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 ⓘ

Nov 19, 2022 – 11:16 AM EST

PDB ID	:	3J0K
EMDB ID	:	EMD-5343
Title	:	Orientation of RNA polymerase II within the human VP16-Mediator-pol II-TFIIF assembly
Authors	:	Bernecky, C.; Grob, P.; Ebmeier, C.C.; Nogales, E.; Taatjes, D.J.
Deposited on	:	2011-10-04
Resolution	:	36.00 Å(reported)
Based on initial model	:	1Y1V

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

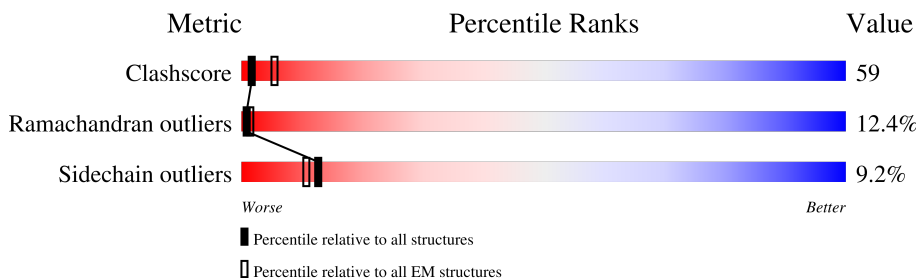|		
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 36.00 Å.

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

Metric	Percentile Ranks	Value
Clashscore		59
Ramachandran outliers		12.4%
Sidechain outliers		9.2%

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	1455	9% / 26% 55% 16% ••
2	B	1224	21% / 25% 52% 13% • 9%
3	C	268	60% / 26% 56% 15% ••
4	D	221	18% / 31% 42% 7% 20%
5	E	215	53% / 35% 54% 11%
6	F	84	27% / 29% 56% 15%
7	G	171	21% / 33% 59% 8%
8	H	146	47% / 29% 53% 9% 9%

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Mol	Chain	Length	Quality of chain
9	I	122	36% · 30% · 49% · 13% · 5% ·
10	J	70	26% · 20% · 54% · 17% · 7%
11	K	120	66% · 39% · 50% · 5% · 5%
12	L	46	76% · 9% · 63% · 26% ·

2 Entry composition ⓘ

There are 14 unique types of molecules in this entry. The entry contains 31137 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 DNA-directed RNA polymerase II largest subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1426	Total 11214	C 7069	N 1959	O 2124	S 62	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1112	Total 8837	C 5594	N 1548	O 1640	S 55	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	266	Total 2095	C 1317	N 348	O 417	S 13	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	177	Total 1356	C 840	N 241	O 273	S 2	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total 1752	C 1111	N 309	O 321	S 11	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total 679	C 434	N 115	O 127	S 3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total 1340	C 861	N 222	O 249	S 8	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total 1068	C 673	N 180	O 211	S 4	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	119	Total 971	C 596	N 179	O 186	S 10	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total 532	C 339	N 93	O 94	S 6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	114	Total 919	C 590	N 156	O 171	S 2	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total 364	C 224	N 72	O 64	S 4	0	0

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total 1	Mg 1	0

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	A	3	Total 3	Zn 3	0
14	B	1	Total 1	Zn 1	0
14	C	1	Total 1	Zn 1	0
14	I	2	Total 2	Zn 2	0
14	J	1	Total 1	Zn 1	0
14	L	1	Total 1	Zn 1	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: DNA-directed RNA polymerase II largest subunit

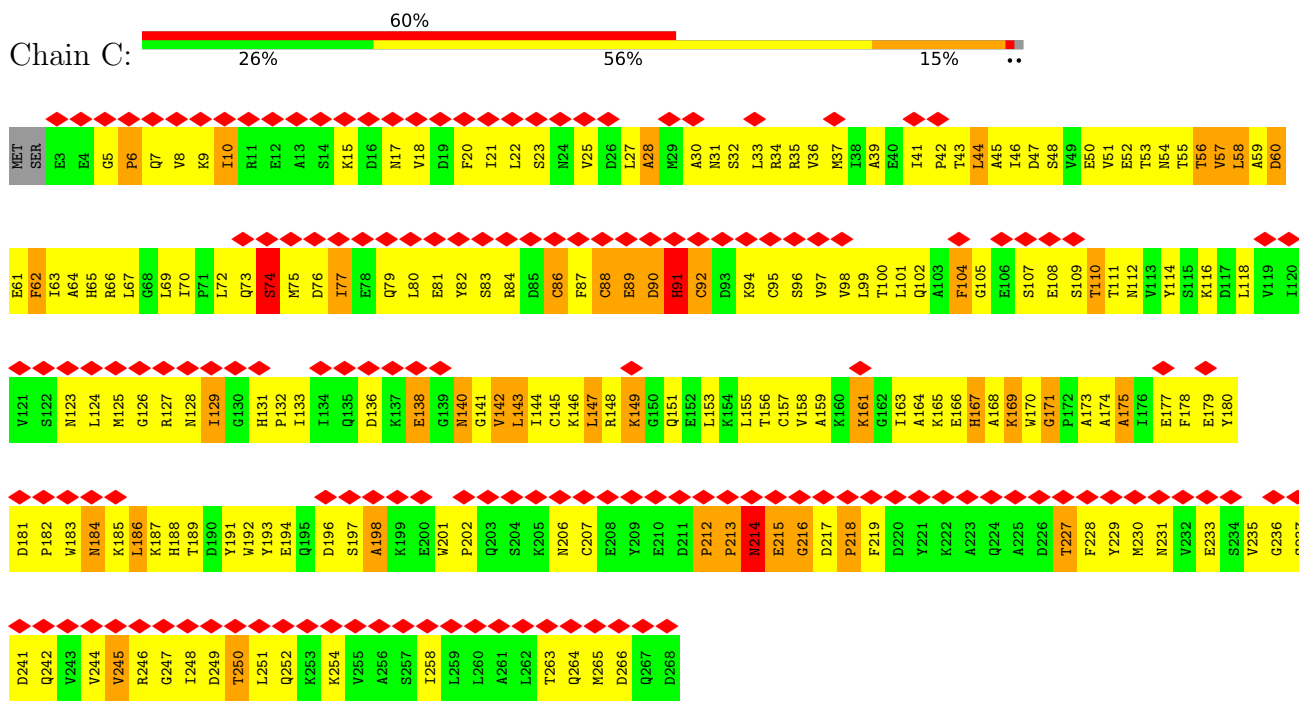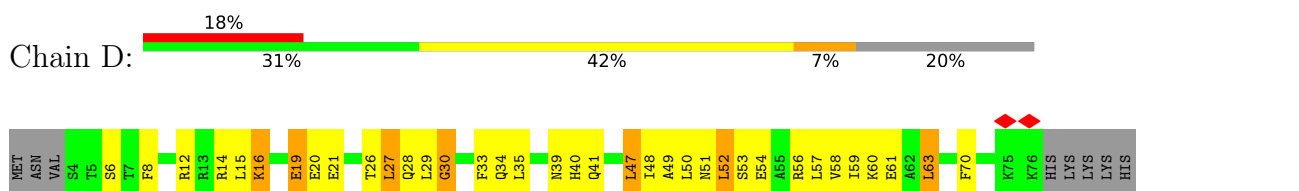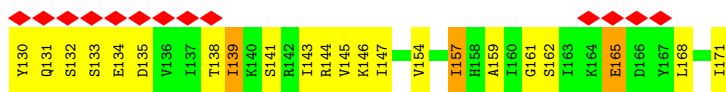• Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

Chain B:

• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

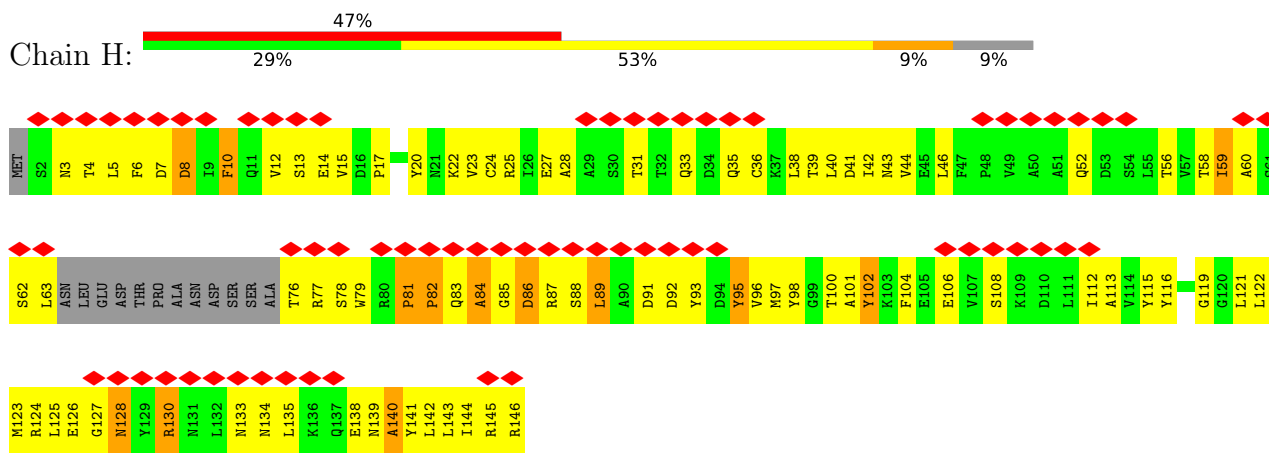• Molecule 4: DNA-directed RNA polymerase II 32 kDa polypeptide

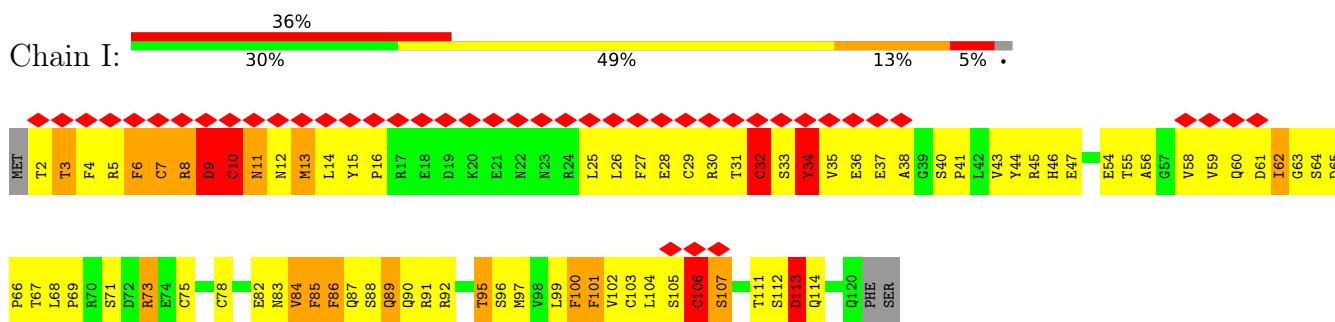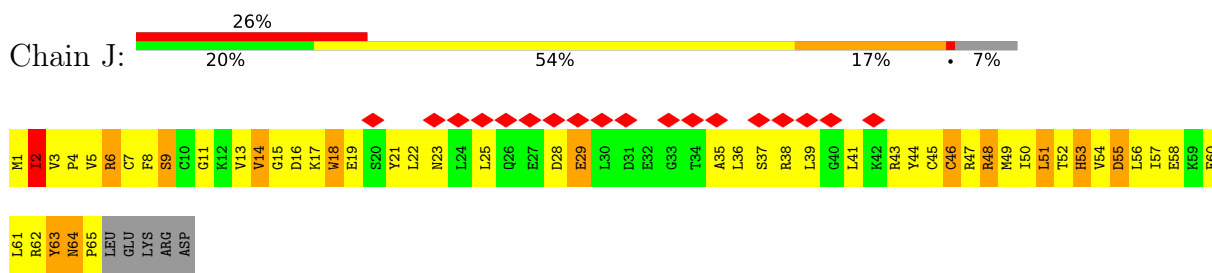LEU LYS HIS GLU ASN ALA ASN ASP GLU THR ALA VAL GLU ASP GLU ASP ASP LEU ASP GLU ASP VAL ASN ALA ASP ASP ASP PHE MET HIS SER GLU T118 E122 L123 E124 S125 I126 D127 V128 L129 L130 E131 Q132 T133 T134 G135 G136 N137 N138 K139 D140 L141 K142 N143

T144 M145 Q146 Y147 L148 T149 N150 F151 S152 R153 F154 R155 D156 Q157 E158 T159 V160 G161 A162 Q165 L166 L167 K168 S169 T170 G171 L172 H173 P174 F175 E176 V177 A178 Q179 L180 G181 S182 C185 D186 T187 A188 D189 E190 A191 K192 T193 L194 I195 P196 S197 L198 N199 N200 K201 I202 S203 D204 D205

E206 L207 E208 R209 I210 L211 K212 E213 L214 S215 N216 L217 E218 T219 L220 Y221

• Molecule 5: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E:

53%
35% 54% 11%

MET D2 Q3 E4 R7 N8 I9 S10 R11 L12 W13 R14 A15 F16 R17 T18 V19 K20 E21 M22 V23 K24 D25 R26 G27 Y28 F29 I30 T31 Q32 E33 E34 V35 E36 L37 P38 L39 E40 D41 F42 K43 A44 K45 Y46 C47 D48 S49 M50 G51 R52 P53 Q54 K55 K56 M57 M58 S59 F60 Q61

A62 N63 P64 T65 E66 E67 S68 I69 S70 K71 F72 P73 D74 M75 G76 S77 L78 W79 V80 E81 F82 C83 D84 E85 P86 V90 K91 T92 M93 K94 T95 F96 V97 I98 H99 I100 Q101 E102 K103 N104 F105 Q106 T107 G108 I109 F110 V111 Y112 Q113 N114 N115 I116 T117 P118 S119 A120 L123 V124

P125 S126 I127 P128 P129 A130 T131 I132 E133 T134 F135 N136 E137 A138 A139 L140 V141 V42 N143 I144 T145 H146 H147 E148 L149 V150 H153 I154 R155 L156 S157 S158 D159 E160 K161 R162 E163 L164 L165 K166 R167 Y168 R169 L170 K171 E172 S173 Q174 L175 P176 R177 I178 D182 P183 V184 A185 L186 Y187

L188 G189 L190 K191 R192 G193 E194 V195 V196 K197 I198 I199 S202 E203 T204 S205 G206 R207 Y208 A209 S210 Y211 R212 I213 C214 M215

• Molecule 6: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

Chain F:

27%
29% 56% 15%

K72 A73 I74 P75 K76 D77 Q78 R79 A80 T81 T82 P83 Y84 M85 T86 K87 Y88 E89 R90 A91 R92 I93 L94 G95 T96 R97 A98 L99 Q100 I101 S102 M103 N104 A105 P106 V107 F108 V109 D110 L111 E112 G113 E114 T115 D116 P117 L118 R119 I120 K123 E124 L125 A126 E127 K128 K129 I130 P131 L132

V133 I134 R135 R136 Y137 L138 P139 D140 G141 S142 F143 E144 D145 W146 S147 V148 E149 E150 L151 I152 V153 D154 L155

• Molecule 7: DNA-directed RNA polymerase II 19 kDa polypeptide

Chain G:

21%
33% 59% 8%

M1 F2 F3 I4 K5 D6 L7 S8 L9 N10 L13 H14 P15 S16 F17 F18 G19 M22 K23 Q24 Y25 L26 K27 T28 K29 L30 L31 V34 C38 T39 G40 K41 F42 G43 Y44 I45 L46 C47 V48 L49 D50 Y51 I54 D55 I56 Q57 R58 G59 R60 I61 L62 P63 T64 D65 G66

S67 A68 E69 F70 N71 V72 K73 Y74 R75 A76 V77 V78 F79 K80 P81 F82 K83 G84 E85 V86 V87 D88 V91 C94 S95 Q96 H97 G98 V101 Q102 V103 G104 P105 M106 K107 V108 F109 V110 T111 K112 H113 L114 M115 P116 Q117 D118 L119 T120 F121 N122 A123 G124 S125 N126 P127 P128 S129

• Molecule 8: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide
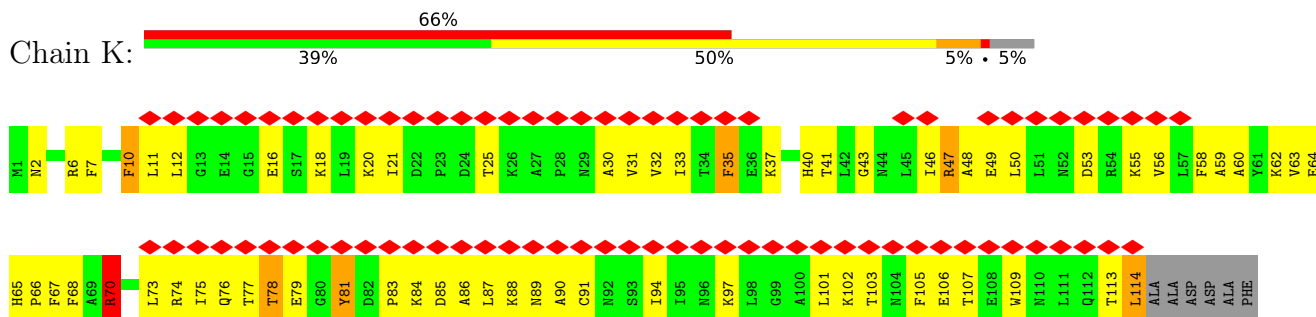
Chain H:
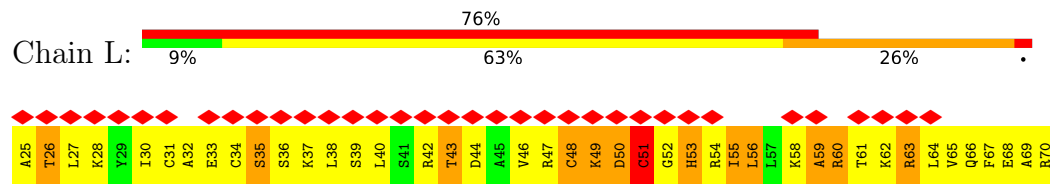

• Molecule 9: DNA-directed RNA polymerase II subunit 9

Chain I:

• Molecule 10: DNA-directed RNA polymerases I/II/III subunit 10

Chain J:

• Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K:

• Molecule 12: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

Chain L:

76%

9%   63%   26%   •

A25 T26 L27 K28 Y29 I30 C31 A32 E33 C34 S35 S36 K37 L38 S39 L40 S41 R42 T43 D44 A45 V46 R47 C48 K49 D50 C51 G52 H53 R54 I55 L56 L57 K58 A59 R60 T61 K62 R63 L64 V65 Q66 F67 E68 A69 R70

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	3146	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	each micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/Å^2)$	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	29000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0284	Depositor
Map size (Å)	690.69, 690.69, 690.69	wwPDB
Map dimensions	161, 161, 161	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	4.29, 4.29, 4.29	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.50	2/11417 (0.0%)	0.78	4/15442 (0.0%)
2	B	0.52	4/9009 (0.0%)	0.76	8/12146 (0.1%)
3	C	0.48	0/2133	0.77	1/2891 (0.0%)
4	D	0.41	0/1365	0.64	0/1837
5	E	0.43	0/1788	0.66	0/2406
6	F	0.52	0/691	0.77	0/933
7	G	0.49	0/1368	0.72	0/1844
8	H	0.38	0/1086	0.65	1/1470 (0.1%)
9	I	0.46	0/989	0.77	1/1331 (0.1%)
10	J	0.48	0/541	0.75	0/727
11	K	0.45	0/937	0.67	0/1265
12	L	0.54	0/366	0.79	0/485
All	All	0.49	6/31690 (0.0%)	0.75	15/42777 (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
2	B	0	2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	467	GLY	C-O	-11.91	1.04	1.23
2	B	468	GLU	CB-CG	8.45	1.68	1.52
2	B	510	LYS	CB-CG	5.58	1.67	1.52
1	A	195	ASP	N-CA	5.49	1.57	1.46
2	B	468	GLU	CG-CD	5.21	1.59	1.51

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	195	ASP	N-CA-C	9.36	136.28	111.00
2	B	510	LYS	CB-CA-C	-7.65	95.10	110.40
2	B	510	LYS	C-N-CD	-7.45	104.21	120.60
3	C	92	CYS	CA-CB-SG	-6.78	101.80	114.00
1	A	1310	GLY	N-CA-C	-6.49	96.88	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	510	LYS	Mainchain
2	B	833	TYR	Sidechain

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	11214	0	11281	1475	0
2	B	8837	0	8871	1203	0
3	C	2095	0	2052	263	0
4	D	1356	0	1319	106	0
5	E	1752	0	1776	189	0
6	F	679	0	701	84	0
7	G	1340	0	1357	161	0
8	H	1068	0	1040	120	0
9	I	971	0	929	113	0
10	J	532	0	542	110	0
11	K	919	0	929	97	0
12	L	364	0	387	68	0
13	A	1	0	0	0	0
14	A	3	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31137	0	31184	3684	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 59.

The worst 5 of 3684 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)
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.28	1.13
4:D:40:HIS:HB3	7:G:73:LYS:HZ3	1.10	1.12
7:G:138:THR:HG22	7:G:139:ILE:H	1.11	1.11
1:A:913:LEU:HD12	1:A:914:GLU:H	1.15	1.11
6:F:82:THR:HG22	6:F:84:TYR:H	1.15	1.11

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	1418/1455 (98%)	914 (64%)	316 (22%)	188 (13%)	0	5
2	B	1096/1224 (90%)	725 (66%)	223 (20%)	148 (14%)	0	4
3	C	264/268 (98%)	169 (64%)	62 (24%)	33 (12%)	0	5
4	D	173/221 (78%)	129 (75%)	27 (16%)	17 (10%)	0	10
5	E	212/215 (99%)	141 (66%)	50 (24%)	21 (10%)	0	9
6	F	82/84 (98%)	60 (73%)	15 (18%)	7 (8%)	1	12
7	G	169/171 (99%)	123 (73%)	34 (20%)	12 (7%)	1	14
8	H	129/146 (88%)	93 (72%)	25 (19%)	11 (8%)	1	12
9	I	117/122 (96%)	80 (68%)	22 (19%)	15 (13%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	63/70 (90%)	36 (57%)	14 (22%)	13 (21%)	0	2
11	K	112/120 (93%)	82 (73%)	25 (22%)	5 (4%)	2	22
12	L	44/46 (96%)	18 (41%)	14 (32%)	12 (27%)	0	0
All	All	3879/4142 (94%)	2570 (66%)	827 (21%)	482 (12%)	1	5

5 of 482 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	48	ALA
1	A	55	ASP
1	A	58	LEU
1	A	62	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	1246/1270 (98%)	1133 (91%)	113 (9%)	9	29
2	B	964/1061 (91%)	880 (91%)	84 (9%)	10	31
3	C	234/236 (99%)	205 (88%)	29 (12%)	4	19
4	D	140/200 (70%)	126 (90%)	14 (10%)	7	26
5	E	196/197 (100%)	184 (94%)	12 (6%)	18	44
6	F	74/74 (100%)	63 (85%)	11 (15%)	3	15
7	G	152/152 (100%)	143 (94%)	9 (6%)	19	45
8	H	117/128 (91%)	110 (94%)	7 (6%)	19	44
9	I	113/116 (97%)	97 (86%)	16 (14%)	3	16
10	J	60/65 (92%)	55 (92%)	5 (8%)	11	34
11	K	99/102 (97%)	91 (92%)	8 (8%)	11	35
12	L	40/40 (100%)	33 (82%)	7 (18%)	2	11
All	All	3435/3641 (94%)	3120 (91%)	315 (9%)	13	29

5 of 315 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	148	LEU
9	I	46	HIS
4	D	197	SER
6	F	143	PHE
11	K	10	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1179	GLN
5	E	101	GLN
3	C	65	HIS
3	C	252	GLN
5	E	147	HIS

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 ⓘ

Of 10 ligands modelled in this entry, 10 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 ⓘ

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-5343. 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 |
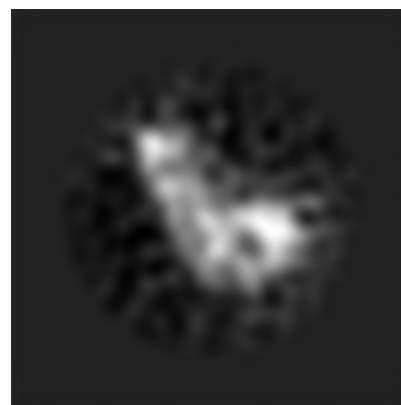
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map

| X Index: 80 | Y Index: 80 | Z Index: 80 |

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: 104 | Y Index: 71 | Z Index: 76 |
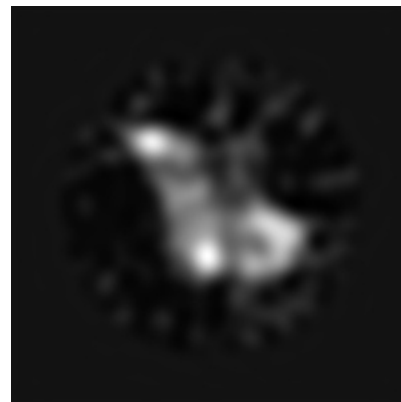
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ
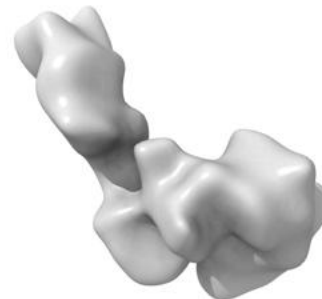
6.4.1 Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.0284. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

6.5 Mask visualisation ⓘ

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

7 Map analysis (i)

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

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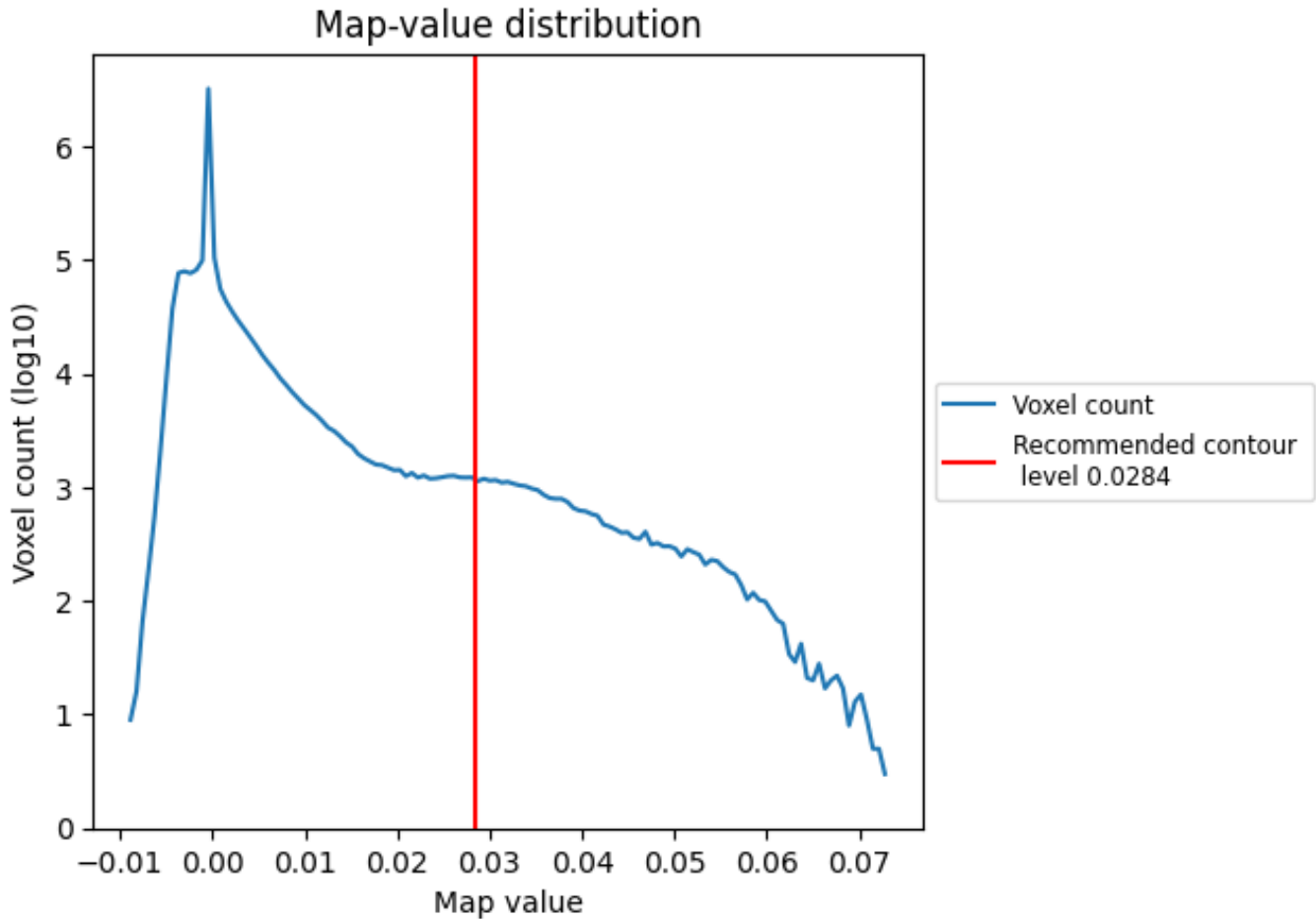
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
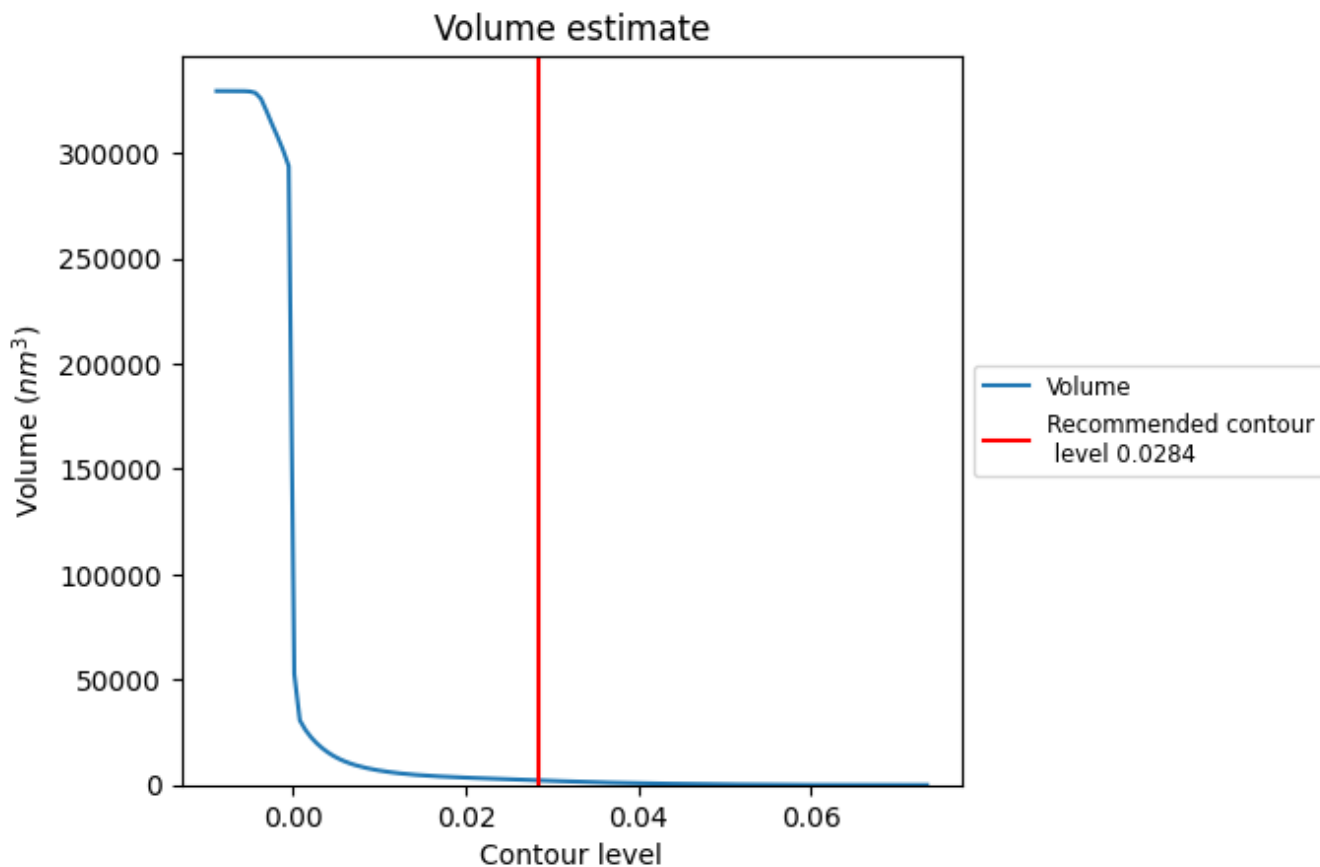
The volume at the recommended contour level is 2188 nm^3; this corresponds to an approximate mass of 1977 kDa.

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 ⓘ
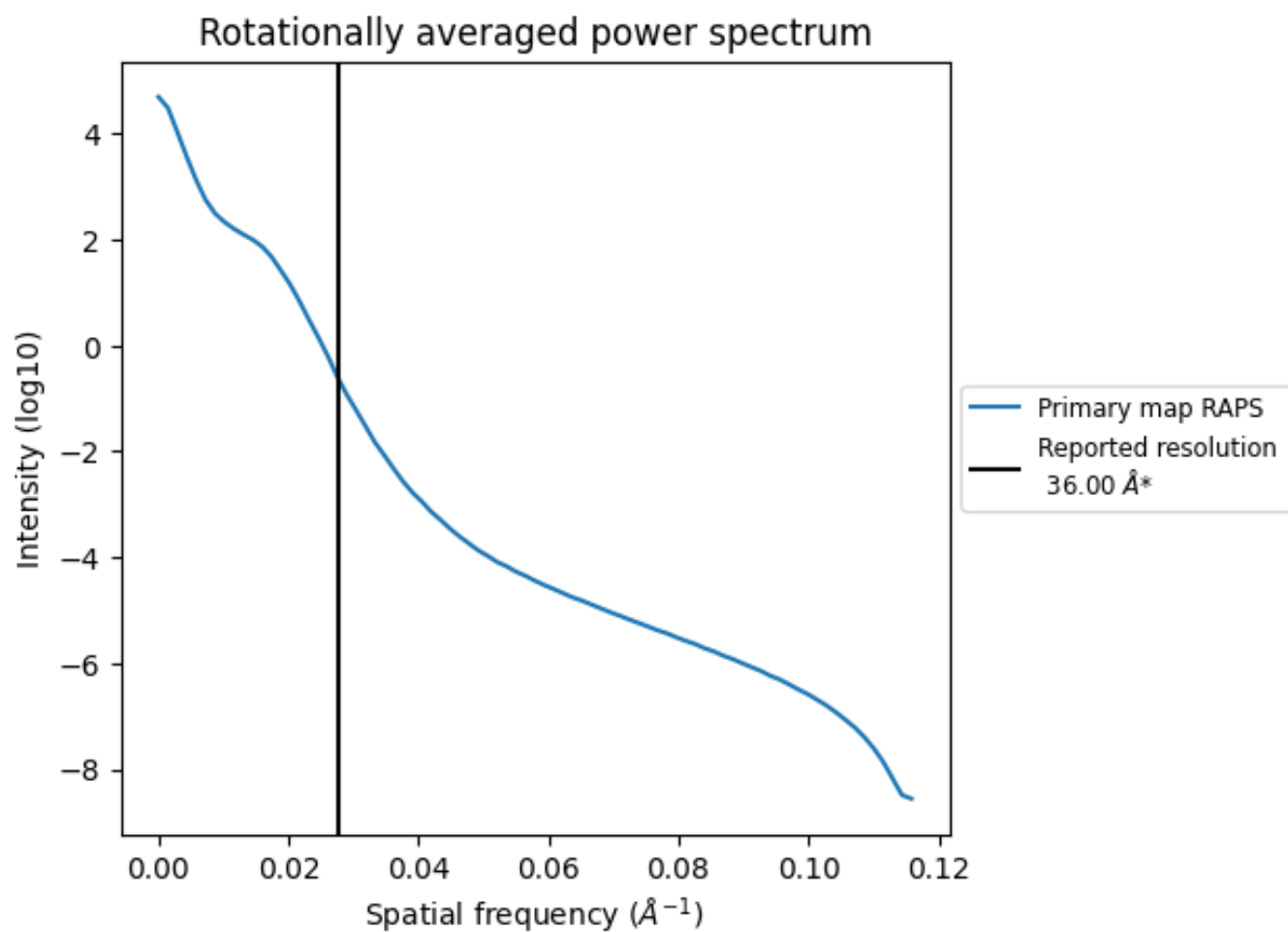
*Reported resolution corresponds to spatial frequency of 0.028 Å^{-1}

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-5343 and PDB model 3J0K. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay ⓘ
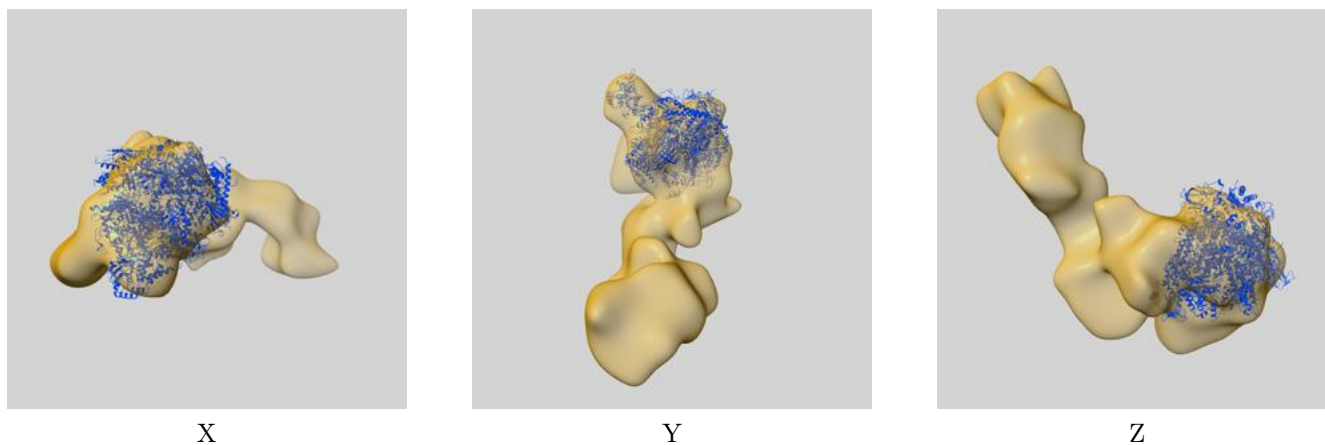
| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.0284 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
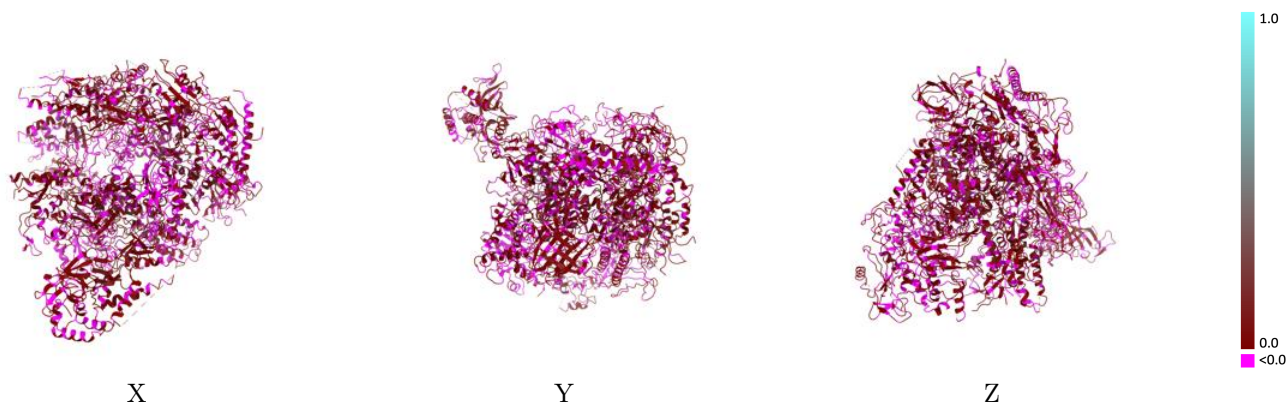
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
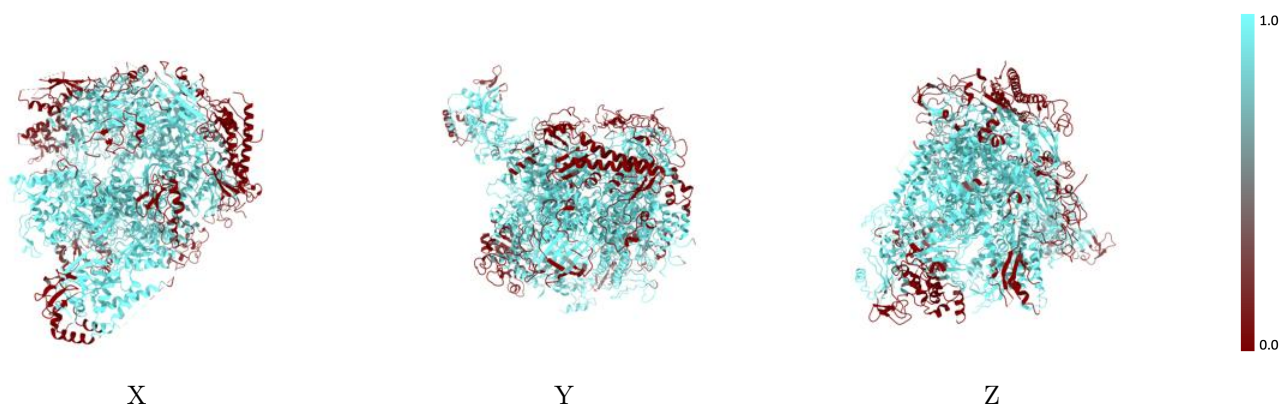
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0284).

9.4   Atom inclusion ⓘ
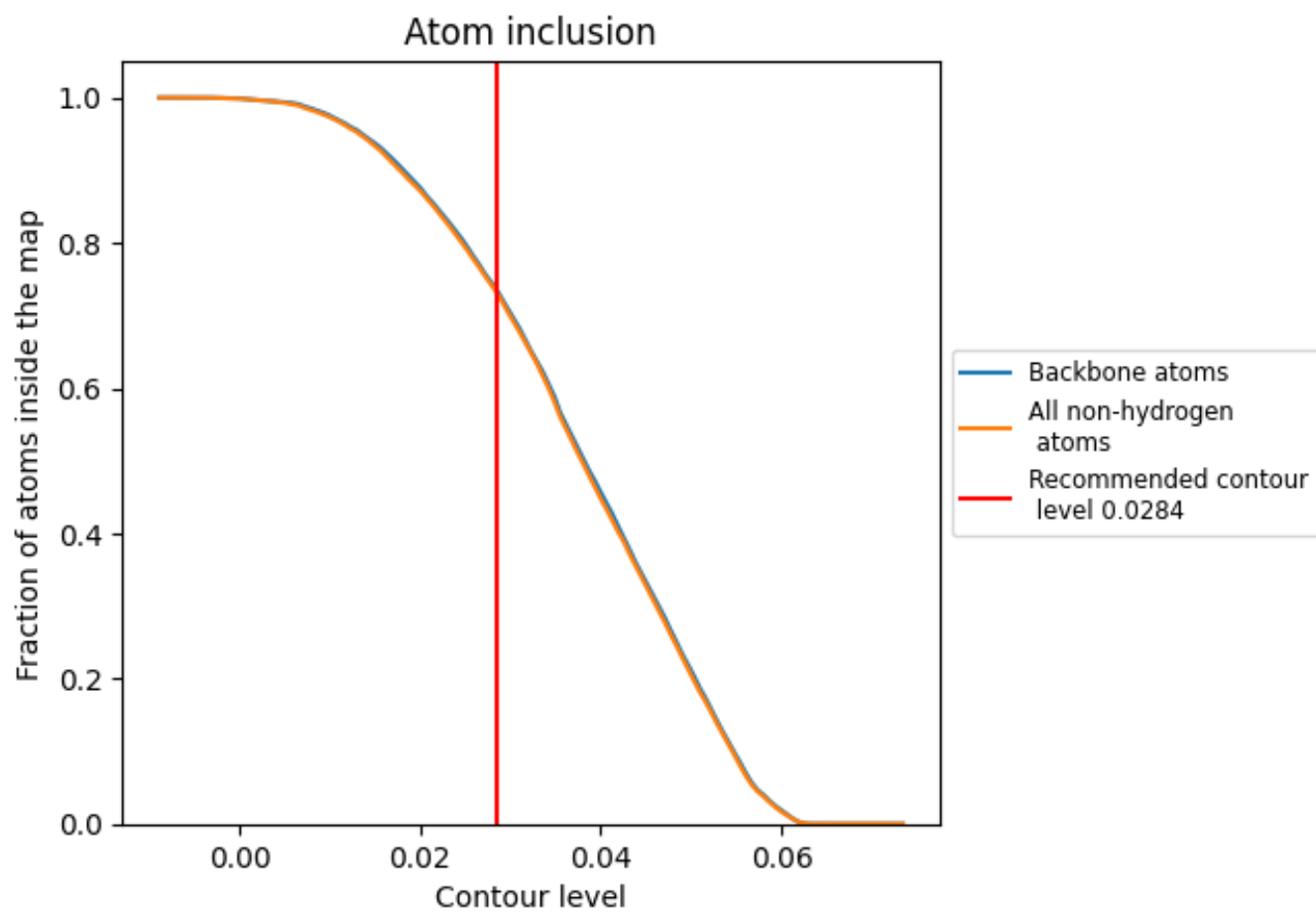
Atom inclusion

At the recommended contour level, 74% of all backbone atoms, 73% 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 (0.0284) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7332	0.0260
A	0.8979	0.0290
B	0.7606	0.0340
C	0.3733	0.0210
D	0.7522	0.0200
E	0.4558	-0.0130
F	0.7489	0.0060
G	0.7882	0.0470
H	0.4846	0.0300
I	0.6205	-0.0000
J	0.7079	0.0350
K	0.3024	0.0000
L	0.2443	0.0090

1.0

0.0
<0.0