



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 09:11 PM EDT

PDB ID : 9YCI / pdb_00009yci
EMDB ID : EMD-72773
Title : Structure of the Adenovirus-7 VLP, Class 3
Authors : Khayat, R.; Madoo, K.
Deposited on : 2025-09-18
Resolution : 3.90 Å(reported)
Based on initial model : .

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:

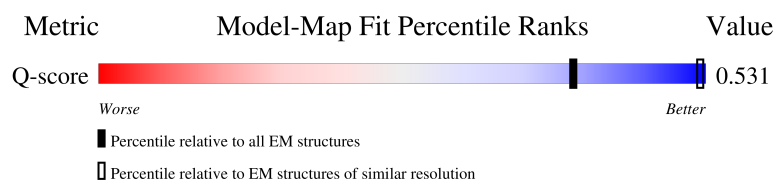
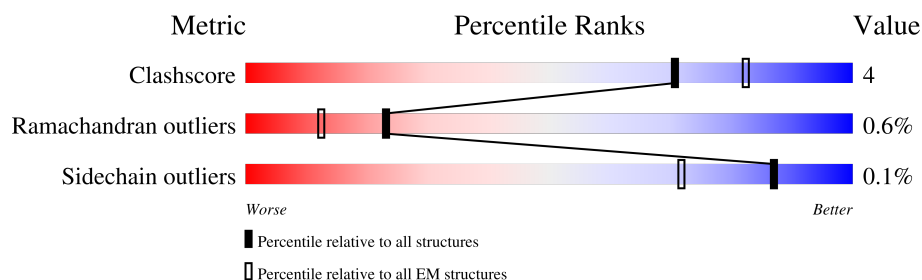
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.90 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.







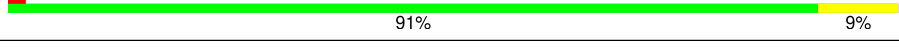


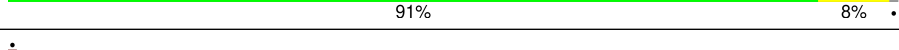
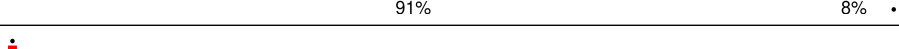
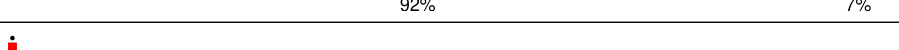

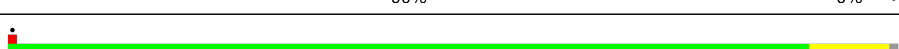


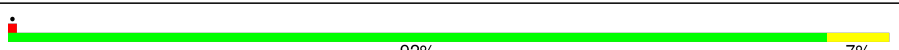





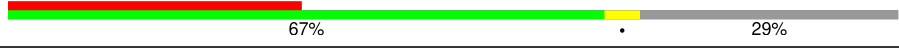
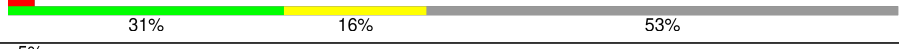
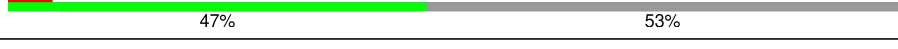

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	0	250	 5% . 94%
1	1	250	 8% . 90%
1	2	250	 8% . 90%
1	3	250	 8% . 93%

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Mol	Chain	Length	Quality of chain
1	4	250	
1	W	250	
1	Y	250	
1	Z	250	
2	A	937	
2	B	937	
2	C	937	
2	D	937	
2	E	937	
2	F	937	
2	G	937	
2	H	937	
2	I	937	
2	J	937	
2	K	937	
2	L	937	
3	M	588	
4	N	544	
5	P	138	
5	Q	138	
5	R	138	
5	S	138	
6	U	227	
6	V	227	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 196022 atoms, of which 95816 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 Pre-protein VI.

Mol	Chain	Residues	Atoms					AltConf	Trace	
1	0	16	Total 227	C 71	H 109	N 24	O 23	0	0	
1	1	25	Total 374	C 118	H 183	N 35	O 37	S 1	0	0
1	2	24	Total 355	C 112	H 172	N 35	O 35	S 1	0	0
1	3	18	Total 285	C 91	H 139	N 29	O 25	S 1	0	0
1	4	24	Total 369	C 120	H 178	N 35	O 35	S 1	0	0
1	W	28	Total 424	C 136	H 206	N 40	O 41	S 1	0	0
1	Y	25	Total 374	C 118	H 183	N 36	O 36	S 1	0	0
1	Z	27	Total 383	C 120	H 185	N 38	O 39	S 1	0	0

- Molecule 2 is a protein called Hexon protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	934	Total 14534	C 4712	H 7104	N 1253	O 1428	S 37	0	0
2	B	932	Total 14509	C 4704	H 7091	N 1251	O 1426	S 37	0	0
2	C	935	Total 14533	C 4714	H 7100	N 1254	O 1428	S 37	0	0
2	D	932	Total 14513	C 4706	H 7093	N 1251	O 1426	S 37	0	0
2	E	929	Total 14474	C 4694	H 7074	N 1248	O 1421	S 37	0	0
2	F	933	Total 14523	C 4708	H 7098	N 1252	O 1428	S 37	0	0
2	G	932	Total 14503	C 4703	H 7087	N 1251	O 1425	S 37	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	932	Total	C	H	N	O	S	0	0
			14510	4705	7092	1251	1425	37		
2	I	931	Total	C	H	N	O	S	0	0
			14495	4700	7084	1250	1424	37		
2	J	931	Total	C	H	N	O	S	0	0
			14495	4700	7084	1250	1424	37		
2	K	933	Total	C	H	N	O	S	0	0
			14524	4708	7099	1252	1428	37		
2	L	933	Total	C	H	N	O	S	0	0
			14523	4709	7098	1252	1427	37		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	PHE	LEU	conflict	UNP P36851
A	61	SER	ARG	conflict	UNP P36851
A	76	ASN	HIS	conflict	UNP P36851
A	266	ALA	ARG	conflict	UNP P36851
A	592	THR	SER	conflict	UNP P36851
B	31	PHE	LEU	conflict	UNP P36851
B	61	SER	ARG	conflict	UNP P36851
B	76	ASN	HIS	conflict	UNP P36851
B	266	ALA	ARG	conflict	UNP P36851
B	592	THR	SER	conflict	UNP P36851
C	31	PHE	LEU	conflict	UNP P36851
C	61	SER	ARG	conflict	UNP P36851
C	76	ASN	HIS	conflict	UNP P36851
C	266	ALA	ARG	conflict	UNP P36851
C	592	THR	SER	conflict	UNP P36851
D	31	PHE	LEU	conflict	UNP P36851
D	61	SER	ARG	conflict	UNP P36851
D	76	ASN	HIS	conflict	UNP P36851
D	266	ALA	ARG	conflict	UNP P36851
D	592	THR	SER	conflict	UNP P36851
E	31	PHE	LEU	conflict	UNP P36851
E	61	SER	ARG	conflict	UNP P36851
E	76	ASN	HIS	conflict	UNP P36851
E	266	ALA	ARG	conflict	UNP P36851
E	592	THR	SER	conflict	UNP P36851
F	31	PHE	LEU	conflict	UNP P36851
F	61	SER	ARG	conflict	UNP P36851
F	76	ASN	HIS	conflict	UNP P36851
F	266	ALA	ARG	conflict	UNP P36851

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Chain	Residue	Modelled	Actual	Comment	Reference
F	592	THR	SER	conflict	UNP P36851
G	31	PHE	LEU	conflict	UNP P36851
G	61	SER	ARG	conflict	UNP P36851
G	76	ASN	HIS	conflict	UNP P36851
G	266	ALA	ARG	conflict	UNP P36851
G	592	THR	SER	conflict	UNP P36851
H	31	PHE	LEU	conflict	UNP P36851
H	61	SER	ARG	conflict	UNP P36851
H	76	ASN	HIS	conflict	UNP P36851
H	266	ALA	ARG	conflict	UNP P36851
H	592	THR	SER	conflict	UNP P36851
I	31	PHE	LEU	conflict	UNP P36851
I	61	SER	ARG	conflict	UNP P36851
I	76	ASN	HIS	conflict	UNP P36851
I	266	ALA	ARG	conflict	UNP P36851
I	592	THR	SER	conflict	UNP P36851
J	31	PHE	LEU	conflict	UNP P36851
J	61	SER	ARG	conflict	UNP P36851
J	76	ASN	HIS	conflict	UNP P36851
J	266	ALA	ARG	conflict	UNP P36851
J	592	THR	SER	conflict	UNP P36851
K	31	PHE	LEU	conflict	UNP P36851
K	61	SER	ARG	conflict	UNP P36851
K	76	ASN	HIS	conflict	UNP P36851
K	266	ALA	ARG	conflict	UNP P36851
K	592	THR	SER	conflict	UNP P36851
L	31	PHE	LEU	conflict	UNP P36851
L	61	SER	ARG	conflict	UNP P36851
L	76	ASN	HIS	conflict	UNP P36851
L	266	ALA	ARG	conflict	UNP P36851
L	592	THR	SER	conflict	UNP P36851

- Molecule 3 is a protein called Pre-hexon-linking protein IIIa.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	M	239	Total	C	H	N	O	S	0	0
			3771	1179	1889	344	355	4		

- Molecule 4 is a protein called Penton protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	N	463	Total	C	H	N	O	S	0	0
			7391	2368	3658	638	713	14		

- Molecule 5 is a protein called Hexon-interlacing protein IX.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	P	99	Total	C	H	N	O	S	0	0
			1190	381	571	113	124	1		
5	Q	97	Total	C	H	N	O	S	0	0
			1172	375	563	111	122	1		
5	R	97	Total	C	H	N	O	S	0	0
			1170	375	561	111	122	1		
5	S	98	Total	C	H	N	O	S	0	0
			1175	378	561	112	123	1		

There are 172 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	92	UNK	PRO	conflict	UNP P68971
P	93	UNK	SER	conflict	UNP P68971
P	94	UNK	THR	conflict	UNP P68971
P	95	UNK	LEU	conflict	UNP P68971
P	96	UNK	ALA	conflict	UNP P68971
P	97	UNK	GLU	conflict	UNP P68971
P	98	UNK	ASP	conflict	UNP P68971
P	99	UNK	LYS	conflict	UNP P68971
P	100	UNK	LEU	conflict	UNP P68971
P	101	UNK	LEU	conflict	UNP P68971
P	102	UNK	VAL	conflict	UNP P68971
P	103	UNK	LEU	conflict	UNP P68971
P	104	UNK	LEU	conflict	UNP P68971
P	105	UNK	ALA	conflict	UNP P68971
P	106	UNK	GLN	conflict	UNP P68971
P	107	UNK	LEU	conflict	UNP P68971
P	108	UNK	GLU	conflict	UNP P68971
P	109	UNK	ALA	conflict	UNP P68971
P	110	UNK	LEU	conflict	UNP P68971
P	111	UNK	THR	conflict	UNP P68971
P	112	UNK	GLN	conflict	UNP P68971
P	113	UNK	ARG	conflict	UNP P68971
P	114	UNK	LEU	conflict	UNP P68971
P	115	UNK	GLY	conflict	UNP P68971
P	116	UNK	GLU	conflict	UNP P68971

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Chain	Residue	Modelled	Actual	Comment	Reference
P	117	UNK	LEU	conflict	UNP P68971
P	118	UNK	SER	conflict	UNP P68971
P	119	UNK	LYS	conflict	UNP P68971
P	120	UNK	GLN	conflict	UNP P68971
P	121	UNK	VAL	conflict	UNP P68971
P	122	UNK	ALA	conflict	UNP P68971
P	123	UNK	GLN	conflict	UNP P68971
P	124	UNK	LEU	conflict	UNP P68971
P	125	UNK	ARG	conflict	UNP P68971
P	126	UNK	GLU	conflict	UNP P68971
P	127	UNK	GLN	conflict	UNP P68971
P	128	UNK	THR	conflict	UNP P68971
P	129	UNK	GLU	conflict	UNP P68971
P	130	UNK	SER	conflict	UNP P68971
P	131	UNK	ALA	conflict	UNP P68971
P	132	UNK	VAL	conflict	UNP P68971
P	133	UNK	ALA	conflict	UNP P68971
P	134	UNK	THR	conflict	UNP P68971
Q	92	UNK	PRO	conflict	UNP P68971
Q	93	UNK	SER	conflict	UNP P68971
Q	94	UNK	THR	conflict	UNP P68971
Q	95	UNK	LEU	conflict	UNP P68971
Q	96	UNK	ALA	conflict	UNP P68971
Q	97	UNK	GLU	conflict	UNP P68971
Q	98	UNK	ASP	conflict	UNP P68971
Q	99	UNK	LYS	conflict	UNP P68971
Q	100	UNK	LEU	conflict	UNP P68971
Q	101	UNK	LEU	conflict	UNP P68971
Q	102	UNK	VAL	conflict	UNP P68971
Q	103	UNK	LEU	conflict	UNP P68971
Q	104	UNK	LEU	conflict	UNP P68971
Q	105	UNK	ALA	conflict	UNP P68971
Q	106	UNK	GLN	conflict	UNP P68971
Q	107	UNK	LEU	conflict	UNP P68971
Q	108	UNK	GLU	conflict	UNP P68971
Q	109	UNK	ALA	conflict	UNP P68971
Q	110	UNK	LEU	conflict	UNP P68971
Q	111	UNK	THR	conflict	UNP P68971
Q	112	UNK	GLN	conflict	UNP P68971
Q	113	UNK	ARG	conflict	UNP P68971
Q	114	UNK	LEU	conflict	UNP P68971
Q	115	UNK	GLY	conflict	UNP P68971

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	116	UNK	GLU	conflict	UNP P68971
Q	117	UNK	LEU	conflict	UNP P68971
Q	118	UNK	SER	conflict	UNP P68971
Q	119	UNK	LYS	conflict	UNP P68971
Q	120	UNK	GLN	conflict	UNP P68971
Q	121	UNK	VAL	conflict	UNP P68971
Q	122	UNK	ALA	conflict	UNP P68971
Q	123	UNK	GLN	conflict	UNP P68971
Q	124	UNK	LEU	conflict	UNP P68971
Q	125	UNK	ARG	conflict	UNP P68971
Q	126	UNK	GLU	conflict	UNP P68971
Q	127	UNK	GLN	conflict	UNP P68971
Q	128	UNK	THR	conflict	UNP P68971
Q	129	UNK	GLU	conflict	UNP P68971
Q	130	UNK	SER	conflict	UNP P68971
Q	131	UNK	ALA	conflict	UNP P68971
Q	132	UNK	VAL	conflict	UNP P68971
Q	133	UNK	ALA	conflict	UNP P68971
Q	134	UNK	THR	conflict	UNP P68971
R	92	UNK	PRO	conflict	UNP P68971
R	93	UNK	SER	conflict	UNP P68971
R	94	UNK	THR	conflict	UNP P68971
R	95	UNK	LEU	conflict	UNP P68971
R	96	UNK	ALA	conflict	UNP P68971
R	97	UNK	GLU	conflict	UNP P68971
R	98	UNK	ASP	conflict	UNP P68971
R	99	UNK	LYS	conflict	UNP P68971
R	100	UNK	LEU	conflict	UNP P68971
R	101	UNK	LEU	conflict	UNP P68971
R	102	UNK	VAL	conflict	UNP P68971
R	103	UNK	LEU	conflict	UNP P68971
R	104	UNK	LEU	conflict	UNP P68971
R	105	UNK	ALA	conflict	UNP P68971
R	106	UNK	GLN	conflict	UNP P68971
R	107	UNK	LEU	conflict	UNP P68971
R	108	UNK	GLU	conflict	UNP P68971
R	109	UNK	ALA	conflict	UNP P68971
R	110	UNK	LEU	conflict	UNP P68971
R	111	UNK	THR	conflict	UNP P68971
R	112	UNK	GLN	conflict	UNP P68971
R	113	UNK	ARG	conflict	UNP P68971
R	114	UNK	LEU	conflict	UNP P68971

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Chain	Residue	Modelled	Actual	Comment	Reference
R	115	UNK	GLY	conflict	UNP P68971
R	116	UNK	GLU	conflict	UNP P68971
R	117	UNK	LEU	conflict	UNP P68971
R	118	UNK	SER	conflict	UNP P68971
R	119	UNK	LYS	conflict	UNP P68971
R	120	UNK	GLN	conflict	UNP P68971
R	121	UNK	VAL	conflict	UNP P68971
R	122	UNK	ALA	conflict	UNP P68971
R	123	UNK	GLN	conflict	UNP P68971
R	124	UNK	LEU	conflict	UNP P68971
R	125	UNK	ARG	conflict	UNP P68971
R	126	UNK	GLU	conflict	UNP P68971
R	127	UNK	GLN	conflict	UNP P68971
R	128	UNK	THR	conflict	UNP P68971
R	129	UNK	GLU	conflict	UNP P68971
R	130	UNK	SER	conflict	UNP P68971
R	131	UNK	ALA	conflict	UNP P68971
R	132	UNK	VAL	conflict	UNP P68971
R	133	UNK	ALA	conflict	UNP P68971
R	134	UNK	THR	conflict	UNP P68971
S	92	UNK	PRO	conflict	UNP P68971
S	93	UNK	SER	conflict	UNP P68971
S	94	UNK	THR	conflict	UNP P68971
S	95	UNK	LEU	conflict	UNP P68971
S	96	UNK	ALA	conflict	UNP P68971
S	97	UNK	GLU	conflict	UNP P68971
S	98	UNK	ASP	conflict	UNP P68971
S	99	UNK	LYS	conflict	UNP P68971
S	100	UNK	LEU	conflict	UNP P68971
S	101	UNK	LEU	conflict	UNP P68971
S	102	UNK	VAL	conflict	UNP P68971
S	103	UNK	LEU	conflict	UNP P68971
S	104	UNK	LEU	conflict	UNP P68971
S	105	UNK	ALA	conflict	UNP P68971
S	106	UNK	GLN	conflict	UNP P68971
S	107	UNK	LEU	conflict	UNP P68971
S	108	UNK	GLU	conflict	UNP P68971
S	109	UNK	ALA	conflict	UNP P68971
S	110	UNK	LEU	conflict	UNP P68971
S	111	UNK	THR	conflict	UNP P68971
S	112	UNK	GLN	conflict	UNP P68971
S	113	UNK	ARG	conflict	UNP P68971

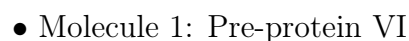
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Chain	Residue	Modelled	Actual	Comment	Reference
S	114	UNK	LEU	conflict	UNP P68971
S	115	UNK	GLY	conflict	UNP P68971
S	116	UNK	GLU	conflict	UNP P68971
S	117	UNK	LEU	conflict	UNP P68971
S	118	UNK	SER	conflict	UNP P68971
S	119	UNK	LYS	conflict	UNP P68971
S	120	UNK	GLN	conflict	UNP P68971
S	121	UNK	VAL	conflict	UNP P68971
S	122	UNK	ALA	conflict	UNP P68971
S	123	UNK	GLN	conflict	UNP P68971
S	124	UNK	LEU	conflict	UNP P68971
S	125	UNK	ARG	conflict	UNP P68971
S	126	UNK	GLU	conflict	UNP P68971
S	127	UNK	GLN	conflict	UNP P68971
S	128	UNK	THR	conflict	UNP P68971
S	129	UNK	GLU	conflict	UNP P68971
S	130	UNK	SER	conflict	UNP P68971
S	131	UNK	ALA	conflict	UNP P68971
S	132	UNK	VAL	conflict	UNP P68971
S	133	UNK	ALA	conflict	UNP P68971
S	134	UNK	THR	conflict	UNP P68971

- Molecule 6 is a protein called Pre-hexon-linking protein VIII.

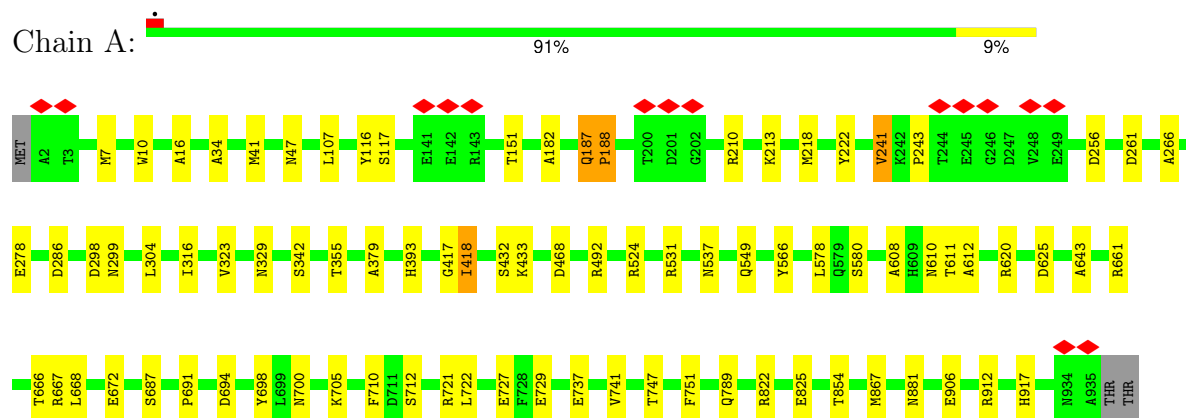
Mol	Chain	Residues	Atoms						AltConf	Trace
6	U	106	Total	C	H	N	O	S	0	0
			1607	531	775	133	164	4		
6	V	107	Total	C	H	N	O	S	0	0
			1619	535	779	134	167	4		



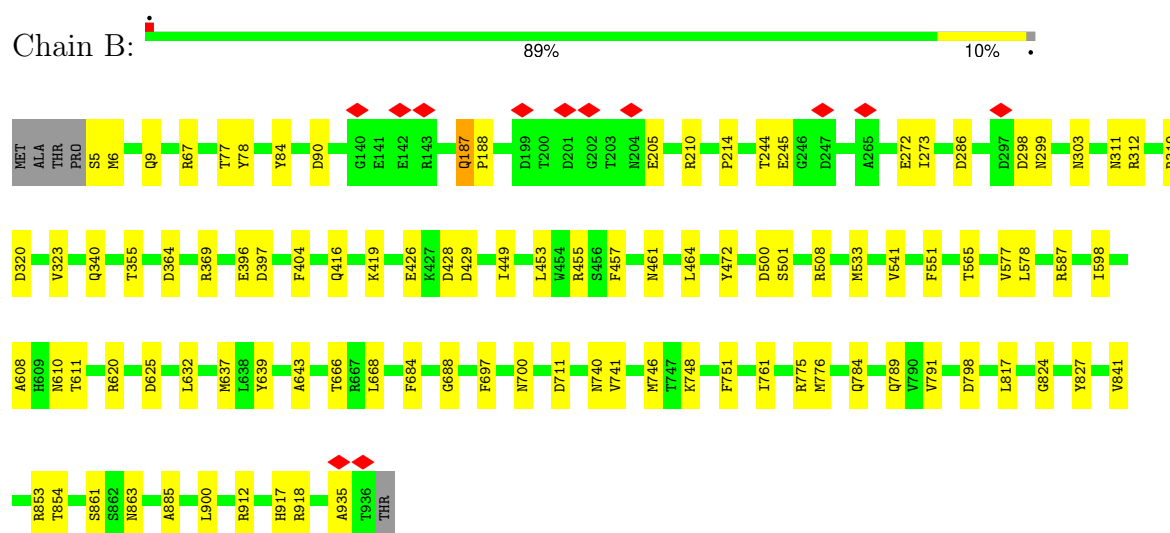
[illegible]

TYR	PRO	GLY	LYS
	PRO	ASP	LEU
	ALA	LYS	LYS
	SER	ARG	GLU
	ALA	PRO	GLN
	LEU	ARG	ASN
	LEU	PRO	PHE
	VAL	GLU	GLN
	PRO	LEU	GLN
	LYS	GLU	LYS
PRO	GLN	VAL	
VAL	THR	VAL	
ALA	LEU	ASP	
THR	VAL	GLY	
ARG	THR	ILE	
LYS	ARG	ALA	
PRO	ALA	SER	
THR	ASP	GLY	
ALA	GLU	ILE	
VAL	PRO	ASN	
GLN	PRO	GLY	
PRO	SER	VAL	
VAL	TYR	VAL	
ALA	GLU	ASP	
VAL	GLU	LEU	
ALA	ALA	ALA	
ARG	VAL	ASN	
PRO	LYS	GLN	
ARG	LEU	ALA	
PRO	GLY	VAL	
GLY	MET	GLN	
GLY	PRO	LYS	
THR	THR	GLN	
PRO	THR	ILE	
ARG	ARG	ASN	
PRO	PRO	SER	
LYS	VAL	ARG	
ALA	ALA	LEU	
ASN	HIS	ASP	
TRP	MET	PRO	
GLN	ALA	PRO	
SER	THR	PRO	
THR	GLY	ALA	
LEU	VAL	THR	
ASN	MET	PRO	
ILE	PRO	GLY	
VAL	SER	MET	
GLY	GLN	GLU	
LEU	SER	VAL	
GLY	HIS	GLU	
VAL	ARG	GLU	
GLN	PRO	GLU	
VAL	ALA	LEU	
LYS	THR	PRO	
ARG	ASP	LEU	
ARG	LEU	GLN	
ARG	PRO	LYS	
CYS	PRO	ARG	
MET	GLU	ASP	ASN
	ILE	GLU	ASN
	LYS	PHE	LYS
	GLN	ASN	GLN
	VAL	GLN	VAL
	THR	THR	THR
	TRP	TRP	THR
	SER	SER	SER
	D24	D24	D24
	I25	I25	I25
G26	G26	G26	
T27	T27	T27	
Q28	Q28	Q28	
L30	L30	L30	
N31	N31	N31	
GLY	GLY	GLY	
ALA	ALA	ALA	
PHE	PHE	PHE	
ASN	ASN	ASN	
TRP	TRP	TRP	
SER	SER	SER	
GLY	GLY	GLY	
LYS	LYS	LYS	
ASN	ASN	ASN	
PHE	PHE	PHE	
SER	SER	SER	
THR	THR	THR	
VAL	VAL	VAL	
LYS	LYS	LYS	
TYR	TYR	TYR	
GLY	GLY	GLY	
ASN	ASN	ASN	
LYS	LYS	LYS	
ALA	ALA	ALA	
TRP	TRP	TRP	
ASN	ASN	ASN	
SER	SER	SER	
SER	SER	SER	
THR	THR	THR	
GLY	GLY	GLY	
ALA	ALA	ALA	
ASN	ASN	ASN	
ARG	ARG	ARG	

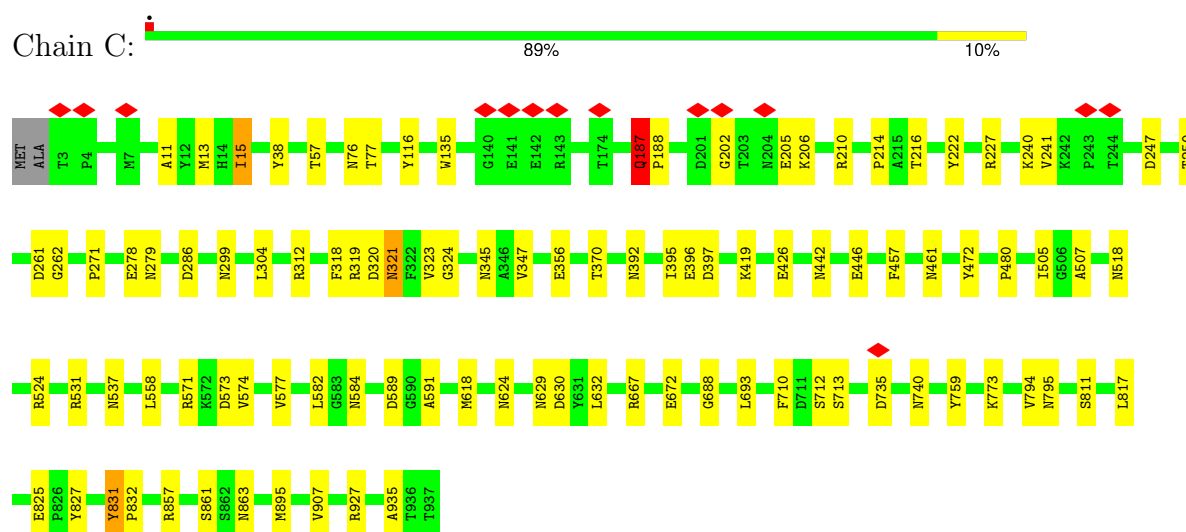
PRO	ASP	LEU	MET
ALA	ARG	GLY	GLU
SER	ARG	GLU	ASP
ALA	PRO	ASN	ILE
ALA	ARG	PHE	N5
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PRO	LEU	GLN	L12
PRO	GLU	VAL	L15
VAL	THR	VAL	L19
ALA	LEU	ASP	L23
THR	VAL	GLY	L25
ARG	THR	ILE	N31
PRO	ARG	ALA	G32
PRO	ALA	SER	G33
THR	ASP	GLY	A34
VAL	GLU	ILE	PHE
ALA	PRO	ASN	ASN
VAL	PRO	GLY	TRP
THR	SER	VAL	TRP
PRO	TYR	VAL	SER
VAL	GLU	ASP	SER
VAL	GLU	LEU	ILE
ALA	ALA	LEU	TRP
ARG	VAL	ASN	SER
PRO	LYS	GLN	GLY
ARG	LEU	ALA	ASN
PRO	GLY	VAL	LEU
ALA	MET	ARG	LYS
ALA	HIS	LEU	ASN
TRP	MET	ASP	PHE
GLN	ALA	PRO	GLY
SER	THR	PRO	SER
THR	GLY	ALA	THR
LEU	VAL	THR	VAL
ASN	MET	PRO	LYS
SER	SER	GLY	THR
ILE	PRO	GLU	TYR
GLY	SER	MET	GLY
LEU	GLN	GLU	LYS
GLY	HIS	VAL	ALA
VAL	ARG	GLU	ALA
PRO	PRO	GLU	TRP
SER	ALA	LEU	ASN
VAL	THR	PRO	SER
LYS	LEU	PRO	THR
ARG	ASP	PRO	GLY
ARG	LEU	LEU	GLN
ARG	PRO	LYS	ALA
CYS	PRO	ARG	LEU
TYR	PRO	GLY	ASN



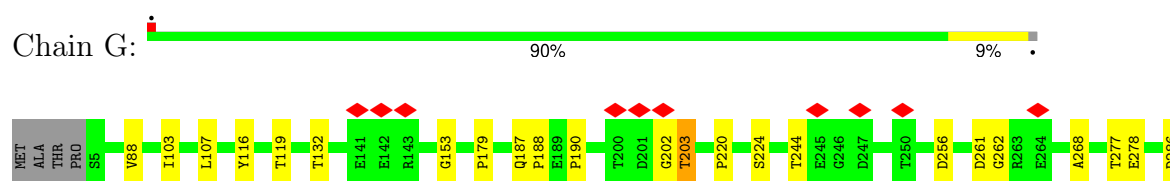
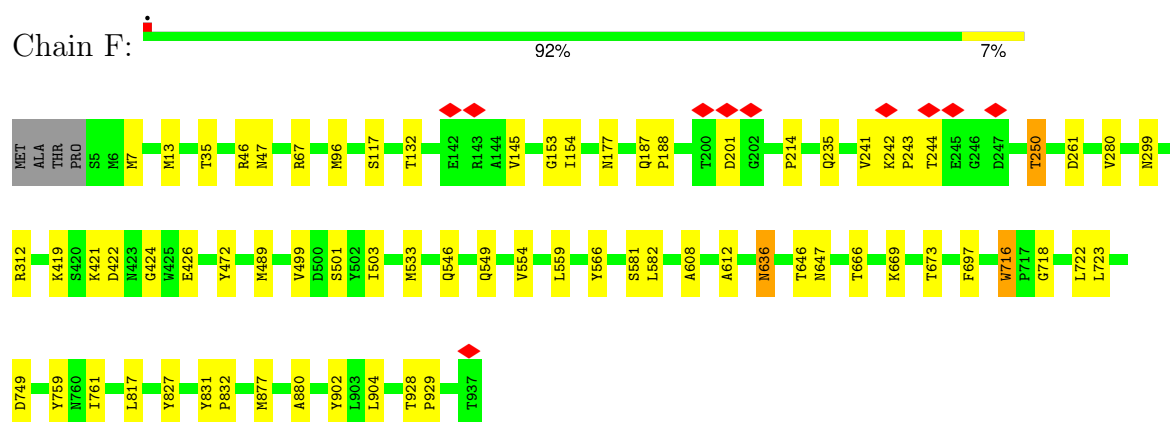
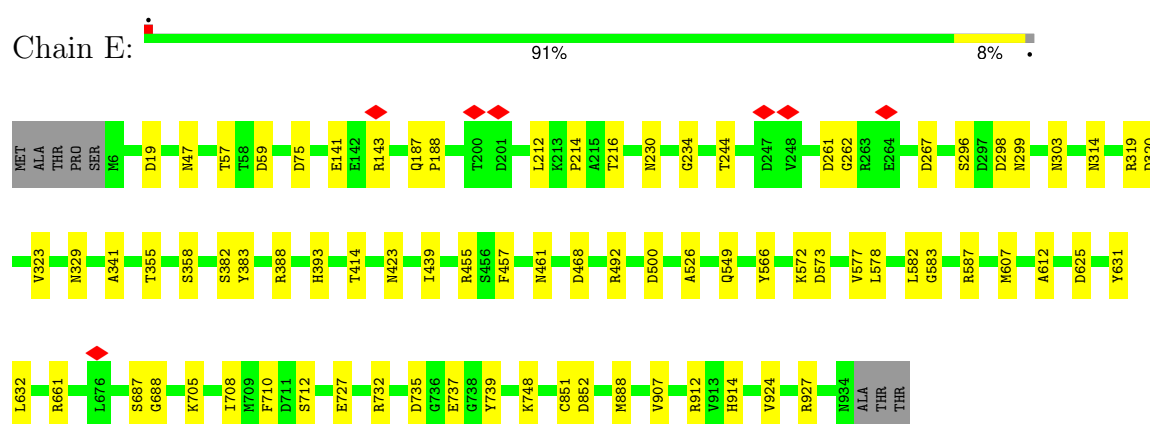
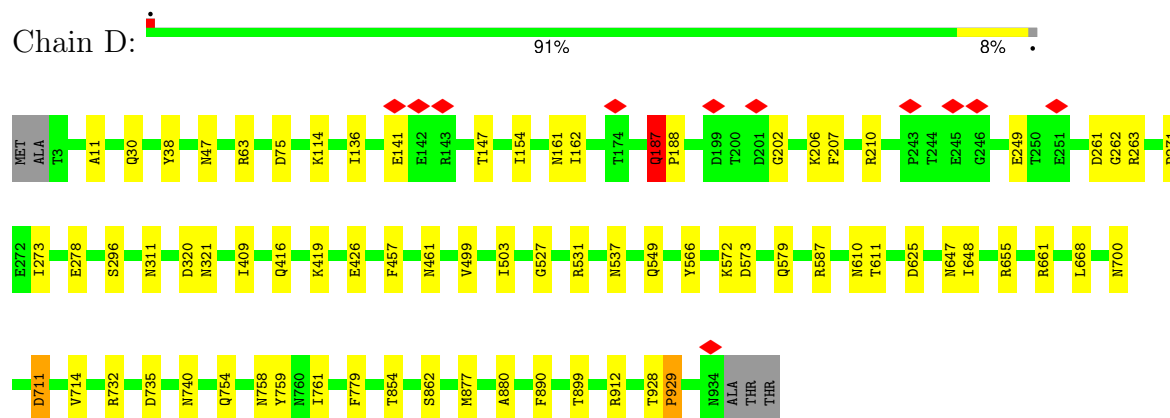
- Molecule 2: Hexon protein

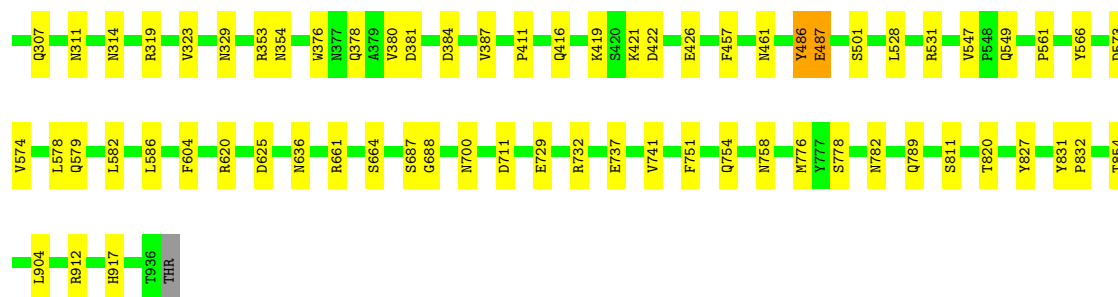


- Molecule 2: Hexon protein

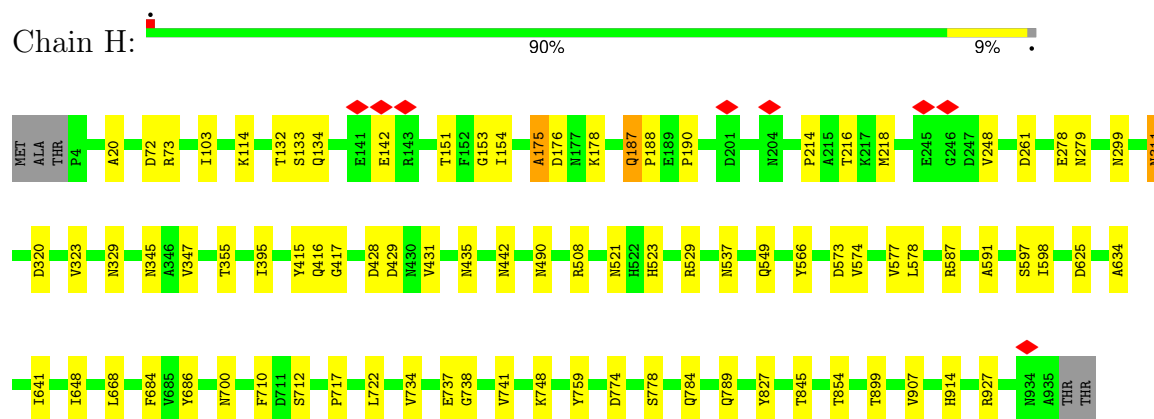


- Molecule 2: Hexon protein

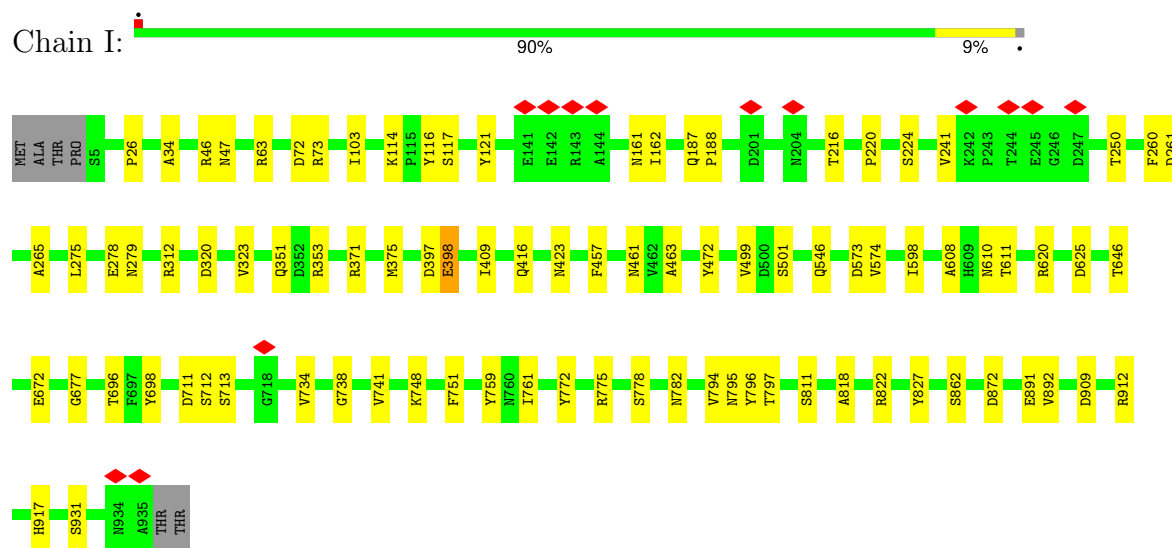




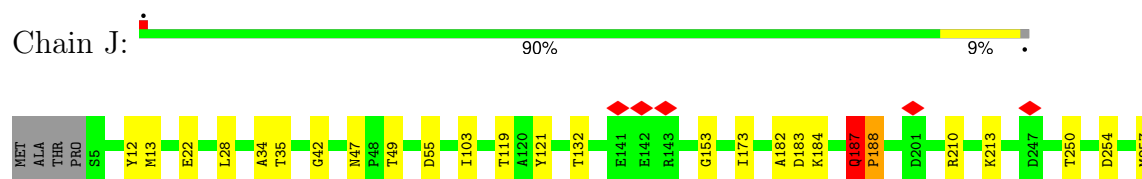
• Molecule 2: Hexon protein

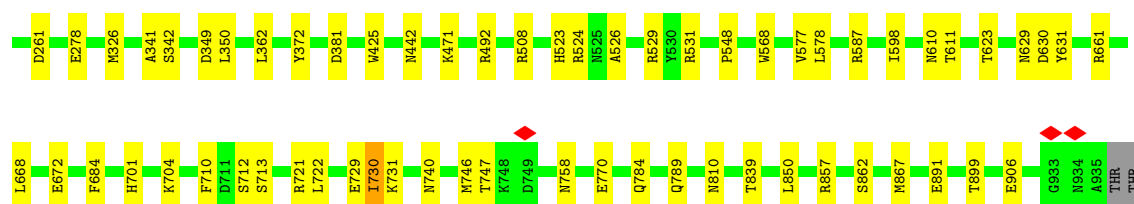


• Molecule 2: Hexon protein

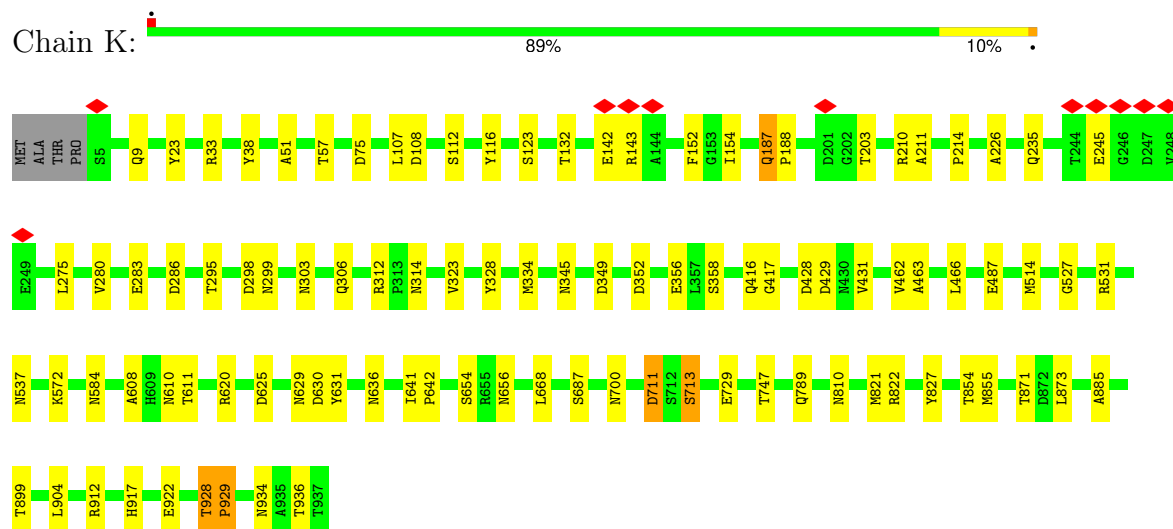


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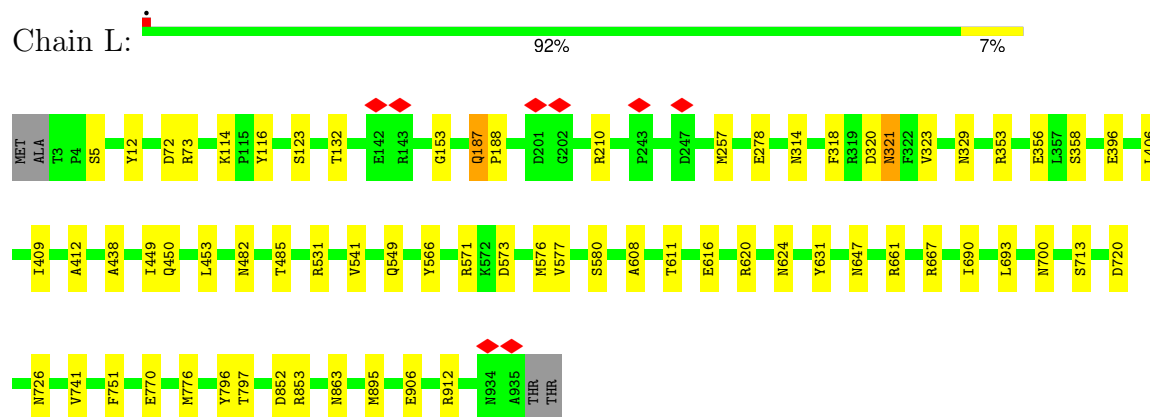




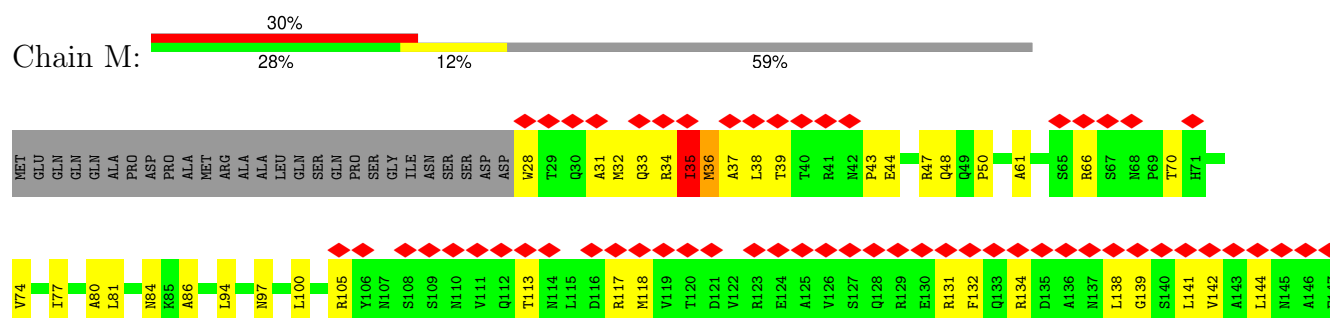
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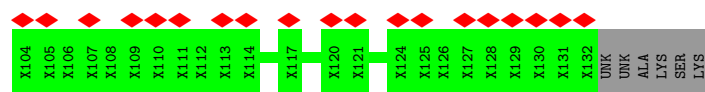


• Molecule 2: Hexon protein

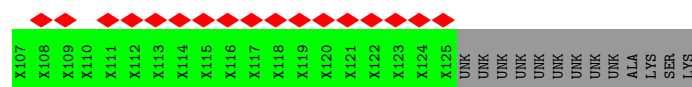
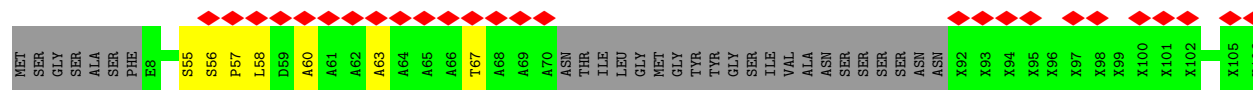


• Molecule 3: Pre-hexon-linking protein IIIa

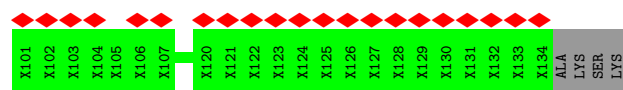
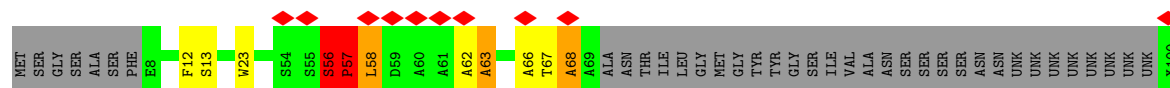




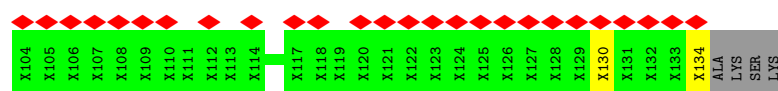
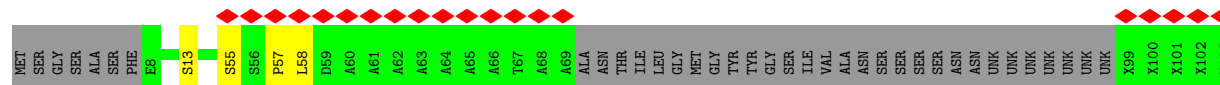
• Molecule 5: Hexon-interlacing protein IX



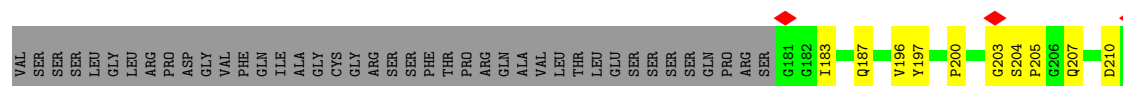
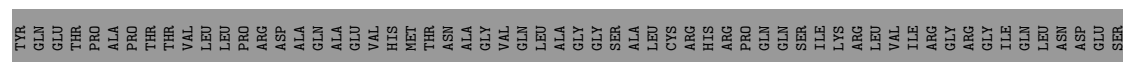
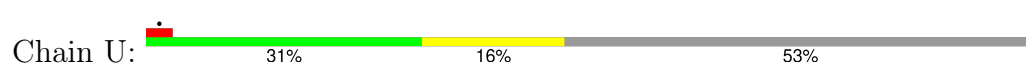
• Molecule 5: Hexon-interlacing protein IX



• Molecule 5: Hexon-interlacing protein IX

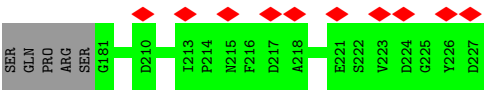
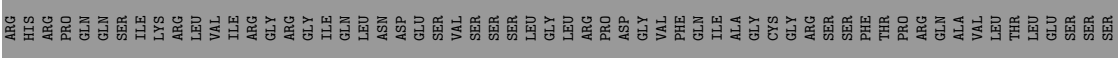
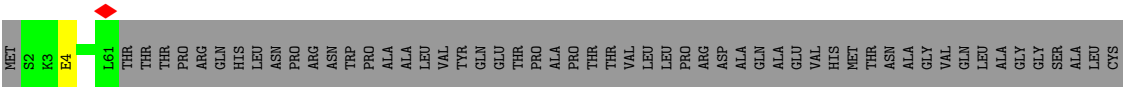


• Molecule 6: Pre-hexon-linking protein VIII





• Molecule 6: Pre-hexon-linking protein VIII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96492	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 ($e^-/\text{\AA}^2$)	53.35	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	10.952	Depositor
Minimum map value	-6.825	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size (Å)	294.576, 461.35797, 252.33899	wwPDB
Map dimensions	233, 426, 272	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	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	0	0.15	0/119	0.24	0/158
1	1	0.15	0/193	0.48	0/257
1	2	0.16	0/186	0.34	0/249
1	3	0.13	0/149	0.34	0/199
1	4	0.15	0/196	0.33	0/264
1	W	0.20	0/224	0.47	0/304
1	Y	0.19	0/194	0.46	0/260
1	Z	0.17	0/201	0.39	0/269
2	A	0.27	0/7631	0.58	2/10387 (0.0%)
2	B	0.27	0/7618	0.56	1/10368 (0.0%)
2	C	0.27	0/7634	0.59	4/10391 (0.0%)
2	D	0.26	0/7621	0.57	4/10373 (0.0%)
2	E	0.27	0/7600	0.56	0/10343
2	F	0.27	0/7625	0.60	7/10378 (0.1%)
2	G	0.29	1/7616 (0.0%)	0.61	11/10365 (0.1%)
2	H	0.28	0/7619	0.57	1/10369 (0.0%)
2	I	0.27	0/7611	0.59	3/10358 (0.0%)
2	J	0.26	0/7611	0.56	4/10358 (0.0%)
2	K	0.26	0/7625	0.55	0/10378
2	L	0.26	0/7626	0.56	1/10380 (0.0%)
3	M	0.19	0/1915	0.50	2/2606 (0.1%)
4	N	0.25	0/3823	0.53	2/5200 (0.0%)
5	P	0.24	0/449	0.52	0/618
5	Q	0.23	0/449	0.52	0/618
5	R	0.57	0/444	1.30	4/611 (0.7%)
5	S	0.25	0/444	0.57	0/611
6	U	0.23	0/856	0.45	0/1164
6	V	0.24	0/864	0.48	0/1175
All	All	0.27	1/102143 (0.0%)	0.57	46/139011 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	3
2	B	0	2
2	C	0	5
2	D	0	5
2	E	0	3
2	F	0	5
2	G	0	3
2	H	0	5
2	I	0	3
2	J	0	2
2	K	0	4
2	L	0	2
3	M	0	1
All	All	0	43

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	179	PRO	CG-CD	-7.08	1.26	1.50

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	57	PRO	N-CA-CB	-15.29	87.19	103.25
5	R	12	PHE	CA-C-N	12.21	151.59	121.80
5	R	12	PHE	C-N-CA	12.21	151.59	121.80
5	R	57	PRO	N-CA-C	11.68	136.53	112.47
2	G	179	PRO	N-CD-CG	-11.67	85.69	103.20
2	F	243	PRO	CA-C-N	11.17	142.88	121.54
2	F	243	PRO	C-N-CA	11.17	142.88	121.54
2	D	202	GLY	CA-C-N	10.64	141.90	122.54
2	D	202	GLY	C-N-CA	10.64	141.90	122.54
2	I	26	PRO	CA-N-CD	-9.07	99.31	112.00
2	I	398	GLU	CB-CG-CD	7.45	125.26	112.60
2	G	179	PRO	CA-CB-CG	-6.93	91.33	104.50
2	G	203	THR	CA-CB-CG2	6.29	121.19	110.50
2	G	244	THR	OG1-CB-CG2	6.17	121.64	109.30
2	F	242	LYS	N-CA-C	6.14	119.62	109.79
2	G	179	PRO	CA-N-CD	-6.11	103.44	112.00
2	G	486	TYR	CA-C-N	6.06	133.12	121.54
2	G	486	TYR	C-N-CA	6.06	133.12	121.54
2	F	244	THR	CA-CB-CG2	6.04	120.77	110.50
2	C	187	GLN	C-N-CD	-5.99	100.44	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	35	ILE	CA-C-N	5.88	132.78	121.54
3	M	35	ILE	C-N-CA	5.88	132.78	121.54
2	A	151	THR	OG1-CB-CG2	5.86	121.01	109.30
2	D	187	GLN	C-N-CD	-5.79	101.27	125.00
2	H	187	GLN	C-N-CD	-5.74	101.46	125.00
2	A	825	GLU	N-CA-C	5.70	116.85	109.72
2	J	187	GLN	C-N-CD	-5.57	102.16	125.00
2	F	250	THR	OG1-CB-CG2	5.54	120.38	109.30
2	C	831	TYR	C-N-CD	-5.48	102.52	125.00
2	B	824	GLY	N-CA-C	5.48	117.44	110.20
2	J	250	THR	OG1-CB-CG2	5.48	120.26	109.30
2	I	398	GLU	N-CA-CB	5.46	119.71	110.49
2	D	154	ILE	CG1-CB-CG2	5.46	127.07	110.70
2	G	203	THR	OG1-CB-CG2	5.44	120.19	109.30
2	L	720	ASP	CA-CB-CG	5.39	117.99	112.60
2	J	250	THR	CA-CB-CG2	5.35	119.60	110.50
2	C	15	ILE	N-CA-C	-5.33	107.58	111.90
2	F	244	THR	OG1-CB-CG2	5.29	119.88	109.30
2	F	250	THR	CA-CB-CG2	5.15	119.26	110.50
4	N	180	PRO	CA-C-N	5.15	131.37	121.54
4	N	180	PRO	C-N-CA	5.15	131.37	121.54
2	G	421	LYS	CA-C-N	5.07	131.22	121.54
2	G	421	LYS	C-N-CA	5.07	131.22	121.54
2	C	935	ALA	CA-C-O	5.04	126.43	120.58
2	J	730	ILE	N-CA-C	-5.04	98.86	109.34
2	G	244	THR	CA-CB-CG2	5.02	119.04	110.50

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	187	GLN	Peptide
2	A	643	ALA	Peptide
2	A	7	MET	Peptide
2	B	187	GLN	Peptide
2	B	935	ALA	Peptide
2	C	11	ALA	Peptide
2	C	187	GLN	Peptide
2	C	247	ASP	Peptide
2	C	321	ASN	Peptide
2	C	831	TYR	Peptide
2	D	187	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	D	321	ASN	Peptide
2	D	711	ASP	Peptide
2	D	779	PHE	Peptide
2	D	928	THR	Peptide
2	E	187	GLN	Peptide
2	E	526	ALA	Peptide
2	E	851	CYS	Peptide
2	F	187	GLN	Peptide
2	F	7	MET	Peptide
2	F	716	TRP	Peptide
2	F	831	TYR	Peptide
2	F	928	THR	Peptide
2	G	187	GLN	Peptide
2	G	711	ASP	Peptide
2	G	831	TYR	Peptide
2	H	175	ALA	Peptide
2	H	176	ASP	Peptide
2	H	187	GLN	Peptide
2	H	311	ASN	Peptide
2	H	717	PRO	Peptide
2	I	121	TYR	Peptide
2	I	187	GLN	Peptide
2	I	397	ASP	Mainchain
2	J	13	MET	Peptide
2	J	187	GLN	Peptide
2	K	187	GLN	Peptide
2	K	328	TYR	Peptide
2	K	711	ASP	Peptide
2	K	928	THR	Peptide
2	L	187	GLN	Peptide
2	L	321	ASN	Peptide
3	M	35	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	118	109	109	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	191	183	183	4	0
1	2	183	172	172	4	0
1	3	146	139	139	10	0
1	4	191	178	178	6	0
1	W	218	206	206	8	0
1	Y	191	183	183	5	0
1	Z	198	185	185	4	0
2	A	7430	7104	7103	53	0
2	B	7418	7091	7091	58	0
2	C	7433	7100	7097	57	0
2	D	7420	7093	7093	42	0
2	E	7400	7074	7074	47	0
2	F	7425	7098	7098	37	0
2	G	7416	7087	7086	51	0
2	H	7418	7092	7092	51	0
2	I	7411	7084	7084	54	0
2	J	7411	7084	7084	55	0
2	K	7425	7099	7098	67	0
2	L	7425	7098	7098	44	0
3	M	1882	1889	1889	68	0
4	N	3733	3658	3658	24	0
5	P	619	571	466	5	0
5	Q	609	563	464	7	0
5	R	609	561	460	9	0
5	S	614	561	461	3	0
6	U	832	775	775	33	0
6	V	840	779	779	0	0
All	All	100206	95816	95405	684	0

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

All (684) 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)
3:M:172:MET:HE1	3:M:243:PHE:HB2	1.52	0.90
6:U:36:ALA:HB1	6:U:40:MET:HB2	1.53	0.89
3:M:33:GLN:HA	3:M:36:MET:HE3	1.58	0.86
3:M:131:ARG:HA	3:M:134:ARG:HE	1.44	0.83
3:M:216:HIS:HA	3:M:253:SER:HA	1.62	0.81
2:K:936:THR:HG21	6:U:5:ILE:HD11	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:412:ALA:HB2	2:L:438:ALA:HB2	1.66	0.78
3:M:217:ALA:HB2	3:M:254:TYR:HA	1.67	0.77
3:M:32:MET:HB3	3:M:61:ALA:HB1	1.68	0.74
2:J:187:GLN:O	2:J:210:ARG:NH1	2.21	0.73
2:B:9:GLN:OE1	2:K:713:SER:OG	2.07	0.73
5:Q:57:PRO:HB2	5:Q:60:ALA:HB3	1.70	0.71
1:3:12:ARG:HG2	1:3:14:GLY:H	1.55	0.71
2:H:587:ARG:NH2	2:H:684:PHE:O	2.23	0.70
3:M:231:PRO:HG2	6:U:4:GLU:HG3	1.71	0.70
2:E:924:VAL:HG23	2:F:13:MET:HE1	1.72	0.70
2:J:839:THR:OG1	2:K:283:GLU:OE2	2.08	0.70
2:F:549:GLN:NE2	2:F:554:VAL:O	2.25	0.70
3:M:138:LEU:HD23	3:M:141:LEU:HD12	1.71	0.70
2:B:508:ARG:NH2	2:B:784:GLN:OE1	2.26	0.69
4:N:185:SER:O	4:N:189:THR:OG1	2.09	0.69
2:I:625:ASP:OD2	2:I:912:ARG:NH1	2.25	0.69
2:K:700:ASN:ND2	2:K:854:THR:O	2.25	0.69
2:A:729:GLU:O	2:A:747:THR:OG1	2.11	0.69
2:D:30:GLN:OE1	1:Z:5:ASN:N	2.25	0.69
2:K:668:LEU:O	2:K:899:THR:OG1	2.10	0.69
2:D:187:GLN:O	2:D:210:ARG:NH1	2.27	0.68
2:H:700:ASN:ND2	2:H:854:THR:O	2.26	0.68
2:D:38:TYR:OH	1:Z:9:LEU:O	2.09	0.68
2:L:776:MET:SD	2:L:853:ARG:NH1	2.66	0.68
2:H:508:ARG:NH2	2:H:784:GLN:OE1	2.27	0.68
2:F:877:MET:O	2:F:880:ALA:O	2.11	0.68
2:D:732:ARG:NE	2:D:735:ASP:OD1	2.26	0.68
2:A:580:SER:OG	2:A:687:SER:O	2.12	0.67
2:K:214:PRO:O	2:K:299:ASN:ND2	2.28	0.67
2:A:620:ARG:NH1	2:A:917:HIS:O	2.27	0.67
2:L:329:ASN:ND2	2:L:353:ARG:O	2.27	0.67
2:J:668:LEU:O	2:J:899:THR:OG1	2.12	0.67
2:L:318:PHE:O	2:L:531:ARG:NH1	2.28	0.67
2:A:278:GLU:OE1	2:C:827:TYR:OH	2.13	0.67
2:K:729:GLU:O	2:K:747:THR:OG1	2.12	0.67
3:M:80:ALA:O	3:M:84:ASN:ND2	2.28	0.67
2:D:668:LEU:O	2:D:899:THR:OG1	2.13	0.67
2:C:318:PHE:O	2:C:531:ARG:NH1	2.28	0.66
2:K:620:ARG:NH1	2:K:917:HIS:O	2.28	0.66
2:D:877:MET:O	2:D:880:ALA:O	2.14	0.66
2:J:471:LYS:O	2:J:492:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:191:GLN:HE21	3:M:196:GLY:HA3	1.61	0.66
2:E:732:ARG:NE	2:E:735:ASP:OD2	2.29	0.66
2:K:654:SER:O	6:U:27:TYR:OH	2.12	0.66
2:G:549:GLN:OE1	2:G:566:TYR:OH	2.14	0.66
2:C:472:TYR:OH	2:C:817:LEU:O	2.12	0.65
1:2:12:ARG:HH22	1:2:15:THR:HA	1.62	0.65
2:K:827:TYR:OH	2:L:278:GLU:OE2	2.12	0.65
2:A:187:GLN:O	2:A:210:ARG:NH1	2.30	0.65
2:I:672:GLU:OE2	2:I:698:TYR:OH	2.12	0.65
2:B:798:ASP:OD2	2:C:227:ARG:NH2	2.30	0.64
2:K:527:GLY:O	2:K:531:ARG:NH1	2.30	0.64
2:B:312:ARG:NH1	2:B:464:LEU:O	2.30	0.64
2:D:531:ARG:NH2	2:D:579:GLN:OE1	2.30	0.64
2:L:571:ARG:NH1	2:L:576:MET:SD	2.69	0.64
2:G:278:GLU:OE2	2:I:827:TYR:OH	2.15	0.64
2:I:759:TYR:HB3	2:I:761:ILE:HD12	1.79	0.64
3:M:34:ARG:O	3:M:39:THR:OG1	2.11	0.64
2:E:358:SER:OG	2:E:631:TYR:O	2.10	0.64
2:F:646:THR:O	2:F:647:ASN:ND2	2.30	0.64
2:J:524:ARG:NH1	2:L:396:GLU:OE2	2.30	0.64
2:G:729:GLU:OE1	2:G:732:ARG:NE	2.31	0.64
2:H:395:ILE:O	2:I:117:SER:OG	2.10	0.64
2:G:220:PRO:O	2:G:224:SER:OG	2.16	0.64
2:B:340:GLN:OE1	2:B:565:THR:OG1	2.16	0.63
2:C:419:LYS:NZ	2:C:426:GLU:OE2	2.26	0.63
3:M:74:VAL:HG11	3:M:100:LEU:HD23	1.81	0.63
5:P:57:PRO:HB3	5:P:60:ALA:HB3	1.79	0.63
3:M:113:THR:HG22	3:M:117:ARG:HH22	1.63	0.63
2:H:577:VAL:HG23	2:H:578:LEU:HD12	1.80	0.63
2:K:298:ASP:O	2:K:303:ASN:ND2	2.32	0.63
2:K:323:VAL:HG23	2:K:356:GLU:OE1	1.99	0.63
2:K:789:GLN:HE22	2:L:541:VAL:HG12	1.62	0.63
2:J:623:THR:OG1	2:K:23:TYR:O	2.16	0.63
2:F:549:GLN:OE1	2:F:566:TYR:OH	2.11	0.62
2:K:116:TYR:OH	2:K:286:ASP:OD2	2.15	0.62
2:G:700:ASN:ND2	2:G:854:THR:O	2.31	0.62
2:D:700:ASN:ND2	2:D:854:THR:O	2.33	0.62
2:F:472:TYR:OH	2:F:817:LEU:O	2.14	0.62
1:Z:12:ARG:NH2	1:Z:15:THR:O	2.31	0.62
2:J:770:GLU:OE1	2:J:770:GLU:N	2.31	0.62
2:K:584:ASN:O	2:K:687:SER:OG	2.10	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:661:ARG:NH2	2:L:906:GLU:OE1	2.32	0.62
3:M:32:MET:SD	3:M:33:GLN:NE2	2.68	0.62
2:J:182:ALA:HB1	2:J:188:PRO:HD3	1.81	0.62
3:M:184:SER:HB2	6:U:203:GLY:HA2	1.82	0.61
1:4:24:ASP:HA	2:J:42:GLY:O	2.00	0.61
2:B:711:ASP:OD1	2:B:885:ALA:N	2.33	0.61
2:I:353:ARG:NH1	2:I:909:ASP:OD2	2.33	0.61
3:M:28:TRP:HB3	3:M:31:ALA:HB3	1.81	0.61
2:C:202:GLY:N	2:C:205:GLU:OE2	2.31	0.61
2:E:577:VAL:HG23	2:E:578:LEU:HD12	1.83	0.61
2:F:214:PRO:O	2:F:299:ASN:ND2	2.34	0.61
4:N:220:ASP:OD1	4:N:221:THR:N	2.33	0.61
5:R:67:THR:O	5:R:68:ALA:HB2	2.00	0.61
1:3:9:LEU:O	2:K:38:TYR:OH	2.12	0.60
2:H:216:THR:OG1	2:H:279:ASN:OD1	2.17	0.60
2:A:625:ASP:OD2	2:A:912:ARG:NH1	2.34	0.60
2:K:463:ALA:HA	2:K:466:LEU:HD13	1.82	0.60
2:B:396:GLU:OE2	2:C:524:ARG:NH2	2.35	0.60
2:G:329:ASN:ND2	2:G:353:ARG:O	2.35	0.60
2:D:278:GLU:OE1	2:F:827:TYR:OH	2.17	0.60
2:K:154:ILE:HG22	2:L:438:ALA:HB3	1.82	0.60
1:4:26:GLY:HA2	2:J:47:ASN:HB2	1.84	0.60
2:C:574:VAL:HG11	2:C:591:ALA:HB3	1.84	0.60
2:D:47:ASN:ND2	1:Z:25:ILE:HA	2.17	0.60
2:K:929:PRO:O	6:U:28:SER:HB2	2.01	0.60
2:B:625:ASP:OD2	2:B:912:ARG:NH1	2.34	0.60
4:N:120:GLY:O	4:N:537:ARG:N	2.35	0.60
5:R:62:ALA:O	5:R:63:ALA:HB2	2.02	0.60
2:H:741:VAL:HG13	2:I:375:MET:HE3	1.83	0.59
3:M:35:ILE:O	3:M:37:ALA:N	2.29	0.59
2:G:319:ARG:NH1	2:G:688:GLY:O	2.34	0.59
2:J:721:ARG:O	2:J:722:LEU:HD22	2.02	0.59
2:B:397:ASP:OD2	2:C:222:TYR:OH	2.19	0.59
2:E:705:LYS:NZ	2:E:727:GLU:OE1	2.28	0.59
2:G:286:ASP:O	2:G:311:ASN:ND2	2.35	0.59
2:B:700:ASN:ND2	2:B:854:THR:O	2.35	0.59
2:C:187:GLN:O	2:C:210:ARG:NH1	2.36	0.59
6:U:197:TYR:CE2	6:U:200:PRO:HA	2.38	0.59
2:A:524:ARG:NH1	2:C:396:GLU:OE2	2.36	0.59
5:S:130:UNK:O	5:S:134:UNK:N	2.36	0.59
2:L:549:GLN:OE1	2:L:566:TYR:OH	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:241:VAL:HG12	2:A:243:PRO:HD3	1.85	0.58
3:M:201:ASN:HB3	3:M:204:GLN:HG3	1.85	0.58
2:J:442:ASN:OD1	2:K:822:ARG:NH1	2.35	0.58
2:G:103:ILE:HD12	2:G:547:VAL:HG21	1.84	0.58
6:U:204:SER:OG	6:U:207:GLN:HB2	2.03	0.58
1:O:27:THR:OG1	2:E:47:ASN:O	2.14	0.58
2:A:705:LYS:NZ	2:A:727:GLU:OE1	2.34	0.58
2:B:827:TYR:OH	2:C:278:GLU:OE1	2.21	0.58
5:R:56:SER:HB2	5:R:57:PRO:CD	2.33	0.58
2:B:741:VAL:HG21	2:B:751:PHE:HB2	1.86	0.57
2:H:549:GLN:OE1	2:H:566:TYR:OH	2.22	0.57
2:E:75:ASP:OD1	2:E:572:LYS:NZ	2.37	0.57
2:I:351:GLN:CD	2:L:726:ASN:HD22	2.13	0.57
5:R:56:SER:CB	5:R:57:PRO:CD	2.83	0.57
2:D:625:ASP:OD2	2:D:912:ARG:NH1	2.37	0.56
2:J:704:LYS:NZ	2:J:891:GLU:OE2	2.25	0.56
2:D:416:GLN:N	2:F:261:ASP:O	2.38	0.56
3:M:162:TYR:CE2	3:M:166:LEU:HD11	2.41	0.56
2:A:47:ASN:HB2	1:W:27:THR:HG23	1.86	0.56
2:H:132:THR:HG23	2:H:153:GLY:HA3	1.88	0.56
2:K:187:GLN:O	2:K:210:ARG:NH1	2.37	0.56
1:4:27:THR:HG23	2:J:47:ASN:O	2.06	0.56
2:A:432:SER:OG	2:A:433:LYS:N	2.39	0.56
2:E:737:GLU:O	2:F:67:ARG:NH1	2.39	0.56
2:L:132:THR:HG23	2:L:153:GLY:HA3	1.88	0.56
1:3:15:THR:OG1	2:J:22:GLU:OE1	2.24	0.56
2:G:625:ASP:OD2	2:G:912:ARG:NH1	2.39	0.56
2:G:687:SER:O	2:G:687:SER:OG	2.21	0.56
2:L:187:GLN:O	2:L:210:ARG:NH1	2.38	0.55
3:M:239:LEU:O	3:M:242:PRO:HD2	2.06	0.55
2:C:857:ARG:NH2	1:W:31:ASN:OD1	2.38	0.55
3:M:81:LEU:O	3:M:86:ALA:N	2.27	0.55
2:I:220:PRO:O	2:I:224:SER:OG	2.23	0.55
1:I:10:ALA:HB2	2:I:34:ALA:HB1	1.88	0.55
1:W:12:ARG:NH1	1:W:17:PRO:HD3	2.21	0.55
2:A:700:ASN:ND2	2:A:854:THR:O	2.39	0.55
2:L:667:ARG:NH1	2:L:895:MET:SD	2.80	0.55
3:M:190:PHE:HB3	3:M:200:VAL:CG2	2.36	0.55
2:C:735:ASP:OD2	2:C:740:ASN:ND2	2.39	0.55
2:D:206:LYS:NZ	2:D:271:PRO:O	2.39	0.55
2:L:114:LYS:NZ	2:L:116:TYR:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:14:GLN:HB3	6:U:19:LEU:O	2.07	0.55
2:C:667:ARG:NH2	2:C:895:MET:SD	2.81	0.54
2:K:358:SER:OG	2:K:631:TYR:O	2.16	0.54
2:L:741:VAL:HG11	2:L:751:PHE:HB2	1.90	0.54
2:H:668:LEU:O	2:H:899:THR:OG1	2.25	0.54
2:A:710:PHE:O	2:A:712:SER:N	2.41	0.54
2:L:770:GLU:N	2:L:770:GLU:OE1	2.41	0.54
2:B:298:ASP:O	2:B:303:ASN:ND2	2.40	0.54
2:J:730:ILE:HG22	2:J:731:LYS:H	1.73	0.54
2:A:379:ALA:O	2:A:531:ARG:NH1	2.41	0.54
2:D:114:LYS:NZ	2:D:311:ASN:O	2.39	0.54
2:J:213:LYS:NZ	2:J:254:ASP:O	2.38	0.54
4:N:50:GLU:HG2	4:N:56:ARG:NH1	2.23	0.54
2:I:772:TYR:O	2:I:775:ARG:NH1	2.41	0.53
3:M:138:LEU:CD2	3:M:141:LEU:HD12	2.38	0.53
2:I:862:SER:OG	2:I:872:ASP:OD2	2.20	0.53
2:K:75:ASP:OD1	2:K:572:LYS:NZ	2.39	0.53
2:A:537:ASN:HB3	2:C:507:ALA:HB2	1.90	0.53
2:B:457:PHE:O	2:B:461:ASN:ND2	2.40	0.53
2:G:319:ARG:HD2	2:G:323:VAL:HG13	1.91	0.53
5:Q:55:SER:HB3	5:Q:58:LEU:HD21	1.90	0.53
3:M:182:TYR:OH	3:M:191:GLN:HB2	2.08	0.53
2:B:741:VAL:HG22	2:B:746:MET:O	2.09	0.53
2:H:774:ASP:OD2	2:I:371:ARG:NH2	2.41	0.53
2:H:789:GLN:OE1	2:H:845:THR:HG22	2.09	0.52
2:K:487:GLU:OE1	2:K:487:GLU:N	2.41	0.52
2:J:867:MET:O	2:K:51:ALA:HB2	2.09	0.52
1:3:9:LEU:HD22	2:J:55:ASP:O	2.10	0.52
2:E:455:ARG:NH1	2:E:500:ASP:OD1	2.43	0.52
2:H:133:SER:OG	2:H:218:MET:SD	2.66	0.52
2:H:634:ALA:HA	2:H:907:VAL:HG22	1.91	0.52
2:J:381:ASP:OD1	2:J:531:ARG:NH2	2.43	0.52
3:M:210:LYS:HA	3:M:213:TRP:HD1	1.75	0.52
3:M:240:VAL:O	3:M:244:THR:OG1	2.16	0.52
1:I:27:THR:HG22	2:I:46:ARG:HD2	1.92	0.52
2:E:214:PRO:O	2:E:299:ASN:ND2	2.42	0.52
4:N:368:LEU:HD21	4:N:375:ALA:HB2	1.92	0.52
2:G:261:ASP:O	2:H:416:GLN:N	2.40	0.52
4:N:50:GLU:HA	4:N:56:ARG:HH12	1.73	0.52
2:D:711:ASP:O	2:D:714:VAL:HG12	2.09	0.52
2:E:388:ARG:NH1	2:E:852:ASP:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:625:ASP:OD2	2:K:912:ARG:NH1	2.43	0.52
2:H:574:VAL:HG21	2:H:591:ALA:CB	2.38	0.52
2:K:711:ASP:OD1	2:K:885:ALA:N	2.43	0.52
2:L:323:VAL:HG12	2:L:356:GLU:CD	2.35	0.52
2:F:419:LYS:O	2:F:426:GLU:N	2.41	0.52
2:I:351:GLN:HE21	2:I:677:GLY:HA3	1.74	0.52
2:E:549:GLN:OE1	2:E:566:TYR:OH	2.28	0.51
2:I:320:ASP:O	2:I:323:VAL:HG23	2.09	0.51
2:L:396:GLU:O	2:L:450:GLN:OE1	2.27	0.51
2:L:700:ASN:ND2	2:L:852:ASP:O	2.42	0.51
2:L:796:TYR:O	2:L:797:THR:OG1	2.28	0.51
3:M:33:GLN:O	3:M:38:LEU:HB2	2.10	0.51
2:E:468:ASP:OD1	2:E:492:ARG:NH1	2.43	0.51
2:F:312:ARG:NH1	2:F:489:MET:O	2.43	0.51
2:J:362:LEU:HD13	2:J:631:TYR:CE2	2.46	0.51
5:P:57:PRO:CB	5:P:60:ALA:HB3	2.39	0.51
3:M:217:ALA:HB2	3:M:254:TYR:CA	2.39	0.51
2:A:182:ALA:HB1	2:A:188:PRO:HD3	1.92	0.51
2:E:19:ASP:OD1	1:Y:14:GLY:HA3	2.09	0.51
2:F:47:ASN:CG	1:Y:26:GLY:HA2	2.36	0.51
2:J:28:LEU:HD23	2:L:624:ASN:ND2	2.25	0.51
5:R:66:ALA:C	5:R:68:ALA:H	2.17	0.51
1:3:31:ASN:ND2	2:J:906:GLU:OE2	2.44	0.51
2:F:501:SER:O	2:F:501:SER:OG	2.28	0.51
3:M:48:GLN:HB2	1:W:8:SER:HB3	1.91	0.51
2:C:76:ASN:OD1	2:C:77:THR:N	2.42	0.51
2:L:5:SER:O	6:U:51:ARG:HG3	2.11	0.51
3:M:242:PRO:HG3	3:M:266:ILE:HG21	1.92	0.51
2:E:710:PHE:O	2:E:712:SER:N	2.42	0.51
2:F:499:VAL:HG23	2:F:503:ILE:HG21	1.93	0.51
2:J:740:ASN:OD1	2:J:746:MET:O	2.29	0.51
2:L:412:ALA:CB	2:L:438:ALA:HB2	2.40	0.51
3:M:172:MET:CE	3:M:243:PHE:HB2	2.34	0.51
2:B:501:SER:O	2:B:501:SER:OG	2.29	0.51
2:D:610:ASN:OD1	2:D:611:THR:N	2.44	0.51
2:E:632:LEU:O	2:E:632:LEU:HD23	2.11	0.50
2:J:326:MET:SD	2:J:568:TRP:NE1	2.84	0.50
6:U:40:MET:O	6:U:44:VAL:HG23	2.11	0.50
2:A:261:ASP:O	2:B:416:GLN:N	2.44	0.50
2:A:468:ASP:O	2:A:492:ARG:NH2	2.43	0.50
2:A:549:GLN:OE1	2:A:566:TYR:OH	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:256:ASP:O	2:G:277:THR:OG1	2.24	0.50
2:B:404:PHE:O	2:C:446:GLU:N	2.43	0.50
2:F:636:ASN:N	2:F:636:ASN:HD22	2.09	0.50
2:J:610:ASN:OD1	2:J:611:THR:N	2.44	0.50
2:K:417:GLY:HA3	2:K:431:VAL:HG21	1.93	0.50
2:G:190:PRO:O	2:I:811:SER:OG	2.30	0.50
2:G:381:ASP:OD1	2:G:531:ARG:NH2	2.45	0.50
2:H:827:TYR:OH	2:I:278:GLU:OE2	2.20	0.50
6:U:4:GLU:O	6:U:6:PRO:HD3	2.12	0.50
2:A:10:TRP:O	2:A:16:ALA:N	2.45	0.50
2:B:577:VAL:HG23	2:B:578:LEU:HD12	1.94	0.50
2:B:620:ARG:NH1	2:B:917:HIS:O	2.44	0.50
2:K:934:ASN:OD1	6:U:34:LEU:HD13	2.11	0.50
2:L:690:ILE:HG21	2:L:693:LEU:HD13	1.93	0.50
6:U:10:MET:HG3	6:U:26:ASP:HB3	1.93	0.50
2:F:96:MET:HE1	2:F:559:LEU:HD22	1.94	0.50
2:J:210:ARG:NH2	2:J:278:GLU:OE2	2.43	0.50
3:M:235:LEU:O	3:M:238:LEU:HG	2.12	0.50
5:Q:55:SER:O	5:Q:58:LEU:HG	2.12	0.50
5:Q:63:ALA:O	5:Q:67:THR:HG23	2.12	0.50
1:I:26:GLY:HA3	2:I:47:ASN:ND2	2.27	0.50
1:2:25:ILE:HG22	2:H:20:ALA:HB3	1.93	0.50
2:C:345:ASN:OD1	2:C:347:VAL:HG22	2.12	0.50
2:I:738:GLY:O	2:I:748:LYS:NZ	2.44	0.50
4:N:292:ILE:HD12	4:N:376:TYR:HB3	1.93	0.50
6:U:210:ASP:HB3	6:U:216:PHE:CE2	2.46	0.50
2:A:213:LYS:NZ	2:A:256:ASP:OD2	2.30	0.49
2:C:457:PHE:O	2:C:461:ASN:ND2	2.43	0.49
2:C:584:ASN:ND2	2:C:589:ASP:OD2	2.45	0.49
2:E:583:GLY:O	2:E:687:SER:OG	2.29	0.49
2:H:214:PRO:O	2:H:299:ASN:ND2	2.45	0.49
3:M:131:ARG:HG2	3:M:134:ARG:HH21	1.77	0.49
2:G:119:THR:HG23	2:G:286:ASP:HB2	1.94	0.49
2:I:216:THR:HG23	2:I:279:ASN:OD1	2.12	0.49
4:N:466:THR:HG22	4:N:468:VAL:HG13	1.93	0.49
2:B:214:PRO:O	2:B:299:ASN:ND2	2.45	0.49
2:J:729:GLU:O	2:J:747:THR:OG1	2.19	0.49
2:K:211:ALA:HB2	2:K:275:LEU:HD12	1.94	0.49
2:B:286:ASP:O	2:B:311:ASN:ND2	2.45	0.49
2:E:607:MET:HE3	2:E:612:ALA:HA	1.95	0.49
2:G:107:LEU:HD11	2:G:578:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:103:ILE:HG12	2:I:598:ILE:HD12	1.93	0.49
2:K:132:THR:HG23	2:K:152:PHE:O	2.13	0.49
2:K:142:GLU:O	2:K:143:ARG:NE	2.45	0.49
2:K:610:ASN:OD1	2:K:611:THR:N	2.46	0.49
2:A:222:TYR:OH	2:C:397:ASP:OD2	2.29	0.49
2:G:261:ASP:OD1	2:G:262:GLY:N	2.45	0.49
2:G:811:SER:OG	2:H:190:PRO:O	2.29	0.49
2:H:759:TYR:OH	2:H:778:SER:OG	2.25	0.49
5:P:55:SER:HB2	5:P:58:LEU:HD12	1.93	0.49
2:G:314:ASN:HD22	2:G:582:LEU:HD12	1.78	0.49
2:F:421:LYS:N	2:F:424:GLY:O	2.45	0.49
2:H:72:ASP:OD1	2:H:73:ARG:N	2.45	0.49
1:3:19:MET:HE3	2:K:33:ARG:HH22	1.78	0.49
2:A:393:HIS:CE1	2:B:533:MET:HE1	2.48	0.49
2:E:661:ARG:NH1	2:E:907:VAL:O	2.45	0.49
2:L:321:ASN:O	2:L:323:VAL:HG13	2.12	0.49
2:B:455:ARG:NH1	2:B:500:ASP:OD1	2.45	0.49
3:M:164:ASN:OD1	3:M:248:SER:O	2.31	0.49
4:N:359:ASP:OD1	4:N:363:ARG:N	2.42	0.49
2:A:218:MET:HE1	2:A:304:LEU:HD22	1.94	0.48
2:C:861:SER:OG	2:C:863:ASN:O	2.26	0.48
2:G:88:VAL:HG23	2:G:604:PHE:HE2	1.78	0.48
2:B:419:LYS:NZ	2:B:426:GLU:OE2	2.46	0.48
2:H:737:GLU:N	2:H:737:GLU:OE1	2.46	0.48
2:C:518:ASN:ND2	2:C:672:GLU:OE1	2.45	0.48
2:G:664:SER:HB2	2:G:904:LEU:HD12	1.94	0.48
2:L:616:GLU:OE2	2:L:620:ARG:NH1	2.46	0.48
2:D:75:ASP:OD1	2:D:572:LYS:NZ	2.45	0.48
2:H:738:GLY:O	2:H:748:LYS:NZ	2.46	0.48
2:K:641:ILE:HG22	2:K:642:PRO:O	2.13	0.48
2:B:610:ASN:OD1	2:B:611:THR:N	2.47	0.48
2:G:620:ARG:NH1	2:G:917:HIS:O	2.46	0.48
6:U:56:LEU:HD21	6:U:196:VAL:HG12	1.95	0.48
2:C:419:LYS:N	2:C:426:GLU:O	2.46	0.48
2:B:449:ILE:HG22	2:B:453:LEU:HD23	1.95	0.48
2:B:666:THR:HG23	2:B:700:ASN:OD1	2.13	0.48
2:G:778:SER:O	2:G:782:ASN:ND2	2.44	0.48
2:H:114:LYS:NZ	2:H:311:ASN:O	2.38	0.48
2:C:710:PHE:O	2:C:712:SER:N	2.44	0.48
2:K:352:ASP:O	2:K:636:ASN:ND2	2.42	0.48
2:G:789:GLN:OE1	2:H:537:ASN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:19:MET:HG2	2:J:34:ALA:HA	1.96	0.48
2:B:608:ALA:HB3	2:B:611:THR:HG22	1.95	0.48
2:C:392:ASN:OD1	2:C:505:ILE:HD13	2.14	0.48
3:M:44:GLU:O	3:M:47:ARG:HG2	2.14	0.48
2:E:625:ASP:OD2	2:E:912:ARG:NH2	2.47	0.47
2:H:103:ILE:HG12	2:H:598:ILE:HD12	1.96	0.47
2:I:646:THR:HG23	2:I:892:VAL:O	2.14	0.47
2:K:334:MET:HE3	2:K:349:ASP:HB2	1.95	0.47
2:B:632:LEU:HD23	2:B:632:LEU:O	2.13	0.47
2:J:103:ILE:HG12	2:J:598:ILE:HD12	1.96	0.47
2:J:523:HIS:O	2:J:529:ARG:NE	2.48	0.47
2:K:112:SER:O	2:K:314:ASN:ND2	2.47	0.47
2:K:871:THR:OG1	2:K:873:LEU:O	2.14	0.47
2:K:936:THR:HG21	6:U:5:ILE:CD1	2.41	0.47
3:M:183:GLN:HB2	3:M:188:TYR:CE2	2.49	0.47
2:C:321:ASN:O	2:C:323:VAL:N	2.46	0.47
2:G:116:TYR:OH	2:G:286:ASP:OD1	2.27	0.47
2:I:891:GLU:OE1	5:R:23:TRP:NE1	2.47	0.47
2:G:202:GLY:O	2:G:203:THR:HB	2.14	0.47
3:M:113:THR:CG2	3:M:117:ARG:HH12	2.28	0.47
2:A:107:LEU:HD11	2:A:578:LEU:CD1	2.44	0.47
2:A:789:GLN:OE1	2:B:541:VAL:HG12	2.14	0.47
2:I:759:TYR:CB	2:I:761:ILE:HD12	2.44	0.47
3:M:182:TYR:CE1	6:U:203:GLY:HA3	2.49	0.47
5:P:8:GLU:N	5:P:8:GLU:OE1	2.48	0.47
1:0:6:PHE:HB3	1:0:9:LEU:HD13	1.97	0.47
2:E:298:ASP:O	2:E:303:ASN:ND2	2.47	0.47
2:G:384:ASP:HB3	2:G:387:VAL:HG22	1.95	0.47
1:3:31:ASN:HB2	2:J:661:ARG:HH12	1.80	0.47
2:B:863:ASN:ND2	2:C:57:THR:OG1	2.48	0.47
2:C:319:ARG:NH1	2:C:688:GLY:O	2.48	0.47
2:D:549:GLN:OE1	2:D:566:TYR:OH	2.32	0.47
2:H:573:ASP:O	2:H:577:VAL:HG22	2.15	0.47
3:M:105:ARG:O	3:M:105:ARG:HG2	2.15	0.47
5:R:56:SER:CB	5:R:57:PRO:HD3	2.45	0.47
2:E:457:PHE:O	2:E:461:ASN:ND2	2.46	0.47
2:J:710:PHE:O	2:J:712:SER:N	2.46	0.47
3:M:241:SER:OG	3:M:242:PRO:HD3	2.15	0.47
2:B:187:GLN:O	2:B:210:ARG:NH1	2.47	0.47
2:B:666:THR:HG21	2:B:697:PHE:CD1	2.49	0.47
2:E:625:ASP:OD1	2:E:914:HIS:ND1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:358:SER:OG	2:L:631:TYR:O	2.28	0.47
3:M:77:ILE:O	3:M:81:LEU:HD13	2.15	0.47
4:N:273:ARG:NH1	4:N:393:ARG:O	2.47	0.47
5:S:55:SER:OG	5:S:58:LEU:HD21	2.15	0.47
2:C:116:TYR:OH	2:C:286:ASP:OD2	2.33	0.46
2:C:135:TRP:CZ3	2:C:304:LEU:HD11	2.50	0.46
2:E:907:VAL:HG21	2:E:927:ARG:HD2	1.97	0.46
4:N:403:VAL:HG13	4:N:404:THR:HG23	1.97	0.46
2:C:794:VAL:HG23	2:C:795:ASN:OD1	2.15	0.46
2:G:827:TYR:OH	2:H:278:GLU:OE1	2.23	0.46
2:E:320:ASP:O	2:E:323:VAL:HG23	2.16	0.46
2:H:415:TYR:N	2:H:435:ASN:O	2.49	0.46
1:3:16:ARG:HG3	1:3:17:PRO:HD2	1.96	0.46
2:A:47:ASN:CG	1:W:26:GLY:HA2	2.40	0.46
2:A:668:LEU:HD22	2:A:691:PRO:HB2	1.98	0.46
2:A:721:ARG:C	2:A:722:LEU:HD12	2.41	0.46
2:J:261:ASP:O	2:K:416:GLN:N	2.45	0.46
4:N:224:PHE:HD2	4:N:381:LEU:HD11	1.81	0.46
1:3:11:PRO:O	1:3:18:TYR:HB2	2.15	0.46
2:B:272:GLU:O	2:B:273:ILE:HD13	2.16	0.46
2:C:629:ASN:OD1	2:C:630:ASP:N	2.48	0.46
2:D:647:ASN:O	5:R:13:SER:OG	2.31	0.46
2:I:608:ALA:HB3	2:I:611:THR:HG22	1.97	0.46
2:K:462:VAL:HG13	2:K:514:MET:HE2	1.96	0.46
4:N:518:ASP:N	4:N:522:ARG:O	2.49	0.46
2:C:214:PRO:O	2:C:299:ASN:ND2	2.48	0.46
2:C:216:THR:OG1	2:C:279:ASN:OD1	2.33	0.46
2:E:59:ASP:OD1	2:E:59:ASP:N	2.49	0.46
5:Q:55:SER:HB3	5:Q:58:LEU:CD2	2.45	0.46
2:A:213:LYS:N	2:A:278:GLU:O	2.47	0.46
2:C:206:LYS:NZ	2:C:271:PRO:O	2.48	0.46
2:I:711:ASP:O	2:I:713:SER:N	2.48	0.46
3:M:77:ILE:HD11	3:M:118:MET:HG2	1.98	0.46
2:B:320:ASP:OD2	2:B:369:ARG:NH2	2.49	0.46
2:E:230:ASN:OD1	2:E:234:GLY:N	2.46	0.46
2:G:119:THR:HG23	2:G:286:ASP:CB	2.46	0.46
2:I:501:SER:O	2:I:501:SER:OG	2.30	0.46
2:J:442:ASN:O	2:K:822:ARG:NH1	2.46	0.46
2:K:656:ASN:ND2	6:U:10:MET:SD	2.89	0.46
2:L:647:ASN:O	5:P:13:SER:OG	2.34	0.46
2:A:608:ALA:O	2:A:612:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:759:TYR:OH	2:C:773:LYS:O	2.23	0.45
2:D:457:PHE:O	2:D:461:ASN:ND2	2.47	0.45
2:B:637:MET:HE2	2:B:639:TYR:OH	2.16	0.45
2:G:419:LYS:NZ	2:G:426:GLU:OE2	2.31	0.45
3:M:132:PHE:CE1	3:M:138:LEU:HB2	2.51	0.45
1:Y:29:GLN:HG2	1:Y:30:LEU:H	1.81	0.45
2:A:672:GLU:OE1	2:A:698:TYR:OH	2.35	0.45
2:E:382:SER:OG	2:E:383:TYR:N	2.48	0.45
2:K:922:GLU:OE1	6:U:40:MET:HG3	2.17	0.45
3:M:33:GLN:HA	3:M:36:MET:CE	2.39	0.45
3:M:188:TYR:O	3:M:202:LEU:N	2.46	0.45
2:B:740:ASN:O	2:B:748:LYS:NZ	2.50	0.45
2:E:319:ARG:NH1	2:E:688:GLY:O	2.48	0.45
2:G:586:LEU:HD13	2:G:687:SER:OG	2.16	0.45
2:I:72:ASP:OD1	2:I:73:ARG:N	2.50	0.45
2:J:758:ASN:OD1	2:J:857:ARG:NH1	2.49	0.45
3:M:31:ALA:O	3:M:34:ARG:HG2	2.17	0.45
2:I:546:GLN:N	2:I:546:GLN:OE1	2.49	0.45
2:J:372:TYR:OH	2:J:526:ALA:O	2.30	0.45
3:M:139:GLY:O	3:M:142:VAL:HG22	2.17	0.45
2:E:708:ILE:HG12	2:E:888:MET:HE3	1.98	0.45
3:M:28:TRP:CB	3:M:31:ALA:HB3	2.44	0.45
2:A:116:TYR:OH	2:A:286:ASP:OD2	2.32	0.45
2:B:789:GLN:OE1	2:C:537:ASN:N	2.46	0.45
2:D:409:ILE:HD13	2:F:154:ILE:HD12	1.98	0.45
2:D:759:TYR:O	2:D:761:ILE:N	2.49	0.45
2:I:931:SER:O	2:L:713:SER:OG	2.31	0.45
4:N:429:GLN:O	4:N:431:ASN:N	2.49	0.45
5:Q:56:SER:OG	5:Q:57:PRO:HD3	2.15	0.45
2:F:669:LYS:O	2:F:673:THR:OG1	2.33	0.45
2:F:902:TYR:CE2	2:F:904:LEU:HD11	2.51	0.45
2:G:103:ILE:HD12	2:G:547:VAL:CG2	2.46	0.45
2:J:587:ARG:NH2	2:J:684:PHE:O	2.49	0.45
2:K:855:MET:HE1	2:K:904:LEU:HD13	1.99	0.45
2:K:928:THR:HG22	2:K:929:PRO:CD	2.47	0.45
3:M:225:VAL:HB	3:M:254:TYR:CE2	2.52	0.45
6:U:183:ILE:HG22	6:U:187:GLN:OE1	2.17	0.45
2:B:84:TYR:OH	2:B:598:ILE:O	2.34	0.44
2:B:320:ASP:O	2:B:323:VAL:HG13	2.17	0.44
2:G:307:GLN:NE2	2:G:820:THR:O	2.50	0.44
2:H:311:ASN:OD1	2:H:490:ASN:ND2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:67:THR:O	5:R:68:ALA:CB	2.65	0.44
2:B:90:ASP:OD2	3:M:94:LEU:HG	2.17	0.44
2:B:918:ARG:NE	3:M:97:ASN:OD1	2.50	0.44
2:D:862:SER:HB3	2:E:57:THR:HG21	1.99	0.44
2:G:132:THR:HG23	2:G:153:GLY:HA3	1.99	0.44
4:N:52:ARG:NH2	4:N:117:SER:OG	2.50	0.44
2:C:573:ASP:O	2:C:577:VAL:HG22	2.17	0.44
2:H:154:ILE:HD12	2:I:409:ILE:HD13	2.00	0.44
2:J:132:THR:HG23	2:J:153:GLY:HA3	2.00	0.44
2:L:608:ALA:HB3	2:L:611:THR:HG22	1.98	0.44
3:M:39:THR:O	3:M:43:PRO:HB3	2.18	0.44
3:M:144:LEU:HD11	3:M:169:LEU:CD2	2.48	0.44
3:M:182:TYR:CE1	3:M:189:PHE:HB2	2.52	0.44
6:U:52:ASN:O	6:U:56:LEU:HG	2.17	0.44
2:I:741:VAL:HG21	2:I:751:PHE:CD1	2.53	0.44
2:J:119:THR:HG22	2:J:121:TYR:H	1.81	0.44
1:3:19:MET:HE3	2:K:33:ARG:NH2	2.32	0.44
2:G:416:GLN:N	2:I:261:ASP:O	2.49	0.44
2:G:501:SER:O	2:G:501:SER:OG	2.34	0.44
2:H:320:ASP:O	2:H:323:VAL:HG23	2.18	0.44
3:M:200:VAL:HG12	3:M:235:LEU:HD23	1.98	0.44
2:B:5:SER:OG	2:B:6:MET:N	2.49	0.44
2:B:587:ARG:NH1	2:B:684:PHE:O	2.49	0.44
2:C:241:VAL:HG22	2:C:250:THR:HA	1.98	0.44
2:F:241:VAL:HG22	2:F:250:THR:O	2.16	0.44
2:K:608:ALA:HB3	2:K:611:THR:HG22	2.00	0.44
2:I:241:VAL:HG12	2:I:250:THR:O	2.18	0.44
2:B:472:TYR:OH	2:B:817:LEU:O	2.26	0.44
2:E:577:VAL:C	2:E:578:LEU:HD12	2.42	0.44
2:J:349:ASP:OD1	2:J:350:LEU:N	2.50	0.44
2:J:629:ASN:OD1	2:J:630:ASP:N	2.51	0.44
2:E:267:ASP:OD1	2:E:267:ASP:N	2.50	0.44
2:H:722:LEU:O	2:I:63:ARG:NH1	2.51	0.44
2:K:428:ASP:OD1	2:K:429:ASP:N	2.51	0.44
3:M:48:GLN:OE1	1:W:7:SER:OG	2.32	0.44
2:C:907:VAL:HG21	2:C:927:ARG:CD	2.48	0.43
2:E:393:HIS:ND1	2:F:533:MET:HE1	2.33	0.43
2:F:608:ALA:O	2:F:612:ALA:N	2.47	0.43
2:J:577:VAL:HG23	2:J:578:LEU:HD13	1.99	0.43
2:K:154:ILE:HG23	2:L:409:ILE:HD12	2.00	0.43
3:M:210:LYS:HA	3:M:213:TRP:CD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:501:THR:C	4:N:502:LEU:HD12	2.43	0.43
2:A:418:ILE:HD11	2:C:261:ASP:HB3	2.00	0.43
2:A:666:THR:OG1	2:A:667:ARG:N	2.50	0.43
2:D:419:LYS:N	2:D:426:GLU:O	2.50	0.43
2:E:296:SER:O	2:E:298:ASP:N	2.51	0.43
2:F:46:ARG:NH1	1:Y:27:THR:OG1	2.45	0.43
2:H:345:ASN:ND2	2:H:347:VAL:O	2.51	0.43
2:L:12:TYR:OH	6:U:40:MET:HE2	2.18	0.43
3:M:155:VAL:HG21	3:M:162:TYR:CD1	2.53	0.43
2:B:791:VAL:HG23	2:B:841:VAL:HG21	2.00	0.43
1:O:31:ASN:HB2	2:D:661:ARG:NH1	2.33	0.43
2:A:117:SER:O	2:C:395:ILE:N	2.51	0.43
2:G:380:VAL:HG21	2:G:776:MET:HE1	2.01	0.43
2:J:341:ALA:O	2:J:342:SER:OG	2.33	0.43
2:B:77:THR:HG23	2:B:78:TYR:CD1	2.54	0.43
2:H:741:VAL:O	2:I:546:GLN:NE2	2.52	0.43
2:K:226:ALA:HB3	2:K:235:GLN:OE1	2.18	0.43
3:M:50:PRO:HD3	1:W:12:ARG:NE	2.32	0.43
4:N:250:VAL:C	4:N:251:LEU:HD12	2.43	0.43
2:D:63:ARG:NH1	2:F:722:LEU:O	2.52	0.43
2:E:329:ASN:OD1	2:E:355:THR:HG22	2.19	0.43
2:E:573:ASP:O	2:E:577:VAL:HG22	2.18	0.43
2:H:134:GLN:HG2	2:H:151:THR:HG23	1.99	0.43
2:K:226:ALA:HB1	2:K:280:VAL:CG2	2.49	0.43
4:N:219:PHE:HD1	4:N:249:ILE:HG22	1.83	0.43
2:D:207:PHE:CD1	2:E:439:ILE:HB	2.53	0.43
2:F:421:LYS:O	2:F:424:GLY:N	2.50	0.43
2:K:936:THR:HG23	6:U:45:ASN:OD1	2.18	0.43
2:C:13:MET:O	2:C:15:ILE:N	2.52	0.43
2:D:537:ASN:O	2:D:537:ASN:ND2	2.50	0.43
2:E:739:TYR:O	2:E:748:LYS:N	2.49	0.43
2:H:329:ASN:OD1	2:H:355:THR:HG22	2.19	0.43
2:A:661:ARG:NH2	2:A:906:GLU:OE1	2.51	0.43
2:B:861:SER:OG	2:B:863:ASN:O	2.32	0.43
2:D:136:ILE:HG23	2:D:147:THR:HG23	2.00	0.43
2:D:573:ASP:OD2	2:D:587:ARG:NH1	2.52	0.43
2:F:759:TYR:O	2:F:761:ILE:N	2.51	0.43
2:L:321:ASN:O	2:L:323:VAL:N	2.52	0.43
2:L:449:ILE:O	2:L:453:LEU:N	2.49	0.43
5:S:13:SER:OG	5:S:13:SER:O	2.36	0.43
2:J:672:GLU:OE1	2:J:672:GLU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:323:VAL:HG12	2:L:356:GLU:OE1	2.19	0.43
2:A:41:MET:HE3	2:C:558:LEU:HD22	2.01	0.42
2:B:761:ILE:HG22	2:B:761:ILE:O	2.18	0.42
2:G:457:PHE:O	2:G:461:ASN:ND2	2.52	0.42
2:I:796:TYR:O	2:I:797:THR:OG1	2.33	0.42
2:K:629:ASN:OD1	2:K:630:ASP:N	2.52	0.42
3:M:191:GLN:NE2	3:M:196:GLY:HA3	2.32	0.42
2:I:573:ASP:OD1	2:I:574:VAL:N	2.49	0.42
2:L:314:ASN:OD1	2:L:580:SER:OG	2.32	0.42
3:M:70:THR:O	3:M:74:VAL:HG23	2.19	0.42
2:A:210:ARG:NH2	2:A:278:GLU:OE2	2.52	0.42
2:A:323:VAL:HG21	2:A:694:ASP:OD1	2.19	0.42
2:A:468:ASP:OD1	2:A:492:ARG:NH2	2.52	0.42
2:K:245:GLU:N	2:K:245:GLU:OE1	2.52	0.42
3:M:235:LEU:HD12	3:M:238:LEU:HD21	2.01	0.42
1:4:9:LEU:HB3	2:J:35:THR:HG22	2.01	0.42
2:A:867:MET:HE2	2:C:38:TYR:HE1	1.85	0.42
2:B:364:ASP:O	2:B:775:ARG:NE	2.52	0.42
2:C:312:ARG:NH1	2:C:582:LEU:HD21	2.34	0.42
2:G:573:ASP:OD1	2:G:574:VAL:N	2.52	0.42
2:H:428:ASP:OD1	2:H:429:ASP:N	2.52	0.42
2:J:183:ASP:OD1	2:J:184:LYS:N	2.52	0.42
2:A:822:ARG:NE	2:C:442:ASN:O	2.51	0.42
2:G:376:TRP:O	2:G:378:GLN:N	2.53	0.42
2:H:523:HIS:O	2:H:529:ARG:NH2	2.46	0.42
2:H:625:ASP:OD1	2:H:914:HIS:ND1	2.53	0.42
2:I:794:VAL:HG23	2:I:795:ASN:OD1	2.20	0.42
2:J:326:MET:HE2	2:J:548:PRO:O	2.20	0.42
2:J:862:SER:HB2	2:K:57:THR:HG21	2.00	0.42
2:K:821:MET:CE	2:L:406:LEU:HD23	2.49	0.42
2:L:72:ASP:OD1	2:L:73:ARG:N	2.53	0.42
2:A:316:ILE:CG2	2:A:578:LEU:HD21	2.50	0.42
2:A:741:VAL:HG11	2:A:751:PHE:HB2	2.00	0.42
2:F:666:THR:HG21	2:F:697:PHE:CD1	2.54	0.42
2:F:723:LEU:N	2:F:749:ASP:OD1	2.46	0.42
2:H:521:ASN:ND2	2:H:686:TYR:OH	2.52	0.42
2:I:610:ASN:OD1	2:I:611:THR:N	2.52	0.42
5:Q:57:PRO:CB	5:Q:60:ALA:HB3	2.43	0.42
2:A:34:ALA:HB1	1:W:10:ALA:HB2	2.02	0.42
2:A:329:ASN:OD1	2:A:355:THR:HG22	2.20	0.42
2:B:428:ASP:OD1	2:B:429:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:648:ILE:HD12	2:D:890:PHE:HB2	2.02	0.42
2:J:701:HIS:CD2	2:J:850:LEU:HD23	2.55	0.42
2:K:810:ASN:OD1	2:L:123:SER:N	2.52	0.42
6:U:215:ASN:O	6:U:223:VAL:HG22	2.20	0.42
2:A:298:ASP:OD1	2:A:299:ASN:N	2.52	0.42
2:C:618:MET:O	2:C:624:ASN:ND2	2.53	0.42
2:E:314:ASN:HD22	2:E:582:LEU:HD12	1.84	0.42
2:F:132:THR:HG23	2:F:153:GLY:HA3	2.01	0.42
2:G:737:GLU:OE1	2:G:737:GLU:N	2.47	0.42
3:M:113:THR:HG22	3:M:117:ARG:HH12	1.85	0.42
2:C:324:GLY:O	2:C:571:ARG:NE	2.47	0.42
2:E:141:GLU:O	2:E:143:ARG:N	2.53	0.42
2:E:261:ASP:OD1	2:E:262:GLY:N	2.52	0.42
2:E:573:ASP:OD2	2:E:587:ARG:NH2	2.52	0.42
2:G:528:LEU:HD21	2:G:579:GLN:CG	2.50	0.42
2:I:260:PHE:CE2	2:I:275:LEU:HD13	2.55	0.42
2:I:463:ALA:HB2	2:I:499:VAL:CG2	2.50	0.42
3:M:184:SER:CB	6:U:203:GLY:HA2	2.48	0.42
2:G:319:ARG:CD	2:G:323:VAL:HG13	2.49	0.42
2:F:35:THR:HG22	1:Y:9:LEU:HB3	2.01	0.41
2:G:741:VAL:HG11	2:G:751:PHE:HB2	2.01	0.41
2:H:574:VAL:HG21	2:H:591:ALA:HB3	2.01	0.41
2:L:482:ASN:O	2:L:485:THR:HG22	2.20	0.41
4:N:205:GLY:O	4:N:210:VAL:N	2.53	0.41
2:A:610:ASN:OD1	2:A:611:THR:N	2.53	0.41
2:A:610:ASN:OD1	2:A:611:THR:HG23	2.19	0.41
2:A:737:GLU:O	2:B:67:ARG:NH1	2.54	0.41
2:B:244:THR:HG22	2:B:245:GLU:OE1	2.20	0.41
2:F:716:TRP:O	2:F:718:GLY:N	2.52	0.41
2:H:641:ILE:HG23	2:H:648:ILE:HD11	2.02	0.41
2:K:345:ASN:O	6:U:35:SER:OG	2.30	0.41
2:C:205:GLU:OE1	2:C:205:GLU:N	2.53	0.41
2:C:632:LEU:O	2:C:632:LEU:HD23	2.21	0.41
2:G:754:GLN:O	2:G:758:ASN:ND2	2.47	0.41
2:J:12:TYR:O	2:L:912:ARG:NH1	2.51	0.41
1:2:29:GLN:OE1	2:G:661:ARG:NH1	2.53	0.41
2:B:776:MET:SD	2:B:853:ARG:NH1	2.92	0.41
2:C:811:SER:OG	2:C:825:GLU:O	2.29	0.41
2:D:141:GLU:OE1	2:D:141:GLU:N	2.54	0.41
2:D:263:ARG:CZ	2:E:414:THR:HG21	2.50	0.41
2:D:499:VAL:HG23	2:D:503:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:486:TYR:O	2:G:487:GLU:HG3	2.20	0.41
2:I:114:LYS:NZ	2:I:116:TYR:O	2.45	0.41
2:D:273:ILE:HD11	2:E:439:ILE:HG23	2.01	0.41
2:F:235:GLN:O	2:F:280:VAL:HG12	2.20	0.41
2:G:354:ASN:N	2:G:636:ASN:OD1	2.53	0.41
2:I:161:ASN:O	2:I:162:ILE:HD13	2.20	0.41
2:I:778:SER:O	2:I:782:ASN:ND2	2.53	0.41
2:D:161:ASN:OD1	2:D:162:ILE:N	2.54	0.41
2:F:117:SER:O	2:F:117:SER:OG	2.36	0.41
2:H:261:ASP:O	2:I:416:GLN:N	2.46	0.41
2:I:472:TYR:OH	2:I:818:ALA:HB2	2.21	0.41
2:I:696:THR:O	2:I:696:THR:OG1	2.36	0.41
2:J:810:ASN:OD1	2:K:123:SER:N	2.53	0.41
6:U:41:ILE:HG22	6:U:45:ASN:ND2	2.35	0.41
2:D:754:GLN:O	2:D:758:ASN:ND2	2.52	0.41
2:K:303:ASN:O	2:K:306:GLN:NE2	2.51	0.41
3:M:66:ARG:HD3	3:M:66:ARG:HA	1.79	0.41
1:2:12:ARG:NH2	1:2:14:GLY:O	2.54	0.41
2:C:240:LYS:NZ	2:C:250:THR:HG21	2.36	0.41
2:C:261:ASP:OD1	2:C:262:GLY:N	2.54	0.41
2:D:735:ASP:OD2	2:D:740:ASN:ND2	2.52	0.41
2:F:581:SER:C	2:F:582:LEU:HD12	2.46	0.41
2:H:442:ASN:O	2:I:822:ARG:NH1	2.54	0.41
2:L:573:ASP:O	2:L:577:VAL:HG22	2.21	0.41
4:N:190:ILE:HA	4:N:193:MET:HE3	2.03	0.41
4:N:236:MET:SD	4:N:236:MET:N	2.94	0.41
2:E:212:LEU:HD23	2:E:216:THR:HG21	2.01	0.41
2:H:175:ALA:O	2:H:178:LYS:NZ	2.54	0.41
2:H:710:PHE:O	2:H:712:SER:N	2.48	0.41
2:I:620:ARG:NH2	2:I:917:HIS:O	2.54	0.41
3:M:190:PHE:HB3	3:M:200:VAL:HG23	2.03	0.41
2:D:261:ASP:OD1	2:D:262:GLY:N	2.54	0.40
2:H:907:VAL:HG21	2:H:927:ARG:HD2	2.03	0.40
2:I:761:ILE:O	2:I:761:ILE:HG22	2.21	0.40
2:J:508:ARG:NH2	2:J:784:GLN:OE1	2.54	0.40
2:K:107:LEU:HD12	2:K:108:ASP:H	1.86	0.40
2:K:928:THR:HG22	2:K:929:PRO:HD3	2.02	0.40
3:M:204:GLN:HE21	3:M:204:GLN:HB2	1.70	0.40
6:U:204:SER:HA	6:U:205:PRO:HD3	1.95	0.40
2:A:881:ASN:ND2	6:U:21:ALA:HA	2.35	0.40
2:B:355:THR:HG21	2:B:551:PHE:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:88:VAL:HG13	2:G:561:PRO:HA	2.02	0.40
2:J:789:GLN:OE1	2:K:537:ASN:N	2.49	0.40
6:U:8:PRO:O	6:U:25:GLN:HA	2.21	0.40
6:U:14:GLN:HG2	6:U:17:MET:HB2	2.03	0.40
1:4:27:THR:OG1	2:J:49:THR:OG1	2.19	0.40
2:D:537:ASN:HD22	2:D:537:ASN:C	2.28	0.40
2:F:546:GLN:OE1	2:F:546:GLN:N	2.54	0.40
2:H:417:GLY:HA3	2:H:431:VAL:HG21	2.03	0.40
2:I:457:PHE:O	2:I:461:ASN:ND2	2.51	0.40
3:M:132:PHE:CZ	3:M:138:LEU:HB2	2.56	0.40
1:I:19:MET:HE3	2:I:34:ALA:HB2	2.03	0.40
2:B:668:LEU:O	2:B:900:LEU:N	2.51	0.40
2:D:527:GLY:O	2:D:531:ARG:NH1	2.55	0.40
2:E:577:VAL:HG23	2:E:578:LEU:CD1	2.50	0.40
2:H:597:SER:O	2:H:598:ILE:HD13	2.22	0.40
4:N:97:GLN:N	4:N:97:GLN:OE1	2.54	0.40
4:N:110:THR:HG22	4:N:509:ARG:HA	2.03	0.40
2:A:881:ASN:HD22	6:U:21:ALA:HA	1.86	0.40
2:B:319:ARG:NH2	2:B:688:GLY:O	2.51	0.40
2:C:356:GLU:OE1	2:C:693:LEU:HD22	2.20	0.40
2:D:655:ARG:NH1	2:D:929:PRO:O	2.55	0.40
4:N:185:SER:OG	4:N:186:ALA:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	12/250 (5%)	12 (100%)	0	0	100	100
1	1	19/250 (8%)	16 (84%)	3 (16%)	0	100	100
1	2	20/250 (8%)	18 (90%)	2 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	14/250 (6%)	11 (79%)	3 (21%)	0	100	100
1	4	20/250 (8%)	18 (90%)	2 (10%)	0	100	100
1	W	26/250 (10%)	21 (81%)	5 (19%)	0	100	100
1	Y	21/250 (8%)	17 (81%)	3 (14%)	1 (5%)	2	18
1	Z	23/250 (9%)	21 (91%)	2 (9%)	0	100	100
2	A	932/937 (100%)	817 (88%)	109 (12%)	6 (1%)	21	55
2	B	930/937 (99%)	839 (90%)	88 (10%)	3 (0%)	36	69
2	C	933/937 (100%)	835 (90%)	91 (10%)	7 (1%)	16	50
2	D	930/937 (99%)	848 (91%)	76 (8%)	6 (1%)	21	55
2	E	927/937 (99%)	835 (90%)	89 (10%)	3 (0%)	36	69
2	F	931/937 (99%)	838 (90%)	87 (9%)	6 (1%)	21	55
2	G	930/937 (99%)	850 (91%)	74 (8%)	6 (1%)	21	55
2	H	930/937 (99%)	831 (89%)	95 (10%)	4 (0%)	30	64
2	I	929/937 (99%)	850 (92%)	73 (8%)	6 (1%)	21	55
2	J	929/937 (99%)	837 (90%)	87 (9%)	5 (0%)	24	59
2	K	931/937 (99%)	839 (90%)	85 (9%)	7 (1%)	16	50
2	L	931/937 (99%)	848 (91%)	80 (9%)	3 (0%)	36	69
3	M	237/588 (40%)	230 (97%)	5 (2%)	2 (1%)	16	50
4	N	459/544 (84%)	423 (92%)	35 (8%)	1 (0%)	43	74
5	P	61/138 (44%)	57 (93%)	3 (5%)	1 (2%)	7	36
5	Q	61/138 (44%)	56 (92%)	5 (8%)	0	100	100
5	R	60/138 (44%)	51 (85%)	4 (7%)	5 (8%)	0	10
5	S	60/138 (44%)	56 (93%)	3 (5%)	1 (2%)	7	35
6	U	102/227 (45%)	98 (96%)	4 (4%)	0	100	100
6	V	103/227 (45%)	95 (92%)	7 (7%)	1 (1%)	12	45
All	All	12461/15382 (81%)	11267 (90%)	1120 (9%)	74 (1%)	23	55

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	188	PRO
2	A	266	ALA
2	A	418	ILE

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Mol	Chain	Res	Type
2	B	188	PRO
2	C	188	PRO
2	C	480	PRO
2	C	713	SER
2	C	832	PRO
2	D	188	PRO
2	E	188	PRO
2	E	341	ALA
2	F	145	VAL
2	F	188	PRO
2	F	832	PRO
2	G	188	PRO
2	G	411	PRO
2	G	487	GLU
2	G	832	PRO
2	H	188	PRO
2	H	248	VAL
2	H	734	VAL
2	I	188	PRO
2	I	265	ALA
2	I	712	SER
2	J	173	ILE
2	J	188	PRO
2	K	9	GLN
2	K	188	PRO
2	K	203	THR
2	K	295	THR
2	K	713	SER
2	K	929	PRO
2	L	188	PRO
3	M	36	MET
5	P	57	PRO
5	R	63	ALA
5	R	68	ALA
5	S	57	PRO
2	A	241	VAL
2	A	342	SER
2	B	205	GLU
2	C	370	THR
2	D	11	ALA
2	F	201	ASP
2	F	422	ASP

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Mol	Chain	Res	Type
2	I	398	GLU
2	I	734	VAL
2	J	713	SER
3	M	35	ILE
5	R	58	LEU
2	D	249	GLU
5	R	57	PRO
1	Y	15	THR
2	C	320	ASP
2	D	296	SER
2	E	244	THR
2	G	268	ALA
2	I	312	ARG
2	J	257	MET
2	J	425	TRP
2	L	320	ASP
6	V	4	GLU
2	A	417	GLY
2	D	320	ASP
2	K	312	ARG
2	L	257	MET
2	B	643	ALA
2	G	422	ASP
2	H	142	GLU
5	R	56	SER
2	C	187	GLN
2	F	929	PRO
4	N	180	PRO
2	D	929	PRO

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	0	13/209 (6%)	13 (100%)	0	100	100
1	1	22/209 (10%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	20/209 (10%)	20 (100%)	0	100	100
1	3	16/209 (8%)	16 (100%)	0	100	100
1	4	21/209 (10%)	21 (100%)	0	100	100
1	W	24/209 (12%)	24 (100%)	0	100	100
1	Y	21/209 (10%)	21 (100%)	0	100	100
1	Z	21/209 (10%)	21 (100%)	0	100	100
2	A	808/811 (100%)	808 (100%)	0	100	100
2	B	807/811 (100%)	807 (100%)	0	100	100
2	C	807/811 (100%)	807 (100%)	0	100	100
2	D	808/811 (100%)	808 (100%)	0	100	100
2	E	805/811 (99%)	804 (100%)	1 (0%)	88	89
2	F	808/811 (100%)	806 (100%)	2 (0%)	87	87
2	G	806/811 (99%)	806 (100%)	0	100	100
2	H	807/811 (100%)	807 (100%)	0	100	100
2	I	806/811 (99%)	805 (100%)	1 (0%)	88	89
2	J	806/811 (99%)	806 (100%)	0	100	100
2	K	808/811 (100%)	808 (100%)	0	100	100
2	L	808/811 (100%)	807 (100%)	1 (0%)	88	89
3	M	206/504 (41%)	205 (100%)	1 (0%)	81	82
4	N	418/485 (86%)	418 (100%)	0	100	100
5	P	44/69 (64%)	44 (100%)	0	100	100
5	Q	44/69 (64%)	44 (100%)	0	100	100
5	R	44/69 (64%)	41 (93%)	3 (7%)	14	41
5	S	44/69 (64%)	44 (100%)	0	100	100
6	U	90/192 (47%)	90 (100%)	0	100	100
6	V	91/192 (47%)	91 (100%)	0	100	100
All	All	10823/13053 (83%)	10814 (100%)	9 (0%)	87	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	423	ASN
2	F	177	ASN

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Mol	Chain	Res	Type
2	F	636	ASN
2	I	423	ASN
2	L	863	ASN
3	M	204	GLN
5	R	56	SER
5	R	57	PRO
5	R	58	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	31	ASN
1	3	29	GLN
2	A	131	ASN
2	A	314	ASN
2	A	644	ASN
2	B	303	ASN
2	B	516	ASN
2	B	523	HIS
2	B	575	ASN
2	B	626	GLN
2	B	644	ASN
2	B	764	GLN
2	B	915	GLN
2	C	187	GLN
2	C	301	HIS
2	C	354	ASN
2	C	624	ASN
2	D	91	ASN
2	D	303	ASN
2	D	311	ASN
2	D	448	ASN
2	D	490	ASN
2	D	537	ASN
2	D	743	GLN
2	D	764	GLN
2	E	314	ASN
2	E	452	ASN
2	E	823	GLN
2	E	846	GLN
2	F	91	ASN
2	F	230	ASN

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Mol	Chain	Res	Type
2	F	647	ASN
2	F	915	GLN
2	G	314	ASN
2	G	740	ASN
2	G	846	GLN
2	G	881	ASN
2	H	299	ASN
2	H	351	GLN
2	H	435	ASN
2	H	584	ASN
2	H	647	ASN
2	H	808	HIS
2	I	62	GLN
2	I	91	ASN
2	I	204	ASN
2	I	351	GLN
2	I	393	HIS
2	I	700	ASN
2	I	764	GLN
2	J	575	ASN
2	J	636	ASN
2	J	701	HIS
2	J	719	ASN
2	J	760	ASN
2	K	30	GLN
2	K	62	GLN
2	K	288	HIS
2	K	490	ASN
2	K	656	ASN
2	K	740	ASN
2	K	754	GLN
2	K	809	ASN
2	K	876	ASN
2	K	915	GLN
2	L	9	GLN
2	L	161	ASN
2	L	235	GLN
2	L	306	GLN
2	L	490	ASN
2	L	584	ASN
2	L	726	ASN
3	M	110	ASN

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Mol	Chain	Res	Type
3	M	112	GLN
3	M	204	GLN
3	M	208	ASN
3	M	232	ASN
4	N	165	HIS
4	N	274	HIS
6	U	16	GLN
6	U	32	ASN
6	U	199	ASN
1	W	5	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.

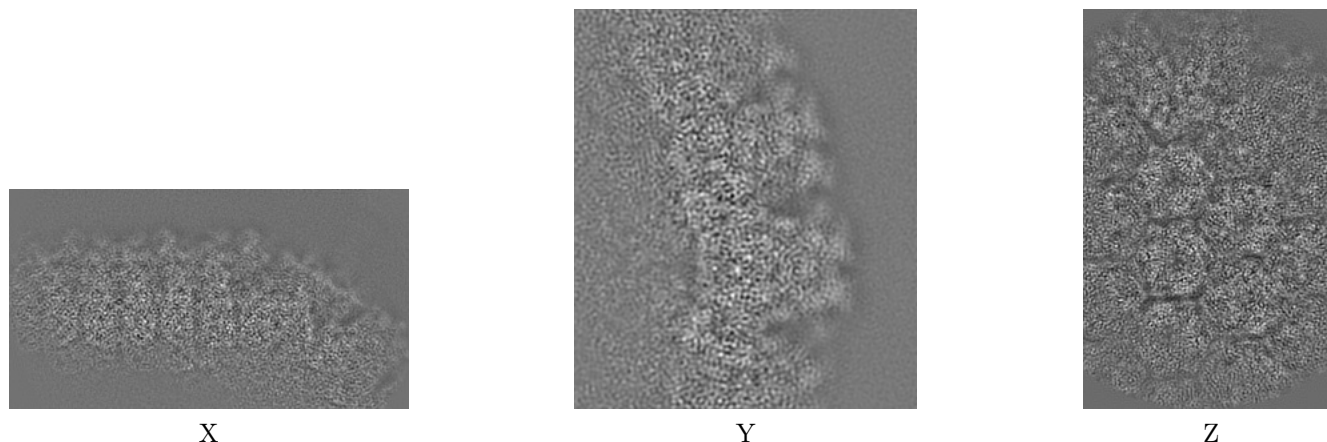
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72773. These allow visual inspection of the internal detail of the map and identification of artifacts.

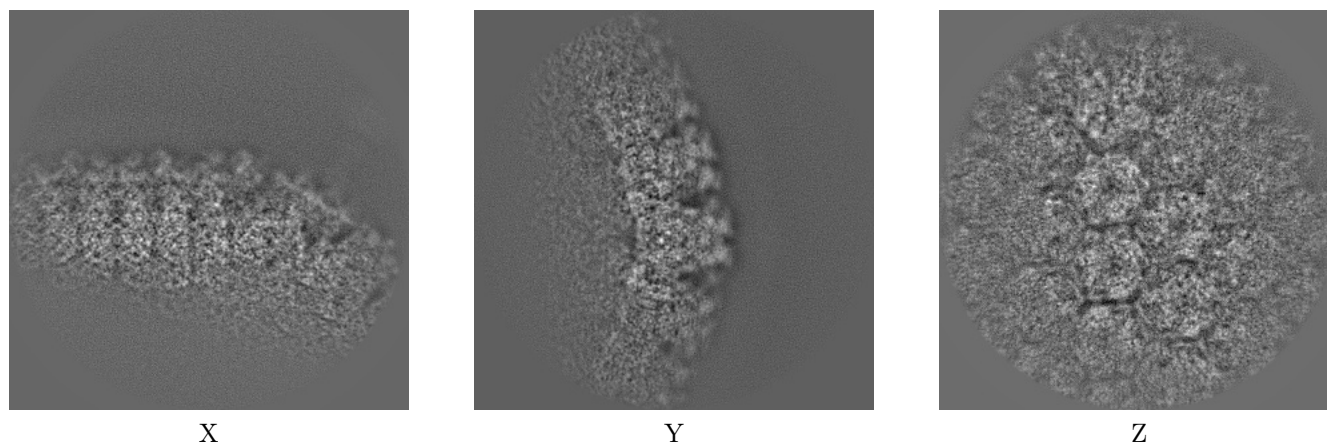
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



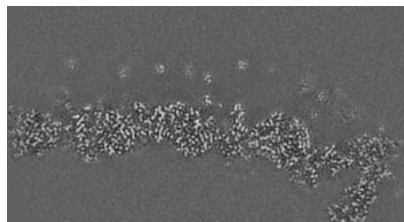
6.1.2 Raw map



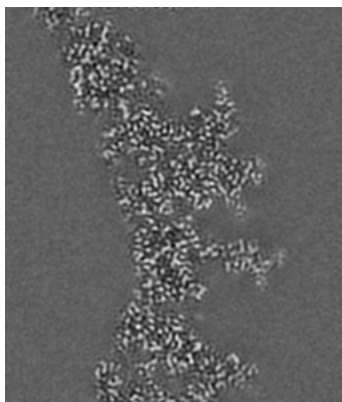
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

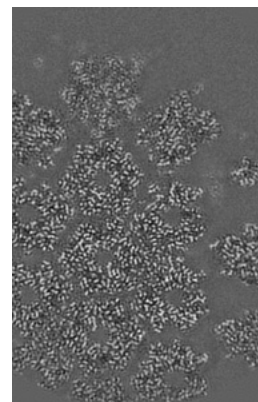
6.2.1 Primary map



X Index: 136

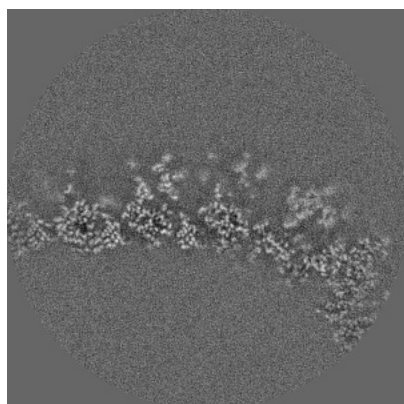


Y Index: 213

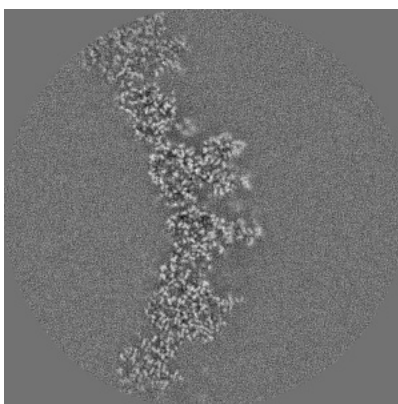


Z Index: 116

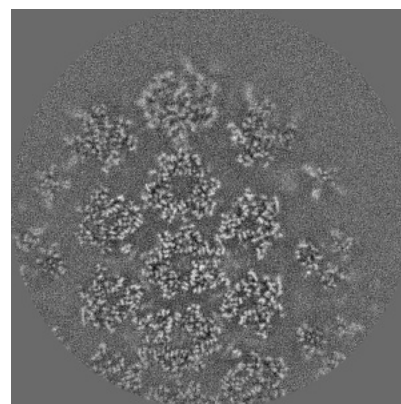
6.2.2 Raw map



X Index: 220



Y Index: 220

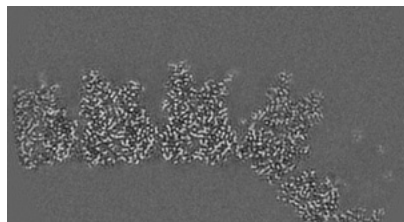


Z Index: 220

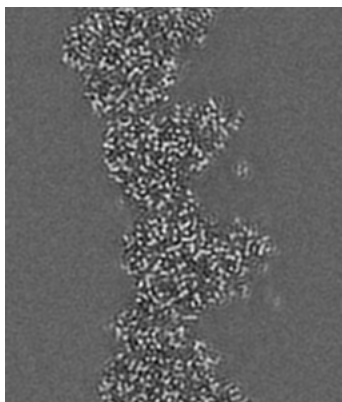
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

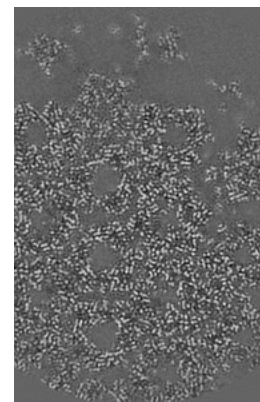
6.3.1 Primary map



X Index: 184

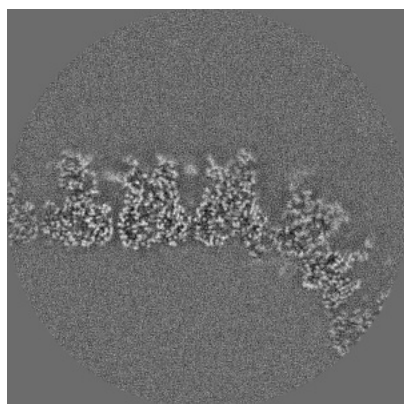


Y Index: 140

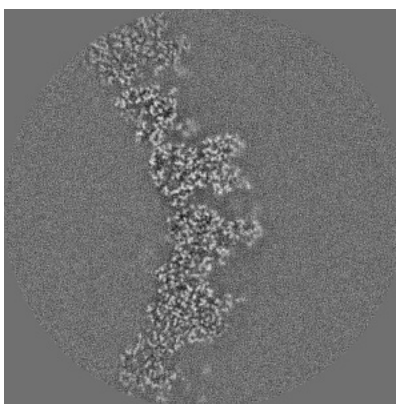


Z Index: 93

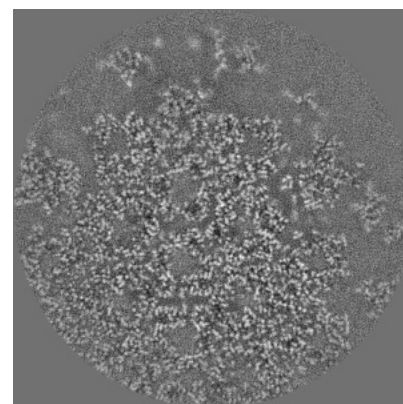
6.3.2 Raw map



X Index: 206



Y Index: 222

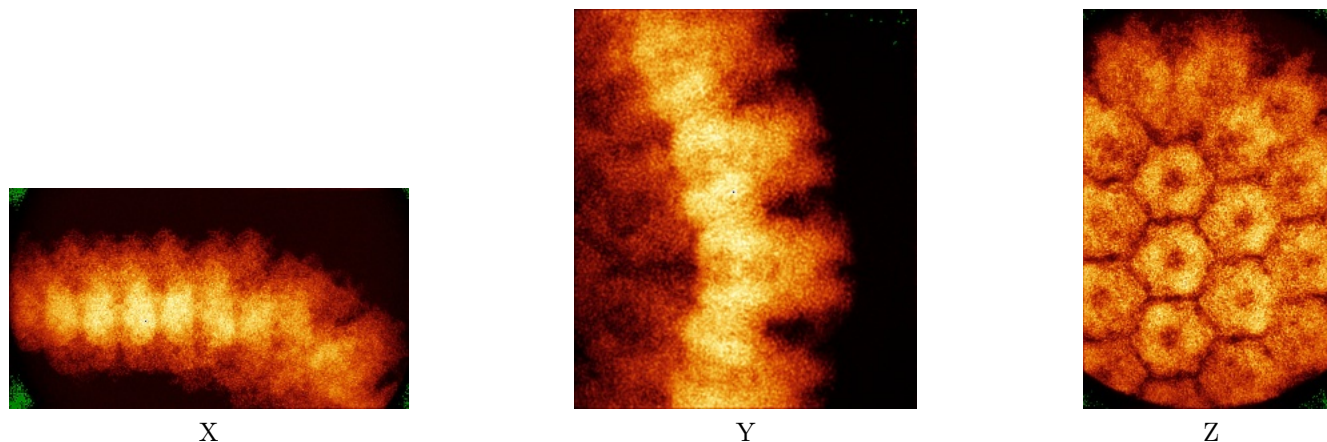


Z Index: 188

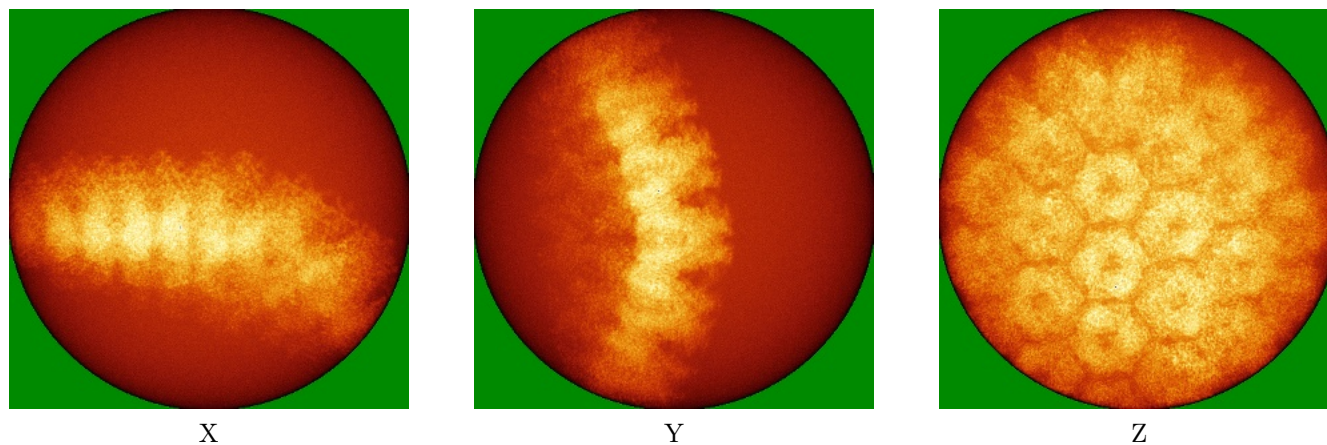
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



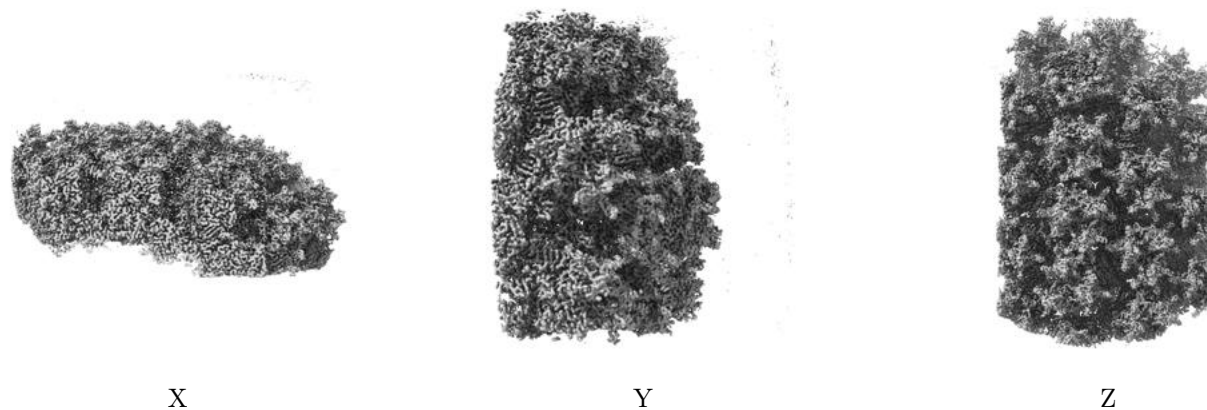
6.4.2 Raw map



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

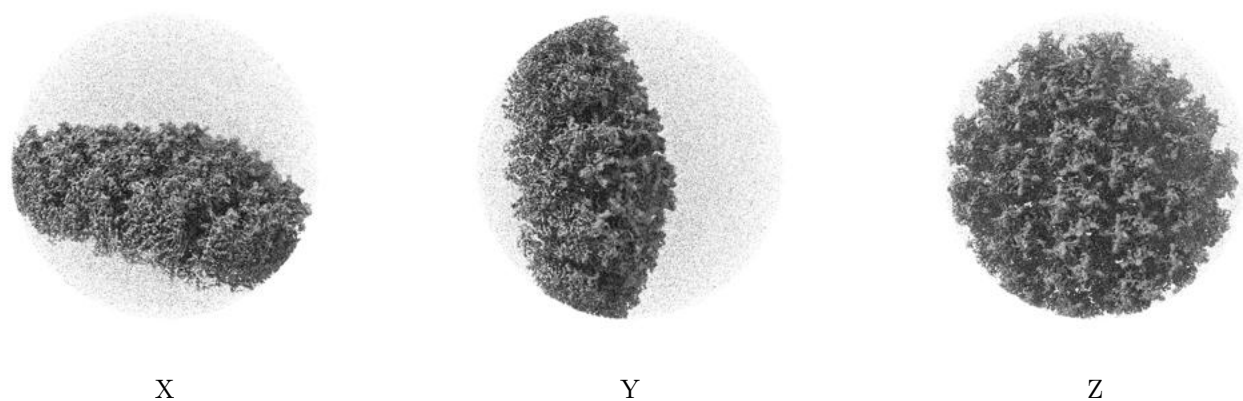
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. 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.

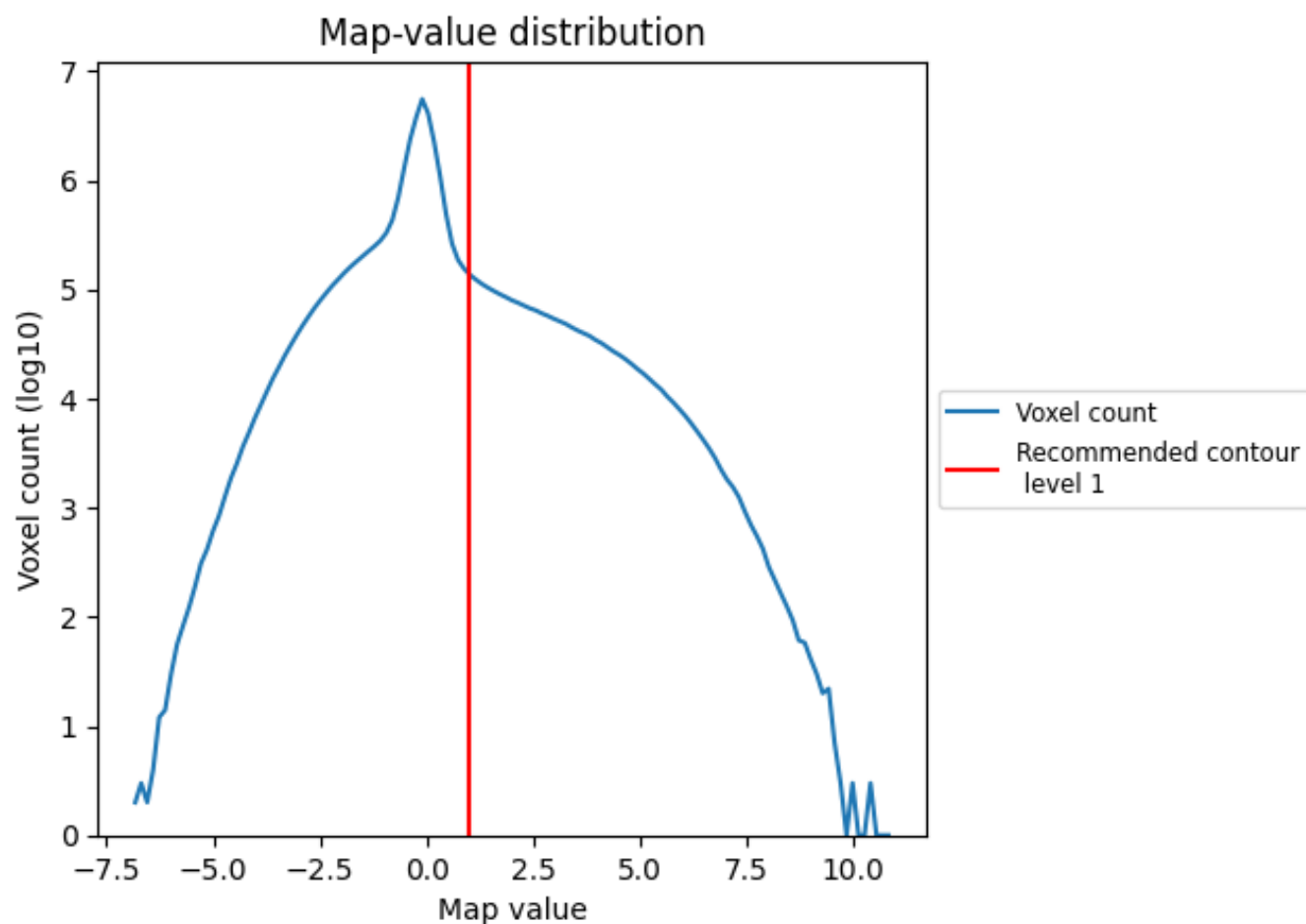
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

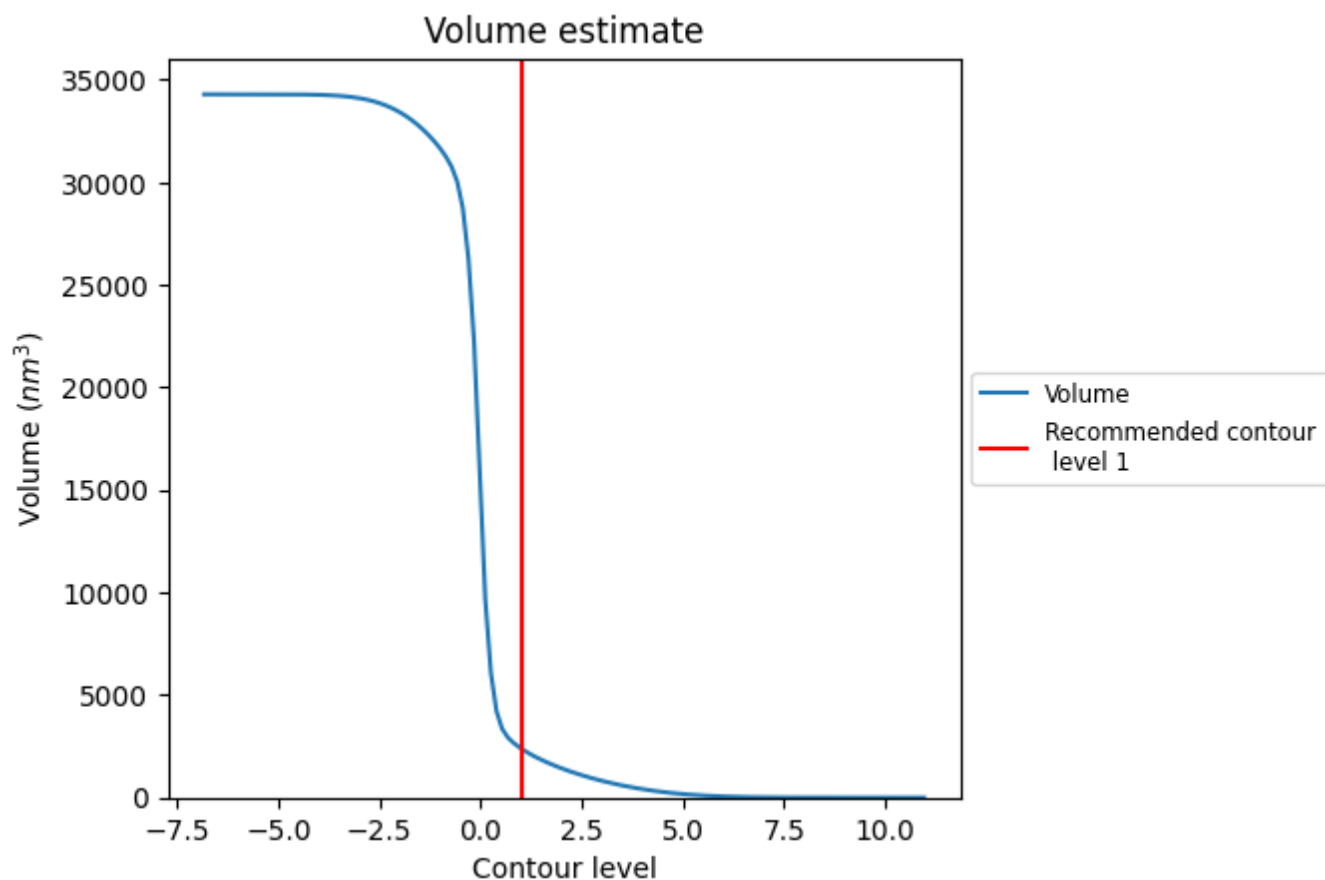
This section contains the results of statistical analysis of the map.

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 2399 nm³; this corresponds to an approximate mass of 2167 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

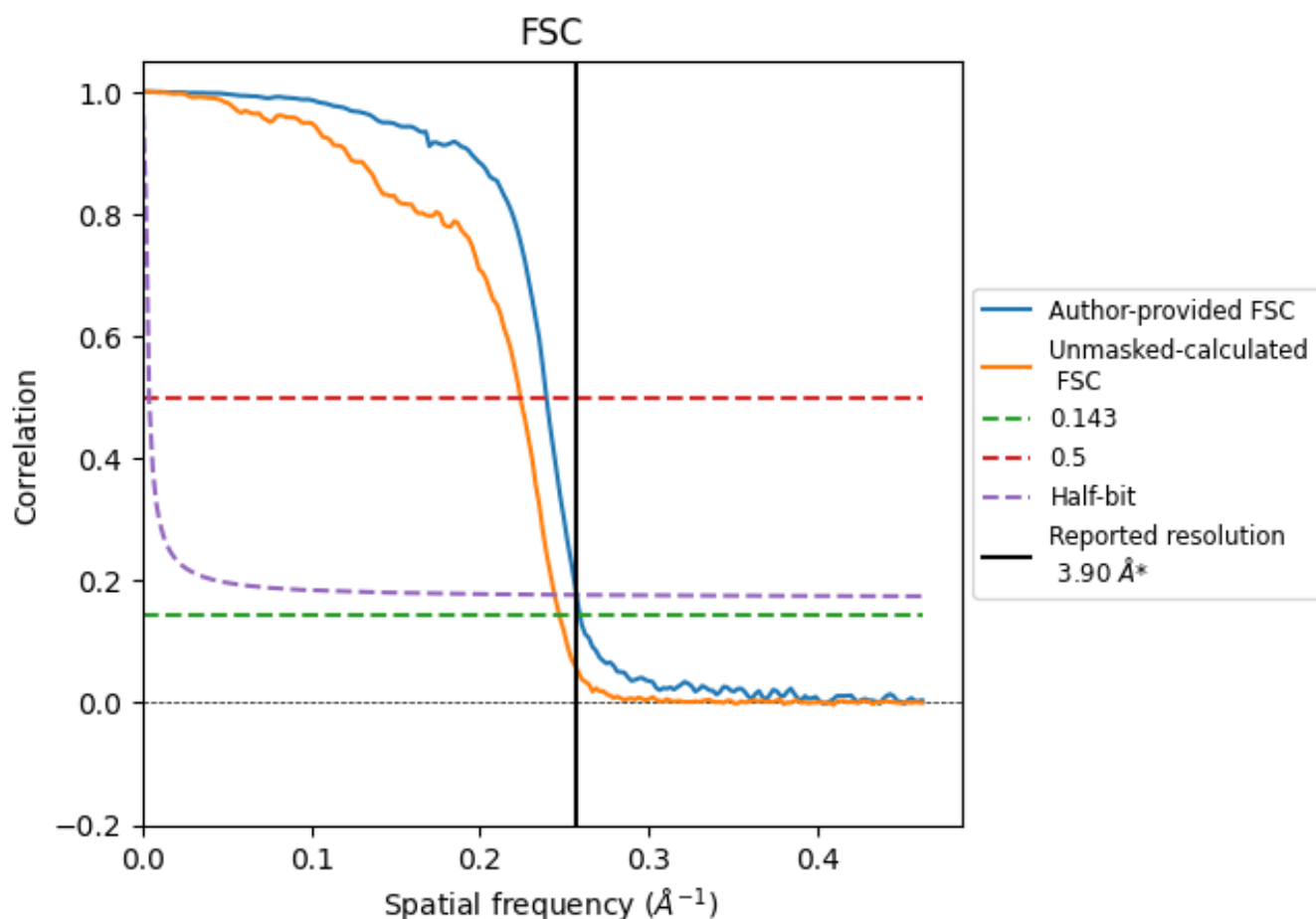
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.256 \AA^{-1}

8.2 Resolution estimates [i](#)

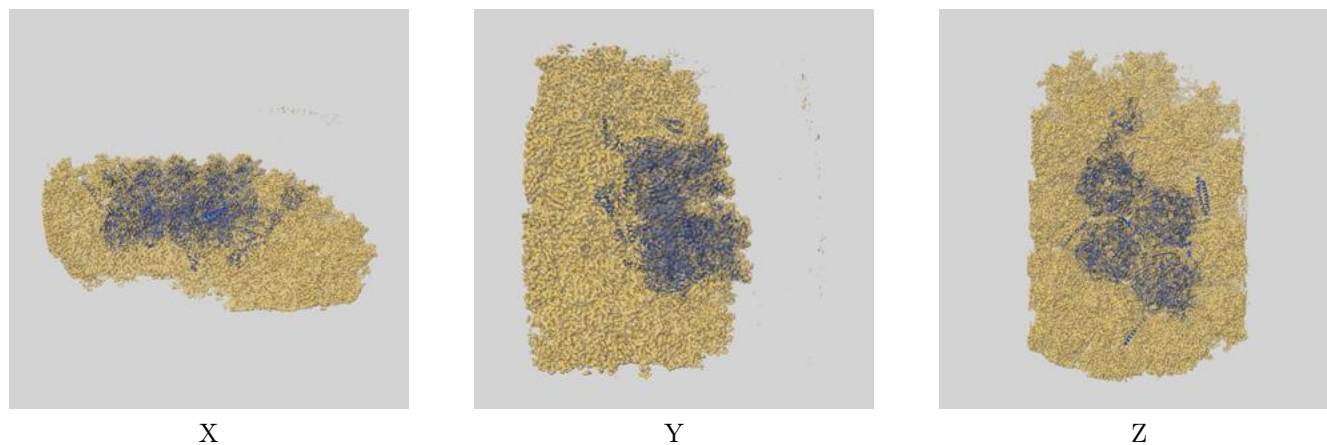
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.86	4.18	3.89
Unmasked-calculated*	4.05	4.47	4.10

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

9 Map-model fit [i](#)

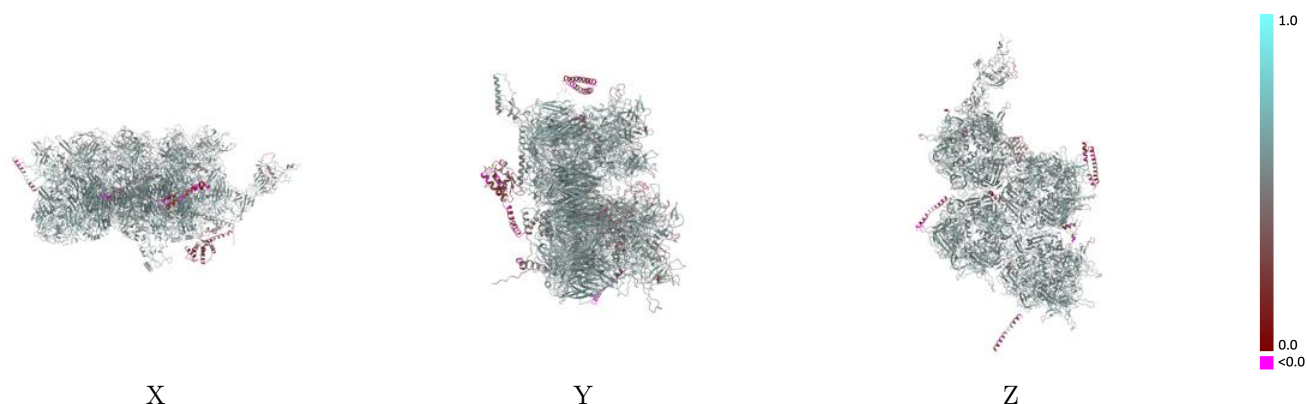
This section contains information regarding the fit between EMDB map EMD-72773 and PDB model 9YCI. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



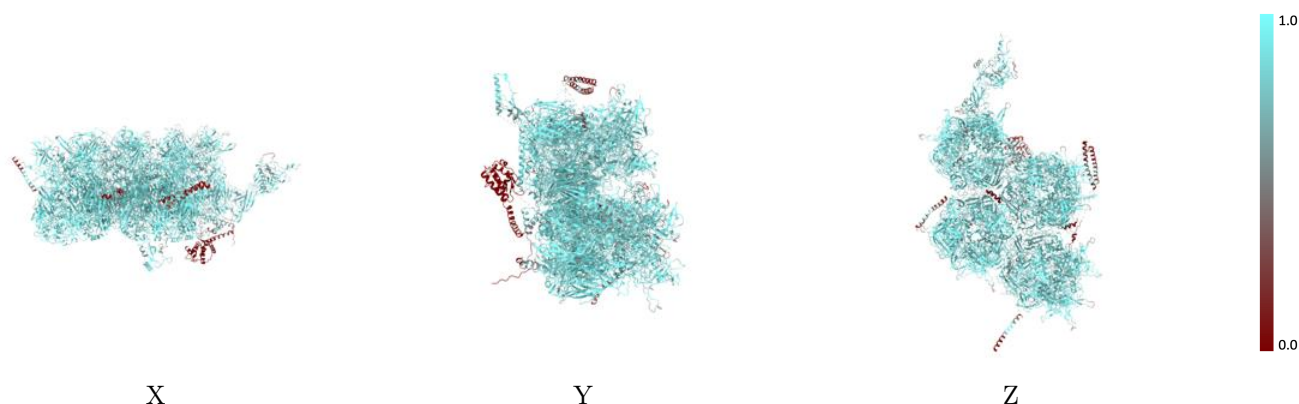
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



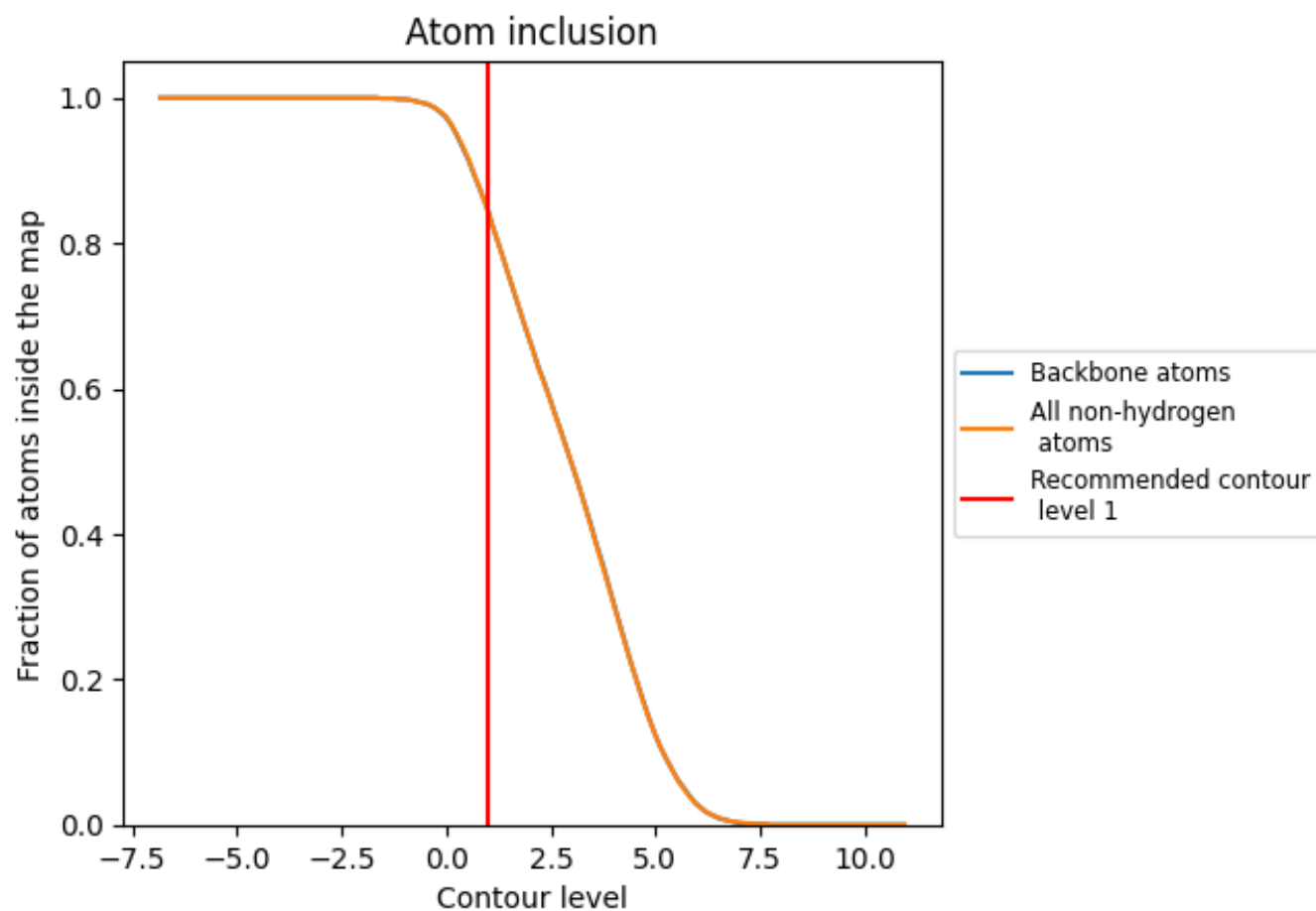
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8440	 0.5310
0	 0.6290	 0.4810
1	 0.6400	 0.4820
2	 0.6290	 0.4520
3	 0.4110	 0.4440
4	 0.5030	 0.3970
A	 0.8650	 0.5360
B	 0.8640	 0.5380
C	 0.8640	 0.5370
D	 0.8810	 0.5480
E	 0.8800	 0.5460
F	 0.8780	 0.5470
G	 0.8790	 0.5440
H	 0.8800	 0.5480
I	 0.8750	 0.5470
J	 0.8790	 0.5480
K	 0.8800	 0.5470
L	 0.8880	 0.5510
M	 0.2050	 0.2690
N	 0.7490	 0.4780
P	 0.5890	 0.3600
Q	 0.5730	 0.3730
R	 0.6680	 0.4280
S	 0.5400	 0.3550
U	 0.7840	 0.5220
V	 0.7270	 0.5120
W	 0.5760	 0.4260
Y	 0.6340	 0.4680
Z	 0.7250	 0.4870

