WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Feb 4, 2024 – 02:48 PM EST

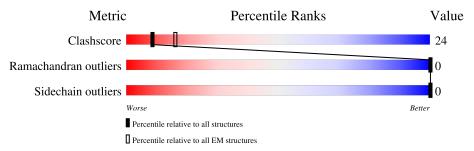|		
PDB ID	:	8CZD
EMDB ID	:	EMD-27095
Title	:	Cryo-EM structure of BCL10 R58Q filament
Authors	:	David, L.; Wu, H.
Deposited on	:	2022-05-24
Resolution	:	4.60 Å(reported)

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 4.60 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	Percentile Ranks	Value
Clashscore		24
Ramachandran outliers		0
Sidechain outliers		0

Worse .... *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	106	54% / 54% green, 46% yellow
1	B	106	42% / 59% green, 41% yellow
1	C	106	46% / 55% green, 45% yellow
1	D	106	53% / 57% green, 43% yellow
1	E	106	45% / 55% green, 45% yellow
1	F	106	42% / 54% green, 46% yellow
1	G	106	45% / 54% green, 46% yellow
1	H	106	39% / 51% green, 49% yellow

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Mol	Chain	Length	Quality of chain
1	I	106	45% / 56% / 44%
1	J	106	38% / 56% / 44%
1	K	106	45% / 55% / 45%
1	L	106	42% / 56% / 44%
1	M	106	40% / 56% / 44%
1	N	106	43% / 54% / 46%
1	O	106	41% / 53% / 47%
1	P	106	40% / 52% / 48%
1	Q	106	46% / 58% / 42%
1	R	106	44% / 60% / 40%
1	S	106	46% / 58% / 42%
1	T	106	46% / 59% / 41%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 17640 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 B-cell lymphoma/leukemia 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	106	Total 882	C 550	N 160	O 170	S 2	0	0
1	Q	106	Total 882	C 550	N 160	O 170	S 2	0	0
1	R	106	Total 882	C 550	N 160	O 170	S 2	0	0
1	S	106	Total 882	C 550	N 160	O 170	S 2	0	0
1	T	106	Total 882	C 550	N 160	O 170	S 2	0	0
1	A	106	Total 882	C 550	N 160	O 170	S 2	0	0
1	B	106	Total 882	C 550	N 160	O 170	S 2	0	0
1	D	106	Total 882	C 550	N 160	O 170	S 2	0	0
1	E	106	Total 882	C 550	N 160	O 170	S 2	0	0
1	F	106	Total 882	C 550	N 160	O 170	S 2	0	0
1	G	106	Total 882	C 550	N 160	O 170	S 2	0	0
1	H	106	Total 882	C 550	N 160	O 170	S 2	0	0
1	I	106	Total 882	C 550	N 160	O 170	S 2	0	0
1	J	106	Total 882	C 550	N 160	O 170	S 2	0	0
1	K	106	Total 882	C 550	N 160	O 170	S 2	0	0
1	L	106	Total 882	C 550	N 160	O 170	S 2	0	0
1	M	106	Total 882	C 550	N 160	O 170	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	106	Total 882	C 550	N 160	O 170	S 2	0	0
1	O	106	Total 882	C 550	N 160	O 170	S 2	0	0
1	P	106	Total 882	C 550	N 160	O 170	S 2	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	58	GLN	ARG	engineered mutation	UNP O95999
Q	58	GLN	ARG	engineered mutation	UNP O95999
R	58	GLN	ARG	engineered mutation	UNP O95999
S	58	GLN	ARG	engineered mutation	UNP O95999
T	58	GLN	ARG	engineered mutation	UNP O95999
A	58	GLN	ARG	engineered mutation	UNP O95999
B	58	GLN	ARG	engineered mutation	UNP O95999
D	58	GLN	ARG	engineered mutation	UNP O95999
E	58	GLN	ARG	engineered mutation	UNP O95999
F	58	GLN	ARG	engineered mutation	UNP O95999
G	58	GLN	ARG	engineered mutation	UNP O95999
H	58	GLN	ARG	engineered mutation	UNP O95999
I	58	GLN	ARG	engineered mutation	UNP O95999
J	58	GLN	ARG	engineered mutation	UNP O95999
K	58	GLN	ARG	engineered mutation	UNP O95999
L	58	GLN	ARG	engineered mutation	UNP O95999
M	58	GLN	ARG	engineered mutation	UNP O95999
N	58	GLN	ARG	engineered mutation	UNP O95999
O	58	GLN	ARG	engineered mutation	UNP O95999
P	58	GLN	ARG	engineered mutation	UNP O95999

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: B-cell lymphoma/leukemia 10

Chain C:

- Molecule 1: B-cell lymphoma/leukemia 10

Chain Q:

- Molecule 1: B-cell lymphoma/leukemia 10

Chain R:

- Molecule 1: B-cell lymphoma/leukemia 10

Chain S:

• Molecule 1: B-cell lymphoma/leukemia 10

Chain T:

• Molecule 1: B-cell lymphoma/leukemia 10

Chain A:

• Molecule 1: B-cell lymphoma/leukemia 10

Chain B:

• Molecule 1: B-cell lymphoma/leukemia 10

Chain D:

E74 N75 P76 L79 L82 V83 E84 S85 I86 R87 R88 E89 K90 T91 Q92 N93 F94 L95 I96 Q97 K98 I99 T100 D101 L104 K105 L106 R107 N108 I109 K110 L111 E112 H113 L114 K115

• Molecule 1: B-cell lymphoma/leukemia 10

Chain E:

45%

55% 45%

E10 E11 D12 L13 V16 L21 E22 N23 L24 R25 L28 C29 E30 K31 I32 I33 A34 E35 R36 H37 F38 D39 H40 L41 R42 A43 K44 K45 I46 L47 S48 R49 E50 D51 E54 I55 S56 C57 Q58 T59 S60 S61 R62 K63 R64 A65 L69 D70 Y71 L72 Q73 E74 L79

L82 V83 E84 S85 I86 R87 R88 E89 K90 T91 Q92 N93 F94 L95 I96 Q97 K98 I99 T100 D101 E102 V103 L104 K105 L106 R107 N108 I109 K110 L111 E112 H113 L114 K115

• Molecule 1: B-cell lymphoma/leukemia 10

Chain F:

42%

54% 46%

E10 E11 D12 L13 T14 E15 V16 A20 L21 L24 R25 L28 C29 E30 K31 I32 I33 A34 E35 R36 H37 F38 D39 H40 L41 R42 A43 K44 K45 I46 L47 S48 R49 E50 D51 T52 E53 E54 I55 S56 C57 Q58 T59 S60 S61 R64 A65 G66 K67 L68 L69 D70 Y71 L72 Q73 E74

N75 P76 D80 T81 L82 V83 E84 S85 I86 R87 R88 E89 K90 T91 Q92 N93 F94 L95 I96 Q97 K98 I99 T100 V103 L104 K105 L106 R107 N108 I109 K110 L111 E112 H113 L114 K115

• Molecule 1: B-cell lymphoma/leukemia 10

Chain G:

45%

54% 46%

E10 E11 D12 L13 T14 E15 V16 D19 A20 L21 E22 N23 L24 R25 L28 C29 E30 K31 I32 I33 A34 E35 R36 H37 F38 D39 H40 L41 R42 A43 K44 K45 I46 L47 S48 R49 E50 D51 T52 E53 E54 I55 S56 C57 Q58 T59 S60 S61 R62 K63 R64 A65 L69 D70 Y71 L72 Q73

E74 N75 P76 V83 E84 S85 I86 R87 R88 E89 K90 T91 Q92 N93 F94 L95 I96 Q97 K98 I99 T100 L104 K105 L106 R107 N108 I109 K110 H113 L114 K115

• Molecule 1: B-cell lymphoma/leukemia 10

Chain H:

39%

51% 49%

E10 E11 D12 L13 T14 E15 V16 K17 K18 D19 A20 L21 E22 N23 L24 R25 L28 K31 I32 I33 A34 E35 R36 H37 F38 D39 H40 L41 R42 A43 K44 K45 I46 L47 S48 R49 E50 D51 E54 I55 S56 C57 Q58 T59 S60 S61 R64 A65 L69 D70 Y71 L72 Q73 E74 N75

P76 E84 S85 I86 R87 R88 E89 K90 T91 Q92 N93 F94 L95 I96 Q97 K98 I99 T100 V103 L104 K105 L106 R107 N108 I109 E112 H113 L114 K115

• Molecule 1: B-cell lymphoma/leukemia 10

Chain I:

- Molecule 1: B-cell lymphoma/leukemia 10

Chain J:

- Molecule 1: B-cell lymphoma/leukemia 10

Chain K:

- Molecule 1: B-cell lymphoma/leukemia 10

Chain L:

- Molecule 1: B-cell lymphoma/leukemia 10

Chain M:

L72 Q73 E74 N75 E84 S85 I86 R87 R88 E89 K90 T91 Q92 N93 F94 L95 I96 Q97 K98 I99 T100 L104 R107 N108 I109 K110 L111 E112 H113 L114 K115

• Molecule 1: B-cell lymphoma/leukemia 10

Chain N:

43%

54% 46%

E10 E11 D12 L13 T14 E15 V16 K17 L21 E22 N23 L24 R25 L28 C29 E30 K31 I32 I33 A34 E35 R36 H37 F38 D39 H40 L41 R42 A43 K44 K45 I46 L47 S48 R49 E50 D51 T52 E53 E54 I55 S56 C57 Q58 T59 S60 S61 R64 A65 L69 D70 Y71 L72 Q73 E74

E84 S85 I86 R87 R88 E89 K90 T91 Q92 N93 F94 L95 I96 Q97 K98 I99 T100 V103 L104 K105 L106 R107 N108 I109 K110 L111 E112 H113 L114 K115

• Molecule 1: B-cell lymphoma/leukemia 10

Chain O:

41%

53% 47%

E10 E11 D12 L13 T14 E15 V16 D19 A20 L21 E22 N23 L24 R25 L28 C29 E30 K31 I32 I33 A34 E35 R36 H37 F38 D39 H40 L41 R42 A43 K44 K45 I46 L47 S48 R49 E50 D51 T52 E53 E54 I55 S56 C57 Q58 T59 S60 S61 R62 K63 R64 A65 G66 L69 D70 Y71 L72

Q73 E74 N75 L82 V83 E84 S85 I86 R87 R88 E89 K90 T91 Q92 N93 F94 L95 I96 Q97 K98 I99 T100 D101 L104 K105 L106 R107 N108 I109 K110 L111 E112 H113 L114 K115

• Molecule 1: B-cell lymphoma/leukemia 10

Chain P:

40%

52% 48%

E10 E11 D12 L13 T14 E15 V16 D19 A20 L21 E22 N23 L24 R25 L28 K31 I32 I33 A34 E35 R36 H37 F38 D39 H40 L41 R42 A43 K44 K45 I46 L47 S48 R49 E50 D51 T52 E53 E54 I55 S56 C57 Q58 T59 S60 S61 R62 K63 R64 A65 L69 D70 Y71 L72 Q73 E74

N75 P76 L82 V83 E84 S85 I86 R87 R88 E89 K90 T91 Q92 N93 F94 L95 I96 Q97 K98 I99 T100 L104 K105 L106 R107 N108 I109 K110 L111 E112 H113 L114 K115

4　Experimental information　ⓘ

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-100.8°, rise=5 Å, axial sym=C1	Depositor
Number of segments used	30000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	38	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.045	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	236.64, 236.64, 236.64	wwPDB
Map dimensions	272, 272, 272	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	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	0.30	0/889	0.49	0/1186
1	B	0.30	0/889	0.49	0/1186
1	C	0.30	0/889	0.49	0/1186
1	D	0.29	0/889	0.49	0/1186
1	E	0.30	0/889	0.49	0/1186
1	F	0.30	0/889	0.49	0/1186
1	G	0.29	0/889	0.49	0/1186
1	H	0.29	0/889	0.49	0/1186
1	I	0.30	0/889	0.49	0/1186
1	J	0.30	0/889	0.49	0/1186
1	K	0.29	0/889	0.49	0/1186
1	L	0.30	0/889	0.49	0/1186
1	M	0.30	0/889	0.49	0/1186
1	N	0.29	0/889	0.49	0/1186
1	O	0.29	0/889	0.49	0/1186
1	P	0.30	0/889	0.49	0/1186
1	Q	0.30	0/889	0.49	0/1186
1	R	0.29	0/889	0.49	0/1186
1	S	0.29	0/889	0.49	0/1186
1	T	0.30	0/889	0.49	0/1186
All	All	0.30	0/17780	0.49	0/23720

There are no bond length outliers.

There are no bond angle outliers.

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	882	0	920	42	0
1	B	882	0	920	42	0
1	C	882	0	920	42	0
1	D	882	0	920	53	0
1	E	882	0	920	61	0
1	F	882	0	920	62	0
1	G	882	0	920	56	0
1	H	882	0	920	69	0
1	I	882	0	920	47	0
1	J	882	0	920	59	0
1	K	882	0	920	56	0
1	L	882	0	920	53	0
1	M	882	0	920	46	0
1	N	882	0	920	44	0
1	O	882	0	920	53	0
1	P	882	0	920	59	0
1	Q	882	0	920	41	0
1	R	882	0	920	40	0
1	S	882	0	920	46	0
1	T	882	0	920	46	0
All	All	17640	0	18400	858	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 24.

The worst 5 of 858 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:25:ARG:HH11	1:H:44:LYS:HD2	1.05	1.14
1:G:25:ARG:HH11	1:J:44:LYS:HD2	1.29	0.97
1:F:49:ARG:H	1:J:90:LYS:HE3	1.30	0.92
1:D:25:ARG:HH11	1:G:44:LYS:HD2	1.36	0.90
1:E:25:ARG:NH1	1:H:44:LYS:HD2	1.87	0.88

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	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	B	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	C	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	D	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	E	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	F	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	G	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	H	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	I	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	J	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	K	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	L	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	M	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	N	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	O	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	P	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	Q	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	R	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	S	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
1	T	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
All	All	2080/2120 (98%)	1900 (91%)	180 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	100/100 (100%)	100 (100%)	0	100	100
1	B	100/100 (100%)	100 (100%)	0	100	100
1	C	100/100 (100%)	100 (100%)	0	100	100
1	D	100/100 (100%)	100 (100%)	0	100	100
1	E	100/100 (100%)	100 (100%)	0	100	100
1	F	100/100 (100%)	100 (100%)	0	100	100
1	G	100/100 (100%)	100 (100%)	0	100	100
1	H	100/100 (100%)	100 (100%)	0	100	100
1	I	100/100 (100%)	100 (100%)	0	100	100
1	J	100/100 (100%)	100 (100%)	0	100	100
1	K	100/100 (100%)	100 (100%)	0	100	100
1	L	100/100 (100%)	100 (100%)	0	100	100
1	M	100/100 (100%)	100 (100%)	0	100	100
1	N	100/100 (100%)	100 (100%)	0	100	100
1	O	100/100 (100%)	100 (100%)	0	100	100
1	P	100/100 (100%)	100 (100%)	0	100	100
1	Q	100/100 (100%)	100 (100%)	0	100	100
1	R	100/100 (100%)	100 (100%)	0	100	100
1	S	100/100 (100%)	100 (100%)	0	100	100
1	T	100/100 (100%)	100 (100%)	0	100	100
All	All	2000/2000 (100%)	2000 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

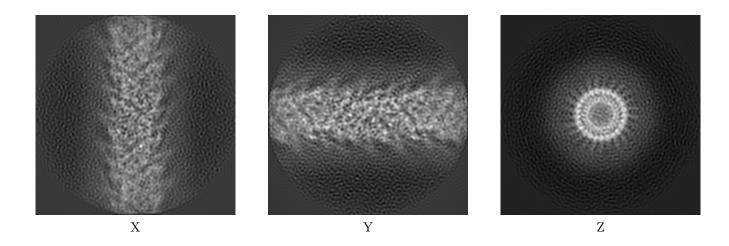## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-27095. These allow visual inspection of the internal detail of the map and identification of artifacts.
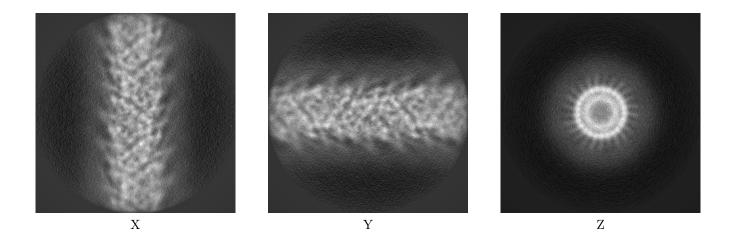
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

X   Y   Z

6.1.2 Raw map

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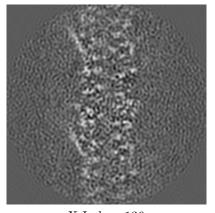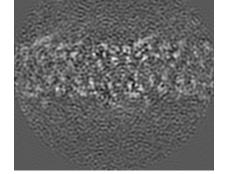
The images above show the map projected in three orthogonal directions.

6.2   Central slices   ⓘ
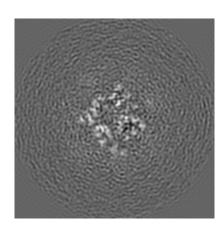
6.2.1   Primary map
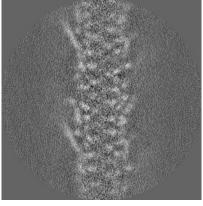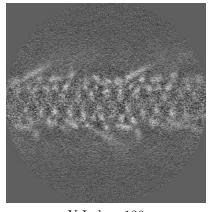
X Index: 136   Y Index: 136   Z Index: 136
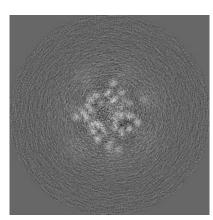
6.2.2   Raw map
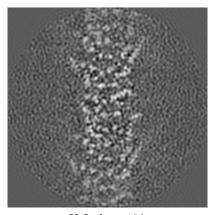

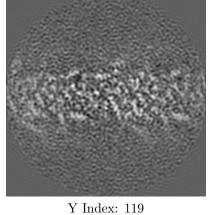X Index: 136   Y Index: 136   Z Index: 136

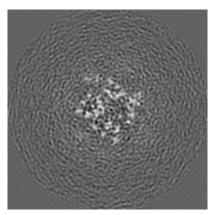The images above show central slices of the map in three orthogonal directions.

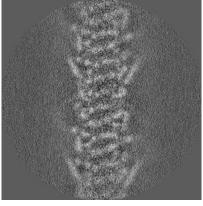## 6.3   Largest variance slices ⓘ

6.3.1   Primary map

<div align="center">

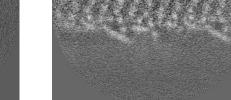X Index: 122   Y Index: 119   Z Index: 126
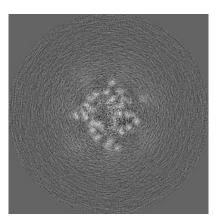
</div>

6.3.2   Raw map

<div align="center">

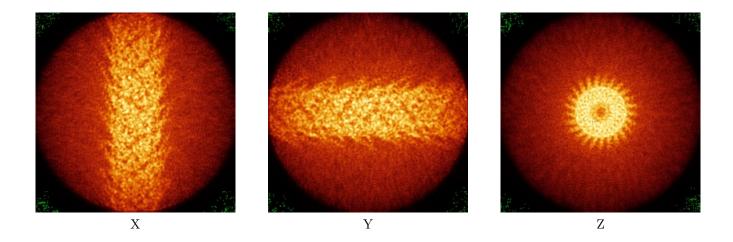X Index: 128   Y Index: 143   Z Index: 135

</div>

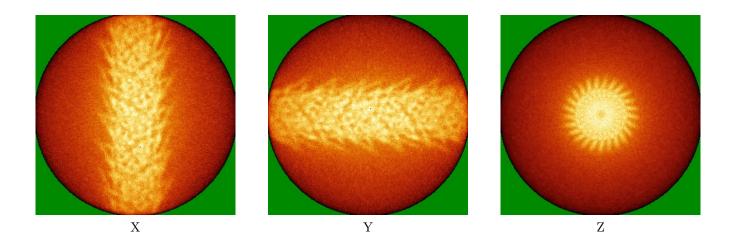The images above show the largest variance slices of the map in three orthogonal directions.

6.4   Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1   Primary map

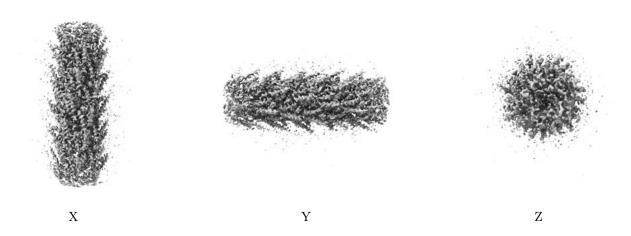| X | Y | Z |

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.
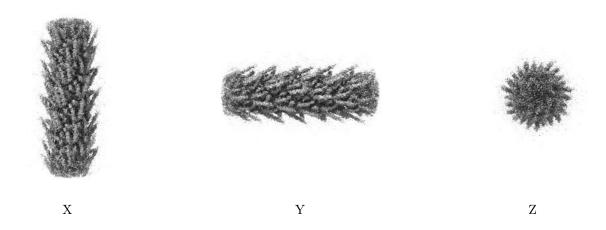
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X	Y	Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. 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.
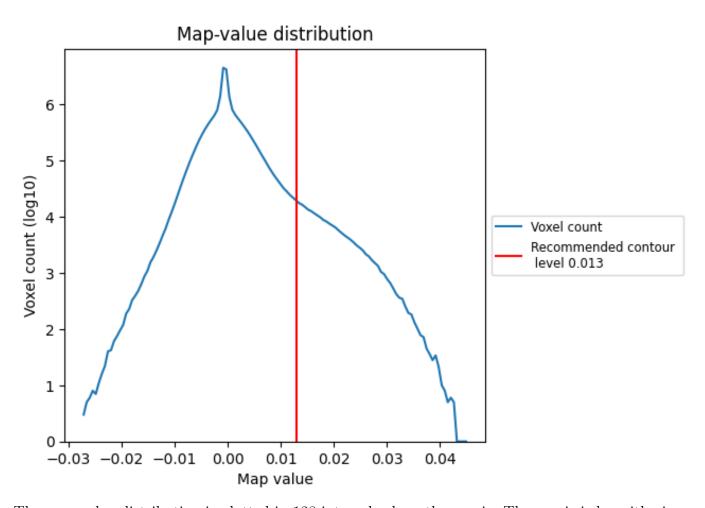
6.6 Mask visualisation (i)

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

7 Map analysis ⓘ

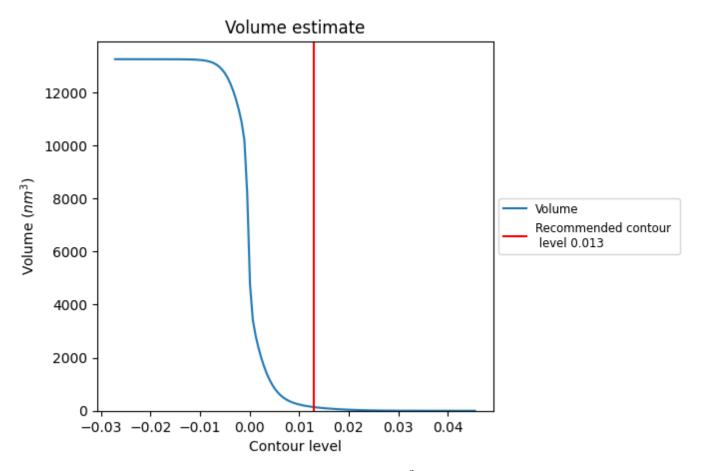This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

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.
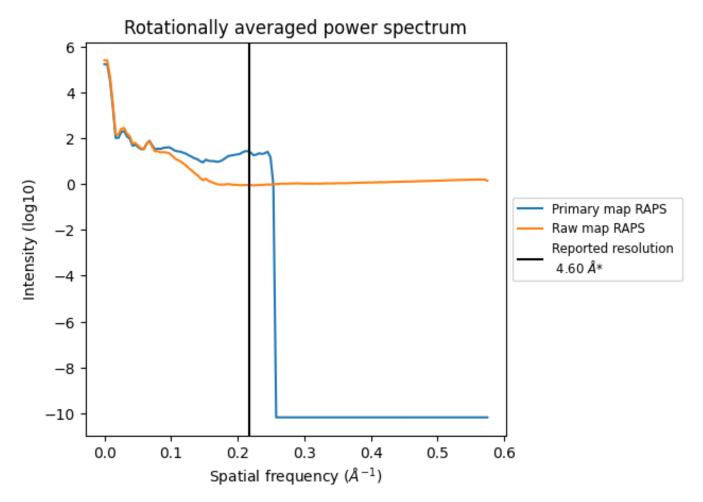
7.2　Volume estimate ⓘ

The volume at the recommended contour level is 139 nm^3; this corresponds to an approximate mass of 125 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.
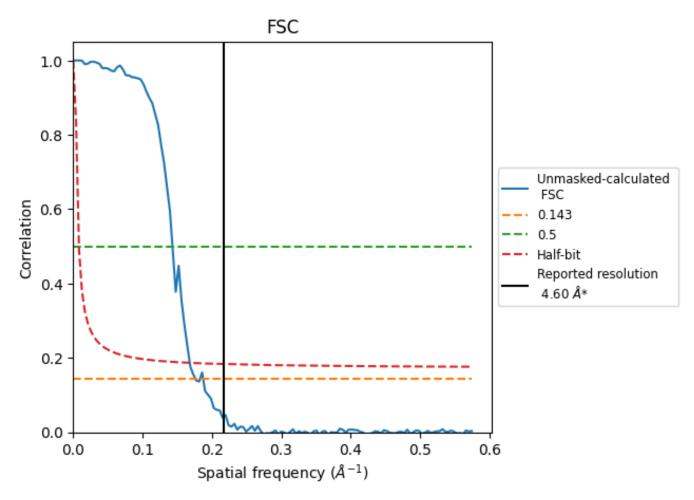
7.3 Rotationally averaged power spectrum ⓘ

*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8   Fourier-Shell correlation ⓘ

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 ⓘ

*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8.2   Resolution estimates (i)

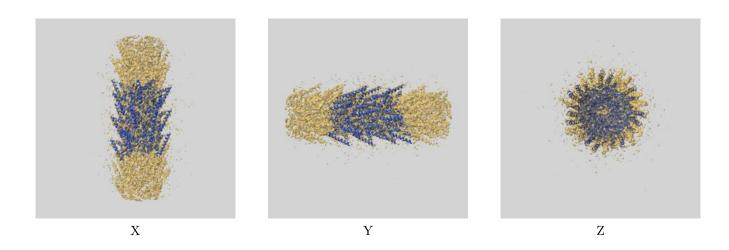| Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.67	6.99	5.95

*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 5.67 differs from the reported value 4.6 by more than 10 %

9　Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-27095 and PDB model 8CZD. Per-residue inclusion information can be found in section 3 on page 6.
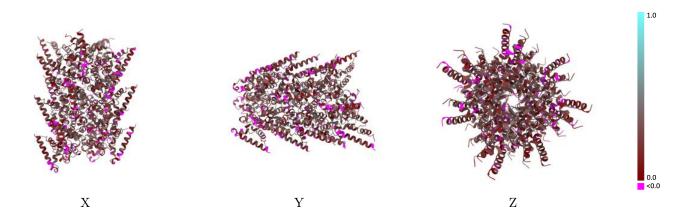
9.1　Map-model overlay ⓘ

X　　　　　　　　　　Y　　　　　　　　　　Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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.
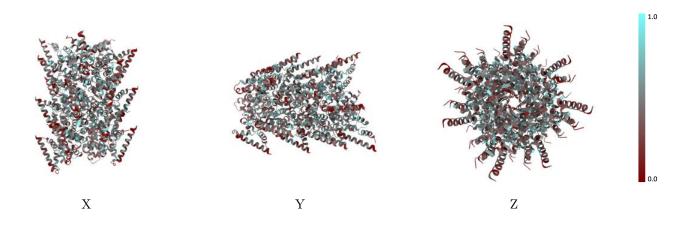
9.2   Q-score mapped to coordinate model ⓘ

The images above show the model with each residue coloured according 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.
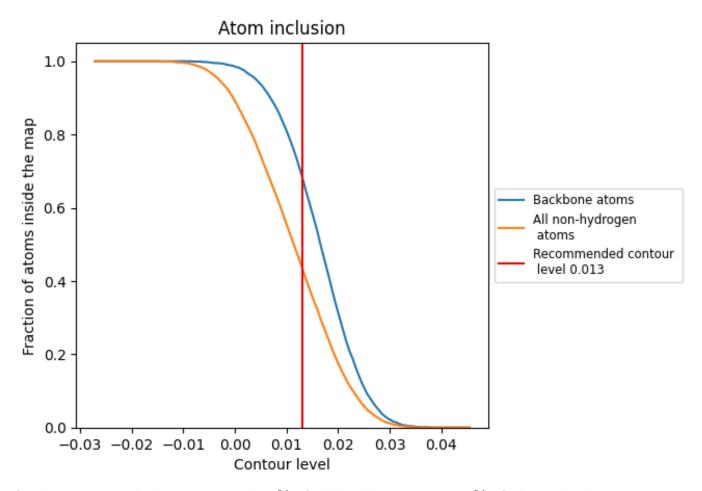
9.3   Atom inclusion mapped to coordinate model ⓘ

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 (0.013).

9.4   Atom inclusion ⓘ

Atom inclusion

At the recommended contour level, 69% of all backbone atoms, 44% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4380	0.2240
A	0.4090	0.2000
B	0.4190	0.2220
C	0.4180	0.2300
D	0.4140	0.2070
E	0.4180	0.2230
F	0.4430	0.2260
G	0.4490	0.2190
H	0.4420	0.2390
I	0.4390	0.2230
J	0.4610	0.2350
K	0.4620	0.2290
L	0.4460	0.2400
M	0.4350	0.2280
N	0.4490	0.2170
O	0.4510	0.2300
P	0.4570	0.2440
Q	0.4220	0.2100
R	0.4440	0.2150
S	0.4420	0.2250
T	0.4320	0.2210

1.0

0.0
<0.0