



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:05 PM UTC

PDB ID : 9B8V / pdb_00009b8v
EMDB ID : EMD-44359
Title : AlphaFold2 informed cryo-EM model of the E. coli cellulose synthase Bc-sAG3B6 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:

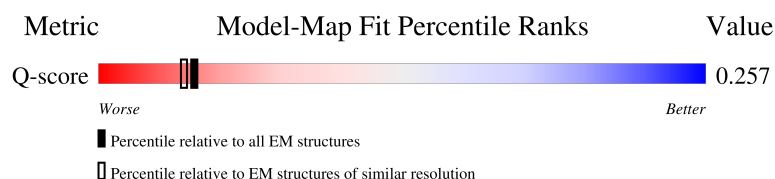
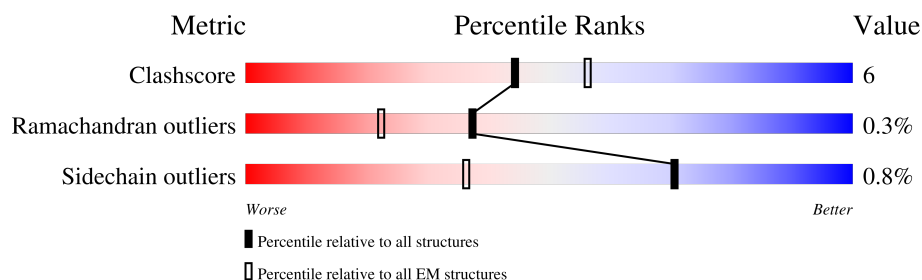
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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

Mol	Chain	Length	Quality of chain
1	A	763	
1	F	763	
1	G	763	
1	H	763	

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Mol	Chain	Length	Quality of chain
1	I	763	21% 79% 6% 15%
1	J	763	19% 79% 9% 13%
2	B	567	10% 11% 76%
2	C	567	7% 12% 11% 75%
2	D	567	7% 12% 11% 75%
3	E	887	37% 78% 15% 5%

2 Entry composition

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

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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		

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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		

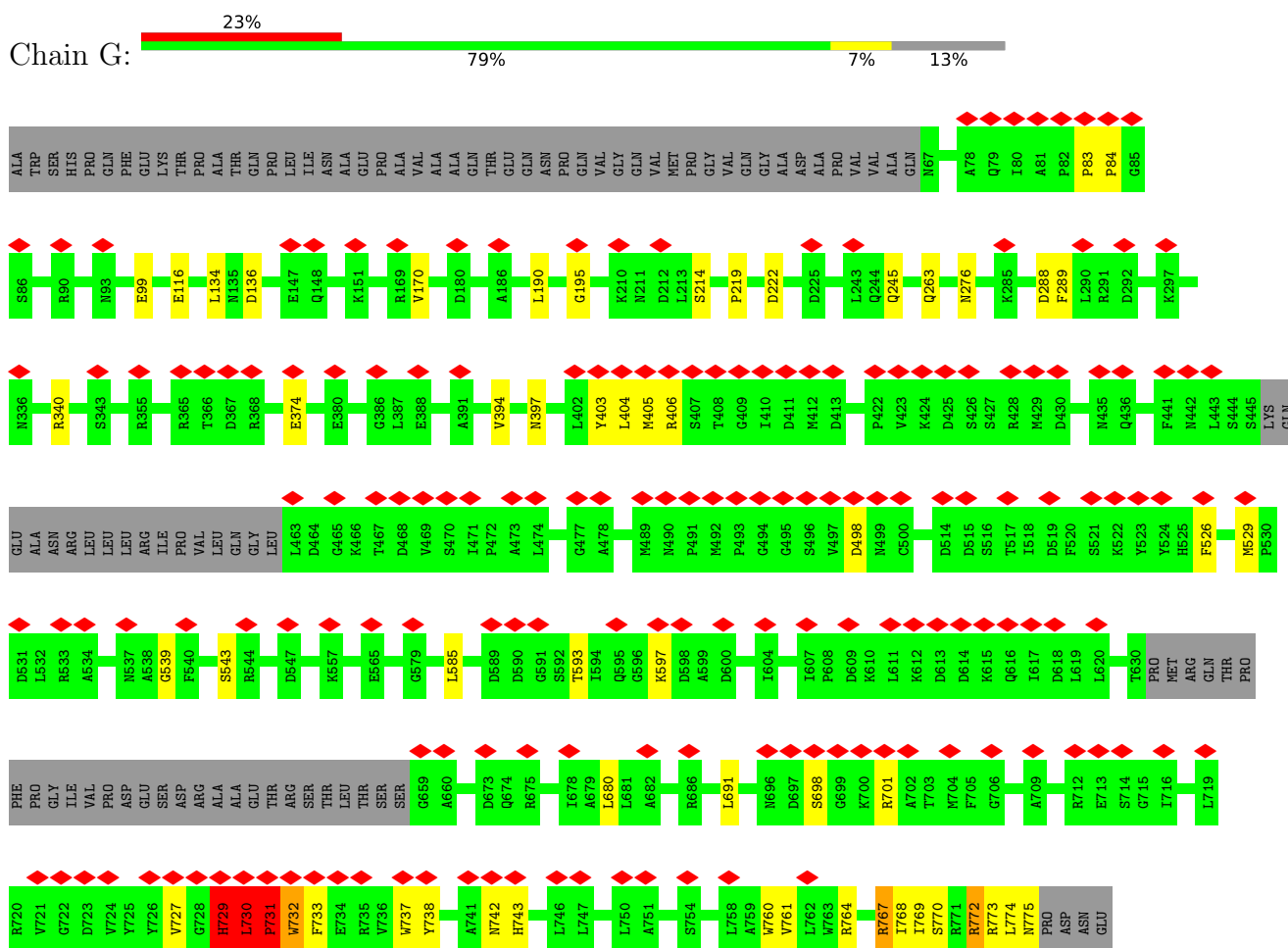
There are 16 discrepancies between the modelled and reference sequences:

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

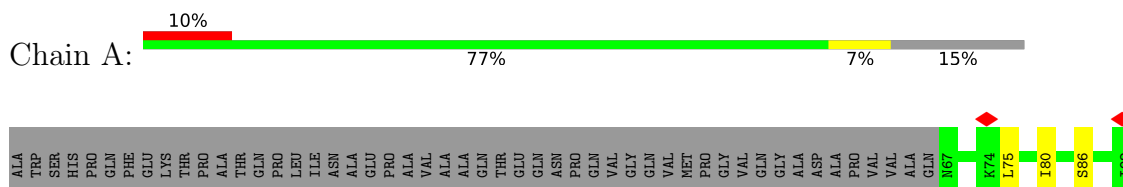
3 Residue-property plots

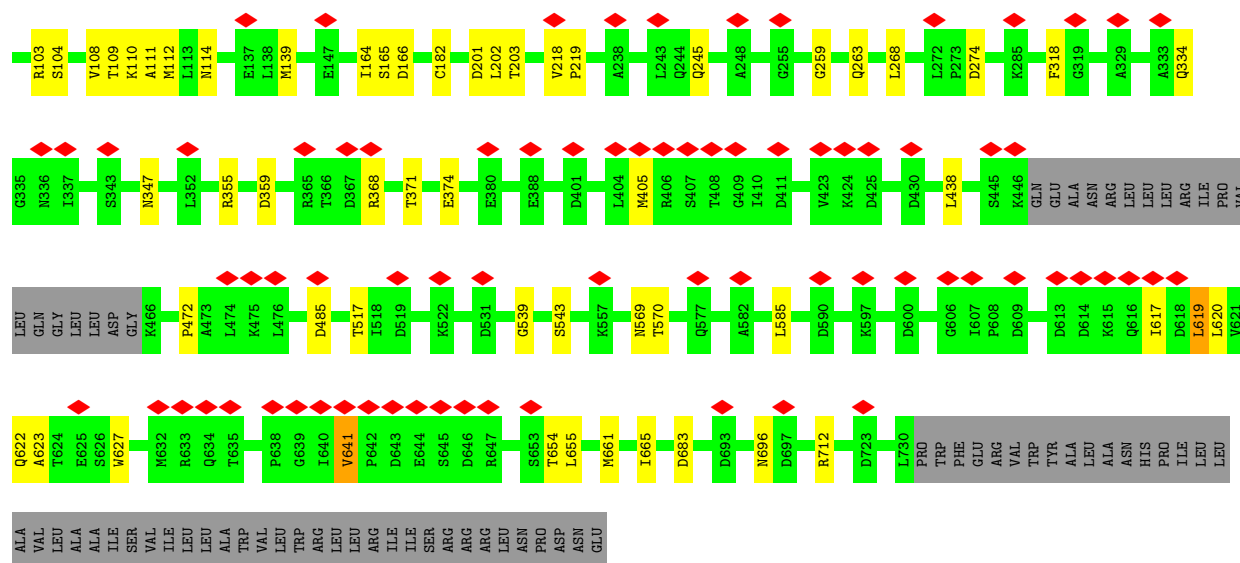
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

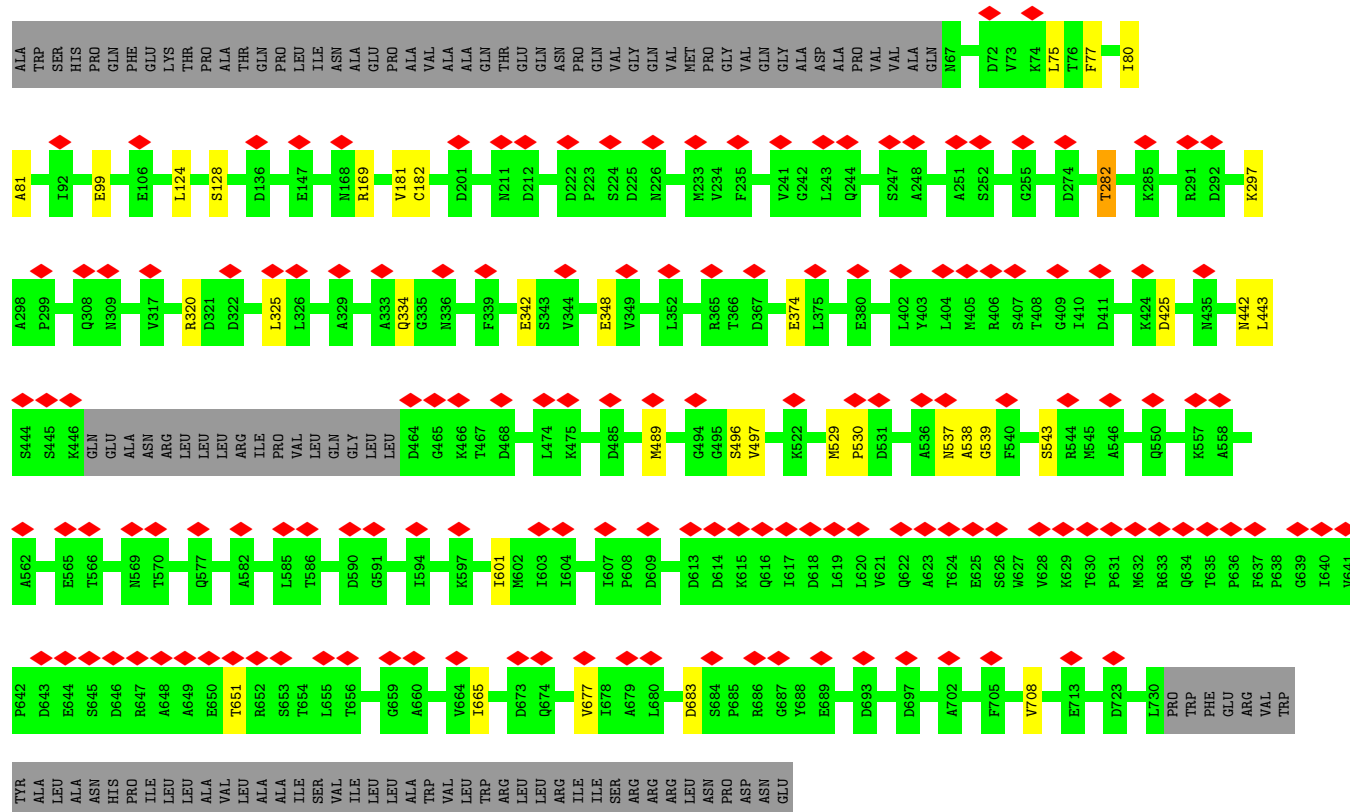


• Molecule 1: Cellulose synthase operon protein B

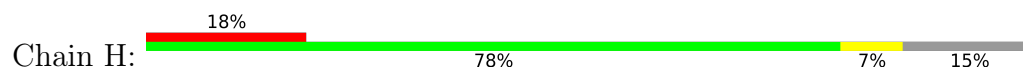


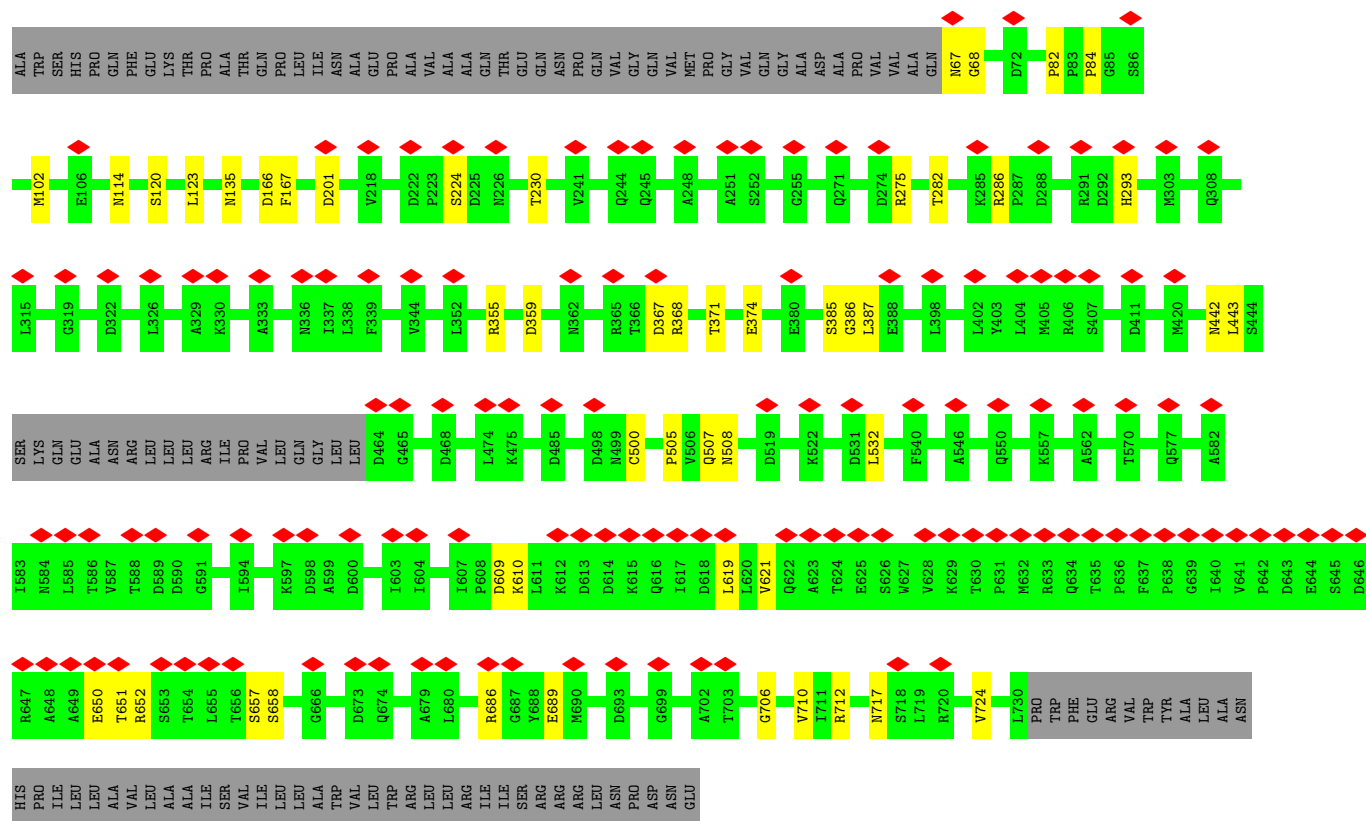


• Molecule 1: Cellulose synthase operon protein B

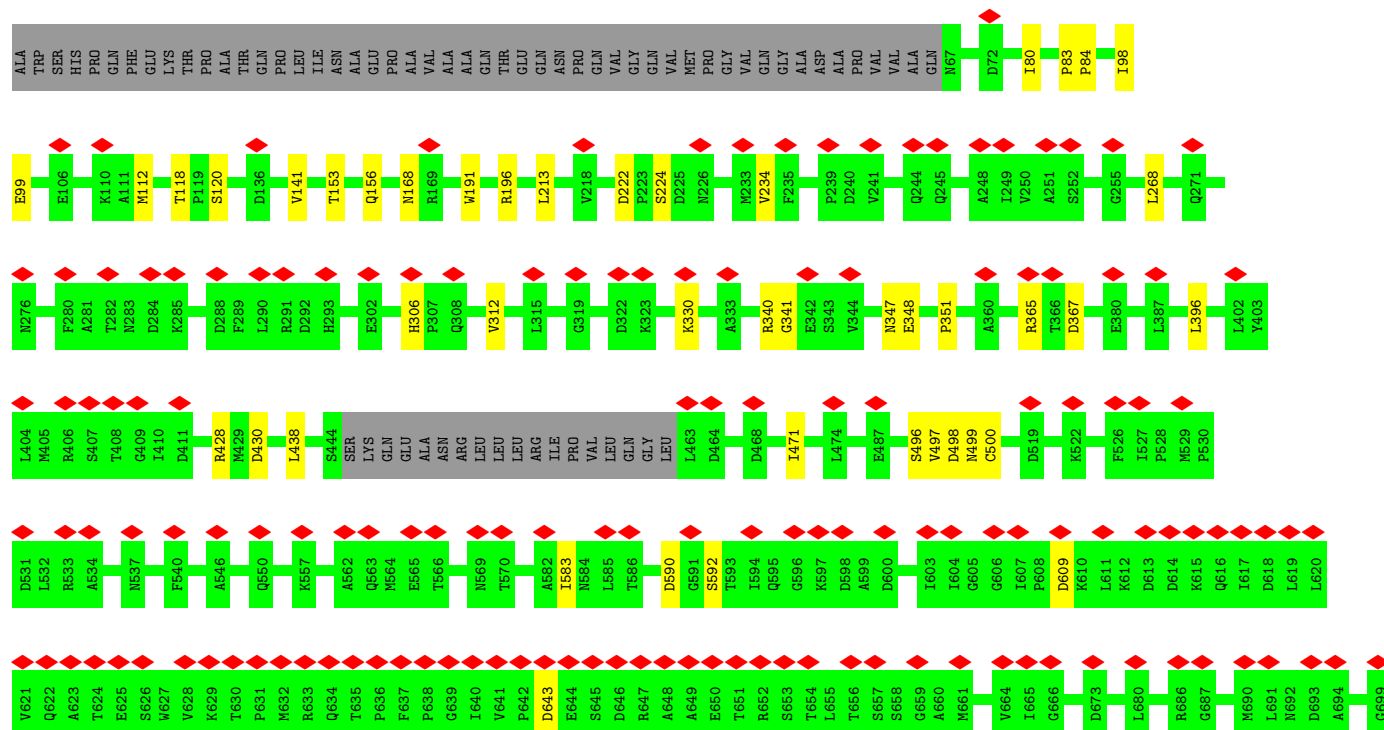
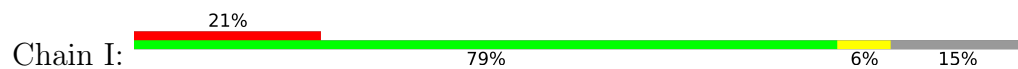


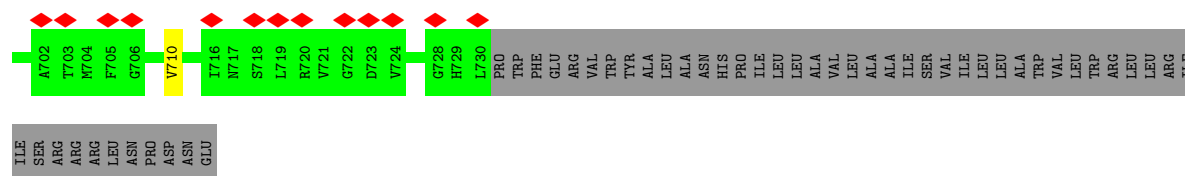
• Molecule 1: Cellulose synthase operon protein B



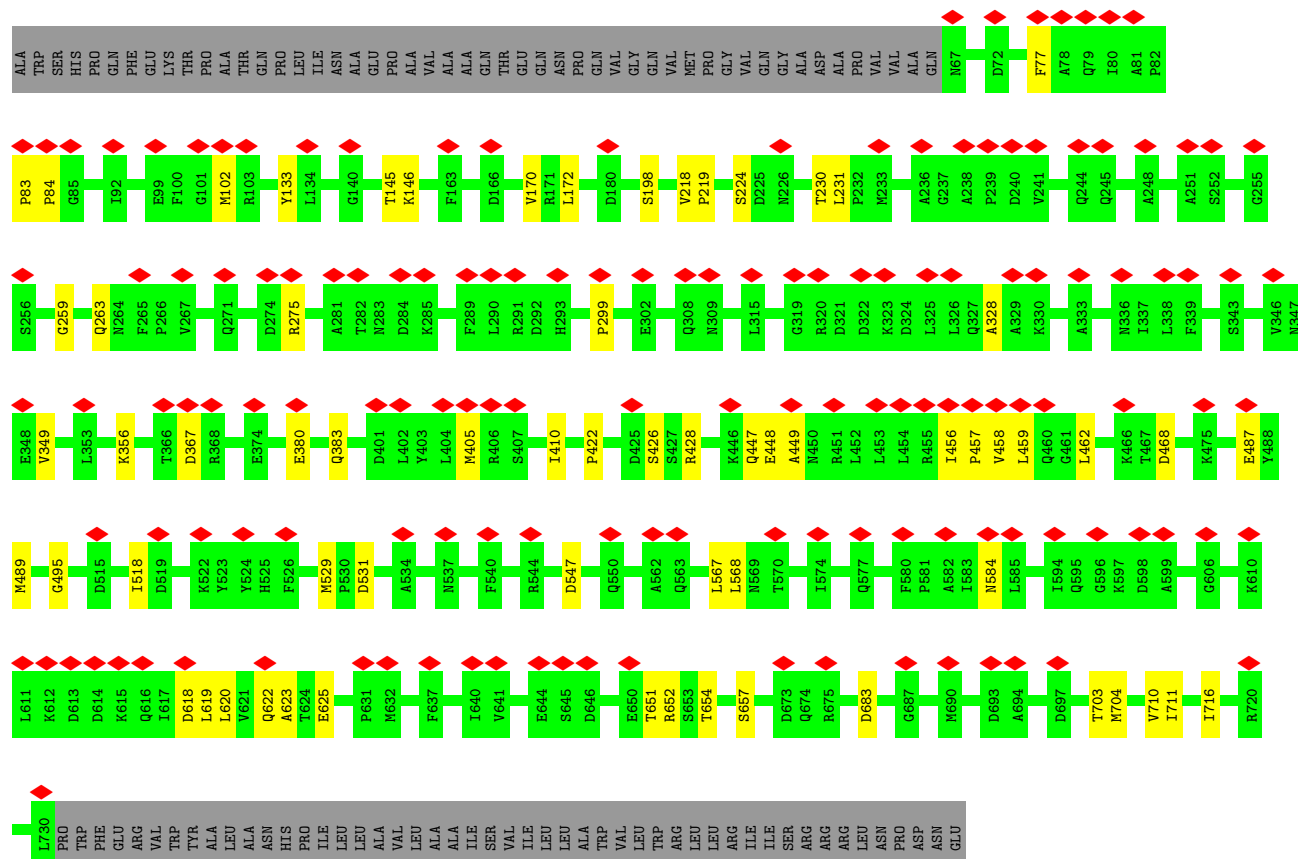
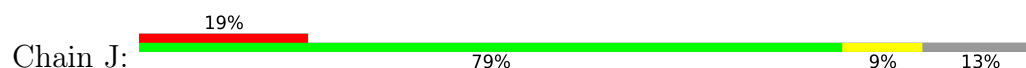


• Molecule 1: Cellulose synthase operon protein B

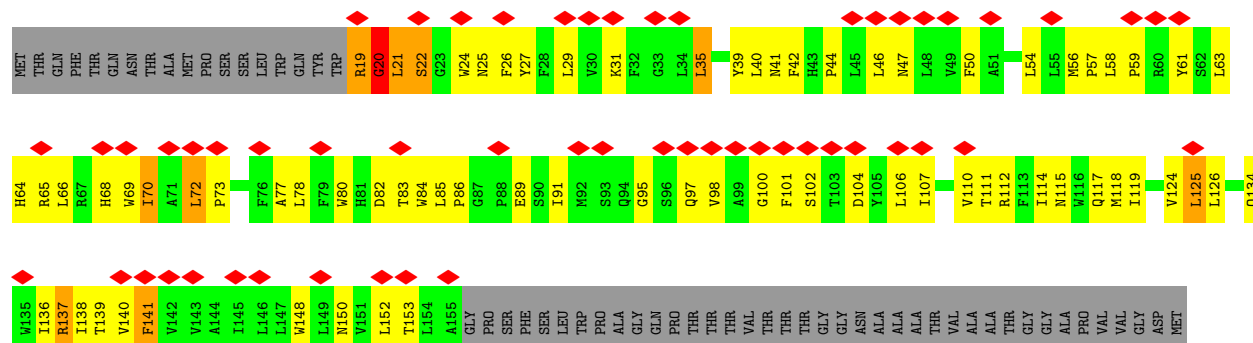




• Molecule 1: Cellulose synthase operon protein B

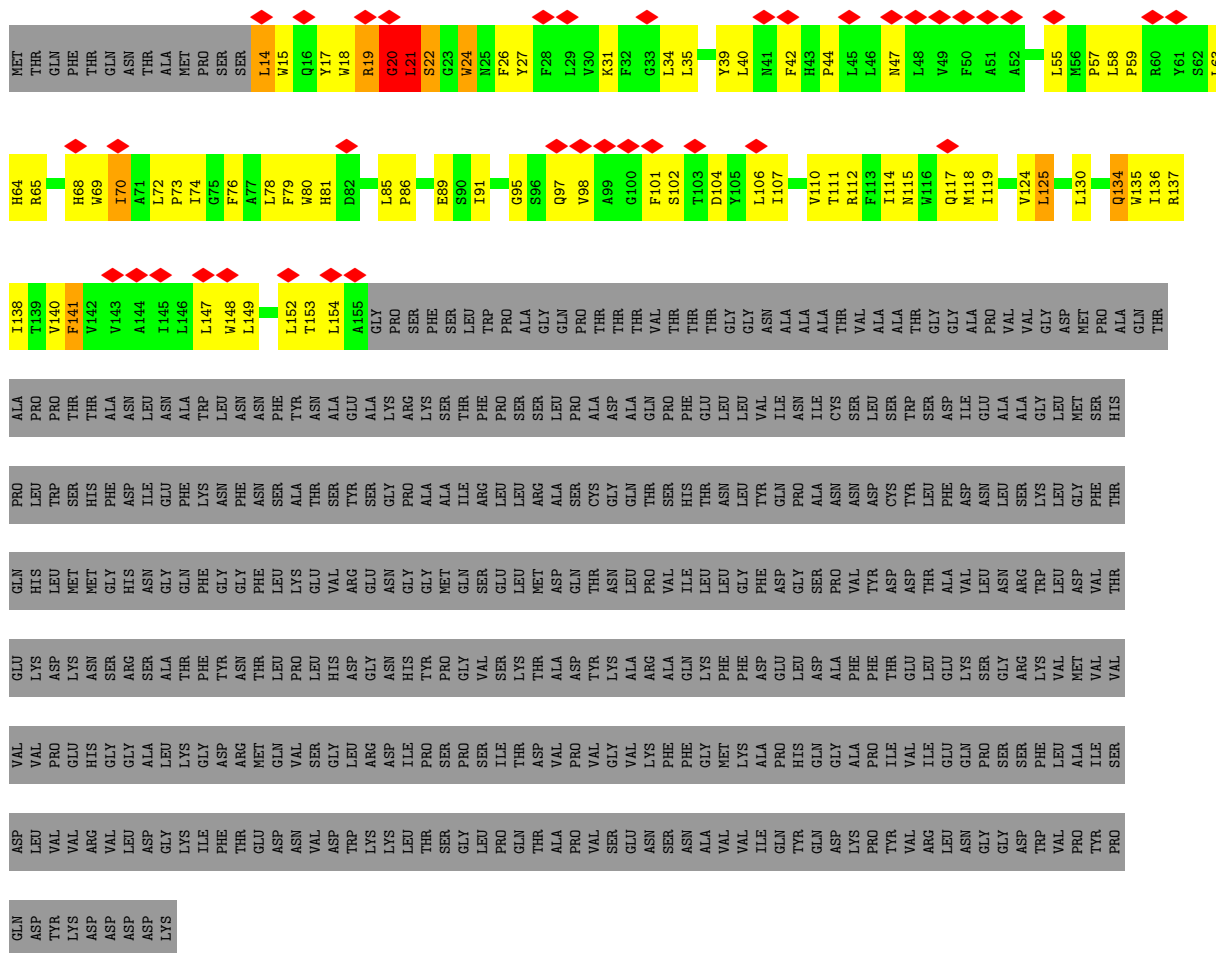


• Molecule 2: Cellulose biosynthesis protein BcsG

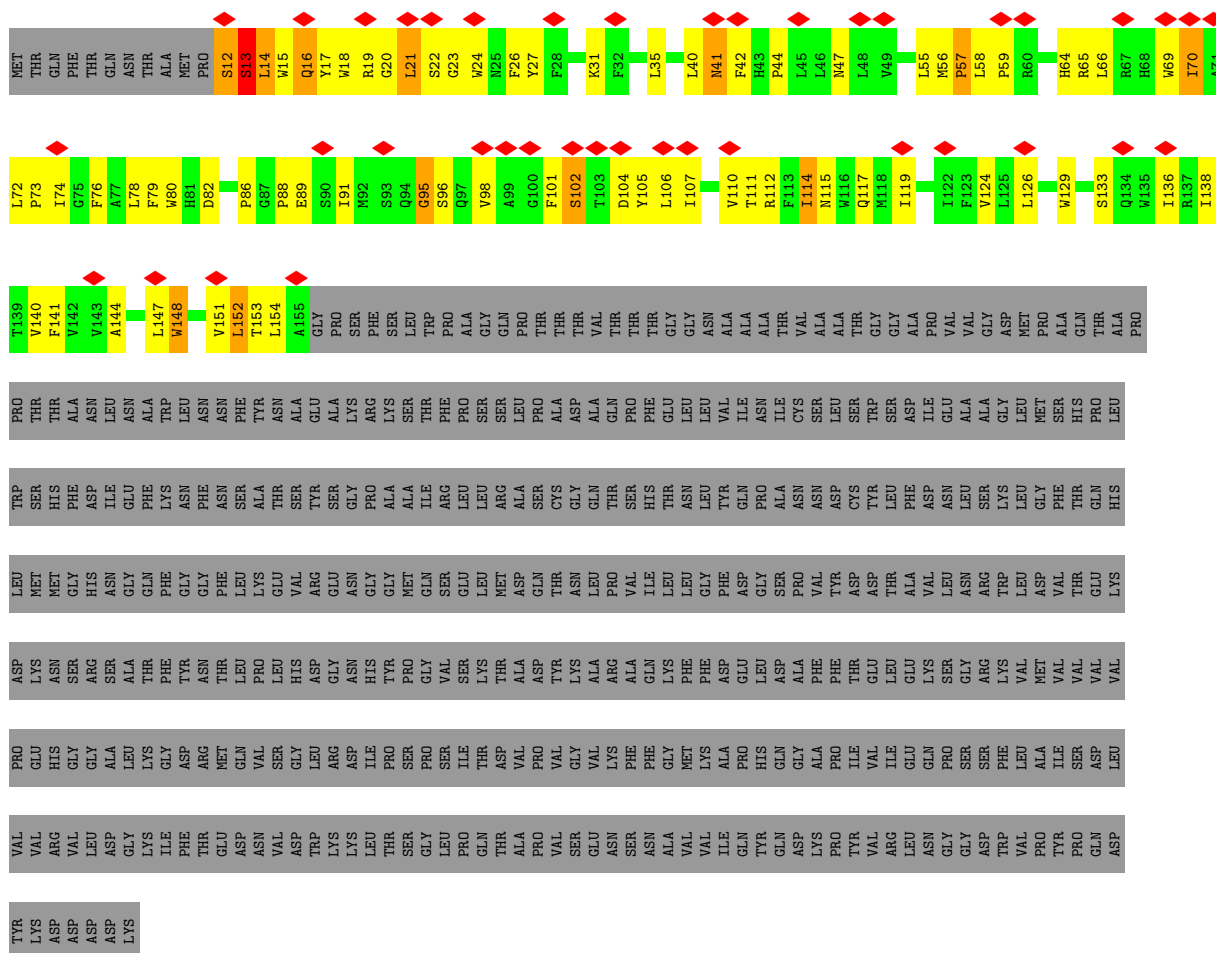


VAL	LEU	VAL	LEU	LEU	LEU	PRO
PRO	ALA	MET	ASP	GLY	GLN	ALA
TYR	ILE	VAL	VAL	PHE	GLN	SER
PRO	SER	VAL	THR	THR	THR	HIS
GLN	ASP	VAL	GLU	GLN	PRO	ALA
ASP	LEU	VAL	LYS	HIS	LEU	PRO
TYR	VAL	PRO	ASP	LEU	TRP	PRO
LYS	VAL	GLU	LYS	MET	SER	THR
ASP	VAL	HIS	ASN	MET	HIS	ALA
ASP	VAL	GLY	SER	GLY	PHE	ALA
ASP	LEU	GLY	ARG	HIS	ASP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

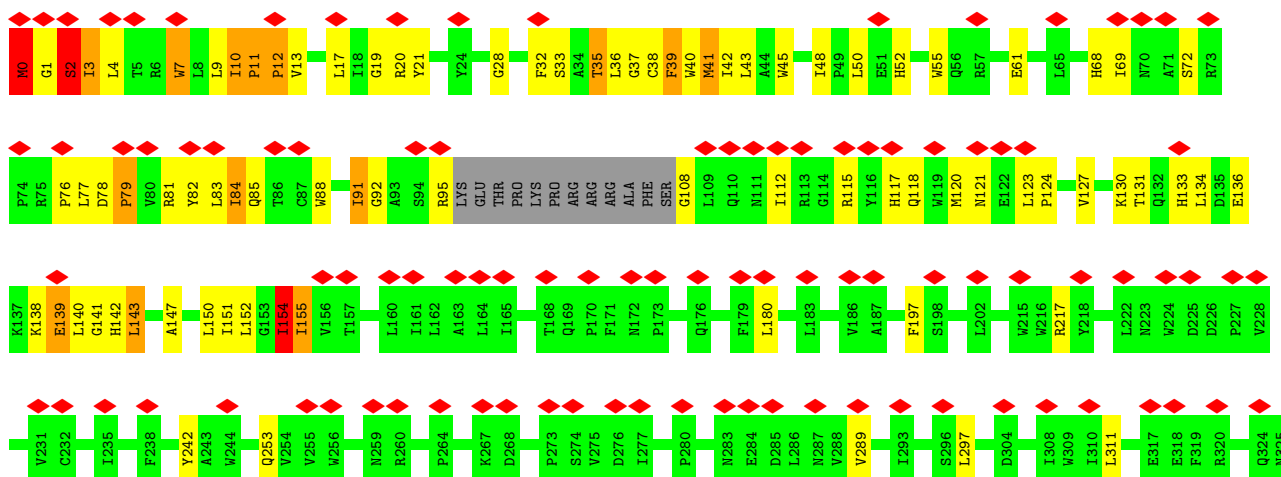
- Molecule 2: Cellulose biosynthesis protein BcsG

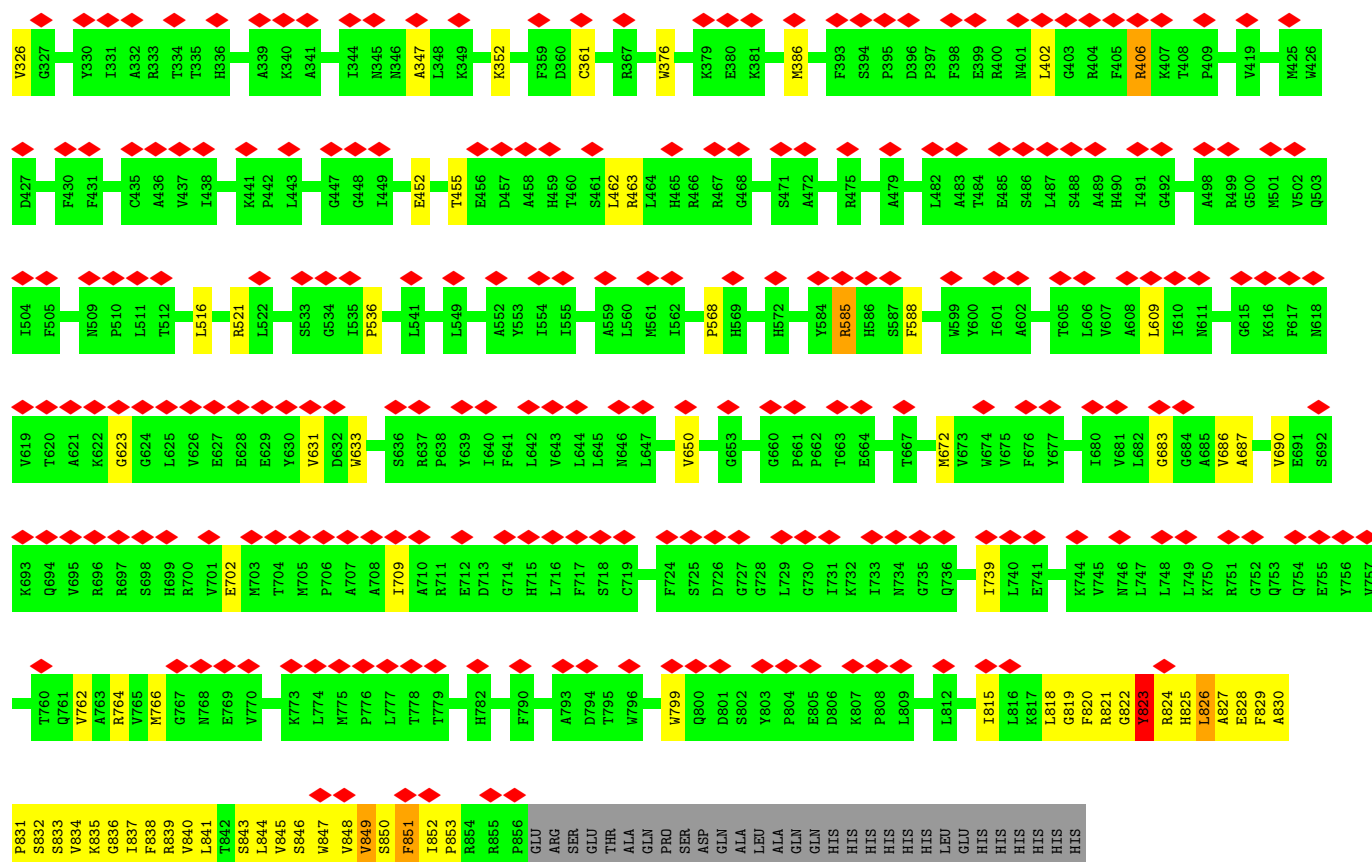


- Molecule 2: Cellulose biosynthesis protein BcsG



Chain E: 37% 78% 15% 5%





4 Experimental information

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 ($e^-/\text{\AA}^2$)	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

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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

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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

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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(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Group
2	D	21	LEU	Mainchain
3	E	0	MET	Peptide,Mainchain
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

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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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	641/763 (84%)	611 (95%)	30 (5%)	0	100	100

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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%)	21	57
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	38
2	C	140/567 (25%)	136 (97%)	1 (1%)	3 (2%)	5	32
2	D	142/567 (25%)	136 (96%)	5 (4%)	1 (1%)	18	54
3	E	841/887 (95%)	816 (97%)	18 (2%)	7 (1%)	16	52
All	All	5145/7166 (72%)	4964 (96%)	164 (3%)	17 (0%)	37	70

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 ⓘ

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%)	65	74
1	F	558/657 (85%)	557 (100%)	1 (0%)	87	87
1	G	574/657 (87%)	571 (100%)	3 (0%)	81	82
1	H	556/657 (85%)	554 (100%)	2 (0%)	84	84
1	I	557/657 (85%)	550 (99%)	7 (1%)	61	72
1	J	573/657 (87%)	569 (99%)	4 (1%)	76	79
2	B	118/480 (25%)	118 (100%)	0	100	100
2	C	123/480 (26%)	122 (99%)	1 (1%)	73	77
2	D	125/480 (26%)	125 (100%)	0	100	100
3	E	729/767 (95%)	718 (98%)	11 (2%)	57	70
All	All	4470/6149 (73%)	4435 (99%)	35 (1%)	70	77

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

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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

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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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

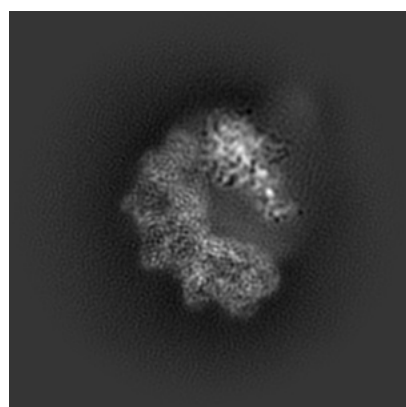
6 Map visualisation [i](#)

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

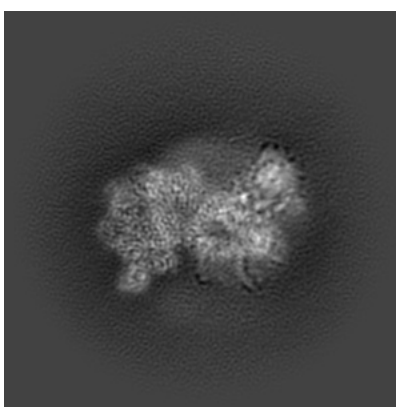
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

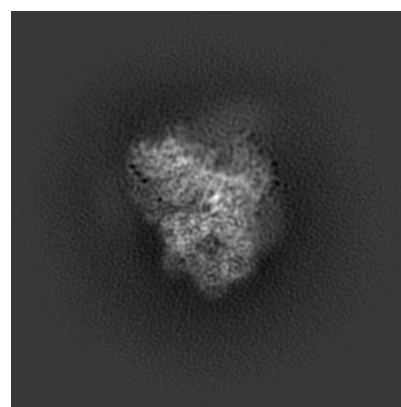
6.1.1 Primary map



X



Y

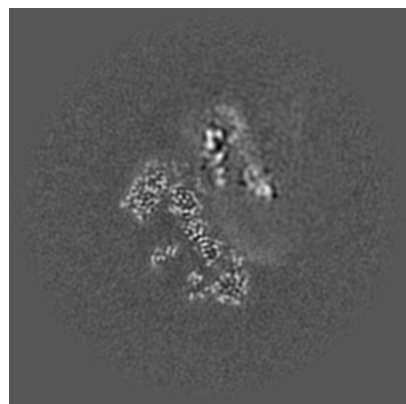


Z

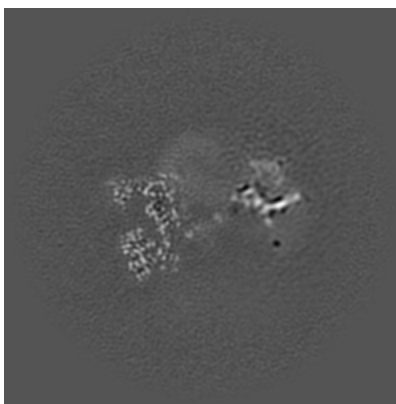
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

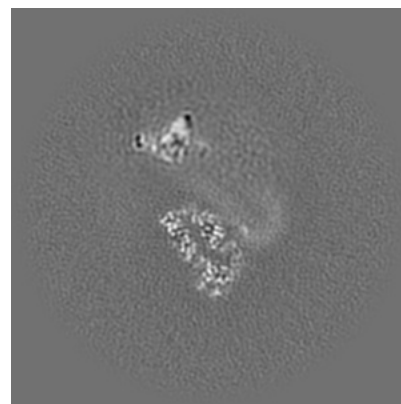
6.2.1 Primary map



X Index: 180



Y Index: 180

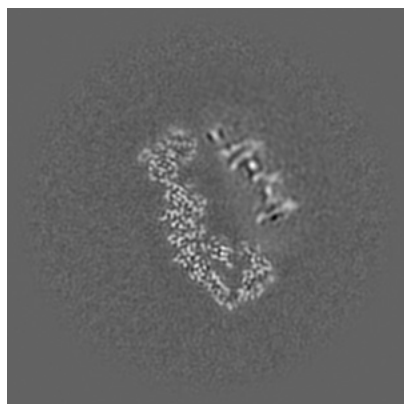


Z Index: 180

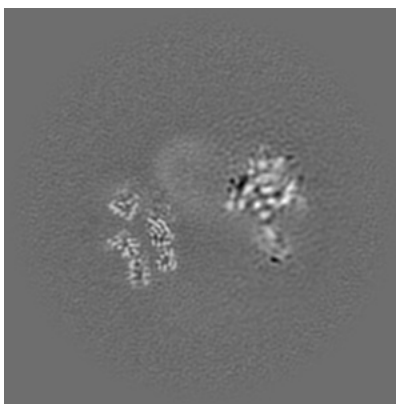
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

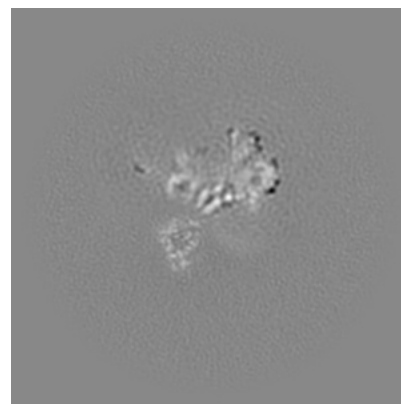
6.3.1 Primary map



X Index: 150



Y Index: 191

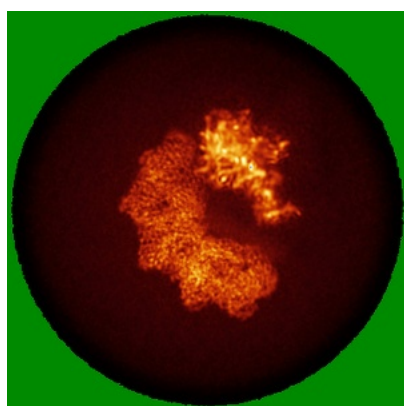


Z Index: 234

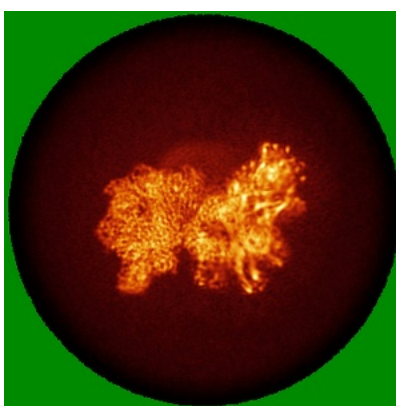
The images above show the largest variance slices of the map in three orthogonal directions.

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

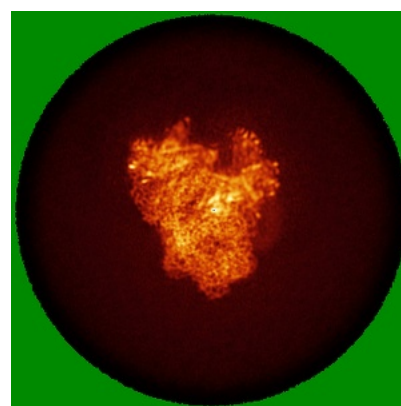
6.4.1 Primary map



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



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.

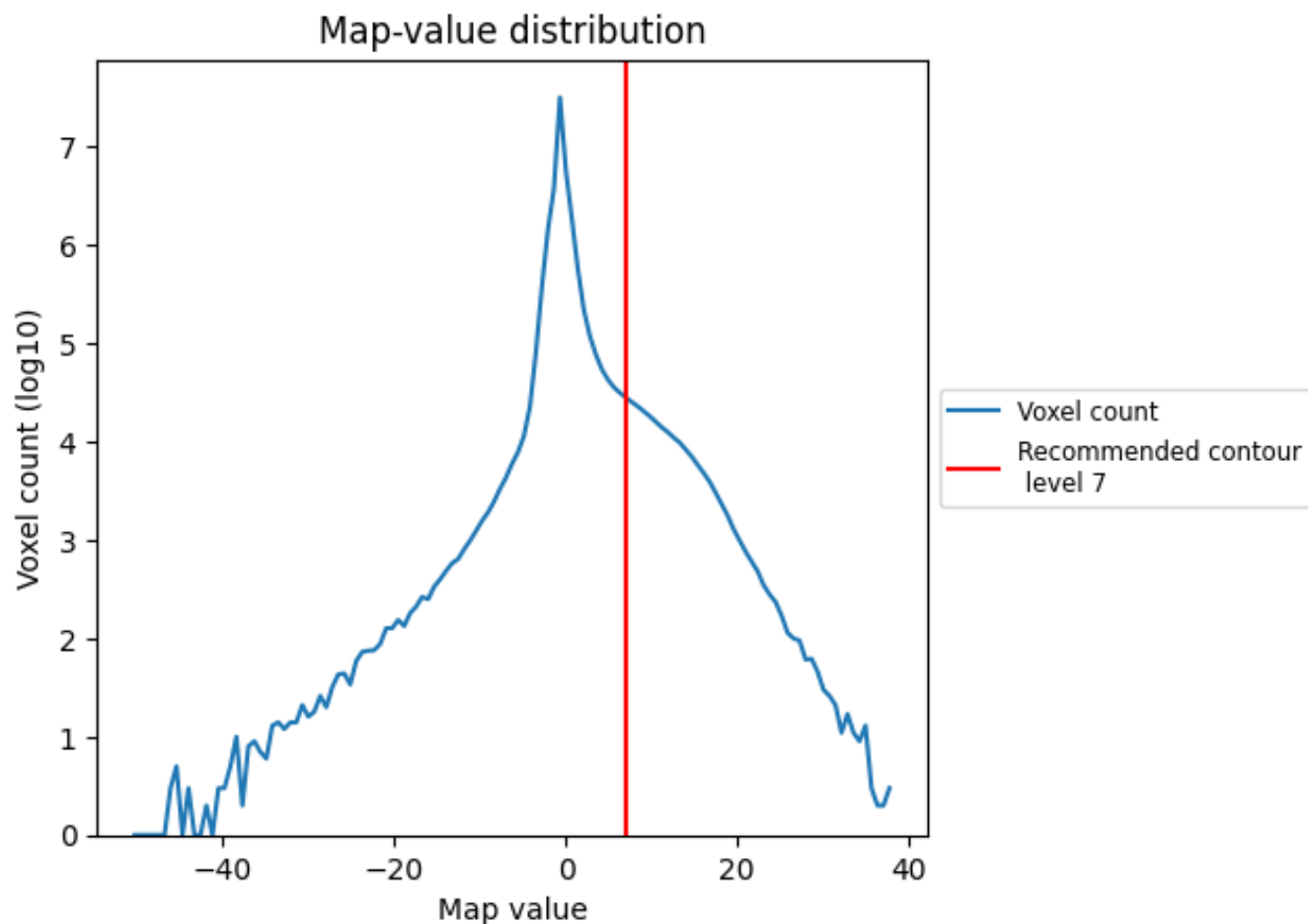
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

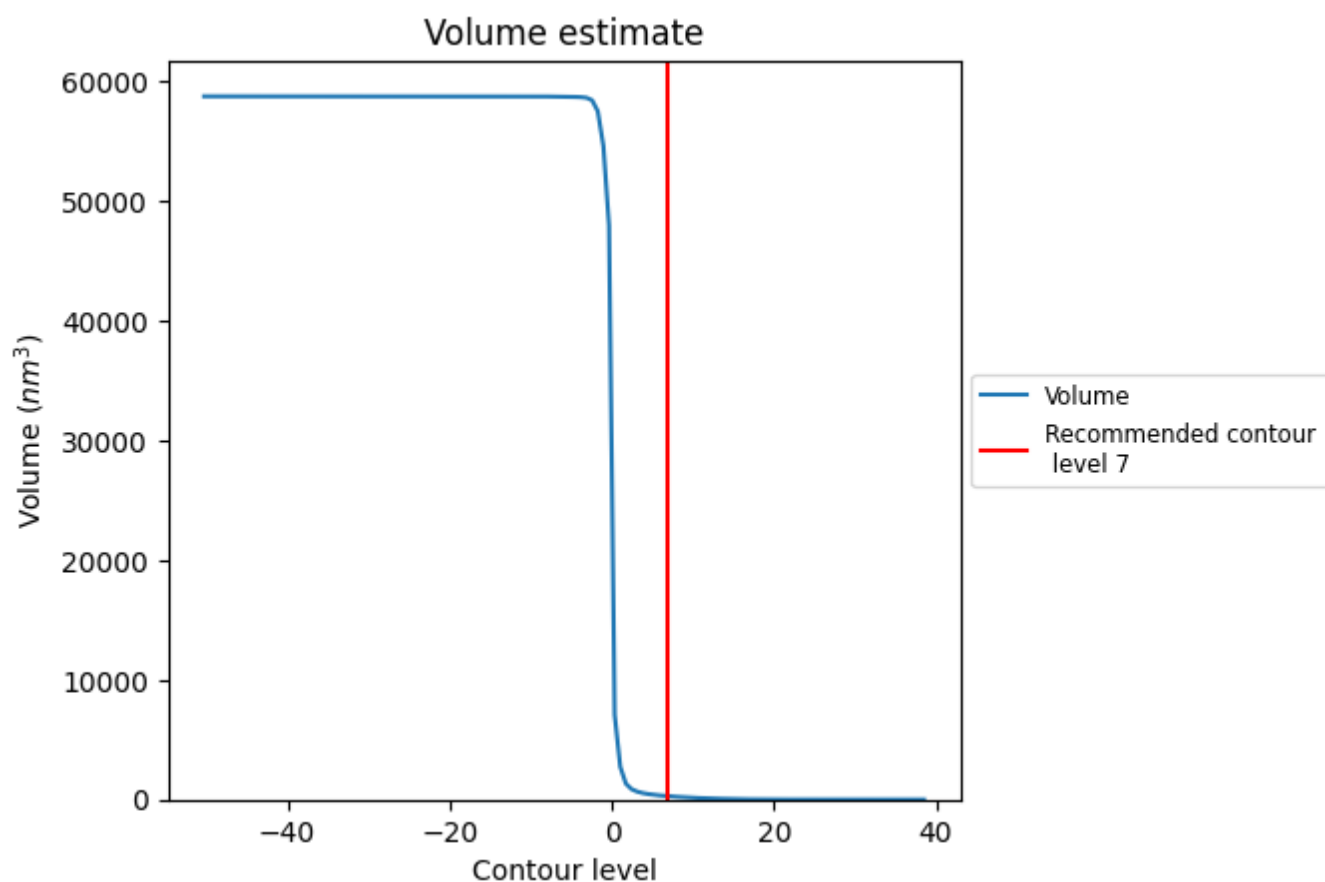
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

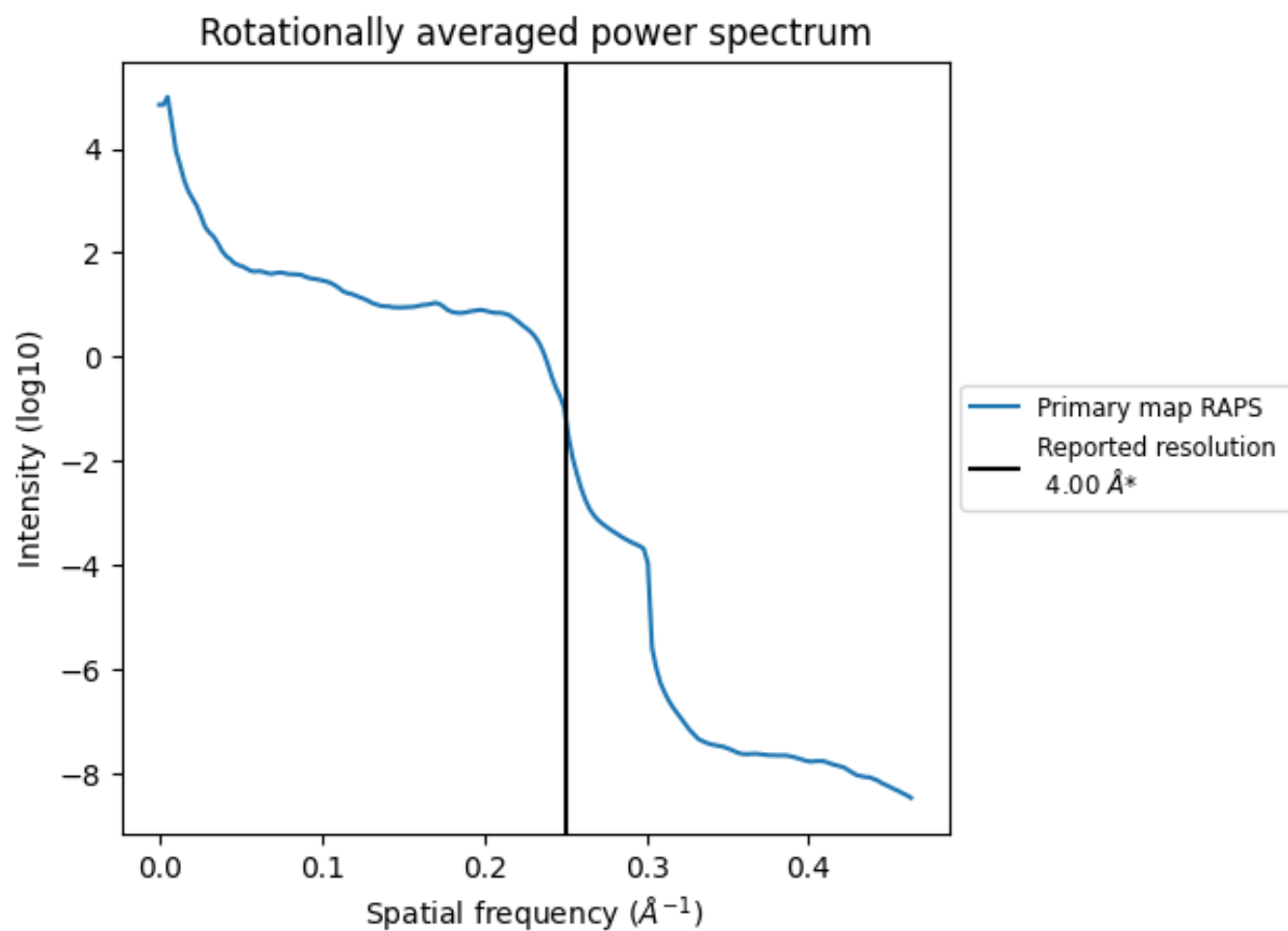
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 282 nm³; 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 ⓘ

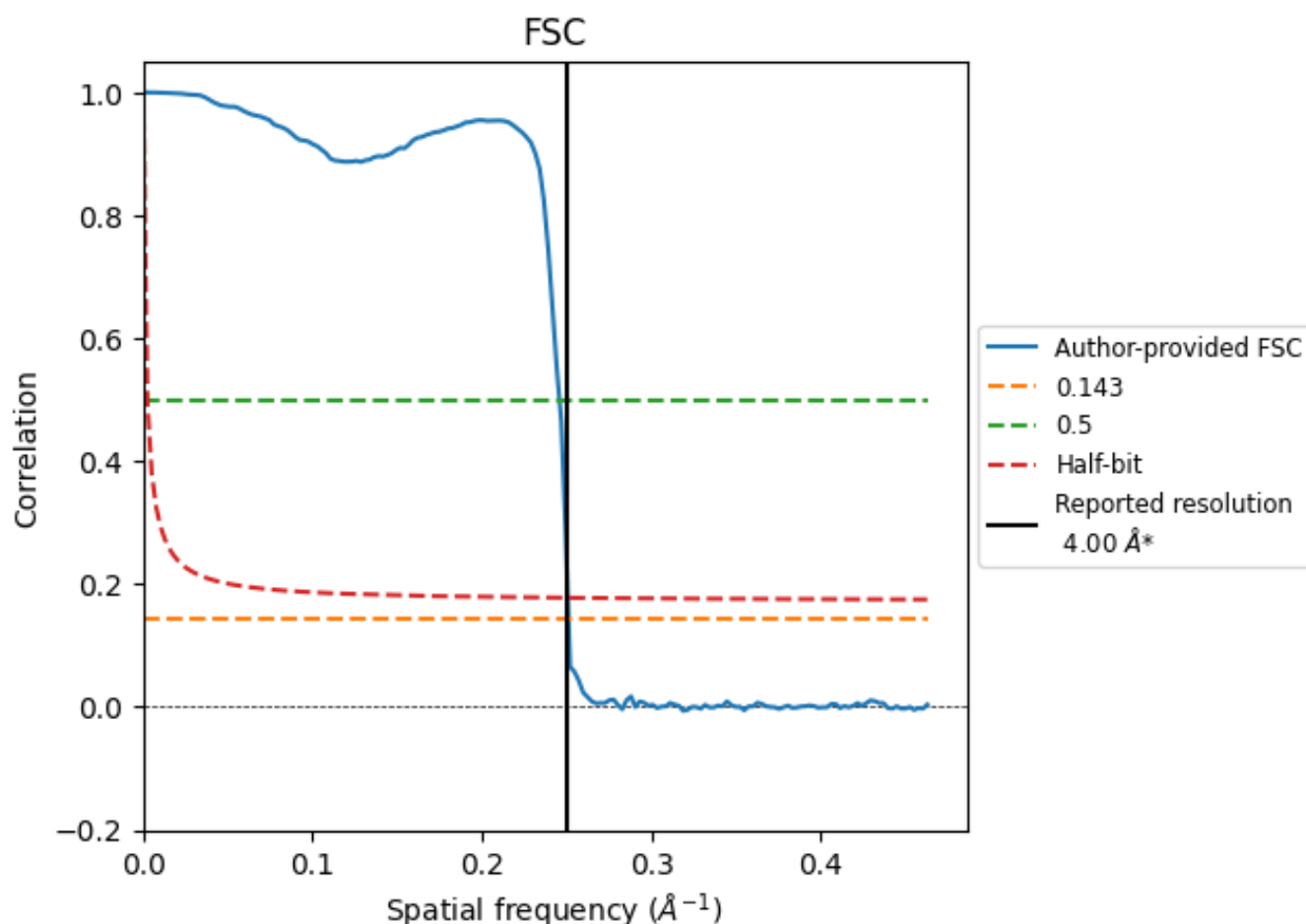


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

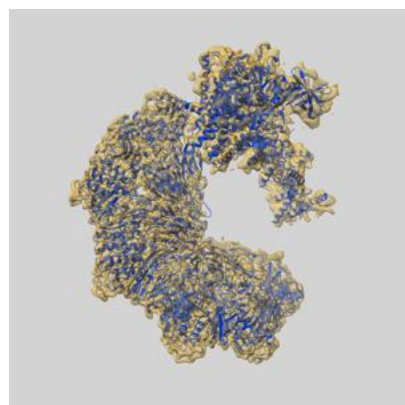
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.98	4.07	3.99
Unmasked-calculated*	-	-	-

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

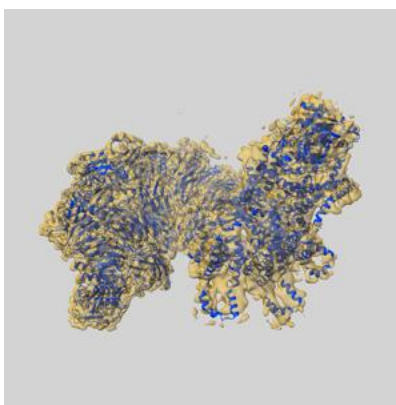
9 Map-model fit [i](#)

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](#).

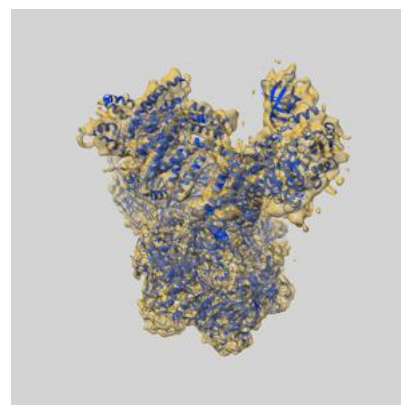
9.1 Map-model overlay [i](#)



X



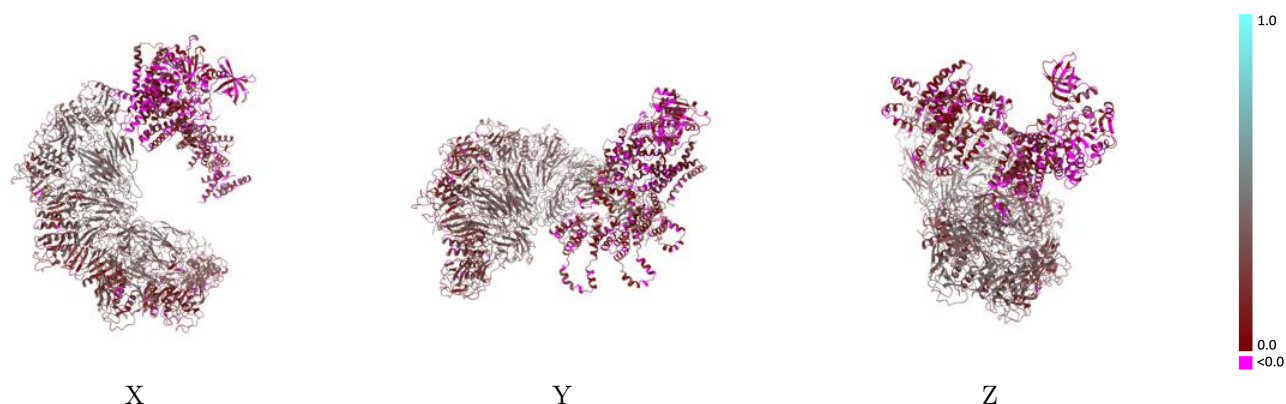
Y



Z

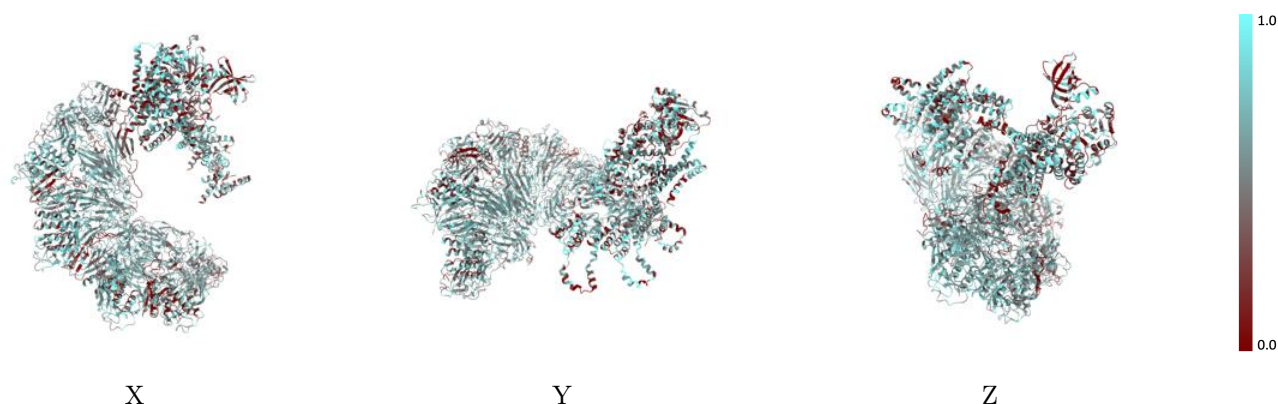
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



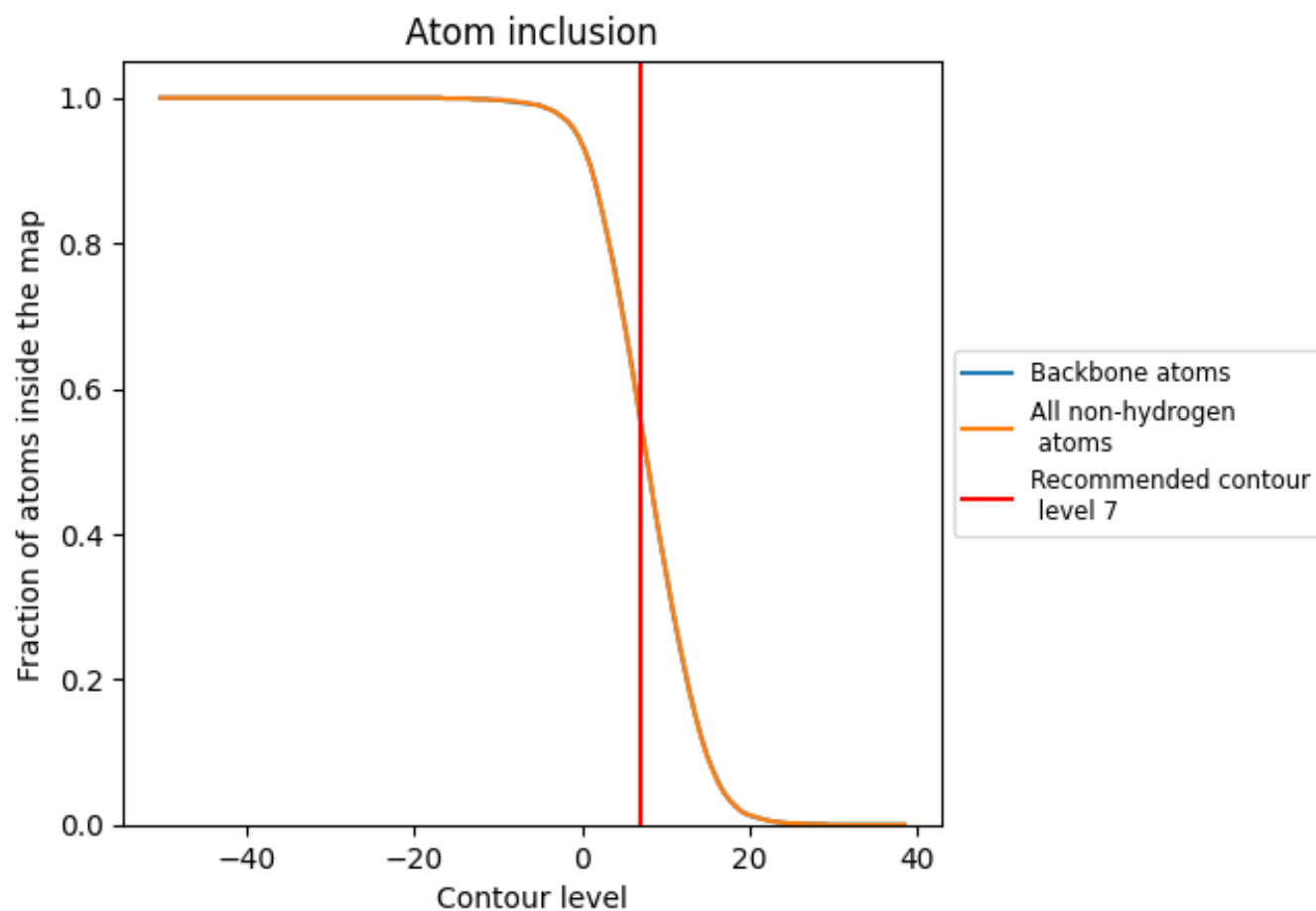
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

1.0

0.0

<0.0