



wwPDB EM Validation Summary Report ⓘ

Nov 12, 2022 – 02:21 PM EST

PDB ID : 6PSW
EMDB ID : EMD-20466
Title : Escherichia coli RNA polymerase promoter unwinding intermediate (TRPo)
with TraR and rpsT P2 promoter
Authors : Chen, J.; Chiu, C.E.; Campbell, E.A.; Darst, S.A.
Deposited on : 2019-07-13
Resolution : 3.70 Å(reported)

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.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
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

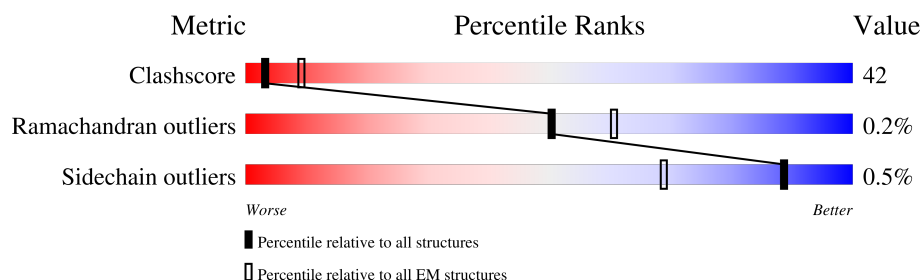
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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 ≥ 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	G	329	
1	H	329	
1	M	329	
2	I	1342	
3	J	1430	
4	K	91	
5	L	616	
6	N	72	

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Mol	Chain	Length	Quality of chain
7	O	85	<div><div><div></div><div></div><div></div></div><div>12%13%60%27%</div></div>
8	P	85	<div><div><div></div><div></div><div></div></div><div>20%11%61%27%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 32773 atoms, of which 78 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	229	Total	C	N	O	S	0	0
			1762	1100	313	343	6		
1	H	219	Total	C	N	O	S	0	0
			1678	1048	295	329	6		
1	M	73	Total	C	N	O	S	0	0
			572	362	100	108	2		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	1341	Total	C	N	O	S	0	0
			10571	6633	1839	2056	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1345	Total	C	N	O	S	0	0
			10460	6574	1864	1972	50		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	VAL	-	expression tag	UNP P0A8T7
J	1408	LEU	-	expression tag	UNP P0A8T7
J	1409	GLU	-	expression tag	UNP P0A8T7
J	1410	LEU	-	expression tag	UNP P0A8T7
J	1411	GLU	-	expression tag	UNP P0A8T7
J	1412	VAL	-	expression tag	UNP P0A8T7
J	1413	LEU	-	expression tag	UNP P0A8T7
J	1414	PHE	-	expression tag	UNP P0A8T7
J	1415	GLN	-	expression tag	UNP P0A8T7
J	1416	GLY	-	expression tag	UNP P0A8T7
J	1417	PRO	-	expression tag	UNP P0A8T7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1418	SER	-	expression tag	UNP P0A8T7
J	1419	SER	-	expression tag	UNP P0A8T7
J	1420	GLY	-	expression tag	UNP P0A8T7
J	1421	HIS	-	expression tag	UNP P0A8T7
J	1422	HIS	-	expression tag	UNP P0A8T7
J	1423	HIS	-	expression tag	UNP P0A8T7
J	1424	HIS	-	expression tag	UNP P0A8T7
J	1425	HIS	-	expression tag	UNP P0A8T7
J	1426	HIS	-	expression tag	UNP P0A8T7
J	1427	HIS	-	expression tag	UNP P0A8T7
J	1428	HIS	-	expression tag	UNP P0A8T7
J	1429	HIS	-	expression tag	UNP P0A8T7
J	1430	HIS	-	expression tag	UNP P0A8T7

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	79	Total	C	N	O	S	0	0
			627	382	118	126	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	473	Total	C	N	O	S	0	0
			3854	2412	687	732	23		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	SER	-	expression tag	UNP Q0P6L9
L	-1	GLU	-	expression tag	UNP Q0P6L9
L	0	PHE	-	expression tag	UNP Q0P6L9

- Molecule 6 is a protein called Protein TraR.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	72	Total	C	N	O	S	0	0
			571	353	105	108	5		

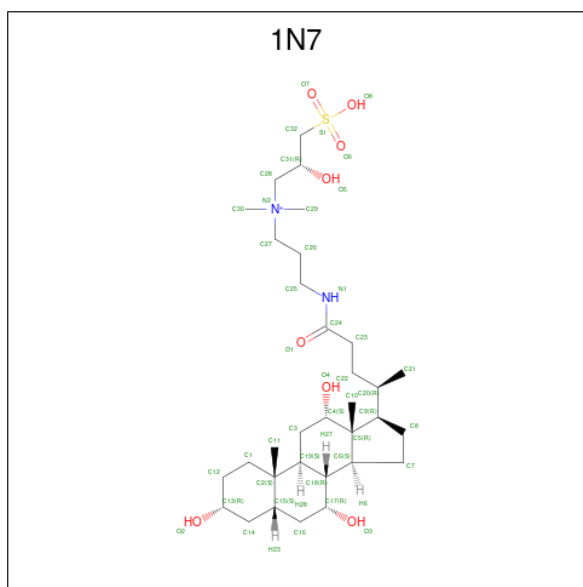
- Molecule 7 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	62	Total	C	N	O	P	0	0
			1270	606	237	365	62		

- Molecule 8 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	62	Total	C	N	O	P	0	0
			1272	609	222	379	62		

- Molecule 9 is CHAPSO (three-letter code: 1N7) (formula: C₃₂H₅₉N₂O₈S).



Mol	Chain	Residues	Atoms				AltConf
9	I	1	Total	C	H	O	0
			66	24	39	3	
9	J	1	Total	C	H	O	0
			66	24	39	3	

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	J	1	Total	Mg	0
			1	1	

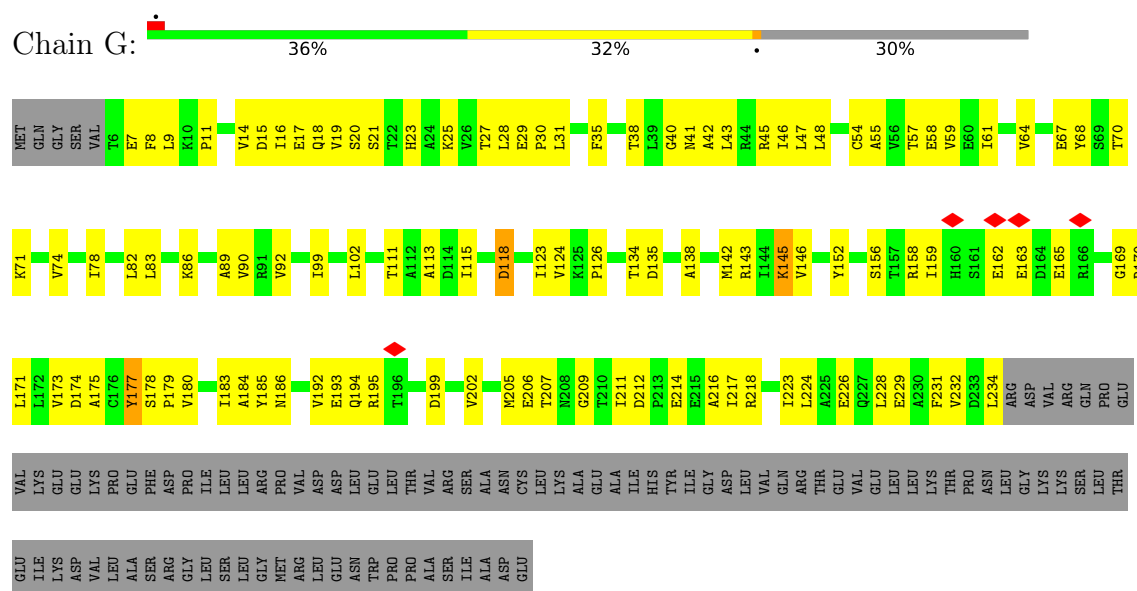
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	J	2	Total 2	Zn 2	0
11	N	1	Total 1	Zn 1	0

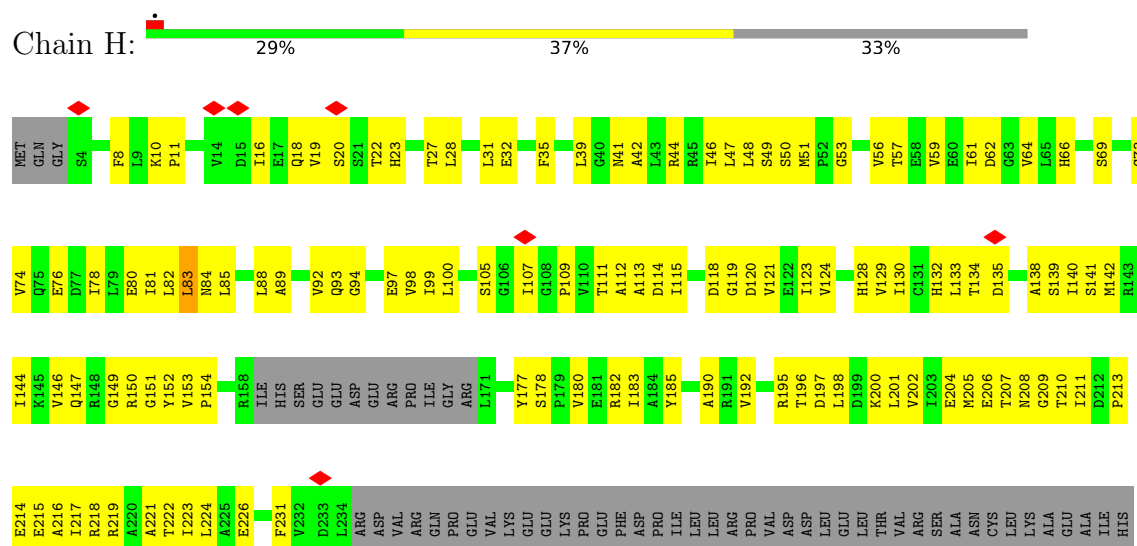
3 Residue-property plots

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: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha



S1057	S1058	S1059	V1060	V1061	L1062	L1063	S1064	A1065	A1066	R1067	T1068	G1070	G1071	K1072	D1073	R1075	P1076	L1077	L1078	K1079	I1080	V1081	D1082	A1083	Q1084	N1086	L1087	V1088	L1089	I1090	P1091	T1092	T1093	D1094	P1095	A1097	Q1098	F1100	L1101	P1102	G1103	K1104	I1105	I1106	V1107	Q1108	L1109	D1110	D1111	G1112	V1113	Q1114	I1115	S1116																																																																																															
Y995	R996	F997	P998	Y999	G1000	A1001	V1002	L1003	A1004	A1005	A1006	G1007	E1008	A1009	A1010	E1011	T1012	V1013	A1014	I1015	T1016	V1017	A1018	N1019	V1020	P1021	H1022	T1023	T1024	M1025	P1026	V1027	I1028	T1029	E1030	S1031	S1032	G1033	F1034	V1035	R1036	F1037	T1038	D1039	M1040	T1041	G1042	G1043	Q1044	T1045	I1046	T1047	R1048	Q1049	T1050	D1051	T991	K992	E993	S994																																																																																									
R933	T934	F935	H936	I937	G1938	A1939	A1940	A1941	A1942	A1943	A1944	A1945	A1946	A1947	A1948	A1949	A1950	A1951	A1952	A1953	A1954	A1955	A1956	A1957	A1958	A1959	A1960	A1961	A1962	A1963	A1964	A1965	A1966	A1967	A1968	A1969	A1970	A1971	A1972	A1973	A1974	A1975	A1976	A1977	A1978	A1979	A1980	A1981	A1982	A1983	A1984	A1985	A1986	A1987	A1988	A1989	A1990	A1991	A1992	A1993																																																																																									
L856	L857	R858	P859	R860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913																																																																																												
L783	A784	T785	T786	K787	T788	T789	A790	A791	L792	L793	L794	L795	L796	L797	L798	L799	L800	V801	A802	Q803	Q804	D805	D806	L807	T808	M809	M810	M811	M812	M813	M814	M815	M816	M817	M818	M819	M820	M821	M822	M823	M824	M825	M826	M827	M828	M829	M830	M831	M832	M833	M834	M835	M836	M837	M838	M839	M840	M841	M842	M843																																																																																									
E714	K715	T716	T717	T718	T719	T720	T721	T722	T723	T724	T725	T726	T727	T728	T729	T730	T731	T732	T733	T734	T735	T736	T737	T738	T739	T740	T741	T742	T743	T744	T745	T746	T747	T748	T749	T750	T751	T752	T753	T754	T755	T756	T757	T758	T759	T760	T761	T762	T763	T764	T765	T766	T767	T768	T769	T770	T771	T772	T773	T774	T775	T776	T777	T778	T779	T780	T781	T782																																																																																	
M644	P645	E646	K647	K648	K649	K650	K651	K652	K653	K654	K655	K656	K657	K658	K659	K660	K661	K662	K663	K664	K665	K666	K667	K668	K669	K670	K671	K672	K673	K674	K675	K676	K677	K678	K679	K680	K681	K682	K683	K684	K685	K686	K687	K688	K689	K690	K691	K692	K693	K694	K695	K696	K697	K698	K699	K700	K701	K702	K703	K704	K705	K706	K707	K708	K709	K710	K711	K712	K713																																																																																
L856	L857	R858	P859	R860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932																																																																									
R933	T934	F935	H936	I937	G1938	A1939	A1940	A1941	A1942	A1943	A1944	A1945	A1946	A1947	A1948	A1949	A1950	A1951	A1952	A1953	A1954	A1955	A1956	A1957	A1958	A1959	A1960	A1961	A1962	A1963	A1964	A1965	A1966	A1967	A1968	A1969	A1970	A1971	A1972	A1973	A1974	A1975	A1976	A1977	A1978	A1979	A1980	A1981	A1982	A1983	A1984	A1985	A1986	A1987	A1988	A1989	A1990	A1991	A1992	A1993	A1994																																																																																								
D67	Y68	E69	C70	L71	C72	G73	K74	Y75	K76	R77	L78	K79	H80	V83	I84	C85	E86	K87	C88	G89	V92	T93	Q94	T95	K96	V97	R98	R99	E100	R101	M102	G103	H104	I105	E106	L107	A108	T111	L114	W115	F116	L117	S122	L123	L124	G125	L126	L127	L128	D129	M130	P131	L132	R133																																																																																															
D134	I135	E136	R137	V138	E142	K143	S144	Y145	V146	I147	L148	G149	G150	M151	T152	N153	L154	Q157	Q158	I159	L160	T161	E162	Q163	Y165	L166	L169	D174	E175	F176	D177	V178	K179	M180	A184	I185	Q186	L189	M192	D193	L194	E195	Q196	E197	Q200	L201	R202	E203	E204	L205																																																																																																			
T208	N209	E211	T212	K213	R214	K215	L216	L217	V218	T219	K220	I221	K222	L223	L224	V228	A302	V303	D304	A305	L306	L307	D308	N309	G310	R311	L316	L324	K325	S326	L327	K334	Q335	G336	F337	F338	R339	L342	L343	G344	K345	R346	V347	D348	Y349	S350	R351	V352	S353	I355	R356																																																																																																		
V357	G358	P359	L363	H364	L368	P369	K370	K371	M372	N373	A374	L374	E375	F376	F377	K378	P379	L385	R388	G389	L390	A391	T392	I393	K394	A395	A396	A397	K398	K399	M400	V401	E402	R403	E404	A405	V407	V408	V409	D410	I411	L412	D413	E414	V415	I416	R417	E418	V421	L422	L423	N424	R425	A426																																																																																															
P427	L428	L429	H430	R431	L432	G433	L434	Q435	A436	P439	V440	L441	L442	E443	G444	K445	L446	L447	Q448	L449	H450	P451	L452	Y457	N458	T393	I394	K395	A396	A397	K398	K399	M400	V401	E402	R403	E404	A405	V407	V408	V409	D410	I411	L412	D413	E414	V415	I416	R417	E418	V421	L422	L423	N424	R425	A426																																																																																													
P498	I499	V500	L501	S502	P503	Q504	G505	V506	L507	G509	L510	M513	T514	R515	D516	C517	V518	N519	A520	G521	G522	M525	V526	L527	P530	K531	E532	A533	E534	R535	L536	Y537	R538	L541	L544	H545	A546	R547	V548	K549	V550	R551	L552	I553	E554	Y555	E556	K557	D558	E562	L563	K566																																																																																																	
T567	S568	L569	K570	T573	V574	G575	R576	A577	L578	L579	V580	M581	I582	V583	P584	K585	P588	Y589	S590	I591	V592	N593	K598	I601	Y609	R610	I611	L612	G613	L614	K615	P616	I619	F620	Q623	I624	M625	Y626	T627	Y631	A632	A633	G636	A637	S638	V639	G640	I641	D642	D643																																																																																																			
M644	P647	E648	K649	K650	K651	K652	K653	K654	K655	K656	K657	K658	K659	K660	K661	K662	K663	K664	K665	K666	K667	K668	K669	K670	K671	K672	K673	K674	K675	K676	K677	K678	K679	K680	K681	K682	K683	K684	K685	K686	K687	K688	K689	K690	K691	K692	K693	K694	K695	K696	K697	K698	K699	K700	K701	K702	K703	K704	K705	K706	K707	K708	K709	K710	K711	K712	K713																																																																																		
E714	K715	T716	T717	T718	T719	T720	T721	T722	T723	T724	T725	T726	T727	T728	T729	T730	T731	T732	T733	T734	T735	T736	T737	T738	T739	T740	T741	T742	T743	T744	T745	T746	T747	T748	T749	T750	T751	T752	T753	T754	T755	T756	T757	T758	T759	T760	T761	T762	T763	T764	T765	T766	T767	T768	T769	T770	T771	T772	T773	T774	T775	T776	T777	T778	T779	T780	T781	T782																																																																																	
L783	A784	T785	T786	K787	T788	T789	A790	A791	L792	L793	L794	L795	L796	L797	L798	L799	L800	V801	A802	Q803	Q804	D805	D806	L807	T808	M809	M810	M811	M812	M813	M814	M815	M816	M817	M818	M819	M820	M821	M822	M823	M824	M825	M826	M827	M828	M829	M830	M831	M832	M833	M834	M835	M836	M837	M838	M839	M840	M841	M842	M843	M844	M845	M846	M847	M848	M849	M850	M851	M852	M853	M854	M855	M856	M857	M858	M859	M860	M861	M862	M863	M864	M865	M866	M867	M868	M869	M870	M871	M872	M873	M874	M875	M876	M877	M878	M879	M880	M881	M882	M883	M884	M885	M886	M887	M888	M889	M890	M891	M892	M893	M894	M895	M896	M897	M898	M899	M900	M901	M902	M903	M904	M905	M906	M907	M908	M909	M910	M911	M912	M913	M914	M915	M916	M917	M918	M919	M920	M921	M922	M923	M924	M925	M926	M927	M928	M929	M930	M931	M932
L856	L857	R858	P859	R860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932																																																																									
R933	T934	F935	H936	I937	G1938	A1939	A1940	A1941	A1942	A1943	A1944	A1945	A1946	A1947	A1948	A1949	A1950	A1951	A1952	A1953	A1954	A1955	A1956	A1957	A1958	A1959	A1960	A1961	A1962	A1963	A1964	A1965	A1966	A1967	A1968	A1969	A1970	A1971	A1972	A1973	A1974	A1975	A1976	A1977	A1978	A1979	A1980	A1981	A1982	A1983	A1984	A1985	A1986	A1987	A1988	A1989	A1990	A1991	A1992	A1993	A1994																																																																																								
Y995	R996	F997	P998	Y999	G1000	A1001	V1002	L1003	A1004	A1005	A1006	G1007	E1008	A1009	A1010	E1011	T1012	V1013	A1014	I1015	T1016	V1017	A1018	N1019	V1020	P1021	H1022	T1023	T1024	M1025	P1026	V1027	I1028	T1029	E1030	S1031	S1032	G1033	F1034	V1035	R1036	F1037	T1038	D1039	M1040	T1041	G1042	G1043	Q1044	T1045	I1046	T1047	R1048	Q1049	T1050	D1051	T991	K992	E993	S994																																																																																									
S1057	S1058	S1059	V1060	V1061	L1062	L1063	S1064	A1065	A1066	R1067	T1068	G1070	G1071	K1072	D1073	R1075	P1076	L1077	L1078	K1079	I1080	V1081	D1082	A1083	Q1084	N1086	L1087	V1088	L1089	I1090	P1091	T1092	T1093	D1094	P1095	A1097	Q																																																																																																																

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46650	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.154	Depositor
Minimum map value	-0.109	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, 1N7

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	G	0.40	0/1784	0.50	0/2419
1	H	0.36	0/1697	0.52	0/2301
1	M	0.25	0/579	0.51	0/784
2	I	0.42	0/10740	0.52	0/14492
3	J	0.40	0/10619	0.53	0/14338
4	K	0.33	0/629	0.49	0/847
5	L	0.31	0/3906	0.49	0/5251
6	N	0.30	0/581	0.52	0/785
7	O	0.59	0/1426	0.94	0/2197
8	P	0.64	0/1424	1.00	1/2197 (0.0%)
All	All	0.41	0/33385	0.58	1/45611 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	I	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	34	DT	O4'-C4'-C3'	-7.22	101.61	104.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	442	VAL	Peptide
2	I	545	PHE	Peptide
2	I	57	PHE	Peptide

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	G	1762	0	1785	112	0
1	H	1678	0	1698	149	0
1	M	572	0	602	56	0
2	I	10571	0	10580	919	0
3	J	10460	0	10679	950	0
4	K	627	0	634	51	0
5	L	3854	0	3911	471	0
6	N	571	0	558	35	0
7	O	1270	0	698	87	0
8	P	1272	0	705	105	0
9	I	27	39	38	5	0
9	J	27	39	38	5	0
10	J	1	0	0	0	0
11	J	2	0	0	0	0
11	N	1	0	0	0	0
All	All	32695	78	31926	2698	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 42.

The worst 5 of 2698 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)
9:J:1504:1N7:C19	9:J:1504:1N7:C3	1.84	1.54
9:I:1401:1N7:C3	9:I:1401:1N7:C19	1.82	1.52
5:L:146:GLU:O	5:L:150:ARG:HG3	1.48	1.10
3:J:145:VAL:HG23	3:J:159:ILE:HG22	1.36	1.05
3:J:965:SER:HB2	3:J:973:LEU:HD11	1.38	1.03

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	G	227/329 (69%)	195 (86%)	32 (14%)	0	100	100
1	H	215/329 (65%)	188 (87%)	26 (12%)	1 (0%)	29	66
1	M	71/329 (22%)	63 (89%)	8 (11%)	0	100	100
2	I	1339/1342 (100%)	1177 (88%)	158 (12%)	4 (0%)	41	74
3	J	1339/1430 (94%)	1187 (89%)	152 (11%)	0	100	100
4	K	77/91 (85%)	69 (90%)	8 (10%)	0	100	100
5	L	467/616 (76%)	422 (90%)	45 (10%)	0	100	100
6	N	70/72 (97%)	62 (89%)	6 (9%)	2 (3%)	4	32
All	All	3805/4538 (84%)	3363 (88%)	435 (11%)	7 (0%)	50	78

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	546	GLU
2	I	974	ARG
6	N	29	ALA
2	I	443	ASP
6	N	30	HIS

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	G	193/286 (68%)	189 (98%)	4 (2%)	53	74
1	H	184/286 (64%)	183 (100%)	1 (0%)	88	94
1	M	65/286 (23%)	65 (100%)	0	100	100
2	I	1155/1157 (100%)	1149 (100%)	6 (0%)	88	94
3	J	1127/1189 (95%)	1122 (100%)	5 (0%)	91	95
4	K	67/75 (89%)	67 (100%)	0	100	100
5	L	421/543 (78%)	420 (100%)	1 (0%)	93	97
6	N	61/61 (100%)	61 (100%)	0	100	100
All	All	3273/3883 (84%)	3256 (100%)	17 (0%)	89	94

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	1167	LYS
5	L	476	ARG
2	I	436	ARG
2	I	443	ASP
2	I	516	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
5	L	227	GLN
5	L	265	GLN
6	N	28	ASN
2	I	1080	ASN
2	I	932	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
9	1N7	J	1504	-	30,30,46	5.06	15 (50%)	47,48,72	2.42	18 (38%)
9	1N7	I	1401	-	30,30,46	4.81	14 (46%)	47,48,72	2.21	14 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	1N7	J	1504	-	-	0/7/72/92	0/4/4/4
9	1N7	I	1401	-	-	2/7/72/92	0/4/4/4

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	1504	1N7	C3-C19	18.59	1.84	1.53
9	I	1401	1N7	C3-C19	17.29	1.82	1.53
9	J	1504	1N7	C3-C4	12.02	1.73	1.53
9	I	1401	1N7	C3-C4	10.88	1.71	1.53
9	I	1401	1N7	C5-C4	-8.87	1.40	1.54

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	1504	1N7	C9-C5-C6	5.92	106.06	100.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	1504	1N7	C9-C5-C4	-5.47	112.67	117.67
9	I	1401	1N7	C19-C3-C4	-4.92	107.80	114.30
9	I	1401	1N7	C7-C6-C18	-4.89	111.49	118.33
9	I	1401	1N7	C9-C5-C4	-4.55	113.51	117.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

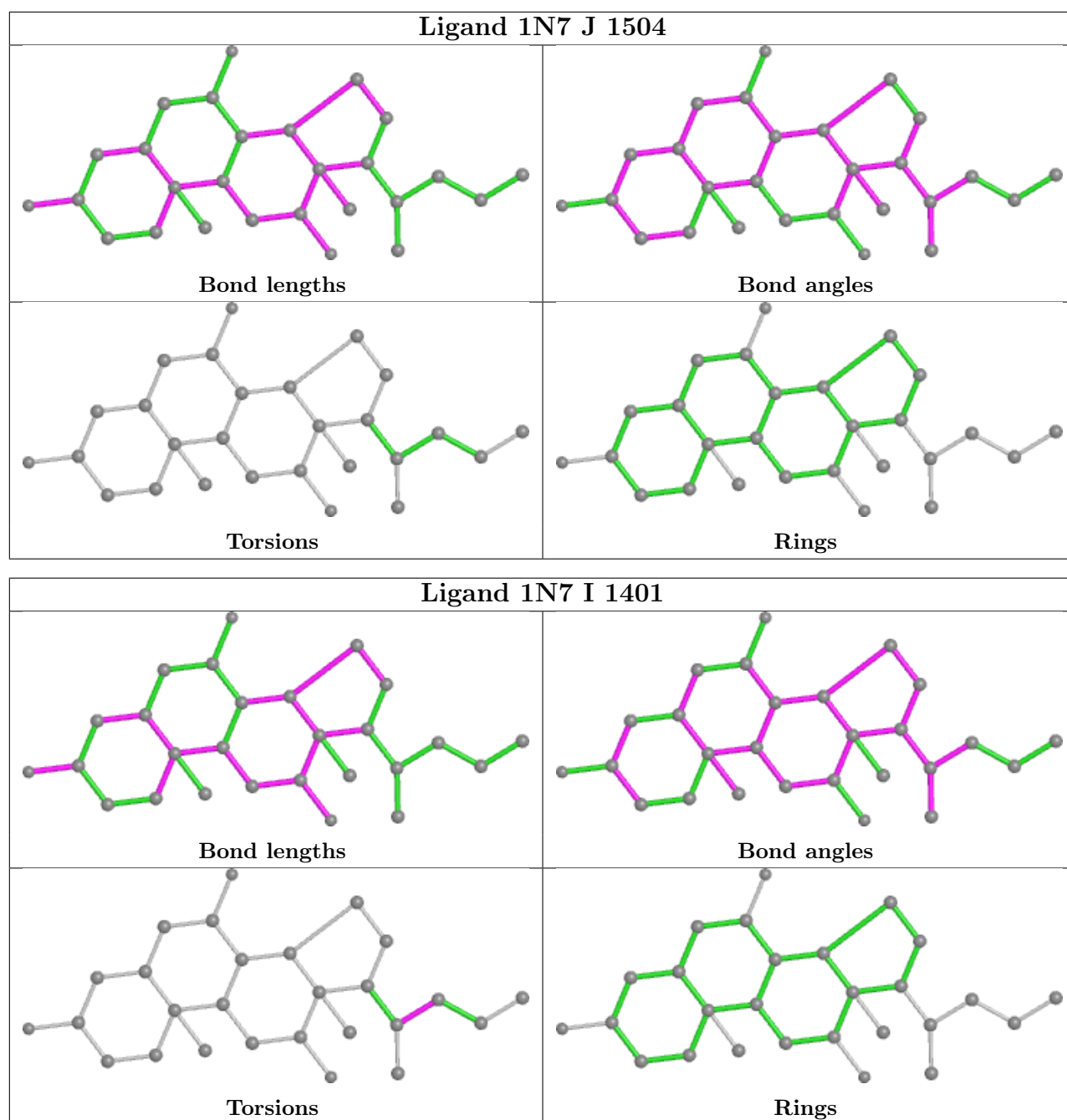
Mol	Chain	Res	Type	Atoms
9	I	1401	1N7	C9-C20-C22-C23
9	I	1401	1N7	C21-C20-C22-C23

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	J	1504	1N7	5	0
9	I	1401	1N7	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

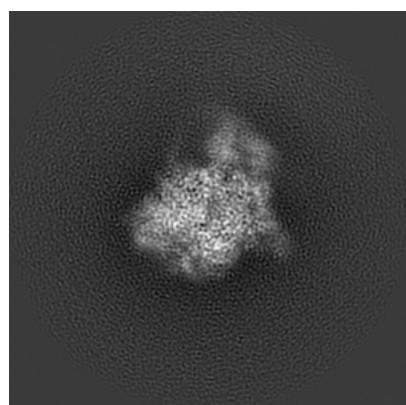
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20466. These allow visual inspection of the internal detail of the map and identification of artifacts.

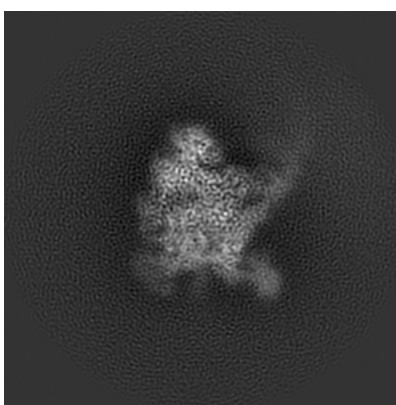
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

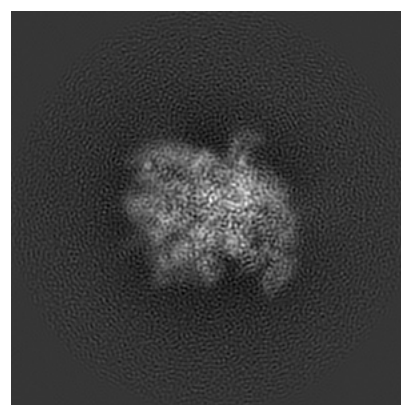
6.1.1 Primary map



X



Y

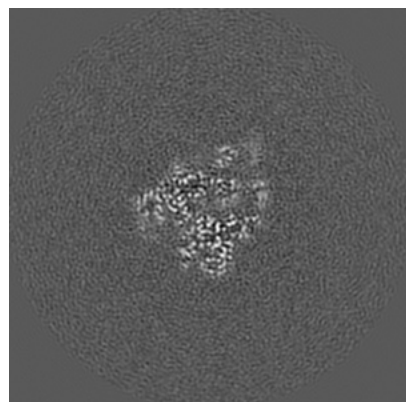


Z

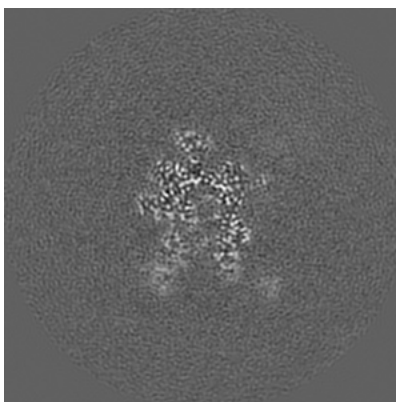
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

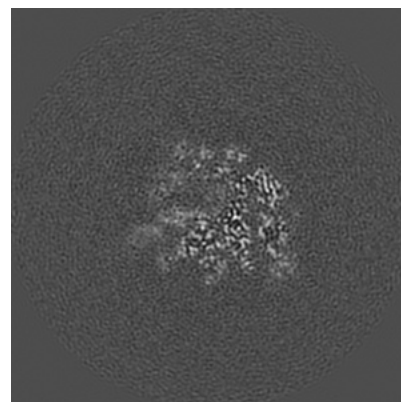
6.2.1 Primary map



X Index: 128



Y Index: 128

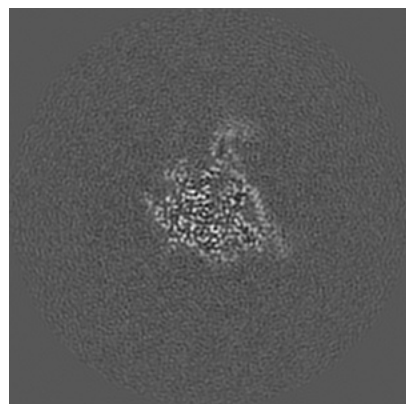


Z Index: 128

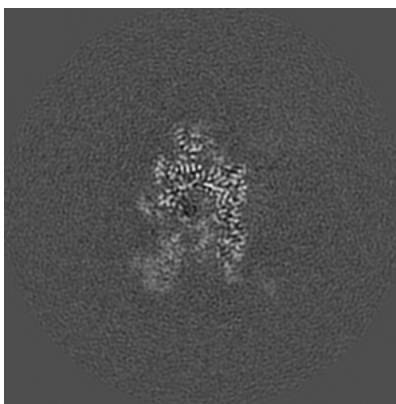
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

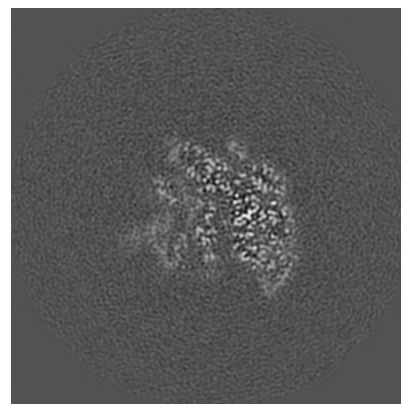
6.3.1 Primary map



X Index: 147



Y Index: 125



Z Index: 121

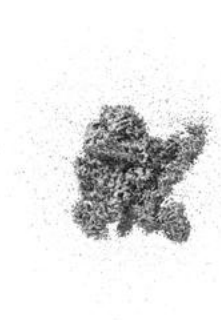
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

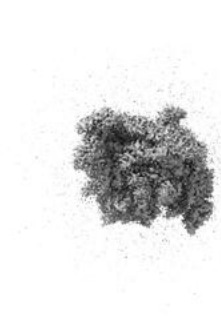
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

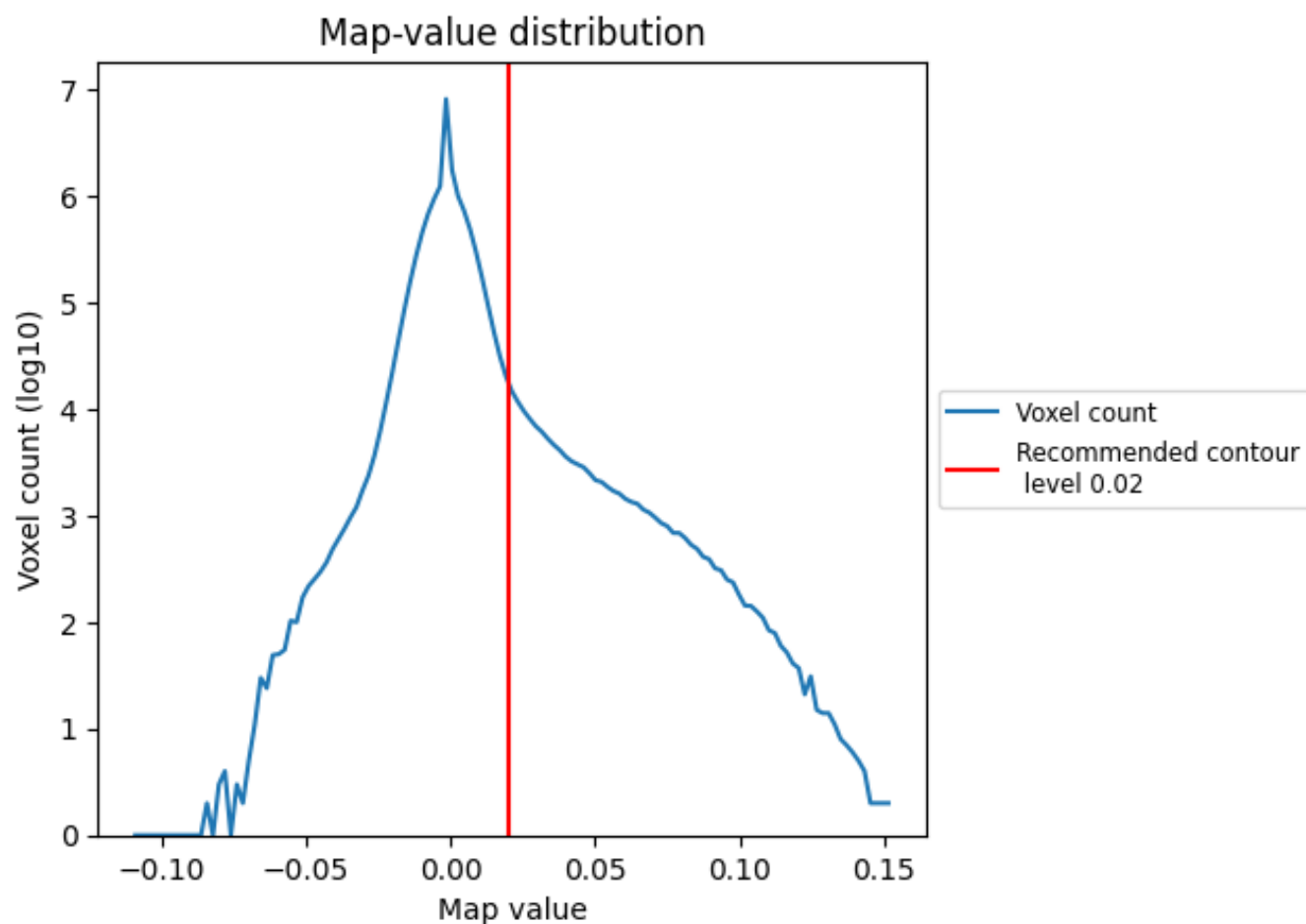
6.5 Mask visualisation

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

7 Map analysis [i](#)

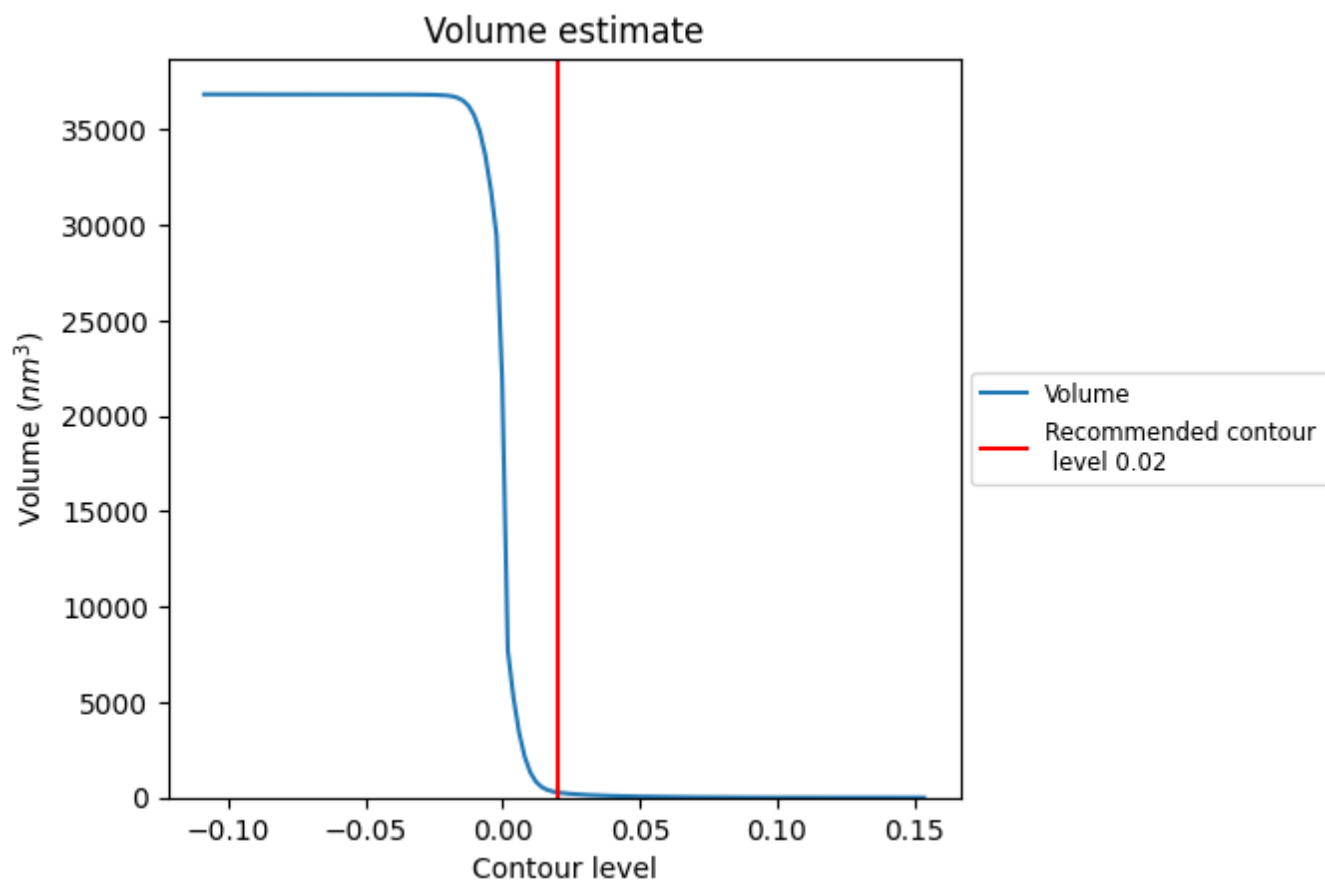
This section contains the results of statistical analysis of the map.

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.

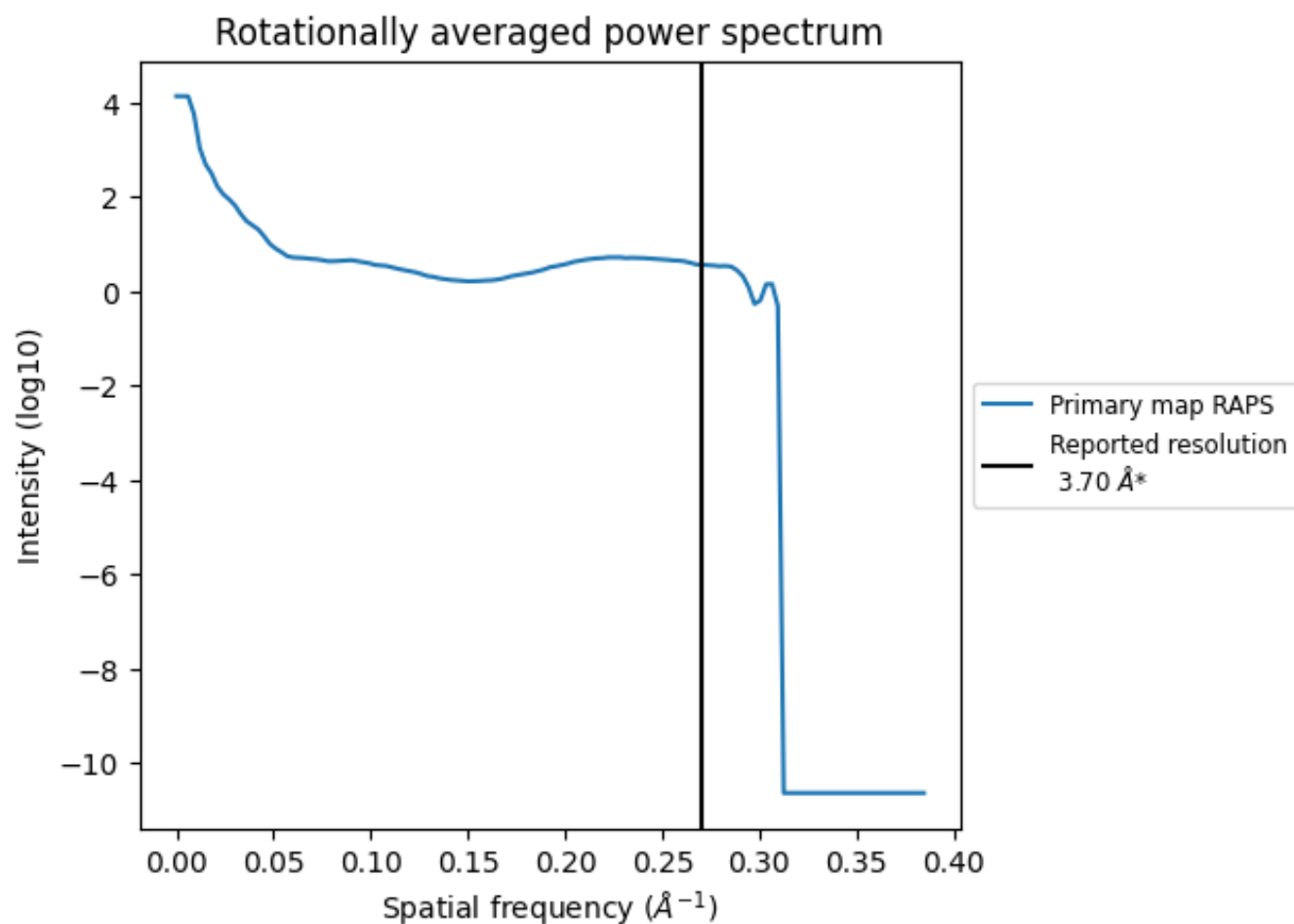
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 270 nm³; this corresponds to an approximate mass of 244 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 ⓘ

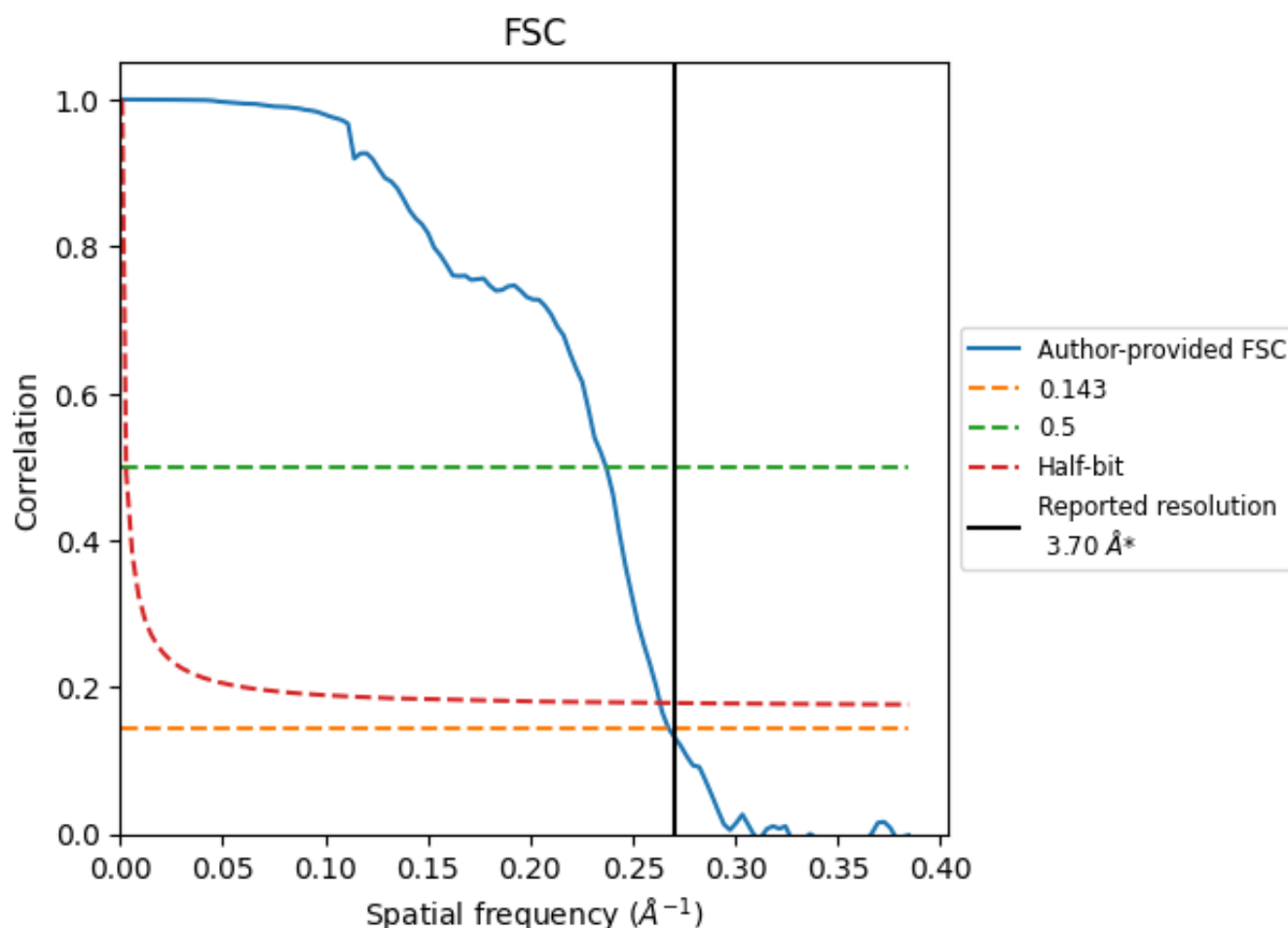


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

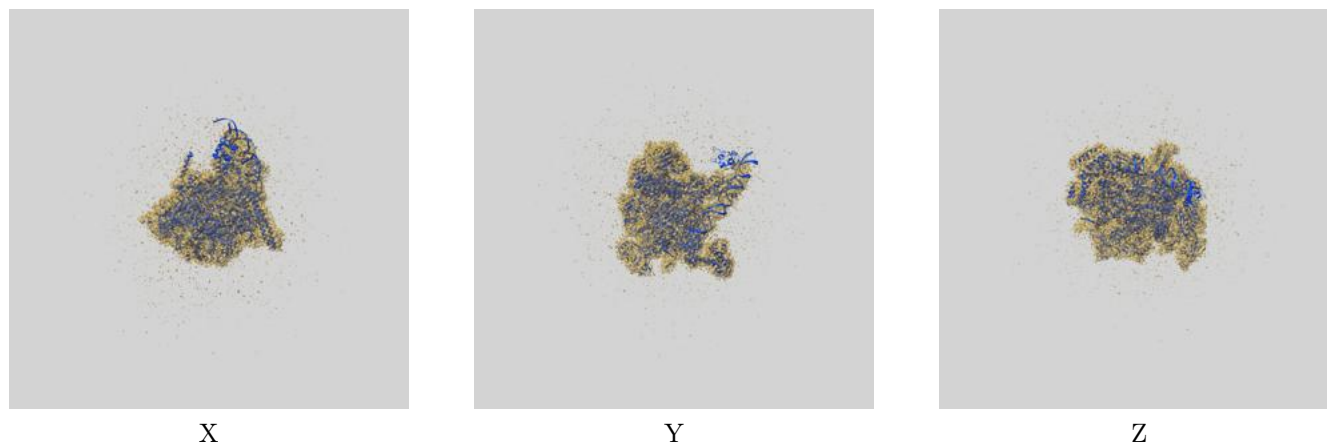
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.74	4.22	3.80
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

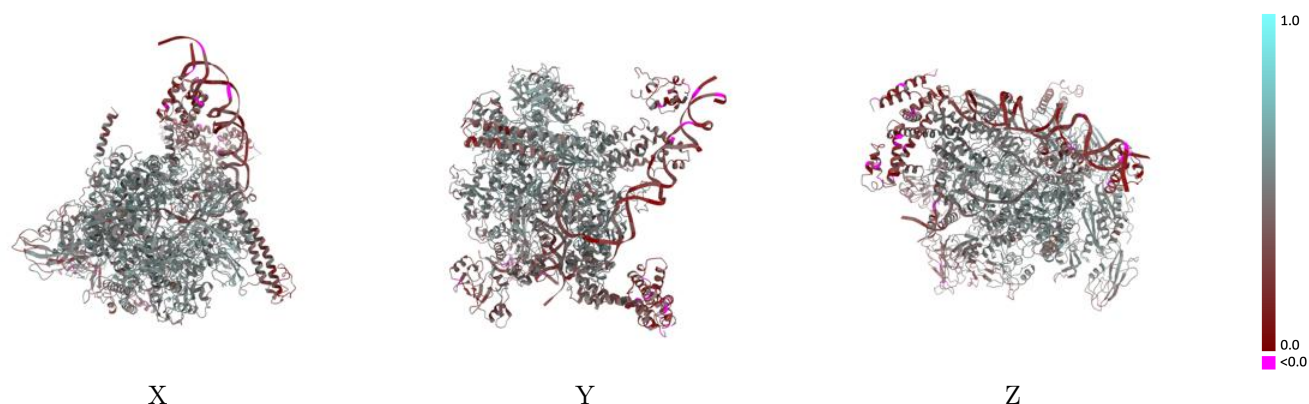
This section contains information regarding the fit between EMDB map EMD-20466 and PDB model 6PSW. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



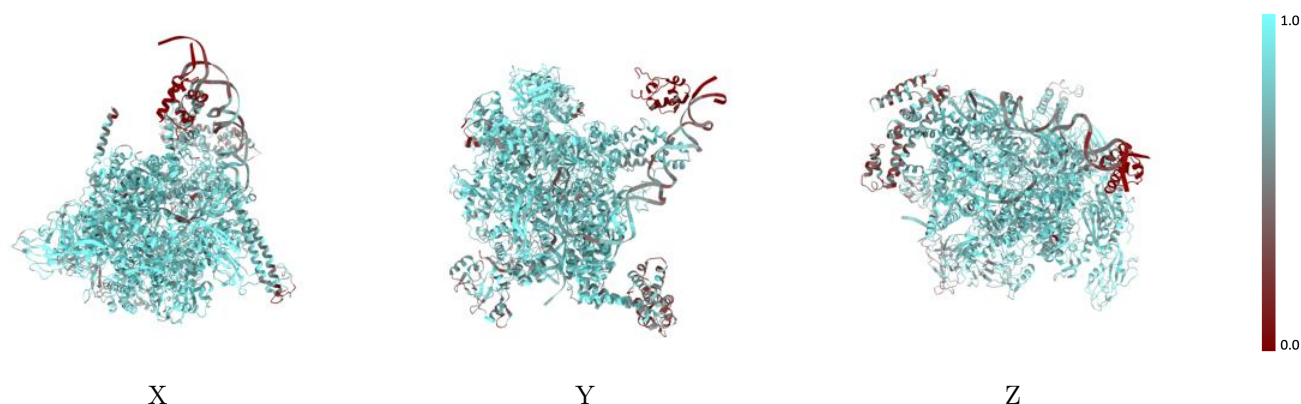
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



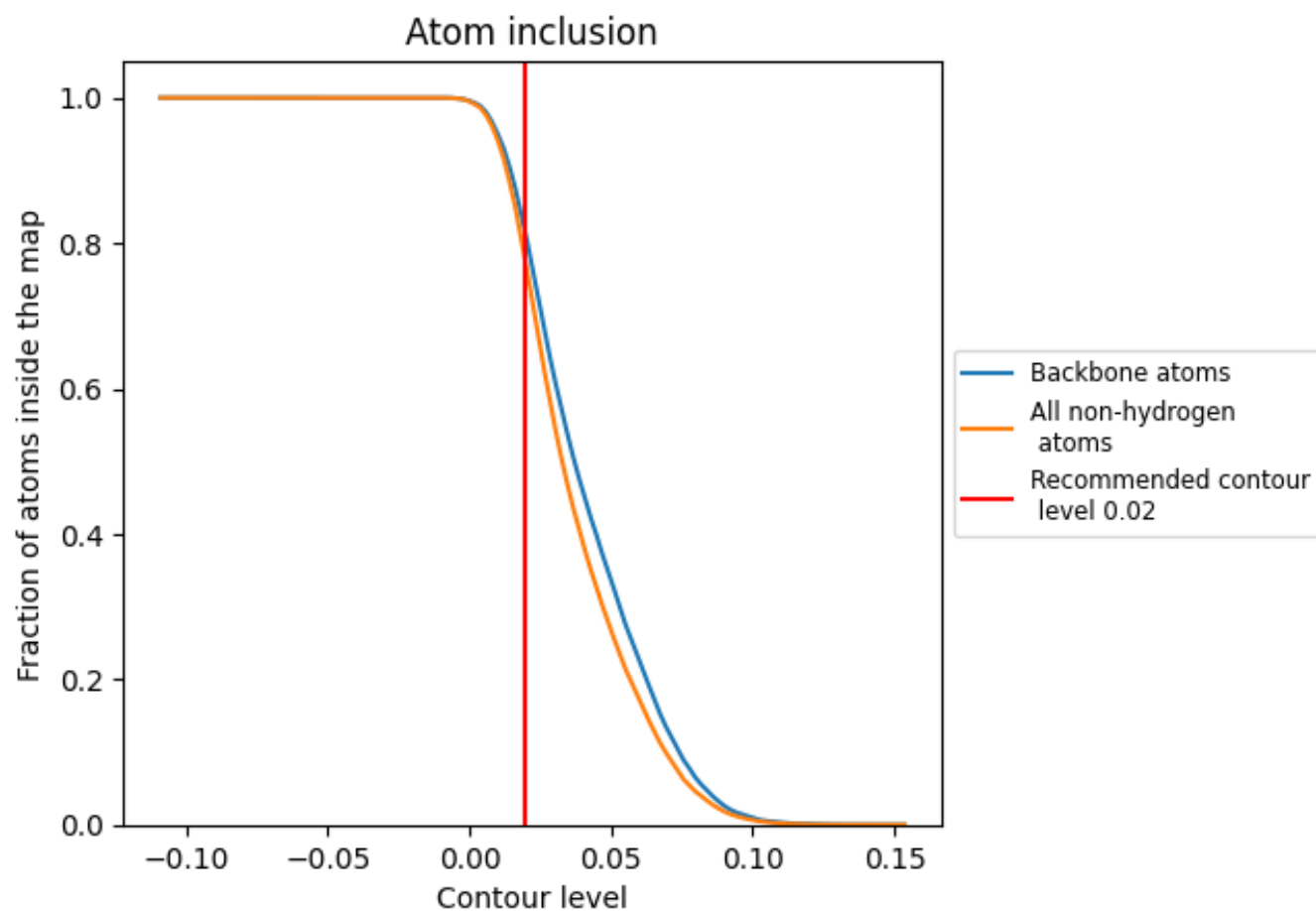
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7703	<div></div> 0.4380
G	<div></div> 0.8586	<div></div> 0.5010
H	<div></div> 0.8262	<div></div> 0.4660
I	<div></div> 0.8268	<div></div> 0.4750
J	<div></div> 0.8218	<div></div> 0.4710
K	<div></div> 0.7381	<div></div> 0.4650
L	<div></div> 0.6766	<div></div> 0.3560
M	<div></div> 0.0464	<div></div> 0.2530
N	<div></div> 0.6888	<div></div> 0.3990
O	<div></div> 0.6260	<div></div> 0.2570
P	<div></div> 0.5653	<div></div> 0.2460

1.0

0.0

<0.0