



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:03 PM BST

PDB ID : 4AU6
EMDB ID: : EMD-2100
Title : Location of the dsRNA-dependent polymerase, VP1, in rotavirus particles
Authors : Estrozi, L.F.; Settembre, E.C.; Goret, G.; McClain, B.; Zhang, X.; Chen, J.Z.; Grigorieff, N.; Harrison, S.C.
Deposited on : 2012-05-14
Resolution : 6.00 Å(reported)
Based on PDB ID : 2R7O

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

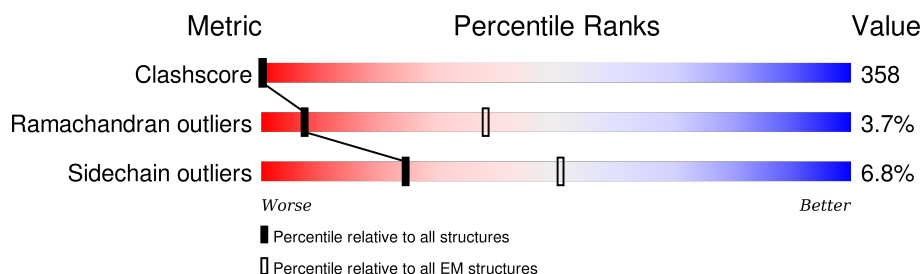
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1095	
1	B	1095	
1	C	1095	
1	D	1095	
1	E	1095	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 43705 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 RNA-DEPENDENT RNA POLYMERASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1071	Total	C	N	O	S	10	0
			8741	5604	1457	1642	38		
1	B	1071	Total	C	N	O	S	10	0
			8741	5604	1457	1642	38		
1	C	1071	Total	C	N	O	S	10	0
			8741	5604	1457	1642	38		
1	D	1071	Total	C	N	O	S	10	0
			8741	5604	1457	1642	38		
1	E	1071	Total	C	N	O	S	10	0
			8741	5604	1457	1642	38		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP O37061
A	-4	HIS	-	EXPRESSION TAG	UNP O37061
A	-3	HIS	-	EXPRESSION TAG	UNP O37061
A	-2	HIS	-	EXPRESSION TAG	UNP O37061
A	-1	HIS	-	EXPRESSION TAG	UNP O37061
A	0	HIS	-	EXPRESSION TAG	UNP O37061
A	1089	PRO	-	EXPRESSION TAG	UNP O37061
B	-5	HIS	-	EXPRESSION TAG	UNP O37061
B	-4	HIS	-	EXPRESSION TAG	UNP O37061
B	-3	HIS	-	EXPRESSION TAG	UNP O37061
B	-2	HIS	-	EXPRESSION TAG	UNP O37061
B	-1	HIS	-	EXPRESSION TAG	UNP O37061
B	0	HIS	-	EXPRESSION TAG	UNP O37061
B	1089	PRO	-	EXPRESSION TAG	UNP O37061
C	-5	HIS	-	EXPRESSION TAG	UNP O37061
C	-4	HIS	-	EXPRESSION TAG	UNP O37061
C	-3	HIS	-	EXPRESSION TAG	UNP O37061
C	-2	HIS	-	EXPRESSION TAG	UNP O37061
C	-1	HIS	-	EXPRESSION TAG	UNP O37061
C	0	HIS	-	EXPRESSION TAG	UNP O37061

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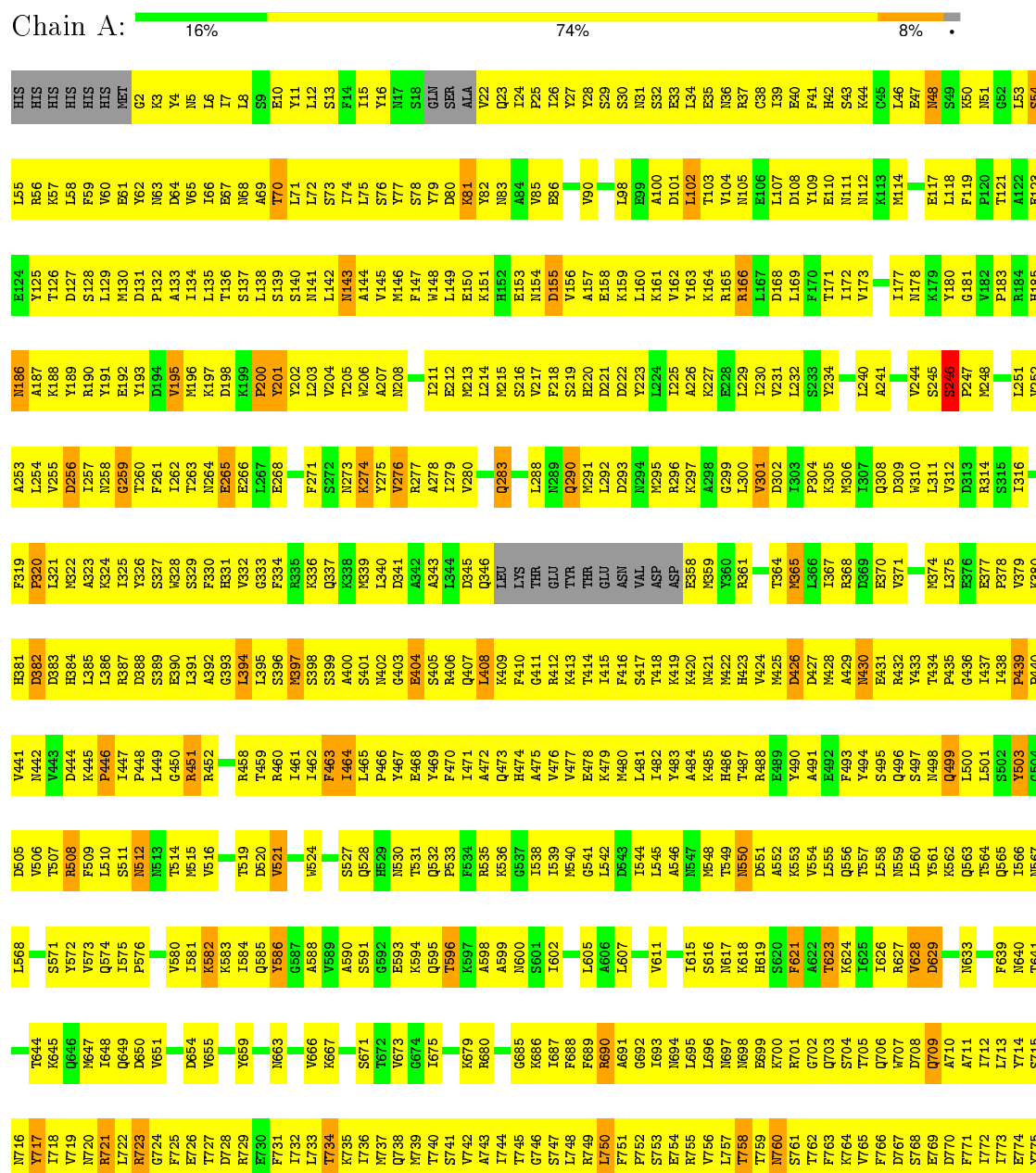
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1089	PRO	-	EXPRESSION TAG	UNP O37061
D	-5	HIS	-	EXPRESSION TAG	UNP O37061
D	-4	HIS	-	EXPRESSION TAG	UNP O37061
D	-3	HIS	-	EXPRESSION TAG	UNP O37061
D	-2	HIS	-	EXPRESSION TAG	UNP O37061
D	-1	HIS	-	EXPRESSION TAG	UNP O37061
D	0	HIS	-	EXPRESSION TAG	UNP O37061
D	1089	PRO	-	EXPRESSION TAG	UNP O37061
E	-5	HIS	-	EXPRESSION TAG	UNP O37061
E	-4	HIS	-	EXPRESSION TAG	UNP O37061
E	-3	HIS	-	EXPRESSION TAG	UNP O37061
E	-2	HIS	-	EXPRESSION TAG	UNP O37061
E	-1	HIS	-	EXPRESSION TAG	UNP O37061
E	0	HIS	-	EXPRESSION TAG	UNP O37061
E	1089	PRO	-	EXPRESSION TAG	UNP O37061

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

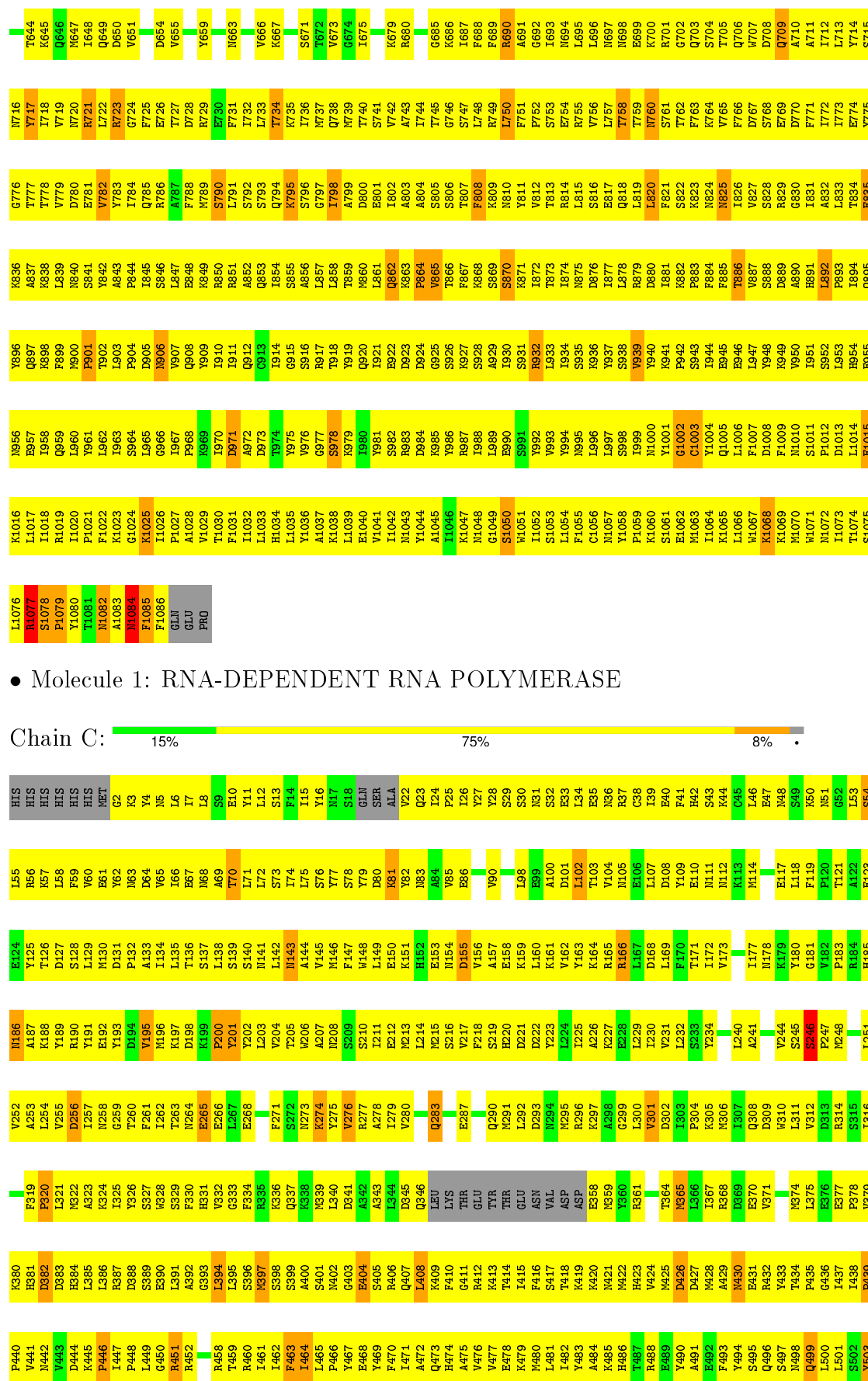
• Molecule 1: RNA-DEPENDENT RNA POLYMERASE



L568	D505	V441	H381	F319	A253	H186	E124	L55	HIS	K1016	Y956	Y896	K836	G776
S571	V506	M442	D382	P320	L254	A187	Y125	R56	HIS	L1017	E957	Q897	A837	T777
V572	T507	V443	D383	L321	V255	K188	D126	K37	HIS	L1018	E958	K898	K338	T778
V573	S508	D444	K384	M322	D266	Y189	D127	L58	HIS	R1019	Q959	F899	L339	V779
Q574	F509	K445	L385	A323	L257	R190	S128	F59	HIS	P1020	L960	N900	N840	D780
S575	L510	P446	L386	K324	N258	Y191	L129	E61	HIS	P1021	Y961	P901	S841	E781
P576	S511	I447	K387	L325	G259	E192	M130	E81	HIS	F1022	L962	T902	Y842	V782
	P512	P448	D388	Y326	T260	Y193	D131	Y62	MET	K1023	L963	L903	A843	V783
	P513	L449	S389	S327	F261	D194	A133	N63		G1024	S964	P904	P844	V784
V580	T514	G450	E390	M328	T262	V195	A133	D64		K1025	L965	D905	K846	V785
L581	M515	R451	L391	S329	T263	M196	I134	V65		P1027	L967	Y907	S846	V786
K582	V516	R452	A392	F330	N264	K197	L136	I66		P1028	P968	Q908	L847	V787
L583	L517		G393	E265	K198	D198	T136	E67		V1029	K969	Y909	K849	V788
	V518	R458	L394	E266	K199	P200	S137	N68		L1030	P970	Y910	K849	V789
Q585	T519	T459	L395	G333	L267	Y201	L138	A69		T1031	D971	Y911	R850	V790
V521	D520	R460	S396	F334	E268	Y202	S139	T70		F1031	A972	Q912	R851	L791
	V524	I461	K397	K335	F271	L203	N140	L71		L1032	K974	Y913	A852	V792
		I462	S398	R336	N272	L204	N142	S73		H1034	V975	G915	Q853	V793
V529	Q528	F463	S399	Q337	N273	T205	N143	I74		L1035	Y976	G916	I854	V794
E529	H529	L465	S401	K338	N274	M206	A144	L75		L1036	Y977	S917	S855	V795
E530	N530	P466	N402	L340	K275	A207	V145	S76		A1037	G977	T918	A856	V796
K594	T531	Y467	G403	D341	V276	N208	M146	Y77		K1038	S978	Y919	L857	V797
Q595	O532	E468	E404	A342	R277		F147	S78		L1039	K979	Q920	T859	V798
P533	P533	F470	S405	A343	A278		M148	Y79		E1040	T980	Q921	M860	V799
			R406	L344	L279		L149	D80		V1041	Y981	T921	L861	D800
K597	F534	V477	Q407	D345	V280	E212	E150	K81		N1042	S982	E922	Q862	E801
A598	R535	A472	L408	Q346		M213	K151	Y82		L1043	S983	D923	K863	L802
A599	K536	H473	F409	LEU	Q283	L214	E152	N83		L1044	D984	D924	P864	A804
N600	G537	H474	F410	LVS	E287	S216	E153	A84			K985	G925	V865	S805
S601	T538	A475	G411	THR		V217	M154	V85		K1047	Y986	S926	T866	S806
L602	T539	V476	R412	GLU		F218	D155	E86		N1048	R987	K927	P867	T807
	P540	V477	K413	THR	Q290	S219	V156	V90		G1049	S988	S928	K868	F808
L605	G541	E478	T414	THR	M291	H220	A157	K81		S1050	L989	A929	S869	K809
L607	L542	K479	L415	GLU	L292	D221	E158	Y28		D1051	E990	T930	S870	N810
	D543	M480	F416	ASN	D293	D222	K159	S30		L1052	S991	S931	K871	V811
	L544	L481	S417	VAL	N294	Y223	L160	N31		S1053	Y992	R932	I872	V812
	L545	I482	T418	ASP	K295	L224	K161	S32		L1054	Y993	L933	T873	T813
I615	A546	Y483	K419	ASP	K296	I225	V162	E33		F1055	Y994	L934	I874	R814
S616	H548	A484	K420	E358	K297	A226	Y163	E33		C1056	N995	S935	N875	L815
N617	T549	K485	N421	M359	A298	K227	K164	E35		N1057	L996	K936	D876	S816
K618	N550	H486	M422	Y360	G299	E228	R165	N36		P1058	L997	Y937	I877	E817
H619	D551	T487	H423	R361	L300	L229	L167	N105		P1059	S998	S938	L878	D818
	A552	R488	V424		V301	I230	L167	E106		K1060	Y999	V939	R879	L819
S620	A553	E489	M425	T364	D302	V231	D168	L107		S1061	N1000	Y940	D880	L820
F621	K553	Y490	D426	M365	L303	L232	L169	D108		E1062	Y1001	P941	I881	F821
A622	V554	A491	D427	L366	F304	S233	F170	Y109		M1063	G1002	P942	K882	S822
T623	L555	E492	M428	L367	K305	Y234	T171	E110		L1064	C1003	S943	K883	K823
K624	O556	F493	A429	K368	N306		N112	H42		K1065	Y1004	Y944	F884	N824
I625	T557	Y494	M430	D369	L307	L240	V173	K44		L1066	Q1005	F945	P885	V825
I626	L558	S495	E431	E370	Q308	A241	K113	G45		M1067	L1006	E946	T886	L826
R627	N559	Q496	R432	V371	D309	V244	I177	L46		K1068	F1007	L947	V887	V827
V628	L560	S497	Y433	M374	N310	S245	M178	E47		M1069	D1008	Y948	S888	S828
D629	V561	M498	T434	L375	L311	S246	K179	N48		N1070	F1009	K949	D889	R829
	K562	Q499	P435	V312	V312	P247	Y180	S49		M1071	N1010	V950	A890	G830
	O563	L500	G436	E376	D313	M248	G181	F119		N1072	S1011	Y951	H891	T831
T641	T564	L501	L437	E377	R314	M248	V182	P120		L1073	P1012	S952	L892	A832
	Q565	S502	L438	P378	S315	L251	P183	T121		S1074	D1013	L953	P893	L833
	V566	Y503	P439	V379	T316	V252	R184	L1014		S1075	L1014	H954	L894	T834
	N567	G504	P440	K380			H185	E123		L1076	E1015	S955	Q895	E835

● Molecule 1: RNA-DEPENDENT RNA POLYMERASE

Chain B:  15% 74% 8%





V252	F319	M186	E124	L55	HIS
	L253	A187	V125	R56	HIS
	L254	K188	T126	K57	HIS
	D255	V189	D127	L58	HIS
	D256	R190	S128	F59	HIS
	T257	V191	L129	V60	HIS
	N258	E192	D130	E61	MET
	G259	F193	M131	Y62	G2
	T260	D194	P132	N63	K3
	F261	V195	A133	D64	K4
V253	K262	M196	L134	V65	N5
	T263	K197	L135	L66	L6
	N264	D198	T136	E67	L7
	F330	K199	S137	N68	L8
	E265	P200	L138	A69	S9
	E266	G201	S139	T70	E10
	L267	Y202	D140	L71	Y11
	E268	L203	M141	L72	L12
	F271	V204	L142	S73	S13
	S272	T205	M143	I74	F14
V254	K273	D206	A144	L75	I15
	K339	A207	V145	S76	Y16
	K274	N208	M146	V77	M17
	V275	S209	F147	S78	S18
	V276	S210	M148	Y79	GLN
	T277	L211	L149	D80	SER
	A278	E212	E150	K81	ALA
	L279	M213	K151	Y82	V22
	V280	L214	M152	N83	Q23
	Q283	M215	E153	A84	L24
V255	L288	S216	M154	V85	P25
	T289	V217	D155	E86	T26
	Q290	F218	V156	Y90	Y27
	K291	S219	A157	Y90	Y28
	L292	H220	E158	S29	S29
	ASN	D221	K159	L98	S30
	D293	D222	L160	E99	N31
	V294	Y223	K161	A100	S32
	ASP	L224	V162	D101	E33
	ASP	L225	Y163	L102	L34
V256	K297	A226	K164	T103	E35
	K369	K227	R165	V104	N36
	G299	E228	R166	N105	R37
	V360	L229	L167	E106	C38
	V301	T230	D168	L107	I39
	N302	V231	L169	D108	E40
	K303	L232	F170	Y109	F41
	F304	S233	T171	E110	H42
	K305	Y234	I172	N111	S43
	N307	L240	V173	N112	K44
V257	Q308	A241	I177	K113	C45
	D309	Y244	M178	M114	L46
	K310	S245	K179	E117	E47
	L311	N48	L118	E117	M48
	V312	E246	K181	F119	S49
	D313	P247	V182	P120	K50
	K314	M248	P183	T121	N51
	S315	L249	K184	E122	G52
	T316	L351	H185	F122	L53
	P370	L352	F186	E123	S54

- Molecule 1: RNA-DEPENDENT RNA POLYMERASE

Chain E:  15% 75% 8%

M186	M187	M188	E124	L55	H15
K438	K439	K440	Y125	R56	H15
K489	K490	K491	K126	K57	H15
K190	K191	K192	L127	L58	H15
E192	E193	E194	L128	L60	H15
L193	L194	L195	M130	B61	NET
L196	L197	L198	D131	V62	G2
L199	L200	L201	P132	N63	K3
L202	L203	L204	A133	D64	K4
L205	L206	L207	L134	V65	N5
L208	L209	L210	L135	L66	L6
L211	L212	L213	L136	B67	L7
L214	L215	L216	P137	N68	L8
L217	L218	L219	L138	A69	S9
L220	L221	L222	S139	T70	E10
L223	L224	L225	S140	L71	E11
L226	L227	L228	M141	L72	L12
L229	L230	L231	L142	S73	S13
L232	L233	L234	M143	T74	F14
L235	L236	L237	A144	L75	L15
L238	L239	L240	V145	S76	L16
L241	L242	L243	M146	V77	L17
L244	L245	L246	F147	S78	L17
L247	L248	L249	M148	V79	S18
L250	L251	L252	E150	D80	GLN
L253	L254	L255	K151	Y82	SER
L256	L257	L258	M152	N83	ALA
L259	L260	L261	E153	A84	V22
L262	L263	L264	M154	B85	Q23
L265	L266	L267	D155	E86	L24
L268	L269	L270	V156	V90	P25
L271	L272	L273	A157	Y90	L26
L274	L275	L276	E158		V27
L277	L278	L279	K159	L98	Y28
L280	L281	L282	L160	E99	S29
L283	L284	L285	V161	A100	S30
L286	L287	L288	D162	D101	N31
L289	L290	L291	V163	L102	S32
L292	L293	L294	K164	T103	E33
L295	L296	L297	R165	V104	L34
L298	L299	L300	R166	E105	E35
L301	L302	L303	L167	N106	N36
L304	L305	L306	D168	D107	R37
L307	L308	L309	L169	L108	C38
L310	L311	L312	F170	Y109	L39
L313	L314	L315	T171	E110	E40
L316	L317	L318	I172	M111	F41
L319	L320	L321	V173	N112	R42
L322	L323	L324	M177	L114	S43
L325	L326	L327	K178	E117	R44
L328	L329	L330	K179	L118	E45
L331	L332	L333	Y180	F119	L46
L334	L335	L336	V182	P120	E47
L337	L338	L339	P183	T121	N48
L340	L341	L342	F184	E122	S49
L343	L344	L345	K185	F123	K50
L346	L347	L348			N51
L349	L350	L351			E52
L352	L353	L354			L53
L355	L356	L357			S54

S1075	E1015	E955	Q895	E835	Y775	S715	T641	N567	G504	P440	K380	F319	A253
L1076	K1016	N956	Y896	K836	G776	N716	T644	L568	D605	V441	H381	P320	L254
S1078	L1017	E957	Q897	K837	T777	T717	T645	S571	V506	N442	D382	D256	V255
P1079	I1018	N958	K898	K838	T778	T718	Q646	Y572	T507	D443	D383	L321	D257
Y1080	R1019	Q959	K899	L839	V779	V719	N508	Y573	B508	K445	H384	K322	N258
T1081	I1020	N960	M900	N840	D780	N720	N546	V574	L510	P446	L385	A323	C259
N1082	P1021	Y961	P901	S841	E781	R721	T648	Q574	S511	I447	L386	K324	T260
F1083	F1022	L962	T902	T842	T782	L722	D650	I575	N512	P449	D388	I325	F261
N1084	K1023	N963	L903	A843	T783	R723	V651	V580	N513	L449	S389	Y326	T262
F1085	G1024	P904	D905	P844	T784	F724	T654	I581	T514	G450	E390	K328	T263
F1086	K1025	N965	N906	I845	Q785	F725	V655	K582	N515	R451	L391	S329	N264
GLN	I1026	G966	N907	S846	R786	T726	T656	K583	V516	R452	A392	F330	E265
GLU	P1027	I967	Q908	E846	T787	D728	T659	I584	T519	R458	G393	H331	E266
PRO	A1028	P968	Q909	E848	F788	R729	T659	Q585	D520	T459	L394	V332	L267
	V1029	K969	I910	K850	S790	E730	N663	Y586	D521	R460	G395	G333	E268
	T1030	T970	I911	R851	T791	F731	N666	G587	N524	I461	N397	F334	F271
	I1032	A972	Q912	A852	S792	T732	K667	E588	N527	F463	S398	K335	S272
	L1033	D973	G913	K853	T793	L733	S671	Y589	B528	I464	A400	Q337	N273
	H1034	T974	I914	I854	Q794	T734	T672	A590	E529	P466	S401	K338	Y275
	L1035	Y975	G915	S855	K795	K735	N573	S591	B529	I465	N402	N339	Y276
	L1036	V976	S916	A856	S796	T736	T674	G592	E530	Y467	G403	L340	D277
	A1037	G977	R917	L857	T797	M737	V673	E593	N530	E404	E403	D341	A278
	S978	S978	T918	L858	T798	Q738	N574	K594	T531	E468	S405	A342	I279
	K979	A799	Y919	T859	D799	T739	G674	Q595	Q532	Y469	R406	A343	V280
	E1040	E1040	Q920	N860	D800	T740	T675	T596	F533	F470	Q407	D345	
	V1041	I981	I921	L861	E801	S741	K679	K597	F534	I471	L408	Q346	Q283
	L1042	S982	E922	K862	T802	F742	N680	A598	N536	A472	K409	LEU	E287
	N1043	K983	D923	K863	A743	A743	T680	A599	K536	Q473	F410	THR	L288
	L1044	D924	A804	P864	A804	T744	G685	N600	G537	H474	G411	GLU	N289
	A1045	K985	G925	V865	S805	T745	K686	G601	E538	A475	G412	THR	N290
	T1046	S986	S926	T866	S806	T746	F688	L602	N540	V476	R413	GLU	D293
	K1047	R987	K927	F867	T807	S747	L605	L606	L542	E478	T414	THR	L292
	N1048	L988	S928	K868	K809	L748	L607	L607	G543	K479	L415	ASN	D293
	G1049	L989	A929	S869	F689	R749	L607	L607	L544	M480	F416	VAL	N294
	S1050	E990	I930	S870	N810	L750	B690	A606	N547	M481	S417	ASP	N295
	H1051	S991	S931	K871	Y811	F751	A691	L607	L545	I481	I418	ASP	R296
	L1052	Y992	R832	I872	N812	F752	G692	V611	L546	I482	K419	ASP	K297
	S1053	Y993	L933	T873	T813	S753	L693	L615	N548	Y490	D426	E358	E298
	L1054	Y994	I934	I874	R814	E754	N694	S616	N549	A491	D427	K359	L300
	F1055	N995	S935	N875	L815	F755	L695	N617	T549	K485	N421	K360	F301
	C1056	L996	K936	D876	S816	V756	L696	K618	N550	H466	H422	R361	D302
	N1057	L997	Y937	I877	E817	L757	N697	H619	T557	T487	V424	T364	D303
	S998	S998	S938	L878	Q818	T758	N698	E699	L554	R488	N423	L366	F304
	P1059	Y999	Y939	R879	L819	T759	E699	S620	T555	E489	A429	R368	K305
	K1060	N1000	Y940	D880	L820	N760	K700	F621	T557	Y494	N430	D699	N306
	S1061	Y1001	K941	I881	F821	S761	R701	F621	L558	Y490	E431	E370	I307
	E1062	K1002	P942	K882	S822	T762	G702	A622	N559	A491	D427	V371	Q308
	M1063	G1003	S943	P883	K823	F763	Q703	T623	L555	E482	N428	I367	D309
	L1064	Y1004	I944	P884	N824	K764	S704	K624	Q556	F493	A429	K306	N310
	K1065	Q1005	E945	F885	N825	V765	T705	T625	T557	Y494	N430	D699	L307
	L1066	E946	E946	T886	I826	F766	Q706	L626	L558	S495	E431	E370	Q308
	M1067	F1007	L947	V887	V827	D767	T707	R627	N559	Q496	R432	V371	D309
	K1068	D1008	Y948	S888	S828	S768	D708	N629	L560	S497	Y433	N374	N310
	M1069	F1009	K949	D889	R829	E769	Q709	D629	N561	Q498	T434	L311	L311
	N1070	N1010	V950	A890	G830	D770	A710	N633	K562	Q499	P435	L375	V312
	W1071	S1011	I851	R891	I831	F771	A711	N633	Q563	L500	G436	E376	E313
	N1072	P1012	S952	L892	A832	T772	L712	F639	T564	L501	I437	E377	R314
	T1073	D1013	L953	P893	L833	T773	L713	N640	T565	S502	I438	P378	S315
	T1074	H954	H954	I894	T834	E774	T714		L566	Y503	P439	V379	I316

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	INDIVIDUAL PARTICLE PHASE FLIPPING	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.41	0/8914	0.62	5/12052 (0.0%)
1	B	0.41	0/8914	0.62	5/12052 (0.0%)
1	C	0.40	0/8914	0.62	5/12052 (0.0%)
1	D	0.41	0/8914	0.62	5/12052 (0.0%)
1	E	0.40	0/8914	0.62	5/12052 (0.0%)
All	All	0.40	0/44570	0.62	25/60260 (0.0%)

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	1082[A]	ASN	N-CA-C	6.33	128.08	111.00
1	E	1082[B]	ASN	N-CA-C	6.33	128.08	111.00
1	C	1082[A]	ASN	N-CA-C	6.31	128.04	111.00
1	C	1082[B]	ASN	N-CA-C	6.31	128.04	111.00
1	A	1082[A]	ASN	N-CA-C	6.30	128.01	111.00

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	8741	0	8343	11726	0
1	B	8741	0	8344	11702	0
1	C	8741	0	8343	11680	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	8741	0	8341	11771	0
1	E	8741	0	8341	11762	0
All	All	43705	0	41712	30580	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 358.

The worst 5 of 30580 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:789:MET:SD	1:C:786:ARG:HD3	1.25	1.77
1:A:786:ARG:HD3	1:D:789:MET:SD	1.25	1.77
1:B:786:ARG:HD3	1:E:789:MET:SD	1.25	1.75
1:C:789:MET:SD	1:E:786:ARG:HD3	1.25	1.75
1:B:789:MET:SD	1:D:786:ARG:HD3	1.25	1.73

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 PDB entries followed by that with respect to all EM entries.

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	1073/1095 (98%)	926 (86%)	105 (10%)	42 (4%)	4	36
1	B	1073/1095 (98%)	927 (86%)	104 (10%)	42 (4%)	4	36
1	C	1073/1095 (98%)	926 (86%)	105 (10%)	42 (4%)	4	36
1	D	1073/1095 (98%)	926 (86%)	105 (10%)	42 (4%)	4	36
1	E	1073/1095 (98%)	926 (86%)	105 (10%)	42 (4%)	4	36
All	All	5365/5475 (98%)	4631 (86%)	524 (10%)	210 (4%)	7	36

5 of 210 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	SER
1	A	397	MET
1	A	401	SER
1	A	864	PRO
1	A	978	SER

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 PDB entries followed by that with respect to all EM entries.

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	979/996 (98%)	911 (93%)	68 (7%)	19	56
1	B	979/996 (98%)	912 (93%)	67 (7%)	20	57
1	C	979/996 (98%)	911 (93%)	68 (7%)	19	56
1	D	979/996 (98%)	911 (93%)	68 (7%)	19	56
1	E	979/996 (98%)	911 (93%)	68 (7%)	19	56
All	All	4895/4980 (98%)	4556 (93%)	339 (7%)	24	56

5 of 339 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	283	GLN
1	C	886	THR
1	E	690	ARG
1	C	320	PRO
1	C	621	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	290	GLN
1	C	810	ASN
1	E	653	ASN
1	C	384	HIS
1	C	556	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.