W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

Nov 23, 2022 – 04:48 AM JST

PDB ID	:	7FEP
EMDB ID	:	EMD-31559
Title	:	Cryo-EM structure of BsClpP-ADEP1 complex at pH 6.5
Authors	:	Kim, L.; Lee, B.-G.; Kim, M.K.; Kwon, D.H.; Kim, H.; Brotz-Oesterhelt, H.; Roh, S.-H.; Song, H.K.
Deposited on	:	2021-07-21
Resolution	:	3.10 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 3.10 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.
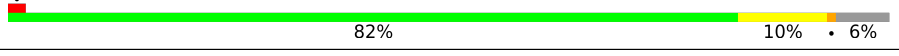
Metric	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0.5%
Sidechain outliers		3.2%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
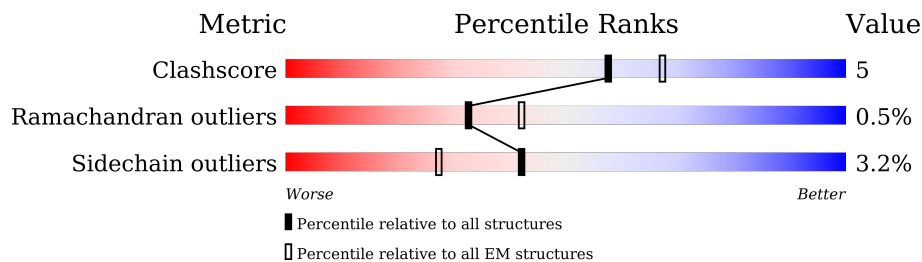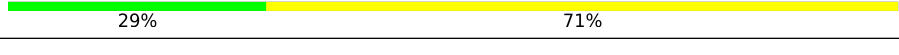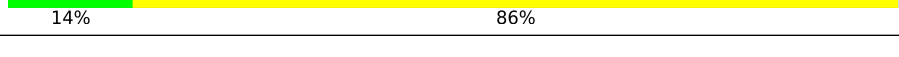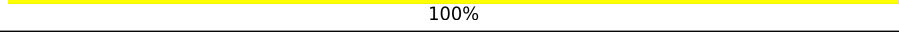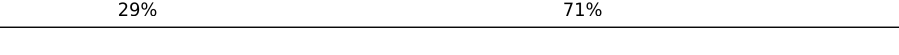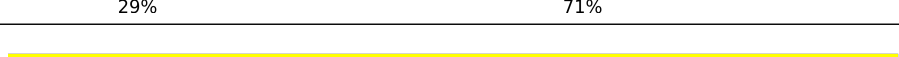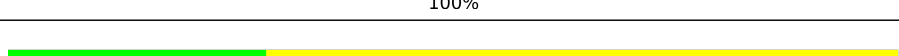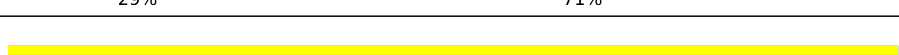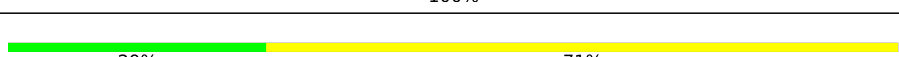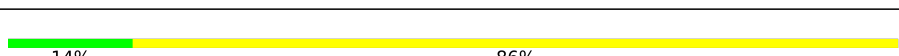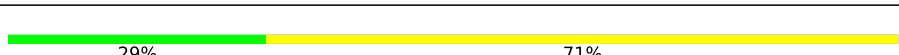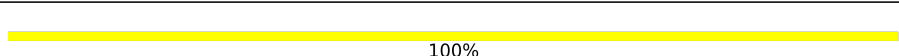
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	202	81% 11% · 6%
1	B	202	82% 10% · 6%
1	C	202	82% 10% · 6%
1	D	202	82% 10% · 6%
1	E	202	82% 10% · 6%
1	F	202	82% 10% · 6%
1	G	202	82% 9% · 6%
1	H	202	82% 9% · 6%

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Mol	Chain	Length	Quality of chain
1	I	202	80% 12% · 6%
1	J	202	80% 11% · 6%
1	K	202	81% 11% · 6%
1	L	202	82% 10% · 6%
1	M	202	83% 9% · 6%
1	N	202	82% 10% · 6%
2	O	7	29% 71%
2	P	7	14% 86%
2	Q	7	100%
2	R	7	29% 71%
2	S	7	29% 71%
2	T	7	100%
2	U	7	29% 71%
2	V	7	100%
2	W	7	29% 71%
2	X	7	14% 86%
2	Y	7	29% 71%
2	Z	7	100%
2	a	7	43% 57%
2	b	7	43% 57%

2   Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 40381 atoms, of which 19353 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	189	Total	C	H	N	O	S	0	0
			2815	916	1365	246	281	7		
1	B	189	Total	C	H	N	O	S	0	0
			2840	916	1390	246	281	7		
1	C	189	Total	C	H	N	O	S	0	0
			2821	916	1371	246	281	7		
1	D	189	Total	C	H	N	O	S	0	0
			2840	916	1390	246	281	7		
1	E	189	Total	C	H	N	O	S	0	0
			2849	916	1399	246	281	7		
1	F	189	Total	C	H	N	O	S	0	0
			2840	916	1390	246	281	7		
1	G	189	Total	C	H	N	O	S	0	0
			2831	916	1381	246	281	7		
1	I	189	Total	C	H	N	O	S	0	0
			2840	916	1390	246	281	7		
1	J	189	Total	C	H	N	O	S	0	0
			2840	916	1390	246	281	7		
1	K	189	Total	C	H	N	O	S	0	0
			2840	916	1390	246	281	7		
1	L	189	Total	C	H	N	O	S	0	0
			2822	916	1372	246	281	7		
1	M	189	Total	C	H	N	O	S	0	0
			2822	916	1372	246	281	7		
1	N	189	Total	C	H	N	O	S	0	0
			2827	916	1377	246	281	7		
1	H	189	Total	C	H	N	O	S	0	0
			2826	916	1376	246	281	7		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	HIS	-	expression tag	UNP P80244
A	198	HIS	-	expression tag	UNP P80244

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Chain	Residue	Modelled	Actual	Comment	Reference
A	199	HIS	-	expression tag	UNP P80244
A	200	HIS	-	expression tag	UNP P80244
A	201	HIS	-	expression tag	UNP P80244
A	202	HIS	-	expression tag	UNP P80244
B	197	HIS	-	expression tag	UNP P80244
B	198	HIS	-	expression tag	UNP P80244
B	199	HIS	-	expression tag	UNP P80244
B	200	HIS	-	expression tag	UNP P80244
B	201	HIS	-	expression tag	UNP P80244
B	202	HIS	-	expression tag	UNP P80244
C	197	HIS	-	expression tag	UNP P80244
C	198	HIS	-	expression tag	UNP P80244
C	199	HIS	-	expression tag	UNP P80244
C	200	HIS	-	expression tag	UNP P80244
C	201	HIS	-	expression tag	UNP P80244
C	202	HIS	-	expression tag	UNP P80244
D	197	HIS	-	expression tag	UNP P80244
D	198	HIS	-	expression tag	UNP P80244
D	199	HIS	-	expression tag	UNP P80244
D	200	HIS	-	expression tag	UNP P80244
D	201	HIS	-	expression tag	UNP P80244
D	202	HIS	-	expression tag	UNP P80244
E	197	HIS	-	expression tag	UNP P80244
E	198	HIS	-	expression tag	UNP P80244
E	199	HIS	-	expression tag	UNP P80244
E	200	HIS	-	expression tag	UNP P80244
E	201	HIS	-	expression tag	UNP P80244
E	202	HIS	-	expression tag	UNP P80244
F	197	HIS	-	expression tag	UNP P80244
F	198	HIS	-	expression tag	UNP P80244
F	199	HIS	-	expression tag	UNP P80244
F	200	HIS	-	expression tag	UNP P80244
F	201	HIS	-	expression tag	UNP P80244
F	202	HIS	-	expression tag	UNP P80244
G	197	HIS	-	expression tag	UNP P80244
G	198	HIS	-	expression tag	UNP P80244
G	199	HIS	-	expression tag	UNP P80244
G	200	HIS	-	expression tag	UNP P80244
G	201	HIS	-	expression tag	UNP P80244
G	202	HIS	-	expression tag	UNP P80244
I	197	HIS	-	expression tag	UNP P80244
I	198	HIS	-	expression tag	UNP P80244

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Chain	Residue	Modelled	Actual	Comment	Reference
I	199	HIS	-	expression tag	UNP P80244
I	200	HIS	-	expression tag	UNP P80244
I	201	HIS	-	expression tag	UNP P80244
I	202	HIS	-	expression tag	UNP P80244
J	197	HIS	-	expression tag	UNP P80244
J	198	HIS	-	expression tag	UNP P80244
J	199	HIS	-	expression tag	UNP P80244
J	200	HIS	-	expression tag	UNP P80244
J	201	HIS	-	expression tag	UNP P80244
J	202	HIS	-	expression tag	UNP P80244
K	197	HIS	-	expression tag	UNP P80244
K	198	HIS	-	expression tag	UNP P80244
K	199	HIS	-	expression tag	UNP P80244
K	200	HIS	-	expression tag	UNP P80244
K	201	HIS	-	expression tag	UNP P80244
K	202	HIS	-	expression tag	UNP P80244
L	197	HIS	-	expression tag	UNP P80244
L	198	HIS	-	expression tag	UNP P80244
L	199	HIS	-	expression tag	UNP P80244
L	200	HIS	-	expression tag	UNP P80244
L	201	HIS	-	expression tag	UNP P80244
L	202	HIS	-	expression tag	UNP P80244
M	197	HIS	-	expression tag	UNP P80244
M	198	HIS	-	expression tag	UNP P80244
M	199	HIS	-	expression tag	UNP P80244
M	200	HIS	-	expression tag	UNP P80244
M	201	HIS	-	expression tag	UNP P80244
M	202	HIS	-	expression tag	UNP P80244
N	197	HIS	-	expression tag	UNP P80244
N	198	HIS	-	expression tag	UNP P80244
N	199	HIS	-	expression tag	UNP P80244
N	200	HIS	-	expression tag	UNP P80244
N	201	HIS	-	expression tag	UNP P80244
N	202	HIS	-	expression tag	UNP P80244
H	197	HIS	-	expression tag	UNP P80244
H	198	HIS	-	expression tag	UNP P80244
H	199	HIS	-	expression tag	UNP P80244
H	200	HIS	-	expression tag	UNP P80244
H	201	HIS	-	expression tag	UNP P80244
H	202	HIS	-	expression tag	UNP P80244

- Molecule 2 is a protein called ADEP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	7	Total 52	C 38	N 6	O 8	0	0
2	P	7	Total 52	C 38	N 6	O 8	0	0
2	Q	7	Total 52	C 38	N 6	O 8	0	0
2	R	7	Total 52	C 38	N 6	O 8	0	0
2	S	7	Total 52	C 38	N 6	O 8	0	0
2	T	7	Total 52	C 38	N 6	O 8	0	0
2	U	7	Total 52	C 38	N 6	O 8	0	0
2	V	7	Total 52	C 38	N 6	O 8	0	0
2	W	7	Total 52	C 38	N 6	O 8	0	0
2	X	7	Total 52	C 38	N 6	O 8	0	0
2	Y	7	Total 52	C 38	N 6	O 8	0	0
2	Z	7	Total 52	C 38	N 6	O 8	0	0
2	a	7	Total 52	C 38	N 6	O 8	0	0
2	b	7	Total 52	C 38	N 6	O 8	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:
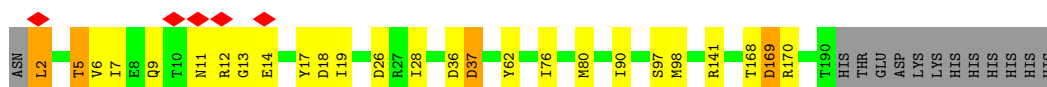
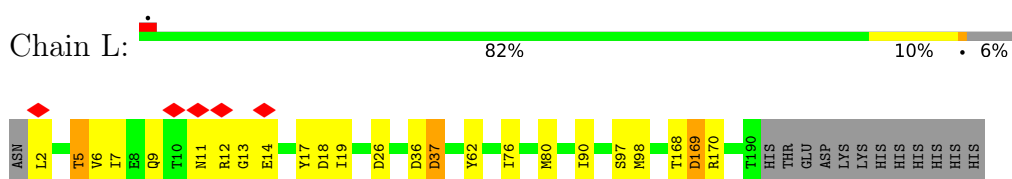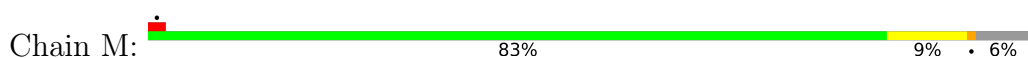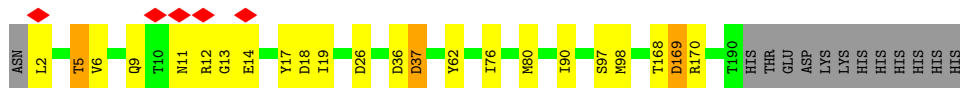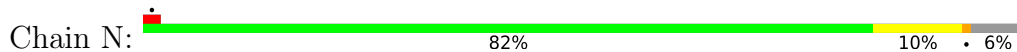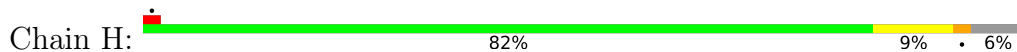• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:
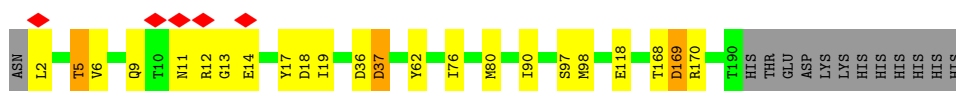
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:

• Molecule 1: ATP-dependent Clp protease proteolytic subunit
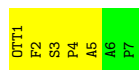
Chain E:

• Molecule 1: ATP-dependent Clp protease proteolytic subunit
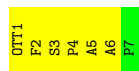
Chain F:

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:

• Molecule 1: ATP-dependent Clp protease proteolytic subunit
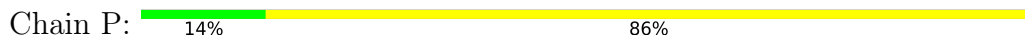
Chain I:

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:

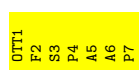• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H:

• Molecule 2: ADEP1

Chain O:

• Molecule 2: ADEP1

Chain P:

• Molecule 2: ADEP1

Chain Q:

• Molecule 2: ADEP1
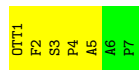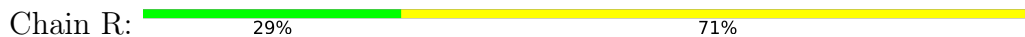
Chain R:

• Molecule 2: ADEP1

Chain S:

• Molecule 2: ADEP1

Chain T: 100%

OTT1 F2 S3 P4 A5 A6 P7

• Molecule 2: ADEP1

Chain U: 29% 71%
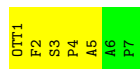
OTT1 F2 S3 P4 A5 A6 P7

• Molecule 2: ADEP1

Chain V: 100%
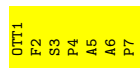
OTT1 F2 S3 P4 A5 A6 P7

• Molecule 2: ADEP1

Chain W: 29% 71%
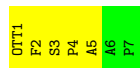
OTT1 F2 S3 P4 A5 A6 P7

• Molecule 2: ADEP1

Chain X: 14% 86%
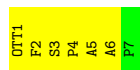
OTT1 F2 S3 P4 A5 A6 P7

• Molecule 2: ADEP1

Chain Y: 29% 71%
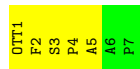
OTT1 F2 S3 P4 A5 A6 P7

• Molecule 2: ADEP1

Chain Z: 100%
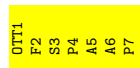
OTT1 F2 S3 P4 A5 A6 P7

• Molecule 2: ADEP1

Chain a: 43% 57%

OTT1 F2 S3 P4 A5 A6 P7

• Molecule 2: ADEP1

Chain b:

43% 57%

OTT1 F2 S3 P4 A5 A6 P7

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138976	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 $(e^-/\text{Å}^2)$	30.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	6.425	Depositor
Minimum map value	-4.100	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.269	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	246.4, 246.4, 246.4	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OTT, MP8, MAA

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	0.42	0/1467	0.63	0/1979
1	B	0.43	0/1467	0.63	0/1979
1	C	0.43	0/1467	0.63	0/1979
1	D	0.42	0/1467	0.63	0/1979
1	E	0.43	0/1467	0.63	0/1979
1	F	0.42	0/1467	0.63	0/1979
1	G	0.42	0/1467	0.63	0/1979
1	H	0.43	0/1467	0.63	0/1979
1	I	0.42	0/1467	0.63	0/1979
1	J	0.42	0/1467	0.63	0/1979
1	K	0.43	0/1467	0.63	0/1979
1	L	0.43	0/1467	0.63	0/1979
1	M	0.43	0/1467	0.63	0/1979
1	N	0.42	0/1467	0.63	0/1979
2	O	3.68	8/29 (27.6%)	2.23	1/37 (2.7%)
2	P	3.68	8/29 (27.6%)	2.23	1/37 (2.7%)
2	Q	3.68	8/29 (27.6%)	2.23	1/37 (2.7%)
2	R	3.68	8/29 (27.6%)	2.23	1/37 (2.7%)
2	S	3.68	8/29 (27.6%)	2.23	1/37 (2.7%)
2	T	3.68	8/29 (27.6%)	2.23	1/37 (2.7%)
2	U	3.68	8/29 (27.6%)	2.23	1/37 (2.7%)
2	V	3.69	8/29 (27.6%)	2.22	1/37 (2.7%)
2	W	3.68	8/29 (27.6%)	2.23	1/37 (2.7%)
2	X	3.68	8/29 (27.6%)	2.23	1/37 (2.7%)
2	Y	3.68	8/29 (27.6%)	2.24	1/37 (2.7%)
2	Z	3.68	8/29 (27.6%)	2.23	1/37 (2.7%)
2	a	3.68	8/29 (27.6%)	2.22	1/37 (2.7%)
2	b	3.68	8/29 (27.6%)	2.23	1/37 (2.7%)
All	All	0.66	112/20944 (0.5%)	0.69	14/28224 (0.0%)

The worst 5 of 112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	2	PHE	CG-CD2	7.65	1.50	1.38
2	Y	2	PHE	CG-CD2	7.64	1.50	1.38
2	R	2	PHE	CG-CD2	7.64	1.50	1.38
2	b	2	PHE	CG-CD2	7.63	1.50	1.38
2	Q	2	PHE	CG-CD2	7.62	1.50	1.38

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	2	PHE	CB-CG-CD2	-5.64	116.85	120.80
2	W	2	PHE	CB-CG-CD2	-5.62	116.87	120.80
2	Y	2	PHE	CB-CG-CD2	-5.62	116.87	120.80
2	b	2	PHE	CB-CG-CD2	-5.60	116.88	120.80
2	O	2	PHE	CB-CG-CD2	-5.59	116.88	120.80

There are no chirality outliers.

There are no planarity outliers.

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	A	1450	1365	1494	20	0
1	B	1450	1390	1494	15	0
1	C	1450	1371	1494	15	0
1	D	1450	1390	1494	17	0
1	E	1450	1399	1494	17	0
1	F	1450	1390	1494	13	0
1	G	1450	1381	1494	16	0
1	H	1450	1376	1494	17	0
1	I	1450	1390	1494	20	0
1	J	1450	1390	1494	20	0
1	K	1450	1390	1494	16	0
1	L	1450	1372	1494	17	0
1	M	1450	1372	1494	13	0
1	N	1450	1377	1494	14	0
2	O	52	0	49	1	0
2	P	52	0	49	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	52	0	49	4	0
2	R	52	0	49	1	0
2	S	52	0	49	1	0
2	T	52	0	49	4	0
2	U	52	0	49	1	0
2	V	52	0	49	3	0
2	W	52	0	49	1	0
2	X	52	0	49	3	0
2	Y	52	0	49	1	0
2	Z	52	0	49	4	0
2	a	52	0	49	0	0
2	b	52	0	49	0	0
All	All	21028	19353	21602	213	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 5.

The worst 5 of 213 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:F:9:GLN:HG2	1:F:14:GLU:H	1.45	0.81
1:H:9:GLN:HG2	1:H:14:GLU:H	1.45	0.81
1:A:9:GLN:HG2	1:A:14:GLU:H	1.45	0.81
1:J:9:GLN:HG2	1:J:14:GLU:H	1.45	0.80
1:N:9:GLN:HG2	1:N:14:GLU:H	1.45	0.80

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	187/202 (93%)	168 (90%)	18 (10%)	1 (0%)	29	64
1	B	187/202 (93%)	168 (90%)	18 (10%)	1 (0%)	29	64
1	C	187/202 (93%)	168 (90%)	18 (10%)	1 (0%)	29	64
1	D	187/202 (93%)	168 (90%)	18 (10%)	1 (0%)	29	64
1	E	187/202 (93%)	168 (90%)	18 (10%)	1 (0%)	29	64
1	F	187/202 (93%)	168 (90%)	18 (10%)	1 (0%)	29	64
1	G	187/202 (93%)	168 (90%)	18 (10%)	1 (0%)	29	64
1	H	187/202 (93%)	168 (90%)	18 (10%)	1 (0%)	29	64
1	I	187/202 (93%)	168 (90%)	18 (10%)	1 (0%)	29	64
1	J	187/202 (93%)	168 (90%)	18 (10%)	1 (0%)	29	64
1	K	187/202 (93%)	168 (90%)	18 (10%)	1 (0%)	29	64
1	L	187/202 (93%)	168 (90%)	18 (10%)	1 (0%)	29	64
1	M	187/202 (93%)	168 (90%)	18 (10%)	1 (0%)	29	64
1	N	187/202 (93%)	168 (90%)	18 (10%)	1 (0%)	29	64
2	O	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	P	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	Q	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	R	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	S	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	T	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	U	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	V	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	W	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	X	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	Y	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	Z	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	a	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	b	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
All	All	2660/2926 (91%)	2380 (90%)	266 (10%)	14 (0%)	32	64

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	ASP
1	B	169	ASP
1	C	169	ASP
1	D	169	ASP
1	E	169	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	155/168 (92%)	150 (97%)	5 (3%)	39	69
1	B	155/168 (92%)	150 (97%)	5 (3%)	39	69
1	C	155/168 (92%)	150 (97%)	5 (3%)	39	69
1	D	155/168 (92%)	150 (97%)	5 (3%)	39	69
1	E	155/168 (92%)	150 (97%)	5 (3%)	39	69
1	F	155/168 (92%)	150 (97%)	5 (3%)	39	69
1	G	155/168 (92%)	150 (97%)	5 (3%)	39	69
1	H	155/168 (92%)	150 (97%)	5 (3%)	39	69
1	I	155/168 (92%)	150 (97%)	5 (3%)	39	69
1	J	155/168 (92%)	150 (97%)	5 (3%)	39	69
1	K	155/168 (92%)	150 (97%)	5 (3%)	39	69
1	L	155/168 (92%)	150 (97%)	5 (3%)	39	69
1	M	155/168 (92%)	150 (97%)	5 (3%)	39	69
1	N	155/168 (92%)	150 (97%)	5 (3%)	39	69
2	O	3/3 (100%)	3 (100%)	0	100	100
2	P	3/3 (100%)	3 (100%)	0	100	100
2	Q	3/3 (100%)	3 (100%)	0	100	100
2	R	3/3 (100%)	3 (100%)	0	100	100
2	S	3/3 (100%)	3 (100%)	0	100	100
2	T	3/3 (100%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	U	3/3 (100%)	3 (100%)	0	100	100
2	V	3/3 (100%)	3 (100%)	0	100	100
2	W	3/3 (100%)	3 (100%)	0	100	100
2	X	3/3 (100%)	3 (100%)	0	100	100
2	Y	3/3 (100%)	3 (100%)	0	100	100
2	Z	3/3 (100%)	3 (100%)	0	100	100
2	a	3/3 (100%)	3 (100%)	0	100	100
2	b	3/3 (100%)	3 (100%)	0	100	100
All	All	2212/2394 (92%)	2142 (97%)	70 (3%)	42	69

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	6	VAL
1	M	37	ASP
1	H	2	LEU
1	E	37	ASP
1	E	36	ASP

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

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

28 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	MP8	O	7	2	5,8,9	0.92	0	3,10,12	1.05	0
2	MAA	O	5	2	4,5,6	3.13	3 (75%)	1,5,7	1.23	0
2	MP8	X	7	2	5,8,9	0.92	0	3,10,12	1.05	0
2	MP8	T	7	2	5,8,9	0.94	0	3,10,12	1.06	0
2	MAA	T	5	2	4,5,6	3.12	3 (75%)	1,5,7	1.25	0
2	MAA	b	5	2	4,5,6	3.13	3 (75%)	1,5,7	1.23	0
2	MP8	U	7	2	5,8,9	0.93	0	3,10,12	1.06	0
2	MAA	S	5	2	4,5,6	3.15	3 (75%)	1,5,7	1.24	0
2	MAA	R	5	2	4,5,6	3.14	3 (75%)	1,5,7	1.25	0
2	MP8	R	7	2	5,8,9	0.93	0	3,10,12	1.06	0
2	MAA	U	5	2	4,5,6	3.14	3 (75%)	1,5,7	1.24	0
2	MP8	V	7	2	5,8,9	0.93	0	3,10,12	1.05	0
2	MAA	Q	5	2	4,5,6	3.15	3 (75%)	1,5,7	1.25	0
2	MAA	V	5	2	4,5,6	3.14	3 (75%)	1,5,7	1.24	0
2	MP8	Z	7	2	5,8,9	0.94	0	3,10,12	1.06	0
2	MAA	W	5	2	4,5,6	3.13	3 (75%)	1,5,7	1.23	0
2	MP8	b	7	2	5,8,9	0.94	0	3,10,12	1.06	0
2	MP8	W	7	2	5,8,9	0.93	0	3,10,12	1.04	0
2	MAA	Y	5	2	4,5,6	3.15	3 (75%)	1,5,7	1.25	0
2	MP8	Q	7	2	5,8,9	0.93	0	3,10,12	1.06	0
2	MAA	P	5	2	4,5,6	3.13	3 (75%)	1,5,7	1.26	0
2	MP8	S	7	2	5,8,9	0.94	0	3,10,12	1.05	0
2	MP8	P	7	2	5,8,9	0.93	0	3,10,12	1.06	0
2	MP8	a	7	2	5,8,9	0.94	0	3,10,12	1.05	0
2	MAA	a	5	2	4,5,6	3.14	3 (75%)	1,5,7	1.24	0
2	MP8	Y	7	2	5,8,9	0.93	0	3,10,12	1.05	0
2	MAA	X	5	2	4,5,6	3.14	3 (75%)	1,5,7	1.24	0
2	MAA	Z	5	2	4,5,6	3.13	3 (75%)	1,5,7	1.25	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	MP8	O	7	2	-	0/0/11/13	0/1/1/1
2	MAA	O	5	2	-	0/1/4/6	-
2	MP8	X	7	2	-	0/0/11/13	0/1/1/1
2	MP8	T	7	2	-	0/0/11/13	0/1/1/1

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PROTEIN DATA BANK

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAA	T	5	2	-	0/1/4/6	-
2	MAA	b	5	2	-	0/1/4/6	-
2	MP8	U	7	2	-	0/0/11/13	0/1/1/1
2	MAA	S	5	2	-	0/1/4/6	-
2	MAA	R	5	2	-	0/1/4/6	-
2	MP8	R	7	2	-	0/0/11/13	0/1/1/1
2	MAA	U	5	2	-	0/1/4/6	-
2	MP8	V	7	2	-	0/0/11/13	0/1/1/1
2	MAA	Q	5	2	-	0/1/4/6	-
2	MAA	V	5	2	-	0/1/4/6	-
2	MP8	Z	7	2	-	0/0/11/13	0/1/1/1
2	MAA	W	5	2	-	0/1/4/6	-
2	MP8	b	7	2	-	0/0/11/13	0/1/1/1
2	MP8	W	7	2	-	0/0/11/13	0/1/1/1
2	MAA	Y	5	2	-	0/1/4/6	-
2	MP8	Q	7	2	-	0/0/11/13	0/1/1/1
2	MAA	P	5	2	-	0/1/4/6	-
2	MP8	S	7	2	-	0/0/11/13	0/1/1/1
2	MP8	P	7	2	-	0/0/11/13	0/1/1/1
2	MP8	a	7	2	-	0/0/11/13	0/1/1/1
2	MAA	a	5	2	-	0/1/4/6	-
2	MP8	Y	7	2	-	0/0/11/13	0/1/1/1
2	MAA	X	5	2	-	0/1/4/6	-
2	MAA	Z	5	2	-	0/1/4/6	-

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	a	5	MAA	CA-N	4.99	1.56	1.47
2	S	5	MAA	CA-N	4.98	1.56	1.47
2	Q	5	MAA	CA-N	4.98	1.56	1.47
2	U	5	MAA	CA-N	4.97	1.56	1.47
2	Z	5	MAA	CA-N	4.96	1.56	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	7	MP8	1	0
2	V	7	MP8	1	0
2	Z	7	MP8	1	0
2	Q	7	MP8	1	0

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-31559. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

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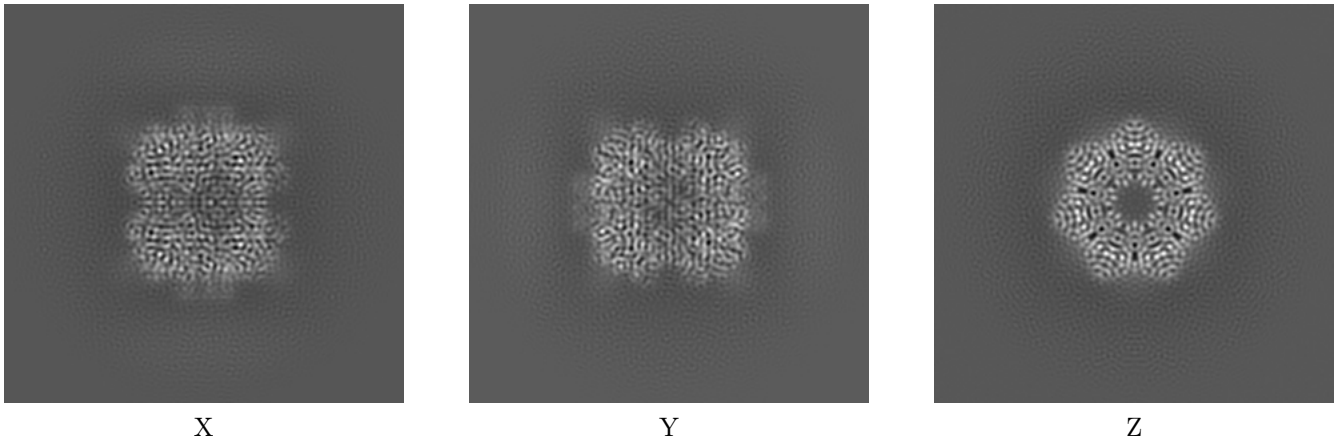
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map

| X Index: 110 | Y Index: 110 | Z Index: 110 |
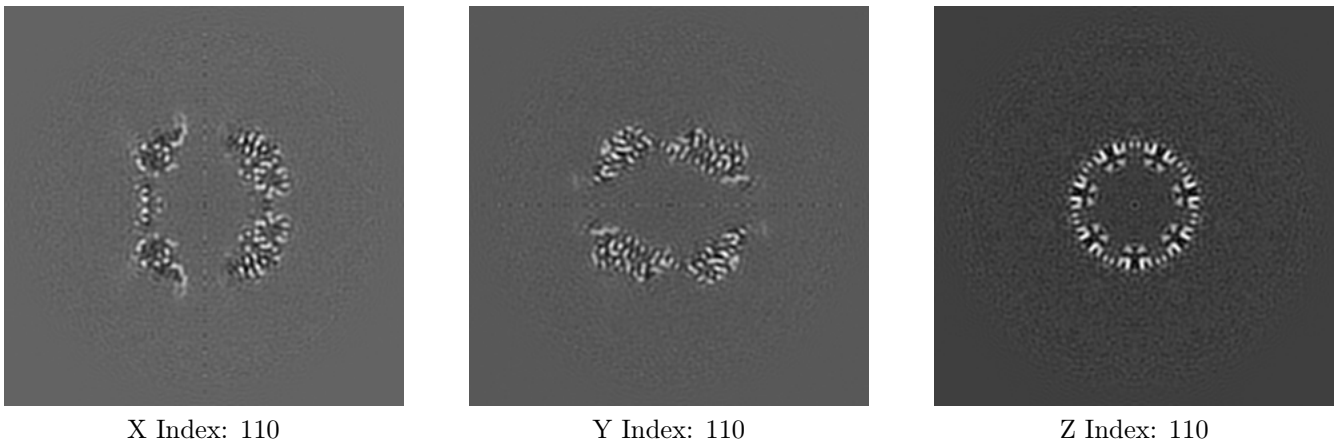
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
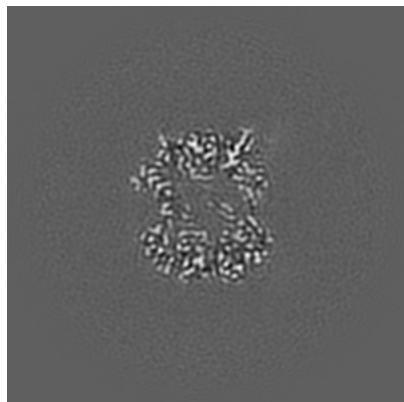
6.3.1 Primary map
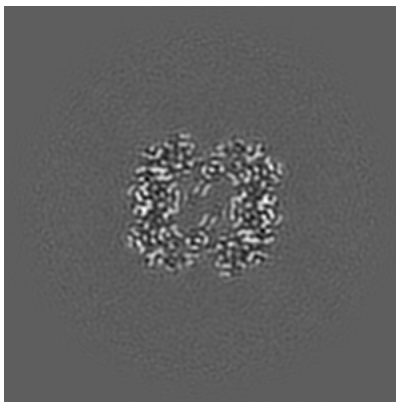
| X Index: 133 | Y Index: 134 | Z Index: 138 |
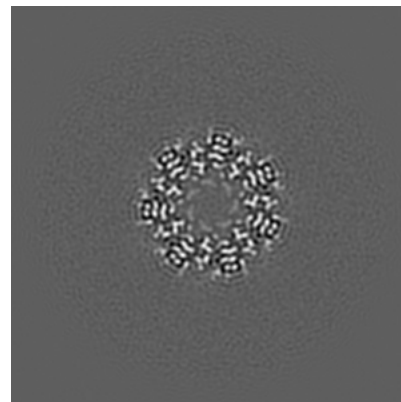
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

| X | Y | Z |
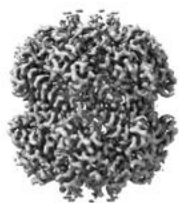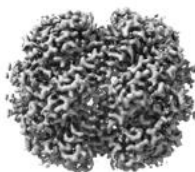
The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5   Mask visualisation ⓘ

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

7   Map analysis ⓘ

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

7.1   Map-value distribution ⓘ
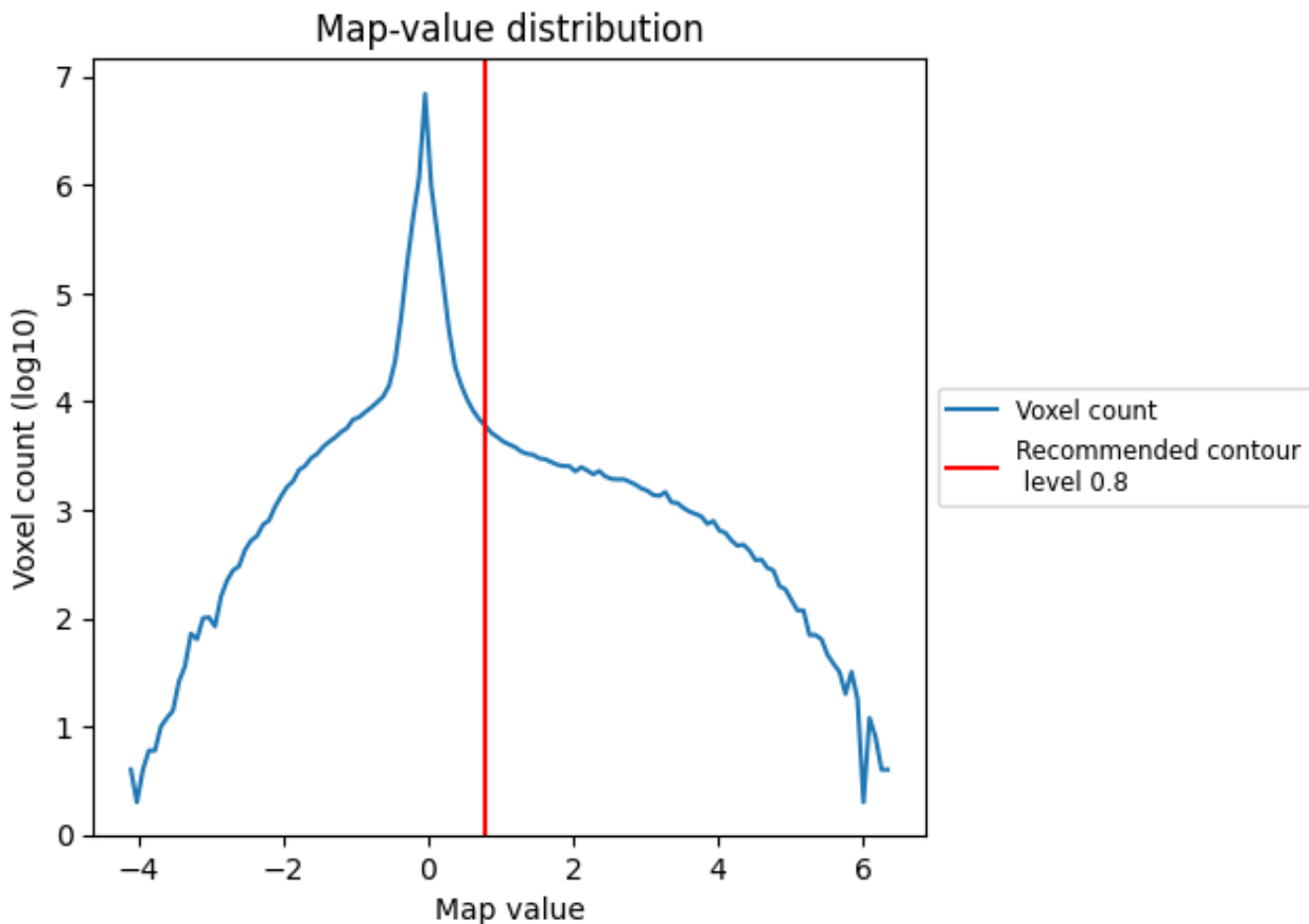
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
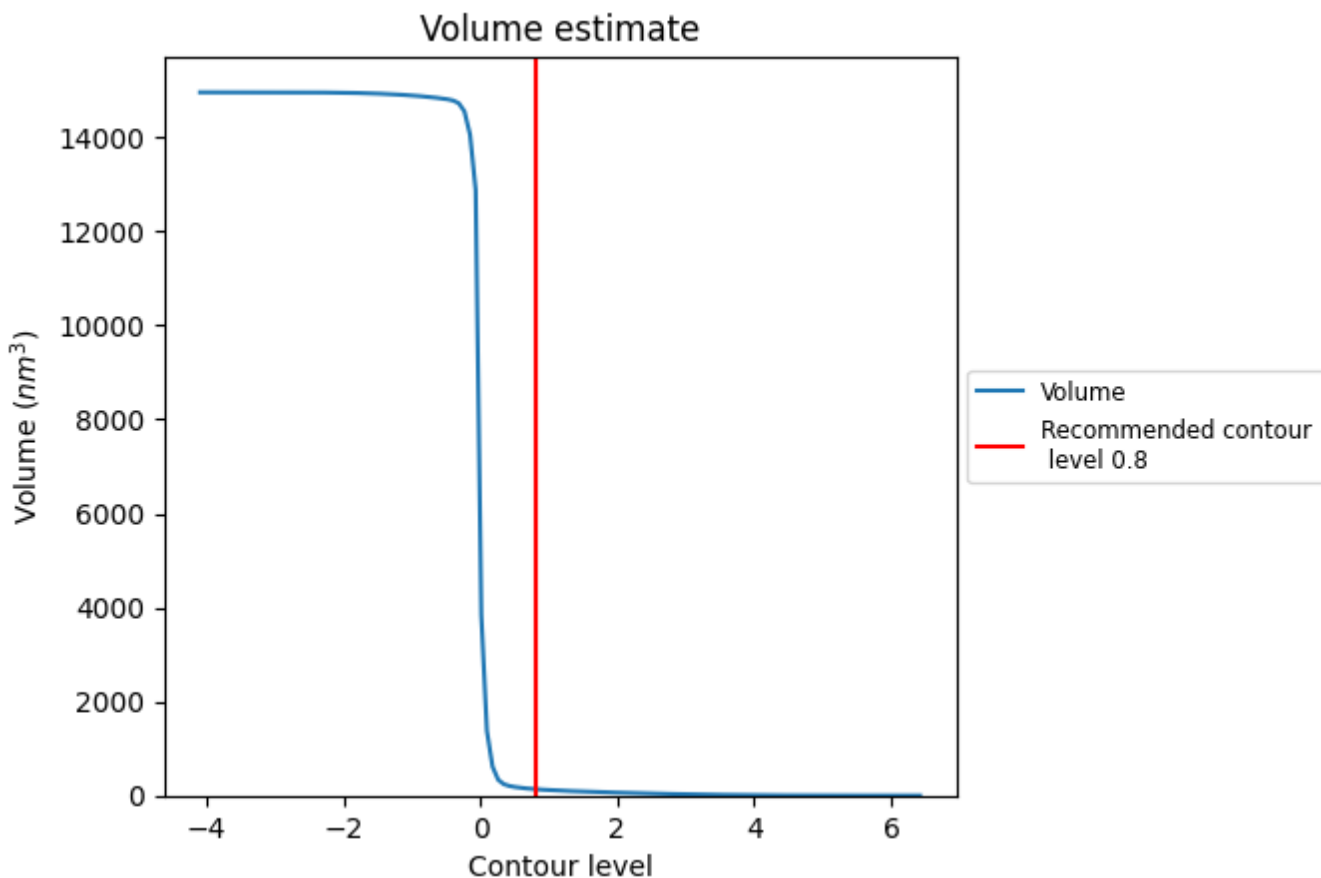
The volume at the recommended contour level is 136 nm^3; this corresponds to an approximate mass of 123 kDa.

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 ⓘ
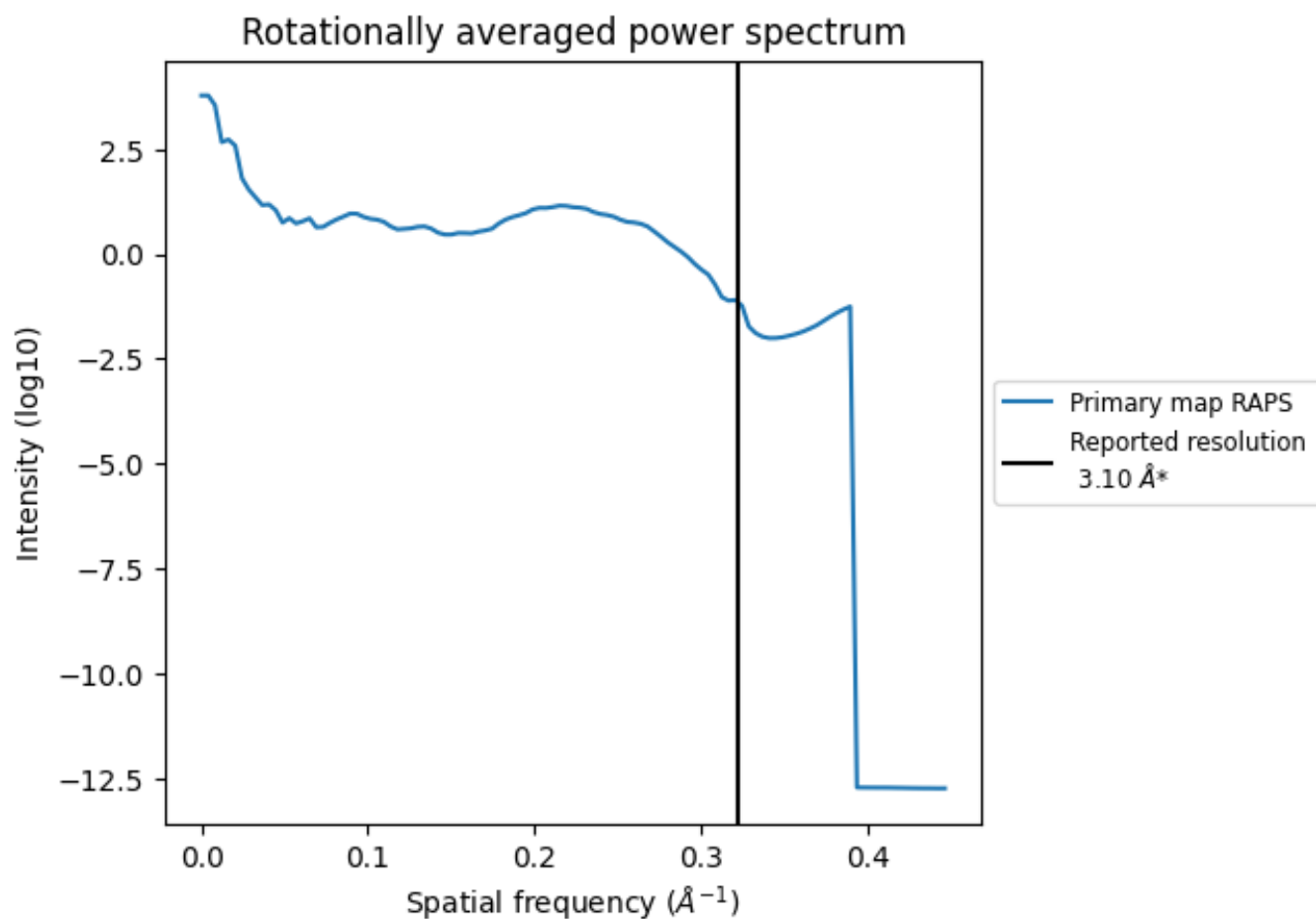
*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-31559 and PDB model 7FEP. Per-residue inclusion information can be found in section 3 on page 8.

9.1   Map-model overlay ⓘ

X	Y	Z
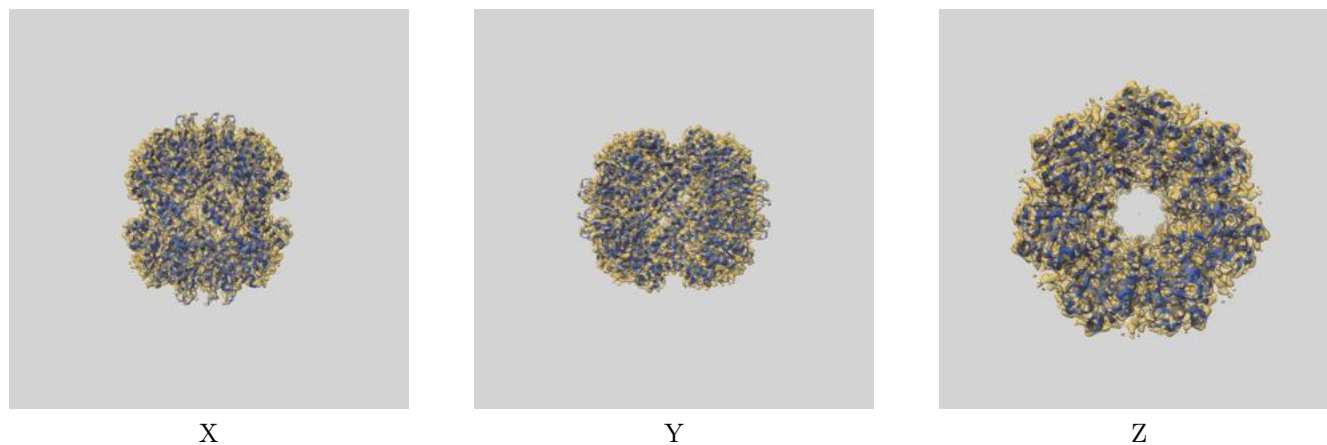
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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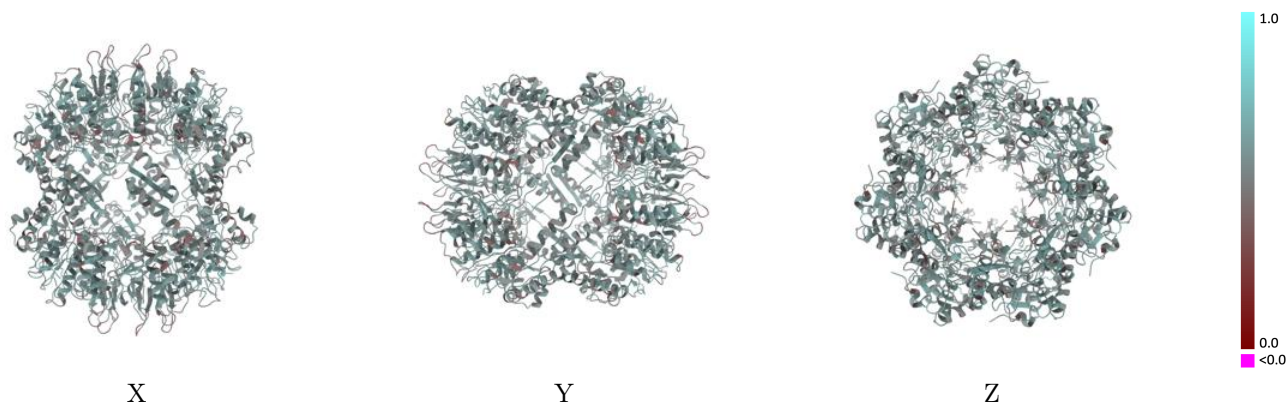
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
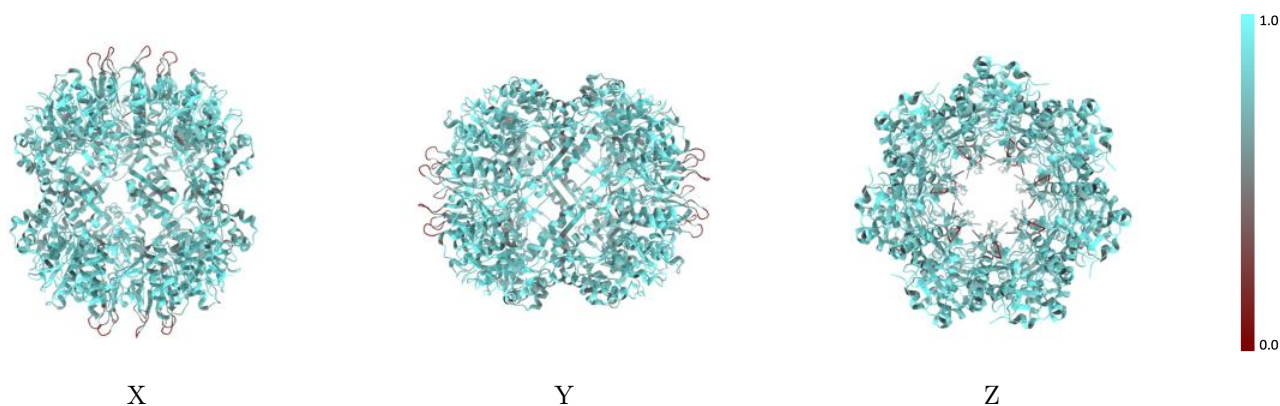
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).

9.4 Atom inclusion ⓘ
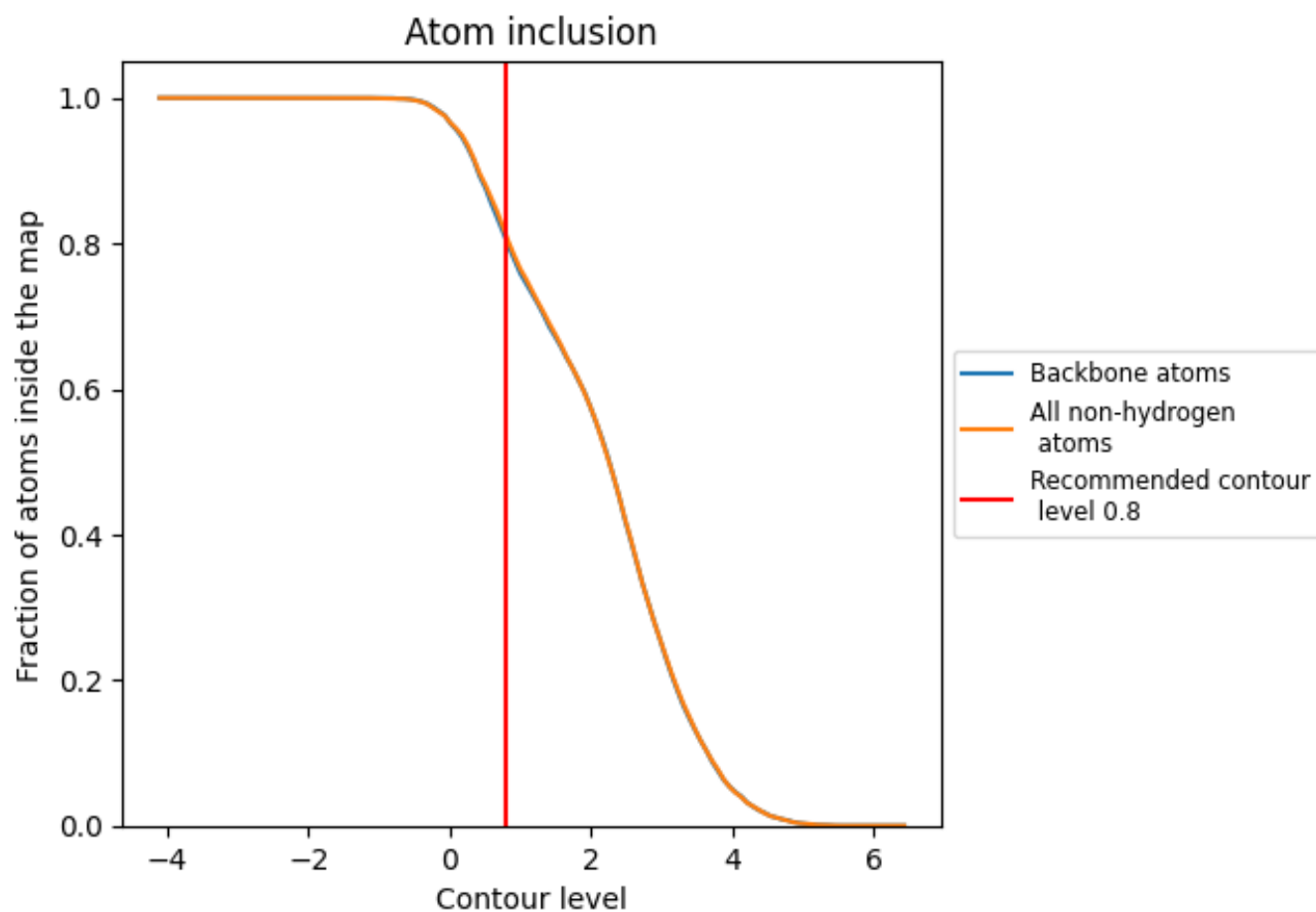
At the recommended contour level, 80% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8108	0.5430
A	0.8034	0.5360
B	0.8097	0.5440
C	0.8076	0.5440
D	0.8041	0.5440
E	0.8069	0.5430
F	0.8090	0.5460
G	0.8069	0.5440
H	0.8048	0.5380
I	0.8174	0.5440
J	0.8132	0.5390
K	0.8013	0.5370
L	0.8055	0.5420
M	0.8167	0.5480
N	0.8097	0.5460
O	0.8846	0.5630
P	0.8846	0.5640
Q	0.8846	0.5700
R	0.9231	0.5530
S	0.8846	0.5590
T	0.8846	0.5770
U	0.9038	0.5710
V	0.8654	0.5590
W	0.9038	0.5460
X	0.8846	0.5510
Y	0.9038	0.5700
Z	0.8846	0.5590
a	0.9038	0.5630
b	0.8846	0.5580

1.0

0.0
<0.0