



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:57 AM UTC

PDB ID : 7QOL / pdb_00007qol
EMDB ID : EMD-14094
Title : Tail assembly of the phicrAss001 virion with C6 symmetry imposed
Authors : Bayfield, O.W.; Shkoporov, A.N.; Yutin, N.; Khokhlova, E.V.; Smith, J.L.R.;
Hawkins, D.E.D.P.; Koonin, E.V.; Hill, C.; Antson, A.A.
Deposited on : 2021-12-24
Resolution : 3.33 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

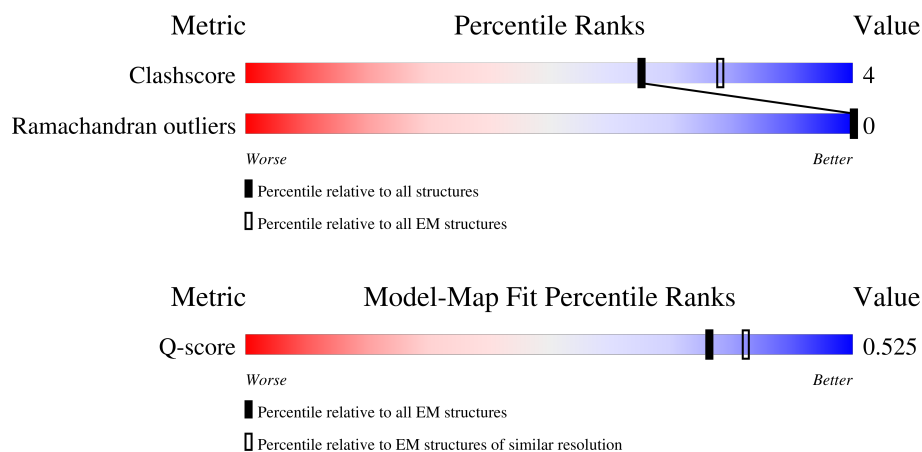
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.33 Å.

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



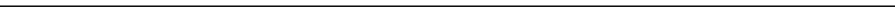
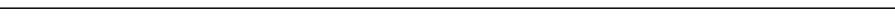
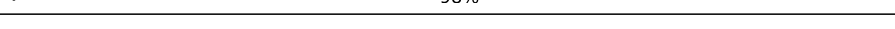
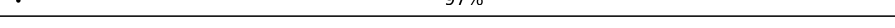
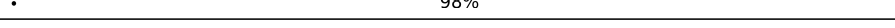
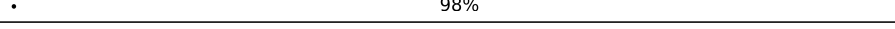
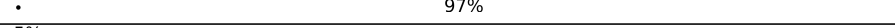
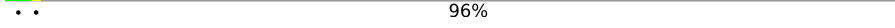
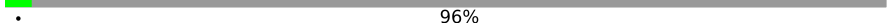
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	14484 (2.83 - 3.83)

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	806	9% 72% 10% 18%
1	O	806	9% 73% 9% 18%
2	B	236	88% 8% •
2	Q	236	89% 7% •
3	C	225	88% 12%

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Mol	Chain	Length	Quality of chain
3	S	225	 89% 11%
4	D	230	 90% 8%
4	T	230	 90% 8%
5	E	238	 90% 10%
5	F	238	 85% 13%
5	U	238	 91% 9%
5	V	238	 88% 12%
6	G	215	 75% 7% 18%
6	H	215	 74% 13% 13%
6	W	215	 72% 9% 19%
6	Z	215	 81% 6% 13%
7	I	114	 81% 13% 6%
7	a	114	 76% 18% 6%
8	J	832	 98%
8	K	832	 98%
8	L	832	 97%
8	b	832	 98%
8	c	832	 98%
8	d	832	 97%
9	M	842	 5% 14% 85%
9	N	842	 96%
9	e	842	 5% 14% 85%
9	f	842	 96%
10	P	1371	 88% 11%
11	R	14	 93% 7%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 51479 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 Portal protein gp20.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	657	Total	C	N	O	S	0	0
			5371	3404	917	1027	23		
1	O	657	Total	C	N	O	S	0	0
			5371	3404	917	1027	23		

- Molecule 2 is a protein called Ring protein 1 gp43.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
2	Q	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		

- Molecule 3 is a protein called Ring protein 2 gp40.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
3	S	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		

- Molecule 4 is a protein called Ring protein 3 gp35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	226	Total	C	N	O	S	0	0
			1805	1151	293	357	4		
4	T	226	Total	C	N	O	S	0	0
			1805	1151	293	357	4		

- Molecule 5 is a protein called Ring protein 4/5 gp34.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	238	Total	C	N	O	S	0	0
			1878	1185	312	377	4		
5	F	238	Total	C	N	O	S	0	0
			1878	1185	312	377	4		
5	U	238	Total	C	N	O	S	0	0
			1878	1185	312	377	4		
5	V	238	Total	C	N	O	S	0	0
			1878	1185	312	377	4		

- Molecule 6 is a protein called Tail hub protein A gp38.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	177	Total	C	N	O	S	0	0
			1441	924	230	276	11		
6	H	188	Total	C	N	O	S	0	0
			1516	968	243	292	13		
6	W	174	Total	C	N	O	S	0	0
			1419	913	225	271	10		
6	Z	188	Total	C	N	O	S	0	0
			1516	968	243	292	13		

- Molecule 7 is a protein called Tail hub protein B gp39.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	107	Total	C	N	O	S	0	0
			878	560	134	175	9		
7	a	107	Total	C	N	O	S	0	0
			878	560	134	175	9		

- Molecule 8 is a protein called Tail fiber protein gp22.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	19	Total	C	N	O	S	0	0
			170	112	27	30	1		
8	K	19	Total	C	N	O	S	0	0
			170	112	27	30	1		
8	L	25	Total	C	N	O	S	0	0
			224	145	37	41	1		
8	b	19	Total	C	N	O	S	0	0
			170	112	27	30	1		
8	c	19	Total	C	N	O	S	0	0
			170	112	27	30	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	25	Total	C	N	O	S	0	0
			224	145	37	41	1		

- Molecule 9 is a protein called Cargo protein 1 gp45.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
9	N	32	Total	C	N	O	S	0	0
			251	157	44	49	1		
9	e	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
9	f	32	Total	C	N	O	S	0	0
			251	157	44	49	1		

- Molecule 10 is a protein called Muzzle protein gp44.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	1354	Total	C	N	O	S	0	0
			10925	6948	1815	2137	25		

- Molecule 11 is a protein called Muzzle bound helix.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	R	14	Total	C	N	O	0	0
			70	42	14	14		

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	Mg	0
			1	1	
12	O	1	Total	Mg	0
			1	1	

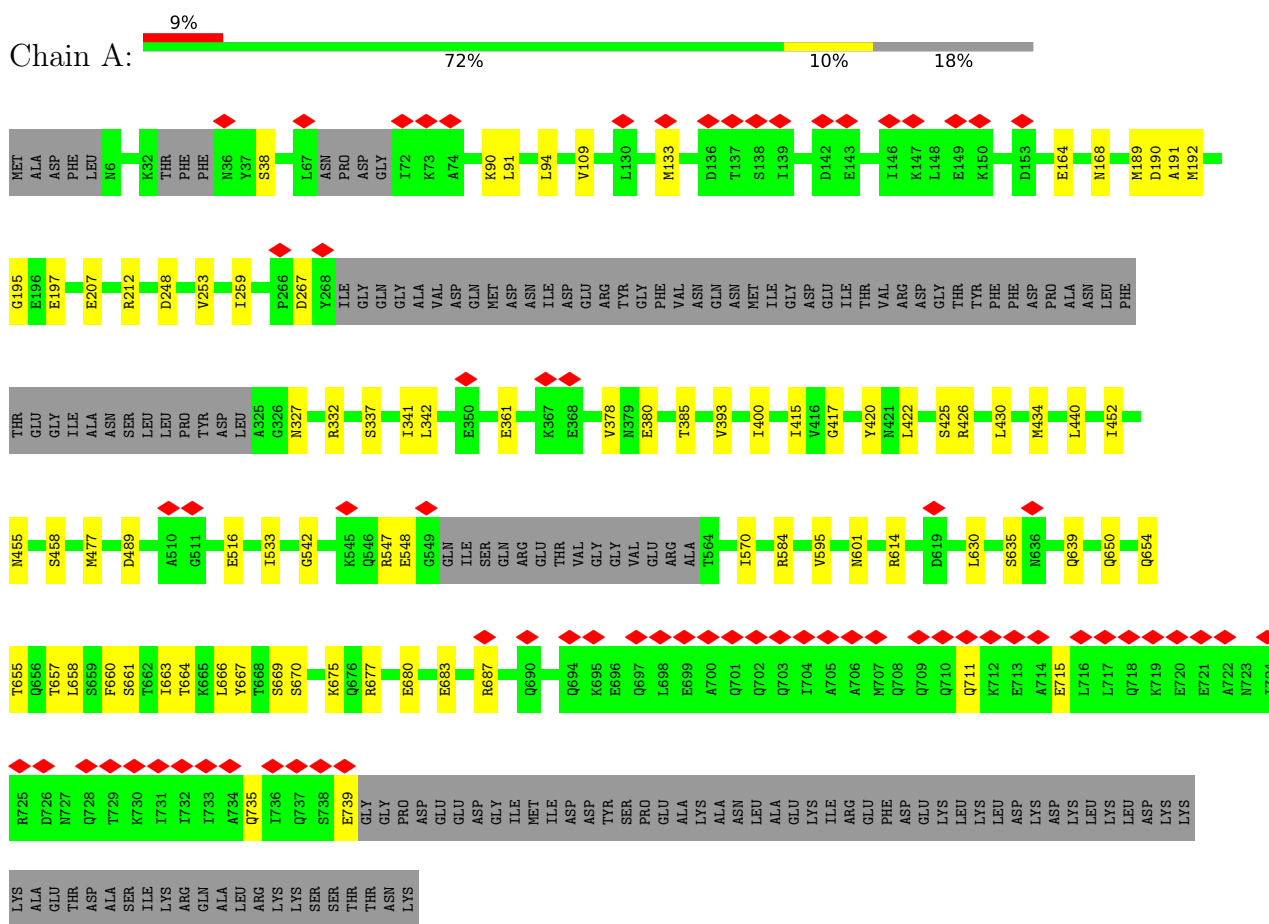
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total	O	0
			1	1	
13	O	1	Total	O	0
			1	1	

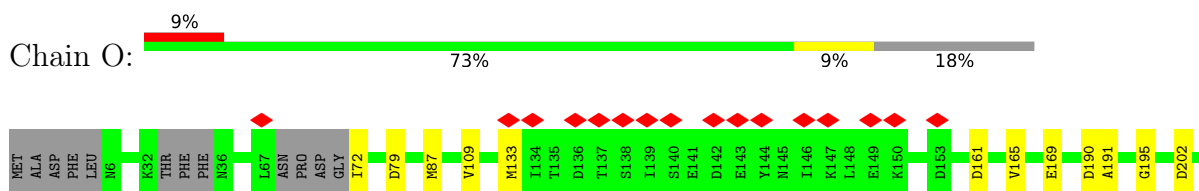
3 Residue-property plots [i](#)

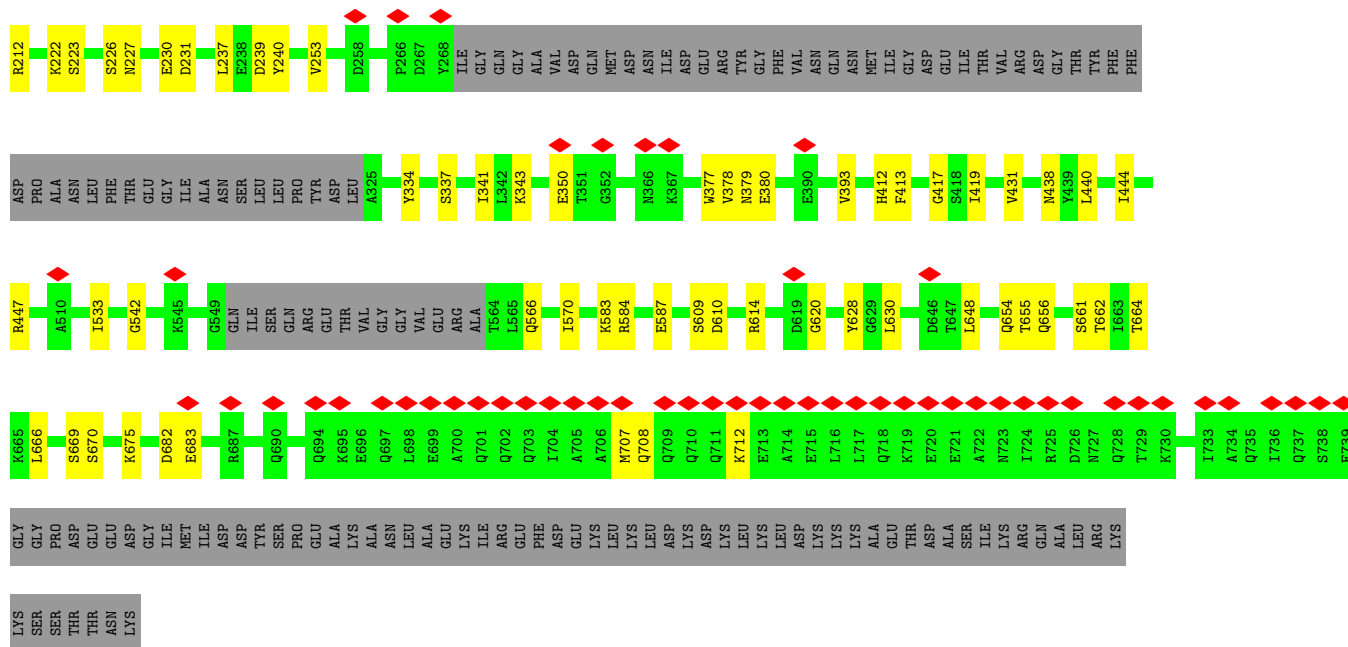
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Portal protein gp20

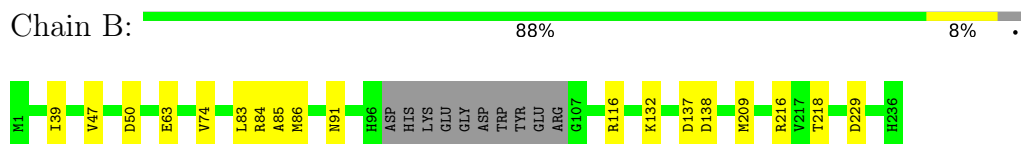


• Molecule 1: Portal protein gp20

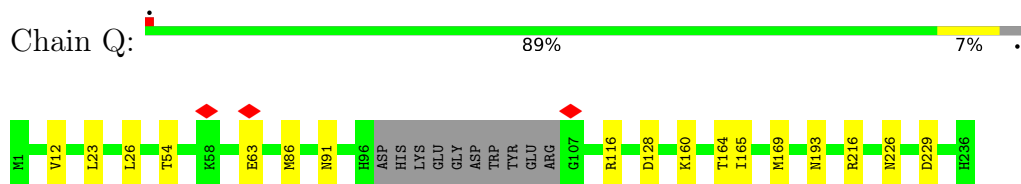




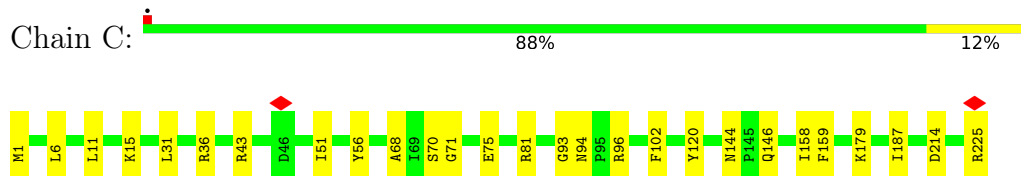
- Molecule 2: Ring protein 1 gp43



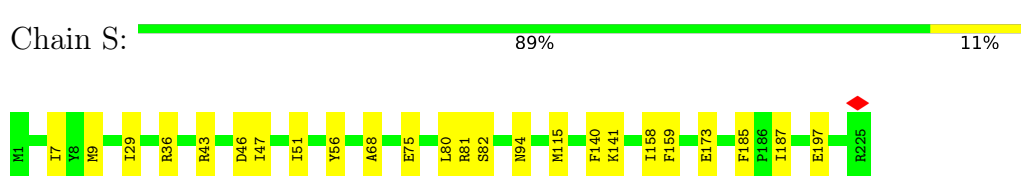
- Molecule 2: Ring protein 1 gp43



- Molecule 3: Ring protein 2 gp40

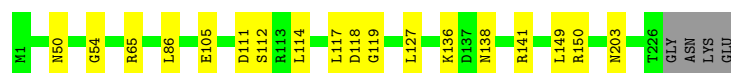


- Molecule 3: Ring protein 2 gp40



- Molecule 4: Ring protein 3 gp35

Chain D:  90% 8% .



- Molecule 4: Ring protein 3 gp35

Chain T:  90% 8% .



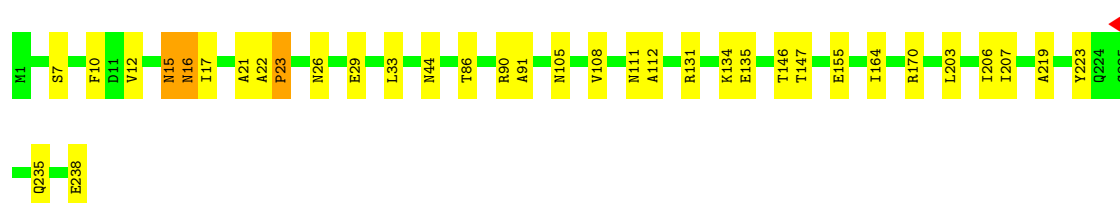
- Molecule 5: Ring protein 4/5 gp34

Chain E:  90% 10%



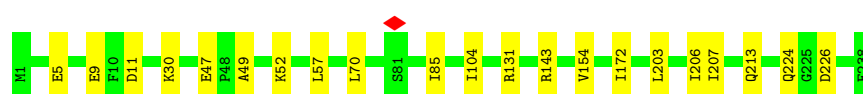
- Molecule 5: Ring protein 4/5 gp34

Chain F:  85% 13% .



- Molecule 5: Ring protein 4/5 gp34

Chain U:  91% 9%



- Molecule 5: Ring protein 4/5 gp34

Chain V:  88% 12%

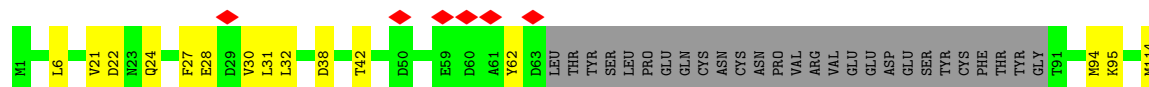
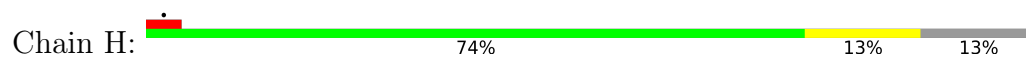


- Molecule 6: Tail hub protein A gp38

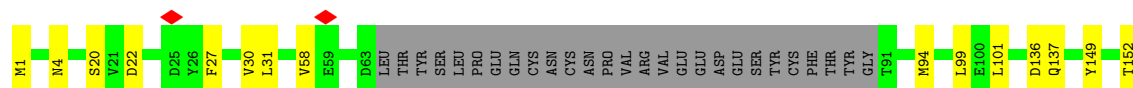
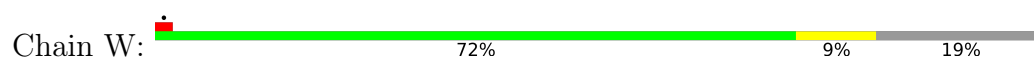
Chain G:  75% 7% 18%



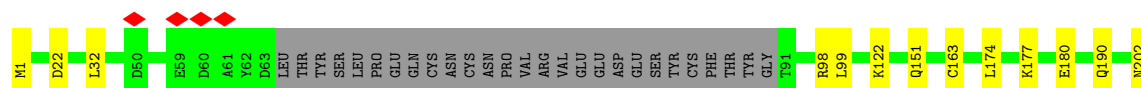
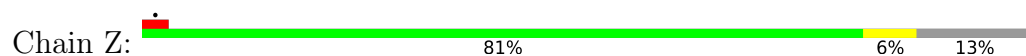
- Molecule 6: Tail hub protein A gp38



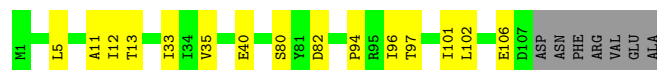
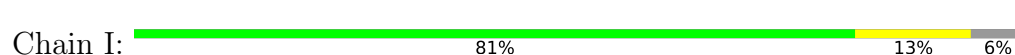
- Molecule 6: Tail hub protein A gp38



- Molecule 6: Tail hub protein A gp38

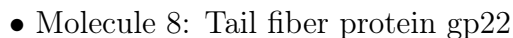


- Molecule 7: Tail hub protein B gp39

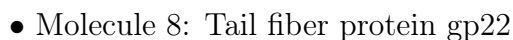


- Molecule 7: Tail hub protein B gp39

Response	Percentage
Yes, the U.S. is a democracy	76%
No, the U.S. is not a democracy	18%
Don't know	6%



98%



98%

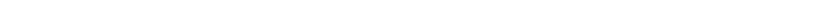






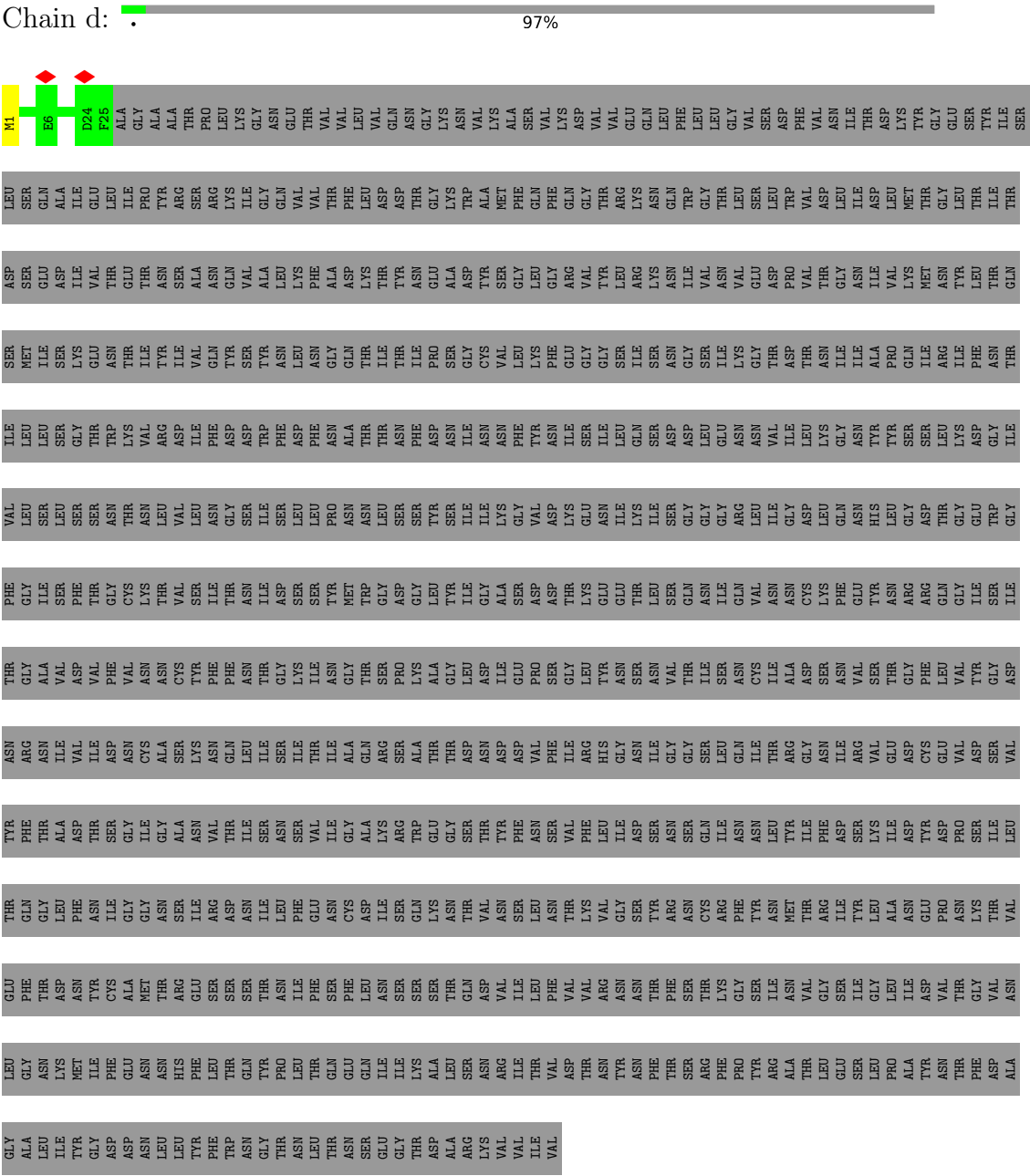
[illegible]

- Molecule 8: Tail fiber protein gp22

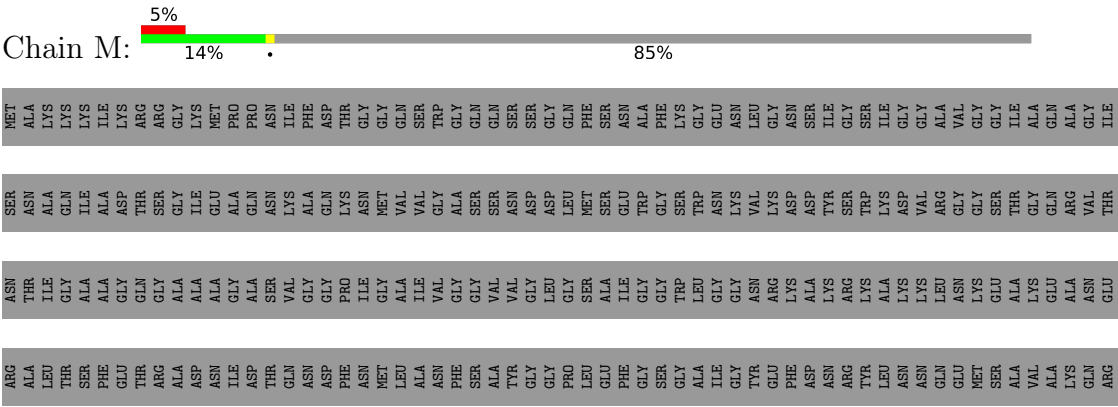
Chain c:  98%

[illegible]

- Molecule 8: Tail fiber protein gp22



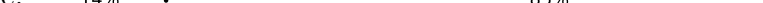
● Molecule 9: Cargo protein 1 gp45





[illegible]

- Molecule 9: Cargo protein 1 gp45

Chain e:  14% 85%

GLU	ARG	ASP	GLY	E541	ARG	GLU	ASP	LEU	ARG	ASN	THR	LEU	ARG	ASN	SER	MET
ARG	ASP	PHE	ASN	A542	ASN	GLN	ALA	THR	ALA	ASN	THR	THR	ALA	THR	ASN	ALA
VAL	THR	GLN	ARG	R543	TRP	THR	ARG	SER	LEU	ILE	ILE	SER	LEU	ILE	ALA	LYS
ALA	ILE	ALA	THR	Q544	A425	VAL	ASP	PRO	THR	GLY	GLY	PRO	THR	GLY	ILE	LYS
PHE	LYS	THR	TRP	R545	F426	ALA	LEU	ASN	PHE	ALA	ALA	ASN	PHE	ALA	ALA	ILE
ASN	LYS	THR	ARG	K546		ALA	ARG	SER	LEU	GLY	GLY	SER	GLU	ASP	ASP	LYS
ARG	MET	THR	ARG	E547	N431	ASN	LEU	ARG	LEU	LEU	THR	PHE	THR	THR	THR	ARG
GLY	ASN	TYR	TYR	A548	T432	ILE	GLY	ALA	ALA	GLY	GLY	GLN	ARG	GLY	GLY	GLY
THR	GLN	THR	ALA	R549	Q433	ALA	ALA	LYS	THR	THR	GLY	ALA	ALA	ALA	ALA	ARG
MET	ALA	PRO	ILE	R550	D436	PRO	ASN	ASP	HEU	GLY	PRO	LEU	ASN	ALA	ILE	LYS
PHE	ALA	ILE	ILE	E551		GLY	GLY	GLY	GLY	GLY	GLU	GLU	ILE	ALA	ALA	PRO
ASN	ALA	GLY	GLY	G552	N445	ASP	ASN	ASP	ASN	ASN	MET	MET	ASP	ALA	GLN	PRO
THR	THR	SER	SER		E446	ILE	SER	GLU	THR	THR	THR	ASN	THR	ASN	ASN	ASN
THR	ARG	GLY	GLY		G447	LYS	VAL	TYR	GLN	GLN	THR	THR	GLN	LYS	LYS	ILE
GLY	GLY	ALA	ALA		G448	ILE	ARG	ASN	PHE	ASN	ASN	ASN	GLY	GLY	ALA	PHE
LEU	LEU	SER	SER		S449	LYS	ARG	ALA	ALA	ALA	ALA	ALA	PHE	GLY	GLN	THR
ALA	ALA	LEU	LEU		R450	GLU	LYS	PHE	ASN	PHE	PHE	ALA	ASN	ILE	ASN	GLY
ALA	ASN	SER	SER		E451	LYS	VAL	VAL	LEU	ALA	ALA	ALA	MET	GLY	MET	GLY
MET	THR	SER	ASP		F452	ASN	ASN	GLU	LEU	GLU	GLU	GLU	LEU	VAL	VAL	VAL
PHE	THR	LEU	PHE		N453	LYS	ALA	GLY	LYS	LYS	GLY	GLY	ASN	ILE	VAL	SER
ASN	GLY	SER	SER		P454	LYS	TYR	GLY	TYR	GLY	GLY	GLY	PHE	VAL	GLY	GLY
ALA	ASN	LYS	LYS		Y455	PHE	PRO	PRO	PRO	PRO	GLY	GLY	SER	GLY	ALA	GLY
GLU	GLU	PRO	ASP		Q456	THR	ALA	ALA	LEU	LYS	GLY	GLY	TYR	VAL	ASN	SER
ARG	ASN	LEU	THR		G457	TYR	TYR	TYR	LYS	GLY	GLY	GLY	ASP	GLY	ASP	SER
ASN	ASN	ALA	ASP		T458	CYS	ALA	ALA	LYS	ALA	LYS	LYS	LEU	LEU	ASP	SER
ALA	GLN	ALA	SER		Q459	GLY	PHE	PHE	ALA	PHE	LYS	LYS	ASN	GLY	ASP	GLY
ALA	ALA	ALA	ALA		R460	GLY	GLY	GLY	GLY	THR	ASN	PRO	LEU	THR	LEU	PHE
LYS	GLY	GLY	ASP		G461	LYS	LYS	LYS	GLY	TYR	GLY	TYR	GLY	ALA	GLY	GLY
ARG	ILE	ILE	LEU		V462	VAL	VAL	VAL	SER	SER	GLY	GLY	PHE	GLY	TRP	ALA
ALA	LEU	ALA	ILE			THR	THR	THR	LEU	LEU	LYS	LYS	SER	GLY	GLY	ALA
ARG	ALA	ALA	SER		D463	GLU	PHE	PHE	LEU	PHE	LYS	LYS	SER	GLY	GLY	PHE
LEU	ALA	ALA	GLY		PRO	ALA	ASP	ASP	ALA	ASP	LYS	LYS	GLY	TRP	TRP	LYS
ARG	ASP	VAL	VAL		GLU	ALA	SER	SER	PRO	PRO	ALA	LEU	ALA	TRP	TRP	GLY
GLN	TYR	TYR	ASP			ILE	ILE	VAL	GLY	GLY	GLY	TYR	ILE	GLY	ASN	PHE
ALA	ASN	ASN	ASN		G466	ARG	GLY	VAL	GLY	GLY	GLY	PRO	GLY	GLY	LYS	ASN
THR	TYR	GLY	GLY		A467	LYS	VAL	VAL	GLY	ASN	ASN	SER	TYR	VAL	VAL	GLY
THR	GLY	ALA	ALA		P468	GLY	ASN	VAL	SER	GLY	GLY	VAL	GLU	LYS	LYS	GLY
VAL	GLN	GLU	GLU			LYS	ASN	PRO	ASN	ASN	PRO	VAL	PHE	ARG	ARG	ASN
ALA	ASN	ALA	ALA		G474	ASN	PHE	PHE	ASN	PHE	ASN	PRO	ASN	LYS	ASP	ASN
GLN	MET	VAL	VAL			GLN	SER	SER	ASN	ASN	GLY	GLY	ASN	GLY	ASP	ASN
LEU	GLY	GLY	GLY		D485	SER	GLN	GLN	ASN	GLY	GLY	GLY	ARG	GLY	GLY	GLY
ARG	ASN	TYR	ALA		R486	ASN	SER	PHE	SER	ASN	ALA	ALA	TYR	LYS	TRP	ILE
GLN	ALA	PRO	PRO			PRO	ASN	THR	PHE	THR	ASN	GLY	LEU	LYS	LYS	ILE
GLY	ALA	ILE	ILE		D491	THR	GLN	THR	GLN	ASN	LYS	GLY	GLY	VAL	VAL	GLY
LYS	GLN	GLY	GLY		D492	ARG	GLY	ARG	GLY	ASN	LYS	PRO	GLN	ARG	VAL	ARG
ASP	ALA	ASN	ASN			LYS	ILE	ILE	GLN	GLU	ASN	ARG	GLU	GLY	GLY	VAL
GLN	GLY	TYR	TYR			ARG	GLY	ARG	GLY	GLY	GLY	SER	GLY	GLY	GLY	GLY
ASP	GLY	LEU	LEU		R495	ALA	GLY	ALA	GLY	GLY	GLY	TYR	SER	SER	SER	GLY
ALA	TYR	SER	SER		E496	THR	GLY	PHE	MET	GLY	GLY	PRO	THR	THR	THR	ILE
ALA	ASN	TYR	TYR		Y497	PHE	THR	THR	ILE	ILE	ALA	ILE	VAL	GLY	GLY	GLY
ARG	GLN	GLN	ARG			ALA	GLN	ALA	GLN	GLN	GLY	PRO	GLN	GLY	GLN	GLN
ARG	GLN	GLN	GLN		R502	ALA	ALA	ALA	GLN	GLN	LYS	THR	LYS	ALA	ALA	ARG
SER	LEU	LEU	ASP			PRO	SER	GLU	GLY	GLY	VAL	LYS	GLN	VAL	VAL	GLY
SER	ASP	THR	THR			ALA	THR	ALA	THR	THR	THR	ALA	ARG	THR	THR	THR

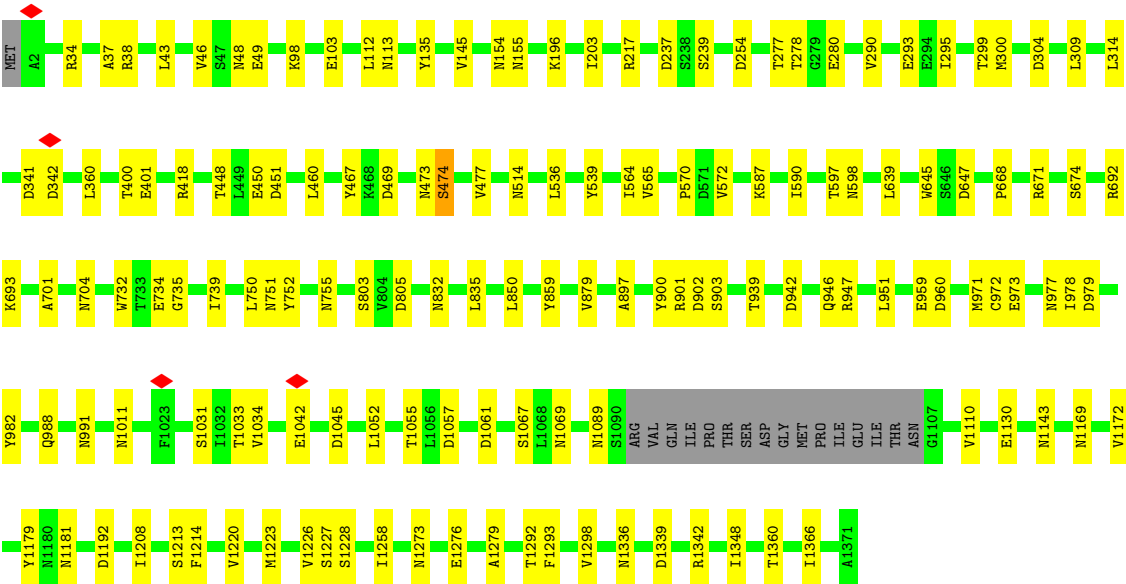
- Molecule 9: Cargo protein 1 gp45

Chain f: 96%

[illegible]

- Molecule 10: Muzzle protein gp44

Chain P: 88% 11%



• Molecule 11: Muzzle bound helix



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	46280	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.457	Depositor
Minimum map value	-0.290	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	892.2228, 892.2228, 892.2228	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.394098, 1.394098, 1.394098	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.16	0/5468	0.36	0/7374
1	O	0.16	0/5468	0.34	0/7374
2	B	0.18	0/1881	0.37	0/2548
2	Q	0.17	0/1881	0.36	0/2548
3	C	0.19	0/1886	0.38	0/2552
3	S	0.18	0/1886	0.37	0/2552
4	D	0.17	0/1837	0.37	0/2491
4	T	0.16	0/1837	0.35	0/2491
5	E	0.16	0/1910	0.33	0/2594
5	F	0.47	2/1910 (0.1%)	0.67	6/2594 (0.2%)
5	U	0.16	0/1910	0.33	0/2594
5	V	0.18	0/1910	0.38	0/2594
6	G	0.31	1/1469 (0.1%)	0.42	0/1989
6	H	0.26	0/1546	0.50	0/2093
6	W	0.18	0/1447	0.39	0/1959
6	Z	0.16	0/1546	0.38	0/2093
7	I	0.20	0/895	0.46	0/1208
7	a	0.31	0/895	0.60	0/1208
8	J	0.24	0/174	0.51	0/232
8	K	0.23	0/174	0.42	0/232
8	L	0.30	0/229	0.48	0/305
8	b	0.24	0/174	0.54	0/232
8	c	0.21	0/174	0.35	0/232
8	d	0.22	0/229	0.52	0/305
9	M	0.15	0/1003	0.32	0/1347
9	N	0.19	0/255	0.38	0/342
9	e	0.16	0/1003	0.38	0/1347
9	f	0.18	0/255	0.38	0/342
10	P	0.14	0/11197	0.32	0/15227
All	All	0.20	3/52449 (0.0%)	0.38	6/70999 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	P	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	51	ASN	C-O	-7.08	1.20	1.23
5	F	7	SER	CA-CB	-5.66	1.44	1.53
5	F	15	ASN	C-O	-5.12	1.17	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	23	PRO	N-CA-C	6.94	123.18	113.53
5	F	26	ASN	CA-C-O	-6.66	115.02	122.01
5	F	23	PRO	CB-CA-C	-6.58	101.76	112.62
5	F	10	PHE	N-CA-C	-6.34	104.45	111.36
5	F	16	ASN	CA-C-O	-5.35	116.07	122.27
5	F	12	VAL	N-CA-C	-5.17	105.99	113.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	P	1061	ASP	Mainchain
10	P	474	SER	Peptide

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	5371	0	5331	57	0
1	O	5371	0	5333	50	0
2	B	1841	0	1863	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	1841	0	1863	11	0
3	C	1841	0	1799	18	0
3	S	1841	0	1802	15	0
4	D	1805	0	1813	11	0
4	T	1805	0	1813	13	0
5	E	1878	0	1870	13	0
5	F	1878	0	1870	26	0
5	U	1878	0	1870	14	0
5	V	1878	0	1870	18	0
6	G	1441	0	1425	12	0
6	H	1516	0	1492	25	0
6	W	1419	0	1410	11	0
6	Z	1516	0	1492	12	0
7	I	878	0	844	15	0
7	a	878	0	843	27	0
8	J	170	0	167	3	0
8	K	170	0	167	1	0
8	L	224	0	217	6	0
8	b	170	0	167	1	0
8	c	170	0	167	2	0
8	d	224	0	217	1	0
9	M	987	0	930	7	0
9	N	251	0	239	4	0
9	e	987	0	930	6	0
9	f	251	0	239	3	0
10	P	10925	0	10447	86	0
11	R	70	0	16	1	0
12	A	1	0	0	0	0
12	O	1	0	0	0	0
13	A	1	0	0	0	0
13	O	1	0	0	0	0
All	All	51479	0	50506	406	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.

All (406) 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)
8:L:20:ARG:NH1	7:a:103:ARG:HD3	1.58	1.16
6:Z:190:GLN:HE22	7:a:13:THR:HG22	1.12	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:190:GLN:HE22	7:a:13:THR:CG2	1.64	1.09
6:H:190:GLN:HE22	7:I:13:THR:HG22	1.19	1.05
6:H:190:GLN:HE22	7:I:13:THR:CG2	1.72	1.01
6:Z:190:GLN:NE2	7:a:13:THR:HG22	1.75	1.00
6:H:190:GLN:NE2	7:I:13:THR:HG22	1.82	0.93
5:E:45:TYR:OH	5:E:210:GLU:OE1	1.87	0.92
8:L:20:ARG:HH12	7:a:103:ARG:HD3	1.33	0.90
8:L:20:ARG:NH1	7:a:103:ARG:CD	2.38	0.86
4:T:29:GLU:OE2	5:U:131:ARG:NH2	2.08	0.85
5:F:223:TYR:OH	10:P:1273:ASN:ND2	2.11	0.84
3:S:51:ILE:HG21	3:S:158:ILE:HD11	1.60	0.83
5:U:203:LEU:HD23	5:U:207:ILE:HD11	1.63	0.81
5:E:191:THR:OG1	5:U:5:GLU:OE2	1.98	0.81
3:C:51:ILE:HG21	3:C:158:ILE:HD11	1.64	0.78
5:F:22:ALA:HB1	5:F:23:PRO:HD2	1.66	0.78
1:O:341:ILE:HD11	1:O:378:VAL:HG21	1.65	0.77
1:A:455:ASN:O	1:O:447:ARG:NH1	2.18	0.76
5:F:235:GLN:O	5:V:52:LYS:NZ	2.18	0.76
1:A:341:ILE:HD11	1:A:378:VAL:HG21	1.66	0.76
5:V:228:GLN:NE2	5:V:232:GLU:OE2	2.18	0.76
1:A:267:ASP:OD2	1:O:222:LYS:NZ	2.20	0.74
9:N:226:ARG:NH2	9:f:229:ASN:OD1	2.19	0.74
5:E:36:LYS:NZ	5:U:213:GLN:OE1	2.21	0.74
2:B:116:ARG:NH1	6:H:163:CYS:SG	2.62	0.73
1:O:190:ASP:OD2	1:O:212:ARG:NH1	2.20	0.73
1:O:654:GLN:O	1:O:655:THR:OG1	2.06	0.73
10:P:304:ASP:OD2	10:P:1089:ASN:ND2	2.21	0.73
1:O:226:SER:OG	1:O:231:ASP:OD2	2.06	0.73
5:E:235:GLN:O	5:U:52:LYS:NZ	2.21	0.72
1:A:677:ARG:NH2	1:A:680:GLU:OE1	2.21	0.72
7:a:79:GLU:OE2	7:a:81:TYR:OH	2.06	0.72
5:F:23:PRO:HB3	5:F:223:TYR:CE1	2.24	0.72
10:P:34:ARG:NE	10:P:49:GLU:OE1	2.24	0.71
6:G:48:PRO:O	8:b:1:MET:N	2.22	0.69
10:P:1172:VAL:O	10:P:1181:ASN:ND2	2.25	0.69
10:P:692:ARG:NH1	10:P:960:ASP:OD1	2.26	0.69
1:A:164:GLU:OE2	1:A:168:ASN:ND2	2.26	0.69
5:E:206:ILE:HG23	5:E:207:ILE:HG23	1.75	0.68
10:P:299:THR:HG21	10:P:1067:SER:HA	1.75	0.68
5:F:17:ILE:HG22	5:F:17:ILE:O	1.94	0.68
2:Q:216:ARG:NH2	2:Q:229:ASP:O	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:701:ALA:O	10:P:947:ARG:NH1	2.27	0.68
3:C:31:LEU:HD21	3:S:9:MET:HE2	1.76	0.68
10:P:832:ASN:ND2	10:P:951:LEU:O	2.27	0.67
1:A:650:GLN:OE1	1:A:667:TYR:OH	2.13	0.67
10:P:217:ARG:NH1	10:P:982:TYR:O	2.28	0.67
2:B:216:ARG:NH2	2:B:229:ASP:O	2.28	0.67
3:S:36:ARG:NH2	3:S:159:PHE:O	2.28	0.67
5:F:203:LEU:HD13	5:F:207:ILE:HD11	1.77	0.67
5:E:224:GLN:NE2	5:E:226:ASP:OD2	2.28	0.66
6:Z:190:GLN:HE22	7:a:13:THR:HG21	1.57	0.66
1:A:248:ASP:OD1	1:O:379:ASN:ND2	2.29	0.66
9:M:497:TYR:O	9:M:534:ARG:NH1	2.28	0.66
6:H:62:TYR:O	6:H:94:MET:HE2	1.95	0.66
2:Q:63:GLU:OE2	2:Q:116:ARG:NH2	2.29	0.66
3:C:36:ARG:NH2	3:C:159:PHE:O	2.29	0.65
10:P:237:ASP:OD1	10:P:239:SER:OG	2.11	0.65
10:P:565:VAL:HG11	10:P:850:LEU:HD11	1.79	0.65
1:A:133:MET:SD	1:A:614:ARG:NH2	2.69	0.65
6:Z:190:GLN:NE2	7:a:13:THR:CG2	2.45	0.65
9:M:463:ASP:O	9:M:466:GLY:N	2.30	0.64
9:e:463:ASP:O	9:e:466:GLY:N	2.31	0.64
6:G:199:PHE:O	6:G:202:ASN:ND2	2.31	0.64
3:C:81:ARG:NH2	3:S:173:GLU:OE2	2.30	0.64
1:O:417:GLY:O	1:O:584:ARG:NH2	2.30	0.64
4:T:100:TRP:NE1	4:T:176:GLN:OE1	2.29	0.64
3:S:43:ARG:NH1	9:f:221:TYR:OH	2.30	0.64
7:a:101:ILE:HD13	7:a:101:ILE:N	2.13	0.64
2:B:50:ASP:OD1	2:B:132:LYS:NZ	2.32	0.63
9:M:445:ASN:OD1	9:M:446:GLU:N	2.31	0.63
5:V:203:LEU:HD13	5:V:207:ILE:HD11	1.80	0.63
5:V:44:ASN:ND2	5:V:238:GLU:O	2.31	0.63
6:H:181:LEU:CD1	7:I:12:ILE:HD12	2.29	0.63
1:O:666:LEU:HD22	1:O:675:LYS:HB2	1.80	0.63
9:N:216:SER:OG	3:S:197:GLU:OE1	2.17	0.63
1:A:422:LEU:O	1:A:425:SER:OG	2.15	0.63
10:P:803:SER:OG	10:P:805:ASP:OD1	2.10	0.62
2:Q:86:MET:SD	2:Q:91:ASN:ND2	2.73	0.62
1:O:661:SER:O	1:O:664:THR:OG1	2.17	0.62
1:A:430:LEU:HG	1:A:434:MET:HE2	1.81	0.62
10:P:587:LYS:O	10:P:900:TYR:N	2.33	0.62
1:A:666:LEU:HD22	1:A:675:LYS:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:58:VAL:HG23	6:W:94:MET:HE1	1.82	0.62
9:e:529:GLN:NE2	9:e:533:GLU:OE2	2.31	0.61
1:A:489:ASP:OD1	2:Q:193:ASN:ND2	2.32	0.61
5:F:44:ASN:ND2	5:F:238:GLU:O	2.32	0.61
10:P:514:ASN:OD1	10:P:539:TYR:OH	2.19	0.61
10:P:1143:ASN:OD1	10:P:1169:ASN:ND2	2.33	0.61
1:A:458:SER:OG	1:A:516:GLU:OE1	2.11	0.61
6:H:181:LEU:HD11	7:I:12:ILE:HD12	1.83	0.61
4:T:167:ASP:OD1	4:T:168:LYS:N	2.33	0.61
10:P:1179:TYR:OH	10:P:1220:VAL:O	2.16	0.61
2:B:218:THR:HG22	2:B:218:THR:O	2.00	0.61
4:D:114:LEU:HD12	4:D:114:LEU:O	2.00	0.61
6:H:148:ILE:HG21	6:H:176:LEU:HD13	1.83	0.61
10:P:671:ARG:NH2	10:P:674:SER:O	2.33	0.61
6:H:38:ASP:OD1	6:H:42:THR:OG1	2.20	0.60
9:e:497:TYR:O	9:e:534:ARG:NH1	2.35	0.60
5:F:16:ASN:HB2	5:F:21:ALA:HB3	1.82	0.60
3:C:1:MET:HE1	3:C:6:LEU:HD13	1.83	0.60
3:S:115:MET:HE2	3:S:141:LYS:HB3	1.83	0.60
9:e:514:GLU:OE2	9:e:515:SER:OG	2.19	0.60
4:D:105:GLU:OE1	4:D:150:ARG:NH2	2.35	0.60
7:a:1:MET:N	8:c:1:MET:O	2.23	0.59
1:A:654:GLN:O	1:A:655:THR:OG1	2.13	0.59
6:H:190:GLN:HE22	7:I:13:THR:HG21	1.62	0.59
6:H:190:GLN:NE2	7:I:13:THR:CG2	2.52	0.59
8:J:16:LEU:HD21	7:a:97:THR:HG22	1.85	0.59
1:O:583:LYS:NZ	1:O:587:GLU:OE2	2.34	0.59
6:W:99:LEU:HD23	6:W:101:LEU:HD21	1.85	0.59
1:A:658:LEU:HD23	1:A:663:ILE:HD11	1.85	0.58
3:C:51:ILE:HG21	3:C:158:ILE:CD1	2.32	0.58
5:E:221:ALA:HB2	5:E:233:LEU:HD22	1.86	0.58
3:C:96:ARG:NH2	3:C:102:PHE:O	2.36	0.58
1:O:707:MET:SD	1:O:708:GLN:NE2	2.77	0.58
5:V:15:ASN:O	10:P:1342:ARG:NH2	2.37	0.57
1:A:259:ILE:HD13	1:O:377:TRP:HB2	1.86	0.57
9:M:436:ASP:OD1	1:O:343:LYS:NZ	2.36	0.57
3:S:68:ALA:HB3	3:S:75:GLU:OE1	2.05	0.57
10:P:293:GLU:N	10:P:293:GLU:OE1	2.38	0.57
10:P:474:SER:O	10:P:751:ASN:ND2	2.38	0.57
10:P:668:PRO:O	10:P:693:LYS:NZ	2.38	0.56
5:F:23:PRO:HB3	5:F:223:TYR:CZ	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:74:ASP:OD1	7:a:75:PHE:N	2.38	0.56
10:P:418:ARG:NH1	10:P:939:THR:O	2.39	0.56
10:P:645:TRP:NE1	10:P:647:ASP:OD2	2.38	0.56
5:V:206:ILE:HG23	5:V:207:ILE:HG23	1.88	0.56
6:Z:32:LEU:O	6:Z:122:LYS:NZ	2.39	0.56
5:F:203:LEU:HD13	5:F:207:ILE:CD1	2.35	0.56
1:O:609:SER:OG	1:O:610:ASP:N	2.38	0.56
1:O:253:VAL:HG21	1:O:393:VAL:HG13	1.87	0.56
10:P:477:VAL:HG21	10:P:564:ILE:HG21	1.88	0.56
5:U:11:ASP:OD1	5:U:30:LYS:NZ	2.28	0.55
10:P:460:LEU:HD21	10:P:897:ALA:HB3	1.89	0.55
10:P:154:ASN:OD1	10:P:155:ASN:ND2	2.40	0.55
1:A:191:ALA:HB2	1:A:197:GLU:HB2	1.88	0.55
1:A:711:GLN:OE1	1:O:712:LYS:NZ	2.24	0.55
2:B:137:ASP:OD1	2:B:138:ASP:N	2.38	0.55
1:O:72:ILE:HG23	1:O:79:ASP:OD2	2.06	0.55
10:P:469:ASP:O	10:P:473:ASN:N	2.38	0.55
1:A:635:SER:O	1:A:639:GLN:NE2	2.40	0.55
10:P:48:ASN:OD1	10:P:1360:THR:N	2.40	0.55
1:A:417:GLY:O	1:A:584:ARG:NH2	2.41	0.54
1:A:253:VAL:HG21	1:A:393:VAL:HG13	1.88	0.54
5:V:79:ASN:ND2	5:V:95:ASP:OD2	2.39	0.54
3:C:36:ARG:HG3	3:C:187:ILE:HD12	1.88	0.54
5:E:7:SER:HB2	5:E:180:THR:HG21	1.89	0.54
1:A:658:LEU:HD23	1:A:663:ILE:CD1	2.36	0.54
5:F:23:PRO:HD3	5:F:223:TYR:CE2	2.43	0.54
1:O:239:ASP:OD1	1:O:240:TYR:N	2.41	0.54
3:C:68:ALA:HB3	3:C:75:GLU:OE1	2.07	0.54
5:F:238:GLU:OE2	5:V:63:ARG:NH1	2.40	0.54
5:U:57:LEU:CD2	5:U:104:ILE:HG21	2.38	0.54
10:P:448:THR:OG1	10:P:451:ASP:OD2	2.26	0.54
2:B:84:ARG:NH1	2:B:85:ALA:O	2.40	0.53
6:H:184:ARG:NH2	7:I:40:GLU:OE1	2.38	0.53
5:F:23:PRO:HG3	5:F:223:TYR:CG	2.43	0.53
1:O:227:ASN:ND2	1:O:419:ILE:H	2.07	0.53
10:P:1069:ASN:ND2	10:P:1130:GLU:OE2	2.38	0.53
10:P:1336:ASN:ND2	10:P:1339:ASP:OD2	2.40	0.53
4:T:154:LYS:O	4:T:155:SER:OG	2.26	0.53
10:P:113:ASN:C	10:P:113:ASN:OD1	2.50	0.53
5:V:11:ASP:OD1	5:V:30:LYS:NZ	2.41	0.53
9:M:462:VAL:N	1:O:350:GLU:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:PHE:CD2	1:O:648:LEU:HD11	2.44	0.52
6:W:152:THR:HG22	6:W:172:MET:HE1	1.91	0.52
10:P:739:ILE:N	10:P:750:LEU:O	2.42	0.52
1:A:669:SER:O	1:A:670:SER:OG	2.21	0.52
5:V:212:LEU:O	5:V:216:VAL:HG23	2.09	0.52
10:P:732:TRP:NE1	10:P:735:GLY:O	2.41	0.52
1:A:660:PHE:HD2	1:O:648:LEU:HD11	1.74	0.52
3:S:51:ILE:HG21	3:S:158:ILE:CD1	2.35	0.52
5:U:206:ILE:HG23	5:U:207:ILE:HG23	1.92	0.52
10:P:477:VAL:HG23	10:P:752:TYR:HD1	1.75	0.52
1:A:190:ASP:OD2	1:A:212:ARG:NH1	2.43	0.51
10:P:467:TYR:OH	10:P:536:LEU:O	2.22	0.51
10:P:1276:GLU:O	10:P:1366:ILE:N	2.42	0.51
2:Q:116:ARG:NH1	6:Z:163:CYS:SG	2.83	0.51
4:D:111:ASP:OD1	4:D:112:SER:N	2.43	0.51
5:F:86:THR:O	5:V:168:LYS:NZ	2.27	0.51
1:A:191:ALA:HB1	1:A:420:TYR:CE2	2.46	0.51
3:C:93:GLY:HA3	3:C:158:ILE:HD12	1.93	0.51
5:F:131:ARG:O	5:F:134:LYS:NZ	2.35	0.51
1:O:87:MET:SD	1:O:438:ASN:ND2	2.83	0.51
10:P:1033:THR:HG22	10:P:1055:THR:HG22	1.93	0.51
1:O:666:LEU:HD22	1:O:675:LYS:CB	2.41	0.51
4:D:138:ASN:OD1	4:D:141:ARG:N	2.42	0.50
6:Z:98:ARG:C	6:Z:99:LEU:HD12	2.35	0.50
10:P:98:LYS:NZ	10:P:103:GLU:OE1	2.29	0.50
6:H:151:GLN:NE2	6:H:202:ASN:OD1	2.43	0.50
6:Z:177:LYS:NZ	6:Z:180:GLU:OE2	2.43	0.50
7:a:80:SER:OG	7:a:82:ASP:OD1	2.30	0.50
10:P:959:GLU:N	10:P:959:GLU:OE1	2.45	0.50
1:A:735:GLN:NE2	1:A:739:GLU:OE2	2.44	0.50
5:F:15:ASN:O	5:F:16:ASN:C	2.52	0.50
1:O:412:HIS:ND1	1:O:413:PHE:O	2.45	0.49
1:O:669:SER:O	1:O:670:SER:OG	2.24	0.49
4:T:25:LEU:HD22	4:T:29:GLU:OE1	2.12	0.49
3:S:56:TYR:OH	3:S:94:ASN:N	2.45	0.49
10:P:1292:THR:HG22	10:P:1293:PHE:CD2	2.47	0.49
1:O:133:MET:HE3	1:O:614:ARG:HH22	1.77	0.49
10:P:300:MET:HG2	10:P:309:LEU:HD23	1.93	0.49
10:P:1298:VAL:HG13	10:P:1348:ILE:HD13	1.95	0.49
10:P:1031:SER:OG	10:P:1057:ASP:OD1	2.30	0.49
1:O:109:VAL:HG22	1:O:630:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:203:LEU:HD13	5:V:207:ILE:CD1	2.43	0.49
6:W:136:ASP:OD1	6:W:137:GLN:N	2.46	0.49
2:B:86:MET:SD	2:B:91:ASN:ND2	2.86	0.49
3:C:43:ARG:NH1	9:N:221:TYR:OH	2.46	0.49
1:O:662:THR:HG21	1:O:682:ASP:OD2	2.12	0.49
10:P:38:ARG:NH1	10:P:1192:ASP:OD2	2.46	0.49
10:P:254:ASP:OD1	10:P:1011:ASN:ND2	2.45	0.49
10:P:704:ASN:ND2	10:P:971:MET:O	2.41	0.49
1:A:660:PHE:N	1:O:683:GLU:OE2	2.42	0.49
2:Q:165:ILE:HG22	2:Q:169:MET:CE	2.43	0.49
5:V:105:ASN:OD1	5:V:170:ARG:NH1	2.46	0.49
10:P:360:LEU:HD11	10:P:977:ASN:HD21	1.78	0.49
1:A:342:LEU:HD13	1:A:361:GLU:HA	1.95	0.48
4:D:136:LYS:NZ	4:T:121:GLU:OE2	2.45	0.48
1:A:440:LEU:HD23	1:A:533:ILE:HD12	1.95	0.48
6:G:50:ASP:OD2	7:a:53:GLN:NE2	2.47	0.48
6:H:30:VAL:C	6:H:31:LEU:HD22	2.39	0.48
4:D:50:ASN:O	4:D:54:GLY:N	2.45	0.48
4:D:86:LEU:HD22	4:T:104:TYR:CD2	2.48	0.48
1:O:109:VAL:HG22	1:O:630:LEU:CD2	2.44	0.48
6:H:28:GLU:N	6:H:28:GLU:OE1	2.46	0.48
1:O:440:LEU:HD23	1:O:533:ILE:HD12	1.95	0.48
1:O:542:GLY:HA3	1:O:570:ILE:HG21	1.96	0.48
10:P:639:LEU:HD23	10:P:639:LEU:O	2.13	0.48
1:O:656:GLN:N	1:O:656:GLN:OE1	2.46	0.48
10:P:196:LYS:HE2	10:P:196:LYS:HA	1.96	0.48
10:P:460:LEU:CD2	10:P:897:ALA:HB3	2.43	0.48
6:G:180:GLU:CG	7:a:84:LEU:HD12	2.44	0.48
6:H:27:PHE:O	6:H:95:LYS:NZ	2.40	0.48
9:e:431:ASN:ND2	9:e:436:ASP:OD1	2.45	0.48
5:E:106:GLU:OE2	5:E:167:TYR:OH	2.31	0.48
10:P:135:TYR:CD2	10:P:145:VAL:HG22	2.49	0.48
1:O:237:LEU:HD12	1:O:334:TYR:HE2	1.78	0.47
6:G:30:VAL:O	6:G:95:LYS:NZ	2.43	0.47
6:H:114:MET:HE1	6:H:116:PHE:CZ	2.49	0.47
1:O:202:ASP:OD1	9:e:433:GLN:NE2	2.46	0.47
5:F:105:ASN:OD1	5:F:170:ARG:NH1	2.48	0.47
8:c:1:MET:HE1	8:d:1:MET:SD	2.55	0.47
6:G:149:TYR:O	6:G:153:LEU:HD23	2.14	0.47
6:W:4:ASN:OD1	6:W:20:SER:OG	2.09	0.47
3:C:144:ASN:O	3:C:146:GLN:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:1:MET:N	6:Z:22:ASP:OD1	2.39	0.47
5:U:85:ILE:HG23	5:U:85:ILE:O	2.15	0.47
10:P:597:THR:OG1	10:P:598:ASN:OD1	2.33	0.47
5:F:16:ASN:CB	5:F:21:ALA:HB3	2.45	0.47
8:L:20:ARG:HH11	7:a:103:ARG:HD3	1.65	0.47
10:P:46:VAL:HG21	10:P:1258:ILE:HD12	1.97	0.47
10:P:295:ILE:HG22	10:P:314:LEU:HD23	1.96	0.47
6:G:36:VAL:HG11	6:G:48:PRO:HB3	1.97	0.46
6:W:30:VAL:C	6:W:31:LEU:HD22	2.40	0.46
6:Z:174:LEU:HD13	7:a:15:TYR:CE2	2.50	0.46
10:P:1213:SER:OG	10:P:1214:PHE:N	2.47	0.46
10:P:572:VAL:HG21	10:P:835:LEU:HG	1.97	0.46
1:A:542:GLY:HA3	1:A:570:ILE:HG21	1.97	0.46
1:A:666:LEU:HD22	1:A:675:LYS:CB	2.45	0.46
10:P:1033:THR:HG21	10:P:1052:LEU:CD2	2.44	0.46
1:A:109:VAL:HG22	1:A:630:LEU:CD2	2.45	0.46
6:H:6:LEU:HG	6:H:142:VAL:HG22	1.97	0.46
4:T:45:ILE:CG2	4:T:63:ILE:HG23	2.46	0.46
4:T:50:ASN:O	4:T:54:GLY:N	2.43	0.46
10:P:570:PRO:CB	10:P:978:ILE:HD11	2.45	0.46
2:B:63:GLU:OE2	2:B:116:ARG:NH2	2.49	0.46
1:A:661:SER:O	1:A:664:THR:OG1	2.29	0.46
7:I:80:SER:OG	7:I:82:ASP:OD1	2.34	0.46
4:T:113:ARG:NH2	4:T:163:LYS:O	2.49	0.46
3:C:11:LEU:O	3:C:15:LYS:N	2.49	0.46
6:H:22:ASP:HB3	6:H:24:GLN:OE1	2.16	0.46
2:Q:54:THR:OG1	2:Q:128:ASP:OD1	2.30	0.46
6:Z:151:GLN:NE2	6:Z:202:ASN:OD1	2.48	0.46
3:S:80:LEU:O	3:S:140:PHE:N	2.45	0.46
10:P:280:GLU:N	10:P:280:GLU:OE1	2.49	0.46
1:A:207:GLU:OE2	1:A:601:ASN:ND2	2.46	0.46
4:D:65:ARG:O	4:D:203:ASN:ND2	2.45	0.46
6:H:114:MET:HE1	6:H:116:PHE:CE1	2.50	0.46
3:S:185:PHE:HD2	3:S:187:ILE:HG22	1.81	0.46
1:A:657:THR:O	1:A:657:THR:HG22	2.16	0.45
3:C:120:TYR:HB3	2:Q:12:VAL:HG22	1.97	0.45
1:O:337:SER:N	1:O:380:GLU:O	2.48	0.45
5:V:120:ILE:HD11	5:V:124:ASP:HB3	1.97	0.45
10:P:341:ASP:OD1	10:P:342:ASP:N	2.48	0.45
7:I:96:ILE:O	7:I:97:THR:OG1	2.31	0.45
10:P:946:GLN:OE1	10:P:978:ILE:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:108:VAL:CG2	5:V:164:ILE:HG23	2.46	0.45
10:P:135:TYR:OH	10:P:1045:ASP:OD2	2.33	0.45
10:P:1034:VAL:HG21	10:P:1110:VAL:HG21	1.99	0.45
6:G:169:PHE:CE2	7:I:35:VAL:HG22	2.52	0.45
5:U:143:ARG:HD3	5:U:154:VAL:HG13	1.98	0.45
1:A:332:ARG:HG2	1:A:385:THR:HG22	1.98	0.45
1:A:415:ILE:HD12	1:A:415:ILE:H	1.82	0.45
5:U:224:GLN:NE2	5:U:226:ASP:OD2	2.50	0.45
10:P:112:LEU:O	10:P:113:ASN:C	2.59	0.45
10:P:203:ILE:HG13	10:P:290:VAL:HG21	1.98	0.45
6:H:114:MET:SD	6:H:141:THR:HG23	2.56	0.45
7:I:101:ILE:C	7:I:102:LEU:HD22	2.42	0.45
1:A:477:MET:HB2	2:B:209:MET:HE1	1.97	0.44
5:F:206:ILE:HG23	5:F:207:ILE:HG23	1.98	0.44
1:O:87:MET:HE1	1:O:431:VAL:HG13	1.99	0.44
1:A:90:LYS:NZ	1:A:548:GLU:OE2	2.47	0.44
6:G:181:LEU:HD22	6:H:152:THR:HG22	1.99	0.44
10:P:360:LEU:HD11	10:P:977:ASN:ND2	2.33	0.44
10:P:1042:GLU:OE1	10:P:1042:GLU:N	2.50	0.44
6:H:184:ARG:HG3	7:I:5:LEU:HD11	1.99	0.44
1:O:230:GLU:OE1	1:O:230:GLU:N	2.49	0.44
6:W:27:PHE:HD1	6:W:30:VAL:HG21	1.82	0.44
2:B:39:ILE:HD12	2:B:47:VAL:HG11	1.99	0.44
3:C:56:TYR:OH	3:C:94:ASN:N	2.50	0.44
5:U:47:GLU:OE1	5:U:49:ALA:HB3	2.18	0.44
1:O:620:GLY:O	1:O:628:TYR:OH	2.35	0.44
7:a:105:THR:O	7:a:105:THR:OG1	2.36	0.43
4:T:10:PHE:CE2	4:T:25:LEU:HD12	2.53	0.43
6:H:208:THR:O	6:H:208:THR:OG1	2.30	0.43
9:M:489:ILE:HG21	9:M:494:ARG:HD3	2.00	0.43
2:Q:160:LYS:O	2:Q:164:THR:OG1	2.32	0.43
1:A:400:ILE:HG12	1:A:595:VAL:HG11	2.00	0.43
2:B:74:VAL:CG1	2:B:83:LEU:HD12	2.49	0.43
1:O:165:VAL:O	1:O:169:GLU:HG3	2.19	0.43
10:P:590:ILE:HG12	10:P:897:ALA:HB2	2.01	0.43
5:E:90:ARG:NH2	5:E:134:LYS:O	2.50	0.43
1:O:227:ASN:HD22	1:O:227:ASN:C	2.27	0.43
10:P:1208:ILE:HG22	11:R:3:UNK:CB	2.49	0.43
1:A:337:SER:N	1:A:380:GLU:O	2.51	0.43
6:G:180:GLU:HG3	7:a:84:LEU:HD12	2.01	0.43
4:D:127:LEU:CD2	4:D:149:LEU:HD13	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:91:ALA:HB1	5:F:155:GLU:HB3	2.01	0.43
10:P:1279:ALA:HB3	10:P:1292:THR:HG21	2.00	0.43
1:O:341:ILE:CD1	1:O:378:VAL:HG21	2.43	0.42
6:G:40:GLN:HB2	6:G:192:ILE:HG23	2.00	0.42
7:a:93:VAL:O	7:a:93:VAL:HG12	2.19	0.42
1:A:341:ILE:CD1	1:A:378:VAL:HG21	2.43	0.42
1:A:547:ARG:NH1	1:O:566:GLN:OE1	2.52	0.42
3:C:70:SER:OG	3:C:71:GLY:N	2.52	0.42
1:A:452:ILE:HG21	1:O:444:ILE:HD11	2.00	0.42
1:A:683:GLU:OE1	1:A:687:ARG:NH1	2.53	0.42
1:A:715:GLU:CG	1:O:712:LYS:HZ1	2.32	0.42
9:N:243:SER:OG	9:N:244:LEU:N	2.52	0.42
10:P:277:THR:OG1	10:P:278:THR:N	2.51	0.42
1:O:161:ASP:O	1:O:165:VAL:HG23	2.20	0.42
3:S:46:ASP:OD1	3:S:47:ILE:N	2.46	0.42
6:W:149:TYR:CE2	6:W:153:LEU:HD11	2.55	0.42
5:F:108:VAL:CG2	5:F:164:ILE:HG23	2.49	0.42
7:a:8:SER:O	7:a:12:ILE:HD12	2.20	0.42
3:C:179:LYS:HG2	4:D:117:LEU:HD21	2.01	0.42
5:F:29:GLU:HG2	5:V:12:VAL:HG13	2.01	0.42
1:A:91:LEU:HD23	1:A:189:MET:HE3	2.01	0.42
8:J:1:MET:HE1	8:L:1:MET:HE2	2.01	0.42
6:W:169:PHE:CE2	7:a:35:VAL:HG22	2.55	0.42
10:P:360:LEU:HD13	10:P:979:ASP:HB3	2.00	0.42
10:P:400:THR:OG1	10:P:401:GLU:OE1	2.37	0.42
8:J:16:LEU:CD2	7:a:97:THR:HG22	2.47	0.41
8:K:19:SER:OG	7:a:97:THR:O	2.27	0.41
9:M:453:ASN:OD1	9:M:455:TYR:N	2.50	0.41
3:C:214:ASP:OD2	3:C:225:ARG:NH1	2.49	0.41
6:H:21:VAL:HG23	6:H:32:LEU:HD11	2.01	0.41
3:S:7:ILE:HD11	3:S:29:ILE:HG12	2.02	0.41
10:P:1220:VAL:HG11	10:P:1223:MET:SD	2.60	0.41
1:A:94:LEU:HD12	1:A:192:MET:SD	2.60	0.41
1:A:109:VAL:HG22	1:A:630:LEU:HD21	2.03	0.41
1:A:440:LEU:HD23	1:A:533:ILE:CD1	2.51	0.41
5:E:117:ILE:HG23	5:E:143:ARG:HB2	2.02	0.41
5:F:146:THR:OG1	5:F:147:THR:N	2.54	0.41
6:W:1:MET:N	6:W:22:ASP:OD2	2.30	0.41
9:f:243:SER:OG	9:f:244:LEU:N	2.52	0.41
5:F:90:ARG:NH2	5:F:135:GLU:OE1	2.53	0.41
7:I:11:ALA:HB1	7:I:33:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:972:CYS:SG	10:P:973:GLU:N	2.94	0.41
5:E:100:LEU:O	5:E:174:ARG:NH2	2.54	0.41
4:D:118:ASP:OD1	4:D:119:GLY:N	2.54	0.41
1:O:191:ALA:O	1:O:195:GLY:N	2.49	0.41
10:P:1228:SER:O	10:P:1228:SER:OG	2.33	0.41
1:A:91:LEU:CD1	1:A:434:MET:HE1	2.50	0.41
10:P:942:ASP:OD1	10:P:942:ASP:N	2.52	0.41
5:F:111:ASN:OD1	5:F:112:ALA:N	2.54	0.41
6:G:51:ASN:N	6:G:52:PRO:HD3	2.36	0.41
3:S:81:ARG:NH1	3:S:82:SER:O	2.53	0.41
5:V:146:THR:OG1	5:V:147:THR:N	2.53	0.41
10:P:37:ALA:HB2	10:P:43:LEU:HB2	2.02	0.41
1:A:38:SER:O	1:A:426:ARG:NH1	2.54	0.41
1:A:327:ASN:ND2	1:O:223:SER:O	2.54	0.41
2:Q:23:LEU:HB3	2:Q:26:LEU:HD12	2.02	0.41
4:T:10:PHE:HE2	4:T:25:LEU:HD12	1.86	0.41
5:U:5:GLU:O	5:U:9:GLU:OE1	2.39	0.41
10:P:734:GLU:O	10:P:755:ASN:ND2	2.54	0.41
10:P:1226:VAL:O	10:P:1227:SER:OG	2.32	0.41
1:A:458:SER:HG	1:A:516:GLU:CD	2.17	0.41
2:Q:226:ASN:ND2	2:Q:229:ASP:OD2	2.48	0.41
10:P:988:GLN:O	10:P:991:ASN:ND2	2.54	0.41
5:U:70:LEU:HD23	5:U:172:ILE:CG2	2.51	0.40
5:F:33:LEU:HD13	5:F:219:ALA:HB2	2.03	0.40
10:P:450:GLU:O	10:P:901:ARG:NH1	2.51	0.40
10:P:859:TYR:CD2	10:P:879:VAL:HG11	2.57	0.40
5:E:38:GLN:HE21	5:E:203:LEU:HD13	1.87	0.40
7:I:94:PRO:HA	7:I:106:GLU:HA	2.03	0.40
8:L:9:ARG:NH2	7:a:90:ARG:O	2.54	0.40
10:P:902:ASP:OD1	10:P:903:SER:N	2.52	0.40
4:T:206:VAL:HG22	4:T:206:VAL:O	2.21	0.40
5:V:111:ASN:OD1	5:V:112:ALA:N	2.55	0.40
6:W:165:ILE:HD12	7:a:35:VAL:HG21	2.03	0.40
1:A:191:ALA:O	1:A:195:GLY:N	2.47	0.40
10:P:859:TYR:CG	10:P:879:VAL:HG11	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	647/806 (80%)	632 (98%)	15 (2%)	0	100	100
1	O	647/806 (80%)	632 (98%)	15 (2%)	0	100	100
2	B	222/236 (94%)	216 (97%)	6 (3%)	0	100	100
2	Q	222/236 (94%)	216 (97%)	6 (3%)	0	100	100
3	C	223/225 (99%)	217 (97%)	6 (3%)	0	100	100
3	S	223/225 (99%)	218 (98%)	5 (2%)	0	100	100
4	D	224/230 (97%)	218 (97%)	6 (3%)	0	100	100
4	T	224/230 (97%)	217 (97%)	7 (3%)	0	100	100
5	E	236/238 (99%)	226 (96%)	10 (4%)	0	100	100
5	F	236/238 (99%)	221 (94%)	15 (6%)	0	100	100
5	U	236/238 (99%)	225 (95%)	11 (5%)	0	100	100
5	V	236/238 (99%)	227 (96%)	9 (4%)	0	100	100
6	G	173/215 (80%)	169 (98%)	4 (2%)	0	100	100
6	H	184/215 (86%)	180 (98%)	4 (2%)	0	100	100
6	W	170/215 (79%)	167 (98%)	3 (2%)	0	100	100
6	Z	184/215 (86%)	180 (98%)	4 (2%)	0	100	100
7	I	105/114 (92%)	101 (96%)	4 (4%)	0	100	100
7	a	105/114 (92%)	100 (95%)	5 (5%)	0	100	100
8	J	17/832 (2%)	16 (94%)	1 (6%)	0	100	100
8	K	17/832 (2%)	16 (94%)	1 (6%)	0	100	100
8	L	23/832 (3%)	23 (100%)	0	0	100	100
8	b	17/832 (2%)	16 (94%)	1 (6%)	0	100	100
8	c	17/832 (2%)	17 (100%)	0	0	100	100
8	d	23/832 (3%)	23 (100%)	0	0	100	100
9	M	122/842 (14%)	117 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	N	30/842 (4%)	28 (93%)	2 (7%)	0	100	100
9	e	122/842 (14%)	116 (95%)	6 (5%)	0	100	100
9	f	30/842 (4%)	28 (93%)	2 (7%)	0	100	100
10	P	1350/1371 (98%)	1297 (96%)	53 (4%)	0	100	100
All	All	6265/14765 (42%)	6059 (97%)	206 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

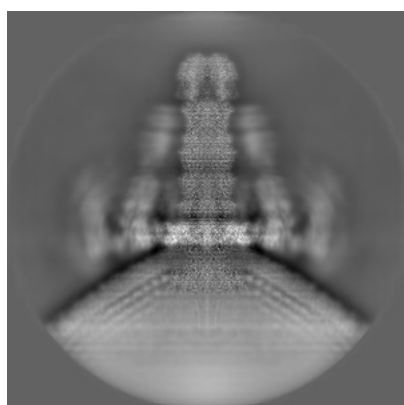
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14094. These allow visual inspection of the internal detail of the map and identification of artifacts.

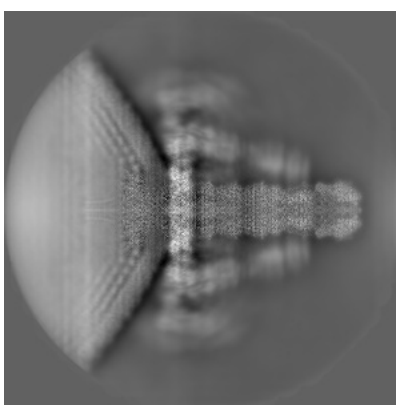
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

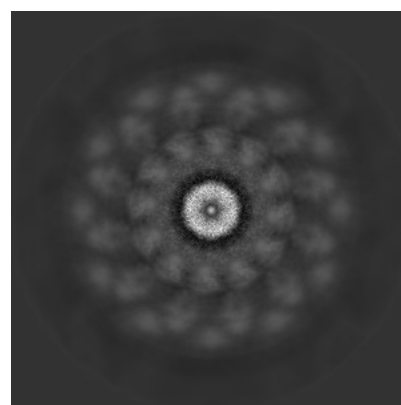
6.1.1 Primary map



X



Y

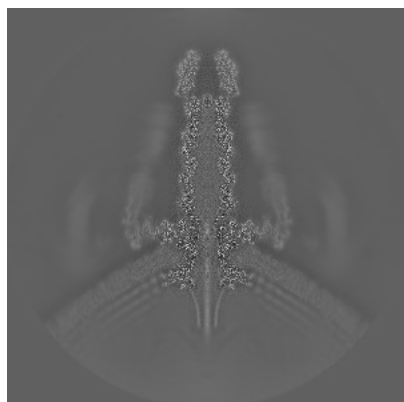


Z

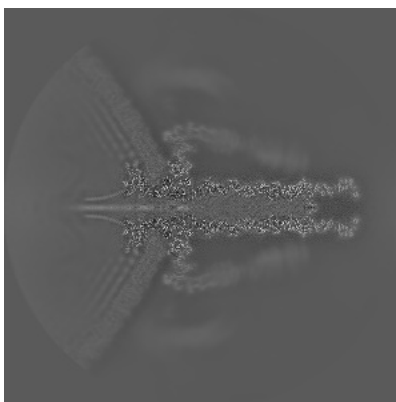
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

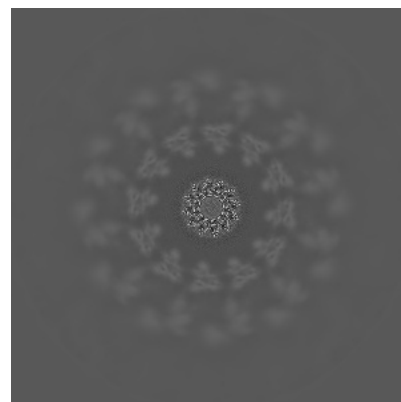
6.2.1 Primary map



X Index: 320



Y Index: 320



Z Index: 320

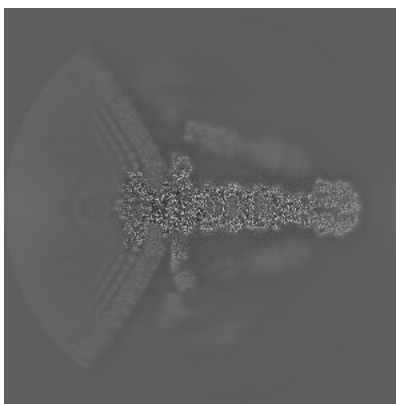
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

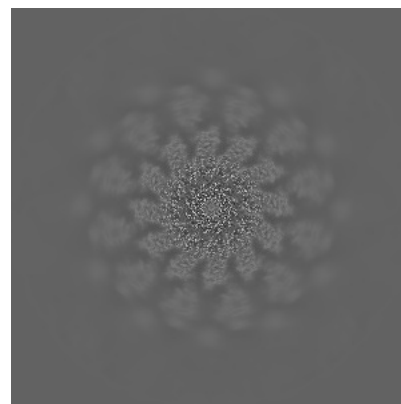
6.3.1 Primary map



X Index: 342



Y Index: 298

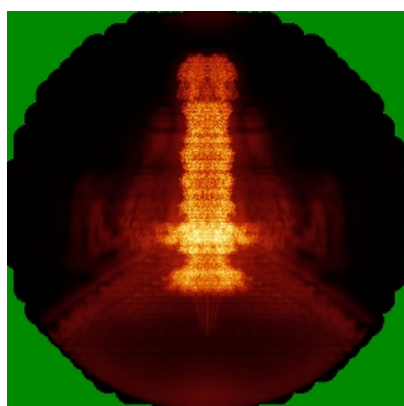


Z Index: 274

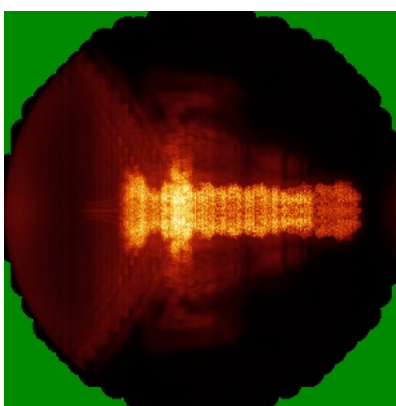
The images above show the largest variance slices of the map in three orthogonal directions.

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

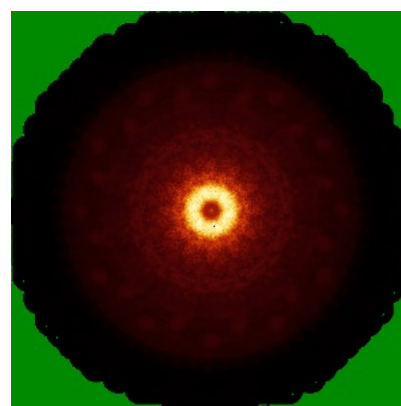
6.4.1 Primary map



X



Y

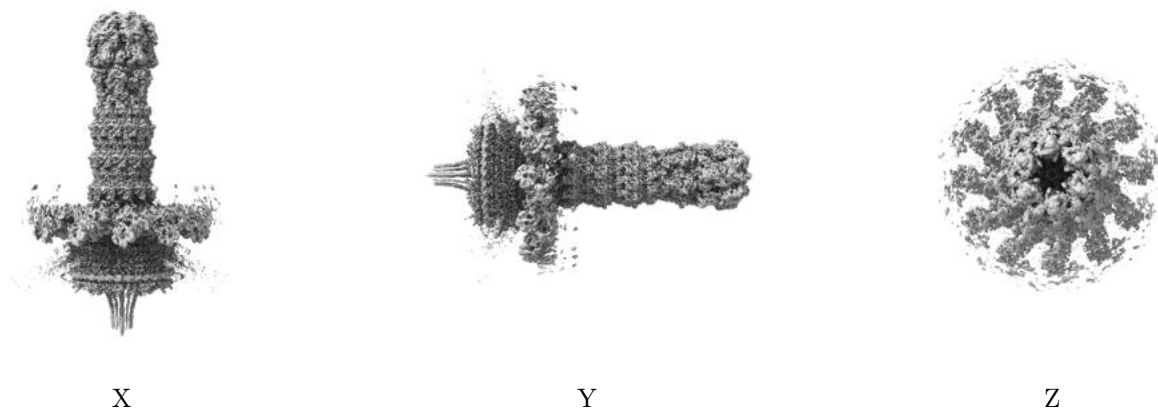


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

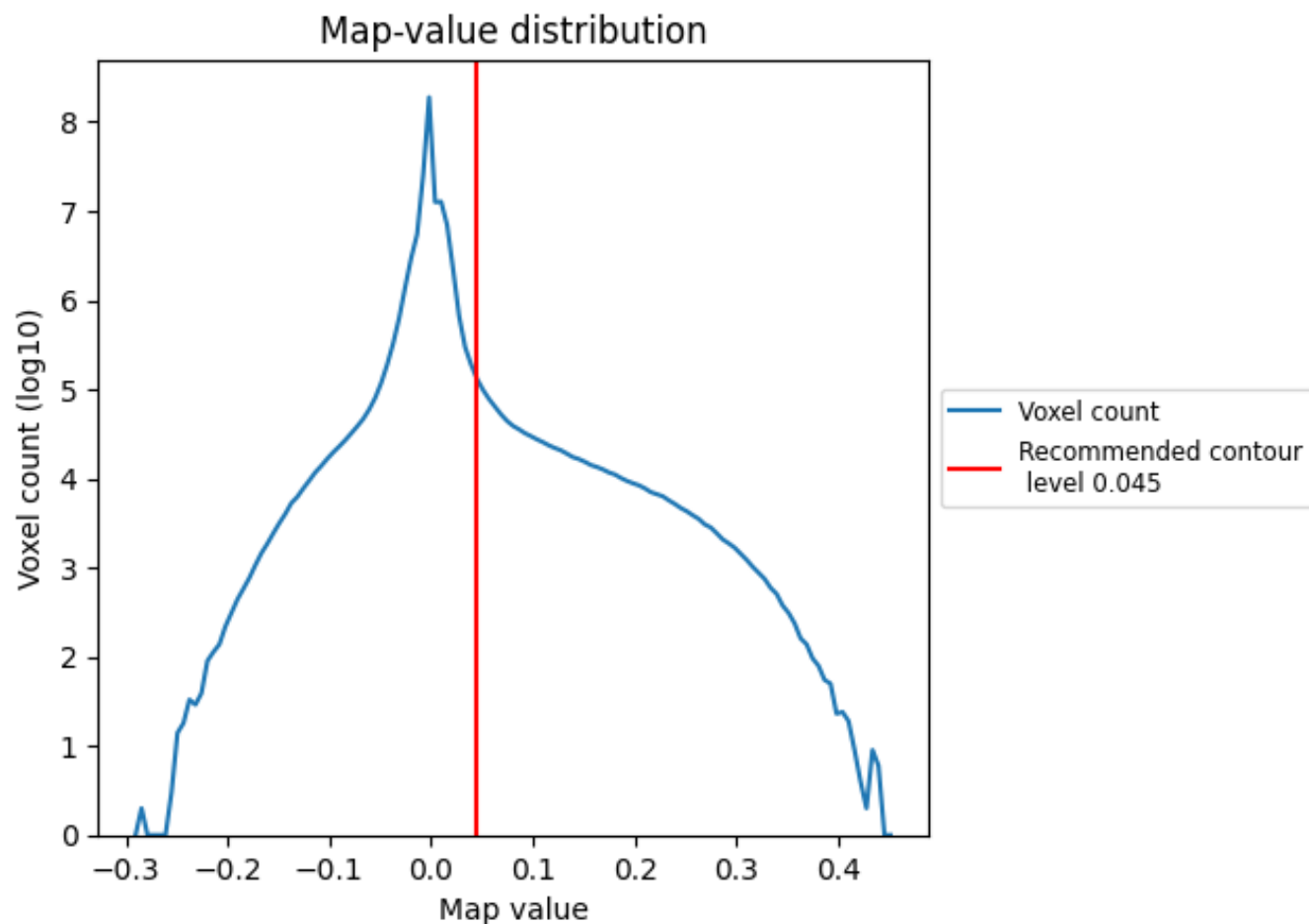
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

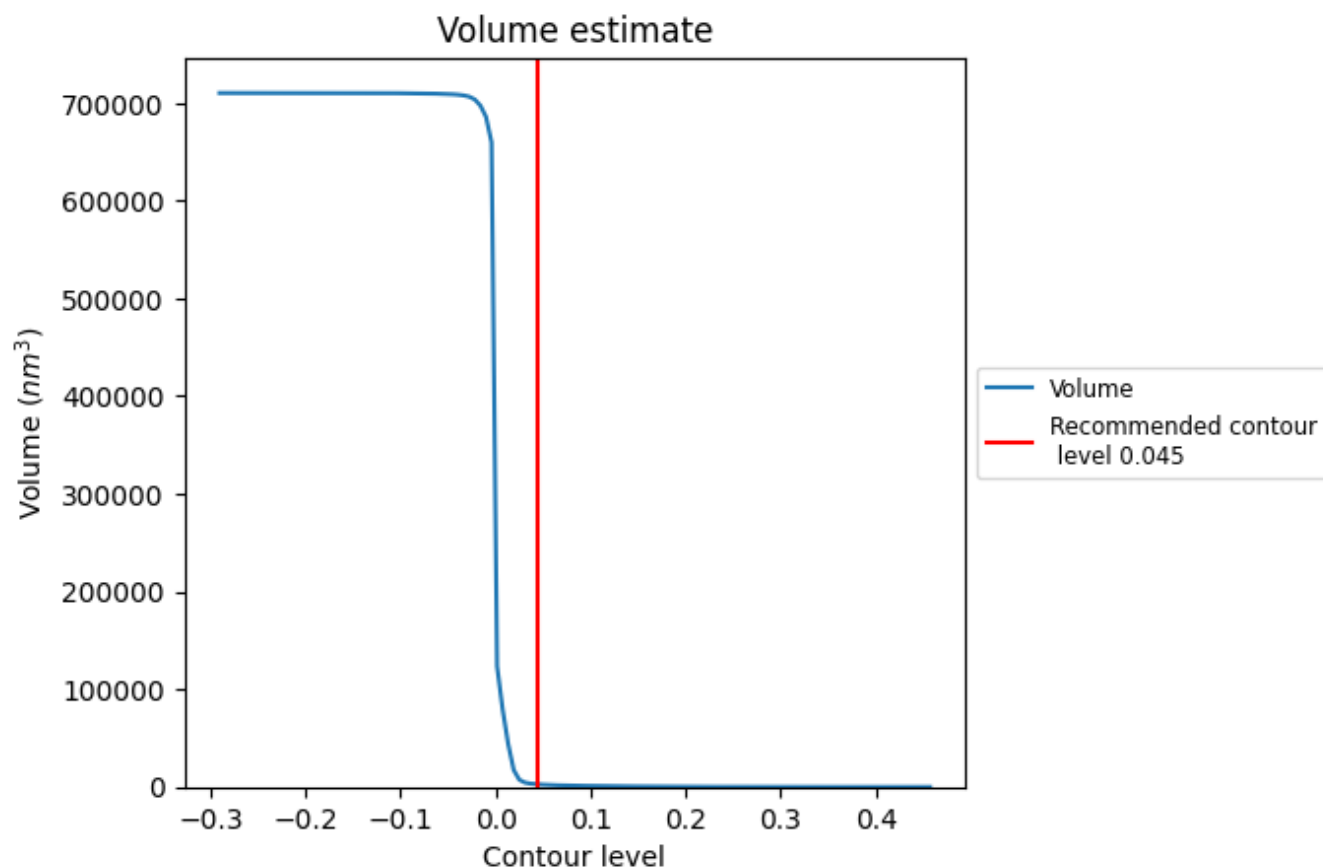
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

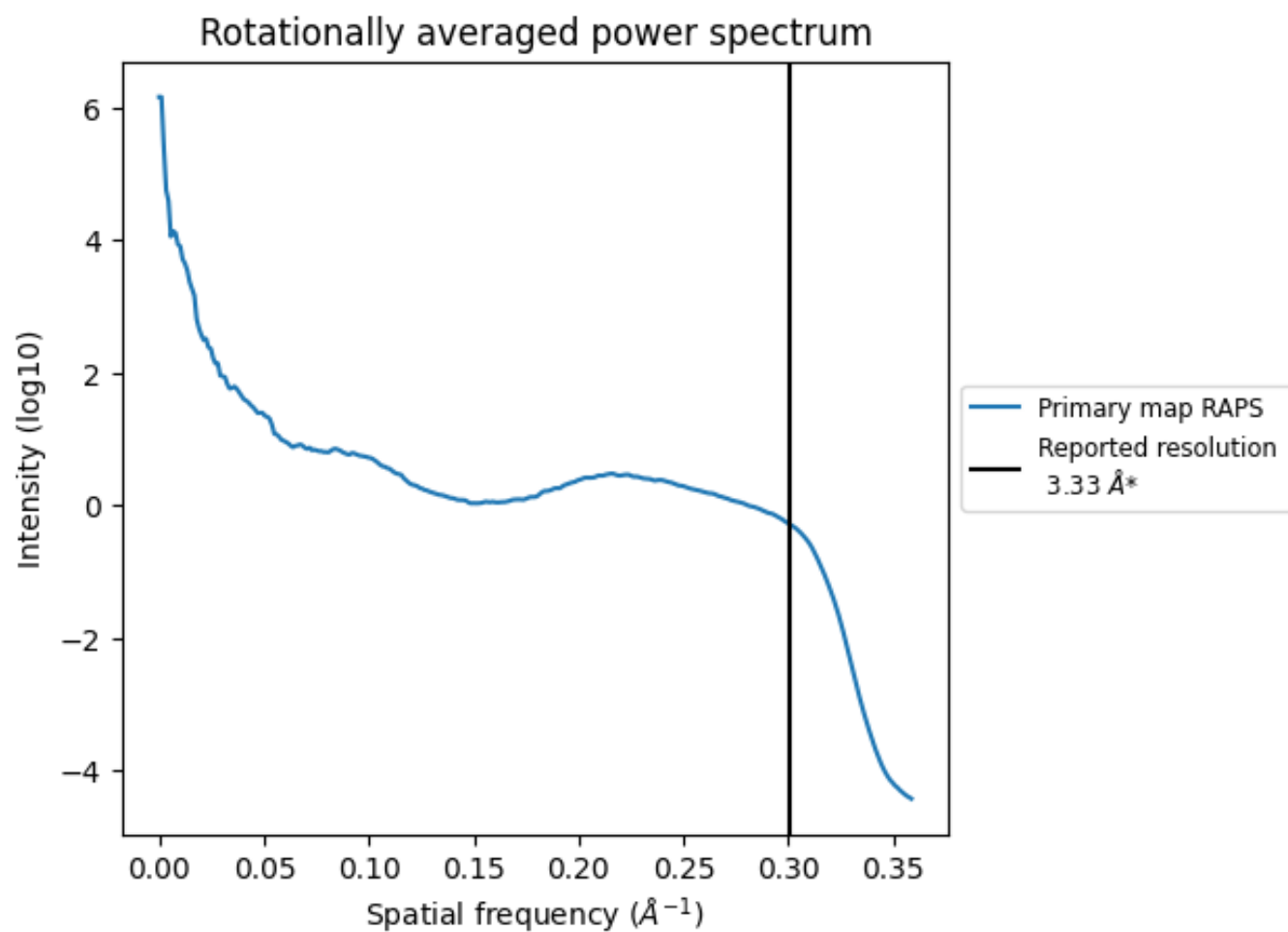
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2647 nm^3 ; this corresponds to an approximate mass of 2391 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 ⓘ

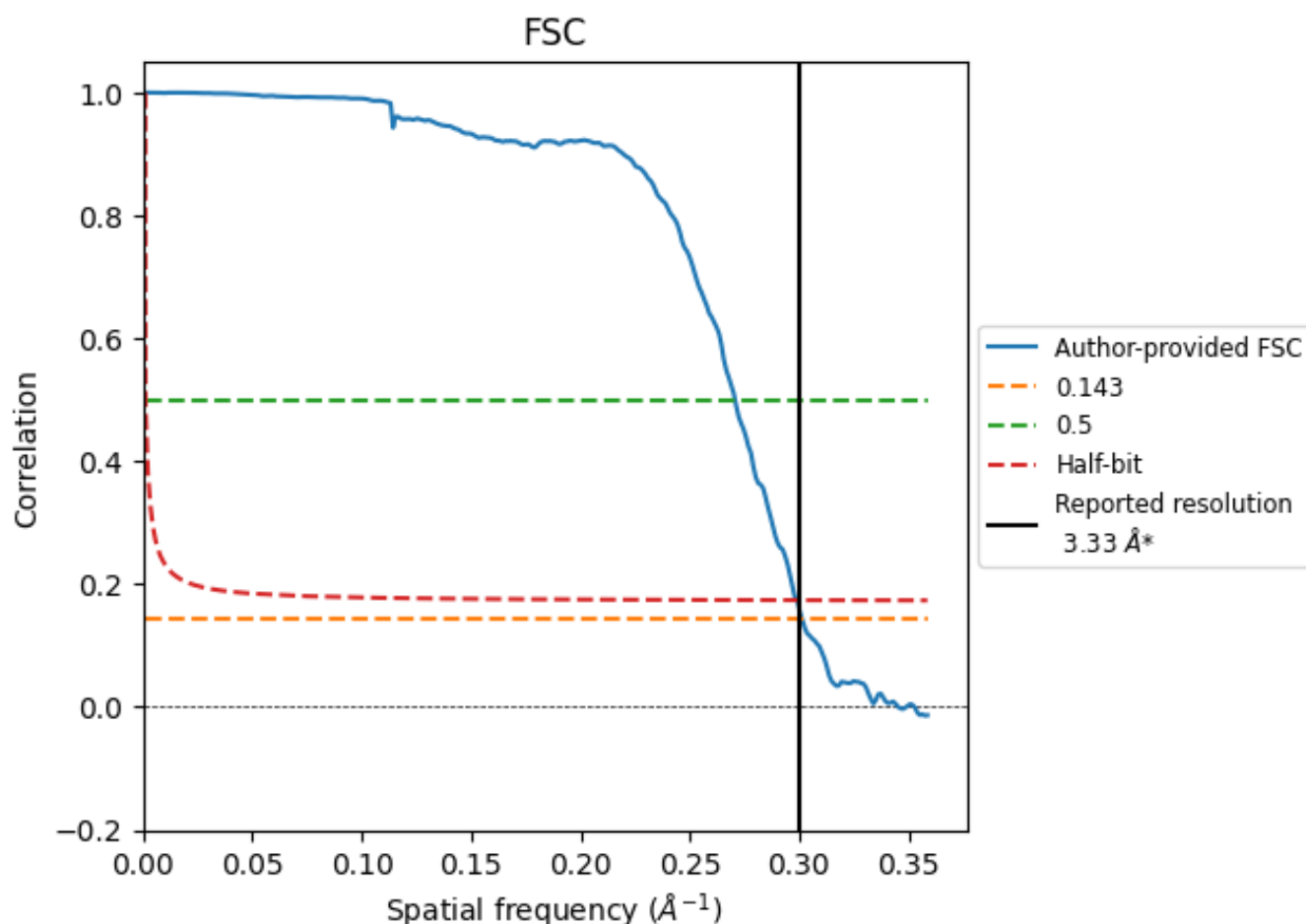


*Reported resolution corresponds to spatial frequency of 0.300 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.300 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	3.32	3.69	3.35
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14094 and PDB model 7QOL. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

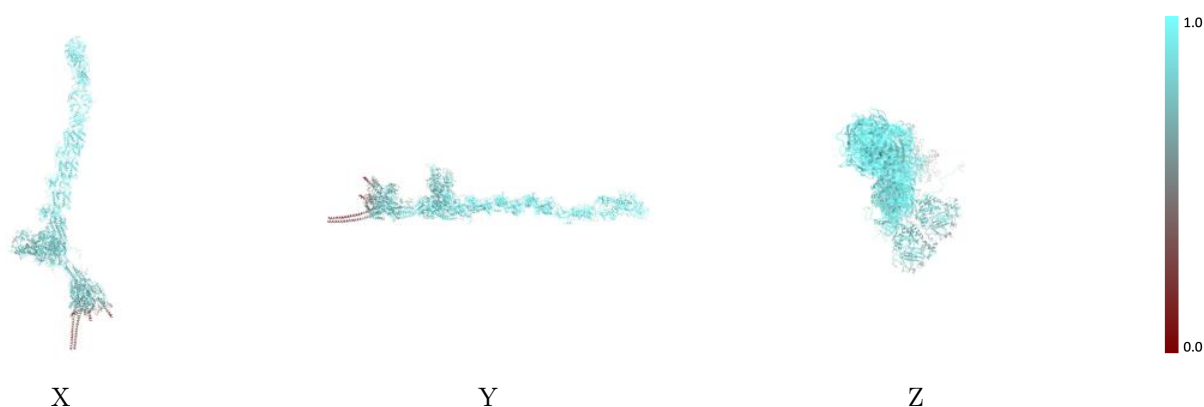
This section was not generated.

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



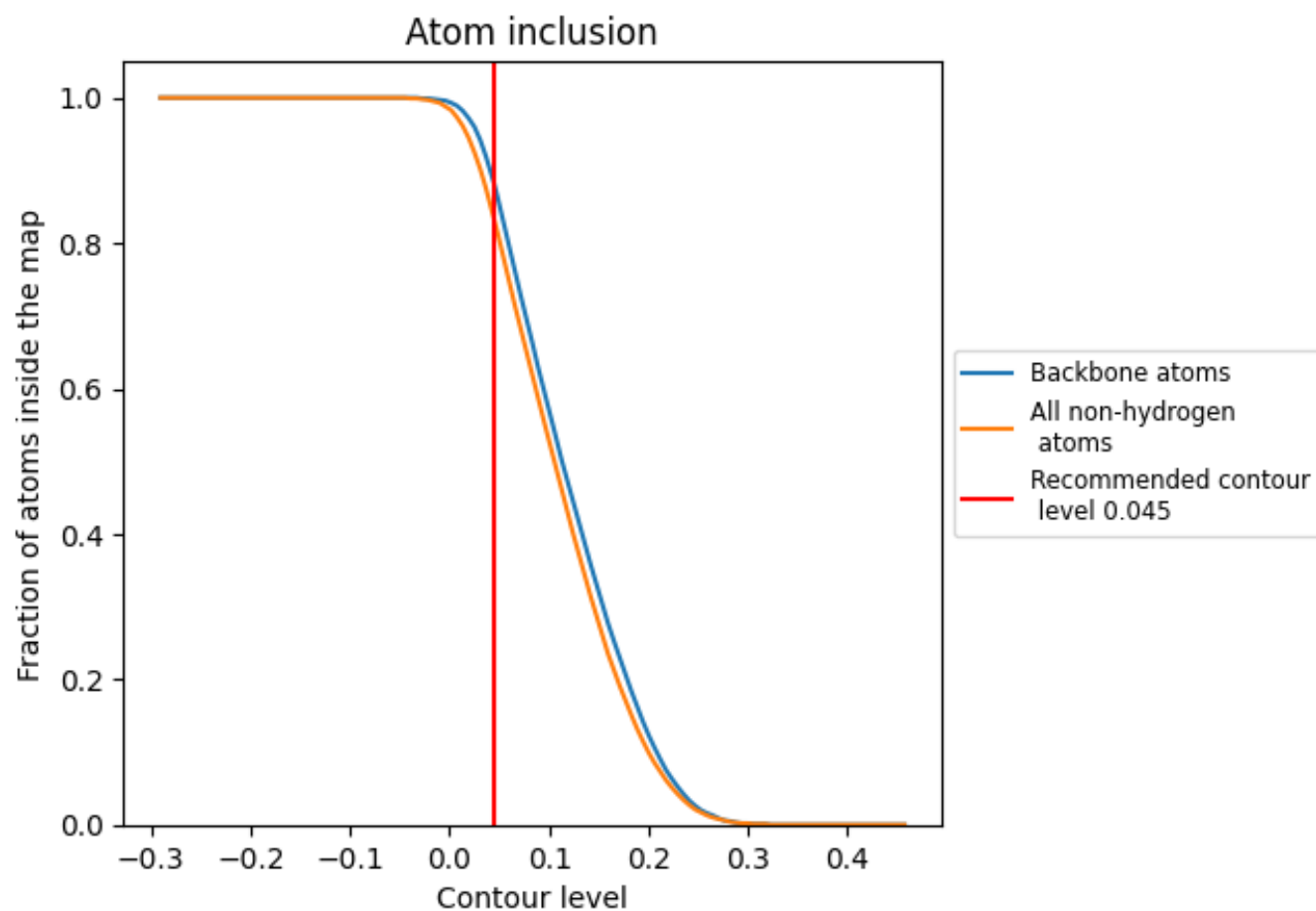
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 83% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8320	 0.5250
A	 0.7260	 0.5110
B	 0.8740	 0.5730
C	 0.9030	 0.5730
D	 0.9110	 0.5550
E	 0.9260	 0.5630
F	 0.9200	 0.5540
G	 0.7760	 0.5020
H	 0.7990	 0.4810
I	 0.8360	 0.5080
J	 0.7230	 0.4210
K	 0.7590	 0.4460
L	 0.7110	 0.4440
M	 0.5060	 0.4530
N	 0.7590	 0.5160
O	 0.7320	 0.5110
P	 0.9190	 0.5170
Q	 0.8600	 0.5660
R	 0.8710	 0.5060
S	 0.9050	 0.5730
T	 0.9180	 0.5600
U	 0.9320	 0.5610
V	 0.9340	 0.5610
W	 0.7940	 0.4950
Z	 0.8120	 0.4930
a	 0.8300	 0.5150
b	 0.7050	 0.4220
c	 0.7890	 0.4780
d	 0.7110	 0.4820
e	 0.5240	 0.4340
f	 0.7220	 0.5120

