	S1215	Y1144	K1079	M1019	E957	H889	I762	I762
HIS	N1216	R1145	K1080	G1020		F990	K828	N763
GLU	ASP		T1081	Y1021	V960	D891	I829	Y764
ALA	GLY	P1149	F1082	T1022	T961	I892	L832	L765
HIS	LEU	K1150	S1083	F1023	N962	R893	L832	K766
HIS	PRO	G1151	E1084	E1024	N963	I894	I833	A767
HIS	LEU	L1152	G1085	L1025	L964	S895	G834	E768
HIS	ARG		P1086	E1026	A965	D896	D835	I769
HIS	GLY	I1157	F1087	S1027	T966	I897	V836	M770
PRO	PRO	P1158	R1088	L1028	V967	S938	P837	S771
SER	SER	D1159	E1089	I1029	D968	P999	S838	K772
GLY	GLY	G1160	S1090	F1030	L969	F900	V839	Y773
CYS		Y1161		A1031	S970	N901	E840	D774
ASP		G1162	K1093	S1032	A971		G841	D775
SER	SER	D1163	H1094	L1033	A872	V904	M842	F776
ALA	ALA	G1164	Y1095	A1034	S973	T905	L843	S777
ASP	ASP	A1165	Y1096	R1035	D974	V906	R844	F778
LEU	PHE	L1166		S1036	S975		H845	G779
PHE	LEU	V1167	V1099	V1037	S910	S910	C946	I780
A1234	A1234		D1100	C1038	S977		R847	D781
I1235	I1235	L1171	V1101	E1039	L978	D913	F848	T782
D1236	D1236	I1172	T1102	I1040	A879	R914	S849	E783
		N1173	P1103	L1041	L980	C915	G850	
		P1174		D1042	C981	I916	G851	A784
		F1175	I1106	L1043	R982	A917	A852	A786
		A1176	R1107	D1044	L983	I918	T853	W785
		K1177	H1108	S1045	L984		T854	A787
		N1178	R1109	S1046	L985		T855	E788
		R1179	I1110	E1047	L986		T856	K789
		G1180	V1111	V1048	P987	N923	N857	F790
		Y1181	S1112	T1049	G988	M924	R858	L791
		L1182	R1183	V1050	F925	S859	S859	A792
		R1245	D1115	Y1051	N990	F326	Y860	A793
		T1251	L1116	G1052	E991	Q927	G861	E796
		Y1184	I1117	D1053	Y992	L928	H862	C797
		V1185	L1118	T1054	R993	G929	P863	A798
		F1252	G1253	I1055	M994	I930	S864	L799
		F1254	V1187	I1056	G995	G931	F865	T800
		L1188	L1120	I1056	D995	L932	K866	N801
		D1255	L1121	L1057	L996	G932	K867	A802
			N1122	P1059	P997	T902	N802	
		T1260						

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	138.77Å 255.12Å 100.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.22 20.00 – 3.22	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-3.22) 97.1 (20.00-3.22)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.24Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.251 , 0.317 (Not available) , 0.272	Depositor DCC
R_{free} test set	1452 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	86.5	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.077 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.022 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9257	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.54	2/9421 (0.0%)	0.98	36/12741 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1062	VAL	CA-CB	14.54	1.62	1.54
1	A	717	ILE	CA-CB	6.12	1.60	1.54

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	SER	CA-C-O	-23.09	81.55	120.80
1	A	998	SER	CA-C-N	9.27	131.42	119.84
1	A	998	SER	C-N-CA	9.27	131.42	119.84
1	A	833	ILE	N-CA-C	8.27	118.32	110.30
1	A	869	LEU	CA-C-N	7.68	128.13	119.83

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	9252	0	9234	882	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	4	0	0	0	0
All	All	9257	0	9234	882	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 48.

The worst 5 of 882 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:930:ILE:HD11	1:A:1021:TYR:HD2	1.17	1.07
1:A:893:ARG:HH11	1:A:893:ARG:HB3	1.20	1.06
1:A:133:ARG:HG2	1:A:134:ARG:H	1.20	1.04
1:A:198:GLN:HA	1:A:201:ILE:HG12	1.37	1.04
1:A:399:GLN:H	1:A:399:GLN:HE21	1.06	1.02

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	1189/1289 (92%)	944 (79%)	179 (15%)	66 (6%)	1 10

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	GLU
1	A	134	ARG
1	A	150	ALA
1	A	176	SER
1	A	209	LYS

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	991/1060 (94%)	788 (80%)	203 (20%)	1 6

5 of 203 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	780	ILE
1	A	924	MET
1	A	1235	ILE
1	A	791	LEU
1	A	843	LEU

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

Mol	Chain	Res	Type
1	A	640	ASN
1	A	1121	ASN
1	A	714	ASN
1	A	1155	ASN
1	A	962	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

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 [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	1199/1289 (93%)	-0.27	0 100 100	72, 137, 182, 211	0

There are no RSRZ outliers to report.

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](#)

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	2001	1/1	0.46	0.15	84,84,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.