



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 26, 2023 – 02:09 AM EDT

PDB ID : 3AGQ
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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

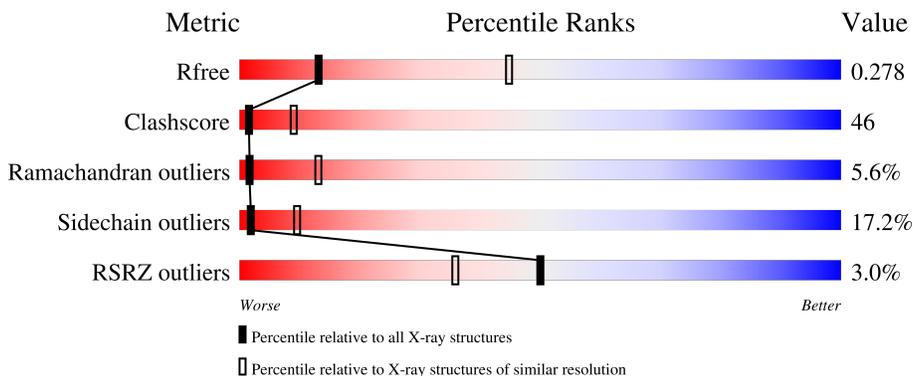
1 Overall quality at a glance

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}	130704	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (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	

2 Entry composition

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
			Total	C	N	O	S			
1	A	1199	9252	5843	1600	1764	45	0	0	0

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 (three-letter code: MG) (formula: Mg).

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

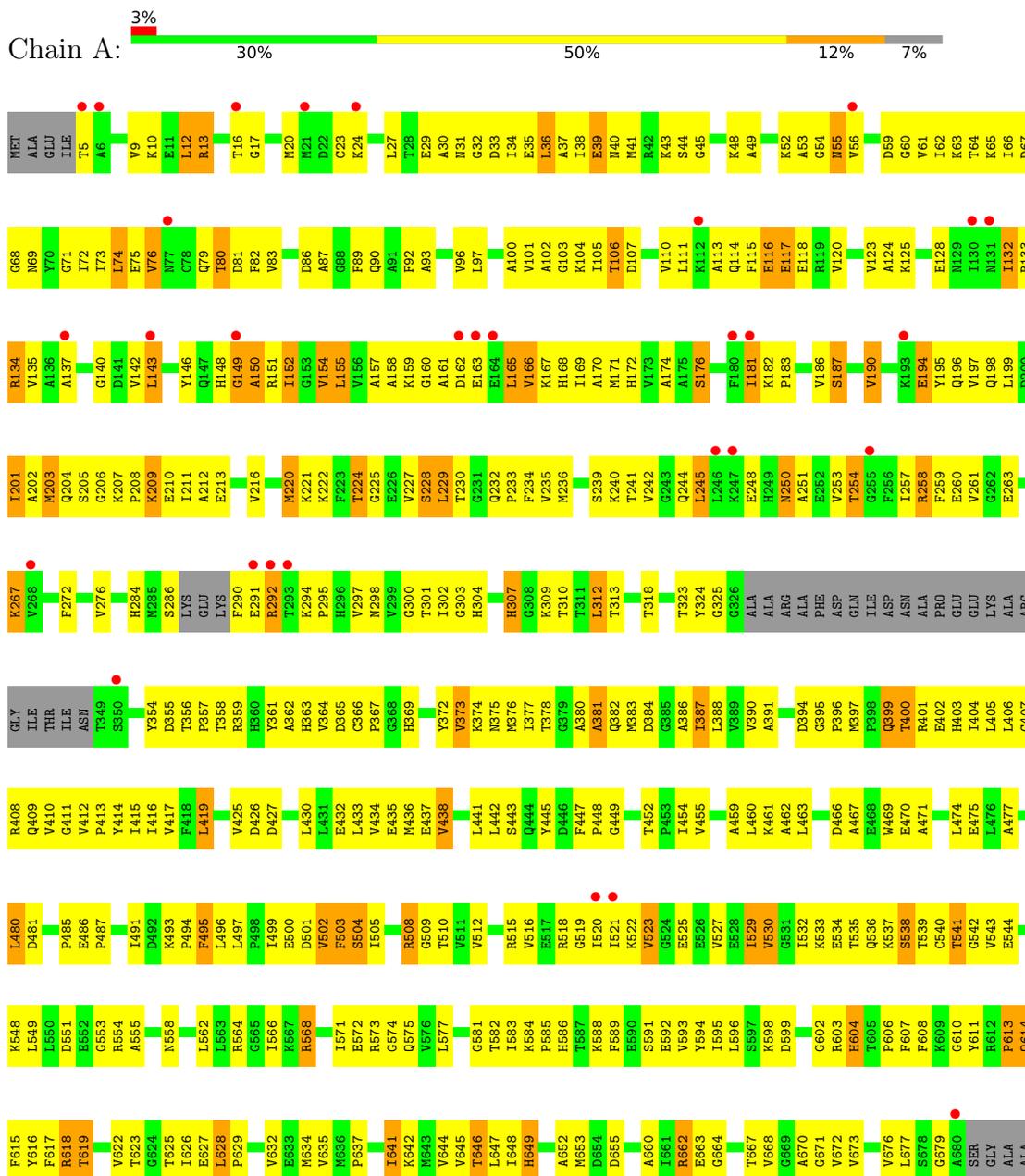
- Molecule 3 is water.

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



GLN	L1207	D1134	Y1071	V1008	D944	P875	S810	E745	GLY	S700
GLY	F1208	P1135	V1072	V1009	L945	R876	E811	C746	GLY	S701
THR	S1209	R1136	G1073	T1010	Q948	A877	D812	L747	GLY	R702
LYS	R1210	A1137	F1074	Y1011	T949	L878	F813	S748	GLY	N703
VAL	C1211	H1138	T1075	K1012	K982	K879	N814	F749	SER	S704
ALA	L1212	S1139	T1076	K1013	R983	Y880	L817	F750	GLY	L705
SER	S1213	V1140	M1077	I1014	R984	V881	G818	D754	GLY	L706
LEU	E1214	K1143	T1078	S1015	A955	L884	E819	G755	GLY	S706
HIS	S1215	Y1144	K1079	S1016	H956	R885	E820	T756	SER	S707
HIS	N1216	K1080	K1080	G1018	H957	A886	C821	S757	MET	S708
ALA	ASP	P1149	F1081	G1019	V960	S887	H822	D759	SER	S709
HIS	LEU	K1150	F1082	G1020	T961	T888	H823	F760	LYS	S710
HIS	PRO	Q1151	S1083	Y1021	N962	H889	M824	K761	THR	S711
HIS	LEU	L1152	G1084	T1022	F990	P900	K628	L762	ALA	R712
HIS	LEU	L1153	G1085	F1023	D891	K629	I629	M763		A712
HIS	GLY	I1157	F1086	E1024	N963	I892	L843	M764		A713
PRO	PRO	P1158	F1087	L1025	L964	R893	R844	M765		A714
SER	SER	D1159	R1088	E1026	A965	I894	H845	M766		A715
GLY	GLY	G1160	E1089	S1027	T986	S935	I833	K767		A716
CYS	CYS	Y1161	S1090	L1028	V967	D896	G834	E768		A717
ASP	ASP	G1162	K1093	I1029	D968	I897	D835	I769		A718
ALA	ALA	D1163	H1094	F1030	L969	S898	V836	M770		A719
ASP	ASP	A1165	Y1095	A1031	S970	P899	P837	S771		A720
LEU	LEU	L1166	Y1096	L1033	A971	F900	S838	K772		A721
PHE	PHE	V1167	Y1034	L1034	A972	N901	V839	M773		A722
	A1234	V1099	V1035	R1035	D974	V904	E840	D774		A723
	I1235	D1100	S1036	S975	S975	T905	L843	D775		A724
	I1236	I1172	V1037	I976	S976	V906	R844	F776		A725
	I1238	M1173	C1038	S977	S977	V906	F777	M714		A726
	M1243	P1174	E1039	L1040	L978	D813	C846	L778		A727
	P1244	F1175	I1040	I1041	A979	R914	G847	G779		A728
	T1245	K1177	L1042	D1042	L980	C915	F848	L780		A729
	K1246	H1108	L1043	L1043	C981	R916	S849	D781		A730
	L1247	R1179	D1044	D1044	E982	A917	T882	V719		A731
	S1248	G1180	S1045	S1045	L984	I918	G850	E720		A732
	R1249	W1181	S1046	S1046	L985	G921	A852	G721		A733
	S1250	I1182	E1047	E1047	P986	W922	T853	M722		A734
	T1251	R1183	V1048	V1048	P987	N923	T854	L723		A735
	F1254	Y1184	T1049	T1049	P988	N924	T855	L732		A736
	D1255	V1185	V1050	V1050	G988	F925	N856	L733		A737
	I1259	P1186	Y1051	Y1051	W989	F926	F925	A734		A738
	A1260	V1187	G1052	G1052	E991	Q927	R857	Y727		A739
	C1261	I1111	D1053	D1053	V992	L928	S858	L791		A740
	S1263	V1119	D1054	D1054	L993	L928	Y860	A792		A741
	R1264	L1120	I1055	I1055	L994	C929	G861	A793		A742
VAL	VAL	N1122	I1056	I1056	N994	I930	H862	E796		A743
LEU	LEU	H1123	L1057	L1057	D995	G931	P863	C797		A744
LEU	LEU	Y1124	P1058	P1058	L996	G932	S864			
ALA	ALA	R1125	S1059	S1059	R997	I933	F865	T800		
PRO	PRO	M1126	C1060	C1060	P999	L934	K866	R801		
TTR	TTR	T1127	P1063	P1063	K1000	R937	F867	A802		
GLY	GLY	A1064	A1064	A1064	L938	L938	A868	R803		
VAL	VAL	D1130	L1065	L1065	R939	P870	L869	S738		
PHE	PHE	G1131	R1066	R1066	C940	Q871	L804	P739		
		W1132	E1067	E1067	W941	A872	Y805	F740		
		M1133	V1068	V1068	G942	C873	R806	N741		
					I943	T874	D808	S742		
							E743	E743		
							Y809	Y809		

4 Data and refinement statistics i

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 30.28 – 3.22	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-3.22) 97.6 (30.28-3.22)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.24Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.251 , 0.317 0.222 , 0.278	Depositor DCC
R_{free} test set	1452 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	86.5	Xtrriage
Anisotropy	0.572	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtrriage
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	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9257	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtrriage'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	0.40	0/9421	0.62	1/12741 (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	A	286	SER	CA-C-O	-18.36	81.55	120.10

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	845	0
2	A	1	0	0	0	0
3	A	4	0	0	0	0
All	All	9257	0	9234	845	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 46.

The worst 5 of 845 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%)	2 13

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 [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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
-----	-------	----------	-----------	----------	-------------

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	991/1060 (94%)	821 (83%)	170 (17%)	2 9

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	905	THR
1	A	1049	THR
1	A	933	ILE
1	A	991	GLU
1	A	1102	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	649	HIS
1	A	1155	ASN
1	A	741	ASN
1	A	1094	HIS
1	A	729	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](#)

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 [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	1199/1289 (93%)	-0.02	36 (3%) 50 36	72, 137, 182, 211	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	700	SER	5.3
1	A	5	THR	4.3
1	A	701	SER	4.0
1	A	6	ALA	3.6
1	A	812	ASP	3.5

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 monosaccharides 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	0.67	0.34	84,84,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.