



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 08:01 PM UTC

PDB ID : 6QG5 / pdb_00006qg5
EMDB ID : EMD-4547
Title : Structure of eIF2B-eIF2 (phosphorylated at Ser51) complex (model C)
Authors : Llacer, J.L.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on : 2019-01-10
Resolution : 10.10 Å (reported)
Based on initial models : 5B04, 6FYX

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

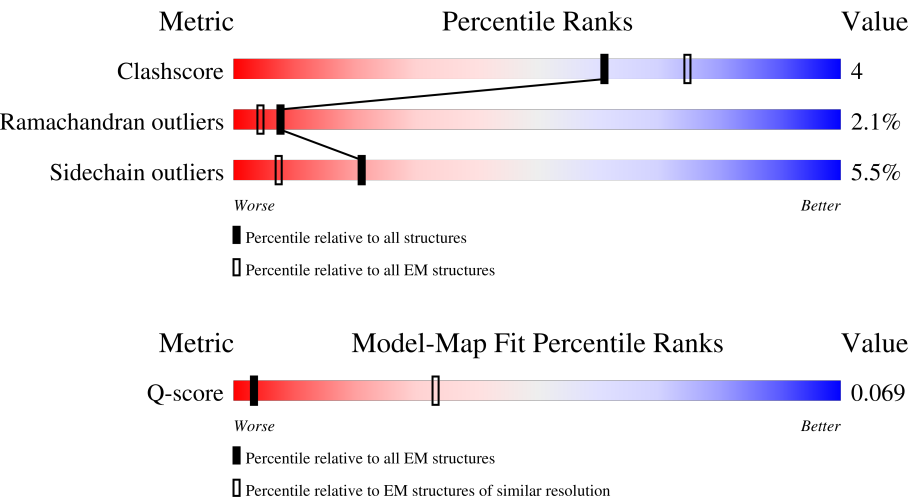
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 10.10 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	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	127 (9.60 - 10.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	305	
1	B	305	
2	C	381	
2	D	381	

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Mol	Chain	Length	Quality of chain
3	E	578	
3	F	578	
4	G	651	
4	H	651	
5	I	712	
5	J	712	
6	K	304	
6	L	304	
7	M	527	
7	N	527	
8	O	285	
8	P	285	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 37875 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 Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	302	Total	C	N	O	S	0	0
			2351	1504	394	443	10		
1	B	302	Total	C	N	O	S	0	0
			2351	1504	394	443	10		

- Molecule 2 is a protein called Translation initiation factor eIF-2B subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	345	Total	C	N	O	S	0	0
			2665	1694	463	502	6		
2	D	345	Total	C	N	O	S	0	0
			2665	1694	463	502	6		

- Molecule 3 is a protein called Translation initiation factor eIF-2B subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	267	Total	C	N	O	S	0	0
			2164	1391	363	400	10		
3	F	267	Total	C	N	O	S	0	0
			2164	1391	363	400	10		

- Molecule 4 is a protein called Translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	355	Total	C	N	O	S	0	0
			2744	1738	474	521	11		
4	H	355	Total	C	N	O	S	0	0
			2744	1738	474	521	11		

- Molecule 5 is a protein called Translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	431	Total	C	N	O	S	0	0
			3406	2147	573	666	20		
5	J	431	Total	C	N	O	S	0	0
			3406	2147	573	666	20		

- Molecule 6 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	246	Total	C	N	O	P S	0	0
			1974	1259	324	382	1 8		
6	L	246	Total	C	N	O	P S	0	0
			1974	1259	324	382	1 8		

- Molecule 7 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	408	Total	C	N	O	S	0	0
			3044	1934	546	548	16		
7	N	408	Total	C	N	O	S	0	0
			3044	1934	546	548	16		

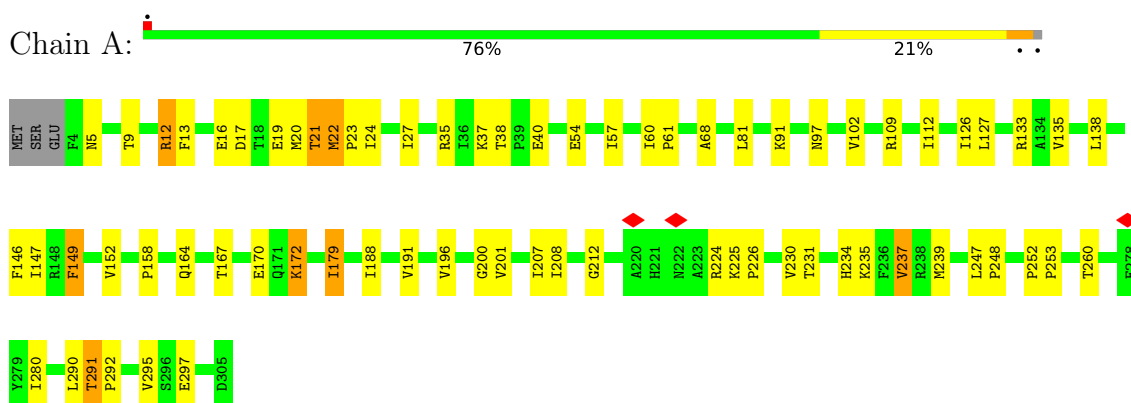
- Molecule 8 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	17	Total	C	N	O		0	0
			143	96	24	23			
8	P	128	Total	C	N	O	S	0	0
			1036	661	186	182	7		

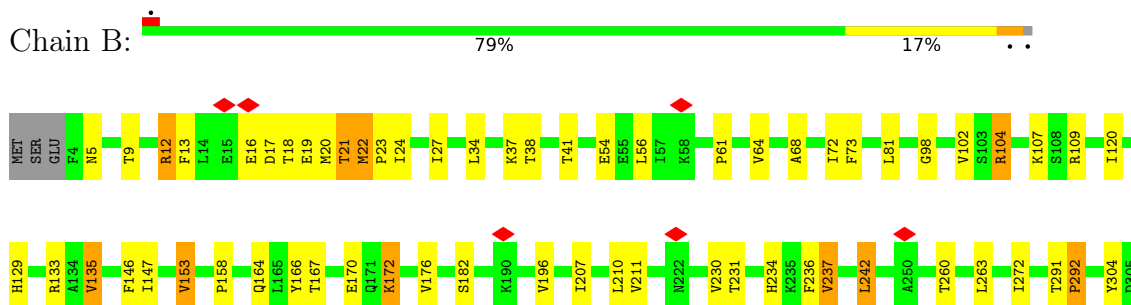
3 Residue-property plots

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.

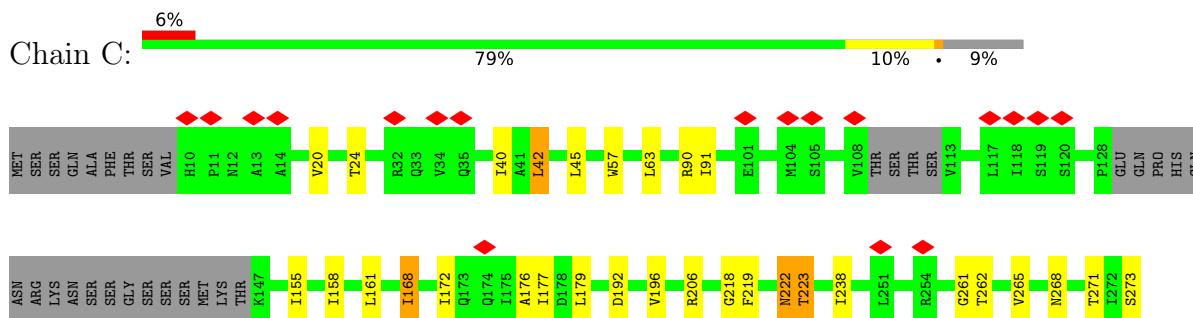
- Molecule 1: Translation initiation factor eIF-2B subunit alpha

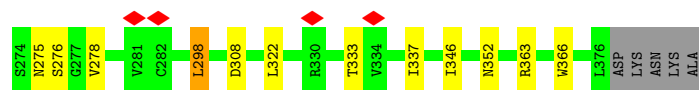


- Molecule 1: Translation initiation factor eIF-2B subunit alpha

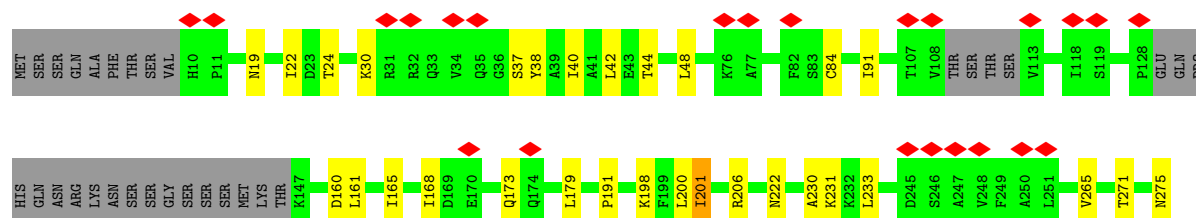
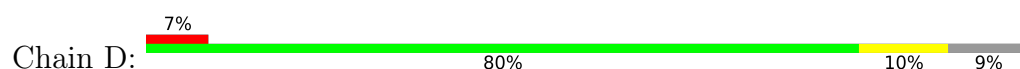


- Molecule 2: Translation initiation factor eIF-2B subunit beta

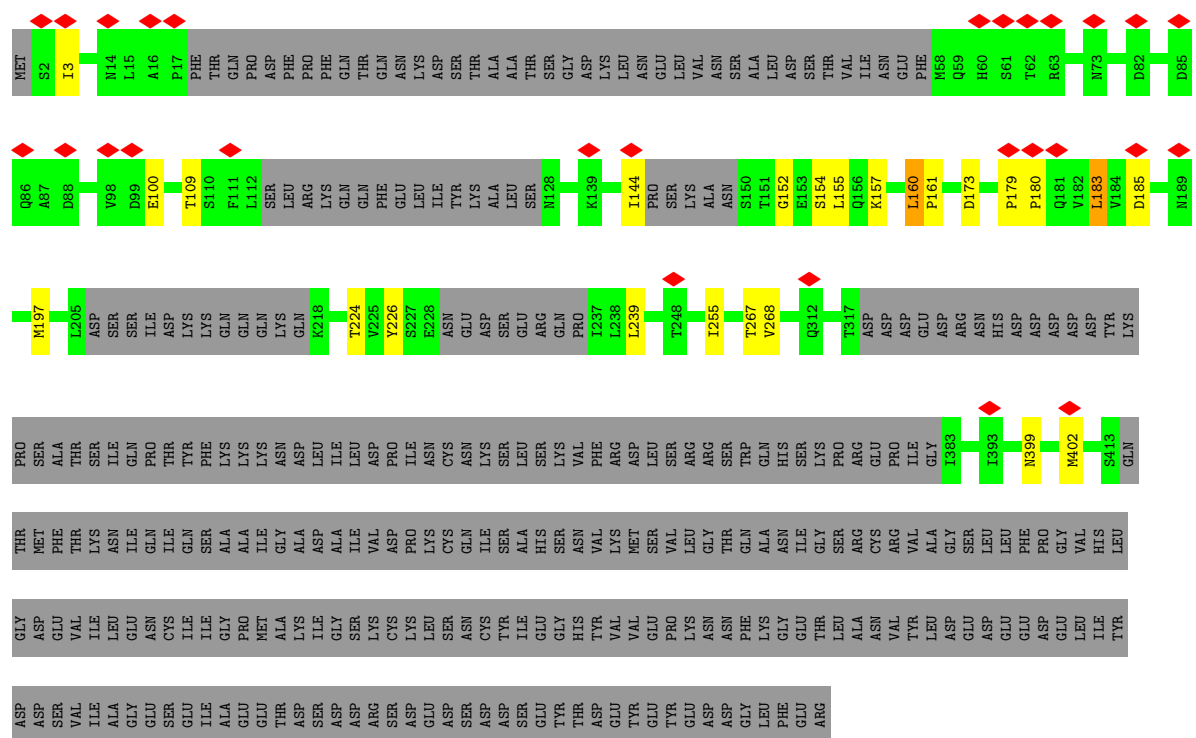
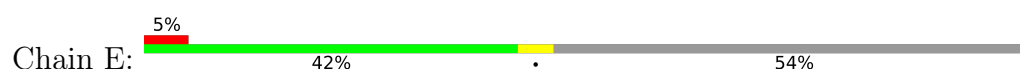




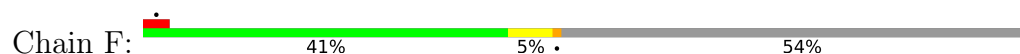
- Molecule 2: Translation initiation factor eIF-2B subunit beta



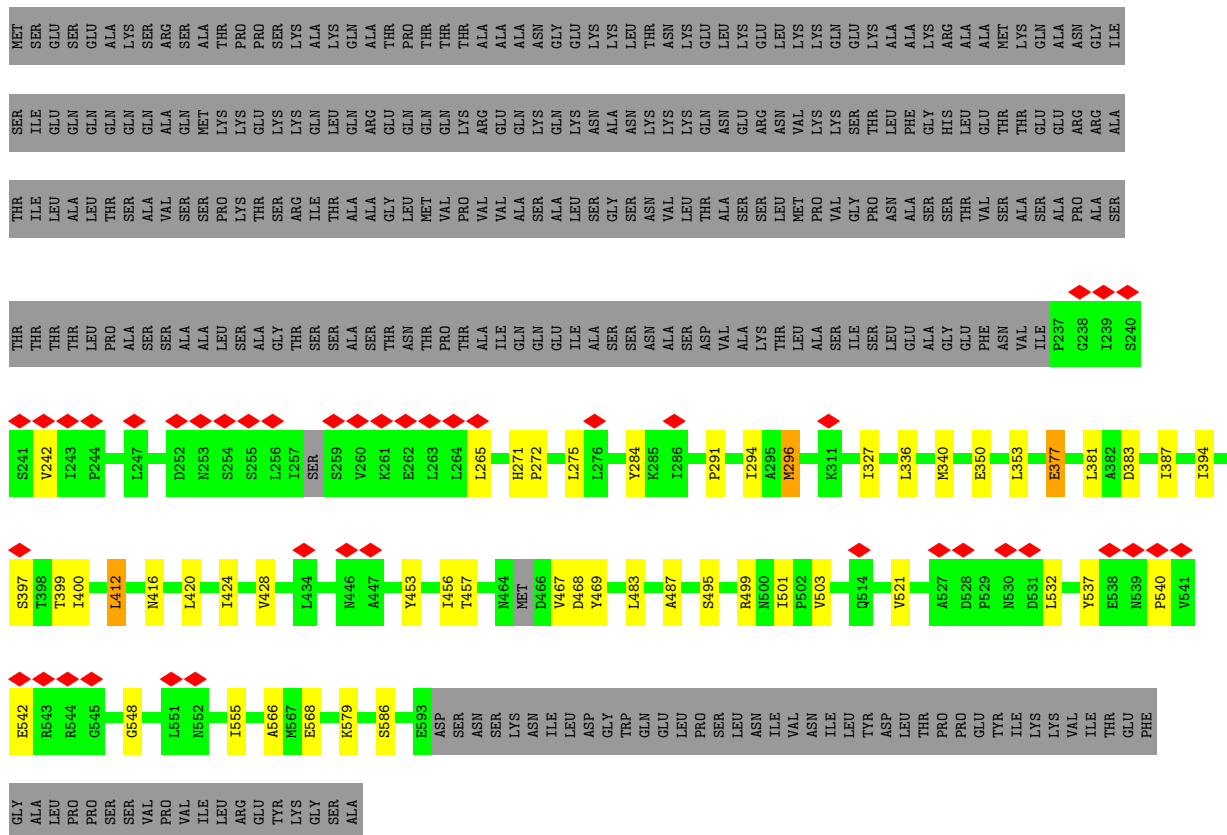
- Molecule 3: Translation initiation factor eIF-2B subunit gamma



- Molecule 3: Translation initiation factor eIF-2B subunit gamma



- Molecule 4: Translation initiation factor eIF-2B subunit delta



- Chain H:

Sequence logo for Chain H. The y-axis represents information content in bits (0.00 to 0.15). The x-axis shows positions 1 to 100. A bar at the top indicates the average conservation: 6% (red), 48% (green), 7% (yellow), and 45% (grey).

Key residues (high conservation) include: E593, L412, I424, V429, E436, N446, A447, I456, M464, MET, D466, L483, N500, V503, L518, F523, N530, D536, Y537, E538, N639, P540, V541, E542, R543, R544, G545, N546, K547, G548, N552, I555, K563, K564, L565, A566, K570, P571, I576.

- [illegible]

- 

LEU
LEU
GLU
SER
SER
LYS
GLY
LEU
ASP
ASN
ASP
SER
SER
ASP
SER
GLU
ASP
ASP
GLU

• Molecule 7: Eukaryotic translation initiation factor 2 subunit gamma

Chain M: 

MET
SER
ASP
LEU
LEU
GLN
ASP
GLN
GLU
PRO
SER
ILE
ILE
ILE
ASN
GLY
ASP
ASN
LEU
GLU
GLU
PRO
VAL
GLY
GLU
GLU
ASP
PRO
ILE
VAL
GLU
GLU
THR
THR
VAL
VAL
ALA
ALA
GLN
GLU
THR
GLN
GLU
THR
THR
LYS
ASP
ALA
ASP
GLU
LYS
PRO
LYS
LYS
VAL
ALA
PHE
THR
THR
GLY
LEU
GLU
GLU
ASP
GLY
THR

GLU
GLU
GLU
LYS
ARG
LYS
LYS
ARG
GLU
PHE
GLU
GLU
GLY
GLY
GLY
ASN
LEU
PRO
GLN
GLN
PRO
LEU
ASN
ASP
PHE
SER
LYS
LYS
ASN
GLU
LEU
PRO
SER
ALA
GLU
I94
Q98
R127
F128
LYS
ASP
GLU
L132
E133
I136
G141
Y142
K149
C150
Q151
E152
PRO
THR
CYS
PRO
PRO

ASP
CYS
TYR
ARG
F164
K168
E169
I170
S171
P172
K173
C174
Q175
R176
P177
C178
C179
P180
G181
R182
Y183
K184
A209
L215
L216
E237
I238
M239
K240
H243
V244
I245
I246
K268
R271
Q272
T273
I274
A275
D276
I291
M295
V299
K300
T301
I302
R307

M310
I311
P312
P313
R319
V337
G345
G350
I353
R356
D363
ASP
K365
I368
E383
P392
I396
G399
V402
L406
C407
R408
A409
D410
R411
V416
Y427
I430
E431
I432
F435
L436
L437
R438
R439
K444
THR
ASP
GLY
GLN
K449

Q450
A451
K452
V461
L462
M463
V464
M465
I466
G467
A470
T471
G472
A473
V474
V475
T488
S489
P490
A491
C492
T493
E494
I495
M496
E497
K498
I499
R503
R504
I505
E506
K507
H508
W509
R510
T516
I517
F518
K519
GLY
THR
THR
LEU
GLU
PRO
ILE
ALA

• Molecule 7: Eukaryotic translation initiation factor 2 subunit gamma

Chain N: 

MET
SER
ASP
LEU
LEU
GLN
ASP
GLN
GLU
PRO
SER
ILE
ILE
ILE
ASN
GLY
ASP
ASN
LEU
GLU
GLU
PRO
VAL
GLY
GLU
GLU
ASP
PRO
ILE
VAL
GLU
THR
THR
VAL
VAL
ALA
GLN
THR
GLN
GLU
THR
THR
GLN
ASP
ALA
ASP
LYS
PRO
LYS
LYS
LYS
VAL
ALA
PHE
THR
THR
GLY
LEU
GLU
GLU
ASP
GLY
GLY
THR

GLU
GLU
GLU
LYS
LYS
ARG
GLU
PHE
GLU
GLU
GLY
GLY
GLY
ASN
LEU
PRO
GLN
GLU
PRO
LEU
ASN
ASP
PHE
SER
LYS
LEU
LEU
PRO
SER
ALA
GLU
I94
I101
K113
S114
R118
Q124
T125
V126
R127
F128
LYS
ASP
GLU
L132
E133
R134
M135
I136
E152
PRO
THR
CYS

PRO
GLU
PRO
ASP
CYS
TYR
ARG
S163
R176
P177
G178
V189
G196
H197
L200
M204
V210
L215
Q226
P227
I245
I246
L247
V251
R255
I302
P305
P306
R307
D308
F309
M310
I311
S312
P313
R314
L315
I316
I330
E331
D332
L333
V337
I342

L343
N344
G345
V346
L349
I353
E354
I355
R356
P357
G358
I359
K362
D363
ASP
K365
I368
K371
E383
G399
D403
L406
C407
R408
A409
D410
R411
L412
Q415
V416
V417
K420
G421
H422
L423
P424
N425
I426
Y427
T428
D429
I430
D431
E431
I432
V443
K444
THR
ASP

GLY
GLN
K449
Q450
I466
T469
L485
Q486
L487
T488
S489
P490
A491
C492
T493
E494
E497
K498
I499
I505
E506
K507
H508
A515
T516
I517
K518
K519
GLY
THR
THR
LEU
GLU
PRO
ILE
ALA

• Molecule 8: Eukaryotic translation initiation factor 2 subunit beta

Chain O: 

MET
SER
SER
ASP
LEU
LEU
ALA
ALA
GLU
LEU
GLY
PHE
ASP
ASP
PRO
ALA
LEU
LYS
LYS
LYS
LYS
LYS
THR
LYS
LYS
LYS
VAL
ILE
PRO
ASP
ASP
PHE
ASP
ALA
ALA
VAL
ASN
GLY
GLU
ASN
GLY
SER
GLY
ASP
ASP
LEU
PHE
ALA
GLY
LEU
LYS
LYS
LYS
LYS
LYS
SER
SER
SER
VAL
SER
ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23909	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.126	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	375.2, 375.2, 375.2	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.53	0/2395	0.94	0/3251
1	B	0.53	0/2395	0.93	0/3251
2	C	0.58	0/2714	1.02	0/3693
2	D	0.56	0/2714	0.99	1/3693 (0.0%)
3	E	0.56	0/2209	0.90	1/2989 (0.0%)
3	F	0.56	0/2209	0.92	0/2989
4	G	0.55	0/2781	0.97	1/3747 (0.0%)
4	H	0.55	0/2781	0.98	0/3747
5	I	0.57	1/3468 (0.0%)	0.91	0/4704
5	J	0.58	0/3468	0.91	2/4704 (0.0%)
6	K	0.55	0/1989	0.96	2/2675 (0.1%)
6	L	0.55	0/1989	0.96	1/2675 (0.0%)
7	M	0.57	0/3087	0.90	2/4173 (0.0%)
7	N	0.56	0/3087	0.88	3/4173 (0.1%)
8	O	0.56	0/146	0.97	0/196
8	P	0.50	0/1051	0.83	0/1402
All	All	0.56	1/38483 (0.0%)	0.94	13/52062 (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
7	N	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	242	VAL	CA-CB	5.03	1.56	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	300	LYS	N-CA-C	6.85	118.44	110.97
7	N	489	SER	CA-C-N	6.53	128.00	119.84
7	N	489	SER	C-N-CA	6.53	128.00	119.84
7	M	356	ARG	N-CA-C	6.34	120.84	112.35
6	K	254	VAL	N-CA-C	6.01	116.67	110.36
4	G	377	GLU	N-CA-C	5.55	117.20	111.03
6	K	118	LYS	N-CA-C	5.46	117.09	111.03
6	L	254	VAL	N-CA-C	5.29	115.91	110.36
3	E	109	THR	N-CA-C	5.20	116.81	111.03
7	N	492	CYS	N-CA-C	5.15	115.33	108.38
5	J	57	VAL	CA-C-N	5.14	125.14	119.89
5	J	57	VAL	C-N-CA	5.14	125.14	119.89
2	D	173	GLN	N-CA-C	5.14	117.55	111.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	N	423	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2351	0	2367	45	0
1	B	2351	0	2367	56	0
2	C	2665	0	2626	14	0
2	D	2665	0	2626	12	0
3	E	2164	0	2154	9	0
3	F	2164	0	2154	11	0
4	G	2744	0	2819	18	0
4	H	2744	0	2819	15	0
5	I	3406	0	3359	20	0
5	J	3406	0	3359	27	0
6	K	1974	0	2020	13	0
6	L	1974	0	2020	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	3044	0	3126	23	0
7	N	3044	0	3126	71	0
8	O	143	0	148	1	0
8	P	1036	0	1080	18	0
All	All	37875	0	38170	337	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 4.

All (337) 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:B:20:MET:SD	1:B:102:VAL:HG13	1.27	1.70
7:N:312:SER:HB2	7:N:422:HIS:CE1	1.47	1.49
1:B:20:MET:SD	1:B:102:VAL:CG1	2.22	1.27
7:N:314:ARG:HH21	7:N:423:LEU:C	1.47	1.23
1:A:20:MET:SD	1:A:102:VAL:CG1	2.34	1.16
1:B:21:THR:HB	1:B:24:ILE:CD1	1.74	1.15
1:A:20:MET:SD	1:A:102:VAL:HG13	1.87	1.14
7:N:314:ARG:NH2	7:N:423:LEU:O	1.78	1.14
7:N:429:ASP:O	7:N:430:ILE:HG13	1.44	1.13
7:N:429:ASP:O	7:N:430:ILE:CG1	1.98	1.11
7:M:142:TYR:HB2	7:M:319:ARG:HH22	1.03	1.08
7:N:314:ARG:HH22	7:N:423:LEU:HG	1.12	1.08
1:B:20:MET:SD	1:B:24:ILE:HG21	1.95	1.06
7:M:142:TYR:HB2	7:M:319:ARG:NH2	1.71	1.05
7:N:368:ILE:HD13	7:N:428:THR:HG21	1.39	1.04
1:B:21:THR:HB	1:B:24:ILE:HD12	1.41	1.03
7:N:312:SER:CB	7:N:422:HIS:CE1	2.43	1.01
8:P:226:LEU:O	8:P:230:ILE:HG13	1.59	1.00
1:A:146:PHE:HB3	5:J:332:VAL:HG13	1.42	0.98
7:M:142:TYR:CB	7:M:319:ARG:HH22	1.76	0.97
1:B:21:THR:CB	1:B:24:ILE:HD13	1.94	0.97
1:B:21:THR:HB	1:B:24:ILE:HD13	1.48	0.96
1:B:120:ILE:HG21	1:B:147:ILE:HG21	1.51	0.93
7:N:314:ARG:NH2	7:N:423:LEU:C	2.22	0.92
1:B:9:THR:HA	1:B:12:ARG:HD2	1.52	0.92
1:B:20:MET:SD	1:B:24:ILE:CG2	2.58	0.91
7:N:312:SER:CB	7:N:422:HIS:HE1	1.78	0.91
1:A:146:PHE:CB	5:J:332:VAL:HG13	2.01	0.91
7:N:426:ILE:HD12	7:N:426:ILE:H	1.32	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:PHE:HB3	5:I:332:VAL:HG13	1.51	0.91
1:B:120:ILE:HG21	1:B:147:ILE:CG2	2.00	0.90
1:B:21:THR:CB	1:B:24:ILE:CD1	2.50	0.90
7:N:314:ARG:NH2	7:N:423:LEU:HG	1.85	0.90
1:A:9:THR:O	1:A:12:ARG:HB2	1.73	0.88
1:B:9:THR:O	1:B:12:ARG:HB2	1.75	0.86
1:B:120:ILE:CG2	1:B:147:ILE:HG21	2.04	0.86
1:B:20:MET:CE	1:B:102:VAL:CG1	2.52	0.86
8:P:238:THR:HG22	8:P:266:ARG:HH21	1.41	0.84
1:B:20:MET:CE	1:B:102:VAL:HG13	2.07	0.84
1:A:21:THR:HG22	1:A:23:PRO:HD2	1.60	0.83
7:N:428:THR:O	7:N:487:LEU:HD12	1.79	0.83
1:A:20:MET:SD	1:A:102:VAL:HG11	2.19	0.81
7:N:368:ILE:HD13	7:N:428:THR:CG2	2.12	0.79
7:N:429:ASP:O	7:N:430:ILE:HG12	1.82	0.79
1:B:146:PHE:CB	5:I:332:VAL:HG13	2.14	0.78
6:L:198:ILE:HG12	7:N:333:LEU:HB2	1.63	0.78
1:A:9:THR:HA	1:A:12:ARG:HD2	1.63	0.78
6:L:202:LYS:CE	7:N:331:GLU:HA	2.14	0.78
7:N:429:ASP:C	7:N:430:ILE:HG12	2.10	0.76
7:N:422:HIS:HB3	7:N:424:PRO:HD2	1.68	0.75
6:L:198:ILE:HG23	7:N:333:LEU:HD12	1.69	0.75
7:N:312:SER:HB2	7:N:422:HIS:HE1	0.99	0.74
1:B:120:ILE:CG2	1:B:147:ILE:CG2	2.65	0.74
1:B:21:THR:HG22	1:B:23:PRO:HD2	1.69	0.74
7:N:429:ASP:C	7:N:430:ILE:CG1	2.57	0.73
1:A:112:ILE:HG22	1:A:138:LEU:HD21	1.70	0.73
7:N:368:ILE:CD1	7:N:428:THR:HG21	2.18	0.72
8:P:169:GLY:HA3	8:P:216:LYS:HG3	1.72	0.72
7:N:314:ARG:HH22	7:N:423:LEU:CG	1.99	0.71
1:B:20:MET:CE	1:B:102:VAL:HG11	2.21	0.71
3:E:160:LEU:H	3:E:161:PRO:HD2	1.55	0.70
6:L:198:ILE:CG2	7:N:330:ILE:O	2.40	0.69
7:M:142:TYR:HB2	7:M:319:ARG:CZ	2.21	0.69
3:F:160:LEU:H	3:F:161:PRO:HD2	1.58	0.68
1:B:21:THR:OG1	1:B:24:ILE:HD13	1.94	0.68
1:A:164:GLN:O	1:A:167:THR:OG1	2.09	0.67
1:B:164:GLN:O	1:B:167:THR:OG1	2.12	0.67
5:J:414:ILE:HG12	5:J:432:ILE:HD12	1.77	0.66
4:H:387:ILE:HD13	4:H:412:LEU:HD22	1.76	0.66
7:M:142:TYR:HB2	7:M:319:ARG:HH12	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:198:ILE:HG23	7:N:330:ILE:O	1.98	0.64
7:M:142:TYR:HB2	7:M:319:ARG:NH1	2.12	0.64
4:H:383:ASP:O	4:H:387:ILE:HG12	1.98	0.63
1:B:23:PRO:O	1:B:27:ILE:HD12	1.98	0.63
6:L:146:LYS:O	6:L:149:ILE:HG13	1.99	0.62
2:C:333:THR:HG22	4:G:453:TYR:HB3	1.81	0.62
7:N:210:VAL:HG22	7:N:343:LEU:HA	1.81	0.62
1:B:9:THR:HA	1:B:12:ARG:CD	2.28	0.61
6:L:194:SER:N	7:N:403:ASP:OD2	2.33	0.61
1:A:260:THR:O	1:B:170:GLU:HG2	2.01	0.61
8:P:233:TYR:OH	8:P:269:SER:C	2.43	0.61
6:K:149:ILE:HG21	6:K:173:ILE:HG21	1.84	0.60
7:N:427:TYR:OH	7:N:519:LYS:HG3	2.02	0.60
5:J:464:VAL:HB	5:J:467:VAL:HG23	1.84	0.60
1:B:20:MET:SD	1:B:24:ILE:HG22	2.42	0.60
6:L:198:ILE:HG12	7:N:333:LEU:CD1	2.32	0.59
1:B:20:MET:HE1	1:B:102:VAL:HG11	1.83	0.59
5:I:459:ASP:H	5:I:466:ILE:HD12	1.68	0.59
1:B:120:ILE:HG21	1:B:147:ILE:HG22	1.80	0.58
2:C:196:VAL:HG21	2:C:261:GLY:HA2	1.85	0.58
6:K:146:LYS:O	6:K:149:ILE:HG13	2.03	0.58
3:F:255:ILE:H	8:P:216:LYS:HD3	1.69	0.58
1:A:208:ILE:HD12	1:A:247:LEU:HD21	1.85	0.57
1:B:109:ARG:HH22	1:B:133:ARG:HB3	1.69	0.57
7:N:101:ILE:HD12	7:N:305:PRO:HG3	1.87	0.56
1:B:135:VAL:HG22	1:B:230:VAL:HB	1.87	0.56
1:A:149:PHE:HD1	1:A:149:PHE:O	1.88	0.56
6:L:198:ILE:CG1	7:N:333:LEU:CD1	2.84	0.56
6:L:198:ILE:HG13	7:N:333:LEU:HD13	1.87	0.56
6:L:202:LYS:HE2	7:N:331:GLU:HA	1.86	0.56
4:G:468:ASP:HA	4:G:501:ILE:HD13	1.87	0.56
6:L:198:ILE:CG2	7:N:333:LEU:HD12	2.35	0.56
2:D:317:GLY:HA2	5:J:301:ARG:HB3	1.88	0.55
6:K:92:SER:HA	6:K:95:ILE:HD12	1.88	0.55
4:G:394:ILE:HD13	4:G:416:ASN:HD21	1.71	0.55
8:P:186:ARG:NH2	8:P:234:VAL:HG22	2.22	0.55
1:A:21:THR:HG21	1:A:234:HIS:CE1	2.42	0.55
1:A:23:PRO:O	1:A:27:ILE:HD12	2.07	0.54
5:I:351:ILE:HG12	5:I:368:ILE:HD12	1.88	0.54
3:F:190:ARG:HH22	3:F:238:LEU:HD12	1.73	0.54
1:A:291:THR:H	1:A:292:PRO:HD3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:165:THR:HA	5:J:274:TYR:HB2	1.90	0.53
1:B:153:VAL:HG11	1:B:166:TYR:HB2	1.90	0.53
1:A:22:MET:HB2	1:A:23:PRO:HD3	1.89	0.53
2:D:231:LYS:HD2	4:H:546:ASN:HD21	1.74	0.53
2:D:318:SER:HA	2:D:321:ILE:HD12	1.91	0.53
4:G:483:LEU:HB3	4:G:566:ALA:HB3	1.91	0.52
6:L:111:ILE:HG23	6:L:169:LEU:HD21	1.92	0.52
1:B:22:MET:CB	1:B:23:PRO:HD3	2.40	0.52
7:N:499:ILE:HB	7:N:515:ALA:HB3	1.91	0.52
8:P:186:ARG:HH21	8:P:234:VAL:HG22	1.75	0.52
8:P:189:GLU:HA	8:P:192:ILE:HD12	1.92	0.52
1:A:57:ILE:HA	1:A:60:ILE:HD12	1.92	0.52
7:N:466:ILE:HG12	7:N:499:ILE:HG12	1.92	0.52
7:N:313:PRO:HA	7:N:344:ASN:O	2.10	0.52
6:L:70:VAL:HG21	6:L:95:ILE:HA	1.90	0.51
7:N:469:THR:HG21	7:N:491:ALA:HA	1.93	0.51
6:L:198:ILE:CG1	7:N:333:LEU:HD13	2.41	0.51
1:A:146:PHE:HB3	5:J:332:VAL:CG1	2.30	0.51
4:H:377:GLU:HA	4:H:381:LEU:HD12	1.92	0.51
1:B:19:GLU:HA	1:B:19:GLU:OE1	2.11	0.51
1:B:129:HIS:HB3	1:B:196:VAL:HG22	1.92	0.51
4:H:330:LEU:HB3	4:H:336:LEU:HD21	1.93	0.51
3:E:226:TYR:HB3	3:E:239:LEU:H	1.75	0.50
8:P:237:LYS:HB2	8:P:266:ARG:CZ	2.41	0.50
6:L:198:ILE:HG12	7:N:333:LEU:HD12	1.92	0.50
7:M:142:TYR:CB	7:M:319:ARG:HH12	2.24	0.50
7:M:237:GLU:HB3	7:M:274:ILE:HD12	1.93	0.50
1:A:68:ALA:HB2	1:A:237:VAL:HG22	1.93	0.50
1:A:224:ARG:HH22	2:D:286:ARG:HE	1.60	0.49
5:J:414:ILE:HA	5:J:432:ILE:HB	1.93	0.49
6:L:198:ILE:HG12	7:N:333:LEU:CB	2.38	0.49
1:A:22:MET:CB	1:A:23:PRO:HD3	2.42	0.49
5:I:414:ILE:HG12	5:I:432:ILE:HD12	1.93	0.49
1:B:21:THR:HG21	1:B:234:HIS:CE1	2.48	0.49
4:H:291:PRO:HA	4:H:294:ILE:HD12	1.93	0.49
2:C:168:ILE:HG23	2:C:352:ASN:HD22	1.77	0.49
5:J:340:GLY:HA3	5:J:358:GLU:HG3	1.95	0.49
8:P:233:TYR:OH	8:P:269:SER:O	2.29	0.49
2:C:90:ARG:HH22	2:C:298:LEU:HD13	1.77	0.48
5:I:178:ARG:HH22	5:I:229:ASP:HA	1.78	0.48
5:J:396:ILE:HG13	5:J:414:ILE:HD12	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:426:ILE:HD12	7:N:426:ILE:N	2.13	0.48
1:A:152:VAL:HG13	1:A:179:ILE:HD13	1.94	0.48
1:A:135:VAL:HG22	1:A:230:VAL:HB	1.95	0.48
1:A:146:PHE:HB2	5:J:332:VAL:HG13	1.90	0.48
1:B:21:THR:O	1:B:24:ILE:HB	2.14	0.48
7:N:113:LYS:HE3	7:N:196:GLY:H	1.78	0.48
7:N:426:ILE:H	7:N:426:ILE:CD1	2.01	0.48
5:I:168:LEU:HB3	5:I:230:LEU:HD22	1.96	0.48
8:P:236:CYS:SG	8:P:237:LYS:N	2.86	0.48
1:A:149:PHE:HD1	1:A:149:PHE:C	2.22	0.47
1:A:260:THR:OG1	1:B:170:GLU:OE2	2.07	0.47
4:G:291:PRO:HA	4:G:294:ILE:HD12	1.95	0.47
5:I:163:ILE:HD11	5:I:271:LYS:HB3	1.96	0.47
5:I:304:TYR:HB3	5:I:305:PRO:HD3	1.96	0.47
7:N:307:ARG:HD3	7:N:307:ARG:HA	1.75	0.47
1:A:149:PHE:C	1:A:149:PHE:CD1	2.92	0.47
1:B:242:LEU:HB3	4:H:393:GLN:HG2	1.96	0.47
3:F:101:ILE:HG23	3:F:102:GLU:HG3	1.97	0.47
5:J:458:ASP:HB3	5:J:466:ILE:HD11	1.96	0.47
6:K:133:PRO:HG2	6:K:134:LEU:HD12	1.97	0.47
7:N:428:THR:O	7:N:487:LEU:CD1	2.59	0.47
1:A:127:LEU:HB2	1:A:191:VAL:HG11	1.95	0.47
7:N:310:MET:HB3	7:N:311:ILE:H	1.57	0.47
7:N:356:ARG:O	7:N:426:ILE:HG23	2.14	0.47
3:E:267:THR:HG23	5:J:225:VAL:HA	1.96	0.47
3:F:171:PRO:HD2	3:F:174:PHE:HE1	1.80	0.47
5:J:139:VAL:HG11	5:J:235:ILE:HD11	1.97	0.47
8:P:238:THR:HG22	8:P:266:ARG:NH2	2.21	0.47
4:H:483:LEU:HB3	4:H:566:ALA:HB3	1.97	0.47
5:I:32:LEU:HB2	5:I:136:SER:HA	1.97	0.47
7:N:315:LEU:CD1	7:N:342:ILE:HG12	2.45	0.47
8:P:187:SER:H	8:P:246:LEU:HD13	1.80	0.47
7:N:197:HIS:HB3	7:N:200:LEU:H	1.78	0.47
5:J:200:LEU:HD11	5:J:211:ILE:HD11	1.96	0.46
3:F:152:GLY:HA2	3:F:155:LEU:HD12	1.97	0.46
1:B:13:PHE:CD1	1:B:13:PHE:N	2.81	0.46
7:N:429:ASP:HA	7:N:486:GLN:HA	1.97	0.46
8:P:227:ARG:O	8:P:231:LEU:HD12	2.15	0.46
8:O:129:LEU:H	8:O:130:PRO:HD2	1.80	0.46
1:B:292:PRO:HG3	2:C:268:ASN:HA	1.98	0.46
5:I:165:THR:HA	5:I:274:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:272:PRO:HA	4:H:275:LEU:HD12	1.98	0.46
5:I:296:GLN:HA	5:I:299:LEU:HD12	1.97	0.46
4:H:403:TYR:HD1	4:H:429:VAL:HB	1.80	0.46
5:J:385:ILE:HG12	5:J:402:LEU:HD12	1.96	0.46
6:L:198:ILE:CG1	7:N:333:LEU:HD12	2.46	0.46
4:G:495:SER:HB2	4:G:499:ARG:HH21	1.81	0.45
1:B:17:ASP:HB3	1:B:18:THR:H	1.50	0.45
7:N:226:GLN:HA	7:N:227:PRO:HD3	1.83	0.45
1:B:22:MET:HB3	1:B:23:PRO:HD3	1.99	0.45
3:F:406:ARG:HA	3:F:409:LEU:HD12	1.99	0.45
8:P:237:LYS:HB2	8:P:266:ARG:NH2	2.31	0.45
4:G:377:GLU:HA	4:G:381:LEU:HD12	1.99	0.45
6:K:20:VAL:HG12	6:K:38:GLU:HB3	1.98	0.45
6:L:147:LEU:O	6:L:150:ILE:HG13	2.16	0.45
7:M:313:PRO:HA	7:M:345:GLY:HA3	1.98	0.45
2:C:42:LEU:HA	2:C:45:LEU:HD12	1.99	0.45
2:C:192:ASP:HB2	2:C:222:ASN:HD21	1.82	0.45
5:J:357:ILE:HA	5:J:374:ILE:HB	1.99	0.45
6:K:220:VAL:HG13	6:K:230:LEU:HB3	1.98	0.45
6:L:202:LYS:HG3	7:N:330:ILE:HG22	1.98	0.45
7:N:245:ILE:HD11	7:N:302:ILE:HD11	1.98	0.45
2:C:262:THR:HA	2:C:273:SER:HA	1.98	0.45
3:E:179:PRO:HA	3:E:180:PRO:HD3	1.78	0.45
1:A:19:GLU:OE1	1:A:19:GLU:HA	2.17	0.44
2:D:30:LYS:HD3	5:J:312:ILE:HA	1.98	0.44
4:G:350:GLU:HA	4:G:353:LEU:HD12	1.99	0.44
4:H:381:LEU:HD22	6:K:64:ARG:HD3	1.99	0.44
5:I:339:ILE:HG22	5:I:357:ILE:HB	2.00	0.44
2:C:218:GLY:HA2	4:G:457:THR:HG21	1.98	0.44
1:A:21:THR:HG21	1:A:234:HIS:NE2	2.33	0.44
1:A:23:PRO:HG2	1:A:234:HIS:CD2	2.53	0.44
1:B:9:THR:CA	1:B:12:ARG:HD2	2.37	0.44
7:M:462:LEU:HD22	7:M:503:ARG:HG2	1.99	0.44
5:J:83:ALA:HA	5:J:86:ILE:HD12	1.99	0.44
7:M:216:LEU:HD23	7:M:246:ILE:HG12	2.00	0.44
7:M:337:VAL:HA	7:M:399:GLY:HA2	1.99	0.44
7:N:427:TYR:OH	7:N:519:LYS:CG	2.66	0.44
1:B:72:ILE:HD11	1:B:236:PHE:HB2	1.99	0.44
4:G:399:THR:HB	4:G:467:VAL:HA	1.99	0.44
7:M:168:LYS:CB	7:M:295:ASN:HB3	2.48	0.44
7:M:243:HIS:HB3	7:M:302:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:232:GLU:HG3	8:P:233:TYR:HD1	1.83	0.44
1:A:170:GLU:HG2	1:B:260:THR:O	2.18	0.43
1:A:225:LYS:HA	1:A:226:PRO:HD3	1.88	0.43
2:D:230:ALA:HA	2:D:233:LEU:HD12	2.00	0.43
2:D:37:SER:HA	2:D:40:ILE:HD12	2.00	0.43
4:G:387:ILE:HD13	4:G:412:LEU:HD22	2.00	0.43
5:J:37:GLU:C	5:J:39:ARG:H	2.26	0.43
7:N:337:VAL:HA	7:N:399:GLY:HA2	1.99	0.43
2:C:219:PHE:HA	2:C:223:THR:HG23	2.00	0.43
3:E:154:SER:HA	3:E:157:LYS:HE3	1.98	0.43
4:H:405:SER:HB3	4:H:436:GLU:HB3	2.01	0.43
5:J:168:LEU:HD22	5:J:230:LEU:HD13	2.01	0.43
5:J:255:LEU:HD12	5:J:256:ARG:HG2	2.01	0.43
7:N:314:ARG:NE	7:N:424:PRO:HD3	2.33	0.43
7:M:141:GLY:O	7:M:319:ARG:NH2	2.52	0.43
1:A:40:GLU:HG3	1:A:91:LYS:HE3	2.01	0.43
4:G:296:MET:HG3	4:G:340:MET:HE3	2.01	0.43
7:N:316:ILE:HD11	7:N:343:LEU:HD12	2.00	0.43
7:N:357:PRO:O	7:N:426:ILE:CG2	2.67	0.43
2:C:155:ILE:HA	2:C:158:ILE:HD12	2.00	0.43
2:D:179:LEU:HD13	2:D:293:PHE:HE2	1.84	0.43
6:L:112:LEU:HD21	6:L:130:ILE:HG13	2.01	0.43
1:A:109:ARG:HH22	1:A:133:ARG:HB3	1.84	0.43
1:A:200:GLY:HA2	1:A:235:LYS:HB3	2.01	0.43
6:K:77:ASP:HB3	6:K:82:TYR:HB2	1.99	0.43
1:B:41:THR:HG22	6:K:75:ARG:HB3	2.00	0.43
6:L:159:GLU:HA	6:L:160:PRO:HD3	1.88	0.43
6:L:202:LYS:HE2	7:N:331:GLU:HG2	2.00	0.43
3:E:183:LEU:HB3	3:E:197:MET:HE3	2.01	0.42
6:L:21:MET:HG2	6:L:102:TYR:HB2	2.01	0.42
7:M:312:SER:HA	7:M:313:PRO:HD3	1.93	0.42
2:C:265:VAL:HA	2:C:271:THR:HG22	1.99	0.42
3:E:173:ASP:HB2	3:E:399:ASN:HD21	1.84	0.42
7:N:309:PHE:HB3	7:N:346:VAL:HG23	2.02	0.42
3:F:252:TYR:HE1	5:I:215:PRO:HG3	1.85	0.42
4:G:271:HIS:HA	4:G:272:PRO:HD3	1.89	0.42
6:K:71:ALA:HB3	6:K:85:LEU:HD23	2.02	0.42
8:P:229:TYR:O	8:P:229:TYR:CG	2.71	0.42
1:B:16:GLU:HB3	1:B:17:ASP:H	1.69	0.42
4:G:272:PRO:HA	4:G:275:LEU:HD12	2.00	0.42
4:G:327:ILE:HG23	4:G:336:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:186:VAL:HG22	5:I:226:ILE:HG23	2.00	0.42
1:B:68:ALA:HB2	1:B:237:VAL:HG22	2.02	0.42
4:G:416:ASN:HA	4:G:420:LEU:HD12	2.02	0.42
1:A:212:GLY:HA3	1:B:182:SER:HB2	2.01	0.42
1:B:210:LEU:HB3	1:B:211:VAL:H	1.63	0.42
3:E:224:THR:HG22	3:E:268:VAL:HG22	2.01	0.42
1:B:21:THR:OG1	1:B:24:ILE:CD1	2.63	0.42
7:M:215:LEU:HD23	7:M:245:ILE:HB	2.02	0.42
2:D:265:VAL:HA	2:D:271:THR:HG22	2.01	0.42
3:F:198:THR:HB	3:F:272:LEU:HB3	2.02	0.42
5:I:344:ALA:HB3	5:I:361:VAL:HG13	2.02	0.42
5:J:135:VAL:HG22	5:J:235:ILE:HG23	2.02	0.42
7:M:149:LYS:HE3	7:M:299:VAL:HG21	2.01	0.42
1:B:34:LEU:HD22	1:B:73:PHE:HZ	1.84	0.42
5:I:37:GLU:C	5:I:39:ARG:H	2.28	0.42
1:A:201:VAL:HG11	1:A:295:VAL:HG21	2.01	0.42
2:D:48:LEU:HD13	2:D:91:ILE:HD13	2.02	0.42
5:J:231:ILE:HG21	5:J:283:VAL:HG22	2.02	0.42
7:N:432:ILE:HG12	7:N:499:ILE:HD13	2.02	0.41
1:B:104:ARG:HA	1:B:107:LYS:HE3	2.02	0.41
3:E:152:GLY:HA2	3:E:155:LEU:HD12	2.02	0.41
5:I:338:LYS:HE3	5:I:356:LYS:HE2	2.01	0.41
5:J:418:VAL:HG22	5:J:461:THR:HG22	2.03	0.41
7:N:357:PRO:HB2	7:N:490:PRO:HB3	2.02	0.41
1:A:252:PRO:HA	1:A:253:PRO:HD3	1.94	0.41
5:I:368:ILE:HG12	5:I:385:ILE:HD12	2.02	0.41
7:N:423:LEU:N	7:N:424:PRO:HD2	2.35	0.41
1:A:239:MET:HE3	1:A:248:PRO:HG2	2.02	0.41
1:B:172:LYS:HE2	1:B:172:LYS:HA	2.01	0.41
7:N:309:PHE:CD1	7:N:309:PHE:N	2.88	0.41
7:N:359:ILE:HD11	7:N:411:ARG:HH11	1.86	0.41
6:K:207:SER:HB2	6:K:250:LYS:HD2	2.01	0.41
7:M:98:GLN:HE22	7:M:396:ILE:HD11	1.85	0.41
7:M:307:ARG:HD3	7:M:392:PRO:HB2	2.02	0.41
2:C:172:ILE:HG22	2:C:176:ALA:HB2	2.02	0.41
7:M:430:ILE:HD12	7:M:432:ILE:HD12	2.03	0.41
2:D:19:ASN:HB2	2:D:22:ILE:HD11	2.03	0.41
3:F:183:LEU:HD22	3:F:197:MET:HE3	2.02	0.41
8:P:211:LEU:HD13	8:P:213:ILE:HD11	2.02	0.41
1:A:109:ARG:HH12	1:A:133:ARG:HB3	1.85	0.41
1:B:166:TYR:HE1	1:B:176:VAL:HG23	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:161:ASP:HB3	5:I:271:LYS:HG2	2.03	0.41
5:J:186:VAL:HG22	5:J:226:ILE:HG12	2.02	0.41
6:K:247:ALA:HA	6:K:250:LYS:HE3	2.03	0.41
1:A:21:THR:HG21	1:A:234:HIS:HE2	1.86	0.41
4:G:400:ILE:HG12	4:G:469:TYR:HB2	2.03	0.41
4:H:271:HIS:HA	4:H:272:PRO:HD3	1.86	0.41
4:H:570:LYS:HB2	4:H:571:PRO:HD3	2.03	0.41
4:G:383:ASP:O	4:G:387:ILE:HG12	2.20	0.40
7:M:461:VAL:HG22	7:M:474:ARG:HE	1.86	0.40
7:N:412:LEU:HA	7:N:415:GLN:HE21	1.86	0.40
2:D:198:LYS:O	2:D:201:ILE:HG22	2.20	0.40
7:N:215:LEU:HD22	7:N:247:LEU:HD11	2.03	0.40
1:A:291:THR:H	1:A:292:PRO:CD	2.34	0.40
5:J:32:LEU:HB2	5:J:136:SER:HA	2.02	0.40
6:K:126:LEU:O	6:K:129:THR:HG22	2.21	0.40
7:M:356:ARG:HB2	7:M:416:VAL:HG23	2.03	0.40
1:A:172:LYS:HD3	1:A:172:LYS:HA	1.75	0.40
2:C:57:TRP:HB3	2:C:63:LEU:HD13	2.04	0.40
3:F:69:LEU:HA	3:F:70:PRO:HD3	1.98	0.40
4:H:539:ASN:HB2	4:H:540:PRO:HD3	2.03	0.40
7:N:499:ILE:HD11	7:N:517:ILE:HB	2.03	0.40

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	300/305 (98%)	254 (85%)	39 (13%)	7 (2%)	5	28
1	B	300/305 (98%)	256 (85%)	35 (12%)	9 (3%)	3	23
2	C	339/381 (89%)	308 (91%)	28 (8%)	3 (1%)	14	51
2	D	339/381 (89%)	309 (91%)	25 (7%)	5 (2%)	8	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	253/578 (44%)	217 (86%)	34 (13%)	2 (1%)	16	54
3	F	253/578 (44%)	211 (83%)	37 (15%)	5 (2%)	6	31
4	G	349/651 (54%)	303 (87%)	35 (10%)	11 (3%)	3	21
4	H	349/651 (54%)	302 (86%)	36 (10%)	11 (3%)	3	21
5	I	427/712 (60%)	379 (89%)	41 (10%)	7 (2%)	7	38
5	J	427/712 (60%)	365 (86%)	45 (10%)	17 (4%)	2	18
6	K	237/304 (78%)	208 (88%)	27 (11%)	2 (1%)	16	54
6	L	237/304 (78%)	211 (89%)	25 (10%)	1 (0%)	30	67
7	M	398/527 (76%)	345 (87%)	48 (12%)	5 (1%)	9	42
7	N	398/527 (76%)	330 (83%)	55 (14%)	13 (3%)	3	21
8	O	15/285 (5%)	13 (87%)	1 (7%)	1 (7%)	1	12
8	P	120/285 (42%)	100 (83%)	18 (15%)	2 (2%)	7	36
All	All	4741/7486 (63%)	4111 (87%)	529 (11%)	101 (2%)	8	30

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	61	PRO
3	E	100	GLU
3	F	100	GLU
4	G	487	ALA
4	H	536	ASP
5	J	202	LEU
1	B	158	PRO
1	B	304	TYR
2	C	275	ASN
2	C	276	SER
2	C	337	ILE
2	D	275	ASN
2	D	276	SER
2	D	337	ILE
4	G	579	LYS
4	H	537	TYR
4	H	579	LYS
5	I	173	THR
5	I	464	VAL
5	J	201	PRO
5	J	459	ASP

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Mol	Chain	Res	Type
5	J	464	VAL
7	M	507	LYS
7	N	311	ILE
7	N	430	ILE
1	A	97	ASN
1	A	158	PRO
1	A	291	THR
1	B	38	THR
1	B	98	GLY
1	B	291	THR
3	E	160	LEU
4	G	265	LEU
4	G	397	SER
4	G	537	TYR
4	G	586	SER
4	H	397	SER
5	I	112	ALA
5	I	423	ASN
5	J	112	ALA
5	J	173	THR
5	J	182	PRO
5	J	355	THR
5	J	371	ASN
5	J	388	ASN
5	J	423	ASN
6	K	225	ALA
6	L	132	TRP
7	M	127	ARG
7	M	164	PHE
7	M	383	GLU
7	N	178	GLY
7	N	255	ARG
7	N	497	GLU
7	N	507	LYS
1	A	5	ASN
1	A	38	THR
1	B	5	ASN
1	B	263	LEU
3	F	160	LEU
3	F	311	GLN
4	H	251	PHE
5	I	311	ASN

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Mol	Chain	Res	Type
5	I	459	ASP
5	J	26	ARG
5	J	192	SER
5	J	421	ASP
8	O	129	LEU
7	N	176	ARG
7	N	306	PRO
8	P	129	LEU
1	A	61	PRO
2	D	324	ARG
3	F	238	LEU
4	G	242	VAL
4	G	542	GLU
4	G	548	GLY
4	H	242	VAL
4	H	248	GLU
4	H	500	ASN
4	H	548	GLY
4	H	555	ILE
5	J	369	GLY
6	K	81	GLY
7	M	497	GLU
7	N	383	GLU
7	N	420	LYS
8	P	200	GLY
1	A	35	ARG
2	D	191	PRO
3	F	180	PRO
4	H	245	THR
5	J	38	THR
7	N	494	GLU
4	G	555	ILE
5	I	466	ILE
5	J	467	VAL
7	N	490	PRO
4	G	540	PRO
7	N	177	PRO
1	B	292	PRO

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	257/265 (97%)	234 (91%)	23 (9%)	9	28
1	B	257/265 (97%)	240 (93%)	17 (7%)	15	37
2	C	286/338 (85%)	266 (93%)	20 (7%)	14	35
2	D	286/338 (85%)	270 (94%)	16 (6%)	19	40
3	E	249/529 (47%)	243 (98%)	6 (2%)	43	64
3	F	249/529 (47%)	241 (97%)	8 (3%)	34	56
4	G	305/561 (54%)	295 (97%)	10 (3%)	33	55
4	H	305/561 (54%)	295 (97%)	10 (3%)	33	55
5	I	389/649 (60%)	372 (96%)	17 (4%)	25	47
5	J	389/649 (60%)	372 (96%)	17 (4%)	25	47
6	K	219/273 (80%)	198 (90%)	21 (10%)	8	25
6	L	219/273 (80%)	198 (90%)	21 (10%)	8	25
7	M	319/449 (71%)	309 (97%)	10 (3%)	35	56
7	N	319/449 (71%)	298 (93%)	21 (7%)	15	37
8	O	16/246 (6%)	16 (100%)	0	100	100
8	P	119/246 (48%)	106 (89%)	13 (11%)	6	21
All	All	4183/6620 (63%)	3953 (94%)	230 (6%)	21	41

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	13	PHE
1	A	16	GLU
1	A	17	ASP
1	A	21	THR
1	A	22	MET
1	A	24	ILE
1	A	37	LYS

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Mol	Chain	Res	Type
1	A	54	GLU
1	A	81	LEU
1	A	126	ILE
1	A	147	ILE
1	A	149	PHE
1	A	172	LYS
1	A	179	ILE
1	A	188	ILE
1	A	196	VAL
1	A	207	ILE
1	A	231	THR
1	A	237	VAL
1	A	280	ILE
1	A	290	LEU
1	A	297	GLU
1	B	12	ARG
1	B	21	THR
1	B	22	MET
1	B	37	LYS
1	B	54	GLU
1	B	56	LEU
1	B	64	VAL
1	B	81	LEU
1	B	104	ARG
1	B	135	VAL
1	B	153	VAL
1	B	172	LYS
1	B	207	ILE
1	B	231	THR
1	B	237	VAL
1	B	242	LEU
1	B	272	ILE
2	C	20	VAL
2	C	24	THR
2	C	40	ILE
2	C	42	LEU
2	C	91	ILE
2	C	161	LEU
2	C	168	ILE
2	C	177	ILE
2	C	179	LEU
2	C	206	ARG

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Mol	Chain	Res	Type
2	C	222	ASN
2	C	223	THR
2	C	238	ILE
2	C	278	VAL
2	C	298	LEU
2	C	308	ASP
2	C	322	LEU
2	C	346	ILE
2	C	363	ARG
2	C	366	TRP
2	D	24	THR
2	D	38	TYR
2	D	42	LEU
2	D	44	THR
2	D	84	CYS
2	D	160	ASP
2	D	161	LEU
2	D	165	ILE
2	D	168	ILE
2	D	200	LEU
2	D	201	ILE
2	D	206	ARG
2	D	222	ASN
2	D	278	VAL
2	D	298	LEU
2	D	366	TRP
3	E	3	ILE
3	E	144	ILE
3	E	183	LEU
3	E	185	ASP
3	E	255	ILE
3	E	402	MET
3	F	3	ILE
3	F	134	HIS
3	F	141	ILE
3	F	173	ASP
3	F	237	ILE
3	F	255	ILE
3	F	258	HIS
3	F	260	LEU
4	G	284	TYR
4	G	296	MET

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Mol	Chain	Res	Type
4	G	412	LEU
4	G	424	ILE
4	G	428	VAL
4	G	456	ILE
4	G	503	VAL
4	G	521	VAL
4	G	532	LEU
4	G	568	GLU
4	H	286	ILE
4	H	388	ASP
4	H	412	LEU
4	H	424	ILE
4	H	456	ILE
4	H	503	VAL
4	H	523	PHE
4	H	563	LYS
4	H	565	LEU
4	H	576	ILE
5	I	41	MET
5	I	51	LEU
5	I	88	ASP
5	I	97	LEU
5	I	106	THR
5	I	113	ARG
5	I	122	LEU
5	I	127	ILE
5	I	139	VAL
5	I	181	GLU
5	I	231	ILE
5	I	273	ILE
5	I	307	VAL
5	I	333	LEU
5	I	339	ILE
5	I	345	ILE
5	I	374	ILE
5	J	32	LEU
5	J	41	MET
5	J	51	LEU
5	J	60	ILE
5	J	88	ASP
5	J	97	LEU
5	J	113	ARG

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Mol	Chain	Res	Type
5	J	122	LEU
5	J	128	ILE
5	J	173	THR
5	J	213	ILE
5	J	247	GLN
5	J	273	ILE
5	J	333	LEU
5	J	339	ILE
5	J	357	ILE
5	J	467	VAL
6	K	11	ASN
6	K	16	ILE
6	K	19	ILE
6	K	45	MET
6	K	47	LEU
6	K	54	ARG
6	K	59	ILE
6	K	79	GLU
6	K	97	LYS
6	K	112	LEU
6	K	124	GLU
6	K	129	THR
6	K	143	GLU
6	K	154	VAL
6	K	163	LYS
6	K	166	LEU
6	K	168	GLU
6	K	169	LEU
6	K	235	LEU
6	K	244	LEU
6	K	251	ILE
6	L	16	ILE
6	L	19	ILE
6	L	45	MET
6	L	46	ILE
6	L	47	LEU
6	L	54	ARG
6	L	59	ILE
6	L	79	GLU
6	L	88	ARG
6	L	97	LYS
6	L	119	PHE

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Mol	Chain	Res	Type
6	L	124	GLU
6	L	127	TYR
6	L	143	GLU
6	L	163	LYS
6	L	165	VAL
6	L	168	GLU
6	L	169	LEU
6	L	235	LEU
6	L	244	LEU
6	L	251	ILE
7	M	169	GLU
7	M	291	ILE
7	M	311	ILE
7	M	353	ILE
7	M	368	ILE
7	M	402	VAL
7	M	406	LEU
7	M	432	ILE
7	M	475	VAL
7	M	508	HIS
7	N	189	VAL
7	N	204	MET
7	N	251	VAL
7	N	309	PHE
7	N	310	MET
7	N	311	ILE
7	N	315	LEU
7	N	353	ILE
7	N	354	GLU
7	N	368	ILE
7	N	371	LYS
7	N	406	LEU
7	N	417	VAL
7	N	420	LYS
7	N	422	HIS
7	N	425	ASN
7	N	426	ILE
7	N	429	ASP
7	N	485	LEU
7	N	492	CYS
7	N	493	THR
8	P	159	ARG

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Mol	Chain	Res	Type
8	P	166	LEU
8	P	170	LYS
8	P	171	LYS
8	P	174	PHE
8	P	180	ILE
8	P	191	LEU
8	P	213	ILE
8	P	221	GLN
8	P	229	TYR
8	P	234	VAL
8	P	235	THR
8	P	238	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	89	ASN
1	A	144	ASN
1	A	161	GLN
1	A	163	ASN
1	A	171	GLN
1	A	222	ASN
1	A	277	GLN
1	B	80	ASN
1	B	82	HIS
1	B	171	GLN
1	B	222	ASN
2	C	59	HIS
2	C	156	GLN
2	C	167	ASN
2	C	222	ASN
2	C	235	GLN
2	C	237	ASN
2	C	335	ASN
2	C	352	ASN
2	D	222	ASN
2	D	275	ASN
2	D	336	GLN
2	D	371	GLN
3	E	86	GLN
3	E	133	HIS

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Mol	Chain	Res	Type
3	E	156	GLN
3	E	164	ASN
3	E	181	GLN
3	E	258	HIS
3	E	262	ASN
3	E	265	ASN
3	E	310	GLN
3	E	313	ASN
3	E	388	ASN
3	E	399	ASN
3	F	86	GLN
3	F	156	GLN
3	F	164	ASN
3	F	186	GLN
3	F	219	GLN
3	F	221	GLN
3	F	254	GLN
3	F	262	ASN
3	F	274	ASN
3	F	309	GLN
3	F	313	ASN
3	F	399	ASN
4	G	266	ASN
4	G	342	ASN
4	G	416	ASN
4	G	475	HIS
4	G	574	ASN
4	H	446	ASN
4	H	500	ASN
4	H	524	ASN
5	I	28	GLN
5	I	73	HIS
5	I	85	GLN
5	I	87	ASN
5	I	124	ASN
5	I	212	GLN
5	I	228	ASN
5	I	296	GLN
5	I	405	ASN
5	I	423	ASN
5	J	87	ASN
5	J	142	ASN

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Mol	Chain	Res	Type
5	J	156	HIS
5	J	212	GLN
5	J	228	ASN
5	J	387	ASN
5	J	405	ASN
5	J	423	ASN
5	J	460	GLN
6	K	41	ASN
6	K	68	ASN
6	L	23	ASN
6	L	68	ASN
6	L	103	GLN
7	M	98	GLN
7	M	111	HIS
7	M	151	GLN
7	M	197	HIS
7	M	226	GLN
7	M	248	GLN
7	M	295	ASN
7	M	415	GLN
7	M	433	ASN
7	M	450	GLN
7	M	465	ASN
7	M	508	HIS
8	O	140	ASN
7	N	243	HIS
7	N	248	GLN
7	N	263	GLN
7	N	295	ASN
7	N	324	ASN
7	N	376	ASN
7	N	422	HIS
7	N	425	ASN
7	N	433	ASN
7	N	465	ASN
8	P	140	ASN
8	P	193	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
6	SEP	L	52	6	8,9,10	0.66	0	7,12,14	1.23	1 (14%)
6	SEP	K	52	6	8,9,10	0.66	0	7,12,14	1.18	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
6	SEP	L	52	6	-	2/6/8/10	-
6	SEP	K	52	6	-	2/6/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	L	52	SEP	OG-CB-CA	2.01	110.11	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	52	SEP	N-CA-CB-OG
6	K	52	SEP	C-CA-CB-OG
6	L	52	SEP	N-CA-CB-OG
6	L	52	SEP	C-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.

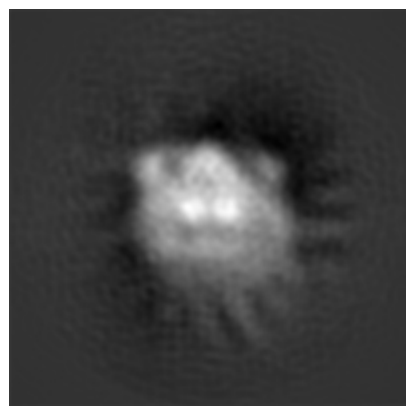
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4547. These allow visual inspection of the internal detail of the map and identification of artifacts.

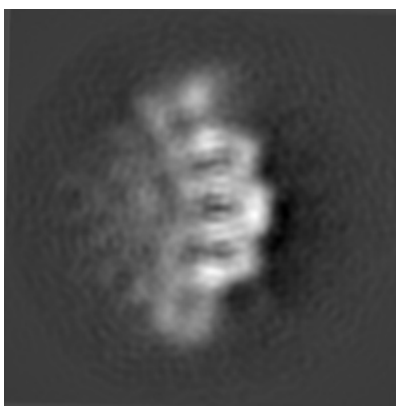
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

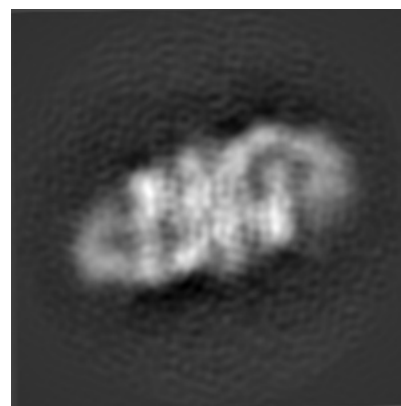
6.1.1 Primary map



X

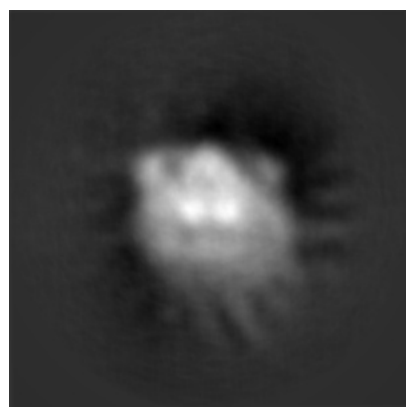


Y

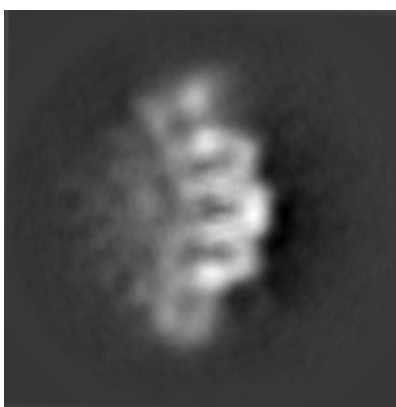


Z

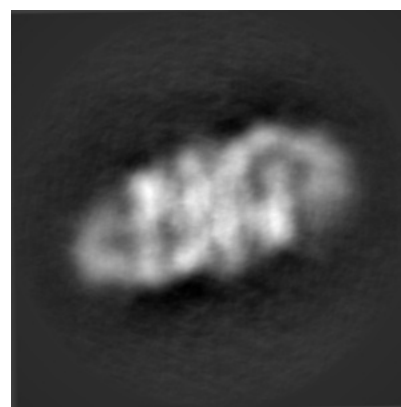
6.1.2 Raw map



X



Y

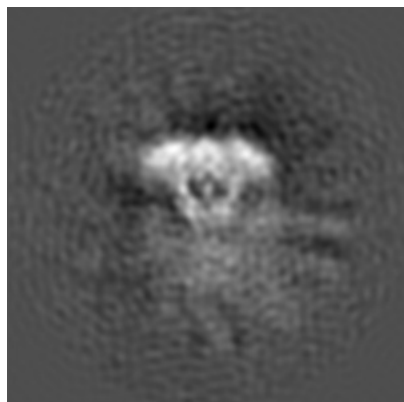


Z

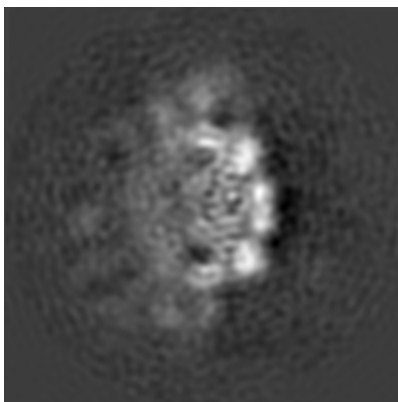
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

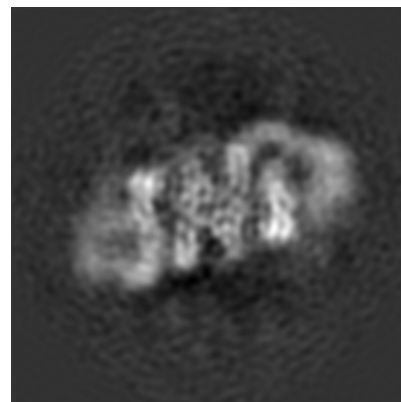
6.2.1 Primary map



X Index: 140

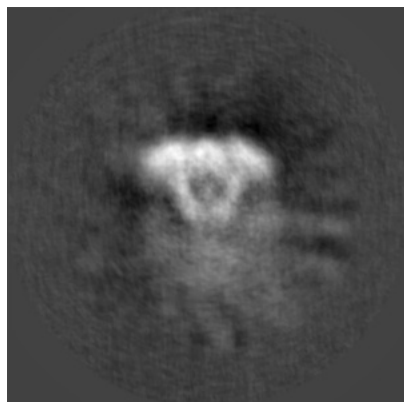


Y Index: 140

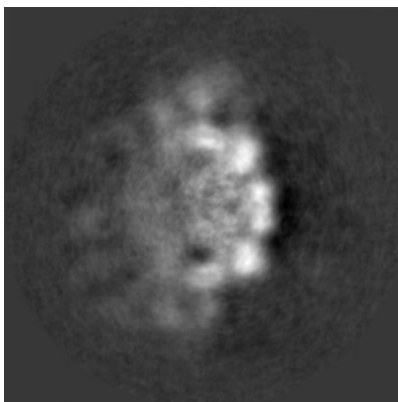


Z Index: 140

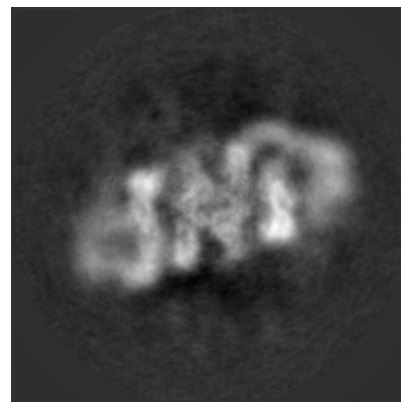
6.2.2 Raw map



X Index: 140



Y Index: 140

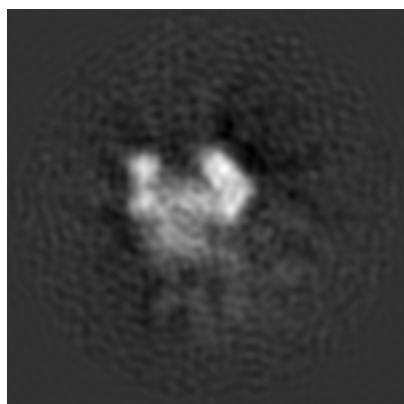


Z Index: 140

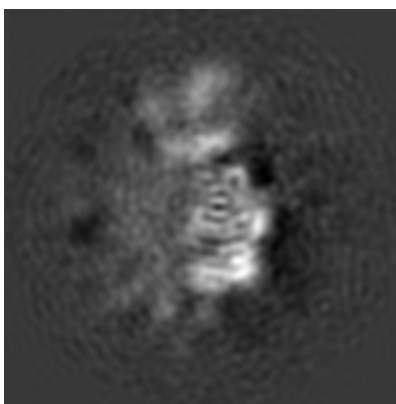
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

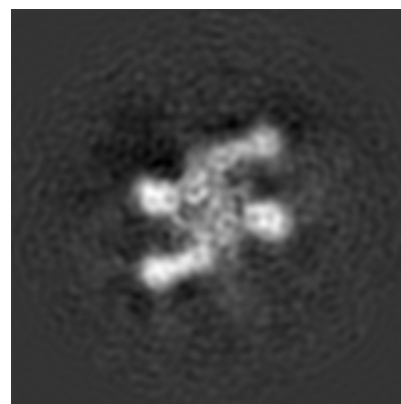
6.3.1 Primary map



X Index: 96

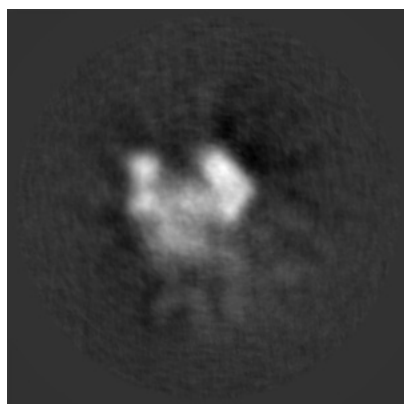


Y Index: 152

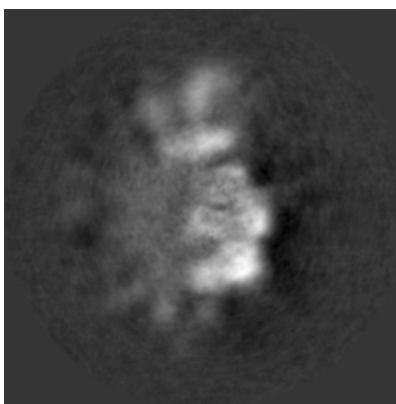


Z Index: 169

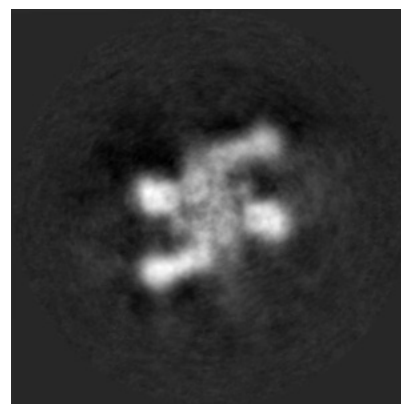
6.3.2 Raw map



X Index: 96



Y Index: 150

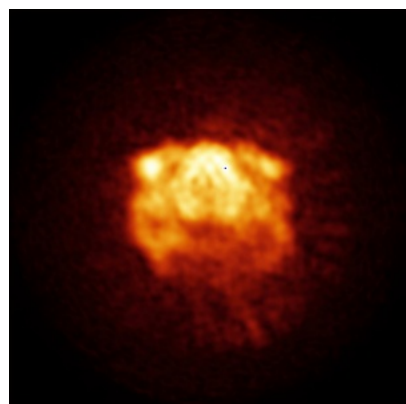


Z Index: 168

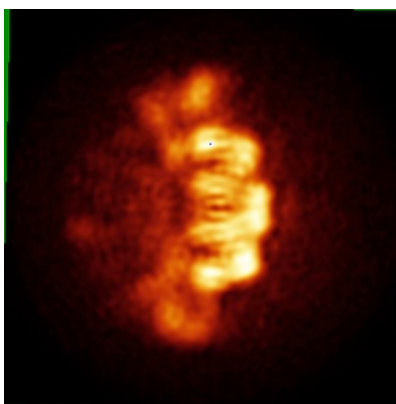
The images above show the largest variance slices of the map in three orthogonal directions.

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

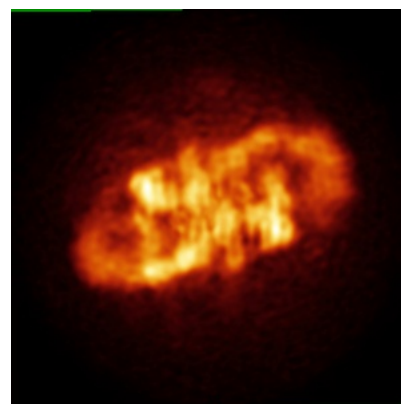
6.4.1 Primary map



X

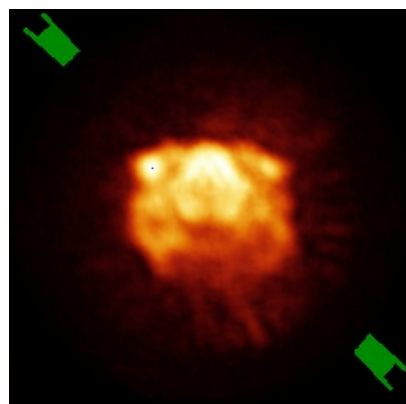


Y

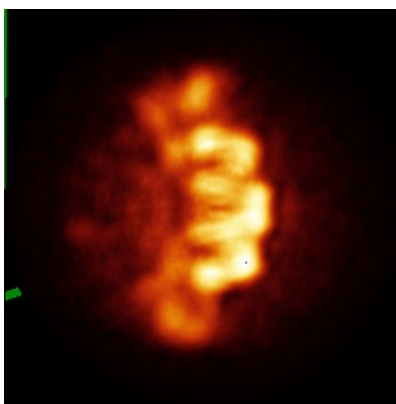


Z

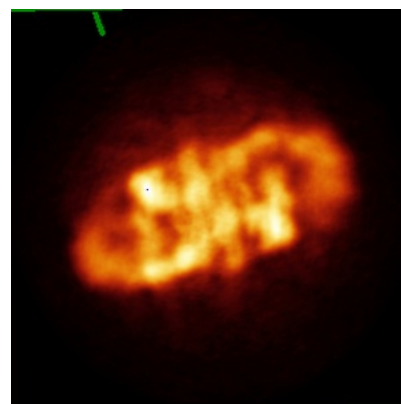
6.4.2 Raw map



X



Y



Z

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

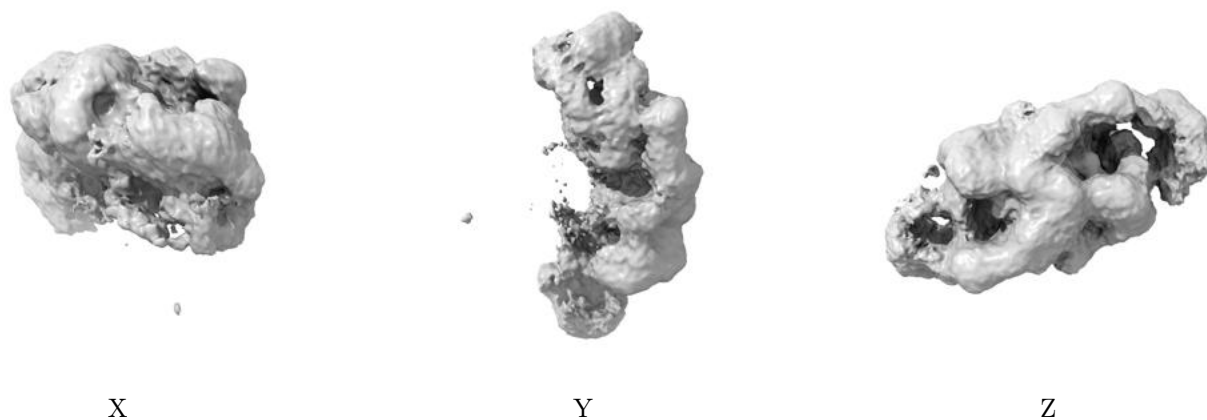
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

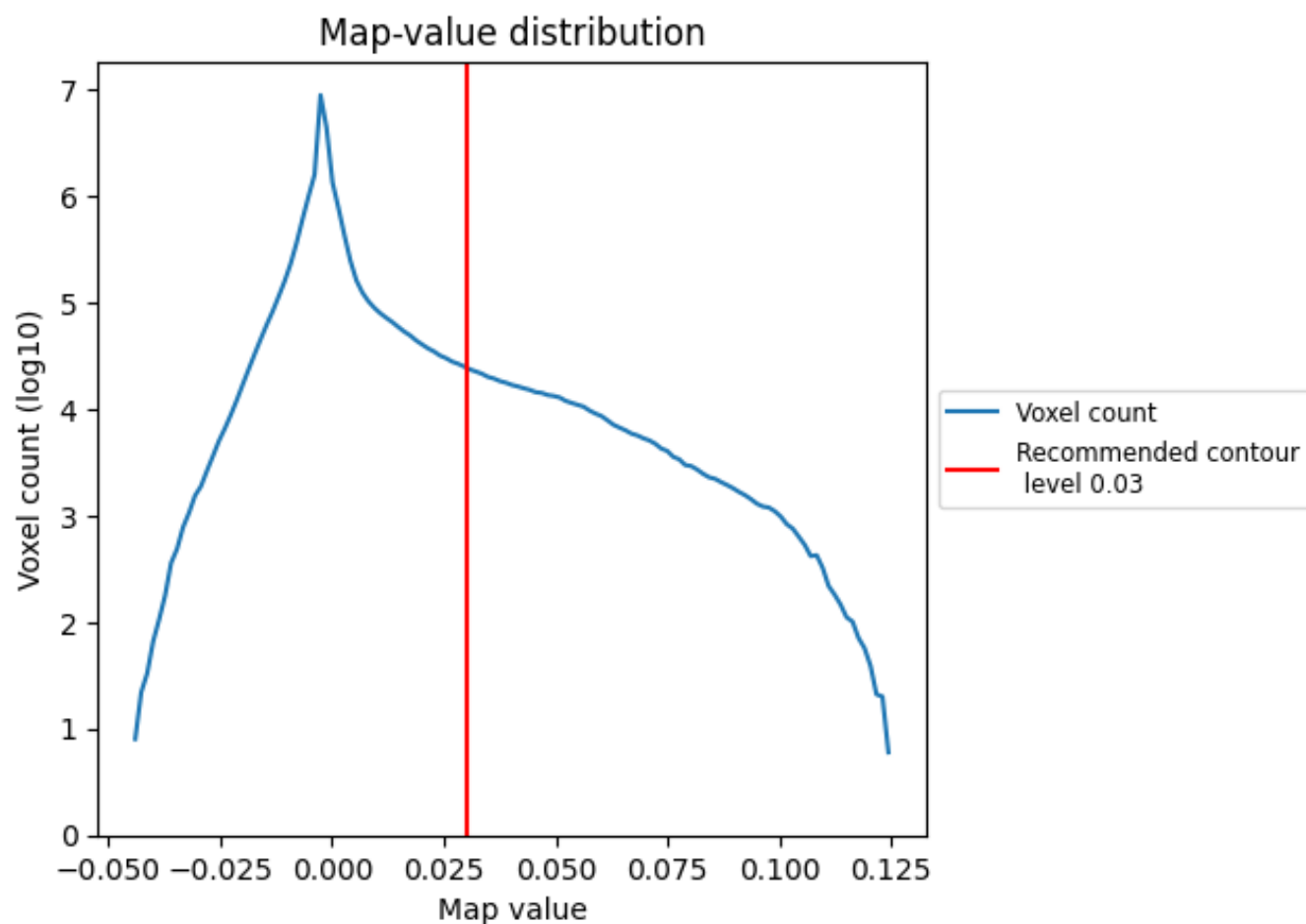
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

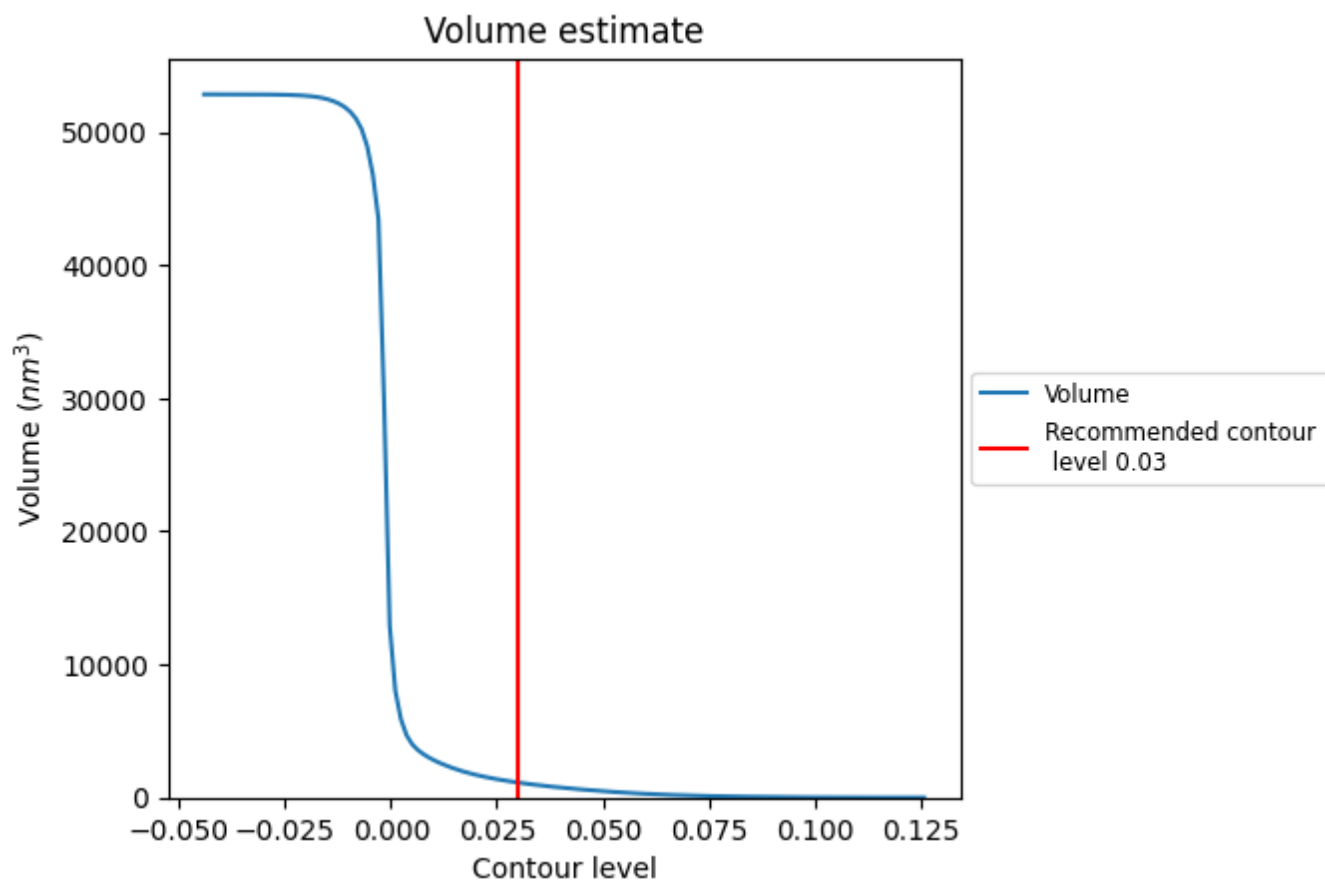
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

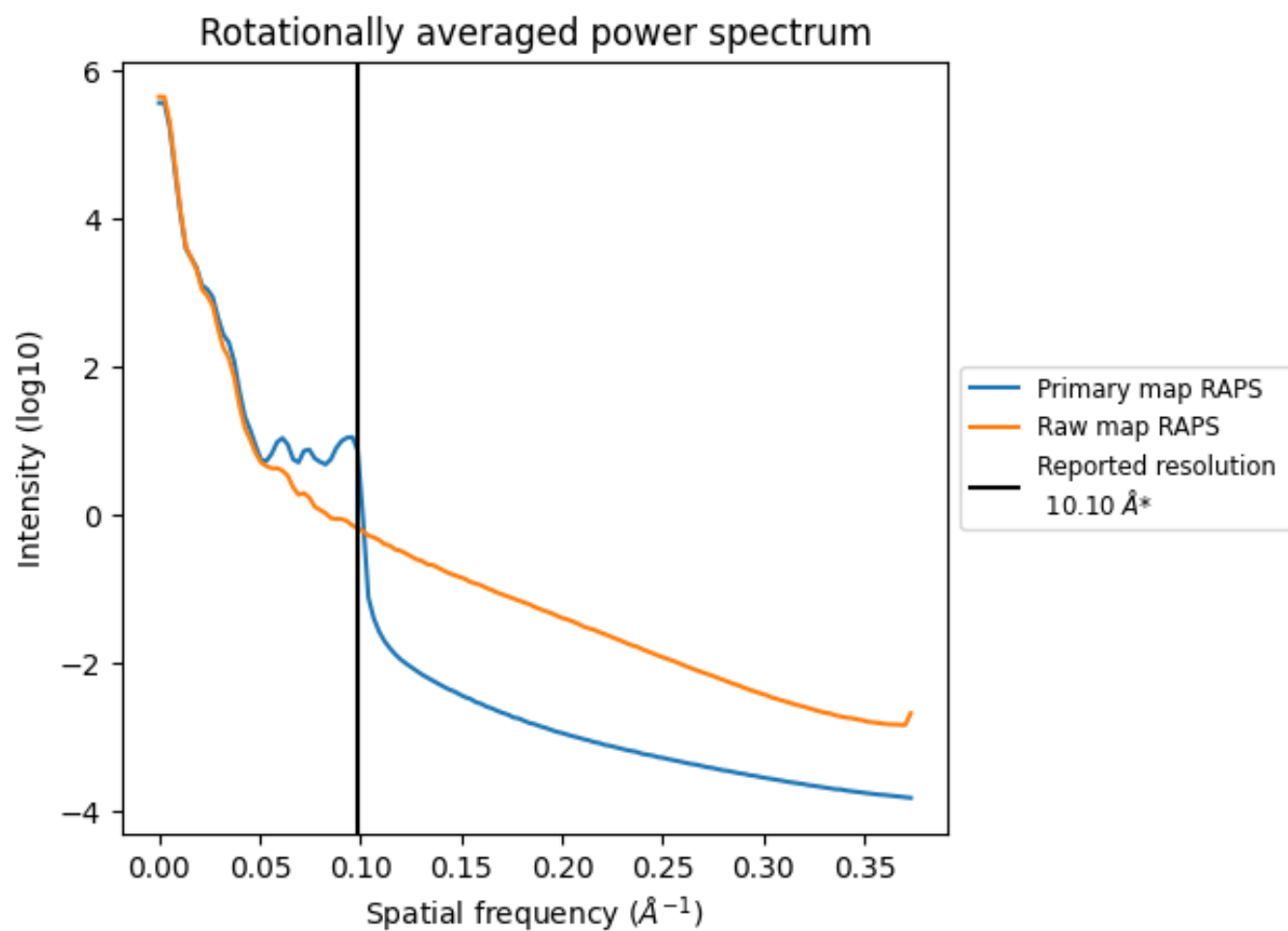
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1127 nm³; this corresponds to an approximate mass of 1018 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 ⓘ

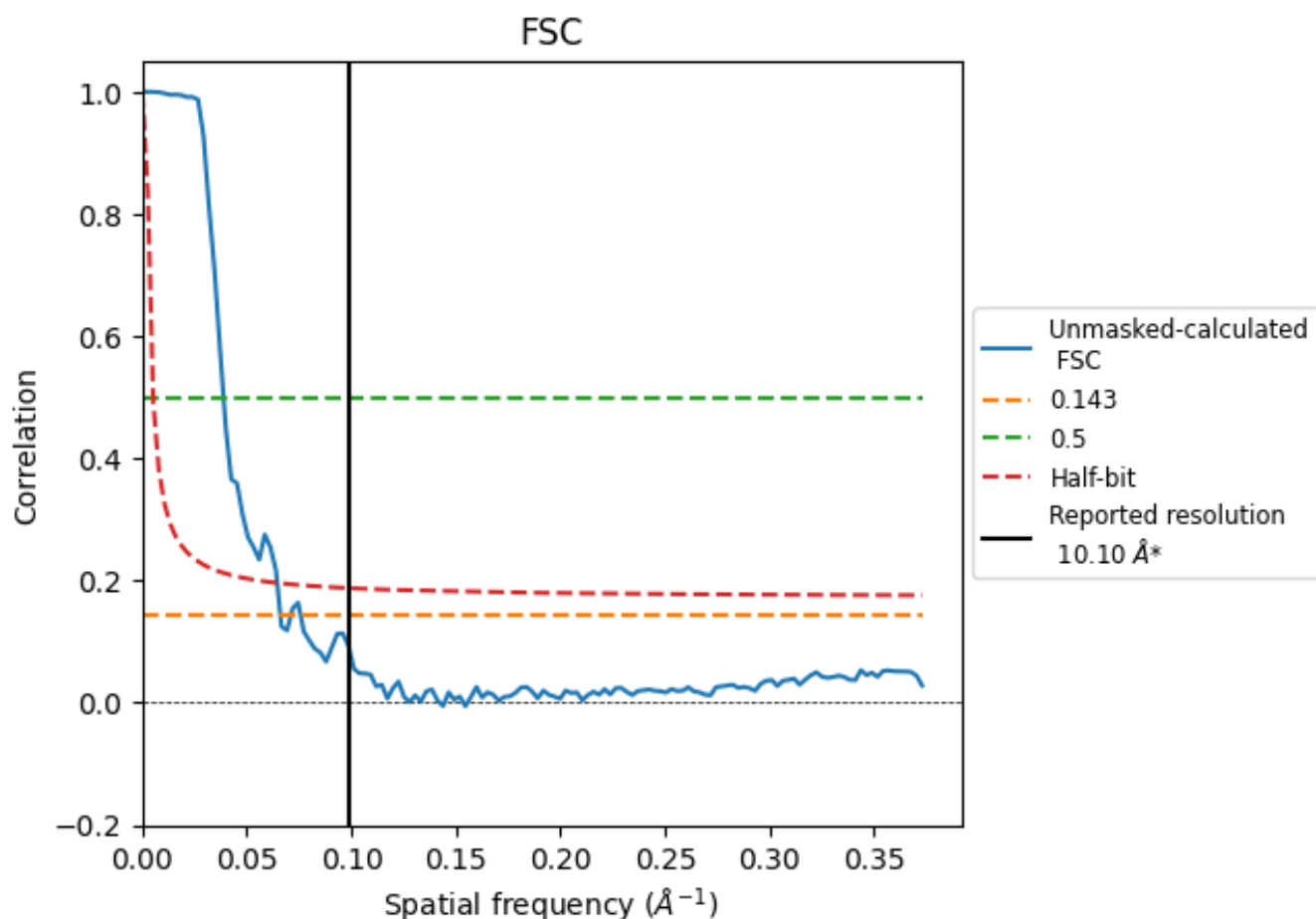


*Reported resolution corresponds to spatial frequency of 0.099 $\text{\AA}^{-1}$

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 0.099 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

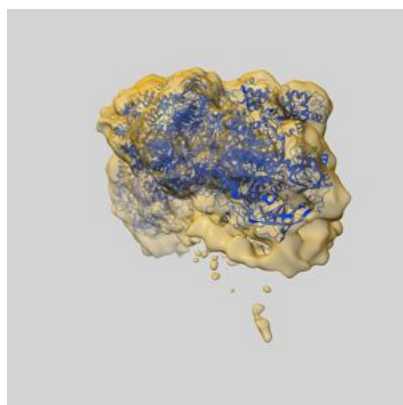
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	15.13	25.71	15.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 15.13 differs from the reported value 10.1 by more than 10 %

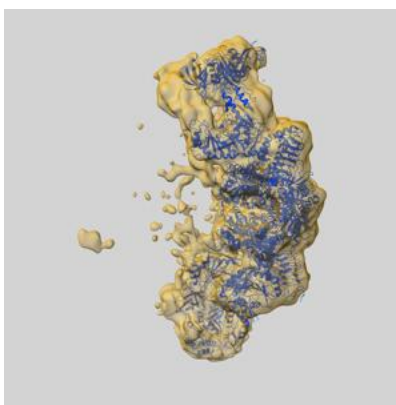
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4547 and PDB model 6QG5. Per-residue inclusion information can be found in section 3 on page 6.

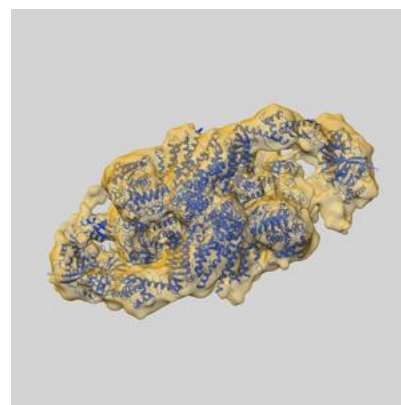
9.1 Map-model overlay [i](#)



X



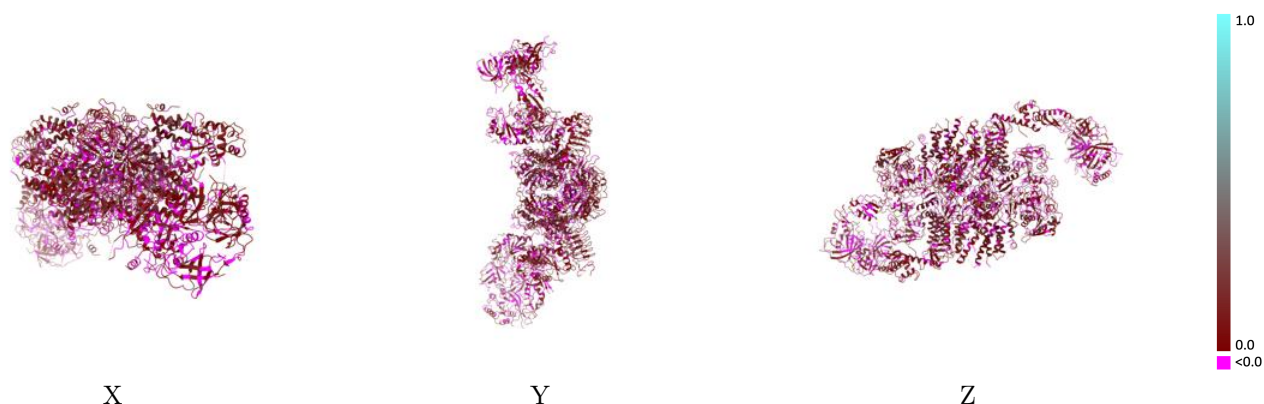
Y



Z

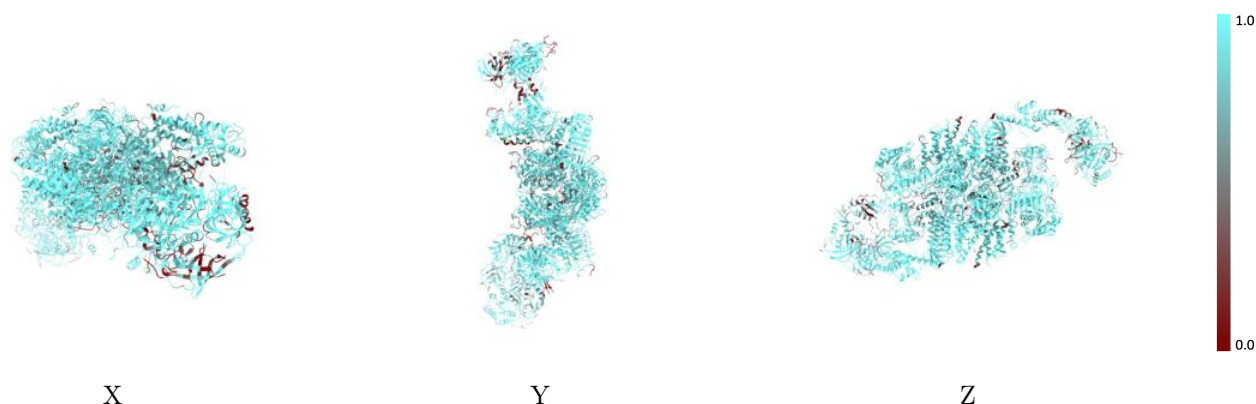
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



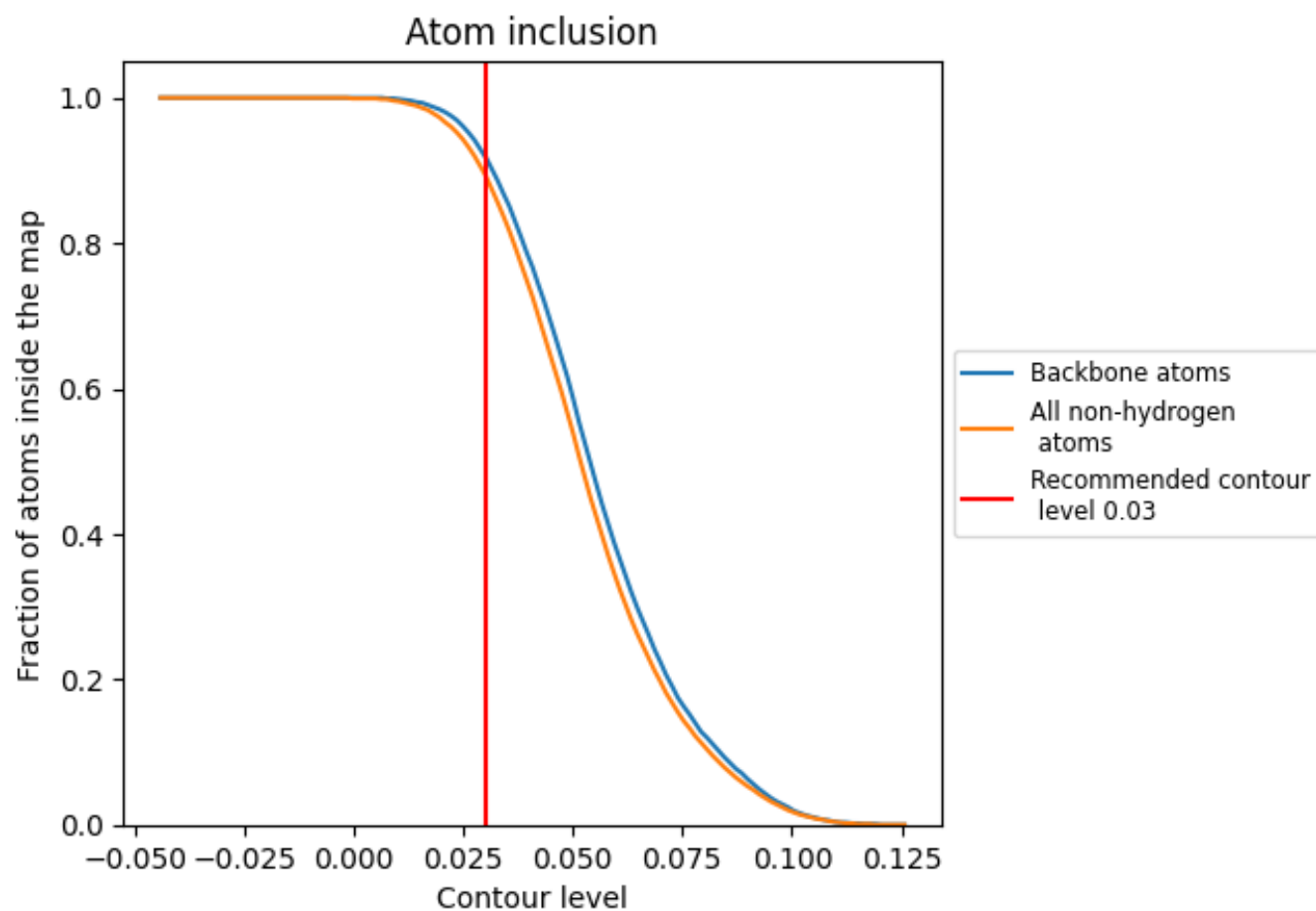
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8940	0.0690
A	0.9750	0.0770
B	0.9600	0.0810
C	0.9020	0.0750
D	0.8880	0.0740
E	0.8670	0.0430
F	0.9120	0.0500
G	0.8500	0.0880
H	0.8390	0.0890
I	0.9590	0.0820
J	0.9620	0.0820
K	0.8280	0.0670
L	0.9840	0.0760
M	0.7870	0.0350
N	0.8860	0.0430
O	0.9130	0.0540
P	0.6850	0.0590

