



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 05:34 PM UTC

PDB ID : 9LU5 / pdb_00009lu5
EMDB ID : EMD-63388
Title : Structure of bacteriophage T4 neck protein gp13 and gp14 and Hfq assembled
in vitro in C6 symmetry
Authors : Han, L.; Mao, Q.; Sun, L.
Deposited on : 2025-02-07
Resolution : 2.79 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

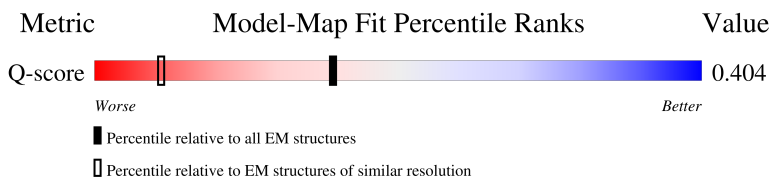
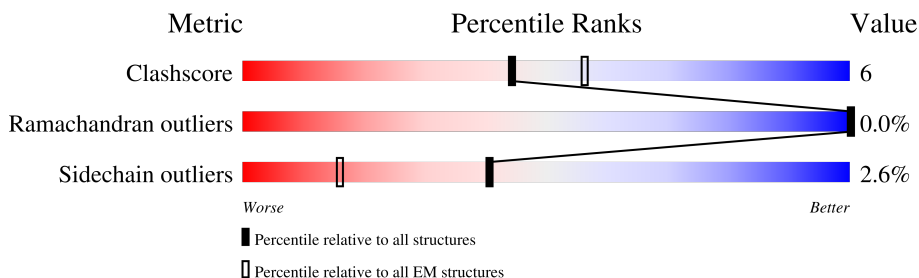
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.79 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10811 (2.29 - 3.29)

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	315	 6% 66% 12% • 21%
1	B	315	 6% 62% 16% • 21%
1	C	315	 7% 62% 17% • 21%
1	D	315	 7% 63% 15% • 21%

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Mol	Chain	Length	Quality of chain
1	E	315	
1	F	315	
1	G	315	
1	H	315	
1	I	315	
1	J	315	
1	K	315	
1	L	315	
2	S	114	
2	T	114	
2	U	114	
2	V	114	
2	W	114	
2	X	114	
3	M	265	
3	N	265	
3	O	265	
3	P	265	
3	Q	265	
3	R	265	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34464 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 Neck protein gp13.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	248	Total 1990	C 1280	N 333	O 366	S 11	0	0
1	I	248	Total 1990	C 1280	N 333	O 366	S 11	0	0
1	G	248	Total 1990	C 1280	N 333	O 366	S 11	0	0
1	E	248	Total 1990	C 1280	N 333	O 366	S 11	0	0
1	A	248	Total 1990	C 1280	N 333	O 366	S 11	0	0
1	B	248	Total 1990	C 1280	N 333	O 366	S 11	0	0
1	D	248	Total 1990	C 1280	N 333	O 366	S 11	0	0
1	F	248	Total 1990	C 1280	N 333	O 366	S 11	0	0
1	H	248	Total 1990	C 1280	N 333	O 366	S 11	0	0
1	J	248	Total 1990	C 1280	N 333	O 366	S 11	0	0
1	K	248	Total 1990	C 1280	N 333	O 366	S 11	0	0
1	L	248	Total 1990	C 1280	N 333	O 366	S 11	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	310	HIS	-	expression tag	UNP P11110
C	311	HIS	-	expression tag	UNP P11110
C	312	HIS	-	expression tag	UNP P11110
C	313	HIS	-	expression tag	UNP P11110
C	314	HIS	-	expression tag	UNP P11110
C	315	HIS	-	expression tag	UNP P11110

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Chain	Residue	Modelled	Actual	Comment	Reference
I	310	HIS	-	expression tag	UNP P11110
I	311	HIS	-	expression tag	UNP P11110
I	312	HIS	-	expression tag	UNP P11110
I	313	HIS	-	expression tag	UNP P11110
I	314	HIS	-	expression tag	UNP P11110
I	315	HIS	-	expression tag	UNP P11110
G	310	HIS	-	expression tag	UNP P11110
G	311	HIS	-	expression tag	UNP P11110
G	312	HIS	-	expression tag	UNP P11110
G	313	HIS	-	expression tag	UNP P11110
G	314	HIS	-	expression tag	UNP P11110
G	315	HIS	-	expression tag	UNP P11110
E	310	HIS	-	expression tag	UNP P11110
E	311	HIS	-	expression tag	UNP P11110
E	312	HIS	-	expression tag	UNP P11110
E	313	HIS	-	expression tag	UNP P11110
E	314	HIS	-	expression tag	UNP P11110
E	315	HIS	-	expression tag	UNP P11110
A	310	HIS	-	expression tag	UNP P11110
A	311	HIS	-	expression tag	UNP P11110
A	312	HIS	-	expression tag	UNP P11110
A	313	HIS	-	expression tag	UNP P11110
A	314	HIS	-	expression tag	UNP P11110
A	315	HIS	-	expression tag	UNP P11110
B	310	HIS	-	expression tag	UNP P11110
B	311	HIS	-	expression tag	UNP P11110
B	312	HIS	-	expression tag	UNP P11110
B	313	HIS	-	expression tag	UNP P11110
B	314	HIS	-	expression tag	UNP P11110
B	315	HIS	-	expression tag	UNP P11110
D	310	HIS	-	expression tag	UNP P11110
D	311	HIS	-	expression tag	UNP P11110
D	312	HIS	-	expression tag	UNP P11110
D	313	HIS	-	expression tag	UNP P11110
D	314	HIS	-	expression tag	UNP P11110
D	315	HIS	-	expression tag	UNP P11110
F	310	HIS	-	expression tag	UNP P11110
F	311	HIS	-	expression tag	UNP P11110
F	312	HIS	-	expression tag	UNP P11110
F	313	HIS	-	expression tag	UNP P11110
F	314	HIS	-	expression tag	UNP P11110
F	315	HIS	-	expression tag	UNP P11110

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Chain	Residue	Modelled	Actual	Comment	Reference
H	310	HIS	-	expression tag	UNP P11110
H	311	HIS	-	expression tag	UNP P11110
H	312	HIS	-	expression tag	UNP P11110
H	313	HIS	-	expression tag	UNP P11110
H	314	HIS	-	expression tag	UNP P11110
H	315	HIS	-	expression tag	UNP P11110
J	310	HIS	-	expression tag	UNP P11110
J	311	HIS	-	expression tag	UNP P11110
J	312	HIS	-	expression tag	UNP P11110
J	313	HIS	-	expression tag	UNP P11110
J	314	HIS	-	expression tag	UNP P11110
J	315	HIS	-	expression tag	UNP P11110
K	310	HIS	-	expression tag	UNP P11110
K	311	HIS	-	expression tag	UNP P11110
K	312	HIS	-	expression tag	UNP P11110
K	313	HIS	-	expression tag	UNP P11110
K	314	HIS	-	expression tag	UNP P11110
K	315	HIS	-	expression tag	UNP P11110
L	310	HIS	-	expression tag	UNP P11110
L	311	HIS	-	expression tag	UNP P11110
L	312	HIS	-	expression tag	UNP P11110
L	313	HIS	-	expression tag	UNP P11110
L	314	HIS	-	expression tag	UNP P11110
L	315	HIS	-	expression tag	UNP P11110

- Molecule 2 is a protein called RNA-binding protein Hfq.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	64	Total	C	N	O	S	0	0
			513	331	90	91	1		
2	S	64	Total	C	N	O	S	0	0
			513	331	90	91	1		
2	X	64	Total	C	N	O	S	0	0
			513	331	90	91	1		
2	W	64	Total	C	N	O	S	0	0
			513	331	90	91	1		
2	V	64	Total	C	N	O	S	0	0
			513	331	90	91	1		
2	U	64	Total	C	N	O	S	0	0
			513	331	90	91	1		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-11	MET	-	initiating methionine	UNP A7ZV41
T	-10	TRP	-	expression tag	UNP A7ZV41
T	-9	SER	-	expression tag	UNP A7ZV41
T	-8	HIS	-	expression tag	UNP A7ZV41
T	-7	PRO	-	expression tag	UNP A7ZV41
T	-6	GLN	-	expression tag	UNP A7ZV41
T	-5	PHE	-	expression tag	UNP A7ZV41
T	-4	GLU	-	expression tag	UNP A7ZV41
T	-3	LYS	-	expression tag	UNP A7ZV41
T	-2	GLY	-	expression tag	UNP A7ZV41
T	-1	SER	-	expression tag	UNP A7ZV41
T	0	SER	-	expression tag	UNP A7ZV41
S	-11	MET	-	initiating methionine	UNP A7ZV41
S	-10	TRP	-	expression tag	UNP A7ZV41
S	-9	SER	-	expression tag	UNP A7ZV41
S	-8	HIS	-	expression tag	UNP A7ZV41
S	-7	PRO	-	expression tag	UNP A7ZV41
S	-6	GLN	-	expression tag	UNP A7ZV41
S	-5	PHE	-	expression tag	UNP A7ZV41
S	-4	GLU	-	expression tag	UNP A7ZV41
S	-3	LYS	-	expression tag	UNP A7ZV41
S	-2	GLY	-	expression tag	UNP A7ZV41
S	-1	SER	-	expression tag	UNP A7ZV41
S	0	SER	-	expression tag	UNP A7ZV41
X	-11	MET	-	initiating methionine	UNP A7ZV41
X	-10	TRP	-	expression tag	UNP A7ZV41
X	-9	SER	-	expression tag	UNP A7ZV41
X	-8	HIS	-	expression tag	UNP A7ZV41
X	-7	PRO	-	expression tag	UNP A7ZV41
X	-6	GLN	-	expression tag	UNP A7ZV41
X	-5	PHE	-	expression tag	UNP A7ZV41
X	-4	GLU	-	expression tag	UNP A7ZV41
X	-3	LYS	-	expression tag	UNP A7ZV41
X	-2	GLY	-	expression tag	UNP A7ZV41
X	-1	SER	-	expression tag	UNP A7ZV41
X	0	SER	-	expression tag	UNP A7ZV41
W	-11	MET	-	initiating methionine	UNP A7ZV41
W	-10	TRP	-	expression tag	UNP A7ZV41
W	-9	SER	-	expression tag	UNP A7ZV41
W	-8	HIS	-	expression tag	UNP A7ZV41
W	-7	PRO	-	expression tag	UNP A7ZV41
W	-6	GLN	-	expression tag	UNP A7ZV41
W	-5	PHE	-	expression tag	UNP A7ZV41

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Chain	Residue	Modelled	Actual	Comment	Reference
W	-4	GLU	-	expression tag	UNP A7ZV41
W	-3	LYS	-	expression tag	UNP A7ZV41
W	-2	GLY	-	expression tag	UNP A7ZV41
W	-1	SER	-	expression tag	UNP A7ZV41
W	0	SER	-	expression tag	UNP A7ZV41
V	-11	MET	-	initiating methionine	UNP A7ZV41
V	-10	TRP	-	expression tag	UNP A7ZV41
V	-9	SER	-	expression tag	UNP A7ZV41
V	-8	HIS	-	expression tag	UNP A7ZV41
V	-7	PRO	-	expression tag	UNP A7ZV41
V	-6	GLN	-	expression tag	UNP A7ZV41
V	-5	PHE	-	expression tag	UNP A7ZV41
V	-4	GLU	-	expression tag	UNP A7ZV41
V	-3	LYS	-	expression tag	UNP A7ZV41
V	-2	GLY	-	expression tag	UNP A7ZV41
V	-1	SER	-	expression tag	UNP A7ZV41
V	0	SER	-	expression tag	UNP A7ZV41
U	-11	MET	-	initiating methionine	UNP A7ZV41
U	-10	TRP	-	expression tag	UNP A7ZV41
U	-9	SER	-	expression tag	UNP A7ZV41
U	-8	HIS	-	expression tag	UNP A7ZV41
U	-7	PRO	-	expression tag	UNP A7ZV41
U	-6	GLN	-	expression tag	UNP A7ZV41
U	-5	PHE	-	expression tag	UNP A7ZV41
U	-4	GLU	-	expression tag	UNP A7ZV41
U	-3	LYS	-	expression tag	UNP A7ZV41
U	-2	GLY	-	expression tag	UNP A7ZV41
U	-1	SER	-	expression tag	UNP A7ZV41
U	0	SER	-	expression tag	UNP A7ZV41

- Molecule 3 is a protein called Neck protein gp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	154	Total	C	N	O	S	0	0
			1251	814	201	233	3		
3	N	154	Total	C	N	O	S	0	0
			1251	814	201	233	3		
3	M	154	Total	C	N	O	S	0	0
			1251	814	201	233	3		
3	R	154	Total	C	N	O	S	0	0
			1251	814	201	233	3		
3	Q	154	Total	C	N	O	S	0	0
			1251	814	201	233	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	154	Total	C	N	O	S	0	0
			1251	814	201	233	3		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-8	HIS	-	expression tag	UNP P11111
O	-7	HIS	-	expression tag	UNP P11111
O	-6	HIS	-	expression tag	UNP P11111
O	-5	HIS	-	expression tag	UNP P11111
O	-4	HIS	-	expression tag	UNP P11111
O	-3	HIS	-	expression tag	UNP P11111
O	-2	SER	-	expression tag	UNP P11111
O	-1	SER	-	expression tag	UNP P11111
O	0	GLY	-	expression tag	UNP P11111
N	-8	HIS	-	expression tag	UNP P11111
N	-7	HIS	-	expression tag	UNP P11111
N	-6	HIS	-	expression tag	UNP P11111
N	-5	HIS	-	expression tag	UNP P11111
N	-4	HIS	-	expression tag	UNP P11111
N	-3	HIS	-	expression tag	UNP P11111
N	-2	SER	-	expression tag	UNP P11111
N	-1	SER	-	expression tag	UNP P11111
N	0	GLY	-	expression tag	UNP P11111
M	-8	HIS	-	expression tag	UNP P11111
M	-7	HIS	-	expression tag	UNP P11111
M	-6	HIS	-	expression tag	UNP P11111
M	-5	HIS	-	expression tag	UNP P11111
M	-4	HIS	-	expression tag	UNP P11111
M	-3	HIS	-	expression tag	UNP P11111
M	-2	SER	-	expression tag	UNP P11111
M	-1	SER	-	expression tag	UNP P11111
M	0	GLY	-	expression tag	UNP P11111
R	-8	HIS	-	expression tag	UNP P11111
R	-7	HIS	-	expression tag	UNP P11111
R	-6	HIS	-	expression tag	UNP P11111
R	-5	HIS	-	expression tag	UNP P11111
R	-4	HIS	-	expression tag	UNP P11111
R	-3	HIS	-	expression tag	UNP P11111
R	-2	SER	-	expression tag	UNP P11111
R	-1	SER	-	expression tag	UNP P11111
R	0	GLY	-	expression tag	UNP P11111

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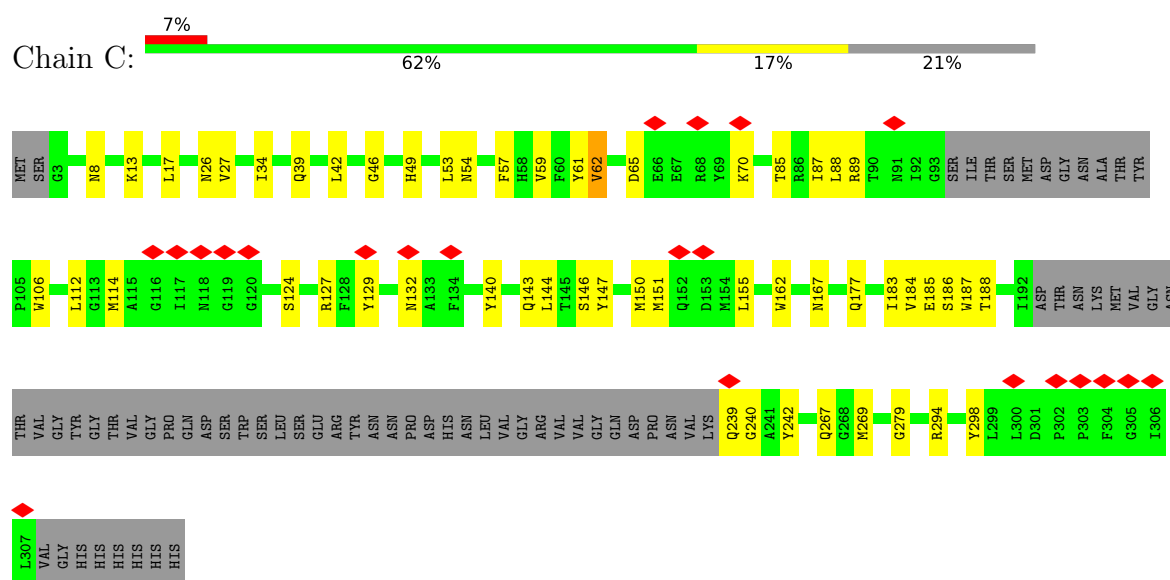
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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-8	HIS	-	expression tag	UNP P11111
Q	-7	HIS	-	expression tag	UNP P11111
Q	-6	HIS	-	expression tag	UNP P11111
Q	-5	HIS	-	expression tag	UNP P11111
Q	-4	HIS	-	expression tag	UNP P11111
Q	-3	HIS	-	expression tag	UNP P11111
Q	-2	SER	-	expression tag	UNP P11111
Q	-1	SER	-	expression tag	UNP P11111
Q	0	GLY	-	expression tag	UNP P11111
P	-8	HIS	-	expression tag	UNP P11111
P	-7	HIS	-	expression tag	UNP P11111
P	-6	HIS	-	expression tag	UNP P11111
P	-5	HIS	-	expression tag	UNP P11111
P	-4	HIS	-	expression tag	UNP P11111
P	-3	HIS	-	expression tag	UNP P11111
P	-2	SER	-	expression tag	UNP P11111
P	-1	SER	-	expression tag	UNP P11111
P	0	GLY	-	expression tag	UNP P11111

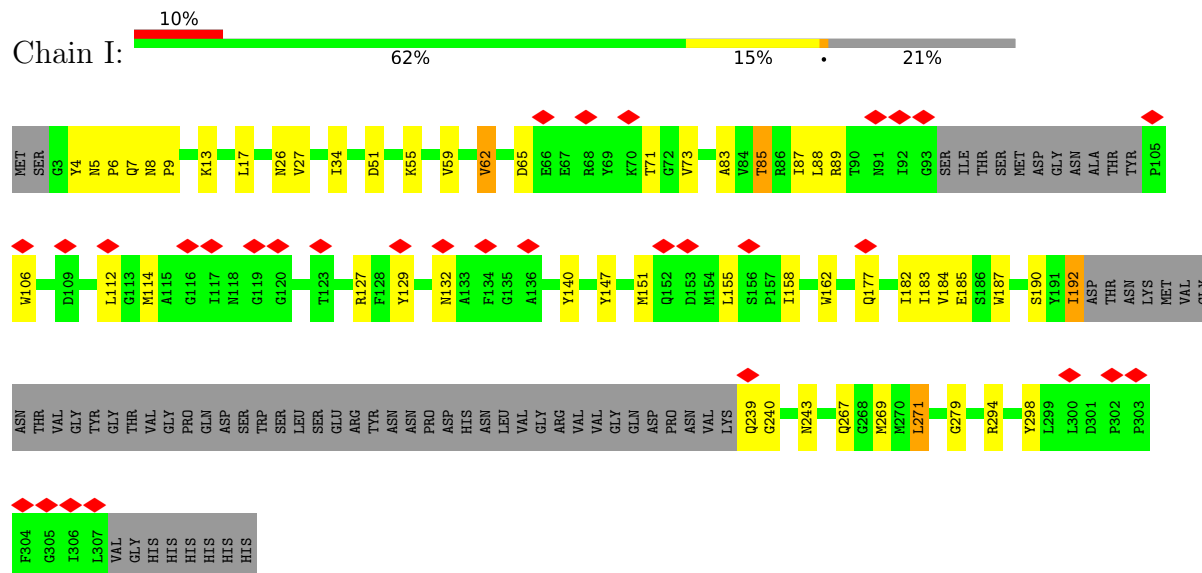
3 Residue-property plots

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

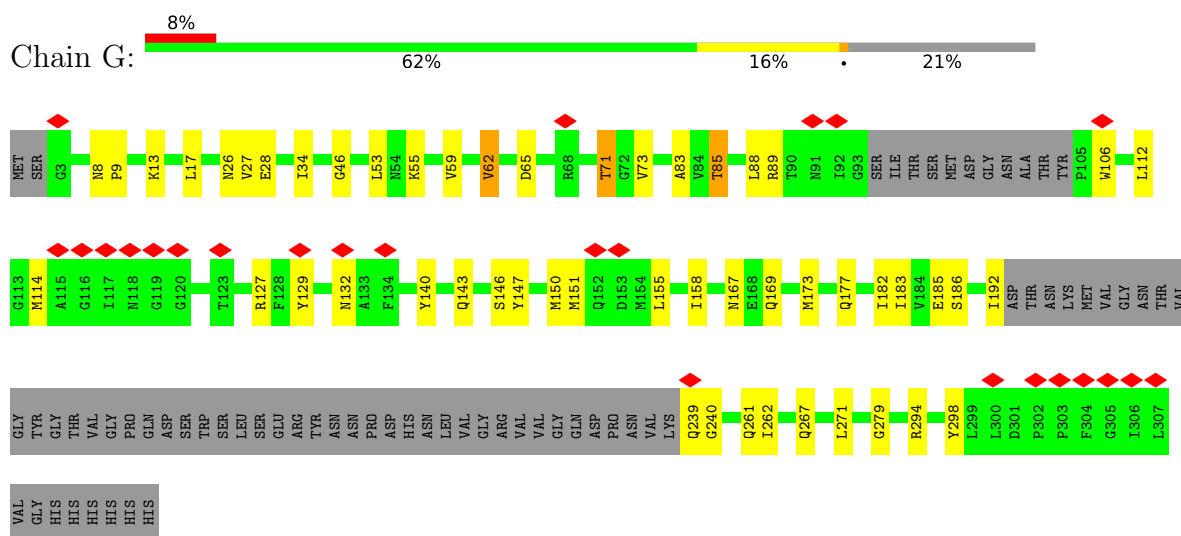
• Molecule 1: Neck protein gp13



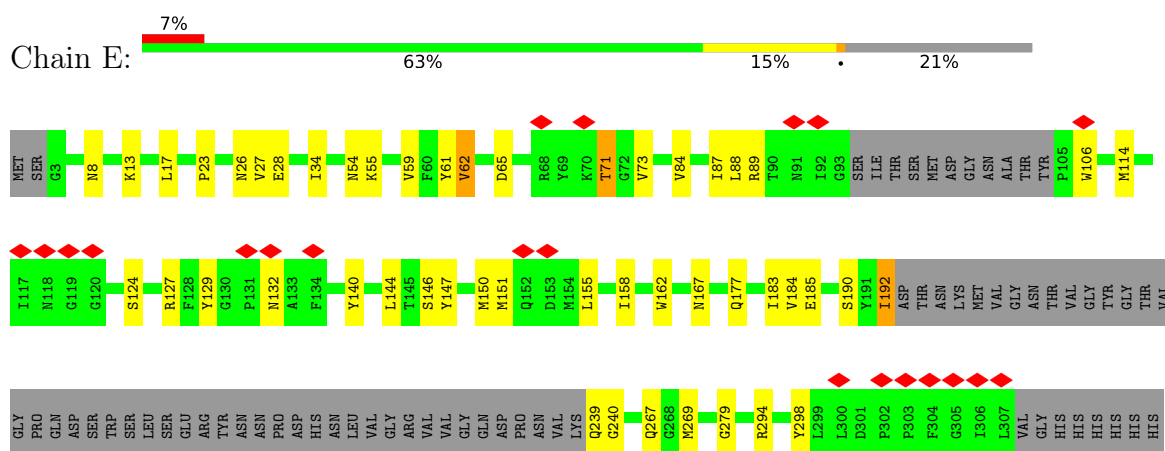
• Molecule 1: Neck protein gp13



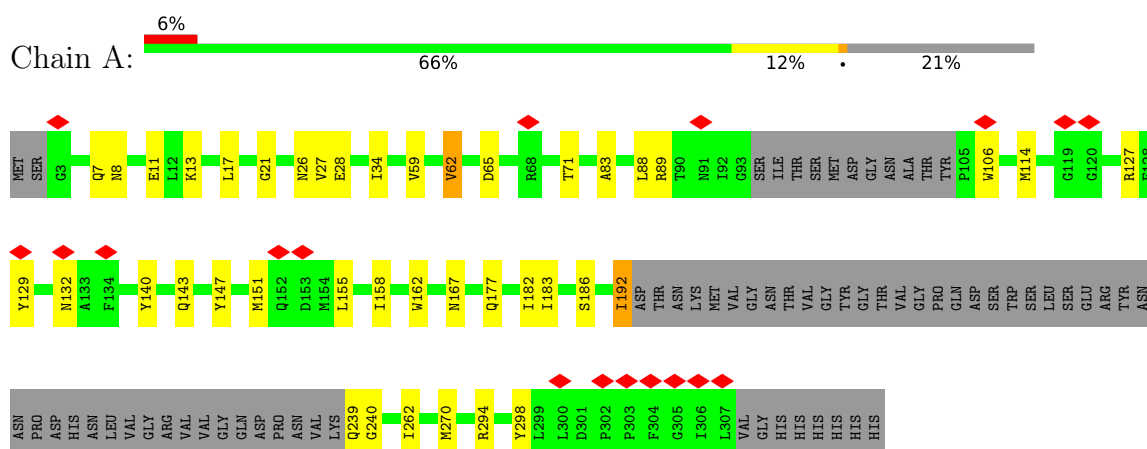
• Molecule 1: Neck protein gp13



• Molecule 1: Neck protein gp13

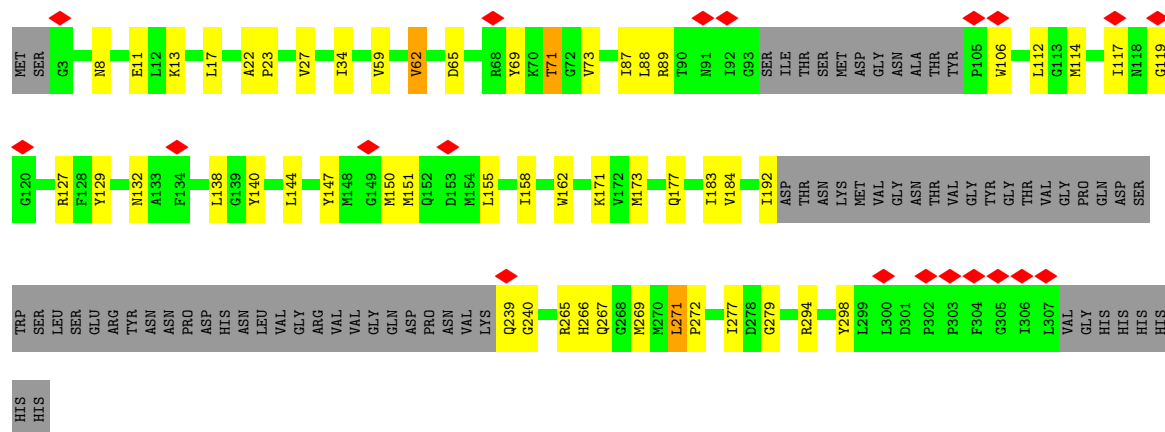


• Molecule 1: Neck protein gp13

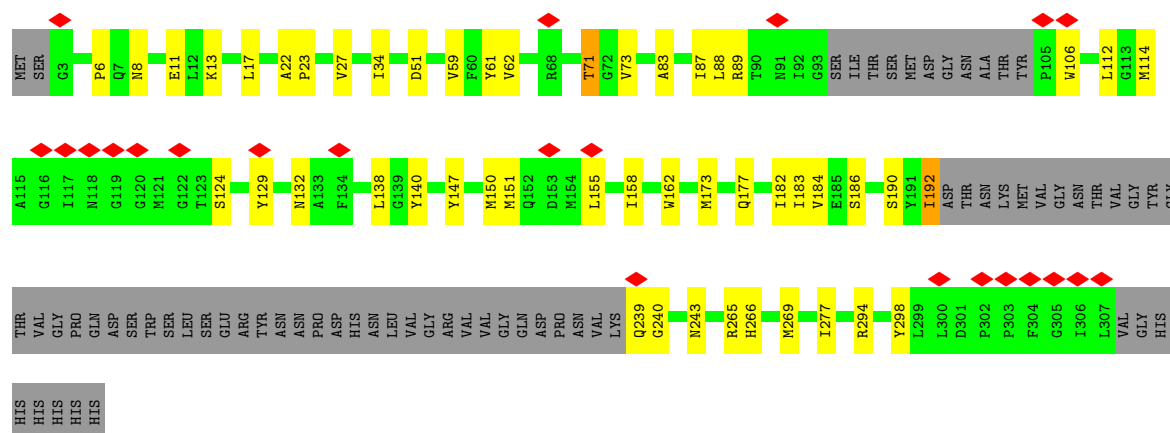


• Molecule 1: Neck protein gp13

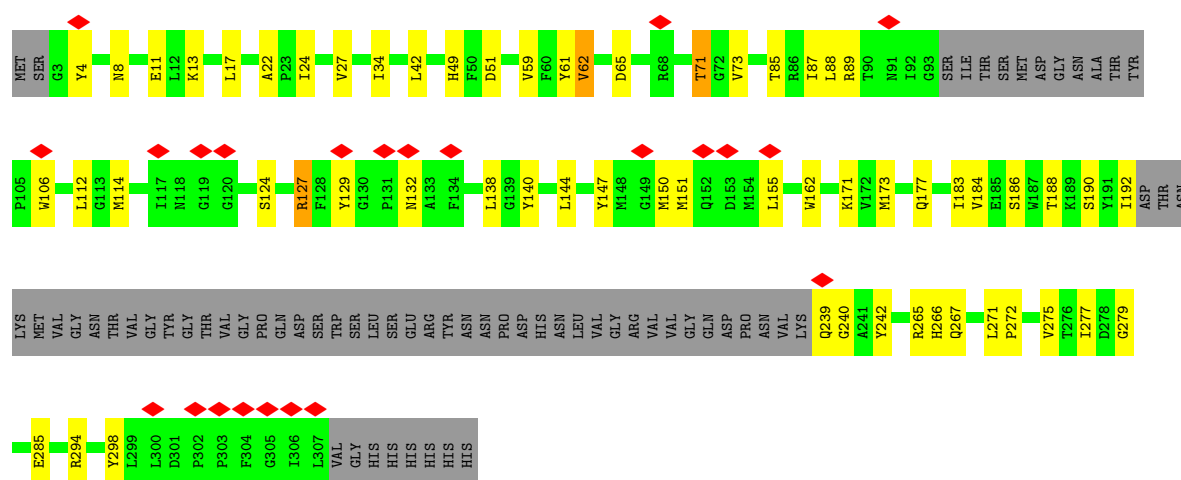




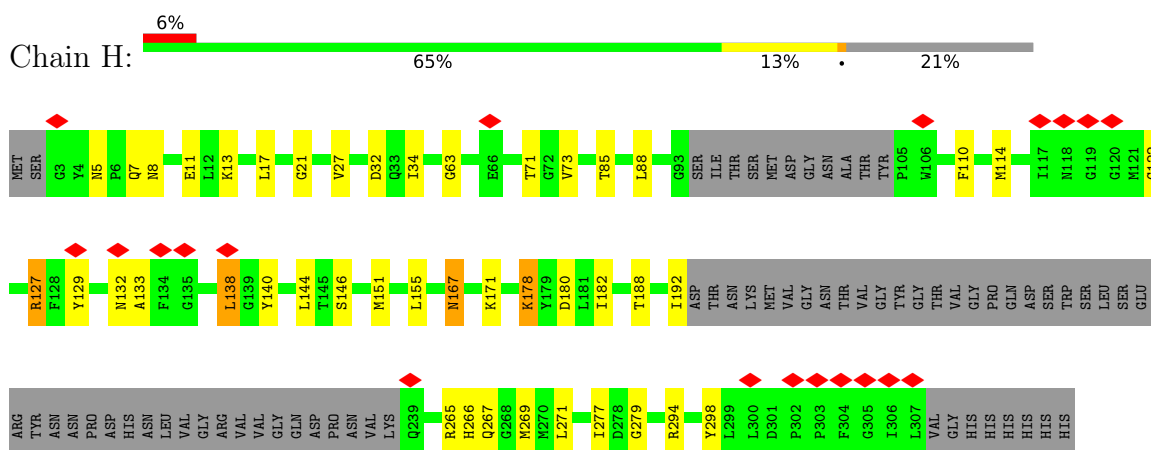
• Molecule 1: Neck protein gp13



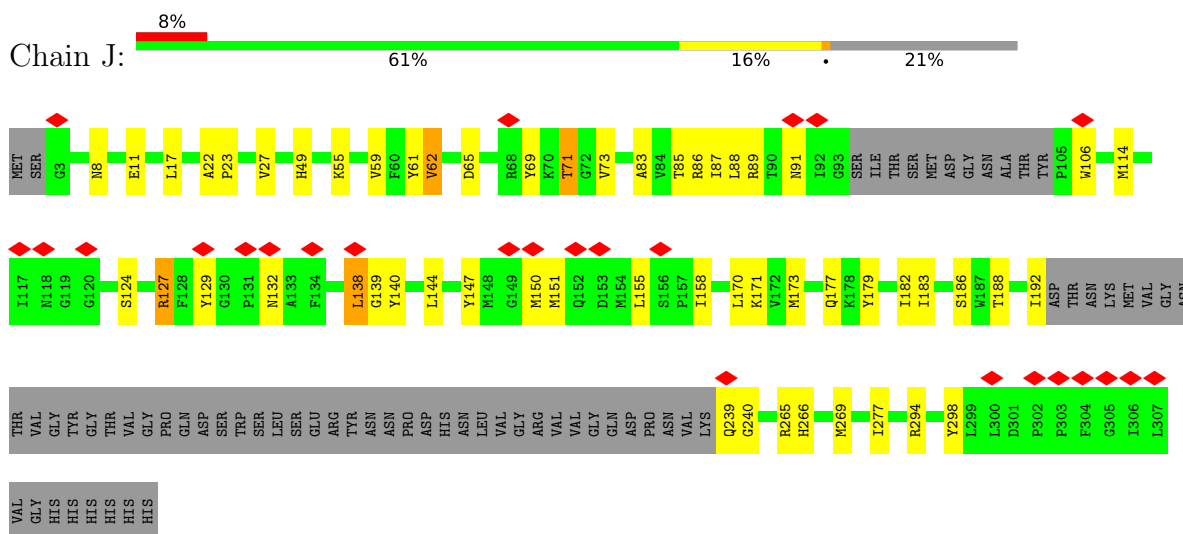
• Molecule 1: Neck protein gp13



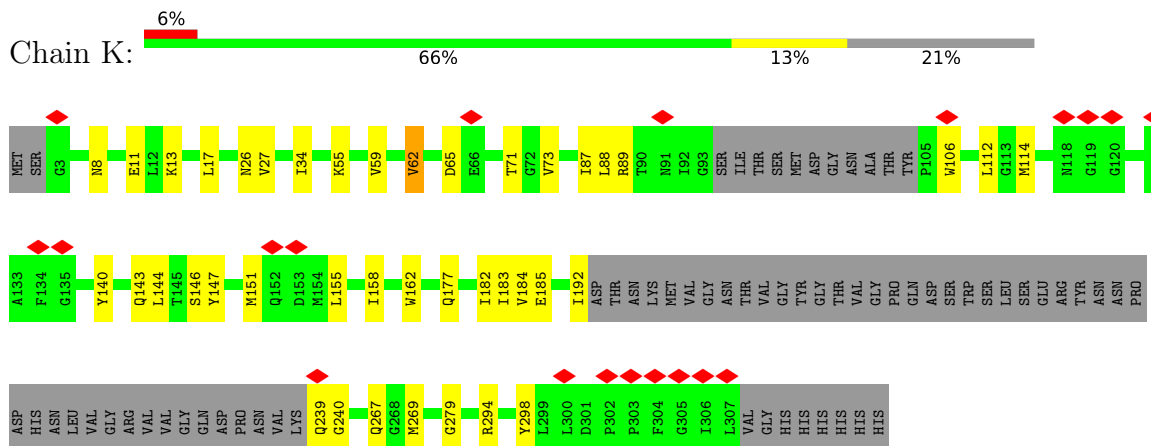
• Molecule 1: Neck protein gp13



- Molecule 1: Neck protein gp13

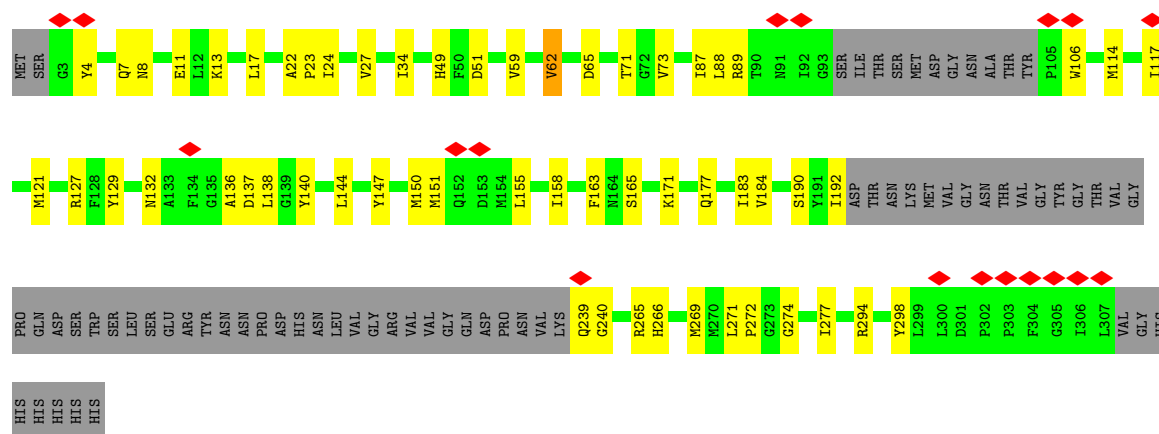


- Molecule 1: Neck protein gp13



- Molecule 1: Neck protein gp13

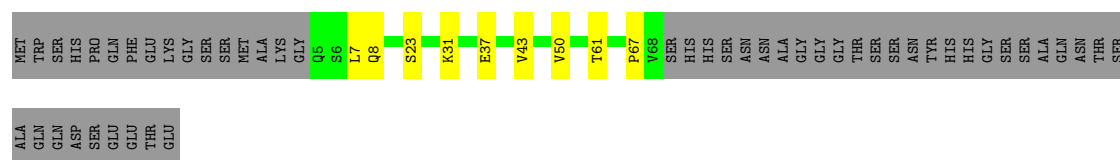




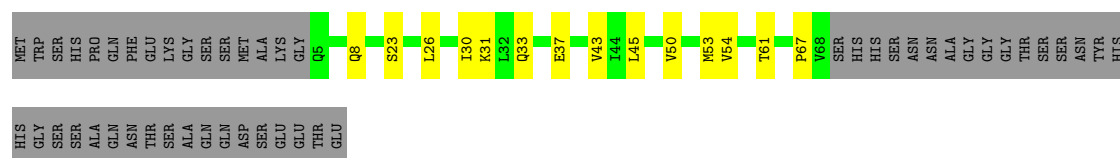
• Molecule 2: RNA-binding protein Hfq



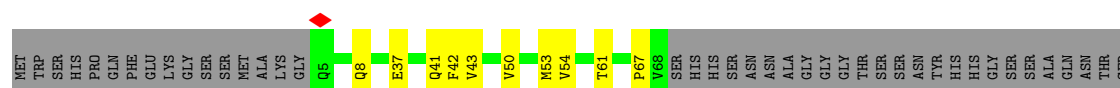
• Molecule 2: RNA-binding protein Hfq



• Molecule 2: RNA-binding protein Hfq



• Molecule 2: RNA-binding protein Hfq



ALA
GLN
GLN
ASP
SER
GLU
GLU
THR
GLU

• Molecule 2: RNA-binding protein Hfq

Chain V: 47% 9% 44%

MET TRP SER HIS HIS PRO GLN PHE GLU LYS GLY SER SER MET ALA LYS GLY Q5 S6 L7 Q8 S23 K31 E37 V50 M53 V54 T61 P67 V68 SER HIS HIS SER SER ASN ASN ALA GLY GLY THR THR SER SER ASN TYR HIS HIS GLY GLY SER SER ALA GLN ASN THR

SER
ALA
GLN
ASP
SER
GLU
THR
GLU

• Molecule 2: RNA-binding protein Hfq

Chain U: 46% 10% 44%

MET TRP SER HIS HIS PRO GLN PHE GLU LYS GLY SER SER MET ALA LYS GLY Q5 S23 K31 L32 Q33 E37 V43 I44 L45 V50 M53 V54 T61 P67 V68 SER HIS HIS SER SER ASN ASN ALA GLY GLY THR THR SER SER ASN TYR HIS HIS GLY GLY SER SER ALA

GLN
ASN
THR
SER
ALA
GLN
GLN
SER
ASP
SER
GLU
THR
GLU

• Molecule 3: Neck protein gp14

Chain O: 5% 50% 8% 42%

HIS HIS HIS HIS HIS HIS SER GLY MET MET ALA TYR D5 K6 L12 E13 E14 ARG THR GLY TYR SER GLN THR ASN GLU T24 E25 I26 L27 N28 V31 L42 R54 V61 D75 L76 K77 N78 K79 F80 N91 S92 F93 E94 G95 TYR GLU ALA LYS SER

PHE PHE SER ASN F106 G107 M108 Q109 V110 Q111 N119 L122 F123 K124 E127 N128 G129 K130 L137 L146 E153 R167 S177 GLY GLU ILE ASN PRO VAL LEU LYS ASN PRO PHE SER GLU LEU LEU ALA VAL ASN

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

• Molecule 3: Neck protein gp14

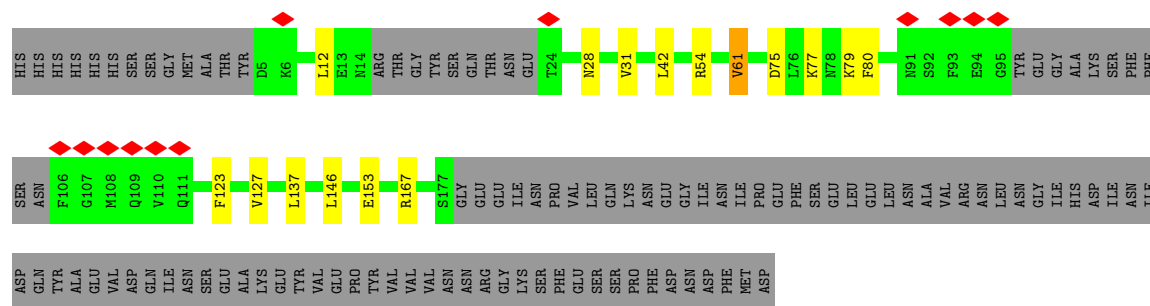
Chain N: 5% 49% 9% 42%

HIS HIS HIS HIS HIS HIS SER GLY MET MET ALA TYR D5 K6 L12 E13 E14 ARG THR GLY TYR SER GLN THR ASN GLU T24 L42 E49 M53 R54 E57 V61 D69 L70 I71 F72 K77 N78 K79 F80 Y89 I90 N91 S92 F93 E94 G95 TYR GLU

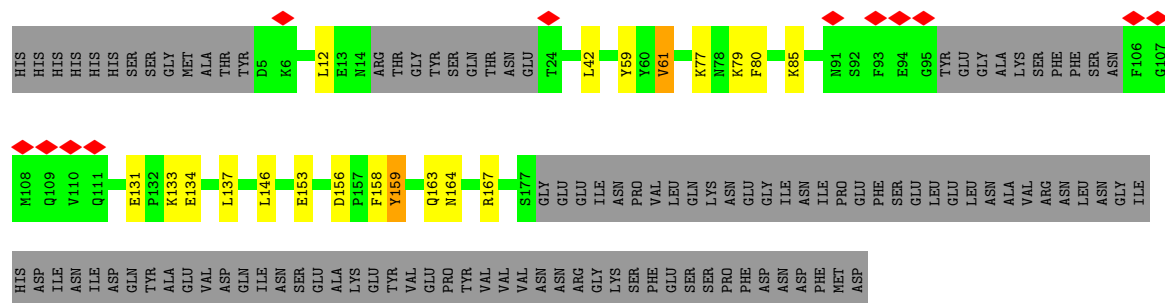
GLY ALA LYS SER PHE PHE ASN F106 G107 M108 Q109 Q111 S117 F123 V127 L137 L146 E153 D156 P157 F158 Q163 R167 S177 GLY GLU ILE ASN PRO PHE VAL LEU LYS GLN ASN GLU TYR ASP ASN ILE ASN ILE PRO GLU PHE SER PHE GLU LEU LEU

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

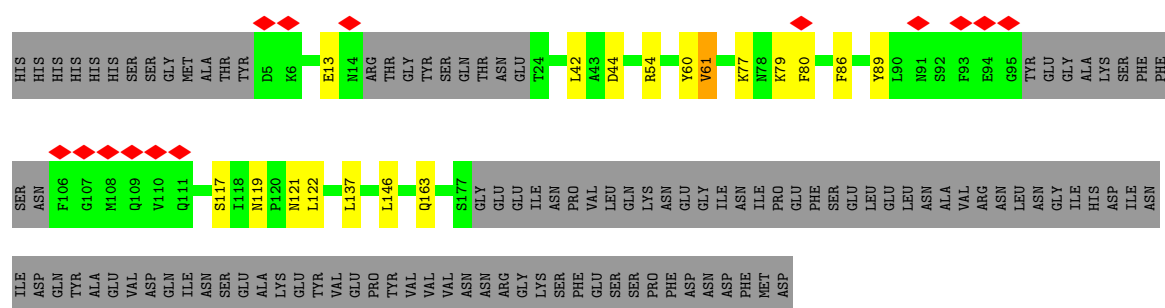
• Molecule 3: Neck protein gp14



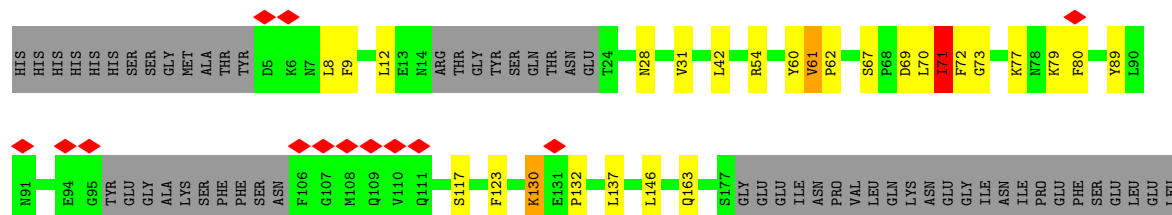
• Molecule 3: Neck protein gp14



• Molecule 3: Neck protein gp14



• Molecule 3: Neck protein gp14



ASN	ALA	VAL	ARG	ASN	LEU	ASN	GLY	ILE	HIS	ASP	ILE	ASN	ASP	GLN	TYR	ALA	GLU	VAL	ASP	GLN	ILE	ASN	SER	GLU	ALA	LYS	GLU	TYR	VAL	GLU	PRO	TYR	VAL	VAL	VAL	ASN	ASN	ARG	GLY	LYS	SER	PHE	GLU	SER	SER	PRO	PHE	ASP	ASN	ASP	PHE	MET	ASP
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	381536	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.582	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.0109	Depositor
Map size (Å)	340.48, 340.48, 340.48	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	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	0.09	0/2037	0.25	0/2752
1	B	0.09	0/2037	0.25	0/2752
1	C	0.09	0/2037	0.25	0/2752
1	D	0.09	0/2037	0.26	0/2752
1	E	0.09	0/2037	0.25	0/2752
1	F	0.10	0/2037	0.26	0/2752
1	G	0.09	0/2037	0.25	0/2752
1	H	0.10	0/2037	0.24	0/2752
1	I	0.09	0/2037	0.26	0/2752
1	J	0.10	0/2037	0.25	0/2752
1	K	0.09	0/2037	0.25	0/2752
1	L	0.15	0/2037	0.35	1/2752 (0.0%)
2	S	0.08	0/522	0.23	0/708
2	T	0.08	0/522	0.23	0/708
2	U	0.08	0/522	0.23	0/708
2	V	0.08	0/522	0.23	0/708
2	W	0.08	0/522	0.24	0/708
2	X	0.08	0/522	0.23	0/708
3	M	0.08	0/1283	0.21	0/1737
3	N	0.20	0/1283	0.31	0/1737
3	O	0.08	0/1283	0.21	0/1737
3	P	0.15	0/1283	0.31	0/1737
3	Q	0.08	0/1283	0.21	0/1737
3	R	0.08	0/1283	0.21	0/1737
All	All	0.10	0/35274	0.26	1/47694 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	136	ALA	N-CA-C	-8.86	100.35	114.09

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	1990	0	1938	26	0
1	B	1990	0	1938	33	0
1	C	1990	0	1938	33	0
1	D	1990	0	1938	31	0
1	E	1990	0	1938	28	0
1	F	1990	0	1938	36	0
1	G	1990	0	1938	32	0
1	H	1990	0	1938	28	0
1	I	1990	0	1938	32	0
1	J	1990	0	1938	32	0
1	K	1990	0	1938	23	0
1	L	1990	0	1938	35	0
2	S	513	0	538	9	0
2	T	513	0	538	5	0
2	U	513	0	538	10	0
2	V	513	0	538	10	0
2	W	513	0	538	9	0
2	X	513	0	538	13	0
3	M	1251	0	1195	11	0
3	N	1251	0	1195	14	0
3	O	1251	0	1195	16	0
3	P	1251	0	1195	19	0
3	Q	1251	0	1195	10	0
3	R	1251	0	1195	16	0
All	All	34464	0	33654	437	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (437) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:88:LEU:HB3	1:K:155:LEU:HD11	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:LEU:HB3	1:C:155:LEU:HD11	1.73	0.70
1:G:88:LEU:HB3	1:G:155:LEU:HD11	1.73	0.70
3:O:119:ASN:HD22	3:O:122:LEU:H	1.38	0.70
1:E:88:LEU:HB3	1:E:155:LEU:HD11	1.74	0.69
1:A:88:LEU:HB3	1:A:155:LEU:HD11	1.73	0.69
1:D:17:LEU:HD22	1:D:27:VAL:HG21	1.75	0.69
1:L:17:LEU:HD22	1:L:27:VAL:HG21	1.75	0.69
3:Q:42:LEU:HD12	1:J:266:HIS:HD2	1.58	0.69
1:L:88:LEU:HB3	1:L:155:LEU:HD11	1.74	0.69
1:I:88:LEU:HB3	1:I:155:LEU:HD11	1.74	0.68
3:P:42:LEU:HD12	1:H:266:HIS:HD2	1.59	0.68
1:J:17:LEU:HD22	1:J:27:VAL:HG21	1.74	0.68
1:F:17:LEU:HD22	1:F:27:VAL:HG21	1.75	0.68
3:N:42:LEU:HD12	1:D:266:HIS:HD2	1.59	0.68
1:H:180:ASP:HB3	1:H:182:ILE:HG13	1.76	0.67
3:O:42:LEU:HD12	1:F:266:HIS:HD2	1.60	0.67
3:P:28:ASN:HD22	3:P:31:VAL:H	1.43	0.67
3:M:28:ASN:HD22	3:M:31:VAL:H	1.42	0.66
1:F:88:LEU:HB3	1:F:155:LEU:HD11	1.77	0.66
3:R:42:LEU:HD12	1:L:266:HIS:HD2	1.61	0.66
1:D:88:LEU:HB3	1:D:155:LEU:HD11	1.78	0.66
3:M:42:LEU:HD12	1:B:266:HIS:HD2	1.60	0.65
1:B:17:LEU:HD22	1:B:27:VAL:HG21	1.78	0.65
3:Q:119:ASN:HD22	3:Q:122:LEU:H	1.44	0.65
1:B:88:LEU:HB3	1:B:155:LEU:HD11	1.77	0.65
1:K:17:LEU:HD22	1:K:27:VAL:HG21	1.80	0.64
1:I:17:LEU:HD22	1:I:27:VAL:HG21	1.79	0.64
1:D:6:PRO:HD2	1:D:243:ASN:HD22	1.62	0.63
1:C:17:LEU:HD22	1:C:27:VAL:HG21	1.81	0.63
1:A:17:LEU:HD22	1:A:27:VAL:HG21	1.81	0.63
1:G:169:GLN:HE22	1:H:138:LEU:HD13	1.63	0.63
3:O:28:ASN:HD22	3:O:31:VAL:H	1.47	0.62
3:R:158:PHE:O	3:R:163:GLN:NE2	2.33	0.62
1:E:17:LEU:HD22	1:E:27:VAL:HG21	1.81	0.62
1:G:114:MET:HE1	1:G:140:TYR:HB3	1.81	0.62
1:J:88:LEU:HB3	1:J:155:LEU:HD11	1.81	0.60
3:M:61:VAL:HG13	3:M:137:LEU:HB2	1.84	0.60
1:G:17:LEU:HD22	1:G:27:VAL:HG21	1.82	0.60
1:B:114:MET:HE1	1:B:140:TYR:HB3	1.83	0.60
3:R:159:TYR:HD1	3:R:159:TYR:H	1.49	0.60
1:E:114:MET:HE1	1:E:140:TYR:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:VAL:HG22	1:D:183:ILE:HG22	1.84	0.59
1:F:59:VAL:HG22	1:F:183:ILE:HG22	1.85	0.59
1:C:59:VAL:HG22	1:C:183:ILE:HG22	1.84	0.59
1:D:114:MET:HE1	1:D:140:TYR:HB3	1.84	0.58
3:N:61:VAL:HG13	3:N:137:LEU:HB2	1.86	0.58
1:F:114:MET:HE1	1:F:140:TYR:HB3	1.85	0.58
3:R:61:VAL:HG13	3:R:137:LEU:HB2	1.85	0.58
3:R:12:LEU:HD21	1:J:22:ALA:HB1	1.86	0.58
1:C:42:LEU:HD11	1:C:242:TYR:HE1	1.69	0.58
1:L:129:TYR:HB3	1:L:132:ASN:HB2	1.86	0.58
1:I:59:VAL:HG22	1:I:183:ILE:HG22	1.86	0.57
3:O:61:VAL:HG13	3:O:137:LEU:HB2	1.86	0.57
3:P:61:VAL:HG13	3:P:137:LEU:HB2	1.84	0.57
1:L:59:VAL:HG22	1:L:183:ILE:HG22	1.85	0.57
2:W:8:GLN:HA	2:V:53:MET:HE1	1.87	0.57
3:Q:61:VAL:HG13	3:Q:137:LEU:HB2	1.87	0.57
1:G:59:VAL:HG22	1:G:183:ILE:HG22	1.86	0.57
1:G:89:ARG:NH2	1:G:177:GLN:OE1	2.38	0.57
3:R:159:TYR:HB2	3:R:164:ASN:HB3	1.87	0.57
1:J:129:TYR:HB3	1:J:132:ASN:HB2	1.86	0.57
1:A:167:ASN:HD21	1:B:138:LEU:HD22	1.69	0.57
1:F:271:LEU:HD13	1:F:277:ILE:HD11	1.87	0.57
1:K:59:VAL:HG22	1:K:183:ILE:HG22	1.87	0.56
1:F:42:LEU:HD11	1:F:242:TYR:HE1	1.69	0.56
1:A:59:VAL:HG22	1:A:183:ILE:HG22	1.86	0.56
1:A:89:ARG:NH2	1:A:177:GLN:OE1	2.38	0.56
1:B:59:VAL:HG22	1:B:183:ILE:HG22	1.87	0.56
1:J:89:ARG:NH2	1:J:177:GLN:OE1	2.39	0.56
2:V:8:GLN:HA	2:U:53:MET:HE1	1.88	0.56
1:J:59:VAL:HG22	1:J:183:ILE:HG22	1.86	0.56
1:J:61:TYR:HB3	1:J:124:SER:H	1.70	0.56
1:K:114:MET:HE1	1:K:140:TYR:HB3	1.88	0.55
1:D:61:TYR:HB3	1:D:124:SER:H	1.70	0.55
1:J:127:ARG:HH22	1:J:188:THR:HG21	1.70	0.55
1:L:117:ILE:HG23	1:L:121:MET:HG2	1.87	0.55
1:C:239:GLN:NE2	1:C:240:GLY:O	2.40	0.55
1:D:129:TYR:HB3	1:D:132:ASN:HB2	1.88	0.55
1:I:89:ARG:NH2	1:I:177:GLN:OE1	2.40	0.55
1:D:89:ARG:NH2	1:D:177:GLN:OE1	2.39	0.55
1:K:89:ARG:NH2	1:K:177:GLN:OE1	2.40	0.55
1:F:239:GLN:NE2	1:F:240:GLY:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:MET:HE1	1:A:140:TYR:HB3	1.89	0.54
2:S:8:GLN:HA	2:X:53:MET:HE1	1.88	0.54
1:F:87:ILE:HG12	1:F:184:VAL:HG13	1.90	0.54
1:I:26:ASN:O	1:J:265:ARG:NH1	2.41	0.54
1:E:59:VAL:HG22	1:E:183:ILE:HG22	1.87	0.54
1:I:114:MET:HE1	1:I:140:TYR:HB3	1.89	0.54
1:D:239:GLN:NE2	1:D:240:GLY:O	2.41	0.54
1:G:239:GLN:NE2	1:G:240:GLY:O	2.41	0.53
3:M:61:VAL:HG21	3:M:79:LYS:HD2	1.90	0.53
3:P:137:LEU:HD13	3:P:146:LEU:HD21	1.89	0.53
1:H:294:ARG:NH2	1:H:298:TYR:OH	2.41	0.53
3:M:12:LEU:HD21	1:L:22:ALA:HB1	1.90	0.53
1:E:167:ASN:HD21	1:F:138:LEU:HD22	1.74	0.53
3:N:12:LEU:HD21	1:B:22:ALA:HB1	1.90	0.53
1:E:89:ARG:NH2	1:E:177:GLN:OE1	2.42	0.53
1:B:129:TYR:HB3	1:B:132:ASN:HB2	1.91	0.53
1:F:271:LEU:HB3	1:F:275:VAL:HB	1.89	0.53
1:A:294:ARG:NH2	1:A:298:TYR:OH	2.42	0.53
1:C:89:ARG:NH2	1:C:177:GLN:OE1	2.42	0.53
1:I:5:ASN:HB2	1:J:55:LYS:HE3	1.91	0.53
1:G:294:ARG:NH2	1:G:298:TYR:OH	2.42	0.52
1:B:89:ARG:NH2	1:B:177:GLN:OE1	2.42	0.52
1:K:294:ARG:NH2	1:K:298:TYR:OH	2.42	0.52
3:N:153:GLU:O	3:N:167:ARG:NE	2.35	0.52
1:B:117:ILE:HG13	1:B:119:GLY:H	1.74	0.52
1:H:88:LEU:HB3	1:H:155:LEU:HD11	1.92	0.52
1:C:87:ILE:HG12	1:C:184:VAL:HG13	1.92	0.52
3:P:89:TYR:HB3	3:P:117:SER:HB3	1.92	0.52
1:E:294:ARG:NH2	1:E:298:TYR:OH	2.43	0.52
1:E:26:ASN:O	1:F:265:ARG:NH1	2.43	0.52
1:C:114:MET:HE1	1:C:140:TYR:HB3	1.92	0.52
1:J:294:ARG:NH2	1:J:298:TYR:OH	2.43	0.52
1:I:267:GLN:HE22	1:I:279:GLY:H	1.58	0.51
1:I:294:ARG:NH2	1:I:298:TYR:OH	2.43	0.51
1:L:87:ILE:HG23	1:L:184:VAL:HG22	1.92	0.51
1:I:55:LYS:NZ	1:I:185:GLU:OE1	2.42	0.51
1:I:71:THR:HG23	1:I:73:VAL:HG12	1.92	0.51
1:C:294:ARG:NH2	1:C:298:TYR:OH	2.44	0.51
2:X:8:GLN:HA	2:W:53:MET:HE1	1.90	0.51
3:O:124:LYS:HG3	3:O:129:GLY:HA2	1.92	0.51
1:L:71:THR:HG23	1:L:73:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:89:ARG:NH2	1:L:177:GLN:OE1	2.44	0.51
3:O:137:LEU:HD13	3:O:146:LEU:HD21	1.91	0.51
3:R:156:ASP:OD2	3:R:163:GLN:NE2	2.44	0.51
3:R:159:TYR:O	3:R:164:ASN:ND2	2.43	0.51
1:A:239:GLN:NE2	1:A:240:GLY:O	2.43	0.51
1:B:294:ARG:NH2	1:B:298:TYR:OH	2.44	0.51
2:X:23:SER:OG	2:X:31:LYS:NZ	2.41	0.51
3:R:153:GLU:O	3:R:167:ARG:NE	2.35	0.51
1:G:129:TYR:HB3	1:G:132:ASN:HB2	1.93	0.51
1:F:129:TYR:HB3	1:F:132:ASN:HB2	1.91	0.51
1:H:129:TYR:HB3	1:H:132:ASN:HB2	1.93	0.51
1:C:26:ASN:O	1:D:265:ARG:NH1	2.44	0.51
1:G:83:ALA:O	1:G:186:SER:OG	2.20	0.51
2:S:8:GLN:HE21	2:X:43:VAL:HG13	1.75	0.51
3:R:137:LEU:HD13	3:R:146:LEU:HD21	1.93	0.51
2:T:8:GLN:HE21	2:S:43:VAL:HG13	1.76	0.50
3:N:61:VAL:HG21	3:N:79:LYS:HD2	1.94	0.50
3:M:137:LEU:HD13	3:M:146:LEU:HD21	1.93	0.50
3:Q:89:TYR:HB3	3:Q:117:SER:HB3	1.91	0.50
3:Q:137:LEU:HD13	3:Q:146:LEU:HD21	1.93	0.50
1:A:129:TYR:HB3	1:A:132:ASN:HB2	1.92	0.50
1:J:8:ASN:HD21	1:J:11:GLU:HG3	1.75	0.50
1:I:62:VAL:HG12	1:I:65:ASP:HA	1.93	0.50
1:K:26:ASN:O	1:L:265:ARG:NH1	2.45	0.50
1:L:294:ARG:NH2	1:L:298:TYR:OH	2.44	0.50
3:O:12:LEU:HD21	1:D:22:ALA:HB1	1.93	0.50
1:E:62:VAL:HG12	1:E:65:ASP:HA	1.93	0.50
1:I:129:TYR:HB3	1:I:132:ASN:HB2	1.94	0.50
1:G:62:VAL:HG12	1:G:65:ASP:HA	1.94	0.50
1:K:71:THR:HG23	1:K:73:VAL:HG12	1.94	0.50
1:D:294:ARG:NH2	1:D:298:TYR:OH	2.44	0.50
1:J:114:MET:HE1	1:J:140:TYR:HB3	1.92	0.50
1:G:167:ASN:ND2	1:H:133:ALA:O	2.44	0.50
3:O:127:VAL:HG23	3:O:130:LYS:H	1.76	0.50
1:K:162:TRP:HH2	1:L:150:MET:HE3	1.77	0.50
3:N:54:ARG:HD3	1:E:269:MET:HE3	1.94	0.50
3:P:12:LEU:HD21	1:F:22:ALA:HB1	1.94	0.50
1:E:162:TRP:HH2	1:F:150:MET:HE3	1.77	0.50
1:L:271:LEU:HD13	1:L:277:ILE:HD11	1.94	0.50
1:C:269:MET:HE3	3:M:54:ARG:HG3	1.93	0.50
1:J:138:LEU:HD12	1:J:139:GLY:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:ARG:HH22	1:F:188:THR:HG21	1.77	0.49
1:F:294:ARG:NH2	1:F:298:TYR:OH	2.45	0.49
1:I:83:ALA:HB3	1:I:187:TRP:HB2	1.95	0.49
2:U:23:SER:OG	2:U:31:LYS:NZ	2.43	0.49
1:H:5:ASN:OD1	1:H:7:GLN:NE2	2.44	0.49
1:L:114:MET:HE1	1:L:140:TYR:HB3	1.95	0.49
1:D:106:TRP:H	1:D:106:TRP:CD1	2.30	0.49
1:G:127:ARG:HH12	1:G:129:TYR:HB2	1.76	0.49
3:R:61:VAL:HG21	3:R:79:LYS:HD2	1.94	0.49
3:O:61:VAL:HG21	3:O:79:LYS:HD2	1.93	0.49
1:D:83:ALA:O	1:D:186:SER:OG	2.22	0.49
1:F:71:THR:HG23	1:F:73:VAL:HG12	1.95	0.49
1:F:87:ILE:HG23	1:F:184:VAL:HG22	1.94	0.49
1:B:106:TRP:H	1:B:106:TRP:CD1	2.30	0.49
1:K:55:LYS:NZ	1:K:185:GLU:OE1	2.43	0.49
3:O:153:GLU:O	3:O:167:ARG:NE	2.36	0.49
1:E:71:THR:HG23	1:E:73:VAL:HG12	1.95	0.48
1:G:150:MET:HE3	1:F:162:TRP:HH2	1.78	0.48
1:F:106:TRP:CD1	1:F:106:TRP:H	2.30	0.48
1:G:106:TRP:H	1:G:106:TRP:CD1	2.31	0.48
1:K:239:GLN:NE2	1:K:240:GLY:O	2.46	0.48
1:C:62:VAL:HG12	1:C:65:ASP:HA	1.95	0.48
1:C:167:ASN:HD21	1:D:138:LEU:HD22	1.79	0.48
1:E:106:TRP:H	1:E:106:TRP:CD1	2.31	0.48
1:A:26:ASN:O	1:B:265:ARG:NH1	2.46	0.48
3:M:153:GLU:O	3:M:167:ARG:NE	2.35	0.48
3:R:131:GLU:OE2	3:R:133:LYS:NZ	2.39	0.48
1:H:127:ARG:HH22	1:H:188:THR:HG21	1.78	0.48
1:K:106:TRP:CD1	1:K:106:TRP:H	2.31	0.48
1:C:85:THR:O	1:C:185:GLU:HG3	2.13	0.48
1:C:129:TYR:HB3	1:C:132:ASN:HB2	1.95	0.48
1:C:162:TRP:HH2	1:D:150:MET:HE3	1.79	0.48
1:J:87:ILE:HD11	1:J:170:LEU:HD21	1.94	0.48
1:A:106:TRP:CD1	1:A:106:TRP:H	2.31	0.48
1:A:162:TRP:HH2	1:B:150:MET:HE3	1.79	0.48
1:D:88:LEU:HD22	1:D:155:LEU:HD21	1.96	0.48
2:V:8:GLN:HE21	2:U:43:VAL:HG13	1.77	0.48
1:F:85:THR:HB	1:F:186:SER:HA	1.95	0.48
1:L:138:LEU:HD12	1:L:138:LEU:H	1.79	0.48
1:G:71:THR:HG23	1:G:73:VAL:HG12	1.95	0.47
2:V:23:SER:OG	2:V:31:LYS:NZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:137:LEU:HD13	3:N:146:LEU:HD21	1.96	0.47
1:E:129:TYR:HB3	1:E:132:ASN:HB2	1.96	0.47
1:H:88:LEU:HD13	1:H:155:LEU:HD21	1.95	0.47
1:A:62:VAL:HG12	1:A:65:ASP:HA	1.96	0.47
1:I:239:GLN:NE2	1:I:240:GLY:O	2.48	0.47
2:S:23:SER:OG	2:S:31:LYS:NZ	2.45	0.47
3:M:123:PHE:O	3:M:127:VAL:HG22	2.14	0.47
1:B:71:THR:HG23	1:B:73:VAL:HG12	1.96	0.47
1:F:8:ASN:HD21	1:F:11:GLU:HG3	1.79	0.47
1:H:267:GLN:HE22	1:H:279:GLY:H	1.61	0.47
1:C:61:TYR:HB3	1:C:124:SER:H	1.79	0.47
1:C:106:TRP:H	1:C:106:TRP:CD1	2.31	0.47
1:I:106:TRP:H	1:I:106:TRP:CD1	2.31	0.47
3:Q:54:ARG:HG3	1:K:269:MET:HE3	1.97	0.47
1:E:61:TYR:HB3	1:E:124:SER:H	1.79	0.47
1:B:271:LEU:HG	1:B:272:PRO:HD2	1.97	0.47
1:L:62:VAL:HG12	1:L:65:ASP:HA	1.96	0.47
3:Q:61:VAL:HG21	3:Q:79:LYS:HD2	1.95	0.47
3:P:61:VAL:HG21	3:P:79:LYS:HD2	1.97	0.47
1:E:150:MET:HE3	1:D:162:TRP:HH2	1.80	0.47
1:J:106:TRP:H	1:J:106:TRP:CD1	2.31	0.47
1:L:106:TRP:H	1:L:106:TRP:CD1	2.30	0.47
1:F:89:ARG:NH2	1:F:177:GLN:OE1	2.47	0.47
1:K:267:GLN:HE22	1:K:279:GLY:H	1.63	0.47
1:H:17:LEU:HD22	1:H:27:VAL:HG11	1.97	0.47
3:N:158:PHE:O	3:N:163:GLN:NE2	2.48	0.46
3:P:71:ILE:HB	3:P:72:PHE:H	1.57	0.46
1:E:239:GLN:NE2	1:E:240:GLY:O	2.47	0.46
1:H:110:PHE:O	1:H:114:MET:HB2	2.14	0.46
1:H:151:MET:HG2	1:H:155:LEU:HD22	1.97	0.46
1:I:9:PRO:HG3	1:I:85:THR:HG22	1.97	0.46
1:B:8:ASN:HD21	1:B:11:GLU:HG3	1.81	0.46
1:B:88:LEU:HD22	1:B:155:LEU:HD21	1.98	0.46
1:G:26:ASN:O	1:H:265:ARG:NH1	2.48	0.46
1:J:71:THR:HG23	1:J:73:VAL:HG12	1.97	0.46
1:L:271:LEU:HG	1:L:272:PRO:HD2	1.96	0.46
1:J:88:LEU:HD22	1:J:155:LEU:HD21	1.98	0.46
1:C:127:ARG:HH12	1:C:129:TYR:HB2	1.80	0.46
2:X:8:GLN:HE21	2:W:43:VAL:HG13	1.80	0.46
1:B:13:LYS:HG3	1:B:34:ILE:HG21	1.98	0.46
1:K:62:VAL:HG12	1:K:65:ASP:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:LEU:HD13	1:B:277:ILE:HD11	1.98	0.46
1:J:239:GLN:NE2	1:J:240:GLY:O	2.49	0.46
1:J:85:THR:HG22	1:J:86:ARG:HG2	1.98	0.45
2:S:7:LEU:HD13	2:X:45:LEU:HD13	1.98	0.45
1:D:87:ILE:HG23	1:D:184:VAL:HG22	1.99	0.45
1:H:269:MET:HB3	1:H:277:ILE:HD12	1.99	0.45
1:J:89:ARG:HB3	1:J:182:ILE:HG12	1.98	0.45
1:L:8:ASN:HD21	1:L:11:GLU:HG3	1.82	0.45
1:I:127:ARG:HH12	1:I:129:TYR:HB2	1.82	0.45
1:F:51:ASP:HB3	1:F:190:SER:HB2	1.99	0.45
1:A:8:ASN:HD21	1:A:11:GLU:HG3	1.82	0.45
1:A:89:ARG:HB3	1:A:182:ILE:HG12	1.98	0.45
1:C:85:THR:HB	1:C:186:SER:HA	1.98	0.45
3:N:89:TYR:HB3	3:N:117:SER:HB3	1.99	0.45
1:L:147:TYR:O	1:L:151:MET:HB2	2.17	0.45
1:G:262:ILE:HD13	1:F:24:ILE:HD12	1.98	0.45
1:F:267:GLN:HE22	1:F:279:GLY:H	1.64	0.45
1:L:88:LEU:HD22	1:L:155:LEU:HD21	1.99	0.45
1:C:8:ASN:N	1:C:8:ASN:OD1	2.49	0.45
1:B:147:TYR:O	1:B:151:MET:HB2	2.17	0.45
1:D:8:ASN:HD21	1:D:11:GLU:HG3	1.82	0.45
1:D:89:ARG:HB3	1:D:182:ILE:HG12	1.99	0.45
1:I:89:ARG:HB3	1:I:182:ILE:HG12	1.99	0.45
1:G:89:ARG:HB3	1:G:182:ILE:HG12	1.99	0.45
1:H:8:ASN:HD21	1:H:11:GLU:HG3	1.81	0.45
1:H:32:ASP:OD1	1:H:32:ASP:N	2.50	0.45
2:S:61:THR:HG23	2:X:54:VAL:HG22	1.99	0.44
2:V:61:THR:HG23	2:U:54:VAL:HG22	1.99	0.44
1:J:269:MET:HB3	1:J:277:ILE:HD12	1.99	0.44
1:G:261:GLN:NE2	1:F:285:GLU:OE1	2.41	0.44
3:P:60:TYR:HE2	3:P:130:LYS:HG2	1.82	0.44
1:B:239:GLN:NE2	1:B:240:GLY:O	2.50	0.44
1:D:13:LYS:HG3	1:D:34:ILE:HG21	1.99	0.44
1:C:150:MET:HE3	1:B:162:TRP:HH2	1.82	0.44
2:W:61:THR:HG23	2:V:54:VAL:HG22	1.99	0.44
1:K:8:ASN:HD21	1:K:11:GLU:HG3	1.82	0.44
1:L:137:ASP:HA	1:L:140:TYR:CD2	2.52	0.44
1:C:143:GLN:HA	1:B:171:LYS:HZ2	1.82	0.44
1:I:162:TRP:HH2	1:J:150:MET:HE3	1.83	0.44
1:G:271:LEU:HD21	3:O:54:ARG:HH21	1.82	0.44
1:H:171:LYS:HA	1:H:171:LYS:HD2	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:147:TYR:O	1:K:151:MET:HB2	2.18	0.44
1:L:165:SER:HG	1:L:239:GLN:N	2.15	0.44
1:L:239:GLN:NE2	1:L:240:GLY:O	2.51	0.44
1:I:8:ASN:OD1	1:I:8:ASN:N	2.51	0.44
1:H:63:GLY:N	1:H:122:GLY:O	2.51	0.44
2:T:37:GLU:N	2:T:37:GLU:OE1	2.51	0.44
2:W:37:GLU:OE1	2:W:37:GLU:N	2.51	0.44
1:E:127:ARG:HH12	1:E:129:TYR:HB2	1.82	0.44
1:I:147:TYR:O	1:I:151:MET:HB2	2.18	0.44
1:A:239:GLN:HE21	1:A:239:GLN:HB3	1.66	0.44
1:G:267:GLN:HE22	1:G:279:GLY:H	1.65	0.43
3:Q:44:ASP:OD2	3:Q:121:ASN:ND2	2.51	0.43
3:Q:77:LYS:H	3:Q:77:LYS:HD3	1.83	0.43
1:A:147:TYR:O	1:A:151:MET:HB2	2.18	0.43
1:B:127:ARG:HH12	1:B:129:TYR:HB2	1.83	0.43
1:I:7:GLN:HG3	1:I:162:TRP:HD1	1.83	0.43
1:J:171:LYS:HZ2	1:K:143:GLN:HA	1.83	0.43
1:C:112:LEU:HD23	1:C:112:LEU:H	1.84	0.43
1:E:55:LYS:NZ	1:E:185:GLU:OE1	2.49	0.43
1:E:147:TYR:O	1:E:151:MET:HB2	2.18	0.43
2:S:67:PRO:HG3	2:X:50:VAL:HG12	2.00	0.43
2:V:67:PRO:HG3	2:U:50:VAL:HG12	2.00	0.43
1:B:62:VAL:HG12	1:B:65:ASP:HA	2.01	0.43
1:D:269:MET:HB3	1:D:277:ILE:HD12	1.98	0.43
1:G:143:GLN:HA	1:F:171:LYS:HZ2	1.83	0.43
2:S:37:GLU:N	2:S:37:GLU:OE1	2.52	0.43
1:B:267:GLN:HE22	1:B:279:GLY:H	1.65	0.43
1:H:167:ASN:O	1:H:167:ASN:ND2	2.49	0.43
1:H:178:LYS:HE2	1:H:178:LYS:HB2	1.91	0.43
1:C:57:PHE:CD2	1:C:185:GLU:HB3	2.54	0.43
1:L:51:ASP:HB3	1:L:190:SER:HB2	2.00	0.43
3:N:77:LYS:H	3:N:77:LYS:HD3	1.84	0.43
1:A:83:ALA:O	1:A:186:SER:OG	2.21	0.43
1:B:87:ILE:HG23	1:B:184:VAL:HG22	2.00	0.43
1:C:146:SER:HB2	1:B:173:MET:HE2	2.01	0.42
1:I:87:ILE:HG23	1:I:184:VAL:HG22	2.01	0.42
1:E:192:ILE:H	1:E:192:ILE:HG13	1.56	0.42
1:G:173:MET:HE2	1:H:146:SER:HB2	2.01	0.42
2:V:7:LEU:HD13	2:U:45:LEU:HD13	2.01	0.42
1:G:9:PRO:HG3	1:G:85:THR:HG22	2.00	0.42
1:C:267:GLN:HE22	1:C:279:GLY:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:TYR:O	1:G:151:MET:HB2	2.19	0.42
1:B:112:LEU:HD23	1:B:112:LEU:H	1.84	0.42
1:I:13:LYS:HG3	1:I:34:ILE:HG21	2.02	0.42
1:G:8:ASN:OD1	1:G:8:ASN:N	2.52	0.42
1:B:269:MET:HB3	1:B:277:ILE:HD12	2.01	0.42
1:F:147:TYR:O	1:F:151:MET:HB2	2.18	0.42
1:L:7:GLN:NE2	1:L:163:PHE:O	2.53	0.42
1:L:127:ARG:HH12	1:L:129:TYR:HB2	1.85	0.42
1:G:13:LYS:HG3	1:G:34:ILE:HG21	2.02	0.42
2:X:37:GLU:N	2:X:37:GLU:OE1	2.53	0.42
3:N:123:PHE:O	3:N:127:VAL:HG22	2.19	0.42
1:E:54:ASN:OD1	1:E:190:SER:OG	2.35	0.42
1:D:112:LEU:H	1:D:112:LEU:HD23	1.83	0.42
1:J:91:ASN:HA	1:J:179:TYR:HD2	1.85	0.42
1:I:6:PRO:HD2	1:I:243:ASN:HD22	1.84	0.42
2:T:54:VAL:HG22	2:U:61:THR:HG23	2.01	0.42
1:E:87:ILE:HG23	1:E:184:VAL:HG22	2.02	0.42
1:A:17:LEU:O	1:A:21:GLY:N	2.53	0.42
1:H:71:THR:HG23	1:H:73:VAL:HG12	2.02	0.42
1:L:87:ILE:HG12	1:L:184:VAL:HG13	2.01	0.42
2:U:37:GLU:OE1	2:U:37:GLU:N	2.52	0.42
3:N:49:GLU:HG2	3:N:53:MET:HE2	2.01	0.42
3:M:75:ASP:HB3	3:M:79:LYS:NZ	2.35	0.42
1:A:270:MET:HE2	1:L:274:GLY:HA3	2.02	0.42
1:J:173:MET:HE2	1:K:146:SER:HB2	2.01	0.42
1:C:39:GLN:HE22	1:C:187:TRP:HE1	1.66	0.42
2:X:67:PRO:HG3	2:W:50:VAL:HG12	2.01	0.42
1:H:178:LYS:H	1:H:178:LYS:HG3	1.72	0.42
2:T:67:PRO:HG3	2:S:50:VAL:HG12	2.02	0.42
2:X:31:LYS:HE3	2:X:33:GLN:HE21	1.85	0.42
3:O:26:ILE:HD12	3:N:57:GLU:HG2	2.02	0.42
3:R:133:LYS:HG3	3:R:134:GLU:H	1.83	0.42
1:D:22:ALA:HB3	1:D:23:PRO:HD3	2.02	0.42
1:F:13:LYS:HG3	1:F:34:ILE:HG21	2.01	0.42
1:F:112:LEU:H	1:F:112:LEU:HD23	1.85	0.42
1:F:271:LEU:HG	1:F:272:PRO:HD2	2.02	0.42
1:I:192:ILE:H	1:I:192:ILE:HG13	1.57	0.41
2:T:50:VAL:HG12	2:U:67:PRO:HG3	2.02	0.41
2:X:61:THR:HG23	2:W:54:VAL:HG22	2.01	0.41
2:V:37:GLU:N	2:V:37:GLU:OE1	2.52	0.41
3:R:77:LYS:HD3	3:R:77:LYS:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:123:PHE:CE2	3:P:132:PRO:HG3	2.55	0.41
1:K:87:ILE:HG23	1:K:184:VAL:HG22	2.01	0.41
1:L:269:MET:HB3	1:L:277:ILE:HD12	2.01	0.41
1:C:87:ILE:HG23	1:C:184:VAL:HG22	2.00	0.41
1:G:146:SER:HB2	1:F:173:MET:HE2	2.02	0.41
3:P:62:PRO:HB3	3:P:130:LYS:HD3	2.02	0.41
1:A:127:ARG:HH12	1:A:129:TYR:HB2	1.85	0.41
1:B:22:ALA:HB3	1:B:23:PRO:HD3	2.02	0.41
1:J:62:VAL:HG12	1:J:65:ASP:HA	2.01	0.41
1:C:147:TYR:O	1:C:151:MET:HB2	2.20	0.41
1:E:13:LYS:HG3	1:E:34:ILE:HG21	2.02	0.41
1:J:83:ALA:C	1:J:186:SER:HG	2.27	0.41
1:E:267:GLN:HE22	1:E:279:GLY:H	1.67	0.41
1:A:13:LYS:HG3	1:A:34:ILE:HG21	2.03	0.41
3:P:79:LYS:HE3	3:P:146:LEU:HD13	2.03	0.41
1:L:13:LYS:HG3	1:L:34:ILE:HG21	2.02	0.41
1:C:46:GLY:HA3	1:C:53:LEU:HD13	2.02	0.41
1:E:8:ASN:OD1	1:E:8:ASN:N	2.52	0.41
1:F:61:TYR:HB3	1:F:124:SER:H	1.86	0.41
1:C:13:LYS:HG3	1:C:34:ILE:HG21	2.02	0.41
1:I:269:MET:HE3	3:P:54:ARG:HG3	2.02	0.41
1:I:271:LEU:HD11	3:P:54:ARG:HH21	1.86	0.41
3:P:8:LEU:HD11	1:E:23:PRO:HB2	2.02	0.41
1:A:143:GLN:HA	1:L:171:LYS:HZ2	1.86	0.41
1:B:62:VAL:HG13	1:B:69:TYR:HD2	1.85	0.41
1:D:71:THR:HG23	1:D:73:VAL:HG12	2.01	0.41
1:H:114:MET:HE1	1:H:140:TYR:HB3	2.02	0.41
1:J:22:ALA:HB3	1:J:23:PRO:HD3	2.03	0.41
1:K:112:LEU:H	1:K:112:LEU:HD23	1.85	0.41
1:I:51:ASP:HB3	1:I:190:SER:HB2	2.02	0.41
3:P:130:LYS:HE3	3:P:130:LYS:HA	2.03	0.41
1:A:7:GLN:HG3	1:A:162:TRP:HD1	1.86	0.41
1:F:62:VAL:HG12	1:F:65:ASP:HA	2.03	0.41
1:H:13:LYS:HG3	1:H:34:ILE:HG21	2.03	0.41
1:C:54:ASN:O	1:C:188:THR:N	2.39	0.41
1:G:46:GLY:HA3	1:G:53:LEU:HD13	2.02	0.41
1:G:112:LEU:H	1:G:112:LEU:HD23	1.86	0.41
2:U:31:LYS:HE3	2:U:33:GLN:HE21	1.85	0.41
1:I:112:LEU:H	1:I:112:LEU:HD23	1.86	0.41
2:X:26:LEU:HD12	2:X:30:ILE:HB	2.02	0.41
1:K:89:ARG:HB3	1:K:182:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:59:TYR:CZ	3:R:85:LYS:HD3	2.57	0.40
3:Q:60:TYR:HB2	3:Q:86:PHE:CE1	2.56	0.40
1:E:146:SER:HB2	1:D:173:MET:HE2	2.03	0.40
1:A:192:ILE:H	1:A:192:ILE:HG13	1.56	0.40
1:D:51:ASP:HB3	1:D:190:SER:HB2	2.04	0.40
1:K:13:LYS:HG3	1:K:34:ILE:HG21	2.03	0.40
1:J:62:VAL:HG13	1:J:69:TYR:HD2	1.86	0.40
1:L:22:ALA:HB3	1:L:23:PRO:HD3	2.04	0.40
3:O:123:PHE:O	3:O:127:VAL:HG22	2.22	0.40
2:W:41:GLN:HG3	2:W:42:PHE:CD2	2.56	0.40
3:O:42:LEU:HD23	3:P:9:PHE:CZ	2.56	0.40
3:O:77:LYS:H	3:O:77:LYS:HD3	1.86	0.40
3:N:156:ASP:OD1	3:N:156:ASP:N	2.53	0.40
3:R:137:LEU:HB3	3:R:146:LEU:HD11	2.03	0.40
3:P:137:LEU:HB3	3:P:146:LEU:HD11	2.03	0.40
1:A:262:ILE:HD13	1:L:24:ILE:HD12	2.02	0.40
1:I:239:GLN:HE21	1:I:239:GLN:HB3	1.67	0.40
1:G:55:LYS:NZ	1:G:185:GLU:OE1	2.51	0.40
2:W:67:PRO:HG3	2:V:50:VAL:HG12	2.04	0.40
3:O:75:ASP:HB3	3:O:79:LYS:NZ	2.36	0.40
3:M:77:LYS:HD3	3:M:77:LYS:H	1.87	0.40
3:P:77:LYS:HD3	3:P:77:LYS:H	1.86	0.40
1:D:147:TYR:O	1:D:151:MET:HB2	2.22	0.40
1:D:192:ILE:H	1:D:192:ILE:HG13	1.56	0.40
1:H:17:LEU:O	1:H:21:GLY:N	2.55	0.40
1:J:147:TYR:O	1:J:151:MET:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/315 (77%)	231 (96%)	11 (4%)	0	100	100
1	B	242/315 (77%)	227 (94%)	15 (6%)	0	100	100
1	C	242/315 (77%)	226 (93%)	16 (7%)	0	100	100
1	D	242/315 (77%)	226 (93%)	16 (7%)	0	100	100
1	E	242/315 (77%)	230 (95%)	12 (5%)	0	100	100
1	F	242/315 (77%)	223 (92%)	19 (8%)	0	100	100
1	G	242/315 (77%)	231 (96%)	11 (4%)	0	100	100
1	H	242/315 (77%)	234 (97%)	8 (3%)	0	100	100
1	I	242/315 (77%)	230 (95%)	12 (5%)	0	100	100
1	J	242/315 (77%)	229 (95%)	13 (5%)	0	100	100
1	K	242/315 (77%)	229 (95%)	13 (5%)	0	100	100
1	L	242/315 (77%)	225 (93%)	17 (7%)	0	100	100
2	S	62/114 (54%)	61 (98%)	1 (2%)	0	100	100
2	T	62/114 (54%)	61 (98%)	1 (2%)	0	100	100
2	U	62/114 (54%)	61 (98%)	1 (2%)	0	100	100
2	V	62/114 (54%)	61 (98%)	1 (2%)	0	100	100
2	W	62/114 (54%)	61 (98%)	1 (2%)	0	100	100
2	X	62/114 (54%)	61 (98%)	1 (2%)	0	100	100
3	M	148/265 (56%)	139 (94%)	9 (6%)	0	100	100
3	N	148/265 (56%)	138 (93%)	10 (7%)	0	100	100
3	O	148/265 (56%)	140 (95%)	8 (5%)	0	100	100
3	P	148/265 (56%)	138 (93%)	8 (5%)	2 (1%)	9	30
3	Q	148/265 (56%)	139 (94%)	9 (6%)	0	100	100
3	R	148/265 (56%)	140 (95%)	8 (5%)	0	100	100
All	All	4164/6054 (69%)	3941 (95%)	221 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	P	73	GLY
3	P	71	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	208/266 (78%)	203 (98%)	5 (2%)	43	77
1	B	208/266 (78%)	202 (97%)	6 (3%)	37	73
1	C	208/266 (78%)	204 (98%)	4 (2%)	50	81
1	D	208/266 (78%)	204 (98%)	4 (2%)	50	81
1	E	208/266 (78%)	201 (97%)	7 (3%)	32	68
1	F	208/266 (78%)	201 (97%)	7 (3%)	32	68
1	G	208/266 (78%)	202 (97%)	6 (3%)	37	73
1	H	208/266 (78%)	200 (96%)	8 (4%)	29	64
1	I	208/266 (78%)	202 (97%)	6 (3%)	37	73
1	J	208/266 (78%)	200 (96%)	8 (4%)	29	64
1	K	208/266 (78%)	204 (98%)	4 (2%)	50	81
1	L	208/266 (78%)	202 (97%)	6 (3%)	37	73
2	S	60/100 (60%)	60 (100%)	0	100	100
2	T	60/100 (60%)	60 (100%)	0	100	100
2	U	60/100 (60%)	60 (100%)	0	100	100
2	V	60/100 (60%)	60 (100%)	0	100	100
2	W	60/100 (60%)	60 (100%)	0	100	100
2	X	60/100 (60%)	60 (100%)	0	100	100
3	M	133/237 (56%)	131 (98%)	2 (2%)	57	84
3	N	133/237 (56%)	128 (96%)	5 (4%)	29	64
3	O	133/237 (56%)	130 (98%)	3 (2%)	44	78
3	P	133/237 (56%)	125 (94%)	8 (6%)	17	47
3	Q	133/237 (56%)	129 (97%)	4 (3%)	36	72
3	R	133/237 (56%)	130 (98%)	3 (2%)	44	78
All	All	3654/5214 (70%)	3558 (97%)	96 (3%)	41	75

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	49	HIS
1	C	62	VAL
1	C	70	LYS
1	C	144	LEU
1	I	4	TYR
1	I	62	VAL
1	I	85	THR
1	I	158	ILE
1	I	192	ILE
1	I	271	LEU
1	G	28	GLU
1	G	62	VAL
1	G	71	THR
1	G	85	THR
1	G	158	ILE
1	G	192	ILE
3	O	61	VAL
3	O	80	PHE
3	O	124	LYS
3	N	61	VAL
3	N	69	ASP
3	N	71	ILE
3	N	72	PHE
3	N	80	PHE
3	M	61	VAL
3	M	80	PHE
3	R	61	VAL
3	R	80	PHE
3	R	159	TYR
3	Q	13	GLU
3	Q	61	VAL
3	Q	80	PHE
3	Q	163	GLN
3	P	61	VAL
3	P	67	SER
3	P	69	ASP
3	P	70	LEU
3	P	71	ILE
3	P	80	PHE
3	P	130	LYS
3	P	163	GLN
1	E	28	GLU
1	E	62	VAL

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Mol	Chain	Res	Type
1	E	71	THR
1	E	84	VAL
1	E	144	LEU
1	E	158	ILE
1	E	192	ILE
1	A	28	GLU
1	A	62	VAL
1	A	71	THR
1	A	158	ILE
1	A	192	ILE
1	B	62	VAL
1	B	71	THR
1	B	144	LEU
1	B	158	ILE
1	B	192	ILE
1	B	271	LEU
1	D	62	VAL
1	D	71	THR
1	D	158	ILE
1	D	192	ILE
1	F	4	TYR
1	F	49	HIS
1	F	62	VAL
1	F	71	THR
1	F	127	ARG
1	F	144	LEU
1	F	192	ILE
1	H	85	THR
1	H	127	ARG
1	H	138	LEU
1	H	144	LEU
1	H	167	ASN
1	H	178	LYS
1	H	192	ILE
1	H	271	LEU
1	J	49	HIS
1	J	62	VAL
1	J	71	THR
1	J	127	ARG
1	J	138	LEU
1	J	144	LEU
1	J	158	ILE

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Mol	Chain	Res	Type
1	J	192	ILE
1	K	62	VAL
1	K	144	LEU
1	K	158	ILE
1	K	192	ILE
1	L	4	TYR
1	L	49	HIS
1	L	62	VAL
1	L	144	LEU
1	L	158	ILE
1	L	192	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	39	GLN
1	C	175	ASN
1	C	239	GLN
1	C	267	GLN
1	I	39	GLN
1	I	169	GLN
1	I	239	GLN
1	I	267	GLN
1	G	91	ASN
1	G	169	GLN
1	G	239	GLN
1	G	267	GLN
2	T	5	GLN
2	T	33	GLN
2	S	5	GLN
2	S	33	GLN
2	X	5	GLN
2	X	33	GLN
2	X	35	GLN
2	W	5	GLN
2	W	33	GLN
2	W	35	GLN
2	V	5	GLN
2	V	35	GLN
2	U	5	GLN
2	U	33	GLN
3	O	28	ASN

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Mol	Chain	Res	Type
3	O	34	ASN
3	O	40	GLN
3	O	119	ASN
3	O	163	GLN
3	N	34	ASN
3	N	40	GLN
3	M	14	ASN
3	M	28	ASN
3	M	34	ASN
3	M	40	GLN
3	R	34	ASN
3	R	163	GLN
3	Q	34	ASN
3	Q	119	ASN
3	Q	163	GLN
3	P	28	ASN
3	P	34	ASN
3	P	40	GLN
3	P	163	GLN
1	E	91	ASN
1	E	167	ASN
1	E	175	ASN
1	E	239	GLN
1	E	267	GLN
1	A	8	ASN
1	A	26	ASN
1	A	91	ASN
1	A	267	GLN
1	B	8	ASN
1	B	33	GLN
1	B	126	ASN
1	B	169	GLN
1	B	175	ASN
1	B	239	GLN
1	B	243	ASN
1	B	259	ASN
1	B	266	HIS
1	B	267	GLN
1	D	8	ASN
1	D	33	GLN
1	D	39	GLN
1	D	169	GLN

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Mol	Chain	Res	Type
1	D	175	ASN
1	D	239	GLN
1	D	243	ASN
1	D	266	HIS
1	D	267	GLN
1	F	8	ASN
1	F	33	GLN
1	F	39	GLN
1	F	126	ASN
1	F	169	GLN
1	F	175	ASN
1	F	239	GLN
1	F	266	HIS
1	F	267	GLN
1	H	5	ASN
1	H	7	GLN
1	H	8	ASN
1	H	33	GLN
1	H	39	GLN
1	H	175	ASN
1	H	239	GLN
1	H	266	HIS
1	H	267	GLN
1	J	8	ASN
1	J	33	GLN
1	J	39	GLN
1	J	169	GLN
1	J	175	ASN
1	J	243	ASN
1	J	266	HIS
1	J	267	GLN
1	K	8	ASN
1	K	239	GLN
1	K	267	GLN
1	L	7	GLN
1	L	8	ASN
1	L	33	GLN
1	L	126	ASN
1	L	169	GLN
1	L	175	ASN
1	L	239	GLN
1	L	266	HIS

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Mol	Chain	Res	Type
1	L	267	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.

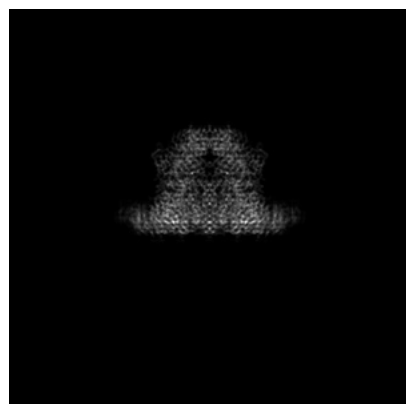
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63388. These allow visual inspection of the internal detail of the map and identification of artifacts.

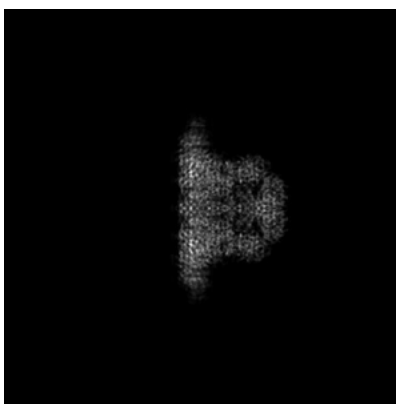
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

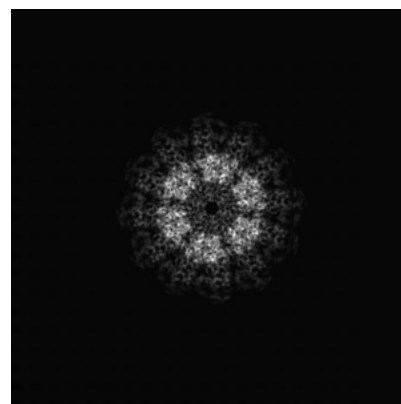
6.1.1 Primary map



X

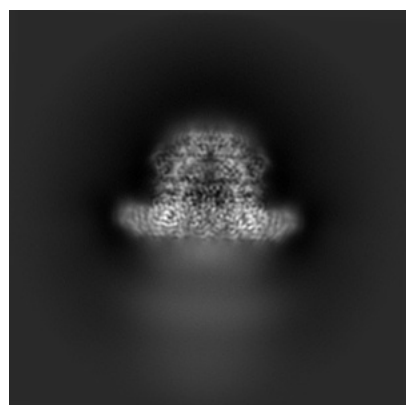


Y

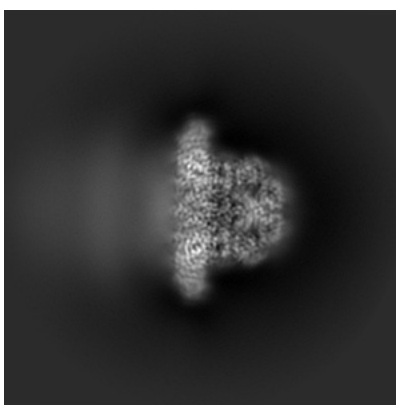


Z

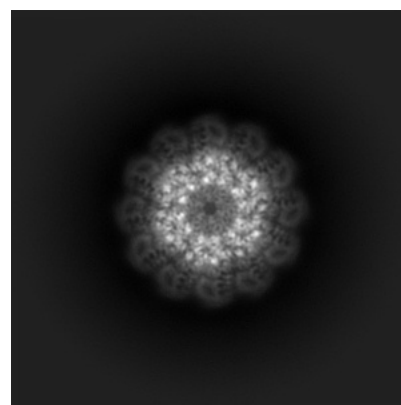
6.1.2 Raw map



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: 160

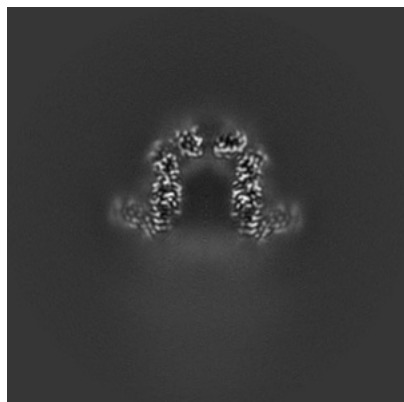


Y Index: 160

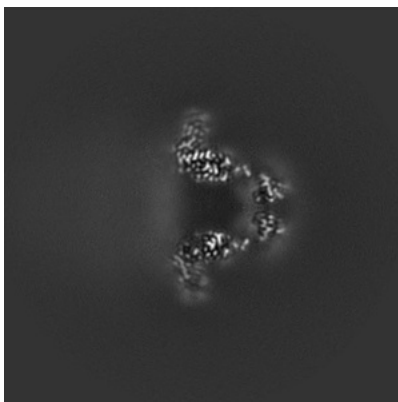


Z Index: 160

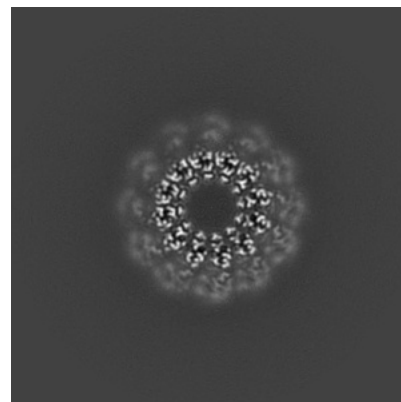
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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

6.3 Largest variance slices [i](#)

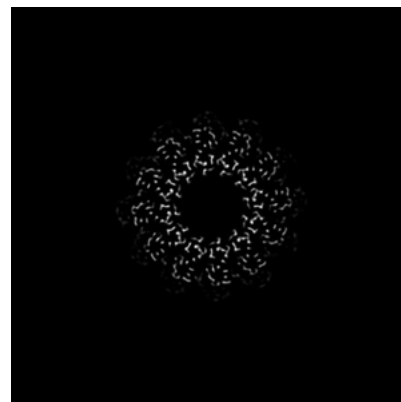
6.3.1 Primary map



X Index: 182

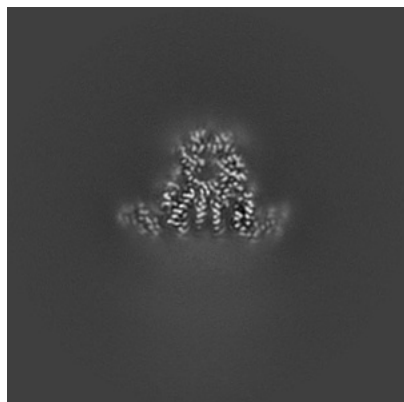


Y Index: 182

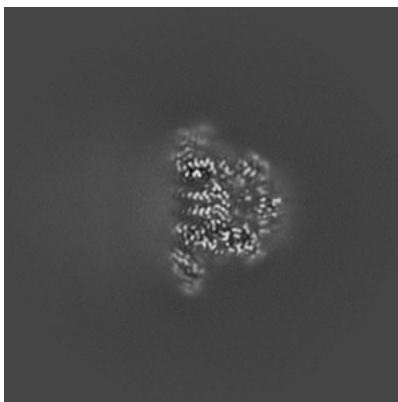


Z Index: 149

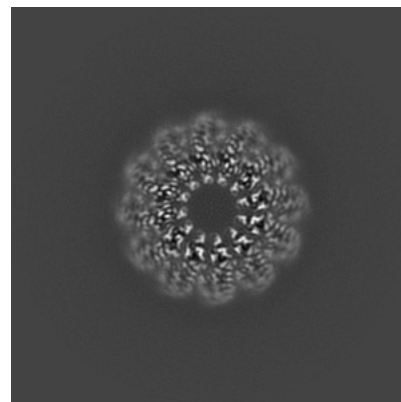
6.3.2 Raw map



X Index: 136



Y Index: 182

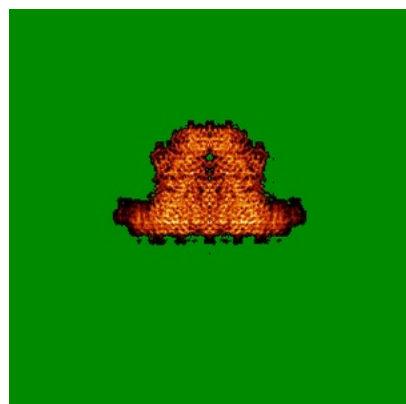


Z Index: 153

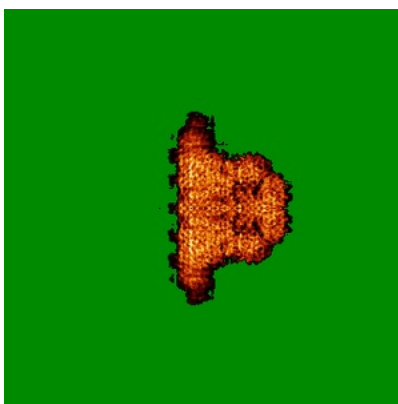
The images above show the largest variance slices of the map in three orthogonal directions.

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

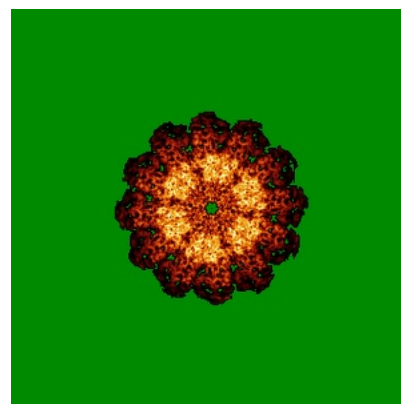
6.4.1 Primary map



X



Y

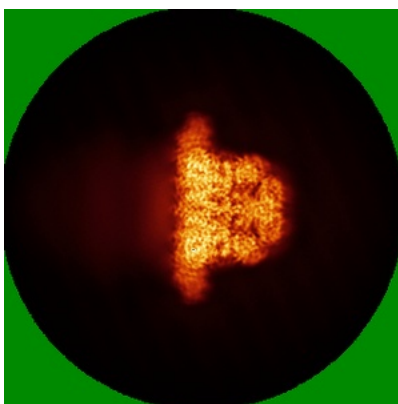


Z

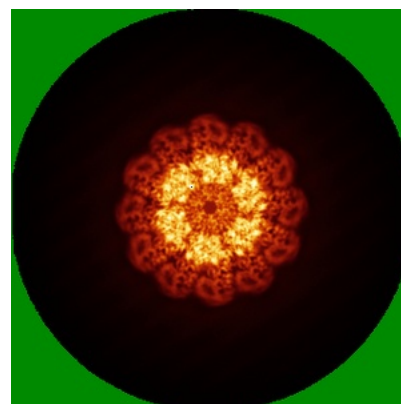
6.4.2 Raw map



X



Y

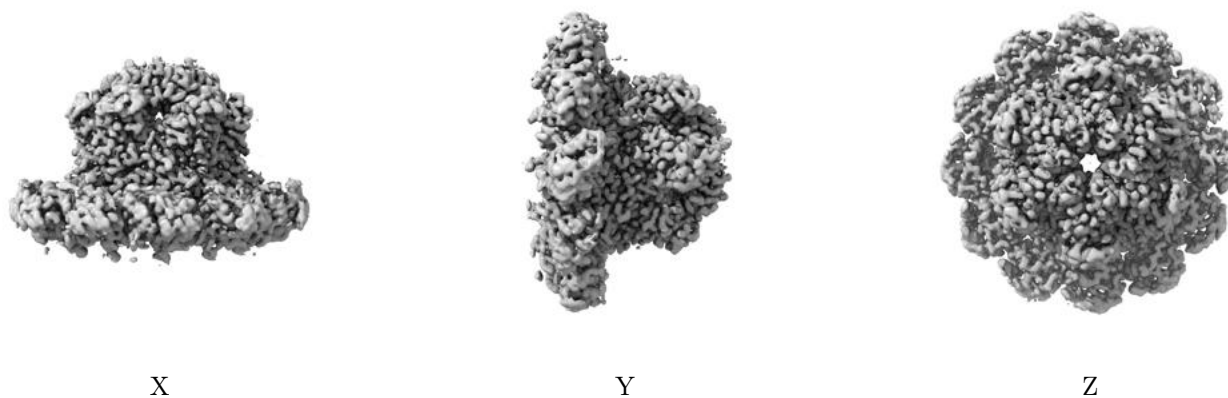


Z

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.

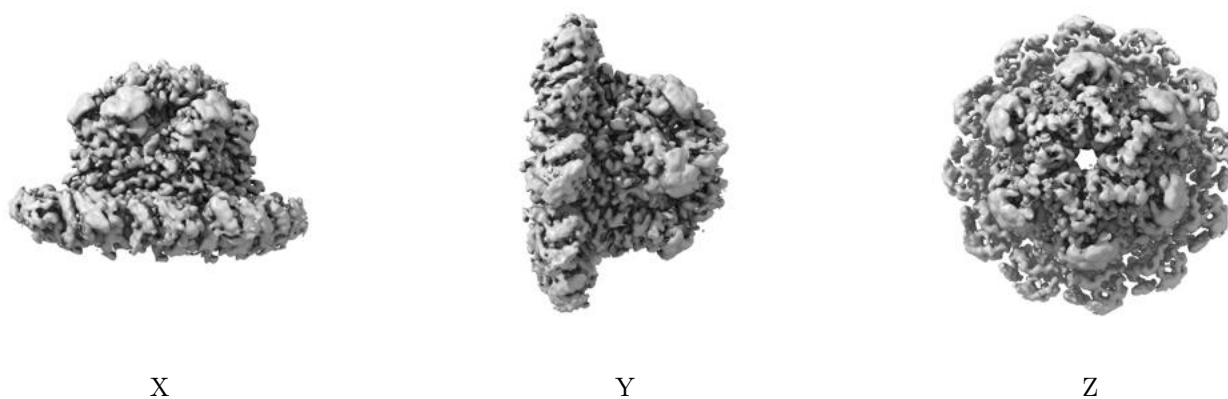
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0109. 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



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.

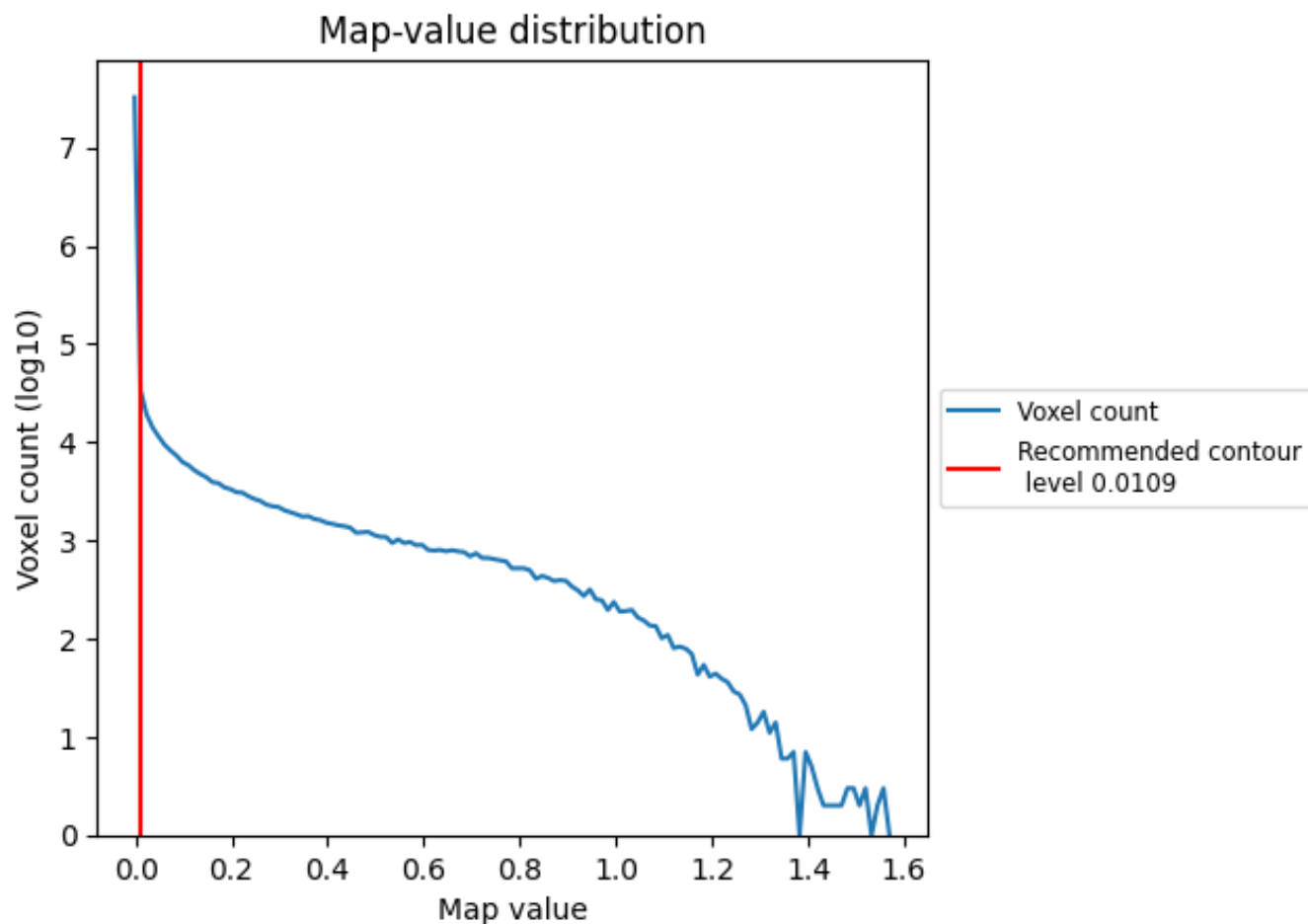
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

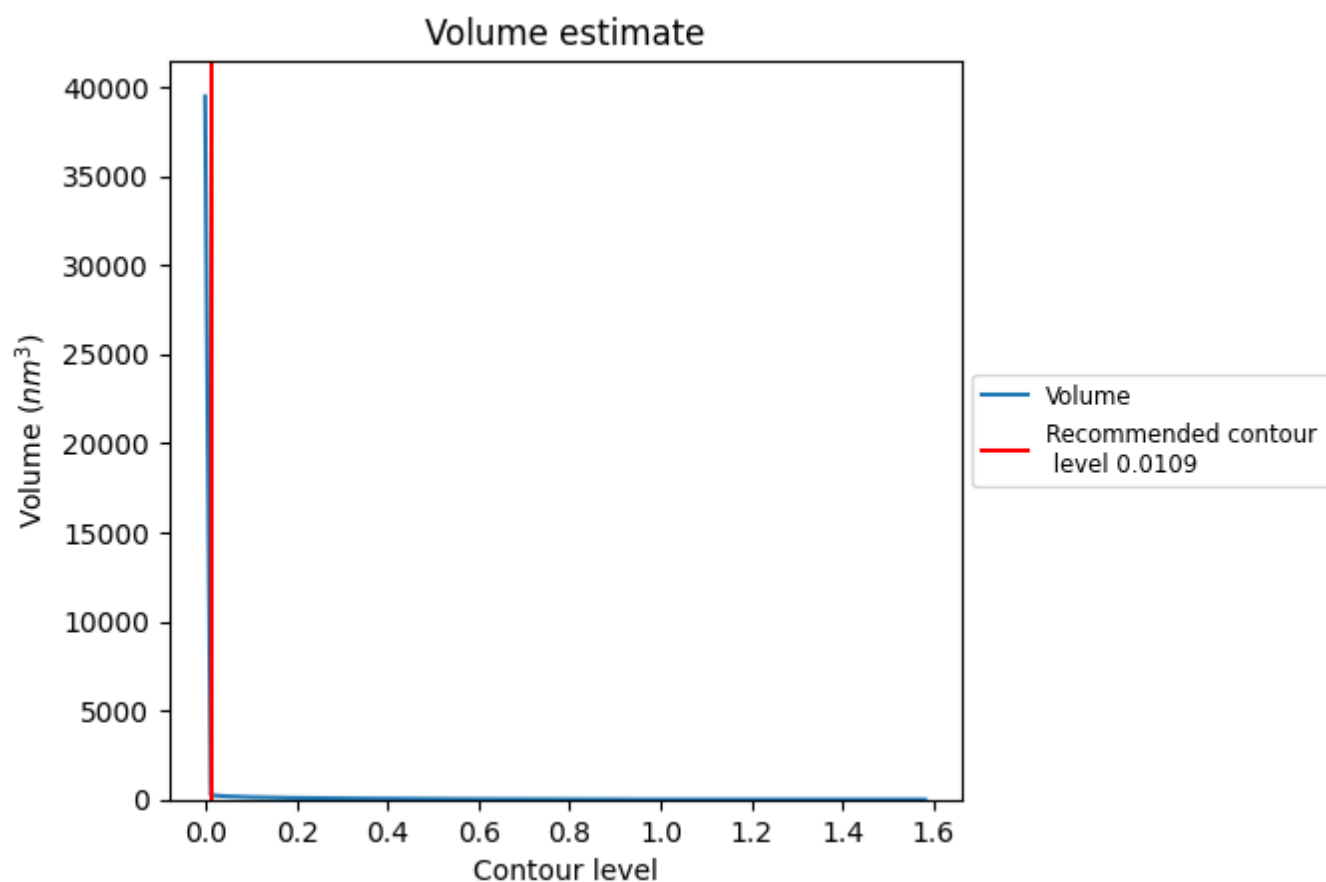
This section contains the results of statistical analysis of the map.

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.

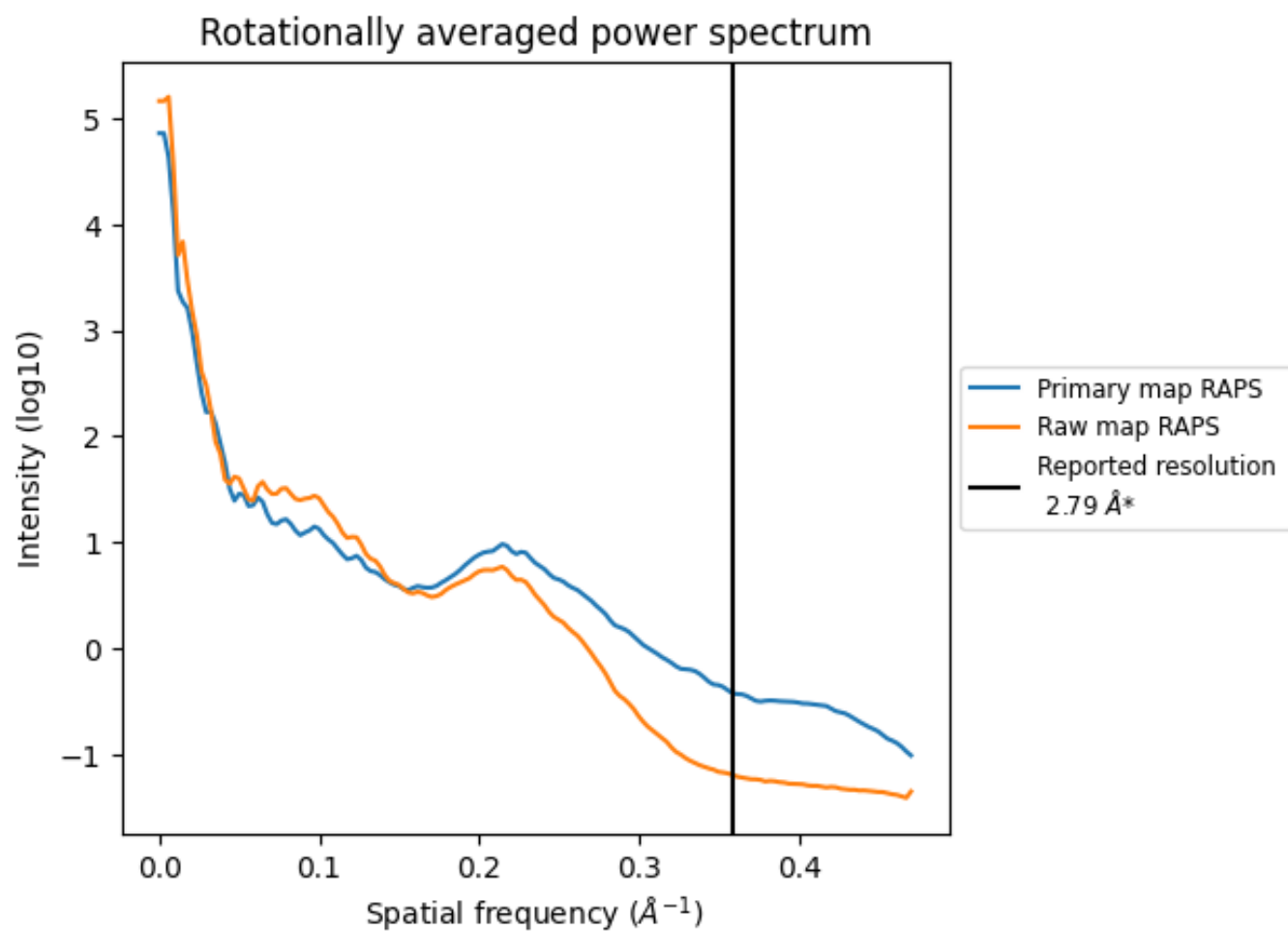
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 261 nm³; this corresponds to an approximate mass of 236 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 ⓘ

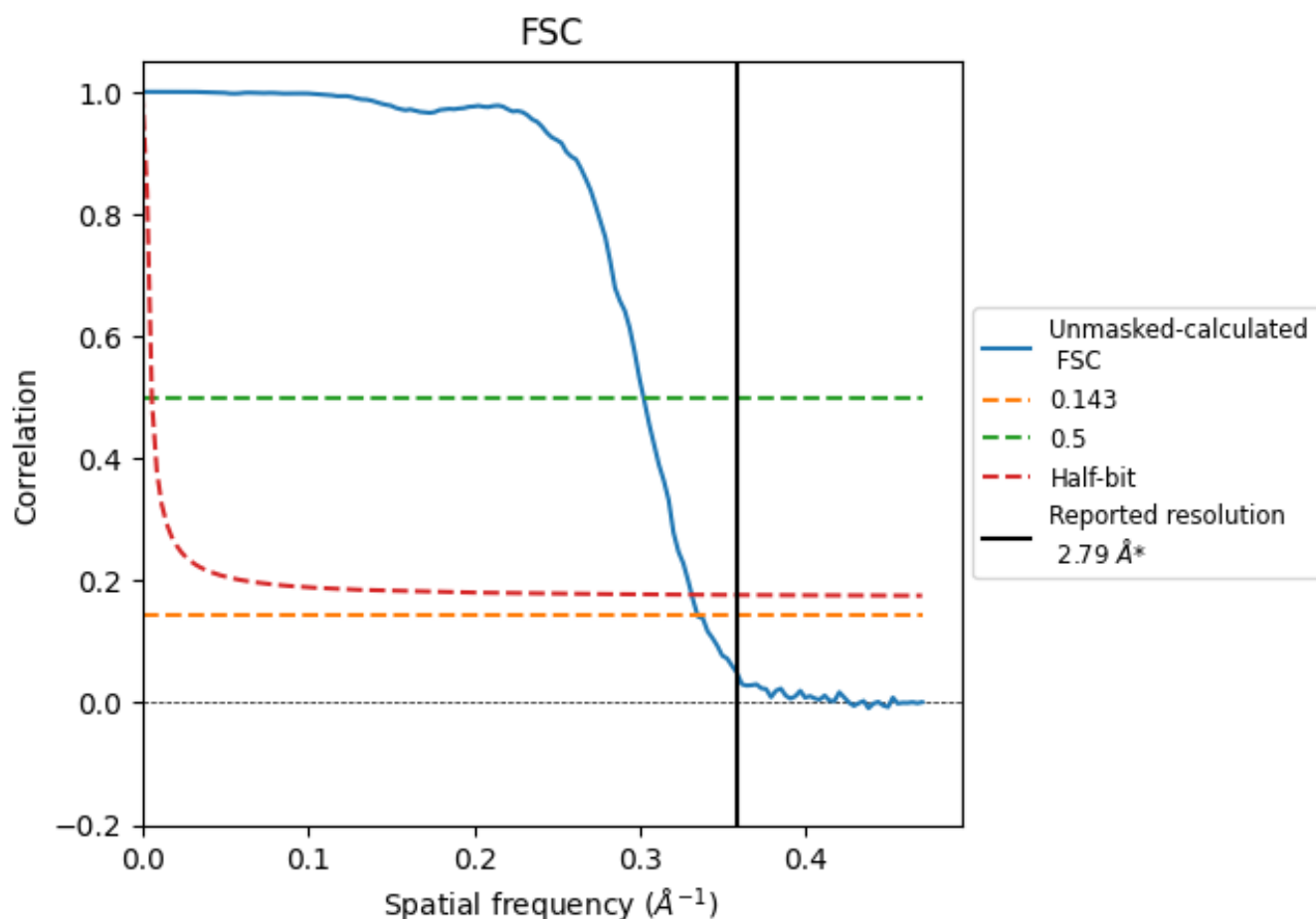


*Reported resolution corresponds to spatial frequency of 0.358 Å⁻¹

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 0.358 Å⁻¹

8.2 Resolution estimates [i](#)

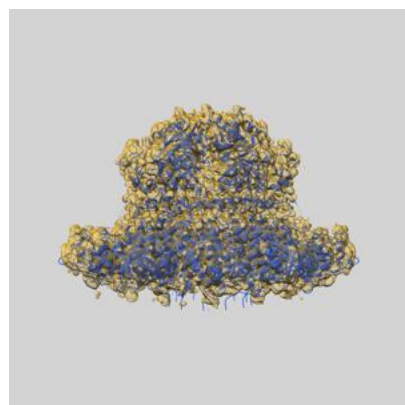
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.99	3.31	3.02

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

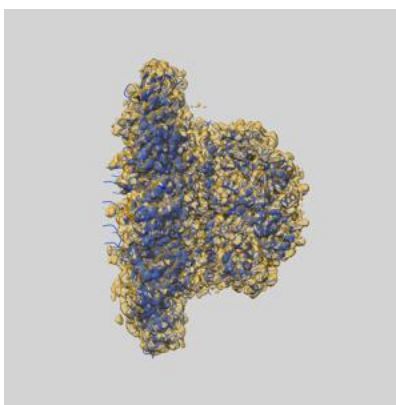
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63388 and PDB model 9LU5. Per-residue inclusion information can be found in section [3](#) on page [11](#).

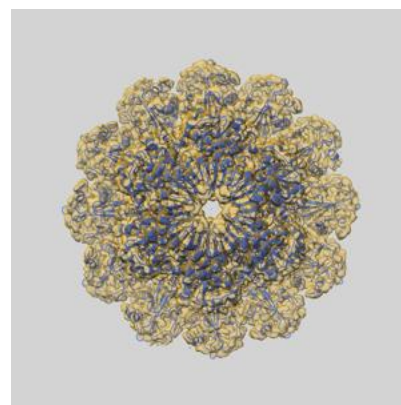
9.1 Map-model overlay [i](#)



X



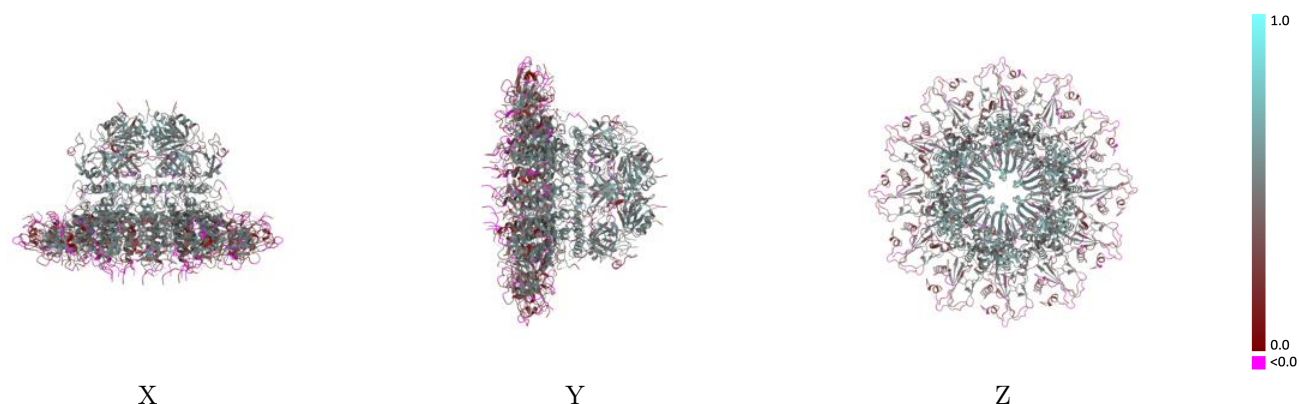
Y



Z

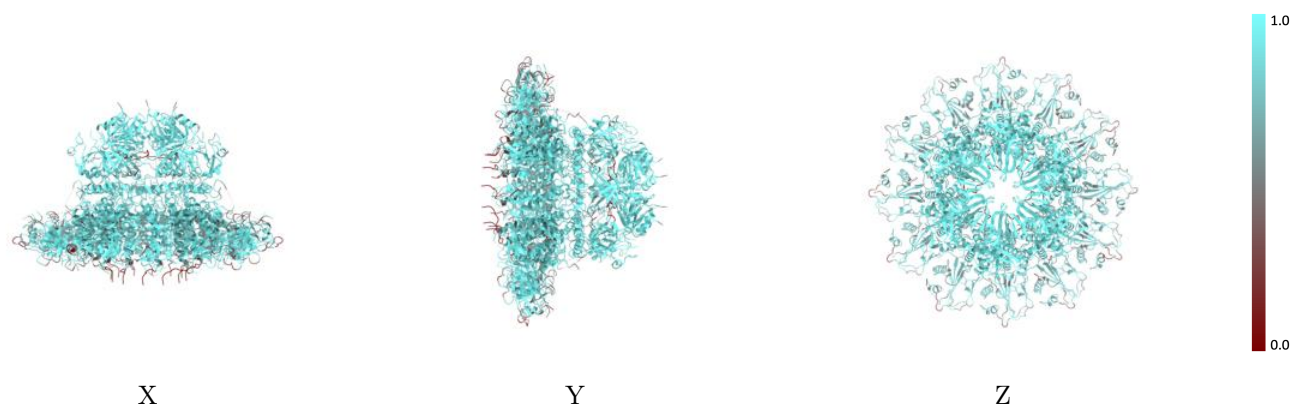
The images above show the 3D surface view of the map at the recommended contour level 0.0109 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



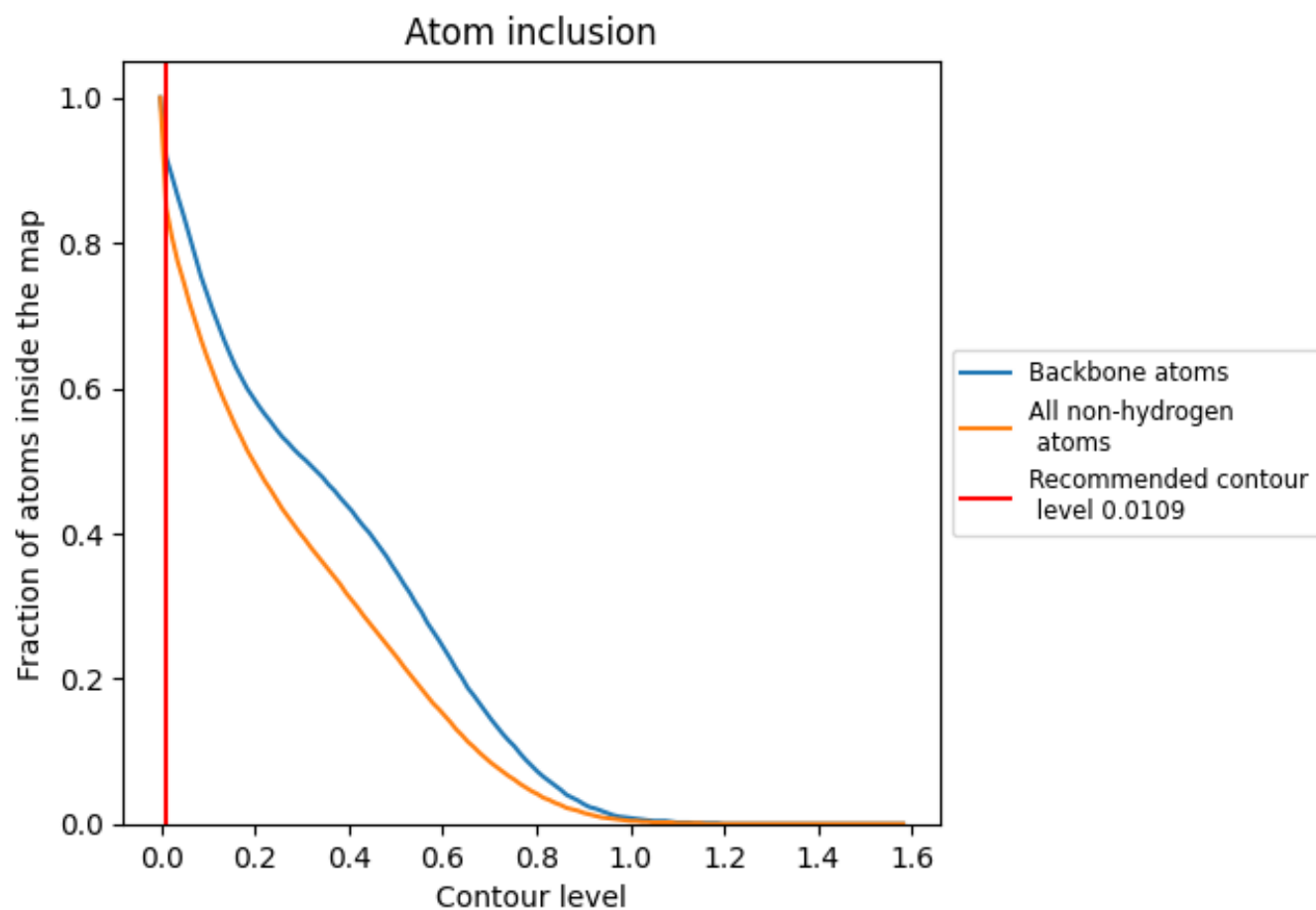
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0109).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 85% 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 (0.0109) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8480	 0.4040
A	 0.8410	 0.3860
B	 0.8380	 0.3840
C	 0.8380	 0.3730
D	 0.8290	 0.3870
E	 0.8380	 0.3770
F	 0.8300	 0.3760
G	 0.8140	 0.3740
H	 0.8350	 0.3990
I	 0.8050	 0.3670
J	 0.8230	 0.3870
K	 0.8410	 0.3760
L	 0.8340	 0.3860
M	 0.8600	 0.4390
N	 0.8660	 0.4440
O	 0.8650	 0.4370
P	 0.8540	 0.4320
Q	 0.8620	 0.4240
R	 0.8590	 0.4280
S	 0.9540	 0.5080
T	 0.9540	 0.5100
U	 0.9580	 0.5140
V	 0.9580	 0.5160
W	 0.9540	 0.5120
X	 0.9580	 0.5180

