



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 02:38 AM UTC

PDB ID : 9CLI / pdb_00009cli
EMDB ID : EMD-45675
Title : Cryo-EM model derived from localized reconstruction of human adenovirus (Ad5)-hexon-FX complex at 3.6Å resolution
Authors : Reddy, V.S.; Ma, O.X.
Deposited on : 2024-07-11
Resolution : 3.61 Å(reported)
Based on initial model : 6BIT

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

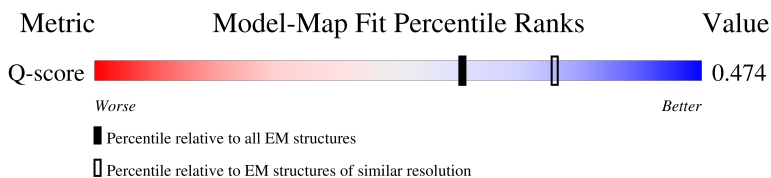
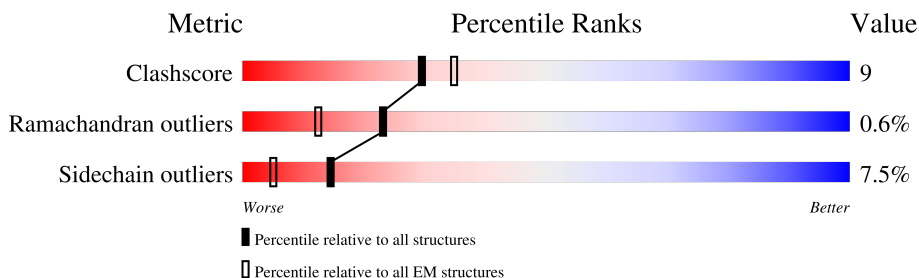
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.61 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11801 (3.11 - 4.10)

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	J	952	
1	K	952	
1	L	952	
2	Z	488	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25186 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 Hexon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	925	Total	C	N	O	S	0	0
			7401	4703	1253	1409	36		
1	K	922	Total	C	N	O	S	0	0
			7382	4691	1250	1405	36		
1	L	924	Total	C	N	O	S	0	0
			7394	4699	1252	1407	36		

- Molecule 2 is a protein called Coagulation factor X.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	377	Total	C	N	O	S	0	0
			3002	1849	516	606	31		

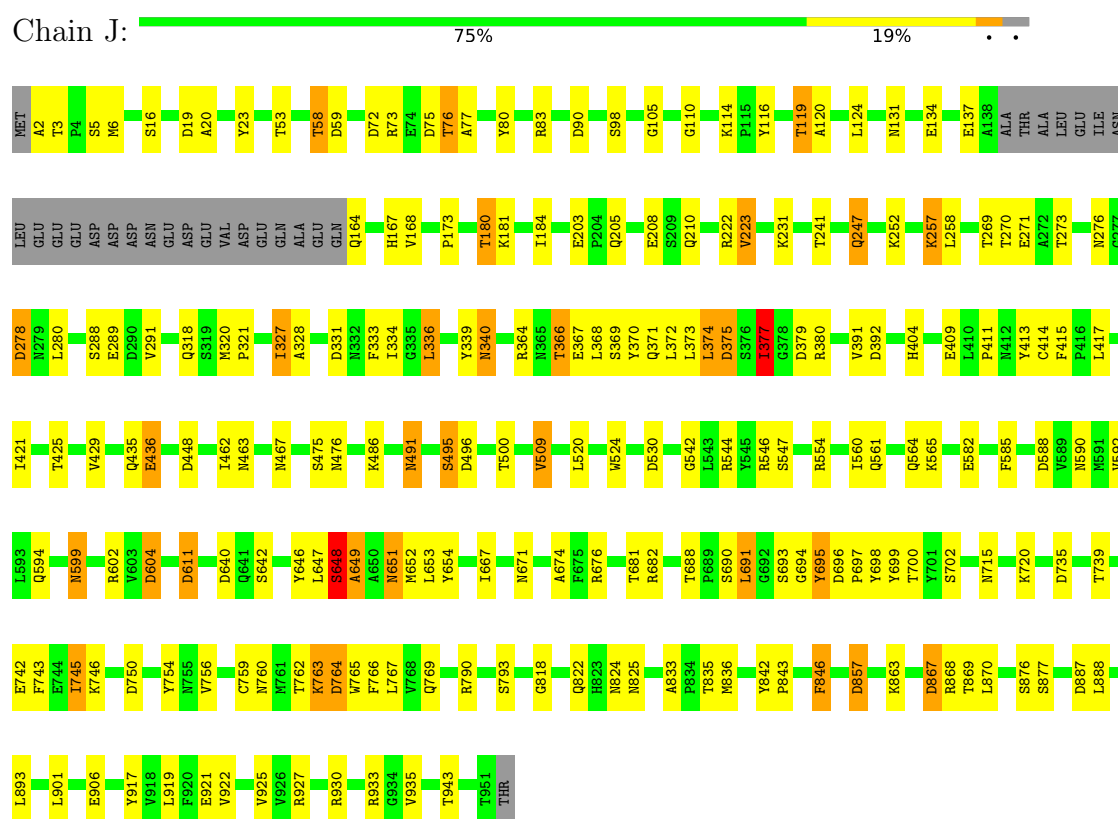
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	L	1	Total	Ca	0
			1	1	
3	Z	6	Total	Ca	0
			6	6	

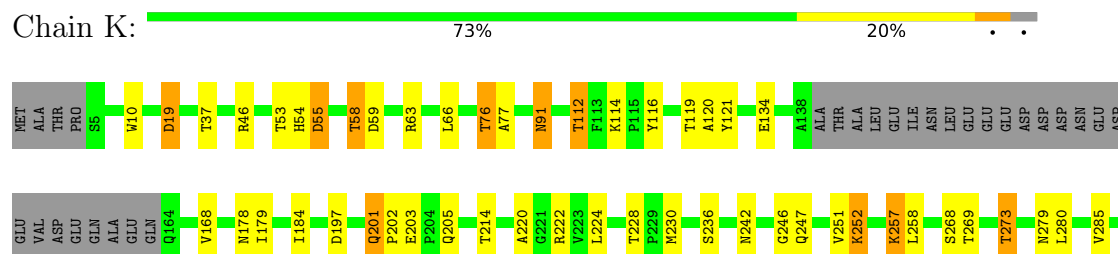
3 Residue-property plots

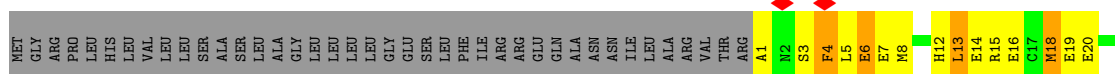
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Hexon protein



- Molecule 1: Hexon protein





LYS	K388	D389	T390	Y391	F392	V393	T394	G395	I396	V397	S398	W399	G400	E401	G402	C403	A404	R405	K406	G407	K408	Y409	G410	I411	Y412	T413	K414	V415	T416	A417	F418	L419	K420	W421	I422	D423	R424	S425	M426	K427	T428	R429	G430	LEU	PRO	LYS	ALA	LYS	SER	HIS	ALA	PRO	PRO	GLU	VAL	ILE	THR	SER	SER	PRO	PRO	LEU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
	H328	E329	K330	G331	R332	Q333	S334	T335	R336	L337	K338	M339	L340	E341	V342	P343	Y344	V345	D346	R347	N348	S349	C350	K351	L352	S353	S354	S355	F356	I357	T358	T359	Q360	N361	M362	F363	C364	A365	G366	Y367	D368	T369	K370	Q371	E372	D373	A374	G375	Q376	Q377	D378	S379	G380	P382	H383	V384	T385	R386	F387																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
	V268	L269	K270	H271	N272	R273	F274	T275	K276	E277	T278	Y279	D280	F281	D282	I283	A284	V285	L286	R287	L288	K289	T290	P291	I292	T293	F294	R295	M296	N297	V298	A299	P300	A301	C302	L303	P304	C305	R306	D307	W308	A309	E310	S311	S312	L313	M314	T315	Q316	K317	T318	G319	I320	V321	S322	G323	F324	G325	R326	T327																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
	W208	Q209	A210	L211	L212	I213	N214	E215	E216	N217	E218	G219	F220	C221	G222	G223	T224	I225	L226	S227	E228	F229	Y230	I231	L232	T233	A234	A235	H236	C237	L238	Y239	Q240	A241	K242	R243	F244	K245	V246	R247	V248	G249	D250	R251	N252	T253	E254	Q255	E256	E257	G258	G259	E260	A261	V262	H263	E264	V265																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
	THR	SER	SER	SER	GLY	GLU	ALA	PRO	ASP	ASP	SER	ILE	THR	THR	LYS	PRO	TYR	ASP	ALA	ALA	ASP	LEU	PRO	THR	GLU	ASN	PRO	PHE	ASN	GLN	THR	GLN	PRO	GLU	GLY	ASP	N190	N191	L192	T193	R194	I195	V196	G197	G198	Q199	E200	C201	K202	D203	G204	E205	C206	P207																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
	L38	C89	S90	L91	D92	N93	G94	D95	C96	THR	D97	Q98	F99	C100	H101	E102	E103	Q104	N105	S106	V107	V108	C109	S110	C111	A112	R113	G114	Y115	T116	L117	A118	D119	N120	G121	K122	A123	C124	I125	P126	T127	G128	P129	Y130	P131	C132	G133	K134	Q135	T136	LEU	GLU	ARG	ARG	LYS	ARG	SER	VAL	ALA	GLN	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
	E25	E26	A27	R28	E29	V30	F31	E32	D33	S34	D35	K36	T37	N38	E39	K43	Y44	K45	D46	G47	D48	Q49	C50	E51	T52	S53	P54	C55	Q56	N57	Q58	G59	K60	C61	K62	D63	G66	E67	Y68	T69	C70	T71	C72	L73	E74	G75	F76	E77	G78	K79	N80	C81	E82	L83	F84	T85	R86	K87																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
	LYS	PRO	LYS	ALA	LYS	SER	HIS	ALA	PRO	PRO	GLU	VAL	ILE	THR	SER	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	LEU	THR	SER	PRO	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	81	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.161	Depositor
Minimum map value	-0.091	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.01	Depositor
Map size (\AA)	116.864, 205.568, 129.536	wwPDB
Map dimensions	146, 92, 83	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.408, 1.408, 1.408	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CGU, CA

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	J	0.47	2/7600 (0.0%)	0.51	4/10336 (0.0%)
1	K	0.44	1/7580 (0.0%)	0.49	4/10307 (0.0%)
1	L	0.45	0/7593	0.48	2/10326 (0.0%)
2	Z	0.13	0/2918	0.40	0/3912
All	All	0.43	3/25691 (0.0%)	0.48	10/34881 (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	J	0	1
1	K	0	2
1	L	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	649	ALA	CA-C	-5.07	1.46	1.52
1	K	763	LYS	CA-C	-5.06	1.46	1.52
1	J	648	SER	CA-C	-5.05	1.46	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	763	LYS	N-CA-C	-6.67	103.62	111.03
1	J	743	PHE	N-CA-C	-6.48	101.36	110.50
1	L	704	SER	N-CA-C	-5.78	101.91	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	374	LEU	N-CA-C	-5.76	104.19	111.11
1	J	377	ILE	N-CA-C	5.67	119.95	112.76

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	846	PHE	Peptide
1	K	201	GLN	Peptide
1	K	731	TRP	Peptide
1	L	201	GLN	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	J	7401	0	7105	135	0
1	K	7382	0	7086	148	0
1	L	7394	0	7097	146	0
2	Z	3002	0	2796	57	0
3	L	1	0	0	0	0
3	Z	6	0	0	0	0
All	All	25186	0	24084	455	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 9.

The worst 5 of 455 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:L:759:CYS:SG	1:L:760:ASN:N	2.36	0.96
1:K:759:CYS:SG	1:K:760:ASN:N	2.39	0.94
1:J:759:CYS:SG	1:J:760:ASN:N	2.45	0.89
2:Z:3:SER:HB3	2:Z:6:CGU:HB3	1.60	0.81
1:L:415:PHE:HB3	1:L:416:PRO:HD2	1.64	0.77

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	J	921/952 (97%)	843 (92%)	75 (8%)	3 (0%)	36	64
1	K	918/952 (96%)	848 (92%)	64 (7%)	6 (1%)	18	49
1	L	920/952 (97%)	847 (92%)	63 (7%)	10 (1%)	11	40
2	Z	362/488 (74%)	347 (96%)	14 (4%)	1 (0%)	36	64
All	All	3121/3344 (93%)	2885 (92%)	216 (7%)	20 (1%)	23	51

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	646	TYR
1	L	437	ASN
1	L	596	SER
1	L	764	ASP
1	L	435	GLN

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	J	805/829 (97%)	746 (93%)	59 (7%)	13	37
1	K	803/829 (97%)	732 (91%)	71 (9%)	9	31
1	L	804/829 (97%)	735 (91%)	69 (9%)	10	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	Z	313/408 (77%)	308 (98%)	5 (2%)	55 66
All	All	2725/2895 (94%)	2521 (92%)	204 (8%)	14 37

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	759	CYS
1	L	124	LEU
2	Z	4	PHE
1	K	854	THR
1	L	11	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	758	GLN
1	L	435	GLN
1	L	861	GLN
1	L	325	ASN
1	L	476	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 non-standard protein/DNA/RNA residues are modelled in this entry.

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
2	CGU	Z	7	2,3	9,11,12	1.44	1 (11%)	10,14,16	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CGU	Z	39	2	9,11,12	1.65	1 (11%)	10,14,16	0.82	0
2	CGU	Z	20	2	9,11,12	1.28	0	10,14,16	0.75	0
2	CGU	Z	29	2,3	9,11,12	1.70	2 (22%)	10,14,16	1.06	0
2	CGU	Z	16	2,3	9,11,12	1.15	0	10,14,16	0.85	0
2	CGU	Z	26	2,3	9,11,12	1.46	0	10,14,16	0.86	0
2	CGU	Z	32	2	9,11,12	1.70	2 (22%)	10,14,16	0.83	0
2	CGU	Z	14	2	9,11,12	1.45	1 (11%)	10,14,16	0.79	0
2	CGU	Z	25	2,3	9,11,12	1.39	0	10,14,16	0.76	0
2	CGU	Z	6	2,3	9,11,12	1.62	1 (11%)	10,14,16	0.97	0
2	CGU	Z	19	2	9,11,12	1.53	1 (11%)	10,14,16	0.83	0

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
2	CGU	Z	7	2,3	-	8/13/14/16	-
2	CGU	Z	39	2	-	3/13/14/16	-
2	CGU	Z	20	2	-	7/13/14/16	-
2	CGU	Z	29	2,3	-	6/13/14/16	-
2	CGU	Z	16	2,3	-	4/13/14/16	-
2	CGU	Z	26	2,3	-	4/13/14/16	-
2	CGU	Z	32	2	-	6/13/14/16	-
2	CGU	Z	14	2	-	6/13/14/16	-
2	CGU	Z	25	2,3	-	7/13/14/16	-
2	CGU	Z	6	2,3	-	2/13/14/16	-
2	CGU	Z	19	2	-	4/13/14/16	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	6	CGU	CG-CD1	2.93	1.55	1.52
2	Z	39	CGU	CG-CD2	2.88	1.55	1.52
2	Z	32	CGU	CG-CD1	2.69	1.55	1.52
2	Z	29	CGU	CG-CD2	2.53	1.55	1.52
2	Z	32	CGU	CG-CD2	2.43	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Z	6	CGU	N-CA-CB-CG
2	Z	6	CGU	C-CA-CB-CG
2	Z	7	CGU	C-CA-CB-CG
2	Z	14	CGU	CA-CB-CG-CD1
2	Z	14	CGU	CA-CB-CG-CD2

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Z	20	CGU	1	0
2	Z	29	CGU	1	0
2	Z	16	CGU	1	0
2	Z	26	CGU	2	0
2	Z	32	CGU	1	0
2	Z	25	CGU	2	0
2	Z	6	CGU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

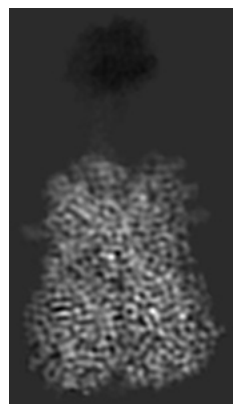
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45675. These allow visual inspection of the internal detail of the map and identification of artifacts.

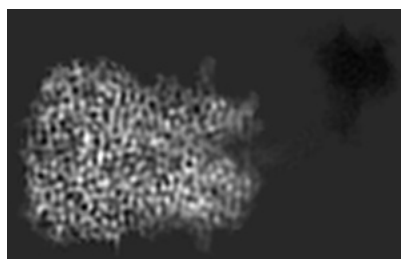
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

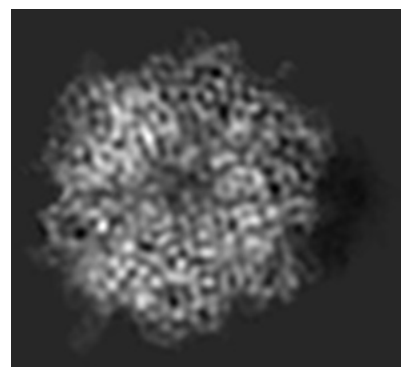
6.1.1 Primary map



X

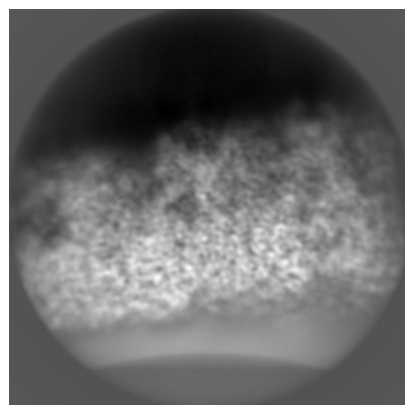


Y

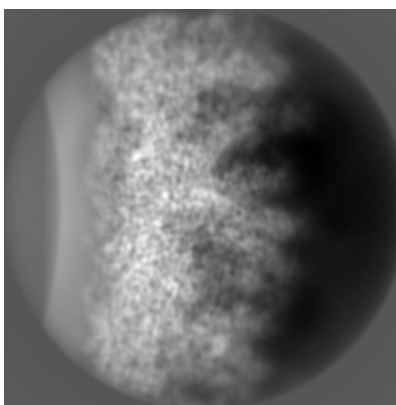


Z

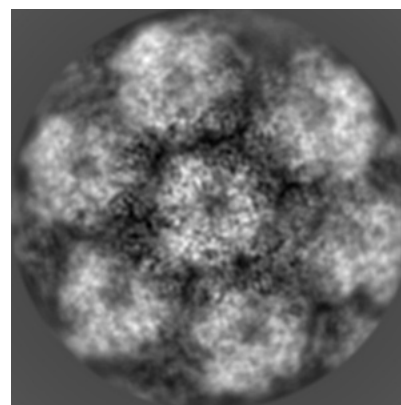
6.1.2 Raw map



X



Y

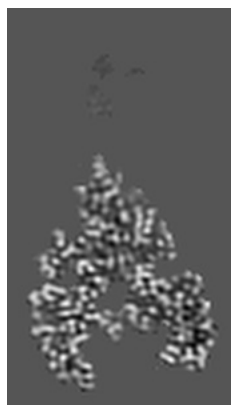


Z

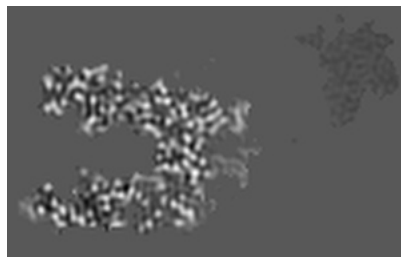
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

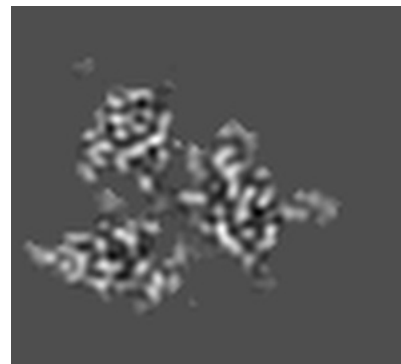
6.2.1 Primary map



X Index: 46

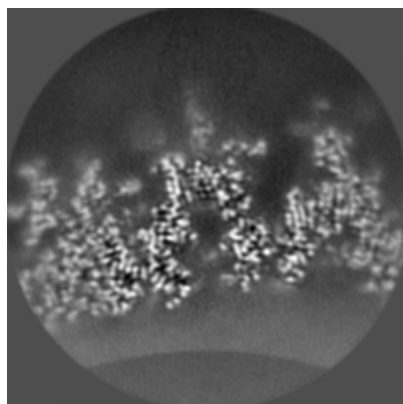


Y Index: 41

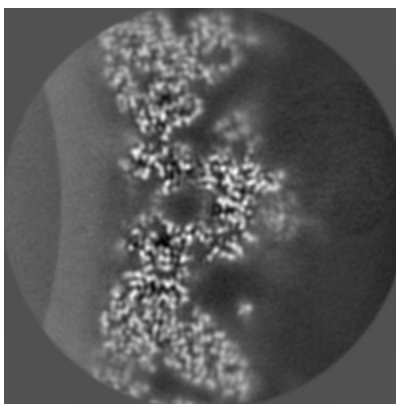


Z Index: 73

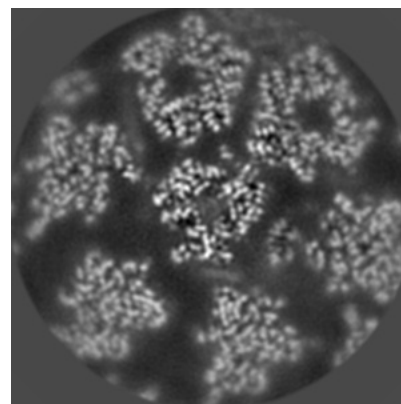
6.2.2 Raw map



X Index: 100



Y Index: 100

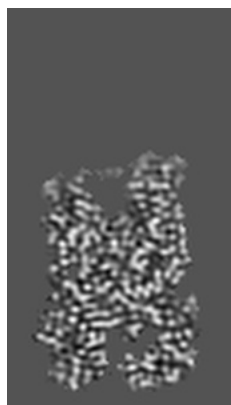


Z Index: 100

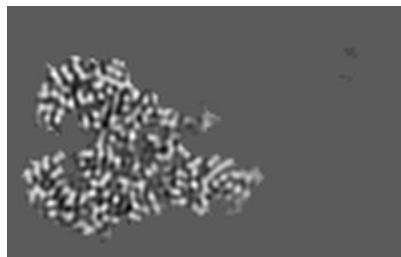
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 27

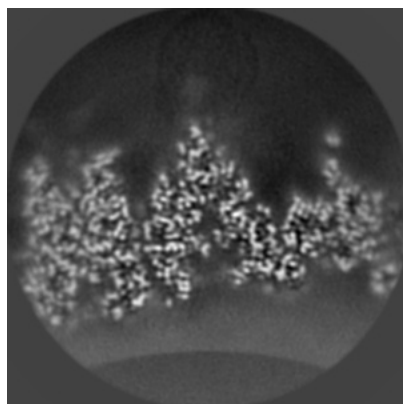


Y Index: 54

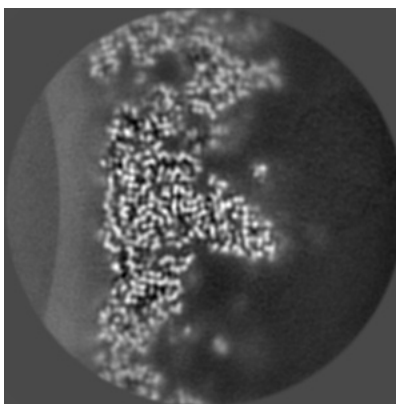


Z Index: 34

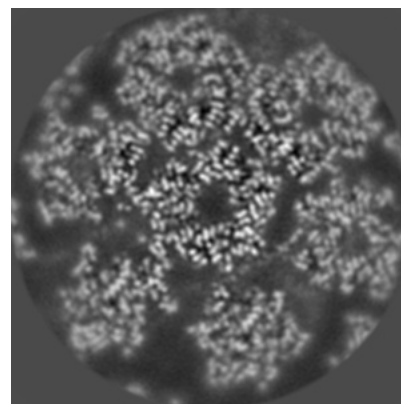
6.3.2 Raw map



X Index: 107



Y Index: 81

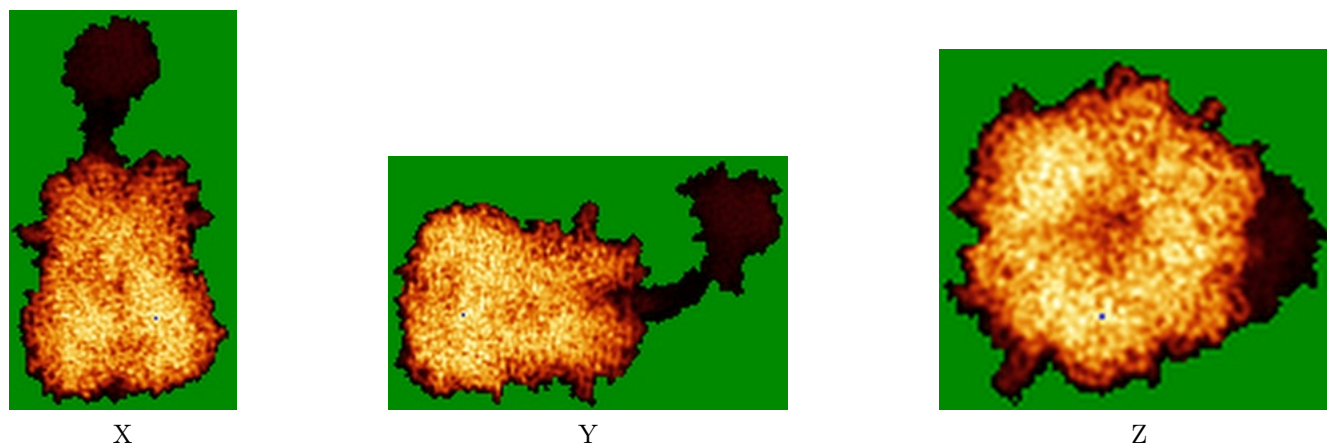


Z Index: 91

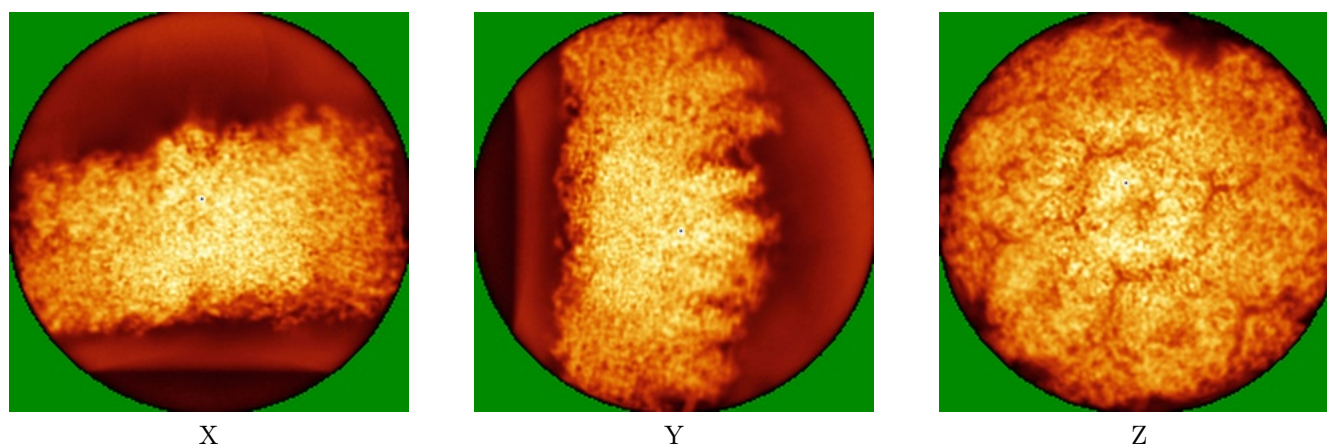
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



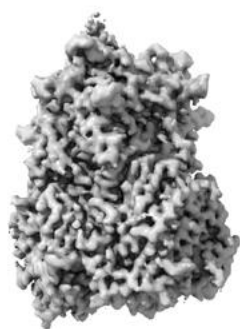
6.4.2 Raw map



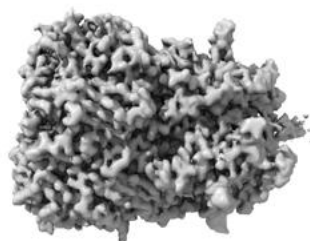
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

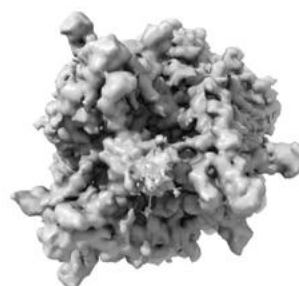
6.5.1 Primary map



X



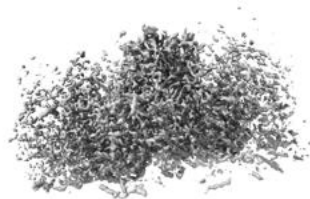
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. 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



X



Y



Z

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.

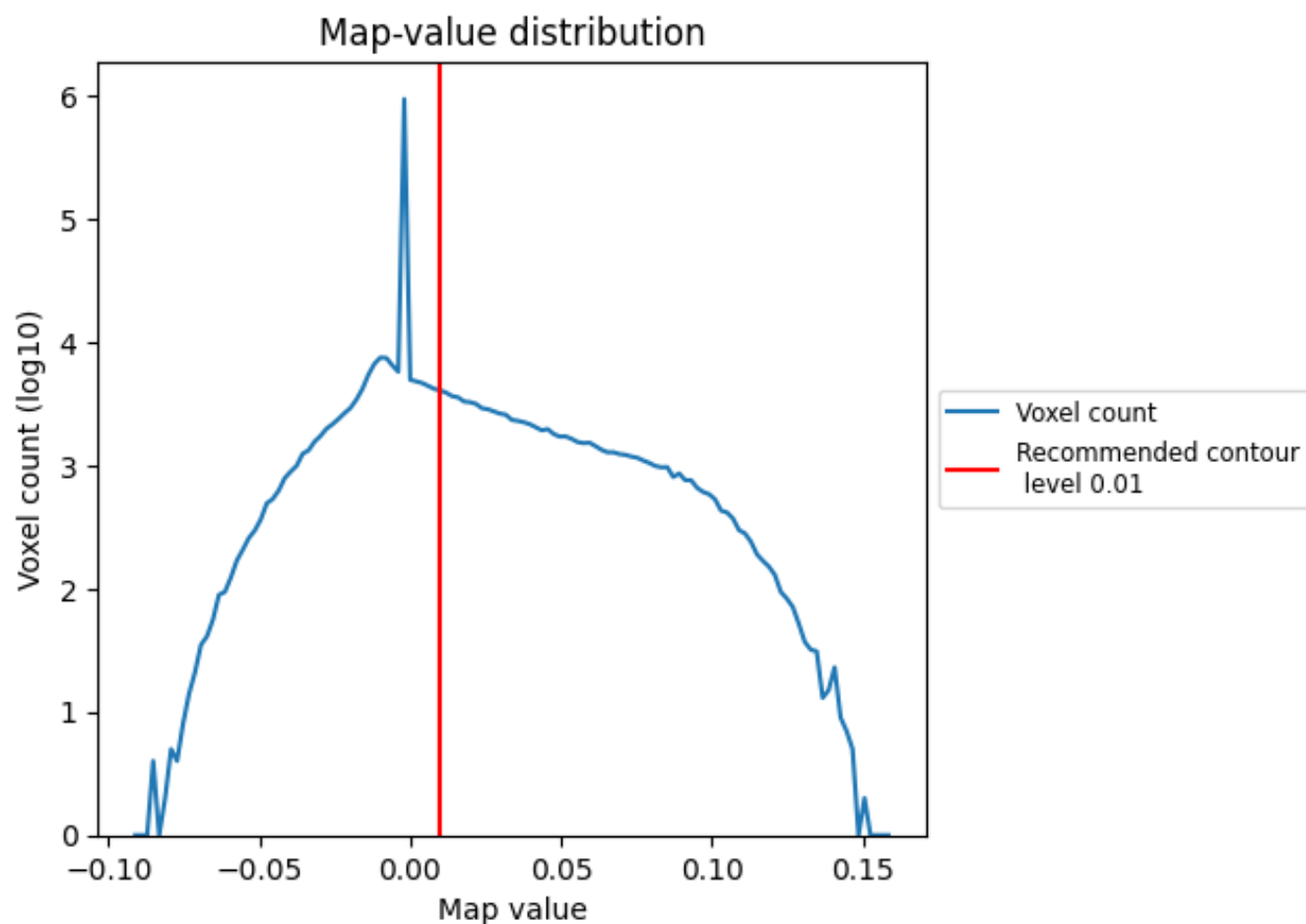
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

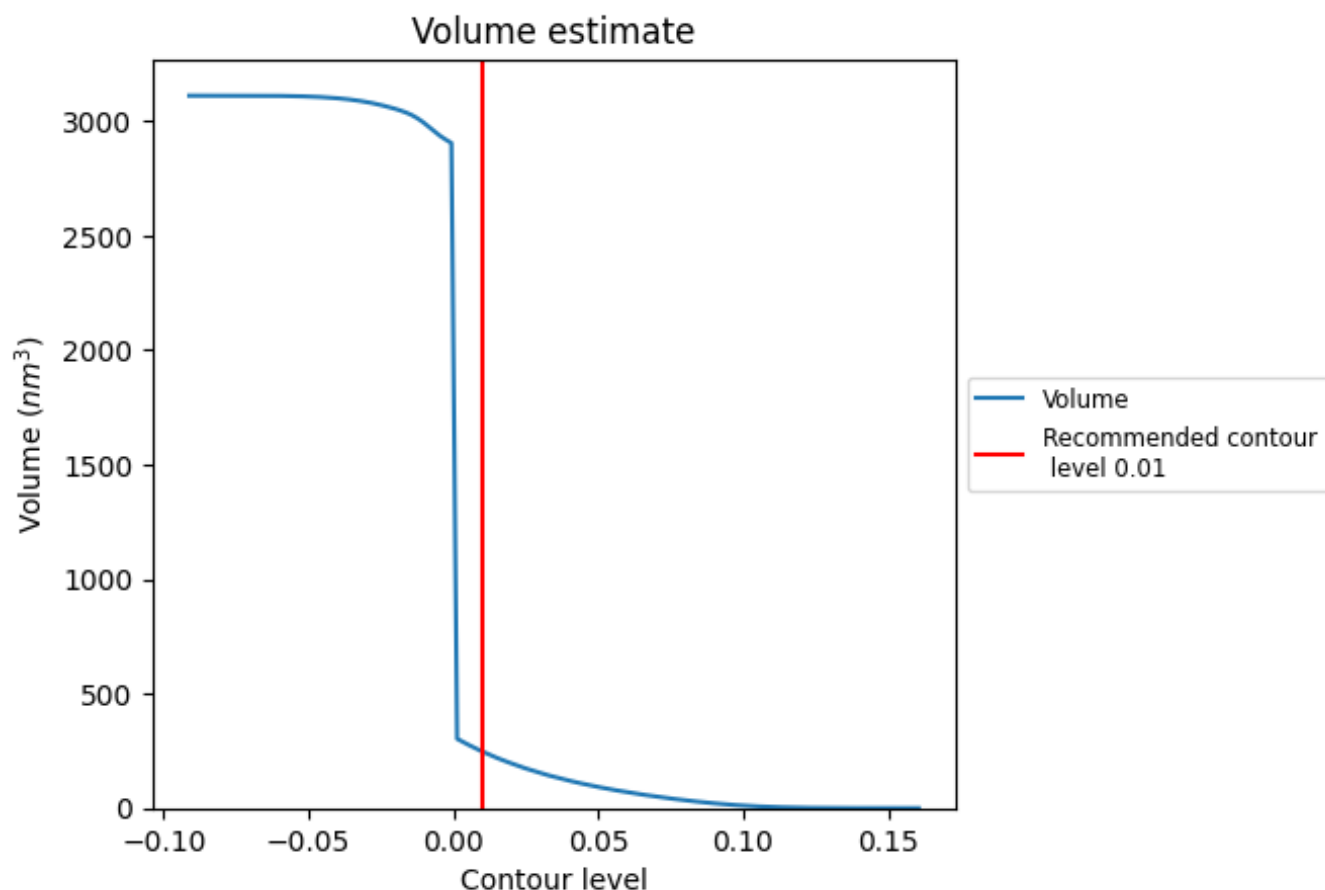
This section contains the results of statistical analysis of the map.

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 247 nm³; this corresponds to an approximate mass of 223 kDa.

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

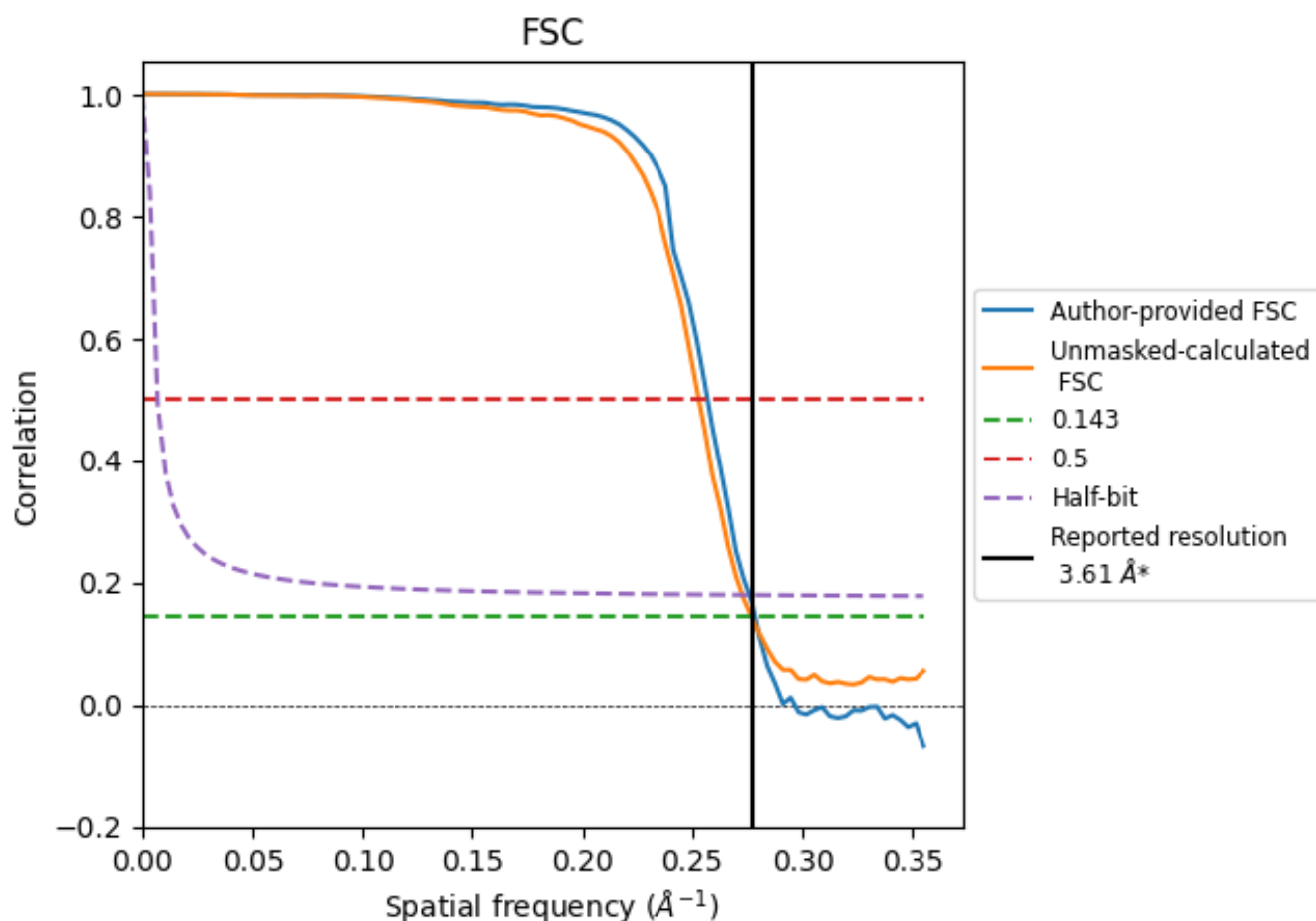
7.3 Rotationally averaged power spectrum [i](#)

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

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.277 Å⁻¹

8.2 Resolution estimates [i](#)

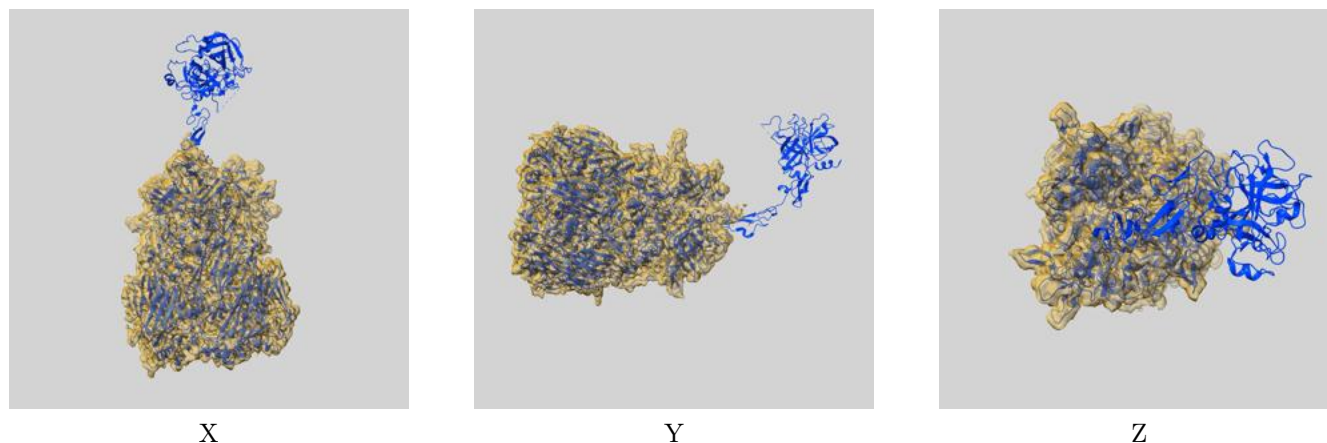
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.61	-	-
Author-provided FSC curve	3.59	3.89	3.62
Unmasked-calculated*	3.61	3.95	3.67

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

9 Map-model fit [i](#)

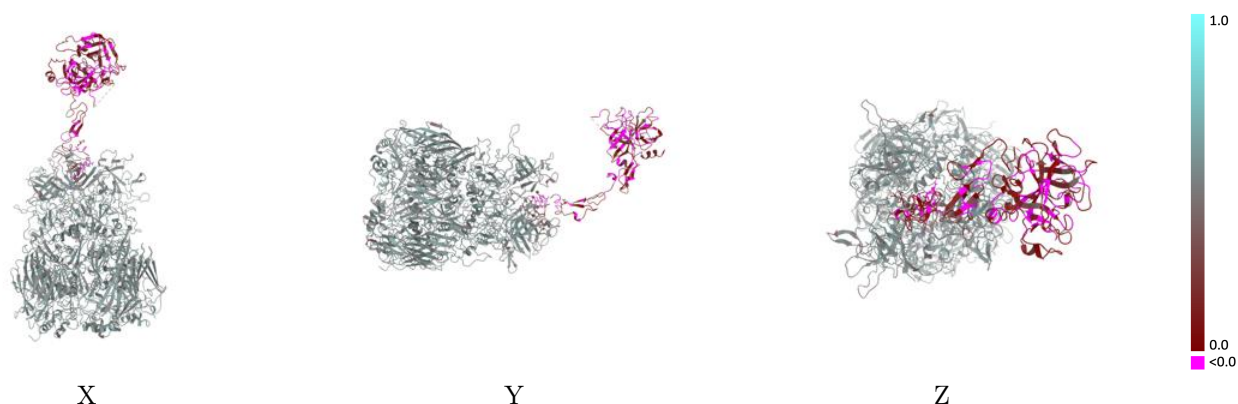
This section contains information regarding the fit between EMDB map EMD-45675 and PDB model 9CLI. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



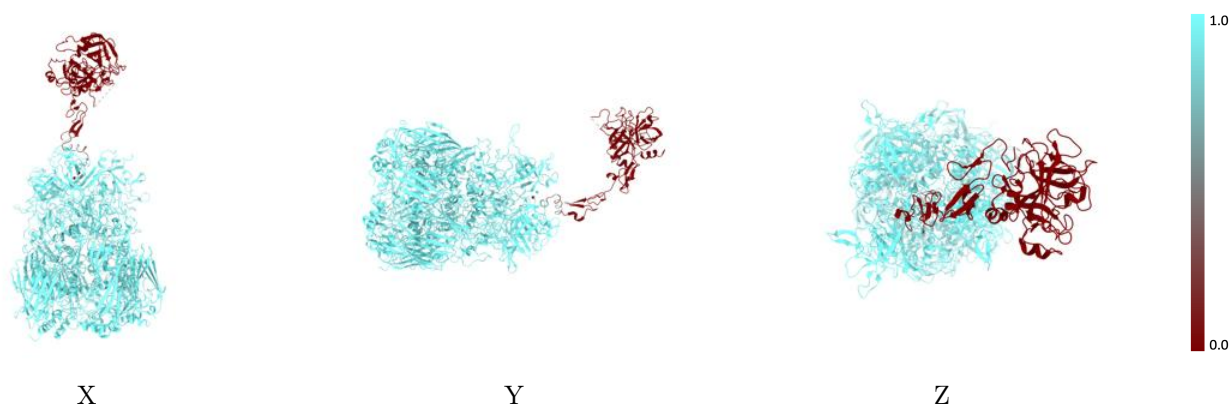
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



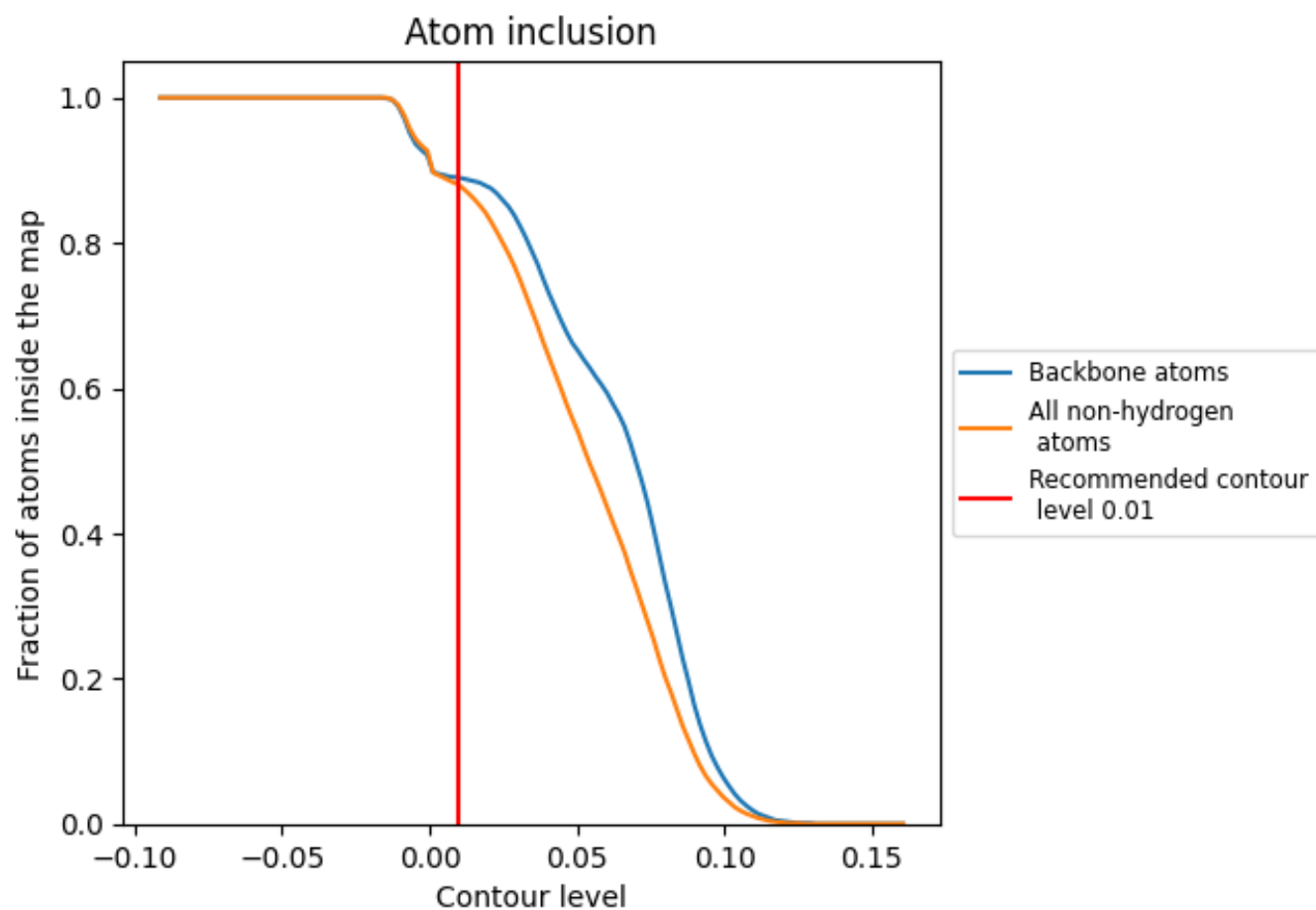
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8800	<div></div> 0.4740
J	<div></div> 0.9860	<div></div> 0.5240
K	<div></div> 0.9860	<div></div> 0.5260
L	<div></div> 0.9870	<div></div> 0.5280
Z	<div></div> 0.0970	<div></div> 0.0870

