wwPDB EM Validation Summary Report (i)

Dec 11, 2022 – 02:52 pm GMT

PDB ID	:	6SMH
EMDB ID	:	EMD-10235
Title	:	Cryo-electron microscopy structure of a RbcL-Raf1 supercomplex from Synechococcus elongatus PCC 7942
Authors	:	Huang, F.; Kong, W.-W.; Sun, Y.; Chen, T.; Dykes, G.F.; Jiang, Y.L.; Liu, L.N.
Deposited on	:	2019-08-21
Resolution	:	4.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

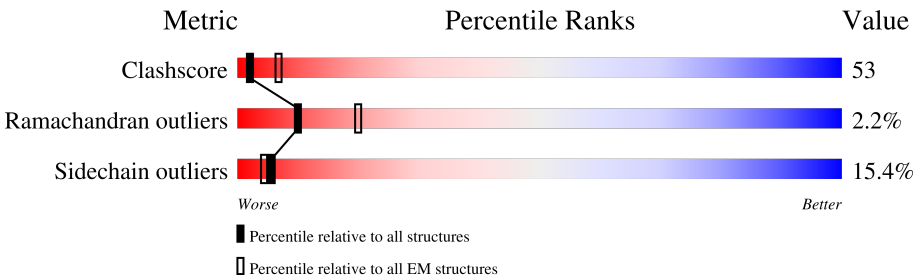
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	447	78% 21%
1	B	447	59% 32% 8%
1	C	447	48% 37% 14%
1	D	447	50% 36% 13%
1	E	447	54% 33% 10%
1	F	447	40% 41% 17%
1	G	447	53% 36% 9%
1	H	447	56% 34% 10%

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Mol	Chain	Length	Quality of chain
2	I	188	74% 70% 23% 5%
2	J	188	73% 43% 41% 9% 7%
2	K	188	71% 48% 35% 9% 5%
2	L	188	72% 39% 40% 13% 5%
2	M	188	69% 49% 36% 7%
2	N	188	73% 59% 34%
2	O	188	71% 46% 38% 9%
2	P	188	70% 66% 29%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 39744 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 Ribulose bisphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	447	3495	2220	614	644	17	0	0
1	B	447	3495	2220	614	644	17	0	0
1	C	447	3495	2220	614	644	17	0	0
1	D	447	3495	2220	614	644	17	0	0
1	E	447	3495	2220	614	644	17	0	0
1	F	447	3495	2220	614	644	17	0	0
1	G	447	3495	2220	614	644	17	0	0
1	H	447	3495	2220	614	644	17	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	PRO	ASP	conflict	UNP Q31NB3
A	78	ASP	LYS	conflict	UNP Q31NB3
A	100	ASP	TYR	conflict	UNP Q31NB3
B	48	PRO	ASP	conflict	UNP Q31NB3
B	78	ASP	LYS	conflict	UNP Q31NB3
B	100	ASP	TYR	conflict	UNP Q31NB3
C	48	PRO	ASP	conflict	UNP Q31NB3
C	78	ASP	LYS	conflict	UNP Q31NB3
C	100	ASP	TYR	conflict	UNP Q31NB3
D	48	PRO	ASP	conflict	UNP Q31NB3
D	78	ASP	LYS	conflict	UNP Q31NB3
D	100	ASP	TYR	conflict	UNP Q31NB3
E	48	PRO	ASP	conflict	UNP Q31NB3
E	78	ASP	LYS	conflict	UNP Q31NB3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	100	ASP	TYR	conflict	UNP Q31NB3
F	48	PRO	ASP	conflict	UNP Q31NB3
F	78	ASP	LYS	conflict	UNP Q31NB3
F	100	ASP	TYR	conflict	UNP Q31NB3
G	48	PRO	ASP	conflict	UNP Q31NB3
G	78	ASP	LYS	conflict	UNP Q31NB3
G	100	ASP	TYR	conflict	UNP Q31NB3
H	48	PRO	ASP	conflict	UNP Q31NB3
H	78	ASP	LYS	conflict	UNP Q31NB3
H	100	ASP	TYR	conflict	UNP Q31NB3

- Molecule 2 is a protein called Rubisco accumulation factor 1 (RAF1) peptide.

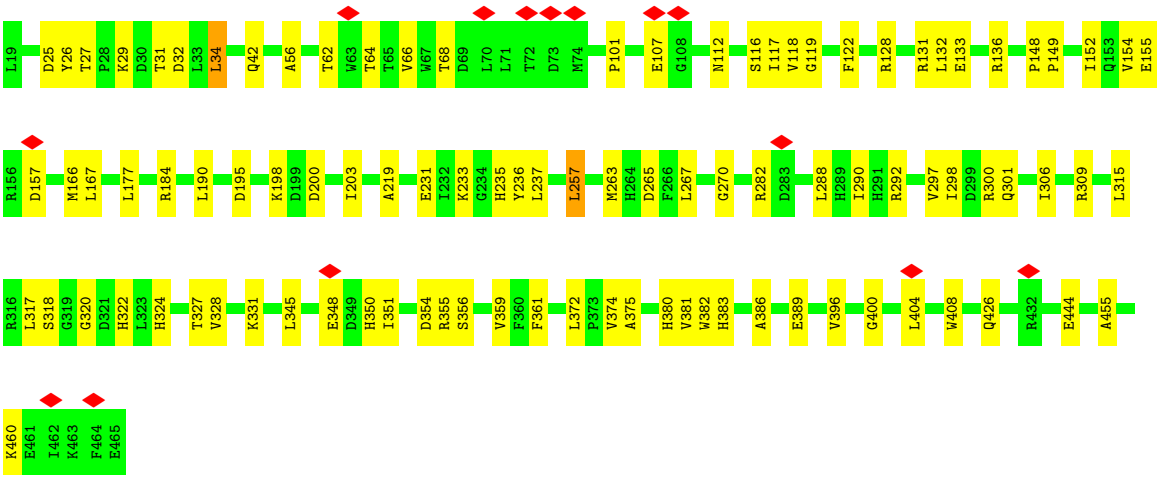
Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	179	Total	C	N	O	S	0	0
			1457	907	275	270	5		
2	J	188	Total	C	N	O	S	0	0
			1523	947	288	283	5		
2	K	179	Total	C	N	O	S	0	0
			1457	907	275	270	5		
2	L	179	Total	C	N	O	S	0	0
			1457	907	275	270	5		
2	M	180	Total	C	N	O	S	0	0
			1465	911	276	273	5		
2	N	181	Total	C	N	O	S	0	0
			1473	917	277	274	5		
2	O	181	Total	C	N	O	S	0	0
			1473	917	277	274	5		
2	P	182	Total	C	N	O	S	0	0
			1479	920	278	276	5		

3 Residue-property plots (i)

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.

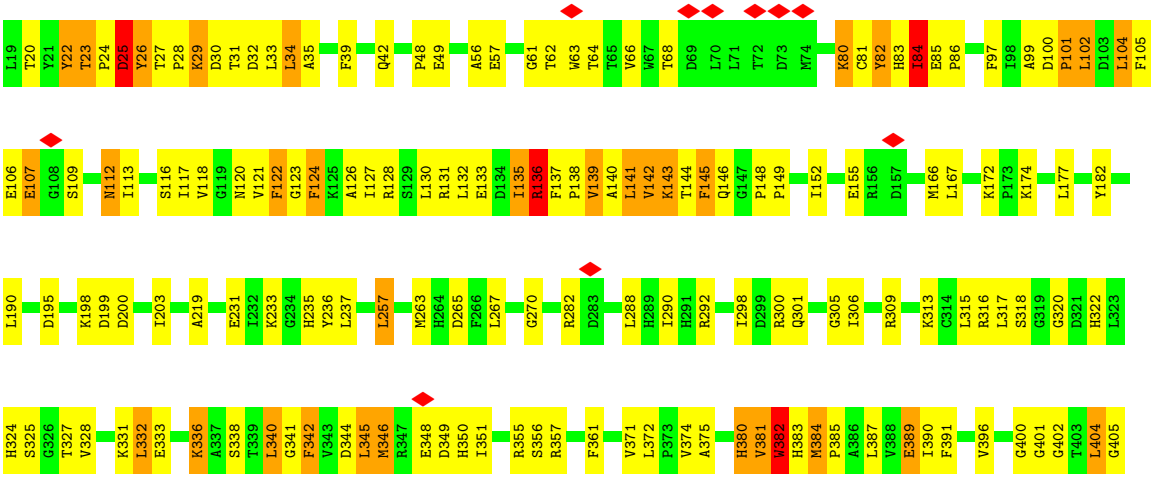
• Molecule 1: Ribulose bisphosphate carboxylase large chain

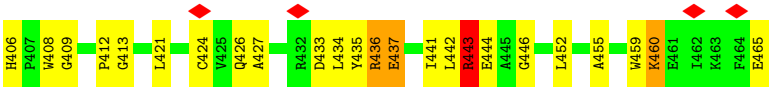
Chain A: 78% 21%



• Molecule 1: Ribulose bisphosphate carboxylase large chain

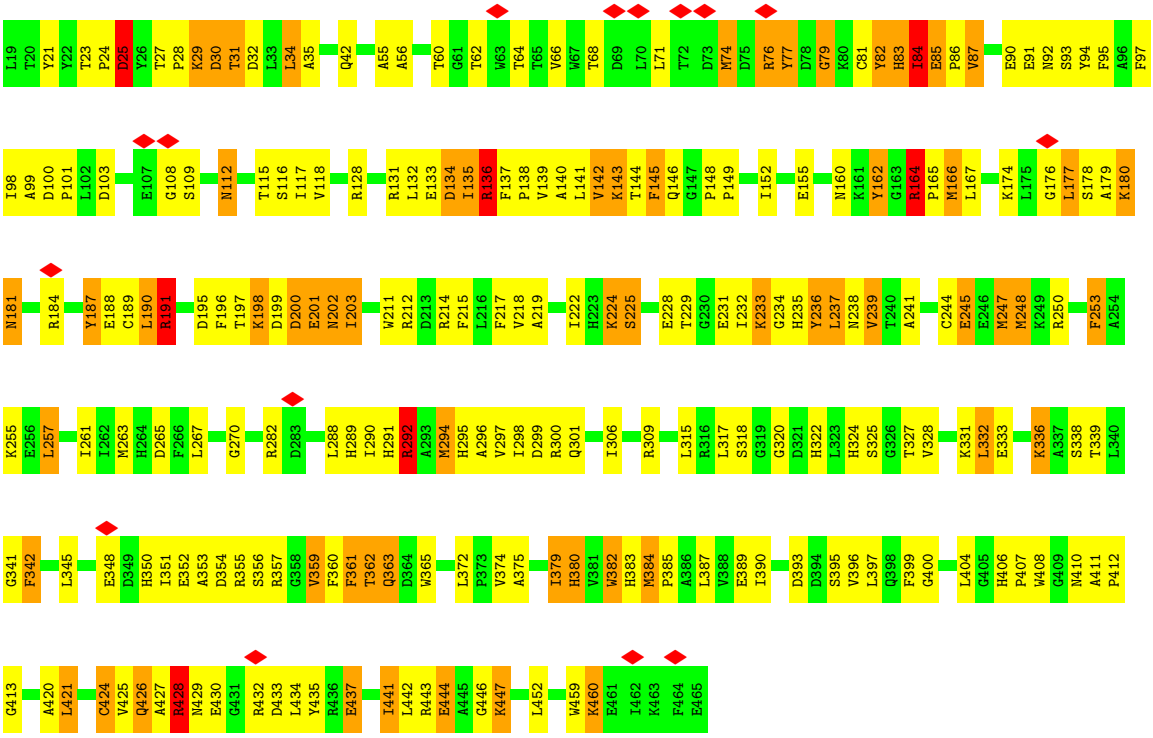
Chain B: 59% 32% 8%





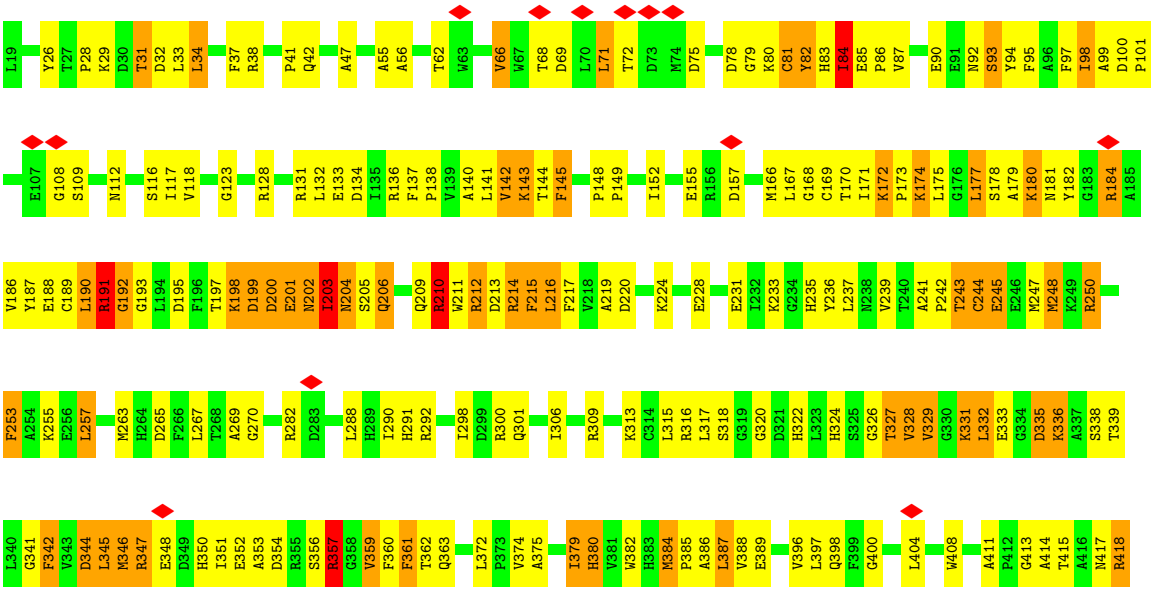
• Molecule 1: Ribulose bisphosphate carboxylase large chain

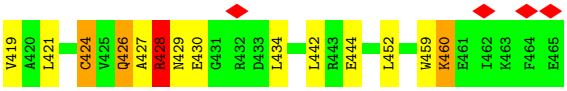
Chain C:



• Molecule 1: Ribulose bisphosphate carboxylase large chain

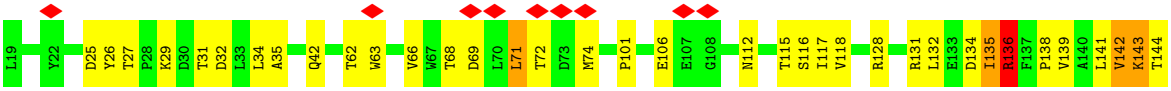
Chain D:

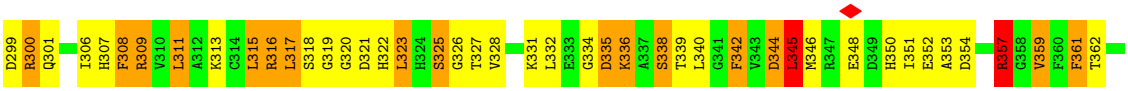


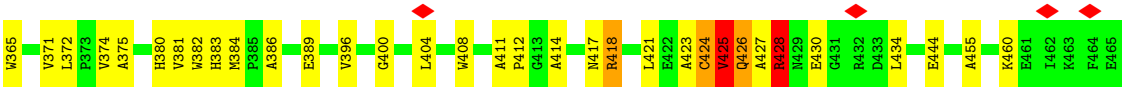


- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain E:

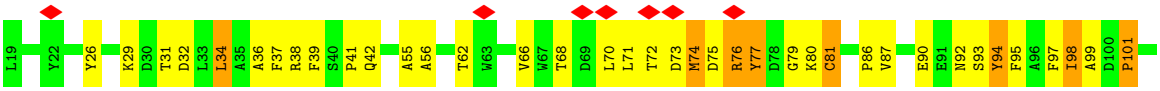


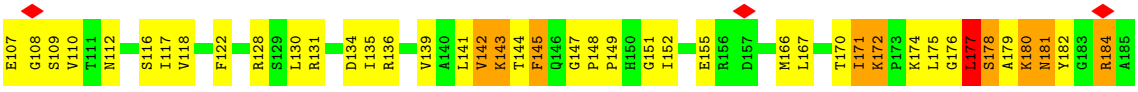


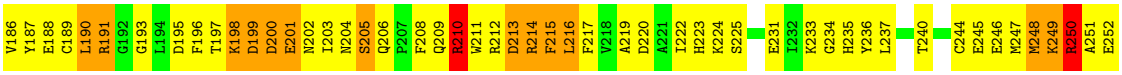


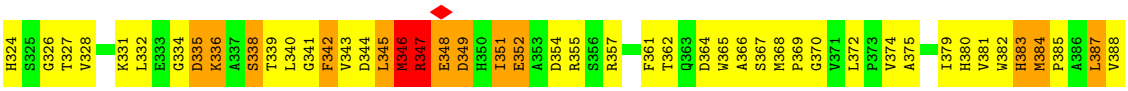
- Molecule 1: Ribulose bisphosphate carboxylase large chain

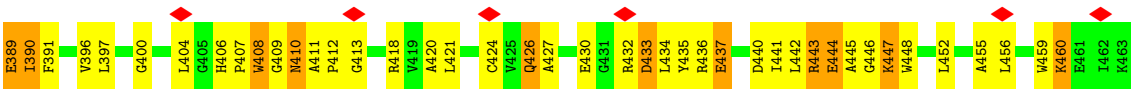
Chain F:

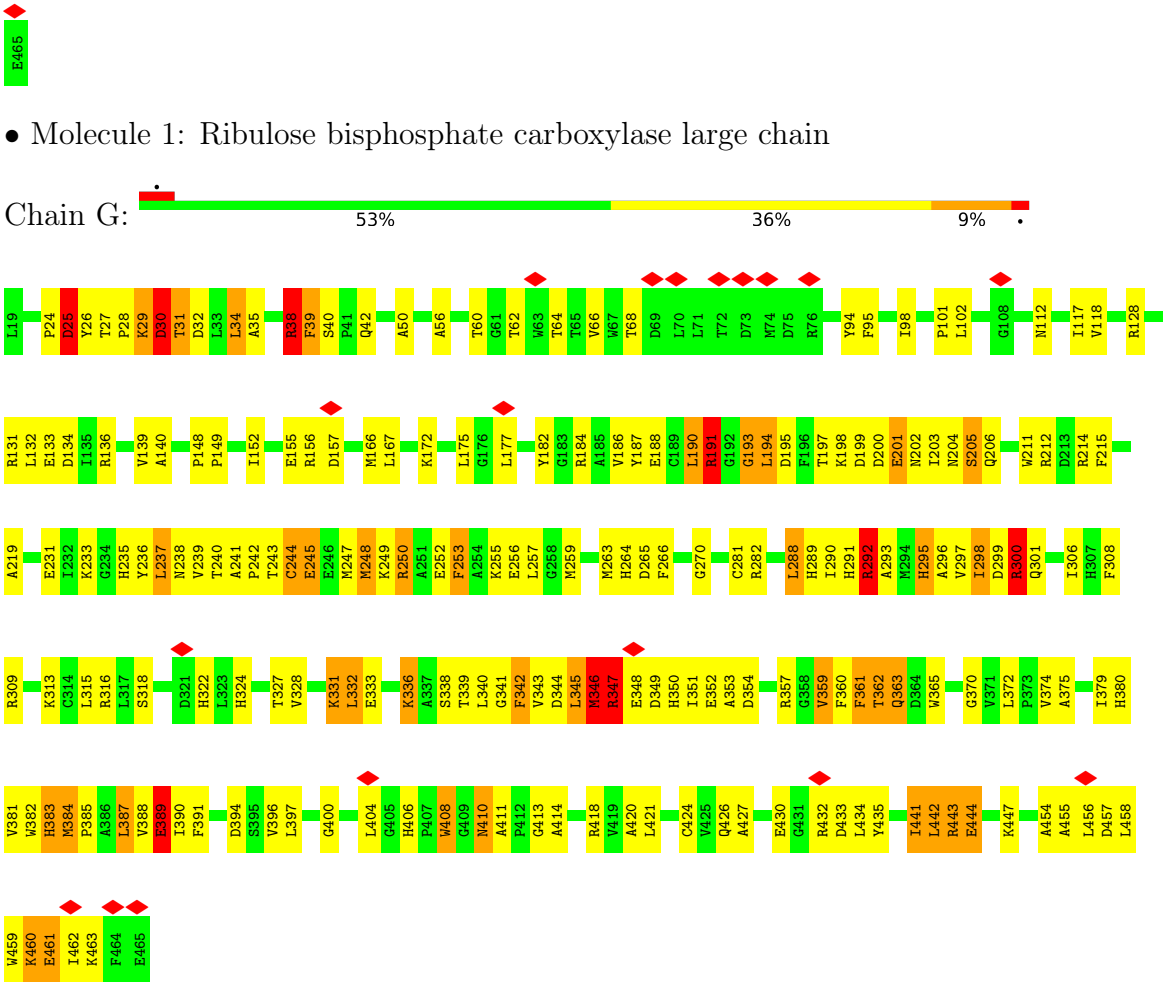






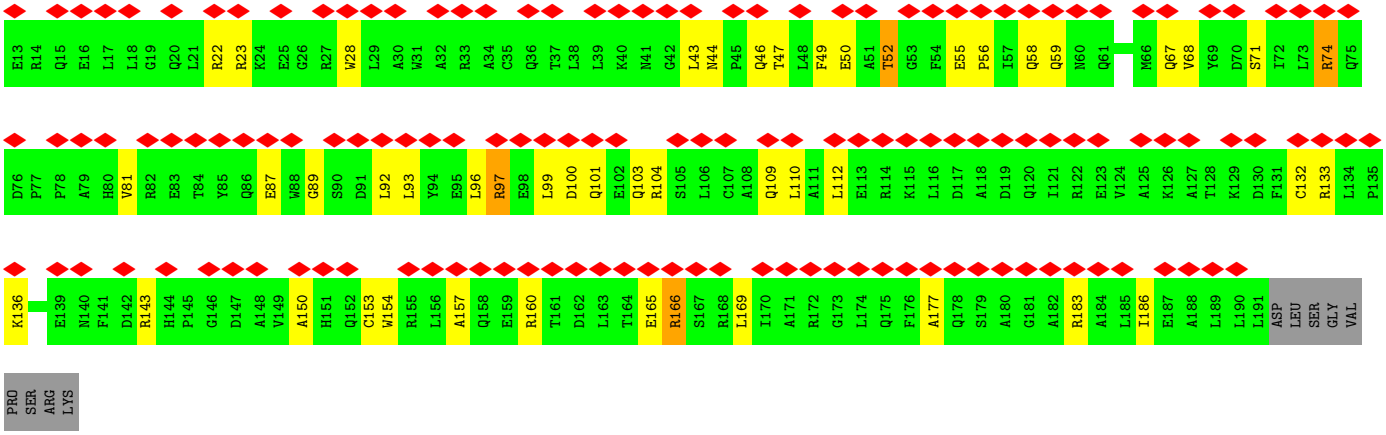





E465
• Molecule 1: Ribulose bisphosphate carboxylase large chain
Chain G:
53%
36%
9%
L19 P24 D25 Y26 T27 P28 K29 D30 T31 D32 L33 L34 A35 R38 F39 S40 P41 Q42 A50 A56 T60 G61 T62 W63 T64 T65 V66 W67 T68 D69 L70 L71 T72 D73 M74 D75 R76 Y94 F95 I98 P101 L102 G108 N112 I117 V118 R128
R131 L132 E133 D134 I135 R136 V139 A140 P148 P149 I152 E155 R156 D157 M166 L167 K172 L175 G176 L177 Y182 G183 R184 A185 V186 Y187 E188 C189 L190 R191 G192 G193 L194 D195 F196 T197 K198 D199 D200 E201 N202 I203 N204 S205 Q206 W211 R212 D213 R214 F215
A219 E231 I232 K233 G234 H235 Y236 L237 N238 V239 T240 A241 P242 T243 C244 E245 E246 M247 M248 K249 R250 A251 E252 F253 A254 K255 E256 L257 G258 M259 M263 H264 D265 F266 G270 C281 R282 L288 H289 I290 H291 R292 A293 M294 H295 A296 V297 I298 D299 R300 Q301 I306 H307 F308
R309 K313 C314 L315 R316 L317 S318 D321 H322 L323 H324 T327 V328 K331 L332 E333 K336 A337 S338 T339 L340 G341 F342 V343 D344 L345 M346 R347 E348 D349 H350 I351 E352 A353 D354 R357 G358 V359 F360 F361 T362 Q363 D364 W365 G370 V371 L372 P373 V374 A375 I379 H380
V381 W382 H383 M384 P385 A386 L387 V388 E389 I390 F391 D394 S395 V396 L397 G400 L404 G405 H406 P407 W408 G409 N410 A411 P412 G413 A414 R418 V419 A420 L421 C424 V425 Q426 A427 E430 G431 R432 D433 L434 Y435 I441 L442 R443 E444 K447 A454 A455 L456 D457 L458
W459 K460 E461 I462 K463 F464 E465
• Molecule 1: Ribulose bisphosphate carboxylase large chain
Chain H:
56%
34%
10%
L19 T20 Y21 Y22 T23 P24 D25 Y26 T27 P28 K29 D30 T31 D32 L33 L34 F37 R38 P41 Q42 A47 P48 E49 A55 A56 T62 W63 V66 W67 T68 D69 L70 L71 T72 D73 M74 D75 D78 G79 K80 C81 Y82 H83 I84 E85 P86 V87 E90 E91 N92 S93 Y94
F95 A96 F97 I98 A99 D100 P101 E107 G108 N112 I117 V118 F122 R128 R131 L132 E133 R136 A140 P148 P149 I152 E155 R156 D157 M166 L167 K172 P173 K174 L177 S178 A179 K180 N181 Y182 G183 R184 Y187 E188 C189 L190 R191 G192 G193
L194 D195 K198 D199 D200 E201 N202 I203 R210 W211 R212 D213 R214 F217 Y218 A219 D220 A221 I222 H223 K224 S225 E231 I232 K233 G234 H235 Y236 L237 K249 L257 M263 H264 D265 F266 L267 G270 R282 L288 H289 I290 H291 R292 A293 M294 H295 A296 V297 I298 D299
R300 Q301 I306 R309 K313 C314 L315 R316 L317 S318 G319 G320 D321 H322 L323 H324 T327 V328 K331 L332 E333 G334 D335 K336 A337 S338 T339 L340 G341 F342 V343 D344 L345 M346 R347 E348 D349 H350 I351 R357 F361 V371 L372 P373 V374 A375 I379 H380 V381 W382 H383
M384 P385 A386 L387 V388 E389 V396 L397 G400 L404 W408 G409 N410 A411 C424 V425 Q426 A427 R428 M429 E430 G431 R432 D433 L434 Y435 R436 E437 I441 L442 R443 E444 A445 G446 K447 A455 L456 W459 K460 E461 I462 K463 F464 E465

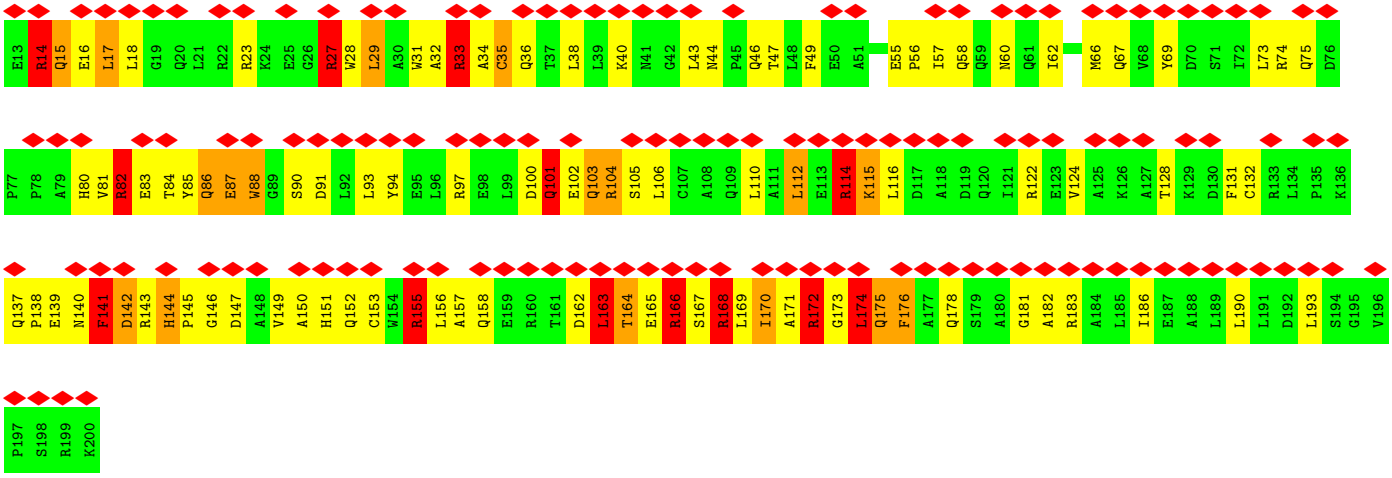
• Molecule 2: Rubisco accumulation factor 1 (RAF1) peptide

Chain I:



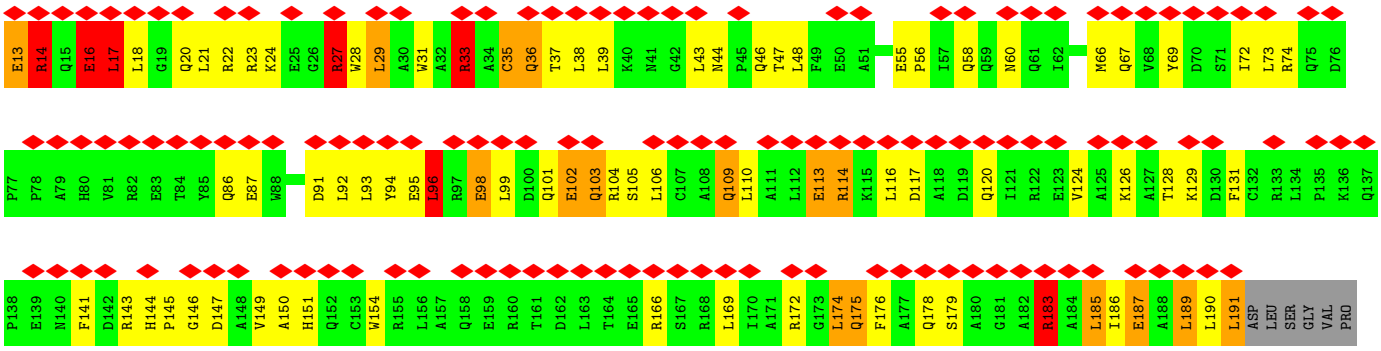
• Molecule 2: Rubisco accumulation factor 1 (RAF1) peptide

Chain J:



• Molecule 2: Rubisco accumulation factor 1 (RAF1) peptide

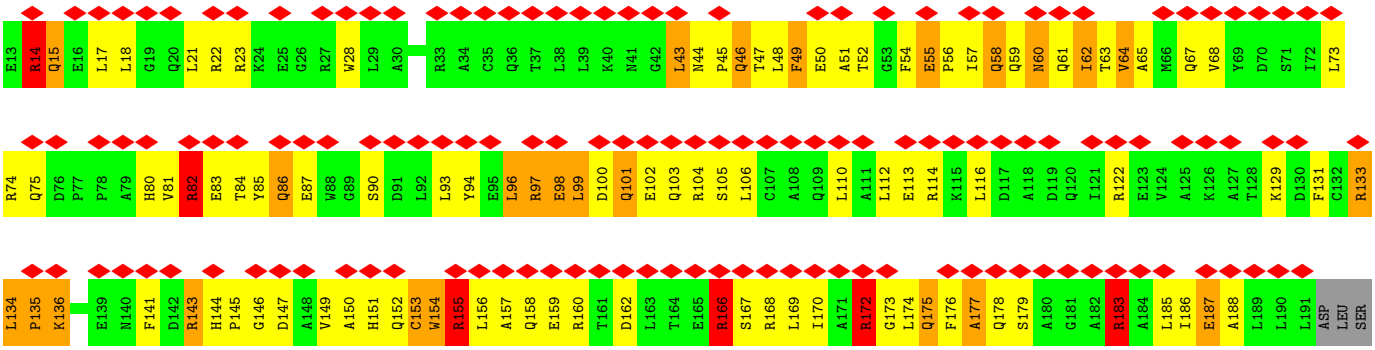
Chain K:



SER ARG LYS

• Molecule 2: Rubisco accumulation factor 1 (RAF1) peptide

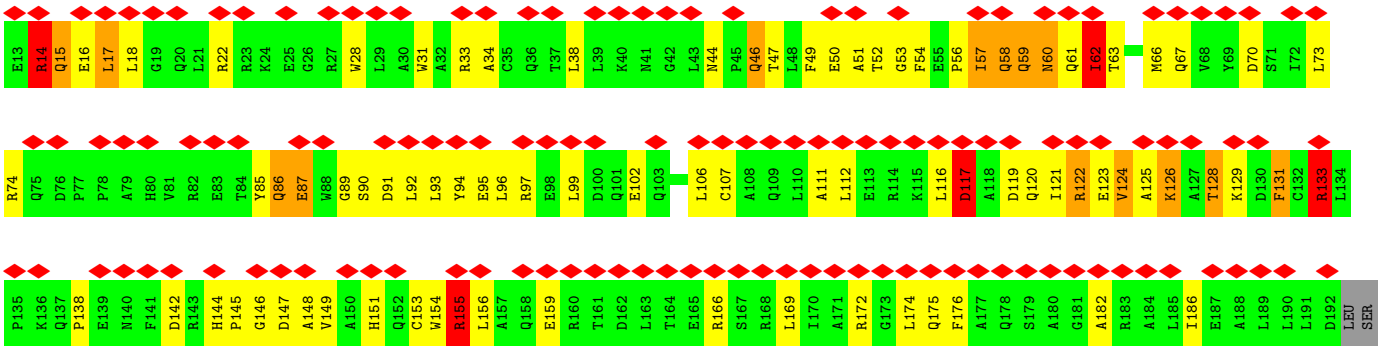
Chain L:



GLY VAL PRO SER ARG LYS

• Molecule 2: Rubisco accumulation factor 1 (RAF1) peptide

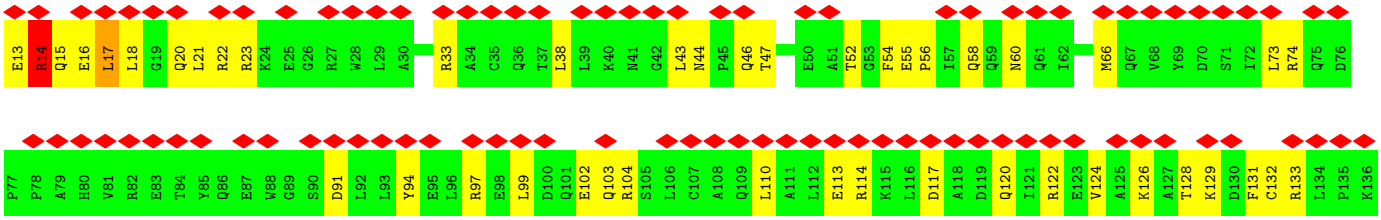
Chain M:

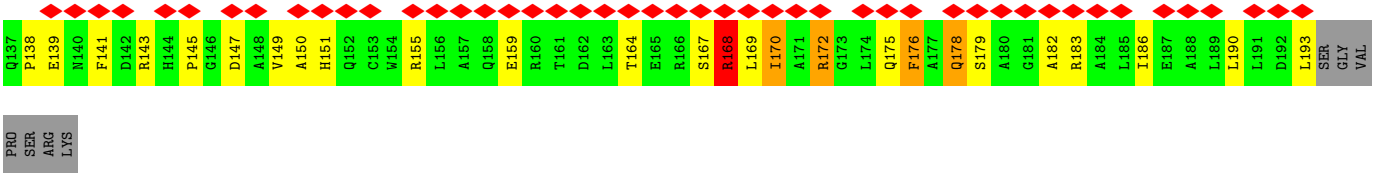


GLY VAL PRO SER ARG LYS

• Molecule 2: Rubisco accumulation factor 1 (RAF1) peptide

Chain N:





• Molecule 2: Rubisco accumulation factor 1 (RAF1) peptide

Chain O:

• Molecule 2: Rubisco accumulation factor 1 (RAF1) peptide

Chain P:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16022	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	300.0, 300.0, 300.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.25, 1.25, 1.25	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	0.37	0/3584	0.62	1/4860 (0.0%)
1	B	0.44	0/3584	0.60	1/4860 (0.0%)
1	C	0.48	0/3584	0.60	1/4860 (0.0%)
1	D	0.47	0/3584	0.60	0/4860
1	E	0.46	0/3584	0.60	0/4860
1	F	0.49	0/3584	0.59	0/4860
1	G	0.45	0/3584	0.59	0/4860
1	H	0.45	0/3584	0.59	1/4860 (0.0%)
2	I	0.37	0/1482	0.76	2/2002 (0.1%)
2	J	0.47	0/1549	0.69	2/2092 (0.1%)
2	K	0.46	0/1482	0.65	1/2002 (0.0%)
2	L	0.49	0/1482	0.65	2/2002 (0.1%)
2	M	0.43	0/1490	0.70	3/2013 (0.1%)
2	N	0.39	0/1498	0.68	1/2024 (0.0%)
2	O	0.46	0/1498	0.68	3/2024 (0.1%)
2	P	0.37	0/1504	0.68	2/2032 (0.1%)
All	All	0.45	0/40657	0.63	20/55071 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	8
1	D	0	11
1	E	0	9
1	F	0	12
1	G	0	8
1	H	0	6
2	I	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	J	0	9
2	K	0	6
2	L	0	9
2	M	0	4
2	N	0	2
2	O	0	6
2	P	0	1
All	All	0	98

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	73	LEU	CA-CB-CG	6.58	130.43	115.30
2	O	73	LEU	CA-CB-CG	6.28	129.75	115.30
2	P	73	LEU	CA-CB-CG	6.20	129.56	115.30
2	N	73	LEU	CA-CB-CG	6.19	129.54	115.30
2	K	73	LEU	CA-CB-CG	6.15	129.45	115.30

There are no chirality outliers.

5 of 98 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	THR	Peptide
1	A	318	SER	Peptide
1	B	136	ARG	Sidechain
1	B	318	SER	Peptide
1	B	443	ARG	Sidechain

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	3495	0	3408	94	0
1	B	3495	0	3405	385	0
1	C	3495	0	3398	554	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3495	0	3399	493	0
1	E	3495	0	3402	404	0
1	F	3495	0	3396	586	0
1	G	3495	0	3401	476	0
1	H	3495	0	3404	374	0
2	I	1457	0	1449	58	0
2	J	1523	0	1511	271	0
2	K	1457	0	1446	190	0
2	L	1457	0	1448	247	0
2	M	1465	0	1452	144	0
2	N	1473	0	1464	84	0
2	O	1473	0	1463	139	0
2	P	1479	0	1469	69	0
All	All	39744	0	38915	4195	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 53.

The worst 5 of 4195 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:236:TYR:CE2	1:F:289:HIS:CE1	1.78	1.67
1:C:408:TRP:CH2	2:J:23:ARG:HD2	1.14	1.64
1:F:236:TYR:CD2	1:F:289:HIS:CE1	1.85	1.64
1:F:219:ALA:HB1	1:F:257:LEU:CD1	1.26	1.64
1:A:122:PHE:CD2	1:H:297:VAL:HG23	1.29	1.62

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	445/447 (100%)	402 (90%)	41 (9%)	2 (0%)	34	72
1	B	445/447 (100%)	389 (87%)	44 (10%)	12 (3%)	5	34
1	C	445/447 (100%)	384 (86%)	50 (11%)	11 (2%)	5	35
1	D	445/447 (100%)	379 (85%)	56 (13%)	10 (2%)	6	38
1	E	445/447 (100%)	388 (87%)	45 (10%)	12 (3%)	5	34
1	F	445/447 (100%)	362 (81%)	69 (16%)	14 (3%)	4	31
1	G	445/447 (100%)	383 (86%)	49 (11%)	13 (3%)	4	32
1	H	445/447 (100%)	387 (87%)	50 (11%)	8 (2%)	8	42
2	I	177/188 (94%)	146 (82%)	31 (18%)	0	100	100
2	J	186/188 (99%)	147 (79%)	30 (16%)	9 (5%)	2	23
2	K	177/188 (94%)	155 (88%)	17 (10%)	5 (3%)	5	33
2	L	177/188 (94%)	143 (81%)	27 (15%)	7 (4%)	3	26
2	M	178/188 (95%)	147 (83%)	26 (15%)	5 (3%)	5	33
2	N	179/188 (95%)	159 (89%)	20 (11%)	0	100	100
2	O	179/188 (95%)	153 (86%)	24 (13%)	2 (1%)	14	52
2	P	180/188 (96%)	162 (90%)	18 (10%)	0	100	100
All	All	4993/5080 (98%)	4286 (86%)	597 (12%)	110 (2%)	10	38

5 of 110 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	32	ASP
1	B	84	ILE
1	C	30	ASP
1	C	84	ILE
1	D	84	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/363 (100%)	353 (97%)	10 (3%)	43	65
1	B	363/363 (100%)	315 (87%)	48 (13%)	4	20
1	C	363/363 (100%)	292 (80%)	71 (20%)	1	9
1	D	363/363 (100%)	288 (79%)	75 (21%)	1	7
1	E	363/363 (100%)	296 (82%)	67 (18%)	1	11
1	F	363/363 (100%)	269 (74%)	94 (26%)	0	4
1	G	363/363 (100%)	303 (84%)	60 (16%)	2	14
1	H	363/363 (100%)	312 (86%)	51 (14%)	3	19
2	I	151/159 (95%)	147 (97%)	4 (3%)	46	67
2	J	159/159 (100%)	124 (78%)	35 (22%)	1	6
2	K	151/159 (95%)	122 (81%)	29 (19%)	1	9
2	L	151/159 (95%)	122 (81%)	29 (19%)	1	9
2	M	152/159 (96%)	131 (86%)	21 (14%)	3	20
2	N	153/159 (96%)	141 (92%)	12 (8%)	12	38
2	O	153/159 (96%)	130 (85%)	23 (15%)	3	17
2	P	154/159 (97%)	147 (96%)	7 (4%)	27	54
All	All	4128/4176 (99%)	3492 (85%)	636 (15%)	6	16

5 of 636 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	346	MET
2	M	14	ARG
2	I	46	GLN
1	H	345	LEU
2	K	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	75	GLN
2	N	175	GLN
2	L	103	GLN
2	M	60	ASN
2	O	67	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

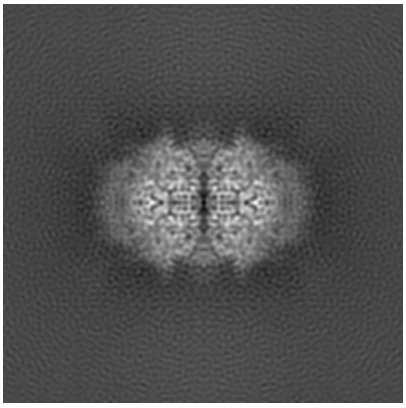
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10235. These allow visual inspection of the internal detail of the map and identification of artifacts.

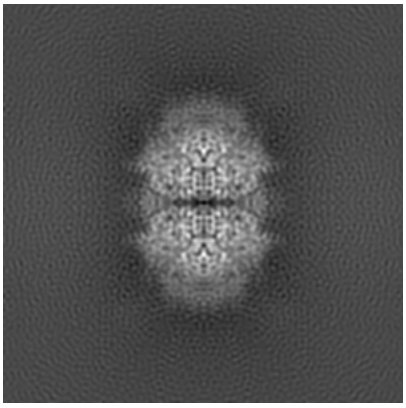
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

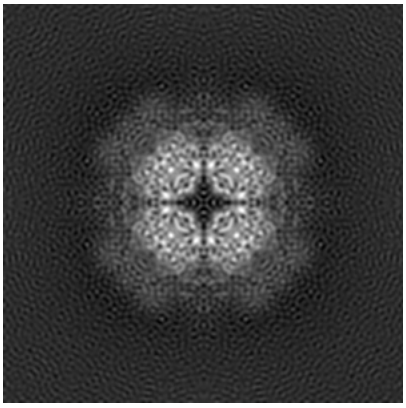
6.1.1 Primary map



X



Y

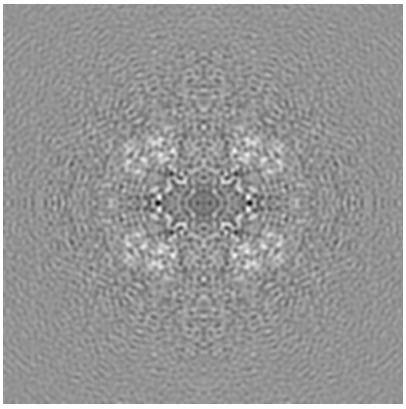


Z

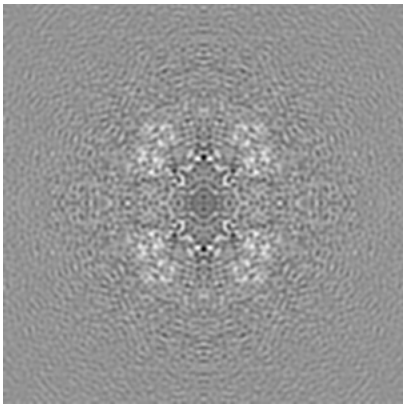
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

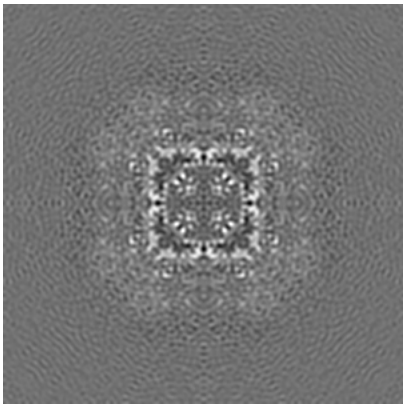
6.2.1 Primary map



X Index: 120



Y Index: 120

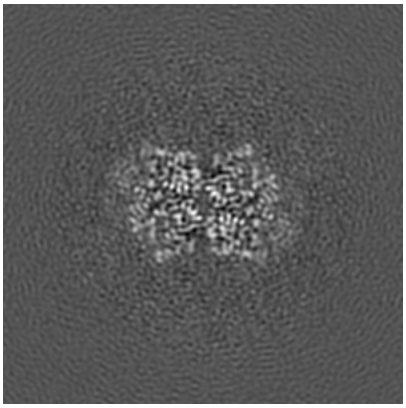


Z Index: 120

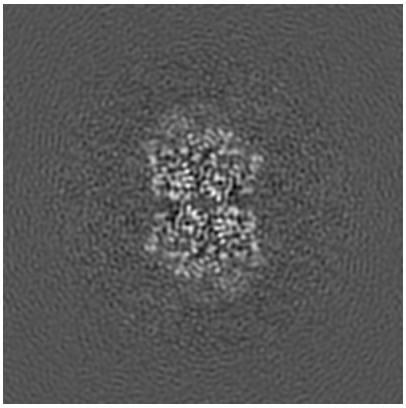
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

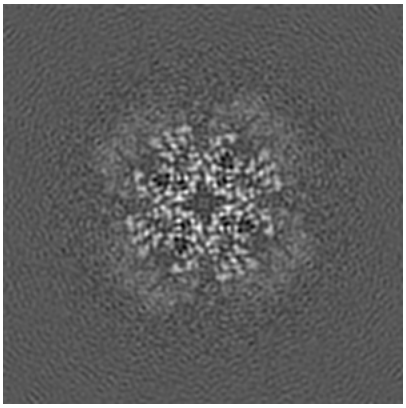
6.3.1 Primary map



X Index: 105



Y Index: 135



Z Index: 129

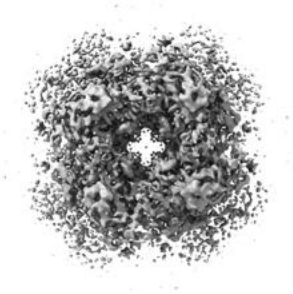
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

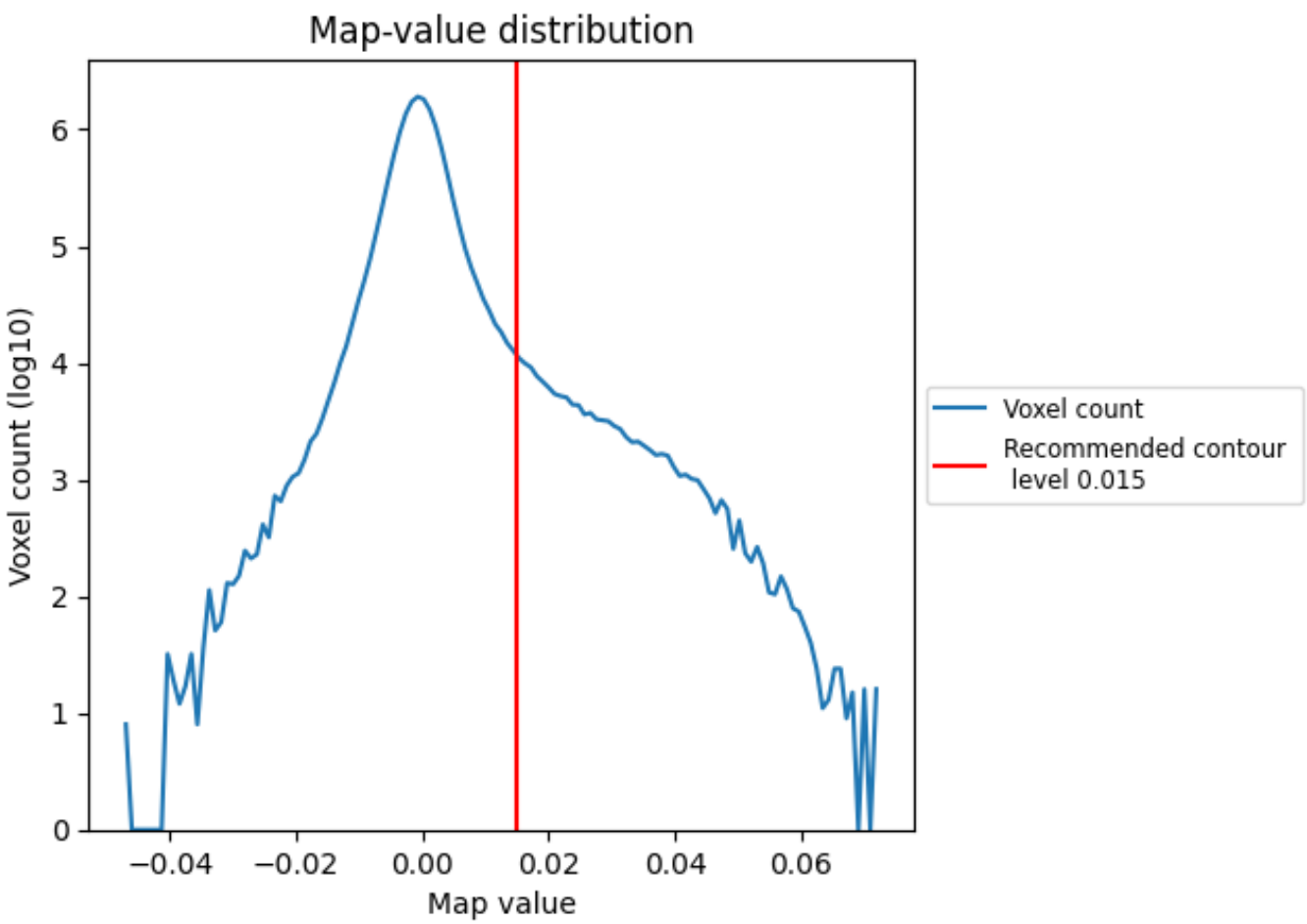
6.5 Mask visualisation (i)

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

7 Map analysis (i)

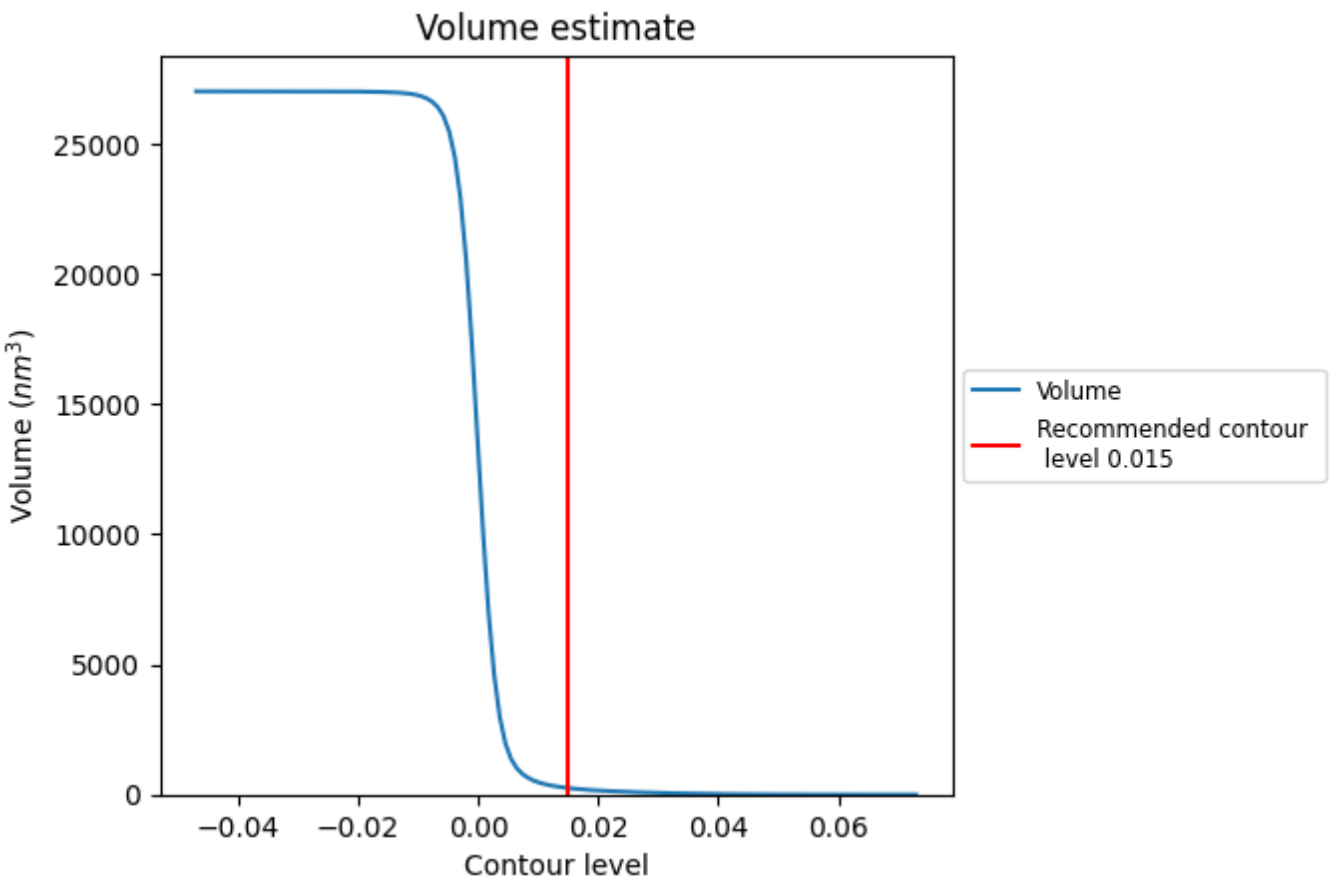
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

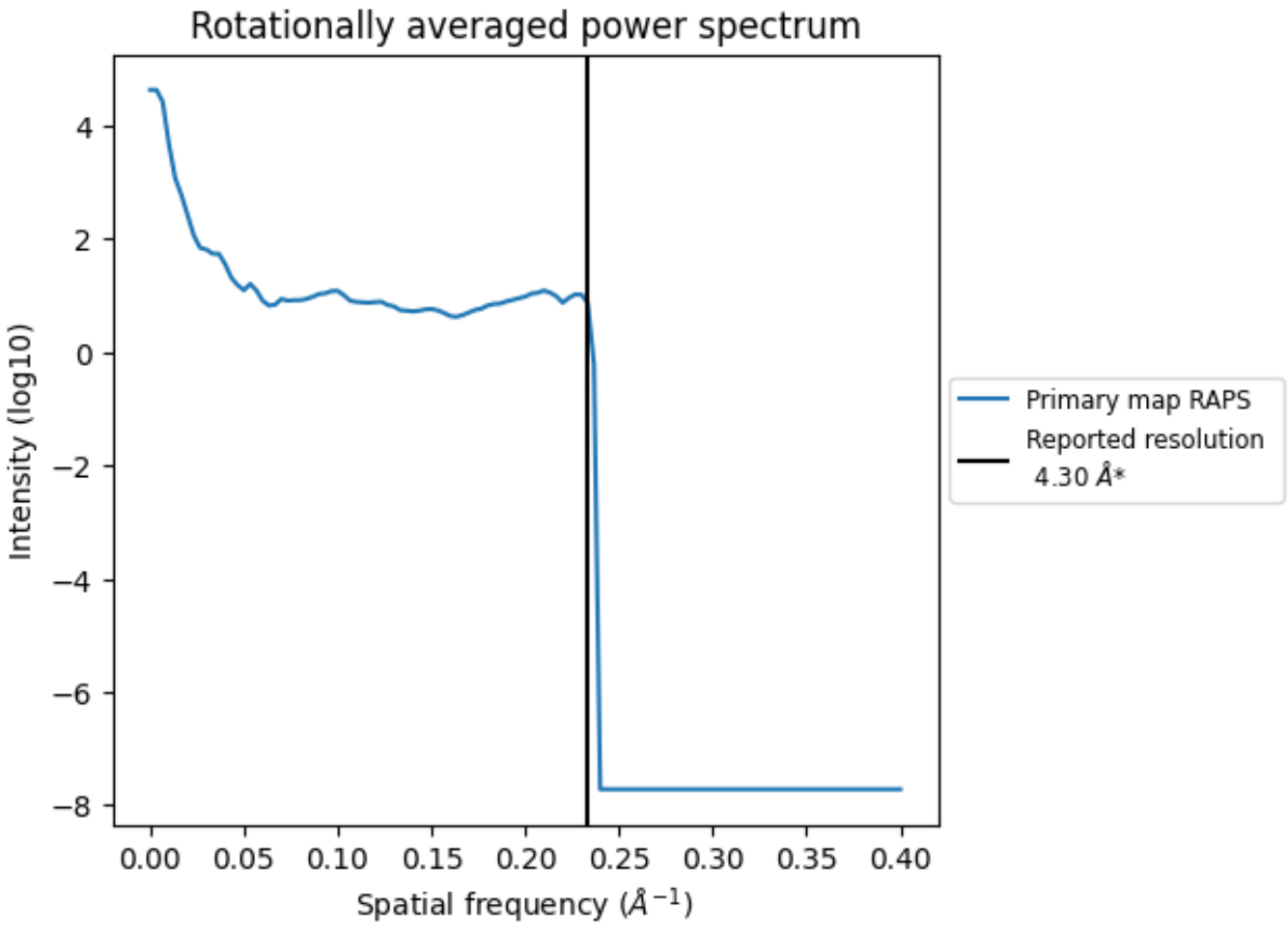
7.2 Volume estimate (i)



The volume at the recommended contour level is 252 nm^3; this corresponds to an approximate mass of 227 kDa.

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

7.3 Rotationally averaged power spectrum (i)

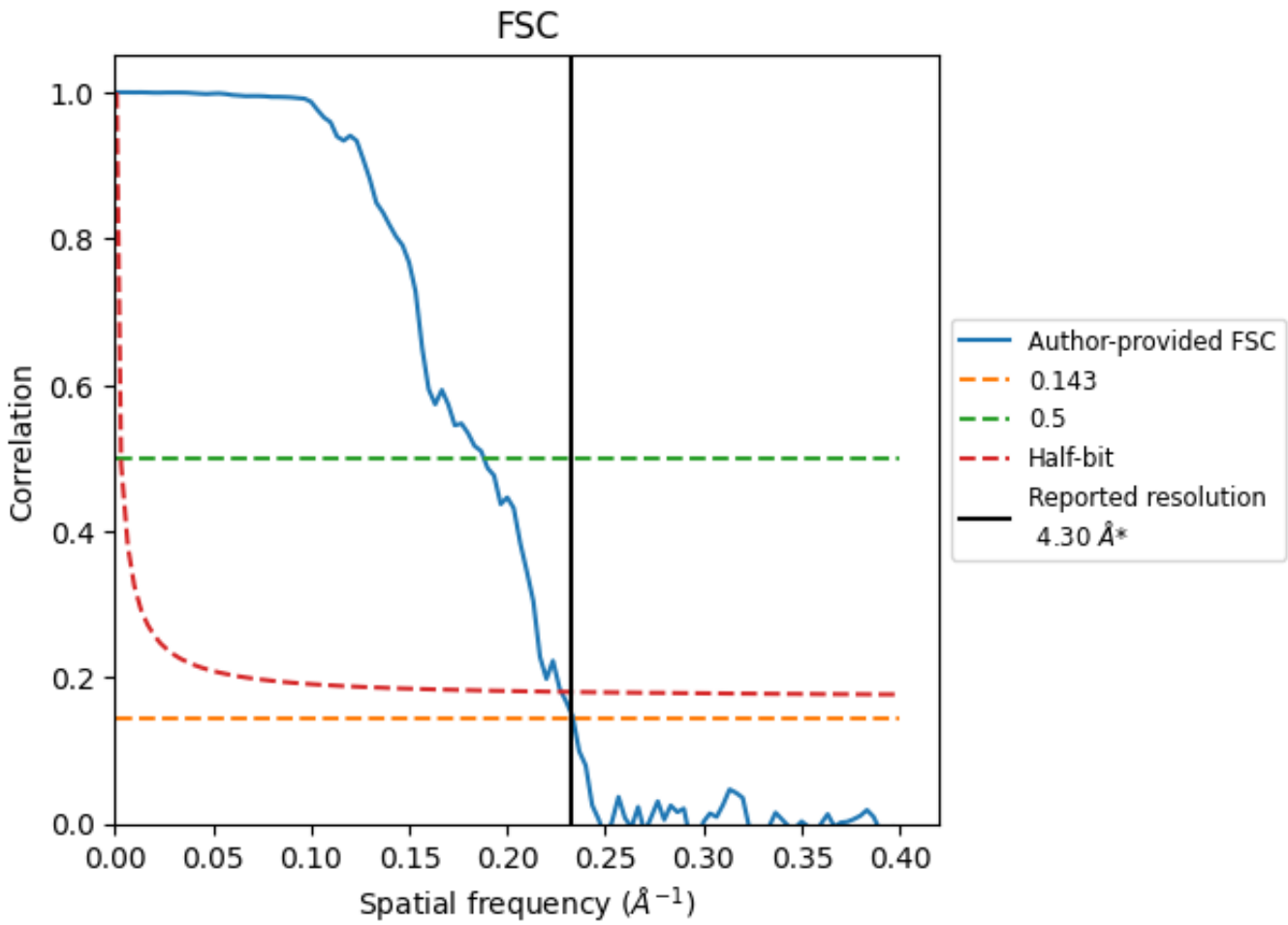


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8.2 Resolution estimates (i)

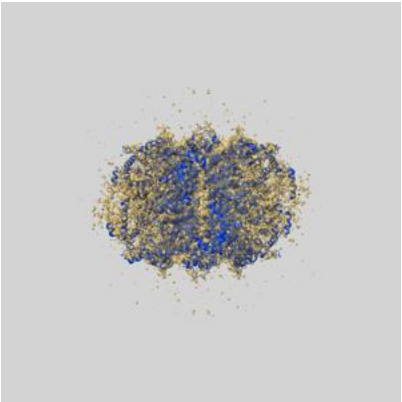
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.28	5.32	4.40
Unmasked-calculated*	-	-	-

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

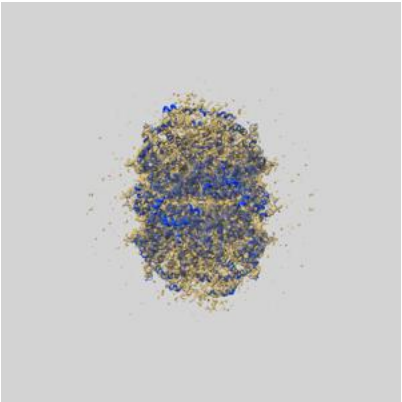
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10235 and PDB model 6SMH. Per-residue inclusion information can be found in section 3 on page 6.

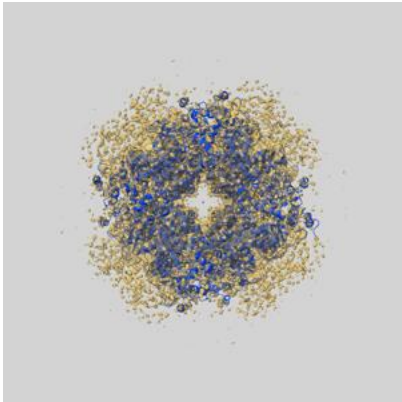
9.1 Map-model overlay (i)



X



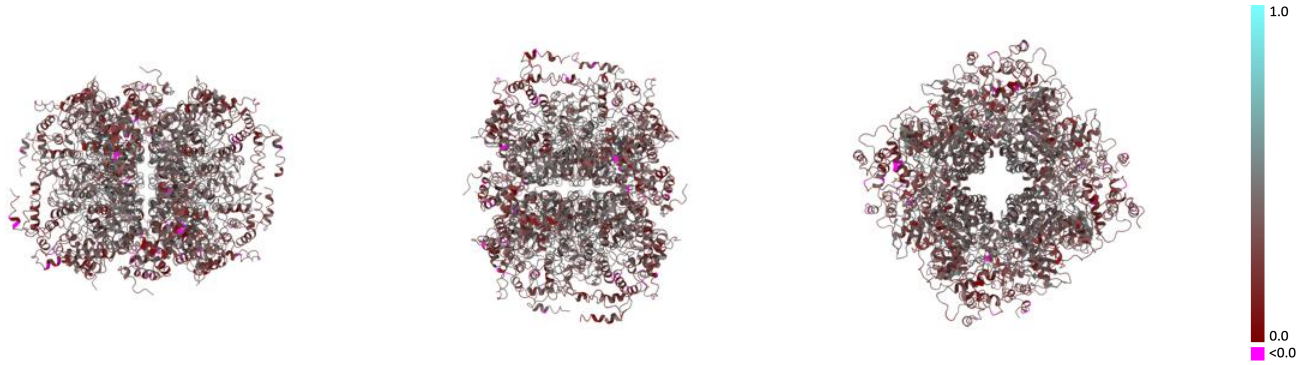
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

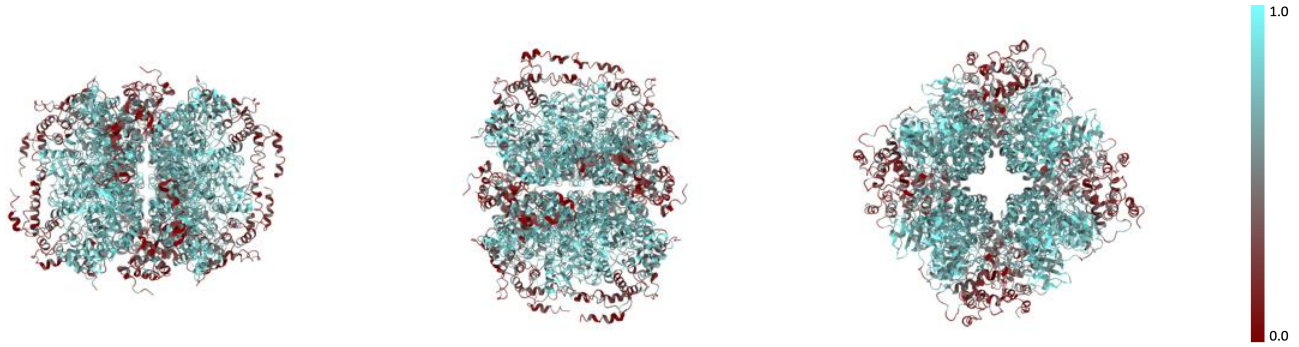
9.2 Q-score mapped to coordinate model (i)



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.

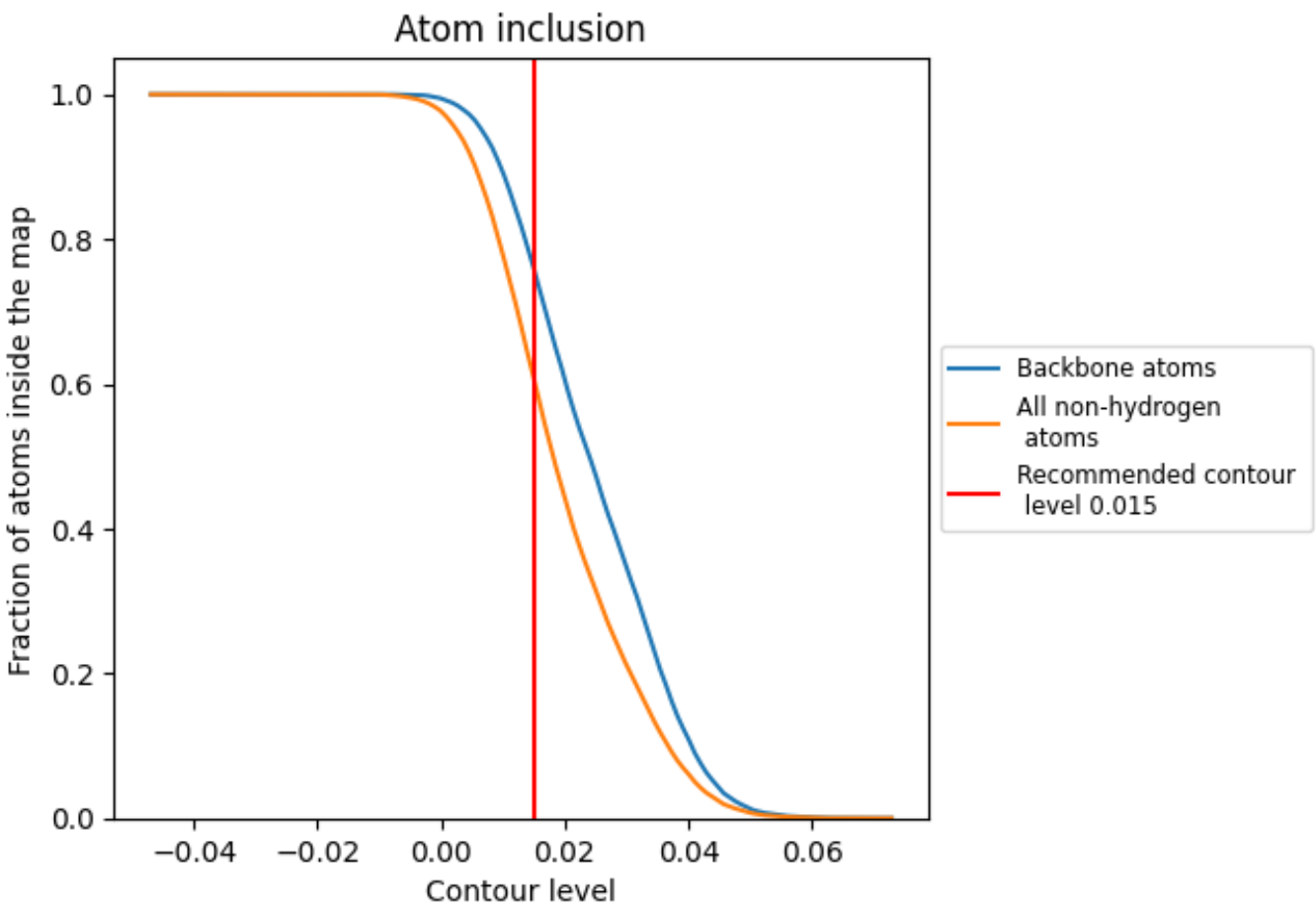
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 61% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6084	0.3540
A	0.7331	0.3700
B	0.7419	0.3830
C	0.7559	0.3890
D	0.7515	0.3890
E	0.7530	0.3880
F	0.7510	0.3880
G	0.7565	0.3880
H	0.7507	0.3870
I	0.2578	0.2460
J	0.2724	0.2960
K	0.2684	0.2870
L	0.2812	0.3100
M	0.2803	0.2930
N	0.2661	0.2700
O	0.2794	0.2870
P	0.2629	0.2640