



wwPDB EM Validation Summary Report ⓘ

Dec 9, 2025 – 01:37 PM JST

PDB ID : 9M8O / pdb_00009m8o
EMDB ID : EMD-63716
Title : Cryo-EM structure of bacteriophage NF5 baseplate
Authors : Peng, Y.N.; Liu, H.R.
Deposited on : 2025-03-12
Resolution : 3.44 Å(reported)

This is a wwPDB EM Validation Summary 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:

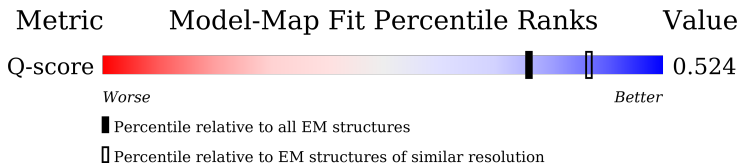
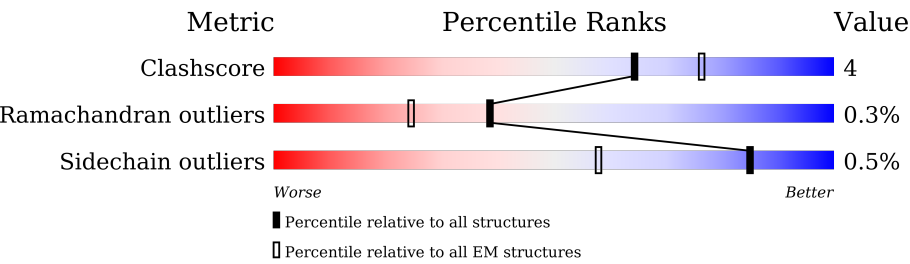
EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.47

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 3.44 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.



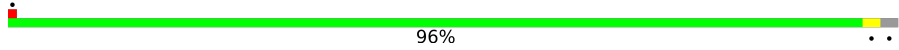
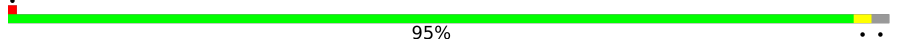
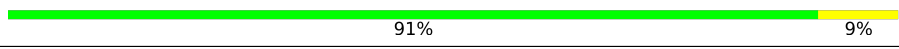

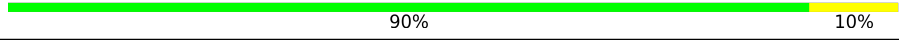
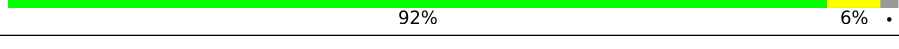
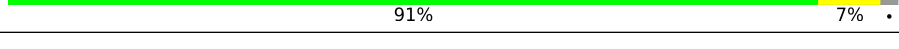
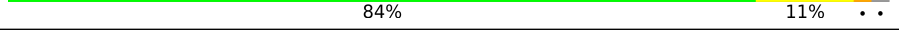
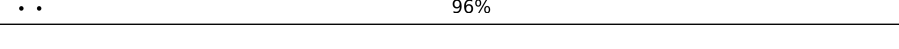
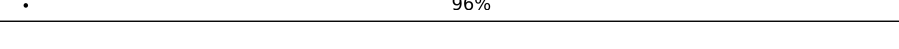
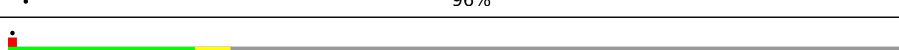














Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13877 (2.94 - 3.94)

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	169	<div><div></div><div>92%</div><div>6%</div><div></div></div>
1	B	169	<div><div></div><div>95%</div><div></div><div></div></div>
1	C	169	<div><div></div><div>92%</div><div>6%</div><div></div></div>
1	D	169	<div><div></div><div>92%</div><div>5%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	E	169	
1	F	169	
2	G	255	
2	H	255	
2	I	255	
2	J	255	
2	K	255	
2	L	255	
3	M	674	
3	N	674	
3	O	674	
4	P	639	
4	Q	639	
4	R	639	
4	S	639	
4	T	639	
4	U	639	
4	V	639	
4	W	639	
4	X	639	
4	Y	639	
4	Z	639	
4	a	639	
4	b	639	
4	c	639	

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Mol	Chain	Length	Quality of chain
4	d	639	<div><div><div></div><div></div><div></div></div><div>13%84%</div></div>
4	e	639	<div><div><div></div><div></div><div></div></div><div>21%76%</div></div>
4	f	639	<div><div><div></div><div></div><div></div></div><div>22%75%</div></div>
4	g	639	<div><div><div></div><div></div><div></div></div><div>12%84%</div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 40205 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 Gp11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	166	Total	C	N	O	S	0	0
			1297	817	206	272	2		
1	B	166	Total	C	N	O	S	0	0
			1297	817	206	272	2		
1	C	165	Total	C	N	O	S	0	0
			1285	808	205	270	2		
1	D	164	Total	C	N	O	S	0	0
			1281	807	204	268	2		
1	E	166	Total	C	N	O	S	0	0
			1297	817	206	272	2		
1	F	165	Total	C	N	O	S	0	0
			1292	814	205	271	2		

- Molecule 2 is a protein called Gp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	255	Total	C	N	O	S	0	0
			2023	1289	327	397	10		
2	H	255	Total	C	N	O	S	0	0
			2023	1289	327	397	10		
2	I	254	Total	C	N	O	S	0	0
			2015	1284	326	396	9		
2	J	250	Total	C	N	O	S	0	0
			1986	1266	322	389	9		
2	K	250	Total	C	N	O	S	0	0
			1986	1266	322	389	9		
2	L	250	Total	C	N	O	S	0	0
			1986	1266	322	389	9		

- Molecule 3 is a protein called Gp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	27	Total	C	N	O	S	0	0
			220	139	35	45	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	27	Total	C	N	O	S	0	0
			220	139	35	45	1		
3	O	26	Total	C	N	O	S	0	0
			209	130	34	44	1		

- Molecule 4 is a protein called Gp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	156	Total	C	N	O	S	0	0
			1246	791	209	243	3		
4	Q	158	Total	C	N	O	S	0	0
			1259	800	211	245	3		
4	R	100	Total	C	N	O	S	0	0
			793	505	133	154	1		
4	S	156	Total	C	N	O	S	0	0
			1246	791	209	243	3		
4	T	158	Total	C	N	O	S	0	0
			1259	800	211	245	3		
4	U	100	Total	C	N	O	S	0	0
			793	505	133	154	1		
4	V	156	Total	C	N	O	S	0	0
			1246	791	209	243	3		
4	W	158	Total	C	N	O	S	0	0
			1259	800	211	245	3		
4	X	100	Total	C	N	O	S	0	0
			793	505	133	154	1		
4	Y	156	Total	C	N	O	S	0	0
			1246	791	209	243	3		
4	Z	158	Total	C	N	O	S	0	0
			1259	800	211	245	3		
4	a	100	Total	C	N	O	S	0	0
			793	505	133	154	1		
4	b	156	Total	C	N	O	S	0	0
			1246	791	209	243	3		
4	c	158	Total	C	N	O	S	0	0
			1259	800	211	245	3		
4	d	100	Total	C	N	O	S	0	0
			793	505	133	154	1		
4	e	156	Total	C	N	O	S	0	0
			1246	791	209	243	3		
4	f	158	Total	C	N	O	S	0	0
			1259	800	211	245	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	100	Total	C	N	O	S	0	0
			793	505	133	154	1		

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: Gp11



- Molecule 1: Gp11



- Molecule 1: Gp11



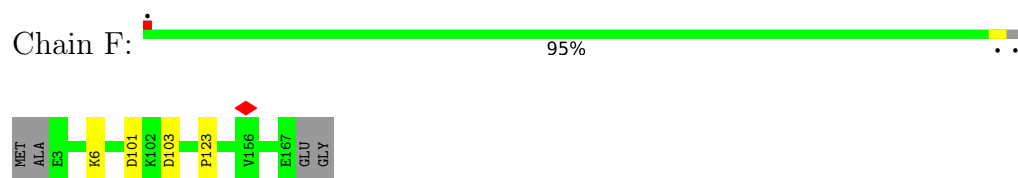
- Molecule 1: Gp11



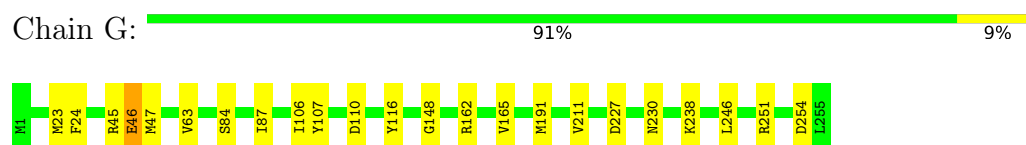
- Molecule 1: Gp11



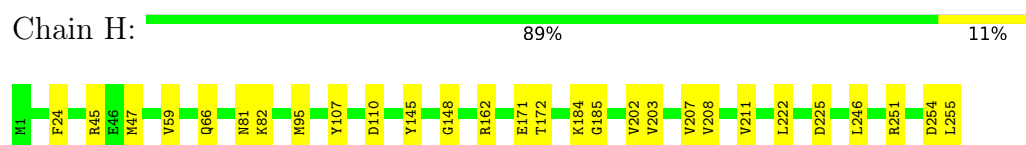
● Molecule 1: Gp11



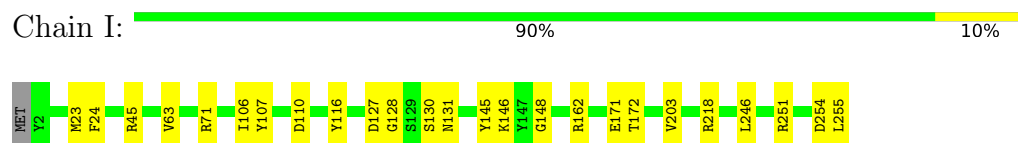
● Molecule 2: Gp15



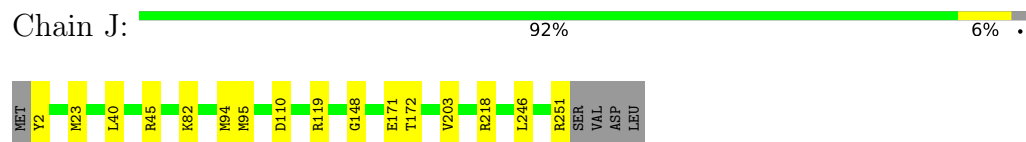
● Molecule 2: Gp15



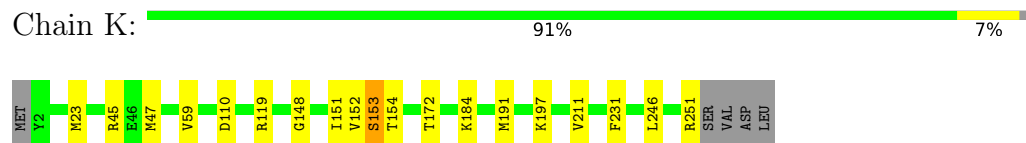
● Molecule 2: Gp15



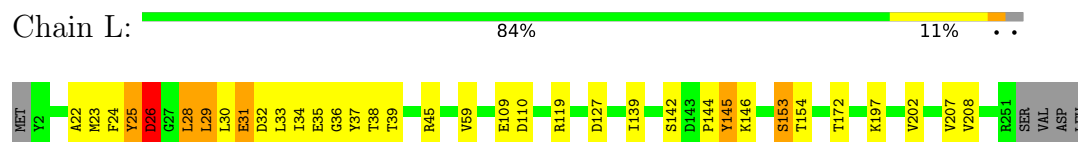
● Molecule 2: Gp15



● Molecule 2: Gp15



● Molecule 2: Gp15



- Molecule 4: Gp18

Chain R: 13% 84%



[illegible]

- Molecule 4: Gp18

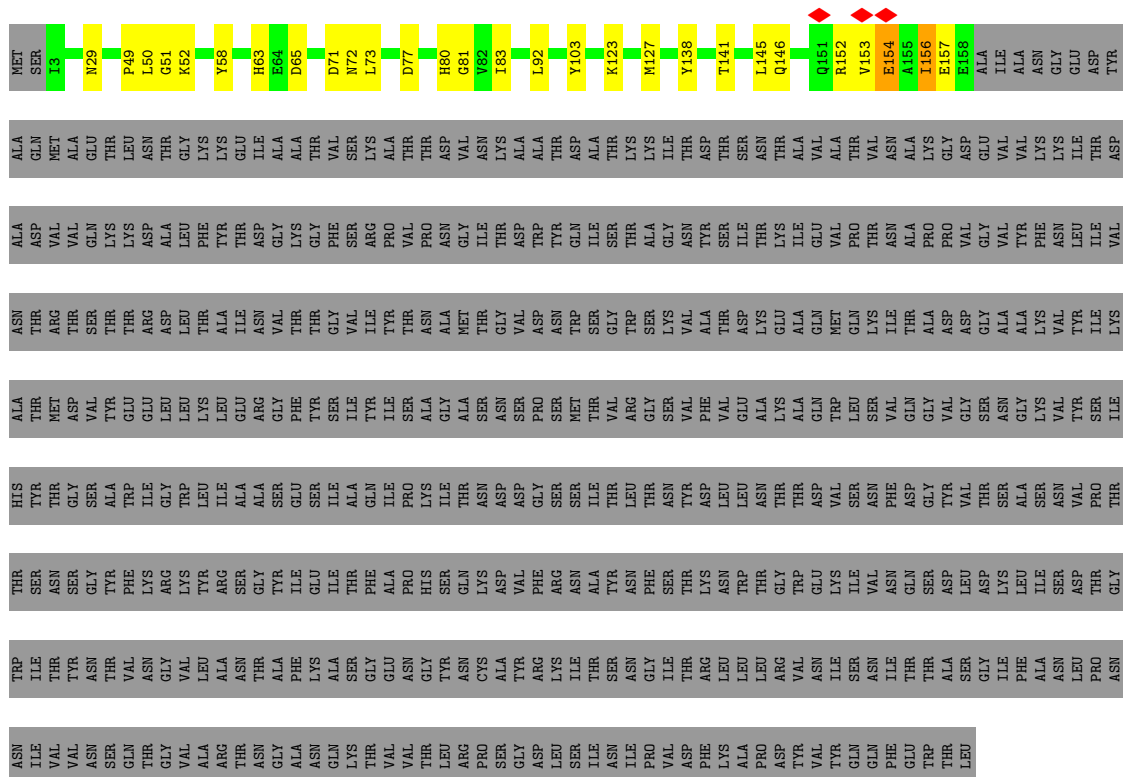
[illegible]

- Molecule 4: Gp18

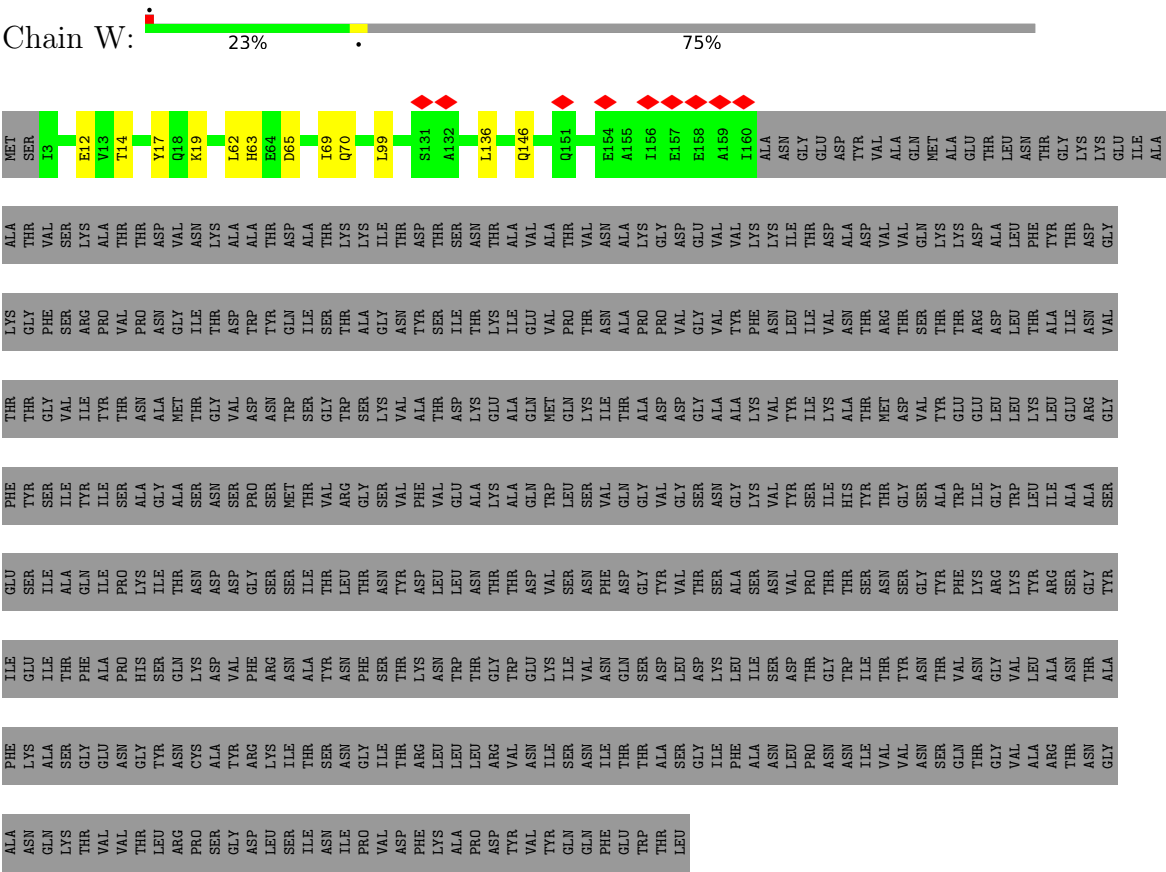


VAL	ILE	GLN	THR	TYS	ILE	PRO	ARG	GLU	PHE	LEU	LVS	HIS	THR	GLY	LVS	V98	Y103	I104	R109	D110	M115	R116	K117	I118	SER	PHE	ASP	LVS	GLN	ASP	LEU	MET	THR	ALA	ALA	ALA	V134	K135	L136	T141	F142	D143	K150	Q151	R152	V153	I156	E157	E158
MET	SER	ILE	THR	LVS	ILE	SER	LVS	SER	VAL	MET	E12	K19	D22	V25	Y28	D31	I32	N33	T34	N40	V41	T42	R43	L50	G51	K52	S53	N54	Y58	L61	LEU	HIS	GLU	ASP	GLY	SER	ARG	ILE	GLN	ASP	ASN	LEU	VAL	ILE	GLU	ASP	GLU	HIS	

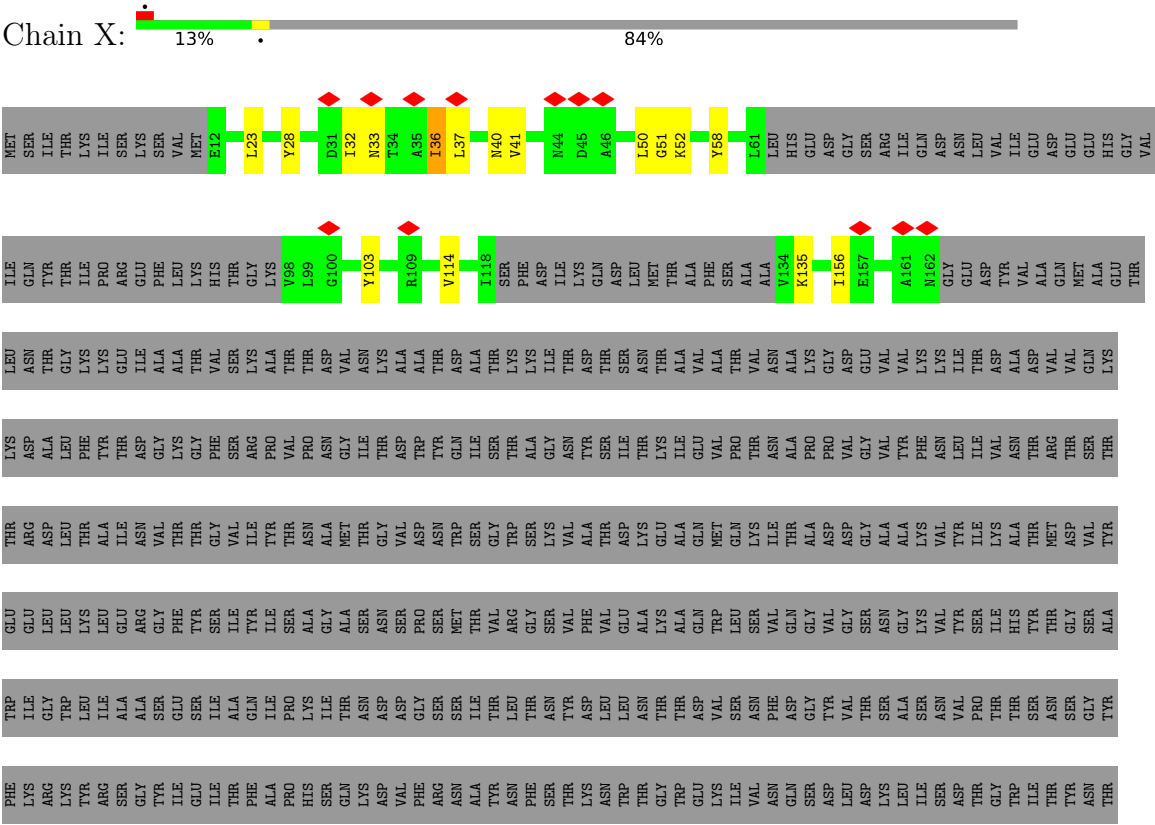
- Molecule 4: Gp18



- Molecule 4: Gp18



• Molecule 4: Gp18





[illegible]

- Molecule 4: Gp18

Chain c:  22% 75%

THR	ASN	SER	ALA	GLU	ILE	THR	GLU	MET
ASN	THR	GLY	ALA	ARG	ASN	ASP	ILE	SER
GLY	ALA	TYR	SER	GLY	VAL	GLY	ALA	I3
ASN	PHE	ILE	GLU	PHE	THR	LYS	ALA	T4
LYS	ASN	GLU	SER	SER	THR	THR	THR	K5
GLN	ALA	ILE	ILE	SER	GLY	PHE	VAL	
LYS	SER	THR	ALA	ILE	VAL	SER	SER	M11
THR	GLY	PHE	GLN	TYR	ILE	ARG	LYS	
VAL	GLU	ALA	ILE	ILE	THR	PRO	ALA	Y17
VAL	ASN	PRO	PRO	SER	THR	VAL	THR	
THR	GLY	HIS	LYS	ALA	ASN	PRO	THR	L62
LEU	THR	SER	ILE	GLY	ALA	ASN	ASP	H63
ARG	ASN	GLN	THR	ALA	MET	GLY	VAL	E64
PRO	CYS	LYS	ASN	SER	THR	ILE	ASN	D65
ALA	ALA	ASP	ASP	ASN	GLY	THR	LYS	
GLY	TYR	VAL	GLY	PRO	VAL	ASP	ALA	R68
ASP	ARG	PHE	GLY	SER	TRP	TRP	ALA	I69
LYS	LYS	ARG	SER	MET	ASN	GLN	THR	Q70
SER	ILE	ASN	SER	THR	TRP	ASP	ASP	
ILE	THR	ALA	ILE	VAL	SER	ILE	ALA	L99
ASN	SER	TYR	THR	VAL	GLY	SER	THR	
ASN	ASN	ASN	LEU	THR	TRP	THR	LYS	M115
PRO	GLY	PHE	THR	GLY	SER	ALA	ILE	
VAL	ILE	SER	ASN	SER	LYS	GLY	ILE	S131
ASP	THR	THR	TYR	VAL	VAL	ASN	THR	A132
ARG	ARG	LYS	ASP	PHE	ALA	LYS	ASP	
LEU	ASN	ASN	LEU	VAL	THR	SER	SER	K135
LEU	LEU	TRP	LEU	GLU	ASP	ILE	THR	
PRO	LEU	THR	ASN	ALA	LYS	THR	ASN	L136
ASP	ARG	GLY	THR	LYS	GLU	THR	THR	
VAL	ASN	GLU	THR	ALA	ALA	ILE	ALA	Q146
TYR	ILE	LYS	VAL	TRP	MET	VAL	VAL	
GLN	SER	ILE	SER	LEU	GLN	PRO	THR	
ASN	ASN	VAL	ASN	SER	LYS	THR	VAL	
PHE	ILE	ASN	PHE	VAL	ILE	ASN	ASN	Q151
GLU	THR	GLN	ASP	VAL	THR	ALA	ALA	R152
TRP	THR	SER	GLY	GLY	THR	PRO	LYS	V153
THR	ALA	SER	TYR	VAL	ASP	PRO	GLY	A155
LEU	SER	LEU	VAL	GLY	ASP	VAL	ASP	I156
	GLY	ASP	THR	SER	GLY	GLY	GLU	E157
	ILE	LYS	SER	ASN	ALA	VAL	VAL	E158
	PHE	LEU	ALA	GLY	ALA	THR	VAL	A159
	ALA	ILE	SER	LYS	LYS	PHE	LYS	I160
	ASN	SER	ASN	VAL	VAL	ASN	LYS	ALA
	PRO	ASP	PRO	TYR	TYR	LEU	ILE	ASN
	ASN	GLY	THR	ILE	LYS	ILE	THR	GLY
	ASN	TRP	THR	HIS	ALA	VAL	ASP	GLU
	ILE	ILE	SER	THR	THR	ASN	ALA	ASP
	VAL	THR	ASN	THR	MET	ARG	VAL	VAL
	VAL	TYR	SER	GLY	ASP	THR	VAL	GLN
	ASN	ASN	GLY	SER	VAL	SER	LYS	MET
	SER	THR	TYR	ALA	TYR	THR	LYS	ALA
	GLN	VAL	PHE	TRP	GLU	THR	LYS	GLU
	THR	VAL	LYS	ILE	GLU	ARG	ASP	THR
	GLY	ASN	ARG	GLY	LEU	ASP	ALA	LEU
	VAL	GLY	LYS	TRP	LEU	LEU	ASN	THR
	ALA	LEU	TYR	LEU	LYS	THR	PHE	GLY
	ARG	ALA	ARG	ILE	THR	ALA	TYR	THR

- Molecule 4: Gp18

Chain d:  13% 84%



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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38436	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.561	Depositor
Minimum map value	-0.797	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.26	Depositor
Map size (\AA)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.2, 1.2, 1.2	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.30	2/1318 (0.2%)	0.36	2/1780 (0.1%)
1	B	0.13	0/1318	0.28	0/1780
1	C	0.13	0/1304	0.27	0/1759
1	D	0.44	4/1302 (0.3%)	0.47	3/1758 (0.2%)
1	E	0.13	0/1318	0.27	0/1780
1	F	0.30	2/1313 (0.2%)	0.29	0/1773
2	G	0.13	0/2059	0.33	2/2779 (0.1%)
2	H	0.12	0/2059	0.26	0/2779
2	I	0.12	0/2051	0.25	0/2769
2	J	0.12	0/2022	0.27	0/2729
2	K	0.30	2/2022 (0.1%)	0.35	2/2729 (0.1%)
2	L	0.99	24/2022 (1.2%)	0.76	9/2729 (0.3%)
3	M	0.14	0/223	0.32	0/296
3	N	0.10	0/223	0.22	0/296
3	O	0.12	0/211	0.21	0/280
4	P	0.41	0/1263	0.53	0/1706
4	Q	0.24	0/1276	0.32	0/1724
4	R	0.34	0/800	0.59	0/1081
4	S	0.49	1/1263 (0.1%)	0.59	2/1706 (0.1%)
4	T	0.14	0/1276	0.31	0/1724
4	U	0.37	0/800	0.50	1/1081 (0.1%)
4	V	0.29	0/1263	0.50	1/1706 (0.1%)
4	W	0.13	0/1276	0.29	0/1724
4	X	0.27	0/800	0.57	0/1081
4	Y	0.34	1/1263 (0.1%)	0.58	4/1706 (0.2%)
4	Z	0.14	0/1276	0.31	0/1724
4	a	0.33	0/800	0.53	0/1081
4	b	0.29	0/1263	0.53	1/1706 (0.1%)
4	c	0.13	0/1276	0.29	0/1724
4	d	0.29	0/800	0.55	0/1081
4	e	0.34	2/1263 (0.2%)	0.62	4/1706 (0.2%)
4	f	0.14	0/1276	0.30	0/1724
4	g	0.30	0/800	0.47	0/1081
All	All	0.33	38/40799 (0.1%)	0.43	31/55082 (0.1%)

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	26	ASP	CA-C	-10.25	1.43	1.53
2	L	144	PRO	CA-CB	-7.48	1.44	1.53
2	L	24	PHE	C-O	-7.33	1.15	1.24
2	L	142	SER	CA-C	-7.06	1.43	1.52
2	L	39	THR	C-O	-7.00	1.15	1.23

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	e	154	GLU	N-CA-C	10.68	122.92	111.28
2	L	35	GLU	N-CA-C	9.94	122.12	111.28
4	e	153	VAL	CA-C-N	8.35	131.47	120.28
4	e	153	VAL	C-N-CA	8.35	131.47	120.28
4	Y	154	GLU	N-CA-C	7.72	120.44	111.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1297	0	1249	8	0
1	B	1297	0	1249	3	0
1	C	1285	0	1239	6	0
1	D	1281	0	1234	6	0
1	E	1297	0	1249	3	0
1	F	1292	0	1244	3	0
2	G	2023	0	2032	15	0
2	H	2023	0	2032	18	0
2	I	2015	0	2020	15	0
2	J	1986	0	1991	13	0
2	K	1986	0	1991	10	0
2	L	1986	0	1991	11	0
3	M	220	0	201	5	0
3	N	220	0	201	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	209	0	192	1	0
4	P	1246	0	1261	14	0
4	Q	1259	0	1277	12	0
4	R	793	0	808	10	0
4	S	1246	0	1261	18	0
4	T	1259	0	1277	11	0
4	U	793	0	808	18	0
4	V	1246	0	1261	18	0
4	W	1259	0	1277	8	0
4	X	793	0	808	10	0
4	Y	1246	0	1261	19	0
4	Z	1259	0	1277	9	0
4	a	793	0	808	15	0
4	b	1246	0	1261	25	0
4	c	1259	0	1277	13	0
4	d	793	0	808	13	0
4	e	1246	0	1261	14	0
4	f	1259	0	1277	11	0
4	g	793	0	808	12	0
All	All	40205	0	40191	317	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 317 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)
4:V:154:GLU:HA	4:V:157:GLU:HB2	1.51	0.92
4:b:154:GLU:HA	4:b:157:GLU:HB2	1.56	0.86
4:S:149:ILE:HD11	4:T:153:VAL:HG11	1.62	0.80
4:b:127:MET:HE1	4:c:70:GLN:HG3	1.64	0.79
4:P:127:MET:HE1	4:Q:70:GLN:HG3	1.72	0.72

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	164/169 (97%)	156 (95%)	8 (5%)	0	100	100
1	B	164/169 (97%)	156 (95%)	8 (5%)	0	100	100
1	C	161/169 (95%)	156 (97%)	5 (3%)	0	100	100
1	D	162/169 (96%)	156 (96%)	6 (4%)	0	100	100
1	E	164/169 (97%)	159 (97%)	5 (3%)	0	100	100
1	F	163/169 (96%)	159 (98%)	4 (2%)	0	100	100
2	G	253/255 (99%)	247 (98%)	6 (2%)	0	100	100
2	H	253/255 (99%)	247 (98%)	6 (2%)	0	100	100
2	I	252/255 (99%)	247 (98%)	5 (2%)	0	100	100
2	J	248/255 (97%)	240 (97%)	8 (3%)	0	100	100
2	K	248/255 (97%)	240 (97%)	8 (3%)	0	100	100
2	L	248/255 (97%)	242 (98%)	6 (2%)	0	100	100
3	M	25/674 (4%)	25 (100%)	0	0	100	100
3	N	25/674 (4%)	24 (96%)	1 (4%)	0	100	100
3	O	24/674 (4%)	24 (100%)	0	0	100	100
4	P	154/639 (24%)	150 (97%)	3 (2%)	1 (1%)	22	54
4	Q	156/639 (24%)	155 (99%)	1 (1%)	0	100	100
4	R	94/639 (15%)	86 (92%)	6 (6%)	2 (2%)	5	29
4	S	154/639 (24%)	151 (98%)	2 (1%)	1 (1%)	22	54
4	T	156/639 (24%)	155 (99%)	1 (1%)	0	100	100
4	U	94/639 (15%)	90 (96%)	3 (3%)	1 (1%)	12	42
4	V	154/639 (24%)	151 (98%)	2 (1%)	1 (1%)	22	54
4	W	156/639 (24%)	155 (99%)	1 (1%)	0	100	100
4	X	94/639 (15%)	88 (94%)	4 (4%)	2 (2%)	5	29
4	Y	154/639 (24%)	152 (99%)	1 (1%)	1 (1%)	22	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Z	156/639 (24%)	152 (97%)	4 (3%)	0	100	100
4	a	94/639 (15%)	88 (94%)	5 (5%)	1 (1%)	12	42
4	b	154/639 (24%)	151 (98%)	2 (1%)	1 (1%)	22	54
4	c	156/639 (24%)	155 (99%)	1 (1%)	0	100	100
4	d	94/639 (15%)	87 (93%)	5 (5%)	2 (2%)	5	29
4	e	154/639 (24%)	150 (97%)	3 (2%)	1 (1%)	22	54
4	f	156/639 (24%)	154 (99%)	2 (1%)	0	100	100
4	g	94/639 (15%)	91 (97%)	2 (2%)	1 (1%)	12	42
All	All	4978/16068 (31%)	4839 (97%)	124 (2%)	15 (0%)	38	68

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	R	36	ILE
4	R	51	GLY
4	X	36	ILE
4	X	51	GLY
4	d	36	ILE

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	138/140 (99%)	138 (100%)	0	100	100
1	B	138/140 (99%)	138 (100%)	0	100	100
1	C	137/140 (98%)	137 (100%)	0	100	100
1	D	136/140 (97%)	136 (100%)	0	100	100
1	E	138/140 (99%)	138 (100%)	0	100	100
1	F	138/140 (99%)	138 (100%)	0	100	100
2	G	233/233 (100%)	233 (100%)	0	100	100
2	H	233/233 (100%)	233 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	232/233 (100%)	232 (100%)	0	100	100
2	J	228/233 (98%)	228 (100%)	0	100	100
2	K	228/233 (98%)	226 (99%)	2 (1%)	75	86
2	L	228/233 (98%)	222 (97%)	6 (3%)	41	67
3	M	23/523 (4%)	23 (100%)	0	100	100
3	N	23/523 (4%)	23 (100%)	0	100	100
3	O	22/523 (4%)	22 (100%)	0	100	100
4	P	139/543 (26%)	136 (98%)	3 (2%)	47	70
4	Q	140/543 (26%)	140 (100%)	0	100	100
4	R	87/543 (16%)	87 (100%)	0	100	100
4	S	139/543 (26%)	138 (99%)	1 (1%)	81	89
4	T	140/543 (26%)	140 (100%)	0	100	100
4	U	87/543 (16%)	85 (98%)	2 (2%)	45	69
4	V	139/543 (26%)	138 (99%)	1 (1%)	81	89
4	W	140/543 (26%)	140 (100%)	0	100	100
4	X	87/543 (16%)	87 (100%)	0	100	100
4	Y	139/543 (26%)	137 (99%)	2 (1%)	62	79
4	Z	140/543 (26%)	140 (100%)	0	100	100
4	a	87/543 (16%)	86 (99%)	1 (1%)	70	82
4	b	139/543 (26%)	137 (99%)	2 (1%)	62	79
4	c	140/543 (26%)	140 (100%)	0	100	100
4	d	87/543 (16%)	86 (99%)	1 (1%)	70	82
4	e	139/543 (26%)	137 (99%)	2 (1%)	62	79
4	f	140/543 (26%)	140 (100%)	0	100	100
4	g	87/543 (16%)	86 (99%)	1 (1%)	70	82
All	All	4471/13581 (33%)	4447 (100%)	24 (0%)	85	92

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	V	156	ILE
4	a	34	THR
4	Y	158	GLU

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Mol	Chain	Res	Type
4	b	152	ARG
2	L	145	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
4	T	38	GLN
4	Z	29	ASN
4	e	94	HIS
4	b	38	GLN
4	Y	30	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 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.

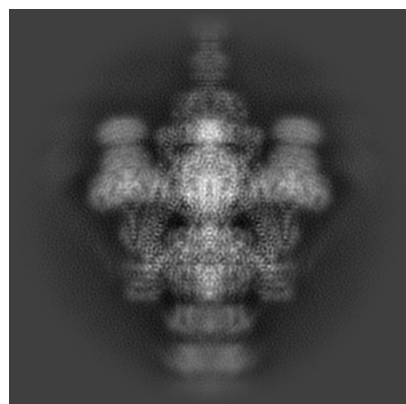
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63716. These allow visual inspection of the internal detail of the map and identification of artifacts.

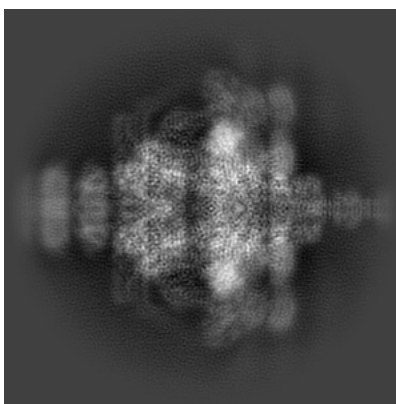
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

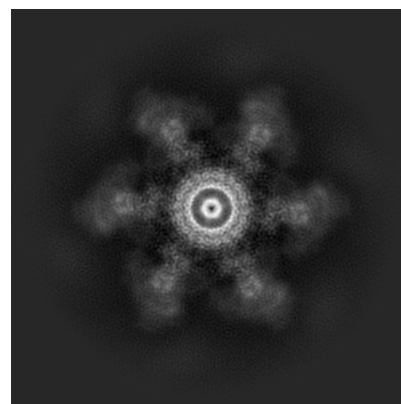
6.1.1 Primary map



X

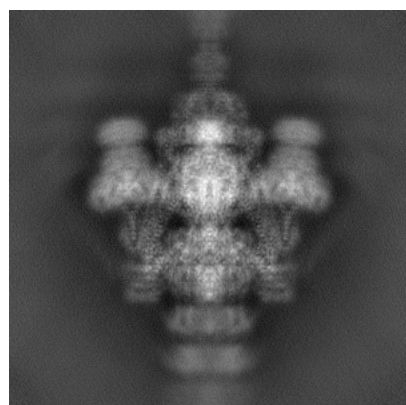


Y

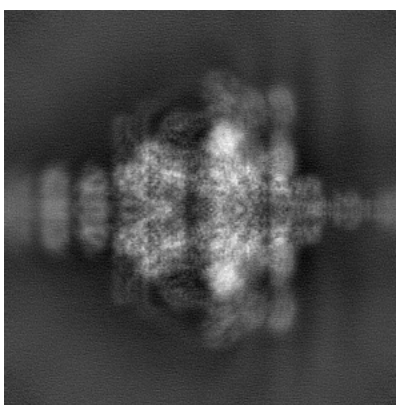


Z

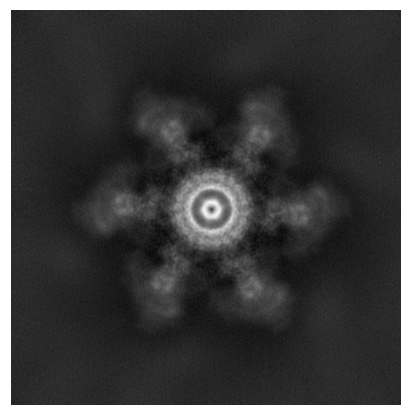
6.1.2 Raw map



X



Y

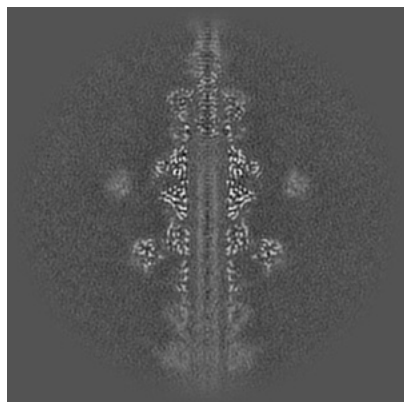


Z

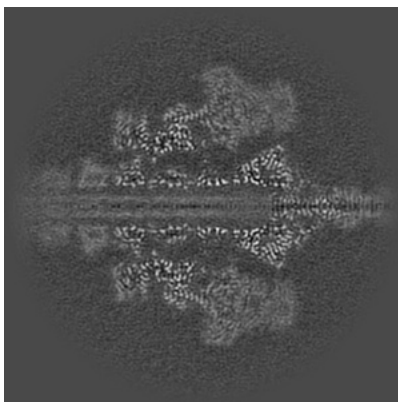
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

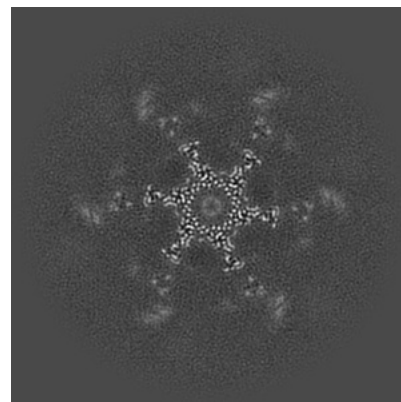
6.2.1 Primary map



X Index: 180

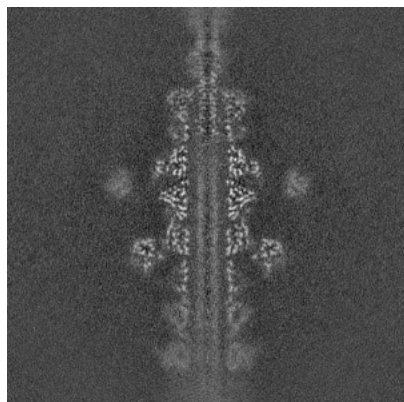


Y Index: 180

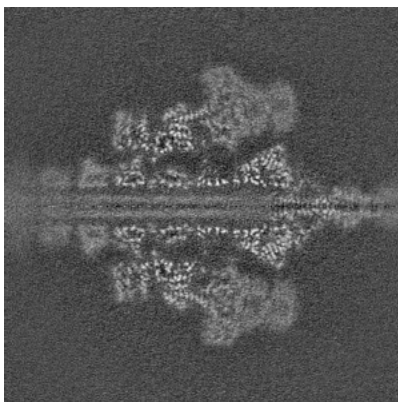


Z Index: 180

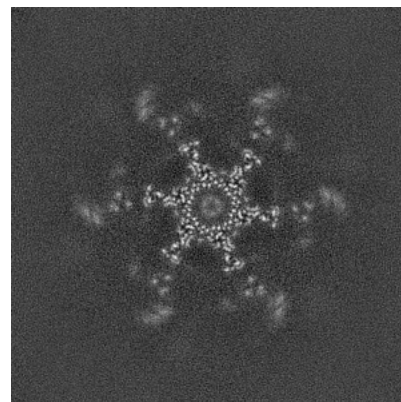
6.2.2 Raw map



X Index: 180



Y Index: 180

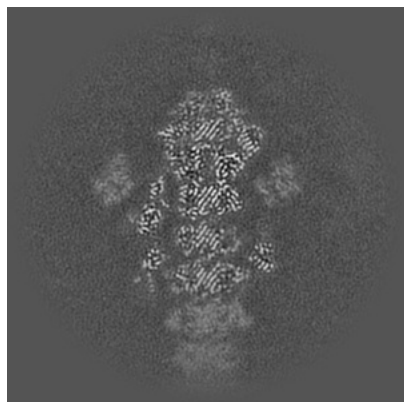


Z Index: 180

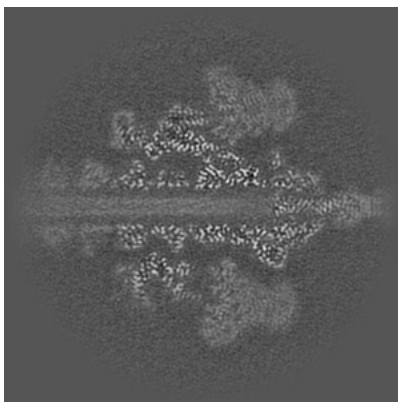
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

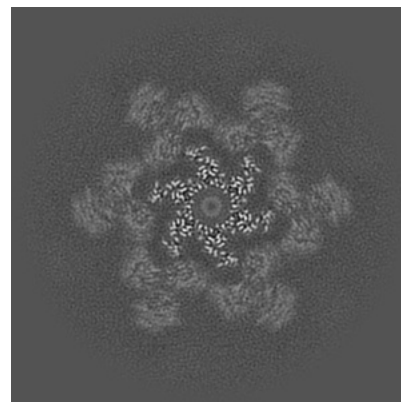
6.3.1 Primary map



X Index: 199

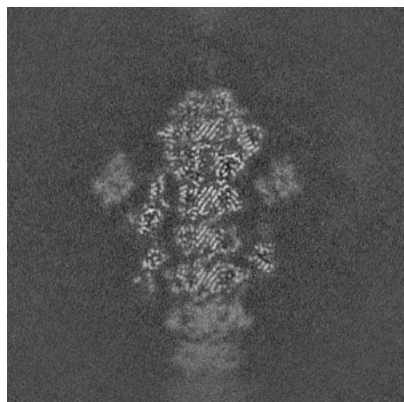


Y Index: 175

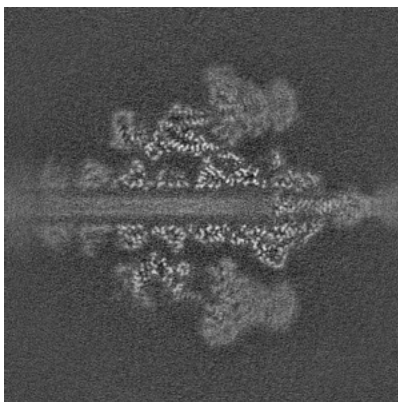


Z Index: 192

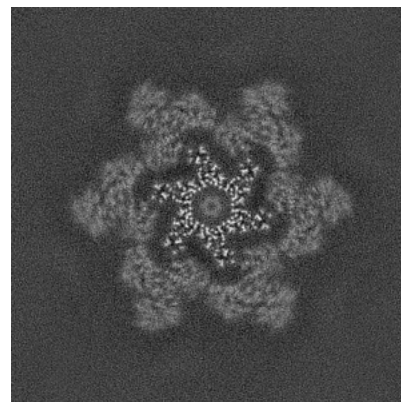
6.3.2 Raw map



X Index: 199



Y Index: 175

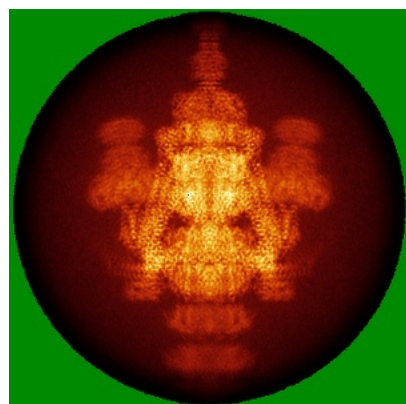


Z Index: 194

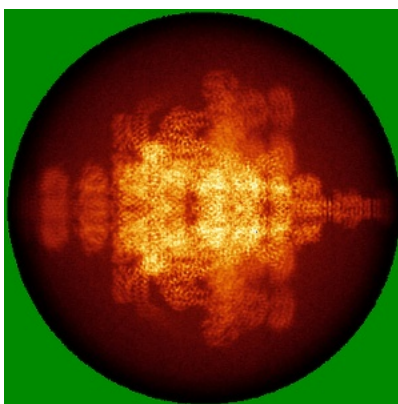
The images above show the largest variance slices of the map in three orthogonal directions.

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

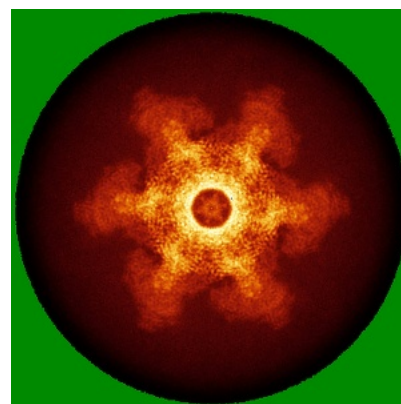
6.4.1 Primary map



X

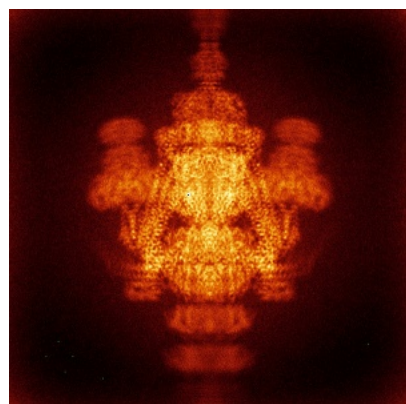


Y

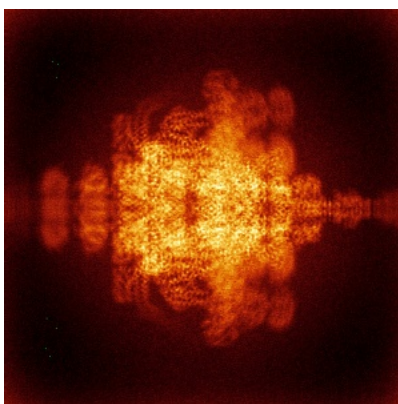


Z

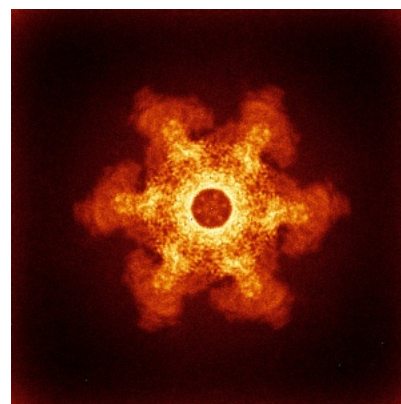
6.4.2 Raw map



X



Y

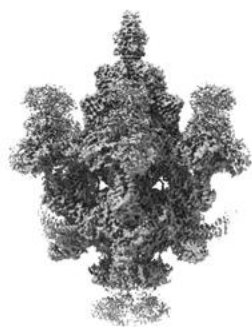


Z

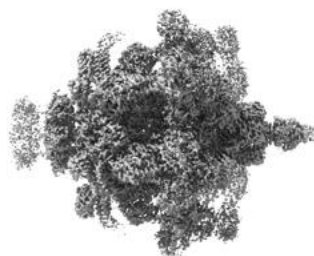
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

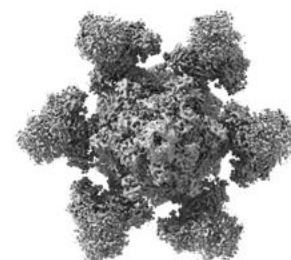
6.5.1 Primary map



X



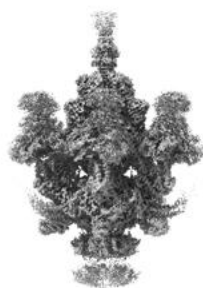
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.26. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

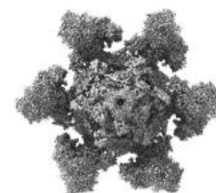
6.5.2 Raw map



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.

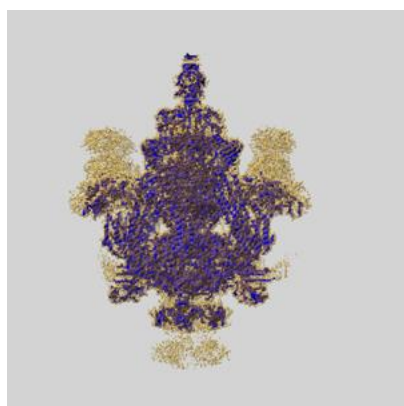
6.6 Mask visualisation [i](#)

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

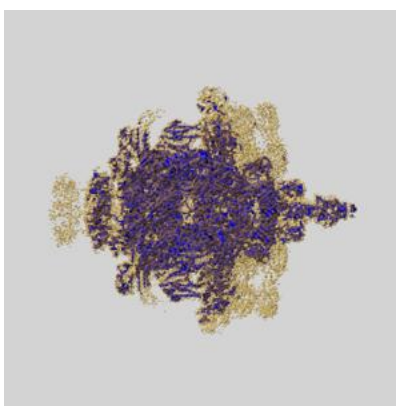
A mask typically either:

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

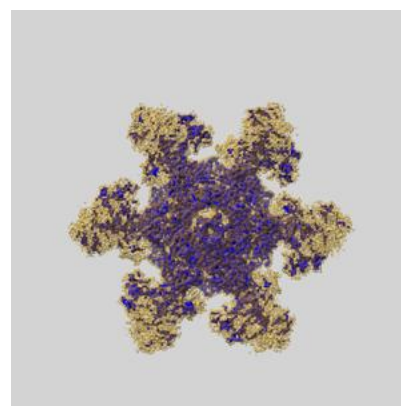
6.6.1 emd_63716_msk_1.map [i](#)



X



Y

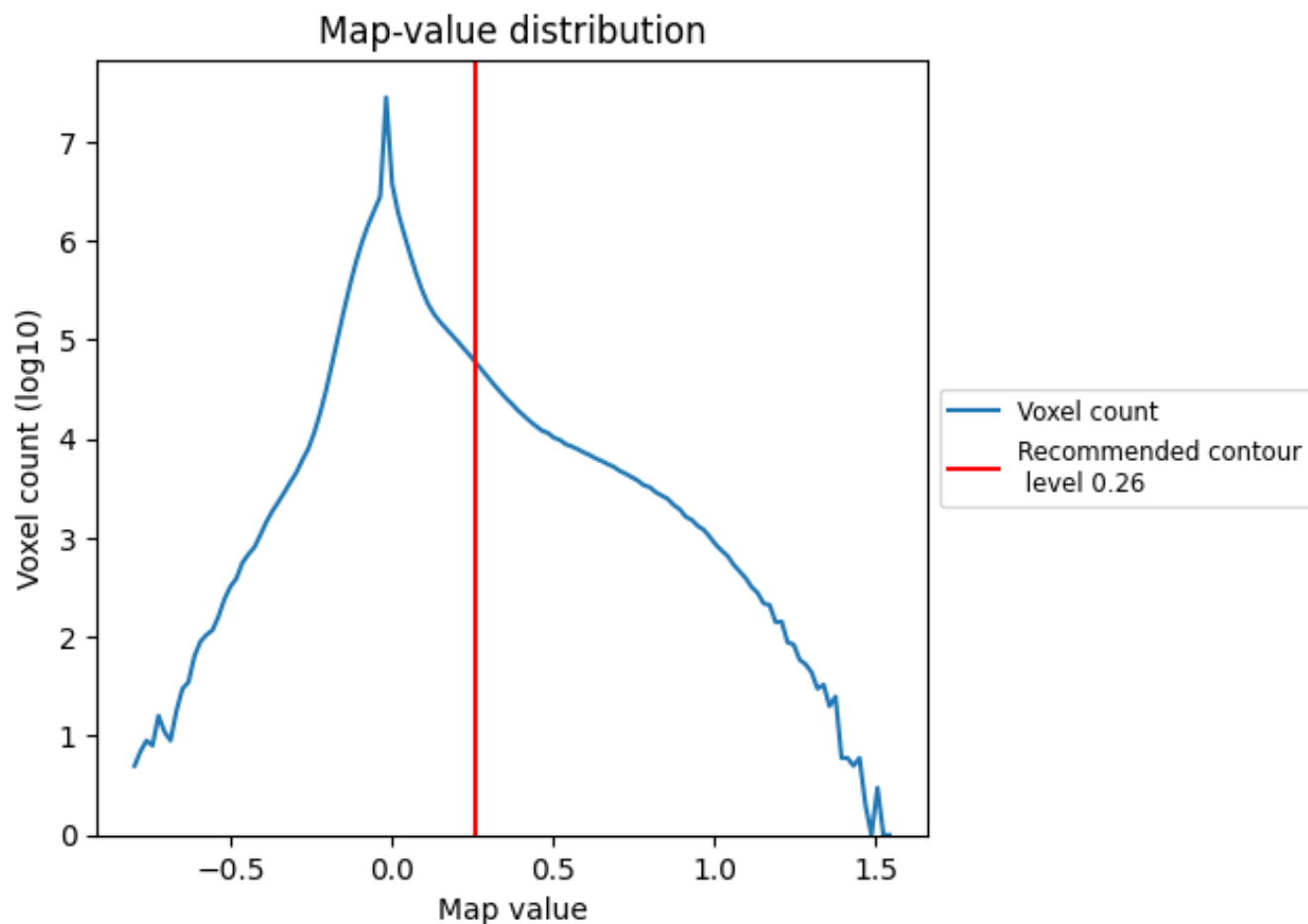


Z

7 Map analysis [i](#)

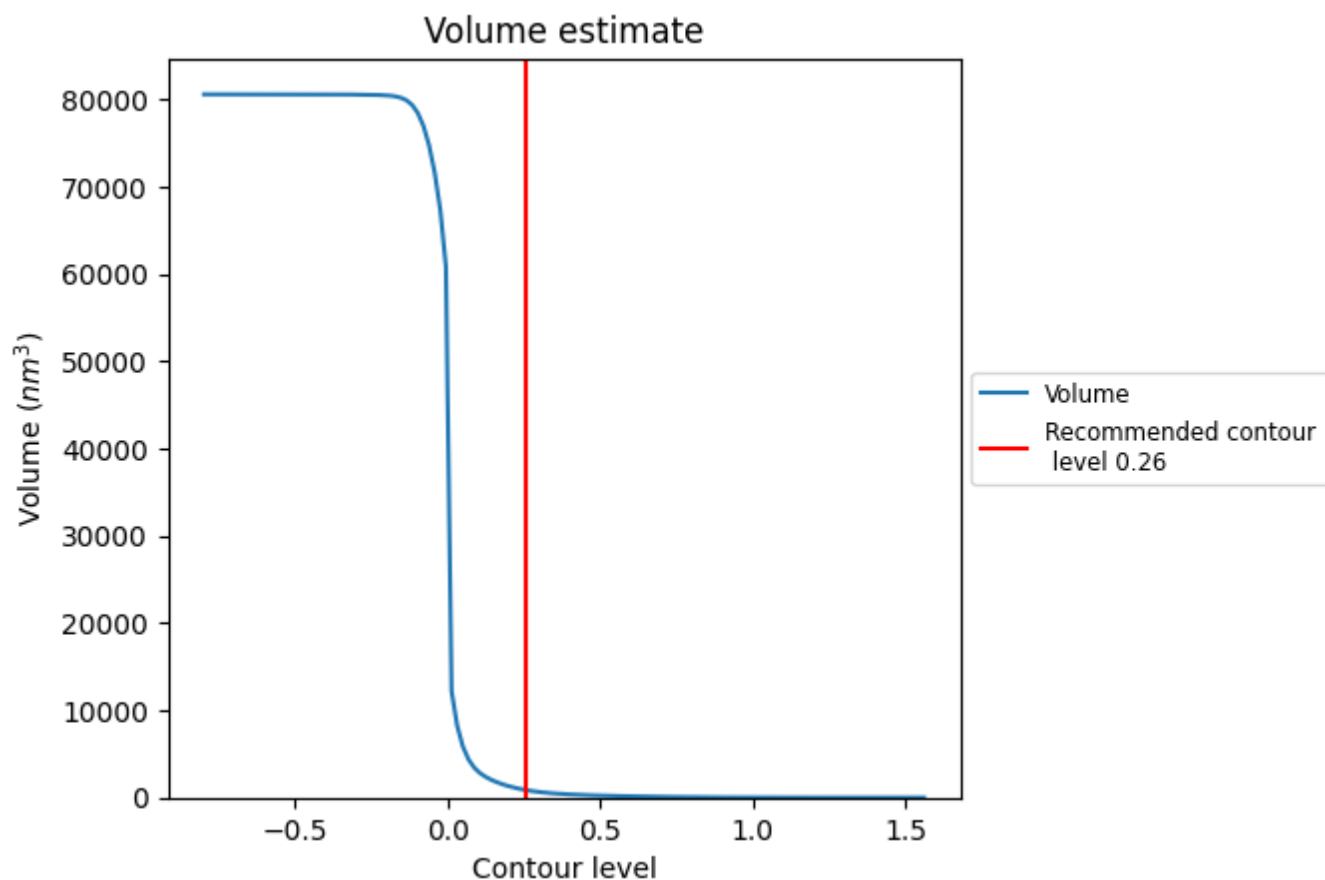
This section contains the results of statistical analysis of the map.

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.

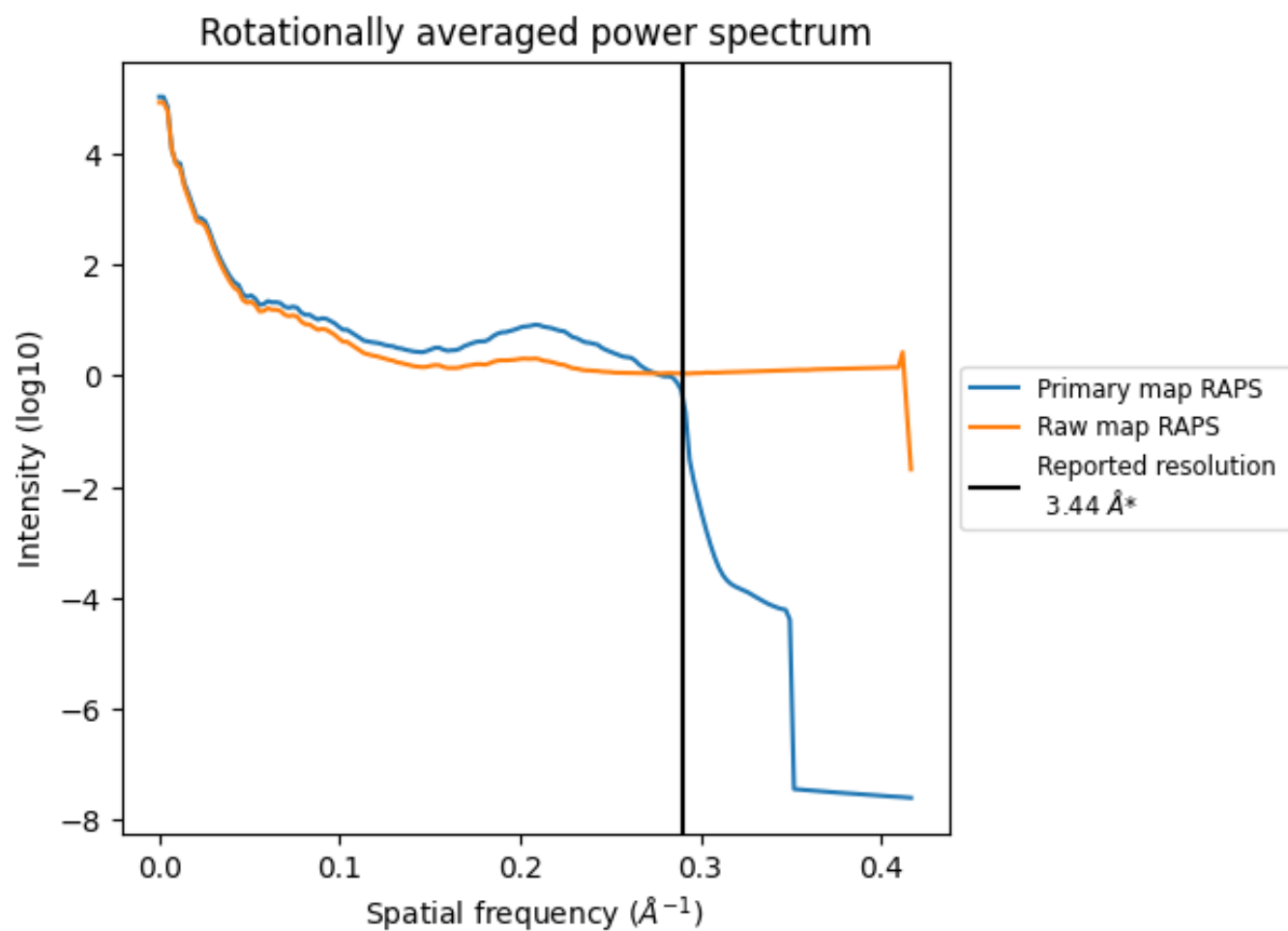
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 844 nm³; this corresponds to an approximate mass of 763 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 ⓘ

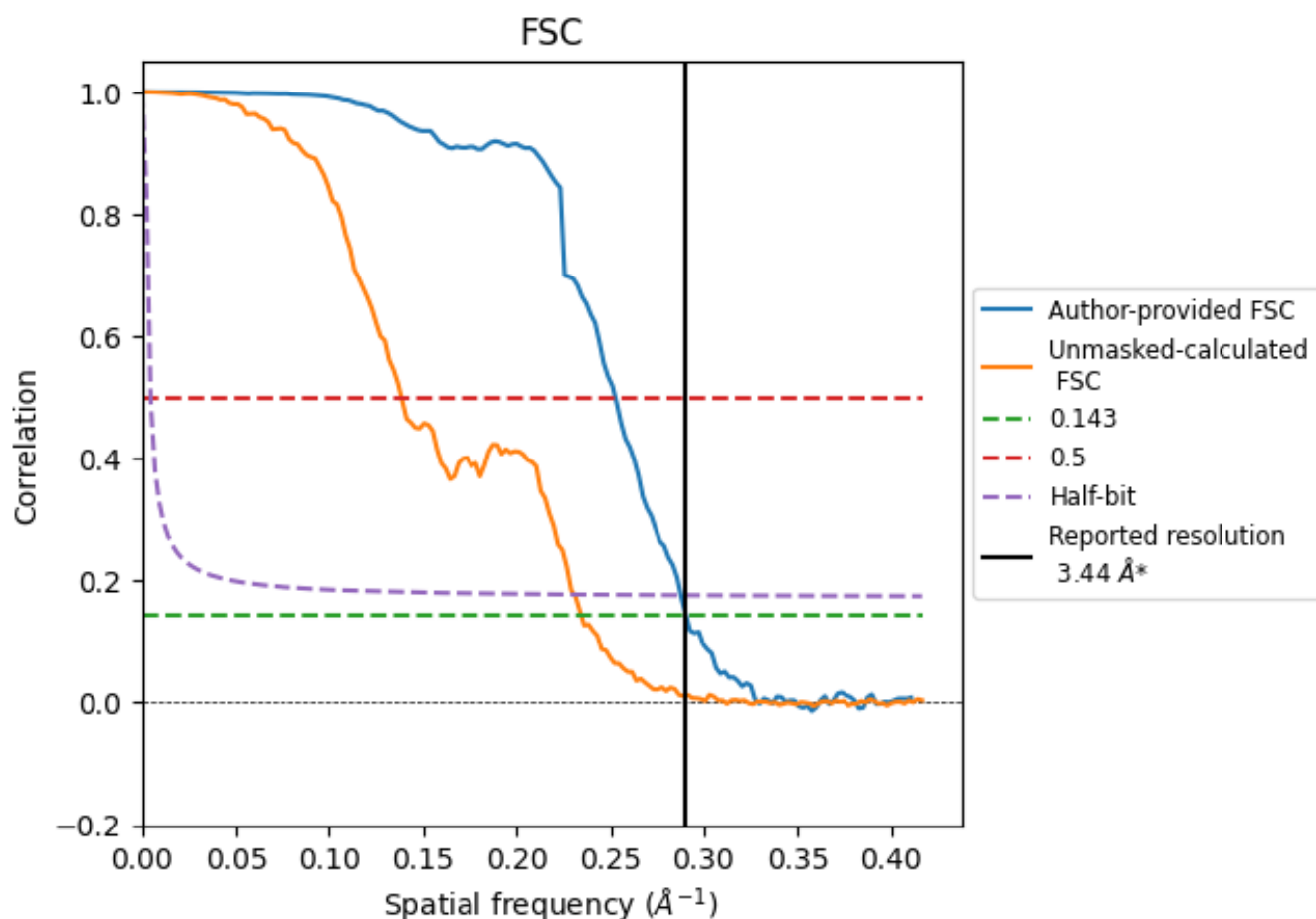


*Reported resolution corresponds to spatial frequency of 0.291 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.291 \AA^{-1}

8.2 Resolution estimates [i](#)

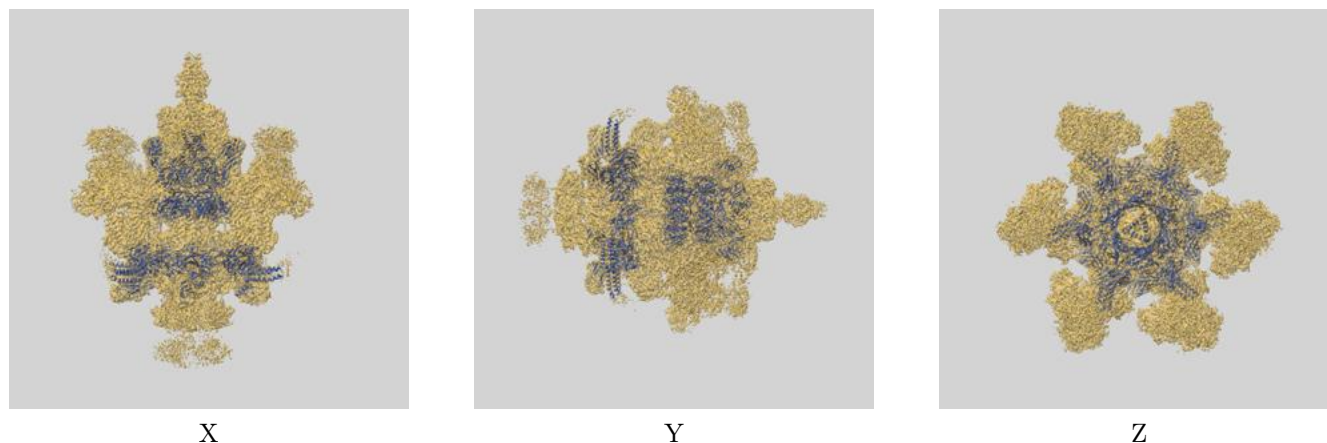
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	3.44	3.96	3.47
Unmasked-calculated*	4.26	7.23	4.33

*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 4.26 differs from the reported value 3.44 by more than 10 %

9 Map-model fit [i](#)

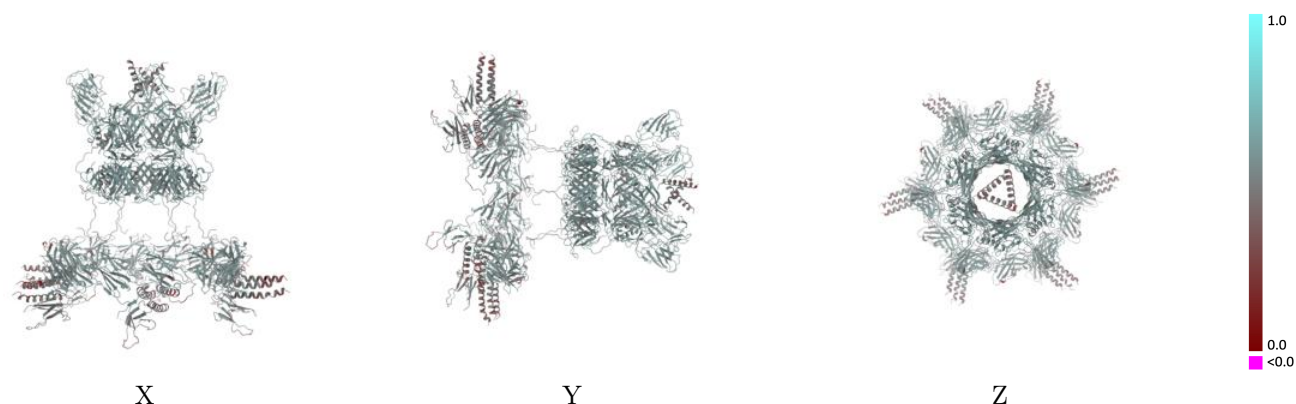
This section contains information regarding the fit between EMDB map EMD-63716 and PDB model 9M8O. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



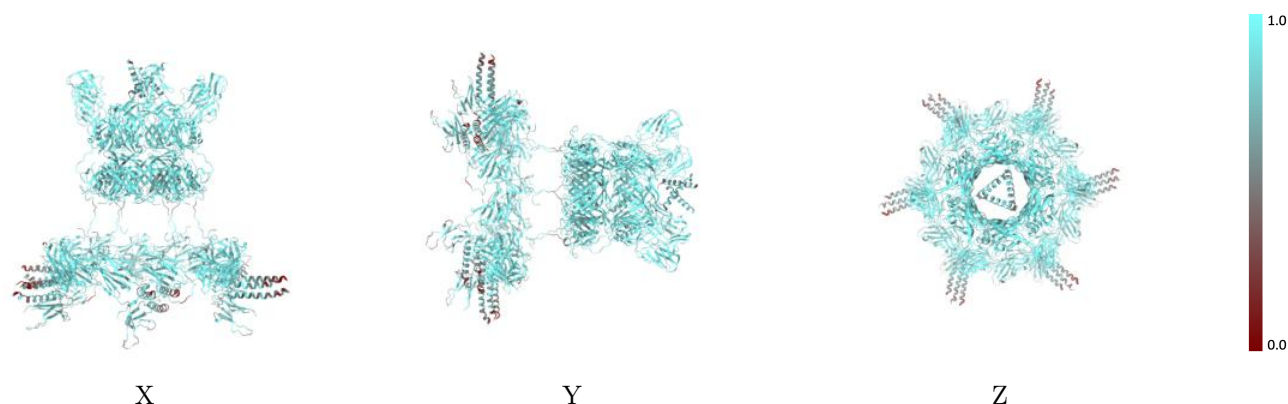
The images above show the 3D surface view of the map at the recommended contour level 0.26 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



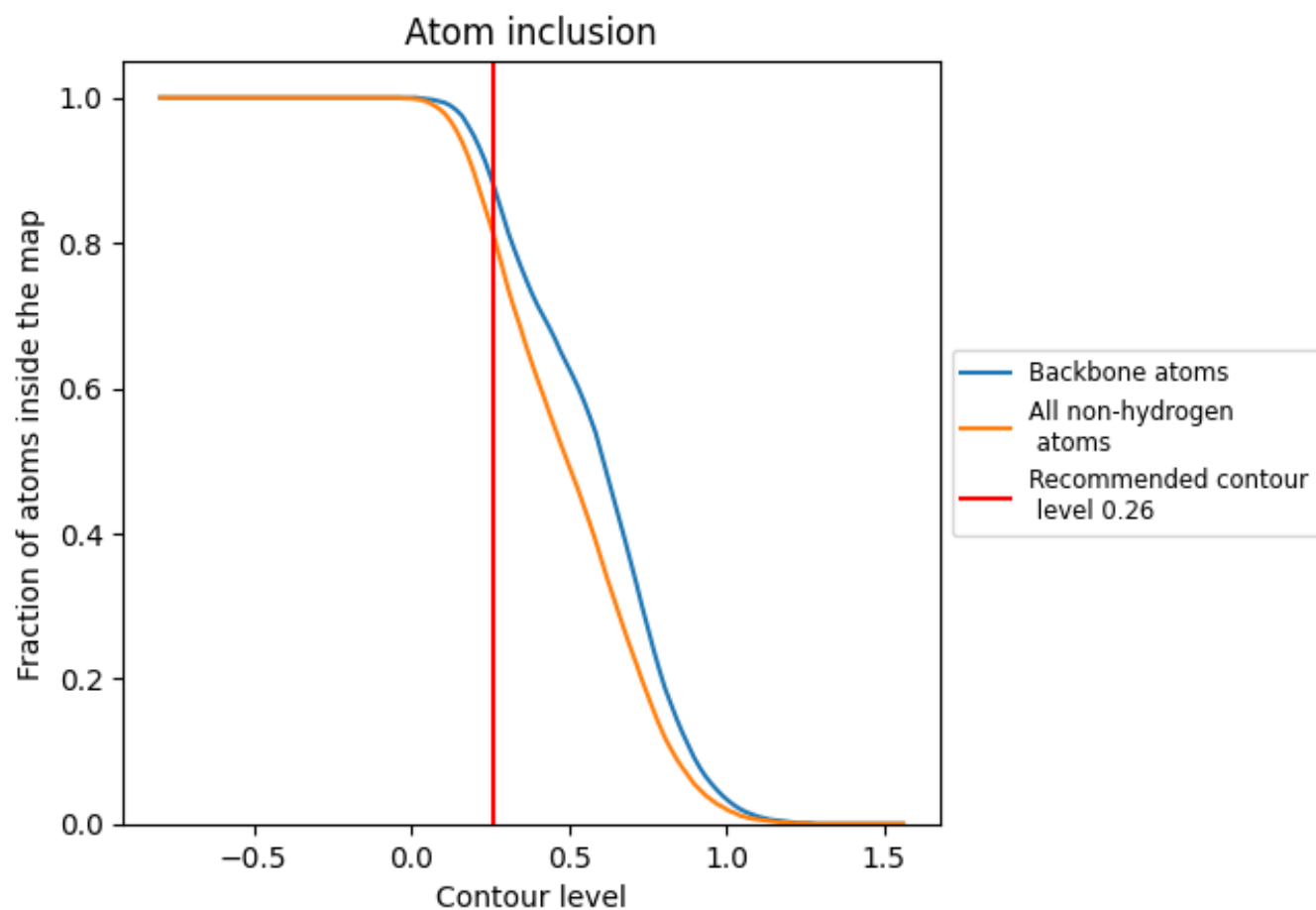
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.26).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 81% 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 (0.26) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8130	 0.5240
A	 0.8260	 0.5430
B	 0.8290	 0.5380
C	 0.8330	 0.5460
D	 0.8270	 0.5460
E	 0.8290	 0.5460
F	 0.8340	 0.5390
G	 0.8730	 0.5460
H	 0.8740	 0.5470
I	 0.8750	 0.5460
J	 0.8720	 0.5450
K	 0.8740	 0.5470
L	 0.8740	 0.5500
M	 0.6710	 0.4630
N	 0.6710	 0.4600
O	 0.6590	 0.4350
P	 0.8070	 0.5180
Q	 0.8020	 0.5220
R	 0.6810	 0.4710
S	 0.7990	 0.5080
T	 0.7880	 0.5140
U	 0.6890	 0.4730
V	 0.8140	 0.5180
W	 0.7980	 0.5220
X	 0.6890	 0.4680
Y	 0.8120	 0.5090
Z	 0.7860	 0.5120
a	 0.6920	 0.4680
b	 0.8090	 0.5140
c	 0.8010	 0.5230
d	 0.6920	 0.4680
e	 0.8040	 0.5070
f	 0.7790	 0.5090
g	 0.7000	 0.4770

