



# wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 01:24 AM EDT

PDB ID : 8EYX  
EMDB ID : EMD-28723  
Title : Cryo-EM structure of 4 insulins bound full-length mouse IR mutant with physically decoupled alpha CTs (C684S/C685S/C687S; denoted as IR-3CS) Asymmetric conformation 1  
Authors : Li, J.; Wu, J.Y.; Hall, C.; Bai, X.C.; Choi, E.  
Deposited on : 2022-10-29  
Resolution : 4.50 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.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

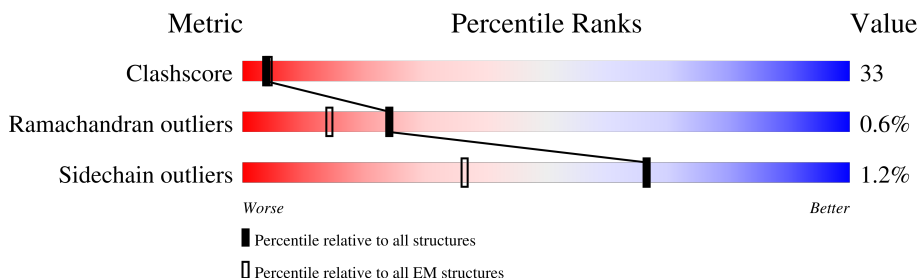
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1345	
1	B	1345	
2	D	110	
2	E	110	
2	F	110	
2	G	110	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14298 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 Insulin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	815	Total	C	N	O	S	0	0
			6572	4171	1135	1217	49		
1	B	772	Total	C	N	O	S	0	0
			6263	3983	1075	1165	40		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	684	SER	CYS	engineered mutation	UNP P15208
A	685	SER	CYS	engineered mutation	UNP P15208
A	687	SER	CYS	engineered mutation	UNP P15208
B	684	SER	CYS	engineered mutation	UNP P15208
B	685	SER	CYS	engineered mutation	UNP P15208
B	687	SER	CYS	engineered mutation	UNP P15208

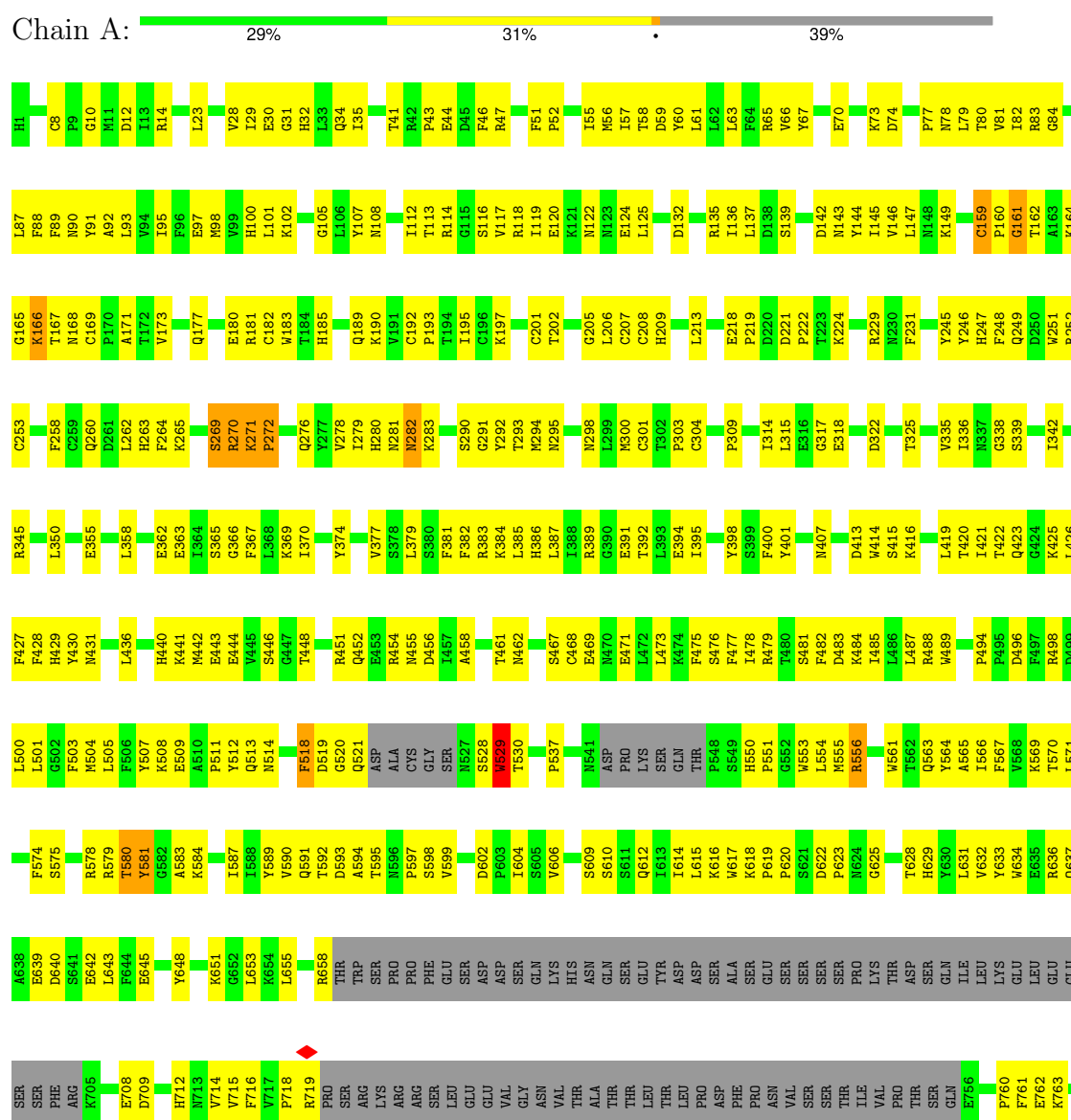
- Molecule 2 is a protein called Insulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	44	Total	C	N	O	S	0	0
			347	220	56	65	6		
2	E	48	Total	C	N	O	S	0	0
			376	238	61	71	6		
2	F	47	Total	C	N	O	S	0	0
			370	235	60	69	6		
2	G	47	Total	C	N	O	S	0	0
			370	235	60	69	6		

### 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.

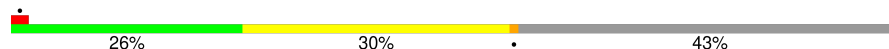
#### • Molecule 1: Insulin receptor



LEU	THR	LEU	LEU	PRO	PRO	SER	TYR	GLY	GLN	GLU	ASP	ILE	L843	K767
LEU	THR	LEU	LEU	PRO	PRO	GLU	ASP	GLY	MET	ALA	GLU	ALA	L844	E768
PRO	PRO	LEU	LEU	LEU	LEU	GLU	PRO	VAL	GLY	SER	TRP	LYS	V845	S769
ARG	ARG	GLU	LEU	VAL	GLN	GLN	PRO	MET	ILE	MET	VAL	ILE	L846	L770
SER	SER	MET	ASP	PRO	MET	PRO	ASP	THR	MET	LYS	PRO	ILE	E848	V771
ASN	ASN	GLU	ASN	VAL	THR	ASN	ASN	ARG	THR	GLY	ARG	GLY	V849	I772
PRO	PRO	GLU	GLU	GLU	GLU	GLU	CYS	ARG	ALA	PHE	GLU	PRO		R776
SER	SER	ASP	ASP	TRP	GLU	TRP	GLU	MET	ILE	THR	LYS	LEU		H777
		MET	ARG	SER	ALA	SER	ARG	SER	HIS	HIS	THR	PHE	Y854	F778
GLU	GLU	MET	LEU	PRO	ASP	PRO	GLU	GLY	VAL	VAL	LEU	VAL	G855	G780
ASN	ASN	VAL	THR	GLU	GLY	THR	GLU	VAL	VAL	GLU	LEU	PHE	D856	Y781
VAL	VAL	GLU	ASP	SER	MET	ASP	SER	ARG	VAL	ARG	GLU	LEU	E857	R782
PRO	PRO	PRO	LEU	LEU	LEU	LEU	LEU	ALA	ARG	ALA	ARG	PHE	I783	I783
LEU	LEU	LEU	MET	LYS	TYR	TYR	LYS	TYR	GLY	LEU	GLY	SER	L859	E784
ASP	ASP	ASP	ARG	ASP	LEU	LEU	ASP	LEU	LEU	GLY	GLY	VAL	H860	
ARG	ARG	ARG	MET	GLY	ASN	GLY	GLN	VAL	VAL	VAL	GLN	VAL	L861	A787
SER	SER	SER	CYS	VAL	ALA	ALA	VAL	VAL	LYS	VAL	SER	ILE	C862	C788
SER	SER	TRP	TRP	PHE	LYS	VAL	GLY	GLY	SER	GLY	GLY	ILE		N789
HIS	HIS	GLN	GLN	THR	THR	THR	THR	PHE	PHE	PHE	SER	SER	K866	Q790
CYS	CYS	CYS	PHE	ALA	LYS	ALA	LYS	GLY	PHE	GLY	GLY	ILE	H867	D791
GLN	GLN	ASN	ASN	VAL	VAL	VAL	VAL	GLY	VAL	MET	MET	TYR	F868	S792
ARG	ARG	PRO	PRO	SER	HIS	ASN	ASN	GLN	THR	GLN	VAL	LEU	A869	P793
GLU	GLU	GLY	LYS	ASP	ARG	ASP	PRO	PRO	PRO	TYR	VAL	PHE		D794
GLU	GLU	GLU	MET	ASP	ASP	ASP	THR	THR	GLY	GLY	GLY	LEU	R872	E795
ALA	ALA	ALA	ARG	TRP	LEU	LEU	LEU	LEU	LEU	ARG	ASN	LYS	G873	R796
GLY	GLY	GLY	PRO	SER	ALA	VAL	VAL	VAL	VAL	ALA	ASN	GLY	C874	C797
GLY	GLY	THR	THR	PHE	ALA	ALA	VAL	ARG	ARG	ARG	ALA	ARG	R875	S798
ARG	ARG	PHE	PHE	GLY	ARG	GLY	MET	GLN	LYS	GLN	LYS	TYR		V799
GLU	GLU	LEU	LEU	VAL	CYS	ASN	ASN	PRO	ASP	PRO	ASP	PRO	P881	A800
GLY	GLY	GLY	GLU	VAL	GLY	LEU	LEU	LEU	ILE	ILE	ILE	ASP	G882	
GLY	GLY	ILE	ILE	VAL	MET	LEU	LEU	MET	ILE	ILE	ILE	GLY	N883	S804
SER	SER	VAL	VAL	VAL	VAL	VAL	VAL	VAL	LYS	PRO	LYS	PRO	Y884	A805
SER	SER	ASN	ASN	ALA	HIS	ALA	HIS	GLY	GLY	MET	GLY	MET	S885	R806
LEU	LEU	LEU	LEU	ILE	HIS	GLY	GLY	ILE	GLY	GLY	GLY	GLY	V886	T807
SER	SER	LEU	THR	THR	THR	THR	THR	ASP	ALA	PRO	ALA	PRO	R887	M808
ILE	ILE	ILE	LYS	SER	PHE	LEU	LYS	LEU	GLU	GLU	LEU	LEU	V888	P809
LYS	LYS	ARG	ASP	ALA	VAL	SER	LYS	THR	THR	THR	TYR	TYR	R889	
THR	THR	THR	THR	LYS	GLY	LEU	GLY	ARG	ALA	ALA	ALA	SER		I816
TYR	TYR	LEU	LEU	GLY	VAL	GLY	HIS	VAL	VAL	SER	VAL	SER	S892	
ASP	ASP	PRO	PRO	PRO	ILE	GLY	LEU	ALA	ALA	SER	ALA	SER	L893	H822
GLU	GLU	SER	SER	ASP	ASP	GLY	ARG	VAL	VAL	VAL	VAL	ASN		E823
HIS	HIS	PHE	PHE	GLN	THR	PHE	THR	LYS	LYS	PRO	PRO	PRO	N896	I824
ILE	ILE	PRO	PRO	GLY	GLY	GLY	ARG	THR	THR	GLU	GLU	GLU		F825
PRO	PRO	PRO	GLU	GLY	LEU	LEU	PRO	ARG	VAL	TYR	TYR	TYR	W899	E826
TYR	TYR	VAL	VAL	MET	MET	MET	ASP	ASN	ASN	ASN	ASN	SER	T900	N827
THR	THR	SER	SER	THR	THR	THR	ASP	GLU	GLU	GLU	SER	LEU		E827
THR	THR	ASN	ASN	VAL	VAL	VAL	THR	GLY	ARG	ALA	ALA	VAL	T903	N828
HIS	HIS	MET	PHE	GLN	GLN	GLN	ASP	ALA	ASN	SER	SER	ALA	V907	V829
ASN	ASN	ASN	TYR	VAL	THR	THR	TYR	TYR	TYR	ASN	ASN	VAL	T908	V830
GLY	GLY	GLY	SER	LEU	LEU	LEU	GLY	PRO	PRO	PRO	VAL	PHE		H831
GLY	GLY	LYS	GLU	LYS	THR	THR	THR	GLY	GLY	GLY	ARG	PRO	ASP	Q835
LYS	LYS	ASN	GLU	VAL	VAL	VAL	PHE	ASP	THR	SER	GLU	SER	LEU	E836
ASN	ASN	ASN	PHE	VAL	VAL	THR	TYR	PRO	PRO	ILE	ILE	ASP	ASP	P837
GLY	GLY	GLY	ALA	ASP	MET	THR	TYR	PRO	TYR	PRO	GLU	VAL	VAL	K838
ARG	ARG	ARG	ARG	GLY	GLY	GLY	ARG	PRO	ARG	PRO	PHE	TYR	PRO	E839
VAL	VAL	VAL	VAL	GLY	GLY	GLY	LYS	THR	LYS	THR	VAL	VAL	LEU	P840
				GLU	GLU	GLU	PRO	GLY	ASN	ASN	ASN	VAL	SER	N841

● Molecule 1: Insulin receptor

Chain B:



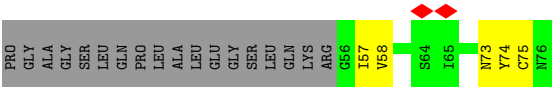
K310	V311	C312	Q313	L314	L315	E316	G317	E318	K319	T320	L321	D322	S323	S326	E329	L330	R331	G332	C333	T334	V335	L336	N337	G338	S339	L340	I341	I342	N343	I344	L354	A355	A356	N357	L358	G359	L360	I361	E362	E363	I364	S365	G366	F367	L368	K369	I370	R371	K372	S373	L376	V377	S378	L379	S380
F231	T232	L233	Q236	Y245	Y246	H247	F248	V251	R252	C253	V254	C259	Q260	D261	L262	H263	F264	K265	C266	R267	N268	S269	R270	K271	P272	G273	C274	H275	Q276	Y277	T278	L279	H280	N281	N282	K283	C284	L285	P286	P289	Y292	T293	K294	N295	N298	L299	M300	C301	P307	C308	P309				
LYS	THR	ASN	CYS	PRO	ALA	THR	VAL	ILE	ASN	GLN	PHE	VAL	GLU	ARG	CYS	TRP	THR	HIS	SER	HIS	CYS	ILE	ILE	CYS	LYS	SER	GLY	HIS	GLY	THR	ALA	GLU	GLY	LEU	CYS	C208	H209	C212	C216	S217	E218	P219	D220	D221	P222	T223	K224	C225	V226	A227					
G84	S85	R86	L87	F88	A82	L93	F96	L101	K102	N108	N111	I112	T113	R114	G115	S116	V117	H118	I119	E120	E124	L125	C126	S134	R135	S139	V140	E141	D142	R143	Y144	I145	V146	K149	D150	D151	ASN	GLU	GLU	CYS	GLY	ASP	VAL	CYS	PRO	GLY	THR	ALA	LYS						
HIS	LEU	TYR	PRO	G5	E6	V7	C8	G9	M11	D12	I13	R14	N15	N16	L23	C26	S27	V28	I29	E30	G31	H32	L33	Q34	I35	L36	L37	P43	E44	D45	F46	R47	D48	P52	K53	L54	I55	M56	I57	T58	D59	Y60	L61	R65	E70	N78	L79	T80	V81	I82	R83				

F381	T448	Q513	D586	THR	GLU	Q790	K866	VAL	GLY	LEU	LEU	ASP	ARG	ASP
F382	K449	T516	I587	TRP	GLU	D791	H867	VAL	GLN	GLY	ASN	GLY	MET	ARG
R383	G450	T516	I588	SER	VAL	P792	P868	ILE	GLY	VAL	ALA	VAL	CYS	SER
K384	E451	GLY	Y589	PRO	GLY	P793	F793	GLY	SER	VAL	LYS	PHE	TRP	SER
L385	Q452	F518	V590	PRO	ASN	D794	R872	SER	PHE	LYS	PHE	ALA	GLN	CYS
H386	E453	D519	Q591	PHE	VAL	R796	R875	ILE	GLY	LYS	VAL	SER	ASN	GLN
L387	R454	G520	T592	GLU	THR	C797	L876	THR	MET	GLY	VAL	SER	PRO	ARG
M455	M455	Q521	T595	SER	ALA	R798	R877	LEU	THR	GLN	HIS	ASP	GLY	ARG
I388	D456	D522	T596	ASP	THR	S798	R877	PHE	TYR	GLU	ASN	ASP	LEU	GLU
R389	M457	A523	N596	ASP	THR	P799	Y800	LEU	GLY	LEU	GLY	ASP	LEU	GLU
G390	E458	A523	P597	SER	LEU	A800	P881	ARG	GLY	LEU	ASN	TRP	ALA	ALA
E391	L459	CYS	S598	SER	THR	A801	G882	LYS	ASN	VAL	ALA	SER	ALA	GLY
T392	L459	GLY	S598	GLN	LEU	Y802	N883	GLN	LYS	VAL	ARG	ARG	THR	ARG
L393	K460	SER	S598	LYS	LEU	Y802	Y884	GLN	LYS	VAL	ARG	ARG	THR	ARG
E394	T461	N527	L601	HIS	PRO	T807	S885	PRO	ASP	GLU	ASN	GLY	THR	GLY
I395	T461	ASP	D602	ASP	ASP	M808	S886	ASP	ASP	GLU	CYS	VAL	GLU	GLY
G396	M462	S528	P603	GLN	PHE	P809	R887	LEU	ILE	LEU	ILE	VAL	GLU	GLY
N397	D464	W529	P603	ASN	THR	P809	R887	GLY	THR	LEU	ILE	VAL	GLU	GLY
Y398	Q465	T530	I604	GLU	GLU	E810	R889	MET	LYS	VAL	VAL	TRP	VAL	VAL
S399	Q465	I534	S607	TYR	VAL	A813	R890	GLY	GLY	ALA	ALA	ILE	ALA	ALA
F400	C468	S540	S610	ASP	SER	D814	T891	PRO	ALA	PRO	ASP	THR	THR	THR
Y401	E469	ASN	S611	SER	THR	D815	S892	THR	GLY	GLU	ASP	THR	THR	THR
A402	M470	ASP	Q612	ALA	ILE	I816	L893	ILE	THR	THR	LYS	THR	THR	THR
L403	E471	PRO	I613	SER	VAL	E823	N896	ALA	VAL	VAL	LYS	VAL	THR	THR
D404	L472	LYS	I614	GLU	PRO	I824	N896	SER	VAL	VAL	LYS	VAL	THR	THR
M405	L473	SER	L615	SER	THR	F825	N899	ILE	ALA	ALA	ILE	ALA	THR	THR
Q406	K474	GLN	K616	SER	SER	F825	N899	SER	VAL	VAL	LYS	VAL	THR	THR
M407	F475	GLN	M617	SER	GLN	N828	E901	GLY	THR	THR	GLY	THR	THR	THR
L408	F477	GLN	K618	SER	GLN	N828	E901	GLY	THR	THR	GLY	THR	THR	THR
R409	L478	GLN	P619	SER	PRO	H831	T903	LEU	ASN	PRO	PRO	ASP	THR	THR
Q410	L478	GLN	P620	LYS	LYS	H831	T903	SER	GLU	ASP	ASP	THR	THR	THR
L411	T480	P551	S621	GLN	T690	L832	Y904	ALA	SER	ALA	ALA	THR	THR	THR
G412	F482	W552	D622	GLN	D691	L832	F905	SER	ALA	SER	ALA	THR	THR	THR
D413	S481	L554	N623	GLN	S692	P837	Y906	ALA	SER	ALA	ALA	THR	THR	THR
M414	D483	M555	N624	GLN	L695	P837	Y906	ALA	SER	ALA	ALA	THR	THR	THR
H417	K484	R556	N624	GLN	K696	K838	T908	VAL	ARG	PRO	ASN	GLY	THR	THR
M418	L485	G557	N624	GLN	E697	K838	T908	PHE	ARG	PRO	ASN	GLY	THR	THR
L419	L486	L558	N624	GLN	L698	P840	T908	PRO	GLY	GLY	ASN	GLY	THR	THR
T420	L487	L558	N624	GLN	E698	P840	T908	PRO	GLY	GLY	ASN	GLY	THR	THR
I421	R488	W561	N624	GLN	L698	P840	T908	PRO	GLY	GLY	ASN	GLY	THR	THR
T422	W489	T562	N624	GLN	E699	G842	Y851	TRP	ILE	VAL	VAL	VAL	VAL	VAL
Q423	E490	Q563	N624	GLN	E700	L843	Y851	TRP	ILE	VAL	VAL	VAL	VAL	VAL
G424	P491	Y564	N624	GLN	S701	I844	R852	TRP	ILE	VAL	VAL	VAL	VAL	VAL
K425	Y492	A565	N624	GLN	S702	V845	R853	TRP	ILE	VAL	VAL	VAL	VAL	VAL
L426	W493	I566	N624	GLN	R703	E848	D856	TRP	ILE	VAL	VAL	VAL	VAL	VAL
F427	P494	V567	N624	GLN	K705	V849	E857	TRP	ILE	VAL	VAL	VAL	VAL	VAL
F428	R498	V568	N624	GLN	Y710	V849	E857	TRP	ILE	VAL	VAL	VAL	VAL	VAL
H429	R498	V568	N624	GLN	Y710	V849	E857	TRP	ILE	VAL	VAL	VAL	VAL	VAL
Y430	L501	D576	N624	GLN	V715	V849	E857	TRP	ILE	VAL	VAL	VAL	VAL	VAL
P432	G502	E577	N624	GLN	V715	V849	E857	TRP	ILE	VAL	VAL	VAL	VAL	VAL
L436	F503	R578	N624	GLN	R719	V849	E857	TRP	ILE	VAL	VAL	VAL	VAL	VAL
I439	M504	R579	N624	GLN	R719	V849	E857	TRP	ILE	VAL	VAL	VAL	VAL	VAL
H440	L505	T580	N624	GLN	R719	V849	E857	TRP	ILE	VAL	VAL	VAL	VAL	VAL
K441	F506	Y581	N624	GLN	R719	V849	E857	TRP	ILE	VAL	VAL	VAL	VAL	VAL
M442	Y507	G582	N624	GLN	R719	V849	E857	TRP	ILE	VAL	VAL	VAL	VAL	VAL
G447	K508	L653	N624	GLN	R719	V849	E857	TRP	ILE	VAL	VAL	VAL	VAL	VAL
	A510	K584	N624	GLN	R719	V849	E857	TRP	ILE	VAL	VAL	VAL	VAL	VAL
		S585	N624	GLN	R719	V849	E857	TRP	ILE	VAL	VAL	VAL	VAL	VAL

● Molecule 2: Insulin



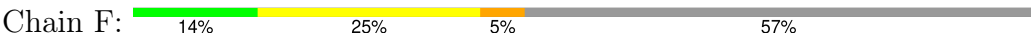
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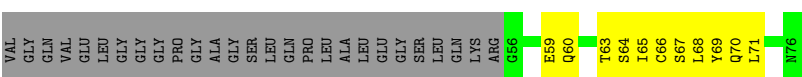
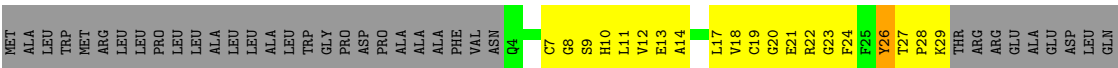
● Molecule 2: Insulin



● Molecule 2: Insulin



● Molecule 2: Insulin



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	101391	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.41	1/6736 (0.0%)	0.55	2/9133 (0.0%)
1	B	0.32	0/6415	0.55	6/8693 (0.1%)
2	D	0.25	0/353	0.38	0/475
2	E	0.38	0/383	0.50	0/518
2	F	0.27	0/377	0.46	0/508
2	G	0.33	0/377	0.52	0/508
All	All	0.36	1/14641 (0.0%)	0.54	8/19835 (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
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	529	TRP	CB-CG	14.81	1.76	1.50

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	548	PRO	CA-N-CD	-8.52	99.58	111.50
1	B	379	LEU	CA-CB-CG	5.32	127.53	115.30
1	B	794	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	691	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	794	ASP	CB-CG-OD2	5.22	123.00	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	580	THR	Peptide
1	B	272	PRO	Peptide

## 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	6572	0	6387	435	0
1	B	6263	0	6099	440	0
2	D	347	0	317	9	0
2	E	376	0	346	13	0
2	F	370	0	344	37	0
2	G	370	0	344	26	0
All	All	14298	0	13837	932	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 33.

The worst 5 of 932 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:529:TRP:CB	1:A:529:TRP:CG	1.76	1.61
1:B:506:PHE:HB3	1:B:529:TRP:CD1	1.10	1.59
1:A:260:GLN:HG2	1:A:264:PHE:CE2	1.40	1.54
1:A:260:GLN:CG	1:A:264:PHE:HE2	1.22	1.52
1:B:506:PHE:CB	1:B:529:TRP:CD1	1.93	1.52

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	805/1345 (60%)	712 (88%)	87 (11%)	6 (1%)	19	56
1	B	760/1345 (56%)	691 (91%)	68 (9%)	1 (0%)	48	83
2	D	40/110 (36%)	37 (92%)	3 (8%)	0	100	100
2	E	44/110 (40%)	40 (91%)	4 (9%)	0	100	100
2	F	43/110 (39%)	38 (88%)	3 (7%)	2 (5%)	2	17
2	G	43/110 (39%)	38 (88%)	4 (9%)	1 (2%)	5	29
All	All	1735/3130 (55%)	1556 (90%)	169 (10%)	10 (1%)	24	60

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	LYS
1	A	272	PRO
2	F	28	PRO
1	A	529	TRP
1	B	794	ASP

### 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	739/1211 (61%)	729 (99%)	10 (1%)	62	75
1	B	704/1211 (58%)	697 (99%)	7 (1%)	73	81
2	D	39/88 (44%)	39 (100%)	0	100	100
2	E	43/88 (49%)	43 (100%)	0	100	100
2	F	42/88 (48%)	39 (93%)	3 (7%)	12	32
2	G	42/88 (48%)	42 (100%)	0	100	100
All	All	1609/2774 (58%)	1589 (99%)	20 (1%)	66	79

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	700	GLU
2	F	24	PHE
2	F	29	LYS
2	F	25	PHE
1	A	518	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	591	GLN
1	B	32	HIS
1	B	276	GLN
1	A	276	GLN
1	A	108	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 ⓘ

There are no chain breaks in this entry.

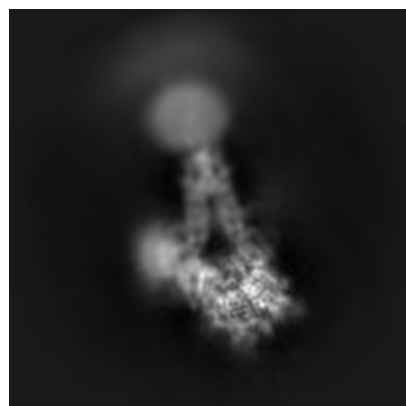
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28723. These allow visual inspection of the internal detail of the map and identification of artifacts.

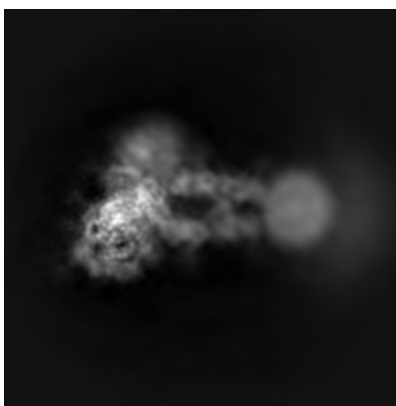
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

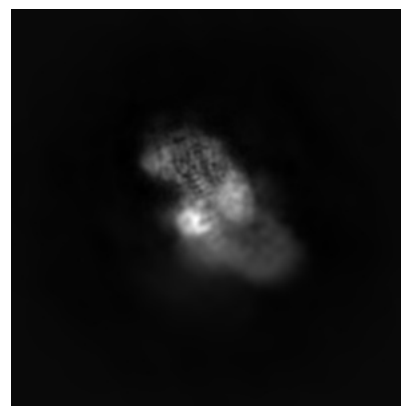
#### 6.1.1 Primary map



X

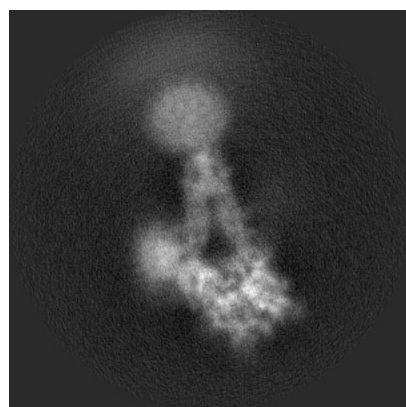


Y

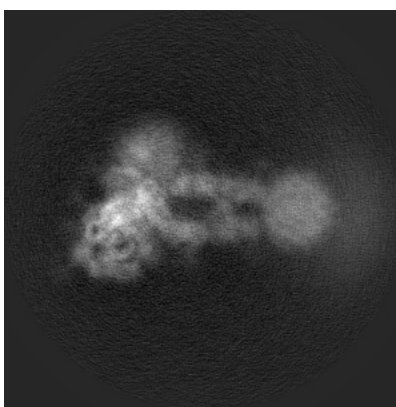


Z

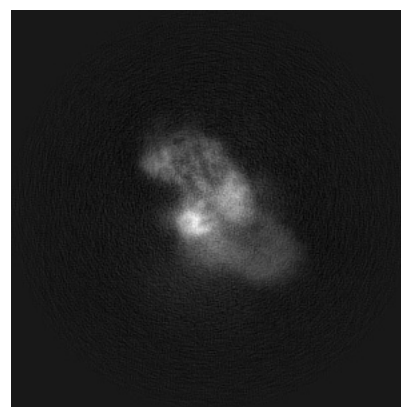
#### 6.1.2 Raw map



X



Y

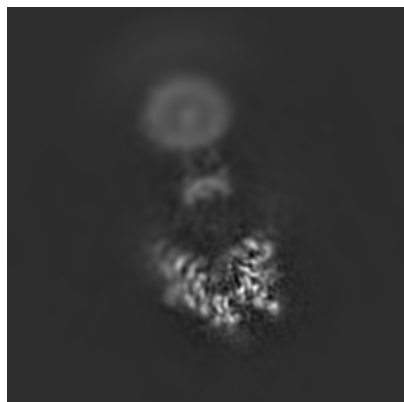


Z

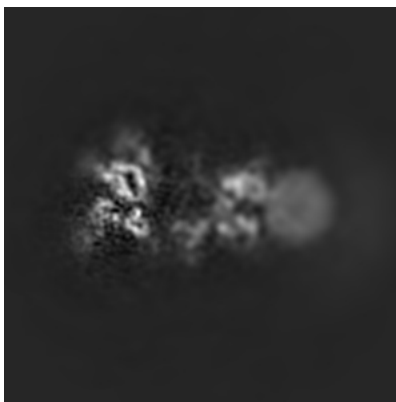
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

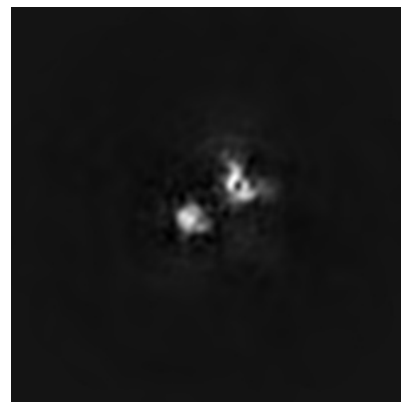
### 6.2.1 Primary map



X Index: 150

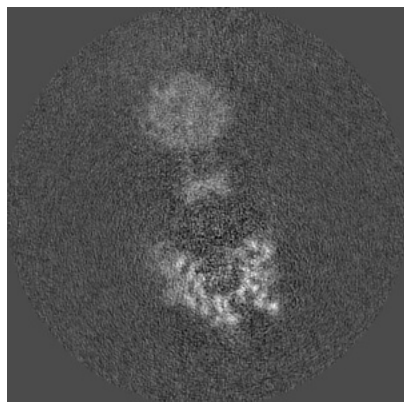


Y Index: 150

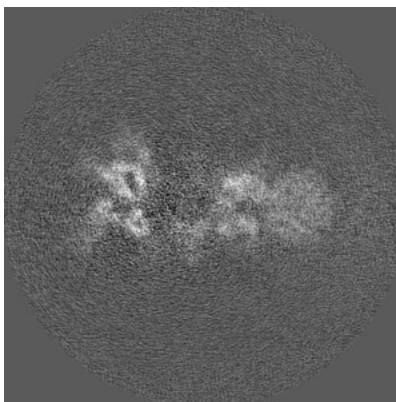


Z Index: 150

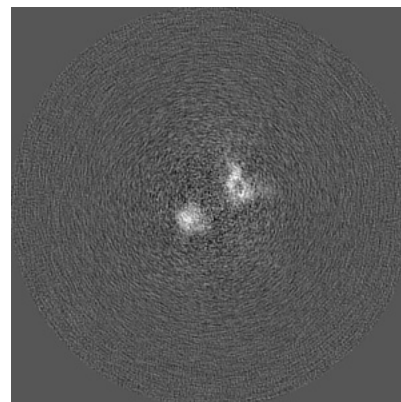
### 6.2.2 Raw map



X Index: 150



Y Index: 150

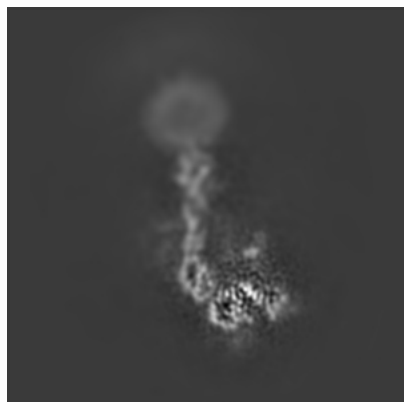


Z Index: 150

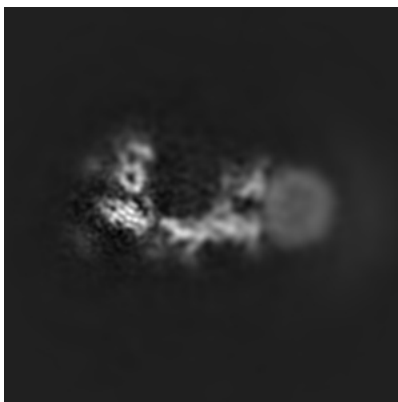
The images above show central slices of the map in three orthogonal directions.

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

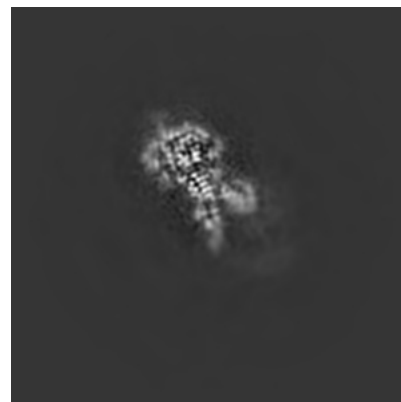
### 6.3.1 Primary map



X Index: 140

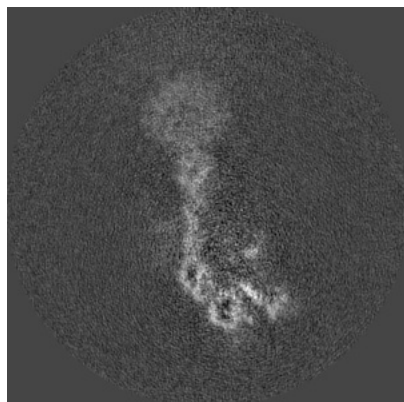


Y Index: 144

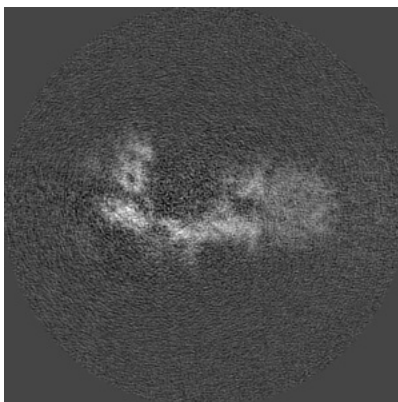


Z Index: 81

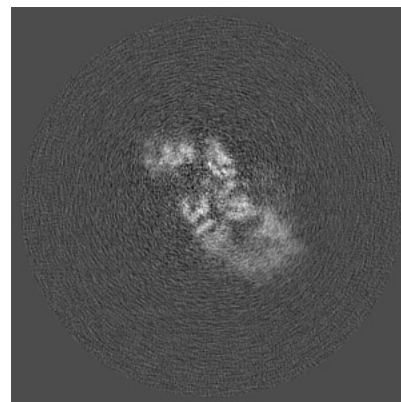
### 6.3.2 Raw map



X Index: 140



Y Index: 144



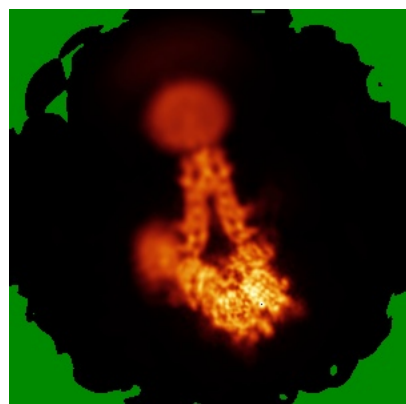
Z Index: 101

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

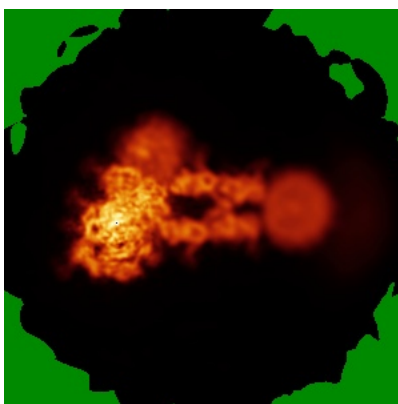


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

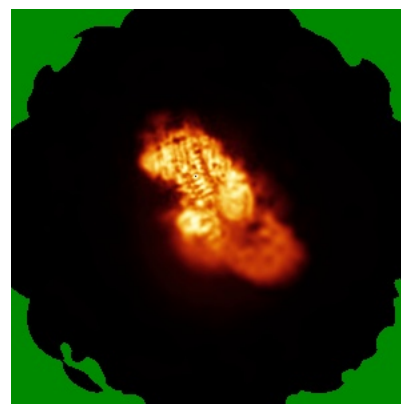
### 6.4.1 Primary map



X

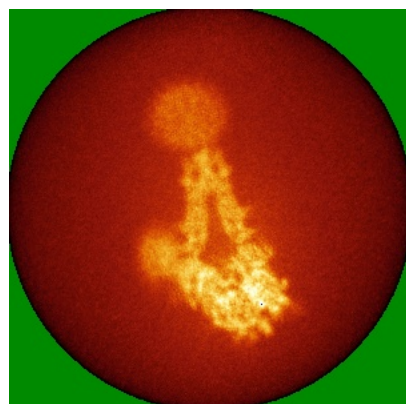


Y

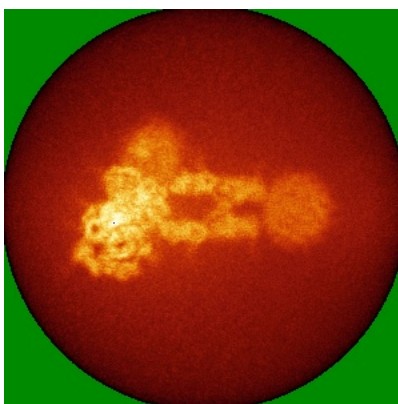


Z

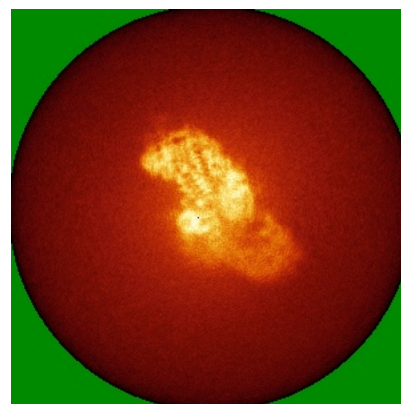
### 6.4.2 Raw map



X



Y

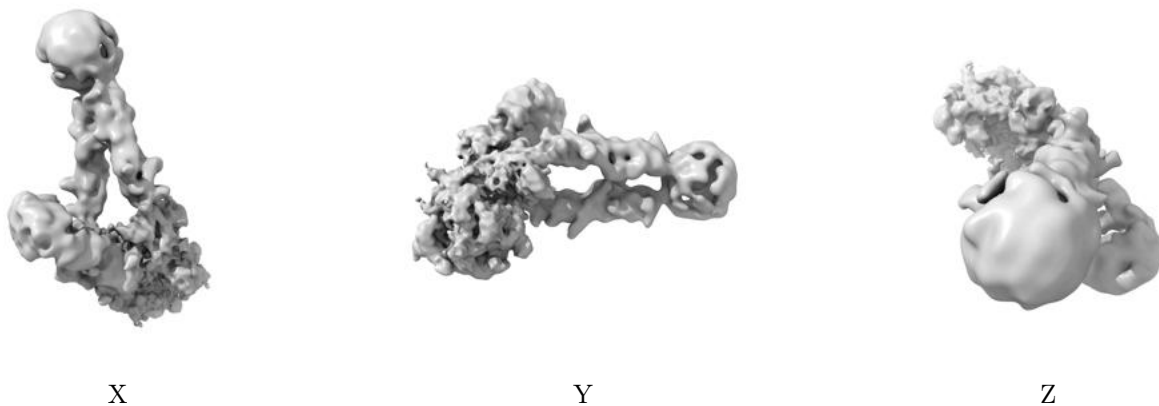


Z

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.

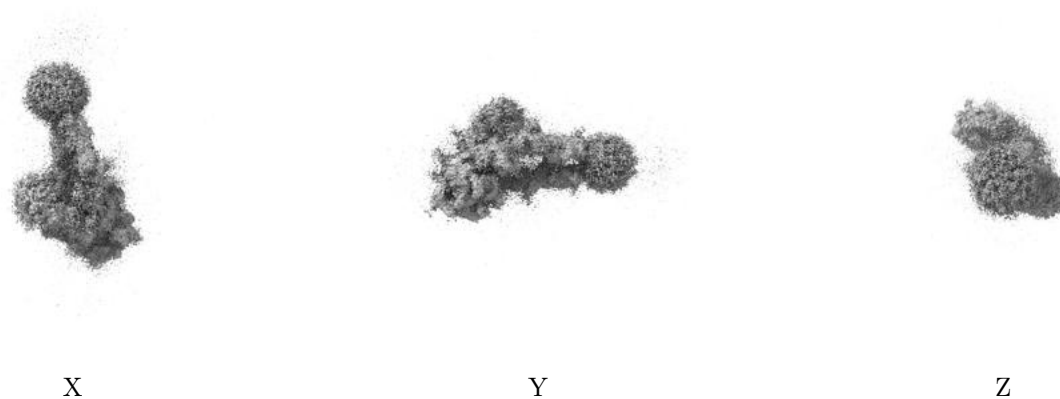
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

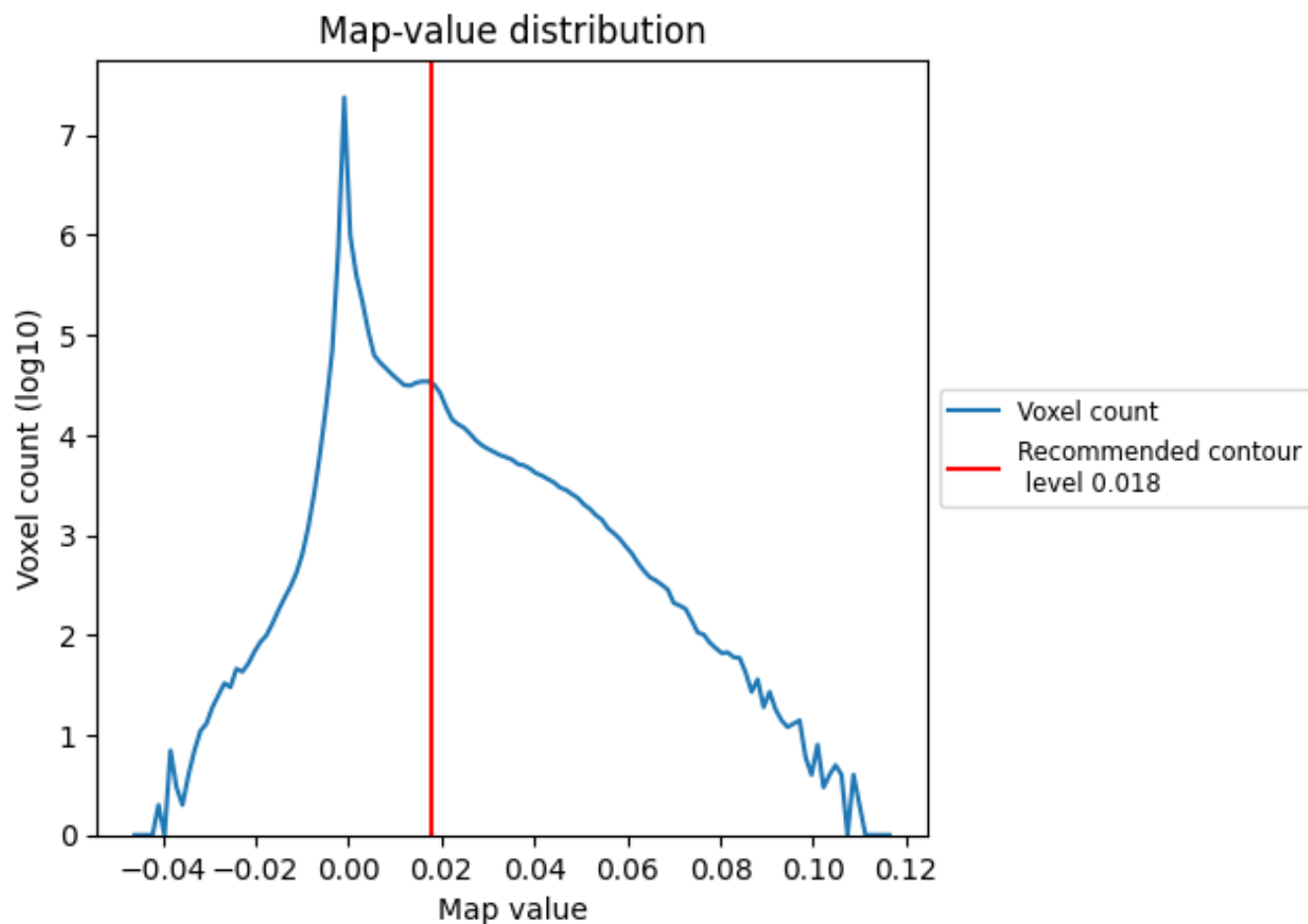
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

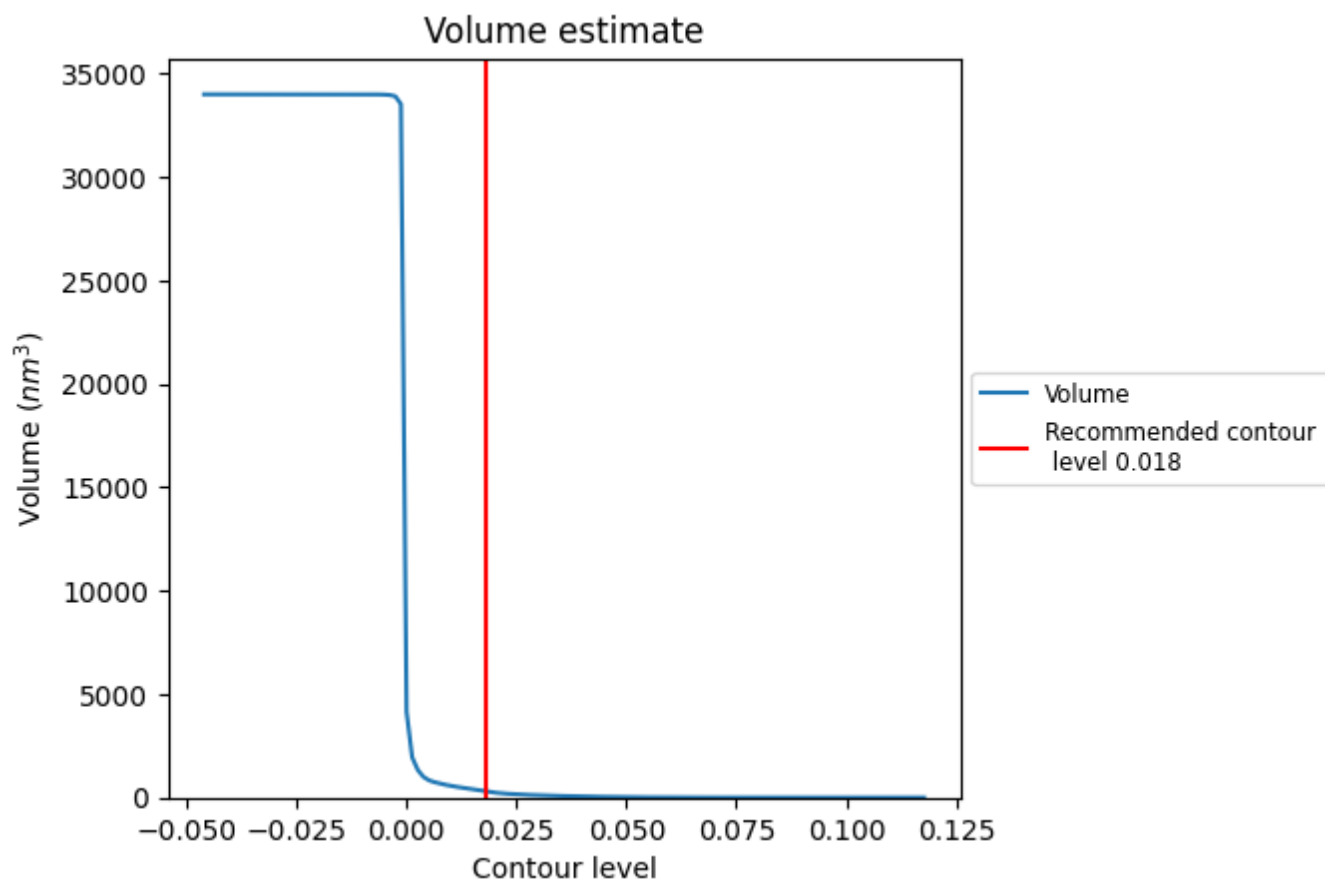
This section contains the results of statistical analysis of the map.

### 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.

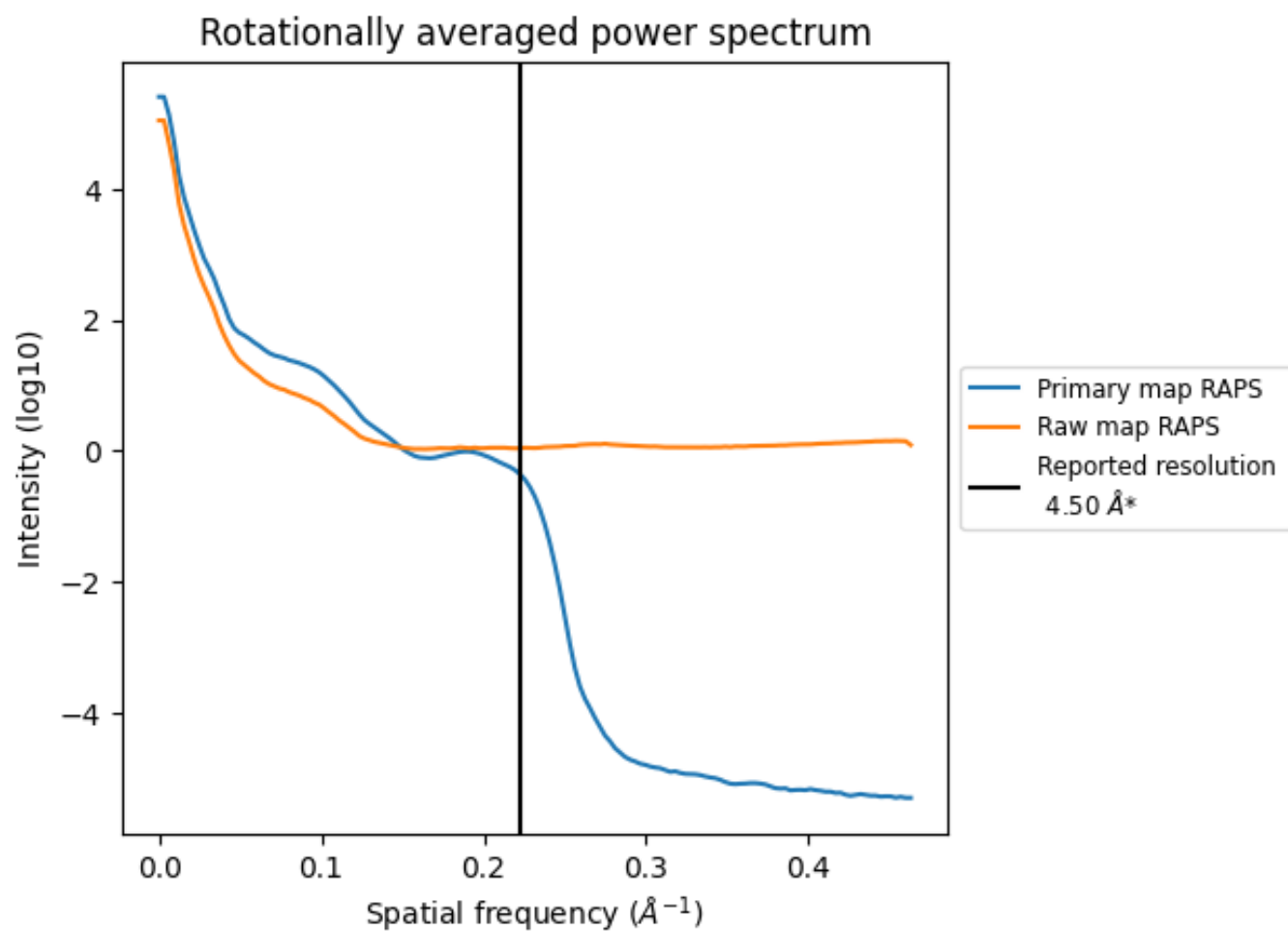
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 306 nm<sup>3</sup>; this corresponds to an approximate mass of 276 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 ⓘ

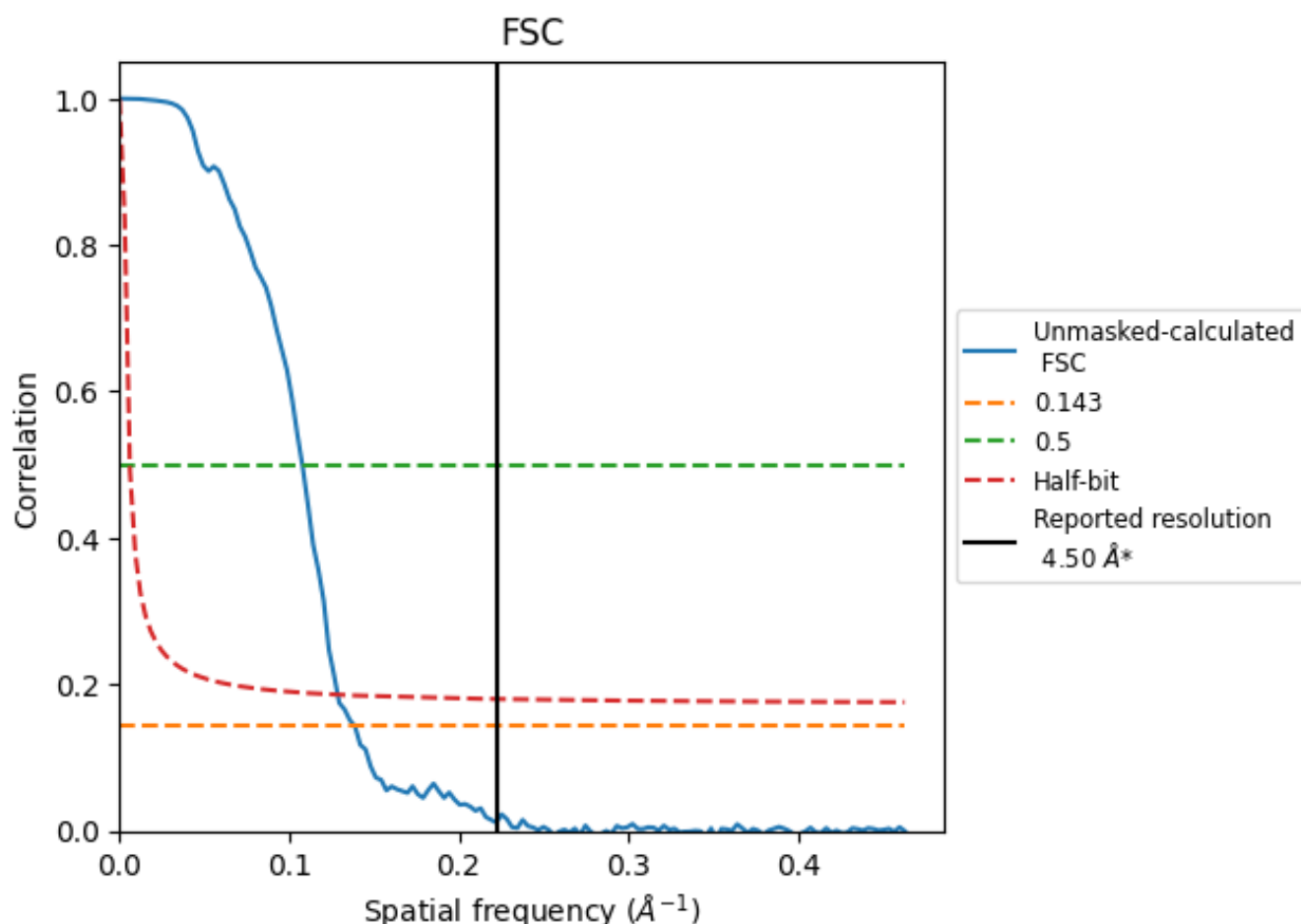


\*Reported resolution corresponds to spatial frequency of 0.222  $\text{\AA}^{-1}$

## 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 0.222 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

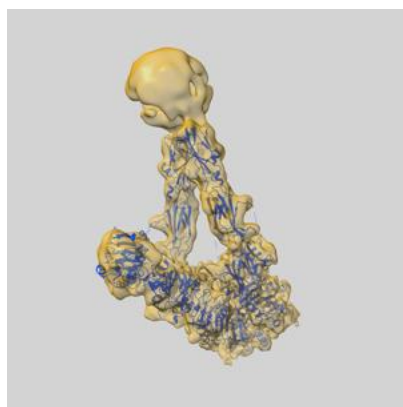
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.22	9.28	7.77

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.22 differs from the reported value 4.5 by more than 10 %

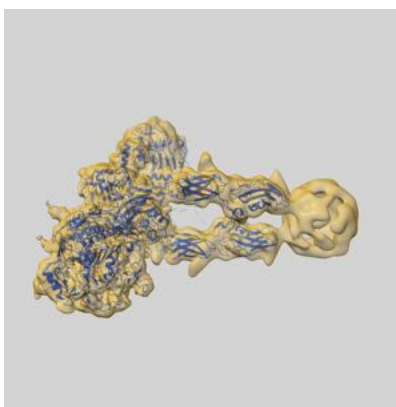
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28723 and PDB model 8EYX. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

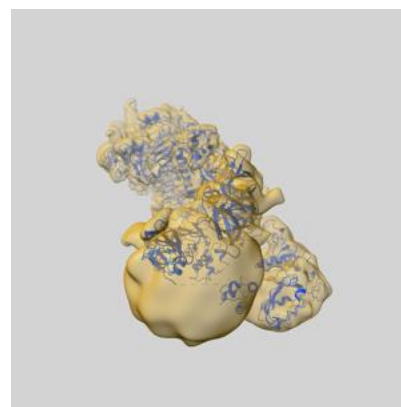
### 9.1 Map-model overlay [i](#)



X



Y

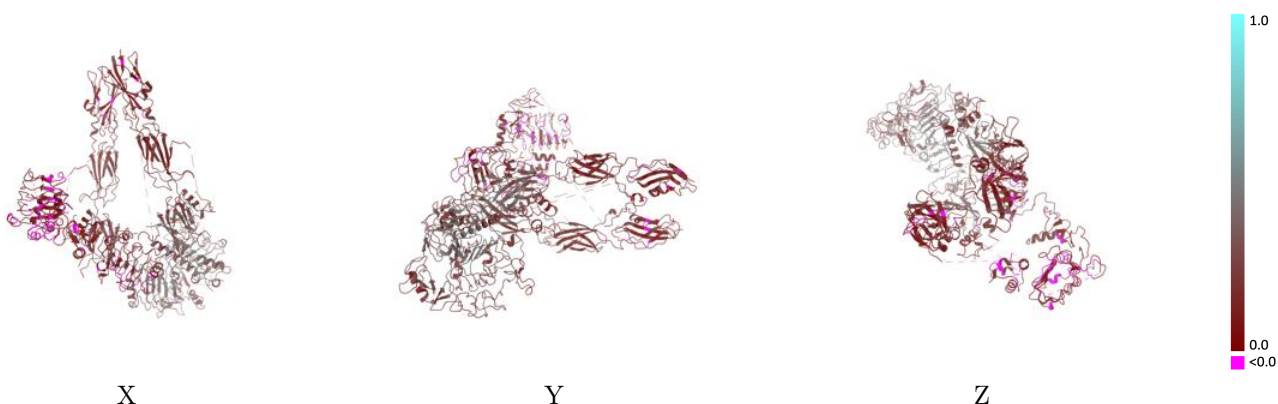


Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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.

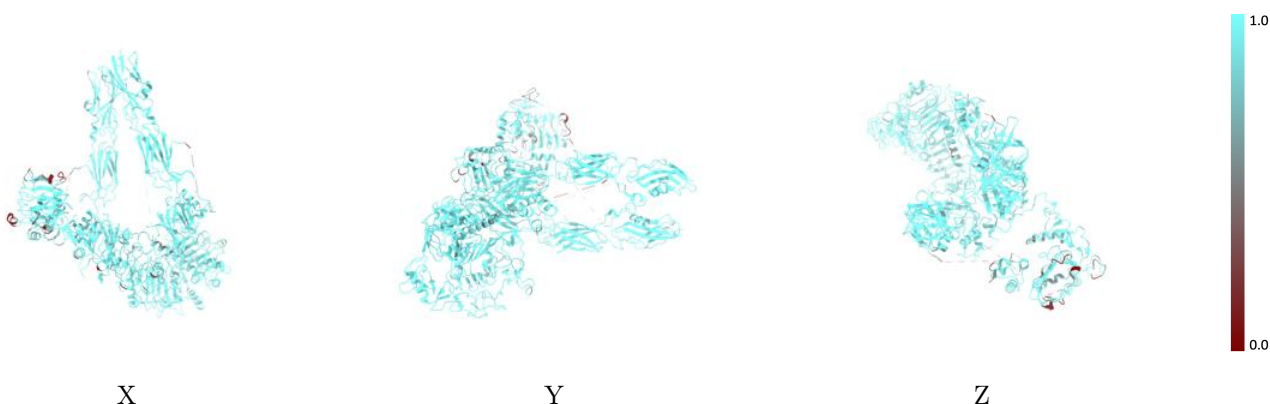


## 9.2 Q-score mapped to coordinate model [i](#)



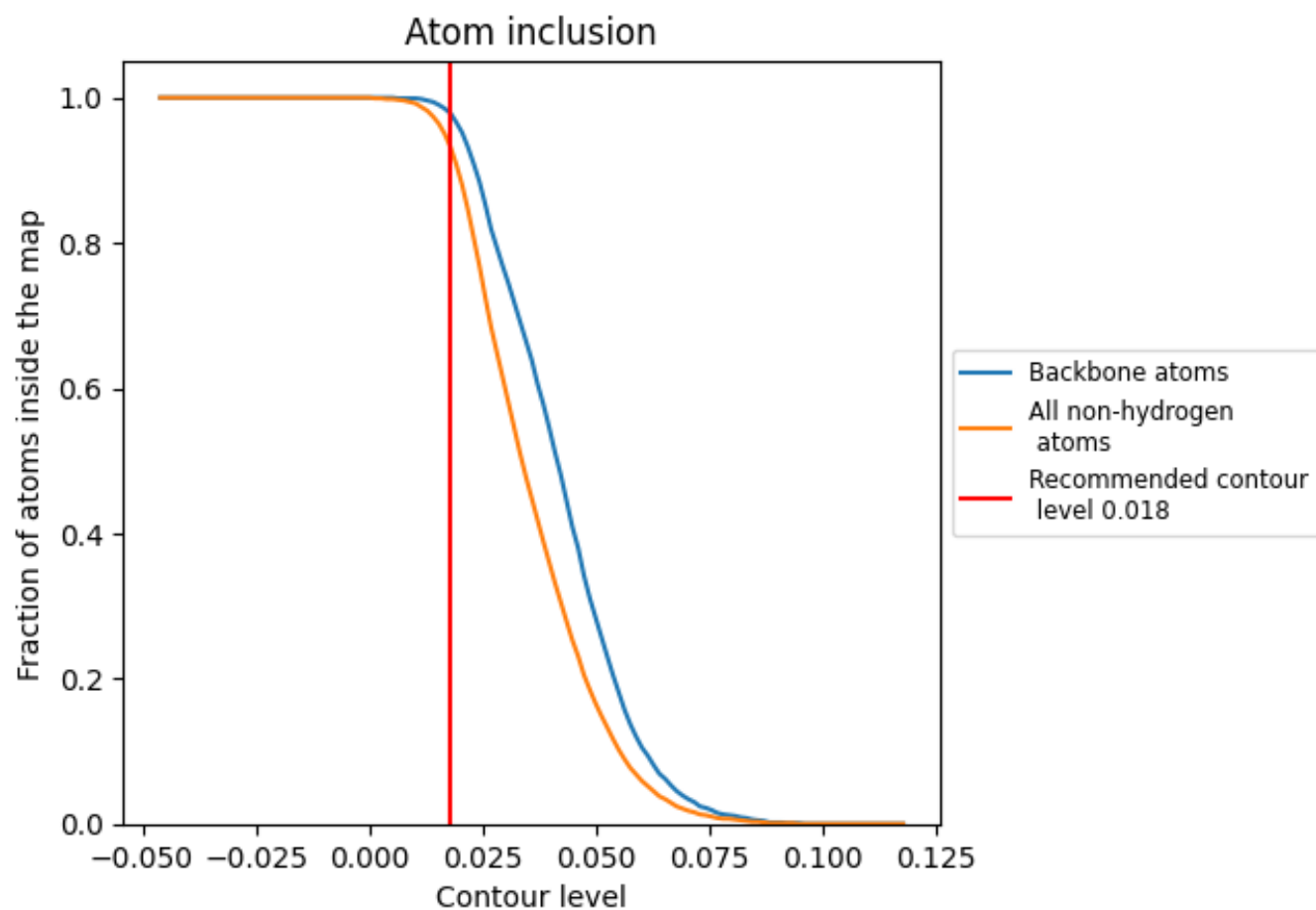
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9310	<div></div> 0.2370
A	<div></div> 0.9550	<div></div> 0.2840
B	<div></div> 0.9030	<div></div> 0.1910
D	<div></div> 0.8890	<div></div> 0.0890
E	<div></div> 0.9780	<div></div> 0.3360
F	<div></div> 0.9510	<div></div> 0.1920
G	<div></div> 0.9480	<div></div> 0.2620

