



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 05:34 pm GMT

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 initial model : 2R7O

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

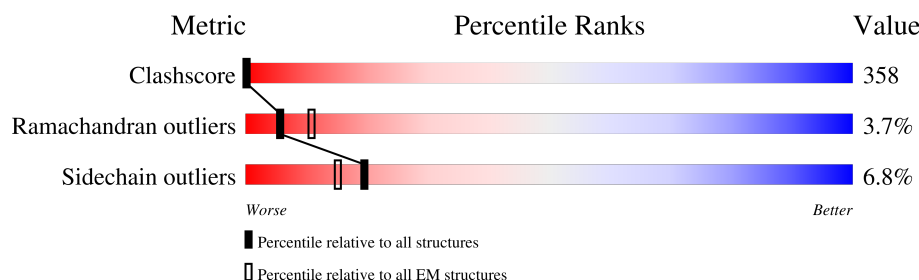
# 1 Overall quality at a glance

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1095	<div> <div>45%</div> <div>16%</div> <div>74%</div> <div>8%</div> <div>.</div> </div>
1	B	1095	<div> <div>46%</div> <div>15%</div> <div>74%</div> <div>8%</div> <div>.</div> </div>
1	C	1095	<div> <div>46%</div> <div>15%</div> <div>75%</div> <div>8%</div> <div>.</div> </div>
1	D	1095	<div> <div>46%</div> <div>15%</div> <div>74%</div> <div>8%</div> <div>.</div> </div>
1	E	1095	<div> <div>46%</div> <div>15%</div> <div>75%</div> <div>8%</div> <div>.</div> </div>

## 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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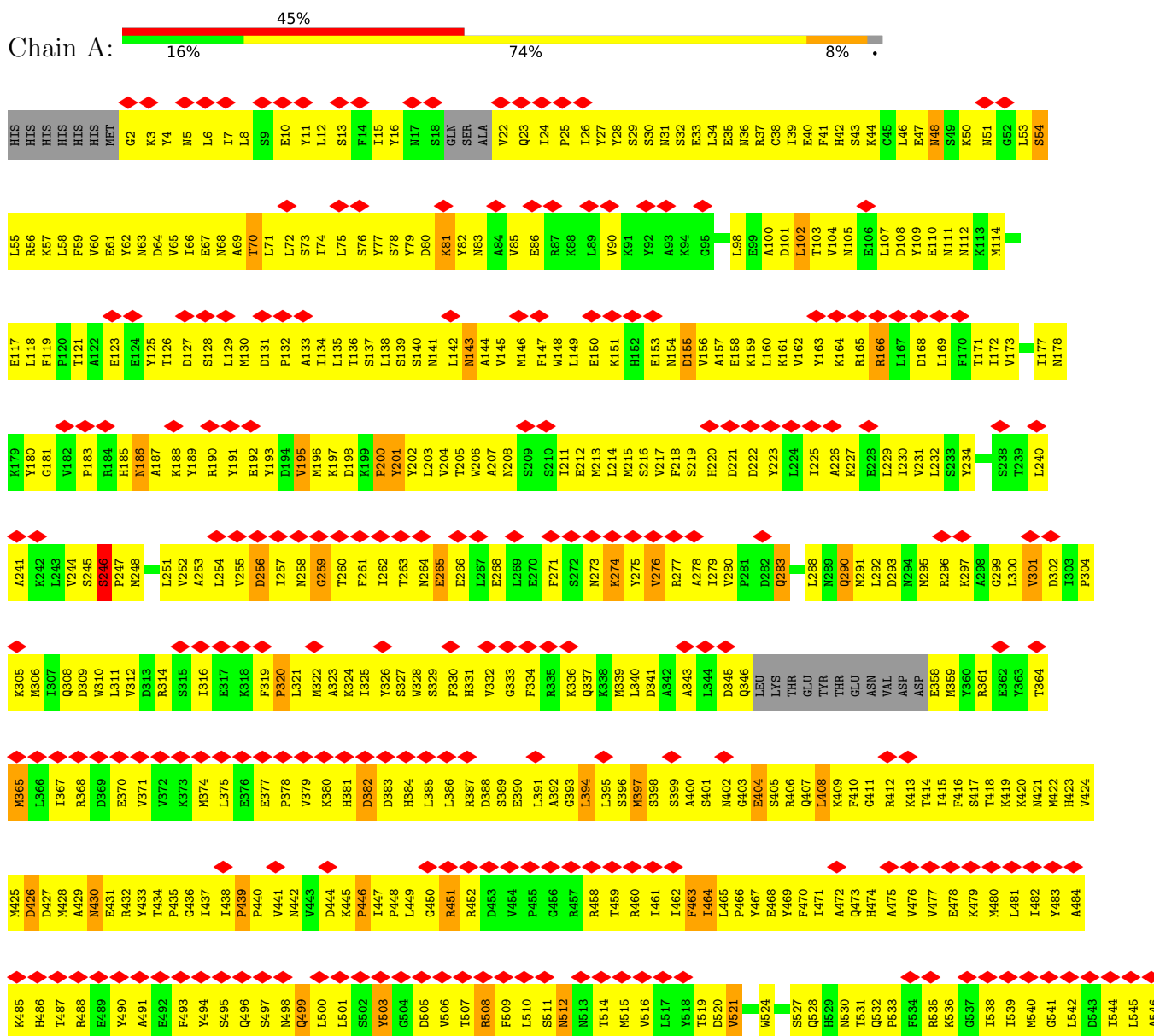
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1089	PRO	-	expression tag	UNP O37061
D	-5	HIS	-	expression tag	UNP O37061
D	-4	HIS	-	expression tag	UNP O37061
D	-3	HIS	-	expression tag	UNP O37061
D	-2	HIS	-	expression tag	UNP O37061
D	-1	HIS	-	expression 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

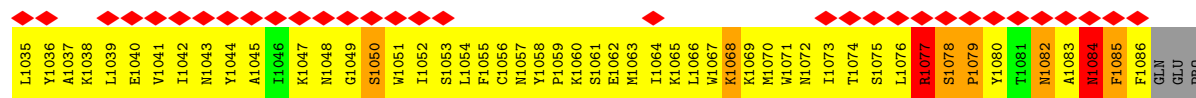
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

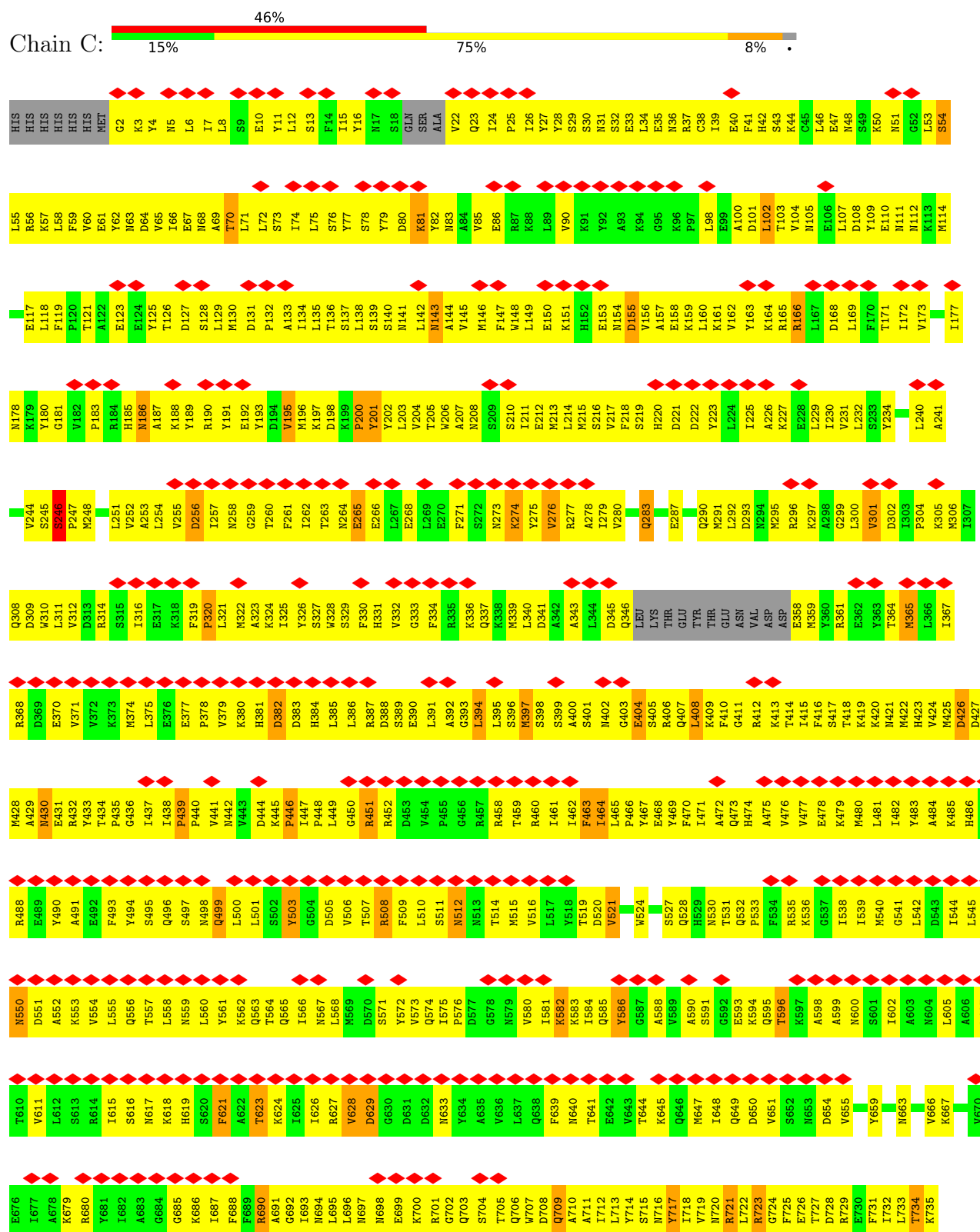




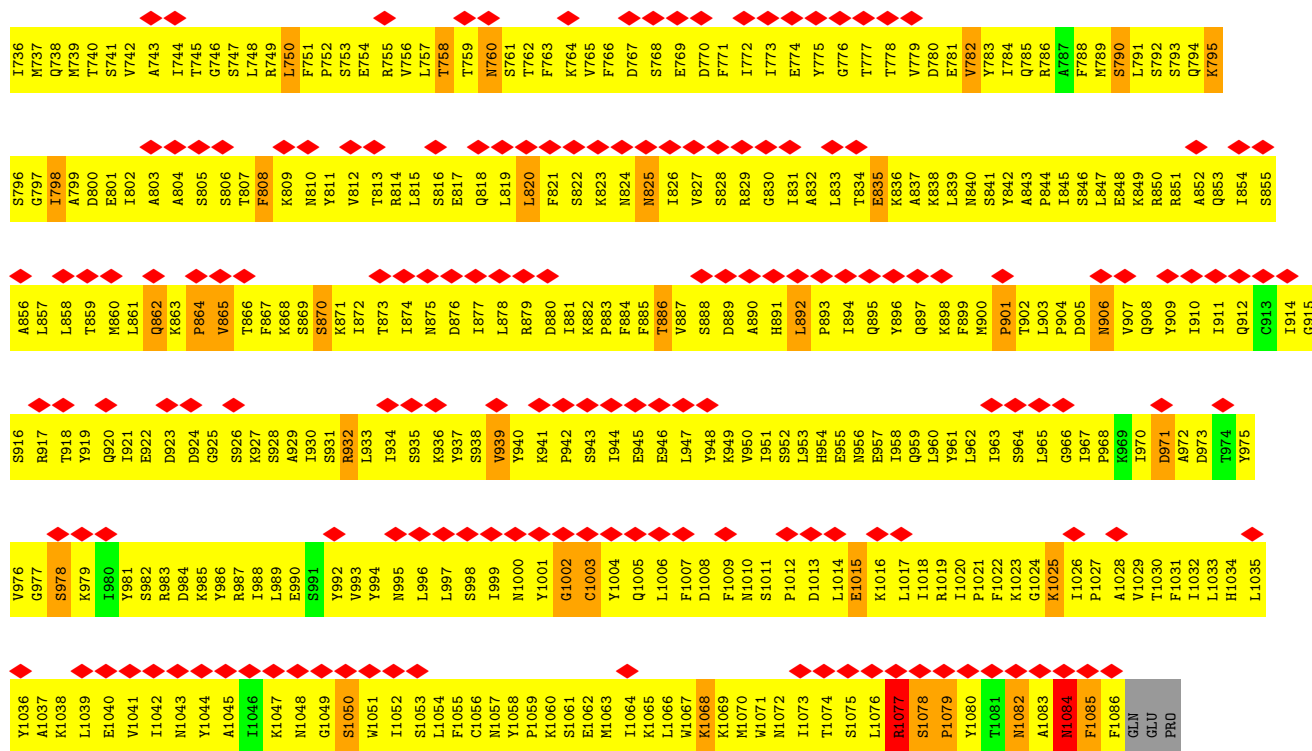
Y975	L240	M306	L366	D426	H486	T549	K609	1675	K735	K795	S855	G915	Y975
V976	A241	I307	I367	D427	T487	N550	T610	E676	L736	S796	A856	S916	V976
S977		Q308	R368	M428	R488	D551	V611	1677	Q737	G797	L857	R917	S977
K978	V244	Q309	R369	A429	E489	A552	L612	E678	Q738	L798	L858	T918	K978
Y980	S246	W310	D370	E431	Y490	K553	R614	K679	T740	D800	T859	Q920	Y980
Y981	P247	L311	V371	E432	A491	V554	R615	R680	S741	E801	M860	L861	Y981
S982	M248	D313	V372	T434	E492	L555	I615	1681	V742	L802	Q862	E922	S982
R983	L251	S315	K373	G436	F493	Q556	S616	1682	A743	A803	K863	D923	R983
D984	V252	I316	M374	I437	Y494	T557	N617	E683	I744	A804	P864	D924	D984
K985	A253	E317	L375	I438	S495	L558	K618	E684	T745	S805	T865	Q925	K985
Y986	L254	K318	E376	I439	Q496	N559	H619	G685	G746	S806	W866	S926	Y986
R987	V255	F319	E377	P440	S497	L560	S620	G686	S747	T807	T866	S927	R987
L988	D256	D320	E378	P441	N498	Y561	F621	K687	L748	K808	F867	K927	L988
E990	L257	L321	V379	N442	Q499	K562	A622	1687	R749	K809	K868	A929	E990
S991	M258	M322	K380	N443	L500	Q563	T623	F688	L750	M810	F751	S931	S991
Y992	Q259	A323	H381	D444	S502	T564	K624	F689	P752	W811	P753	R932	Y992
Y993	T260	K324	D382	K445	Y503	Q565	I625	E690	S753	B612	T813	L933	Y993
Y994	F261	I325	D383	P446	S504	L566	I626	A691	R754	T814	T873	I934	Y994
N995	I262	Y326	D384	I447	G504	N567	R627	G692	R755	L815	T874	S935	N995
L996	T263	W328	H384	P448	D505	L568	V628	1694	W756	L816	T875	K936	L996
L997	T263	S329	L385	L449	D506	N567	V629	1695	L757	S816	N875	Y937	L997
S998	N264	F330	L386	G450	V506	M569	D629	1696	T758	E817	D876	S938	S998
Y999	E265	H331	L387	R451	T507	D570	D630	1697	T759	L818	T877	Y939	Y999
Y1000	E266	V332	R387	R452	R508	S571	D631	N698	W760	L820	R878	Y940	Y1000
Y1001	L267	G333	D388	D453	F509	Y572	D632	E699	S761	R821	R879	K941	Y1001
C1003	E268	E390	S389	V454	L510	Q574	N633	K700	F763	S822	D880	P942	C1003
Y1004	L269	F334	E392	P455	S511	I575	Y634	R701	K764	K823	T881	S943	Y1004
Q1005	E270	R335	G393	G456	N512	P576	A635	G702	W765	N824	K882	S944	Q1005
L1006	F271	K336	C393	G457	N513	D577	V636	Q703	F766	M825	F885	E945	L1006
F1007	S272	Q337	L394	R457	T514	G578	L637	S704	D767	I826	T886	E946	F1007
D1008	N273	K338	L395	R458	T515	N579	L638	T705	S768	W827	V887	L947	D1008
F1009	K274	M339	S396	T459	M515	V580	Q638	Q706	E769	R828	S888	Y948	F1009
N1010	Y275	D341	M397	R460	V516	I581	F639	W707	D770	R829	D889	Y950	N1010
S1011	V276	A342	S398	I461	L517	K582	N640	Q709	F771	Q830	A890	I951	S1011
P1012	R277	A343	S399	I462	Y518	K583	T641	A710	I772	I773	H891	S952	P1012
D1013	A278	L344	N402	A400	T519	I584	E642	A711	I773	E774	L831	L892	D1013
E1015	I279	D345	S401	A463	D520	Q585	V643	I712	E775	G776	A832	P893	E1015
K1016	V280	Q346	G403	L465	Y521	Y586	T644	L713	W775	G776	T834	E955	K1016
L1017	Q283	L345	E404	P466	W524	G587	K645	S715	T777	T777	E835	E957	L1017
I1018	E287	L345	S405	Y467	Q528	V589	Q646	Y117	T778	T778	A837	I958	I1018
R1019	Q290	L345	R406	E468	H529	A590	N647	T718	V779	V779	K838	Q959	R1019
I1020	M291	GLU	Q407	Y469	N530	S591	I648	T719	D780	D780	L839	L960	I1020
F1021	L292	THR	L408	F470	T531	G592	Q649	N720	E781	E781	N840	P961	F1021
F1022	M292	THR	K409	A472	Q532	E593	D650	R721	W782	W782	S841	L962	F1022
K1025	D293	THR	G411	I471	P533	K594	V651	L722	I783	I783	Y842	I963	K1025
I1026	N294	ASP	R412	A475	F534	Q595	S652	R723	Q724	Q724	A843	S964	I1026
P1027	M295	ASP	K413	V476	R535	T596	N653	F725	W726	W726	P844	L965	P1027
A1028	R296	ASP	I415	V477	K536	K597	V655	E726	E727	E727	R786	Q966	A1028
V1029	A298	E358	F416	E478	G537	A598	D654	T727	F788	F788	L847	P967	V1029
T1030	G299	M359	S417	K479	I538	A599	V655	D728	W789	W789	K848	P968	T1030
F1031	L300	Y360	T418	M480	I539	N600	Y659	E730	R729	R729	R849	R969	F1031
I1032	I303	R361	S417	K479	I539	N600	N663	F731	D729	D729	R851	D971	I1032
L1033	D302	E362	T418	M480	I539	N600	N663	I732	E732	E732	R851	A972	L1033
H1034	I304	Y363	S417	M480	I539	N600	N663	L733	S792	S792	R851	T974	H1034
	M305	T364	K419	L482	G541	A603	V666	T734	Q794	Q794	A852	D973	
		M365	K420	L482	G541	A603	V666	T734	Q794	Q794	A852	D973	
			M425	A484	Y483	N543	V670						
							S671						
							T672						
							V673						
							G674						



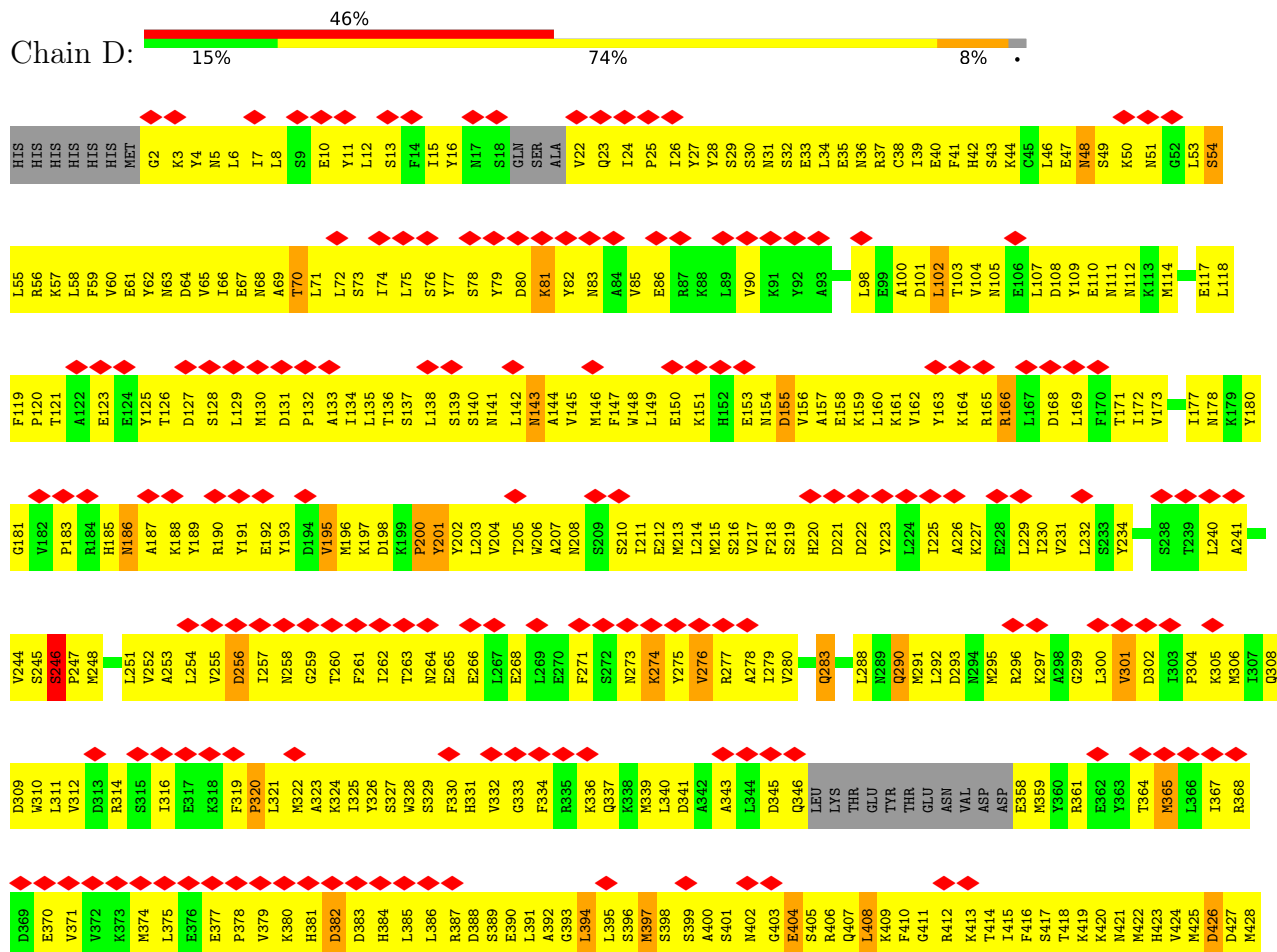
# Molecule 1: RNA-DEPENDENT RNA POLYMERASE







### • Molecule 1: RNA-DEPENDENT RNA POLYMERASE





C913	I914	G915	S916	R917	T918	Y919	Q920	R921	E922	D923	D924	G925	S926	K927	S928	A929	I930	S931	R932	L933	I934	S935	K936	D937	S938	V939	K941	P942	S943	I944	E945	E946	L947	Y948	K949	V950	I951	S952	L953	P954	E955	N956	E957	I958	Q959	L960	Y961	L962	N963	S964	L965	G966	I967	P968	K969	D970	A971	A972								
L733	T734	K735	T736	L737	T738	T739	T740	T741	T742	A743	T744	T745	T746	T747	T748	T749	L750	F751	F752	S753	E754	T755	T756	L757	T758	T759	M760	S761	T762	F763	K764	T765	F766	D767	S768	E769	D770	T771	T772	T773	E774	Y775	G776	T777	T778	T779	D780	E781	T782	N783	T784	Q785	T786	A787	F788	M789	S790	L791	S792							
S793	Q794	K795	S796	G797	T798	T799	D800	E801	I802	A803	T804	S805	S806	T807	F808	K809	M810	F811	S753	V812	T813	T814	L815	S816	D817	Q818	L819	L820	F821	S822	K823	M824	N825	I826	T827	S828	D829	T830	G831	I832	L833	E834	E835	K836	A837	K838	L839	M840	T841	L722	T842	Q785	P844	T845	S846	L847	P848	K849	R850	A851	A852					
Q853	I854	S855	A856	L857	L858	T859	M860	L861	E922	K862	K863	P864	V865	T866	K927	K868	S869	S870	K871	L872	T873	I874	N875	D876	L877	L878	L879	D880	I881	K882	P883	F884	T885	T886	L887	S888	D889	A890	I891	S952	L953	P893	I894	N955	E956	E957	I958	Q959	L960	Y961	L962	N963	S964	L965	G966	I967	P968	K969	D970	A971	A972					
E117	L118	F119	P120	T121	A122	E123	E124	E125	Y126	D127	S128	L129	M130	D131	P132	A133	I134	L135	T136	S137	L138	S139	S140	M141	L142	N143	A144	V145	M146	F147	W148	S209	S210	T211	E212	L213	L214	M215	S216	V217	F218	S219	A157	E158	K159	L160	K161	Y163	K164	R165	R166	L167	D168	I230	V231	L232	S233	Y234	S238	T239	L240					
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A241	K242	L243	V244	S245	S246	P247	M248	L251	V252	A253	L254	V255	D256	I257	N258	M196	G259	T260	F261	I262	S263	N264	S265	E266	L267	E268	L269	E270	F271	S272	K336	N273	K274	Y275	V276	R277	A278	F278	H220	D221	Y222	Y223	L224	I225	A226	K227	E228	L229	I230	V231	L232	S233	Y234	S238	T239	L240										
K305	M306	I307	Q308	D309	W310	L311	V312	D313	R314	S315	I316	E317	K318	F319	P320	L321	M322	K323	K324	I325	V326	S327	W328	S329	F330	H331	V332	G333	F334	R335	K336	Q337	K338	M339	L340	Y275	V276	R277	A278	F278	H220	D221	Y222	Y223	L224	I225	A226	K227	E228	L229	I230	V231	L232	S233	Y234	S238	T239	L240								
M365	L366	T367	R368	D369	E370	V371	V372	K373	K374	L375	E376	E377	P378	V379	K380	H381	S382	D383	H384	L385	L386	R387	D388	S389	E390	L391	A392	G393	L394	L395	S396	M397	S398	S399	A400	S401	M402	G403	E404	S405	R406	Q407	L408	K409	Q410	G411	R412	K413	T414	L415	F416	S417	T418	K419	L420	M421	N422	H423	V424							
M425	D426	D427	M428	A429	M430	E431	R432	Y433	T434	P435	G436	L437	L438	P439	P440	V441	M442	V443	D444	K445	P446	L447	P448	L449	G450	R451	R452	D453	V454	P455	G456	R457	R458	T459	R460	L461	L462	F463	L464	L465	P466	Y467	E468	Y469	F470	L471	A472	Q473	G474	H475	A476	V476	V477	E478	K479	M480	L481	L482	Y483	A484						
K485	H486	T487	R488	E489	Y490	A491	E492	F493	Y494	S495	Q496	S497	N498	Q499	L500	L501	S502	Y503	G504	D505	V506	T507	R508	F509	L510	S511	N512	N513	T514	N515	V516	L517	Y518	T519	D520	V521	W524	S527	Q528	H529	N530	T531	U532	P533	F534	R535	K536	G537	L538	I539	N540	G541	L542	D543	L544	L545	A546									
N547	H548	T549	N550	D551	A552	K553	V554	L555	Q556	T557	L558	N559	L560	Y561	K562	Q563	T564	Q565	L566	N567	L568	N569	D570	S571	Y572	V573	U574	L575	P576	D577	N578	N579	V580	L581	K582	K583	L584	Q585	Y586	G587	V588	Q589	A590	S591	G592	E593	K594	Q595	T596	K597	A598	A599	M600	S601	L602	A603	N604	L605	A606							
L607	T608	K609	T610	V611	L612	S613	R614	L615	S616	N617	K618	S619	R620	F621	A622	T623	K624	L625	T626	R627	V628	D629	G630	D631	D632	N633	V634	A635	V636	L637	G638	F639	N640	T641	E642	V643	T644	K645	Q646	M647	L648	N530	Q649	D650	V651	S652	N653	D654	V655	Y656	N657	A658	L659	K660	L661	S662	T663	L664	L665	L666	L667	S668	L669	L670	S671	T672
V673	G674	I675	E676	L677	A678	K679	R680	V681	T682	A683	G684	G685	K686	T687	F688	R689	K690	A691	G692	T693	N694	L695	L696	L697	N698	E699	K700	R701	G702	Q703	S704	T705	Q706	T707	D708	A710	I711	L712	L713	S715	N716	Y717	I718	Y719	N720	R721	L722	R723	G724	F725	T727	D728	R729	E730	F731	I732										
L733	T734	K735	T736	L737	T738	T739	T740	T741	T742	A743	T744	T745	T746	T747	T748	T749	L750	F751	F752	S753	E754	T755	T756	L757	T758	T759	M760	S761	T762	F763	K764	T765	F766	D767	S768	E769	D770	T771	T772	T773	E774	Y775	G776	T777	T778	T779	D780	E781	T782	N783	T784	Q785	T786	A787	F788	M789	S790	L791	S792							
S793	Q794	K795	S796	G797	T798	T799	D800	E801	I802	A803	T804	S805	S806	T807	F808	K809	M810	F811	S753	V812	T813	T814	L815	S816	D817	Q818	L819	L820	F821	S822	K823	M824	N825	I826	T827	S828	D829	T830	G831	I832	L833	E834	E835	K836	A837	K838	L839	M840	T841	L722	T842	Q785	P844	T845	S846	L847	P848	K849	R850	A851	A852					
Q853	I854	S855	A856	L857	L858	T859	M860	L861	E922	K862	K863	P864	V865	T866	K927	K868	S869	S870	K871	L872	T873	I874	N875	D876	L877	L878	L879	D880	I881	K882	P883	F884	T885	T886	L887	S888	D889	A890	I891	S952	L953	P893	I894	N955	E956	E957	I958	Q959	L960	Y961	L962	N963	S964	L965	G966	I967	P968	K969	D970	A971	A972					

D973	D974	D975	D976	D977	D978	D979	D980	D981	D982	D983	D984	D985	D986	D987	D988	D989	D990	D991	D992	D993	D994	D995	D996	D997	D998	D999	D1000	D1001	D1002	D1003	D1004	D1005	D1006	D1007	D1008	D1009	D1010	D1011	D1012	D1013	D1014	D1015	D1016	D1017	D1018	D1019	D1020	D1021	D1022	D1023	D1024	D1025	D1026	D1027	D1028	D1029	D1030	D1031	D1032																																								
L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	7000	Depositor
Resolution determination method	Not provided	
CTF correction method	INDIVIDUAL PARTICLE PHASE FLIPPING	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	15	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	56540	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.008	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0004844	Depositor
Map size (Å)	237.5, 473.30356, 237.5	wwPDB
Map dimensions	140, 279, 140	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.696428571, 1.696428571, 1.696428571	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	$\# Z  > 5$	RMSZ	$\# Z  > 5$
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

*Continued on next page...*

*Continued from previous page...*

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%)	3	23
1	B	1073/1095 (98%)	927 (86%)	104 (10%)	42 (4%)	3	23
1	C	1073/1095 (98%)	926 (86%)	105 (10%)	42 (4%)	3	23
1	D	1073/1095 (98%)	926 (86%)	105 (10%)	42 (4%)	3	23
1	E	1073/1095 (98%)	926 (86%)	105 (10%)	42 (4%)	3	23
All	All	5365/5475 (98%)	4631 (86%)	524 (10%)	210 (4%)	6	23

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%)	15	40
1	B	979/996 (98%)	912 (93%)	67 (7%)	16	41
1	C	979/996 (98%)	911 (93%)	68 (7%)	15	40
1	D	979/996 (98%)	911 (93%)	68 (7%)	15	40
1	E	979/996 (98%)	911 (93%)	68 (7%)	15	40
All	All	4895/4980 (98%)	4556 (93%)	339 (7%)	19	40

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

Mol	Chain	Res	Type
1	D	426	ASP
1	E	274	LYS
1	D	550	ASN
1	D	932	ARG
1	E	430	ASN

Sometimes 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	308	GLN
1	E	498	ASN
1	C	853	GLN
1	E	473	GLN
1	E	709	GLN



### 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](#)

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.

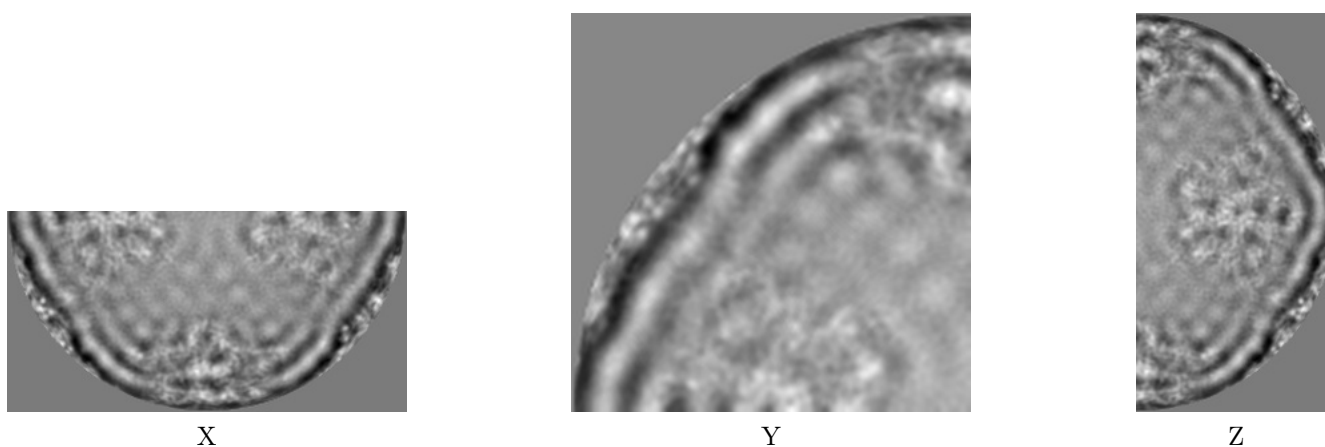
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2100. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

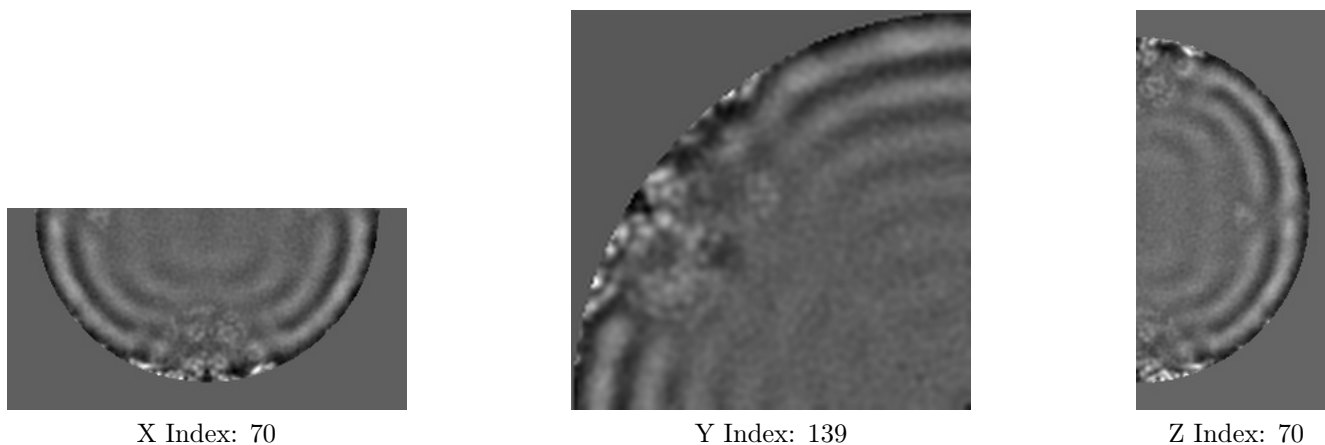
#### 6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

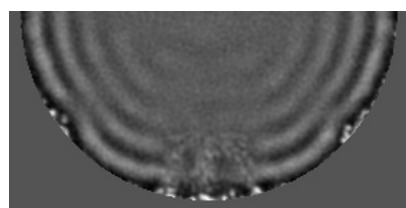
#### 6.2.1 Primary map



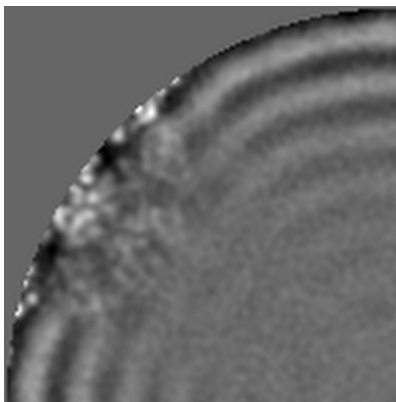
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

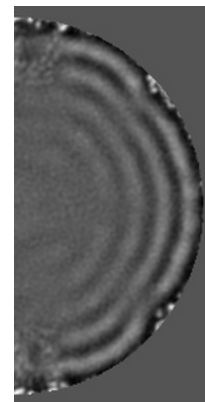
### 6.3.1 Primary map



X Index: 45



Y Index: 145



Z Index: 94

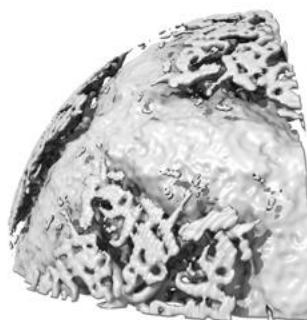
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

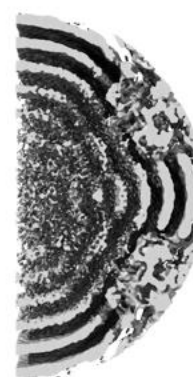
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0004844. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

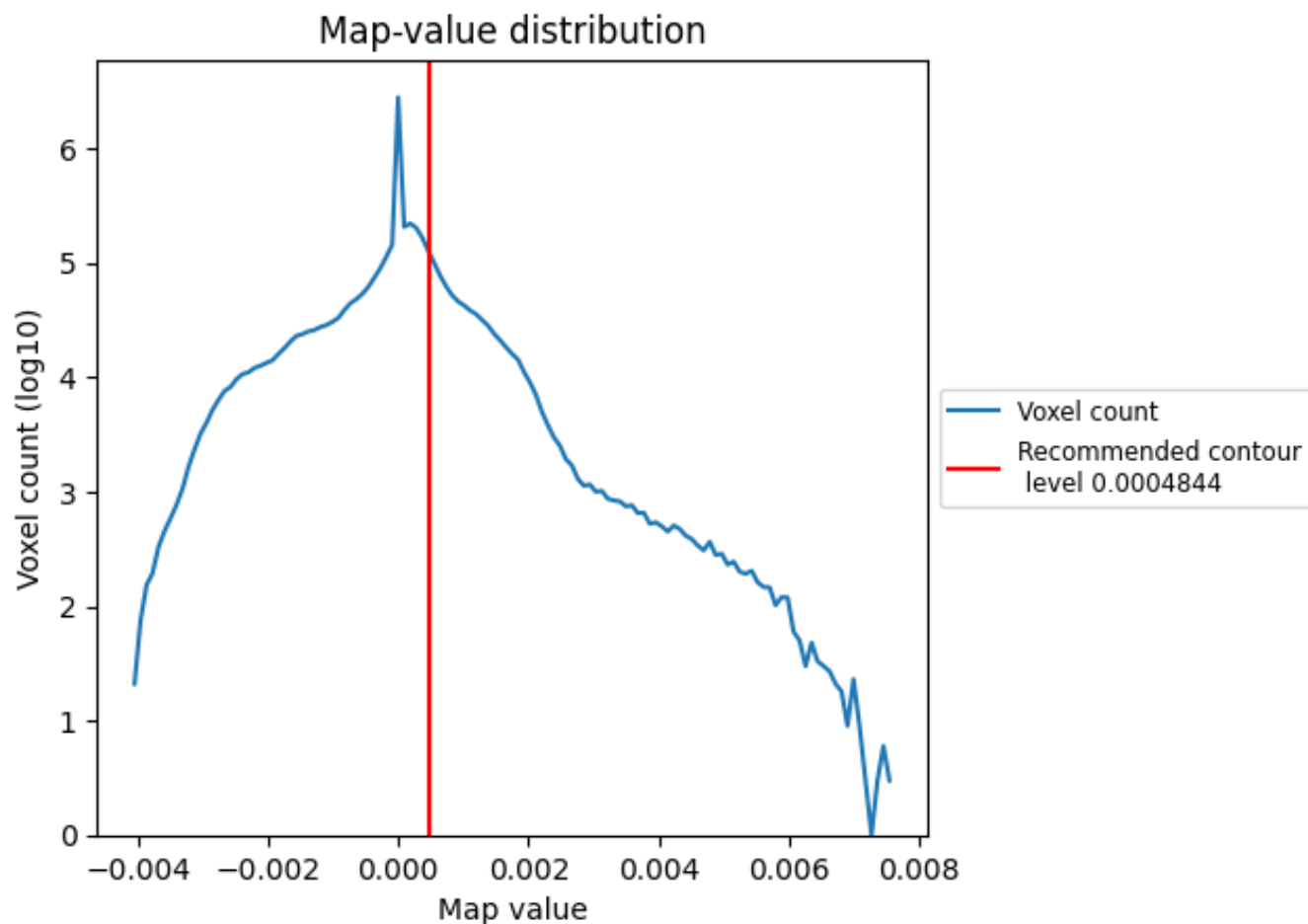
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

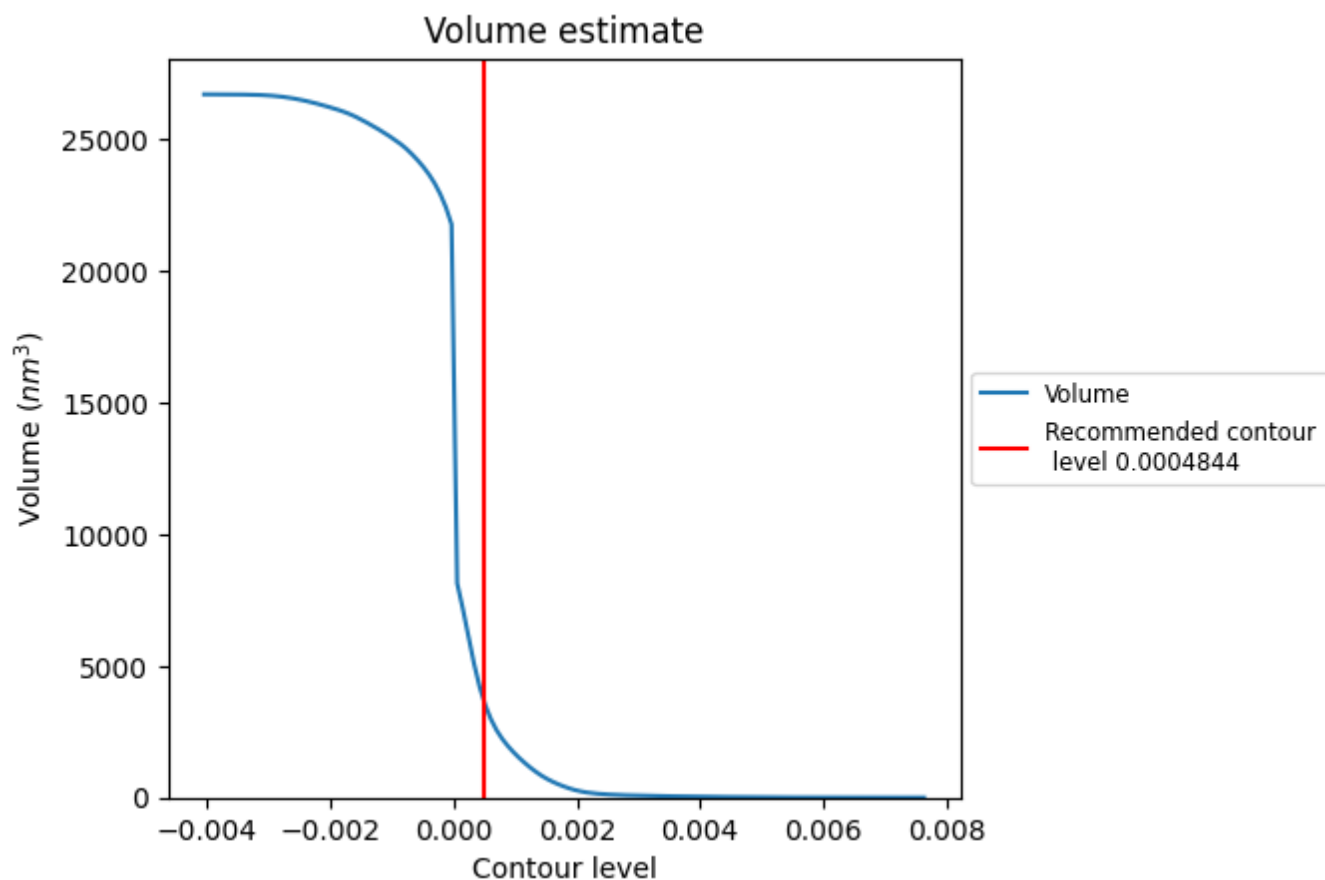
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3732 nm<sup>3</sup>; this corresponds to an approximate mass of 3371 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

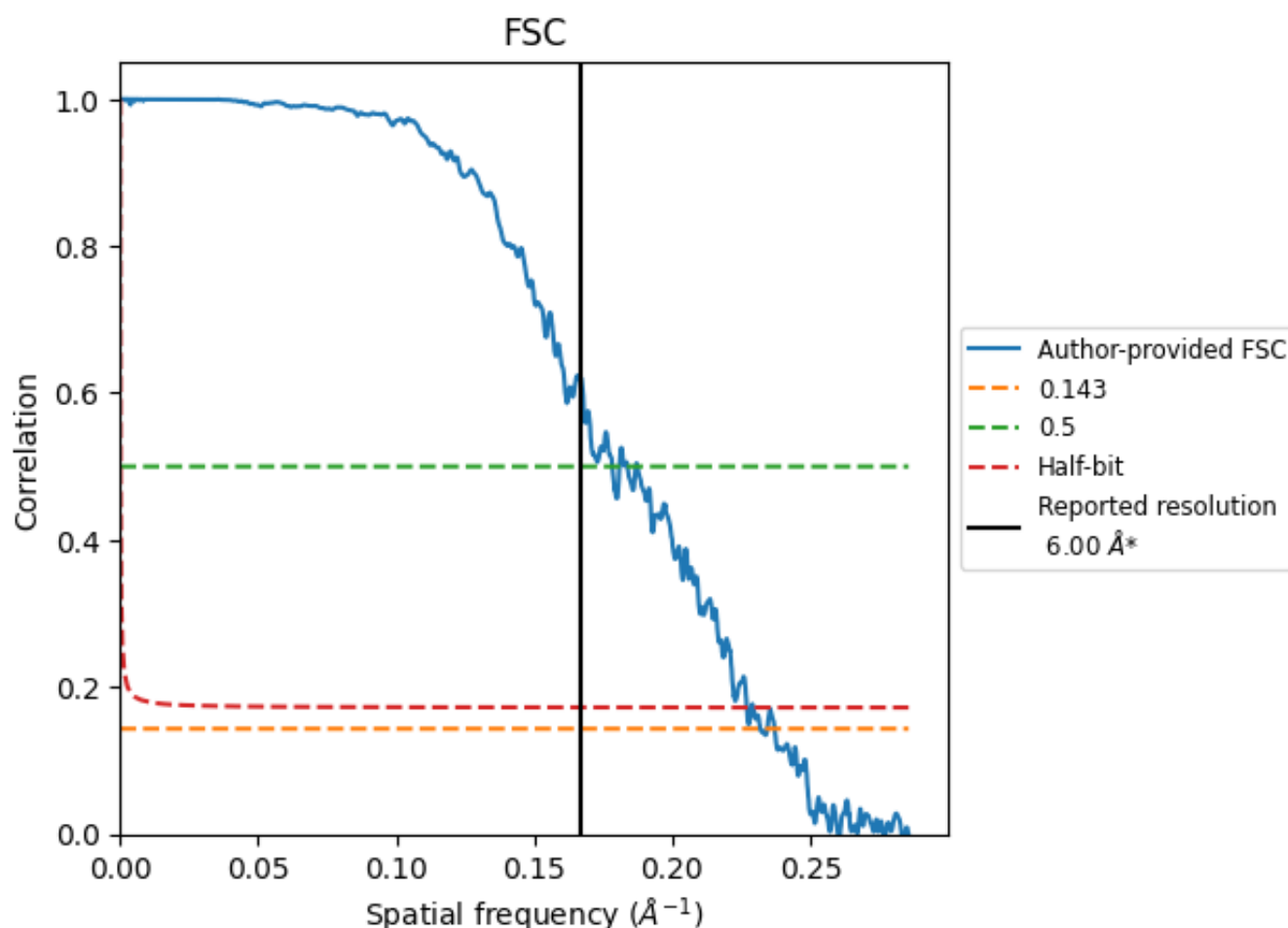
## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.167  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	4.31	5.61	4.40
Unmasked-calculated*	-	-	-

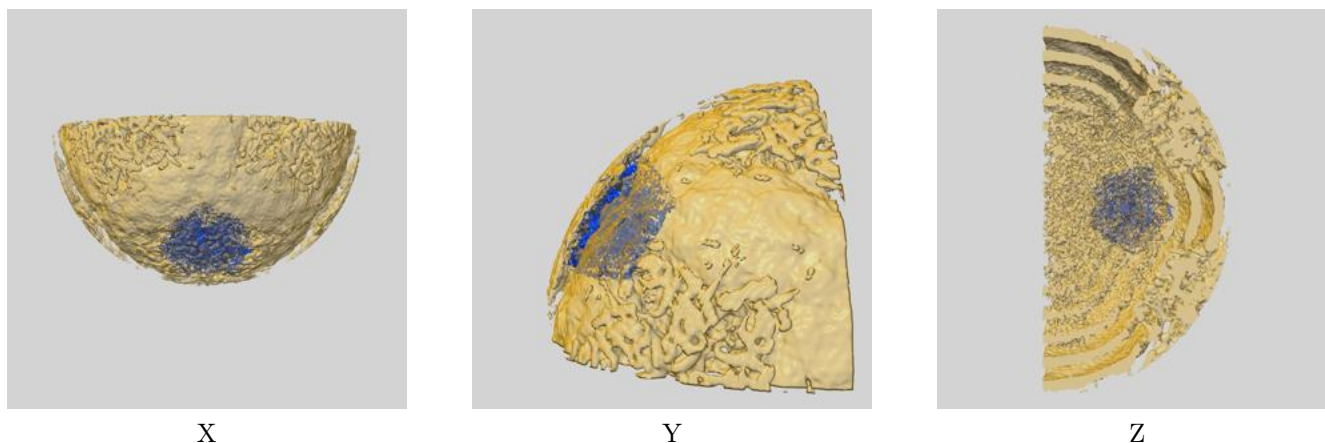
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



## 9 Map-model fit [i](#)

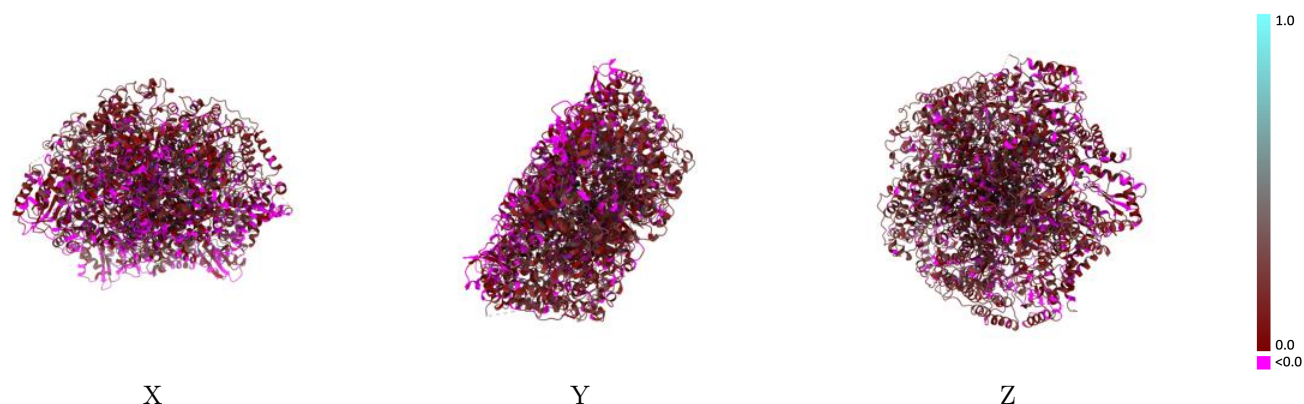
This section contains information regarding the fit between EMDB map EMD-2100 and PDB model 4AU6. Per-residue inclusion information can be found in section [3](#) on page [5](#).

### 9.1 Map-model overlay [i](#)



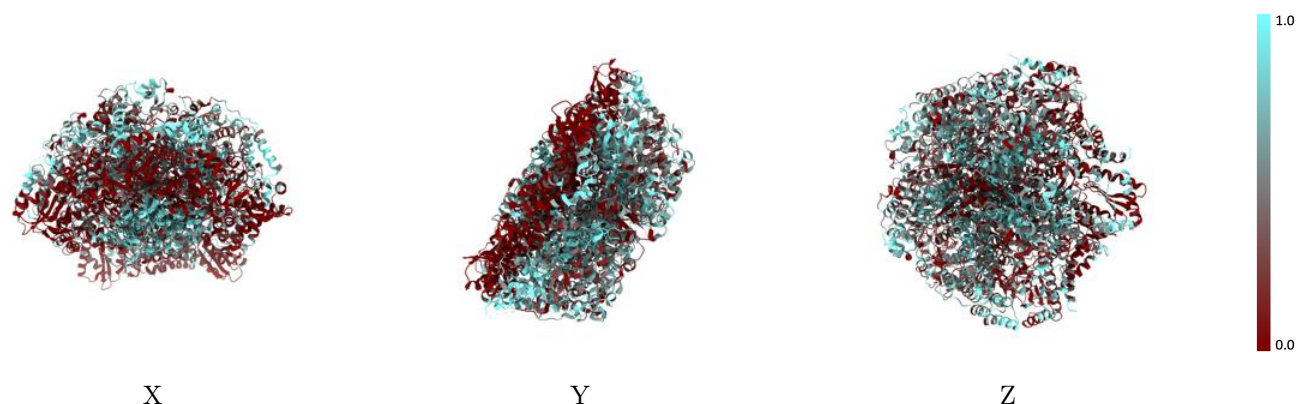
The images above show the 3D surface view of the map at the recommended contour level 0.0004844 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



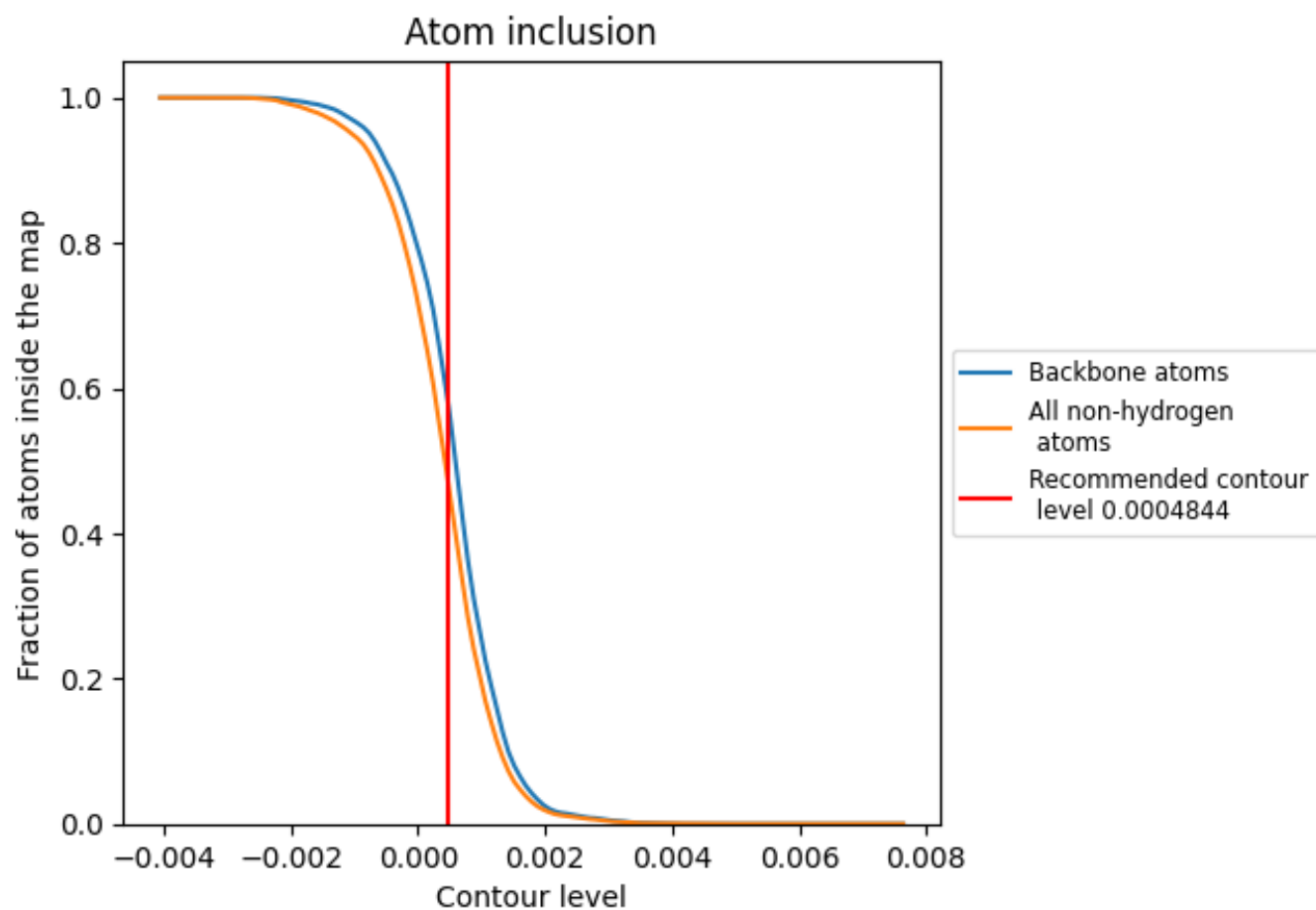
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0004844).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0004844) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.4662	<div><div></div></div> 0.1190
A	<div><div></div></div> 0.4675	<div><div></div></div> 0.1180
B	<div><div></div></div> 0.4665	<div><div></div></div> 0.1190
C	<div><div></div></div> 0.4697	<div><div></div></div> 0.1180
D	<div><div></div></div> 0.4638	<div><div></div></div> 0.1190
E	<div><div></div></div> 0.4636	<div><div></div></div> 0.1200

1.0

0.0

<0.0