



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 10:38 PM UTC

PDB ID : 9LU6 / pdb_00009lu6
EMDB ID : EMD-63389
Title : Structure of bacteriophage T4 protal-neck protein gp20-gp13-gp14-Hfq assembled in vitro in C6 symmetry
Authors : Han, L.; Mao, Q.; Sun, L.
Deposited on : 2025-02-07
Resolution : 2.91 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

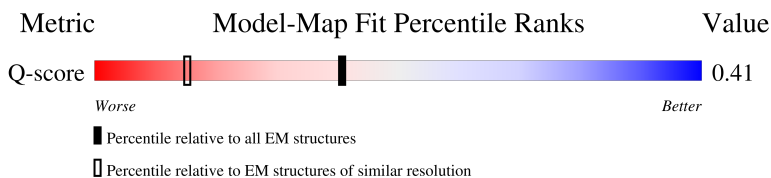
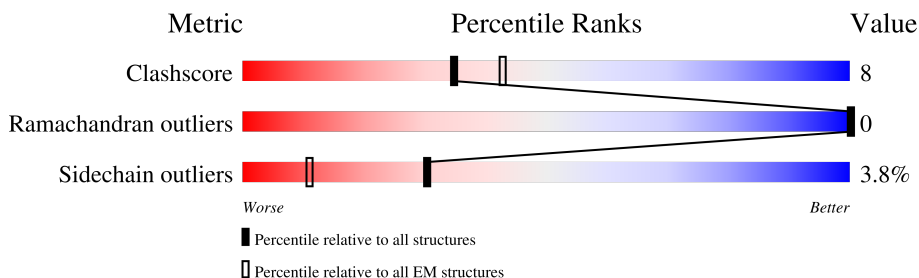
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 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.









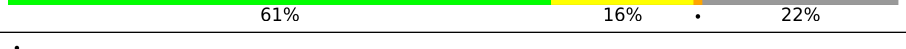
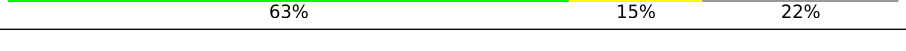
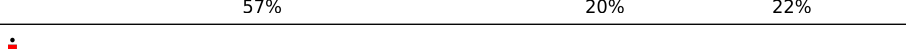
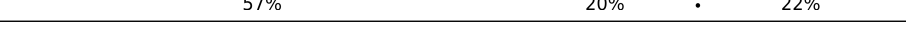
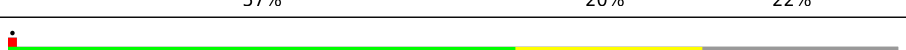

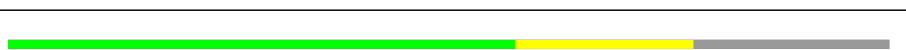

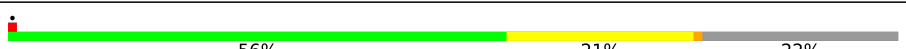




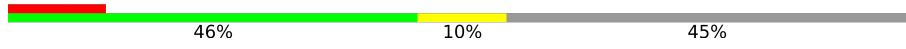
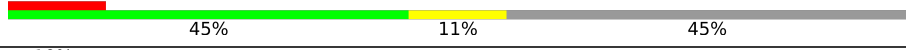
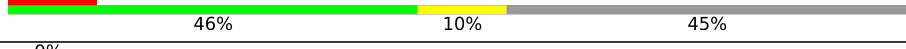
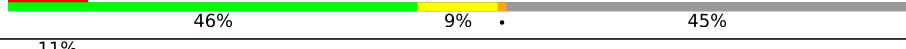
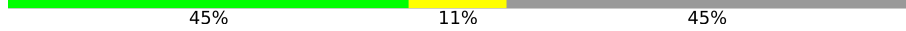

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12972 (2.41 - 3.41)

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	
1	B	315	
1	C	315	
1	D	315	

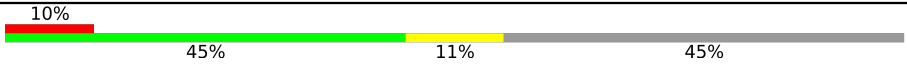

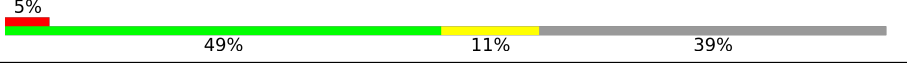
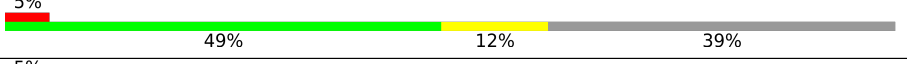
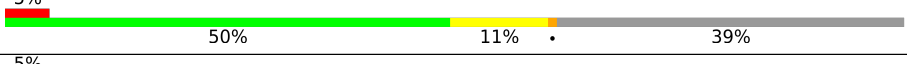
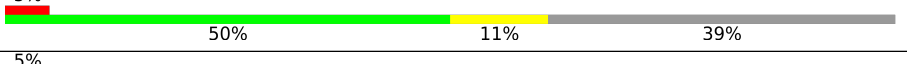

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Mol	Chain	Length	Quality of chain
1	E	315	
1	F	315	
1	G	315	
1	H	315	
1	I	315	
1	J	315	
1	K	315	
1	L	315	
2	a	533	
2	b	533	
2	c	533	
2	d	533	
2	e	533	
2	f	533	
2	g	533	
2	h	533	
2	i	533	
2	j	533	
2	k	533	
2	l	533	
3	S	114	
3	T	114	
3	U	114	
3	V	114	
3	W	114	

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Mol	Chain	Length	Quality of chain
3	X	114	
4	M	265	
4	N	265	
4	O	265	
4	P	265	
4	Q	265	
4	R	265	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 75102 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	B	246	Total 1977	C 1273	N 330	O 363	S 11	0	0
1	L	246	Total 1977	C 1273	N 330	O 363	S 11	0	0
1	A	246	Total 1977	C 1273	N 330	O 363	S 11	0	0
1	C	246	Total 1977	C 1273	N 330	O 363	S 11	0	0
1	D	246	Total 1977	C 1273	N 330	O 363	S 11	0	0
1	E	246	Total 1977	C 1273	N 330	O 363	S 11	0	0
1	F	246	Total 1977	C 1273	N 330	O 363	S 11	0	0
1	G	246	Total 1977	C 1273	N 330	O 363	S 11	0	0
1	H	246	Total 1977	C 1273	N 330	O 363	S 11	0	0
1	I	246	Total 1977	C 1273	N 330	O 363	S 11	0	0
1	J	246	Total 1977	C 1273	N 330	O 363	S 11	0	0
1	K	246	Total 1977	C 1273	N 330	O 363	S 11	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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
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
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
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

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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
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
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

- Molecule 2 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	l	415	Total	C	N	O	S	0	0
			3385	2138	593	635	19		
2	k	415	Total	C	N	O	S	0	0
			3385	2138	593	635	19		
2	j	415	Total	C	N	O	S	0	0
			3385	2138	593	635	19		
2	i	415	Total	C	N	O	S	0	0
			3385	2138	593	635	19		
2	h	415	Total	C	N	O	S	0	0
			3385	2138	593	635	19		
2	g	415	Total	C	N	O	S	0	0
			3385	2138	593	635	19		
2	f	415	Total	C	N	O	S	0	0
			3385	2138	593	635	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	e	415	Total	C	N	O	S	0	0
			3385	2138	593	635	19		
2	d	415	Total	C	N	O	S	0	0
			3385	2138	593	635	19		
2	c	415	Total	C	N	O	S	0	0
			3385	2138	593	635	19		
2	b	415	Total	C	N	O	S	0	0
			3385	2138	593	635	19		
2	a	415	Total	C	N	O	S	0	0
			3385	2138	593	635	19		

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	525	SER	-	expression tag	UNP A0A7S9SW10
l	526	SER	-	expression tag	UNP A0A7S9SW10
l	527	GLY	-	expression tag	UNP A0A7S9SW10
l	528	HIS	-	expression tag	UNP A0A7S9SW10
l	529	HIS	-	expression tag	UNP A0A7S9SW10
l	530	HIS	-	expression tag	UNP A0A7S9SW10
l	531	HIS	-	expression tag	UNP A0A7S9SW10
l	532	HIS	-	expression tag	UNP A0A7S9SW10
l	533	HIS	-	expression tag	UNP A0A7S9SW10
k	525	SER	-	expression tag	UNP A0A7S9SW10
k	526	SER	-	expression tag	UNP A0A7S9SW10
k	527	GLY	-	expression tag	UNP A0A7S9SW10
k	528	HIS	-	expression tag	UNP A0A7S9SW10
k	529	HIS	-	expression tag	UNP A0A7S9SW10
k	530	HIS	-	expression tag	UNP A0A7S9SW10
k	531	HIS	-	expression tag	UNP A0A7S9SW10
k	532	HIS	-	expression tag	UNP A0A7S9SW10
k	533	HIS	-	expression tag	UNP A0A7S9SW10
j	525	SER	-	expression tag	UNP A0A7S9SW10
j	526	SER	-	expression tag	UNP A0A7S9SW10
j	527	GLY	-	expression tag	UNP A0A7S9SW10
j	528	HIS	-	expression tag	UNP A0A7S9SW10
j	529	HIS	-	expression tag	UNP A0A7S9SW10
j	530	HIS	-	expression tag	UNP A0A7S9SW10
j	531	HIS	-	expression tag	UNP A0A7S9SW10
j	532	HIS	-	expression tag	UNP A0A7S9SW10
j	533	HIS	-	expression tag	UNP A0A7S9SW10
i	525	SER	-	expression tag	UNP A0A7S9SW10
i	526	SER	-	expression tag	UNP A0A7S9SW10

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Chain	Residue	Modelled	Actual	Comment	Reference
i	527	GLY	-	expression tag	UNP A0A7S9SW10
i	528	HIS	-	expression tag	UNP A0A7S9SW10
i	529	HIS	-	expression tag	UNP A0A7S9SW10
i	530	HIS	-	expression tag	UNP A0A7S9SW10
i	531	HIS	-	expression tag	UNP A0A7S9SW10
i	532	HIS	-	expression tag	UNP A0A7S9SW10
i	533	HIS	-	expression tag	UNP A0A7S9SW10
h	525	SER	-	expression tag	UNP A0A7S9SW10
h	526	SER	-	expression tag	UNP A0A7S9SW10
h	527	GLY	-	expression tag	UNP A0A7S9SW10
h	528	HIS	-	expression tag	UNP A0A7S9SW10
h	529	HIS	-	expression tag	UNP A0A7S9SW10
h	530	HIS	-	expression tag	UNP A0A7S9SW10
h	531	HIS	-	expression tag	UNP A0A7S9SW10
h	532	HIS	-	expression tag	UNP A0A7S9SW10
h	533	HIS	-	expression tag	UNP A0A7S9SW10
g	525	SER	-	expression tag	UNP A0A7S9SW10
g	526	SER	-	expression tag	UNP A0A7S9SW10
g	527	GLY	-	expression tag	UNP A0A7S9SW10
g	528	HIS	-	expression tag	UNP A0A7S9SW10
g	529	HIS	-	expression tag	UNP A0A7S9SW10
g	530	HIS	-	expression tag	UNP A0A7S9SW10
g	531	HIS	-	expression tag	UNP A0A7S9SW10
g	532	HIS	-	expression tag	UNP A0A7S9SW10
g	533	HIS	-	expression tag	UNP A0A7S9SW10
f	525	SER	-	expression tag	UNP A0A7S9SW10
f	526	SER	-	expression tag	UNP A0A7S9SW10
f	527	GLY	-	expression tag	UNP A0A7S9SW10
f	528	HIS	-	expression tag	UNP A0A7S9SW10
f	529	HIS	-	expression tag	UNP A0A7S9SW10
f	530	HIS	-	expression tag	UNP A0A7S9SW10
f	531	HIS	-	expression tag	UNP A0A7S9SW10
f	532	HIS	-	expression tag	UNP A0A7S9SW10
f	533	HIS	-	expression tag	UNP A0A7S9SW10
e	525	SER	-	expression tag	UNP A0A7S9SW10
e	526	SER	-	expression tag	UNP A0A7S9SW10
e	527	GLY	-	expression tag	UNP A0A7S9SW10
e	528	HIS	-	expression tag	UNP A0A7S9SW10
e	529	HIS	-	expression tag	UNP A0A7S9SW10
e	530	HIS	-	expression tag	UNP A0A7S9SW10
e	531	HIS	-	expression tag	UNP A0A7S9SW10
e	532	HIS	-	expression tag	UNP A0A7S9SW10

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Chain	Residue	Modelled	Actual	Comment	Reference
e	533	HIS	-	expression tag	UNP A0A7S9SW10
d	525	SER	-	expression tag	UNP A0A7S9SW10
d	526	SER	-	expression tag	UNP A0A7S9SW10
d	527	GLY	-	expression tag	UNP A0A7S9SW10
d	528	HIS	-	expression tag	UNP A0A7S9SW10
d	529	HIS	-	expression tag	UNP A0A7S9SW10
d	530	HIS	-	expression tag	UNP A0A7S9SW10
d	531	HIS	-	expression tag	UNP A0A7S9SW10
d	532	HIS	-	expression tag	UNP A0A7S9SW10
d	533	HIS	-	expression tag	UNP A0A7S9SW10
c	525	SER	-	expression tag	UNP A0A7S9SW10
c	526	SER	-	expression tag	UNP A0A7S9SW10
c	527	GLY	-	expression tag	UNP A0A7S9SW10
c	528	HIS	-	expression tag	UNP A0A7S9SW10
c	529	HIS	-	expression tag	UNP A0A7S9SW10
c	530	HIS	-	expression tag	UNP A0A7S9SW10
c	531	HIS	-	expression tag	UNP A0A7S9SW10
c	532	HIS	-	expression tag	UNP A0A7S9SW10
c	533	HIS	-	expression tag	UNP A0A7S9SW10
b	525	SER	-	expression tag	UNP A0A7S9SW10
b	526	SER	-	expression tag	UNP A0A7S9SW10
b	527	GLY	-	expression tag	UNP A0A7S9SW10
b	528	HIS	-	expression tag	UNP A0A7S9SW10
b	529	HIS	-	expression tag	UNP A0A7S9SW10
b	530	HIS	-	expression tag	UNP A0A7S9SW10
b	531	HIS	-	expression tag	UNP A0A7S9SW10
b	532	HIS	-	expression tag	UNP A0A7S9SW10
b	533	HIS	-	expression tag	UNP A0A7S9SW10
a	525	SER	-	expression tag	UNP A0A7S9SW10
a	526	SER	-	expression tag	UNP A0A7S9SW10
a	527	GLY	-	expression tag	UNP A0A7S9SW10
a	528	HIS	-	expression tag	UNP A0A7S9SW10
a	529	HIS	-	expression tag	UNP A0A7S9SW10
a	530	HIS	-	expression tag	UNP A0A7S9SW10
a	531	HIS	-	expression tag	UNP A0A7S9SW10
a	532	HIS	-	expression tag	UNP A0A7S9SW10
a	533	HIS	-	expression tag	UNP A0A7S9SW10

- Molecule 3 is a protein called RNA-binding protein Hfq.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	X	63	Total	C	N	O	S	0	0
			504	326	88	89	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	63	Total	C	N	O	S	0	0
			504	326	88	89	1		
3	V	63	Total	C	N	O	S	0	0
			504	326	88	89	1		
3	U	63	Total	C	N	O	S	0	0
			504	326	88	89	1		
3	T	63	Total	C	N	O	S	0	0
			504	326	88	89	1		
3	S	63	Total	C	N	O	S	0	0
			504	326	88	89	1		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
S	0	SER	-	expression tag	UNP A7ZV41

- Molecule 4 is a protein called Neck protein gp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	162	Total	C	N	O	S	0	0
			1289	832	212	242	3		
4	M	162	Total	C	N	O	S	0	0
			1289	832	212	242	3		
4	O	162	Total	C	N	O	S	0	0
			1289	832	212	242	3		
4	P	162	Total	C	N	O	S	0	0
			1289	832	212	242	3		
4	Q	162	Total	C	N	O	S	0	0
			1289	832	212	242	3		
4	R	162	Total	C	N	O	S	0	0
			1289	832	212	242	3		

There are 54 discrepancies between the modelled and reference sequences:

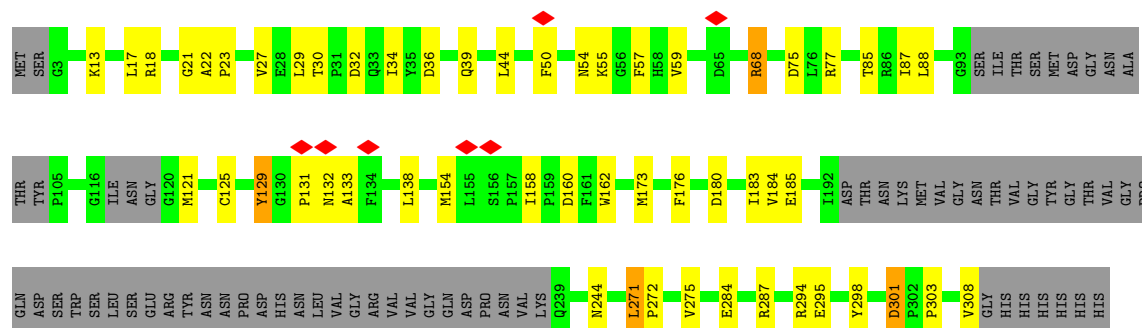
Chain	Residue	Modelled	Actual	Comment	Reference
N	-8	HIS	-	expression tag	UNP P11111
N	-7	HIS	-	expression tag	UNP P11111
N	-6	HIS	-	expression tag	UNP P11111
N	-5	HIS	-	expression tag	UNP P11111
N	-4	HIS	-	expression tag	UNP P11111
N	-3	HIS	-	expression tag	UNP P11111
N	-2	SER	-	expression tag	UNP P11111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

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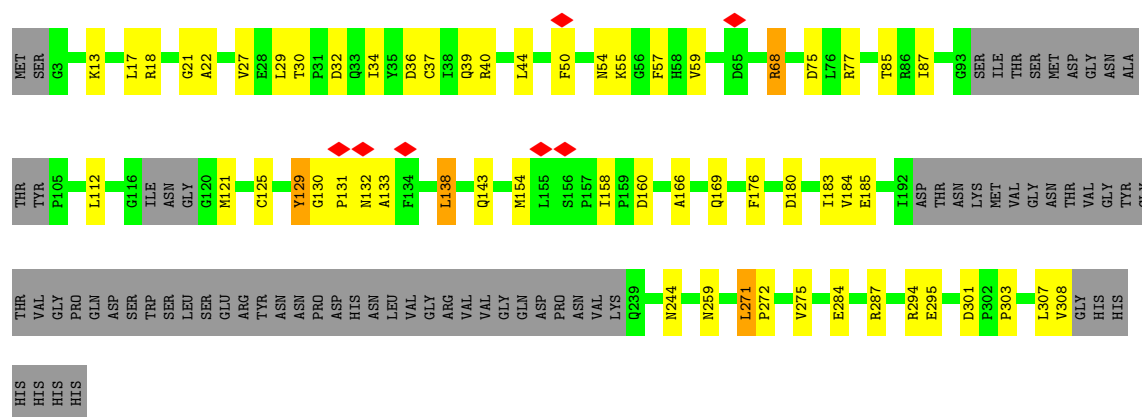
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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

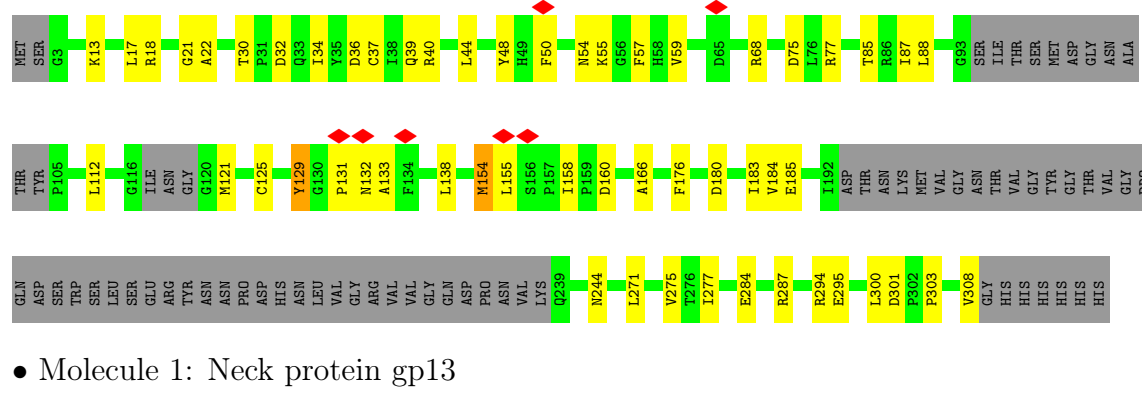




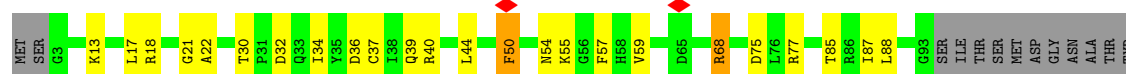
• Molecule 1: Neck protein gp13

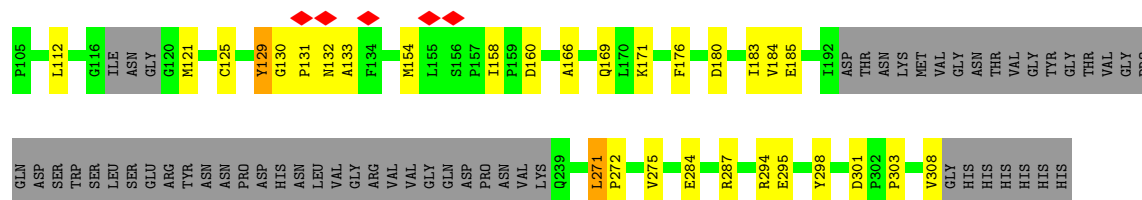


• Molecule 1: Neck protein gp13

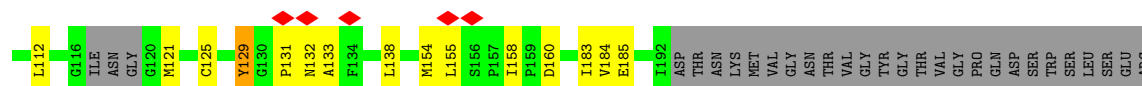
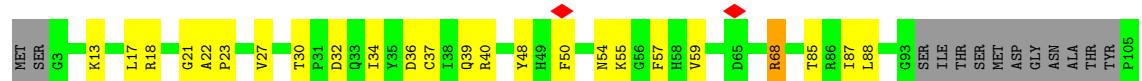


• Molecule 1: Neck protein gp13

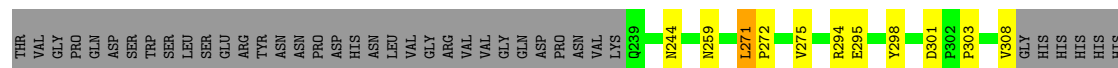
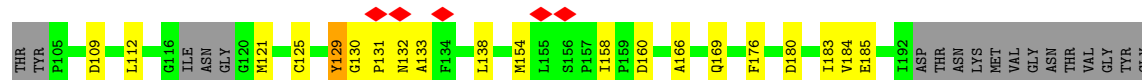




• Molecule 1: Neck protein gp13

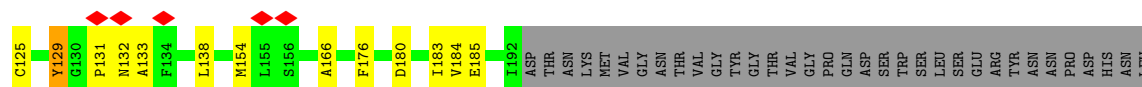


• Molecule 1: Neck protein gp13



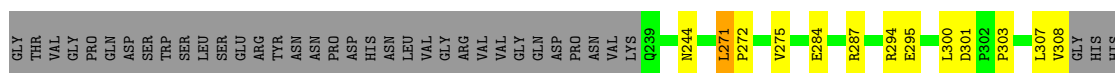
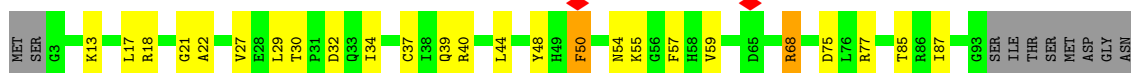
HIS

• Molecule 1: Neck protein gp13





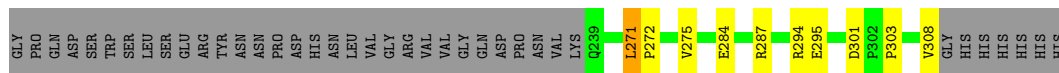
• Molecule 1: Neck protein gp13



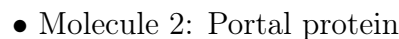
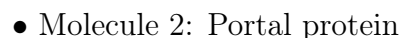
• Molecule 1: Neck protein gp13

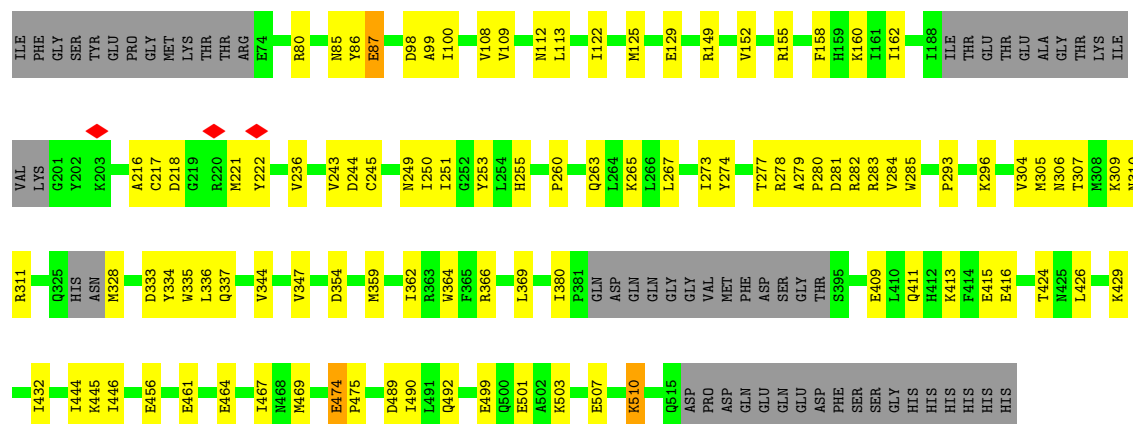


• Molecule 1: Neck protein gp13



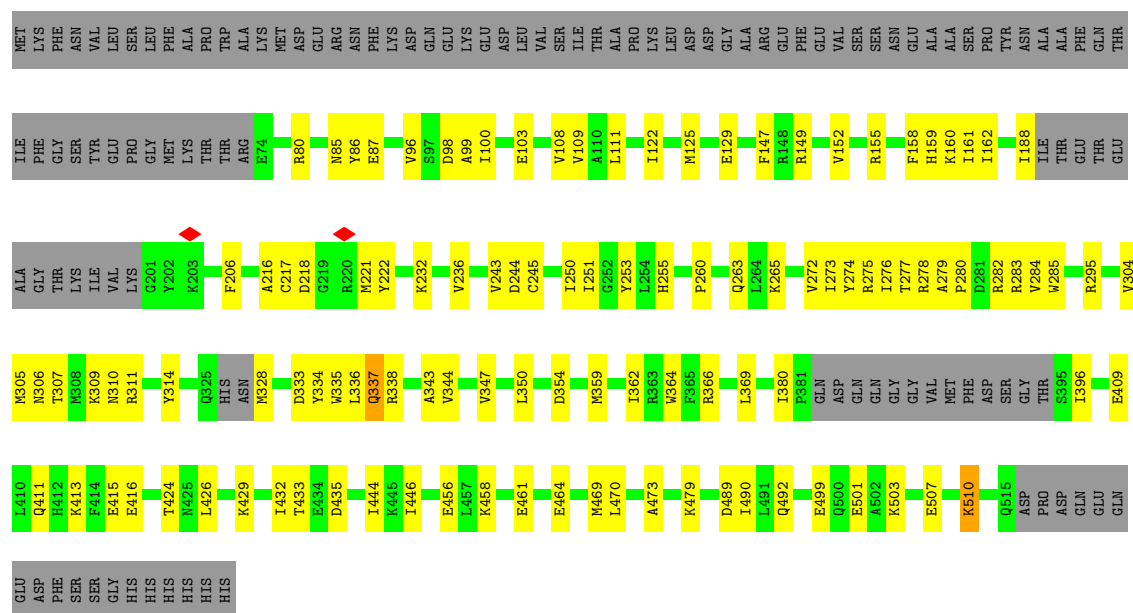
• Molecule 2: Portal protein





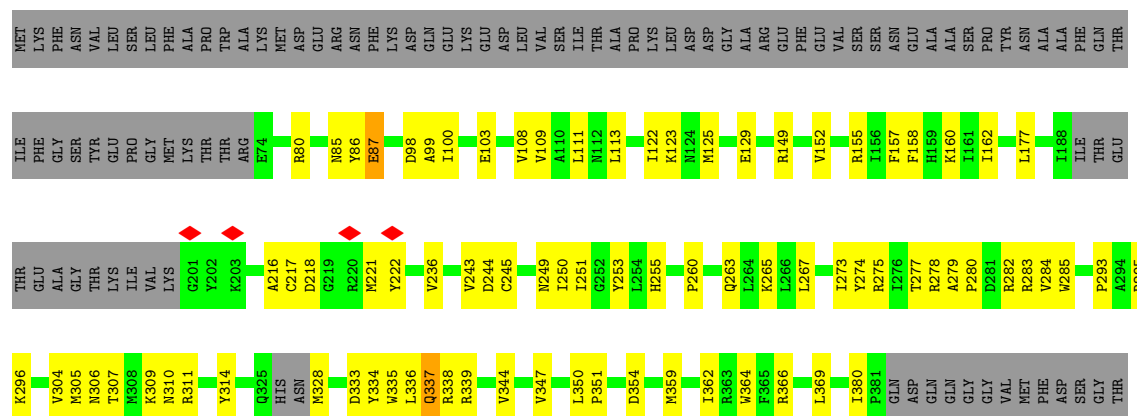
• Molecule 2: Portal protein

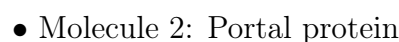
Chain i:



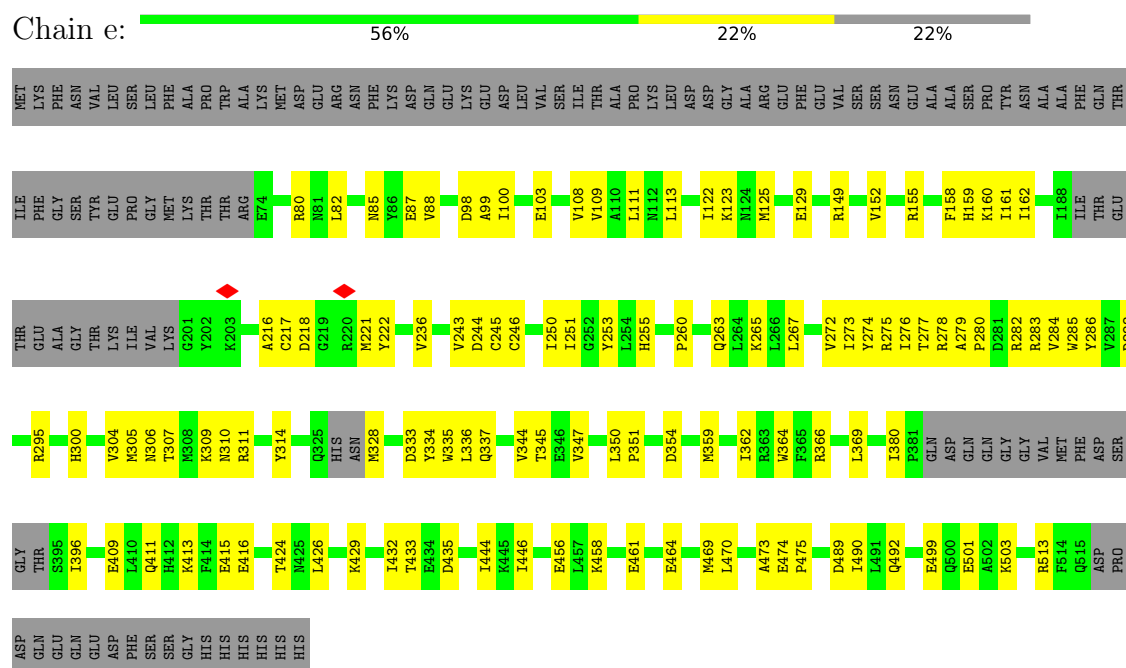
• Molecule 2: Portal protein

Chain h:



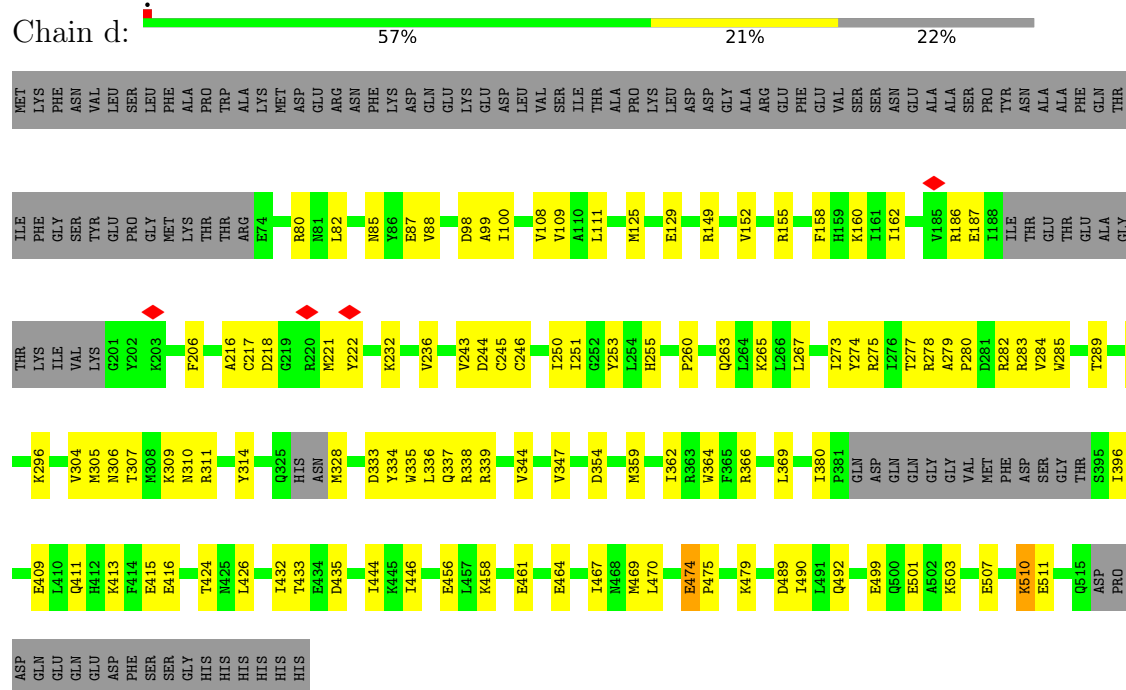


Chain e:



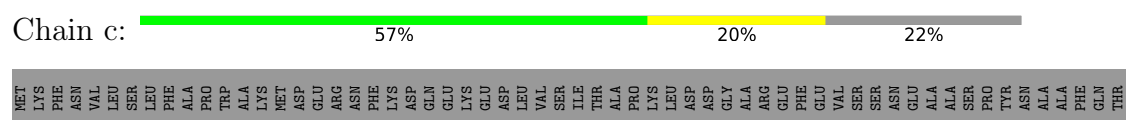
• Molecule 2: Portal protein

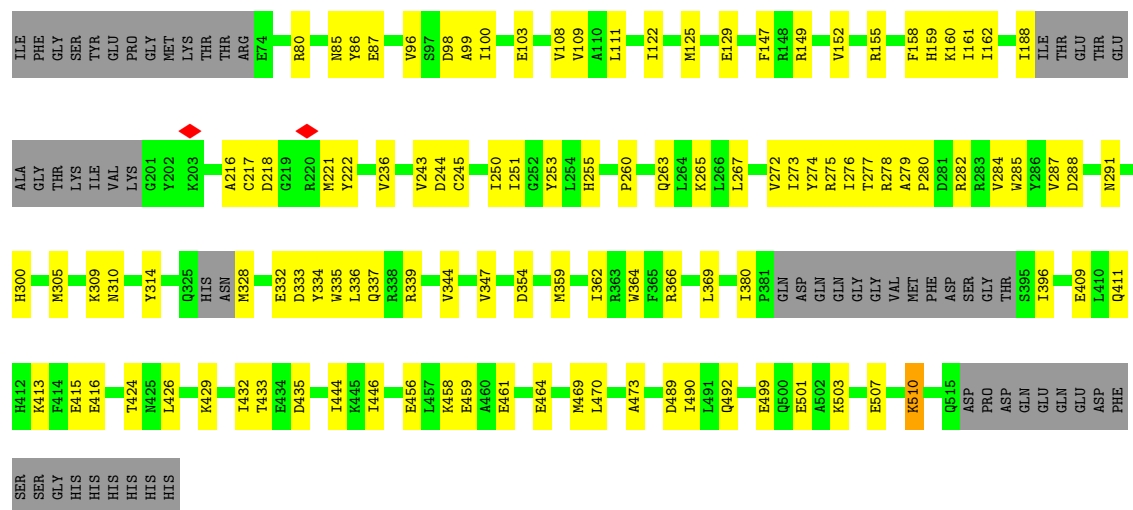
Chain d:



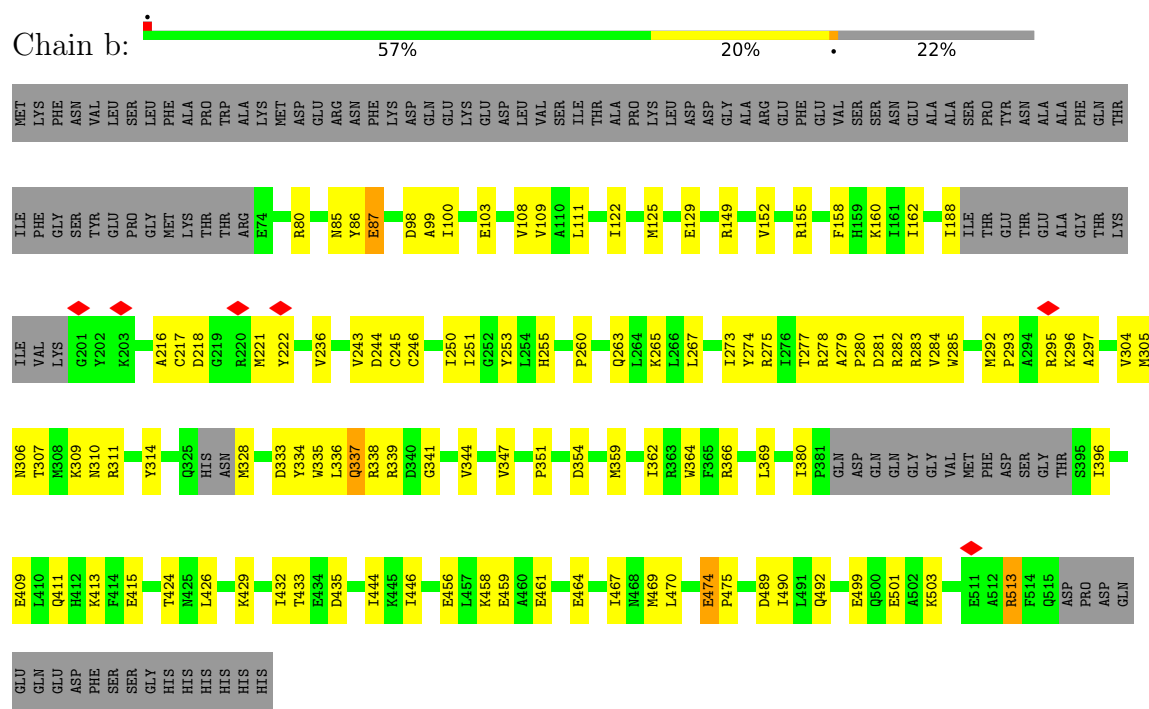
• Molecule 2: Portal protein

Chain c:

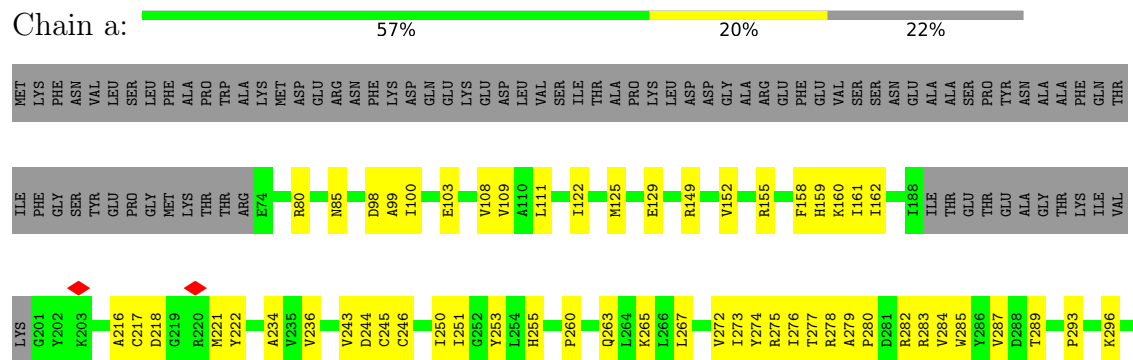


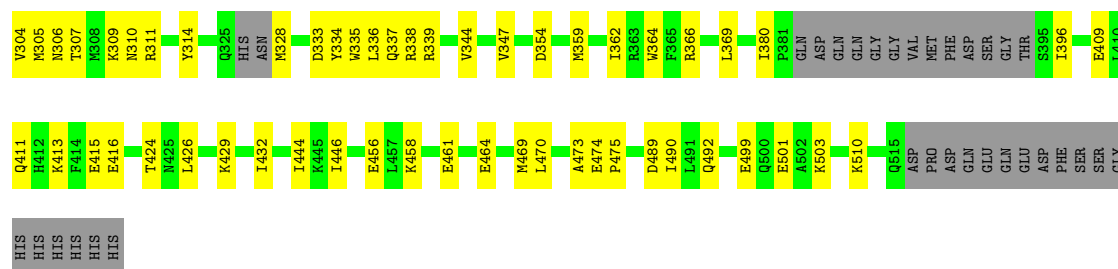


• Molecule 2: Portal protein

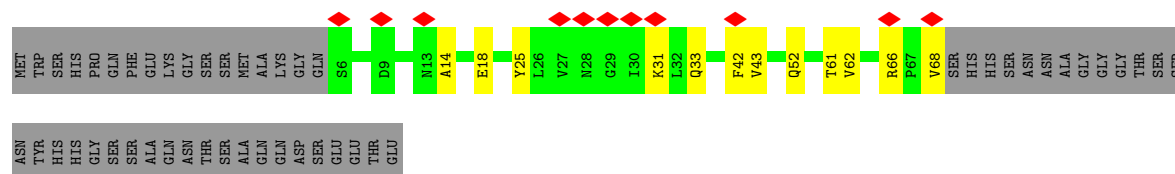


• Molecule 2: Portal protein

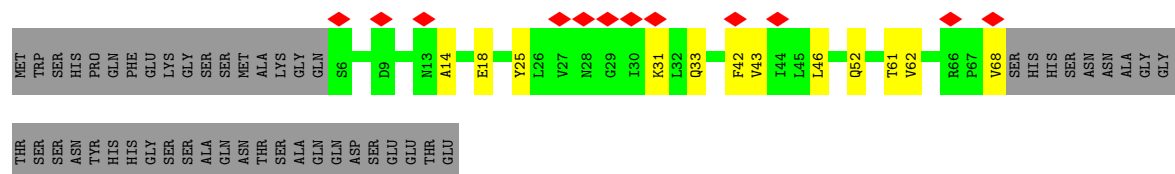




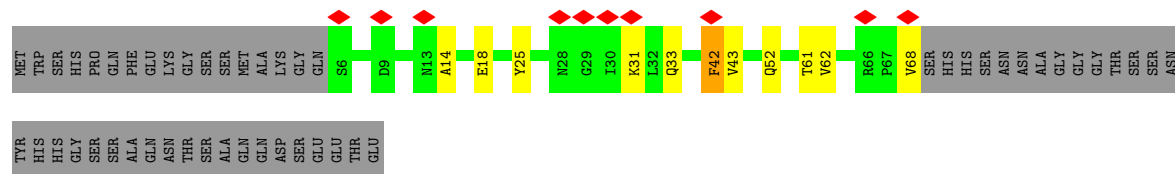
- Molecule 3: RNA-binding protein Hfq



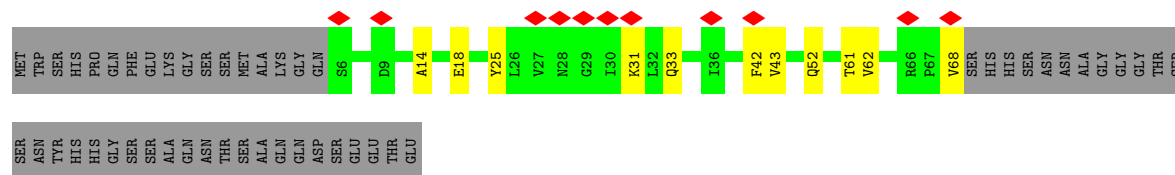
- Molecule 3: RNA-binding protein Hfq



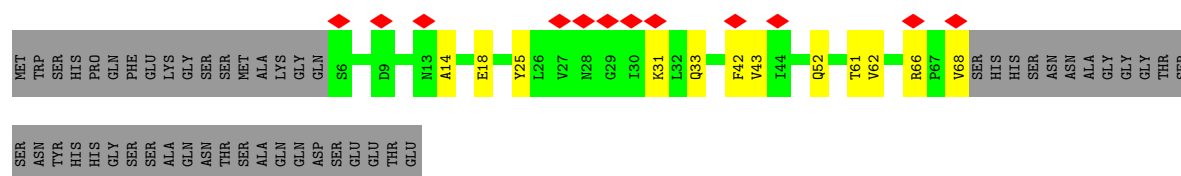
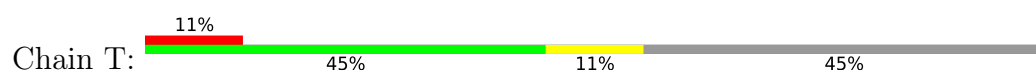
- Molecule 3: RNA-binding protein Hfq



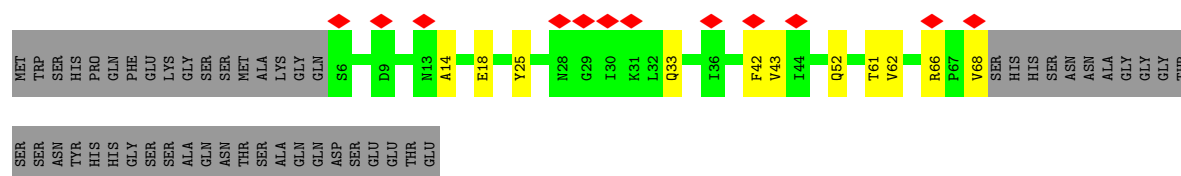
- Molecule 3: RNA-binding protein Hfq



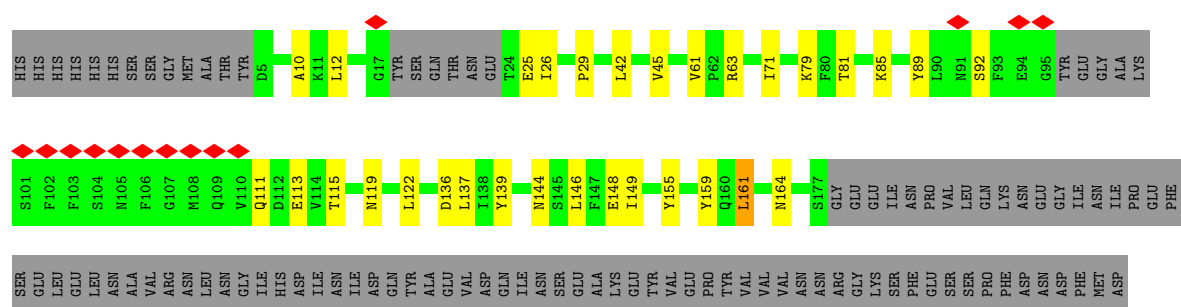
- Molecule 3: RNA-binding protein Hfq



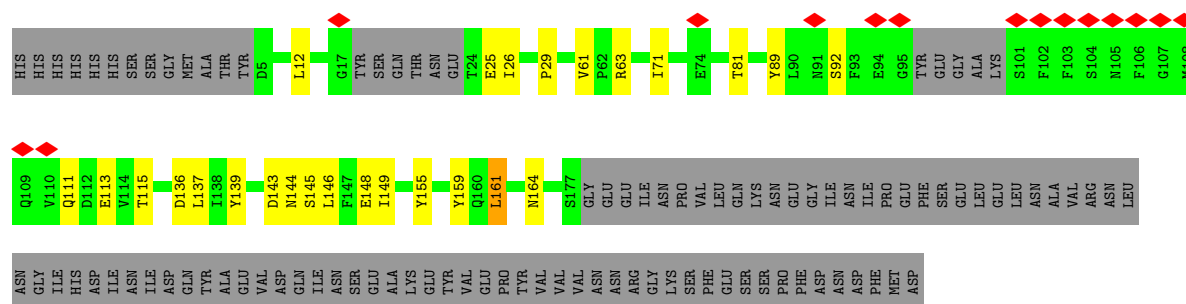
• Molecule 3: RNA-binding protein Hfq



• Molecule 4: Neck protein gp14

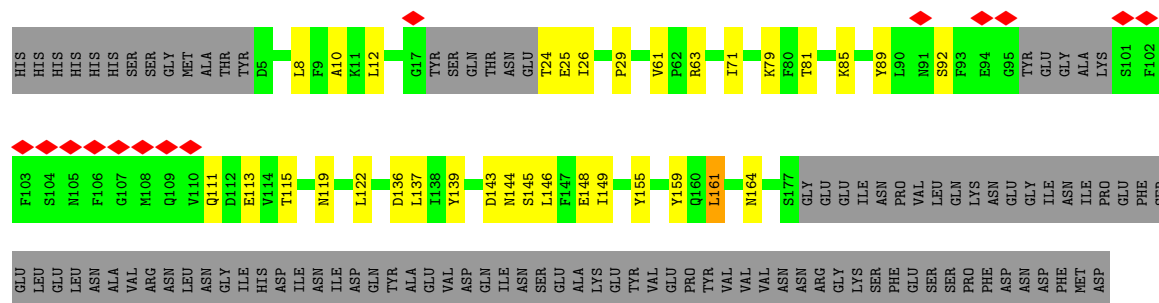


• Molecule 4: Neck protein gp14

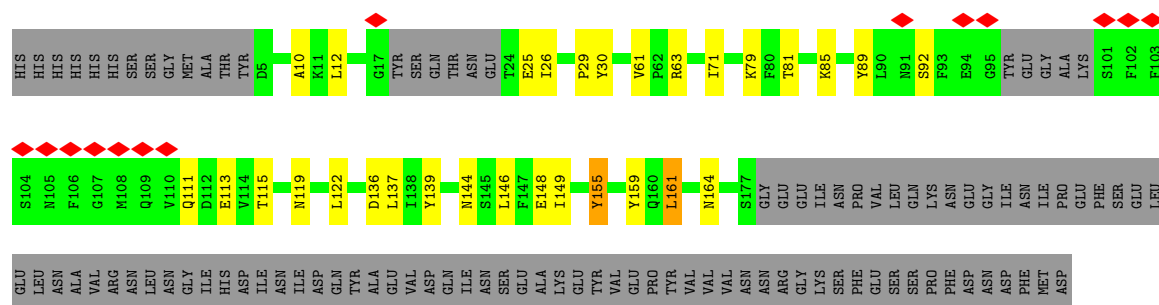


• Molecule 4: Neck protein gp14

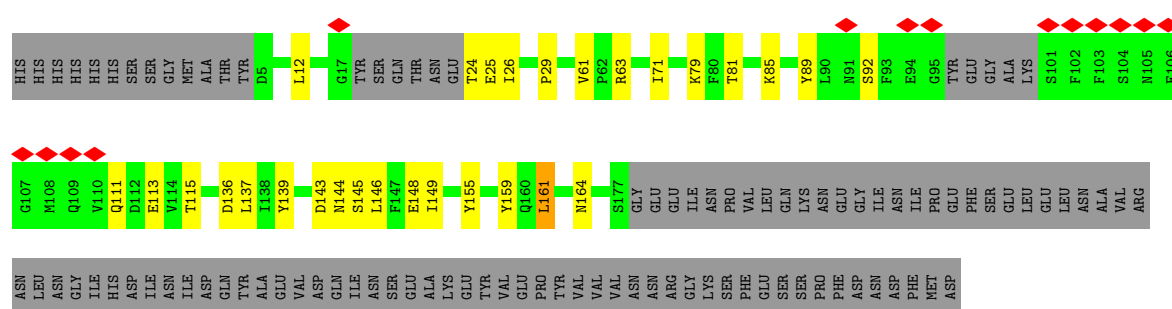




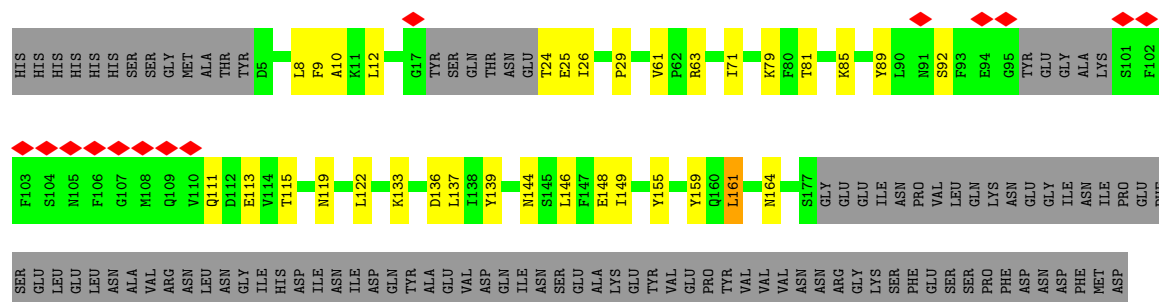
• Molecule 4: Neck protein gp14



• Molecule 4: Neck protein gp14



• Molecule 4: Neck protein gp14



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80622	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 ($e^-/\text{\AA}^2$)	53.00, 53, 53, 53, 53, 53, 53	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), FEI FALCON IV (4k x 4k), FEI FALCON IV (4k x 4k), FEI FALCON IV (4k x 4k), FEI FALCON IV (4k x 4k), FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00591	Depositor
Map size (Å)	334.72, 334.72, 334.72	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.046, 1.046, 1.046	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.11	0/2023	0.26	0/2732
1	B	0.23	0/2023	0.36	0/2732
1	C	0.11	0/2023	0.26	0/2732
1	D	0.10	0/2023	0.26	0/2732
1	E	0.10	0/2023	0.26	0/2732
1	F	0.11	0/2023	0.27	0/2732
1	G	0.10	0/2023	0.26	0/2732
1	H	0.11	0/2023	0.26	0/2732
1	I	0.10	0/2023	0.26	0/2732
1	J	0.10	0/2023	0.27	0/2732
1	K	0.10	0/2023	0.25	0/2732
1	L	0.10	0/2023	0.26	0/2732
2	a	0.10	0/3447	0.26	0/4644
2	b	0.11	0/3447	0.27	0/4644
2	c	0.10	0/3447	0.26	0/4644
2	d	0.11	0/3447	0.27	0/4644
2	e	0.10	0/3447	0.26	0/4644
2	f	0.11	0/3447	0.27	0/4644
2	g	0.10	0/3447	0.26	0/4644
2	h	0.11	0/3447	0.27	0/4644
2	i	0.10	0/3447	0.26	0/4644
2	j	0.11	0/3447	0.27	0/4644
2	k	0.10	0/3447	0.26	0/4644
2	l	0.11	0/3447	0.27	0/4644
3	S	0.10	0/513	0.26	0/696
3	T	0.09	0/513	0.25	0/696
3	U	0.09	0/513	0.24	0/696
3	V	0.11	0/513	0.26	0/696
3	W	0.09	0/513	0.25	0/696
3	X	0.09	0/513	0.24	0/696
4	M	0.11	0/1320	0.27	0/1788
4	N	0.11	0/1320	0.27	0/1788
4	O	0.10	0/1320	0.27	0/1788
4	P	0.11	0/1320	0.27	0/1788

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	Q	0.11	0/1320	0.27	0/1788
4	R	0.11	0/1320	0.27	0/1788
All	All	0.11	0/76638	0.27	0/103416

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1977	0	1926	31	0
1	B	1977	0	1926	46	0
1	C	1977	0	1926	34	0
1	D	1977	0	1926	31	0
1	E	1977	0	1926	33	0
1	F	1977	0	1926	29	0
1	G	1977	0	1926	33	0
1	H	1977	0	1926	26	0
1	I	1977	0	1926	34	0
1	J	1977	0	1926	31	0
1	K	1977	0	1926	33	0
1	L	1977	0	1926	29	0
2	a	3385	0	3331	70	0
2	b	3385	0	3331	74	0
2	c	3385	0	3331	74	0
2	d	3385	0	3331	71	0
2	e	3385	0	3331	75	0
2	f	3385	0	3331	69	0
2	g	3385	0	3331	72	0
2	h	3385	0	3331	72	0
2	i	3385	0	3331	69	0
2	j	3385	0	3331	62	0
2	k	3385	0	3331	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	3385	0	3331	73	0
3	S	504	0	530	7	0
3	T	504	0	530	9	0
3	U	504	0	530	7	0
3	V	504	0	530	8	0
3	W	504	0	530	9	0
3	X	504	0	530	9	0
4	M	1289	0	1212	20	0
4	N	1289	0	1212	23	0
4	O	1289	0	1212	26	0
4	P	1289	0	1212	23	0
4	Q	1289	0	1212	23	0
4	R	1289	0	1212	29	0
All	All	75102	0	73536	1194	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 8.

All (1194) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:PRO:HB3	2:c:300:HIS:NE2	1.94	0.82
1:D:59:VAL:O	1:D:125:CYS:HA	1.80	0.81
1:L:59:VAL:O	1:L:125:CYS:HA	1.82	0.79
1:B:28:GLU:OE2	4:N:42:LEU:HG	1.83	0.79
1:H:59:VAL:O	1:H:125:CYS:HA	1.84	0.78
2:e:286:TYR:O	2:e:345:THR:HA	1.84	0.78
1:J:59:VAL:O	1:J:125:CYS:HA	1.83	0.77
4:P:159:TYR:HB3	4:P:164:ASN:HD22	1.49	0.77
1:F:59:VAL:O	1:F:125:CYS:HA	1.85	0.77
1:I:59:VAL:O	1:I:125:CYS:HA	1.85	0.77
1:K:59:VAL:O	1:K:125:CYS:HA	1.84	0.77
1:C:59:VAL:O	1:C:125:CYS:HA	1.86	0.76
4:M:159:TYR:HB3	4:M:164:ASN:HD22	1.51	0.75
4:R:159:TYR:HB3	4:R:164:ASN:HD22	1.51	0.75
4:Q:159:TYR:HB3	4:Q:164:ASN:HD22	1.51	0.74
4:O:159:TYR:HB3	4:O:164:ASN:HD22	1.52	0.73
4:N:159:TYR:HB3	4:N:164:ASN:HD22	1.54	0.71
1:B:266:HIS:HB3	1:B:269:MET:HB2	1.71	0.70
1:G:59:VAL:O	1:G:125:CYS:HA	1.91	0.70
1:B:59:VAL:O	1:B:125:CYS:HA	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:VAL:O	1:A:125:CYS:HA	1.92	0.69
1:B:308:VAL:HA	2:b:305:MET:HE2	1.76	0.67
1:A:271:LEU:HD22	1:A:272:PRO:HD2	1.77	0.67
2:a:160:LYS:HE3	2:a:424:THR:HG21	1.77	0.66
1:I:271:LEU:HD22	1:I:272:PRO:HD2	1.77	0.66
1:K:271:LEU:HD22	1:K:272:PRO:HD2	1.78	0.66
2:l:160:LYS:HE3	2:l:424:THR:HG21	1.77	0.66
2:k:314:TYR:OH	2:i:263:GLN:NE2	2.29	0.66
1:G:271:LEU:HD22	1:G:272:PRO:HD2	1.77	0.66
2:k:155:ARG:HH21	2:k:250:ILE:HB	1.60	0.66
2:g:160:LYS:HE3	2:g:424:THR:HG21	1.76	0.66
1:C:271:LEU:HD22	1:C:272:PRO:HD2	1.78	0.65
2:j:160:LYS:HE3	2:j:424:THR:HG21	1.77	0.65
2:j:337:GLN:HE21	2:j:344:VAL:HG11	1.61	0.65
1:C:68:ARG:O	1:C:68:ARG:NH1	2.29	0.65
1:E:271:LEU:HD22	1:E:272:PRO:HD2	1.77	0.65
2:d:160:LYS:HE3	2:d:424:THR:HG21	1.79	0.65
2:i:160:LYS:HE3	2:i:424:THR:HG21	1.79	0.65
2:h:160:LYS:HE3	2:h:424:THR:HG21	1.79	0.65
2:g:334:TYR:HB2	2:f:284:VAL:HG12	1.78	0.65
2:e:160:LYS:HE3	2:e:424:THR:HG21	1.78	0.65
2:c:160:LYS:HE3	2:c:424:THR:HG21	1.77	0.65
1:J:129:TYR:HB3	1:J:133:ALA:HB2	1.79	0.65
2:k:160:LYS:HE3	2:k:424:THR:HG21	1.79	0.64
2:f:160:LYS:HE3	2:f:424:THR:HG21	1.78	0.64
1:B:301:ASP:O	1:B:303:PRO:HD3	1.98	0.64
1:B:68:ARG:O	1:B:68:ARG:NH1	2.29	0.64
1:A:301:ASP:O	1:A:303:PRO:HD3	1.98	0.64
2:l:284:VAL:HG12	2:a:334:TYR:HB2	1.80	0.64
3:X:52:GLN:HE22	3:S:62:VAL:H	1.46	0.64
2:d:334:TYR:HB2	2:c:284:VAL:HG12	1.80	0.64
2:c:155:ARG:HH21	2:c:250:ILE:HB	1.63	0.64
2:e:314:TYR:OH	2:c:263:GLN:NE2	2.31	0.64
1:H:301:ASP:O	1:H:303:PRO:HD3	1.98	0.64
4:Q:137:LEU:HB3	4:Q:146:LEU:HD11	1.80	0.64
2:b:155:ARG:HH21	2:b:250:ILE:HB	1.63	0.64
3:V:25:TYR:HB2	3:V:61:THR:HB	1.79	0.63
1:F:17:LEU:HB3	1:F:22:ALA:HB2	1.79	0.63
1:A:68:ARG:NH1	1:A:68:ARG:O	2.29	0.63
1:F:129:TYR:HB3	1:F:133:ALA:HB2	1.81	0.63
1:F:301:ASP:O	1:F:303:PRO:HD3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:TYR:HB3	1:D:133:ALA:HB2	1.81	0.63
1:H:17:LEU:HB3	1:H:22:ALA:HB2	1.81	0.63
2:i:334:TYR:HB2	2:h:284:VAL:HG12	1.81	0.63
1:J:301:ASP:O	1:J:303:PRO:HD3	1.99	0.63
2:h:283:ARG:HH22	2:h:311:ARG:HH22	1.46	0.63
1:H:129:TYR:HB3	1:H:133:ALA:HB2	1.81	0.63
1:J:17:LEU:HB3	1:J:22:ALA:HB2	1.81	0.63
2:b:337:GLN:HE21	2:b:344:VAL:HG11	1.63	0.63
3:T:25:TYR:HB2	3:T:61:THR:HB	1.80	0.63
2:i:155:ARG:HH21	2:i:250:ILE:HB	1.64	0.63
1:G:68:ARG:O	1:G:68:ARG:NH1	2.30	0.63
3:X:25:TYR:HB2	3:X:61:THR:HB	1.81	0.62
2:h:155:ARG:HH21	2:h:250:ILE:HB	1.63	0.62
3:W:25:TYR:HB2	3:W:61:THR:HB	1.80	0.62
2:b:160:LYS:HE3	2:b:424:THR:HG21	1.79	0.62
1:L:39:GLN:HE22	1:L:85:THR:HG21	1.64	0.62
1:E:301:ASP:O	1:E:303:PRO:HD3	2.00	0.62
2:j:334:TYR:HB2	2:i:284:VAL:HG12	1.81	0.62
2:l:334:TYR:HB2	2:k:284:VAL:HG12	1.81	0.62
3:U:25:TYR:HB2	3:U:61:THR:HB	1.81	0.62
3:S:25:TYR:HB2	3:S:61:THR:HB	1.81	0.62
1:K:301:ASP:O	1:K:303:PRO:HD3	2.00	0.62
2:l:335:TRP:NE1	2:k:305:MET:SD	2.73	0.62
2:e:155:ARG:HH21	2:e:250:ILE:HB	1.63	0.62
1:L:129:TYR:HB3	1:L:133:ALA:HB2	1.81	0.62
4:O:137:LEU:HD13	4:O:146:LEU:HD21	1.82	0.62
4:M:137:LEU:HB3	4:M:146:LEU:HD11	1.81	0.61
2:f:335:TRP:NE1	2:e:305:MET:SD	2.73	0.61
2:c:334:TYR:HB2	2:b:284:VAL:HG12	1.82	0.61
2:h:334:TYR:HB2	2:g:284:VAL:HG12	1.82	0.61
1:G:301:ASP:O	1:G:303:PRO:HD3	2.00	0.61
4:R:137:LEU:HD13	4:R:146:LEU:HD21	1.82	0.61
2:k:263:GLN:NE2	2:a:314:TYR:OH	2.29	0.61
1:D:17:LEU:HB3	1:D:22:ALA:HB2	1.81	0.61
1:B:54:ASN:ND2	1:B:132:ASN:OD1	2.34	0.61
1:D:301:ASP:O	1:D:303:PRO:HD3	2.01	0.61
1:E:59:VAL:O	1:E:125:CYS:HA	2.01	0.61
4:N:137:LEU:HB3	4:N:146:LEU:HD11	1.82	0.61
1:L:17:LEU:HB3	1:L:22:ALA:HB2	1.81	0.61
1:C:301:ASP:O	1:C:303:PRO:HD3	2.00	0.61
1:A:54:ASN:ND2	1:A:132:ASN:OD1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:HIS:HA	1:A:275:VAL:HG13	1.82	0.61
4:P:137:LEU:HB3	4:P:146:LEU:HD11	1.82	0.61
4:R:161:LEU:HD12	1:C:271:LEU:HD11	1.83	0.61
4:O:137:LEU:HB3	4:O:146:LEU:HD11	1.83	0.61
2:k:335:TRP:NE1	2:j:305:MET:SD	2.74	0.61
2:i:216:ALA:HB1	2:i:222:TYR:HA	1.83	0.61
2:g:283:ARG:HH22	2:g:311:ARG:HH22	1.46	0.61
1:L:301:ASP:O	1:L:303:PRO:HD3	2.00	0.61
4:N:137:LEU:HD13	4:N:146:LEU:HD21	1.82	0.60
4:P:139:TYR:OH	4:P:144:ASN:ND2	2.34	0.60
2:g:216:ALA:HB1	2:g:222:TYR:HA	1.83	0.60
4:M:139:TYR:OH	4:M:144:ASN:ND2	2.34	0.60
2:i:489:ASP:O	2:i:492:GLN:NE2	2.35	0.60
2:f:149:ARG:HH21	2:f:152:VAL:HG11	1.67	0.60
1:I:301:ASP:O	1:I:303:PRO:HD3	2.01	0.60
2:e:334:TYR:HB2	2:d:284:VAL:HG12	1.83	0.60
4:Q:139:TYR:OH	4:Q:144:ASN:ND2	2.34	0.60
2:l:474:GLU:HG3	2:l:475:PRO:HD3	1.83	0.60
2:j:335:TRP:NE1	2:i:305:MET:SD	2.74	0.60
4:P:161:LEU:HD12	1:G:271:LEU:HD11	1.84	0.60
2:b:334:TYR:HB2	2:a:284:VAL:HG12	1.84	0.60
4:O:161:LEU:HD12	1:I:271:LEU:HD11	1.84	0.60
2:k:334:TYR:HB2	2:j:284:VAL:HG12	1.84	0.60
2:b:149:ARG:HH21	2:b:152:VAL:HG11	1.66	0.60
4:R:137:LEU:HB3	4:R:146:LEU:HD11	1.84	0.60
4:R:139:TYR:OH	4:R:144:ASN:ND2	2.35	0.60
2:i:335:TRP:NE1	2:h:305:MET:SD	2.74	0.60
2:h:149:ARG:HH21	2:h:152:VAL:HG11	1.67	0.60
2:h:507:GLU:O	2:h:510:LYS:NZ	2.35	0.60
2:a:489:ASP:O	2:a:492:GLN:NE2	2.35	0.60
4:N:139:TYR:OH	4:N:144:ASN:ND2	2.34	0.59
4:M:137:LEU:HD13	4:M:146:LEU:HD21	1.83	0.59
4:P:137:LEU:HD13	4:P:146:LEU:HD21	1.82	0.59
4:N:161:LEU:HD12	1:A:271:LEU:HD11	1.84	0.59
4:O:139:TYR:OH	4:O:144:ASN:ND2	2.35	0.59
2:f:334:TYR:HB2	2:e:284:VAL:HG12	1.84	0.59
2:d:186:ARG:HE	2:d:187:GLU:H	1.49	0.59
4:M:161:LEU:HD12	1:K:271:LEU:HD11	1.84	0.59
4:Q:137:LEU:HD13	4:Q:146:LEU:HD21	1.83	0.59
1:I:54:ASN:ND2	1:I:132:ASN:OD1	2.35	0.59
3:X:14:ALA:HB1	3:X:68:VAL:HG11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:ASN:ND2	1:E:132:ASN:OD1	2.35	0.59
3:V:14:ALA:HB1	3:V:68:VAL:HG11	1.84	0.59
2:k:489:ASP:O	2:k:492:GLN:NE2	2.35	0.59
2:h:489:ASP:O	2:h:492:GLN:NE2	2.35	0.59
2:c:489:ASP:O	2:c:492:GLN:NE2	2.35	0.59
2:j:283:ARG:HH22	2:j:311:ARG:HH22	1.48	0.59
2:d:474:GLU:HG3	2:d:475:PRO:HD3	1.84	0.59
1:G:54:ASN:ND2	1:G:132:ASN:OD1	2.35	0.59
3:S:14:ALA:HB1	3:S:68:VAL:HG11	1.84	0.59
2:a:499:GLU:OE2	2:a:503:LYS:NZ	2.36	0.59
2:l:489:ASP:O	2:l:492:GLN:NE2	2.36	0.59
1:C:54:ASN:ND2	1:C:132:ASN:OD1	2.35	0.59
1:F:39:GLN:HE22	1:F:85:THR:HG21	1.66	0.59
1:G:129:TYR:HB3	1:G:133:ALA:HB2	1.85	0.59
4:Q:161:LEU:HD12	1:E:271:LEU:HD11	1.84	0.58
2:d:507:GLU:O	2:d:510:LYS:NZ	2.36	0.58
2:b:335:TRP:NE1	2:a:305:MET:SD	2.75	0.58
2:b:489:ASP:O	2:b:492:GLN:NE2	2.36	0.58
2:i:499:GLU:OE2	2:i:503:LYS:NZ	2.36	0.58
2:d:337:GLN:HE21	2:d:344:VAL:HG11	1.68	0.58
2:c:288:ASP:HB2	2:c:344:VAL:HG13	1.83	0.58
1:K:54:ASN:ND2	1:K:132:ASN:OD1	2.35	0.58
2:j:149:ARG:HH21	2:j:152:VAL:HG11	1.68	0.58
1:D:271:LEU:HB2	1:D:275:VAL:HB	1.85	0.58
2:j:489:ASP:O	2:j:492:GLN:NE2	2.36	0.58
2:g:489:ASP:O	2:g:492:GLN:NE2	2.36	0.58
2:e:149:ARG:HH21	2:e:152:VAL:HG11	1.69	0.58
2:f:489:ASP:O	2:f:492:GLN:NE2	2.36	0.58
2:e:489:ASP:O	2:e:492:GLN:NE2	2.36	0.58
2:g:335:TRP:NE1	2:f:305:MET:SD	2.76	0.58
2:c:499:GLU:OE2	2:c:503:LYS:NZ	2.36	0.58
1:E:129:TYR:HB3	1:E:133:ALA:HB2	1.86	0.58
3:U:14:ALA:HB1	3:U:68:VAL:HG11	1.85	0.58
1:E:68:ARG:O	1:E:68:ARG:NH1	2.31	0.58
3:T:14:ALA:HB1	3:T:68:VAL:HG11	1.85	0.58
1:L:54:ASN:ND2	1:L:132:ASN:OD1	2.36	0.58
2:l:186:ARG:HE	2:l:187:GLU:H	1.50	0.58
2:b:499:GLU:OE2	2:b:503:LYS:NZ	2.36	0.58
2:l:86:TYR:O	2:l:87:GLU:HG3	2.04	0.57
2:l:263:GLN:NE2	2:b:314:TYR:OH	2.30	0.57
4:O:63:ARG:NH2	4:O:148:GLU:OE1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:63:ARG:NH2	4:R:148:GLU:OE1	2.36	0.57
2:j:277:THR:O	2:j:282:ARG:NH1	2.37	0.57
2:i:149:ARG:HH21	2:i:152:VAL:HG11	1.67	0.57
2:d:149:ARG:HH21	2:d:152:VAL:HG11	1.69	0.57
2:d:489:ASP:O	2:d:492:GLN:NE2	2.37	0.57
2:a:283:ARG:HH22	2:a:311:ARG:HH22	1.52	0.57
1:J:54:ASN:ND2	1:J:132:ASN:OD1	2.37	0.57
2:h:335:TRP:NE1	2:g:305:MET:SD	2.77	0.57
2:d:277:THR:O	2:d:282:ARG:NH1	2.37	0.57
2:a:216:ALA:HB1	2:a:222:TYR:HA	1.85	0.57
2:e:499:GLU:OE2	2:e:503:LYS:NZ	2.36	0.57
2:c:253:TYR:OH	2:c:413:LYS:NZ	2.30	0.57
1:H:54:ASN:ND2	1:H:132:ASN:OD1	2.36	0.57
2:k:149:ARG:HH21	2:k:152:VAL:HG11	1.69	0.57
2:g:499:GLU:OE2	2:g:503:LYS:NZ	2.36	0.57
2:f:499:GLU:OE2	2:f:503:LYS:NZ	2.36	0.57
2:l:149:ARG:HH21	2:l:152:VAL:HG11	1.68	0.57
4:N:63:ARG:NH2	4:N:148:GLU:OE1	2.37	0.57
2:f:283:ARG:HH22	2:f:311:ARG:HH22	1.53	0.57
2:c:426:LEU:HD23	2:c:432:ILE:HD12	1.87	0.57
2:k:469:MET:HE3	2:k:490:ILE:HG23	1.87	0.57
2:c:216:ALA:HB1	2:c:222:TYR:HA	1.86	0.57
2:a:99:ALA:O	2:a:411:GLN:NE2	2.38	0.57
1:F:54:ASN:ND2	1:F:132:ASN:OD1	2.37	0.57
1:I:39:GLN:HE22	1:I:85:THR:HG21	1.69	0.57
3:W:14:ALA:HB1	3:W:68:VAL:HG11	1.86	0.57
3:W:62:VAL:H	3:V:52:GLN:HE22	1.51	0.57
2:j:499:GLU:OE2	2:j:503:LYS:NZ	2.36	0.57
2:f:99:ALA:O	2:f:411:GLN:NE2	2.38	0.57
1:I:129:TYR:HB3	1:I:133:ALA:HB2	1.87	0.57
3:T:33:GLN:NE2	4:R:113:GLU:OE2	2.38	0.57
2:k:283:ARG:HH22	2:k:311:ARG:HH22	1.52	0.57
1:K:68:ARG:O	1:K:68:ARG:NH1	2.31	0.57
2:l:469:MET:HE3	2:l:490:ILE:HG23	1.87	0.57
2:d:283:ARG:HH22	2:d:311:ARG:HH22	1.50	0.57
2:c:335:TRP:NE1	2:b:305:MET:SD	2.76	0.57
2:l:206:PHE:HE2	2:l:232:LYS:HD3	1.68	0.57
4:M:63:ARG:NH2	4:M:148:GLU:OE1	2.37	0.57
4:Q:63:ARG:NH2	4:Q:148:GLU:OE1	2.37	0.57
2:i:469:MET:HE3	2:i:490:ILE:HG23	1.86	0.57
3:T:62:VAL:H	3:S:52:GLN:HE22	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:63:ARG:NH2	4:P:148:GLU:OE1	2.38	0.56
2:i:426:LEU:HD23	2:i:432:ILE:HD12	1.87	0.56
2:h:86:TYR:O	2:h:87:GLU:HG3	2.04	0.56
2:h:99:ALA:O	2:h:411:GLN:NE2	2.38	0.56
2:g:336:LEU:HD11	2:g:347:VAL:HG23	1.87	0.56
2:d:335:TRP:NE1	2:c:305:MET:SD	2.77	0.56
2:l:305:MET:SD	2:a:335:TRP:NE1	2.78	0.56
2:l:499:GLU:OE2	2:l:503:LYS:NZ	2.36	0.56
3:X:62:VAL:H	3:W:52:GLN:HE22	1.53	0.56
2:j:86:TYR:O	2:j:87:GLU:HG3	2.04	0.56
2:h:499:GLU:OE2	2:h:503:LYS:NZ	2.36	0.56
2:d:499:GLU:OE2	2:d:503:LYS:NZ	2.36	0.56
1:C:129:TYR:HB3	1:C:133:ALA:HB2	1.87	0.56
1:F:271:LEU:HB2	1:F:275:VAL:HB	1.87	0.56
1:B:299:LEU:HD23	2:c:291:ASN:ND2	2.20	0.56
2:l:99:ALA:O	2:l:411:GLN:NE2	2.38	0.56
2:k:499:GLU:OE2	2:k:503:LYS:NZ	2.36	0.56
2:e:335:TRP:NE1	2:d:305:MET:SD	2.77	0.56
2:c:314:TYR:OH	2:a:263:GLN:NE2	2.27	0.56
2:c:366:ARG:HE	2:b:364:TRP:HH2	1.53	0.56
2:l:314:TYR:OH	2:j:263:GLN:NE2	2.29	0.56
1:D:54:ASN:ND2	1:D:132:ASN:OD1	2.38	0.56
3:W:33:GLN:NE2	4:O:113:GLU:OE2	2.39	0.56
2:k:253:TYR:OH	2:k:413:LYS:NZ	2.29	0.56
2:e:99:ALA:O	2:e:411:GLN:NE2	2.39	0.56
2:b:469:MET:HE3	2:b:490:ILE:HG23	1.87	0.56
2:l:253:TYR:OH	2:l:413:LYS:NZ	2.29	0.56
2:a:469:MET:HE3	2:a:490:ILE:HG23	1.87	0.56
1:B:129:TYR:HB3	1:B:133:ALA:HB2	1.87	0.56
2:l:283:ARG:HH22	2:l:311:ARG:HH22	1.53	0.56
3:X:33:GLN:NE2	4:M:113:GLU:OE2	2.39	0.56
3:V:62:VAL:H	3:U:52:GLN:HE22	1.52	0.56
4:N:25:GLU:HG3	4:N:29:PRO:HG3	1.87	0.56
4:P:61:VAL:HG23	4:P:137:LEU:HB2	1.88	0.56
2:g:277:THR:O	2:g:282:ARG:NH1	2.39	0.56
2:d:336:LEU:HD11	2:d:347:VAL:HG23	1.88	0.56
1:H:271:LEU:HB2	1:H:275:VAL:HB	1.88	0.56
2:j:336:LEU:HD11	2:j:347:VAL:HG23	1.88	0.56
2:i:507:GLU:O	2:i:510:LYS:NZ	2.39	0.56
2:d:216:ALA:HB1	2:d:222:TYR:HA	1.88	0.56
2:c:469:MET:HE3	2:c:490:ILE:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:277:THR:O	2:a:282:ARG:NH1	2.39	0.56
1:J:271:LEU:HB2	1:J:275:VAL:HB	1.87	0.56
1:B:191:TYR:CE1	2:b:295:ARG:HD2	2.41	0.55
2:k:99:ALA:O	2:k:411:GLN:NE2	2.38	0.55
2:k:337:GLN:HE21	2:k:344:VAL:HG11	1.70	0.55
2:i:99:ALA:O	2:i:411:GLN:NE2	2.39	0.55
2:l:155:ARG:HH21	2:l:250:ILE:HB	1.70	0.55
2:l:217:CYS:SG	2:l:218:ASP:N	2.80	0.55
4:O:61:VAL:HG23	4:O:137:LEU:HB2	1.88	0.55
3:U:33:GLN:NE2	4:Q:113:GLU:OE2	2.39	0.55
2:j:279:ALA:O	2:i:278:ARG:NH1	2.38	0.55
2:h:469:MET:HE3	2:h:490:ILE:HG23	1.87	0.55
2:a:337:GLN:HE21	2:a:344:VAL:HG11	1.71	0.55
4:N:61:VAL:HG23	4:N:137:LEU:HB2	1.88	0.55
2:k:186:ARG:HE	2:k:187:GLU:H	1.53	0.55
2:j:469:MET:HE3	2:j:490:ILE:HG23	1.88	0.55
2:g:149:ARG:HH21	2:g:152:VAL:HG11	1.71	0.55
1:A:129:TYR:HB3	1:A:133:ALA:HB2	1.87	0.55
1:I:18:ARG:HH12	1:J:36:ASP:HB2	1.71	0.55
1:K:129:TYR:HB3	1:K:133:ALA:HB2	1.88	0.55
3:U:62:VAL:H	3:T:52:GLN:HE22	1.53	0.55
3:S:33:GLN:NE2	4:N:113:GLU:OE2	2.40	0.55
2:k:216:ALA:HB1	2:k:222:TYR:HA	1.87	0.55
2:k:513:ARG:NH1	2:i:479:LYS:O	2.39	0.55
2:j:474:GLU:HG3	2:j:475:PRO:HD3	1.87	0.55
2:i:456:GLU:OE2	2:h:492:GLN:NE2	2.40	0.55
2:f:216:ALA:HB1	2:f:222:TYR:HA	1.88	0.55
2:b:99:ALA:O	2:b:411:GLN:NE2	2.38	0.55
4:R:61:VAL:HG23	4:R:137:LEU:HB2	1.89	0.55
2:h:217:CYS:SG	2:h:218:ASP:N	2.80	0.55
2:e:217:CYS:SG	2:e:218:ASP:N	2.80	0.55
2:a:149:ARG:HH21	2:a:152:VAL:HG11	1.70	0.55
1:H:37:CYS:SG	1:H:40:ARG:NH2	2.79	0.55
2:i:366:ARG:HE	2:h:364:TRP:HH2	1.54	0.55
2:h:216:ALA:HB1	2:h:222:TYR:HA	1.88	0.55
2:e:253:TYR:OH	2:e:413:LYS:NZ	2.29	0.55
4:M:26:ILE:HD12	4:O:85:LYS:HG3	1.89	0.55
2:c:99:ALA:O	2:c:411:GLN:NE2	2.39	0.55
2:j:217:CYS:SG	2:j:218:ASP:N	2.80	0.55
2:g:337:GLN:HE21	2:g:344:VAL:HG11	1.71	0.55
2:f:277:THR:O	2:f:282:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:415:GLU:HB2	2:b:446:ILE:HD12	1.88	0.55
1:E:17:LEU:HB3	1:E:22:ALA:HB2	1.88	0.55
2:g:426:LEU:HD23	2:g:432:ILE:HD12	1.88	0.55
2:f:155:ARG:HH21	2:f:250:ILE:HB	1.72	0.55
2:e:277:THR:O	2:e:282:ARG:NH1	2.40	0.55
2:d:366:ARG:HE	2:c:364:TRP:HH2	1.55	0.55
4:M:25:GLU:HG3	4:M:29:PRO:HG3	1.89	0.54
4:O:25:GLU:HG3	4:O:29:PRO:HG3	1.89	0.54
2:g:99:ALA:O	2:g:411:GLN:NE2	2.39	0.54
2:b:217:CYS:SG	2:b:218:ASP:N	2.80	0.54
2:l:277:THR:O	2:l:282:ARG:NH1	2.41	0.54
2:k:277:THR:O	2:k:282:ARG:NH1	2.40	0.54
2:j:99:ALA:O	2:j:411:GLN:NE2	2.39	0.54
2:f:474:GLU:HG3	2:f:475:PRO:HD3	1.89	0.54
2:e:216:ALA:HB1	2:e:222:TYR:HA	1.87	0.54
2:e:469:MET:HE3	2:e:490:ILE:HG23	1.88	0.54
2:l:456:GLU:OE2	2:k:492:GLN:NE2	2.40	0.54
2:b:216:ALA:HB1	2:b:222:TYR:HA	1.89	0.54
2:b:366:ARG:HE	2:a:364:TRP:HH2	1.55	0.54
1:F:37:CYS:SG	1:F:40:ARG:NH2	2.80	0.54
1:B:304:PHE:CD1	2:c:337:GLN:NE2	2.76	0.54
4:Q:26:ILE:HD12	4:R:85:LYS:HG3	1.89	0.54
2:d:99:ALA:O	2:d:411:GLN:NE2	2.40	0.54
2:d:217:CYS:SG	2:d:218:ASP:N	2.80	0.54
2:a:426:LEU:HD23	2:a:432:ILE:HD12	1.88	0.54
1:J:39:GLN:HE22	1:J:85:THR:HG21	1.73	0.54
2:l:216:ALA:HB1	2:l:222:TYR:HA	1.88	0.54
3:V:33:GLN:NE2	4:P:113:GLU:OE2	2.40	0.54
3:S:18:GLU:HG3	3:S:68:VAL:HG13	1.89	0.54
4:Q:61:VAL:HG23	4:Q:137:LEU:HB2	1.90	0.54
2:g:314:TYR:HH	2:e:263:GLN:HE21	1.53	0.54
2:b:277:THR:O	2:b:282:ARG:NH1	2.40	0.54
1:L:271:LEU:HB2	1:L:275:VAL:HB	1.89	0.54
4:P:25:GLU:HG3	4:P:29:PRO:HG3	1.89	0.54
2:f:244:ASP:OD1	2:f:245:CYS:N	2.41	0.54
2:c:149:ARG:HH21	2:c:152:VAL:HG11	1.72	0.54
1:K:17:LEU:HB3	1:K:22:ALA:HB2	1.90	0.54
2:l:85:ASN:HB3	2:l:265:LYS:HE2	1.89	0.54
2:g:244:ASP:OD1	2:g:245:CYS:N	2.40	0.54
2:e:336:LEU:HD11	2:e:347:VAL:HG23	1.90	0.54
2:a:309:LYS:NZ	2:a:310:ASN:OD1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:61:VAL:HG23	4:M:137:LEU:HB2	1.90	0.54
2:k:309:LYS:NZ	2:k:310:ASN:OD1	2.41	0.54
2:h:277:THR:O	2:h:282:ARG:NH1	2.40	0.54
2:f:456:GLU:OE2	2:e:492:GLN:NE2	2.41	0.54
2:f:469:MET:HE3	2:f:490:ILE:HG23	1.88	0.54
2:f:513:ARG:NH1	2:d:479:LYS:O	2.40	0.54
2:d:469:MET:HE3	2:d:490:ILE:HG23	1.88	0.54
2:c:456:GLU:OE2	2:b:492:GLN:NE2	2.41	0.54
2:j:244:ASP:OD1	2:j:245:CYS:N	2.41	0.54
2:e:366:ARG:HE	2:d:364:TRP:HH2	1.54	0.54
2:e:426:LEU:HD23	2:e:432:ILE:HD12	1.90	0.54
1:H:39:GLN:HE22	1:H:85:THR:HG21	1.73	0.54
1:I:68:ARG:O	1:I:68:ARG:NH1	2.32	0.54
1:G:75:ASP:OD2	1:G:77:ARG:NH1	2.41	0.54
1:B:27:VAL:HG11	4:R:10:ALA:O	2.08	0.53
2:i:314:TYR:OH	2:g:263:GLN:NE2	2.27	0.53
2:g:279:ALA:O	2:f:278:ARG:NH1	2.42	0.53
2:f:366:ARG:HE	2:e:364:TRP:HH2	1.56	0.53
2:d:206:PHE:HE2	2:d:232:LYS:HD3	1.73	0.53
2:b:283:ARG:HH22	2:b:311:ARG:HH22	1.54	0.53
1:A:271:LEU:HB3	1:A:275:VAL:HB	1.90	0.53
2:k:426:LEU:HD23	2:k:432:ILE:HD12	1.89	0.53
2:j:456:GLU:OE2	2:i:492:GLN:NE2	2.41	0.53
2:h:366:ARG:HE	2:g:364:TRP:HH2	1.55	0.53
2:g:469:MET:HE3	2:g:490:ILE:HG23	1.89	0.53
2:l:278:ARG:NH1	2:a:279:ALA:O	2.40	0.53
2:j:216:ALA:HB1	2:j:222:TYR:HA	1.89	0.53
2:e:309:LYS:NZ	2:e:310:ASN:OD1	2.41	0.53
2:b:309:LYS:NZ	2:b:310:ASN:OD1	2.41	0.53
1:B:271:LEU:HB2	1:B:275:VAL:HB	1.90	0.53
1:C:55:LYS:NZ	1:C:185:GLU:OE2	2.41	0.53
4:N:85:LYS:HG3	4:R:26:ILE:HD12	1.90	0.53
2:i:336:LEU:HD11	2:i:347:VAL:HG23	1.91	0.53
2:h:336:LEU:HD11	2:h:347:VAL:HG23	1.91	0.53
2:h:474:GLU:HG3	2:h:475:PRO:HD3	1.91	0.53
2:f:274:TYR:OH	2:f:354:ASP:OD1	2.27	0.53
2:a:415:GLU:HB2	2:a:446:ILE:HD12	1.90	0.53
2:l:336:LEU:HD11	2:l:347:VAL:HG23	1.91	0.53
2:k:85:ASN:HB3	2:k:265:LYS:HE2	1.91	0.53
2:i:277:THR:O	2:i:282:ARG:NH1	2.41	0.53
2:e:85:ASN:HB3	2:e:265:LYS:HE2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:GLN:HE22	1:C:85:THR:HG21	1.74	0.53
1:D:39:GLN:HE22	1:D:85:THR:HG21	1.72	0.53
2:l:274:TYR:OH	2:l:354:ASP:OD1	2.26	0.53
3:T:18:GLU:HG3	3:T:68:VAL:HG13	1.91	0.53
2:i:309:LYS:NZ	2:i:310:ASN:OD1	2.41	0.53
2:f:426:LEU:HD23	2:f:432:ILE:HD12	1.90	0.53
2:d:279:ALA:O	2:c:278:ARG:NH1	2.41	0.53
1:F:55:LYS:NZ	1:F:185:GLU:OE2	2.42	0.53
4:R:8:LEU:HD11	1:A:23:PRO:HB2	1.90	0.53
2:j:158:PHE:H	2:j:236:VAL:HG22	1.73	0.53
2:j:366:ARG:HE	2:i:364:TRP:HH2	1.56	0.53
2:c:314:TYR:HH	2:a:263:GLN:HE21	1.55	0.53
2:b:456:GLU:OE2	2:a:492:GLN:NE2	2.41	0.53
1:B:36:ASP:HB2	1:A:18:ARG:HH12	1.73	0.53
2:k:456:GLU:OE2	2:j:492:GLN:NE2	2.42	0.53
2:k:508:GLU:OE1	2:k:510:LYS:NZ	2.38	0.53
3:U:18:GLU:HG3	3:U:68:VAL:HG13	1.91	0.52
4:N:136:ASP:HB2	4:N:149:ILE:HD12	1.91	0.52
2:k:244:ASP:OD1	2:k:245:CYS:N	2.41	0.52
2:h:253:TYR:OH	2:h:413:LYS:NZ	2.29	0.52
2:g:158:PHE:H	2:g:236:VAL:HG22	1.74	0.52
2:g:456:GLU:OE2	2:f:492:GLN:NE2	2.42	0.52
2:f:336:LEU:HD11	2:f:347:VAL:HG23	1.91	0.52
2:b:338:ARG:NH2	2:b:341:GLY:O	2.41	0.52
1:G:271:LEU:HB3	1:G:275:VAL:HB	1.90	0.52
1:J:87:ILE:HG22	1:J:184:VAL:HG13	1.91	0.52
3:V:18:GLU:HG3	3:V:68:VAL:HG13	1.92	0.52
2:h:309:LYS:NZ	2:h:310:ASN:OD1	2.41	0.52
2:f:279:ALA:O	2:e:278:ARG:NH1	2.42	0.52
2:d:456:GLU:OE2	2:c:492:GLN:NE2	2.42	0.52
2:c:277:THR:O	2:c:282:ARG:NH1	2.42	0.52
2:b:244:ASP:OD1	2:b:245:CYS:N	2.41	0.52
1:K:271:LEU:HB3	1:K:275:VAL:HB	1.92	0.52
4:R:136:ASP:HB2	4:R:149:ILE:HD12	1.91	0.52
2:b:279:ALA:O	2:a:278:ARG:NH1	2.41	0.52
2:a:158:PHE:H	2:a:236:VAL:HG22	1.74	0.52
3:X:18:GLU:HG3	3:X:68:VAL:HG13	1.90	0.52
4:N:92:SER:O	4:N:115:THR:OG1	2.27	0.52
2:g:309:LYS:NZ	2:g:310:ASN:OD1	2.41	0.52
2:f:158:PHE:H	2:f:236:VAL:HG22	1.74	0.52
1:I:57:PHE:HB3	1:I:183:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:55:LYS:NZ	1:J:185:GLU:OE2	2.42	0.52
2:l:279:ALA:O	2:k:278:ARG:NH1	2.42	0.52
2:j:253:TYR:OH	2:j:413:LYS:NZ	2.30	0.52
2:j:309:LYS:NZ	2:j:310:ASN:OD1	2.41	0.52
2:i:470:LEU:HB2	2:i:490:ILE:HG21	1.92	0.52
2:f:309:LYS:NZ	2:f:310:ASN:OD1	2.42	0.52
2:c:244:ASP:OD1	2:c:245:CYS:N	2.41	0.52
2:b:292:MET:HG2	2:b:297:ALA:HB2	1.91	0.52
4:Q:25:GLU:HG3	4:Q:29:PRO:HG3	1.90	0.52
2:i:253:TYR:OH	2:i:413:LYS:NZ	2.29	0.52
2:h:279:ALA:O	2:g:278:ARG:NH1	2.42	0.52
2:d:158:PHE:H	2:d:236:VAL:HG22	1.75	0.52
2:a:155:ARG:HH21	2:a:250:ILE:HB	1.74	0.52
2:l:288:ASP:HA	2:a:338:ARG:HB2	1.91	0.52
2:l:492:GLN:NE2	2:a:456:GLU:OE2	2.43	0.52
2:b:474:GLU:HG3	2:b:475:PRO:HD3	1.91	0.52
2:h:415:GLU:HB2	2:h:446:ILE:HD12	1.92	0.52
2:e:108:VAL:HG23	2:e:109:VAL:HG22	1.92	0.52
2:b:274:TYR:OH	2:b:354:ASP:OD1	2.26	0.52
1:A:57:PHE:HB3	1:A:183:ILE:HD11	1.92	0.52
1:K:55:LYS:NZ	1:K:185:GLU:OE2	2.43	0.52
2:l:366:ARG:HE	2:k:364:TRP:HH2	1.57	0.52
1:E:57:PHE:HB3	1:E:183:ILE:HD11	1.90	0.52
4:O:92:SER:OG	4:O:115:THR:O	2.28	0.52
4:Q:143:ASP:OD1	4:Q:145:SER:OG	2.22	0.52
2:h:337:GLN:HE21	2:h:344:VAL:HG11	1.75	0.52
2:e:158:PHE:H	2:e:236:VAL:HG22	1.75	0.52
2:c:415:GLU:HB2	2:c:446:ILE:HD12	1.91	0.52
2:l:158:PHE:H	2:l:236:VAL:HG22	1.75	0.51
2:k:217:CYS:SG	2:k:218:ASP:N	2.83	0.51
2:c:507:GLU:O	2:c:510:LYS:NZ	2.42	0.51
1:G:57:PHE:HB3	1:G:183:ILE:HD11	1.92	0.51
1:B:57:PHE:HB3	1:B:183:ILE:HD11	1.91	0.51
2:l:309:LYS:NZ	2:l:310:ASN:OD1	2.42	0.51
4:O:136:ASP:HB2	4:O:149:ILE:HD12	1.92	0.51
2:i:244:ASP:OD1	2:i:245:CYS:N	2.40	0.51
2:c:336:LEU:HD11	2:c:347:VAL:HG23	1.92	0.51
4:M:92:SER:O	4:M:115:THR:OG1	2.28	0.51
4:Q:136:ASP:HB2	4:Q:149:ILE:HD12	1.93	0.51
2:k:158:PHE:H	2:k:236:VAL:HG22	1.75	0.51
2:j:85:ASN:HB3	2:j:265:LYS:HE2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:217:CYS:SG	2:i:218:ASP:N	2.84	0.51
2:f:85:ASN:HB3	2:f:265:LYS:HE2	1.92	0.51
2:d:309:LYS:NZ	2:d:310:ASN:OD1	2.41	0.51
2:a:85:ASN:HB3	2:a:265:LYS:HE2	1.93	0.51
1:G:55:LYS:NZ	1:G:185:GLU:OE2	2.43	0.51
1:I:55:LYS:NZ	1:I:185:GLU:OE2	2.43	0.51
2:l:364:TRP:HH2	2:a:366:ARG:HE	1.59	0.51
2:k:415:GLU:HB2	2:k:446:ILE:HD12	1.92	0.51
2:i:158:PHE:H	2:i:236:VAL:HG22	1.76	0.51
2:h:244:ASP:OD1	2:h:245:CYS:N	2.41	0.51
2:g:217:CYS:SG	2:g:218:ASP:N	2.84	0.51
2:g:274:TYR:OH	2:g:354:ASP:OD1	2.28	0.51
2:c:158:PHE:H	2:c:236:VAL:HG22	1.75	0.51
2:b:337:GLN:OE1	2:a:289:THR:OG1	2.28	0.51
2:a:336:LEU:HD11	2:a:347:VAL:HG23	1.92	0.51
3:W:18:GLU:HG3	3:W:68:VAL:HG13	1.93	0.51
2:h:314:TYR:OH	2:f:263:GLN:NE2	2.28	0.51
2:f:433:THR:OG1	2:f:435:ASP:OD1	2.29	0.51
2:d:85:ASN:HB3	2:d:265:LYS:HE2	1.91	0.51
1:K:57:PHE:HB3	1:K:183:ILE:HD11	1.92	0.51
2:k:366:ARG:HE	2:j:364:TRP:HH2	1.57	0.51
1:C:17:LEU:HB3	1:C:22:ALA:HB2	1.93	0.51
2:c:217:CYS:SG	2:c:218:ASP:N	2.84	0.51
2:c:274:TYR:OH	2:c:354:ASP:OD1	2.28	0.51
2:a:244:ASP:OD1	2:a:245:CYS:N	2.40	0.51
1:I:37:CYS:SG	1:I:40:ARG:NH2	2.84	0.51
2:j:507:GLU:O	2:j:510:LYS:NZ	2.44	0.51
2:i:415:GLU:HB2	2:i:446:ILE:HD12	1.93	0.51
2:h:456:GLU:OE2	2:g:492:GLN:NE2	2.43	0.51
2:c:333:ASP:OD2	2:b:285:TRP:NE1	2.44	0.51
2:a:217:CYS:SG	2:a:218:ASP:N	2.83	0.51
2:l:244:ASP:OD1	2:l:245:CYS:N	2.40	0.51
1:G:18:ARG:HH12	1:H:36:ASP:HB2	1.75	0.51
2:k:336:LEU:HD11	2:k:347:VAL:HG23	1.93	0.51
2:h:158:PHE:H	2:h:236:VAL:HG22	1.76	0.51
2:g:366:ARG:HE	2:f:364:TRP:HH2	1.58	0.51
2:a:274:TYR:OH	2:a:354:ASP:OD1	2.28	0.51
1:L:154:MET:SD	1:L:155:LEU:N	2.80	0.51
1:G:39:GLN:HE22	1:G:85:THR:HG21	1.76	0.51
1:K:17:LEU:O	1:K:21:GLY:N	2.44	0.51
4:R:92:SER:OG	4:R:115:THR:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:85:ASN:HB3	2:i:265:LYS:HE2	1.93	0.50
2:e:456:GLU:OE2	2:d:492:GLN:NE2	2.44	0.50
2:b:336:LEU:HD11	2:b:347:VAL:HG23	1.93	0.50
4:P:136:ASP:HB2	4:P:149:ILE:HD12	1.94	0.50
2:k:108:VAL:HG23	2:k:109:VAL:HG22	1.94	0.50
2:h:274:TYR:OH	2:h:354:ASP:OD1	2.26	0.50
2:b:426:LEU:HD23	2:b:432:ILE:HD12	1.93	0.50
2:a:253:TYR:OH	2:a:413:LYS:NZ	2.30	0.50
1:B:18:ARG:HH12	1:C:36:ASP:HB2	1.75	0.50
4:M:136:ASP:HB2	4:M:149:ILE:HD12	1.94	0.50
4:Q:92:SER:OG	4:Q:115:THR:O	2.28	0.50
1:E:17:LEU:O	1:E:21:GLY:N	2.44	0.50
2:i:283:ARG:HH22	2:i:311:ARG:HH22	1.58	0.50
2:f:217:CYS:SG	2:f:218:ASP:N	2.84	0.50
2:e:274:TYR:OH	2:e:354:ASP:OD1	2.27	0.50
1:B:55:LYS:NZ	1:B:185:GLU:OE2	2.44	0.50
2:g:253:TYR:OH	2:g:413:LYS:NZ	2.31	0.50
2:e:415:GLU:HB2	2:e:446:ILE:HD12	1.93	0.50
2:c:309:LYS:NZ	2:c:310:ASN:OD1	2.45	0.50
1:L:36:ASP:HB2	1:K:18:ARG:HH12	1.76	0.50
2:b:85:ASN:HB3	2:b:265:LYS:HE2	1.92	0.50
1:C:57:PHE:HB3	1:C:183:ILE:HD11	1.93	0.50
1:B:39:GLN:HE22	1:B:85:THR:HG21	1.75	0.50
2:k:470:LEU:HB2	2:k:490:ILE:HG21	1.92	0.50
2:i:338:ARG:HG2	2:i:343:ALA:HA	1.93	0.50
1:E:18:ARG:HH12	1:F:36:ASP:HB2	1.77	0.50
4:P:92:SER:OG	4:P:115:THR:O	2.29	0.50
2:i:159:HIS:NE2	2:i:218:ASP:OD1	2.40	0.50
2:h:337:GLN:OE1	2:g:289:THR:OG1	2.29	0.50
2:c:279:ALA:O	2:b:278:ARG:NH1	2.44	0.50
1:L:55:LYS:NZ	1:L:185:GLU:OE2	2.44	0.50
1:A:39:GLN:HE22	1:A:85:THR:HG21	1.75	0.50
2:h:282:ARG:NH2	2:h:351:PRO:O	2.45	0.49
2:e:470:LEU:HB2	2:e:490:ILE:HG21	1.93	0.49
2:d:244:ASP:OD1	2:d:245:CYS:N	2.40	0.49
1:L:37:CYS:SG	1:L:40:ARG:NH2	2.82	0.49
1:C:18:ARG:HH12	1:D:36:ASP:HB2	1.75	0.49
1:E:271:LEU:HB3	1:E:275:VAL:HB	1.94	0.49
2:f:253:TYR:OH	2:f:413:LYS:NZ	2.30	0.49
2:f:359:MET:HE3	2:f:362:ILE:HD12	1.94	0.49
2:e:282:ARG:NH2	2:e:351:PRO:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:470:LEU:HB2	2:c:490:ILE:HG21	1.93	0.49
1:D:17:LEU:O	1:D:21:GLY:N	2.46	0.49
2:i:108:VAL:HG23	2:i:109:VAL:HG22	1.95	0.49
2:g:333:ASP:OD2	2:f:285:TRP:NE1	2.45	0.49
2:b:359:MET:HE3	2:b:362:ILE:HD12	1.95	0.49
1:L:138:LEU:HD13	1:K:169:GLN:HG3	1.94	0.49
1:D:37:CYS:SG	1:D:40:ARG:NH2	2.84	0.49
4:R:25:GLU:HG3	4:R:29:PRO:HG3	1.92	0.49
2:h:426:LEU:HD23	2:h:432:ILE:HD12	1.94	0.49
1:H:57:PHE:HB3	1:H:183:ILE:HD11	1.94	0.49
2:l:415:GLU:HB2	2:l:446:ILE:HD12	1.95	0.49
2:j:415:GLU:HB2	2:j:446:ILE:HD12	1.95	0.49
2:e:244:ASP:OD1	2:e:245:CYS:N	2.41	0.49
2:c:359:MET:HE3	2:c:362:ILE:HD12	1.94	0.49
1:A:55:LYS:NZ	1:A:185:GLU:OE2	2.44	0.49
4:O:143:ASP:OD1	4:O:145:SER:OG	2.26	0.49
2:i:279:ALA:O	2:h:278:ARG:NH1	2.46	0.49
2:c:159:HIS:NE2	2:c:218:ASP:OD1	2.40	0.49
2:c:337:GLN:HG3	2:c:344:VAL:HB	1.94	0.49
1:A:44:LEU:HD21	1:A:294:ARG:HD3	1.95	0.49
1:E:55:LYS:NZ	1:E:185:GLU:OE2	2.43	0.49
1:I:166:ALA:HB2	1:J:131:PRO:HA	1.95	0.49
1:F:17:LEU:O	1:F:21:GLY:N	2.45	0.49
4:N:79:LYS:HE3	4:N:146:LEU:HD13	1.95	0.49
2:k:359:MET:HE3	2:k:362:ILE:HD12	1.94	0.49
2:i:359:MET:HE3	2:i:362:ILE:HD12	1.95	0.49
2:b:158:PHE:H	2:b:236:VAL:HG22	1.78	0.49
1:B:17:LEU:HB3	1:B:22:ALA:HB2	1.95	0.49
1:A:17:LEU:HB3	1:A:22:ALA:HB2	1.95	0.49
1:G:87:ILE:HG22	1:G:184:VAL:HG13	1.94	0.49
4:O:26:ILE:HD12	4:P:85:LYS:HG3	1.94	0.49
2:c:108:VAL:HG23	2:c:109:VAL:HG22	1.95	0.49
2:h:359:MET:HE3	2:h:362:ILE:HD12	1.95	0.48
2:g:415:GLU:HB2	2:g:446:ILE:HD12	1.95	0.48
2:d:274:TYR:OH	2:d:354:ASP:OD1	2.28	0.48
1:B:44:LEU:HD21	1:B:294:ARG:HD3	1.95	0.48
4:N:92:SER:OG	4:N:115:THR:O	2.29	0.48
2:k:282:ARG:NH2	2:k:351:PRO:O	2.46	0.48
2:i:328:MET:HE3	2:g:273:ILE:HD12	1.95	0.48
1:K:39:GLN:HE22	1:K:85:THR:HG21	1.77	0.48
1:G:17:LEU:HB3	1:G:22:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:85:ASN:HB3	2:h:265:LYS:HE2	1.96	0.48
2:e:359:MET:HE3	2:e:362:ILE:HD12	1.94	0.48
1:L:17:LEU:O	1:L:21:GLY:N	2.46	0.48
1:E:169:GLN:HG3	1:F:138:LEU:HD13	1.94	0.48
1:F:154:MET:SD	1:F:155:LEU:N	2.80	0.48
1:I:13:LYS:HG3	1:I:34:ILE:HG21	1.96	0.48
2:l:111:LEU:HD11	2:l:444:ILE:HG22	1.96	0.48
2:k:274:TYR:OH	2:k:354:ASP:OD1	2.26	0.48
2:j:274:TYR:OH	2:j:354:ASP:OD1	2.27	0.48
2:j:281:ASP:OD1	2:j:281:ASP:N	2.47	0.48
2:b:108:VAL:HG23	2:b:109:VAL:HG22	1.96	0.48
1:G:44:LEU:HD21	1:G:294:ARG:HD3	1.95	0.48
1:H:17:LEU:O	1:H:21:GLY:N	2.46	0.48
2:i:274:TYR:OH	2:i:354:ASP:OD1	2.28	0.48
2:h:328:MET:HE3	2:f:273:ILE:HD12	1.96	0.48
2:g:85:ASN:HB3	2:g:265:LYS:HE2	1.96	0.48
2:g:328:MET:HE3	2:e:273:ILE:HD12	1.95	0.48
2:a:359:MET:HE3	2:a:362:ILE:HD12	1.96	0.48
1:C:17:LEU:O	1:C:21:GLY:N	2.47	0.48
1:G:169:GLN:HG3	1:H:138:LEU:HD13	1.96	0.48
4:M:159:TYR:HB3	4:M:164:ASN:ND2	2.26	0.48
2:k:433:THR:OG1	2:k:435:ASP:OD1	2.30	0.48
2:c:305:MET:HE2	1:C:308:VAL:HA	1.96	0.48
2:b:281:ASP:OD1	2:b:281:ASP:N	2.47	0.48
3:S:18:GLU:O	3:S:66:ARG:NH2	2.46	0.48
2:j:333:ASP:OD2	2:i:285:TRP:NE1	2.47	0.48
2:g:243:VAL:O	2:g:251:ILE:N	2.47	0.48
2:d:426:LEU:HD23	2:d:432:ILE:HD12	1.94	0.48
2:b:304:VAL:O	2:b:307:THR:OG1	2.31	0.48
4:M:92:SER:OG	4:M:115:THR:O	2.28	0.48
4:Q:92:SER:O	4:Q:115:THR:OG1	2.28	0.48
2:h:108:VAL:HG23	2:h:109:VAL:HG22	1.95	0.48
2:h:433:THR:OG1	2:h:435:ASP:OD1	2.30	0.48
2:c:433:THR:OG1	2:c:435:ASP:OD1	2.30	0.48
1:I:169:GLN:HG3	1:J:138:LEU:HD13	1.96	0.48
4:N:45:VAL:HG21	4:R:9:PHE:HE2	1.79	0.48
2:d:333:ASP:OD2	2:c:285:TRP:NE1	2.47	0.48
4:P:25:GLU:OE1	4:P:26:ILE:N	2.47	0.47
2:e:279:ALA:O	2:d:278:ARG:NH1	2.47	0.47
2:c:461:GLU:O	2:c:464:GLU:HG3	2.14	0.47
1:L:57:PHE:HB3	1:L:183:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ALA:HB2	1:D:131:PRO:HA	1.96	0.47
1:L:131:PRO:HA	1:K:166:ALA:HB2	1.95	0.47
1:J:176:PHE:HB3	1:J:180:ASP:HB3	1.96	0.47
2:k:461:GLU:O	2:k:464:GLU:HG3	2.15	0.47
2:i:461:GLU:O	2:i:464:GLU:HG3	2.15	0.47
2:h:461:GLU:O	2:h:464:GLU:HG3	2.14	0.47
2:g:470:LEU:HB2	2:g:490:ILE:HG21	1.96	0.47
2:f:304:VAL:O	2:f:307:THR:OG1	2.33	0.47
2:d:243:VAL:O	2:d:251:ILE:N	2.47	0.47
1:G:13:LYS:HG3	1:G:34:ILE:HG21	1.97	0.47
1:H:55:LYS:NZ	1:H:185:GLU:OE2	2.48	0.47
2:d:415:GLU:HB2	2:d:446:ILE:HD12	1.96	0.47
1:C:75:ASP:OD2	1:C:77:ARG:NH1	2.47	0.47
1:E:39:GLN:HE22	1:E:85:THR:HG21	1.79	0.47
1:I:17:LEU:HB3	1:I:22:ALA:HB2	1.97	0.47
2:g:278:ARG:HA	2:g:282:ARG:HH12	1.78	0.47
2:b:111:LEU:HD11	2:b:444:ILE:HG22	1.97	0.47
1:E:166:ALA:HB2	1:F:131:PRO:HA	1.95	0.47
1:J:37:CYS:SG	1:J:40:ARG:NH2	2.85	0.47
2:l:273:ILE:HD12	2:b:328:MET:HE3	1.95	0.47
4:R:79:LYS:HE3	4:R:146:LEU:HD13	1.95	0.47
2:f:337:GLN:HE21	2:f:344:VAL:HG11	1.79	0.47
2:b:86:TYR:O	2:b:87:GLU:HG3	2.14	0.47
1:B:75:ASP:OD2	1:B:77:ARG:NH1	2.48	0.47
4:M:143:ASP:OD1	4:M:145:SER:OG	2.23	0.47
4:R:25:GLU:OE1	4:R:26:ILE:N	2.47	0.47
2:j:461:GLU:O	2:j:464:GLU:HG3	2.15	0.47
2:h:333:ASP:OD2	2:g:285:TRP:NE1	2.48	0.47
2:g:461:GLU:O	2:g:464:GLU:HG3	2.15	0.47
2:e:461:GLU:O	2:e:464:GLU:HG3	2.15	0.47
2:d:306:ASN:HA	2:d:309:LYS:HB2	1.97	0.47
2:c:328:MET:HE3	2:a:273:ILE:HD12	1.95	0.47
2:a:461:GLU:O	2:a:464:GLU:HG3	2.15	0.47
2:a:470:LEU:HB2	2:a:490:ILE:HG21	1.96	0.47
1:A:13:LYS:HG3	1:A:34:ILE:HG21	1.97	0.47
1:D:55:LYS:NZ	1:D:185:GLU:OE2	2.44	0.47
1:G:166:ALA:HB2	1:H:131:PRO:HA	1.96	0.47
1:H:87:ILE:HG22	1:H:184:VAL:HG13	1.96	0.47
1:J:57:PHE:HB3	1:J:183:ILE:HD11	1.96	0.47
1:B:171:LYS:NZ	1:C:143:GLN:HA	2.29	0.47
2:l:328:MET:HE3	2:j:273:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:306:ASN:HA	2:j:309:LYS:HB2	1.97	0.47
2:g:159:HIS:NE2	2:g:218:ASP:OD1	2.42	0.47
2:f:108:VAL:HG23	2:f:109:VAL:HG22	1.97	0.47
2:f:415:GLU:HB2	2:f:446:ILE:HD12	1.96	0.47
2:b:253:TYR:OH	2:b:413:LYS:NZ	2.30	0.47
2:a:243:VAL:O	2:a:251:ILE:N	2.47	0.47
1:I:271:LEU:HB3	1:I:275:VAL:HB	1.96	0.47
4:P:119:ASN:HB3	4:P:122:LEU:HB3	1.97	0.47
2:g:359:MET:HE3	2:g:362:ILE:HD12	1.96	0.47
2:d:359:MET:HE3	2:d:362:ILE:HD12	1.96	0.47
2:a:108:VAL:HG23	2:a:109:VAL:HG22	1.97	0.47
1:C:271:LEU:HB3	1:C:275:VAL:HB	1.97	0.47
1:E:13:LYS:HG3	1:E:34:ILE:HG21	1.97	0.47
1:J:17:LEU:O	1:J:21:GLY:N	2.46	0.47
1:K:13:LYS:HG3	1:K:34:ILE:HG21	1.97	0.47
1:K:75:ASP:OD2	1:K:77:ARG:NH1	2.48	0.47
2:l:359:MET:HE3	2:l:362:ILE:HD12	1.96	0.47
2:k:273:ILE:HD12	2:a:328:MET:HE3	1.97	0.47
2:h:304:VAL:O	2:h:307:THR:OG1	2.33	0.47
2:f:461:GLU:O	2:f:464:GLU:HG3	2.15	0.47
2:e:243:VAL:O	2:e:251:ILE:N	2.48	0.47
2:d:328:MET:HE3	2:b:273:ILE:HD12	1.97	0.47
1:D:87:ILE:HG22	1:D:184:VAL:HG13	1.96	0.47
1:B:22:ALA:HB3	4:R:12:LEU:HD22	1.97	0.46
2:l:260:PRO:O	2:l:263:GLN:HB2	2.15	0.46
4:O:159:TYR:HB3	4:O:164:ASN:ND2	2.27	0.46
2:k:293:PRO:HD2	2:k:296:LYS:HD2	1.97	0.46
2:i:243:VAL:O	2:i:251:ILE:N	2.48	0.46
2:e:328:MET:HE3	2:c:273:ILE:HD12	1.97	0.46
1:D:75:ASP:OD2	1:D:77:ARG:NH1	2.49	0.46
1:E:87:ILE:HG22	1:E:184:VAL:HG13	1.98	0.46
1:I:75:ASP:OD2	1:I:77:ARG:NH1	2.48	0.46
4:Q:25:GLU:OE1	4:Q:26:ILE:N	2.49	0.46
2:f:328:MET:HE3	2:d:273:ILE:HD12	1.97	0.46
2:d:461:GLU:O	2:d:464:GLU:HG3	2.15	0.46
2:k:328:MET:HE3	2:i:273:ILE:HD12	1.97	0.46
2:j:243:VAL:O	2:j:251:ILE:N	2.48	0.46
2:d:111:LEU:HD11	2:d:444:ILE:HG22	1.97	0.46
2:d:433:THR:OG1	2:d:435:ASP:OD1	2.30	0.46
1:B:13:LYS:HB3	1:B:13:LYS:HE3	1.45	0.46
2:l:433:THR:OG1	2:l:435:ASP:OD1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:25:GLU:OE1	4:M:26:ILE:N	2.48	0.46
4:P:26:ILE:HD12	4:Q:85:LYS:HG3	1.97	0.46
2:g:108:VAL:HG23	2:g:109:VAL:HG22	1.96	0.46
2:f:111:LEU:HD11	2:f:444:ILE:HG22	1.96	0.46
2:b:333:ASP:OD2	2:a:285:TRP:NE1	2.49	0.46
1:C:169:GLN:HG3	1:D:138:LEU:HD13	1.96	0.46
1:J:18:ARG:HH12	1:K:36:ASP:HB2	1.80	0.46
1:B:27:VAL:HG11	4:R:10:ALA:HB3	1.96	0.46
1:B:87:ILE:HG22	1:B:184:VAL:HG13	1.96	0.46
2:l:461:GLU:O	2:l:464:GLU:HG3	2.15	0.46
4:N:159:TYR:HB3	4:N:164:ASN:ND2	2.27	0.46
2:j:359:MET:HE3	2:j:362:ILE:HD12	1.97	0.46
2:i:337:GLN:HE21	2:i:344:VAL:HG11	1.80	0.46
2:d:293:PRO:HD2	2:d:296:LYS:HD2	1.95	0.46
2:c:275:ARG:HD2	2:b:267:LEU:HD22	1.96	0.46
1:A:87:ILE:HG22	1:A:184:VAL:HG13	1.96	0.46
1:G:17:LEU:O	1:G:21:GLY:N	2.48	0.46
2:l:108:VAL:HG23	2:l:109:VAL:HG22	1.98	0.46
1:A:75:ASP:OD2	1:A:77:ARG:NH1	2.48	0.46
2:l:285:TRP:NE1	2:a:333:ASP:OD2	2.48	0.46
4:O:25:GLU:OE1	4:O:26:ILE:N	2.49	0.46
2:k:251:ILE:HD11	2:k:255:HIS:CD2	2.51	0.46
2:k:263:GLN:HE21	2:a:314:TYR:HH	1.60	0.46
2:f:305:MET:HE2	1:F:308:VAL:HA	1.98	0.46
1:L:284:GLU:OE2	1:L:287:ARG:NH2	2.47	0.46
1:B:30:THR:HG22	1:B:32:ASP:H	1.81	0.46
2:f:314:TYR:OH	2:d:263:GLN:NE2	2.28	0.46
2:b:461:GLU:O	2:b:464:GLU:HG3	2.15	0.46
2:l:479:LYS:O	2:b:513:ARG:NE	2.49	0.46
3:W:31:LYS:O	4:O:111:GLN:NE2	2.48	0.46
2:k:279:ALA:O	2:j:278:ARG:NH1	2.49	0.46
2:i:122:ILE:HD11	2:i:432:ILE:HG12	1.98	0.46
1:L:18:ARG:HH12	1:A:36:ASP:HB2	1.80	0.46
2:l:243:VAL:O	2:l:251:ILE:N	2.48	0.46
2:l:333:ASP:OD2	2:k:285:TRP:NE1	2.49	0.46
2:f:243:VAL:O	2:f:251:ILE:N	2.49	0.46
2:d:155:ARG:HH21	2:d:250:ILE:HB	1.81	0.46
2:b:260:PRO:O	2:b:263:GLN:HB2	2.16	0.46
1:F:68:ARG:O	1:F:68:ARG:NH1	2.36	0.46
4:O:10:ALA:HB3	1:H:27:VAL:HG11	1.97	0.45
4:O:111:GLN:HB3	4:O:113:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:80:ARG:HD3	2:h:245:CYS:O	2.16	0.45
2:e:305:MET:HE2	1:E:308:VAL:HA	1.98	0.45
2:d:253:TYR:OH	2:d:413:LYS:NZ	2.31	0.45
2:b:251:ILE:HD11	2:b:255:HIS:CD2	2.51	0.45
1:A:30:THR:HG22	1:A:32:ASP:H	1.81	0.45
1:D:88:LEU:HB2	1:D:183:ILE:HG23	1.98	0.45
1:E:75:ASP:OD2	1:E:77:ARG:NH1	2.48	0.45
1:J:88:LEU:HB2	1:J:183:ILE:HG23	1.98	0.45
2:l:304:VAL:O	2:l:307:THR:OG1	2.32	0.45
2:e:251:ILE:HD11	2:e:255:HIS:CD2	2.52	0.45
2:e:283:ARG:HH22	2:e:311:ARG:HH22	1.63	0.45
2:e:295:ARG:NH2	1:E:50:PHE:O	2.41	0.45
1:L:48:TYR:HE2	1:L:300:LEU:HD12	1.82	0.45
1:C:13:LYS:HG3	1:C:34:ILE:HG21	1.97	0.45
1:G:176:PHE:HB3	1:G:180:ASP:HB3	1.98	0.45
2:h:221:MET:SD	2:h:221:MET:N	2.90	0.45
1:D:154:MET:SD	1:D:155:LEU:N	2.83	0.45
1:F:88:LEU:HB2	1:F:183:ILE:HG23	1.97	0.45
1:B:17:LEU:O	1:B:21:GLY:N	2.49	0.45
1:B:308:VAL:CG1	2:c:333:ASP:H	2.30	0.45
4:N:119:ASN:HB3	4:N:122:LEU:HB3	1.99	0.45
4:M:111:GLN:HB3	4:M:113:GLU:HG2	1.99	0.45
4:P:79:LYS:HE3	4:P:146:LEU:HD13	1.98	0.45
2:g:80:ARG:HD3	2:f:245:CYS:O	2.17	0.45
2:g:474:GLU:HG3	2:g:475:PRO:HD3	1.97	0.45
2:f:470:LEU:HB2	2:f:490:ILE:HG21	1.98	0.45
2:e:221:MET:SD	2:e:221:MET:N	2.90	0.45
2:c:122:ILE:HD11	2:c:432:ILE:HG12	1.99	0.45
1:D:18:ARG:HH12	1:E:36:ASP:HB2	1.81	0.45
2:l:122:ILE:O	2:l:125:MET:HG3	2.17	0.45
2:l:221:MET:SD	2:l:221:MET:N	2.90	0.45
2:h:251:ILE:HD11	2:h:255:HIS:CD2	2.52	0.45
2:e:80:ARG:HD3	2:d:245:CYS:O	2.17	0.45
2:e:288:ASP:HB2	2:e:344:VAL:HG13	1.99	0.45
2:c:111:LEU:HD11	2:c:444:ILE:HG22	1.98	0.45
2:b:80:ARG:HD3	2:a:245:CYS:O	2.17	0.45
1:F:13:LYS:HG3	1:F:34:ILE:HG21	1.99	0.45
1:G:158:ILE:HG22	1:G:160:ASP:H	1.80	0.45
1:I:30:THR:HG22	1:I:32:ASP:H	1.82	0.45
1:J:284:GLU:OE2	1:J:287:ARG:NH2	2.47	0.45
2:l:305:MET:HE2	1:L:308:VAL:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:221:MET:N	2:k:221:MET:SD	2.90	0.45
2:j:108:VAL:HG23	2:j:109:VAL:HG22	1.99	0.45
2:i:275:ARG:HD2	2:h:267:LEU:HD22	1.97	0.45
2:h:80:ARG:HD3	2:g:245:CYS:O	2.17	0.45
2:h:243:VAL:O	2:h:251:ILE:N	2.50	0.45
2:f:221:MET:N	2:f:221:MET:SD	2.89	0.45
2:e:304:VAL:O	2:e:307:THR:OG1	2.34	0.45
2:c:85:ASN:HB3	2:c:265:LYS:HE2	1.99	0.45
2:c:243:VAL:O	2:c:251:ILE:N	2.49	0.45
1:K:87:ILE:HG22	1:K:184:VAL:HG13	1.98	0.45
2:j:155:ARG:HH21	2:j:250:ILE:HB	1.82	0.45
2:h:111:LEU:HD11	2:h:444:ILE:HG22	1.97	0.45
2:f:275:ARG:HD2	2:e:267:LEU:HD22	1.98	0.45
2:f:306:ASN:HA	2:f:309:LYS:HB2	1.99	0.45
2:e:125:MET:HE2	2:e:125:MET:HB2	1.85	0.45
4:N:25:GLU:OE1	4:N:26:ILE:N	2.50	0.45
2:k:282:ARG:HB2	2:k:350:LEU:HB2	1.99	0.45
2:j:122:ILE:O	2:j:125:MET:HG3	2.17	0.45
2:j:279:ALA:HB3	2:j:280:PRO:HD3	1.99	0.45
2:i:279:ALA:HB3	2:i:280:PRO:HD3	1.99	0.45
2:g:314:TYR:OH	2:e:263:GLN:NE2	2.29	0.45
2:e:337:GLN:OE1	2:d:289:THR:OG1	2.34	0.45
2:b:243:VAL:O	2:b:251:ILE:N	2.49	0.45
2:b:433:THR:OG1	2:b:435:ASP:OD1	2.29	0.45
1:L:88:LEU:HB2	1:L:183:ILE:HG23	1.98	0.45
1:A:17:LEU:O	1:A:21:GLY:N	2.49	0.45
1:K:158:ILE:HG22	1:K:160:ASP:H	1.82	0.45
4:P:111:GLN:HB3	4:P:113:GLU:HG2	1.98	0.45
2:j:221:MET:SD	2:j:221:MET:N	2.90	0.45
2:h:306:ASN:HA	2:h:309:LYS:HB2	1.99	0.45
2:h:470:LEU:HB2	2:h:490:ILE:HG21	1.98	0.45
2:f:260:PRO:O	2:f:263:GLN:HB2	2.17	0.45
2:f:396:ILE:HD13	2:f:458:LYS:HG3	1.99	0.45
2:d:221:MET:SD	2:d:221:MET:N	2.90	0.45
2:b:338:ARG:N	2:a:287:VAL:O	2.50	0.45
1:L:87:ILE:HG22	1:L:184:VAL:HG13	1.99	0.45
1:E:44:LEU:HD21	1:E:294:ARG:HD3	1.98	0.45
1:F:18:ARG:HH12	1:G:36:ASP:HB2	1.82	0.45
1:G:30:THR:HG22	1:G:32:ASP:H	1.82	0.45
1:I:17:LEU:O	1:I:21:GLY:N	2.49	0.45
2:l:306:ASN:HA	2:l:309:LYS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:396:ILE:HD13	2:l:458:LYS:HG3	1.99	0.45
2:j:260:PRO:O	2:j:263:GLN:HB2	2.17	0.45
2:h:260:PRO:O	2:h:263:GLN:HB2	2.16	0.45
2:g:245:CYS:SG	2:g:246:CYS:N	2.90	0.45
2:g:251:ILE:HD11	2:g:255:HIS:CD2	2.52	0.45
2:g:304:VAL:O	2:g:307:THR:OG1	2.35	0.45
2:d:80:ARG:HD3	2:c:245:CYS:O	2.17	0.45
2:c:80:ARG:HD3	2:b:245:CYS:O	2.17	0.45
2:a:306:ASN:HA	2:a:309:LYS:HB2	1.99	0.45
1:A:27:VAL:HG22	1:A:29:LEU:HB2	1.98	0.45
1:B:27:VAL:CG1	4:R:10:ALA:O	2.65	0.44
2:k:243:VAL:O	2:k:251:ILE:N	2.49	0.44
2:k:306:ASN:HA	2:k:309:LYS:HB2	2.00	0.44
2:j:80:ARG:HD3	2:i:245:CYS:O	2.17	0.44
2:h:125:MET:HE2	2:h:125:MET:HB2	1.88	0.44
2:f:333:ASP:OD2	2:e:285:TRP:NE1	2.49	0.44
2:e:433:THR:OG1	2:e:435:ASP:OD1	2.32	0.44
1:A:158:ILE:HG22	1:A:160:ASP:H	1.82	0.44
1:D:13:LYS:HG3	1:D:34:ILE:HG21	1.99	0.44
1:D:48:TYR:HE2	1:D:300:LEU:HD12	1.82	0.44
1:B:158:ILE:HG22	1:B:160:ASP:H	1.82	0.44
2:l:245:CYS:O	2:a:80:ARG:HD3	2.17	0.44
2:l:279:ALA:HB3	2:l:280:PRO:HD3	1.99	0.44
2:h:282:ARG:HB2	2:h:350:LEU:HB2	2.00	0.44
2:h:338:ARG:N	2:g:287:VAL:O	2.51	0.44
2:f:80:ARG:HD3	2:e:245:CYS:O	2.17	0.44
2:d:108:VAL:HG23	2:d:109:VAL:HG22	1.99	0.44
2:b:221:MET:SD	2:b:221:MET:N	2.90	0.44
2:a:396:ILE:HD13	2:a:458:LYS:HG3	1.99	0.44
1:D:57:PHE:HB3	1:D:183:ILE:HD11	1.98	0.44
1:I:44:LEU:HD21	1:I:294:ARG:HD3	1.99	0.44
1:I:158:ILE:HG22	1:I:160:ASP:H	1.82	0.44
1:K:30:THR:HG22	1:K:32:ASP:H	1.82	0.44
1:K:284:GLU:OE2	1:K:287:ARG:NH2	2.48	0.44
1:B:27:VAL:HG22	1:B:29:LEU:HB2	1.98	0.44
2:l:337:GLN:OE1	2:k:289:THR:OG1	2.34	0.44
4:Q:111:GLN:HB3	4:Q:113:GLU:HG2	1.99	0.44
2:k:80:ARG:HD3	2:j:245:CYS:O	2.17	0.44
2:j:251:ILE:HD11	2:j:255:HIS:CD2	2.53	0.44
2:e:159:HIS:NE2	2:e:218:ASP:OD1	2.50	0.44
1:C:87:ILE:HG22	1:C:184:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:PHE:HB3	1:F:183:ILE:HD11	1.99	0.44
1:I:48:TYR:HE2	1:I:300:LEU:HD12	1.83	0.44
1:B:171:LYS:HZ2	1:C:143:GLN:HA	1.83	0.44
2:l:125:MET:HE2	2:l:125:MET:HB2	1.93	0.44
3:V:31:LYS:O	4:P:111:GLN:NE2	2.51	0.44
2:i:305:MET:HE2	1:I:308:VAL:HA	1.99	0.44
2:i:333:ASP:OD2	2:h:285:TRP:NE1	2.51	0.44
2:c:396:ILE:HD13	2:c:458:LYS:HG3	2.00	0.44
1:D:284:GLU:OE2	1:D:287:ARG:NH2	2.48	0.44
2:l:80:ARG:HD3	2:k:245:CYS:O	2.18	0.44
2:l:470:LEU:HB2	2:l:490:ILE:HG21	1.98	0.44
4:R:92:SER:O	4:R:115:THR:OG1	2.28	0.44
2:k:122:ILE:O	2:k:125:MET:HG3	2.18	0.44
2:d:125:MET:HE2	2:d:125:MET:HB2	1.90	0.44
2:d:314:TYR:OH	2:b:263:GLN:NE2	2.30	0.44
2:a:221:MET:SD	2:a:221:MET:N	2.91	0.44
2:a:278:ARG:HA	2:a:282:ARG:HH12	1.81	0.44
2:l:275:ARG:HD2	2:k:267:LEU:HD22	1.98	0.44
2:g:433:THR:OG1	2:g:435:ASP:OD1	2.33	0.44
2:e:87:GLU:OE1	2:e:366:ARG:HG2	2.18	0.44
2:a:304:VAL:O	2:a:307:THR:OG1	2.34	0.44
2:k:279:ALA:HB3	2:k:280:PRO:HD3	1.99	0.44
2:k:333:ASP:OD2	2:j:285:TRP:NE1	2.50	0.44
2:i:111:LEU:HD11	2:i:444:ILE:HG22	2.00	0.44
2:h:279:ALA:HB3	2:h:280:PRO:HD3	1.99	0.44
2:g:111:LEU:HD11	2:g:444:ILE:HG22	2.00	0.44
2:e:111:LEU:HD11	2:e:444:ILE:HG22	2.00	0.44
2:a:245:CYS:SG	2:a:246:CYS:N	2.91	0.44
2:a:260:PRO:O	2:a:263:GLN:HB2	2.18	0.44
2:k:305:MET:HE2	1:K:308:VAL:HA	2.00	0.44
2:i:306:ASN:HA	2:i:309:LYS:HB2	2.00	0.44
2:g:275:ARG:HD2	2:f:267:LEU:HD22	2.00	0.44
2:g:293:PRO:HD2	2:g:296:LYS:HD2	1.99	0.44
2:g:306:ASN:HA	2:g:309:LYS:HB2	2.00	0.44
2:d:304:VAL:O	2:d:307:THR:OG1	2.35	0.44
1:J:13:LYS:HG3	1:J:34:ILE:HG21	2.00	0.44
1:J:48:TYR:HE2	1:J:300:LEU:HD12	1.82	0.44
2:l:293:PRO:HD2	2:l:296:LYS:HD2	1.99	0.44
4:O:8:LEU:HD11	1:G:23:PRO:HB2	2.00	0.44
4:O:12:LEU:HD22	1:H:22:ALA:HB3	2.00	0.44
4:O:119:ASN:HB3	4:O:122:LEU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:295:ARG:NH2	1:K:50:PHE:O	2.44	0.44
2:j:113:LEU:HD22	2:j:444:ILE:HD12	2.00	0.44
2:i:122:ILE:O	2:i:125:MET:HG3	2.18	0.44
2:i:251:ILE:HD11	2:i:255:HIS:CD2	2.53	0.44
2:g:279:ALA:HB3	2:g:280:PRO:HD3	2.00	0.44
2:e:306:ASN:HA	2:e:309:LYS:HB2	2.00	0.44
2:d:245:CYS:SG	2:d:246:CYS:N	2.90	0.44
2:b:125:MET:HE2	2:b:125:MET:HB2	1.89	0.44
2:a:279:ALA:HB3	2:a:280:PRO:HD3	2.00	0.44
1:E:284:GLU:OE2	1:E:287:ARG:NH2	2.49	0.44
4:O:79:LYS:HE3	4:O:146:LEU:HD13	1.98	0.43
2:j:125:MET:HE2	2:j:125:MET:HB2	1.94	0.43
2:i:433:THR:OG1	2:i:435:ASP:OD1	2.31	0.43
2:f:279:ALA:HB3	2:f:280:PRO:HD3	1.98	0.43
2:e:282:ARG:HB2	2:e:350:LEU:HB2	2.00	0.43
2:b:279:ALA:HB3	2:b:280:PRO:HD3	1.99	0.43
2:a:305:MET:HE2	1:A:308:VAL:HA	2.00	0.43
1:C:176:PHE:HB3	1:C:180:ASP:HB3	2.00	0.43
1:E:30:THR:HG22	1:E:32:ASP:H	1.82	0.43
1:I:27:VAL:HG22	1:I:29:LEU:HB2	2.00	0.43
2:g:122:ILE:O	2:g:125:MET:HG3	2.18	0.43
1:E:176:PHE:HB3	1:E:180:ASP:HB3	2.00	0.43
4:Q:159:TYR:HB3	4:Q:164:ASN:ND2	2.26	0.43
2:k:86:TYR:O	2:k:87:GLU:HG2	2.18	0.43
2:k:304:VAL:O	2:k:307:THR:OG1	2.34	0.43
2:i:86:TYR:O	2:i:87:GLU:HG2	2.18	0.43
2:i:260:PRO:O	2:i:263:GLN:HB2	2.18	0.43
2:h:305:MET:HE2	1:H:308:VAL:HA	2.00	0.43
2:e:474:GLU:HG3	2:e:475:PRO:HD3	1.99	0.43
1:A:176:PHE:HB3	1:A:180:ASP:HB3	1.99	0.43
1:C:44:LEU:HD21	1:C:294:ARG:HD3	1.99	0.43
1:E:37:CYS:SG	1:E:40:ARG:NH2	2.89	0.43
2:l:251:ILE:HD11	2:l:255:HIS:CD2	2.53	0.43
2:g:281:ASP:OD1	2:g:281:ASP:N	2.46	0.43
2:d:279:ALA:HB3	2:d:280:PRO:HD3	1.99	0.43
2:c:279:ALA:HB3	2:c:280:PRO:HD3	1.99	0.43
2:b:339:ARG:HH21	1:A:298:TYR:HB3	1.83	0.43
1:K:112:LEU:H	1:K:112:LEU:HD23	1.83	0.43
1:B:176:PHE:HB3	1:B:180:ASP:HB3	1.99	0.43
3:T:31:LYS:O	4:R:111:GLN:NE2	2.51	0.43
4:N:111:GLN:HB3	4:N:113:GLU:HG2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:221:MET:SD	2:i:221:MET:N	2.92	0.43
2:i:295:ARG:NH2	1:I:50:PHE:O	2.40	0.43
2:g:86:TYR:O	2:g:87:GLU:HG2	2.18	0.43
2:f:251:ILE:HD11	2:f:255:HIS:CD2	2.53	0.43
2:c:260:PRO:O	2:c:263:GLN:HB2	2.19	0.43
1:J:166:ALA:HB2	1:K:131:PRO:HA	2.01	0.43
4:R:111:GLN:HB3	4:R:113:GLU:HG2	2.00	0.43
2:e:396:ILE:HD13	2:e:458:LYS:HG3	2.01	0.43
1:C:30:THR:HG22	1:C:32:ASP:H	1.83	0.43
1:C:158:ILE:HG22	1:C:160:ASP:H	1.83	0.43
2:k:111:LEU:HD11	2:k:444:ILE:HG22	2.01	0.43
2:h:295:ARG:NH2	1:H:50:PHE:O	2.39	0.43
2:e:275:ARG:HD2	2:d:267:LEU:HD22	2.01	0.43
2:e:279:ALA:HB3	2:e:280:PRO:HD3	1.99	0.43
2:c:122:ILE:O	2:c:125:MET:HG3	2.18	0.43
2:a:293:PRO:HD2	2:a:296:LYS:HD2	2.00	0.43
1:H:88:LEU:HB2	1:H:183:ILE:HG23	1.99	0.43
2:l:267:LEU:HD22	2:a:275:ARG:HD2	2.00	0.43
2:g:221:MET:SD	2:g:221:MET:N	2.92	0.43
2:f:293:PRO:HD2	2:f:296:LYS:HD2	2.01	0.43
2:e:333:ASP:OD2	2:d:285:TRP:NE1	2.52	0.43
1:I:87:ILE:HG22	1:I:184:VAL:HG13	2.01	0.43
1:B:298:TYR:HB3	2:c:339:ARG:HH21	1.84	0.43
4:P:89:TYR:HD2	4:P:92:SER:HB3	1.84	0.43
2:k:278:ARG:HA	2:k:282:ARG:HH12	1.83	0.43
2:d:275:ARG:HD2	2:c:267:LEU:HD22	2.01	0.43
2:c:251:ILE:HD11	2:c:255:HIS:CD2	2.54	0.43
2:b:470:LEU:HB2	2:b:490:ILE:HG21	2.01	0.43
2:a:251:ILE:HD11	2:a:255:HIS:CD2	2.53	0.43
1:I:275:VAL:HG13	1:J:266:HIS:HA	2.01	0.43
2:l:467:ILE:HG13	2:k:473:ALA:HB2	2.01	0.43
2:j:304:VAL:O	2:j:307:THR:OG1	2.35	0.43
2:d:251:ILE:HD11	2:d:255:HIS:CD2	2.53	0.43
2:c:221:MET:SD	2:c:221:MET:N	2.92	0.43
2:b:278:ARG:HA	2:b:282:ARG:HH12	1.83	0.43
2:b:467:ILE:HG13	2:a:473:ALA:HB2	2.00	0.43
1:F:87:ILE:HG22	1:F:184:VAL:HG13	2.00	0.43
4:P:155:TYR:HD1	4:P:155:TYR:HA	1.74	0.42
2:k:113:LEU:HB2	2:k:123:LYS:HE3	2.01	0.42
2:j:278:ARG:HA	2:j:282:ARG:HH12	1.82	0.42
2:h:396:ILE:HD13	2:h:458:LYS:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:111:LEU:HD11	2:a:444:ILE:HG22	2.01	0.42
1:I:176:PHE:HB3	1:I:180:ASP:HB3	2.01	0.42
1:K:88:LEU:HB2	1:K:183:ILE:HG23	2.01	0.42
2:l:232:LYS:HE2	2:l:232:LYS:HB2	1.87	0.42
4:N:89:TYR:HD2	4:N:92:SER:HB3	1.84	0.42
4:O:89:TYR:HD2	4:O:92:SER:HB3	1.83	0.42
4:Q:79:LYS:HE3	4:Q:146:LEU:HD13	2.00	0.42
2:j:293:PRO:HD2	2:j:296:LYS:HD2	2.01	0.42
2:d:467:ILE:HG13	2:c:473:ALA:HB2	1.99	0.42
1:L:75:ASP:OD2	1:L:77:ARG:NH1	2.53	0.42
1:L:112:LEU:HD23	1:L:112:LEU:H	1.84	0.42
1:K:44:LEU:HD21	1:K:294:ARG:HD3	2.01	0.42
1:B:303:PRO:CB	2:c:300:HIS:NE2	2.75	0.42
2:l:426:LEU:HB3	2:l:432:ILE:HB	2.01	0.42
4:R:133:LYS:N	4:R:136:ASP:OD2	2.52	0.42
2:e:278:ARG:HA	2:e:282:ARG:HH12	1.84	0.42
2:c:86:TYR:O	2:c:87:GLU:HG2	2.19	0.42
1:B:169:GLN:HG3	1:C:138:LEU:HD13	2.01	0.42
2:l:282:ARG:HB2	2:l:350:LEU:HB2	2.02	0.42
2:l:337:GLN:HE21	2:l:344:VAL:HG11	1.84	0.42
3:T:18:GLU:O	3:T:66:ARG:NH2	2.53	0.42
2:f:281:ASP:OD1	2:f:281:ASP:N	2.45	0.42
2:e:122:ILE:O	2:e:125:MET:HG3	2.19	0.42
2:e:245:CYS:SG	2:e:246:CYS:N	2.92	0.42
2:e:300:HIS:HE1	1:D:303:PRO:HB3	1.84	0.42
2:d:396:ILE:HD13	2:d:458:LYS:HG3	2.02	0.42
2:b:122:ILE:O	2:b:125:MET:HG3	2.20	0.42
1:B:284:GLU:OE2	1:B:287:ARG:NH2	2.50	0.42
4:M:89:TYR:HD2	4:M:92:SER:HB3	1.84	0.42
4:P:10:ALA:HB3	1:F:27:VAL:HG11	2.02	0.42
2:g:305:MET:HE2	1:G:308:VAL:HA	2.00	0.42
2:a:122:ILE:O	2:a:125:MET:HG3	2.19	0.42
1:H:284:GLU:OE2	1:H:287:ARG:NH2	2.46	0.42
1:I:284:GLU:OE2	1:I:287:ARG:NH2	2.50	0.42
1:K:176:PHE:HB3	1:K:180:ASP:HB3	2.00	0.42
1:B:171:LYS:NZ	1:C:143:GLN:HG2	2.35	0.42
2:f:122:ILE:O	2:f:125:MET:HG3	2.20	0.42
2:f:125:MET:HE2	2:f:125:MET:HB2	1.86	0.42
2:b:275:ARG:HD2	2:a:267:LEU:HD22	2.02	0.42
1:D:30:THR:HG22	1:D:32:ASP:H	1.84	0.42
1:J:44:LEU:HD21	1:J:294:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ASN:HB2	1:B:131:PRO:HD2	2.01	0.42
1:B:308:VAL:HG11	2:c:332:GLU:HA	2.01	0.42
2:l:272:VAL:O	2:l:276:ILE:HG12	2.20	0.42
3:X:25:TYR:HE2	3:X:31:LYS:HE2	1.84	0.42
3:X:31:LYS:O	4:M:111:GLN:NE2	2.52	0.42
2:j:328:MET:HE3	2:h:273:ILE:HD12	2.01	0.42
2:i:304:VAL:O	2:i:307:THR:OG1	2.35	0.42
2:b:306:ASN:HA	2:b:309:LYS:HB2	2.02	0.42
2:d:260:PRO:O	2:d:263:GLN:HB2	2.20	0.42
2:d:305:MET:HE2	1:D:308:VAL:HA	2.02	0.42
1:D:44:LEU:HD21	1:D:294:ARG:HD3	2.02	0.42
1:E:158:ILE:HG22	1:E:160:ASP:H	1.85	0.42
1:G:88:LEU:HB2	1:G:183:ILE:HG23	2.02	0.42
1:H:112:LEU:HD23	1:H:112:LEU:H	1.84	0.42
4:R:89:TYR:HD2	4:R:92:SER:HB3	1.85	0.42
2:i:396:ILE:HD13	2:i:458:LYS:HG3	2.01	0.42
2:g:82:LEU:HG	2:g:88:VAL:HG11	2.01	0.42
2:g:155:ARG:HH21	2:g:250:ILE:HB	1.85	0.42
1:C:112:LEU:HD23	1:C:112:LEU:H	1.85	0.42
1:D:112:LEU:H	1:D:112:LEU:HD23	1.85	0.42
1:F:48:TYR:HE2	1:F:300:LEU:HD12	1.84	0.42
1:F:112:LEU:H	1:F:112:LEU:HD23	1.85	0.42
1:J:30:THR:HG22	1:J:32:ASP:H	1.85	0.42
1:B:303:PRO:HB3	2:c:300:HIS:CE1	2.54	0.42
2:h:293:PRO:HD2	2:h:296:LYS:HD2	2.01	0.42
2:d:339:ARG:HG3	2:d:344:VAL:HG21	2.00	0.42
1:A:284:GLU:OE2	1:A:287:ARG:NH2	2.50	0.42
1:F:30:THR:HG22	1:F:32:ASP:H	1.85	0.42
2:j:467:ILE:HG13	2:i:473:ALA:HB2	2.01	0.41
2:f:510:LYS:HE2	2:f:510:LYS:HB2	1.92	0.41
2:e:260:PRO:O	2:e:263:GLN:HB2	2.20	0.41
1:E:112:LEU:HD23	1:E:112:LEU:H	1.84	0.41
4:M:12:LEU:HD22	1:J:22:ALA:HB3	2.02	0.41
2:k:275:ARG:HD2	2:j:267:LEU:HD22	2.01	0.41
2:h:339:ARG:HH21	1:G:298:TYR:HB3	1.85	0.41
1:L:85:THR:OG1	1:L:185:GLU:OE1	2.37	0.41
1:C:37:CYS:SG	1:C:40:ARG:NH2	2.92	0.41
3:W:25:TYR:HE2	3:W:31:LYS:HE2	1.86	0.41
2:j:305:MET:HE2	1:J:308:VAL:HA	2.02	0.41
2:g:96:VAL:HG23	2:g:147:PHE:HB3	2.03	0.41
2:f:272:VAL:O	2:f:276:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:282:ARG:NH2	2:b:351:PRO:O	2.53	0.41
2:b:396:ILE:HD13	2:b:458:LYS:HG3	2.02	0.41
2:a:339:ARG:HH21	1:L:298:TYR:HB3	1.85	0.41
1:L:13:LYS:HG3	1:L:34:ILE:HG21	2.02	0.41
1:C:130:GLY:HA3	1:C:131:PRO:HD3	1.96	0.41
1:D:166:ALA:HB2	1:E:131:PRO:HA	2.01	0.41
1:H:166:ALA:HB2	1:I:131:PRO:HA	2.02	0.41
1:J:294:ARG:HH21	1:J:298:TYR:HH	1.61	0.41
2:h:275:ARG:HD2	2:g:267:LEU:HD22	2.03	0.41
1:G:27:VAL:HG22	1:G:29:LEU:HB2	2.02	0.41
3:W:46:LEU:HB3	3:W:52:GLN:HB3	2.01	0.41
2:d:338:ARG:N	2:c:287:VAL:O	2.54	0.41
2:a:272:VAL:O	2:a:276:ILE:HG12	2.21	0.41
1:H:44:LEU:HD21	1:H:294:ARG:HD3	2.02	0.41
1:H:176:PHE:HB3	1:H:180:ASP:HB3	2.02	0.41
4:Q:89:TYR:HD2	4:Q:92:SER:HB3	1.86	0.41
2:i:206:PHE:HE2	2:i:232:LYS:HD3	1.86	0.41
2:h:467:ILE:HG13	2:g:473:ALA:HB2	2.03	0.41
2:g:122:ILE:HD11	2:g:432:ILE:HG12	2.02	0.41
2:f:467:ILE:HG13	2:e:473:ALA:HB2	2.03	0.41
1:L:30:THR:HG22	1:L:32:ASP:H	1.86	0.41
1:A:54:ASN:HB2	1:A:131:PRO:HD2	2.01	0.41
3:V:42:PHE:HD1	3:V:42:PHE:HA	1.80	0.41
4:N:10:ALA:HB3	1:L:27:VAL:HG11	2.01	0.41
4:O:24:THR:OG1	4:O:25:GLU:N	2.54	0.41
4:P:30:TYR:CE1	1:F:23:PRO:HB2	2.56	0.41
4:R:24:THR:OG1	4:R:25:GLU:N	2.53	0.41
4:R:159:TYR:HB3	4:R:164:ASN:ND2	2.26	0.41
2:k:260:PRO:O	2:k:263:GLN:HB2	2.20	0.41
2:j:112:ASN:OD1	2:j:445:LYS:HB2	2.21	0.41
2:i:96:VAL:HG23	2:i:147:PHE:HB3	2.03	0.41
2:g:264:LEU:HD23	2:g:369:LEU:HD12	2.03	0.41
2:f:339:ARG:HH21	1:E:298:TYR:HB3	1.85	0.41
2:c:96:VAL:HG23	2:c:147:PHE:HB3	2.03	0.41
2:a:160:LYS:N	2:a:234:ALA:O	2.45	0.41
1:F:284:GLU:OE2	1:F:287:ARG:NH2	2.52	0.41
1:K:27:VAL:HG22	1:K:29:LEU:HB2	2.03	0.41
2:k:125:MET:HE2	2:k:125:MET:HB2	1.87	0.41
2:j:426:LEU:HB3	2:j:432:ILE:HB	2.03	0.41
2:h:122:ILE:O	2:h:125:MET:HG3	2.21	0.41
2:f:146:HIS:HD2	2:f:176:ARG:HH21	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:456:GLU:O	2:b:459:GLU:HG3	2.21	0.41
1:K:37:CYS:SG	1:K:40:ARG:NH2	2.91	0.41
2:l:245:CYS:SG	2:l:246:CYS:N	2.94	0.41
3:X:18:GLU:O	3:X:66:ARG:NH2	2.54	0.41
3:T:25:TYR:HE2	3:T:31:LYS:HE2	1.86	0.41
4:P:12:LEU:HD22	1:F:22:ALA:HB3	2.03	0.41
4:Q:12:LEU:HD22	1:D:22:ALA:HB3	2.01	0.41
4:R:119:ASN:HB3	4:R:122:LEU:HB3	2.03	0.41
2:i:125:MET:HE2	2:i:125:MET:HB2	1.85	0.41
2:g:260:PRO:O	2:g:263:GLN:HB2	2.21	0.41
2:f:86:TYR:O	2:f:87:GLU:HG2	2.20	0.41
2:e:272:VAL:O	2:e:276:ILE:HG12	2.21	0.41
2:d:87:GLU:OE1	2:d:366:ARG:HG2	2.21	0.41
2:d:278:ARG:HA	2:d:282:ARG:HH12	1.84	0.41
2:c:125:MET:HE2	2:c:125:MET:HB2	1.85	0.41
1:D:158:ILE:HG22	1:D:160:ASP:H	1.86	0.41
1:D:176:PHE:HB3	1:D:180:ASP:HB3	2.02	0.41
1:I:112:LEU:HD23	1:I:112:LEU:H	1.85	0.41
1:K:54:ASN:HB2	1:K:131:PRO:HD2	2.03	0.41
2:k:245:CYS:SG	2:k:246:CYS:N	2.94	0.41
2:c:272:VAL:O	2:c:276:ILE:HG12	2.20	0.41
2:b:245:CYS:SG	2:b:246:CYS:N	2.94	0.41
1:B:88:LEU:HB2	1:B:183:ILE:HG23	2.04	0.40
2:h:113:LEU:HB2	2:h:123:LYS:HE3	2.02	0.40
2:h:157:PHE:HB2	2:h:177:LEU:HB2	2.02	0.40
2:f:146:HIS:CD2	2:f:176:ARG:HH21	2.39	0.40
1:G:130:GLY:HA3	1:G:131:PRO:HD3	1.96	0.40
2:l:426:LEU:HD23	2:l:432:ILE:HG13	2.03	0.40
3:U:31:LYS:O	4:Q:111:GLN:NE2	2.53	0.40
4:Q:24:THR:OG1	4:Q:25:GLU:N	2.55	0.40
2:k:474:GLU:N	2:k:475:PRO:HD2	2.36	0.40
2:e:251:ILE:HD11	2:e:255:HIS:CG	2.56	0.40
1:C:27:VAL:HG22	1:C:29:LEU:HB2	2.03	0.40
1:J:75:ASP:OD2	1:J:77:ARG:NH1	2.54	0.40
2:h:456:GLU:O	2:h:459:GLU:HG3	2.21	0.40
2:g:456:GLU:O	2:g:459:GLU:HG3	2.21	0.40
2:d:82:LEU:HG	2:d:88:VAL:HG11	2.04	0.40
2:b:293:PRO:HD2	2:b:296:LYS:HD2	2.04	0.40
2:a:159:HIS:NE2	2:a:218:ASP:OD1	2.41	0.40
2:a:474:GLU:HG3	2:a:475:PRO:HD3	2.02	0.40
1:A:162:TRP:HZ3	1:A:173:MET:HG3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:GLU:OE2	1:C:287:ARG:NH2	2.52	0.40
1:G:112:LEU:HD23	1:G:112:LEU:H	1.85	0.40
1:B:162:TRP:HZ3	1:B:173:MET:HG3	1.87	0.40
2:l:456:GLU:O	2:l:459:GLU:HG3	2.21	0.40
4:O:92:SER:O	4:O:115:THR:OG1	2.28	0.40
2:j:249:ASN:OD1	2:j:249:ASN:N	2.54	0.40
2:h:249:ASN:OD1	2:h:249:ASN:N	2.54	0.40
2:e:82:LEU:HG	2:e:88:VAL:HG11	2.03	0.40
2:d:470:LEU:HB2	2:d:490:ILE:HG21	2.02	0.40
2:c:456:GLU:O	2:c:459:GLU:HG3	2.21	0.40
1:E:130:GLY:HA3	1:E:131:PRO:HD3	1.97	0.40
1:I:54:ASN:HB2	1:I:131:PRO:HD2	2.04	0.40
1:I:109:ASP:OD1	1:I:109:ASP:N	2.55	0.40
1:J:154:MET:SD	1:J:155:LEU:N	2.83	0.40
4:N:12:LEU:HD22	1:L:22:ALA:HB3	2.04	0.40
2:k:396:ILE:HD13	2:k:458:LYS:HG3	2.03	0.40
2:i:272:VAL:O	2:i:276:ILE:HG12	2.21	0.40
2:i:282:ARG:HB2	2:i:350:LEU:HB2	2.03	0.40
2:e:113:LEU:HB2	2:e:123:LYS:HE3	2.03	0.40
1:A:88:LEU:HB2	1:A:183:ILE:HG23	2.04	0.40
1:E:88:LEU:HB2	1:E:183:ILE:HG23	2.02	0.40
1:F:158:ILE:HG22	1:F:160:ASP:H	1.87	0.40
1:G:54:ASN:HB2	1:G:131:PRO:HD2	2.03	0.40
1:G:109:ASP:OD1	1:G:109:ASP:N	2.55	0.40
1:H:37:CYS:HA	1:H:40:ARG:HE	1.87	0.40
1:J:112:LEU:HD23	1:J:112:LEU:H	1.85	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	238/315 (76%)	224 (94%)	14 (6%)	0	100	100
1	B	238/315 (76%)	222 (93%)	16 (7%)	0	100	100
1	C	238/315 (76%)	225 (94%)	13 (6%)	0	100	100
1	D	238/315 (76%)	225 (94%)	13 (6%)	0	100	100
1	E	238/315 (76%)	225 (94%)	13 (6%)	0	100	100
1	F	238/315 (76%)	222 (93%)	16 (7%)	0	100	100
1	G	238/315 (76%)	227 (95%)	11 (5%)	0	100	100
1	H	238/315 (76%)	222 (93%)	16 (7%)	0	100	100
1	I	238/315 (76%)	225 (94%)	13 (6%)	0	100	100
1	J	238/315 (76%)	224 (94%)	14 (6%)	0	100	100
1	K	238/315 (76%)	224 (94%)	14 (6%)	0	100	100
1	L	238/315 (76%)	222 (93%)	16 (7%)	0	100	100
2	a	407/533 (76%)	394 (97%)	13 (3%)	0	100	100
2	b	407/533 (76%)	393 (97%)	14 (3%)	0	100	100
2	c	407/533 (76%)	393 (97%)	14 (3%)	0	100	100
2	d	407/533 (76%)	392 (96%)	15 (4%)	0	100	100
2	e	407/533 (76%)	391 (96%)	16 (4%)	0	100	100
2	f	407/533 (76%)	394 (97%)	13 (3%)	0	100	100
2	g	407/533 (76%)	393 (97%)	14 (3%)	0	100	100
2	h	407/533 (76%)	394 (97%)	13 (3%)	0	100	100
2	i	407/533 (76%)	394 (97%)	13 (3%)	0	100	100
2	j	407/533 (76%)	394 (97%)	13 (3%)	0	100	100
2	k	407/533 (76%)	392 (96%)	15 (4%)	0	100	100
2	l	407/533 (76%)	393 (97%)	14 (3%)	0	100	100
3	S	61/114 (54%)	61 (100%)	0	0	100	100
3	T	61/114 (54%)	61 (100%)	0	0	100	100
3	U	61/114 (54%)	61 (100%)	0	0	100	100
3	V	61/114 (54%)	61 (100%)	0	0	100	100
3	W	61/114 (54%)	61 (100%)	0	0	100	100
3	X	61/114 (54%)	61 (100%)	0	0	100	100
4	M	156/265 (59%)	144 (92%)	12 (8%)	0	100	100
4	N	156/265 (59%)	146 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	O	156/265 (59%)	143 (92%)	13 (8%)	0	100	100
4	P	156/265 (59%)	146 (94%)	10 (6%)	0	100	100
4	Q	156/265 (59%)	144 (92%)	12 (8%)	0	100	100
4	R	156/265 (59%)	144 (92%)	12 (8%)	0	100	100
All	All	9042/12450 (73%)	8637 (96%)	405 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	207/266 (78%)	197 (95%)	10 (5%)	23	54
1	B	207/266 (78%)	196 (95%)	11 (5%)	20	50
1	C	207/266 (78%)	196 (95%)	11 (5%)	20	50
1	D	207/266 (78%)	199 (96%)	8 (4%)	28	61
1	E	207/266 (78%)	199 (96%)	8 (4%)	28	61
1	F	207/266 (78%)	201 (97%)	6 (3%)	37	69
1	G	207/266 (78%)	197 (95%)	10 (5%)	23	54
1	H	207/266 (78%)	199 (96%)	8 (4%)	28	61
1	I	207/266 (78%)	197 (95%)	10 (5%)	23	54
1	J	207/266 (78%)	198 (96%)	9 (4%)	26	58
1	K	207/266 (78%)	199 (96%)	8 (4%)	28	61
1	L	207/266 (78%)	201 (97%)	6 (3%)	37	69
2	a	363/473 (77%)	350 (96%)	13 (4%)	31	63
2	b	363/473 (77%)	348 (96%)	15 (4%)	27	60
2	c	363/473 (77%)	349 (96%)	14 (4%)	28	61
2	d	363/473 (77%)	351 (97%)	12 (3%)	33	65
2	e	363/473 (77%)	350 (96%)	13 (4%)	31	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	f	363/473 (77%)	350 (96%)	13 (4%)	31	63
2	g	363/473 (77%)	350 (96%)	13 (4%)	31	63
2	h	363/473 (77%)	349 (96%)	14 (4%)	28	61
2	i	363/473 (77%)	348 (96%)	15 (4%)	27	60
2	j	363/473 (77%)	350 (96%)	13 (4%)	31	63
2	k	363/473 (77%)	350 (96%)	13 (4%)	31	63
2	l	363/473 (77%)	351 (97%)	12 (3%)	33	65
3	S	59/100 (59%)	57 (97%)	2 (3%)	32	65
3	T	59/100 (59%)	57 (97%)	2 (3%)	32	65
3	U	59/100 (59%)	57 (97%)	2 (3%)	32	65
3	V	59/100 (59%)	57 (97%)	2 (3%)	32	65
3	W	59/100 (59%)	57 (97%)	2 (3%)	32	65
3	X	59/100 (59%)	57 (97%)	2 (3%)	32	65
4	M	133/237 (56%)	129 (97%)	4 (3%)	36	68
4	N	133/237 (56%)	129 (97%)	4 (3%)	36	68
4	O	133/237 (56%)	129 (97%)	4 (3%)	36	68
4	P	133/237 (56%)	129 (97%)	4 (3%)	36	68
4	Q	133/237 (56%)	129 (97%)	4 (3%)	36	68
4	R	133/237 (56%)	129 (97%)	4 (3%)	36	68
All	All	7992/10890 (73%)	7691 (96%)	301 (4%)	30	62

All (301) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	13	LYS
1	B	14	ASP
1	B	50	PHE
1	B	68	ARG
1	B	121	MET
1	B	129	TYR
1	B	138	LEU
1	B	154	MET
1	B	244	ASN
1	B	295	GLU
1	B	301	ASP

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Mol	Chain	Res	Type
2	1	87	GLU
2	1	98	ASP
2	1	100	ILE
2	1	103	GLU
2	1	162	ILE
2	1	337	GLN
2	1	369	LEU
2	1	380	ILE
2	1	409	GLU
2	1	416	GLU
2	1	425	ASN
2	1	501	GLU
3	X	42	PHE
3	X	43	VAL
3	W	42	PHE
3	W	43	VAL
3	V	42	PHE
3	V	43	VAL
3	U	42	PHE
3	U	43	VAL
3	T	42	PHE
3	T	43	VAL
3	S	42	PHE
3	S	43	VAL
4	N	71	ILE
4	N	81	THR
4	N	155	TYR
4	N	161	LEU
4	M	71	ILE
4	M	81	THR
4	M	155	TYR
4	M	161	LEU
4	O	71	ILE
4	O	81	THR
4	O	155	TYR
4	O	161	LEU
4	P	71	ILE
4	P	81	THR
4	P	155	TYR
4	P	161	LEU
4	Q	71	ILE
4	Q	81	THR

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Mol	Chain	Res	Type
4	Q	155	TYR
4	Q	161	LEU
4	R	71	ILE
4	R	81	THR
4	R	155	TYR
4	R	161	LEU
2	k	98	ASP
2	k	100	ILE
2	k	103	GLU
2	k	129	GLU
2	k	161	ILE
2	k	162	ILE
2	k	185	VAL
2	k	369	LEU
2	k	380	ILE
2	k	409	GLU
2	k	416	GLU
2	k	501	GLU
2	k	510	LYS
2	j	87	GLU
2	j	98	ASP
2	j	100	ILE
2	j	129	GLU
2	j	162	ILE
2	j	369	LEU
2	j	380	ILE
2	j	409	GLU
2	j	416	GLU
2	j	429	LYS
2	j	474	GLU
2	j	501	GLU
2	j	510	LYS
2	i	98	ASP
2	i	100	ILE
2	i	103	GLU
2	i	129	GLU
2	i	161	ILE
2	i	162	ILE
2	i	188	ILE
2	i	337	GLN
2	i	369	LEU
2	i	380	ILE

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Mol	Chain	Res	Type
2	i	409	GLU
2	i	416	GLU
2	i	429	LYS
2	i	501	GLU
2	i	510	LYS
2	h	87	GLU
2	h	98	ASP
2	h	100	ILE
2	h	103	GLU
2	h	129	GLU
2	h	162	ILE
2	h	337	GLN
2	h	369	LEU
2	h	380	ILE
2	h	409	GLU
2	h	429	LYS
2	h	501	GLU
2	h	510	LYS
2	h	511	GLU
2	g	98	ASP
2	g	100	ILE
2	g	129	GLU
2	g	161	ILE
2	g	162	ILE
2	g	337	GLN
2	g	369	LEU
2	g	380	ILE
2	g	409	GLU
2	g	416	GLU
2	g	429	LYS
2	g	501	GLU
2	g	511	GLU
2	f	98	ASP
2	f	100	ILE
2	f	103	GLU
2	f	129	GLU
2	f	162	ILE
2	f	337	GLN
2	f	369	LEU
2	f	380	ILE
2	f	409	GLU
2	f	416	GLU

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Mol	Chain	Res	Type
2	f	429	LYS
2	f	474	GLU
2	f	501	GLU
2	e	98	ASP
2	e	100	ILE
2	e	103	GLU
2	e	129	GLU
2	e	161	ILE
2	e	162	ILE
2	e	369	LEU
2	e	380	ILE
2	e	409	GLU
2	e	416	GLU
2	e	429	LYS
2	e	501	GLU
2	e	513	ARG
2	d	98	ASP
2	d	100	ILE
2	d	129	GLU
2	d	162	ILE
2	d	369	LEU
2	d	380	ILE
2	d	409	GLU
2	d	416	GLU
2	d	474	GLU
2	d	501	GLU
2	d	510	LYS
2	d	511	GLU
2	c	98	ASP
2	c	100	ILE
2	c	103	GLU
2	c	129	GLU
2	c	161	ILE
2	c	162	ILE
2	c	188	ILE
2	c	369	LEU
2	c	380	ILE
2	c	409	GLU
2	c	416	GLU
2	c	429	LYS
2	c	501	GLU
2	c	510	LYS

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Mol	Chain	Res	Type
2	b	87	GLU
2	b	98	ASP
2	b	100	ILE
2	b	103	GLU
2	b	129	GLU
2	b	162	ILE
2	b	188	ILE
2	b	337	GLN
2	b	369	LEU
2	b	380	ILE
2	b	409	GLU
2	b	429	LYS
2	b	474	GLU
2	b	501	GLU
2	b	513	ARG
2	a	98	ASP
2	a	100	ILE
2	a	103	GLU
2	a	129	GLU
2	a	161	ILE
2	a	162	ILE
2	a	369	LEU
2	a	380	ILE
2	a	409	GLU
2	a	416	GLU
2	a	429	LYS
2	a	501	GLU
2	a	510	LYS
1	L	50	PHE
1	L	68	ARG
1	L	121	MET
1	L	129	TYR
1	L	295	GLU
1	L	307	LEU
1	A	50	PHE
1	A	68	ARG
1	A	121	MET
1	A	129	TYR
1	A	138	LEU
1	A	154	MET
1	A	244	ASN
1	A	271	LEU

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Mol	Chain	Res	Type
1	A	295	GLU
1	A	301	ASP
1	C	50	PHE
1	C	68	ARG
1	C	121	MET
1	C	129	TYR
1	C	138	LEU
1	C	154	MET
1	C	244	ASN
1	C	259	ASN
1	C	271	LEU
1	C	295	GLU
1	C	307	LEU
1	D	50	PHE
1	D	68	ARG
1	D	121	MET
1	D	129	TYR
1	D	154	MET
1	D	244	ASN
1	D	277	ILE
1	D	295	GLU
1	E	50	PHE
1	E	68	ARG
1	E	121	MET
1	E	129	TYR
1	E	154	MET
1	E	171	LYS
1	E	271	LEU
1	E	295	GLU
1	F	50	PHE
1	F	68	ARG
1	F	121	MET
1	F	129	TYR
1	F	295	GLU
1	F	307	LEU
1	G	50	PHE
1	G	68	ARG
1	G	121	MET
1	G	129	TYR
1	G	138	LEU
1	G	154	MET
1	G	244	ASN

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Mol	Chain	Res	Type
1	G	259	ASN
1	G	271	LEU
1	G	295	GLU
1	H	50	PHE
1	H	68	ARG
1	H	121	MET
1	H	129	TYR
1	H	154	MET
1	H	259	ASN
1	H	277	ILE
1	H	295	GLU
1	I	50	PHE
1	I	68	ARG
1	I	121	MET
1	I	129	TYR
1	I	138	LEU
1	I	154	MET
1	I	244	ASN
1	I	271	LEU
1	I	295	GLU
1	I	307	LEU
1	J	50	PHE
1	J	68	ARG
1	J	121	MET
1	J	129	TYR
1	J	154	MET
1	J	244	ASN
1	J	277	ILE
1	J	295	GLU
1	J	307	LEU
1	K	50	PHE
1	K	68	ARG
1	K	106	TRP
1	K	121	MET
1	K	129	TYR
1	K	154	MET
1	K	271	LEU
1	K	295	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (171) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	33	GLN
1	B	39	GLN
1	B	80	ASN
1	B	91	ASN
1	B	169	GLN
1	B	244	ASN
2	l	291	ASN
2	l	300	HIS
2	l	323	ASN
2	l	492	GLN
3	X	33	GLN
3	X	35	GLN
3	X	52	GLN
3	W	35	GLN
3	W	52	GLN
3	V	35	GLN
3	V	52	GLN
3	U	35	GLN
3	U	52	GLN
3	T	35	GLN
3	T	52	GLN
3	S	35	GLN
3	S	52	GLN
4	N	14	ASN
4	N	38	ASN
4	N	78	ASN
4	N	128	ASN
4	N	144	ASN
4	N	160	GLN
4	N	164	ASN
4	M	14	ASN
4	M	38	ASN
4	M	78	ASN
4	M	128	ASN
4	M	144	ASN
4	M	160	GLN
4	M	164	ASN
4	O	14	ASN
4	O	38	ASN
4	O	78	ASN
4	O	144	ASN
4	O	160	GLN
4	O	164	ASN

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Mol	Chain	Res	Type
4	P	14	ASN
4	P	38	ASN
4	P	78	ASN
4	P	125	HIS
4	P	128	ASN
4	P	144	ASN
4	P	160	GLN
4	P	164	ASN
4	Q	14	ASN
4	Q	38	ASN
4	Q	78	ASN
4	Q	91	ASN
4	Q	128	ASN
4	Q	144	ASN
4	Q	164	ASN
4	R	14	ASN
4	R	38	ASN
4	R	78	ASN
4	R	128	ASN
4	R	144	ASN
4	R	160	GLN
4	R	164	ASN
2	k	255	HIS
2	k	291	ASN
2	k	300	HIS
2	k	323	ASN
2	k	492	GLN
2	j	181	GLN
2	j	300	HIS
2	j	323	ASN
2	i	300	HIS
2	i	323	ASN
2	i	367	GLN
2	h	135	ASN
2	h	255	HIS
2	h	291	ASN
2	h	306	ASN
2	h	323	ASN
2	g	181	GLN
2	g	255	HIS
2	g	291	ASN
2	g	323	ASN

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Mol	Chain	Res	Type
2	f	181	GLN
2	f	291	ASN
2	f	323	ASN
2	e	90	ASN
2	e	255	HIS
2	e	291	ASN
2	e	306	ASN
2	e	323	ASN
2	e	367	GLN
2	d	90	ASN
2	d	291	ASN
2	d	300	HIS
2	d	323	ASN
2	d	449	HIS
2	c	291	ASN
2	c	323	ASN
2	c	337	GLN
2	c	367	GLN
2	b	135	ASN
2	b	255	HIS
2	b	291	ASN
2	b	323	ASN
2	b	449	HIS
2	a	181	GLN
2	a	291	ASN
2	a	300	HIS
2	a	323	ASN
2	a	443	ASN
1	L	26	ASN
1	L	33	GLN
1	L	39	GLN
1	L	80	ASN
1	L	169	GLN
1	L	244	ASN
1	A	39	GLN
1	A	80	ASN
1	A	91	ASN
1	A	169	GLN
1	A	244	ASN
1	C	80	ASN
1	C	91	ASN
1	C	126	ASN

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Mol	Chain	Res	Type
1	C	169	GLN
1	C	244	ASN
1	D	26	ASN
1	D	33	GLN
1	D	80	ASN
1	D	126	ASN
1	D	169	GLN
1	D	244	ASN
1	E	80	ASN
1	E	169	GLN
1	E	244	ASN
1	F	26	ASN
1	F	33	GLN
1	F	39	GLN
1	F	80	ASN
1	F	126	ASN
1	F	169	GLN
1	F	244	ASN
1	G	33	GLN
1	G	80	ASN
1	G	169	GLN
1	G	244	ASN
1	H	26	ASN
1	H	33	GLN
1	H	39	GLN
1	H	80	ASN
1	H	169	GLN
1	H	244	ASN
1	I	39	GLN
1	I	80	ASN
1	I	169	GLN
1	I	244	ASN
1	J	26	ASN
1	J	33	GLN
1	J	39	GLN
1	J	80	ASN
1	J	169	GLN
1	J	244	ASN
1	K	33	GLN
1	K	39	GLN
1	K	80	ASN
1	K	91	ASN

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Mol	Chain	Res	Type
1	K	169	GLN
1	K	244	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

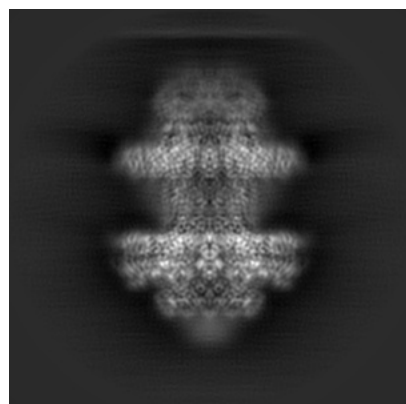
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63389. These allow visual inspection of the internal detail of the map and identification of artifacts.

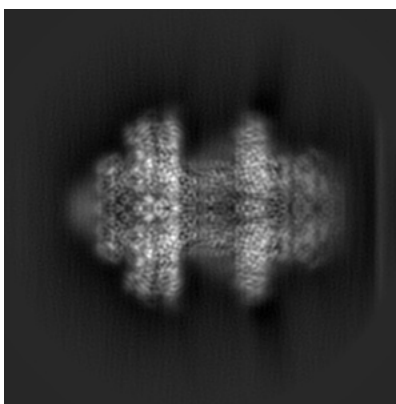
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

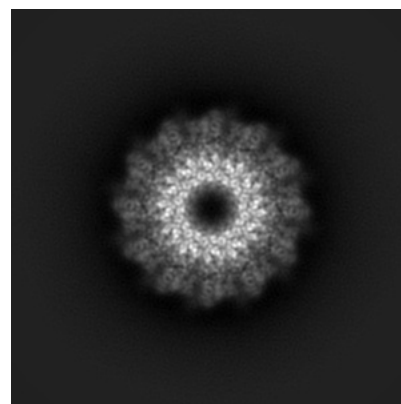
6.1.1 Primary map



X

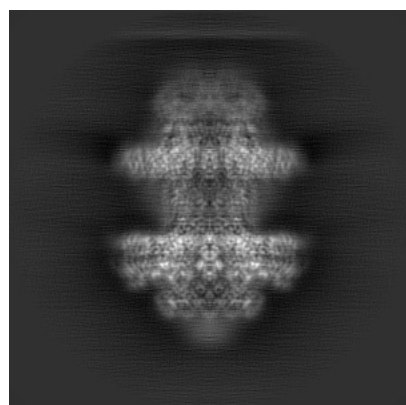


Y

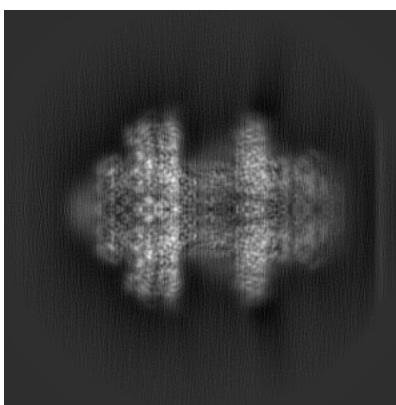


Z

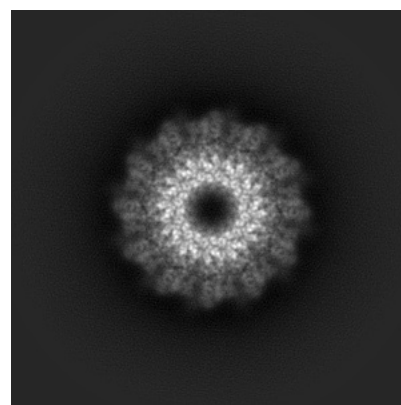
6.1.2 Raw map



X



Y

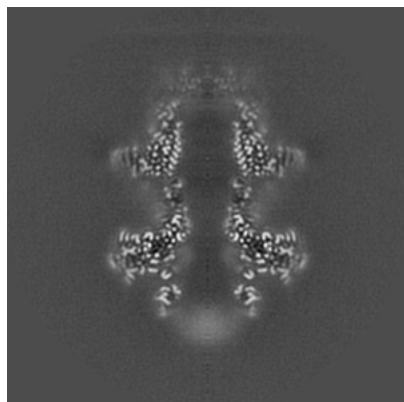


Z

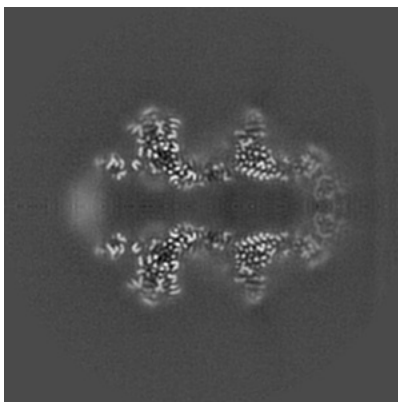
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

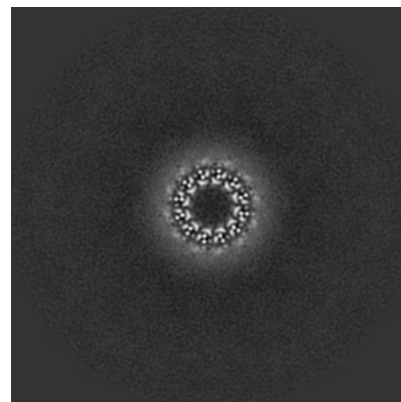
6.2.1 Primary map



X Index: 160

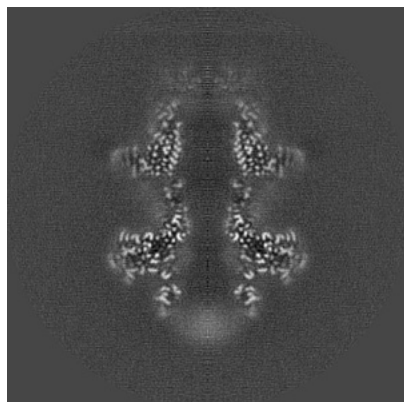


Y Index: 160

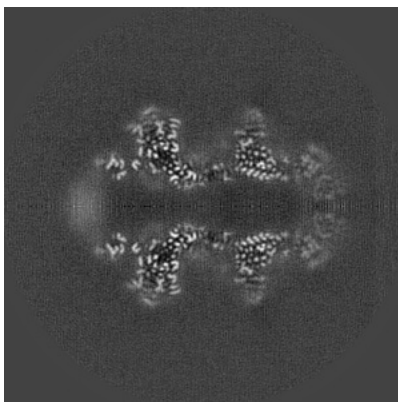


Z Index: 160

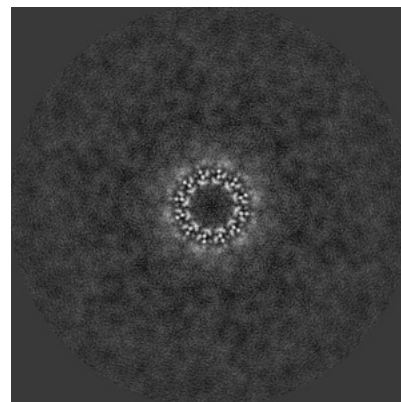
6.2.2 Raw map



X Index: 160



Y Index: 160

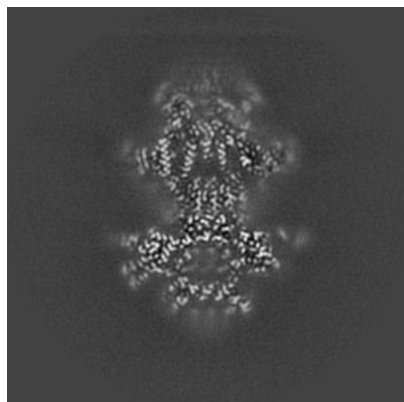


Z Index: 160

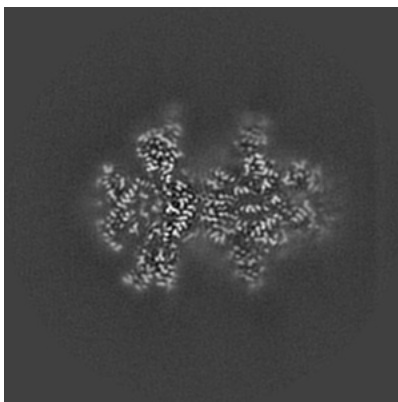
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

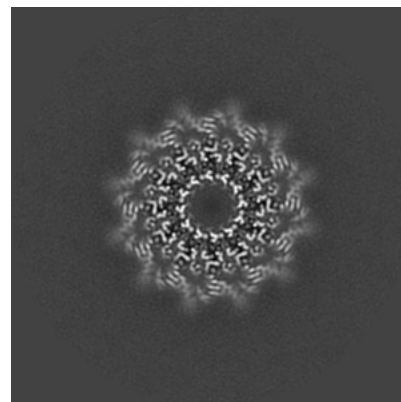
6.3.1 Primary map



X Index: 137

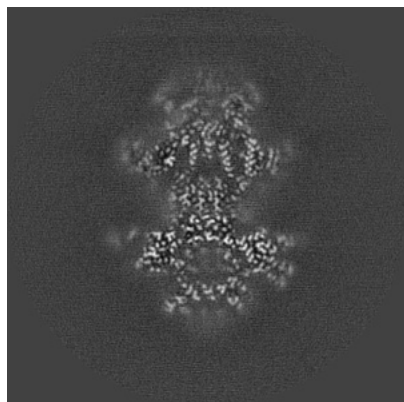


Y Index: 187

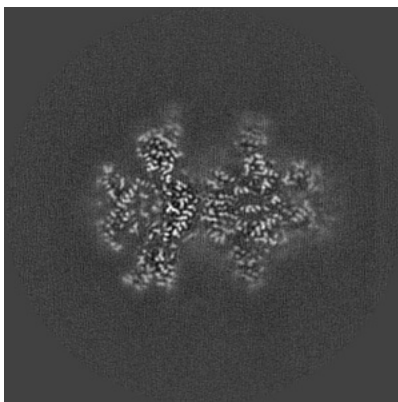


Z Index: 134

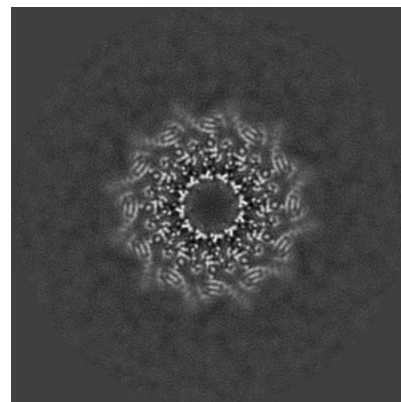
6.3.2 Raw map



X Index: 183



Y Index: 187

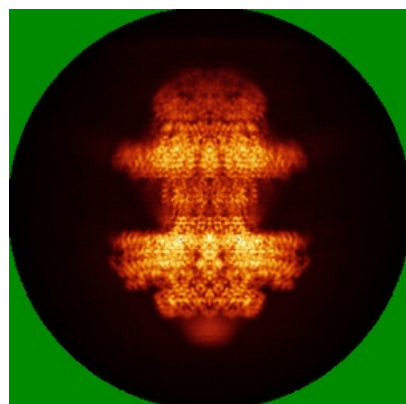


Z Index: 135

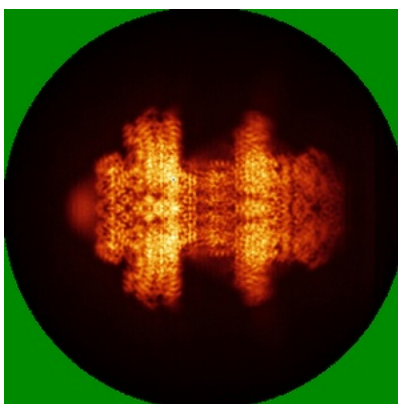
The images above show the largest variance slices of the map in three orthogonal directions.

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

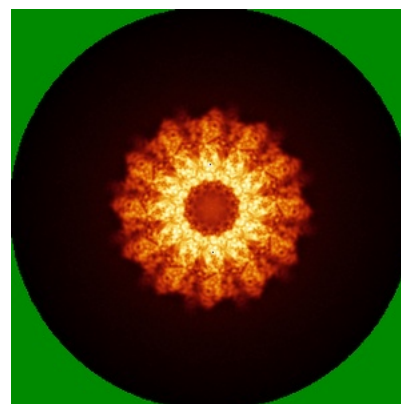
6.4.1 Primary map



X

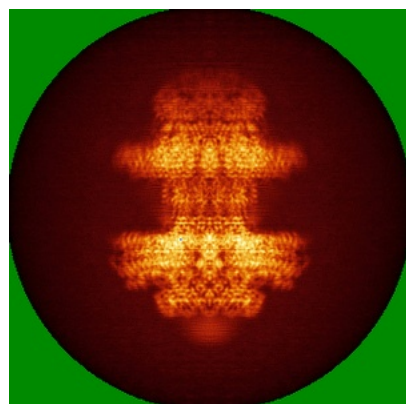


Y

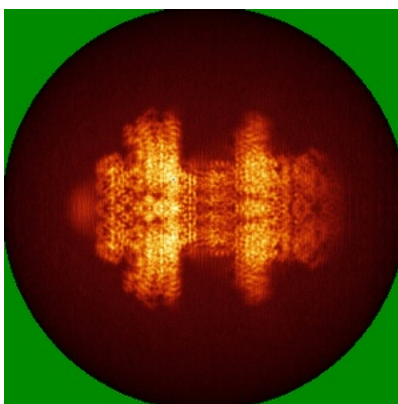


Z

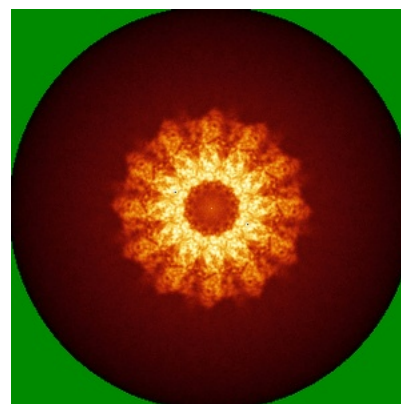
6.4.2 Raw map



X



Y

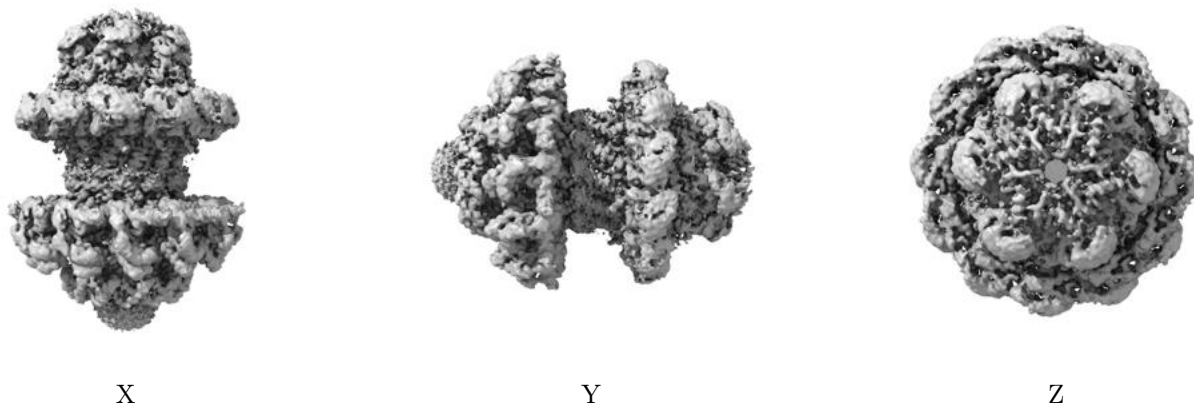


Z

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.

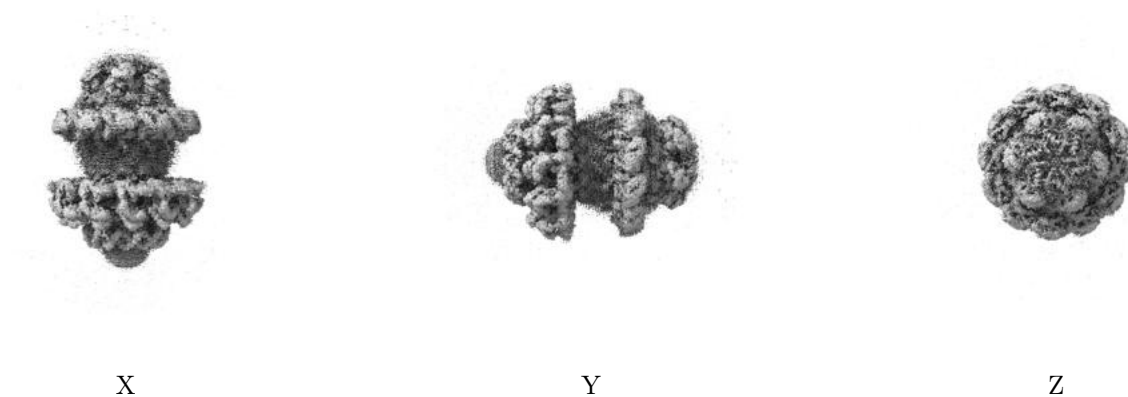
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00591. 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.

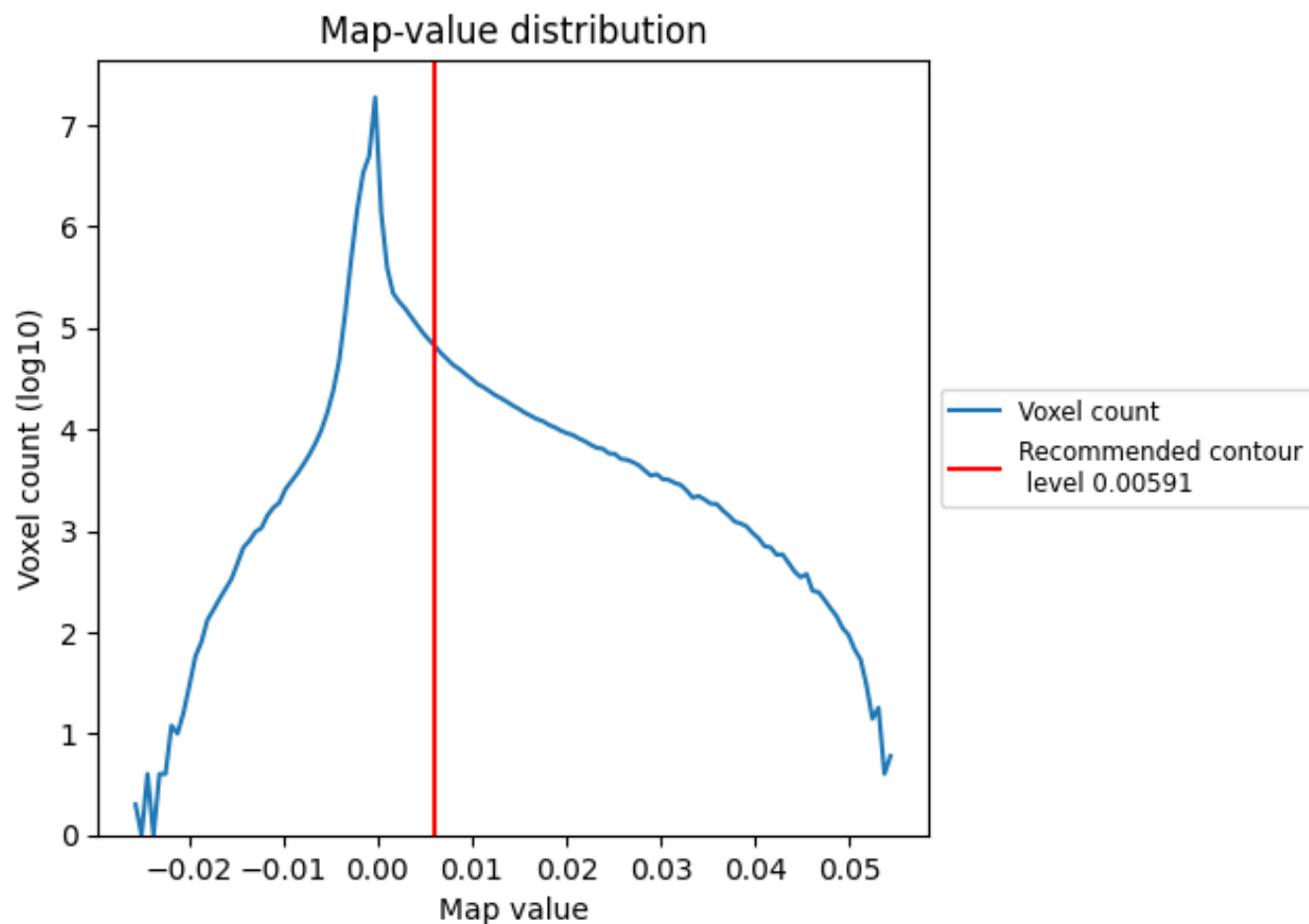
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

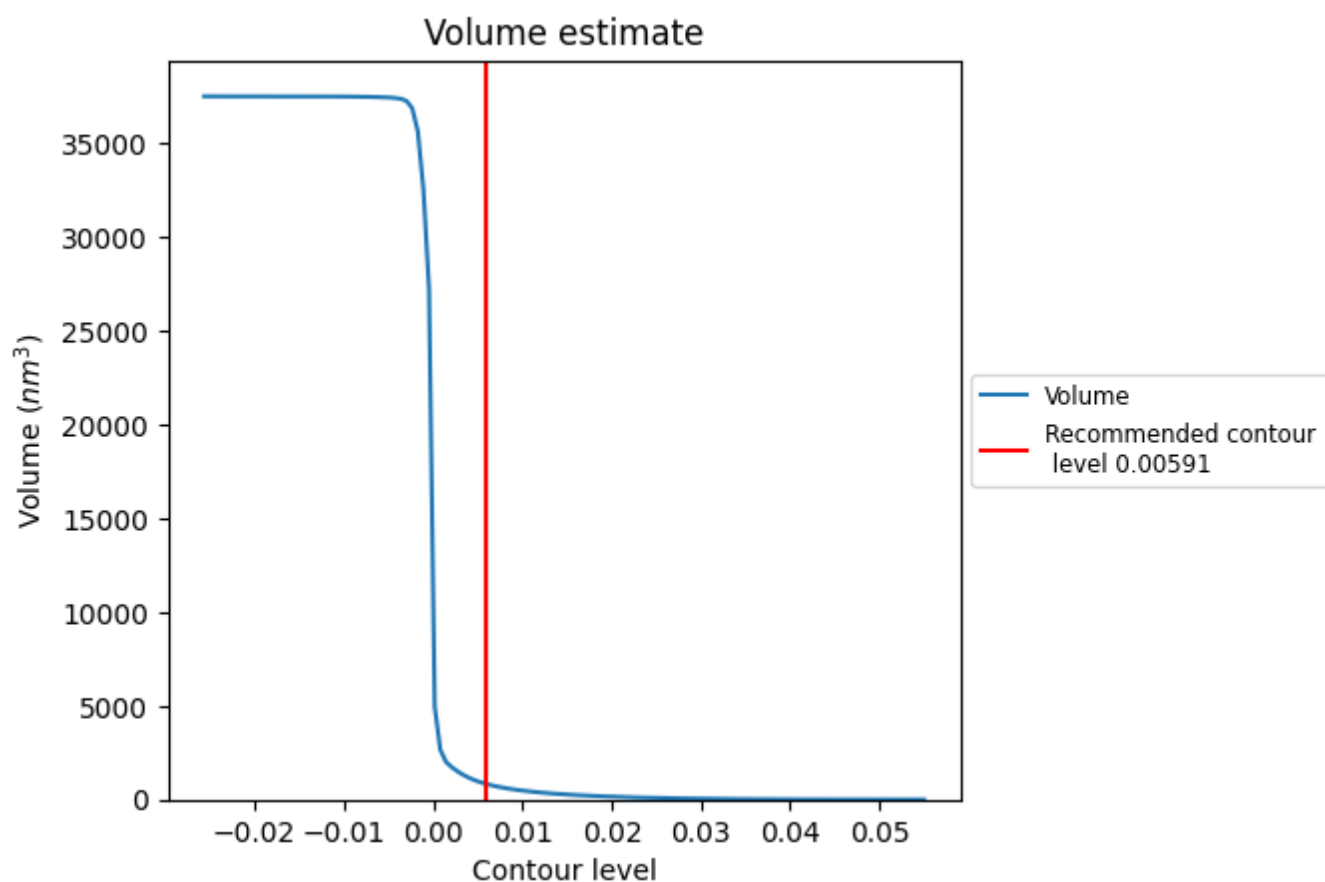
This section contains the results of statistical analysis of the map.

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.

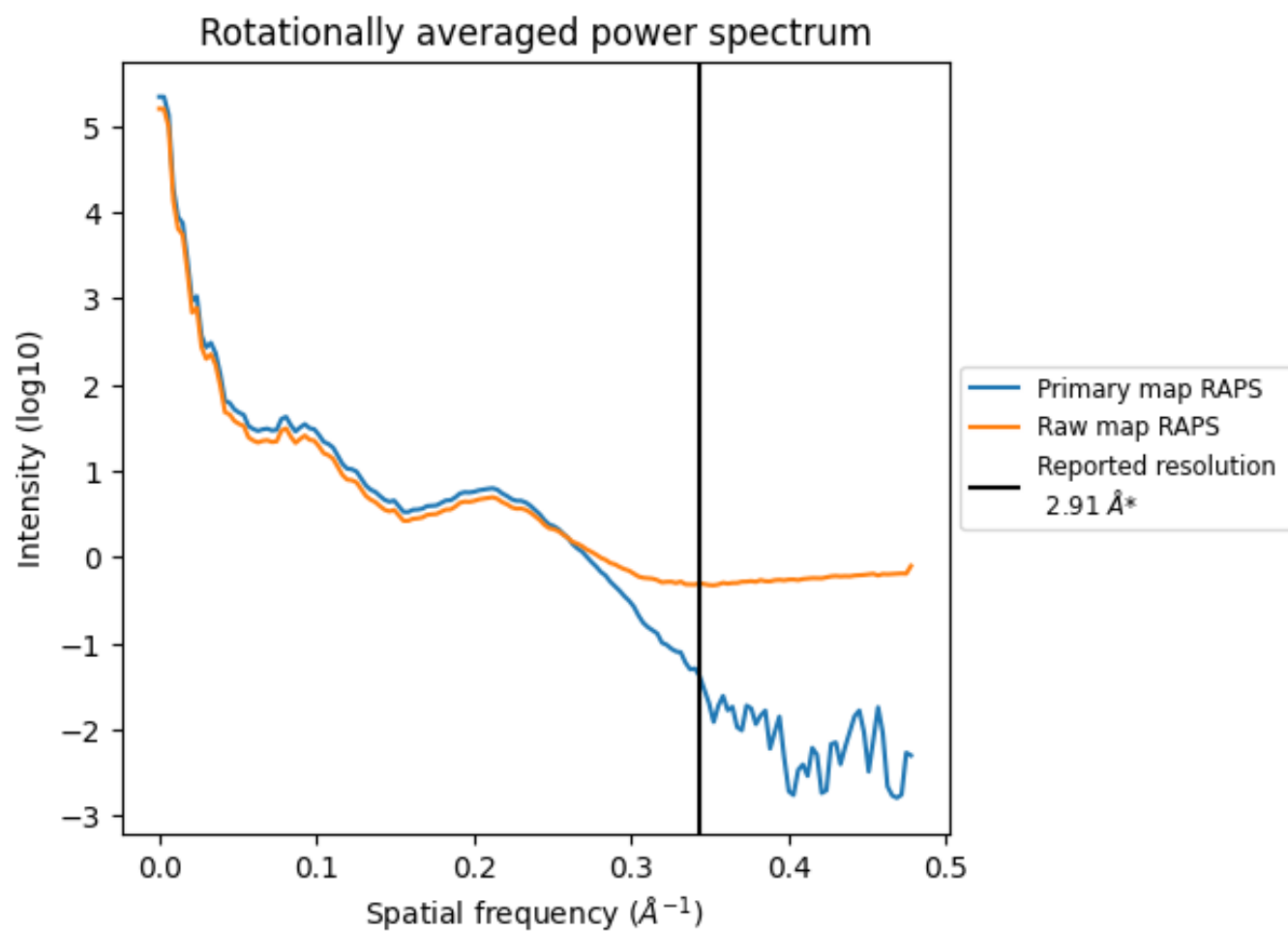
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 838 nm³; this corresponds to an approximate mass of 757 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 ⓘ

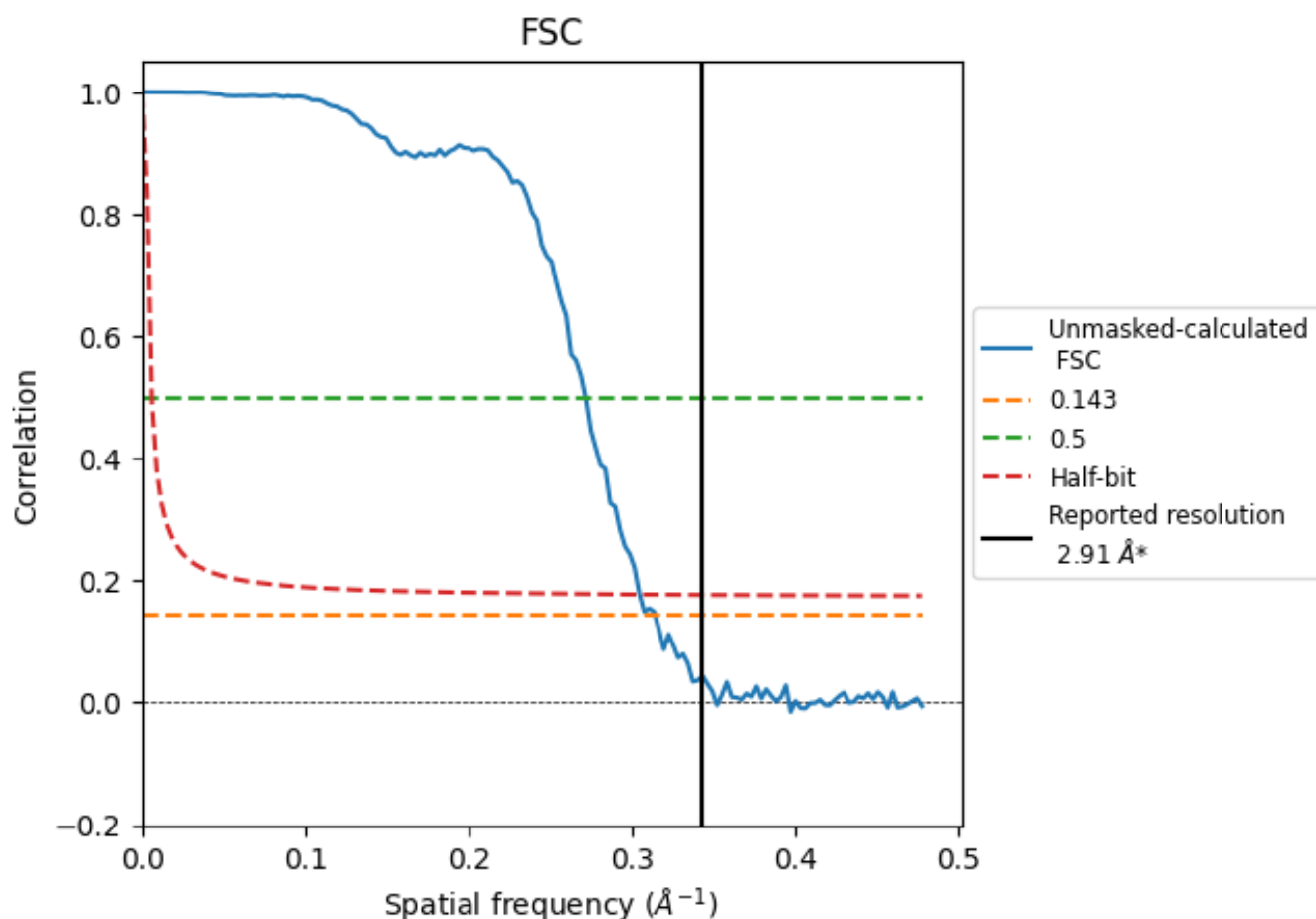


*Reported resolution corresponds to spatial frequency of 0.344 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.344 \AA^{-1}

8.2 Resolution estimates [i](#)

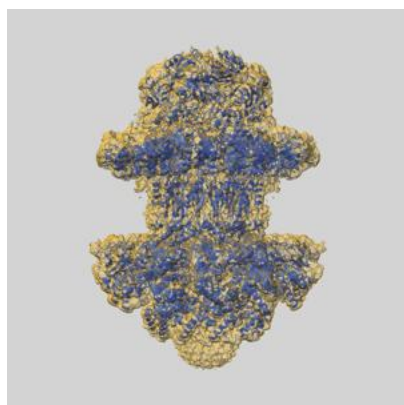
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.18	3.68	3.28

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

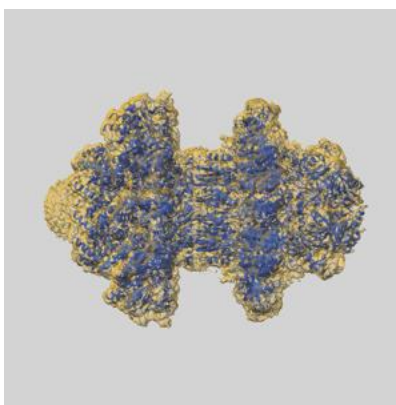
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63389 and PDB model 9LU6. Per-residue inclusion information can be found in section [3](#) on page [15](#).

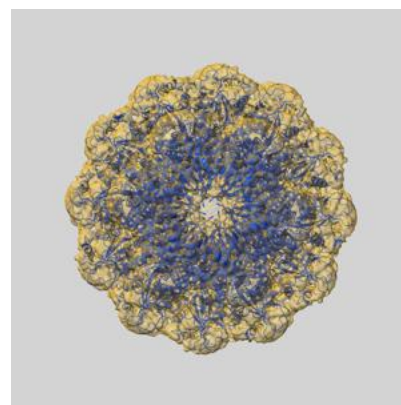
9.1 Map-model overlay [i](#)



X



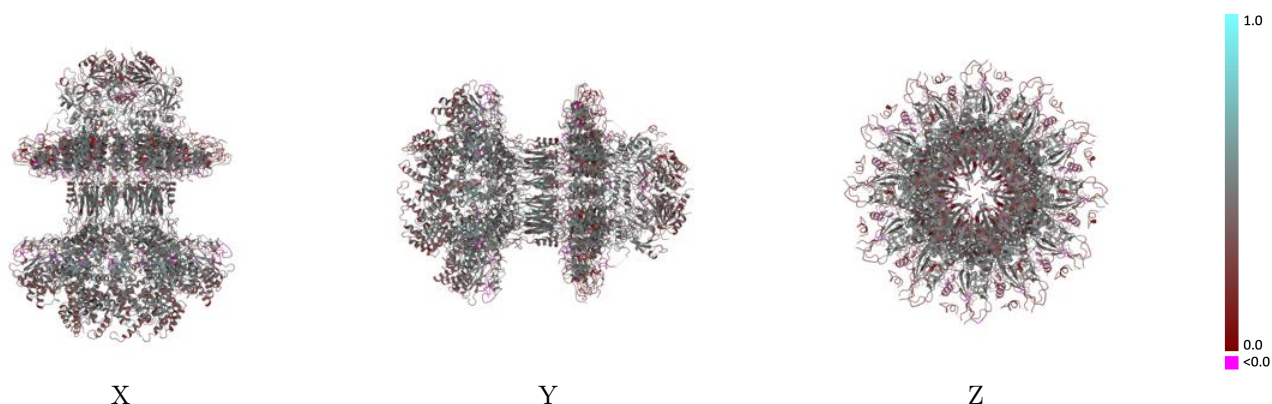
Y



Z

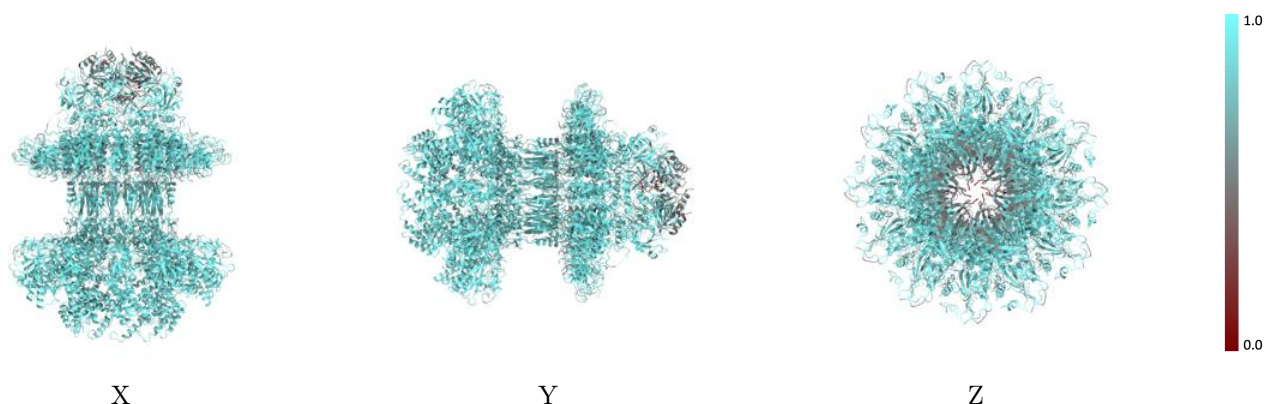
The images above show the 3D surface view of the map at the recommended contour level 0.00591 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



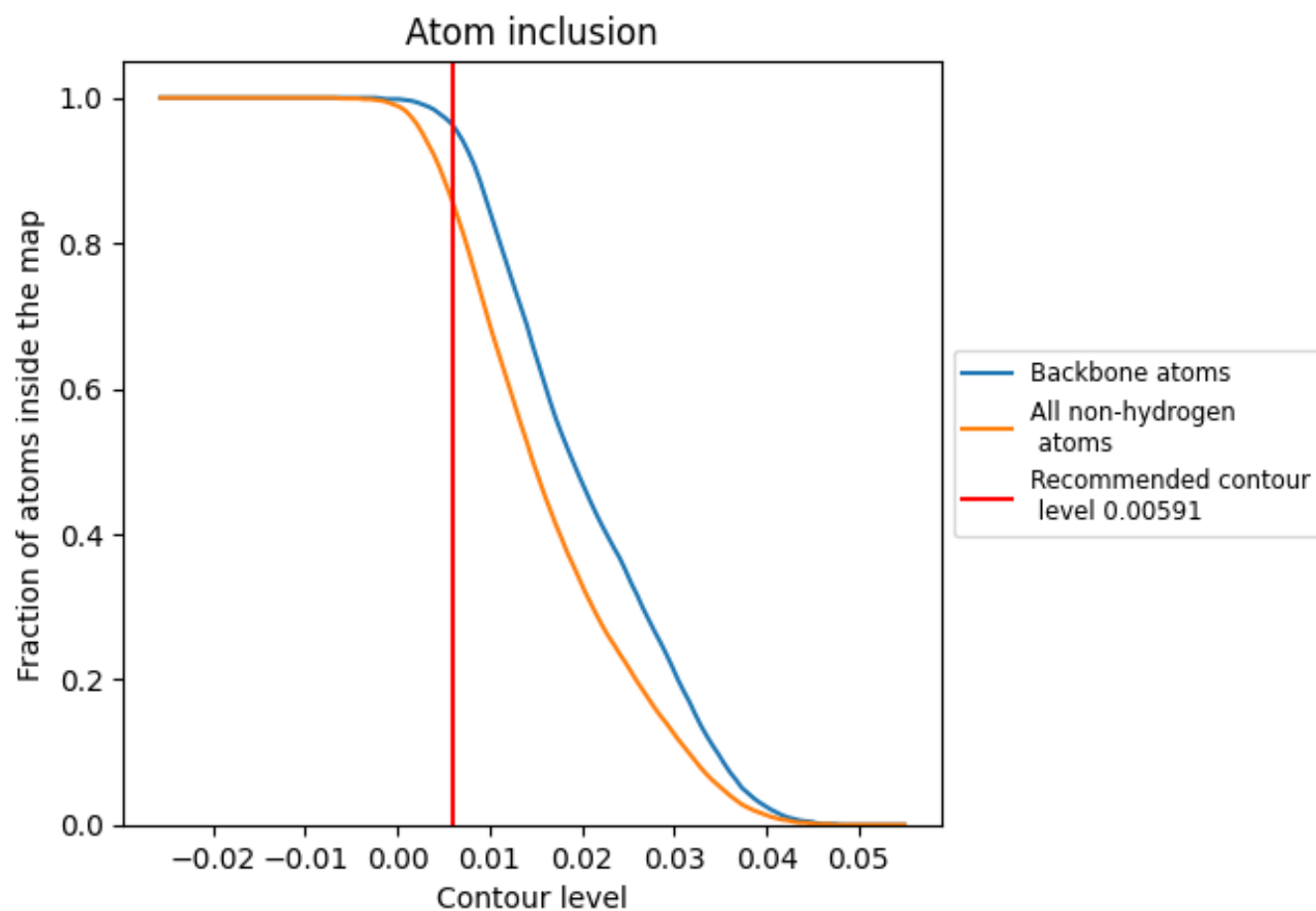
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00591).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 86% 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 (0.00591) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8600	 0.4100
A	 0.8550	 0.3850
B	 0.8440	 0.3810
C	 0.8510	 0.3880
D	 0.8480	 0.3930
E	 0.8550	 0.3870
F	 0.8530	 0.3930
G	 0.8520	 0.3870
H	 0.8480	 0.3940
I	 0.8520	 0.3900
J	 0.8510	 0.3910
K	 0.8560	 0.3880
L	 0.8510	 0.3920
M	 0.8320	 0.3840
N	 0.8350	 0.3870
O	 0.8360	 0.3850
P	 0.8380	 0.3880
Q	 0.8330	 0.3880
R	 0.8350	 0.3820
S	 0.5690	 0.3740
T	 0.5650	 0.3690
U	 0.5610	 0.3700
V	 0.5730	 0.3730
W	 0.5710	 0.3660
X	 0.5610	 0.3650
a	 0.8930	 0.4320
b	 0.8900	 0.4300
c	 0.8940	 0.4320
d	 0.8900	 0.4280
e	 0.8910	 0.4340
f	 0.8920	 0.4300
g	 0.8930	 0.4320
h	 0.8920	 0.4320
i	 0.8930	 0.4320
j	 0.8930	 0.4290



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Chain	Atom inclusion	Q-score
k	 0.8890	 0.4290
l	 0.8860	 0.4280