



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 05:21 pm GMT

PDB ID : 4AV2  
EMDB ID : EMD-2105  
Title : Single particle electron microscopy of PilQ dodecameric complexes from *Neisseria meningitidis*.  
Authors : Berry, J.L.; Phelan, M.M.; Collins, R.F.; Adomavicius, T.; Tonjum, T.; Frye, S.A.; Bird, L.; Owens, R.; Ford, R.C.; Lian, L.Y.; Derrick, J.P.  
Deposited on : 2012-05-23  
Resolution : 26.00 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](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

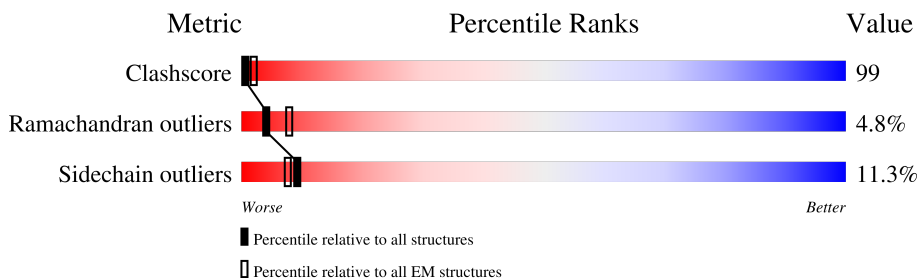
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 26.00 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	745	9% 25% . 63%
1	B	745	9% 25% . 63%
1	C	745	9% 25% . 63%
1	D	745	9% 25% . 63%
1	E	745	9% 25% . 63%
1	F	745	9% 25% . 63%
1	G	745	9% 25% . 63%
1	H	745	9% 25% . 63%

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Mol	Chain	Length	Quality of chain
1	I	745	9% 25% 63%
1	J	745	9% 25% 63%
1	K	745	9% 25% 63%
1	L	745	9% 25% 63%
2	M	181	10% 27% 8% 55%
2	N	181	10% 28% 7% 55%
2	O	181	10% 28% 7% 55%
2	P	181	11% 27% 8% 55%
2	Q	181	12% 25% 8% 55%
2	R	181	10% 28% 8% 55%
2	S	181	11% 26% 8% 55%
2	T	181	10% 28% 7% 55%
2	U	181	12% 25% 8% 55%
2	V	181	11% 27% 8% 55%
2	W	181	12% 26% 8% 55%
2	X	181	11% 27% 8% 55%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 34704 atoms, of which 1152 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 TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	275	2152	1354	379	415	4	0	1
1	B	275	2152	1354	379	415	4	0	1
1	C	275	2152	1354	379	415	4	0	1
1	D	275	2152	1354	379	415	4	0	1
1	E	275	2152	1354	379	415	4	0	1
1	F	275	2152	1354	379	415	4	0	1
1	G	275	2152	1354	379	415	4	0	1
1	H	275	2152	1354	379	415	4	0	1
1	I	275	2152	1354	379	415	4	0	1
1	J	275	2152	1354	379	415	4	0	1
1	K	275	2152	1354	379	415	4	0	1
1	L	275	2152	1354	379	415	4	0	1

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	428	PHE	LEU	variant	UNP Q70M91
B	428	PHE	LEU	variant	UNP Q70M91
C	428	PHE	LEU	variant	UNP Q70M91
D	428	PHE	LEU	variant	UNP Q70M91
E	428	PHE	LEU	variant	UNP Q70M91

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Chain	Residue	Modelled	Actual	Comment	Reference
F	428	PHE	LEU	variant	UNP Q70M91
G	428	PHE	LEU	variant	UNP Q70M91
H	428	PHE	LEU	variant	UNP Q70M91
I	428	PHE	LEU	variant	UNP Q70M91
J	428	PHE	LEU	variant	UNP Q70M91
K	428	PHE	LEU	variant	UNP Q70M91
L	428	PHE	LEU	variant	UNP Q70M91

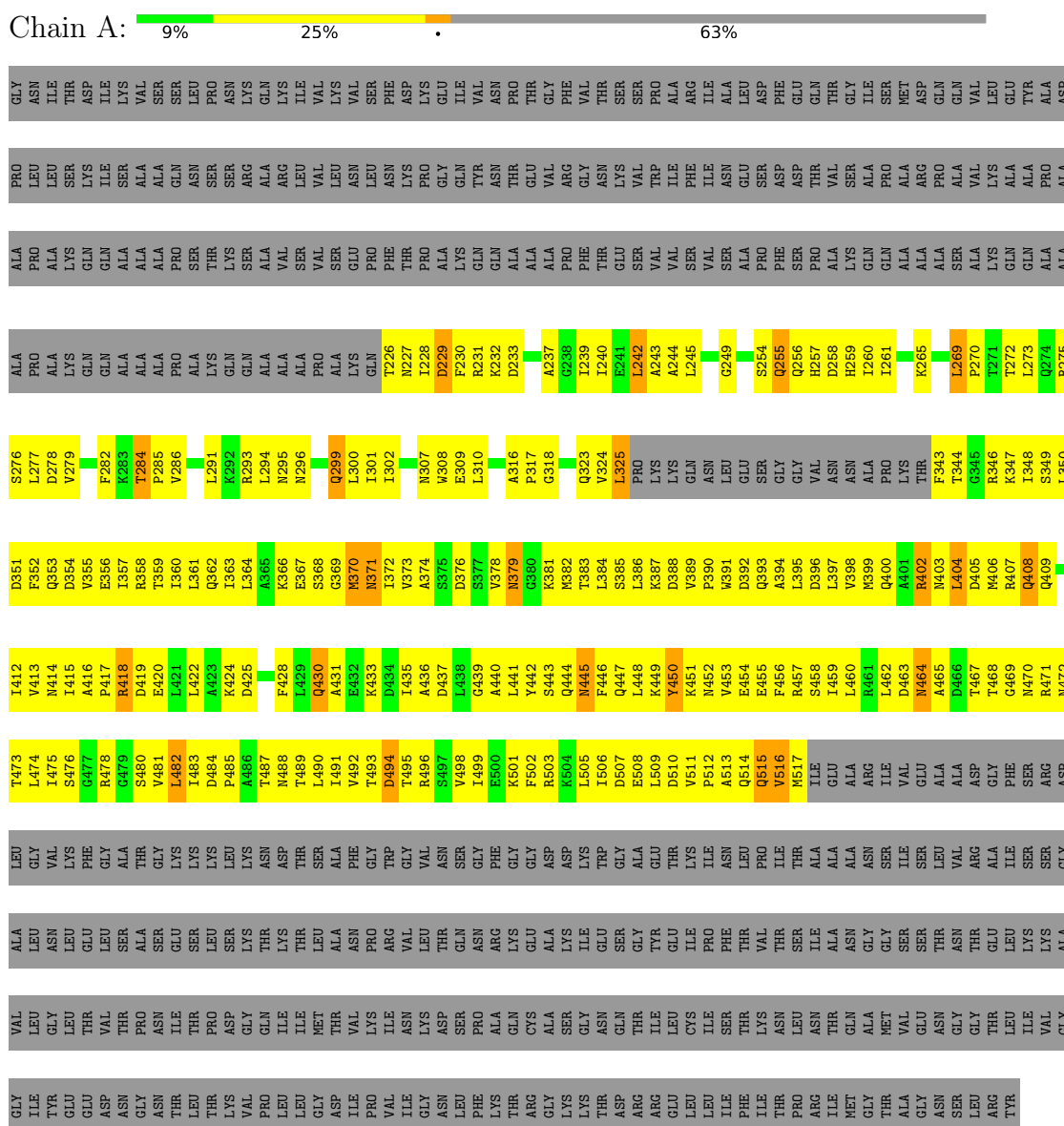
- Molecule 2 is a protein called PILP PROTEIN.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	M	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	N	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	O	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	P	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	Q	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	R	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	S	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	T	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	U	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	V	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	W	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	X	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		

### 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: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ



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S276	D851	I412	L474	LEU	LEU	ILE
L277	F352	V413	I475	ASN	GLY	TYR
D278	Q353	M414	S476	LEU	LEU	GLU
V279	D354	I415	G477	GLU	THR	GLY
F282	V355	A416	R478	VAL	VAL	ASP
K283	E356	P417	G479	THR	THR	ASN
T284	I357	R418	S480	ALA	PRO	GLY
V286	R358	D419	V481	ASN	ASN	THR
L291	T359	E420	L482	GLU	ILE	ASN
K292	I360	L421	I483	LEU	THR	THR
R293	L361	L422	D484	LEU	PRO	THR
L294	L362	L423	P485	LEU	ASP	LEU
N295	L363	K424	A486	LEU	GLY	VAL
N296	L364	D425	T487	THR	GLN	PRO
Q299	A365	F428	M488	LYS	ILE	LEU
L300	K366	L429	T489	THR	THR	LEU
I302	E367	L430	L490	LEU	MET	LEU
N307	S368	Q430	I491	ALA	THR	ALA
E309	G369	A431	I492	ASN	VAL	ASN
L310	M370	E432	V493	PRO	LYS	GLY
A316	N371	K433	D494	ARG	ILE	VAL
G318	I372	D434	T495	ASN	ASN	ILE
Q323	V373	I435	R496	LEU	GLY	GLY
V324	A374	A436	S497	THR	ASN	ASP
L325	A375	A437	V498	GLN	THR	GLY
PRO	L376	L438	I499	ASN	PRO	ILE
LYS	S377	G439	E500	ARG	ALA	GLY
LYS	V378	A440	K501	LYS	GLN	ASP
GLN	N379	L441	F502	LYS	CYS	THR
ASN	K381	L444	R503	ALA	ALA	GLY
ASN	M382	Q444	K504	LYS	SER	LYS
LEU	I383	M445	L505	ILE	GLY	THR
LEU	L384	F446	I506	GLU	THR	LYS
GLY	S385	Q447	D507	SER	GLN	ASP
GLY	L386	L448	E508	THR	THR	ARG
GLY	L387	K449	L509	THR	ILE	ARG
GLY	D388	Y450	D510	GLU	GLU	GLY
GLN	V389	K451	V511	LEU	CYS	LEU
ASN	W391	M452	P512	PRO	ILE	ILE
LEU	D392	V453	A513	PHE	ASN	ASN
GLU	Q393	E454	Q514	THR	THR	THR
SER	Q394	E455	Q515	LEU	VAL	VAL
GLY	A394	F456	V516	THR	THR	THR
GLY	L395	R457	M517	SER	SER	THR
VAL	D396	S458	ILE	ILE	ARG	ARG
ASN	L397	I459	GLU	ALA	THR	THR
ASN	V398	L460	ALA	ASN	GLN	GLN
ALA	M399	R461	GLY	GLY	ALA	ALA
PRO	Q400	D462	ILE	GLY	THR	THR
LYS	A401	M463	VAL	VAL	ALA	ALA
THR	R402	M464	GLY	GLU	GLY	ASP
F343	M403	A465	ALA	ASN	ASN	THR
T344	L404	D466	ASP	GLY	GLY	GLY
R346	D405	T468	THR	THR	THR	THR
K347	M406	G469	ILE	LEU	LEU	LEU
I348	R407	M470	PHE	LEU	ILE	ILE
S349	Q408	R471	SER	LYS	SER	LYS
L350	Q409	N472	ARG	VAL	ARG	VAL
		T473	LEU	GLY	GLY	GLY

• Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ



GLY	PRO	ALA	ALA	ALA	ALA	S276	D851	I412	T473	LEU
ASN	LEU	PRO	ALA	ALA	ALA	L277	F352	V413	L474	GLY
THR	LEU	ALA	ALA	ALA	ALA	D278	Q353	M414	I475	VAL
ILE	SER	LYS	GLN	GLN	GLN	V279	D354	I415	S476	VAL
ASP	LYS	ILE	GLN	GLN	GLN	F282	V355	A416	G477	PHE
LYS	SER	ALA	ALA	ALA	ALA	K283	E356	P417	R478	ALA
VAL	ASN	ALA	ALA	ALA	ALA	T284	I357	R418	G479	ALA
GLN	ASN	ALA	ALA	ALA	ALA	V286	R358	D419	S480	THR
LYS	ASN	ALA	ALA	ALA	ALA	L291	T359	E420	V481	GLY
ASN	ASN	ALA	ALA	ALA	ALA	K292	I360	L421	L482	GLY
THR	THR	ALA	ALA	ALA	ALA	R293	L361	L422	I483	LYS
GLN	ARG	LYS	SER	SER	SER	L294	Q362	A423	D484	LYS
GLN	ARG	GLN	ASN	ASN	ASN	R295	L363	K424	P485	LEU
ALA	ALA	ALA	ALA	ALA	ALA	N296	L364	D425	A486	LYS
ILE	ILE	VAL	VAL	VAL	VAL	Q299	A365	F428	T487	ASN
LYS	VAL	VAL	VAL	VAL	VAL	L300	K366	L429	M488	ASP
GLY	ASN	PHE	THR	THR	THR	I302	E367	L430	T489	THR
THR	PRO	VAL	VAL	VAL	VAL	N307	S368	Q430	L490	SER
GLY	ASN	LYS	LYS	LYS	LYS	E309	G369	A431	I491	ALA
ILE	GLN	ILE	GLY	GLY	GLY	L310	M370	E432	V492	PHE
VAL	THR	VAL	VAL	VAL	VAL	G318	N371	K433	T493	GLY
ARG	PHE	ARG	ARG	ARG	ARG	Q323	I372	D434	D494	TRP
THR	THR	THR	THR	THR	THR	V324	V373	I435	T495	GLY
THR	THR	THR	THR	THR	THR	L325	A374	A436	R496	VAL
THR	THR	THR	THR	THR	THR	PRO	A375	A437	S497	VAL
THR	THR	THR	THR	THR	THR	LYS	N308	D437	V498	ASN
THR	THR	THR	THR	THR	THR	LYS	E309	L438	D376	SER
THR	THR	THR	THR	THR	THR	GLN	L310	G439	S377	GLY
THR	THR	THR	THR	THR	THR	ASN	G318	A440	V378	PHE
THR	THR	THR	THR	THR	THR	ASN	Q323	L441	K501	GLY
THR	THR	THR	THR	THR	THR	ASN	V324	Y442	N379	GLY
THR	THR	THR	THR	THR	THR	ASN	L325	L444	G380	GLY
THR	THR	THR	THR	THR	THR	ASN	PRO	S443	K381	ASP
THR	THR	THR	THR	THR	THR	ASN	LYS	Q444	M382	ASP
THR	THR	THR	THR	THR	THR	ASN	GLN	M445	I383	LYS
THR	THR	THR	THR	THR	THR	ASN	GLN	F446	L384	LYS
THR	THR	THR	THR	THR	THR	ASN	THR	Q447	S385	TRP
THR	THR	THR	THR	THR	THR	ASN	THR	L448	L386	ALA
THR	THR	THR	THR	THR	THR	ASN	THR	K449	L387	ALA
THR	THR	THR	THR	THR	THR	ASN	THR	Y450	D388	ALA
THR	THR	THR	THR	THR	THR	ASN	THR	K451	V389	THR
THR	THR	THR	THR	THR	THR	ASN	THR	M452	P390	LYS
THR	THR	THR	THR	THR	THR	ASN	THR	V453	W391	ILE
THR	THR	THR	THR	THR	THR	ASN	THR	E454	D392	ASN
THR	THR	THR	THR	THR	THR	ASN	THR	E455	Q393	ASN
THR	THR	THR	THR	THR	THR	ASN	THR	F456	Q394	ASN
THR	THR	THR	THR	THR	THR	ASN	THR	R457	L395	ASN
THR	THR	THR	THR	THR	THR	ASN	THR	S458	D396	ALA
THR	THR	THR	THR	THR	THR	ASN	THR	I459	L397	ALA
THR	THR	THR	THR	THR	THR	ASN	THR	L460	V398	ALA
THR	THR	THR	THR	THR	THR	ASN	THR	R461	M399	ALA
THR	THR	THR	THR	THR	THR	ASN	THR	L462	Q400	ALA
THR	THR	THR	THR	THR	THR	ASN	THR	D463	PRO	SER
THR	THR	THR	THR	THR	THR	ASN	THR	M464	LYS	ILE
THR	THR	THR	THR	THR	THR	ASN	THR	M465	THR	ILE
THR	THR	THR	THR	THR	THR	ASN	THR	A465	R402	SER
THR	THR	THR	THR	THR	THR	ASN	THR	D466	M403	SER
THR	THR	THR	THR	THR	THR	ASN	THR	T467	L404	VAL
THR	THR	THR	THR	THR	THR	ASN	THR	G469	D405	ARG
THR	THR	THR	THR	THR	THR	ASN	THR	M470	M406	ALA
THR	THR	THR	THR	THR	THR	ASN	THR	N471	R407	ALA
THR	THR	THR	THR	THR	THR	ASN	THR	R471	Q408	ILE
THR	THR	THR	THR	THR	THR	ASN	THR	N472	Q409	SER
THR	THR	THR	THR	THR	THR	ASN	THR	T473	Q409	SER
THR	THR	THR	THR	THR	THR	ASN	THR			ARG
THR	THR	THR	THR	THR	THR	ASN	THR			ALA
THR	THR	THR	THR	THR	THR	ASN	THR			GLY







V413	M414	I415	A416	P417	R418	D419	E420	L421	A423	K424	D425	F428	L429	Q430	A431	E432	K433	D434	I435	A436	D437	L438	G439	A440	L441	Y442	R503	S443	Q444	M445	F446	Q447	L448	K449	Y450	K451	M452	E453	E454	E455	F456	R457	S458	I459	L460	R461	L462	D463	M464	A465	D466	T467	T468	G469	M470	R471	N472	T473																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
L474	I475	S476	G477	R478	G479	S480	V481	L482	I483	D484	P485	A486	T487	M488	T489	Q490	I491	V492	T493	D494	T495	R496	S497	V498	L499	E500	K501	F502	R503	K504	L505	I506	D507	E508	L509	D510	V511	P512	A513	Q514	Q515	V516	M517	I518	G519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000

● Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ

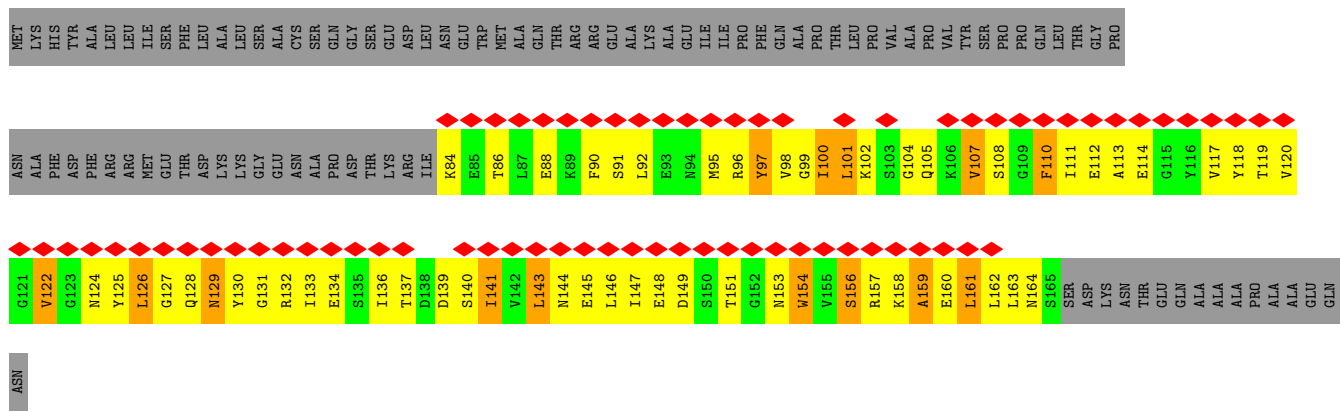
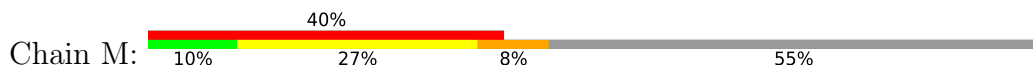


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V413	M414	I415	A416	P417	R418	D419	E420	L421	A422	L423	K424	D425	F428	L429	Q430	A431	E432	K433	D434	I435	A436	D437	L438	G439	A440	L441	Y442	R503	S443	Q444	M445	F446	Q447	L448	K449	Y450	K451	M452	E453	E454	E455	F456	R457	S458	I459	L460	R461	L462	D463	M464	A465	D466	T467	T468	G469	M470	R471	N472	T473																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
L474	I475	S476	G477	R478	G479	S480	V481	L482	I483	D484	P485	A486	T487	M488	T489	Q490	I491	V492	T493	D494	T495	R496	S497	V498	L499	E500	K501	F502	R503	K504	L505	I506	D507	E508	L509	D510	V511	P512	A513	Q514	Q515	V516	M517	I518	G519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000

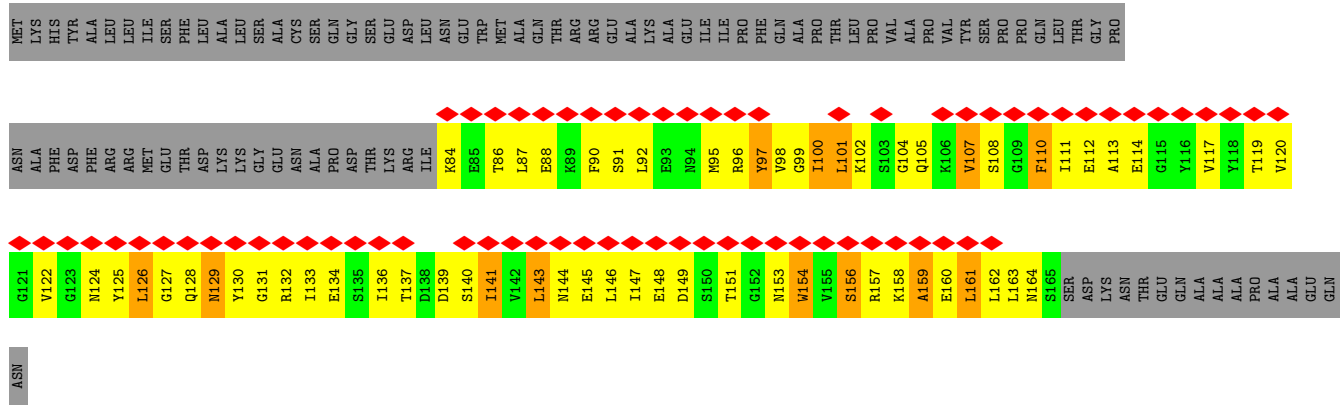
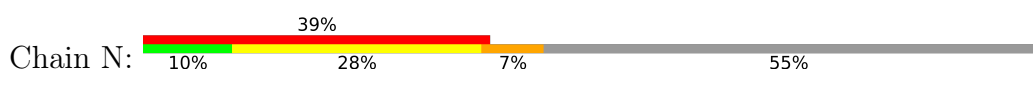




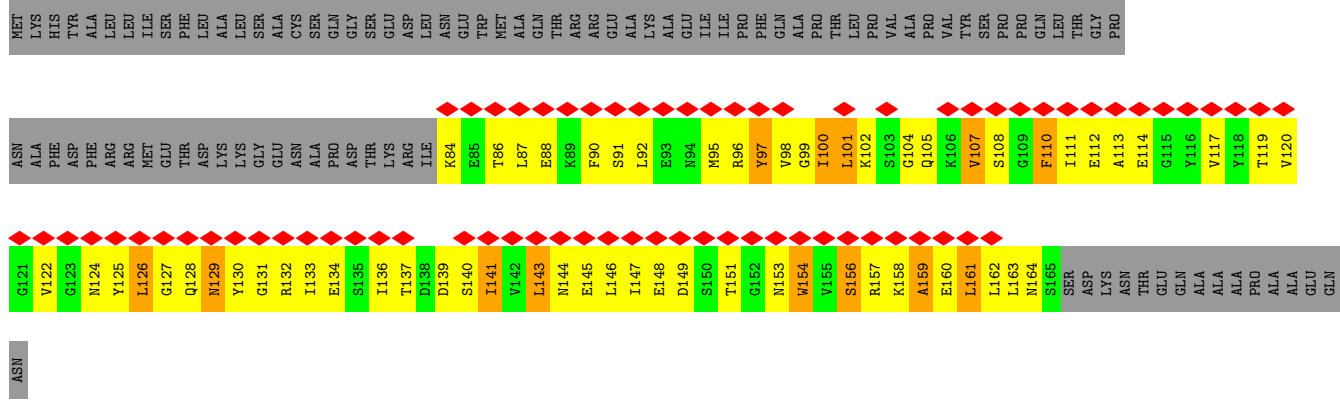
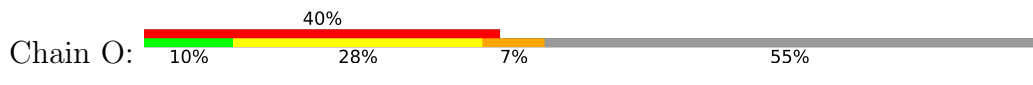




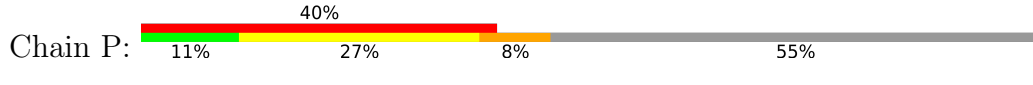
• Molecule 2: PILP PROTEIN



• Molecule 2: PILP PROTEIN

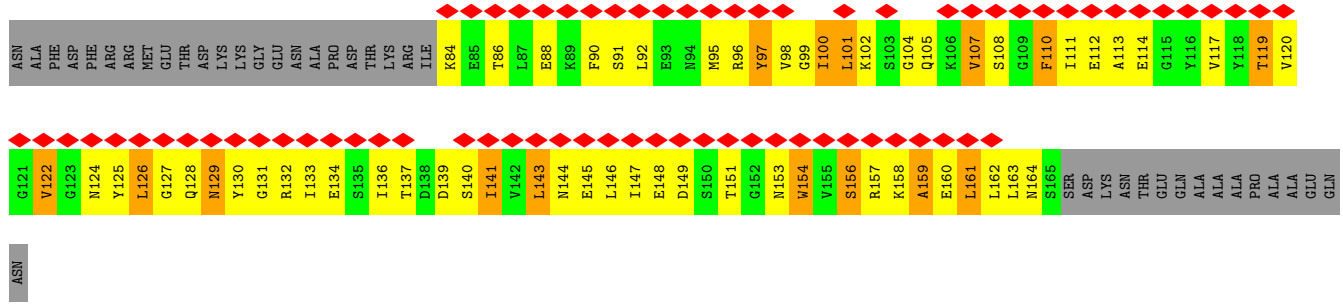


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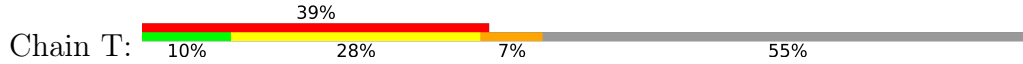




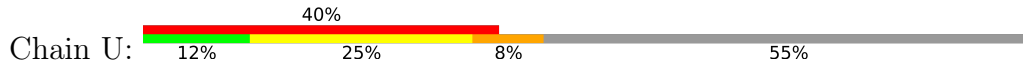




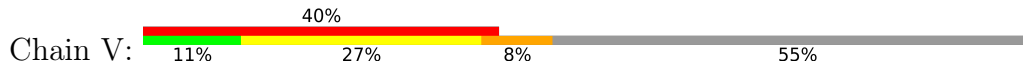
• Molecule 2: PILP PROTEIN



• Molecule 2: PILP PROTEIN



• Molecule 2: PILP PROTEIN





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C12	Depositor
Number of particles used	25303	Depositor
Resolution determination method	Not provided	
CTF correction method	CTFFIT EACH MICROGRAPH	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5100	Depositor
Magnification	33112	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	0.346	Depositor
Minimum map value	-0.113	Depositor
Average map value	0.095	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.28	Depositor
Map size ( $\text{\AA}$ )	289.92, 289.92, 289.92	wwPDB
Map dimensions	64, 64, 64	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	4.53, 4.53, 4.53	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	0.79	0/2179	1.19	4/2950 (0.1%)
1	B	0.79	0/2179	1.19	4/2950 (0.1%)
1	C	0.79	0/2179	1.19	4/2950 (0.1%)
1	D	0.79	0/2179	1.19	4/2950 (0.1%)
1	E	0.79	0/2179	1.19	4/2950 (0.1%)
1	F	0.79	0/2179	1.19	4/2950 (0.1%)
1	G	0.79	0/2179	1.19	4/2950 (0.1%)
1	H	0.79	0/2179	1.19	4/2950 (0.1%)
1	I	0.79	0/2179	1.19	4/2950 (0.1%)
1	J	0.79	0/2179	1.19	4/2950 (0.1%)
1	K	0.79	0/2179	1.19	4/2950 (0.1%)
1	L	0.79	0/2179	1.19	4/2950 (0.1%)
2	M	0.23	0/652	0.40	0/878
2	N	0.23	0/652	0.40	0/878
2	O	0.23	0/652	0.40	0/878
2	P	0.23	0/652	0.40	0/878
2	Q	0.23	0/652	0.40	0/878
2	R	0.23	0/652	0.40	0/878
2	S	0.23	0/652	0.40	0/878
2	T	0.23	0/652	0.40	0/878
2	U	0.23	0/652	0.40	0/878
2	V	0.23	0/652	0.40	0/878
2	W	0.23	0/652	0.40	0/878
2	X	0.23	0/652	0.40	0/878
All	All	0.70	0/33972	1.06	48/45936 (0.1%)

There are no bond length outliers.

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	GLN	CG-CD-OE1	-38.48	44.65	121.60
1	D	408	GLN	CG-CD-OE1	-38.48	44.65	121.60
1	G	408	GLN	CG-CD-OE1	-38.48	44.65	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	408	GLN	CG-CD-OE1	-38.48	44.65	121.60
1	C	408	GLN	CG-CD-OE1	-38.47	44.66	121.60

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	2152	0	2190	607	0
1	B	2152	0	2190	612	0
1	C	2152	0	2190	615	0
1	D	2152	0	2190	610	0
1	E	2152	0	2190	610	0
1	F	2152	0	2190	603	0
1	G	2152	0	2190	601	0
1	H	2152	0	2190	613	0
1	I	2152	0	2190	599	0
1	J	2152	0	2190	605	0
1	K	2152	0	2190	607	0
1	L	2152	0	2190	601	0
2	M	644	96	636	116	0
2	N	644	96	636	115	0
2	O	644	96	636	115	0
2	P	644	96	636	118	0
2	Q	644	96	636	119	0
2	R	644	96	636	119	0
2	S	644	96	636	117	0
2	T	644	96	636	117	0
2	U	644	96	636	113	0
2	V	644	96	636	115	0
2	W	644	96	636	114	0
2	X	644	96	636	117	0
All	All	33552	1152	33912	6674	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 99.

The worst 5 of 6674 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:E:347:LYS:NZ	2:Q:104:GLY:HA2	1.29	1.47
1:C:347:LYS:NZ	2:O:104:GLY:HA2	1.30	1.46
1:G:347:LYS:NZ	2:S:104:GLY:HA2	1.30	1.46
1:A:347:LYS:NZ	2:M:104:GLY:HA2	1.30	1.41
1:I:347:LYS:NZ	2:U:104:GLY:HA2	1.30	1.40

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	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	5	31
1	B	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	5	31
1	C	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	5	31
1	D	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	5	31
1	E	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	5	31
1	F	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	5	31
1	G	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	5	31
1	H	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	5	31
1	I	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	5	31
1	J	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	5	31
1	K	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	5	31
1	L	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	5	31
2	M	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	5
2	O	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	5
2	P	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	5
2	Q	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	5
2	R	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	5
2	S	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	5
2	T	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	5
2	U	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	5
2	V	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	5
2	W	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	5
2	X	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	5
All	All	4212/11112 (38%)	3432 (82%)	576 (14%)	204 (5%)	4	21

5 of 204 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	ASN
1	A	402	ARG
1	B	379	ASN
1	B	402	ARG
1	C	379	ASN

### 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	A	239/615 (39%)	216 (90%)	23 (10%)	8	27
1	B	239/615 (39%)	216 (90%)	23 (10%)	8	27
1	C	239/615 (39%)	216 (90%)	23 (10%)	8	27
1	D	239/615 (39%)	216 (90%)	23 (10%)	8	27
1	E	239/615 (39%)	216 (90%)	23 (10%)	8	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	239/615 (39%)	216 (90%)	23 (10%)	8	27
1	G	239/615 (39%)	216 (90%)	23 (10%)	8	27
1	H	239/615 (39%)	216 (90%)	23 (10%)	8	27
1	I	239/615 (39%)	216 (90%)	23 (10%)	8	27
1	J	239/615 (39%)	216 (90%)	23 (10%)	8	27
1	K	239/615 (39%)	216 (90%)	23 (10%)	8	27
1	L	239/615 (39%)	216 (90%)	23 (10%)	8	27
2	M	71/152 (47%)	59 (83%)	12 (17%)	2	12
2	N	71/152 (47%)	59 (83%)	12 (17%)	2	12
2	O	71/152 (47%)	59 (83%)	12 (17%)	2	12
2	P	71/152 (47%)	59 (83%)	12 (17%)	2	12
2	Q	71/152 (47%)	59 (83%)	12 (17%)	2	12
2	R	71/152 (47%)	59 (83%)	12 (17%)	2	12
2	S	71/152 (47%)	59 (83%)	12 (17%)	2	12
2	T	71/152 (47%)	59 (83%)	12 (17%)	2	12
2	U	71/152 (47%)	59 (83%)	12 (17%)	2	12
2	V	71/152 (47%)	59 (83%)	12 (17%)	2	12
2	W	71/152 (47%)	59 (83%)	12 (17%)	2	12
2	X	71/152 (47%)	59 (83%)	12 (17%)	2	12
All	All	3720/9204 (40%)	3300 (89%)	420 (11%)	9	21

5 of 420 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	233	ASP
2	M	161	LEU
2	W	119	THR
1	K	284	THR
1	L	278	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 157 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	408	GLN

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Mol	Chain	Res	Type
2	R	129	ASN
1	K	515	GLN
1	L	515	GLN
2	V	94	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 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.

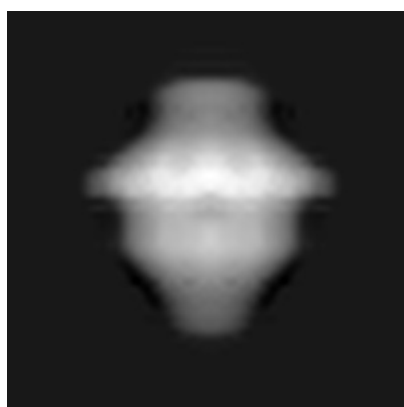
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2105. These allow visual inspection of the internal detail of the map and identification of artifacts.

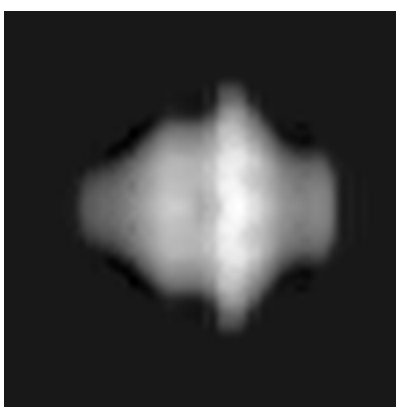
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

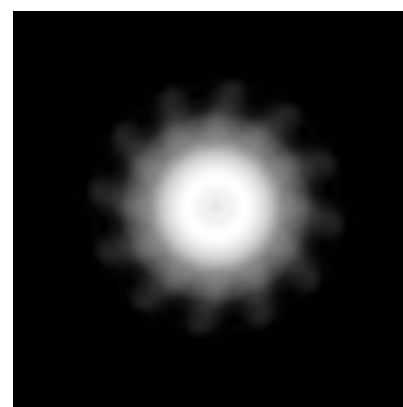
#### 6.1.1 Primary map



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: 32



Y Index: 32



Z Index: 32

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: 32



Y Index: 32



Z Index: 36

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 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

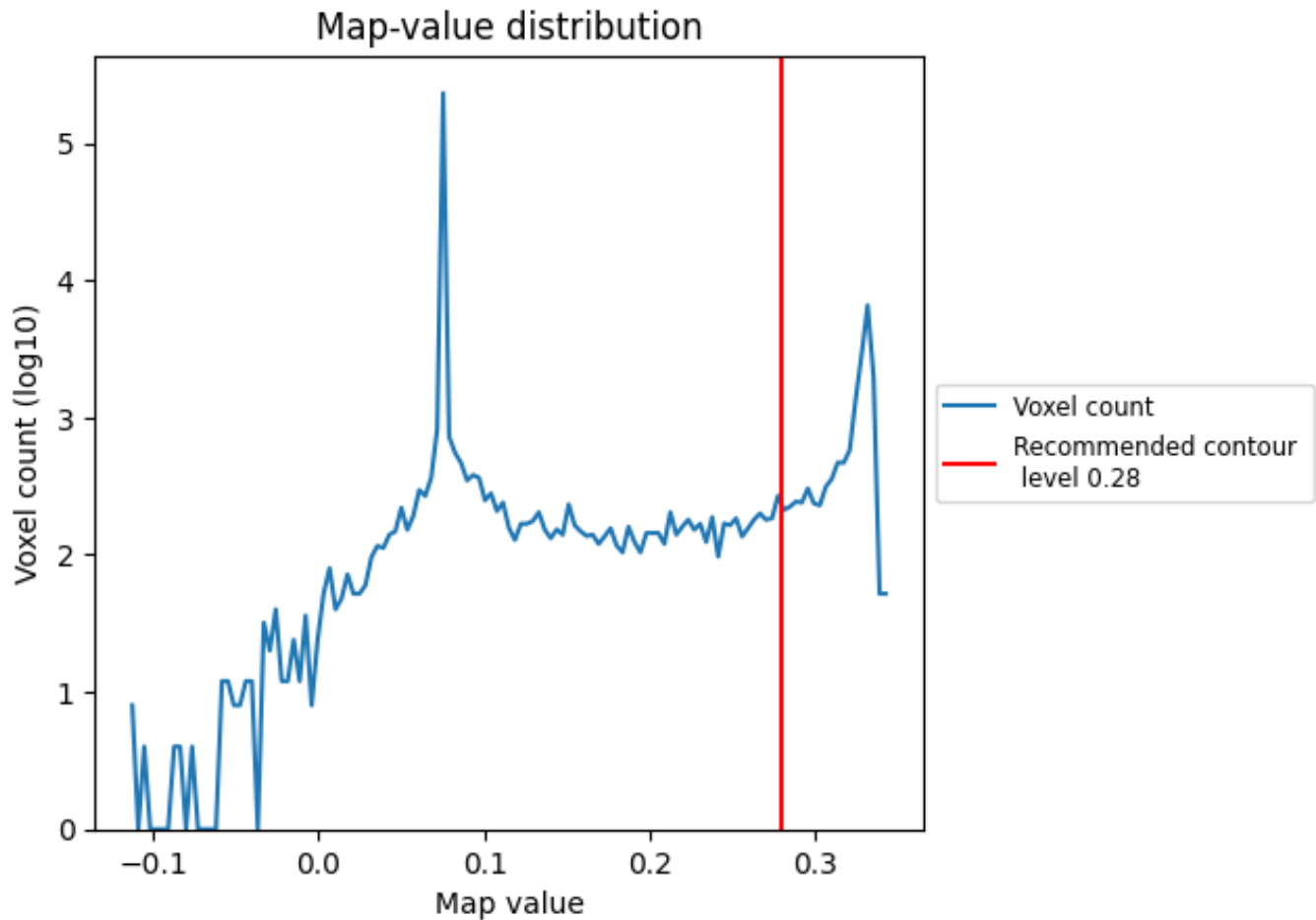
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

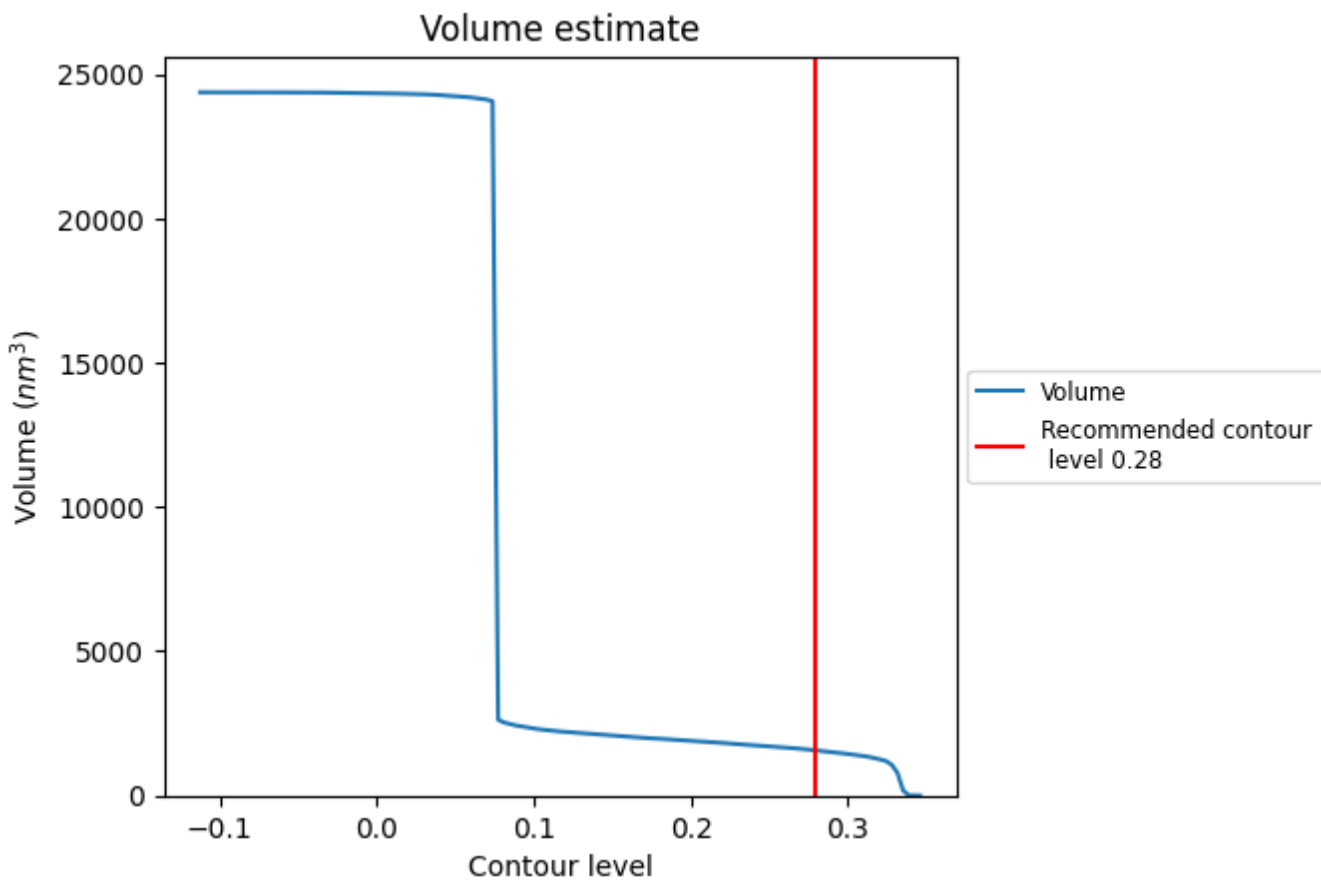
This section contains the results of statistical analysis of the map.

### 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.

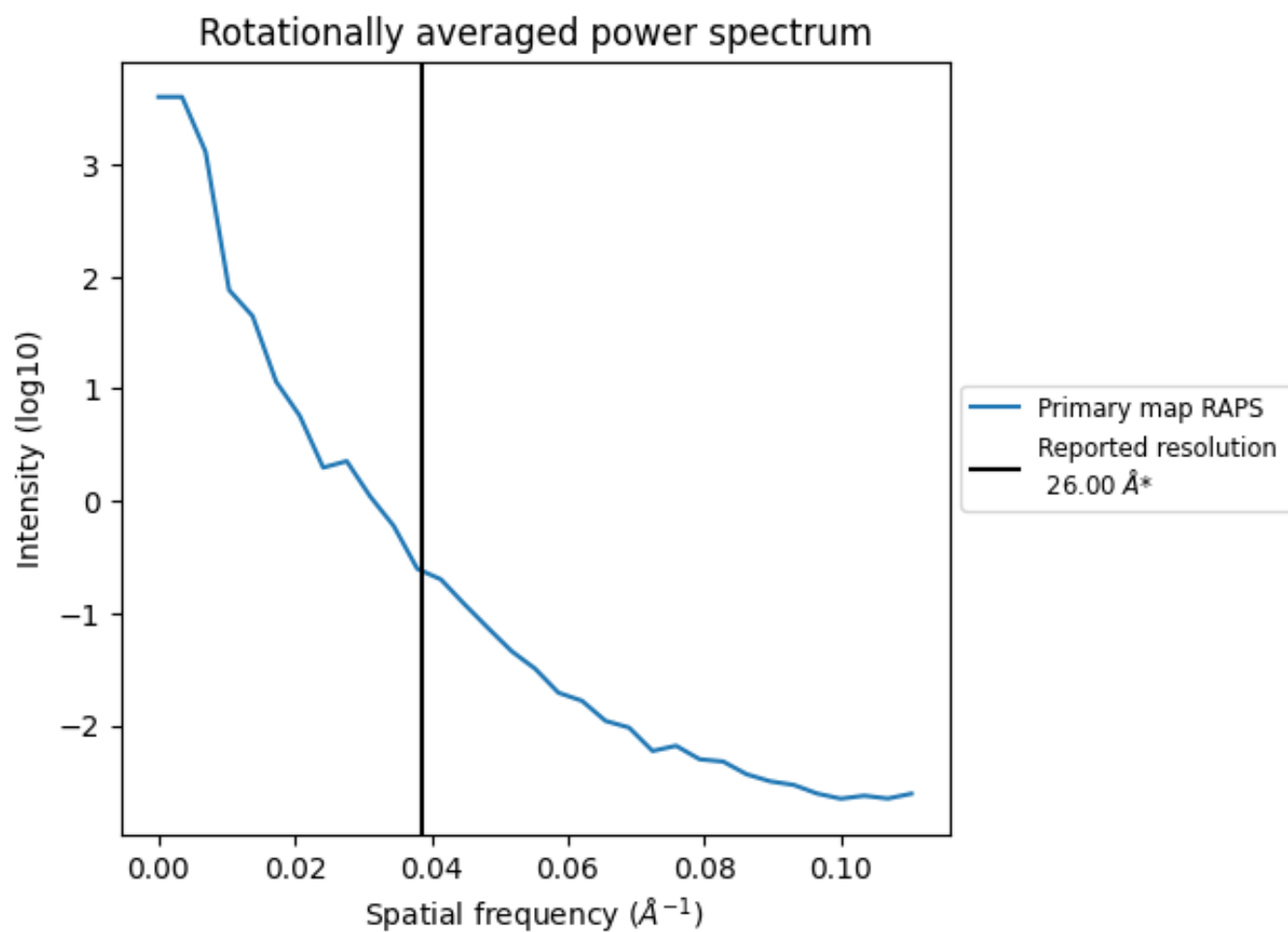
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1565 nm<sup>3</sup>; this corresponds to an approximate mass of 1414 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](#)



\*Reported resolution corresponds to spatial frequency of 0.038 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

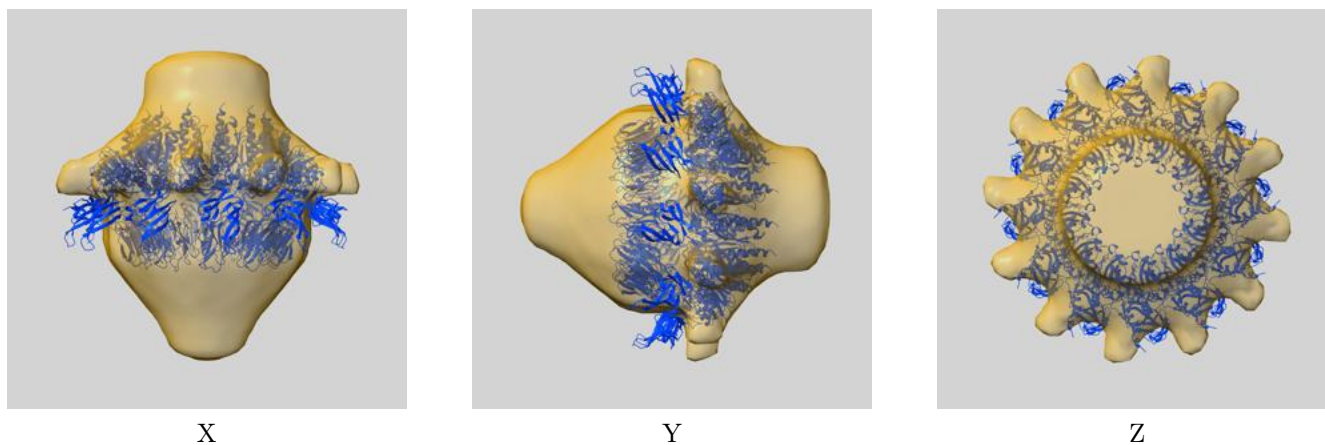
This section was not generated. No FSC curve or half-maps provided.



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

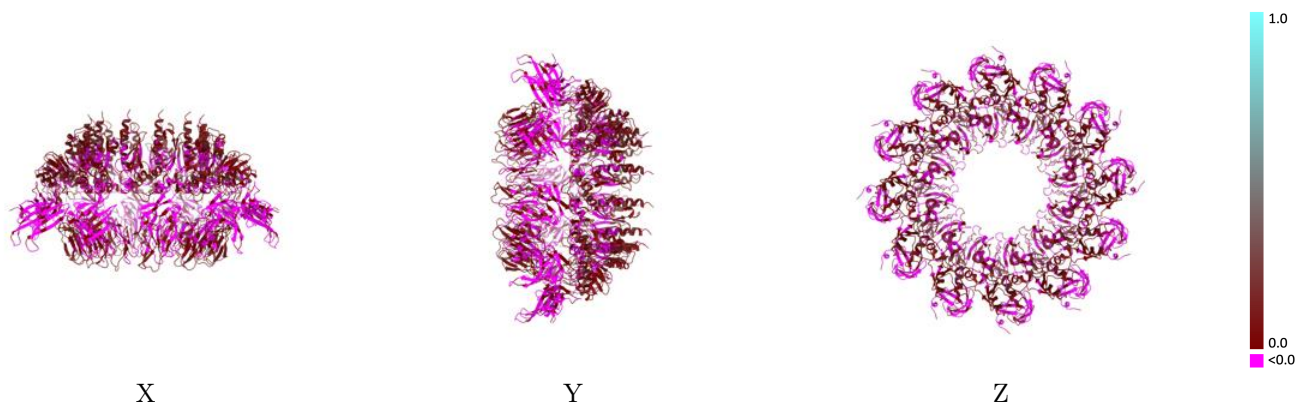
This section contains information regarding the fit between EMDB map EMD-2105 and PDB model 4AV2. Per-residue inclusion information can be found in section 3 on page 6.

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



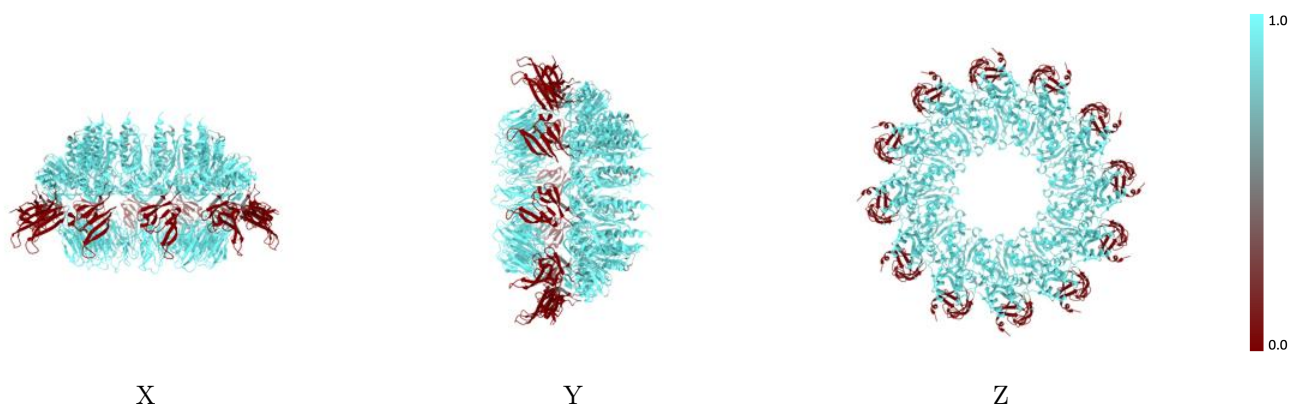
The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



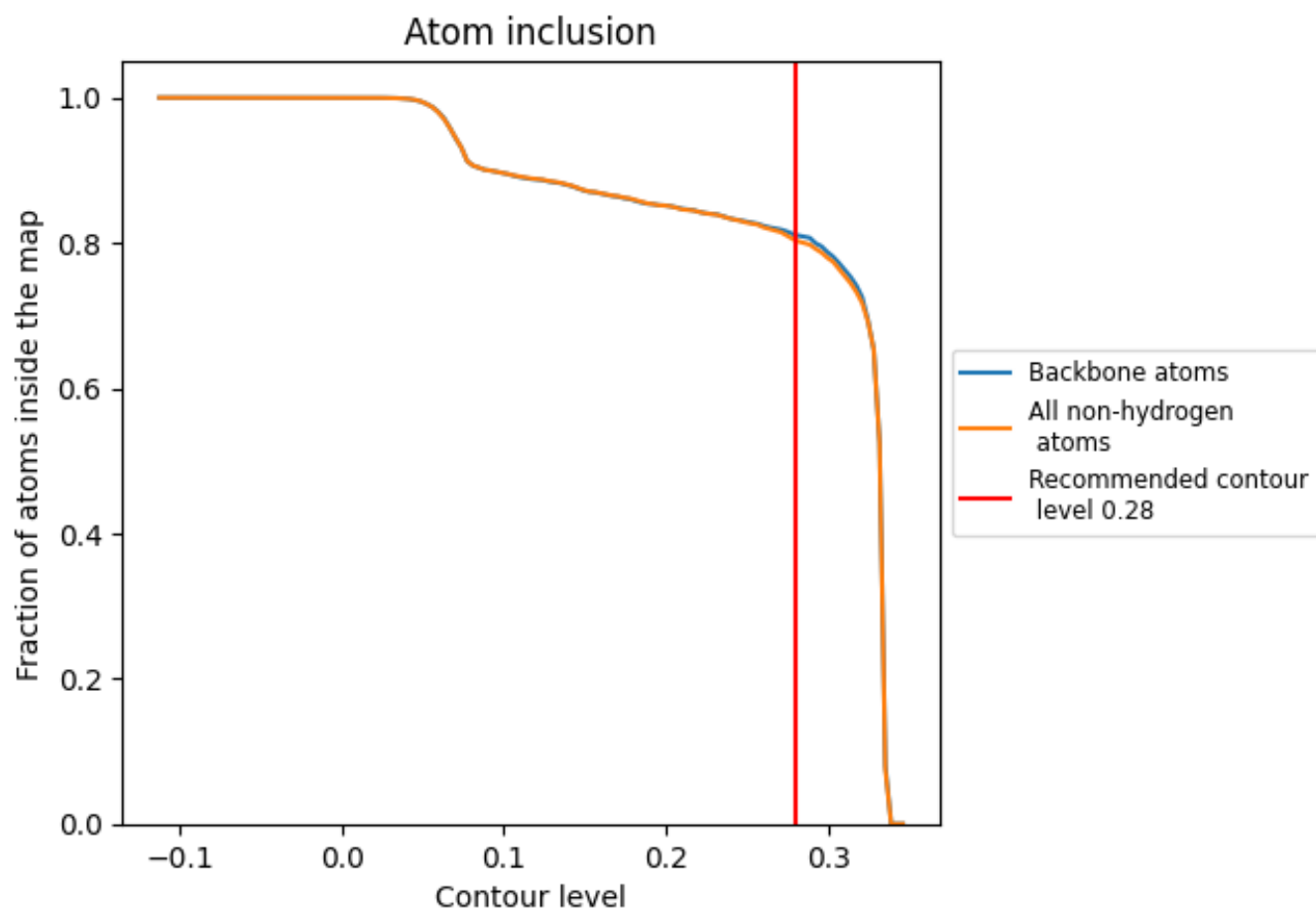
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.28).



















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 80% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8032	 0.0380
A	 0.9891	 0.0630
B	 0.9887	 0.0590
C	 0.9887	 0.0650
D	 0.9891	 0.0620
E	 0.9887	 0.0600
F	 0.9887	 0.0650
G	 0.9891	 0.0620
H	 0.9887	 0.0600
I	 0.9887	 0.0660
J	 0.9891	 0.0640
K	 0.9887	 0.0610
L	 0.9887	 0.0640
M	 0.0902	 -0.0540
N	 0.0902	 -0.0460
O	 0.0902	 -0.0540
P	 0.0902	 -0.0550
Q	 0.0902	 -0.0380
R	 0.0902	 -0.0470
S	 0.0902	 -0.0440
T	 0.0902	 -0.0320
U	 0.0902	 -0.0440
V	 0.0902	 -0.0460
W	 0.0902	 -0.0370
X	 0.0902	 -0.0520

