



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 03:33 AM UTC

PDB ID : 4AU6 / pdb_00004au6
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

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>.

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

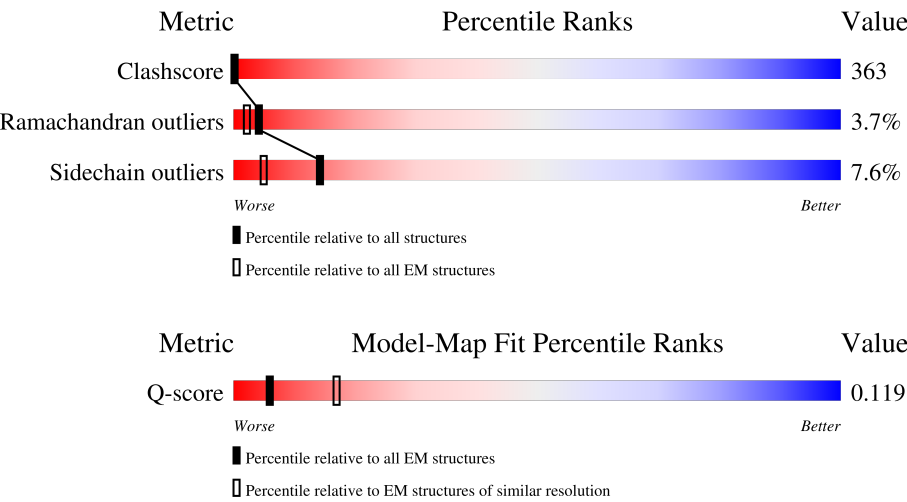
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	525 (5.50 - 6.50)

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 ≥ 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	45% 15%73%10%
1	B	1095	46% 15%73%10%
1	C	1095	46% 15%73%10%
1	D	1095	46% 15%73%10%

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Mol	Chain	Length	Quality of chain
1	E	1095	46% 15% 73% 10%

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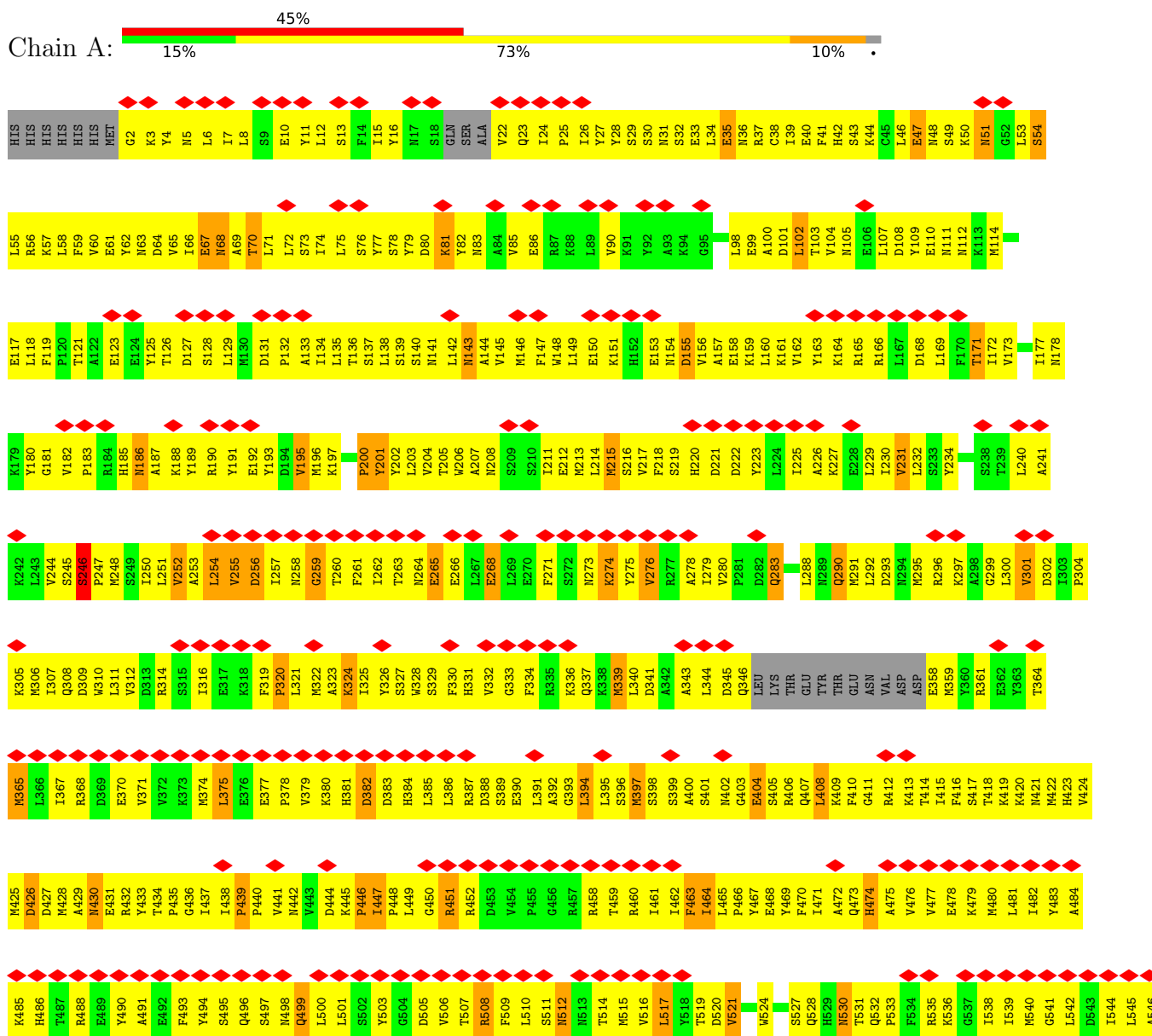
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1089	PRO	-	expression tag	UNP O37061
D	-5	HIS	-	expression tag	UNP O37061
D	-4	HIS	-	expression tag	UNP O37061
D	-3	HIS	-	expression tag	UNP O37061
D	-2	HIS	-	expression tag	UNP O37061
D	-1	HIS	-	expression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

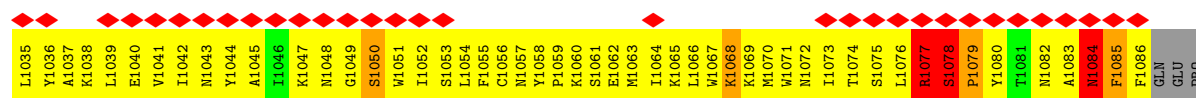
3 Residue-property plots

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.

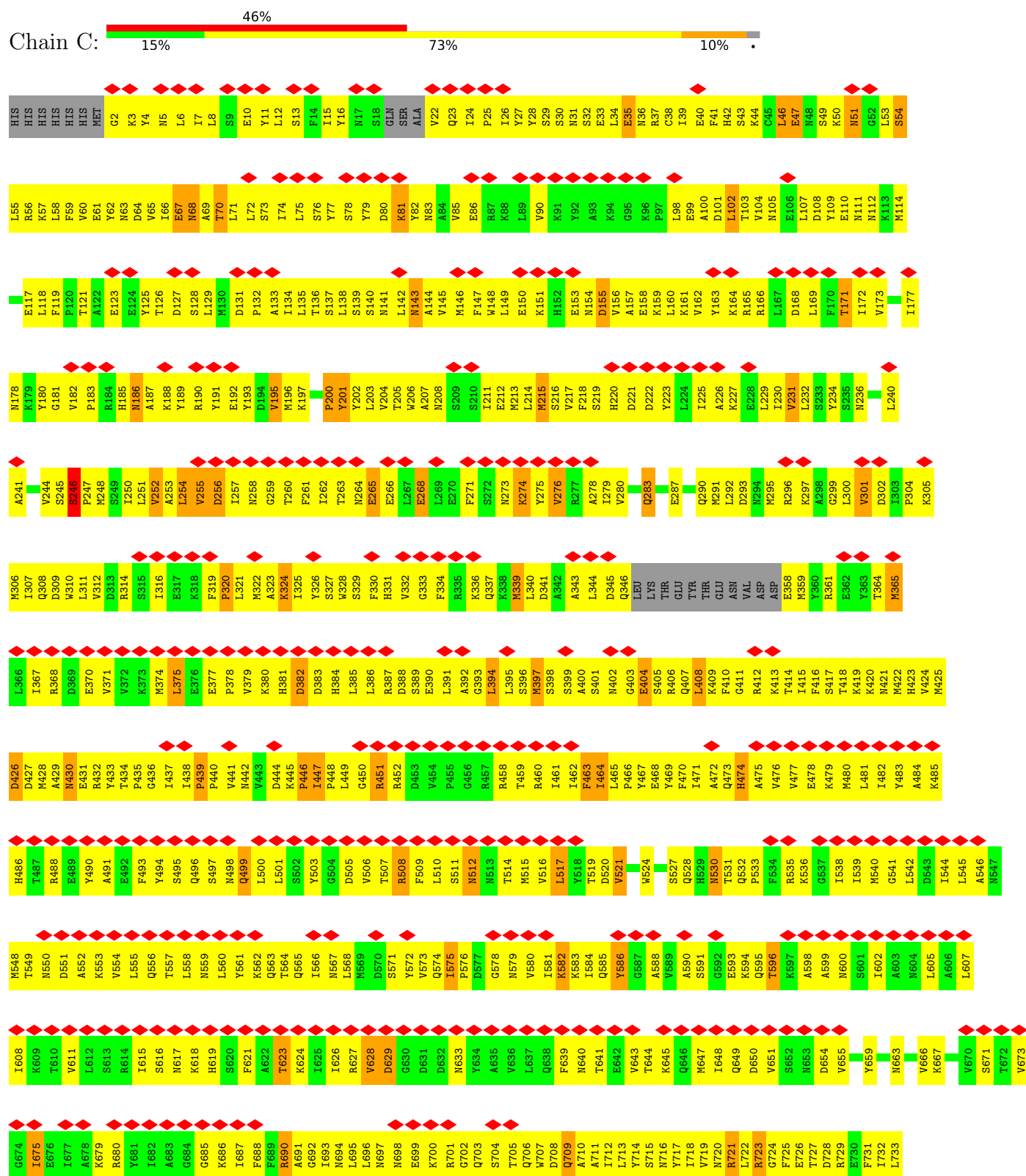
• Molecule 1: RNA-DEPENDENT RNA POLYMERASE

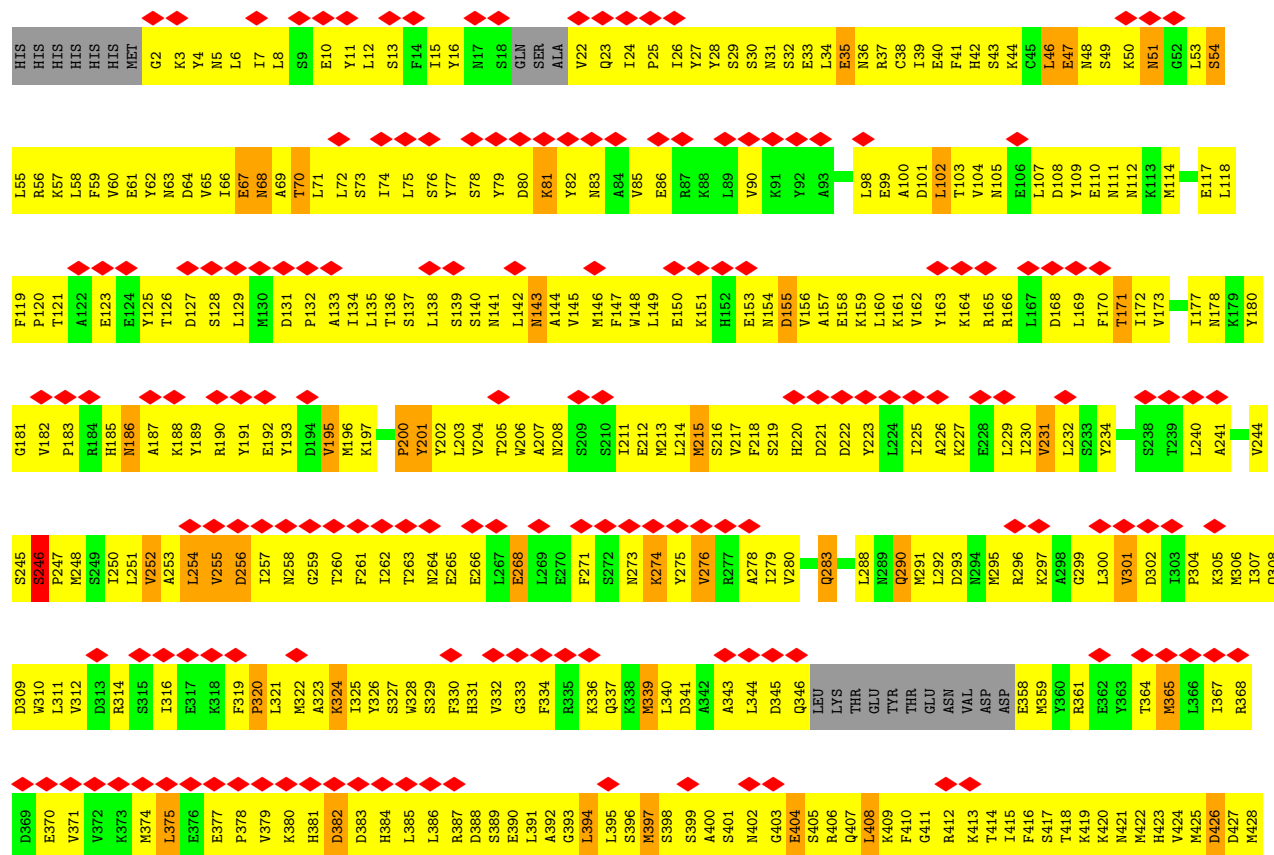


Y975	G915	K795	K609	T549	H486	D426	M306	A241
V976	S916	S796	T610	N550	T487	D427	I307	V244
G977	R917	G797	V611	D551	R488	M428	Q308	S245
S978	T918	T798	L612	A552	E489	A429	W310	S246
K979	T919	A799	R613	K553	Y490	E431	L311	P247
X980	Q920	D800	R614	V554	E492	R432	V312	M248
Y981	R921	E801	I615	L555	F493	T434	D313	S249
S982	E922	L802	S616	Q556	F494	Y433	S315	T250
R983	D923	A804	N617	T557	Y494	G436	S316	L251
D984	D924	S805	K618	L558	S495	I437	E317	V252
K985	C925	S806	H619	N559	Q496	I438	K318	A253
R987	S926	T807	S620	L560	S497	P439	E377	L254
L988	K927	F808	R621	Y561	N498	P440	E378	V255
R989	S928	L748	F622	Y562	Q499	V441	D256	D256
E990	A929	R749	T623	K562	Q499	N442	I257	T257
S991	R930	F751	R624	Q563	L500	Y443	M258	G259
Y992	S931	P752	G625	T564	L501	D444	K324	T260
V993	R932	S753	I626	Q565	S502	K445	I325	F261
Y994	L933	E754	R627	L566	Y503	P446	I326	T262
N995	L934	R755	I628	N567	G504	I447	S327	T263
S996	S935	R756	R629	L568	D505	P448	W328	T263
L997	K936	L757	V628	N567	L568	L449	S329	N264
L998	Y937	T758	D629	M569	V506	G450	F330	E265
S998	S938	T759	D630	S571	T507	R451	H331	E266
Y999	V939	R760	D631	G572	R508	D452	V332	L267
N1000	Y940	S761	D632	V573	F509	D453	G333	E268
Y1001	K941	T762	N633	Q574	L510	V454	E390	L269
G1002	P942	K763	R634	I575	S511	P455	R335	E270
C1003	S943	R764	A635	P576	N512	G456	K336	F271
Y1004	L944	R765	V636	D577	N513	R457	Q337	S272
Q1005	E945	R766	L637	G578	T514	R458	L395	N273
L1006	E946	S767	Q638	N579	M515	T459	S396	K274
F1007	L947	E768	F639	V580	V516	R460	S397	Y275
D1008	Y948	D770	N640	I581	L517	I461	S398	V276
F1009	K949	F771	T641	K582	Y518	I462	S399	R277
N1010	V950	I772	T642	L584	T519	F463	A400	A278
S1011	P951	L773	E642	Q585	D520	I464	N402	I279
P1012	S952	E774	V643	Y586	V521	L465	G403	V280
D1013	L953	G776	K645	G587	W524	P466	E404	Q283
L1014	E955	R777	Q646	A588	Q528	Y467	LVS	Q287
N1015	E956	T778	N647	V589	H529	E468	THR	E287
E1016	E957	A837	I648	A590	N530	F470	GLU	E287
L1017	Q958	R838	Q649	S591	T531	I471	THR	Q290
I1018	L960	L839	D650	G592	Q532	A472	GLU	M291
R1019	Y961	N840	V651	E593	K536	Q473	ASN	L292
I1020	L962	E841	S652	K594	P533	H474	VAL	D293
F1021	P963	R782	R653	Q595	F534	A475	ASP	R294
K1022	S964	L783	N654	T596	R535	V476	ASP	M295
L1023	L965	Q785	R655	K597	K536	V477	M359	R296
G1024	Q966	R786	D654	A598	G537	E478	Y360	K297
K1025	D967	F787	V655	A599	I538	K479	S417	A298
I1026	P968	L847	Y659	N600	I539	M480	T418	G299
P1027	A1028	R848	N663	S601	M540	L481	K419	L300
A1028	V1029	K849	L666	I602	G541	I482	K420	V301
V1029	Q908	R850	S671	A603	L542	Y483	T364	I302
D971	T1030	R851	N667	N604	I544	A484	M365	I303
F1031	A972	R852	V670	G606	L545	K485	M425	P304
T1031	A973	K853	S672	L607	I608			K305
L1032	D973	R854	G674					
L1033	T974							
H1034								



• Molecule 1: RNA-DEPENDENT RNA POLYMERASE





C913	E117	K479	K242	K305	M365	M425	K485	M547	L607	V673	L733	S793	Q853
I914	L118	Y180	K243	M306	L366	D426	H486	M548	L608	G674	T734	Q794	I854
G915	L243	G181	V244	I307	L367	D427	H487	T549	K609	I675	K735	Q795	S855
S916	S245	V182	S246	Q308	R368	M428	R488	N550	T610	E676	M737	S796	A856
R917	T121	P183	S247	D309	R369	A429	R489	D551	V611	I677	Q738	I798	L857
T918	A122	R184	P247	W310	D369	M430	A552	A552	L612	A678	M739	A799	L858
Y919	E123	H185	M248	L311	E431	E431	A553	K553	S613	K679	T740	D800	T859
Q920	E124	M186	S249	L312	R432	Y433	A491	V554	S614	R680	S741	E801	M860
M860	L126	A187	L250	D313	T434	P435	E492	L555	R614	R681	V742	L802	L861
E922	D127	K188	L251	W312	V371	T435	F493	Q556	L615	Y682	A743	A803	Q862
D923	S128	Y189	V252	R314	V372	G436	F494	T557	S616	I683	T744	A804	K863
D924	L129	R190	A253	R315	K374	T437	S495	L558	N617	G685	T745	S805	P864
G925	R130	Y191	L254	E317	L375	L438	Q496	N559	K618	G686	T746	S806	V865
S926	D131	E192	V255	K318	E376	P439	S497	L560	S620	I687	L748	T807	T866
K927	P132	E193	D256	F319	E377	P440	N498	L561	R621	T687	R749	F808	K867
S928	A133	Y194	M258	L321	P378	V441	Q499	K562	F622	F688	L750	K809	K868
A929	I134	V195	G259	M322	V379	M442	L500	Q563	A623	F689	F751	M810	S869
I930	L135	M196	T260	K323	K380	V443	L501	T564	T624	R690	S752	R811	S870
S931	T136	K197	F261	K324	H381	D444	L502	Q565	K624	R691	S753	V812	K871
R932	S137	P200	L262	I325	D382	K445	S502	T565	I625	A692	E754	T813	L872
L933	L138	Y201	T263	Y326	D383	P446	S503	I566	T626	G692	R755	T814	T873
I934	S139	Y202	G263	S327	H384	L447	Y503	L567	I627	I693	V756	T815	I874
S935	S140	L203	M264	W328	H385	L449	D504	L568	T628	I694	L757	L816	N875
K936	Y141	L204	E265	S329	L386	G450	V506	M569	R627	L695	T758	T817	D876
Y937	L142	T205	E266	F330	R387	R451	T507	D570	V628	L696	T759	Q818	I877
S938	M143	V206	L267	H331	D387	R452	R508	S571	D629	N697	M760	L819	L878
V939	A144	A207	E268	G332	D388	D453	F509	F572	G630	N698	S761	L820	R879
K941	V145	N208	L269	G333	S389	V454	L510	W573	D631	E699	T762	R821	D880
P942	M146	S209	L270	F334	E390	V455	S511	Q575	D632	T705	F763	R822	I881
S943	F147	S210	F271	R335	L391	G456	N512	P576	N633	Q702	K764	K823	K882
I944	W148	G211	S272	K336	A392	G457	N513	D577	V634	Q703	A635	N824	P883
E945	L149	E212	N273	Q337	G393	L394	T514	Q578	A636	S704	V636	N825	F884
E946	E150	M213	K274	K338	S396	R458	N515	N579	L637	Q706	L637	N826	T886
L947	K151	M215	Y275	L340	M397	R460	V516	V580	D638	T707	D638	I827	R887
Y948	H152	S216	V276	D341	S398	L461	L517	K582	F639	Q708	F639	R828	S888
K949	E153	S217	R277	A342	S399	L462	Y518	K583	N640	D708	L772	R829	D889
V950	M154	F218	Q276	A343	A400	L464	T519	L584	T641	A710	L773	G830	A890
I951	D155	S219	A278	A343	S401	L465	D520	Q585	T642	A711	E774	I831	I951
S952	V156	H220	I279	A344	M402	L466	V521	V586	E642	L712	Y775	L832	E891
E953	E158	D221	V280	D345	G403	P466	Q528	Y587	V643	L713	G776	L833	L892
L954	K159	D222	Q283	LEU	E404	Y467	W524	A588	T644	L714	T777	L834	P893
E955	L160	Y223	E287	LYS	S405	E468	S527	V589	K645	S715	T778	E835	I894
E956	K161	E224	L288	THR	R406	Y469	Q528	K591	Q646	N716	V779	T836	N956
E957	V162	I225	N289	GLU	Q407	F470	N529	S592	M647	Y717	D780	K836	E957
I958	Y163	A226	Q290	THR	L408	L471	H529	K593	T648	L718	E781	A837	I958
Q959	K164	K227	M291	GLU	K409	A472	N530	E592	L648	Y719	K594	R838	Q959
L960	R165	E228	L292	ASN	F410	Q473	T531	K594	D649	N720	D649	L839	K898
L962	R166	L229	D293	VAL	G411	H474	Q532	O595	D650	R721	V651	M840	F899
I963	L167	ASP	M294	ASP	R412	A475	P533	T596	V651	L722	R723	T841	N900
S964	D168	V231	N295	ASP	R413	V476	F534	K597	S652	R724	R725	Y842	P901
L965	L169	L232	R296	E358	T414	V477	R535	A598	T653	G726	F726	T843	T902
G966	F170	S233	K297	M359	L415	E478	K536	A599	N653	E726	E726	R844	L903
I967	T171	Y234	G299	Y360	F416	K479	G537	A599	D654	T727	T727	T845	P904
K968	L172	S238	Q300	E362	T417	M480	L538	N600	V655	R729	R729	L847	G966
D971	V173	G239	V301	Y363	K419	L481	L539	S601	V655	E730	E730	M848	P967
A972	L177	L240	D302	T364	K420	L482	N540	T602	V659	F731	F731	T849	K968
	M178	A241	I303	T364	M422	Y483	G541	N604	N663	I732	L791	R850	P968
					H423	A484	L542	A606	V666		S792	K851	K969
							L545	L545	V670			R852	A972
							A546	A546	S671			A852	Q912
									T672				

D973	D974	Y975	Y976	G977	S978	K979	I980	Y981	S982	R983	D984	K985	Y986	R987	T988	L989	E990	S991	Y992	Y993	Y994	N995	L996	L997	S998	I999	N1000	Y1001	G1002	C1003	Y1004	Q1005	L1006	F1007	D1008	F1009	N1010	S1011	P1012	D1013	L1014	E1015	K1016	L1017	I1018	R1019	I1020	F1021	F1022	K1023	G1024	K1025	I1026	P1027	A1028	V1029	T1030	F1031	I1032
L1033	H1034	L1035	Y1036	A1037	K1038	L1039	E1040	V1041	I1042	N1043	Y1044	A1045	I1046	K1047	N1048	G1049	S1050	W1051	I1052	S1053	L1054	F1055	C1056	N1057	Y1058	P1059	K1060	S1061	E1062	M1063	I1064	K1065	L1066	W1067	K1068	K1069	M1070	W1071	N1072	I1073	T1074	S1075	L1076	R1077	S1078	P1079	Y1080	T1081	N1082	A1083	N1084	F1085	F1086	GLN	GLU	PRO			

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 ($\text{\AA}$)	237.5, 473.30356, 237.5	wwPDB
Map dimensions	140, 279, 140	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.51	0/8914	0.98	27/12052 (0.2%)
1	B	0.51	0/8914	0.98	27/12052 (0.2%)
1	C	0.51	0/8914	0.98	27/12052 (0.2%)
1	D	0.51	0/8914	0.98	27/12052 (0.2%)
1	E	0.51	0/8914	0.98	27/12052 (0.2%)
All	All	0.51	0/44570	0.98	135/60260 (0.2%)

There are no bond length outliers.

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1078[A]	SER	CA-C-N	8.53	128.26	119.64
1	A	1078[A]	SER	C-N-CA	8.53	128.26	119.64
1	A	1078[B]	SER	CA-C-N	8.53	128.26	119.64
1	A	1078[B]	SER	C-N-CA	8.53	128.26	119.64
1	C	1078[A]	SER	CA-C-N	8.51	128.23	119.64

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	11874	0
1	B	8741	0	8346	11873	0
1	C	8741	0	8345	11827	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	8741	0	8343	11903	0
1	E	8741	0	8344	11890	0
All	All	43705	0	41721	31000	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 363.

The worst 5 of 31000 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%)	2	18
1	B	1073/1095 (98%)	927 (86%)	104 (10%)	42 (4%)	2	18
1	C	1073/1095 (98%)	926 (86%)	105 (10%)	42 (4%)	2	18
1	D	1073/1095 (98%)	926 (86%)	105 (10%)	42 (4%)	2	18
1	E	1073/1095 (98%)	926 (86%)	105 (10%)	42 (4%)	2	18
All	All	5365/5475 (98%)	4631 (86%)	524 (10%)	210 (4%)	4	18

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%)	904 (92%)	75 (8%)	12	32
1	B	979/996 (98%)	903 (92%)	76 (8%)	11	32
1	C	979/996 (98%)	903 (92%)	76 (8%)	11	32
1	D	979/996 (98%)	903 (92%)	76 (8%)	11	32
1	E	979/996 (98%)	903 (92%)	76 (8%)	11	32
All	All	4895/4980 (98%)	4516 (92%)	379 (8%)	14	32

5 of 379 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	70	THR
1	D	835	GLU
1	D	171	THR
1	D	404	GLU
1	D	1078[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 146 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	23	GLN
1	E	1005	GLN
1	E	283	GLN
1	E	547	ASN
1	B	720	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 oligosaccharides 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.

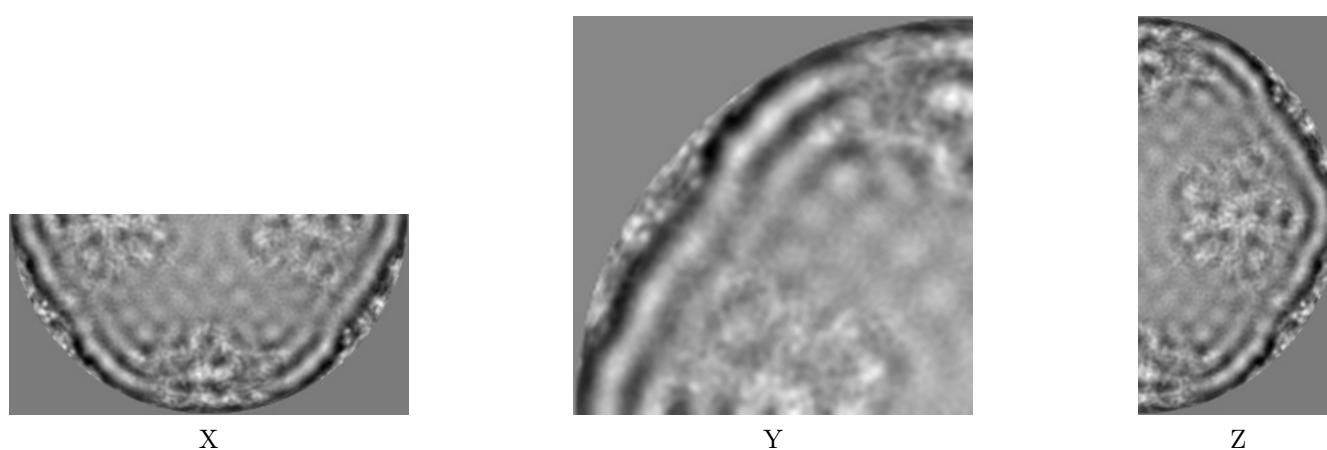
6 Map visualisation [i](#)

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](#)

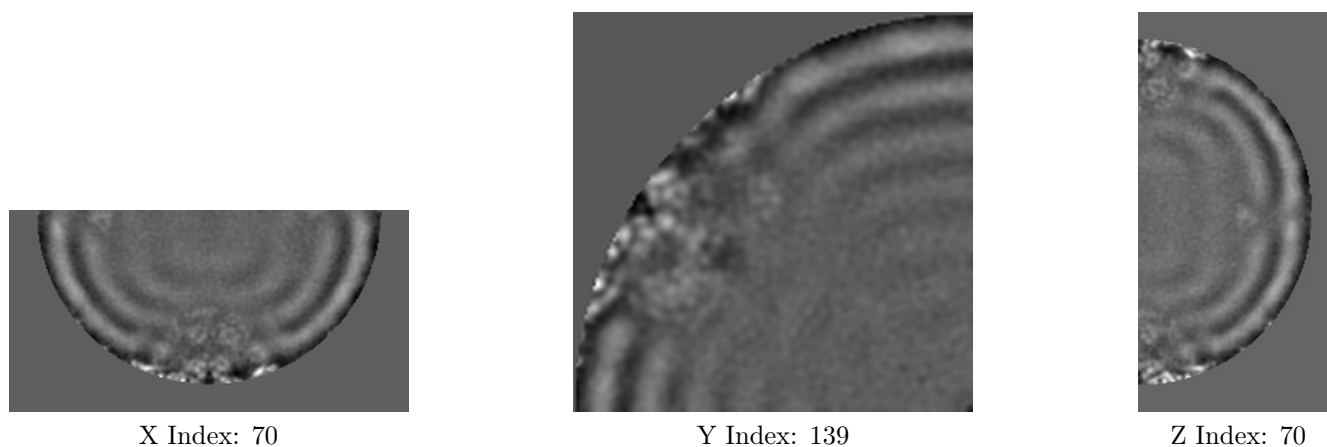
6.1.1 Primary map



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

6.2 Central slices [i](#)

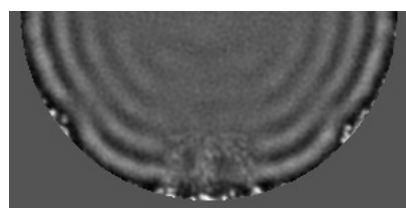
6.2.1 Primary map



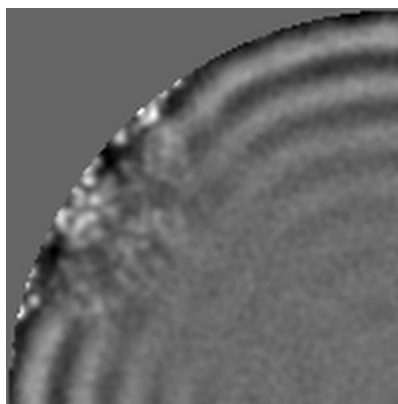
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

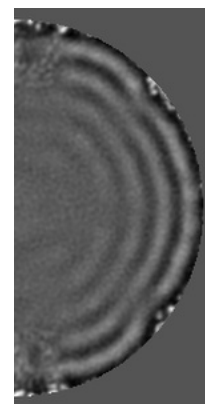
6.3.1 Primary map



X Index: 45



Y Index: 145

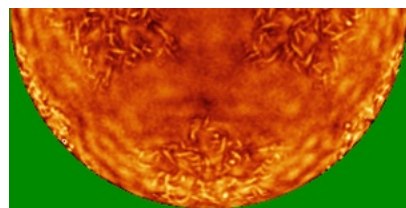


Z Index: 94

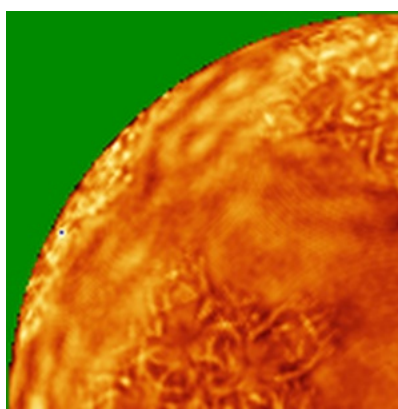
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

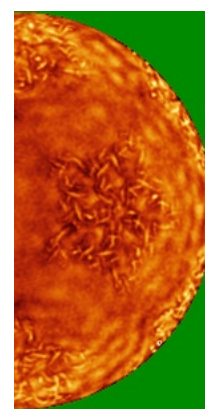
6.4.1 Primary map



X



Y

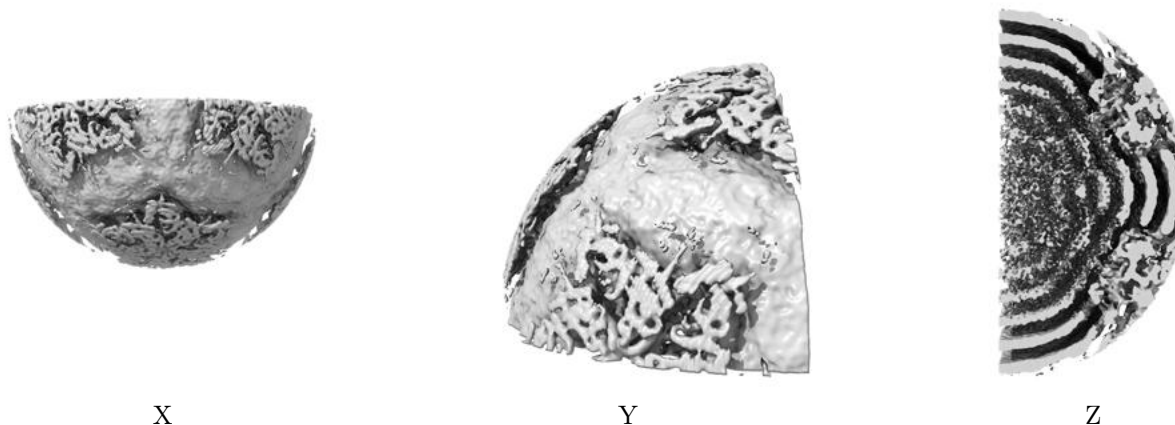


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

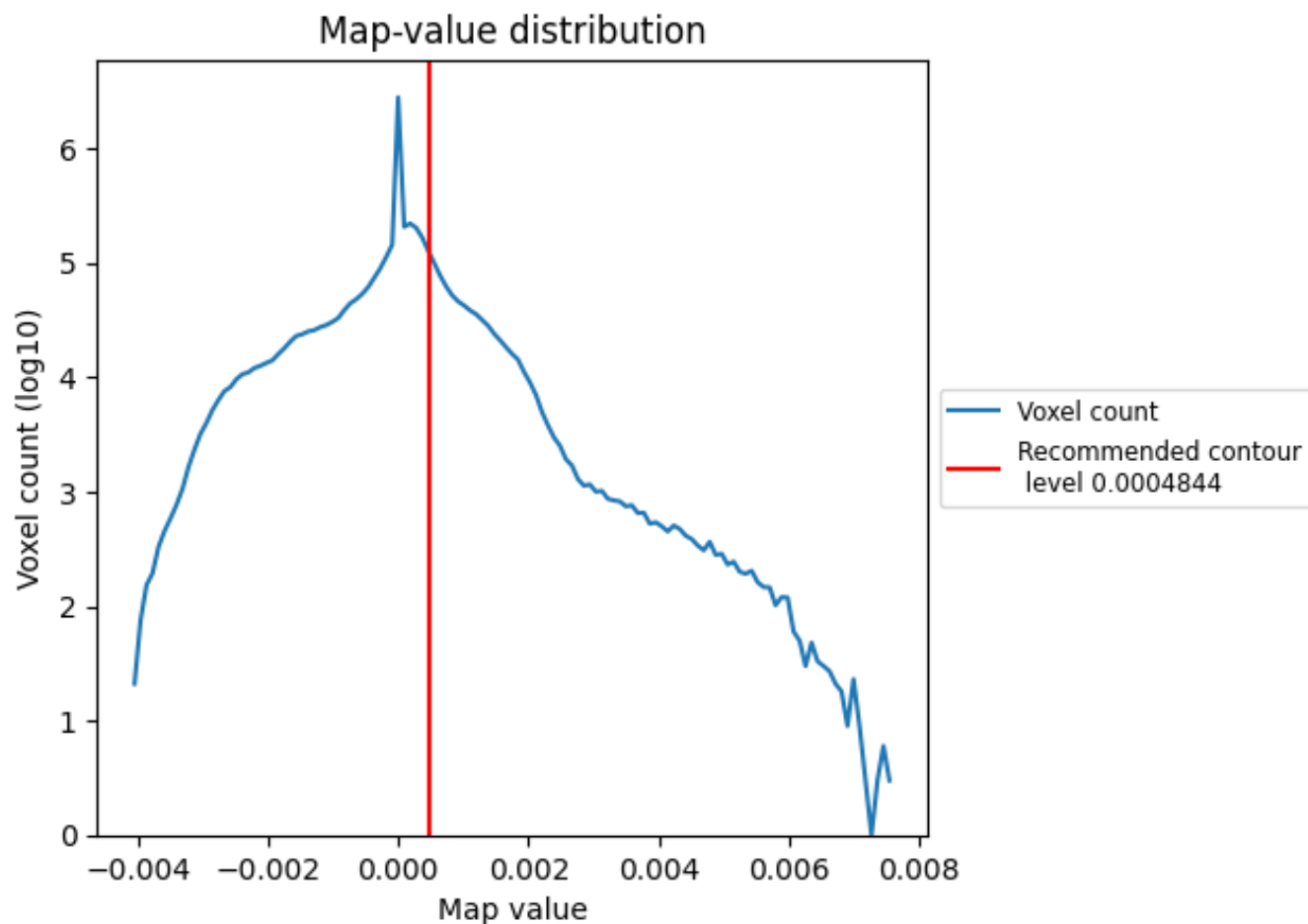
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

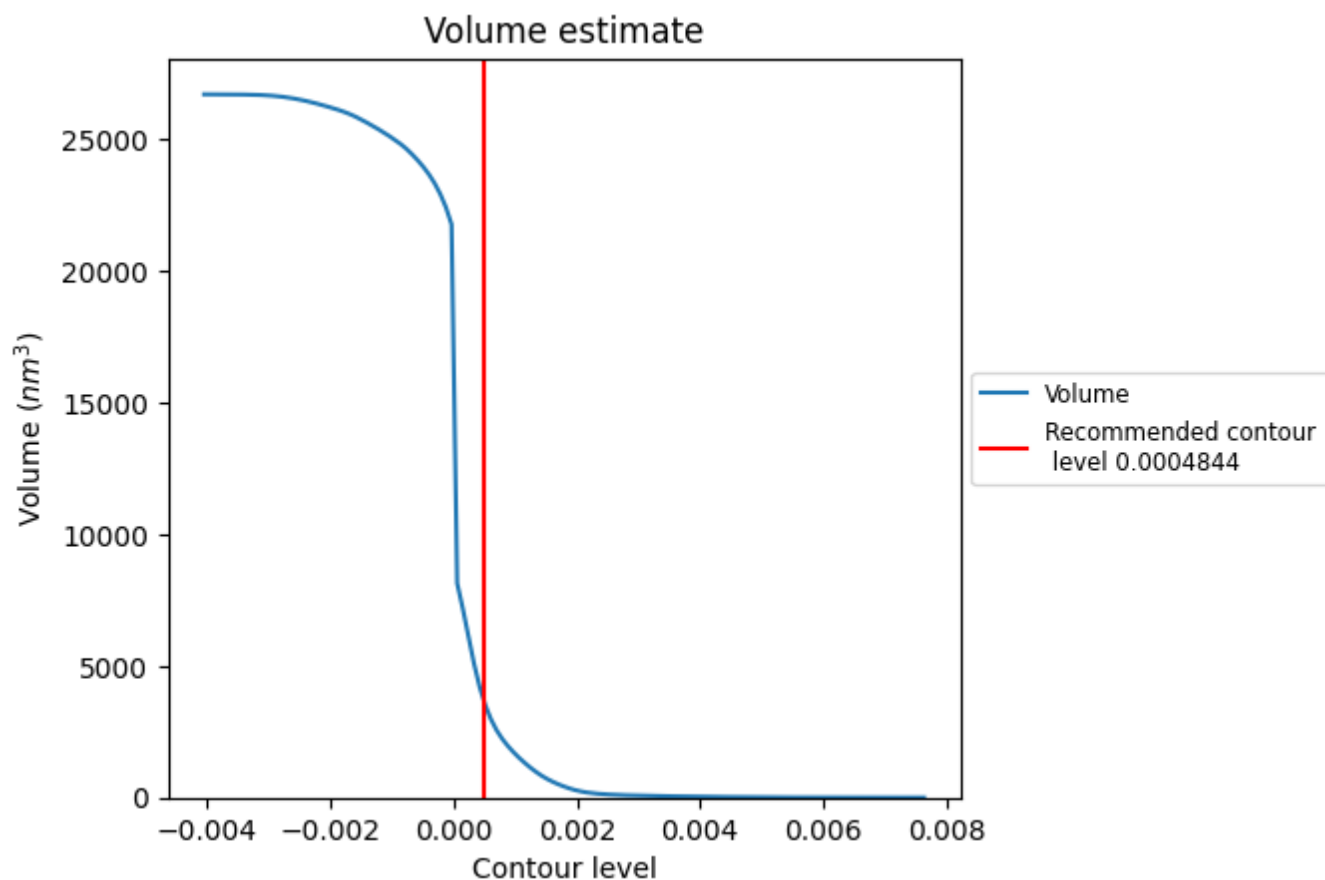
This section contains the results of statistical analysis of the map.

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 nm³; 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.

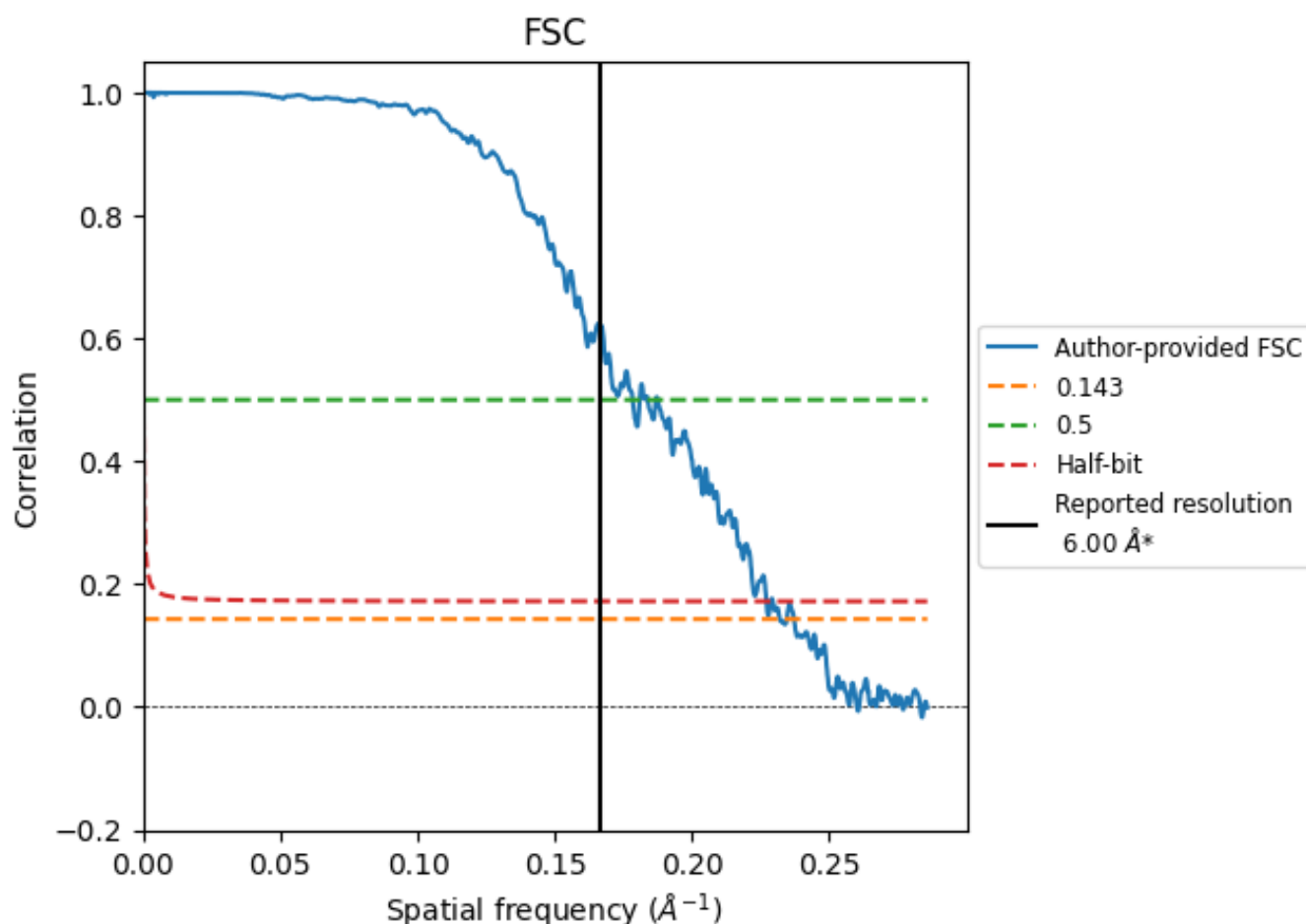
7.3 Rotationally averaged power spectrum [i](#)

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 Å⁻¹

8.2 Resolution estimates [i](#)

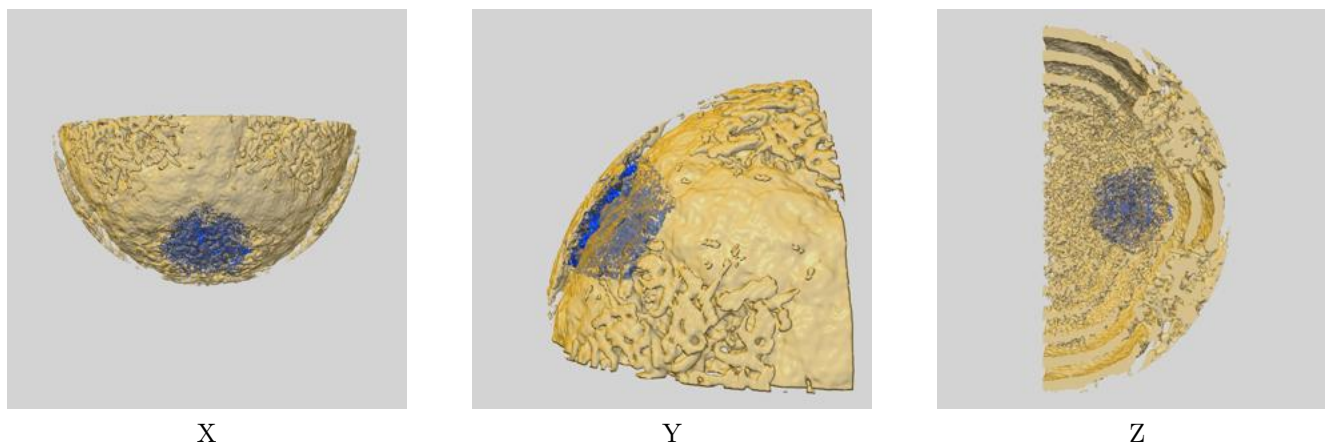
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	4.31	5.61	4.40
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

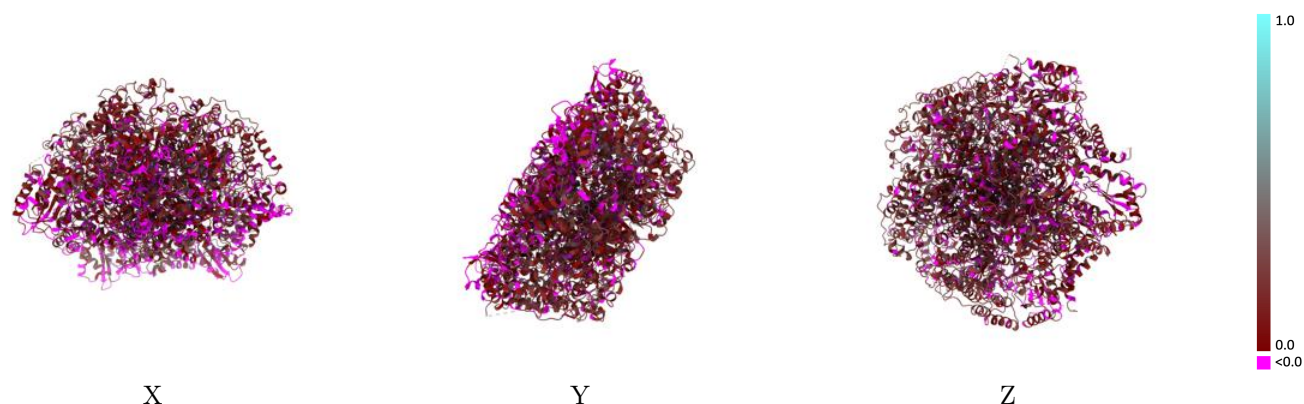
This section contains information regarding the fit between EMDB map EMD-2100 and PDB model 4AU6. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



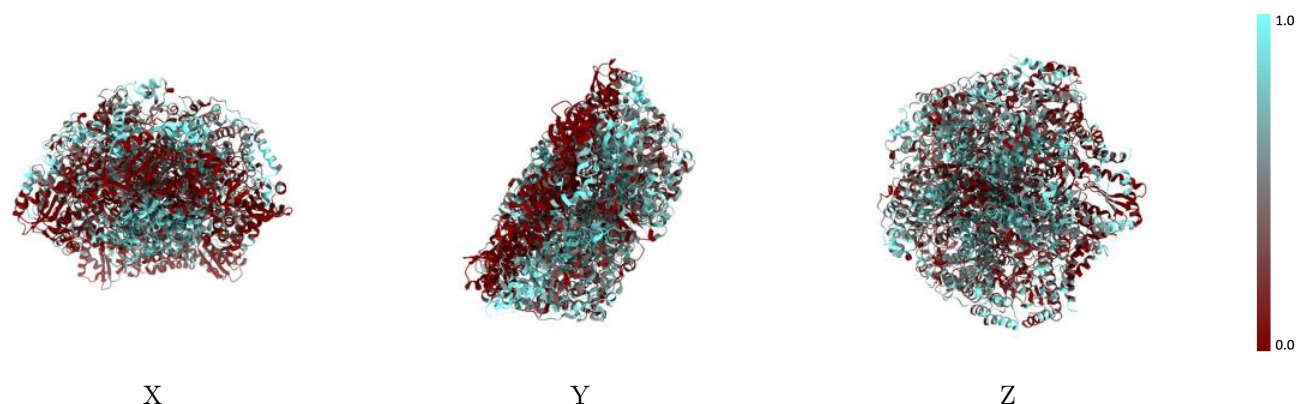
The images above show the 3D surface view of the map at the recommended contour level 0.0004844 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



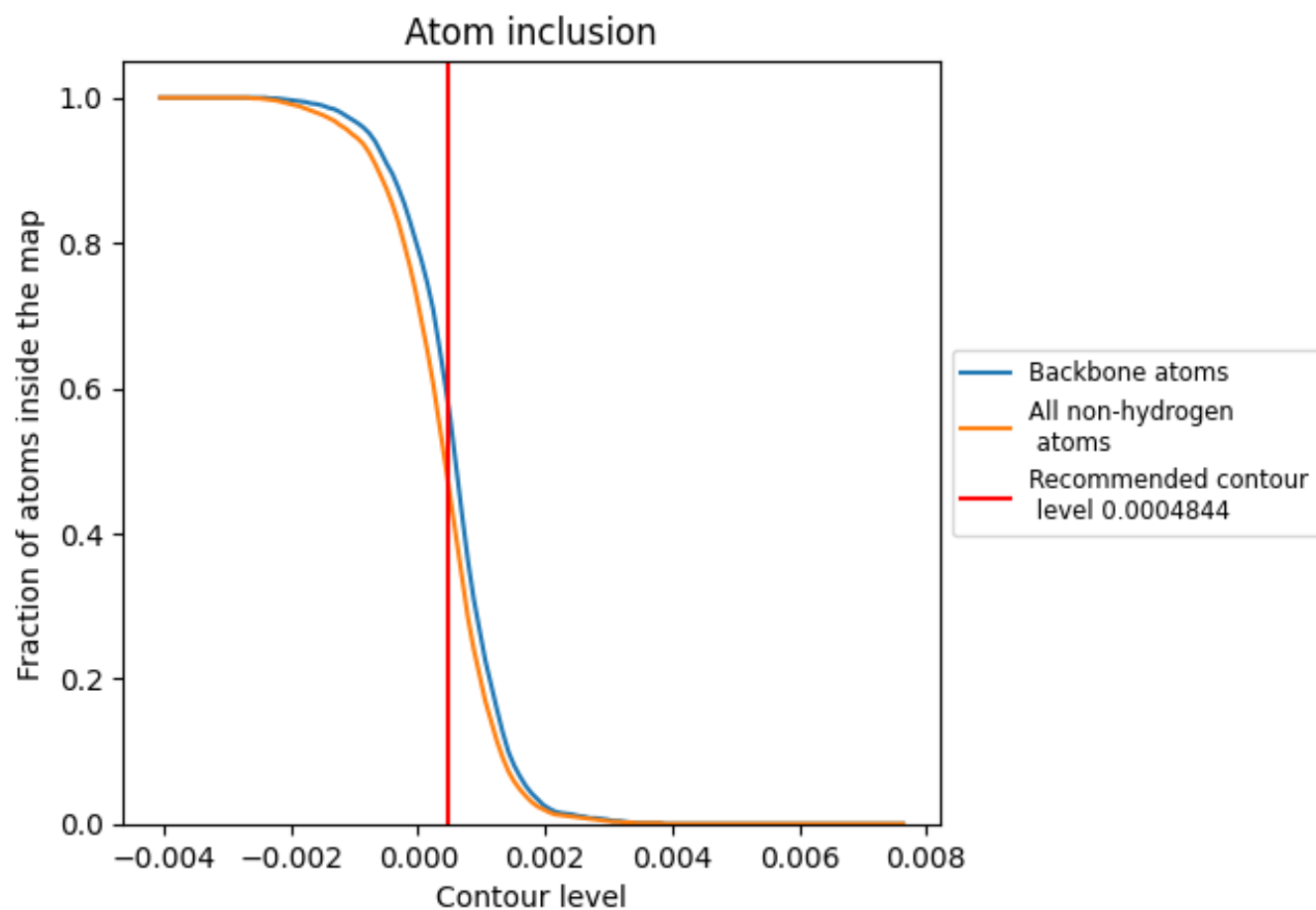
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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	0.4660	0.1190
A	0.4680	0.1180
B	0.4670	0.1190
C	0.4700	0.1180
D	0.4640	0.1190
E	0.4640	0.1200

