



## Full wwPDB EM Validation Report ⓘ

Jul 14, 2024 – 07:54 pm BST

PDB ID : 7ZZQ  
EMDB ID : EMD-15039  
Title : BcsH-BcsD 'beads-on-a-string' filament, local refine  
Authors : Krasteva, P.V.; Abidi, W.; Decossas, M.  
Deposited on : 2022-05-26  
Resolution : 2.60 Å (reported)  
Based on initial model : 3A8E

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

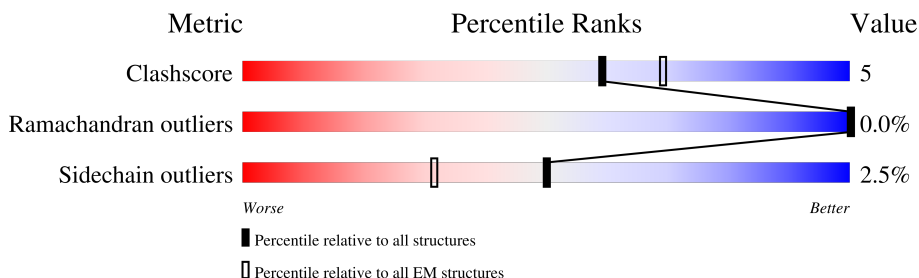
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	158	
1	B	158	
1	C	158	
1	D	158	
1	E	158	
1	F	158	
1	G	158	
1	H	158	

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Mol	Chain	Length	Quality of chain
1	I	158	75% 11% 13%
1	J	158	76% 12% 11%
1	K	158	70% 16% 13%
1	L	158	76% 15% 9%
1	M	158	78% 9% 13%
1	N	158	78% 11% 11%
1	O	158	67% 20% 13%
1	P	158	75% 11% 13%
1	W	158	96%
1	c	158	96%
2	Q	89	31% 7% 62%
2	R	89	35% 0% 61%
2	S	89	26% 0% 72%
2	T	89	28% 0% 69%
2	U	89	16% 0% 83%
2	V	89	10% 0% 89%
2	X	89	15% 0% 84%
2	Y	89	12% 0% 88%
2	Z	89	16% 0% 83%
2	a	89	11% 0% 89%
2	b	89	6% 24% 76%
2	d	89	9% 0% 89%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 19527 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cellulose biosynthesis protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	138	1088	694	185	203	6	1	0
1	B	141	1112	708	191	207	6	1	0
1	C	138	1099	700	189	204	6	2	0
1	D	136	1083	689	186	202	6	1	0
1	E	138	1088	694	185	203	6	1	0
1	F	144	1133	719	197	212	5	1	0
1	G	138	1088	694	185	203	6	1	0
1	H	141	1115	709	194	207	5	1	0
1	I	138	1099	700	189	204	6	2	0
1	J	140	1098	700	189	204	5	0	0
1	K	137	1083	691	184	202	6	1	0
1	L	144	1133	719	197	212	5	1	0
1	M	138	1099	700	189	204	6	2	0
1	N	141	1104	703	190	206	5	0	0
1	O	138	1099	700	189	204	6	2	0
1	P	138	1096	695	191	205	5	1	0
1	W	6	42	24	9	9		0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	c	6	42	24	9	9	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q76KJ6
A	0	GLY	-	expression tag	UNP Q76KJ6
A	1	SER	-	expression tag	UNP Q76KJ6
B	-1	MET	-	initiating methionine	UNP Q76KJ6
B	0	GLY	-	expression tag	UNP Q76KJ6
B	1	SER	-	expression tag	UNP Q76KJ6
C	-1	MET	-	initiating methionine	UNP Q76KJ6
C	0	GLY	-	expression tag	UNP Q76KJ6
C	1	SER	-	expression tag	UNP Q76KJ6
D	-1	MET	-	initiating methionine	UNP Q76KJ6
D	0	GLY	-	expression tag	UNP Q76KJ6
D	1	SER	-	expression tag	UNP Q76KJ6
E	-1	MET	-	initiating methionine	UNP Q76KJ6
E	0	GLY	-	expression tag	UNP Q76KJ6
E	1	SER	-	expression tag	UNP Q76KJ6
F	-1	MET	-	initiating methionine	UNP Q76KJ6
F	0	GLY	-	expression tag	UNP Q76KJ6
F	1	SER	-	expression tag	UNP Q76KJ6
G	-1	MET	-	initiating methionine	UNP Q76KJ6
G	0	GLY	-	expression tag	UNP Q76KJ6
G	1	SER	-	expression tag	UNP Q76KJ6
H	-1	MET	-	initiating methionine	UNP Q76KJ6
H	0	GLY	-	expression tag	UNP Q76KJ6
H	1	SER	-	expression tag	UNP Q76KJ6
I	-1	MET	-	initiating methionine	UNP Q76KJ6
I	0	GLY	-	expression tag	UNP Q76KJ6
I	1	SER	-	expression tag	UNP Q76KJ6
J	-1	MET	-	initiating methionine	UNP Q76KJ6
J	0	GLY	-	expression tag	UNP Q76KJ6
J	1	SER	-	expression tag	UNP Q76KJ6
K	-1	MET	-	initiating methionine	UNP Q76KJ6
K	0	GLY	-	expression tag	UNP Q76KJ6
K	1	SER	-	expression tag	UNP Q76KJ6
L	-1	MET	-	initiating methionine	UNP Q76KJ6
L	0	GLY	-	expression tag	UNP Q76KJ6
L	1	SER	-	expression tag	UNP Q76KJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-1	MET	-	initiating methionine	UNP Q76KJ6
M	0	GLY	-	expression tag	UNP Q76KJ6
M	1	SER	-	expression tag	UNP Q76KJ6
N	-1	MET	-	initiating methionine	UNP Q76KJ6
N	0	GLY	-	expression tag	UNP Q76KJ6
N	1	SER	-	expression tag	UNP Q76KJ6
O	-1	MET	-	initiating methionine	UNP Q76KJ6
O	0	GLY	-	expression tag	UNP Q76KJ6
O	1	SER	-	expression tag	UNP Q76KJ6
P	-1	MET	-	initiating methionine	UNP Q76KJ6
P	0	GLY	-	expression tag	UNP Q76KJ6
P	1	SER	-	expression tag	UNP Q76KJ6
W	-1	MET	-	initiating methionine	UNP Q76KJ6
W	0	GLY	-	expression tag	UNP Q76KJ6
W	1	SER	-	expression tag	UNP Q76KJ6
c	-1	MET	-	initiating methionine	UNP Q76KJ6
c	0	GLY	-	expression tag	UNP Q76KJ6
c	1	SER	-	expression tag	UNP Q76KJ6

- Molecule 2 is a protein called BcsH fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Q	34	Total	C	N	O	S	0	0
			259	160	49	48	2		
2	R	35	Total	C	N	O	S	0	0
			266	165	50	49	2		
2	S	25	Total	C	N	O	S	0	0
			187	116	34	35	2		
2	T	28	Total	C	N	O	S	0	0
			210	130	40	38	2		
2	U	15	Total	C	N	O	S	0	0
			103	64	15	22	2		
2	V	10	Total	C	N	O		0	0
			84	52	19	13			
2	X	14	Total	C	N	O	S	0	0
			99	62	14	21	2		
2	Y	11	Total	C	N	O		0	0
			91	57	20	14			
2	Z	15	Total	C	N	O	S	0	0
			103	64	15	22	2		
2	a	10	Total	C	N	O		0	0
			84	52	19	13			

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	21	Total	C	N	O	S	0	0
			151	94	24	31	2		
2	d	10	Total	C	N	O		0	0
			84	52	19	13			

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	265	MET	-	initiating methionine	UNP D5QCK0
Q	266	SER	-	expression tag	UNP D5QCK0
Q	267	TYR	-	expression tag	UNP D5QCK0
Q	268	TYR	-	expression tag	UNP D5QCK0
Q	269	HIS	-	expression tag	UNP D5QCK0
Q	270	HIS	-	expression tag	UNP D5QCK0
Q	271	HIS	-	expression tag	UNP D5QCK0
Q	272	HIS	-	expression tag	UNP D5QCK0
Q	273	HIS	-	expression tag	UNP D5QCK0
Q	274	HIS	-	expression tag	UNP D5QCK0
Q	275	ASP	-	expression tag	UNP D5QCK0
Q	276	TYR	-	expression tag	UNP D5QCK0
Q	277	ASP	-	expression tag	UNP D5QCK0
Q	278	ILE	-	expression tag	UNP D5QCK0
Q	279	PRO	-	expression tag	UNP D5QCK0
Q	280	THR	-	expression tag	UNP D5QCK0
Q	281	THR	-	expression tag	UNP D5QCK0
Q	282	LEU	-	expression tag	UNP D5QCK0
Q	283	GLU	-	expression tag	UNP D5QCK0
Q	284	VAL	-	expression tag	UNP D5QCK0
Q	285	LEU	-	expression tag	UNP D5QCK0
Q	286	PHE	-	expression tag	UNP D5QCK0
Q	287	GLN	-	expression tag	UNP D5QCK0
Q	288	GLY	-	expression tag	UNP D5QCK0
Q	289	PRO	-	expression tag	UNP D5QCK0
Q	290	MET	-	expression tag	UNP D5QCK0
Q	291	GLY	-	expression tag	UNP D5QCK0
Q	292	SER	-	expression tag	UNP D5QCK0
R	265	MET	-	initiating methionine	UNP D5QCK0
R	266	SER	-	expression tag	UNP D5QCK0
R	267	TYR	-	expression tag	UNP D5QCK0
R	268	TYR	-	expression tag	UNP D5QCK0
R	269	HIS	-	expression tag	UNP D5QCK0
R	270	HIS	-	expression tag	UNP D5QCK0

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Chain	Residue	Modelled	Actual	Comment	Reference
R	271	HIS	-	expression tag	UNP D5QCK0
R	272	HIS	-	expression tag	UNP D5QCK0
R	273	HIS	-	expression tag	UNP D5QCK0
R	274	HIS	-	expression tag	UNP D5QCK0
R	275	ASP	-	expression tag	UNP D5QCK0
R	276	TYR	-	expression tag	UNP D5QCK0
R	277	ASP	-	expression tag	UNP D5QCK0
R	278	ILE	-	expression tag	UNP D5QCK0
R	279	PRO	-	expression tag	UNP D5QCK0
R	280	THR	-	expression tag	UNP D5QCK0
R	281	THR	-	expression tag	UNP D5QCK0
R	282	LEU	-	expression tag	UNP D5QCK0
R	283	GLU	-	expression tag	UNP D5QCK0
R	284	VAL	-	expression tag	UNP D5QCK0
R	285	LEU	-	expression tag	UNP D5QCK0
R	286	PHE	-	expression tag	UNP D5QCK0
R	287	GLN	-	expression tag	UNP D5QCK0
R	288	GLY	-	expression tag	UNP D5QCK0
R	289	PRO	-	expression tag	UNP D5QCK0
R	290	MET	-	expression tag	UNP D5QCK0
R	291	GLY	-	expression tag	UNP D5QCK0
R	292	SER	-	expression tag	UNP D5QCK0
S	265	MET	-	initiating methionine	UNP D5QCK0
S	266	SER	-	expression tag	UNP D5QCK0
S	267	TYR	-	expression tag	UNP D5QCK0
S	268	TYR	-	expression tag	UNP D5QCK0
S	269	HIS	-	expression tag	UNP D5QCK0
S	270	HIS	-	expression tag	UNP D5QCK0
S	271	HIS	-	expression tag	UNP D5QCK0
S	272	HIS	-	expression tag	UNP D5QCK0
S	273	HIS	-	expression tag	UNP D5QCK0
S	274	HIS	-	expression tag	UNP D5QCK0
S	275	ASP	-	expression tag	UNP D5QCK0
S	276	TYR	-	expression tag	UNP D5QCK0
S	277	ASP	-	expression tag	UNP D5QCK0
S	278	ILE	-	expression tag	UNP D5QCK0
S	279	PRO	-	expression tag	UNP D5QCK0
S	280	THR	-	expression tag	UNP D5QCK0
S	281	THR	-	expression tag	UNP D5QCK0
S	282	LEU	-	expression tag	UNP D5QCK0
S	283	GLU	-	expression tag	UNP D5QCK0
S	284	VAL	-	expression tag	UNP D5QCK0

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Chain	Residue	Modelled	Actual	Comment	Reference
S	285	LEU	-	expression tag	UNP D5QCK0
S	286	PHE	-	expression tag	UNP D5QCK0
S	287	GLN	-	expression tag	UNP D5QCK0
S	288	GLY	-	expression tag	UNP D5QCK0
S	289	PRO	-	expression tag	UNP D5QCK0
S	290	MET	-	expression tag	UNP D5QCK0
S	291	GLY	-	expression tag	UNP D5QCK0
S	292	SER	-	expression tag	UNP D5QCK0
T	265	MET	-	initiating methionine	UNP D5QCK0
T	266	SER	-	expression tag	UNP D5QCK0
T	267	TYR	-	expression tag	UNP D5QCK0
T	268	TYR	-	expression tag	UNP D5QCK0
T	269	HIS	-	expression tag	UNP D5QCK0
T	270	HIS	-	expression tag	UNP D5QCK0
T	271	HIS	-	expression tag	UNP D5QCK0
T	272	HIS	-	expression tag	UNP D5QCK0
T	273	HIS	-	expression tag	UNP D5QCK0
T	274	HIS	-	expression tag	UNP D5QCK0
T	275	ASP	-	expression tag	UNP D5QCK0
T	276	TYR	-	expression tag	UNP D5QCK0
T	277	ASP	-	expression tag	UNP D5QCK0
T	278	ILE	-	expression tag	UNP D5QCK0
T	279	PRO	-	expression tag	UNP D5QCK0
T	280	THR	-	expression tag	UNP D5QCK0
T	281	THR	-	expression tag	UNP D5QCK0
T	282	LEU	-	expression tag	UNP D5QCK0
T	283	GLU	-	expression tag	UNP D5QCK0
T	284	VAL	-	expression tag	UNP D5QCK0
T	285	LEU	-	expression tag	UNP D5QCK0
T	286	PHE	-	expression tag	UNP D5QCK0
T	287	GLN	-	expression tag	UNP D5QCK0
T	288	GLY	-	expression tag	UNP D5QCK0
T	289	PRO	-	expression tag	UNP D5QCK0
T	290	MET	-	expression tag	UNP D5QCK0
T	291	GLY	-	expression tag	UNP D5QCK0
T	292	SER	-	expression tag	UNP D5QCK0
U	265	MET	-	initiating methionine	UNP D5QCK0
U	266	SER	-	expression tag	UNP D5QCK0
U	267	TYR	-	expression tag	UNP D5QCK0
U	268	TYR	-	expression tag	UNP D5QCK0
U	269	HIS	-	expression tag	UNP D5QCK0
U	270	HIS	-	expression tag	UNP D5QCK0

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Chain	Residue	Modelled	Actual	Comment	Reference
U	271	HIS	-	expression tag	UNP D5QCK0
U	272	HIS	-	expression tag	UNP D5QCK0
U	273	HIS	-	expression tag	UNP D5QCK0
U	274	HIS	-	expression tag	UNP D5QCK0
U	275	ASP	-	expression tag	UNP D5QCK0
U	276	TYR	-	expression tag	UNP D5QCK0
U	277	ASP	-	expression tag	UNP D5QCK0
U	278	ILE	-	expression tag	UNP D5QCK0
U	279	PRO	-	expression tag	UNP D5QCK0
U	280	THR	-	expression tag	UNP D5QCK0
U	281	THR	-	expression tag	UNP D5QCK0
U	282	LEU	-	expression tag	UNP D5QCK0
U	283	GLU	-	expression tag	UNP D5QCK0
U	284	VAL	-	expression tag	UNP D5QCK0
U	285	LEU	-	expression tag	UNP D5QCK0
U	286	PHE	-	expression tag	UNP D5QCK0
U	287	GLN	-	expression tag	UNP D5QCK0
U	288	GLY	-	expression tag	UNP D5QCK0
U	289	PRO	-	expression tag	UNP D5QCK0
U	290	MET	-	expression tag	UNP D5QCK0
U	291	GLY	-	expression tag	UNP D5QCK0
U	292	SER	-	expression tag	UNP D5QCK0
V	265	MET	-	initiating methionine	UNP D5QCK0
V	266	SER	-	expression tag	UNP D5QCK0
V	267	TYR	-	expression tag	UNP D5QCK0
V	268	TYR	-	expression tag	UNP D5QCK0
V	269	HIS	-	expression tag	UNP D5QCK0
V	270	HIS	-	expression tag	UNP D5QCK0
V	271	HIS	-	expression tag	UNP D5QCK0
V	272	HIS	-	expression tag	UNP D5QCK0
V	273	HIS	-	expression tag	UNP D5QCK0
V	274	HIS	-	expression tag	UNP D5QCK0
V	275	ASP	-	expression tag	UNP D5QCK0
V	276	TYR	-	expression tag	UNP D5QCK0
V	277	ASP	-	expression tag	UNP D5QCK0
V	278	ILE	-	expression tag	UNP D5QCK0
V	279	PRO	-	expression tag	UNP D5QCK0
V	280	THR	-	expression tag	UNP D5QCK0
V	281	THR	-	expression tag	UNP D5QCK0
V	282	LEU	-	expression tag	UNP D5QCK0
V	283	GLU	-	expression tag	UNP D5QCK0
V	284	VAL	-	expression tag	UNP D5QCK0

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Chain	Residue	Modelled	Actual	Comment	Reference
V	285	LEU	-	expression tag	UNP D5QCK0
V	286	PHE	-	expression tag	UNP D5QCK0
V	287	GLN	-	expression tag	UNP D5QCK0
V	288	GLY	-	expression tag	UNP D5QCK0
V	289	PRO	-	expression tag	UNP D5QCK0
V	290	MET	-	expression tag	UNP D5QCK0
V	291	GLY	-	expression tag	UNP D5QCK0
V	292	SER	-	expression tag	UNP D5QCK0
X	265	MET	-	initiating methionine	UNP D5QCK0
X	266	SER	-	expression tag	UNP D5QCK0
X	267	TYR	-	expression tag	UNP D5QCK0
X	268	TYR	-	expression tag	UNP D5QCK0
X	269	HIS	-	expression tag	UNP D5QCK0
X	270	HIS	-	expression tag	UNP D5QCK0
X	271	HIS	-	expression tag	UNP D5QCK0
X	272	HIS	-	expression tag	UNP D5QCK0
X	273	HIS	-	expression tag	UNP D5QCK0
X	274	HIS	-	expression tag	UNP D5QCK0
X	275	ASP	-	expression tag	UNP D5QCK0
X	276	TYR	-	expression tag	UNP D5QCK0
X	277	ASP	-	expression tag	UNP D5QCK0
X	278	ILE	-	expression tag	UNP D5QCK0
X	279	PRO	-	expression tag	UNP D5QCK0
X	280	THR	-	expression tag	UNP D5QCK0
X	281	THR	-	expression tag	UNP D5QCK0
X	282	LEU	-	expression tag	UNP D5QCK0
X	283	GLU	-	expression tag	UNP D5QCK0
X	284	VAL	-	expression tag	UNP D5QCK0
X	285	LEU	-	expression tag	UNP D5QCK0
X	286	PHE	-	expression tag	UNP D5QCK0
X	287	GLN	-	expression tag	UNP D5QCK0
X	288	GLY	-	expression tag	UNP D5QCK0
X	289	PRO	-	expression tag	UNP D5QCK0
X	290	MET	-	expression tag	UNP D5QCK0
X	291	GLY	-	expression tag	UNP D5QCK0
X	292	SER	-	expression tag	UNP D5QCK0
Y	265	MET	-	initiating methionine	UNP D5QCK0
Y	266	SER	-	expression tag	UNP D5QCK0
Y	267	TYR	-	expression tag	UNP D5QCK0
Y	268	TYR	-	expression tag	UNP D5QCK0
Y	269	HIS	-	expression tag	UNP D5QCK0
Y	270	HIS	-	expression tag	UNP D5QCK0

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	271	HIS	-	expression tag	UNP D5QCK0
Y	272	HIS	-	expression tag	UNP D5QCK0
Y	273	HIS	-	expression tag	UNP D5QCK0
Y	274	HIS	-	expression tag	UNP D5QCK0
Y	275	ASP	-	expression tag	UNP D5QCK0
Y	276	TYR	-	expression tag	UNP D5QCK0
Y	277	ASP	-	expression tag	UNP D5QCK0
Y	278	ILE	-	expression tag	UNP D5QCK0
Y	279	PRO	-	expression tag	UNP D5QCK0
Y	280	THR	-	expression tag	UNP D5QCK0
Y	281	THR	-	expression tag	UNP D5QCK0
Y	282	LEU	-	expression tag	UNP D5QCK0
Y	283	GLU	-	expression tag	UNP D5QCK0
Y	284	VAL	-	expression tag	UNP D5QCK0
Y	285	LEU	-	expression tag	UNP D5QCK0
Y	286	PHE	-	expression tag	UNP D5QCK0
Y	287	GLN	-	expression tag	UNP D5QCK0
Y	288	GLY	-	expression tag	UNP D5QCK0
Y	289	PRO	-	expression tag	UNP D5QCK0
Y	290	MET	-	expression tag	UNP D5QCK0
Y	291	GLY	-	expression tag	UNP D5QCK0
Y	292	SER	-	expression tag	UNP D5QCK0
Z	265	MET	-	initiating methionine	UNP D5QCK0
Z	266	SER	-	expression tag	UNP D5QCK0
Z	267	TYR	-	expression tag	UNP D5QCK0
Z	268	TYR	-	expression tag	UNP D5QCK0
Z	269	HIS	-	expression tag	UNP D5QCK0
Z	270	HIS	-	expression tag	UNP D5QCK0
Z	271	HIS	-	expression tag	UNP D5QCK0
Z	272	HIS	-	expression tag	UNP D5QCK0
Z	273	HIS	-	expression tag	UNP D5QCK0
Z	274	HIS	-	expression tag	UNP D5QCK0
Z	275	ASP	-	expression tag	UNP D5QCK0
Z	276	TYR	-	expression tag	UNP D5QCK0
Z	277	ASP	-	expression tag	UNP D5QCK0
Z	278	ILE	-	expression tag	UNP D5QCK0
Z	279	PRO	-	expression tag	UNP D5QCK0
Z	280	THR	-	expression tag	UNP D5QCK0
Z	281	THR	-	expression tag	UNP D5QCK0
Z	282	LEU	-	expression tag	UNP D5QCK0
Z	283	GLU	-	expression tag	UNP D5QCK0
Z	284	VAL	-	expression tag	UNP D5QCK0

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	285	LEU	-	expression tag	UNP D5QCK0
Z	286	PHE	-	expression tag	UNP D5QCK0
Z	287	GLN	-	expression tag	UNP D5QCK0
Z	288	GLY	-	expression tag	UNP D5QCK0
Z	289	PRO	-	expression tag	UNP D5QCK0
Z	290	MET	-	expression tag	UNP D5QCK0
Z	291	GLY	-	expression tag	UNP D5QCK0
Z	292	SER	-	expression tag	UNP D5QCK0
a	265	MET	-	initiating methionine	UNP D5QCK0
a	266	SER	-	expression tag	UNP D5QCK0
a	267	TYR	-	expression tag	UNP D5QCK0
a	268	TYR	-	expression tag	UNP D5QCK0
a	269	HIS	-	expression tag	UNP D5QCK0
a	270	HIS	-	expression tag	UNP D5QCK0
a	271	HIS	-	expression tag	UNP D5QCK0
a	272	HIS	-	expression tag	UNP D5QCK0
a	273	HIS	-	expression tag	UNP D5QCK0
a	274	HIS	-	expression tag	UNP D5QCK0
a	275	ASP	-	expression tag	UNP D5QCK0
a	276	TYR	-	expression tag	UNP D5QCK0
a	277	ASP	-	expression tag	UNP D5QCK0
a	278	ILE	-	expression tag	UNP D5QCK0
a	279	PRO	-	expression tag	UNP D5QCK0
a	280	THR	-	expression tag	UNP D5QCK0
a	281	THR	-	expression tag	UNP D5QCK0
a	282	LEU	-	expression tag	UNP D5QCK0
a	283	GLU	-	expression tag	UNP D5QCK0
a	284	VAL	-	expression tag	UNP D5QCK0
a	285	LEU	-	expression tag	UNP D5QCK0
a	286	PHE	-	expression tag	UNP D5QCK0
a	287	GLN	-	expression tag	UNP D5QCK0
a	288	GLY	-	expression tag	UNP D5QCK0
a	289	PRO	-	expression tag	UNP D5QCK0
a	290	MET	-	expression tag	UNP D5QCK0
a	291	GLY	-	expression tag	UNP D5QCK0
a	292	SER	-	expression tag	UNP D5QCK0
b	265	MET	-	initiating methionine	UNP D5QCK0
b	266	SER	-	expression tag	UNP D5QCK0
b	267	TYR	-	expression tag	UNP D5QCK0
b	268	TYR	-	expression tag	UNP D5QCK0
b	269	HIS	-	expression tag	UNP D5QCK0
b	270	HIS	-	expression tag	UNP D5QCK0

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Chain	Residue	Modelled	Actual	Comment	Reference
b	271	HIS	-	expression tag	UNP D5QCK0
b	272	HIS	-	expression tag	UNP D5QCK0
b	273	HIS	-	expression tag	UNP D5QCK0
b	274	HIS	-	expression tag	UNP D5QCK0
b	275	ASP	-	expression tag	UNP D5QCK0
b	276	TYR	-	expression tag	UNP D5QCK0
b	277	ASP	-	expression tag	UNP D5QCK0
b	278	ILE	-	expression tag	UNP D5QCK0
b	279	PRO	-	expression tag	UNP D5QCK0
b	280	THR	-	expression tag	UNP D5QCK0
b	281	THR	-	expression tag	UNP D5QCK0
b	282	LEU	-	expression tag	UNP D5QCK0
b	283	GLU	-	expression tag	UNP D5QCK0
b	284	VAL	-	expression tag	UNP D5QCK0
b	285	LEU	-	expression tag	UNP D5QCK0
b	286	PHE	-	expression tag	UNP D5QCK0
b	287	GLN	-	expression tag	UNP D5QCK0
b	288	GLY	-	expression tag	UNP D5QCK0
b	289	PRO	-	expression tag	UNP D5QCK0
b	290	MET	-	expression tag	UNP D5QCK0
b	291	GLY	-	expression tag	UNP D5QCK0
b	292	SER	-	expression tag	UNP D5QCK0
d	265	MET	-	initiating methionine	UNP D5QCK0
d	266	SER	-	expression tag	UNP D5QCK0
d	267	TYR	-	expression tag	UNP D5QCK0
d	268	TYR	-	expression tag	UNP D5QCK0
d	269	HIS	-	expression tag	UNP D5QCK0
d	270	HIS	-	expression tag	UNP D5QCK0
d	271	HIS	-	expression tag	UNP D5QCK0
d	272	HIS	-	expression tag	UNP D5QCK0
d	273	HIS	-	expression tag	UNP D5QCK0
d	274	HIS	-	expression tag	UNP D5QCK0
d	275	ASP	-	expression tag	UNP D5QCK0
d	276	TYR	-	expression tag	UNP D5QCK0
d	277	ASP	-	expression tag	UNP D5QCK0
d	278	ILE	-	expression tag	UNP D5QCK0
d	279	PRO	-	expression tag	UNP D5QCK0
d	280	THR	-	expression tag	UNP D5QCK0
d	281	THR	-	expression tag	UNP D5QCK0
d	282	LEU	-	expression tag	UNP D5QCK0
d	283	GLU	-	expression tag	UNP D5QCK0
d	284	VAL	-	expression tag	UNP D5QCK0

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Chain	Residue	Modelled	Actual	Comment	Reference
d	285	LEU	-	expression tag	UNP D5QCK0
d	286	PHE	-	expression tag	UNP D5QCK0
d	287	GLN	-	expression tag	UNP D5QCK0
d	288	GLY	-	expression tag	UNP D5QCK0
d	289	PRO	-	expression tag	UNP D5QCK0
d	290	MET	-	expression tag	UNP D5QCK0
d	291	GLY	-	expression tag	UNP D5QCK0
d	292	SER	-	expression tag	UNP D5QCK0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	AltConf
3	A	8	Total O 8 8	0
3	B	4	Total O 4 4	0
3	C	8	Total O 8 8	0
3	D	7	Total O 7 7	0
3	E	5	Total O 5 5	0
3	F	5	Total O 5 5	0
3	G	5	Total O 5 5	0
3	H	6	Total O 6 6	0
3	I	6	Total O 6 6	0
3	J	7	Total O 7 7	0
3	K	5	Total O 5 5	0
3	L	6	Total O 6 6	0
3	M	11	Total O 11 11	0
3	N	6	Total O 6 6	0
3	O	8	Total O 8 8	0

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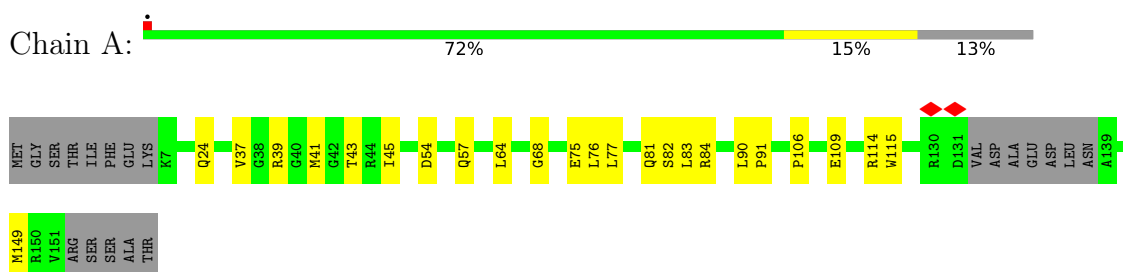
Mol	Chain	Residues	Atoms		AltConf
3	P	8	Total	O	0
			8	8	



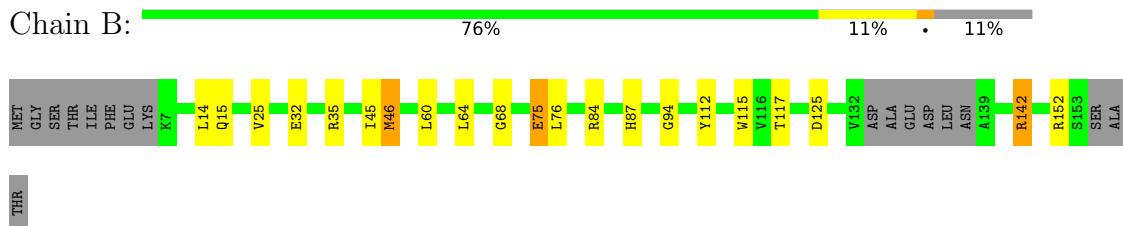
### 3 Residue-property plots [i](#)

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.

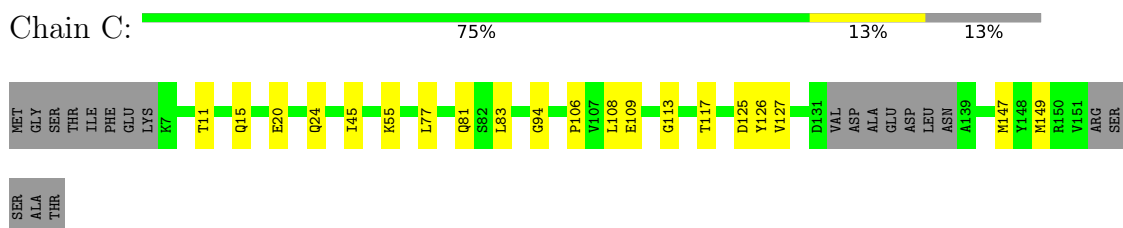
- Molecule 1: Cellulose biosynthesis protein



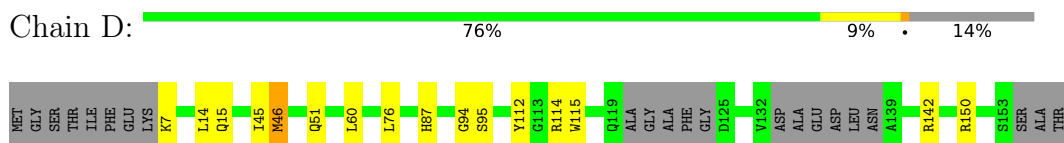
- Molecule 1: Cellulose biosynthesis protein



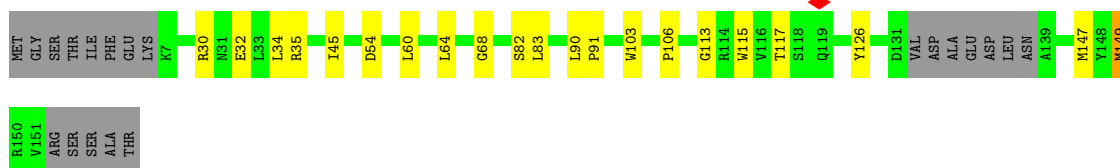
- Molecule 1: Cellulose biosynthesis protein



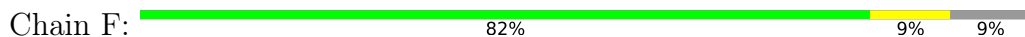
- Molecule 1: Cellulose biosynthesis protein



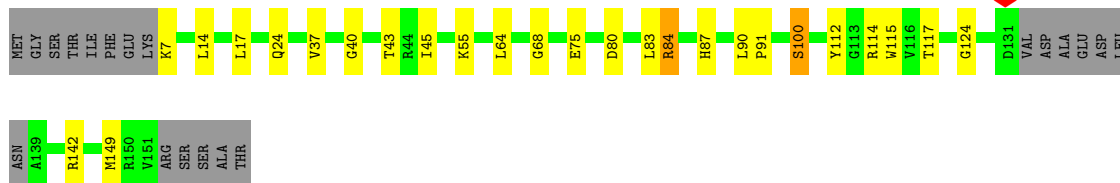
- Molecule 1: Cellulose biosynthesis protein



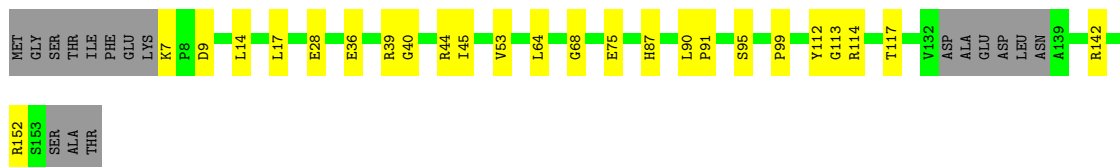
• Molecule 1: Cellulose biosynthesis protein



• Molecule 1: Cellulose biosynthesis protein



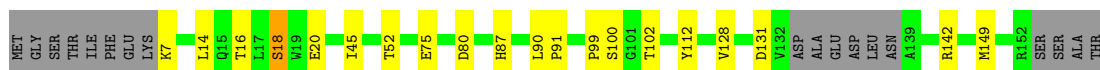
• Molecule 1: Cellulose biosynthesis protein



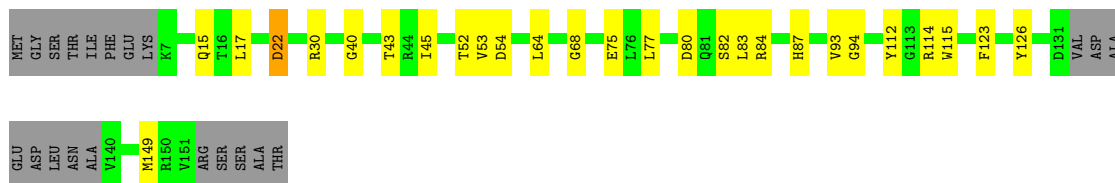
• Molecule 1: Cellulose biosynthesis protein



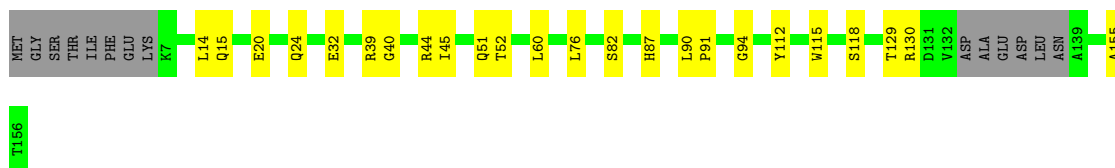
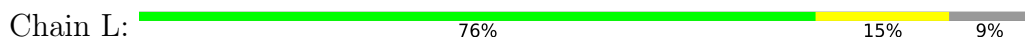
• Molecule 1: Cellulose biosynthesis protein



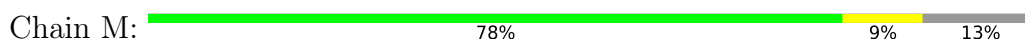
• Molecule 1: Cellulose biosynthesis protein



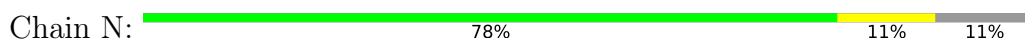
• Molecule 1: Cellulose biosynthesis protein



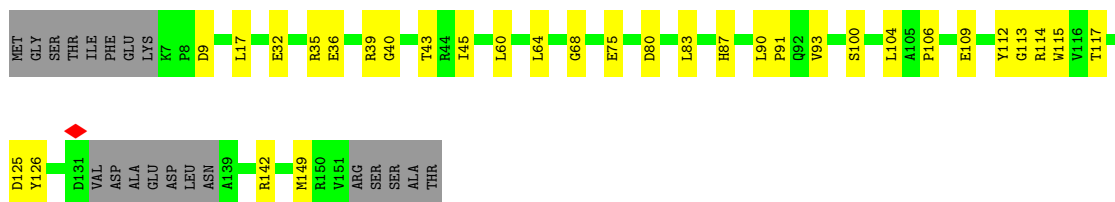
• Molecule 1: Cellulose biosynthesis protein



• Molecule 1: Cellulose biosynthesis protein



• Molecule 1: Cellulose biosynthesis protein



• Molecule 1: Cellulose biosynthesis protein





ASN  
GLU  
GLU  
SER

• Molecule 2: BcsH fragment



MET SER TYR TYR HIS HIS HIS HIS ASP ASP TYR ILE PRO THR THR LEU LEU VAL LEU PHE GLN GLY PRO MET GLY SER THR LYS THR ASP THR ASN SER SER GLN ALA SER ARG PRO GLY SER PRO VAL ALA SER PRO D313 V321 F322 M323 G327 ARG ALA THR LEU

LEU SER PRO ARG P337 R346 ARG GLU ASN ASP TYR LEU LEU SER

• Molecule 2: BcsH fragment



MET SER TYR HIS HIS HIS HIS ASP ASP ILE PRO THR THR LEU LEU VAL LEU PHE GLN GLY PRO MET GLY SER THR LYS THR ASP THR ASN SER SER GLN ALA SER ARG PRO GLY SER PRO VAL ALA SER PRO F312 E320 M323 R328 A329 THR LEU LEU SER

PRO ARG P337 R345 R346 ARG GLU ASN ASP TYR LEU LEU SER

• Molecule 2: BcsH fragment



MET SER TYR TYR HIS HIS HIS HIS ASP ASP ILE PRO THR THR LEU LEU VAL LEU PHE GLN GLY PRO MET GLY SER THR LYS THR ASP THR ASN SER SER GLN ALA SER ARG PRO GLY SER PRO VAL ALA SER PRO D313 V321 G327 ARG ALA THR LEU LEU SER

PRO ARG PRO SER LEU ARG ALA LEU ARG ARG ARG GLU ASN LEU LEU SER

• Molecule 2: BcsH fragment



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

LEU GLY ARG ALA THR LEU SER PRO ARG P337 S338 L339 R345 R346 ARG ASN GLU GLU SER

• Molecule 2: BcsH fragment



MET SER TYR HIS HIS HIS HIS ASP ASP ILE PRO THR THR LEU LEU VAL LEU PHE GLN GLY PRO MET GLY SER THR LYS THR ASP THR ASN SER SER GLN ALA SER ARG PRO GLY SER PRO VAL ALA SER PRO D313 V321 G326 ARG ALA THR LEU LEU SER



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1425195	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 ( $e^-/\text{\AA}^2$ )	49.9	Depositor
Minimum defocus (nm)	480	Depositor
Maximum defocus (nm)	2750	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.037	Depositor
Minimum map value	-0.302	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.23	Depositor
Map size ( $\text{\AA}$ )	377.55, 377.55, 377.55	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.839, 0.839, 0.839	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	0.25	0/1109	0.50	0/1510
1	B	0.25	0/1133	0.49	0/1542
1	C	0.25	0/1120	0.48	0/1524
1	D	0.24	0/1102	0.48	0/1499
1	E	0.24	0/1109	0.48	0/1510
1	F	0.24	0/1154	0.49	0/1570
1	G	0.24	0/1109	0.47	0/1510
1	H	0.24	0/1136	0.48	0/1545
1	I	0.24	0/1120	0.48	0/1524
1	J	0.24	0/1119	0.48	0/1523
1	K	0.24	0/1104	0.48	0/1503
1	L	0.24	0/1154	0.49	0/1570
1	M	0.24	0/1120	0.48	0/1524
1	N	0.24	0/1125	0.48	0/1531
1	O	0.25	0/1120	0.50	0/1524
1	P	0.25	0/1115	0.49	0/1515
1	W	0.23	0/41	0.67	0/54
1	c	0.24	0/41	0.65	0/54
2	Q	0.33	0/262	0.62	0/352
2	R	0.24	0/270	0.55	0/363
2	S	0.24	0/188	0.51	0/249
2	T	0.26	0/212	0.59	0/281
2	U	0.25	0/104	0.42	0/139
2	V	0.22	0/84	0.65	0/110
2	X	0.25	0/100	0.38	0/134
2	Y	0.22	0/92	0.62	0/122
2	Z	0.27	0/104	0.39	0/139
2	a	0.21	0/84	0.62	0/111
2	b	0.25	0/152	0.48	0/204
2	d	0.21	0/84	0.62	0/110
All	All	0.24	0/19767	0.49	0/26846

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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	1088	0	1095	12	0
1	B	1112	0	1122	16	0
1	C	1099	0	1107	12	0
1	D	1083	0	1096	12	0
1	E	1088	0	1095	13	0
1	F	1133	0	1142	7	0
1	G	1088	0	1095	17	0
1	H	1115	0	1125	16	0
1	I	1099	0	1107	12	0
1	J	1098	0	1108	10	0
1	K	1083	0	1090	14	0
1	L	1133	0	1142	15	0
1	M	1099	0	1107	7	0
1	N	1104	0	1113	9	0
1	O	1099	0	1107	18	0
1	P	1096	0	1107	10	0
1	W	42	0	43	1	0
1	c	42	0	43	0	0
2	Q	259	0	269	4	0
2	R	266	0	277	2	0
2	S	187	0	191	1	0
2	T	210	0	217	2	0
2	U	103	0	96	1	0
2	V	84	0	95	2	0
2	X	99	0	93	2	0
2	Y	91	0	102	0	0
2	Z	103	0	96	1	0
2	a	84	0	94	0	0
2	b	151	0	149	0	0
2	d	84	0	95	0	0
3	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	0	0
3	C	8	0	0	0	0
3	D	7	0	0	1	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	6	0	0	0	0
3	I	6	0	0	0	0
3	J	7	0	0	0	0
3	K	5	0	0	0	0
3	L	6	0	0	0	0
3	M	11	0	0	0	0
3	N	6	0	0	0	0
3	O	8	0	0	0	0
3	P	8	0	0	0	0
All	All	19527	0	19618	184	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 5.

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LEU:HD22	2:X:321:VAL:HG22	1.58	0.86
1:G:83:LEU:HB3	1:G:149:MET:HB2	1.64	0.78
1:I:36:GLU:OE2	1:I:39:ARG:NH1	2.21	0.74
1:L:129:THR:HG21	2:Q:328:ARG:HH12	1.53	0.73
1:O:113:GLY:O	1:O:117:THR:OG1	2.09	0.70
1:J:128:VAL:HG22	1:J:149:MET:HG3	1.75	0.68
1:B:87:HIS:ND1	1:B:112:TYR:OH	2.26	0.68
1:K:75:GLU:HG3	1:K:84:ARG:HB3	1.75	0.67
1:E:113:GLY:O	1:E:117:THR:OG1	2.12	0.67
1:A:54:ASP:OD2	1:F:142:ARG:NH2	2.20	0.66
1:K:87:HIS:ND1	1:K:112:TYR:OH	2.30	0.65
1:P:76:LEU:HD22	2:Z:321:VAL:HG22	1.77	0.65
1:C:83:LEU:HB3	1:C:149:MET:HB2	1.79	0.64
1:O:126:TYR:HB3	1:O:149:MET:HB3	1.79	0.64
1:I:54:ASP:OD2	1:N:142:ARG:NH2	2.31	0.64
1:B:45:ILE:HG22	1:D:45:ILE:HG22	1.81	0.63
1:H:36:GLU:OE1	1:H:39:ARG:NH2	2.26	0.62
1:J:45:ILE:HG22	1:L:45:ILE:HG22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:GLU:HG2	1:B:84:ARG:HB3	1.83	0.60
1:B:125:ASP:OD2	1:B:152:ARG:NH1	2.34	0.59
1:E:126:TYR:HB3	1:E:149:MET:HG3	1.83	0.59
1:F:87:HIS:ND1	1:F:112:TYR:OH	2.30	0.59
1:L:87:HIS:ND1	1:L:112:TYR:OH	2.32	0.59
1:N:128:VAL:HG22	1:N:149:MET:HG3	1.85	0.59
2:R:323:MET:HG2	2:R:330:THR:HA	1.84	0.58
1:B:64:LEU:O	1:B:68:GLY:N	2.37	0.58
1:O:80:ASP:OD1	1:O:80:ASP:N	2.36	0.58
1:F:45:ILE:HG22	1:H:45:ILE:HG22	1.86	0.58
1:C:126:TYR:HB3	1:C:149:MET:HB3	1.87	0.56
1:B:32:GLU:OE2	1:B:35:ARG:NH1	2.38	0.56
1:N:45:ILE:HG22	1:P:45:ILE:HG22	1.88	0.56
1:B:15:GLN:HG2	1:B:94:GLY:N	2.21	0.55
1:G:87:HIS:ND1	1:G:112:TYR:OH	2.34	0.55
1:G:90:LEU:HD12	1:G:91:PRO:HD2	1.89	0.55
1:A:64:LEU:O	1:A:68:GLY:N	2.38	0.55
1:E:64:LEU:O	1:E:68:GLY:N	2.39	0.55
1:B:25:VAL:HG11	2:V:339:LEU:HD12	1.87	0.55
1:H:87:HIS:ND1	1:H:112:TYR:OH	2.32	0.55
1:C:45:ILE:HG22	1:G:45:ILE:HG22	1.90	0.54
1:J:87:HIS:ND1	1:J:112:TYR:OH	2.40	0.54
1:G:80:ASP:OD1	1:G:80:ASP:N	2.40	0.54
1:K:53:VAL:HG22	1:K:123:PHE:HZ	1.73	0.54
1:M:87:HIS:ND1	1:M:112:TYR:OH	2.37	0.54
1:N:36:GLU:OE1	1:N:39:ARG:NH1	2.41	0.53
1:O:64:LEU:O	1:O:68:GLY:N	2.41	0.53
1:E:30:ARG:HD2	1:E:103:TRP:NE1	2.24	0.53
1:H:99:PRO:HB2	1:H:142:ARG:HE	1.73	0.53
1:D:94:GLY:HA3	3:D:204:HOH:O	2.09	0.53
2:T:320:GLU:HA	2:T:323:MET:HE2	1.91	0.53
1:I:64:LEU:O	1:I:68:GLY:N	2.42	0.53
1:E:83:LEU:HB3	1:E:149:MET:HB3	1.90	0.52
1:K:64:LEU:O	1:K:68:GLY:N	2.42	0.52
1:N:87:HIS:ND1	1:N:112:TYR:OH	2.35	0.52
1:G:64:LEU:O	1:G:68:GLY:N	2.43	0.51
1:G:117:THR:HA	1:G:124:GLY:HA2	1.93	0.51
1:B:76:LEU:HD13	2:X:321:VAL:HG13	1.93	0.51
1:H:117:THR:HG21	1:L:155:ALA:HB2	1.93	0.51
1:I:35:ARG:O	1:I:39:ARG:HG3	2.10	0.51
1:P:11:THR:O	1:P:15:GLN:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:HIS:ND1	1:D:112:TYR:OH	2.37	0.51
1:P:59:GLU:OE2	1:P:59:GLU:HA	2.11	0.50
1:P:86:VAL:HG22	1:P:146:ILE:HG12	1.94	0.50
1:F:25:VAL:HG13	1:F:29:VAL:HB	1.93	0.50
1:C:106:PRO:O	1:C:109:GLU:HB2	2.11	0.49
1:I:80:ASP:N	1:I:80:ASP:OD1	2.45	0.49
1:O:35:ARG:O	1:O:39:ARG:HG3	2.12	0.49
2:T:345:ARG:HB2	2:T:345:ARG:NH1	2.27	0.49
1:O:93:VAL:O	1:O:93:VAL:HG23	2.12	0.49
1:A:83:LEU:HB3	1:A:149:MET:HB2	1.94	0.49
1:O:90:LEU:HD11	1:O:104:LEU:HB2	1.93	0.49
1:K:52:THR:HG22	1:K:54:ASP:H	1.77	0.49
1:H:90:LEU:HD12	1:H:91:PRO:HD2	1.94	0.49
1:A:90:LEU:HD12	1:A:91:PRO:HD2	1.94	0.49
1:P:87:HIS:ND1	1:P:112:TYR:OH	2.37	0.49
1:A:45:ILE:HG22	1:E:45:ILE:HG22	1.95	0.49
1:D:76:LEU:HD22	2:U:321:VAL:HG22	1.95	0.49
1:C:77:LEU:O	1:C:81:GLN:N	2.46	0.48
1:K:93:VAL:O	1:K:93:VAL:HG23	2.13	0.48
1:O:100:SER:O	1:O:142:ARG:HD2	2.12	0.48
2:Q:319:ALA:O	2:Q:323:MET:HG3	2.13	0.48
1:G:75:GLU:HG2	1:G:84:ARG:HB3	1.95	0.48
1:O:87:HIS:ND1	1:O:112:TYR:OH	2.40	0.48
1:A:45:ILE:HD12	1:A:115:TRP:HZ2	1.79	0.47
1:P:90:LEU:HD12	1:P:91:PRO:HD2	1.95	0.47
1:F:36:GLU:OE2	1:F:39[B]:ARG:NH1	2.47	0.47
1:H:40:GLY:O	1:H:44:ARG:HG2	2.14	0.47
1:P:100:SER:O	1:P:142:ARG:HD2	2.14	0.47
1:K:77:LEU:HD12	1:K:82:SER:HB3	1.97	0.47
1:F:90:LEU:HD12	1:F:91:PRO:HD2	1.97	0.47
1:J:16:THR:O	1:J:20:GLU:HG2	2.14	0.47
1:G:40:GLY:O	1:G:43:THR:OG1	2.28	0.47
1:E:30:ARG:HD2	1:E:103:TRP:HE1	1.79	0.47
1:J:52:THR:HA	2:R:317:THR:HA	1.96	0.46
1:B:142:ARG:NH2	1:E:54:ASP:OD2	2.48	0.46
1:M:93:VAL:HG23	1:M:93:VAL:O	2.15	0.46
1:G:7:LYS:NZ	1:H:9:ASP:OD1	2.48	0.46
1:K:45:ILE:HG22	1:O:45:ILE:HG22	1.97	0.46
1:O:83:LEU:HB3	1:O:149:MET:HB2	1.95	0.46
1:B:117:THR:HG23	1:W:153:SER:OG	2.14	0.46
1:E:90:LEU:HD12	1:E:91:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:PRO:O	1:A:109:GLU:HB2	2.16	0.46
1:D:95:SER:O	1:G:55:LYS:NZ	2.48	0.45
1:E:113:GLY:HA2	1:E:149:MET:HE1	1.98	0.45
1:K:40:GLY:O	1:K:43:THR:OG1	2.30	0.45
1:D:112:TYR:HA	1:D:115:TRP:HB2	1.98	0.45
1:G:37:VAL:HG21	1:H:17:LEU:HD12	1.99	0.45
1:O:17:LEU:HD12	1:P:37:VAL:HG21	1.98	0.45
1:O:32:GLU:O	1:O:36:GLU:HG2	2.16	0.45
1:N:114:ARG:HH11	1:N:114:ARG:HG3	1.82	0.45
1:G:43:THR:HG23	1:G:114:ARG:HE	1.82	0.45
1:J:100:SER:O	1:J:142:ARG:HD2	2.17	0.45
1:L:90:LEU:HD12	1:L:91:PRO:HD2	1.99	0.45
1:B:14:LEU:HD23	1:B:14:LEU:HA	1.84	0.45
1:L:40:GLY:O	1:L:44:ARG:HG2	2.18	0.44
1:H:113:GLY:O	1:H:117:THR:OG1	2.28	0.44
1:J:7:LYS:HB3	1:J:7:LYS:HE3	1.86	0.44
1:E:34:LEU:HB2	1:E:106:PRO:HB2	1.98	0.44
1:M:90:LEU:HD12	1:M:91:PRO:HD2	2.00	0.44
1:B:46[A]:MET:HE1	1:D:46[A]:MET:HB2	2.00	0.44
1:O:40:GLY:O	1:O:43:THR:OG1	2.30	0.44
1:O:106:PRO:HA	1:O:109:GLU:HB2	2.00	0.44
1:K:80:ASP:N	1:K:80:ASP:OD1	2.51	0.44
1:J:90:LEU:HD12	1:J:91:PRO:HD2	2.00	0.44
1:I:20:GLU:OE1	1:I:24:GLN:NE2	2.41	0.44
1:P:46:MET:HE2	1:P:115:TRP:HD1	1.83	0.44
1:A:75:GLU:HG2	1:A:84:ARG:HB3	2.00	0.43
1:K:15:GLN:HG2	1:K:94:GLY:N	2.33	0.43
1:M:14:LEU:HD23	1:M:14:LEU:HA	1.87	0.43
1:A:77:LEU:O	1:A:81:GLN:HA	2.18	0.43
1:E:32:GLU:OE1	1:E:35:ARG:NH1	2.50	0.43
1:A:37:VAL:O	1:A:41:MET:HG3	2.19	0.43
1:G:17:LEU:HD21	1:H:17:LEU:HD21	2.00	0.43
1:M:37:VAL:HG21	1:N:17:LEU:HD12	1.99	0.43
1:G:100:SER:O	1:G:142:ARG:NH1	2.47	0.43
1:L:39[B]:ARG:HG3	1:L:40:GLY:N	2.33	0.43
1:L:51:GLN:HG3	1:L:52:THR:HG23	2.01	0.43
1:G:45:ILE:HD12	1:G:115:TRP:HZ2	1.84	0.43
1:E:60:LEU:HD22	1:E:115:TRP:CE3	2.53	0.42
1:C:15:GLN:HG2	1:C:94:GLY:N	2.34	0.42
1:J:14:LEU:O	1:J:18:SER:OG	2.38	0.42
1:J:99:PRO:O	1:J:102:THR:OG1	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:LEU:HD23	1:D:14:LEU:HA	1.93	0.42
1:M:127:VAL:O	1:M:149:MET:HA	2.19	0.42
1:B:25:VAL:HG11	2:V:339:LEU:CD1	2.49	0.42
1:H:7:LYS:HE3	1:H:7:LYS:HB2	1.72	0.42
1:K:83:LEU:HB3	1:K:149:MET:HB2	2.01	0.42
1:I:42:GLY:HA3	1:I:114[A]:ARG:HG2	2.01	0.42
1:L:60:LEU:HD22	1:L:115:TRP:CE3	2.55	0.42
1:A:39:ARG:O	1:A:43:THR:HG23	2.19	0.41
1:K:45:ILE:HD12	1:K:115:TRP:HZ2	1.84	0.41
1:L:115:TRP:O	1:L:118:SER:OG	2.26	0.41
1:C:55:LYS:HG2	1:H:95:SER:HB2	2.03	0.41
1:L:14:LEU:HD23	1:L:14:LEU:HA	1.87	0.41
1:C:113:GLY:O	1:C:117:THR:OG1	2.29	0.41
1:D:142:ARG:HD3	1:D:142:ARG:HA	1.80	0.41
1:G:14:LEU:HD21	1:H:14:LEU:HD21	2.02	0.41
1:K:22:ASP:OD2	1:K:30:ARG:NH2	2.42	0.41
1:O:60:LEU:HD22	1:O:115:TRP:CE3	2.56	0.41
1:C:20:GLU:O	1:C:24:GLN:HG3	2.21	0.41
1:I:34:LEU:HB2	1:I:106:PRO:HB2	2.02	0.41
1:L:32:GLU:HG2	2:Q:336:ARG:HH21	1.86	0.41
1:C:108:LEU:HB3	1:C:147:MET:HE1	2.02	0.41
1:D:15:GLN:HG2	1:D:94:GLY:N	2.35	0.41
1:I:14:LEU:HD23	1:I:14:LEU:HA	1.87	0.41
1:O:39:ARG:HA	1:O:114[B]:ARG:HG3	2.03	0.41
1:B:60:LEU:HD22	1:B:115:TRP:CE3	2.55	0.41
1:C:11:THR:O	1:C:15:GLN:HG3	2.20	0.41
1:D:7:LYS:HE2	1:D:7:LYS:HB2	1.90	0.41
1:I:60:LEU:HD22	1:I:115:TRP:CE3	2.56	0.41
1:C:127:VAL:O	1:C:149:MET:HA	2.22	0.40
1:F:20:GLU:O	1:F:24:GLN:HG3	2.21	0.40
1:H:53:VAL:HG23	2:Q:316:PRO:O	2.21	0.40
1:O:90:LEU:HD12	1:O:91:PRO:HD2	2.03	0.40
1:I:117:THR:HA	1:I:123:PHE:O	2.21	0.40
1:L:15:GLN:HG2	1:L:94:GLY:N	2.36	0.40
1:A:76:LEU:HD12	1:A:82:SER:O	2.22	0.40
1:I:43:THR:HG22	1:I:114[A]:ARG:HE	1.86	0.40
1:L:20:GLU:O	1:L:24:GLN:HG3	2.21	0.40
1:M:117:THR:HA	1:M:123:PHE:O	2.22	0.40
1:L:76:LEU:HD13	2:S:321:VAL:HG22	2.04	0.40
1:N:20:GLU:O	1:N:24:GLN:HG3	2.21	0.40
1:N:83:LEU:HB3	1:N:149:MET:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:LEU:HD22	1:D:115:TRP:CE3	2.56	0.40
1:H:64:LEU:O	1:H:68:GLY:N	2.54	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	135/158 (85%)	130 (96%)	5 (4%)	0	100	100
1	B	138/158 (87%)	136 (99%)	2 (1%)	0	100	100
1	C	136/158 (86%)	134 (98%)	2 (2%)	0	100	100
1	D	131/158 (83%)	129 (98%)	2 (2%)	0	100	100
1	E	135/158 (85%)	132 (98%)	3 (2%)	0	100	100
1	F	141/158 (89%)	138 (98%)	3 (2%)	0	100	100
1	G	135/158 (85%)	131 (97%)	4 (3%)	0	100	100
1	H	138/158 (87%)	136 (99%)	2 (1%)	0	100	100
1	I	136/158 (86%)	131 (96%)	5 (4%)	0	100	100
1	J	136/158 (86%)	133 (98%)	3 (2%)	0	100	100
1	K	134/158 (85%)	132 (98%)	1 (1%)	1 (1%)	22	43
1	L	141/158 (89%)	138 (98%)	3 (2%)	0	100	100
1	M	136/158 (86%)	132 (97%)	4 (3%)	0	100	100
1	N	137/158 (87%)	136 (99%)	1 (1%)	0	100	100
1	O	136/158 (86%)	133 (98%)	3 (2%)	0	100	100
1	P	133/158 (84%)	131 (98%)	2 (2%)	0	100	100
1	W	4/158 (2%)	4 (100%)	0	0	100	100
1	c	4/158 (2%)	4 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	32/89 (36%)	32 (100%)	0	0	100	100
2	R	33/89 (37%)	33 (100%)	0	0	100	100
2	S	21/89 (24%)	21 (100%)	0	0	100	100
2	T	24/89 (27%)	24 (100%)	0	0	100	100
2	U	13/89 (15%)	13 (100%)	0	0	100	100
2	V	8/89 (9%)	8 (100%)	0	0	100	100
2	X	12/89 (14%)	12 (100%)	0	0	100	100
2	Y	9/89 (10%)	9 (100%)	0	0	100	100
2	Z	13/89 (15%)	13 (100%)	0	0	100	100
2	a	8/89 (9%)	8 (100%)	0	0	100	100
2	b	19/89 (21%)	19 (100%)	0	0	100	100
2	d	8/89 (9%)	8 (100%)	0	0	100	100
All	All	2386/3912 (61%)	2340 (98%)	45 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	126	TYR

### 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	119/135 (88%)	116 (98%)	3 (2%)	47	73
1	B	122/135 (90%)	118 (97%)	4 (3%)	38	64
1	C	120/135 (89%)	119 (99%)	1 (1%)	81	92
1	D	121/135 (90%)	116 (96%)	5 (4%)	30	56
1	E	119/135 (88%)	116 (98%)	3 (2%)	47	73
1	F	124/135 (92%)	122 (98%)	2 (2%)	62	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	119/135 (88%)	116 (98%)	3 (2%)	47	73
1	H	122/135 (90%)	118 (97%)	4 (3%)	38	64
1	I	120/135 (89%)	119 (99%)	1 (1%)	81	92
1	J	120/135 (89%)	116 (97%)	4 (3%)	38	64
1	K	119/135 (88%)	116 (98%)	3 (2%)	47	73
1	L	124/135 (92%)	122 (98%)	2 (2%)	62	82
1	M	120/135 (89%)	115 (96%)	5 (4%)	30	55
1	N	121/135 (90%)	117 (97%)	4 (3%)	38	64
1	O	120/135 (89%)	117 (98%)	3 (2%)	47	73
1	P	122/135 (90%)	118 (97%)	4 (3%)	38	64
1	W	5/135 (4%)	5 (100%)	0	100	100
1	c	5/135 (4%)	5 (100%)	0	100	100
2	Q	28/78 (36%)	27 (96%)	1 (4%)	35	61
2	R	29/78 (37%)	28 (97%)	1 (3%)	37	63
2	S	20/78 (26%)	19 (95%)	1 (5%)	24	47
2	T	22/78 (28%)	22 (100%)	0	100	100
2	U	11/78 (14%)	11 (100%)	0	100	100
2	V	9/78 (12%)	9 (100%)	0	100	100
2	X	11/78 (14%)	11 (100%)	0	100	100
2	Y	10/78 (13%)	10 (100%)	0	100	100
2	Z	11/78 (14%)	11 (100%)	0	100	100
2	a	9/78 (12%)	9 (100%)	0	100	100
2	b	16/78 (20%)	16 (100%)	0	100	100
2	d	9/78 (12%)	7 (78%)	2 (22%)	1	1
All	All	2127/3366 (63%)	2071 (97%)	56 (3%)	50	72

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	57	GLN
1	A	114	ARG
1	B	46[A]	MET
1	B	46[B]	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	75	GLU
1	B	142	ARG
1	C	125	ASP
1	D	46[A]	MET
1	D	46[B]	MET
1	D	51	GLN
1	D	114	ARG
1	D	150	ARG
1	E	82	SER
1	E	147	MET
1	E	149	MET
1	F	9	ASP
1	F	78	SER
1	G	24	GLN
1	G	84	ARG
1	G	100	SER
1	H	28	GLU
1	H	75	GLU
1	H	114	ARG
1	H	152	ARG
1	I	36	GLU
1	J	18	SER
1	J	75	GLU
1	J	80	ASP
1	J	131	ASP
1	K	17	LEU
1	K	22	ASP
1	K	114	ARG
1	L	82	SER
1	L	130	ARG
1	M	9	ASP
1	M	100	SER
1	M	114[A]	ARG
1	M	114[B]	ARG
1	M	125	ASP
1	N	23	ASP
1	N	46	MET
1	N	78	SER
1	N	125	ASP
1	O	9	ASP
1	O	75	GLU
1	O	125	ASP

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Mol	Chain	Res	Type
1	P	51	GLN
1	P	78	SER
1	P	100	SER
1	P	114	ARG
2	Q	313	ASP
2	R	336	ARG
2	S	323	MET
2	d	345	ARG
2	d	346	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	81	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

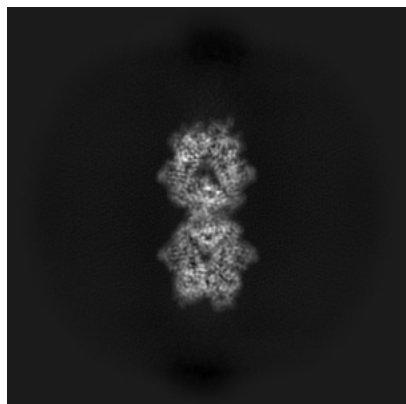
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15039. These allow visual inspection of the internal detail of the map and identification of artifacts.

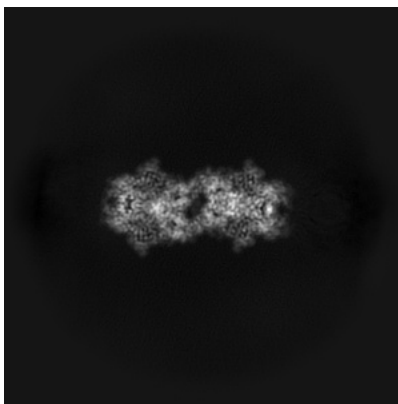
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

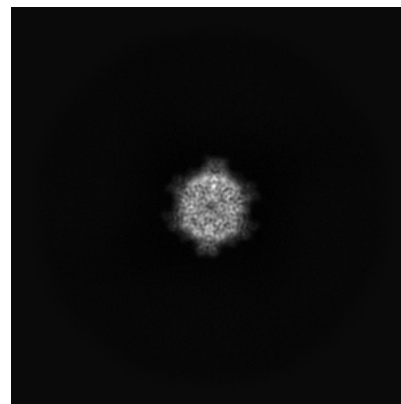
#### 6.1.1 Primary map



X

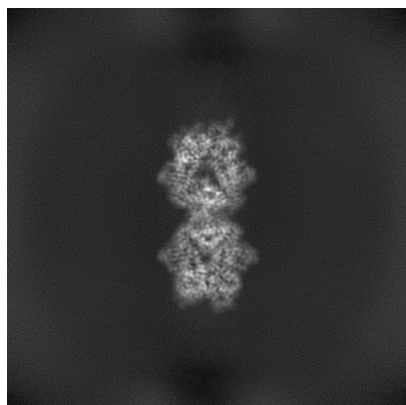


Y

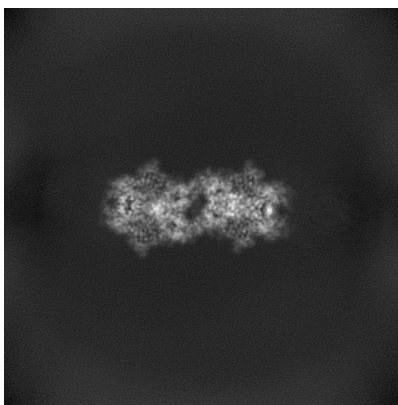


Z

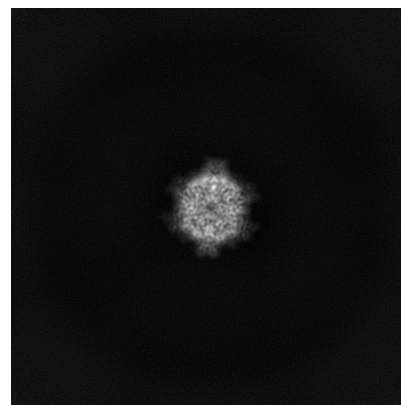
#### 6.1.2 Raw map



X



Y

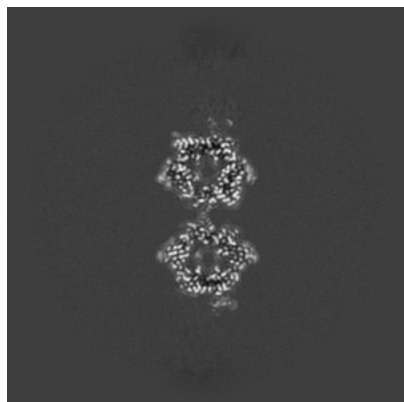


Z

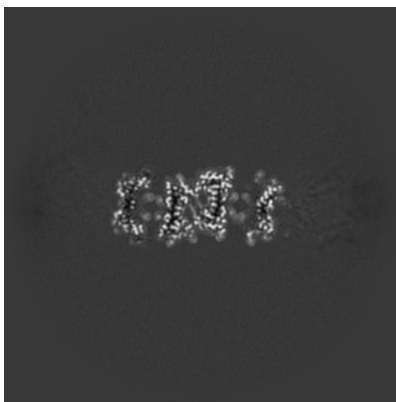
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

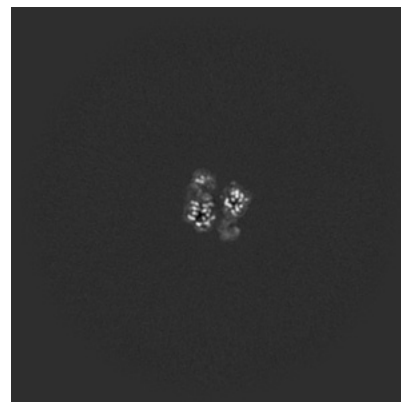
### 6.2.1 Primary map



X Index: 225

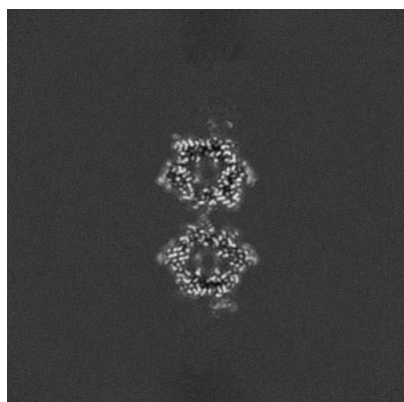


Y Index: 225

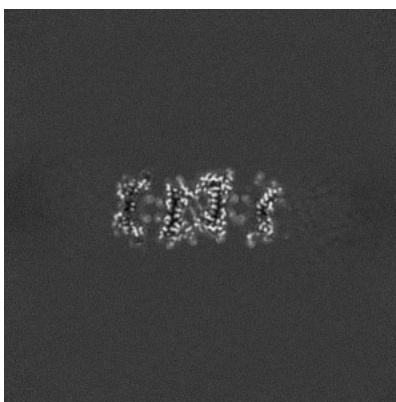


Z Index: 225

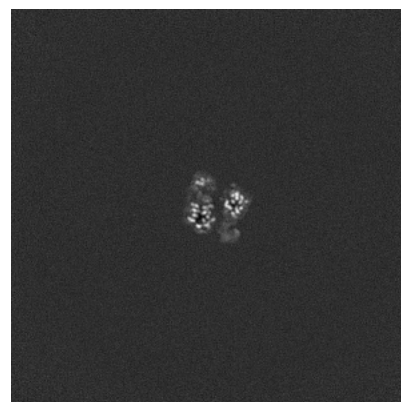
### 6.2.2 Raw map



X Index: 225



Y Index: 225

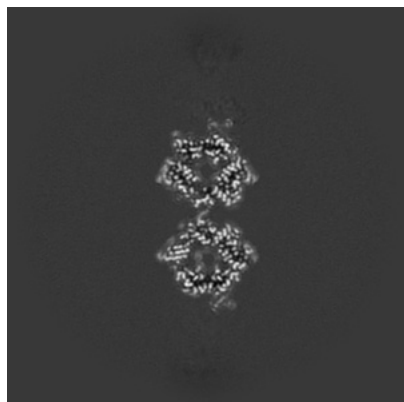


Z Index: 225

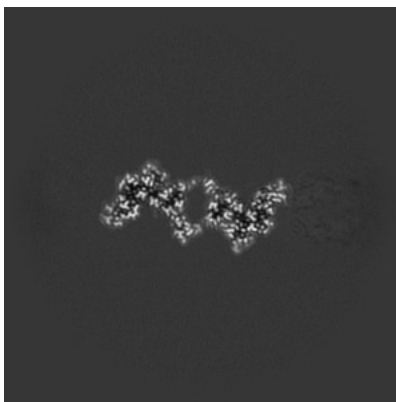
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

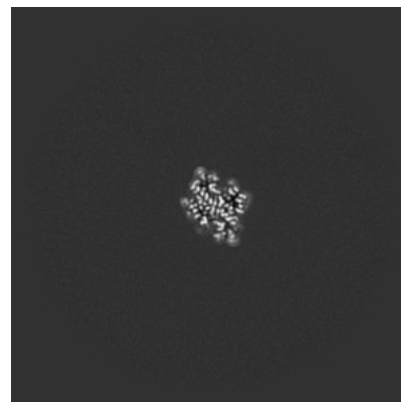
### 6.3.1 Primary map



X Index: 227

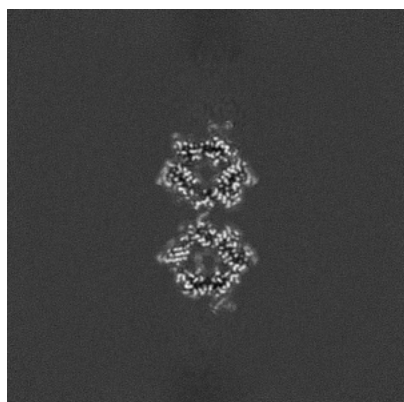


Y Index: 244

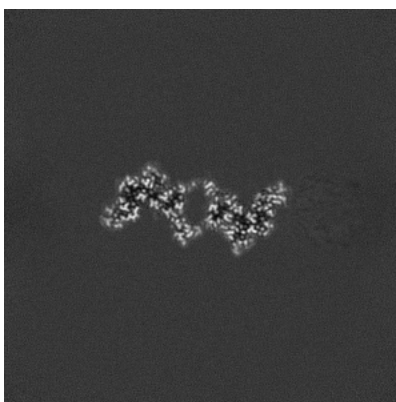


Z Index: 233

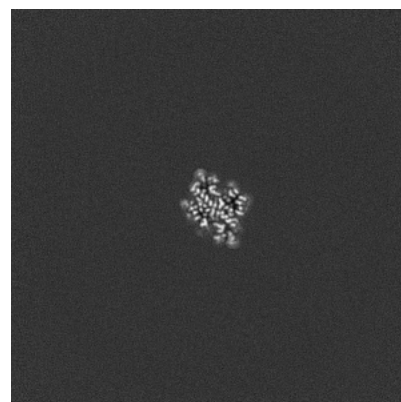
### 6.3.2 Raw map



X Index: 227



Y Index: 244

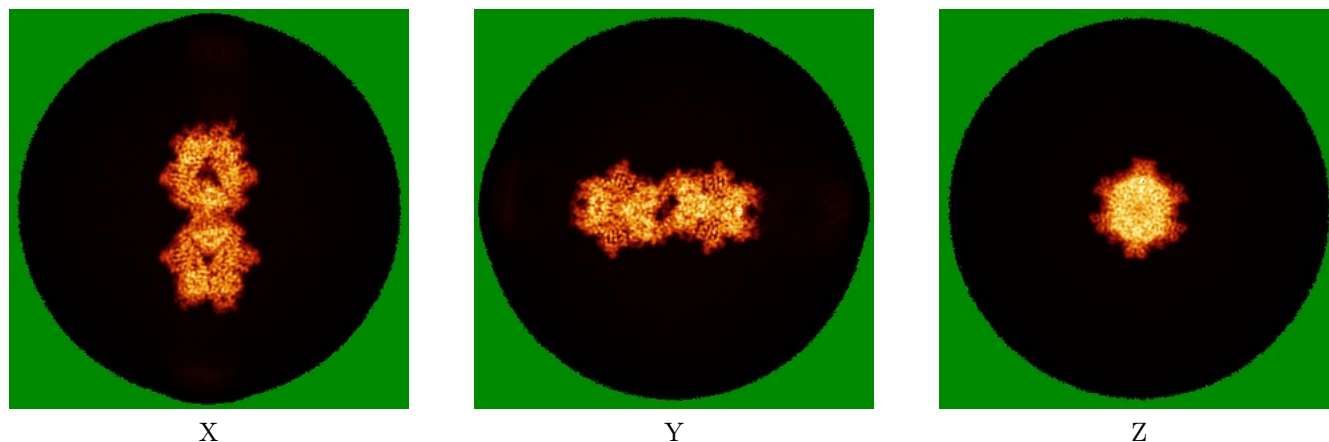


Z Index: 233

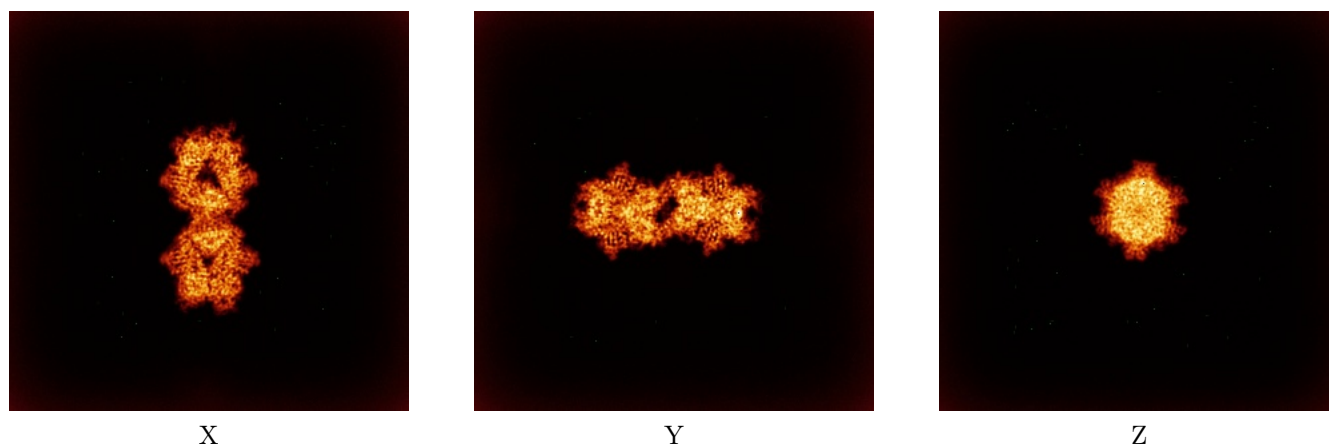
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



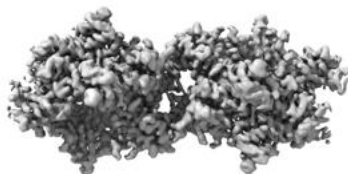
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

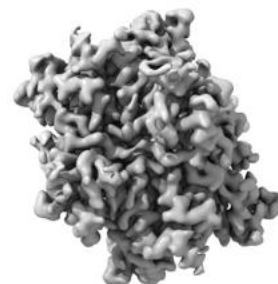
### 6.5.1 Primary map



X



Y



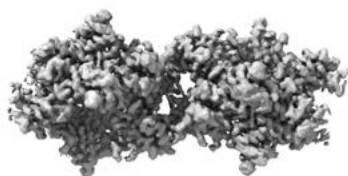
Z

The images above show the 3D surface view of the map at the recommended contour level 0.23. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

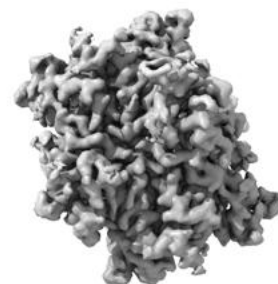
### 6.5.2 Raw map



X



Y



Z

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



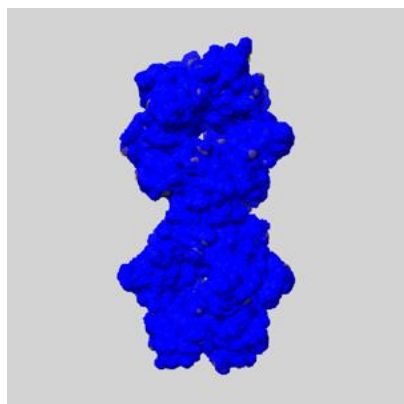
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

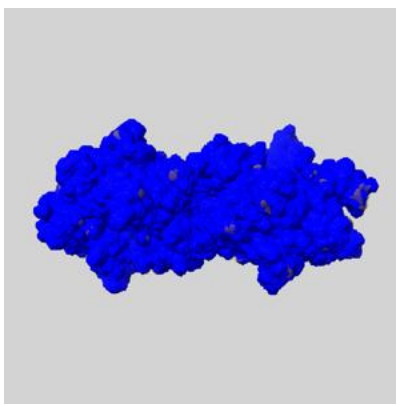
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

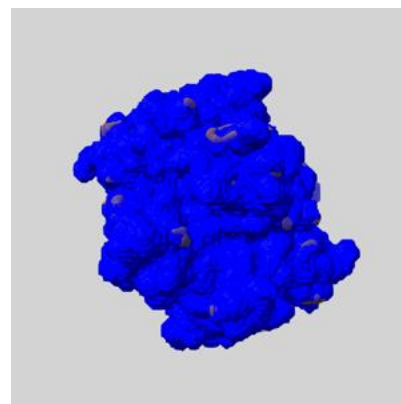
### 6.6.1 emd\_15039\_msk\_1.map [i](#)



X



Y

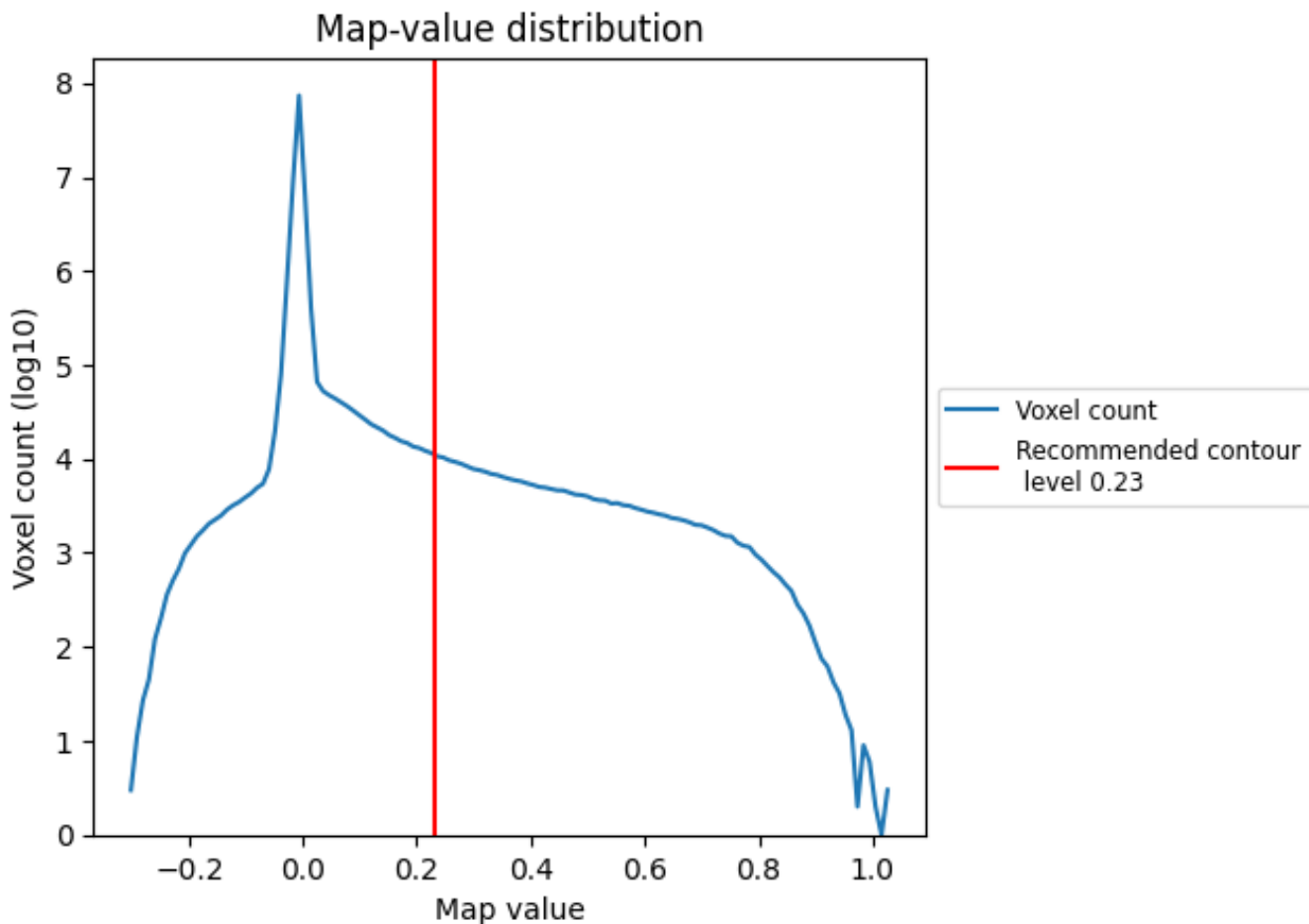


Z

## 7 Map analysis [i](#)

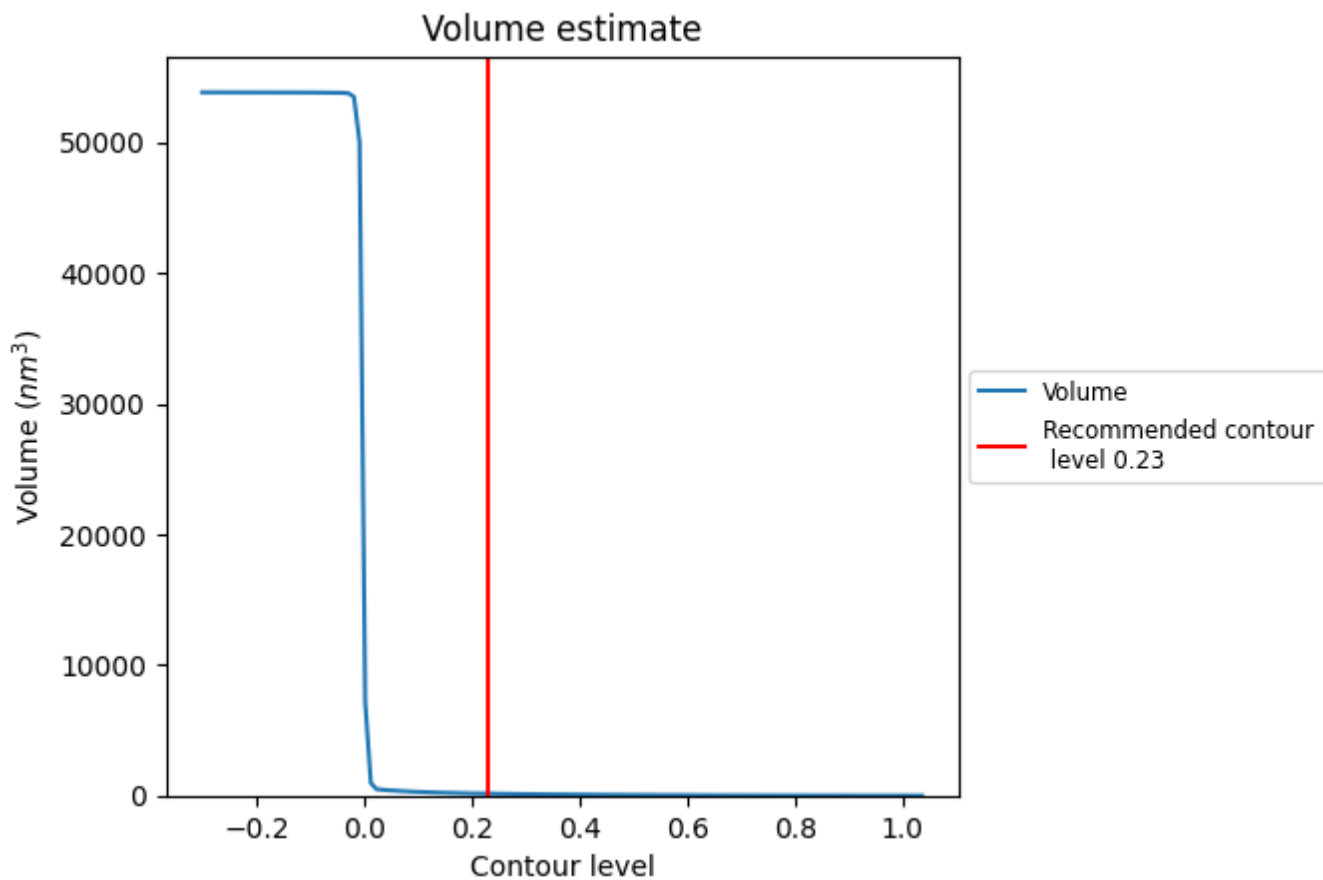
This section contains the results of statistical analysis of the map.

### 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.

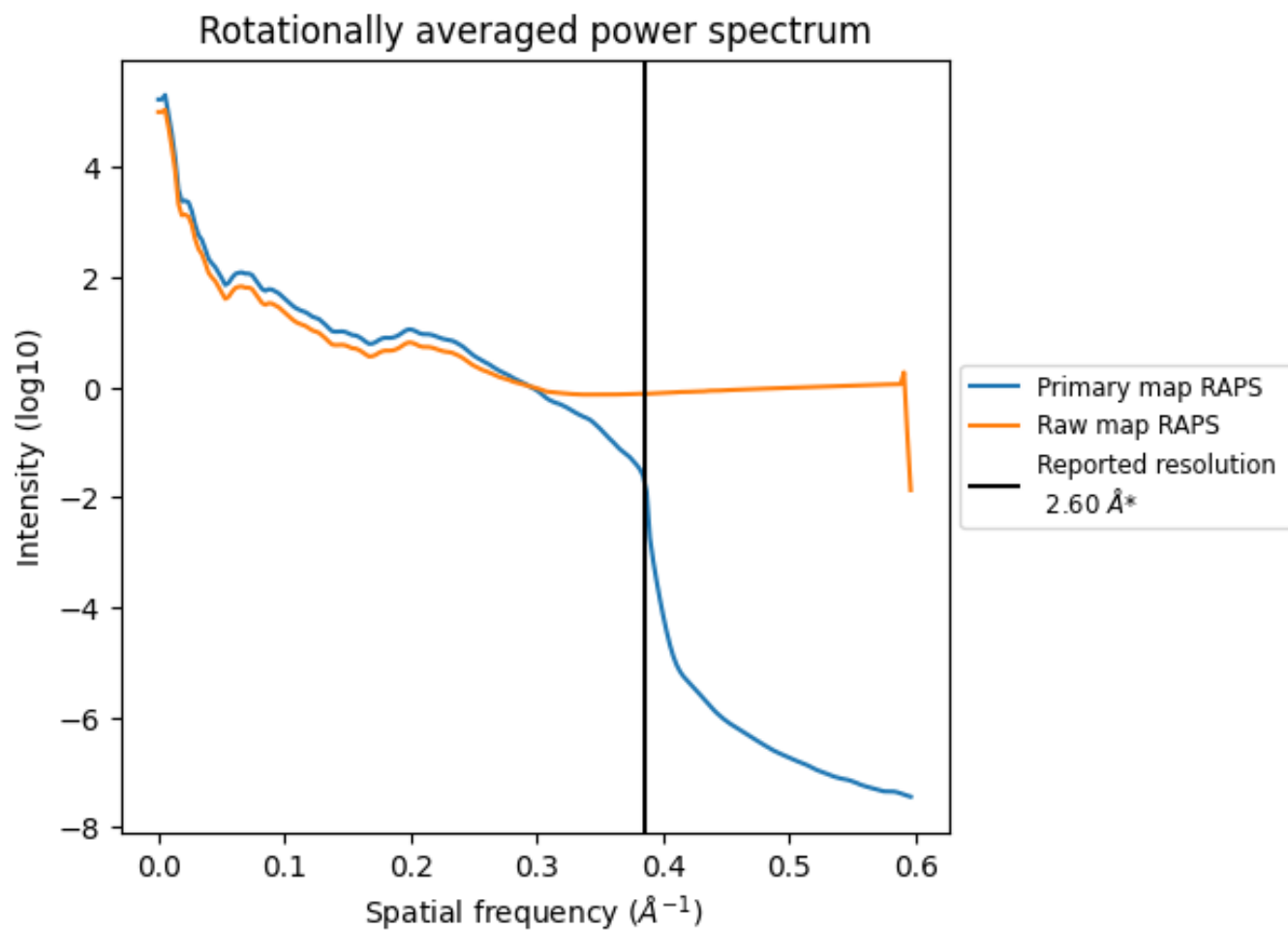
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 146 nm<sup>3</sup>; this corresponds to an approximate mass of 132 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

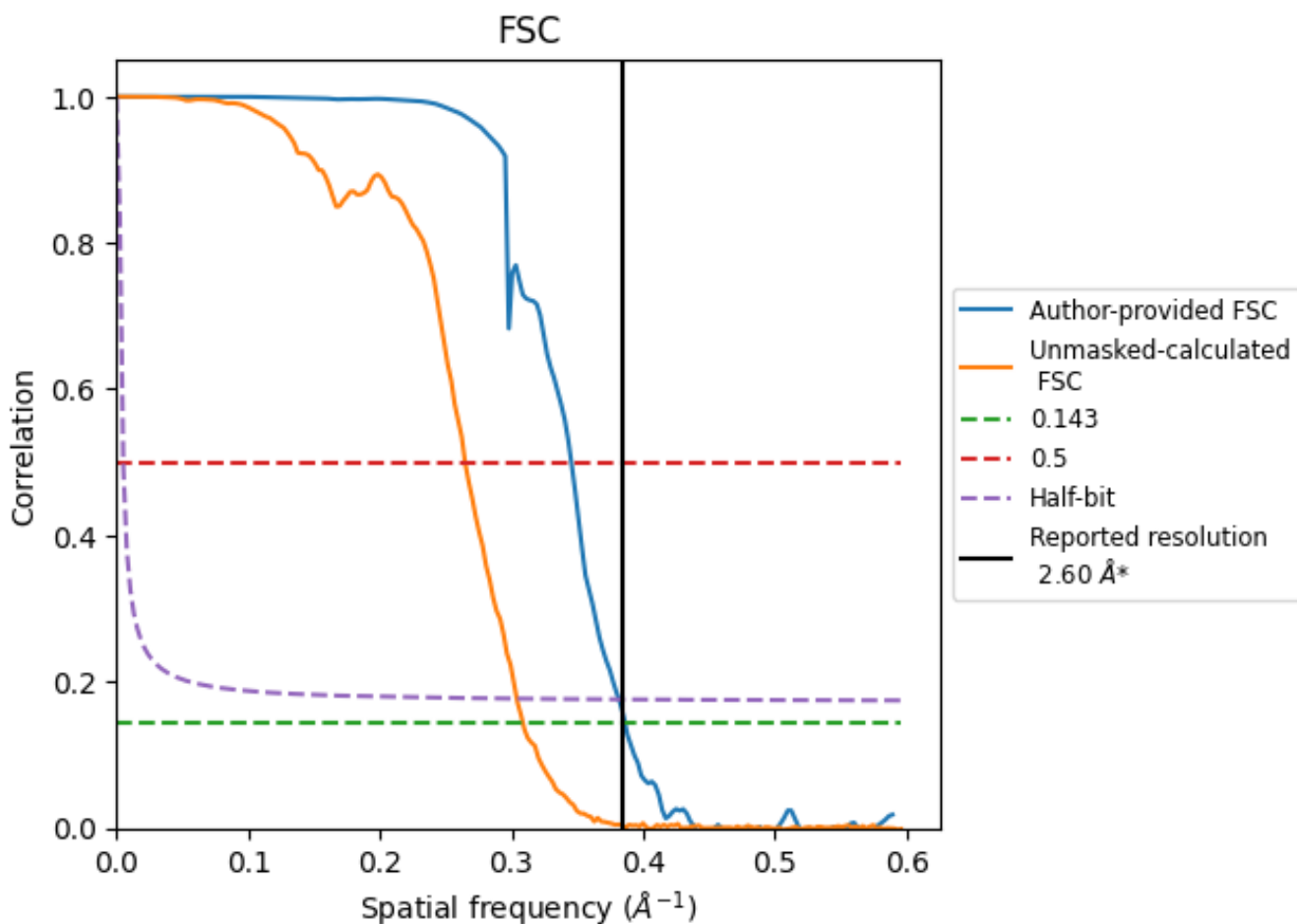


\*Reported resolution corresponds to spatial frequency of 0.385 Å<sup>-1</sup>

## 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 0.385 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

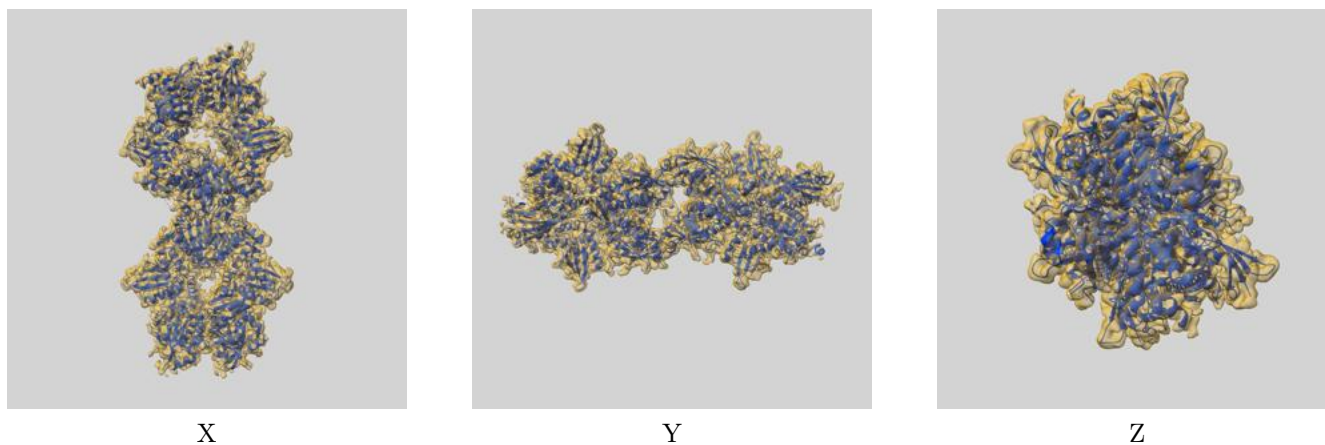
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.59	2.89	2.62
Unmasked-calculated*	3.24	3.78	3.29

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.24 differs from the reported value 2.6 by more than 10 %

## 9 Map-model fit [i](#)

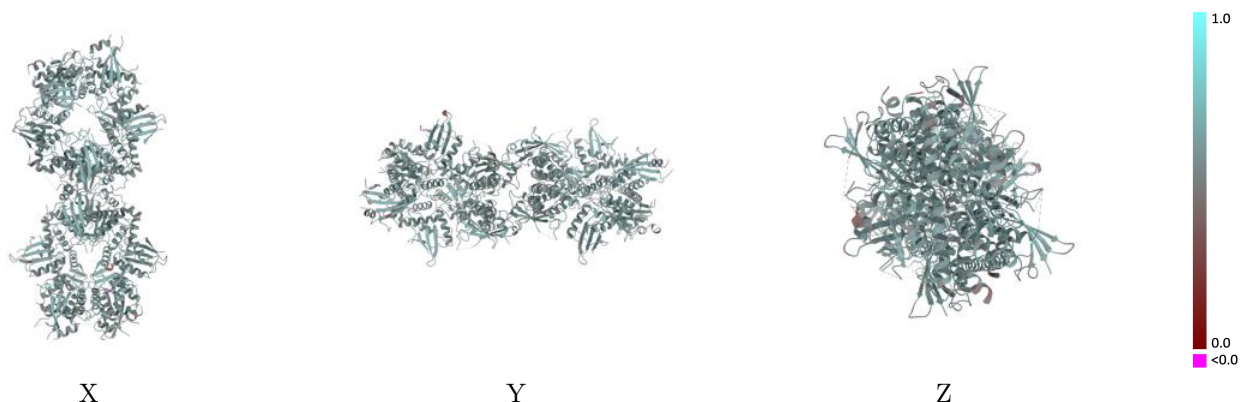
This section contains information regarding the fit between EMDB map EMD-15039 and PDB model 7ZZQ. Per-residue inclusion information can be found in section 3 on page 17.

### 9.1 Map-model overlay [i](#)



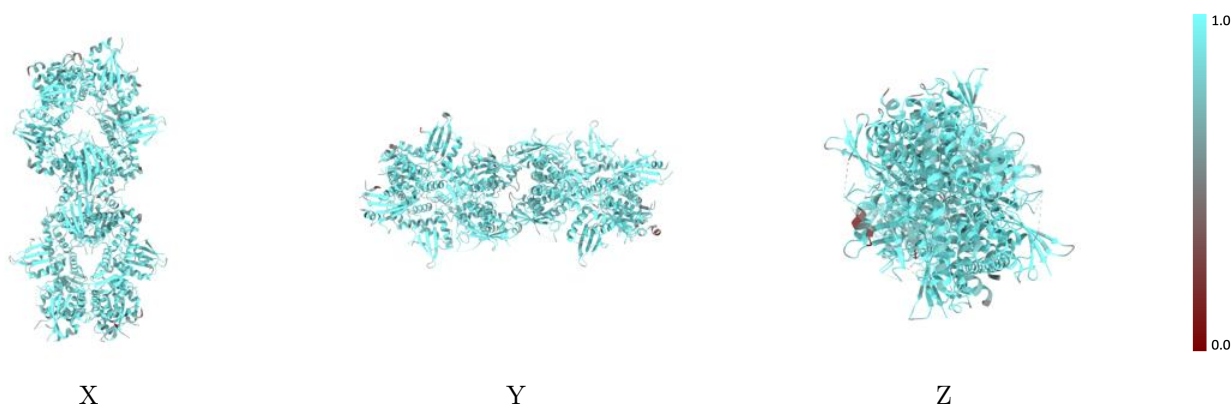
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

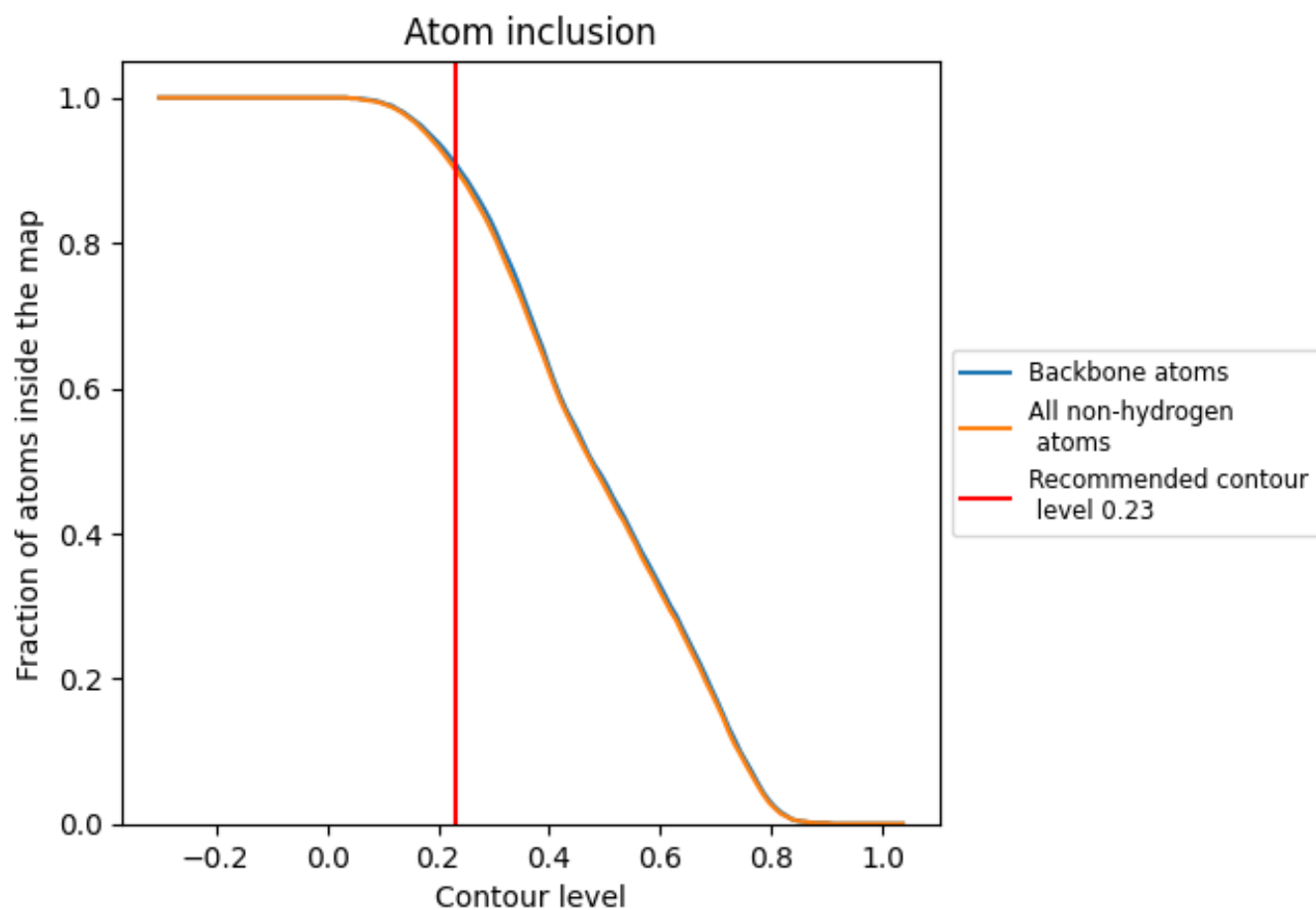
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.23).

































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9020	 0.5680
A	 0.9010	 0.5630
B	 0.9090	 0.5720
C	 0.9270	 0.5710
D	 0.9190	 0.5750
E	 0.9130	 0.5670
F	 0.9120	 0.5740
G	 0.9110	 0.5640
H	 0.9400	 0.5800
I	 0.9250	 0.5670
J	 0.9360	 0.5810
K	 0.9230	 0.5690
L	 0.9110	 0.5760
M	 0.9280	 0.5770
N	 0.9260	 0.5810
O	 0.9190	 0.5730
P	 0.9270	 0.5780
Q	 0.8510	 0.5250
R	 0.8590	 0.5410
S	 0.8560	 0.5160
T	 0.8220	 0.5180
U	 0.8450	 0.5430
V	 0.6670	 0.4740
W	 0.5500	 0.4800
X	 0.8690	 0.5370
Y	 0.6590	 0.4820
Z	 0.8640	 0.5380
a	 0.7440	 0.4690
b	 0.6850	 0.4980
c	 0.6250	 0.5410
d	 0.7310	 0.4920

