Full wwPDB EM Validation Report

May 14, 2025 – 09:40 AM EDT

PDB ID	:	9B8V / pdb_00009b8v
EMDB ID	:	EMD-44359
Title	:	AlphaFold2 informed cryo-EM model of the E. coli cellulose synthase BcsAG3B6 complex
Authors	:	Verma, P.; Zimmer, J.
Deposited on	:	2024-04-01
Resolution	:	4.00 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 ⓘ 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:

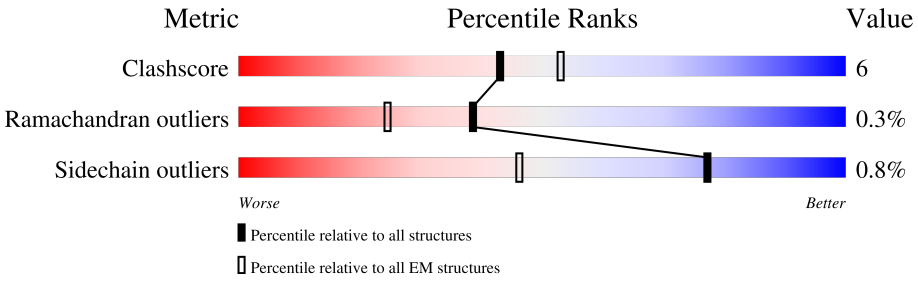
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 Å.

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



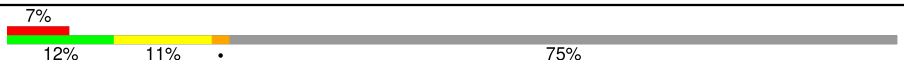
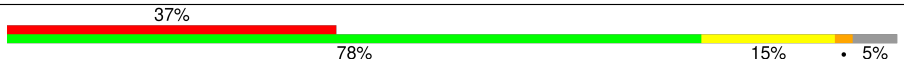
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	763	10% 77% 7% 15%
1	F	763	20% 80% 5% 15%
1	G	763	23% 79% 7% 13%
1	H	763	18% 78% 7% 15%
1	I	763	21% 79% 6% 15%
1	J	763	19% 79% 9% 13%
2	B	567	10% 11% 11% • 76%
2	C	567	7% 12% 11% • 75%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	567	
3	E	887	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 70366 atoms, of which 29654 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 Cellulose synthase operon protein B.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	G	664	Total	C	H	N	O	S	0	0
			9920	3316	4730	887	964	23		
1	A	645	Total	C	H	N	O	S	0	0
			9952	3171	4953	851	953	24		
1	F	647	Total	C	H	N	O	S	0	0
			9971	3177	4960	853	957	24		
1	H	645	Total	C	H	N	O	S	0	0
			9938	3168	4942	850	954	24		
1	I	646	Total	C	H	N	O	S	0	0
			9957	3174	4953	851	955	24		
1	J	664	Total	C	H	N	O	S	0	0
			10263	3265	5116	879	979	24		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	17	ALA	-	expression tag	UNP P37652
G	18	TRP	-	expression tag	UNP P37652
G	19	SER	-	expression tag	UNP P37652
G	20	HIS	-	expression tag	UNP P37652
G	21	PRO	-	expression tag	UNP P37652
G	22	GLN	-	expression tag	UNP P37652
G	23	PHE	-	expression tag	UNP P37652
G	24	GLU	-	expression tag	UNP P37652
G	25	LYS	-	expression tag	UNP P37652
A	17	ALA	-	expression tag	UNP P37652
A	18	TRP	-	expression tag	UNP P37652
A	19	SER	-	expression tag	UNP P37652
A	20	HIS	-	expression tag	UNP P37652
A	21	PRO	-	expression tag	UNP P37652
A	22	GLN	-	expression tag	UNP P37652
A	23	PHE	-	expression tag	UNP P37652
A	24	GLU	-	expression tag	UNP P37652
A	25	LYS	-	expression tag	UNP P37652

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	17	ALA	-	expression tag	UNP P37652
F	18	TRP	-	expression tag	UNP P37652
F	19	SER	-	expression tag	UNP P37652
F	20	HIS	-	expression tag	UNP P37652
F	21	PRO	-	expression tag	UNP P37652
F	22	GLN	-	expression tag	UNP P37652
F	23	PHE	-	expression tag	UNP P37652
F	24	GLU	-	expression tag	UNP P37652
F	25	LYS	-	expression tag	UNP P37652
H	17	ALA	-	expression tag	UNP P37652
H	18	TRP	-	expression tag	UNP P37652
H	19	SER	-	expression tag	UNP P37652
H	20	HIS	-	expression tag	UNP P37652
H	21	PRO	-	expression tag	UNP P37652
H	22	GLN	-	expression tag	UNP P37652
H	23	PHE	-	expression tag	UNP P37652
H	24	GLU	-	expression tag	UNP P37652
H	25	LYS	-	expression tag	UNP P37652
I	17	ALA	-	expression tag	UNP P37652
I	18	TRP	-	expression tag	UNP P37652
I	19	SER	-	expression tag	UNP P37652
I	20	HIS	-	expression tag	UNP P37652
I	21	PRO	-	expression tag	UNP P37652
I	22	GLN	-	expression tag	UNP P37652
I	23	PHE	-	expression tag	UNP P37652
I	24	GLU	-	expression tag	UNP P37652
I	25	LYS	-	expression tag	UNP P37652
J	17	ALA	-	expression tag	UNP P37652
J	18	TRP	-	expression tag	UNP P37652
J	19	SER	-	expression tag	UNP P37652
J	20	HIS	-	expression tag	UNP P37652
J	21	PRO	-	expression tag	UNP P37652
J	22	GLN	-	expression tag	UNP P37652
J	23	PHE	-	expression tag	UNP P37652
J	24	GLU	-	expression tag	UNP P37652
J	25	LYS	-	expression tag	UNP P37652

- Molecule 2 is a protein called Cellulose biosynthesis protein BcsG.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	137	Total	C	N	O	S	0	0
			1136	781	182	170	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	142	Total	C	N	O	S	0	0
			1193	823	190	177	3		
2	D	144	Total	C	N	O	S	0	0
			1205	829	192	181	3		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	560	ASP	-	expression tag	UNP P37659
B	561	TYR	-	expression tag	UNP P37659
B	562	LYS	-	expression tag	UNP P37659
B	563	ASP	-	expression tag	UNP P37659
B	564	ASP	-	expression tag	UNP P37659
B	565	ASP	-	expression tag	UNP P37659
B	566	ASP	-	expression tag	UNP P37659
B	567	LYS	-	expression tag	UNP P37659
C	560	ASP	-	expression tag	UNP P37659
C	561	TYR	-	expression tag	UNP P37659
C	562	LYS	-	expression tag	UNP P37659
C	563	ASP	-	expression tag	UNP P37659
C	564	ASP	-	expression tag	UNP P37659
C	565	ASP	-	expression tag	UNP P37659
C	566	ASP	-	expression tag	UNP P37659
C	567	LYS	-	expression tag	UNP P37659
D	560	ASP	-	expression tag	UNP P37659
D	561	TYR	-	expression tag	UNP P37659
D	562	LYS	-	expression tag	UNP P37659
D	563	ASP	-	expression tag	UNP P37659
D	564	ASP	-	expression tag	UNP P37659
D	565	ASP	-	expression tag	UNP P37659
D	566	ASP	-	expression tag	UNP P37659
D	567	LYS	-	expression tag	UNP P37659

- Molecule 3 is a protein called Cellulose synthase catalytic subunit [UDP-forming].

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	845	Total	C	N	O	S	0	0
			6831	4460	1189	1148	34		

There are 16 discrepancies between the modelled and reference sequences:

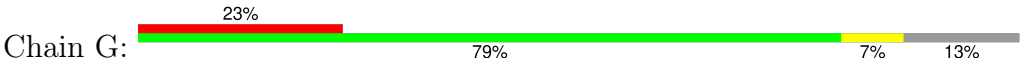
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	MET	-	initiating methionine	UNP P37653
E	1	GLY	-	cloning artifact	UNP P37653
E	873	HIS	-	expression tag	UNP P37653
E	874	HIS	-	expression tag	UNP P37653
E	875	HIS	-	expression tag	UNP P37653
E	876	HIS	-	expression tag	UNP P37653
E	877	HIS	-	expression tag	UNP P37653
E	878	HIS	-	expression tag	UNP P37653
E	879	LEU	-	expression tag	UNP P37653
E	880	GLU	-	expression tag	UNP P37653
E	881	HIS	-	expression tag	UNP P37653
E	882	HIS	-	expression tag	UNP P37653
E	883	HIS	-	expression tag	UNP P37653
E	884	HIS	-	expression tag	UNP P37653
E	885	HIS	-	expression tag	UNP P37653
E	886	HIS	-	expression tag	UNP P37653

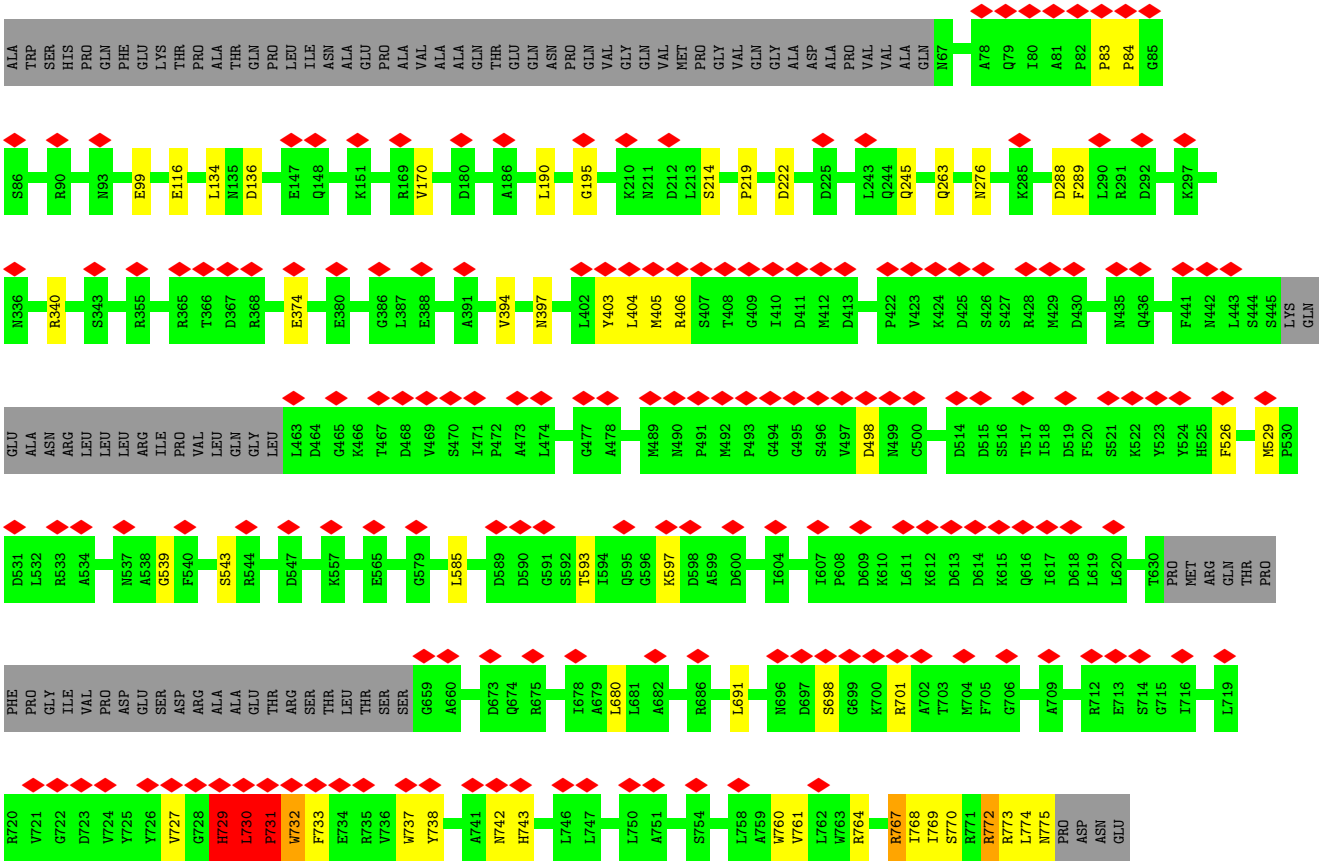
3 Residue-property plots (i)

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

• Molecule 1: Cellulose synthase operon protein B

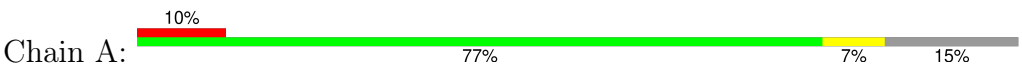
Chain G:

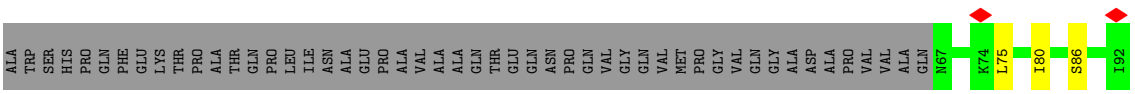


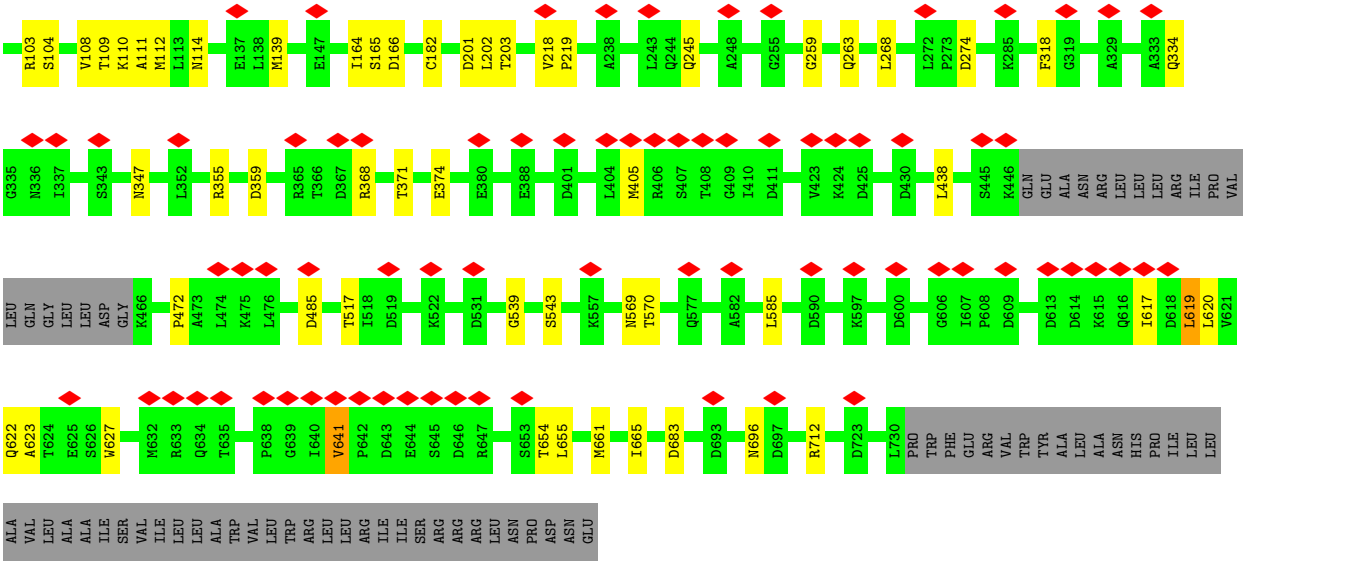


• Molecule 1: Cellulose synthase operon protein B

Chain A:

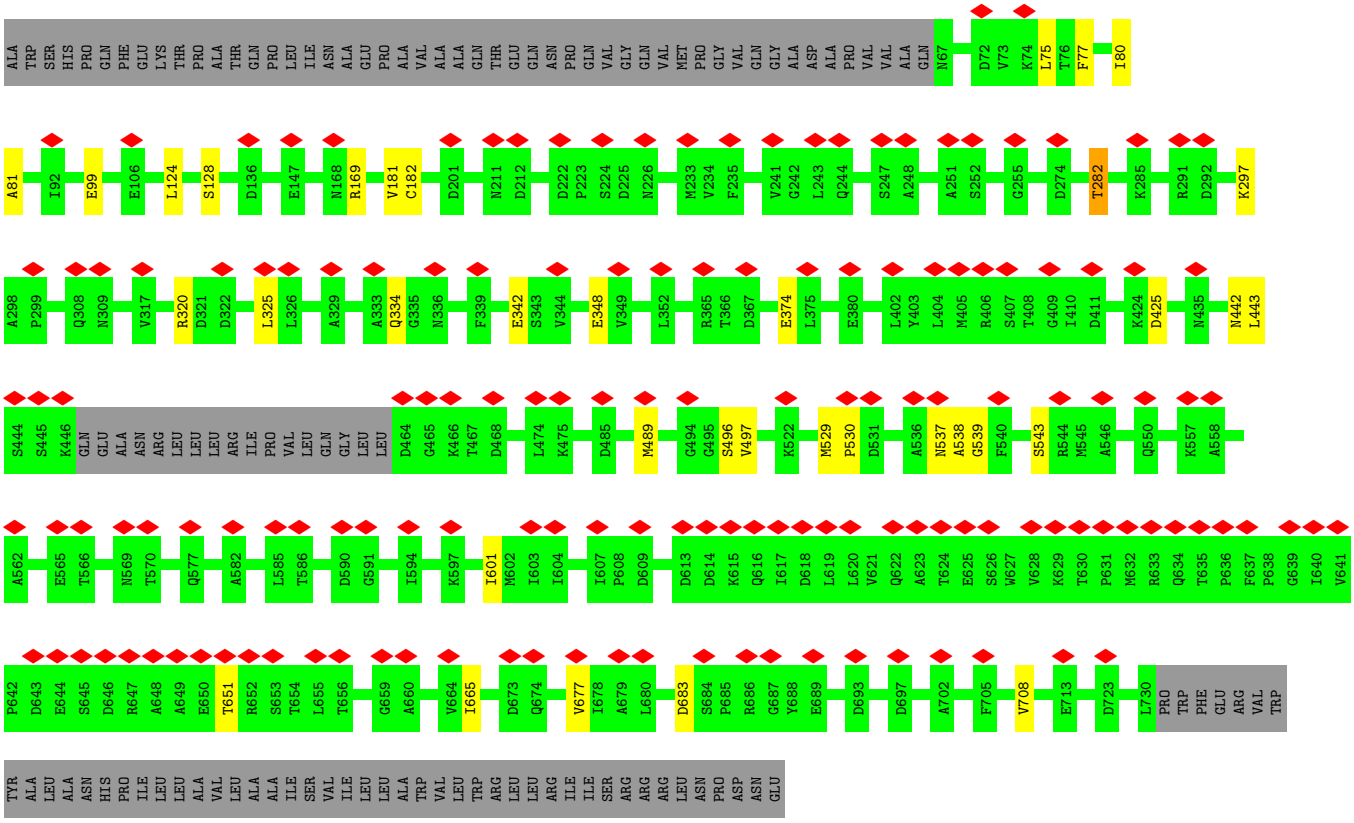






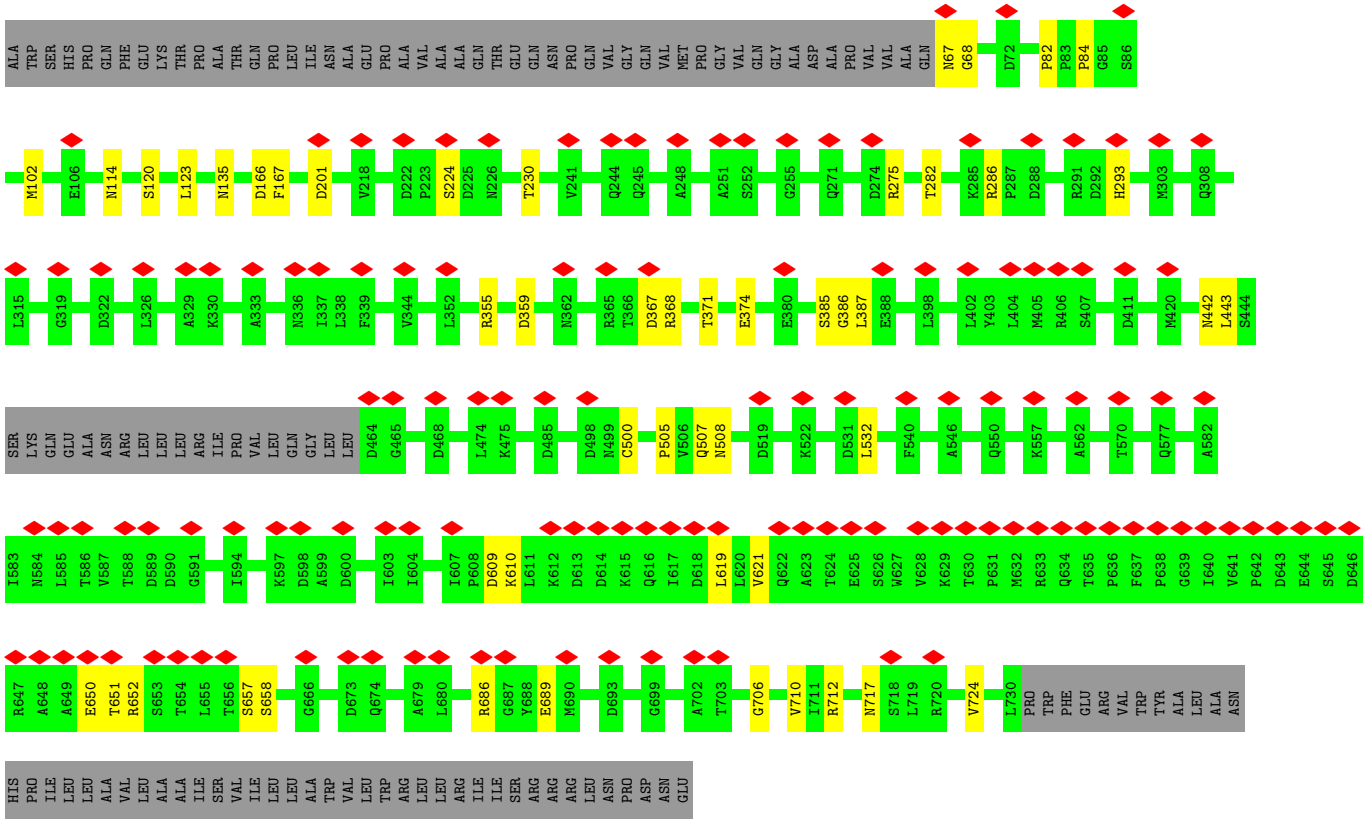
• Molecule 1: Cellulose synthase operon protein B

Chain F:



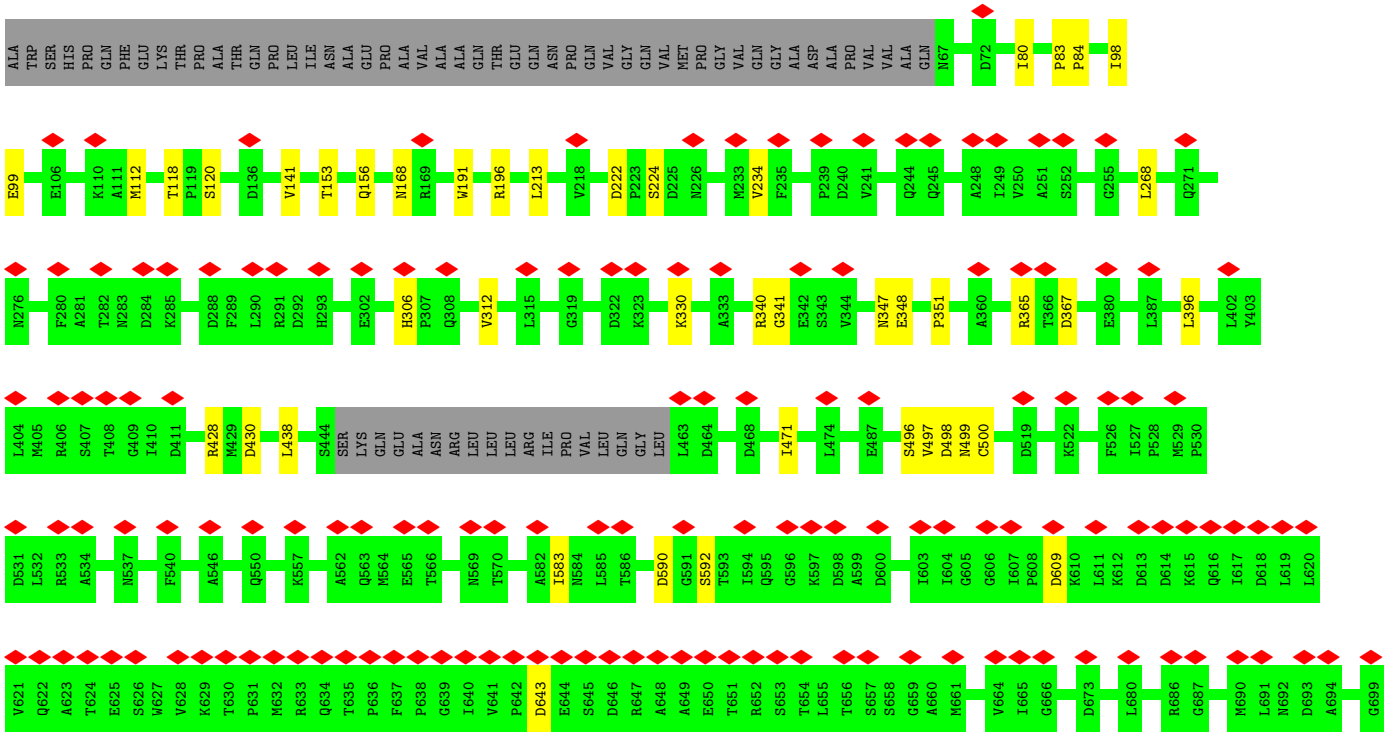
• Molecule 1: Cellulose synthase operon protein B

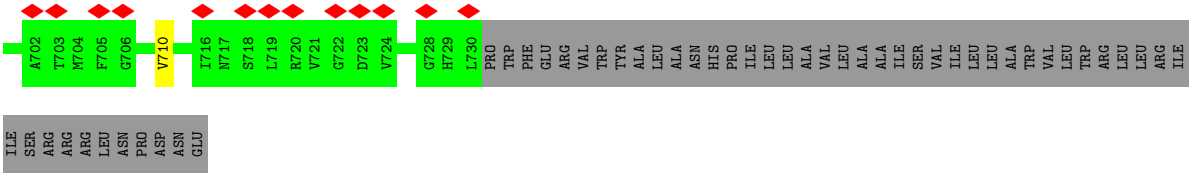
Chain H:



• Molecule 1: Cellulose synthase operon protein B

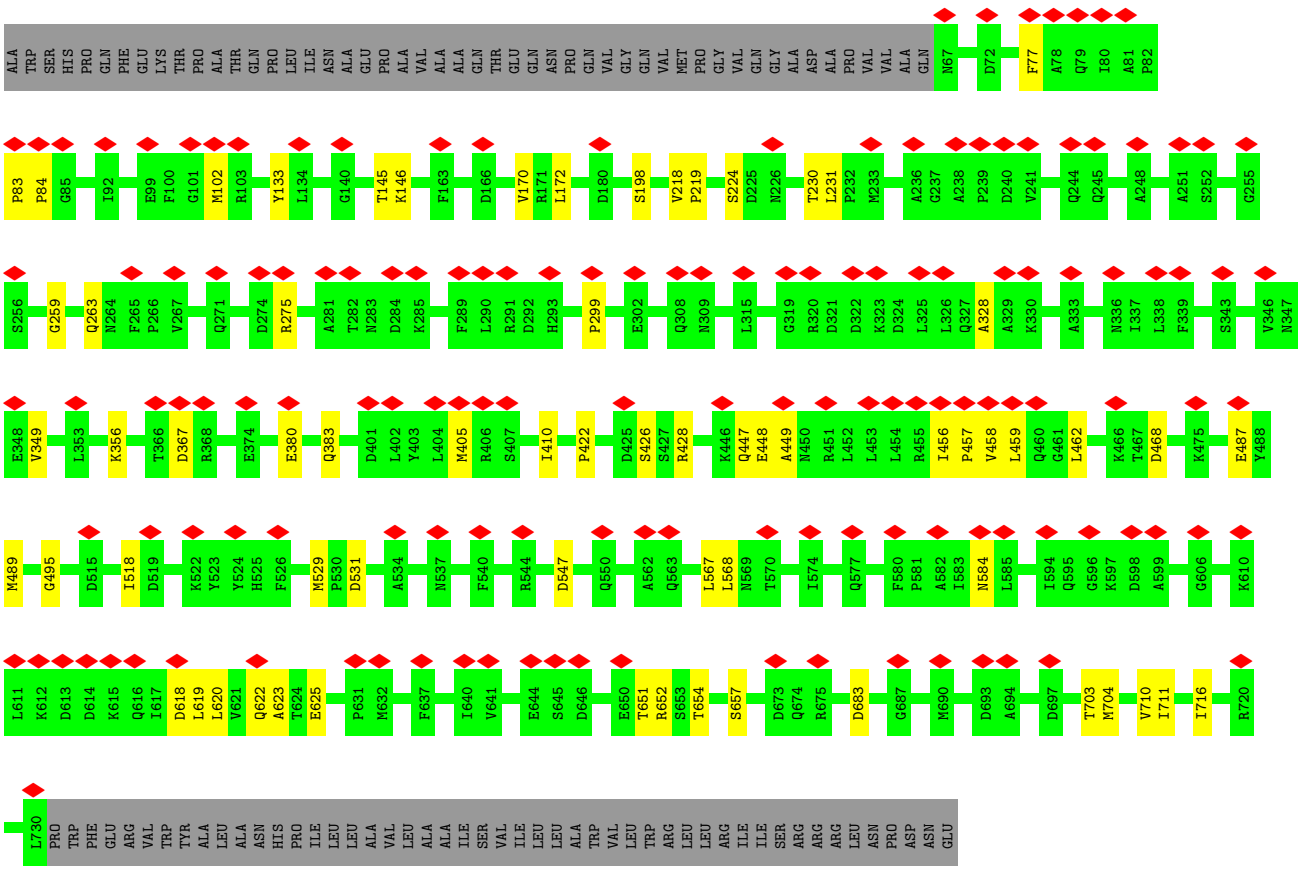
Chain I:





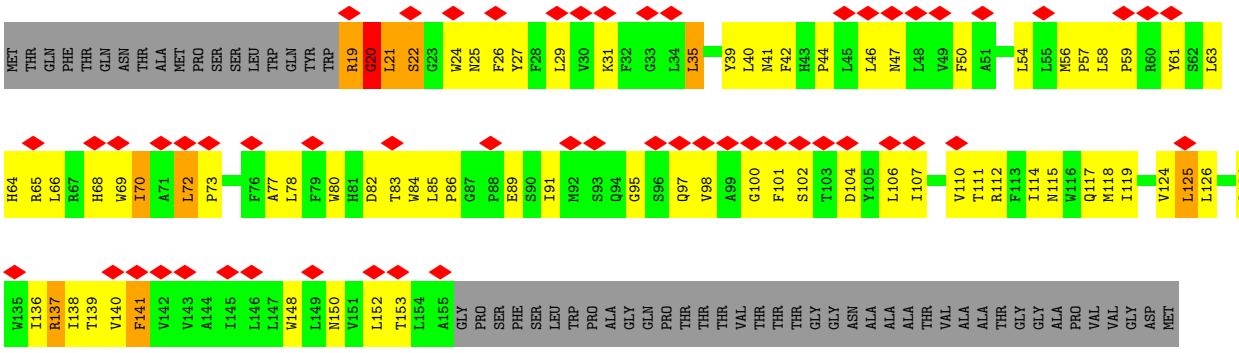
• Molecule 1: Cellulose synthase operon protein B

Chain J:



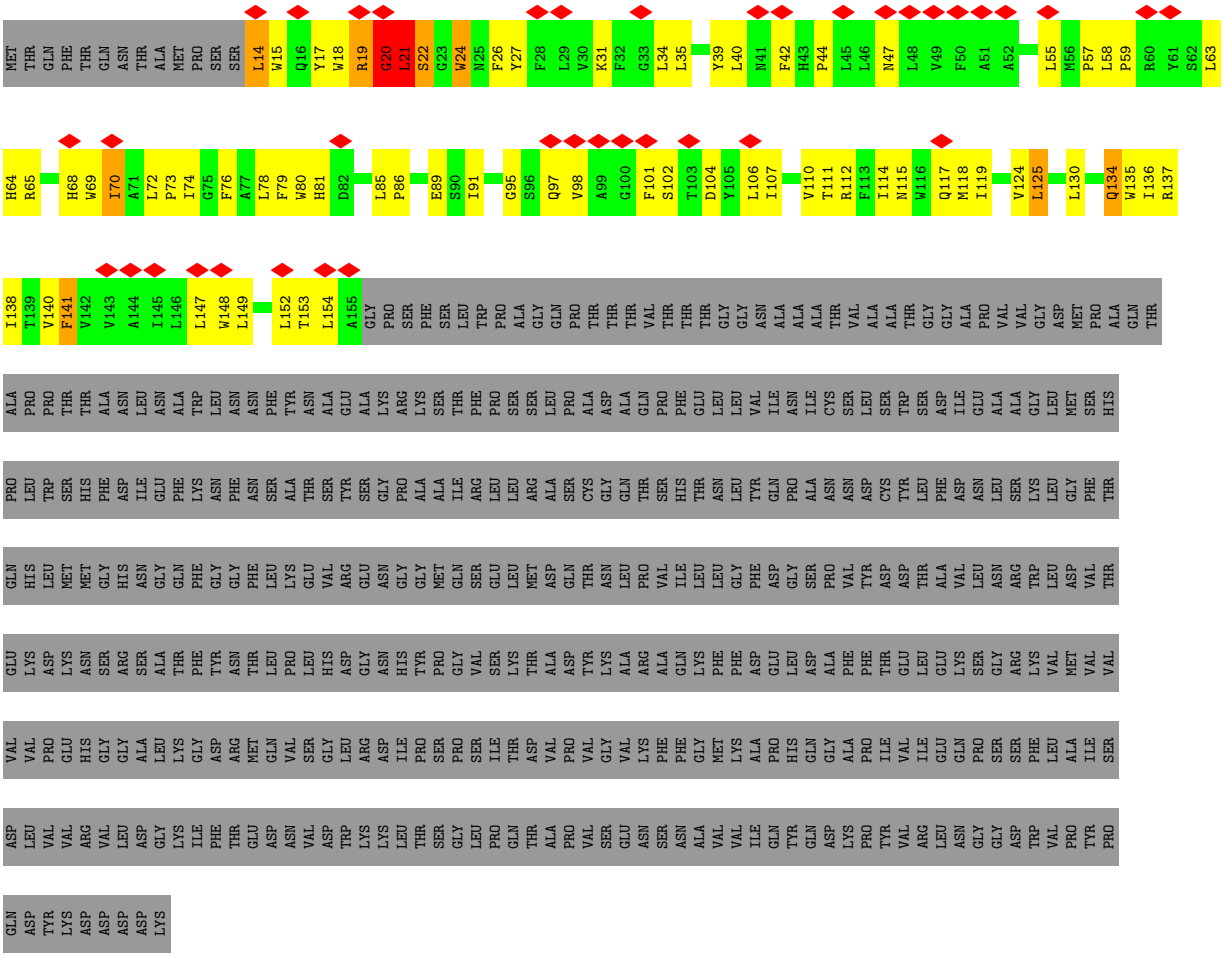
• Molecule 2: Cellulose biosynthesis protein BcsG

Chain B:



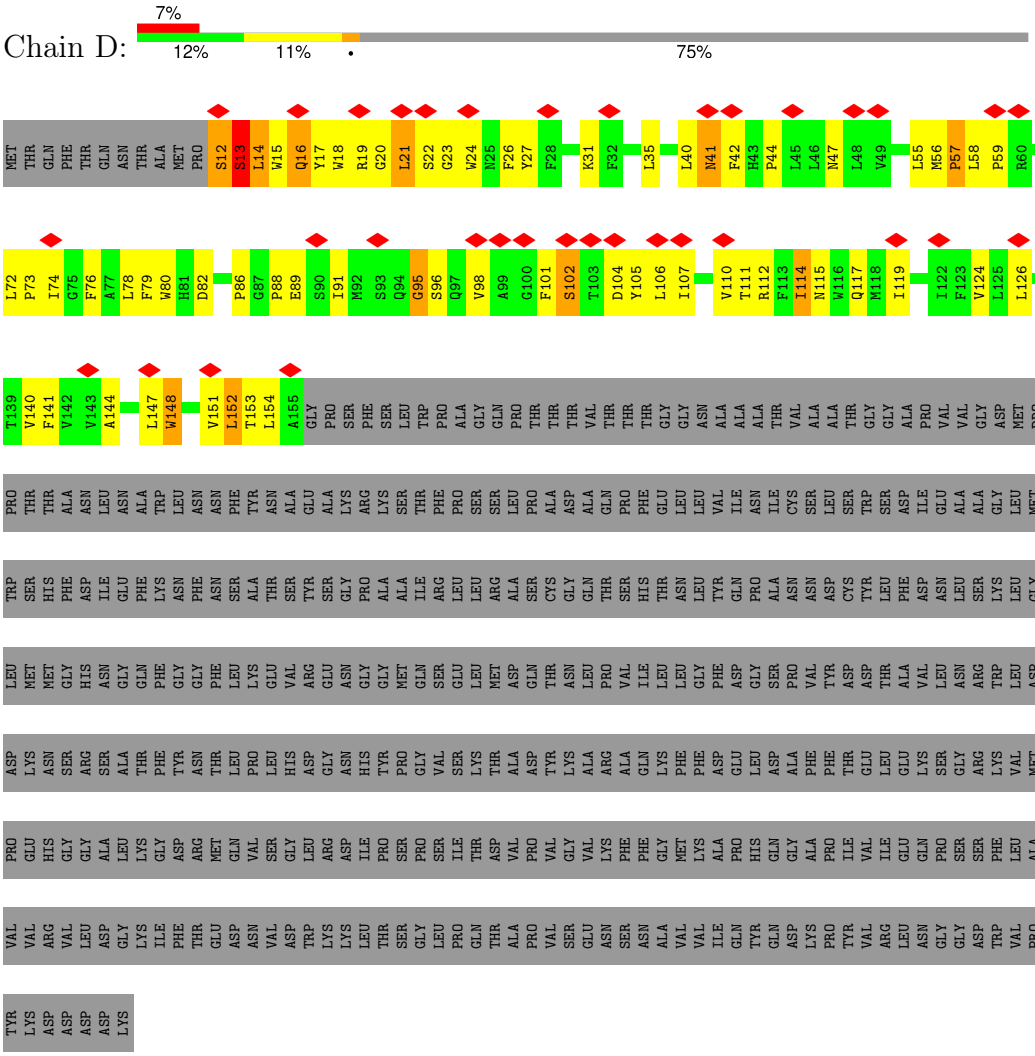
• Molecule 2: Cellulose biosynthesis protein BcsG

Chain C:



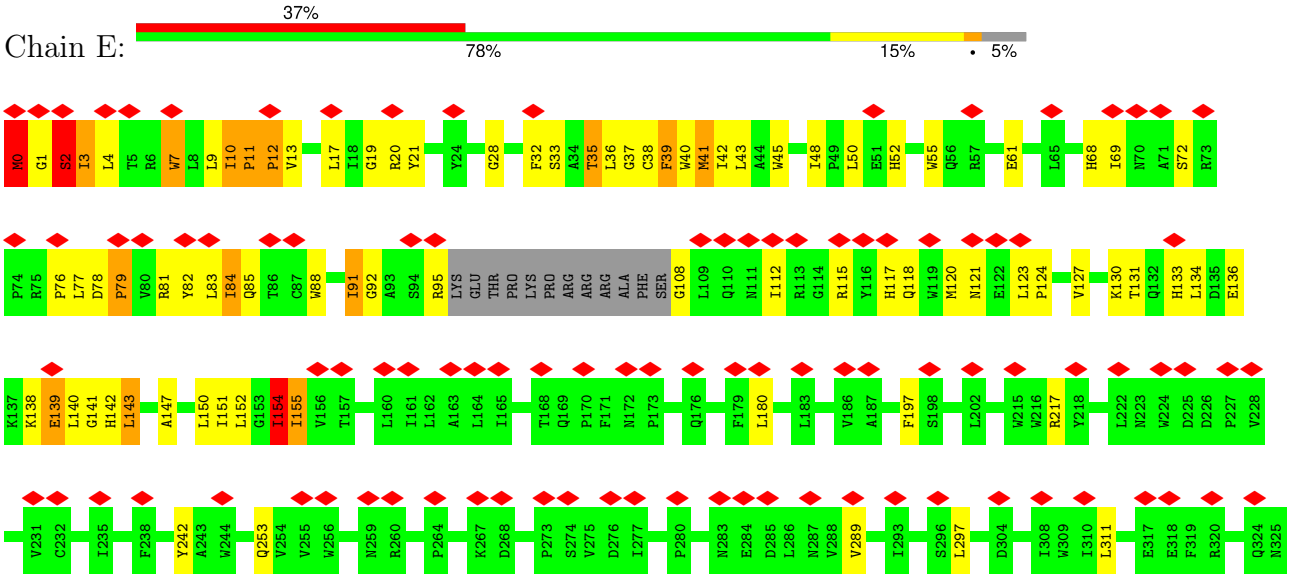
• Molecule 2: Cellulose biosynthesis protein BcsG

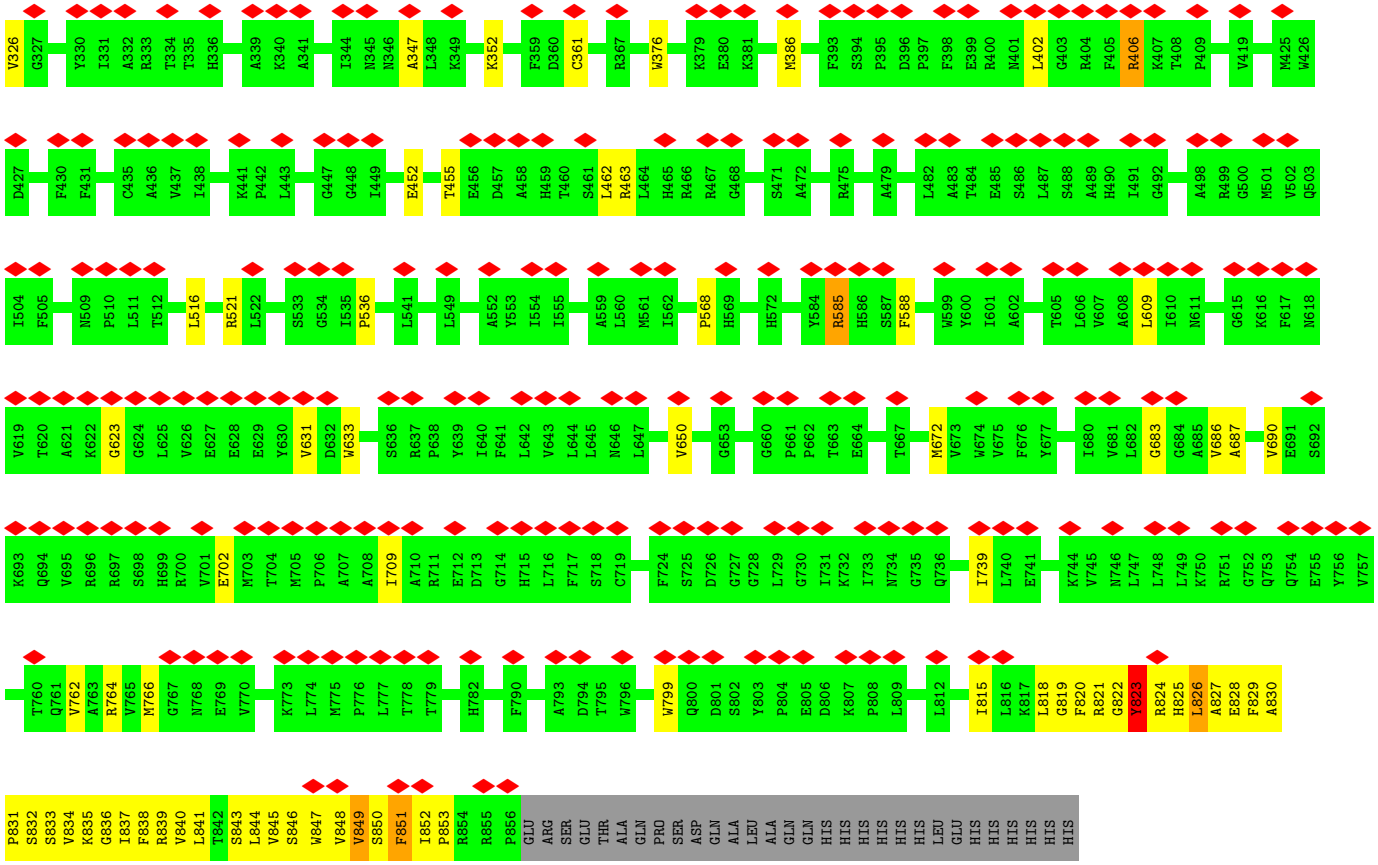
Chain D:



• Molecule 3: Cellulose synthase catalytic subunit [UDP-forming]

Chain E:




V326 G327 Y330 I331 A332 R333 T334 T335 H336 A339 K340 A341 I344 N345 N346 A347 L348 K349 K352 F359 D360 C361 R367 W376 K379 E380 K381 M386 F393 S394 P395 D396 P397 F398 E399 R400 N401 L402 G403 R404 F405 R406 K407 T408 P409 V419 M425 W426
D427 F430 F431 C435 A436 V437 I438 K441 P442 L443 G447 G448 I449 E452 T455 E456 D457 A458 H459 T460 S461 L462 R463 L464 H465 R466 R467 G468 S471 A472 R475 A479 L482 A483 T484 E485 S486 L487 S488 A489 H490 I491 G492 A498 R499 G500 M501 V502 Q503
I504 P505 N509 P510 L511 T512 L516 R521 L522 S533 G534 I535 P536 L541 L549 A552 Y553 I554 I555 A559 L560 M561 I562 P568 H569 H572 Y584 R585 H586 S587 F588 W599 Y600 I601 A602 T605 L606 V607 A608 L609 I610 N611 G615 K616 F617 N618
V619 T620 A621 K622 G623 G624 L625 V626 E627 E628 E629 Y630 V631 D632 W633 S636 R637 P638 Y639 I640 F641 L642 V643 L644 L645 N646 L647 V650 G653 G660 P661 P662 T663 E664 T667 M672 V673 W674 V675 F676 Y677 I680 V681 L682 G683 G684 A685 V686 A687 V690 E691 S692
K693 Q694 V695 R696 R697 S698 H699 R700 V701 E702 M703 T704 M705 P706 A707 A708 I709 A710 R711 E712 D713 G714 H715 L716 F717 S718 C719 F724 S725 D726 G727 G728 L729 G730 I731 K732 I733 N734 G735 Q736 I739 L740 E741 K744 V745 N746 L747 L748 L749 K750 R751 G752 Q753 Q754 E755 Y756 V757
T760 Q761 V762 A763 R764 V765 M766 G767 N768 E769 V770 K773 L774 M775 P776 L777 T778 T779 H782 F790 A793 D794 T795 W796 W799 Q800 D801 S802 Y803 P804 E805 D806 K807 P808 L809 L812 I815 L816 K817 L818 G819 F820 R821 G822 Y823 R824 H825 L826 A827 E828 F829 A830
P831 S832 S833 V834 K835 C836 I837 F838 R839 V840 L841 T842 S843 L844 V845 S846 W847 V848 V849 S850 F851 I852 P853 R854 R855 P856 GLU ARG SER GLU THR ALA GLN PRO SER ASP GLN ALA LEU ALA GLN GLN HIS HIS HIS HIS HIS LEU GLU GLU HIS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39522	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 ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	38.522	Depositor
Minimum map value	-50.281	Depositor
Average map value	-0.009	Depositor
Map value standard deviation	1.122	Depositor
Recommended contour level	7	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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	0.12	0/5113	0.31	2/6959 (0.0%)
1	F	0.12	0/5125	0.27	0/6975
1	G	0.25	0/5312	0.45	2/7233 (0.0%)
1	H	0.11	0/5110	0.28	0/6956
1	I	0.11	0/5118	0.26	0/6967
1	J	0.11	0/5263	0.27	0/7164
2	B	1.36	23/1180 (1.9%)	1.09	9/1617 (0.6%)
2	C	1.34	25/1242 (2.0%)	1.09	11/1704 (0.6%)
2	D	1.29	29/1254 (2.3%)	1.19	10/1720 (0.6%)
3	E	0.85	22/7028 (0.3%)	1.21	18/9560 (0.2%)
All	All	0.54	99/41745 (0.2%)	0.66	52/56855 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	4
2	B	0	3
2	C	0	3
2	D	0	8
3	E	0	6
All	All	0	24

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	85	LEU	C-N	13.33	1.50	1.33
2	C	85	LEU	C-N	11.73	1.48	1.33
3	E	79	PRO	C-N	-10.53	1.20	1.33
3	E	40	TRP	C-N	-10.27	1.20	1.33
2	D	58	LEU	C-N	9.12	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	59	PRO	N-CD	-9.02	1.35	1.47
2	D	104	ASP	C-N	-8.93	1.21	1.33
2	D	86	PRO	N-CD	-8.82	1.35	1.47
3	E	19	GLY	C-N	-8.77	1.22	1.33
2	C	80	TRP	C-N	-8.68	1.22	1.33
2	C	86	PRO	N-CD	-8.60	1.35	1.47
3	E	33	SER	C-N	-8.35	1.22	1.33
2	B	89	GLU	C-N	-8.27	1.22	1.33
2	B	86	PRO	N-CD	-8.00	1.36	1.47
2	B	70	ILE	C-N	-7.99	1.23	1.34
2	C	104	ASP	C-N	-7.95	1.23	1.33
2	D	112	ARG	C-N	-7.95	1.22	1.33
2	B	56	MET	C-N	7.81	1.41	1.33
2	D	80	TRP	C-N	-7.54	1.24	1.33
2	B	140	VAL	C-N	-7.25	1.24	1.33
3	E	85	GLN	C-N	-7.17	1.24	1.33
3	E	2	SER	C-N	-7.00	1.24	1.33
2	B	72	LEU	C-N	6.94	1.42	1.34
2	B	125	LEU	C-N	-6.93	1.25	1.33
2	C	147	LEU	C-N	-6.84	1.25	1.33
2	C	76	PHE	C-N	-6.72	1.25	1.33
2	C	89	GLU	C-N	-6.72	1.24	1.33
2	C	58	LEU	C-N	6.71	1.42	1.34
2	B	80	TRP	C-N	-6.70	1.25	1.33
2	B	97	GLN	C-N	-6.66	1.25	1.33
3	E	20	ARG	C-N	-6.65	1.25	1.33
2	D	88	PRO	N-CD	-6.64	1.38	1.47
2	B	19	ARG	C-N	6.64	1.43	1.33
2	C	70	ILE	C-N	-6.61	1.24	1.34
2	D	23	GLY	C-N	-6.56	1.24	1.33
2	C	112	ARG	C-N	-6.51	1.24	1.33
2	C	64	HIS	C-N	-6.44	1.25	1.33
2	C	124	VAL	C-N	-6.41	1.25	1.33
2	C	141	PHE	C-N	-6.39	1.25	1.33
2	D	151	VAL	C-N	-6.30	1.25	1.34
2	B	112	ARG	C-N	-6.29	1.24	1.33
2	C	68	HIS	C-N	-6.25	1.25	1.33
2	C	97	GLN	C-N	-6.25	1.26	1.33
3	E	10	ILE	C-N	6.20	1.40	1.33
2	D	154	LEU	C-N	6.20	1.42	1.33
2	D	64	HIS	C-N	-6.17	1.25	1.33
2	D	152	LEU	C-N	-6.16	1.25	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	124	VAL	C-N	-6.12	1.25	1.33
2	D	76	PHE	C-N	-6.11	1.25	1.33
2	C	140	VAL	C-N	-6.09	1.25	1.33
2	B	35	LEU	C-N	-6.06	1.25	1.33
2	B	141	PHE	C-N	-6.05	1.26	1.33
2	C	154	LEU	C-N	6.04	1.41	1.33
3	E	32	PHE	C-N	-6.03	1.25	1.33
2	B	57	PRO	C-N	6.03	1.41	1.33
2	D	148	TRP	C-N	-6.03	1.26	1.33
3	E	35	THR	C-N	-6.01	1.26	1.33
2	D	124	VAL	C-N	-6.00	1.26	1.33
2	D	140	VAL	C-N	-6.00	1.25	1.33
2	C	137	ARG	C-N	-5.94	1.26	1.33
2	D	147	LEU	C-N	-5.89	1.26	1.33
2	B	104	ASP	C-N	-5.88	1.25	1.33
3	E	38	CYS	C-N	-5.80	1.26	1.33
3	E	11	PRO	N-CD	5.77	1.55	1.47
2	D	12	SER	C-N	-5.75	1.25	1.33
2	C	134	GLN	C-N	-5.73	1.25	1.33
2	D	89	GLU	C-N	-5.69	1.26	1.33
3	E	21	TYR	C-N	-5.63	1.26	1.33
2	B	138	ILE	C-N	-5.63	1.26	1.33
3	E	83	LEU	C-N	-5.61	1.26	1.33
2	D	65	ARG	C-N	-5.57	1.26	1.33
2	B	102	SER	C-N	5.56	1.41	1.34
2	B	137	ARG	C-N	-5.51	1.27	1.34
2	C	14	LEU	C-N	5.49	1.41	1.33
2	C	15	TRP	C-N	-5.47	1.25	1.33
2	D	114	ILE	C-N	-5.47	1.26	1.33
3	E	39	PHE	C-N	-5.43	1.26	1.33
2	D	57	PRO	C-N	5.40	1.40	1.33
2	D	144	ALA	C-N	-5.39	1.27	1.33
2	B	46	LEU	C-N	-5.39	1.26	1.34
2	D	105	TYR	C-N	-5.35	1.26	1.33
3	E	7	TRP	C-N	5.34	1.41	1.33
2	D	86	PRO	C-N	5.33	1.41	1.33
3	E	61	GLU	C-N	-5.33	1.27	1.33
3	E	12	PRO	C-N	-5.32	1.27	1.33
2	C	81	HIS	C-N	-5.32	1.25	1.33
2	B	100	GLY	C-N	-5.30	1.26	1.33
3	E	77	LEU	C-N	-5.28	1.26	1.33
2	D	41	ASN	C-N	-5.20	1.26	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	79	PRO	N-CD	5.20	1.55	1.47
3	E	84	ILE	C-N	-5.16	1.26	1.33
2	C	86	PRO	C-N	5.16	1.41	1.33
2	D	56	MET	C-N	5.12	1.39	1.33
2	C	138	ILE	C-N	-5.10	1.27	1.33
2	D	95	GLY	C-N	5.08	1.41	1.33
2	D	70	ILE	C-N	-5.07	1.26	1.34
2	C	24	TRP	C-N	5.05	1.40	1.33
3	E	42	ILE	C-N	-5.04	1.27	1.33
2	D	96	SER	C-N	-5.02	1.26	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	13	SER	O-C-N	-18.69	97.73	122.59
3	E	2	SER	O-C-N	-16.16	100.92	122.57
2	D	12	SER	O-C-N	-14.70	99.48	123.00
1	G	729	HIS	O-C-N	-11.37	107.47	122.59
3	E	846	SER	N-CA-C	-10.41	100.02	111.36
3	E	840	VAL	N-CA-C	-8.22	102.42	110.72
3	E	849	VAL	N-CA-C	-8.08	102.56	110.72
2	C	21	LEU	O-C-N	-7.48	112.65	122.59
2	D	16	GLN	CA-C-N	-7.45	110.95	122.49
2	D	16	GLN	C-N-CA	-7.45	110.95	122.49
3	E	623	GLY	CA-C-N	7.24	127.91	120.60
3	E	623	GLY	C-N-CA	7.24	127.91	120.60
2	B	22	SER	CA-C-N	7.05	132.87	120.74
2	B	22	SER	C-N-CA	7.05	132.87	120.74
2	C	22	SER	CA-C-N	7.00	132.79	120.74
2	C	22	SER	C-N-CA	7.00	132.79	120.74
2	C	22	SER	O-C-N	-6.89	113.42	122.59
2	D	22	SER	CA-C-N	6.79	132.42	120.74
2	D	22	SER	C-N-CA	6.79	132.42	120.74
2	C	102	SER	CA-C-N	6.70	130.16	120.38
2	C	102	SER	C-N-CA	6.70	130.16	120.38
3	E	155	ILE	N-CA-C	-6.66	104.03	110.42
2	C	20	GLY	O-C-N	-6.62	114.09	122.70
2	C	20	GLY	CA-C-N	6.43	133.83	121.54
2	C	20	GLY	C-N-CA	6.43	133.83	121.54
2	B	22	SER	O-C-N	-6.37	114.12	122.59
2	B	102	SER	CA-C-N	6.34	129.64	120.38
2	B	102	SER	C-N-CA	6.34	129.64	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	22	SER	O-C-N	-6.24	114.30	122.59
2	B	19	ARG	O-C-N	-6.20	113.07	123.00
2	D	21	LEU	O-C-N	-6.13	114.44	122.59
3	E	843	SER	N-CA-C	-6.04	104.77	111.36
3	E	826	LEU	N-CA-C	-6.02	105.20	112.54
2	D	102	SER	CA-C-N	5.89	128.97	120.38
2	D	102	SER	C-N-CA	5.89	128.97	120.38
3	E	41	MET	O-C-N	5.80	128.27	122.12
2	B	20	GLY	O-C-N	-5.65	115.35	122.70
2	B	63	LEU	O-C-N	5.46	128.98	122.27
2	C	63	LEU	O-C-N	5.45	128.98	122.27
3	E	823	TYR	N-CA-C	-5.44	105.35	111.28
3	E	28	GLY	O-C-N	-5.40	116.50	122.50
3	E	253	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	A	570	THR	CB-CA-C	5.29	119.58	110.79
2	C	130	LEU	O-C-N	5.24	127.67	122.12
1	G	733	PHE	N-CA-C	-5.19	107.08	113.41
3	E	352	LYS	CA-C-N	5.15	124.99	120.10
3	E	352	LYS	C-N-CA	5.15	124.99	120.10
3	E	154	ILE	N-CA-C	-5.15	105.52	110.72
2	B	77	ALA	O-C-N	5.09	127.52	122.12
1	A	570	THR	N-CA-CB	5.09	117.60	110.12
3	E	152	LEU	N-CA-C	-5.08	105.83	111.36
3	E	217	ARG	CD-NE-CZ	5.01	131.41	124.40

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	19	ARG	Mainchain
2	B	20	GLY	Mainchain
2	B	21	LEU	Mainchain
2	C	19	ARG	Mainchain
2	C	20	GLY	Mainchain
2	C	21	LEU	Mainchain
2	D	102	SER	Mainchain
2	D	12	SER	Mainchain
2	D	13	SER	Mainchain
2	D	14	LEU	Mainchain
2	D	16	GLN	Mainchain
2	D	19	ARG	Mainchain
2	D	20	GLY	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	D	21	LEU	Mainchain
3	E	0	MET	Mainchain,Peptide
3	E	2	SER	Mainchain
3	E	406	ARG	Sidechain
3	E	521	ARG	Sidechain
3	E	585	ARG	Sidechain
1	G	729	HIS	Mainchain
1	G	731	PRO	Peptide
1	G	772	ARG	Sidechain
1	G	773	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4999	4953	4951	39	0
1	F	5011	4960	4958	22	0
1	G	5190	4730	5179	53	0
1	H	4996	4942	4940	29	0
1	I	5004	4953	4951	27	0
1	J	5147	5116	5114	39	0
2	B	1136	0	1154	60	0
2	C	1193	0	1202	56	0
2	D	1205	0	1212	67	0
3	E	6831	0	6919	158	0
All	All	40712	29654	40580	520	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 6.

All (520) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:10:ILE:CD1	3:E:12:PRO:HG2	1.65	1.25
1:G:730:LEU:HB3	1:G:731:PRO:HD2	1.23	1.19
2:D:40:LEU:HD21	2:D:82:ASP:HB3	1.22	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:LEU:HD21	2:B:82:ASP:HB3	1.29	1.08
2:C:44:PRO:HG2	2:C:153:THR:HG21	1.36	1.07
2:C:24:TRP:HA	2:C:27:TYR:HD2	1.20	1.06
2:D:24:TRP:HA	2:D:27:TYR:HD2	1.16	1.05
1:G:406:ARG:HH21	1:G:738:TYR:HA	1.16	1.04
2:B:24:TRP:HA	2:B:27:TYR:HD2	1.19	1.02
2:D:44:PRO:HG2	2:D:153:THR:HG21	1.43	1.00
2:D:24:TRP:HA	2:D:27:TYR:CD2	1.98	0.98
1:G:406:ARG:NH2	1:G:738:TYR:HA	1.78	0.97
2:B:24:TRP:HA	2:B:27:TYR:CD2	1.99	0.96
3:E:10:ILE:HD12	3:E:12:PRO:CD	1.95	0.95
2:C:24:TRP:HA	2:C:27:TYR:CD2	2.01	0.95
3:E:10:ILE:CD1	3:E:12:PRO:CG	2.44	0.94
3:E:10:ILE:HD11	3:E:13:VAL:HG23	1.46	0.94
1:G:730:LEU:HB3	1:G:731:PRO:CD	1.98	0.93
2:D:17:TYR:CD1	2:D:59:PRO:HA	2.03	0.93
2:B:44:PRO:HG3	2:B:153:THR:HG21	1.50	0.93
3:E:10:ILE:HD12	3:E:12:PRO:HD2	1.50	0.92
2:B:134:GLN:HE22	2:C:18:TRP:HE1	1.12	0.92
2:D:13:SER:C	2:D:15:TRP:H	1.79	0.90
3:E:68:HIS:O	3:E:81:ARG:NH2	2.03	0.90
1:G:406:ARG:HH21	1:G:738:TYR:CA	1.87	0.88
2:B:31:LYS:NZ	2:B:78:LEU:HD22	1.89	0.88
3:E:10:ILE:HD12	3:E:12:PRO:HG2	1.56	0.88
1:A:109:THR:OG1	1:A:203:THR:O	1.90	0.88
3:E:41:MET:O	3:E:45:TRP:HD1	1.57	0.86
3:E:84:ILE:O	3:E:88:TRP:HD1	1.59	0.85
3:E:10:ILE:HD12	3:E:12:PRO:CG	2.06	0.85
1:G:406:ARG:NH2	1:G:738:TYR:CA	2.40	0.85
3:E:45:TRP:CD2	3:E:50:LEU:HD12	2.13	0.84
2:B:61:TYR:HE1	2:B:65:ARG:HH21	1.24	0.83
2:D:129:TRP:CD1	2:D:138:ILE:CD1	2.61	0.83
3:E:3:ILE:O	3:E:7:TRP:HD1	1.60	0.83
3:E:41:MET:O	3:E:45:TRP:CD1	2.31	0.83
2:B:134:GLN:NE2	2:C:18:TRP:HE1	1.76	0.83
2:D:129:TRP:HD1	2:D:138:ILE:HD13	1.44	0.82
3:E:84:ILE:O	3:E:88:TRP:CD1	2.33	0.82
3:E:138:LYS:C	3:E:140:LEU:H	1.89	0.81
3:E:633:TRP:CZ2	3:E:829:PHE:HB3	2.15	0.81
1:G:526:PHE:HB3	1:G:738:TYR:OH	1.80	0.80
1:G:526:PHE:CG	1:G:738:TYR:CE1	2.70	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:2:SER:C	3:E:4:LEU:H	1.89	0.79
3:E:10:ILE:HD13	3:E:12:PRO:HG2	1.62	0.78
1:H:286:ARG:NH2	1:H:293:HIS:O	2.16	0.78
1:G:729:HIS:O	1:G:730:LEU:HB2	1.84	0.78
2:D:129:TRP:CD1	2:D:138:ILE:HD12	2.18	0.78
2:C:31:LYS:NZ	2:C:78:LEU:CD2	2.48	0.77
1:A:114:ASN:ND2	1:A:201:ASP:OD1	2.18	0.77
2:D:66:LEU:HD23	2:D:70:ILE:HD12	1.67	0.77
3:E:633:TRP:HZ2	3:E:829:PHE:HB3	1.50	0.76
2:D:129:TRP:HD1	2:D:138:ILE:CD1	1.97	0.76
3:E:45:TRP:CE3	3:E:50:LEU:HD12	2.20	0.76
2:B:31:LYS:NZ	2:B:78:LEU:CD2	2.48	0.76
3:E:838:PHE:HA	3:E:841:LEU:HB3	1.65	0.76
3:E:36:LEU:HD23	3:E:76:PRO:HA	1.67	0.76
3:E:10:ILE:HD11	3:E:12:PRO:HG2	1.66	0.76
2:C:134:GLN:NE2	3:E:52:HIS:CE1	2.54	0.76
3:E:68:HIS:C	3:E:81:ARG:HH22	1.94	0.75
2:B:40:LEU:CD2	2:B:82:ASP:HB3	2.13	0.75
2:D:35:LEU:HD13	2:D:42:PHE:HB2	1.68	0.75
3:E:48:ILE:CG2	3:E:55:TRP:CE2	2.70	0.74
2:C:17:TYR:CD1	2:C:59:PRO:HA	2.22	0.74
3:E:402:LEU:HD22	3:E:818:LEU:HD11	1.70	0.73
2:D:40:LEU:CD2	2:D:82:ASP:HB3	2.11	0.73
3:E:2:SER:C	3:E:4:LEU:N	2.46	0.73
2:D:42:PHE:O	2:D:44:PRO:HD3	1.90	0.72
2:C:35:LEU:HD13	2:C:42:PHE:HB2	1.71	0.71
2:B:35:LEU:HD13	2:B:42:PHE:HB2	1.71	0.71
2:C:136:ILE:CG2	2:C:141:PHE:HE2	2.03	0.71
1:A:259:GLY:O	1:A:263:GLN:NE2	2.23	0.71
1:G:526:PHE:CD2	1:G:738:TYR:HE1	2.09	0.70
2:C:31:LYS:NZ	2:C:78:LEU:HD22	2.06	0.70
3:E:631:VAL:CG2	3:E:829:PHE:CD2	2.74	0.70
3:E:845:VAL:HA	3:E:848:VAL:HB	1.72	0.70
1:G:526:PHE:CG	1:G:738:TYR:HE1	2.10	0.69
2:B:134:GLN:HE22	2:C:18:TRP:NE1	1.87	0.69
2:D:15:TRP:C	2:D:17:TYR:H	2.00	0.69
1:G:406:ARG:NH2	1:G:738:TYR:N	2.41	0.69
1:G:761:VAL:HG21	3:E:155:ILE:HG21	1.74	0.69
3:E:10:ILE:CD1	3:E:12:PRO:HD2	2.22	0.69
2:B:31:LYS:HZ3	2:B:78:LEU:CD2	2.07	0.68
1:A:245:GLN:NE2	1:A:585:LEU:O	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:LYS:NZ	2:D:78:LEU:CD2	2.57	0.67
2:D:66:LEU:HD21	2:D:70:ILE:HD11	1.77	0.67
2:C:115:ASN:OD1	2:C:117:GLN:OE1	2.13	0.67
3:E:631:VAL:HG23	3:E:829:PHE:CD2	2.30	0.67
3:E:841:LEU:O	3:E:845:VAL:HG23	1.95	0.67
1:G:403:TYR:CD2	1:G:404:LEU:O	2.47	0.67
2:B:61:TYR:HE1	2:B:65:ARG:NH2	1.92	0.67
3:E:10:ILE:CD1	3:E:12:PRO:CD	2.70	0.67
2:C:31:LYS:HZ3	2:C:78:LEU:HD23	1.58	0.66
3:E:0:MET:SD	3:E:35:THR:CG2	2.83	0.66
2:B:66:LEU:HD23	2:B:70:ILE:HD12	1.78	0.66
3:E:683:GLY:O	3:E:822:GLY:HA3	1.95	0.66
2:D:98:VAL:HA	2:D:101:PHE:CD2	2.31	0.66
2:D:47:ASN:OD1	2:D:78:LEU:HD21	1.95	0.66
1:G:219:PRO:O	1:G:276:ASN:ND2	2.29	0.66
2:C:31:LYS:HZ3	2:C:78:LEU:CD2	2.07	0.66
2:C:134:GLN:HE22	3:E:52:HIS:CE1	2.11	0.65
2:B:66:LEU:HD21	2:B:70:ILE:HD11	1.78	0.65
3:E:851:PHE:O	3:E:852:ILE:C	2.39	0.65
1:J:703:THR:OG1	1:J:716:ILE:HD11	1.96	0.64
2:C:34:LEU:HB2	2:C:40:LEU:HD12	1.78	0.64
1:G:760:TRP:HA	3:E:197:PHE:HE2	1.61	0.64
3:E:138:LYS:C	3:E:140:LEU:N	2.55	0.64
1:G:731:PRO:HB2	1:G:732:TRP:CD1	2.33	0.64
1:H:135:ASN:O	1:I:196:ARG:NH1	2.31	0.64
2:B:98:VAL:HA	2:B:101:PHE:CD2	2.33	0.63
2:C:42:PHE:O	2:C:44:PRO:HD3	1.97	0.63
2:D:17:TYR:CE1	2:D:59:PRO:HA	2.33	0.63
1:J:448:GLU:OE1	1:J:449:ALA:N	2.31	0.63
1:F:348:GLU:OE1	1:H:652:ARG:NH2	2.32	0.63
3:E:84:ILE:CG2	3:E:88:TRP:HE1	2.11	0.63
1:G:680:LEU:HD13	1:G:691:LEU:HD21	1.81	0.63
2:D:18:TRP:CZ3	2:D:55:LEU:O	2.51	0.63
1:F:342:GLU:N	1:F:342:GLU:OE1	2.32	0.63
2:C:47:ASN:OD1	2:C:78:LEU:HD21	1.99	0.63
2:C:136:ILE:HG21	2:C:141:PHE:HE2	1.63	0.62
2:D:31:LYS:NZ	2:D:78:LEU:HD23	2.14	0.62
3:E:835:LYS:HA	3:E:838:PHE:HD2	1.62	0.62
1:A:139:MET:SD	1:A:139:MET:N	2.72	0.62
1:J:77:PHE:N	1:J:198:SER:O	2.32	0.62
1:I:348:GLU:OE2	1:J:652:ARG:NH2	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:123:LEU:HB2	3:E:124:PRO:HD3	1.80	0.62
3:E:838:PHE:HA	3:E:841:LEU:CB	2.29	0.62
2:D:115:ASN:OD1	2:D:117:GLN:OE1	2.17	0.61
2:C:26:PHE:CE2	2:C:125:LEU:HD23	2.35	0.61
2:C:98:VAL:HA	2:C:101:PHE:CD2	2.36	0.61
2:D:66:LEU:CD2	2:D:70:ILE:CD1	2.79	0.61
1:H:387:LEU:HD11	1:H:505:PRO:HB2	1.83	0.61
2:C:136:ILE:HG21	2:C:141:PHE:CE2	2.36	0.61
2:D:66:LEU:CD2	2:D:70:ILE:HD12	2.31	0.61
3:E:117:HIS:HA	3:E:120:MET:HE2	1.81	0.60
3:E:297:LEU:HD11	3:E:326:VAL:CG1	2.32	0.60
3:E:631:VAL:HG21	3:E:829:PHE:CD2	2.35	0.60
1:A:438:LEU:HD11	1:A:472:PRO:HD2	1.82	0.60
1:H:114:ASN:ND2	1:H:201:ASP:OD1	2.34	0.60
2:D:13:SER:C	2:D:15:TRP:N	2.50	0.60
2:C:31:LYS:NZ	2:C:78:LEU:HD23	2.16	0.60
3:E:127:VAL:HA	3:E:130:LYS:HD2	1.82	0.60
1:J:230:THR:OG1	1:J:275:ARG:NH1	2.35	0.59
3:E:180:LEU:HD13	3:E:568:PRO:HG3	1.84	0.59
3:E:588:PHE:HB2	3:E:815:ILE:HD12	1.84	0.59
3:E:48:ILE:HG23	3:E:55:TRP:CE2	2.37	0.59
2:B:47:ASN:OD1	2:B:78:LEU:HD21	2.03	0.59
2:B:114:ILE:HG23	2:B:119:ILE:HD11	1.84	0.59
3:E:376:TRP:HB2	3:E:386:MET:HE1	1.85	0.59
2:B:114:ILE:CG2	2:B:119:ILE:HD11	2.33	0.59
2:D:18:TRP:CH2	2:D:57:PRO:HD3	2.38	0.59
3:E:686:VAL:HG11	3:E:826:LEU:HB2	1.84	0.59
2:D:15:TRP:C	2:D:17:TYR:N	2.59	0.58
2:B:137:ARG:HD2	3:E:7:TRP:O	2.03	0.58
3:E:88:TRP:CE3	3:E:853:PRO:HG3	2.37	0.58
2:C:134:GLN:NE2	3:E:52:HIS:NE2	2.51	0.58
1:A:620:LEU:HD13	1:A:627:TRP:CZ2	2.38	0.58
1:J:428:ARG:NH2	1:J:487:GLU:OE1	2.35	0.58
2:D:91:ILE:O	2:D:95:GLY:N	2.37	0.58
3:E:48:ILE:HG21	3:E:55:TRP:CE2	2.39	0.58
1:F:297:LYS:O	1:F:320:ARG:NH2	2.37	0.58
1:A:619:LEU:C	1:A:620:LEU:HD12	2.29	0.58
3:E:133:HIS:HA	3:E:136:GLU:HB3	1.86	0.57
1:A:109:THR:HG1	1:A:203:THR:HG1	0.89	0.57
2:D:24:TRP:CA	2:D:27:TYR:HD2	2.05	0.57
3:E:68:HIS:C	3:E:81:ARG:NH2	2.60	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:37:GLY:O	3:E:41:MET:HG2	2.04	0.57
2:D:136:ILE:HG21	2:D:141:PHE:HE2	1.69	0.57
1:G:406:ARG:NH2	1:G:737:TRP:C	2.62	0.57
3:E:10:ILE:CD1	3:E:13:VAL:HG23	2.28	0.57
2:C:114:ILE:CG2	2:C:119:ILE:HD11	2.35	0.56
2:B:24:TRP:CA	2:B:27:TYR:HD2	2.07	0.56
2:B:66:LEU:CD2	2:B:70:ILE:HD12	2.35	0.56
2:B:66:LEU:CD2	2:B:70:ILE:CD1	2.83	0.56
2:C:44:PRO:CG	2:C:153:THR:HG21	2.23	0.56
1:H:230:THR:O	1:H:275:ARG:NH1	2.38	0.56
1:J:619:LEU:HD23	1:J:620:LEU:N	2.19	0.56
2:C:18:TRP:CZ3	2:C:55:LEU:O	2.58	0.56
2:B:39:TYR:CE2	2:B:118:MET:CE	2.89	0.56
1:G:593:THR:O	1:G:597:LYS:NZ	2.37	0.56
1:G:761:VAL:CG2	3:E:155:ILE:HG21	2.36	0.56
1:G:764:ARG:O	1:G:768:ILE:HG13	2.06	0.56
1:F:124:LEU:O	1:F:128:SER:OG	2.18	0.56
3:E:832:SER:HB3	3:E:834:VAL:HG23	1.88	0.55
1:H:686:ARG:NH1	1:H:689:GLU:OE1	2.39	0.55
2:D:114:ILE:CG2	2:D:119:ILE:HD11	2.37	0.55
3:E:826:LEU:O	3:E:830:ALA:HB2	2.06	0.55
3:E:84:ILE:HG23	3:E:88:TRP:HE1	1.70	0.55
3:E:633:TRP:HZ3	3:E:831:PRO:HD3	1.72	0.55
2:D:66:LEU:HD21	2:D:70:ILE:CD1	2.37	0.55
3:E:297:LEU:HD11	3:E:326:VAL:HG12	1.87	0.55
2:B:148:TRP:NE1	2:B:152:LEU:HD11	2.22	0.55
1:H:712:ARG:NH1	1:H:717:ASN:OD1	2.37	0.55
3:E:10:ILE:HD13	3:E:12:PRO:CG	2.26	0.55
3:E:115:ARG:HA	3:E:118:GLN:HB3	1.89	0.55
2:D:66:LEU:HD23	2:D:70:ILE:CD1	2.36	0.54
2:D:47:ASN:OD1	2:D:78:LEU:CD2	2.54	0.54
3:E:822:GLY:HA2	3:E:825:HIS:HB2	1.87	0.54
1:G:403:TYR:CE2	1:G:404:LEU:O	2.60	0.54
1:G:772:ARG:O	1:G:775:ASN:HB2	2.06	0.54
2:C:114:ILE:HG23	2:C:119:ILE:HD11	1.89	0.54
3:E:0:MET:SD	3:E:35:THR:HG22	2.47	0.54
2:B:136:ILE:HG21	2:B:141:PHE:HE2	1.72	0.54
3:E:150:LEU:O	3:E:154:ILE:N	2.41	0.54
2:D:133:SER:OG	2:D:138:ILE:HD12	2.07	0.54
3:E:138:LYS:O	3:E:140:LEU:N	2.40	0.54
3:E:11:PRO:N	3:E:12:PRO:HD2	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:835:LYS:HA	3:E:838:PHE:CD2	2.42	0.54
1:J:426:SER:HB3	1:J:489:MET:HE2	1.90	0.54
1:G:729:HIS:O	1:G:730:LEU:CB	2.54	0.54
1:H:609:ASP:OD2	1:H:610:LYS:N	2.41	0.53
1:G:288:ASP:OD1	1:G:289:PHE:N	2.42	0.53
2:C:107:ILE:O	2:C:111:THR:HG23	2.08	0.53
1:A:485:ASP:OD2	1:A:485:ASP:N	2.41	0.53
3:E:838:PHE:HD1	3:E:841:LEU:HD22	1.74	0.53
3:E:142:HIS:O	3:E:143:LEU:HG	2.08	0.53
2:C:106:LEU:O	2:C:110:VAL:HG23	2.09	0.53
2:D:42:PHE:CE1	2:D:44:PRO:HA	2.43	0.53
3:E:3:ILE:O	3:E:7:TRP:CD1	2.52	0.53
3:E:39:PHE:CE1	3:E:43:LEU:HD11	2.44	0.53
1:A:112:MET:N	1:A:201:ASP:O	2.42	0.53
1:J:567:LEU:HD23	1:J:568:LEU:HD12	1.91	0.53
1:G:374:GLU:OE2	1:G:374:GLU:N	2.40	0.53
3:E:824:ARG:O	3:E:828:GLU:N	2.40	0.53
2:D:17:TYR:CG	2:D:59:PRO:HA	2.43	0.53
2:B:106:LEU:O	2:B:110:VAL:HG23	2.09	0.52
3:E:68:HIS:CD2	3:E:81:ARG:NH2	2.77	0.52
1:I:222:ASP:OD2	1:I:224:SER:OG	2.17	0.52
2:B:66:LEU:HD21	2:B:70:ILE:CD1	2.38	0.52
3:E:631:VAL:HG21	3:E:829:PHE:HB2	1.90	0.52
1:A:108:VAL:HG21	1:A:164:ILE:HG21	1.91	0.52
2:C:98:VAL:HA	2:C:101:PHE:CE2	2.45	0.52
3:E:48:ILE:HG23	3:E:55:TRP:NE1	2.25	0.52
1:H:532:LEU:N	1:H:706:GLY:O	2.41	0.52
1:H:619:LEU:HD21	1:H:710:VAL:HG22	1.92	0.52
1:G:539:GLY:O	1:G:543:SER:OG	2.24	0.52
3:E:9:LEU:HD13	3:E:17:LEU:HD12	1.91	0.52
3:E:462:LEU:HD11	3:E:516:LEU:HD11	1.91	0.52
1:G:526:PHE:HB3	1:G:738:TYR:CZ	2.44	0.52
2:C:148:TRP:NE1	2:C:152:LEU:HD11	2.25	0.52
1:I:306:HIS:HB2	1:I:312:VAL:HG13	1.93	0.51
2:C:91:ILE:O	2:C:95:GLY:N	2.44	0.51
2:D:114:ILE:HG23	2:D:119:ILE:HD11	1.93	0.51
1:G:190:LEU:HD23	1:G:190:LEU:H	1.76	0.51
1:J:145:THR:OG1	1:J:146:LYS:N	2.43	0.51
1:G:222:ASP:OD1	1:G:222:ASP:N	2.41	0.51
2:D:31:LYS:NZ	2:D:78:LEU:HD22	2.26	0.50
3:E:68:HIS:CD2	3:E:81:ARG:HH21	2.28	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:GLN:O	1:A:623:ALA:HB3	2.11	0.50
1:H:67:ASN:OD1	1:H:68:GLY:N	2.43	0.50
1:I:120:SER:OG	1:I:191:TRP:O	2.22	0.50
1:G:340:ARG:HD3	1:A:661:MET:HE3	1.93	0.50
1:F:665:ILE:HG22	1:F:708:VAL:HG23	1.93	0.50
1:G:529:MET:SD	1:G:727:VAL:HG11	2.52	0.50
1:F:496:SER:OG	1:F:497:VAL:N	2.44	0.50
1:I:213:LEU:N	1:I:341:GLY:O	2.43	0.50
2:B:115:ASN:OD1	2:B:117:GLN:HB2	2.12	0.50
3:E:48:ILE:HG21	3:E:55:TRP:CZ2	2.47	0.50
2:C:24:TRP:CA	2:C:27:TYR:HD2	2.09	0.50
2:B:40:LEU:HD23	2:B:41:ASN:C	2.37	0.50
2:B:98:VAL:HA	2:B:101:PHE:CE2	2.47	0.50
1:J:422:PRO:O	1:J:447:GLN:NE2	2.45	0.49
1:G:397:ASN:N	1:G:397:ASN:OD1	2.45	0.49
3:E:821:ARG:HG2	3:E:825:HIS:CD2	2.47	0.49
1:A:619:LEU:HB3	1:A:665:ILE:HD11	1.94	0.49
3:E:121:ASN:O	3:E:124:PRO:HD2	2.12	0.49
1:I:351:PRO:HA	1:J:651:THR:HG22	1.94	0.49
1:I:590:ASP:OD1	1:I:592:SER:N	2.38	0.49
2:B:64:HIS:O	2:B:68:HIS:ND1	2.36	0.49
2:D:31:LYS:HZ1	2:D:78:LEU:HD23	1.76	0.49
3:E:633:TRP:CZ3	3:E:831:PRO:HD3	2.47	0.49
1:A:654:THR:C	1:A:655:LEU:HD12	2.38	0.49
1:G:134:LEU:HD12	1:G:170:VAL:HG22	1.95	0.49
1:A:218:VAL:N	1:A:219:PRO:CD	2.76	0.49
1:F:683:ASP:OD1	1:F:683:ASP:N	2.46	0.49
1:J:405:MET:SD	1:J:405:MET:N	2.84	0.49
2:B:44:PRO:HB2	2:B:150:ASN:OD1	2.13	0.48
2:D:136:ILE:CG2	2:D:141:PHE:HE2	2.26	0.48
2:D:148:TRP:NE1	2:D:152:LEU:HD11	2.28	0.48
3:E:834:VAL:HA	3:E:837:ILE:HD12	1.95	0.48
3:E:0:MET:SD	3:E:35:THR:HG21	2.53	0.48
3:E:68:HIS:CD2	3:E:69:ILE:HG13	2.48	0.48
3:E:69:ILE:HG21	3:E:82:TYR:CZ	2.48	0.48
1:G:742:ASN:OD1	1:G:743:HIS:CD2	2.67	0.48
3:E:2:SER:O	3:E:4:LEU:N	2.46	0.48
1:I:643:ASP:N	1:I:643:ASP:OD2	2.45	0.48
3:E:819:GLY:O	3:E:823:TYR:N	2.35	0.48
2:D:44:PRO:CG	2:D:153:THR:HG21	2.31	0.48
3:E:828:GLU:O	3:E:829:PHE:CG	2.67	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ARG:NH2	1:A:359:ASP:OD2	2.40	0.48
1:F:334:GLN:NE2	1:H:651:THR:HG21	2.28	0.48
2:D:40:LEU:HD21	2:D:82:ASP:CB	2.16	0.48
3:E:818:LEU:O	3:E:822:GLY:N	2.43	0.48
2:D:106:LEU:O	2:D:110:VAL:HG23	2.13	0.48
3:E:68:HIS:HD2	3:E:81:ARG:NH2	2.11	0.48
3:E:837:ILE:O	3:E:841:LEU:N	2.45	0.48
2:B:47:ASN:OD1	2:B:78:LEU:CD2	2.61	0.47
2:D:107:ILE:O	2:D:111:THR:HG23	2.14	0.47
1:J:704:MET:HB3	1:J:716:ILE:HD12	1.96	0.47
3:E:289:VAL:HG22	3:E:361:CYS:HB2	1.95	0.47
1:J:458:VAL:HG23	1:J:459:LEU:N	2.29	0.47
2:D:18:TRP:CZ2	2:D:57:PRO:HD3	2.49	0.47
1:I:438:LEU:HD13	1:I:471:ILE:HG23	1.96	0.47
2:B:21:LEU:HD12	2:B:139:THR:HG23	1.96	0.47
2:C:115:ASN:OD1	2:C:117:GLN:HB2	2.15	0.47
1:I:112:MET:SD	1:I:156:GLN:NE2	2.88	0.47
1:J:529:MET:O	1:J:531:ASP:N	2.48	0.47
2:B:114:ILE:CG2	2:B:119:ILE:CD1	2.92	0.47
2:C:42:PHE:CE1	2:C:44:PRO:HA	2.50	0.47
3:E:690:VAL:HG21	3:E:825:HIS:ND1	2.30	0.47
1:J:683:ASP:N	1:J:683:ASP:OD1	2.46	0.47
1:G:761:VAL:HG21	3:E:155:ILE:CG2	2.43	0.47
2:B:107:ILE:O	2:B:111:THR:HG23	2.15	0.47
2:C:134:GLN:HE22	3:E:52:HIS:HE2	1.60	0.47
2:D:31:LYS:HE2	2:D:79:PHE:HD2	1.79	0.47
2:D:70:ILE:HG22	2:D:74:ILE:HD12	1.96	0.47
3:E:633:TRP:HH2	3:E:829:PHE:C	2.23	0.47
3:E:836:GLY:O	3:E:839:ARG:HB3	2.14	0.47
1:J:231:LEU:HD23	1:J:231:LEU:H	1.80	0.47
3:E:48:ILE:CG2	3:E:55:TRP:CZ2	2.98	0.47
1:F:99:GLU:OE2	1:F:169:ARG:NH1	2.46	0.47
2:B:70:ILE:O	2:B:73:PRO:HD2	2.15	0.47
1:I:365:ARG:NH2	1:I:367:ASP:OD2	2.48	0.47
1:G:136:ASP:O	1:A:86:SER:OG	2.26	0.47
3:E:84:ILE:HG22	3:E:88:TRP:CD1	2.50	0.47
1:F:425:ASP:HB2	1:F:489:MET:HE2	1.97	0.47
1:J:380:GLU:OE2	1:J:383:GLN:NE2	2.47	0.47
2:D:98:VAL:HA	2:D:101:PHE:CE2	2.50	0.46
2:C:19:ARG:C	2:C:20:GLY:O	2.57	0.46
2:D:72:LEU:HB3	2:D:73:PRO:HD3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:825:HIS:HD1	3:E:828:GLU:HG3	1.80	0.46
3:E:834:VAL:O	3:E:837:ILE:HB	2.15	0.46
2:D:13:SER:O	2:D:15:TRP:N	2.47	0.46
3:E:690:VAL:HG21	3:E:825:HIS:CG	2.51	0.46
3:E:825:HIS:HA	3:E:828:GLU:HB2	1.97	0.46
1:F:537:ASN:O	1:F:538:ALA:HB3	2.16	0.46
1:I:340:ARG:NE	1:J:657:SER:OG	2.48	0.46
2:C:70:ILE:HG22	2:C:74:ILE:HD12	1.97	0.46
3:E:833:SER:O	3:E:834:VAL:C	2.57	0.46
1:H:507:GLN:O	1:I:428:ARG:NH2	2.49	0.46
1:H:619:LEU:O	1:H:621:VAL:HG23	2.15	0.46
2:C:69:TRP:O	2:C:73:PRO:CD	2.63	0.46
2:D:129:TRP:CD1	2:D:138:ILE:HD13	2.31	0.46
3:E:845:VAL:HG12	3:E:845:VAL:O	2.16	0.46
1:F:529:MET:N	1:F:530:PRO:CD	2.79	0.46
1:G:760:TRP:CA	3:E:197:PHE:HE2	2.27	0.46
2:B:31:LYS:HZ1	2:B:78:LEU:HD22	1.78	0.46
3:E:108:GLY:O	3:E:112:ILE:HG13	2.16	0.46
3:E:130:LYS:O	3:E:134:LEU:HG	2.16	0.46
3:E:406:ARG:NH2	3:E:799:TRP:CH2	2.84	0.46
1:H:120:SER:HB3	1:H:123:LEU:HD13	1.97	0.46
1:J:259:GLY:O	1:J:263:GLN:NE2	2.49	0.46
2:B:44:PRO:HB2	2:B:150:ASN:CG	2.41	0.45
2:B:66:LEU:HD23	2:B:70:ILE:CD1	2.44	0.45
2:C:18:TRP:CH2	2:C:57:PRO:HD3	2.51	0.45
3:E:818:LEU:O	3:E:821:ARG:HB3	2.16	0.45
1:G:99:GLU:OE1	1:G:99:GLU:N	2.48	0.45
1:A:569:ASN:ND2	1:A:696:ASN:OD1	2.49	0.45
1:H:282:THR:O	1:H:282:THR:HG22	2.16	0.45
1:J:218:VAL:N	1:J:219:PRO:CD	2.79	0.45
1:H:166:ASP:OD1	1:H:167:PHE:N	2.49	0.45
1:J:133:TYR:O	1:J:170:VAL:HA	2.17	0.45
1:J:468:ASP:OD1	1:J:468:ASP:N	2.48	0.45
2:C:47:ASN:OD1	2:C:78:LEU:CD2	2.62	0.45
1:A:368:ARG:NH2	1:A:374:GLU:OE2	2.50	0.45
1:G:698:SER:OG	1:G:701:ARG:NH1	2.50	0.45
2:D:115:ASN:OD1	2:D:117:GLN:HB2	2.16	0.45
1:A:75:LEU:HD12	1:A:80:ILE:HD13	1.98	0.45
1:A:109:THR:O	1:A:110:LYS:C	2.60	0.45
1:A:334:GLN:NE2	1:F:651:THR:HG21	2.32	0.45
1:I:83:PRO:N	1:I:84:PRO:HD2	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:458:VAL:HG23	1:J:459:LEU:H	1.80	0.45
3:E:687:ALA:HA	3:E:825:HIS:CD2	2.52	0.45
1:I:268:LEU:HD23	1:I:268:LEU:H	1.82	0.45
2:C:72:LEU:N	2:C:73:PRO:HD2	2.32	0.45
1:A:274:ASP:OD1	1:A:274:ASP:N	2.50	0.45
1:F:601:ILE:HB	1:F:677:VAL:HG13	1.99	0.45
1:G:214:SER:OG	1:A:712:ARG:NH2	2.50	0.45
2:D:31:LYS:HZ3	2:D:78:LEU:CD2	2.30	0.45
1:A:683:ASP:OD1	1:A:683:ASP:N	2.50	0.45
1:I:330:LYS:NZ	1:I:583:ILE:O	2.50	0.45
3:E:151:ILE:HA	3:E:154:ILE:HB	1.98	0.44
3:E:311:LEU:HD22	3:E:347:ALA:HB2	1.99	0.44
1:I:500:CYS:O	1:J:495:GLY:N	2.42	0.44
1:J:102:MET:O	1:J:224:SER:OG	2.14	0.44
1:G:767:ARG:HG2	1:G:768:ILE:N	2.31	0.44
3:E:151:ILE:HD13	3:E:154:ILE:HD12	1.99	0.44
1:H:367:ASP:OD1	1:H:368:ARG:N	2.50	0.44
1:J:547:ASP:OD2	1:J:584:ASN:ND2	2.50	0.44
1:A:111:ALA:HA	1:A:202:LEU:HA	1.99	0.44
1:G:404:LEU:O	1:G:405:MET:HB2	2.17	0.44
2:B:136:ILE:CG2	2:B:141:PHE:HE2	2.30	0.44
1:F:181:VAL:HG13	1:F:182:CYS:N	2.32	0.44
1:I:99:GLU:N	1:I:99:GLU:OE1	2.51	0.44
1:G:770:SER:O	1:G:774:LEU:HG	2.17	0.44
2:B:91:ILE:O	2:B:95:GLY:N	2.50	0.44
3:E:844:LEU:O	3:E:848:VAL:HG23	2.17	0.44
3:E:650:VAL:HG13	3:E:672:MET:HE1	1.99	0.44
2:C:72:LEU:HB3	2:C:73:PRO:HD3	1.99	0.43
3:E:406:ARG:HH12	3:E:702:GLU:HB2	1.83	0.43
1:A:112:MET:O	1:A:201:ASP:N	2.46	0.43
1:J:83:PRO:N	1:J:84:PRO:HD2	2.32	0.43
2:B:148:TRP:HE1	2:B:152:LEU:HD11	1.84	0.43
2:D:136:ILE:HG21	2:D:141:PHE:CE2	2.53	0.43
1:A:108:VAL:HG11	1:A:164:ILE:CD1	2.49	0.43
1:G:263:GLN:N	1:G:263:GLN:OE1	2.51	0.43
1:G:498:ASP:OD1	1:G:498:ASP:N	2.52	0.43
1:G:769:ILE:HA	1:G:772:ARG:HD2	2.01	0.43
2:B:70:ILE:C	2:B:73:PRO:HD2	2.44	0.43
3:E:130:LYS:O	3:E:134:LEU:N	2.44	0.43
3:E:48:ILE:CG2	3:E:55:TRP:NE1	2.82	0.43
3:E:84:ILE:CG2	3:E:88:TRP:NE1	2.79	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:70:ILE:C	2:C:73:PRO:HD2	2.44	0.43
3:E:11:PRO:N	3:E:12:PRO:CD	2.82	0.43
1:A:202:LEU:HD23	1:A:202:LEU:H	1.82	0.43
1:F:282:THR:HG22	1:F:325:LEU:HD11	2.00	0.43
2:B:29:LEU:HB3	2:B:125:LEU:HD21	1.99	0.43
3:E:180:LEU:HD13	3:E:568:PRO:CG	2.48	0.43
3:E:739:ILE:CG2	3:E:762:VAL:HG21	2.48	0.43
1:H:657:SER:OG	1:H:658:SER:N	2.51	0.43
1:I:348:GLU:O	1:J:654:THR:OG1	2.37	0.43
2:B:69:TRP:O	2:B:73:PRO:CD	2.67	0.43
2:B:72:LEU:HB3	2:B:73:PRO:HD3	2.01	0.43
2:C:39:TYR:CE2	2:C:118:MET:HE2	2.54	0.43
2:C:70:ILE:O	2:C:73:PRO:HD2	2.18	0.43
2:D:72:LEU:N	2:D:73:PRO:HD2	2.33	0.43
1:I:80:ILE:HD12	1:I:98:ILE:HD12	2.00	0.43
1:J:218:VAL:HG12	1:J:219:PRO:HD3	2.00	0.43
1:G:730:LEU:CB	1:G:731:PRO:CD	2.81	0.42
3:E:68:HIS:HB2	3:E:81:ARG:HH21	1.84	0.42
3:E:827:ALA:HB2	3:E:838:PHE:CD2	2.54	0.42
1:A:103:ARG:O	1:A:104:SER:OG	2.27	0.42
1:H:371:THR:OG1	1:H:374:GLU:OE1	2.32	0.42
2:B:21:LEU:HB2	2:B:25:ASN:OD1	2.19	0.42
2:C:39:TYR:CE2	2:C:118:MET:CE	3.02	0.42
1:F:539:GLY:O	1:F:543:SER:OG	2.32	0.42
1:A:165:SER:OG	1:A:166:ASP:N	2.53	0.42
1:F:75:LEU:HD12	1:F:80:ILE:HG21	2.02	0.42
1:I:609:ASP:OD1	1:I:609:ASP:N	2.52	0.42
2:D:40:LEU:HD23	2:D:41:ASN:C	2.44	0.42
2:D:69:TRP:O	2:D:73:PRO:CD	2.68	0.42
1:A:371:THR:HG22	1:A:517:THR:HG22	2.02	0.42
1:H:82:PRO:C	1:H:84:PRO:CD	2.91	0.42
1:F:77:PHE:O	1:F:81:ALA:HB3	2.20	0.42
1:F:334:GLN:HE22	1:H:651:THR:HG21	1.83	0.42
1:I:312:VAL:HG13	1:I:312:VAL:O	2.19	0.42
1:J:356:LYS:NZ	1:J:367:ASP:OD1	2.53	0.42
1:J:619:LEU:CD1	1:J:710:VAL:HG12	2.49	0.42
1:J:622:GLN:O	1:J:623:ALA:HB3	2.19	0.42
2:C:65:ARG:O	2:C:69:TRP:HD1	2.01	0.42
1:A:539:GLY:O	1:A:543:SER:OG	2.38	0.42
3:E:764:ARG:CZ	3:E:766:MET:SD	3.08	0.42
3:E:833:SER:O	3:E:836:GLY:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:PRO:N	1:G:84:PRO:HD2	2.35	0.42
1:G:245:GLN:NE2	1:G:585:LEU:O	2.50	0.42
2:C:135:TRP:HZ2	2:D:15:TRP:CH2	2.38	0.42
2:D:15:TRP:HA	2:D:18:TRP:HD1	1.84	0.42
3:E:406:ARG:NH2	3:E:799:TRP:CZ2	2.87	0.42
1:I:234:VAL:HG13	1:I:234:VAL:O	2.20	0.42
1:I:498:ASP:OD1	1:I:499:ASN:N	2.53	0.42
2:B:72:LEU:N	2:B:73:PRO:HD2	2.35	0.42
2:C:31:LYS:HE2	2:C:79:PHE:HD2	1.85	0.42
3:E:69:ILE:HG21	3:E:82:TYR:CE2	2.55	0.42
3:E:242:TYR:CD1	3:E:536:PRO:HG2	2.55	0.42
3:E:838:PHE:CA	3:E:841:LEU:HB3	2.43	0.42
3:E:78:ASP:N	3:E:79:PRO:CD	2.83	0.42
2:D:70:ILE:O	2:D:73:PRO:HD2	2.20	0.41
3:E:131:THR:O	3:E:134:LEU:HB2	2.21	0.41
3:E:633:TRP:CH2	3:E:829:PHE:C	2.98	0.41
3:E:847:TRP:O	3:E:850:SER:HB2	2.21	0.41
1:H:355:ARG:NH2	1:H:359:ASP:OD1	2.53	0.41
1:H:442:ASN:OD1	1:H:443:LEU:N	2.53	0.41
3:E:687:ALA:HB2	3:E:822:GLY:CA	2.50	0.41
1:A:405:MET:SD	1:A:641:VAL:HG22	2.60	0.41
2:B:50:PHE:CE1	2:B:54:LEU:HD11	2.55	0.41
2:B:58:LEU:O	2:B:64:HIS:NE2	2.53	0.41
2:C:114:ILE:CG2	2:C:119:ILE:CD1	2.97	0.41
2:C:149:LEU:O	2:C:153:THR:HG23	2.21	0.41
3:E:633:TRP:HH2	3:E:830:ALA:N	2.19	0.41
3:E:845:VAL:O	3:E:849:VAL:HG23	2.20	0.41
1:G:406:ARG:HH22	1:G:738:TYR:N	2.15	0.41
3:E:147:ALA:O	3:E:151:ILE:HG12	2.19	0.41
3:E:633:TRP:HH2	3:E:830:ALA:CA	2.33	0.41
1:H:385:SER:OG	1:H:386:GLY:N	2.51	0.41
2:B:39:TYR:CD2	2:B:118:MET:CE	3.04	0.41
3:E:84:ILE:C	3:E:88:TRP:HD1	2.26	0.41
3:E:631:VAL:CG2	3:E:829:PHE:HD2	2.32	0.41
3:E:833:SER:O	3:E:837:ILE:N	2.45	0.41
2:B:42:PHE:CE1	2:B:44:PRO:HA	2.55	0.41
2:D:66:LEU:CD2	2:D:70:ILE:HD11	2.43	0.41
3:E:833:SER:O	3:E:837:ILE:HG13	2.21	0.41
1:A:218:VAL:HG22	1:A:219:PRO:HD3	2.03	0.41
1:H:508:ASN:OD1	1:H:508:ASN:N	2.53	0.41
1:J:410:ILE:HD12	1:J:518:ILE:HD11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:LYS:HZ3	2:B:78:LEU:HD23	1.83	0.41
2:D:26:PHE:CE2	2:D:126:LEU:HA	2.56	0.41
3:E:452:GLU:CD	3:E:463:ARG:HH22	2.29	0.41
2:B:83:THR:HG22	2:B:84:TRP:N	2.36	0.41
1:J:711:ILE:HD12	1:J:716:ILE:HG22	2.03	0.41
1:I:347:ASN:ND2	1:J:625:GLU:OE1	2.48	0.40
1:I:496:SER:OG	1:I:497:VAL:N	2.54	0.40
1:J:456:ILE:N	1:J:457:PRO:CD	2.84	0.40
2:B:39:TYR:CD2	2:B:118:MET:HE1	2.56	0.40
3:E:91:ILE:HG22	3:E:92:GLY:N	2.36	0.40
2:B:26:PHE:CE2	2:B:126:LEU:HA	2.56	0.40
1:F:374:GLU:OE2	1:F:374:GLU:N	2.53	0.40
1:F:442:ASN:OD1	1:F:443:LEU:N	2.54	0.40
1:H:102:MET:O	1:H:224:SER:OG	2.30	0.40
1:G:116:GLU:O	1:G:195:GLY:N	2.54	0.40
2:D:18:TRP:CE3	2:D:55:LEU:O	2.74	0.40
3:E:588:PHE:CB	3:E:815:ILE:HD12	2.51	0.40
1:A:108:VAL:HG11	1:A:164:ILE:HD13	2.02	0.40
1:A:617:ILE:O	1:A:617:ILE:HG23	2.22	0.40
1:J:299:PRO:HB3	1:J:328:ALA:HB2	2.04	0.40
2:B:134:GLN:NE2	2:C:18:TRP:NE1	2.55	0.40
2:C:14:LEU:HA	2:C:17:TYR:HD2	1.85	0.40
2:D:70:ILE:C	2:D:73:PRO:HD2	2.46	0.40
3:E:844:LEU:O	3:E:847:TRP:HB3	2.21	0.40
1:H:650:GLU:HG2	1:H:651:THR:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	641/763 (84%)	611 (95%)	30 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	643/763 (84%)	622 (97%)	21 (3%)	0	100	100
1	G	658/763 (86%)	631 (96%)	23 (4%)	4 (1%)	22	58
1	H	641/763 (84%)	620 (97%)	21 (3%)	0	100	100
1	I	642/763 (84%)	625 (97%)	17 (3%)	0	100	100
1	J	662/763 (87%)	636 (96%)	26 (4%)	0	100	100
2	B	135/567 (24%)	131 (97%)	2 (2%)	2 (2%)	8	40
2	C	140/567 (25%)	136 (97%)	1 (1%)	3 (2%)	5	33
2	D	142/567 (25%)	136 (96%)	5 (4%)	1 (1%)	19	55
3	E	841/887 (95%)	816 (97%)	18 (2%)	7 (1%)	16	53
All	All	5145/7166 (72%)	4964 (96%)	164 (3%)	17 (0%)	38	71

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	730	LEU
1	G	732	TRP
2	D	14	LEU
3	E	3	ILE
3	E	139	GLU
3	E	851	PHE
1	G	731	PRO
2	C	20	GLY
3	E	141	GLY
3	E	143	LEU
1	G	729	HIS
2	B	22	SER
2	C	21	LEU
2	C	22	SER
2	B	20	GLY
3	E	91	ILE
3	E	1	GLY

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	557/657 (85%)	551 (99%)	6 (1%)	70 80
1	F	558/657 (85%)	557 (100%)	1 (0%)	92 93
1	G	574/657 (87%)	571 (100%)	3 (0%)	86 89
1	H	556/657 (85%)	554 (100%)	2 (0%)	89 91
1	I	557/657 (85%)	550 (99%)	7 (1%)	65 77
1	J	573/657 (87%)	569 (99%)	4 (1%)	81 86
2	B	118/480 (25%)	118 (100%)	0	100 100
2	C	123/480 (26%)	122 (99%)	1 (1%)	79 84
2	D	125/480 (26%)	125 (100%)	0	100 100
3	E	729/767 (95%)	718 (98%)	11 (2%)	60 75
All	All	4470/6149 (73%)	4435 (99%)	35 (1%)	77 84

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	394	VAL
1	G	730	LEU
1	G	767	ARG
2	C	125	LEU
3	E	0	MET
3	E	72	SER
3	E	95	ARG
3	E	139	GLU
3	E	154	ILE
3	E	455	THR
3	E	585	ARG
3	E	609	LEU
3	E	709	ILE
3	E	820	PHE
3	E	823	TYR
1	A	182	CYS
1	A	268	LEU
1	A	318	PHE
1	A	347	ASN
1	A	619	LEU
1	A	641	VAL
1	F	282	THR
1	H	500	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	724	VAL
1	I	118	THR
1	I	141	VAL
1	I	153	THR
1	I	168	ASN
1	I	396	LEU
1	I	430	ASP
1	I	710	VAL
1	J	172	LEU
1	J	349	VAL
1	J	462	LEU
1	J	618	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	499	ASN
1	G	622	GLN
1	G	674	GLN
1	G	743	HIS
2	B	43	HIS
2	B	134	GLN
2	C	43	HIS
2	C	134	GLN
2	D	43	HIS
3	E	68	HIS
3	E	117	HIS
3	E	121	ASN
3	E	678	ASN
3	E	734	ASN
1	A	270	ASN
1	A	293	HIS
1	A	327	GLN
1	A	383	GLN
1	F	327	GLN
1	F	336	ASN
1	F	397	ASN
1	H	327	GLN
1	H	436	GLN
1	I	156	GLN
1	I	309	ASN
1	I	480	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	293	HIS
1	J	309	ASN
1	J	439	GLN
1	J	480	ASN
1	J	508	ASN

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.

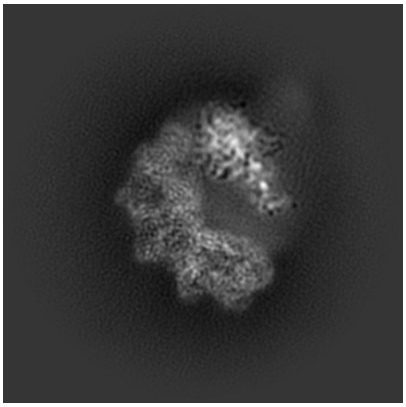
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44359. These allow visual inspection of the internal detail of the map and identification of artifacts.

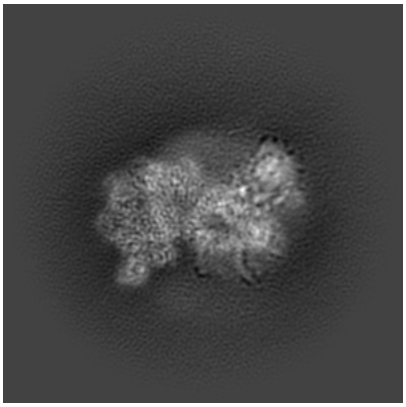
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

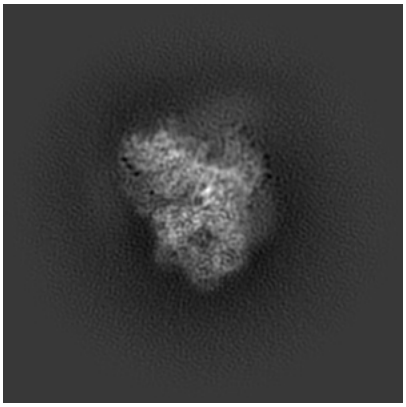
6.1.1 Primary map



X



Y

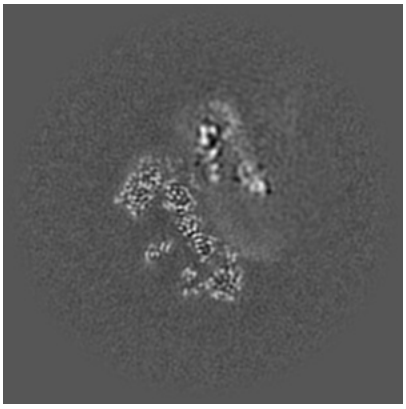


Z

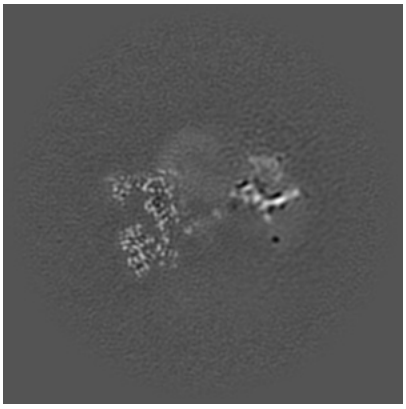
The images above show the map projected in three orthogonal directions.

6.2 Central slices

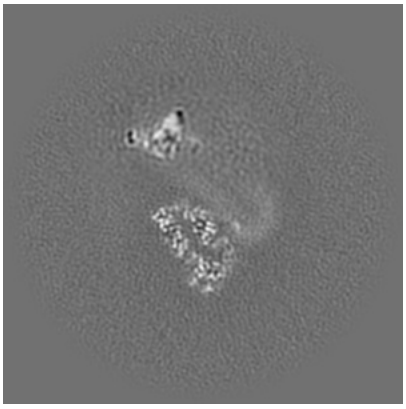
6.2.1 Primary map



X Index: 180



Y Index: 180

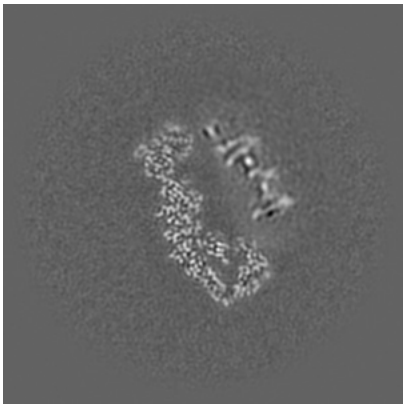


Z Index: 180

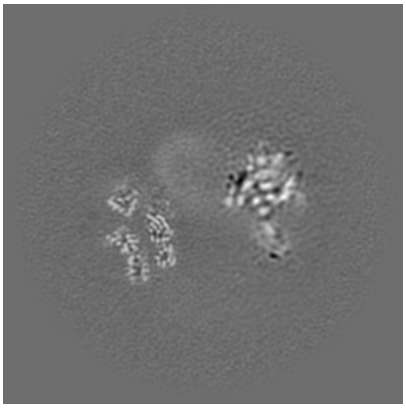
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

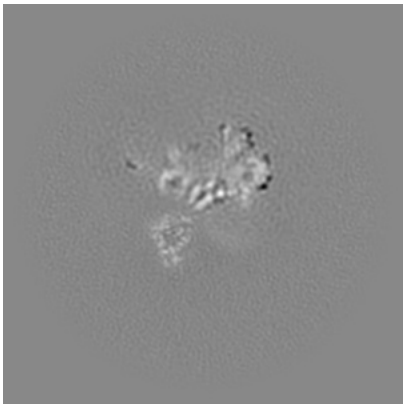
6.3.1 Primary map



X Index: 150



Y Index: 191

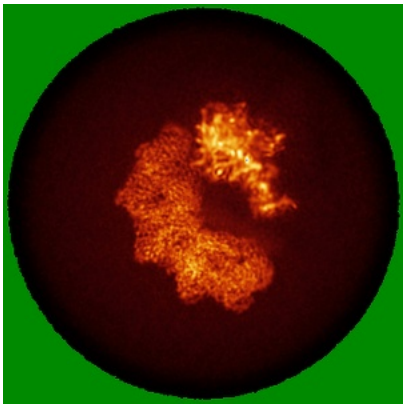


Z Index: 234

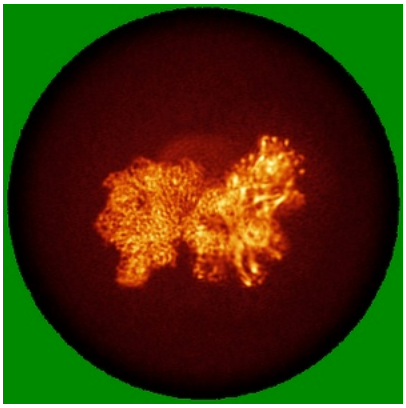
The images above show the largest variance slices of the map in three orthogonal directions.

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

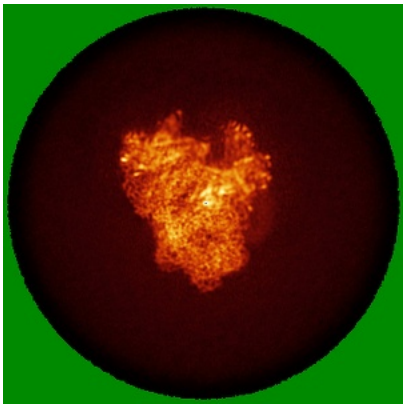
6.4.1 Primary map



X



Y



Z

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 7.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

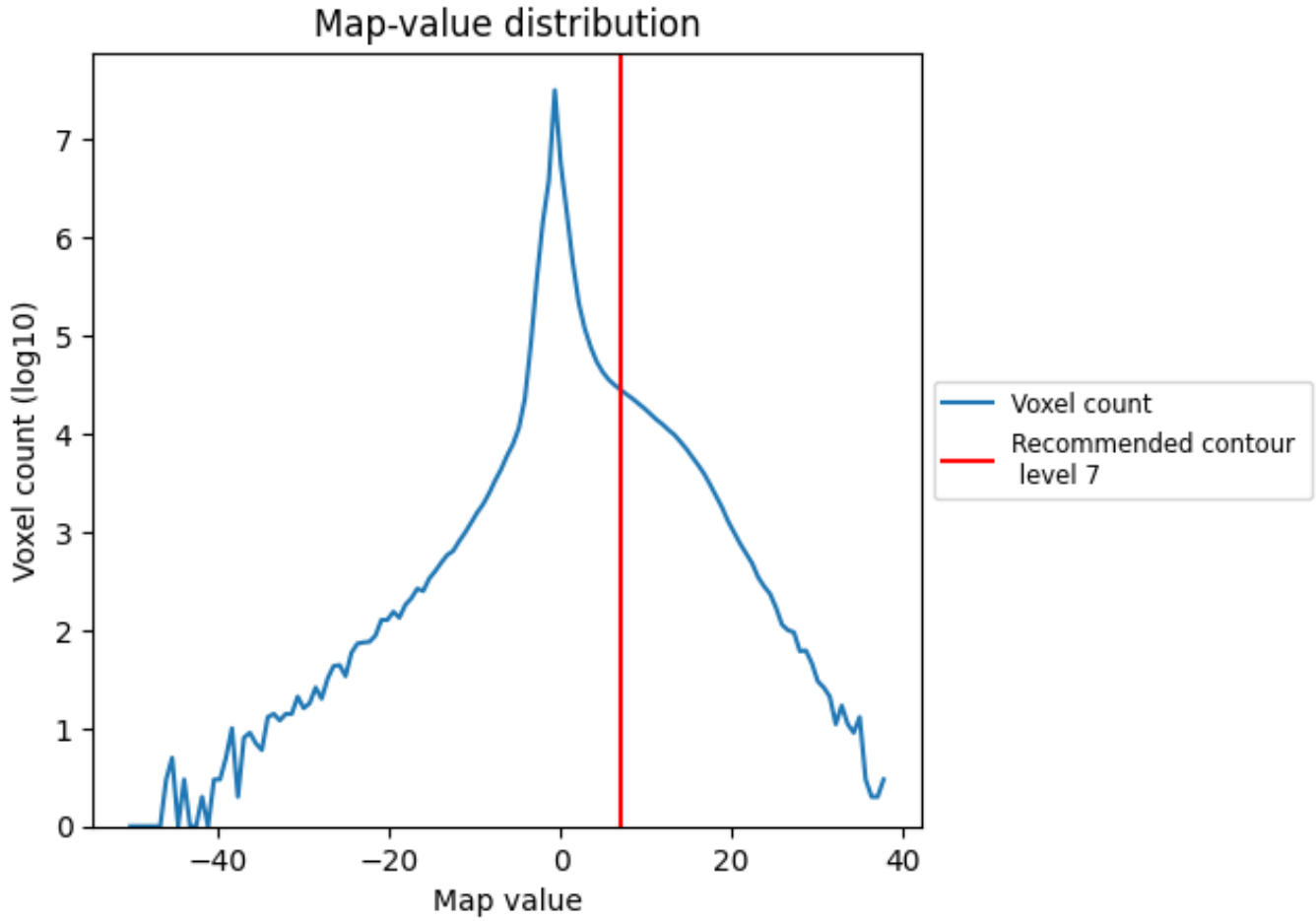
6.6 Mask visualisation (i)

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

7 Map analysis

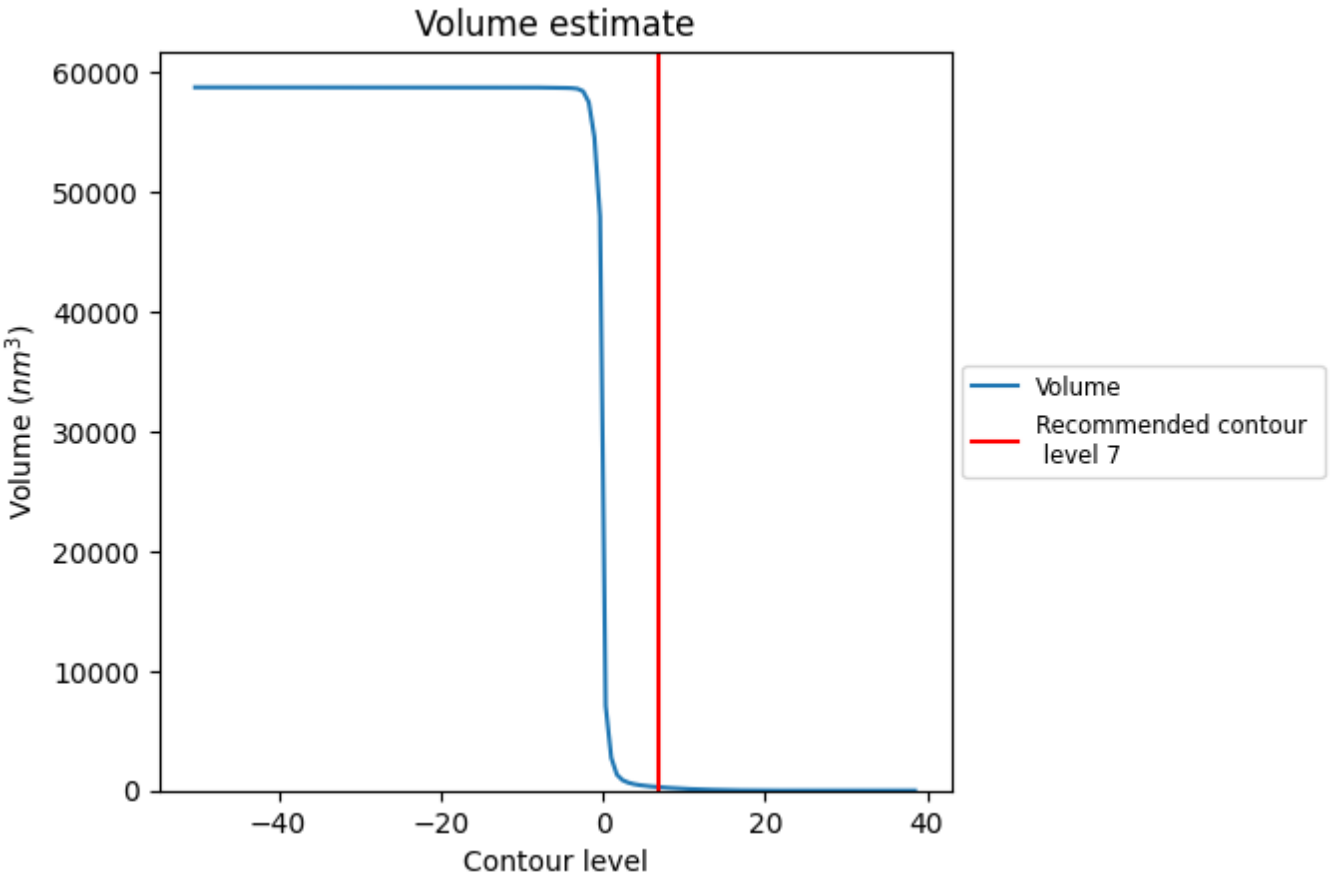
This section contains the results of statistical analysis of the map.

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.

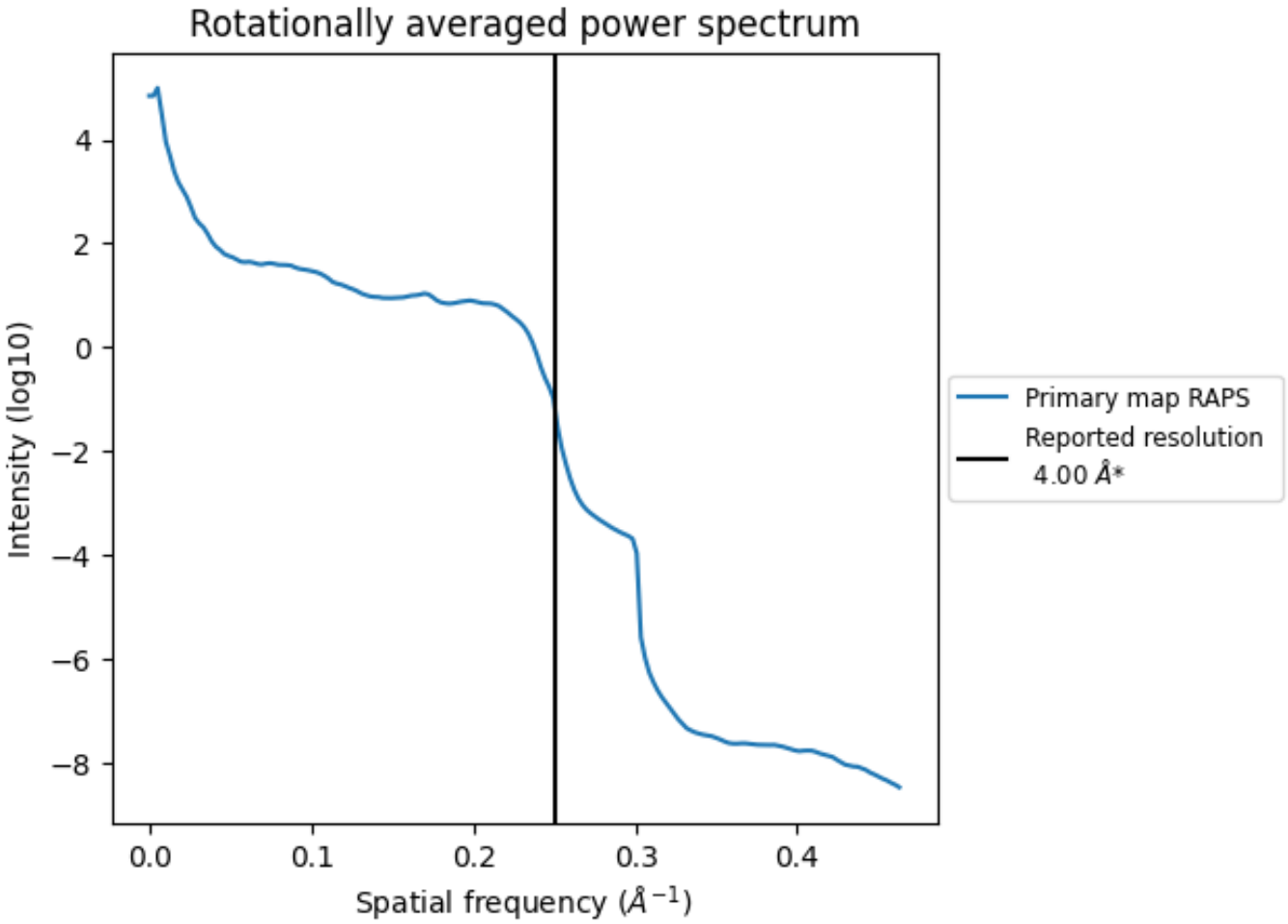
7.2 Volume estimate



The volume at the recommended contour level is 282 nm^3; this corresponds to an approximate mass of 255 kDa.

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

7.3 Rotationally averaged power spectrum (i)

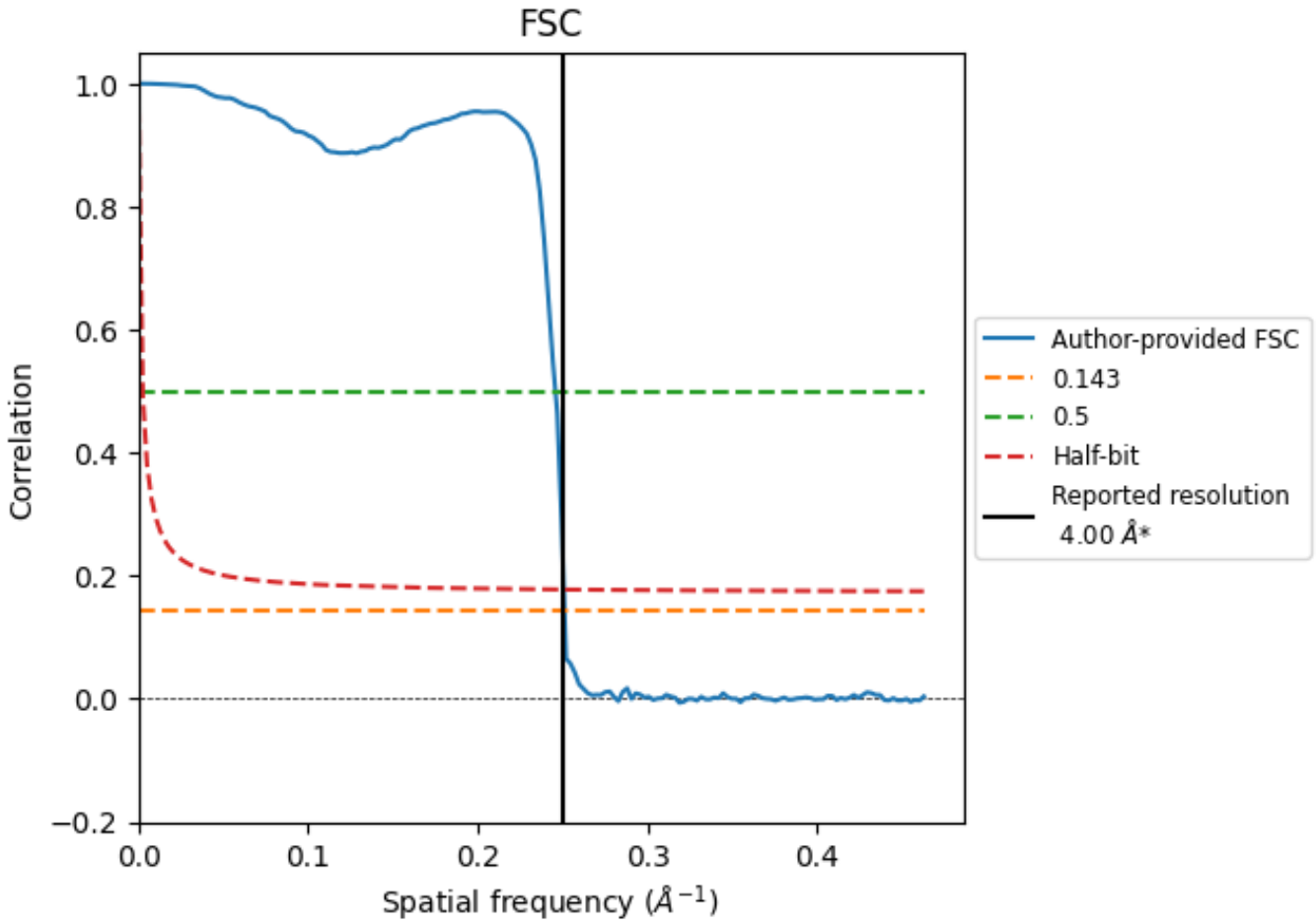


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

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 0.250 Å^{-1}

8.2 Resolution estimates (i)

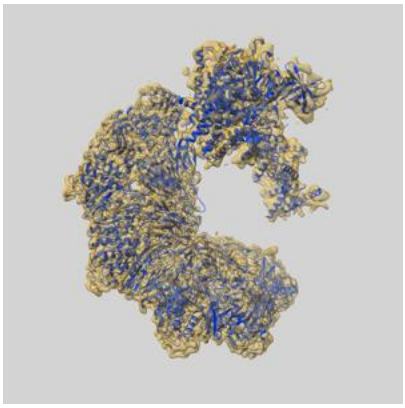
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.98	4.07	3.99
Unmasked-calculated*	-	-	-

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

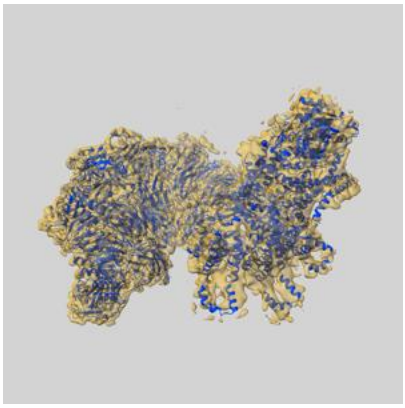
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44359 and PDB model 9B8V. Per-residue inclusion information can be found in section 3 on page 8.

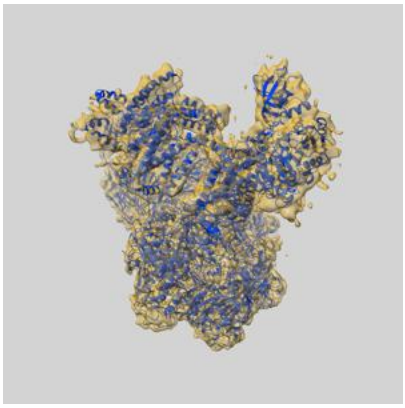
9.1 Map-model overlay



X



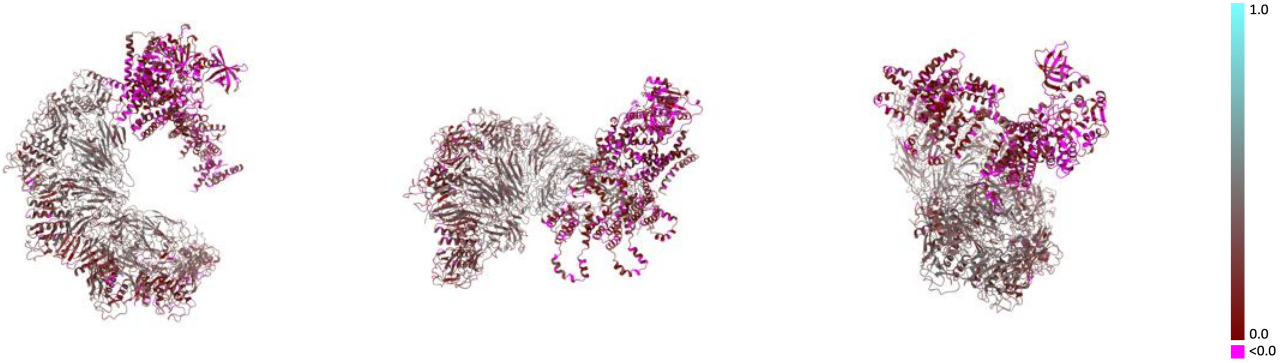
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.0 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.

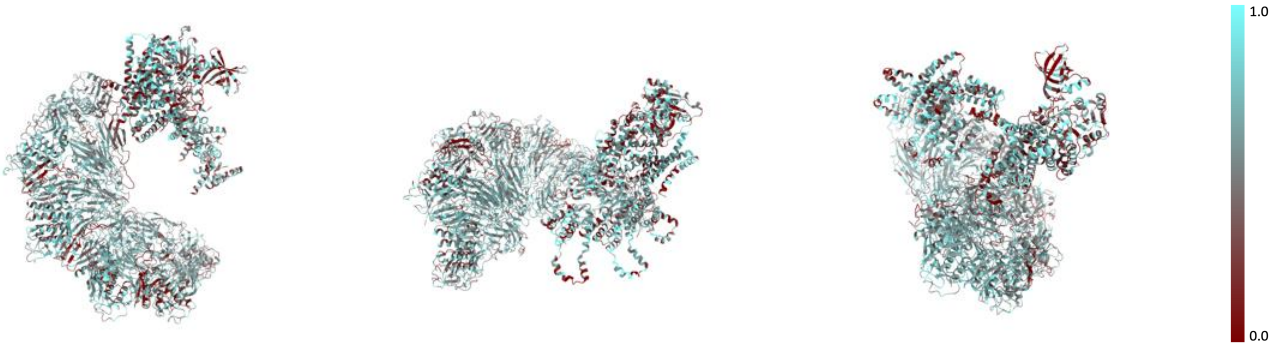
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

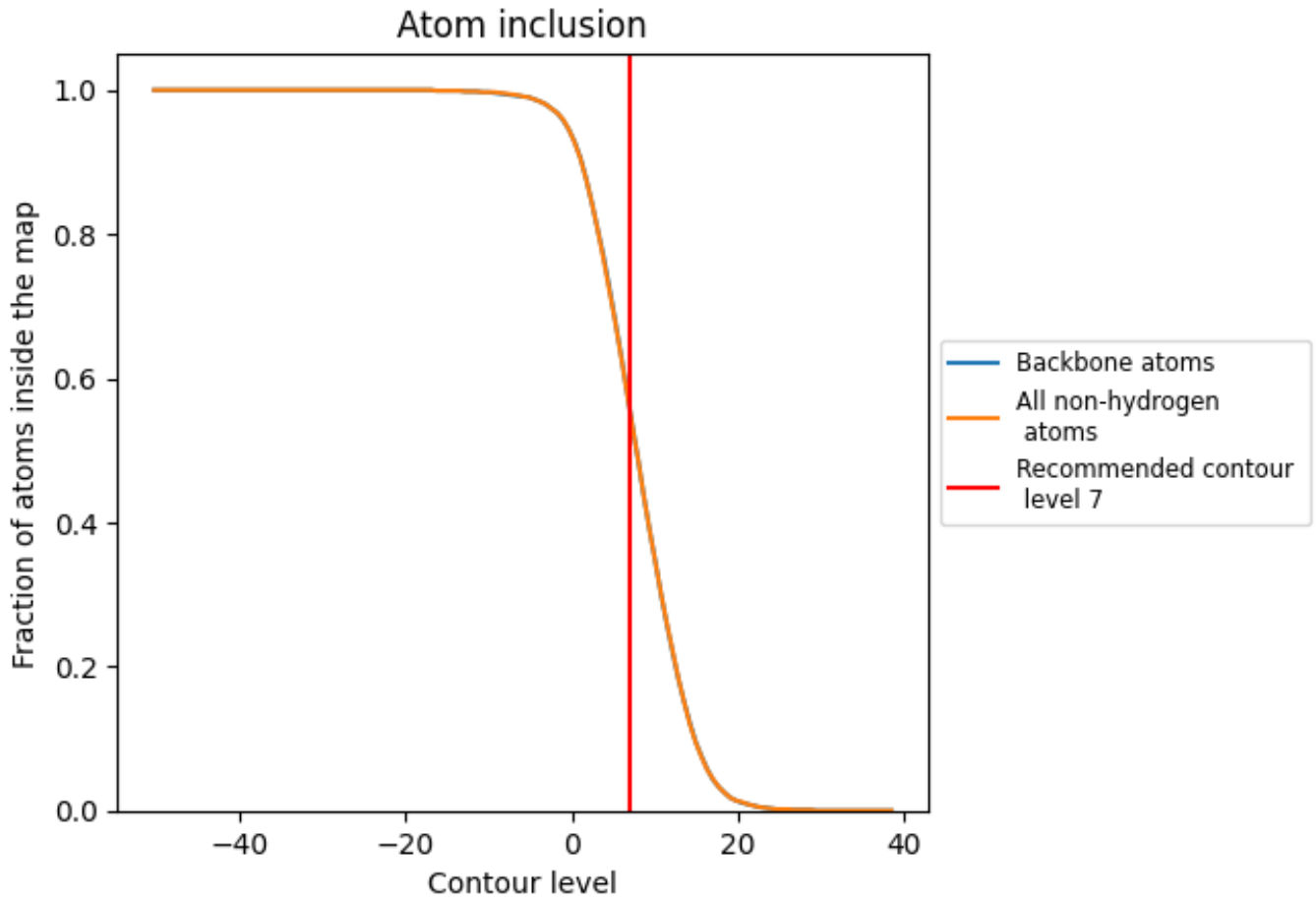
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7).

9.4 Atom inclusion (i)



At the recommended contour level, 56% of all backbone atoms, 56% 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 (7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5560	0.2570
A	0.6260	0.3670
B	0.5070	0.0880
C	0.5810	0.0980
D	0.5680	0.1260
E	0.4970	0.0760
F	0.5790	0.3110
G	0.5650	0.3330
H	0.5840	0.3060
I	0.5560	0.2880
J	0.5670	0.2900