



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:08 AM UTC

PDB ID : 3AVV / pdb_00003avv
Title : Structure of viral RNA polymerase complex 3
Authors : Takeshita, D.; Tomita, K.
Deposited on : 2011-03-08
Resolution : 3.12 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

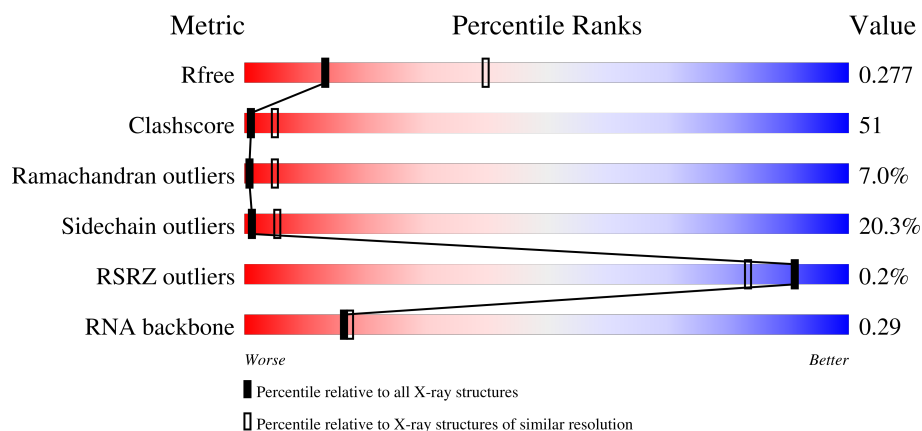
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

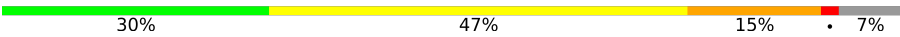
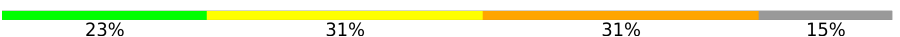
The reported resolution of this entry is 3.12 Å.

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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)
RNA backbone	3983	1017 (3.34-2.90)

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	G	8	
3	T	13	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9702 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, LINKER, Q beta replicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1203	Total	C	N	O	S	0	0	0
			9287	5865	1605	1772	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 a RNA chain called RNA (5'-R(*GP*GP*GP*UP*CP*CP*AP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	8	Total	C	N	O	P	0	0	0
			168	76	30	55	7			

- Molecule 3 is a RNA chain called RNA (5'-R(*AP*AP*CP*GP*AP*UP*GP*GP*AP*CP*CP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	11	Total	C	N	O	P	0	0	0
			235	105	44	75	11			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		

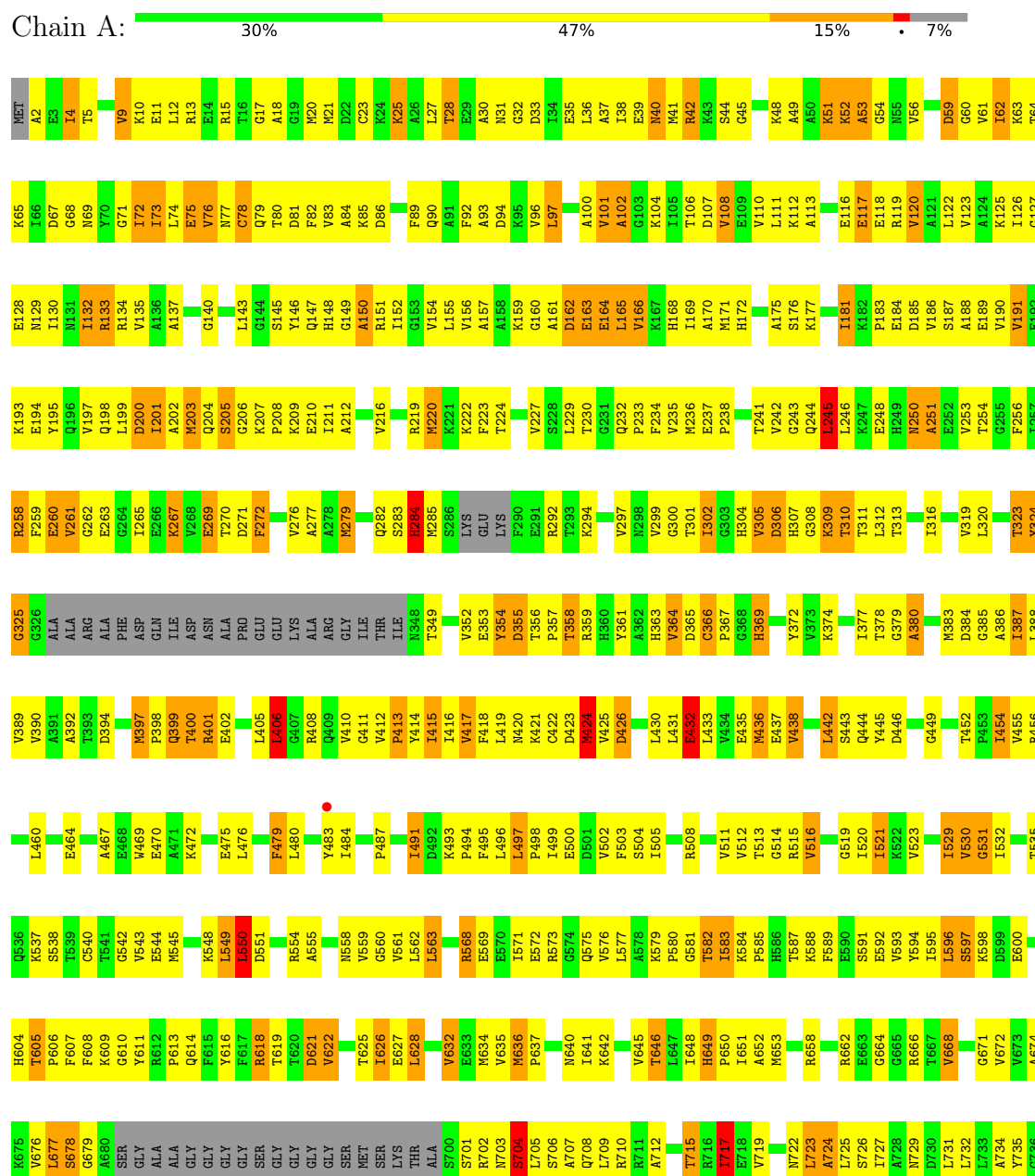
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		

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, LINKER, Q beta replicase



Q737	A802	F867	I933	L1003	V1072	L1142	R1210	LYS
S738	R803	A868	L934	L1003	G1073	K1143	C1211	VAL
P739	L804	L869	R935	D1005	F1074	Y1144	L1212	ALA
F740	Y805	P870	D936	D1005	T1075	Y1145	C2004	SER
	R806	Q871	R937	G1006	T1076	K1146	S1215	LEU
E743	P807	A872	L938	S1007	N1077	L1147	N1216	HIS
A744	D808	C873	R939	V1008	T1078	L1148	ASP	GLU
E745	Y809	T874	C940	V1009	T1081	P1149	GLY	ASP
C746	S810	P875	G941	W911	S1082	K1150	LEU	GLY
S748	E811	G942	G943	E1012	F1083	Q1151	PRO	HIS
F749	D812	I943	I943	E1012	E1084	L1152	LEU	HIS
S750	F813	L878	L878	K1013	G1085	Q1153	ARG	HIS
		Y880	D947	I1014	P1086	N1155	GLY	HIS
		Y881	Q943	I1014	F1087	T1156	PRO	HIS
T756	G818	Y882	T949	M1017	R1088	G1164	SER	
P757	S820	A883	I950	G1018	F1088	A1165	GLY	
D759	H823	L884	N951	M1019	E1089	G1166	CYS	
F760	M824	R885	Q952	G1020	S1090	V1167	ASP	
F761	A825	T888	R953	Y1021	K1093		ALA	
I762	R826		R954	T1022	H1094		ASP	
N763	R827	D891	A955	F1023	Y1095	V1170	PHE	
Y764	K828	I892	H956	E1024	Y1096	L1171	I1234	
L765	I829	R893	E957	L1025	S1097	L1172	I1235	
K766	A830	R894	G958	E1026	G1098	P1174	D1236	
A767	K831	S895	V960	S1027	V1099	F1175		
E768	L832	D896	A965	L1028	D1100	A1176	I1239	
I769	R833	R897	T966	F1030	V1101	K1177	C1240	
M770	G834	S898	V967	S1032	T1102	R1178	R1241	
S771	D835	P899	D968	L1033	F1103	R1179	S1242	
K772	V836	F900	L969	A1034	Y1105	G1180	N1243	
Y773	P837	N901	L969	L1035	I1106	W1181	P1244	
D774	S838	K902	S970	S1036	I1107	L1182	T1245	
D775	V839	A903	A971	V1037	H1108	R1183	K1246	
F776	E840	V904	S973	I1040	R1109	Y1184	I1247	
S777	G841	D974	S975		I1110	V1185	S1248	
L778	M842	P907	S976		V1111	P1186		
G779	L843	K911	S977	D1044	S1112	V1187	T1251	
I780	R844		L976	S1045	L1116	T1189	I1256	
D781	R847		L978	S1046	I1117	D1190	Q1257	
T782	F848		A979	E1047	L1118	Y1191	Y1258	
E783	S849		L980	V1048	V1119	T1192	I1259	
A784	G850		L983	T1049	L1120	R1193	A1260	
V785	G851		L984	V1050	M1121	D1194	C1261	
A786	A852		G988	D1053	W1126	R1195	S1263	
W787	T853		W989	D1054	A1127	R1197	R1264	
E788	T854		F990	I1055	T1128	E1198	VAL	
K789	T855		E991	I1056	T1129	E1199	LEU	
F790	N856		V992	L1057	D1130	L1200	ALA	
L791	N857		E992	V1062	G1131	S1201	PRO	
A792	N858		L993	P1063	V1132	T1202	TYR	
A793	S859		M994	A1064	Y1203	Y1203	GLY	
E794	G861		D995	L1065	P1135	D1206	VAL	
A795	H862		L996	R1066	R1136	L1207	PHE	
E796	C797		S997	K1070	V1140	F1208	GLN	
C797	A798		S998	Y1071	Y1141	S1209	GLY	
L799	P863						THR	
L799	S864							
F865	F865							
T800	K866							

- Molecule 2: RNA (5'-R(*GP*GP*GP*UP*CP*CP*AP*U)-3')

Chain G:  50% 38% 12%

G2001	U2004
C2005	A2007
U2008	

- Molecule 3: RNA (5'-R(*AP*AP*CP*GP*AP*UP*GP*GP*AP*CP*CP*CP*A)-3')

Chain T:  23% 31% 31% 15%

A	C2103	G2104	A2105	U2106	G2107	G2108	A2109	C2110	C2111	C2112	A2113
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	138.99Å 255.09Å 101.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.12 20.00 – 3.12	Depositor EDS
% Data completeness (in resolution range)	90.4 (20.00-3.12) 95.3 (20.00-3.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.226 , 0.298 0.214 , 0.277	Depositor DCC
R_{free} test set	1571 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.079 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.057 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9702	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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

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

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	0.67	2/9456 (0.0%)	1.01	43/12787 (0.3%)
2	G	0.33	0/187	0.41	0/290
3	T	0.39	0/262	0.56	0/406
All	All	0.66	2/9905 (0.0%)	0.99	43/13483 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	717	ILE	CA-CB	5.67	1.61	1.54
1	A	1076	THR	CA-CB	5.45	1.60	1.53

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1018	GLY	N-CA-C	-8.91	104.05	113.58
1	A	1086	PRO	N-CA-C	-8.36	105.98	114.68
1	A	444	GLN	N-CA-C	-8.25	103.24	113.38
1	A	919	GLU	CA-C-N	-7.40	112.13	119.90
1	A	919	GLU	C-N-CA	-7.40	112.13	119.90

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	9287	0	9273	950	0
2	G	168	0	88	9	0
3	T	235	0	121	17	0
4	A	2	0	0	0	0
5	A	10	0	0	0	0
All	All	9702	0	9482	969	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 51.

The worst 5 of 969 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:1189:THR:HG21	1:A:1257:GLN:HE21	1.05	1.11
1:A:72:ILE:HG12	1:A:137:ALA:HB2	1.37	1.07
1:A:198:GLN:HA	1:A:201:ILE:HG12	1.37	1.05
1:A:930:ILE:HD13	1:A:931:GLY:N	1.70	1.05
1:A:930:ILE:HD11	1:A:1021:TYR:HB3	1.32	1.04

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	1193/1289 (93%)	910 (76%)	200 (17%)	83 (7%)	1 5

5 of 83 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	31	ASN
1	A	101	VAL

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Mol	Chain	Res	Type
1	A	150	ALA
1	A	261	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	995/1060 (94%)	793 (80%)	202 (20%)	1 5

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	785	VAL
1	A	939	ARG
1	A	1251	THR
1	A	800	THR
1	A	855	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	871	GLN
1	A	1019	ASN
1	A	952	GLN
1	A	1077	ASN
1	A	586	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	7/8 (87%)	1 (14%)	0
3	T	10/13 (76%)	5 (50%)	0
All	All	17/21 (80%)	6 (35%)	0

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	2008	U
3	T	2106	U
3	T	2108	G
3	T	2109	A
3	T	2110	C

There are no RNA pucker outliers to report.

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](#)

Of 2 ligands modelled in this entry, 2 are 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	1203/1289 (93%)	-0.69	2 (0%) 91 83	26, 65, 111, 136	0
2	G	8/8 (100%)	-0.52	0 100 100	68, 87, 110, 112	0
3	T	11/13 (84%)	-0.65	0 100 100	66, 84, 110, 124	0
All	All	1222/1310 (93%)	-0.68	2 (0%) 91 83	26, 66, 111, 136	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1236	ASP	2.4
1	A	483	TYR	2.1

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
4	CA	A	3001	1/1	0.89	0.09	65,65,65,65	0
4	CA	A	3002	1/1	0.96	0.12	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.