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

Full wwPDB EM Validation Report (i)

Jun 2, 2025 – 02:19 PM EDT

PDB ID	:	9B7L / pdb_00009b7l
EMDB ID	:	EMD-44315
Title	:	Fab2-2 in complex with the capsid of Adeno-associated virus type 9
Authors	:	Mietzsch, M.; McKenna, R.
Deposited on	:	2024-03-27
Resolution	:	2.82 Å(reported)

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 (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:

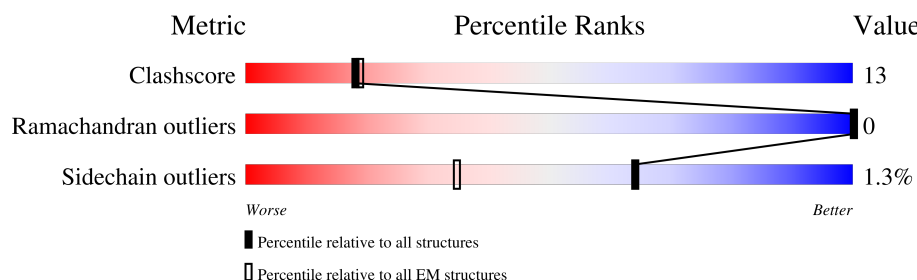|		
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.82 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		13
Ramachandran outliers		0
Sidechain outliers		1.3%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	534	59% 19% • 22%
1	B	534	24% 8% • 67%
1	C	534	70% 23% • 6%
1	D	534	59% 19% • 22%
1	E	534	23% 10% 67%
1	F	534	70% 23% • 6%
2	H	124	65% 34% ••
3	L	111	76% 24%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 19200 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	419	Total 3307	C 2092	N 570	O 632	S 13	0	0
1	B	178	Total 1384	C 857	N 248	O 274	S 5	0	0
1	C	503	Total 4018	C 2537	N 699	O 768	S 14	0	0
1	D	419	Total 3307	C 2092	N 570	O 632	S 13	0	0
1	E	177	Total 1375	C 852	N 247	O 271	S 5	0	0
1	F	503	Total 4018	C 2537	N 699	O 768	S 14	0	0

- Molecule 2 is a protein called Fab2-2 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	124	Total 985	C 628	N 160	O 194	S 3	0	0

- Molecule 3 is a protein called Fab2-2 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	111	Total 804	C 494	N 133	O 174	S 3	0	0

- Molecule 4 is water.

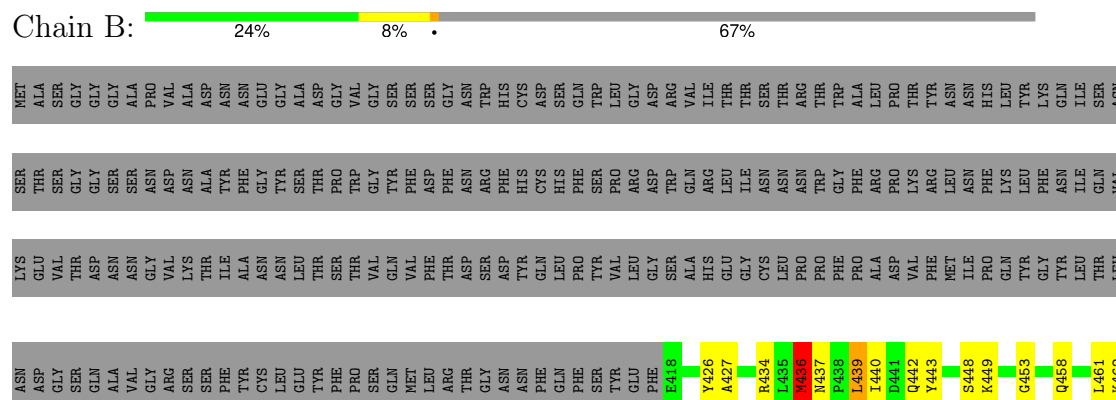| Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total 1	O 1	0
4	L	1	Total 1	O 1	0

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.
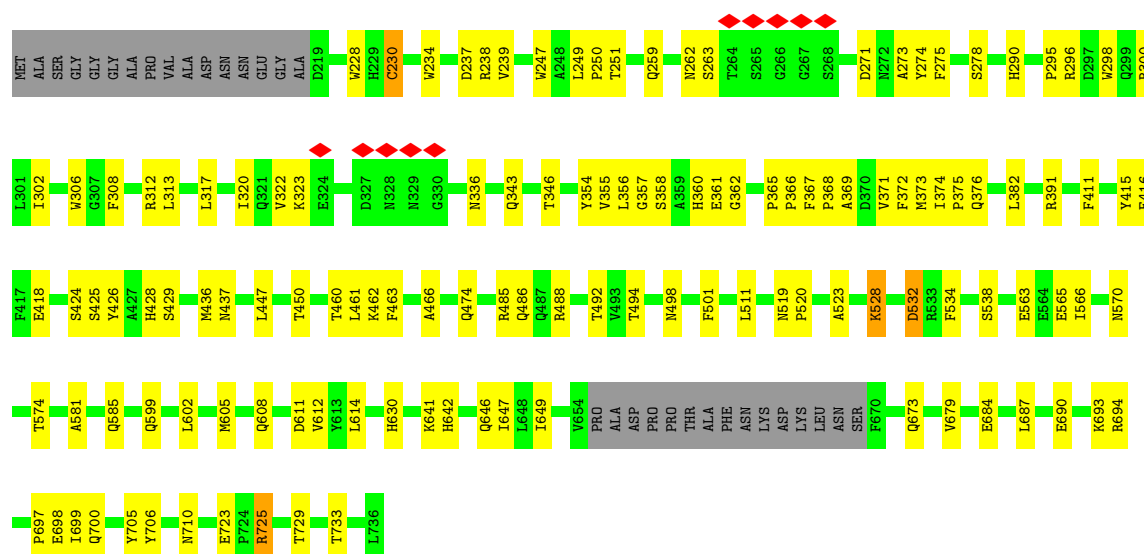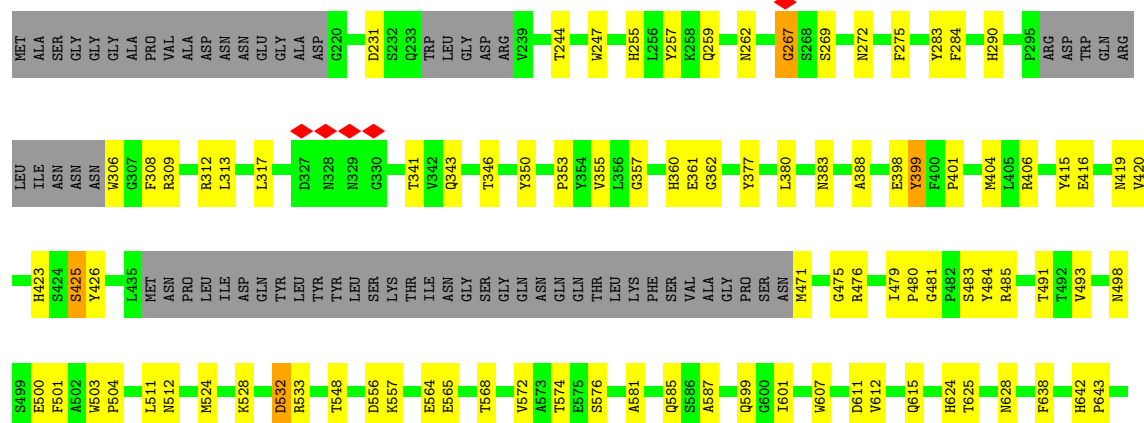
• Molecule 1: Capsid protein VP1
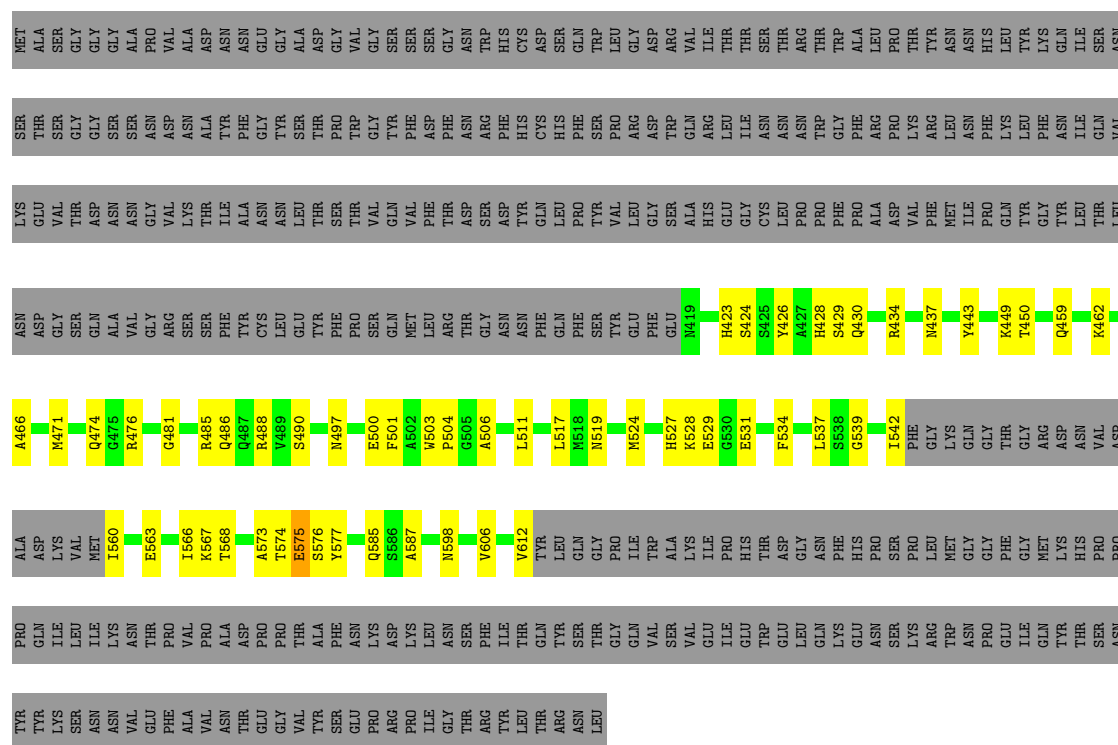
Chain A:

• Molecule 1: Capsid protein VP1

Chain B:

A466 G467 M477 Y478 I479 P480 G481 Y484 R485 S490 W503 P504 W509 A510 L511 L517 M518 N519 M524 A525 E529 D532 R533 F534 F535 P536 L537 S538 G539 I542 PHE GLY LYS GLN GLY THR GLY ARG ASP ASN VAL ASP ALA LYS VAL MET I560

K567 T568 T569 N570 P571 V572 A573 A581 Q585 N598 P603 V612 TYR LEU GLN GLY PRO ILE TRP ALA LYS ILE PRO HIS THR ASP GLY ASN GLN LYS GLU ASN SER SER PRO LEU MET GLY GLY PHE GLY MET LYS HIS PRO PRO GLN LEU ILE LEU LYS ASN THR PRO VAL PRO

ALA ASP PRO PRO THR ALA PHE ASN LYS ASP LYS LEU ASN SER PHE ILE THR GLN TYR SER THR GLY GLN VAL SER VAL GLU ILE GLU TRP GLU LEU GLN LYS GLU ASN SER LYS ARG TRP ASN PRO GLU ILE GLN TYR THR SER ASN TYR TYR LYS SER ASN ASN VAL GLU PHE ALA VAL

ASN THR GLU GLY GLY VAL TYR SER GLU PRO ARG PRO ILE GLY THR ARG TYR LEU THR ARG ASN LEU

• Molecule 1: Capsid protein VP1

Chain C: 70%   23%   • 6%

MET ALA SER GLY GLY ALA PRO VAL ALA ASP ASN ASN GLU GLY ALA D219 W228 H229 C230 W234 D237 R238 V239 W247 A248 L249 P250 T251 Q259 N262 S263 T264 S265 G266 G267 S268 D271 N272 A273 Y274 F275 S278 H290 P295 R296 D297 W298 Q299 R300

L301 I302 W306 G307 F308 R312 L313 L317 I320 Q321 V322 K323 E324 D327 N328 N329 G330 N336 Q343 T346 Y354 V355 L356 G357 S358 A359 H360 E361 G362 P365 P366 F367 P368 A369 D370 V371 F372 M373 I374 P375 Q376 L382 R391 F411 Y415 E416

F417 E418 S424 S425 Y426 A427 H428 S429 M436 N437 L447 T450 T460 L461 K462 F463 A466 Q474 R485 Q486 Q487 R488 T492 V493 T494 N498 F501 L511 N519 P520 A523 K528 D532 R533 F534 S538 E563 E564 E565 I566 N570

T574 A581 Q585 Q599 L602 M605 Q608 D611 V612 Y613 L614 H630 K641 H642 Q646 I647 L648 I649 V654 PRO ALA SER PRO PRO THR ALA PHE ASN LYS ASP LYS LEU ASN SER F670 Q673 V679 E684 L687 E690 K693 R694

P697 E698 I699 Q700 Y705 Y706 N710 E723 P724 R725 T729 T733 L736

• Molecule 1: Capsid protein VP1

Chain D: 59%   19%   •   22%

MET ALA SER GLY GLY ALA PRO VAL ALA ASP ASN ASN GLU GLY ALA ASP G220 D231 S232 Q233 TRP LEU GLY ASP ARG V239 T244 W247 H255 L256 Y257 K258 Q259 N262 G267 S268 S269 N272 F275 Y283 F284 H290 P295 ARG ASP TRP GLN ARG

LEU ILE ASN ASN ASN W306 G307 F308 R309 R312 L313 L317 D327 N328 N329 G330 T341 V342 Q343 T346 Y350 P353 Y354 V355 L356 G357 H360 E361 G362 Y377 L380 N383 A388 E398 Y399 F400 P401 M404 L405 R406 Y415 E416 N419 V420

H423 S424 S425 Y426 L435 MET ASN PRO LEU ILE ASP GLN TYR LEU TYR LEU SER LYS THR ILE ASN GLY SER GLY GLN ASN GLN GLN THR LEU PHE SER VAL ALA GLY PRO SER ASN M471 G475 R476 I479 P480 G481 P482 S483 Y484 R485 T491 T492 V493 N498

S499 E500 F501 A502 W503 P504 L511 N512 M524 K528 D532 R533 T548 D556 K557 E564 E565 T568 V572 A573 E575 S576 A581 Q585 S586 A587 Q599 G600 I601 W607 D611 V612 Q615 H624 T625 N628 F638 H642 P643

Q646 I647 P653 V654 D657 P658 P659 T660 A661 F662 L667 I671 V679 E686 L687 Q688 LYS GLU ASN SER LYS ARG TRP ASN GLU PRO ILE GLN TYR THR SER ASN TYR TYR LYS SER ASN ASN VAL GLU PHE ALA VAL ASN THR GLU GLY VAL TYR SER GLU PRO ARG PRO

ILE GLY THR ARG TYR LEU THR ARG ASN LEU

● Molecule 1: Capsid protein VP1

Chain E:

     23%   10%   67%

MET ALA SER GLY GLY ALA PRO VAL ALA ASP ASN GLU GLY ALA ASP GLY VAL GLY SER SER GLY ASN TRP HIS CYS ASP SER GLN TRP LEU GLY ASP ARG VAL ILE THR THR SER THR ARG THR TRP ALA LEU PRO THR TYR ASN ASN HIS LEU TYR LYS GLN ILE SER ASN

SER THR SER GLY GLY SER SER ASN ASP ASN ALA TYR PHE GLY TYR SER THR PRO TRP GLY TYR PHE ASP PHE ASN ARG PHE HIS CYS HIS PHE SER PRO ARG ASP TRP GLN ARG LEU ILE ASN ASN ASN TRP GLY PHE ARG PRO LYS ARG LEU ASN PHE LYS LEU PHE ASN ILE GLN VAL

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

ASN ASP GLY SER GLN ALA VAL GLY ARG SER SER PHE TYR CYS LEU GLU TYR PHE PRO SER GLN MET LEU ARG THR GLY ASN ASN PHE GLN PHE SER TYR GLU PHE GLU N419 H423 S424 Y425 Y426 A427 H428 S429 Q430 R434 N437 Y443 K449 T450 Q459 K462

A466 M471 Q474 G475 R476 G481 R485 Q486 Q487 R488 V489 S490 N497 E500 F501 A502 W503 P504 G505 A506 L511 L517 M518 N519 M524 H527 K528 E529 G530 E531 F534 L537 S538 G539 I542 PHE GLY LYS GLN GLY THR GLY ARG ASP ASN VAL ASP

ALA ASP LYS VAL MET I560 E563 I566 K567 T568 A573 T574 E575 S576 Y577 Q585 S586 A587 N598 V606 V612 TYR LEU GLN GLY PRO ILE TRP ALA LYS ILE PRO HIS THR ASP GLY ASN PHE HIS PRO SER PRO LEU MET GLY GLY PHE GLY MET LYS HIS PRO

PRO GLN ILE LEU ILE LYS ASN THR PRO VAL PRO ALA ASP PRO PRO THR ALA PHE ASN LYS ASP LYS LEU ASN SER PHE ILE THR GLN TYR SER THR GLY GLN VAL SER VAL GLU ILE GLU TRP GLU LEU GLN LYS GLU ASN SER LYS ARG TRP ASN PRO GLU ILE GLN TYR THR SER ASN

TYR TYR LYS SER ASN ASN VAL GLU PHE ALA VAL ASN THR GLU GLY VAL TYR SER GLU PRO ARG PRO ILE GLY THR ARG TYR LEU THR ARG ASN LEU

● Molecule 1: Capsid protein VP1

Chain F:

         70%   23%   6%

MET ALA SER GLY GLY ALA PRO VAL ALA ASP ASN GLU GLY ALA D219 C230 D231 S232 Q233 W234 L235 V239 S243 T246 W247 P250 T251 Y252 Q259 N262 S265 G266 G267 S268 A273 Y274 F275 W281 F284 R288 F289 H290 P295 R296 D297

W298 Q299 R300 L301 I302 W306 G307 P308 R309 R312 K316 L317 Q321 D327 N328 N329 G330 V331 K332 S340 T346 P353 Y354 V355 S358 A359 H360 E361 G362 P365 F366 F367 P368 A369 D370 V371 F372 M373 I374 N383 Q412 E416 F417 E418 N419 V420

S425 Y426 A427 H428 S429 Q430 S431 R434 Q442 Y443 L447 S448 K449 T450 Q459 T460 L461 K462 A466 Q474 N477 N497 N498 S499 E500 F501 A502 W503 P504 G505 A506 L511 L517 D532 I542 I560 T561 N562 E563 E564 E565 I566 K567 T568 T569 N570

A581 Q585 I601 V606 W607 Q608 D611 V612 Q615 H624 T625 F629 K641 Q646 I647 K650 V654 PRO ALA ASP PRO PRO THR ALA PHE ASN LYS ASP LYS LEU ASN SER F670 Q673 V679 S680 E684 W685 E686 E690 R694 P697 E698

Y701 T702 S703 N704 Y705 Y706 K707 T729 T733 L736

• Molecule 2: Fab2-2 heavy chain

Chain H:

65%   34%

Q20 V21 Q22 L23 Q24 E25 L30 V31 K32 V35 T36 C41 D46 S47 I48 Y52 W53 S54 W66 I67 G68 Y69 I70 Y71 Y72 N75 T76 N77 Y78 L82 K83 S84 R85 V86 T87 M88 N95 Q96 L101 N102 S103 V104 T105 C114 H118 Y121

Y124 S127 V141 S142 S143

• Molecule 3: Fab2-2 light chain

Chain L:

76%   24%

Q21 L24 T25 Q26 V30 S31 P34 G35 Q36 S37 I40 G44 D48 M69 P77 S78 S79 G80 V81 N92 S99 E104 D105 E106 Y109 Y110 C111 S118 T119 G125 T126 K127 L128 T129 V130 L131

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1085751	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	12.388	Depositor
Minimum map value	-6.320	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2	Depositor
Map size (Å)	166.2, 166.2, 166.2	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.831, 0.831, 0.831	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	0/3408	0.58	2/4642 (0.0%)
1	B	0.44	0/1417	1.04	15/1928 (0.8%)
1	C	0.41	0/4138	0.61	3/5636 (0.1%)
1	D	0.39	1/3408 (0.0%)	0.60	1/4642 (0.0%)
1	E	0.39	0/1408	0.69	1/1916 (0.1%)
1	F	0.41	0/4138	0.57	0/5636
2	H	0.46	0/1015	0.80	3/1387 (0.2%)
3	L	0.46	0/819	0.84	0/1114
All	All	0.41	1/19751 (0.0%)	0.66	25/26901 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	399	TYR	C-N	-5.62	1.22	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	539	GLY	N-CA-C	10.73	125.61	112.73
1	B	481	GLY	CA-C-N	7.65	127.64	119.76
1	B	481	GLY	C-N-CA	7.65	127.64	119.76
1	B	440	ILE	N-CA-C	7.56	119.17	108.36
1	B	453	GLY	N-CA-C	7.40	121.43	112.48
1	D	267	GLY	N-CA-C	7.16	124.33	111.02
1	B	467	GLY	CA-C-N	7.02	126.84	119.05
1	B	467	GLY	C-N-CA	7.02	126.84	119.05
1	B	533	ARG	N-CA-C	6.86	118.76	111.28
1	C	705	TYR	N-CA-C	-6.76	97.53	108.41
1	B	448	SER	N-CA-C	6.46	118.40	111.36
1	B	439	LEU	N-CA-C	6.28	118.21	111.36
1	E	539	GLY	N-CA-C	6.06	120.01	112.73
1	B	534	PHE	N-CA-C	5.92	119.04	110.28
1	C	723	GLU	CA-C-N	5.88	125.58	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	723	GLU	C-N-CA	5.88	125.58	119.05
1	B	437	ASN	CA-C-N	5.79	125.48	119.05
1	B	437	ASN	C-N-CA	5.79	125.48	119.05
2	H	86	VAL	N-CA-C	5.59	115.93	108.11
2	H	83	LYS	N-CA-C	5.48	117.26	111.28
1	A	256	LEU	N-CA-C	5.40	117.89	109.52
1	B	436	MET	N-CA-C	5.39	117.65	110.53
1	B	570	ASN	N-CA-C	5.14	116.30	109.93
2	H	85	ARG	N-CA-C	5.08	118.79	112.59
1	A	423	HIS	N-CA-C	-5.05	102.80	110.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3307	0	3095	86	0
1	B	1384	0	1306	49	0
1	C	4018	0	3775	113	0
1	D	3307	0	3095	112	0
1	E	1375	0	1300	59	0
1	F	4018	0	3775	118	0
2	H	985	0	928	35	0
3	L	804	0	767	25	0
4	C	1	0	0	0	0
4	L	1	0	0	0	0
All	All	19200	0	18041	484	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 13.

All (484) 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:D:483:SER:HA	1:D:524:MET:CE	1.40	1.47
1:D:483:SER:CA	1:D:524:MET:CE	2.04	1.35
1:A:524:MET:HE2	1:A:573:ALA:HA	1.22	1.14
1:B:436:MET:H	1:B:436:MET:HE3	1.00	1.13
1:D:483:SER:CA	1:D:524:MET:HE3	1.74	1.10
1:D:483:SER:CB	1:D:524:MET:HE2	1.83	1.09
1:D:483:SER:CB	1:D:524:MET:CE	2.30	1.08
1:E:527:HIS:ND1	1:E:531:GLU:O	1.88	1.06
1:E:524:MET:HE2	1:E:573:ALA:HA	1.05	1.05
1:E:524:MET:CE	1:E:573:ALA:HA	1.86	1.04
1:E:528:LYS:HE2	1:E:575:GLU:CD	1.85	1.01
1:E:529:GLU:OE1	1:E:567:LYS:NZ	1.93	1.00
1:C:725:ARG:HH11	1:C:725:ARG:HB3	1.28	0.98
1:E:528:LYS:HE2	1:E:575:GLU:OE1	1.66	0.95
1:D:483:SER:HB2	1:D:524:MET:CE	1.96	0.92
2:H:105:THR:O	2:H:141:VAL:HG11	1.68	0.91
1:B:436:MET:HE3	1:B:436:MET:N	1.85	0.91
3:L:40:ILE:HG21	3:L:126:THR:HG21	1.52	0.90
1:D:484:TYR:N	1:D:524:MET:HE1	1.87	0.90
1:D:483:SER:CA	1:D:524:MET:HE1	2.00	0.88
1:A:306:TRP:O	1:A:425:SER:OG	1.92	0.88
1:E:506:ALA:HB1	1:E:517:LEU:HD11	1.53	0.87
1:D:483:SER:HB2	1:D:524:MET:HE2	1.54	0.87
1:C:725:ARG:HB3	1:C:725:ARG:NH1	1.91	0.85
1:E:524:MET:HE2	1:E:573:ALA:CA	1.99	0.85
1:E:528:LYS:HE2	1:E:575:GLU:OE2	1.77	0.84
1:F:297:ASP:OD1	1:F:300:ARG:NH1	2.12	0.82
1:E:485:ARG:NH2	1:E:576:SER:OG	2.14	0.80
1:D:483:SER:HA	1:D:524:MET:HE3	0.81	0.79
1:C:699:ILE:HG12	1:F:703:SER:O	1.83	0.79
2:H:105:THR:C	2:H:141:VAL:HG11	2.07	0.78
1:A:524:MET:CE	1:A:573:ALA:HA	2.08	0.78
1:F:431:SER:HA	1:F:568:THR:HB	1.66	0.78
1:B:436:MET:H	1:B:436:MET:CE	1.90	0.77
1:A:381:THR:HG21	1:A:393:SER:H	1.52	0.74
1:A:581:ALA:O	1:B:485:ARG:HD2	1.87	0.74
1:A:306:TRP:C	1:A:425:SER:HG	1.95	0.74
1:D:483:SER:HB2	1:D:524:MET:HE1	1.68	0.74
1:F:259:GLN:HE21	1:F:275:PHE:HE1	1.35	0.73
1:C:230:CYS:HB3	1:D:399:TYR:HA	1.70	0.73
1:D:528:LYS:HG2	1:D:572:VAL:HG21	1.68	0.73
1:C:725:ARG:HH11	1:C:725:ARG:CB	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:SER:HB2	1:C:729:THR:HG22	1.72	0.72
1:D:587:ALA:HA	1:E:497:ASN:HA	1.70	0.72
1:C:361:GLU:HG3	1:C:362:GLY:H	1.55	0.71
1:B:568:THR:HG21	1:C:382:LEU:HD21	1.73	0.71
1:A:485:ARG:NH2	1:A:576:SER:OG	2.23	0.71
1:F:570:ASN:HD21	1:F:608:GLN:H	1.39	0.71
1:A:346:THR:HG22	1:A:647:ILE:HG12	1.72	0.71
2:H:70:ILE:HG13	2:H:76:THR:HG22	1.73	0.71
1:B:525:ALA:HB3	1:B:572:VAL:HA	1.74	0.70
1:D:484:TYR:H	1:D:524:MET:HE1	1.53	0.70
1:C:425:SER:CB	1:C:729:THR:HG22	2.22	0.69
1:F:252:TYR:OH	1:F:374:ILE:O	2.11	0.69
1:D:306:TRP:O	1:D:425:SER:N	2.25	0.69
1:A:566:ILE:HD12	1:A:570:ASN:HD22	1.57	0.69
1:A:322:VAL:HG11	1:A:673:GLN:HE21	1.56	0.69
1:D:475:GLY:CA	1:E:519:ASN:HD22	2.05	0.69
1:A:381:THR:HG22	1:A:382:LEU:H	1.58	0.69
3:L:40:ILE:CG2	3:L:126:THR:HG21	2.22	0.68
1:B:537:LEU:C	1:B:537:LEU:HD23	2.19	0.68
1:D:483:SER:C	1:D:524:MET:HE1	2.18	0.68
1:D:262:ASN:O	1:D:267:GLY:N	2.26	0.67
1:A:247:TRP:CD1	1:A:679:VAL:HG23	2.29	0.67
1:A:343:GLN:HE21	1:A:404:MET:HE3	1.59	0.67
1:D:484:TYR:H	1:D:524:MET:CE	2.08	0.67
1:C:565:GLU:OE1	1:C:565:GLU:N	2.23	0.66
1:D:568:THR:O	1:E:511:LEU:HD11	1.95	0.66
1:C:230:CYS:O	1:D:399:TYR:O	2.13	0.66
1:F:466:ALA:HB1	1:F:474:GLN:HG2	1.76	0.66
1:E:528:LYS:CE	1:E:575:GLU:OE1	2.42	0.66
1:D:532:ASP:OD1	1:D:532:ASP:N	2.28	0.66
1:A:250:PRO:HG3	1:A:373:MET:HE3	1.76	0.65
1:E:542:ILE:HG12	1:E:560:ILE:HG12	1.78	0.65
1:D:498:ASN:HB2	1:F:459:GLN:NE2	2.12	0.65
1:A:568:THR:O	1:B:511:LEU:HD21	1.98	0.64
1:C:693:LYS:NZ	1:F:231:ASP:OD2	2.30	0.64
1:D:565:GLU:N	1:D:565:GLU:OE1	2.28	0.64
1:E:500:GLU:OE1	1:E:500:GLU:HA	1.96	0.64
1:F:312:ARG:NH1	1:F:684:GLU:OE1	2.30	0.64
1:A:325:VAL:HG22	1:A:334:ILE:HG12	1.79	0.64
1:E:585:GLN:OE1	1:F:501:PHE:CZ	2.51	0.64
1:F:503:TRP:N	1:F:504:PRO:CD	2.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ASN:ND2	1:C:599:GLN:OE1	2.30	0.64
1:C:323:LYS:NZ	1:C:336:ASN:OD1	2.19	0.64
1:D:306:TRP:O	1:D:425:SER:HB2	1.98	0.64
1:B:477:ASN:ND2	1:C:357:GLY:O	2.31	0.64
1:D:484:TYR:N	1:D:524:MET:CE	2.58	0.64
1:E:537:LEU:HD23	1:E:537:LEU:O	1.98	0.64
2:H:105:THR:O	2:H:141:VAL:CG1	2.45	0.64
1:D:501:PHE:CZ	1:F:585:GLN:OE1	2.50	0.63
1:D:511:LEU:HD21	1:F:568:THR:O	1.98	0.63
1:B:427:ALA:HB3	1:C:391:ARG:HD3	1.79	0.63
1:D:247:TRP:CD1	1:D:679:VAL:HG23	2.32	0.63
1:D:585:GLN:OE1	1:E:501:PHE:CZ	2.51	0.63
1:A:262:ASN:HD22	1:A:273:ALA:HA	1.63	0.63
1:B:479:ILE:HB	1:B:480:PRO:HD2	1.80	0.63
1:A:399:TYR:O	1:F:230:CYS:O	2.17	0.63
1:D:503:TRP:HB3	1:D:504:PRO:HD3	1.81	0.63
1:C:237:ASP:O	1:C:687:LEU:N	2.29	0.63
1:A:322:VAL:CG1	1:A:673:GLN:HE21	2.12	0.62
1:A:483:SER:HB2	1:A:524:MET:HE3	1.80	0.62
1:C:317:LEU:HB3	1:C:411:PHE:HB3	1.79	0.62
2:H:32:LYS:O	2:H:35:VAL:HG12	1.99	0.62
2:H:47:SER:HA	2:H:95:ASN:HD21	1.63	0.62
1:D:353:PRO:HB3	1:F:430:GLN:NE2	2.14	0.61
1:E:537:LEU:HD23	1:E:537:LEU:C	2.24	0.61
1:D:483:SER:C	1:D:524:MET:CE	2.74	0.61
1:F:565:GLU:CD	1:F:565:GLU:H	2.08	0.61
1:A:513:GLY:HA3	1:C:528:LYS:HD3	1.82	0.61
1:F:425:SER:CB	1:F:729:THR:HG22	2.31	0.61
1:B:458:GLN:O	1:C:498:ASN:OD1	2.18	0.61
1:D:355:VAL:H	1:D:646:GLN:NE2	1.99	0.60
1:B:581:ALA:O	1:C:485:ARG:HD2	2.02	0.60
1:D:475:GLY:HA2	1:E:519:ASN:HD22	1.65	0.60
1:B:537:LEU:HD23	1:B:537:LEU:O	2.01	0.60
1:E:529:GLU:OE1	1:E:567:LYS:CE	2.50	0.60
1:A:361:GLU:HG3	1:A:362:GLY:H	1.66	0.59
1:E:527:HIS:CG	1:E:531:GLU:O	2.54	0.59
1:C:249:LEU:HB2	1:C:374:ILE:HD12	1.84	0.59
1:B:443:TYR:HB3	1:C:361:GLU:OE1	2.03	0.59
1:E:471:MET:O	1:E:476:ARG:NH2	2.31	0.59
1:A:624:HIS:O	1:C:428:HIS:HE1	1.86	0.59
1:C:355:VAL:H	1:C:646:GLN:NE2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:ARG:NH1	1:D:420:VAL:O	2.32	0.59
1:E:528:LYS:CE	1:E:575:GLU:OE2	2.50	0.58
1:A:244:THR:O	1:A:245:ARG:NH2	2.35	0.58
1:C:247:TRP:CD1	1:C:679:VAL:HG23	2.39	0.58
1:D:423:HIS:NE2	1:D:612:VAL:HG22	2.18	0.58
1:D:343:GLN:HG2	1:D:404:MET:HG2	1.84	0.58
1:E:506:ALA:HB1	1:E:517:LEU:CD1	2.28	0.58
1:D:485:ARG:NH2	1:D:576:SER:OG	2.34	0.58
1:E:430:GLN:NE2	1:F:353:PRO:HB3	2.19	0.57
1:A:355:VAL:H	1:A:646:GLN:NE2	2.03	0.57
1:C:488:ARG:HB3	1:C:574:THR:HG21	1.86	0.57
2:H:35:VAL:O	2:H:104:VAL:HG22	2.05	0.57
1:C:346:THR:HG22	1:C:647:ILE:HG12	1.86	0.57
1:F:284:PHE:CE1	1:F:679:VAL:HG21	2.40	0.57
2:H:68:GLY:C	2:H:88:MET:HE1	2.30	0.57
1:B:503:TRP:N	1:B:504:PRO:CD	2.68	0.56
1:E:490:SER:HB2	1:E:534:PHE:CE1	2.40	0.56
1:F:355:VAL:H	1:F:646:GLN:NE2	2.03	0.56
1:C:250:PRO:HG3	1:C:373:MET:HE3	1.87	0.56
1:C:228:TRP:O	1:D:401:PRO:HA	2.06	0.56
1:A:387:GLN:OE1	1:F:707:LYS:HE2	2.06	0.55
1:D:548:THR:HG23	1:D:557:LYS:HB3	1.88	0.55
1:E:466:ALA:HB1	1:E:474:GLN:HG2	1.87	0.55
1:F:340:SER:OG	1:F:673:GLN:NE2	2.37	0.55
1:A:399:TYR:HA	1:F:230:CYS:HB3	1.89	0.55
1:B:585:GLN:OE1	1:C:501:PHE:CZ	2.59	0.55
1:D:483:SER:CB	1:D:524:MET:HE1	2.18	0.55
1:A:228:TRP:HE1	1:A:230:CYS:HB2	1.72	0.55
1:D:483:SER:HA	1:D:524:MET:HE2	1.68	0.55
1:D:624:HIS:O	1:F:428:HIS:HE1	1.90	0.55
1:A:565:GLU:CD	1:A:565:GLU:H	2.15	0.55
1:E:423:HIS:NE2	1:E:612:VAL:HG22	2.23	0.54
1:D:257:TYR:OH	1:D:398:GLU:HG2	2.06	0.54
1:F:503:TRP:H	1:F:504:PRO:CD	2.19	0.54
2:H:78:TYR:HE1	2:H:88:MET:HG3	1.72	0.54
1:B:427:ALA:CB	1:C:391:ARG:HD3	2.37	0.54
3:L:40:ILE:HD13	3:L:126:THR:HG21	1.88	0.54
1:D:231:ASP:N	1:D:231:ASP:OD1	2.41	0.54
1:D:244:THR:HA	1:D:679:VAL:O	2.07	0.54
1:D:346:THR:HG22	1:D:647:ILE:HG12	1.89	0.54
1:A:340:SER:HA	1:F:321:GLN:NE2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:485:ARG:HG2	1:E:486:GLN:N	2.23	0.54
1:A:262:ASN:OD1	1:A:263:SER:N	2.41	0.54
1:D:585:GLN:HE22	1:E:501:PHE:HZ	1.55	0.54
1:F:706:TYR:CD1	1:F:706:TYR:C	2.85	0.54
1:B:442:GLN:NE2	1:C:358:SER:O	2.35	0.54
1:C:694:ARG:HD3	1:C:698:GLU:OE2	2.07	0.54
2:H:31:VAL:CG1	2:H:35:VAL:CG1	2.86	0.54
1:B:436:MET:HB2	1:C:360:HIS:NE2	2.23	0.53
1:D:483:SER:HB3	1:D:524:MET:HE2	1.84	0.53
1:A:388:ALA:O	1:F:707:LYS:HA	2.08	0.53
1:C:313:LEU:HB3	1:C:415:TYR:HB3	1.90	0.53
1:C:308:PHE:HE2	1:C:729:THR:HG21	1.73	0.53
1:C:361:GLU:HG3	1:C:362:GLY:N	2.22	0.53
1:D:512:ASN:ND2	1:F:567:LYS:HD2	2.22	0.53
1:C:368:PRO:HB2	1:D:398:GLU:HB2	1.91	0.53
1:F:302:ILE:HG22	1:F:729:THR:HG23	1.90	0.53
1:F:425:SER:HB2	1:F:729:THR:HG22	1.89	0.53
1:A:306:TRP:C	1:A:425:SER:OG	2.48	0.53
1:F:425:SER:HB3	1:F:729:THR:HG22	1.91	0.53
1:D:360:HIS:HA	1:F:442:GLN:HA	1.91	0.52
1:D:485:ARG:HD2	1:F:581:ALA:O	2.09	0.52
1:C:302:ILE:HG22	1:C:729:THR:HG23	1.90	0.52
1:D:353:PRO:HB3	1:F:430:GLN:HE22	1.73	0.52
1:C:322:VAL:HG11	1:C:673:GLN:HE21	1.75	0.52
1:F:250:PRO:HG3	1:F:373:MET:HE3	1.91	0.52
1:F:262:ASN:HD22	1:F:274:TYR:H	1.56	0.52
1:D:426:TYR:CD1	1:D:426:TYR:C	2.86	0.52
1:F:361:GLU:HG3	1:F:362:GLY:H	1.74	0.52
2:H:23:LEU:HD13	2:H:114:CYS:O	2.10	0.52
1:D:350:TYR:OH	1:D:643:PRO:O	2.27	0.52
1:A:599:GLN:OE1	1:B:598:ASN:ND2	2.40	0.52
1:A:473:VAL:HG12	1:B:503:TRP:HZ3	1.75	0.52
1:D:599:GLN:OE1	1:E:598:ASN:ND2	2.43	0.52
1:B:442:GLN:HB2	1:B:466:ALA:HB3	1.92	0.52
1:A:473:VAL:HG12	1:B:503:TRP:CZ3	2.45	0.51
1:B:568:THR:CG2	1:C:382:LEU:HD21	2.39	0.51
1:E:488:ARG:HB2	1:E:574:THR:HB	1.91	0.51
2:H:36:THR:HA	2:H:101:LEU:O	2.10	0.51
1:B:536:PRO:HB2	1:B:539:GLY:HA3	1.91	0.51
1:C:532:ASP:O	2:H:124:TYR:CE1	2.64	0.51
1:D:275:PHE:HB3	1:D:383:ASN:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:SER:HB3	1:C:729:THR:HG22	1.93	0.51
1:D:361:GLU:HG3	1:D:362:GLY:H	1.74	0.51
1:A:340:SER:HA	1:F:321:GLN:HE22	1.76	0.51
1:D:585:GLN:OE1	1:E:501:PHE:CE2	2.64	0.51
1:E:503:TRP:HB3	1:E:504:PRO:HD3	1.91	0.51
2:H:52:TYR:CE1	2:H:71:TYR:HB2	2.45	0.51
1:B:503:TRP:HB3	1:B:504:PRO:HD3	1.92	0.50
1:A:288:ARG:HH21	1:A:615:GLN:HB3	1.76	0.50
1:A:662:PHE:HA	1:F:373:MET:HE2	1.92	0.50
1:F:694:ARG:HD3	1:F:698:GLU:OE2	2.12	0.50
2:H:23:LEU:HD21	2:H:53:TRP:HZ3	1.76	0.50
1:A:358:SER:HB2	1:A:360:HIS:CD2	2.46	0.50
1:C:485:ARG:HG2	1:C:486:GLN:N	2.26	0.50
3:L:37:SER:HA	3:L:99:SER:HA	1.94	0.50
1:B:568:THR:O	1:C:511:LEU:HD21	2.11	0.50
2:H:86:VAL:CG2	2:H:101:LEU:HD13	2.41	0.50
1:D:528:LYS:CG	1:D:572:VAL:HG21	2.40	0.50
1:A:284:PHE:CE1	1:A:679:VAL:HG21	2.46	0.49
1:D:493:VAL:HG12	1:F:461:LEU:HD13	1.92	0.49
2:H:25:GLU:OE1	2:H:25:GLU:N	2.45	0.49
3:L:109:TYR:O	3:L:125:GLY:HA2	2.13	0.49
1:C:317:LEU:HG	1:C:320:ILE:HD11	1.94	0.49
1:C:466:ALA:HB1	1:C:474:GLN:HG2	1.94	0.49
2:H:77:ASN:ND2	3:L:118:SER:O	2.45	0.49
1:B:517:LEU:HD23	1:B:519:ASN:HB2	1.94	0.49
1:D:309:ARG:NH1	1:D:419:ASN:OD1	2.44	0.49
1:E:443:TYR:HB3	1:F:361:GLU:OE1	2.12	0.49
1:B:503:TRP:H	1:B:504:PRO:CD	2.25	0.49
1:C:488:ARG:HD2	1:C:534:PHE:CD1	2.47	0.49
1:A:306:TRP:O	1:A:425:SER:N	2.43	0.49
2:H:21:VAL:HG22	2:H:46:ASP:CB	2.43	0.49
2:H:66:TRP:CZ2	2:H:68:GLY:HA2	2.47	0.49
1:A:389:VAL:HA	1:F:706:TYR:O	2.12	0.49
1:C:262:ASN:HD22	1:C:274:TYR:H	1.61	0.49
1:C:460:THR:O	1:C:461:LEU:HD12	2.13	0.49
2:H:70:ILE:HG13	2:H:76:THR:CG2	2.43	0.49
1:E:430:GLN:HE22	1:F:353:PRO:HB3	1.78	0.48
1:E:606:VAL:HB	1:F:625:THR:HG21	1.95	0.48
1:F:449:LYS:HB2	1:F:462:LYS:HB2	1.94	0.48
1:C:425:SER:HB3	1:C:729:THR:CG2	2.43	0.48
1:C:532:ASP:OD1	2:H:121:TYR:CE1	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:SER:HB3	1:D:272:ASN:HD22	1.78	0.48
1:A:246:THR:HB	1:A:371:VAL:HG22	1.94	0.48
1:E:563:GLU:O	1:E:566:ILE:HG12	2.13	0.48
1:F:299:GLN:HG3	1:F:701:TYR:HD2	1.78	0.48
3:L:30:VAL:O	3:L:128:LEU:HA	2.13	0.48
3:L:77:PRO:HD2	3:L:81:VAL:HG21	1.96	0.48
1:D:491:THR:HG23	1:D:533:ARG:O	2.14	0.48
1:D:313:LEU:HB3	1:D:415:TYR:HB3	1.94	0.48
1:D:503:TRP:N	1:D:504:PRO:CD	2.77	0.48
1:B:490:SER:HB2	1:B:534:PHE:CE1	2.49	0.48
1:C:365:PRO:HG3	1:C:372:PHE:HB3	1.96	0.48
1:D:585:GLN:NE2	1:E:501:PHE:CZ	2.82	0.48
1:E:481:GLY:O	1:E:577:TYR:HE1	1.96	0.48
1:F:259:GLN:NE2	1:F:275:PHE:HE1	2.09	0.48
1:B:524:MET:HB2	1:B:573:ALA:HB2	1.95	0.48
2:H:85:ARG:HB2	2:H:102:ASN:HB2	1.95	0.48
1:A:244:THR:HA	1:A:679:VAL:O	2.14	0.48
1:F:569:THR:HG22	1:F:736:LEU:HD21	1.96	0.48
1:A:426:TYR:CD1	1:A:426:TYR:C	2.92	0.47
1:A:308:PHE:HA	1:A:686:GLU:O	2.14	0.47
1:C:262:ASN:HD22	1:C:273:ALA:HA	1.78	0.47
1:F:247:TRP:NE1	1:F:679:VAL:HG23	2.30	0.47
3:L:26:GLN:OE1	3:L:125:GLY:CA	2.62	0.47
1:D:611:ASP:OD1	1:D:612:VAL:N	2.48	0.47
1:F:503:TRP:H	1:F:504:PRO:HD3	1.79	0.47
1:A:355:VAL:HB	1:C:437:ASN:HB2	1.95	0.47
1:C:259:GLN:NE2	1:C:275:PHE:HE1	2.13	0.47
1:C:295:PRO:HB2	1:F:697:PRO:HD3	1.97	0.47
1:D:500:GLU:HA	1:F:450:THR:OG1	2.13	0.47
1:D:625:THR:HA	1:F:608:GLN:HE22	1.79	0.47
1:E:537:LEU:C	1:E:537:LEU:CD2	2.88	0.47
3:L:128:LEU:C	3:L:128:LEU:HD23	2.39	0.47
3:L:24:LEU:HD13	3:L:111:CYS:SG	2.55	0.47
1:B:439:LEU:HD21	1:C:278:SER:HB3	1.96	0.47
1:B:439:LEU:HD13	1:C:376:GLN:CD	2.40	0.47
2:H:31:VAL:HG13	2:H:35:VAL:CG1	2.45	0.47
1:B:484:TYR:CE2	1:B:518:MET:HE3	2.50	0.47
1:F:233:GLN:HG2	1:F:235:LEU:HD21	1.97	0.47
1:A:381:THR:HG21	1:A:393:SER:N	2.27	0.46
1:C:492:THR:HG22	1:C:494:THR:HG22	1.97	0.46
1:E:585:GLN:OE1	1:F:501:PHE:CE2	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:690:GLU:OE1	1:C:690:GLU:N	2.47	0.46
1:D:423:HIS:HB2	1:D:638:PHE:CZ	2.50	0.46
1:A:283:TYR:HD2	1:A:377:TYR:HB2	1.81	0.46
1:C:312:ARG:HG2	1:C:416:GLU:OE1	2.16	0.46
1:A:485:ARG:HD2	1:C:581:ALA:O	2.16	0.46
1:F:704:ASN:C	1:F:704:ASN:ND2	2.73	0.46
1:F:565:GLU:OE1	1:F:565:GLU:N	2.33	0.46
1:F:309:ARG:NH1	1:F:420:VAL:O	2.42	0.46
1:A:562:ASN:ND2	1:A:564:GLU:HG2	2.30	0.46
1:C:706:TYR:CD1	1:C:706:TYR:C	2.94	0.46
3:L:44:GLY:O	3:L:92:ASN:HB3	2.15	0.46
1:A:290:HIS:HD2	1:A:615:GLN:HA	1.80	0.46
1:D:255:HIS:CG	1:D:653:PRO:HB3	2.50	0.46
1:F:262:ASN:HD22	1:F:273:ALA:HA	1.81	0.46
1:D:475:GLY:CA	1:E:519:ASN:ND2	2.77	0.46
1:F:281:TRP:HA	1:F:650:LYS:HB3	1.98	0.46
1:F:601:ILE:HG13	1:F:629:PHE:CE2	2.51	0.46
1:A:475:GLY:HA2	1:B:519:ASN:HB3	1.98	0.46
1:A:500:GLU:HA	1:C:450:THR:OG1	2.16	0.46
1:F:275:PHE:HB3	1:F:383:ASN:HB3	1.98	0.46
1:B:524:MET:CB	1:B:573:ALA:HB2	2.45	0.45
1:B:529:GLU:CD	1:B:567:LYS:HE3	2.40	0.45
1:D:341:THR:HG22	1:D:406:ARG:HG3	1.97	0.45
1:D:423:HIS:HB2	1:D:638:PHE:CE1	2.51	0.45
1:F:247:TRP:CD1	1:F:679:VAL:HG23	2.51	0.45
1:F:426:TYR:CD1	1:F:426:TYR:C	2.93	0.45
1:D:343:GLN:HE21	1:D:404:MET:HE3	1.82	0.45
1:A:285:ASP:O	1:A:363:CYS:HA	2.16	0.45
1:A:423:HIS:NE2	1:A:612:VAL:HG22	2.31	0.45
1:F:361:GLU:HG3	1:F:362:GLY:N	2.31	0.45
1:C:698:GLU:HG2	1:F:296:ARG:NE	2.31	0.45
1:F:262:ASN:ND2	1:F:273:ALA:HA	2.31	0.45
1:F:367:PHE:CE2	1:F:369:ALA:HB3	2.52	0.45
1:F:506:ALA:HB1	1:F:517:LEU:HD11	1.99	0.45
2:H:78:TYR:CE1	2:H:88:MET:HG3	2.51	0.45
1:C:523:ALA:O	1:C:570:ASN:ND2	2.47	0.45
1:D:481:GLY:HA3	1:D:607:TRP:HB3	1.99	0.45
1:A:361:GLU:HG3	1:A:362:GLY:N	2.29	0.45
1:C:563:GLU:O	1:C:566:ILE:HG12	2.17	0.45
1:F:611:ASP:OD1	1:F:612:VAL:N	2.50	0.45
1:A:418:GLU:OE2	1:A:641:LYS:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:LEU:C	1:B:537:LEU:CD2	2.89	0.45
1:D:572:VAL:HG12	1:D:574:THR:H	1.82	0.45
3:L:40:ILE:HG21	3:L:126:THR:CG2	2.36	0.45
1:A:480:PRO:HG3	1:B:509:TRP:CE3	2.52	0.44
1:D:312:ARG:HG2	1:D:416:GLU:OE1	2.16	0.44
1:E:428:HIS:CE1	1:F:624:HIS:O	2.71	0.44
1:E:459:GLN:NE2	1:F:498:ASN:HB2	2.33	0.44
1:E:529:GLU:OE1	1:E:567:LYS:HE2	2.16	0.44
2:H:54:SER:OG	2:H:69:TYR:HB3	2.16	0.44
1:A:418:GLU:HG2	1:A:640:MET:HE3	1.99	0.44
1:B:449:LYS:HB3	1:B:462:LYS:HB2	1.99	0.44
2:H:86:VAL:HG23	2:H:101:LEU:CD1	2.47	0.44
1:A:262:ASN:ND2	1:A:273:ALA:HA	2.30	0.44
1:A:281:TRP:NE1	1:A:398:GLU:OE2	2.48	0.44
1:D:501:PHE:CE1	1:F:585:GLN:OE1	2.71	0.44
1:D:624:HIS:O	1:F:428:HIS:CE1	2.70	0.44
1:A:501:PHE:CZ	1:C:585:GLN:OE1	2.71	0.44
1:C:447:LEU:HD12	1:C:462:LYS:O	2.17	0.44
1:D:290:HIS:HD2	1:D:615:GLN:HA	1.80	0.44
1:E:587:ALA:HA	1:F:497:ASN:HA	1.99	0.44
1:A:624:HIS:O	1:C:428:HIS:CE1	2.68	0.44
1:D:654:VAL:HG12	1:D:671:ILE:HD12	1.99	0.44
1:A:255:HIS:ND1	1:A:653:PRO:HB3	2.33	0.44
1:C:298:TRP:CG	1:C:614:LEU:HD12	2.53	0.44
2:H:72:TYR:CD1	2:H:72:TYR:C	2.95	0.44
1:C:262:ASN:OD1	1:C:263:SER:N	2.50	0.44
1:F:312:ARG:HG2	1:F:416:GLU:OE1	2.18	0.44
1:A:525:ALA:HB3	1:A:572:VAL:HA	1.99	0.44
1:B:434:ARG:NH2	1:C:271:ASP:O	2.49	0.44
1:B:436:MET:HE2	1:B:436:MET:HB3	1.72	0.44
1:A:553:VAL:HG22	1:C:463:PHE:O	2.18	0.44
1:B:603:PRO:HB3	1:C:630:HIS:HB3	2.00	0.44
1:C:611:ASP:OD1	1:C:612:VAL:N	2.50	0.43
1:D:262:ASN:HD22	1:D:267:GLY:HA2	1.82	0.43
1:B:426:TYR:CD1	1:B:426:TYR:C	2.96	0.43
1:C:354:TYR:CZ	1:C:356:LEU:HB2	2.53	0.43
1:C:602:LEU:HB2	1:C:605:MET:HE3	2.00	0.43
1:E:568:THR:O	1:F:511:LEU:HD21	2.17	0.43
1:F:243:SER:O	1:F:680:SER:HA	2.17	0.43
3:L:40:ILE:HD13	3:L:126:THR:CG2	2.48	0.43
1:C:306:TRP:CE2	1:C:690:GLU:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ASN:HB3	1:A:682:GLU:HB3	2.00	0.43
2:H:23:LEU:HD21	2:H:53:TRP:CZ3	2.53	0.43
3:L:106:GLU:HA	3:L:128:LEU:CD2	2.48	0.43
1:B:585:GLN:HE22	1:C:501:PHE:HZ	1.63	0.43
1:C:262:ASN:ND2	1:C:273:ALA:HA	2.33	0.43
1:D:380:LEU:HD13	1:F:434:ARG:HD2	2.00	0.43
1:D:568:THR:O	1:E:511:LEU:HD21	2.18	0.43
2:H:30:LEU:HD11	2:H:142:SER:HB3	2.01	0.43
1:C:371:VAL:HG12	1:D:667:LEU:HD12	2.00	0.43
1:F:234:TRP:CE3	1:F:239:VAL:HG22	2.54	0.43
1:F:707:LYS:HG3	1:F:707:LYS:O	2.17	0.43
1:A:382:LEU:HG	1:C:429:SER:O	2.18	0.43
1:F:418:GLU:OE2	1:F:641:LYS:N	2.52	0.43
3:L:37:SER:OG	3:L:99:SER:CB	2.66	0.43
1:C:234:TRP:CE2	1:C:300:ARG:HD2	2.54	0.43
1:F:262:ASN:O	1:F:266:GLY:N	2.52	0.43
1:F:355:VAL:H	1:F:646:GLN:HE22	1.67	0.43
1:A:263:SER:HA	1:A:267:GLY:HA2	2.00	0.43
1:A:367:PHE:CE2	1:A:369:ALA:HB3	2.54	0.43
1:C:460:THR:C	1:C:461:LEU:HD12	2.44	0.43
1:D:471:MET:O	1:D:476:ARG:NH2	2.47	0.43
2:H:66:TRP:HZ3	3:L:119:THR:HG1	1.66	0.43
3:L:26:GLN:OE1	3:L:125:GLY:N	2.52	0.43
1:E:424:SER:HB2	1:E:426:TYR:CE2	2.54	0.43
2:H:85:ARG:NH1	2:H:102:ASN:O	2.51	0.43
2:H:118:HIS:O	2:H:127:SER:OG	2.34	0.43
3:L:69:MET:O	3:L:77:PRO:HD3	2.18	0.43
1:D:357:GLY:O	1:F:477:ASN:ND2	2.52	0.42
1:E:585:GLN:O	1:E:585:GLN:HG3	2.19	0.42
1:A:367:PHE:HA	1:A:368:PRO:HD3	1.90	0.42
1:A:391:ARG:HG3	1:C:733:THR:HG21	2.02	0.42
1:A:485:ARG:HG2	1:A:486:GLN:N	2.35	0.42
1:C:710:ASN:ND2	1:D:259:GLN:OE1	2.42	0.42
1:E:434:ARG:HD3	1:E:434:ARG:HA	1.77	0.42
1:F:542:ILE:HG12	1:F:560:ILE:HG12	2.00	0.42
1:C:343:GLN:O	1:C:649:ILE:HA	2.19	0.42
1:D:247:TRP:NE1	1:D:679:VAL:HG23	2.34	0.42
1:A:493:VAL:HG12	1:C:461:LEU:HD13	2.00	0.42
1:C:418:GLU:OE2	1:C:641:LYS:N	2.53	0.42
1:C:520:PRO:HA	1:C:538:SER:O	2.19	0.42
1:F:358:SER:HB2	1:F:360:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:704:ASN:C	1:F:704:ASN:HD22	2.24	0.42
1:C:424:SER:HB2	1:C:426:TYR:CE2	2.54	0.42
1:D:581:ALA:O	1:E:485:ARG:HD2	2.20	0.42
1:F:704:ASN:ND2	1:F:704:ASN:O	2.52	0.42
1:C:426:TYR:CD1	1:C:426:TYR:C	2.97	0.42
1:D:415:TYR:OH	1:D:642:HIS:O	2.37	0.42
1:F:308:PHE:HA	1:F:686:GLU:O	2.20	0.42
1:A:657:ASP:OD2	1:F:332:LYS:NZ	2.30	0.42
1:B:439:LEU:HD11	1:C:278:SER:HB2	2.02	0.42
1:C:290:HIS:CE1	1:C:366:PRO:HG3	2.54	0.42
1:A:400:PHE:CZ	1:C:693:LYS:HG3	2.55	0.42
1:A:625:THR:HA	1:C:608:GLN:NE2	2.35	0.42
1:F:262:ASN:OD1	1:F:267:GLY:HA3	2.19	0.42
1:C:358:SER:HB2	1:C:360:HIS:CD2	2.54	0.42
1:C:367:PHE:CE2	1:C:369:ALA:HB3	2.54	0.42
1:C:698:GLU:HB2	1:C:700:GLN:NE2	2.34	0.42
1:D:308:PHE:HA	1:D:686:GLU:O	2.20	0.42
3:L:34:PRO:HG3	3:L:130:VAL:HG12	2.02	0.42
1:A:381:THR:HG22	1:A:382:LEU:N	2.31	0.41
3:L:31:SER:HB3	3:L:129:THR:OG1	2.20	0.41
3:L:36:GLN:O	3:L:36:GLN:HG3	2.19	0.41
1:A:288:ARG:NH2	1:A:615:GLN:HB3	2.35	0.41
1:D:275:PHE:CZ	1:D:388:ALA:HB2	2.55	0.41
1:D:479:ILE:HB	1:D:480:PRO:HD2	2.02	0.41
1:D:556:ASP:OD1	1:D:556:ASP:N	2.53	0.41
1:F:532:ASP:OD2	3:L:79:SER:HB3	2.21	0.41
1:C:375:PRO:HA	1:D:662:PHE:CD1	2.56	0.41
1:E:450:THR:OG1	1:F:500:GLU:HA	2.20	0.41
1:C:251:THR:O	1:D:660:THR:HG23	2.20	0.41
1:C:290:HIS:HB3	1:C:614:LEU:HD23	2.01	0.41
1:C:519:ASN:HA	1:C:520:PRO:HA	1.88	0.41
1:D:601:ILE:HG12	1:F:601:ILE:O	2.20	0.41
1:F:704:ASN:HD22	1:F:704:ASN:N	2.17	0.41
1:A:471:MET:O	1:A:476:ARG:NH2	2.41	0.41
1:A:548:THR:HG23	1:A:557:LYS:HB3	2.03	0.41
1:C:415:TYR:OH	1:C:642:HIS:O	2.35	0.41
1:F:308:PHE:HE2	1:F:729:THR:HG21	1.85	0.41
1:A:358:SER:OG	1:C:436:MET:HA	2.20	0.41
1:C:488:ARG:HD2	1:C:534:PHE:CG	2.54	0.41
1:D:657:ASP:HA	1:D:658:PRO:HD3	1.94	0.41
1:E:437:ASN:HB2	1:F:355:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:503:TRP:N	1:E:504:PRO:CD	2.84	0.41
1:F:316:LYS:HE2	1:F:412:GLN:OE1	2.20	0.41
2:H:31:VAL:HG13	2:H:35:VAL:HG11	2.03	0.41
2:H:41:CYS:O	2:H:96:GLN:HB2	2.20	0.41
3:L:26:GLN:HE21	3:L:111:CYS:HB2	1.85	0.41
1:B:524:MET:HB2	1:B:524:MET:HE3	1.95	0.41
1:C:697:PRO:HD3	1:F:295:PRO:HB2	2.03	0.41
1:D:503:TRP:H	1:D:504:PRO:CD	2.34	0.41
1:F:367:PHE:HA	1:F:368:PRO:HD3	1.90	0.41
1:F:447:LEU:HD12	1:F:462:LYS:O	2.20	0.41
1:F:562:ASN:ND2	1:F:564:GLU:HB3	2.36	0.41
1:D:247:TRP:CZ2	1:D:317:LEU:HD11	2.56	0.41
1:F:290:HIS:CG	1:F:366:PRO:HB3	2.56	0.41
1:F:306:TRP:CD2	1:F:690:GLU:HA	2.55	0.41
1:B:442:GLN:HA	1:C:360:HIS:HA	2.03	0.40
1:D:361:GLU:OE1	1:F:443:TYR:HB3	2.21	0.40
1:F:246:THR:HB	1:F:371:VAL:HG22	2.02	0.40
1:C:296:ARG:NE	1:F:698:GLU:HG2	2.37	0.40
1:D:283:TYR:HD2	1:D:377:TYR:HB2	1.86	0.40
1:D:284:PHE:CE1	1:D:679:VAL:HG21	2.55	0.40
1:F:288:ARG:HH21	1:F:615:GLN:HB3	1.86	0.40
3:L:106:GLU:HA	3:L:128:LEU:HD23	2.04	0.40
1:A:354:TYR:CZ	1:A:356:LEU:HB2	2.56	0.40
1:C:238:ARG:HD2	1:C:684:GLU:OE2	2.21	0.40
1:D:625:THR:HA	1:F:608:GLN:NE2	2.36	0.40
1:D:628:ASN:HB3	1:F:606:VAL:HG12	2.04	0.40
1:E:449:LYS:HE2	1:E:462:LYS:HG3	2.02	0.40
1:F:427:ALA:O	1:F:733:THR:HA	2.21	0.40
1:D:361:GLU:HG3	1:D:362:GLY:N	2.36	0.40
1:F:346:THR:HG22	1:F:647:ILE:HG12	2.03	0.40
1:F:365:PRO:HD3	1:F:372:PHE:HB3	2.03	0.40
1:F:247:TRP:CZ2	1:F:317:LEU:HD11	2.56	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	411/534 (77%)	399 (97%)	12 (3%)	0	100	100
1	B	174/534 (33%)	168 (97%)	6 (3%)	0	100	100
1	C	499/534 (93%)	487 (98%)	12 (2%)	0	100	100
1	D	411/534 (77%)	394 (96%)	17 (4%)	0	100	100
1	E	173/534 (32%)	169 (98%)	4 (2%)	0	100	100
1	F	499/534 (93%)	487 (98%)	12 (2%)	0	100	100
2	H	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
3	L	109/111 (98%)	106 (97%)	3 (3%)	0	100	100
All	All	2398/3439 (70%)	2330 (97%)	68 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	362/461 (78%)	359 (99%)	3 (1%)	79	93
1	B	151/461 (33%)	148 (98%)	3 (2%)	50	80
1	C	440/461 (95%)	435 (99%)	5 (1%)	70	90
1	D	362/461 (78%)	359 (99%)	3 (1%)	79	93
1	E	150/461 (32%)	148 (99%)	2 (1%)	65	88
1	F	440/461 (95%)	435 (99%)	5 (1%)	70	90
2	H	110/110 (100%)	105 (96%)	5 (4%)	23	54
3	L	92/92 (100%)	90 (98%)	2 (2%)	47	78
All	All	2107/2968 (71%)	2079 (99%)	28 (1%)	64	88

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	CYS
1	A	432	LEU
1	A	564	GLU
1	B	436	MET
1	B	461	LEU
1	B	485	ARG
1	C	230	CYS
1	C	239	VAL
1	C	528	LYS
1	C	532	ASP
1	C	725	ARG
1	D	425	SER
1	D	532	ASP
1	D	564	GLU
1	E	429	SER
1	E	575	GLU
1	F	230	CYS
1	F	235	LEU
1	F	564	GLU
1	F	704	ASN
1	F	736	LEU
2	H	48	ILE
2	H	75	ASN
2	H	82	LEU
2	H	86	VAL
2	H	103	SER
3	L	48	ASP
3	L	104	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	HIS
1	A	343	GLN
1	A	585	GLN
1	A	608	GLN
1	A	624	HIS
1	A	646	GLN
1	A	651	ASN
1	A	673	GLN
1	B	452	ASN
1	B	458	GLN
1	B	459	GLN

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Mol	Chain	Res	Type
1	B	477	ASN
1	B	497	ASN
1	B	585	GLN
1	B	608	GLN
1	C	497	ASN
1	C	527	HIS
1	C	585	GLN
1	C	608	GLN
1	C	624	HIS
1	C	646	GLN
1	C	673	GLN
1	D	343	GLN
1	D	546	GLN
1	D	585	GLN
1	D	624	HIS
1	D	642	HIS
1	D	646	GLN
1	D	651	ASN
1	D	673	GLN
1	E	430	GLN
1	E	452	ASN
1	E	458	GLN
1	E	519	ASN
1	E	585	GLN
1	E	608	GLN
1	F	259	GLN
1	F	456	GLN
1	F	562	ASN
1	F	570	ASN
1	F	584	HIS
1	F	585	GLN
1	F	608	GLN
1	F	646	GLN
1	F	673	GLN
1	F	700	GLN
1	F	704	ASN
2	H	24	GLN
2	H	118	HIS
3	L	59	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-44315. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ
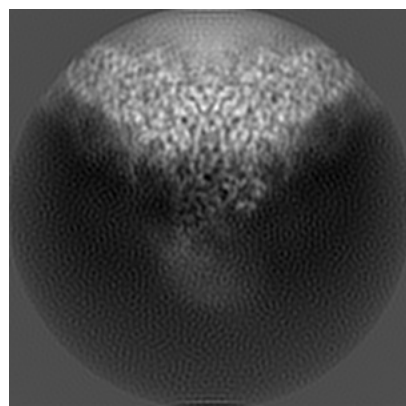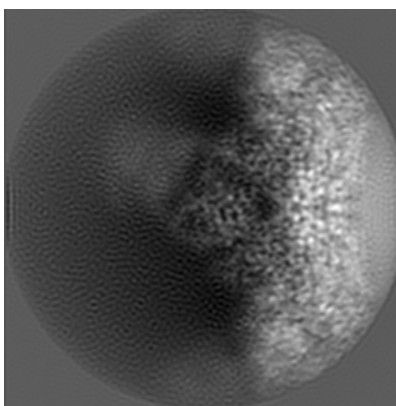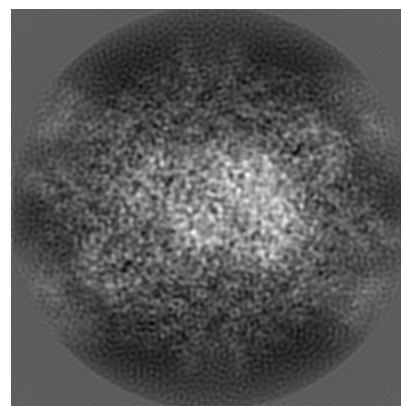
6.1.1 Primary map

X   Y   Z

6.1.2 Raw map

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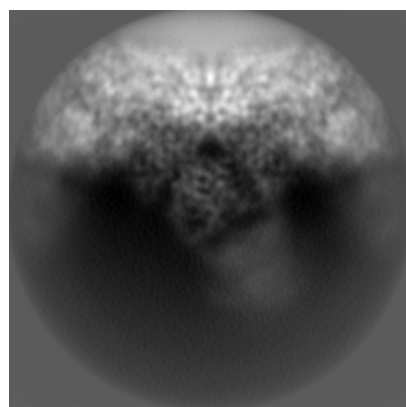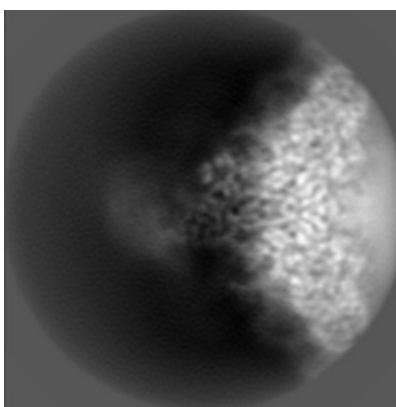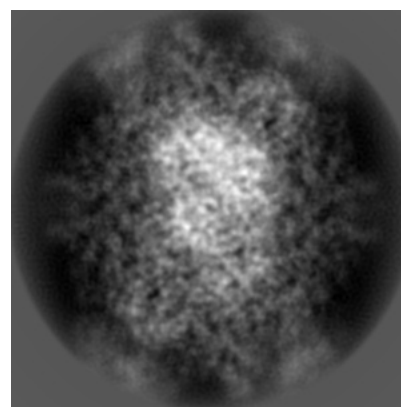
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map
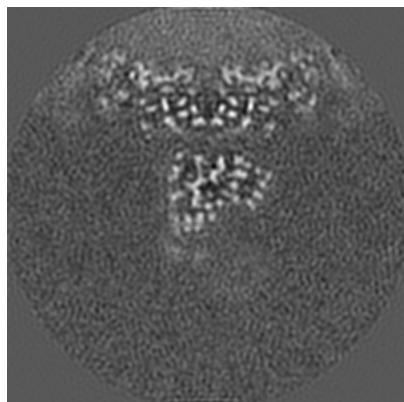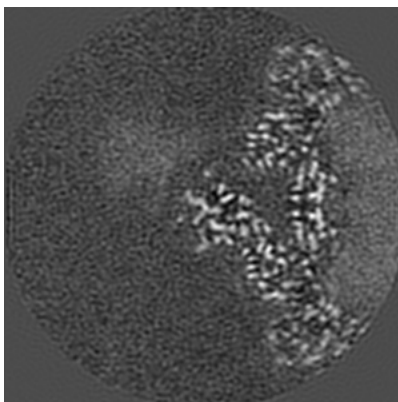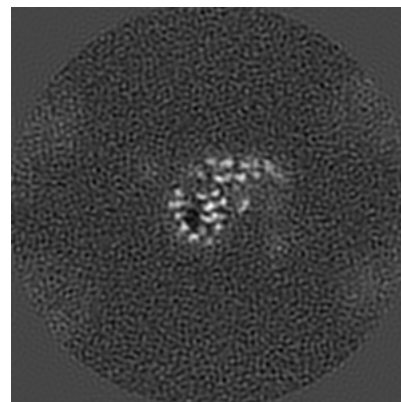
| X Index: 100 | Y Index: 100 | Z Index: 100 |

6.2.2 Raw map
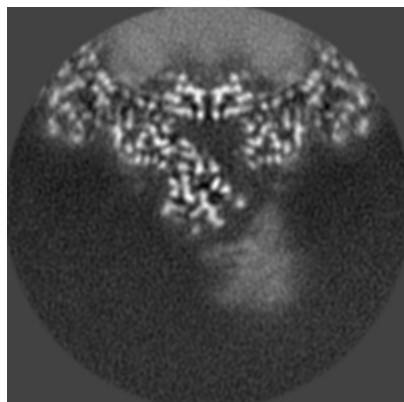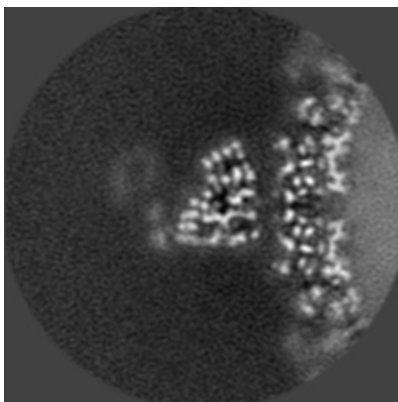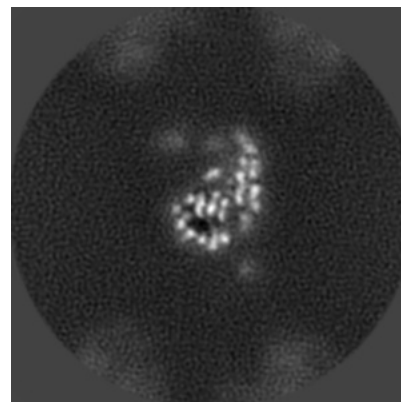
| X Index: 100 | Y Index: 100 | Z Index: 100 |

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

6.3　Largest variance slices ⓘ
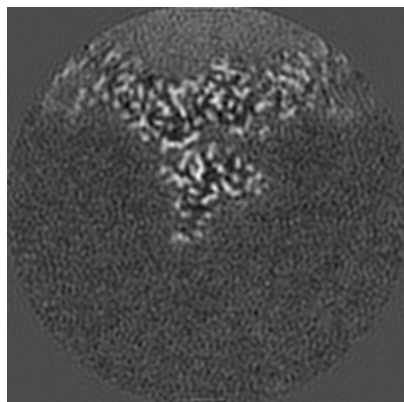
6.3.1　Primary map
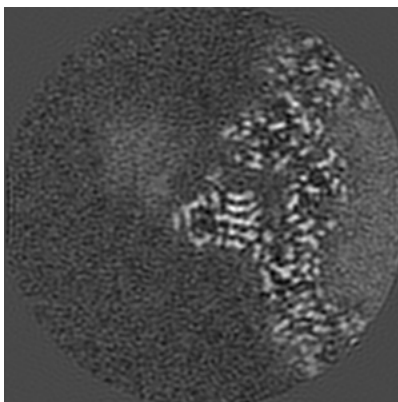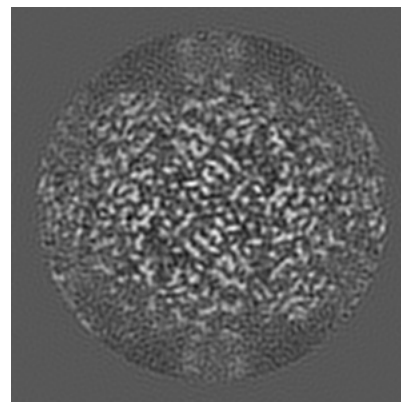
| X Index: 92 | Y Index: 96 | Z Index: 151 |

6.3.2　Raw map
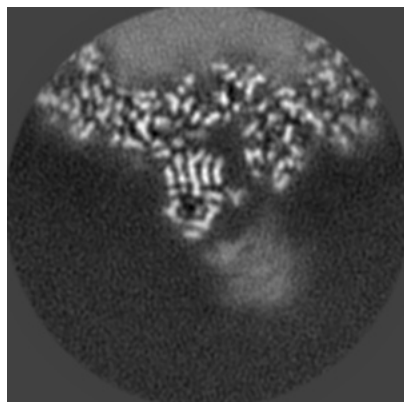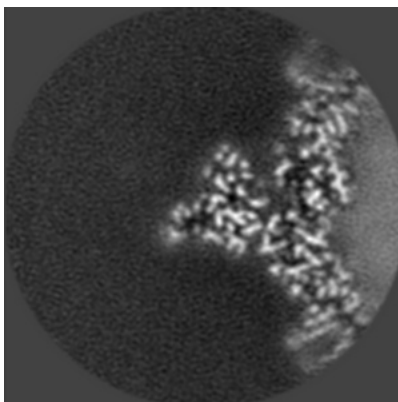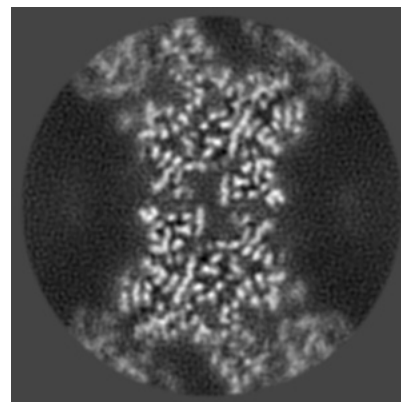
| X Index: 96 | Y Index: 93 | Z Index: 136 |

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

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

6.4.1　Primary map
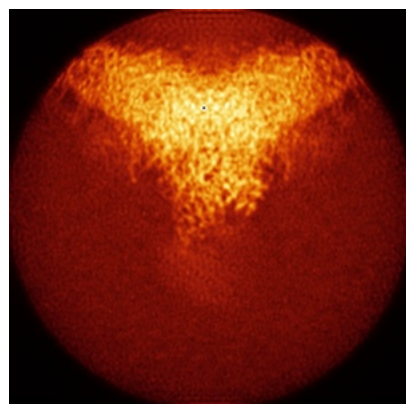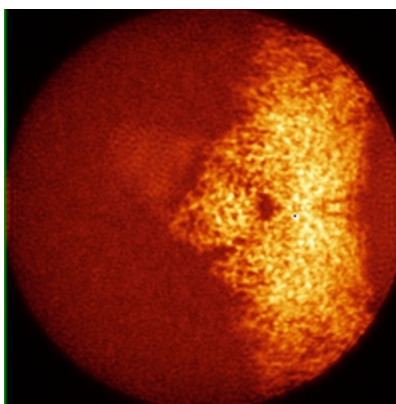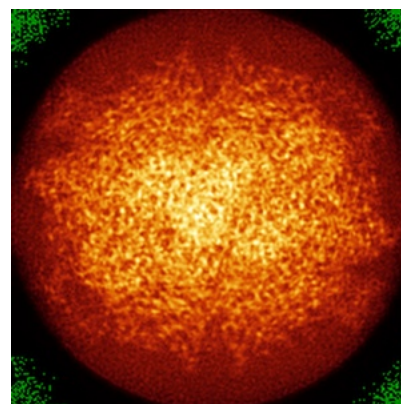
| X | Y | Z |

6.4.2　Raw map

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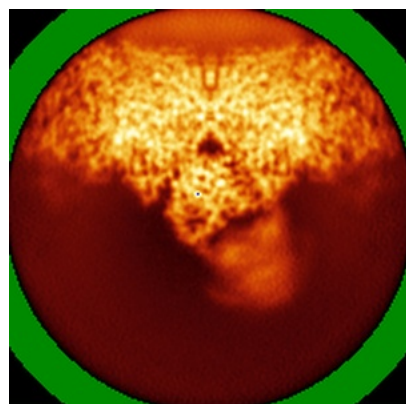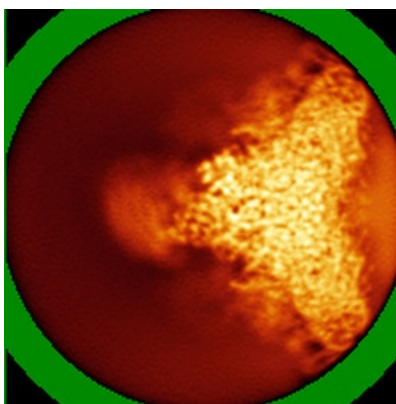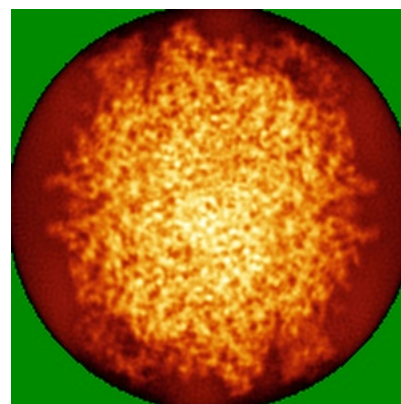
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X   Y   Z
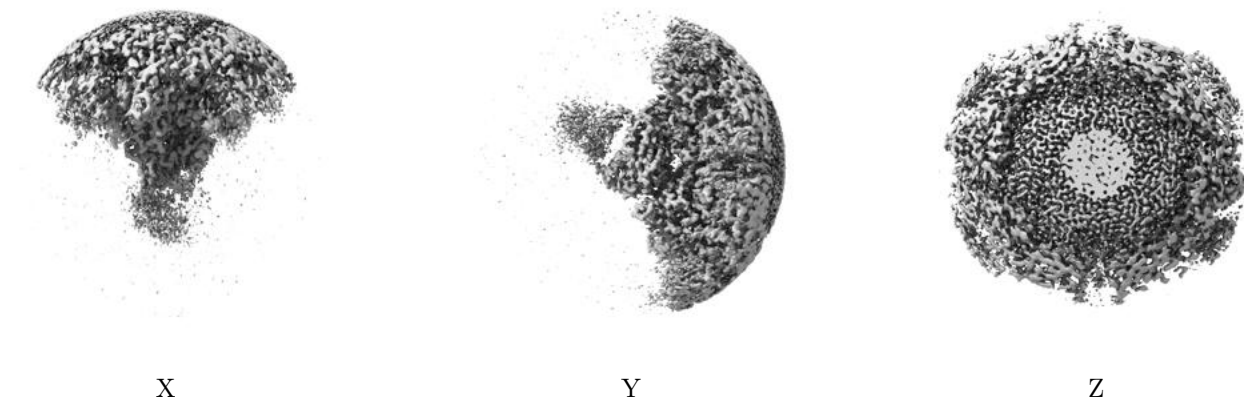
The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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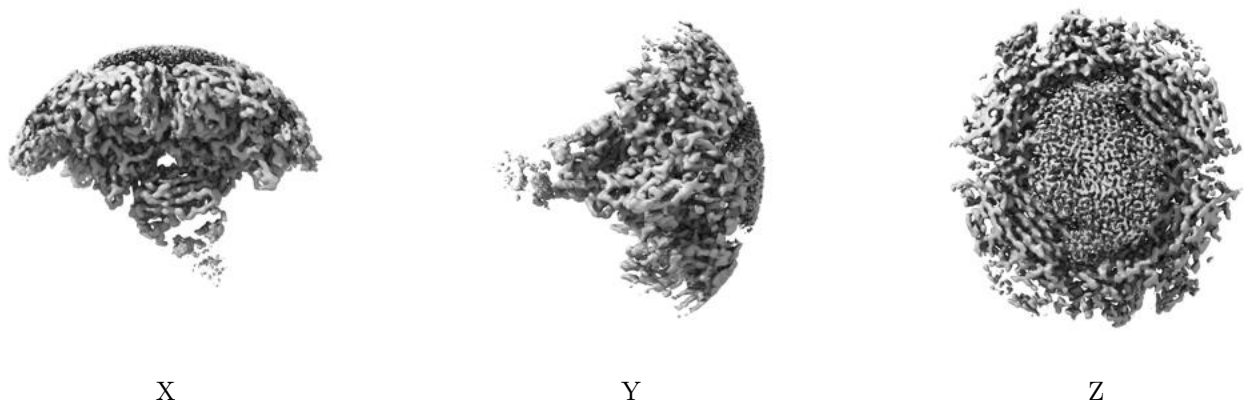
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

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

7 Map analysis ⓘ

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

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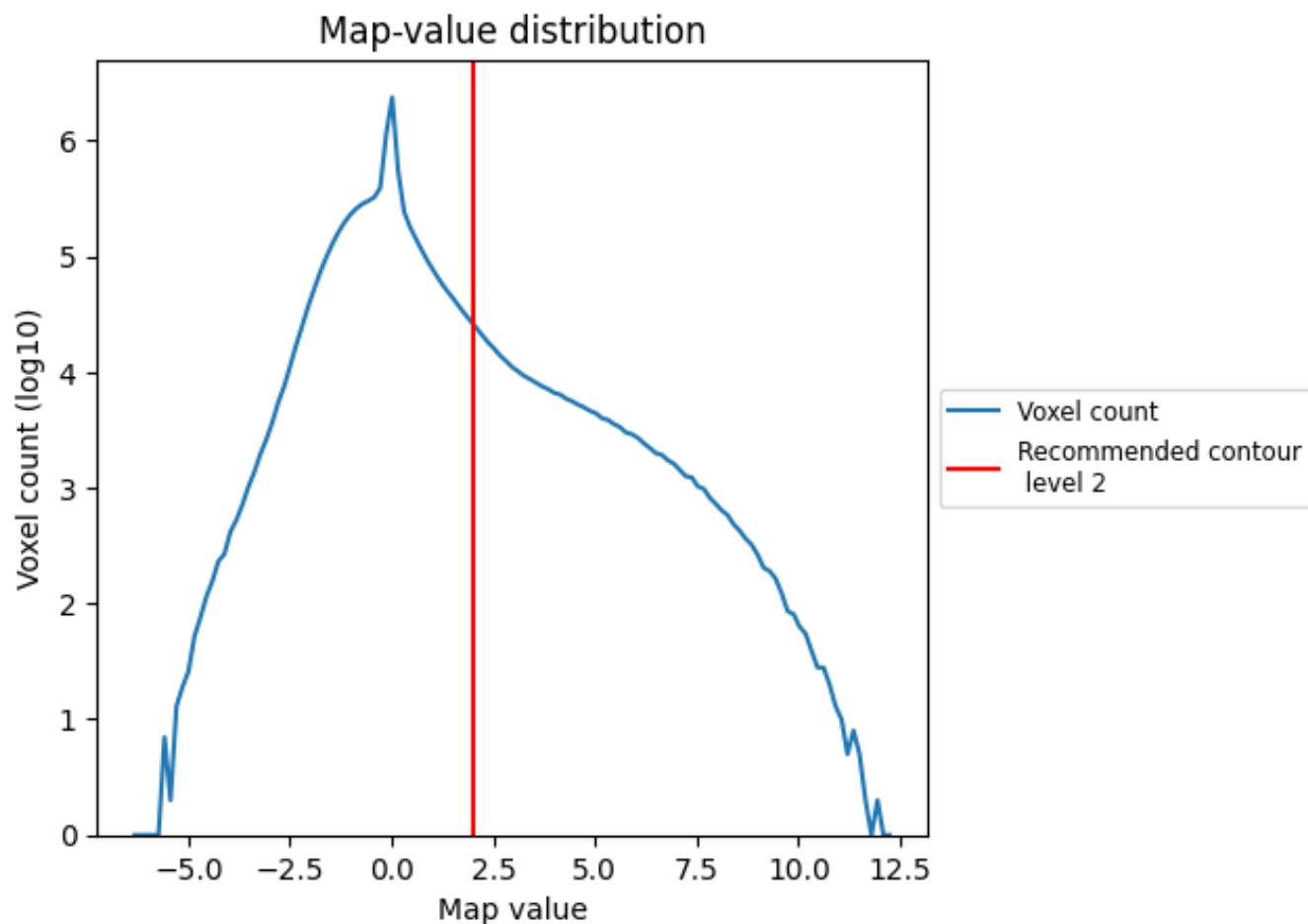
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
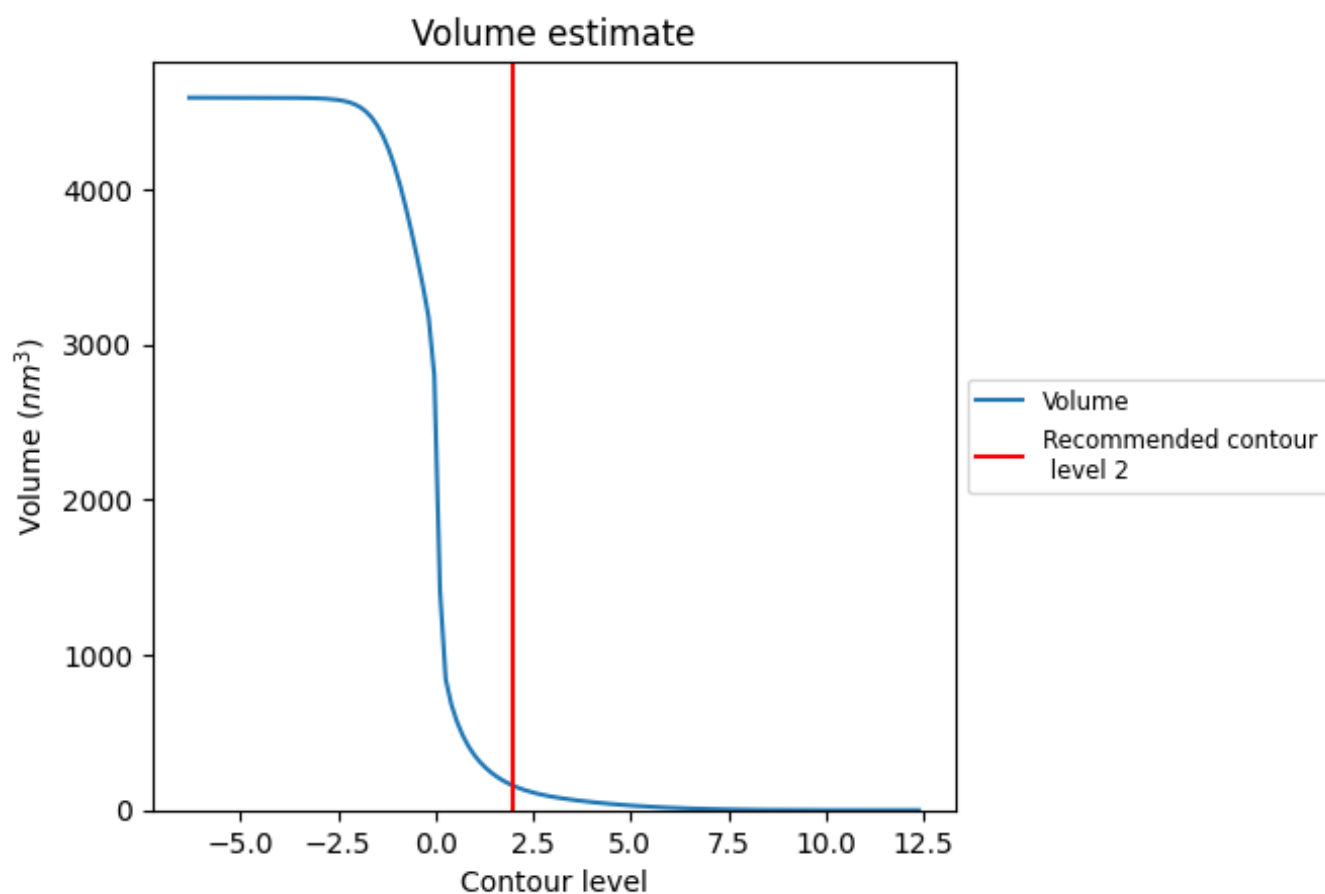
The volume at the recommended contour level is 156 nm^3; this corresponds to an approximate mass of 141 kDa.

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 ⓘ
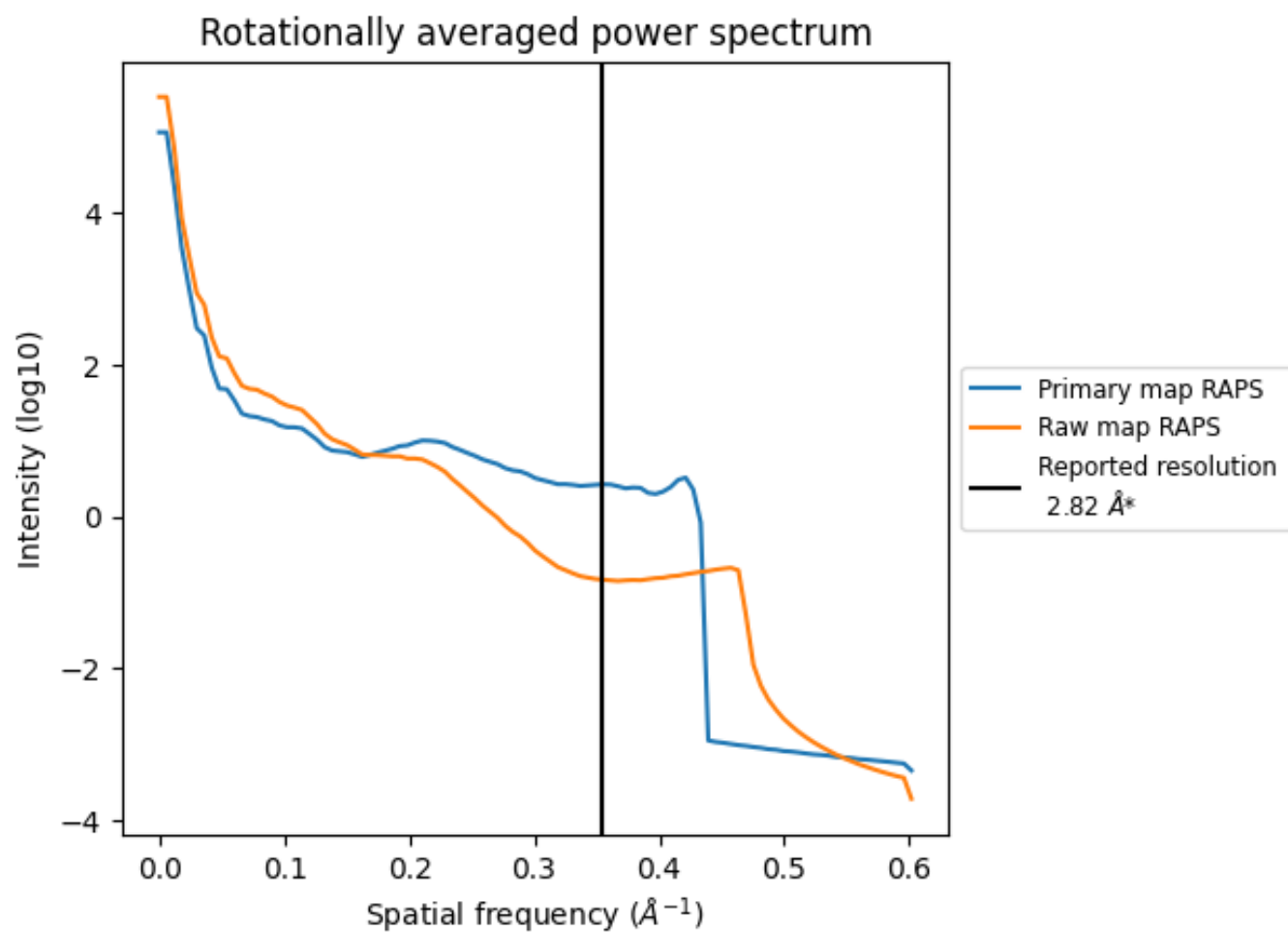
*Reported resolution corresponds to spatial frequency of 0.355 Å^{-1}

8　Fourier-Shell correlation ⓘ

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

8.1　FSC ⓘ
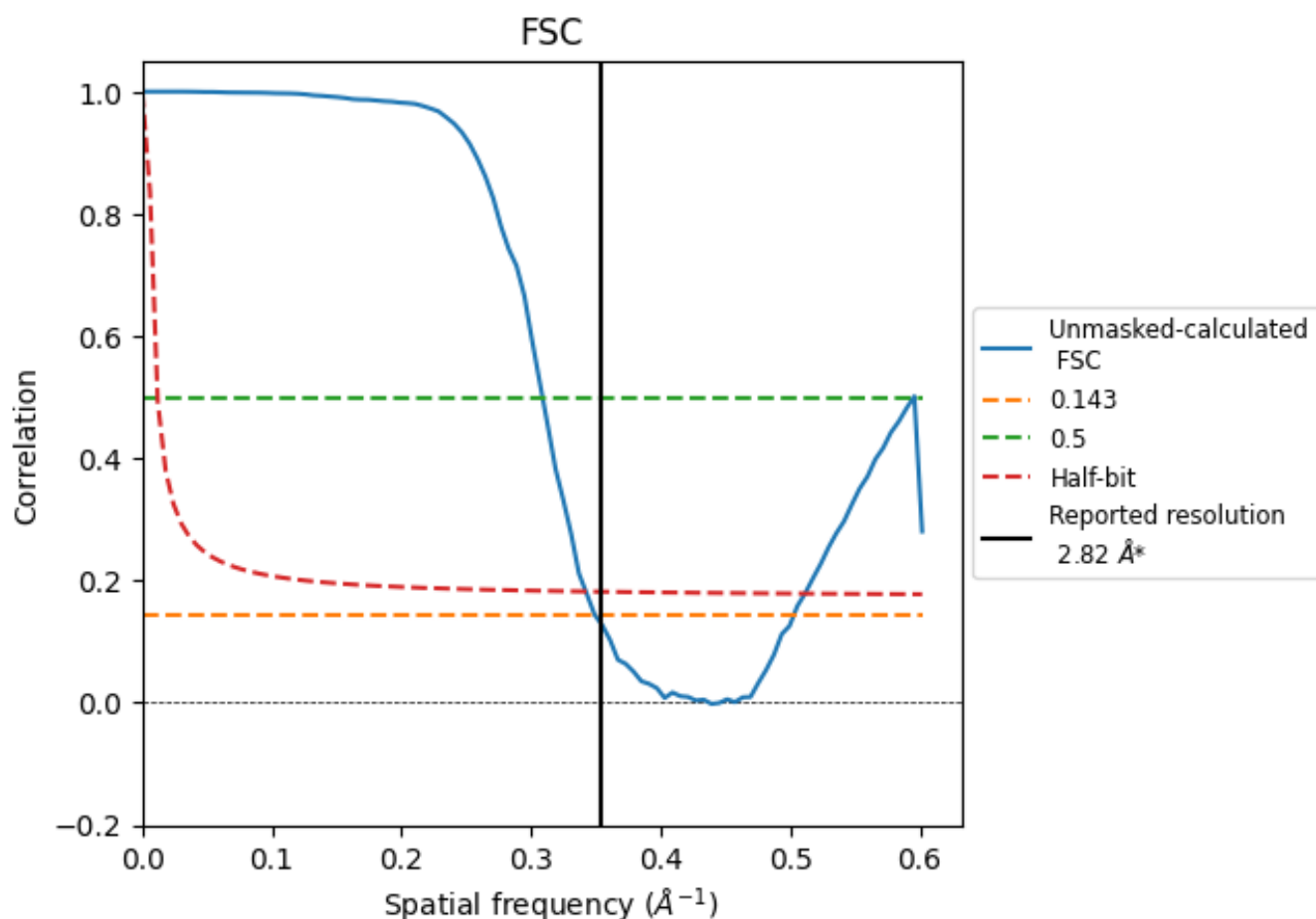
*Reported resolution corresponds to spatial frequency of 0.355 Å^{-1}

8.2　Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.82	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.86	3.24	2.92

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-44315 and PDB model 9B7L. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay ⓘ

| X | Y | Z |
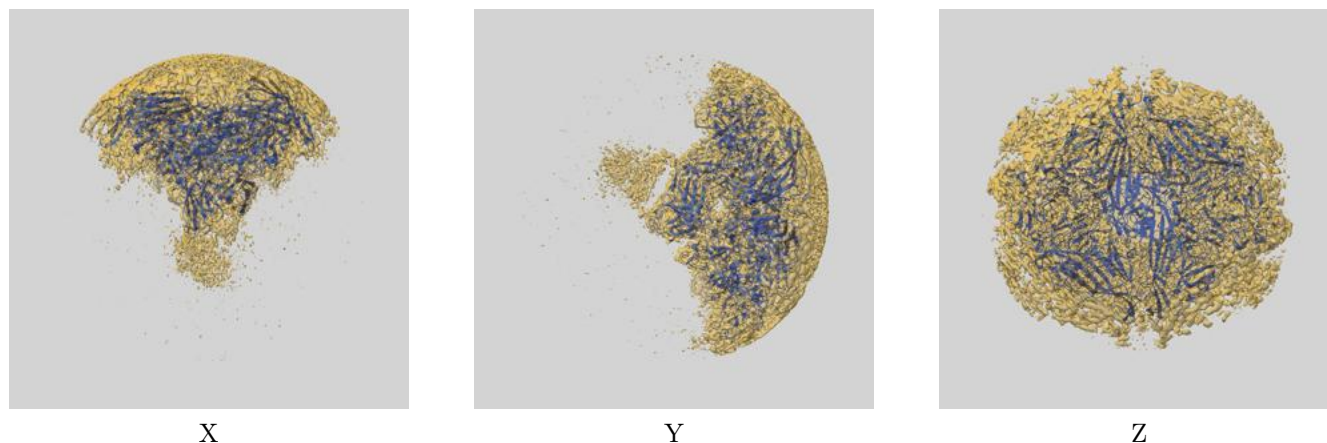
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ

X　　　　　　　　　　　　Y　　　　　　　　　　　　Z
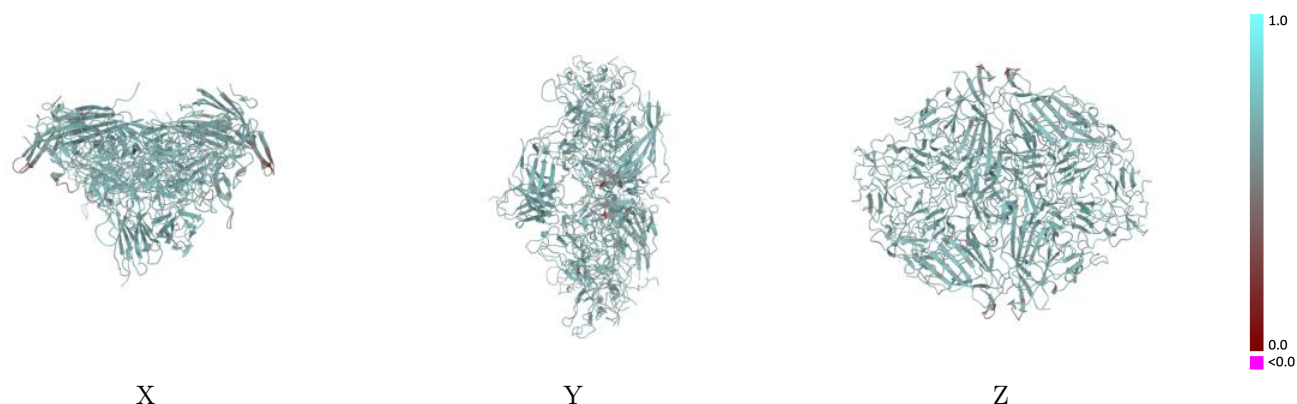
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
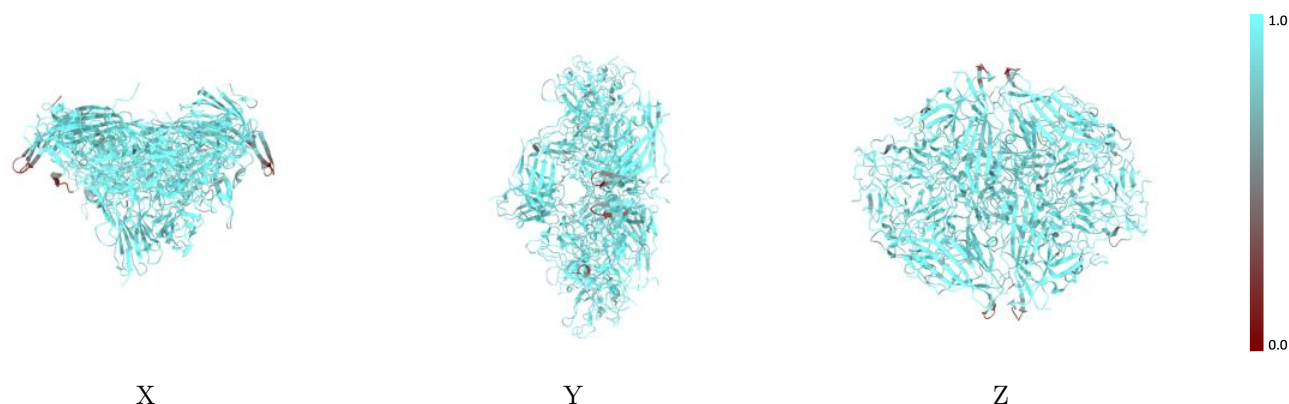
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2).

9.4　Atom inclusion (i)
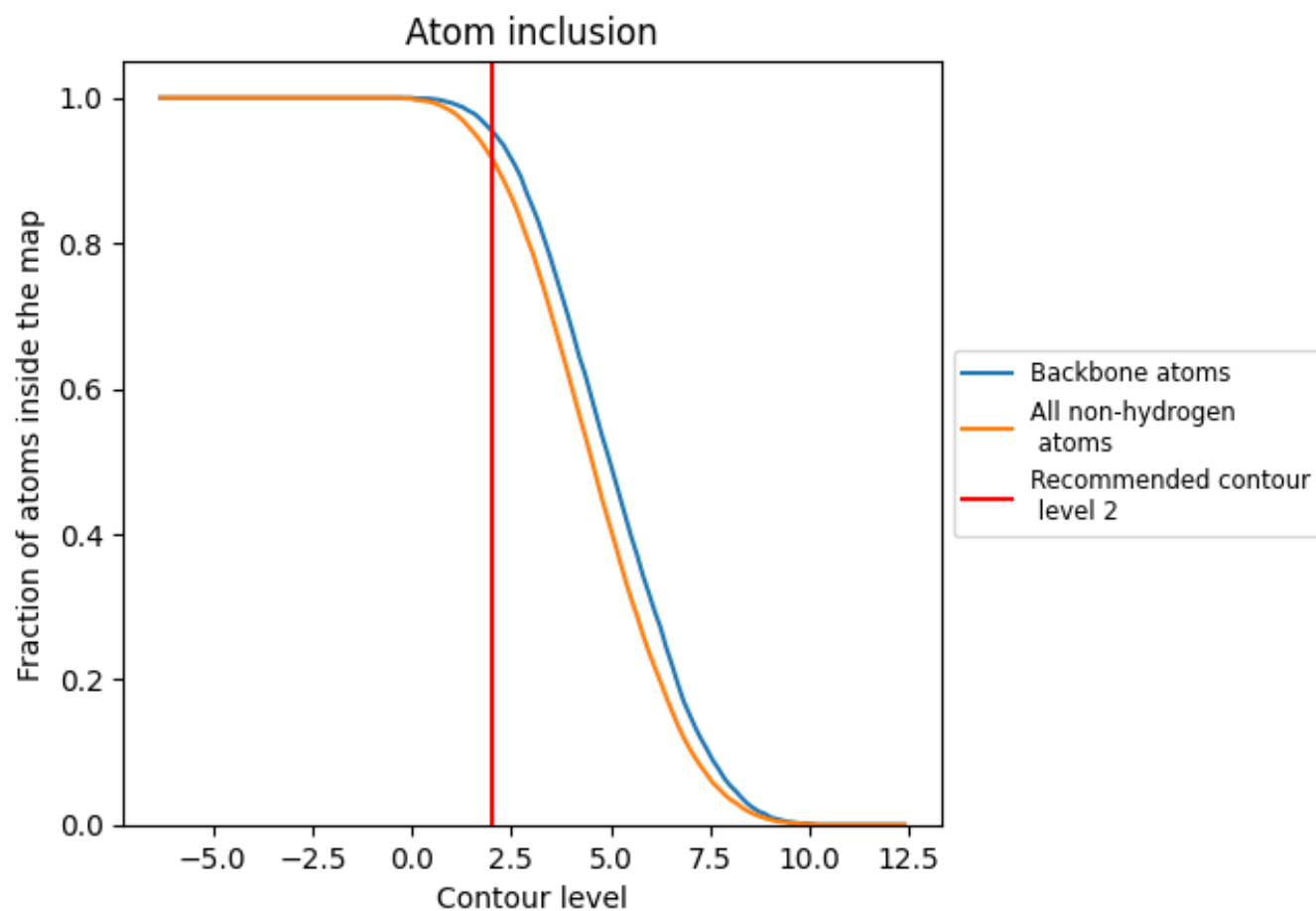
At the recommended contour level, 96% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9180	0.6280
A	0.9040	0.6180
B	0.9150	0.6220
C	0.9270	0.6350
D	0.9070	0.6170
E	0.9230	0.6290
F	0.9290	0.6390
H	0.9230	0.6330
L	0.9270	0.6400

1.0

0.0
<0.0