Full wwPDB EM Validation Report (i)

Nov 27, 2022 – 07:10 AM EST

PDB ID	:	6ODM
EMDB ID	:	EMD-9860
Title	:	Herpes simplex virus type 1 (HSV-1) portal vertex-adjacent capsid/CATC, asymmetric unit
Authors	:	Liu, Y.T.; Jih, J.; Dai, X.H.; Bi, G.Q.; Zhou, Z.H.
Deposited on	:	2019-03-26
Resolution	:	4.30 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 (i) 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 (i)) were used in the production of this report:

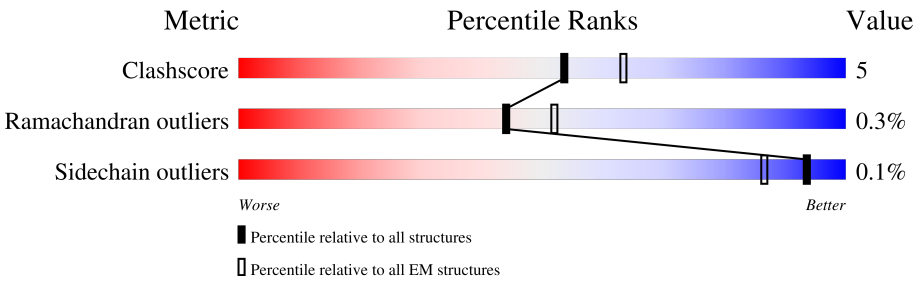
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	S	1374	8% 79% 17% •
1	T	1374	12% 83% 17%
1	W	1374	18% 85% 14% •
1	X	1374	7% 80% 15% 5%
2	E	112	10% 79% 11% 10%
2	F	112	12% 83% 7% 10%
2	L	112	52% 81% 9% 10%
2	P	112	13% 82% 8% 10%

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Mol	Chain	Length	Quality of chain
3	5	465	21% 72% 11% 17%
3	D	465	12% 67% 10% 22%
4	6	318	14% 78% 13% 8%
4	7	318	14% 80% 17%
4	A	318	35% 81% 15%
4	H	318	31% 75% 16% 8%
5	C	703	16% 67% 13% 20%
6	G	580	5% 14% 84%
6	K	580	11% 86%
7	B	3094	98%
7	O	3094	98%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 65560 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	T	1369	10470	6612	1884	1920	54	0	0
1	W	1367	10451	6602	1879	1916	54	0	0
1	S	1328	10151	6418	1823	1858	52	0	0
1	X	1310	10027	6337	1801	1836	53	0	0

- Molecule 2 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	101	774	488	146	137	3	0	0
2	P	101	774	488	146	137	3	0	0
2	E	101	774	488	146	137	3	0	0
2	F	101	774	488	146	137	3	0	0

- Molecule 3 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	5	387	2963	1848	564	532	19	0	0
3	D	363	2786	1741	531	496	18	0	0

- Molecule 4 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	6	291	2216	1413	393	403	7	0	0
			Total	C	N	O	S		
4	7	310	2355	1497	417	432	9	0	0
			Total	C	N	O	S		
4	H	291	2216	1413	393	403	7	0	0
			Total	C	N	O	S		
4	A	310	2355	1497	417	432	9	0	0

- Molecule 5 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	565	4305	2734	783	767	21	0	0

- Molecule 6 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	92	749	475	136	134	4	0	0
			Total	C	N	O	S		
6	K	79	644	407	121	114	2	0	0

- Molecule 7 is a protein called Large tegument protein deneddylase.

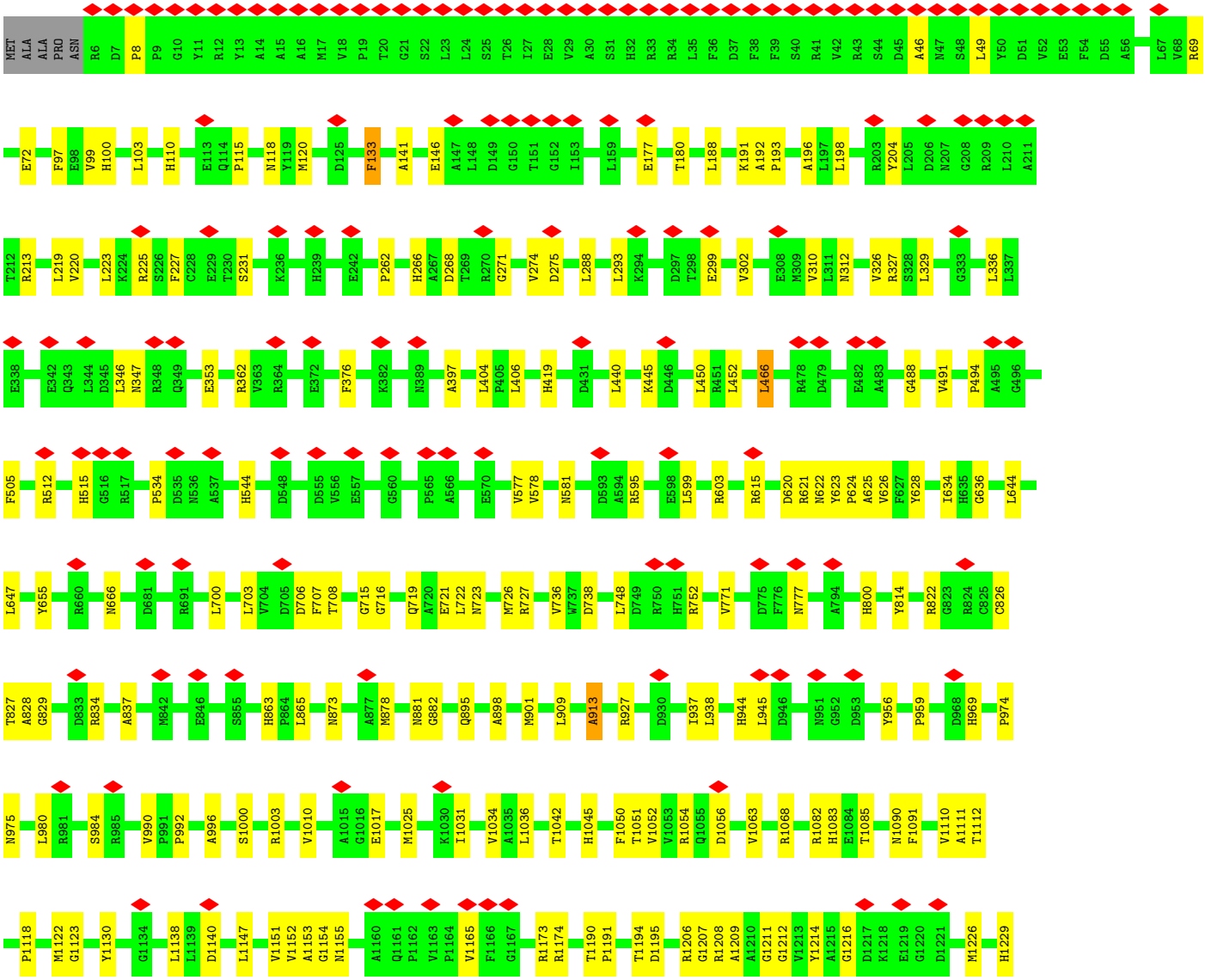
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	O	48	388	239	85	62	2	0	0
			Total	C	N	O	S		
7	B	48	388	239	85	62	2	0	0

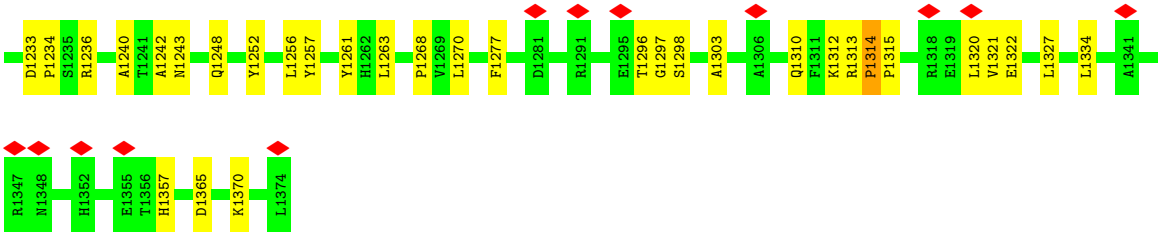
3 Residue-property plots (i)

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

- Molecule 1: Major capsid protein

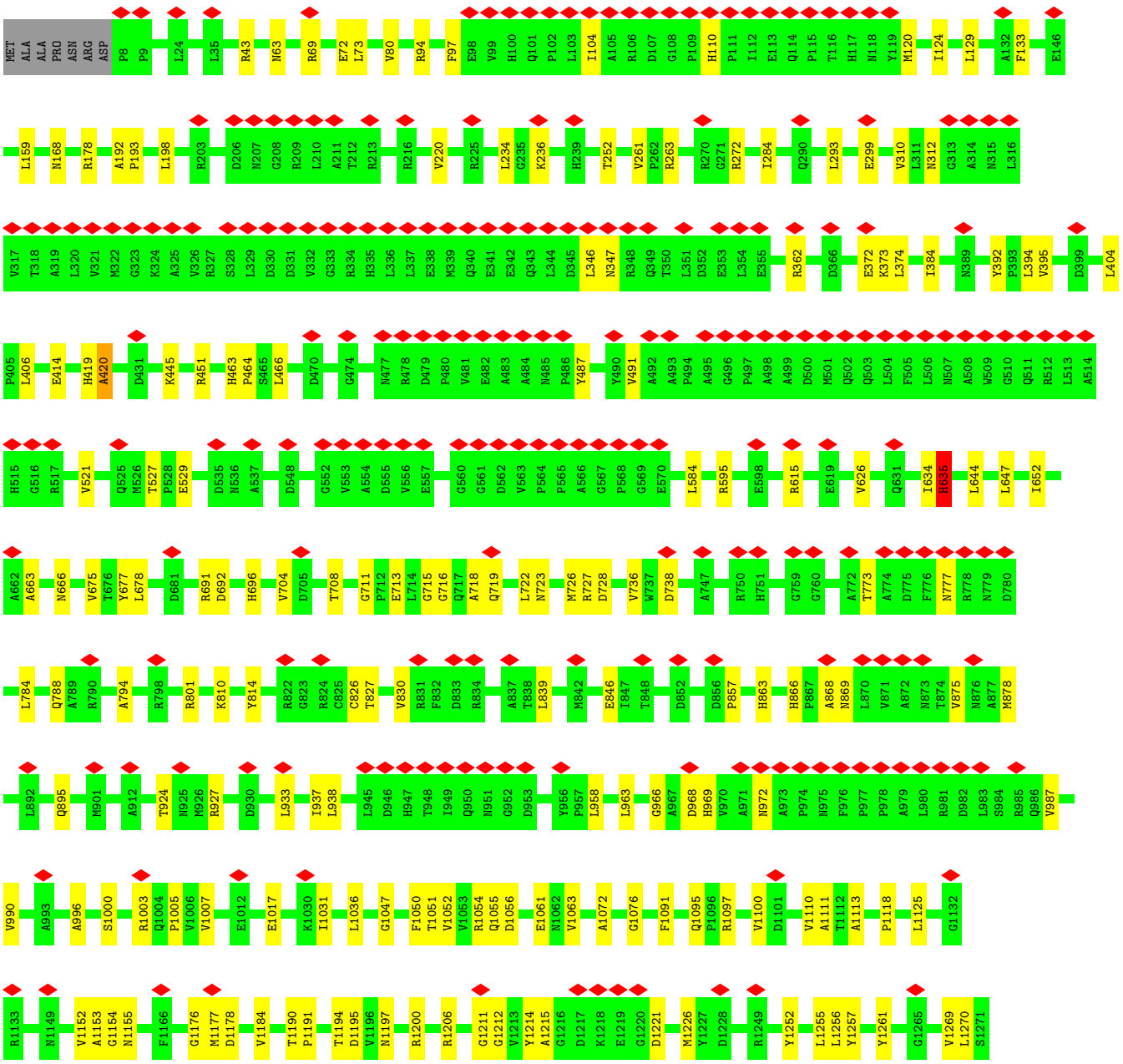
Chain T: 12% 83% 17%

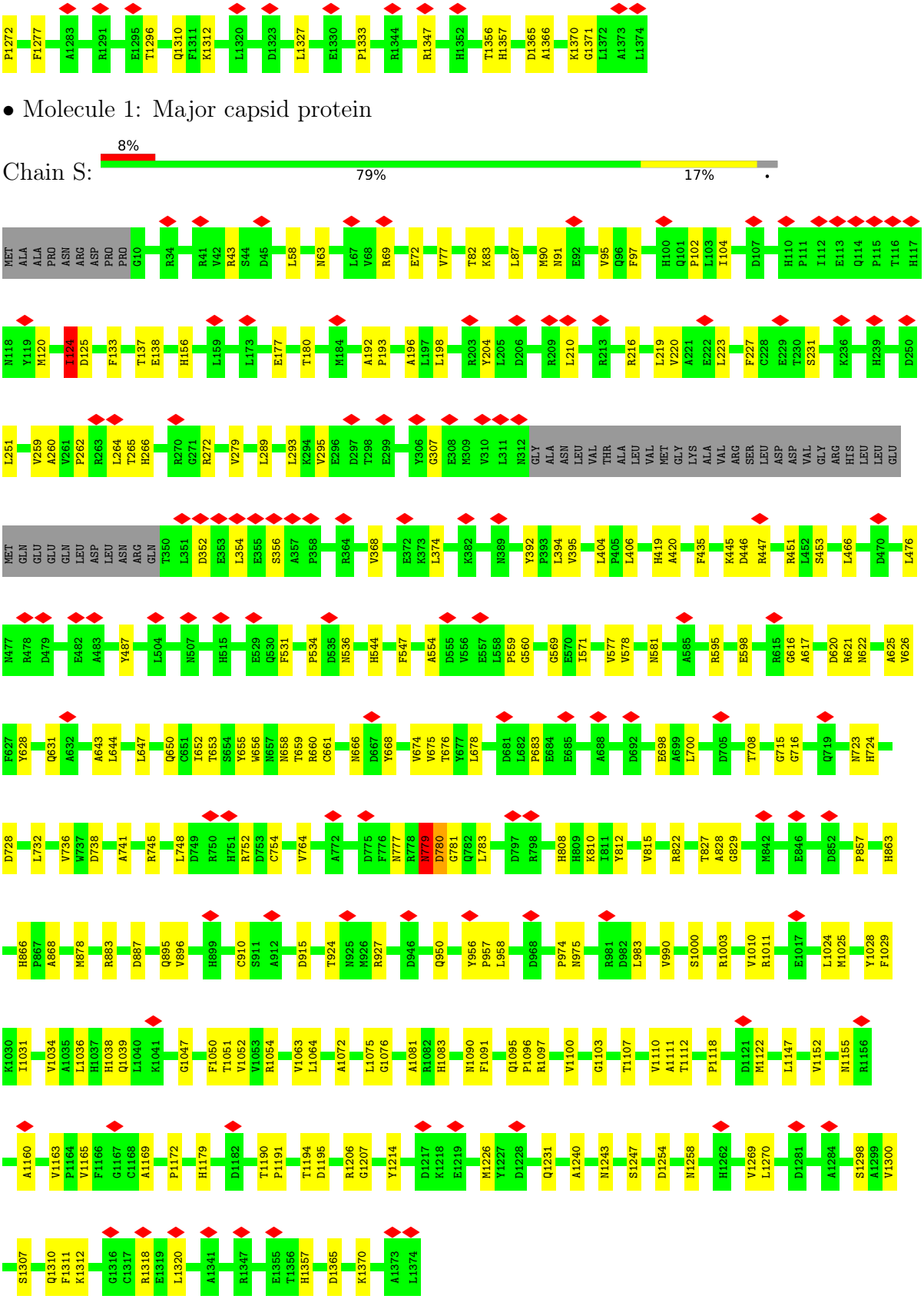




• Molecule 1: Major capsid protein

Chain W:

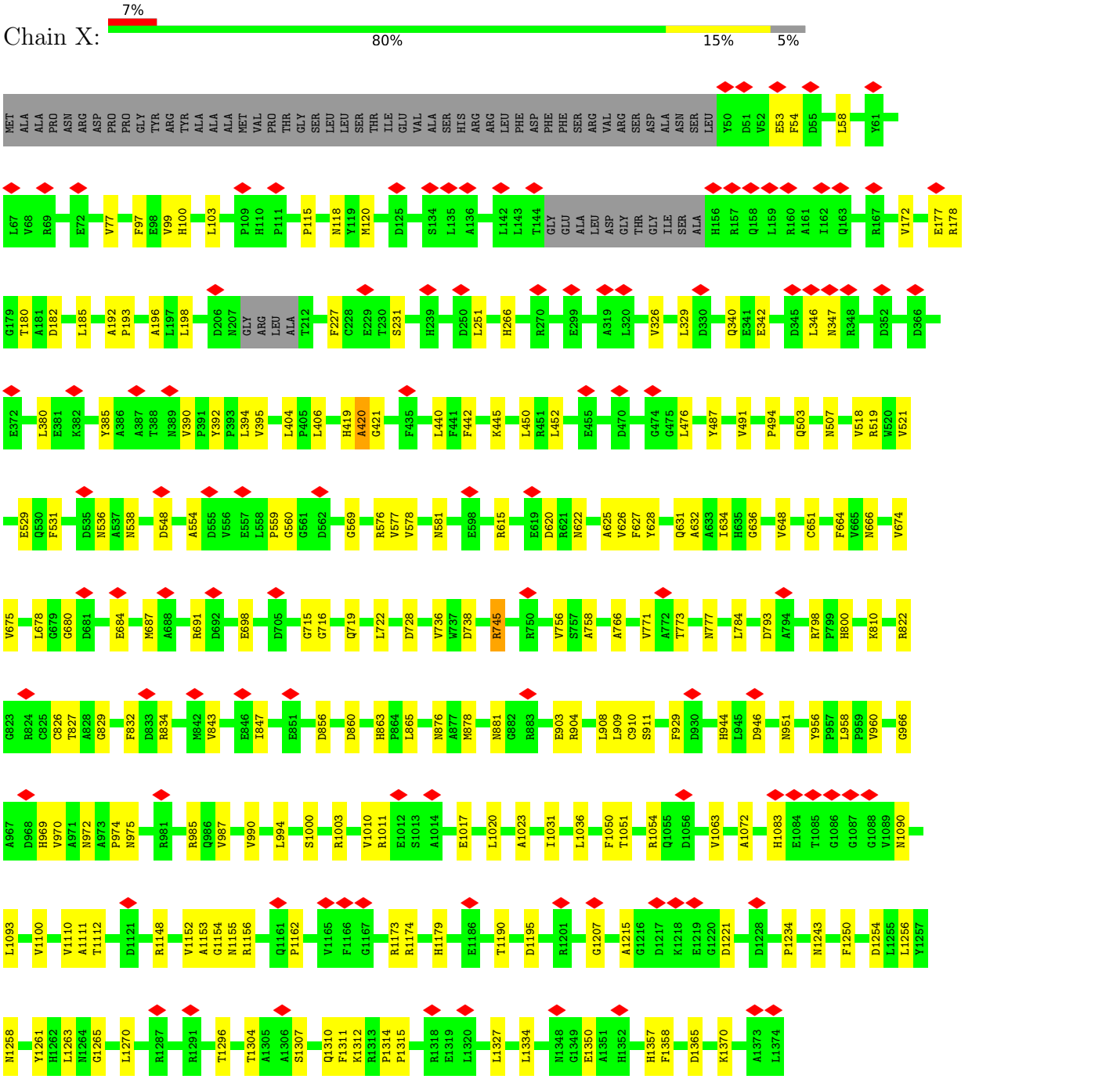




• Molecule 1: Major capsid protein

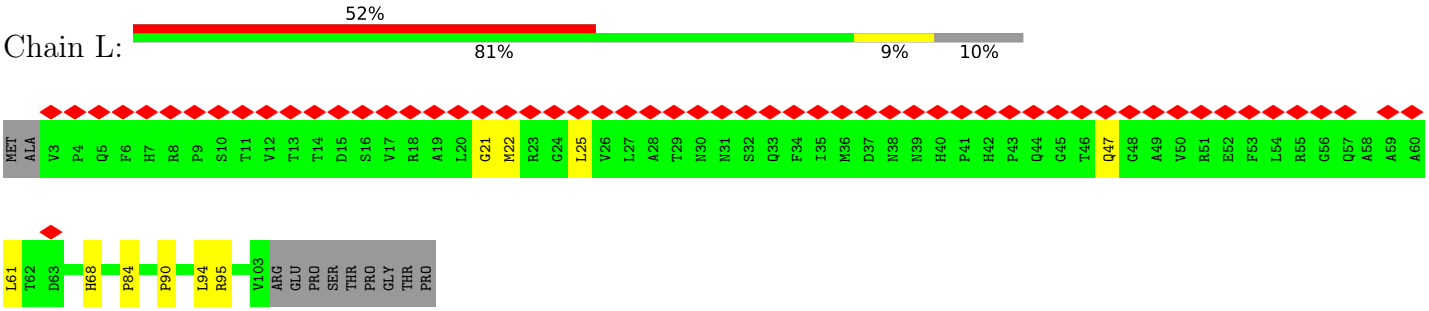
• Molecule 1: Major capsid protein

Chain X:



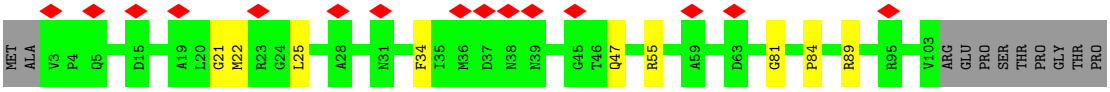
• Molecule 2: Small capsomere-interacting protein

Chain L:



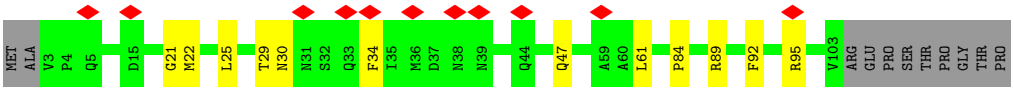
- Molecule 2: Small capsomere-interacting protein

Chain P:



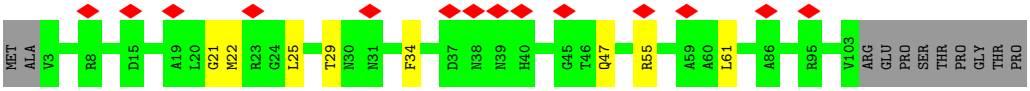
- Molecule 2: Small capsomere-interacting protein

Chain E:



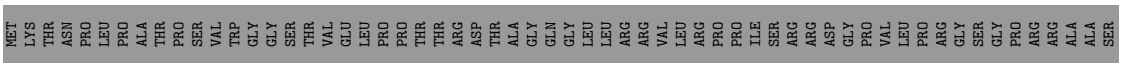
- Molecule 2: Small capsomere-interacting protein

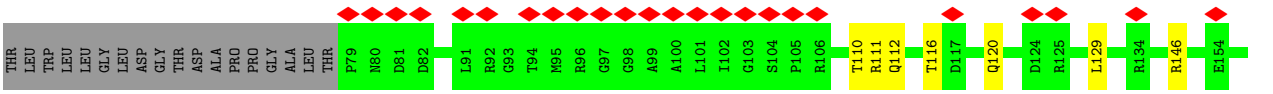
Chain F:

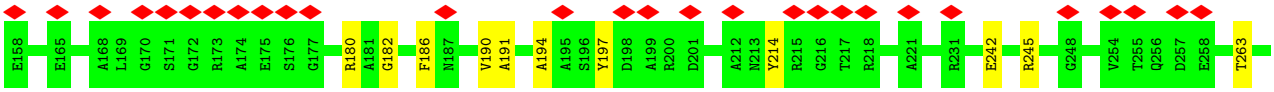


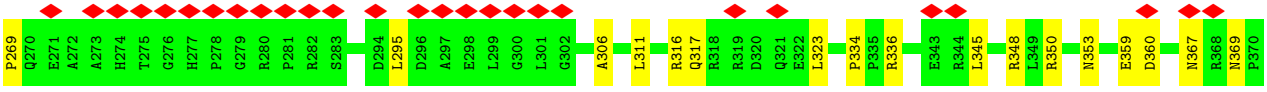
- Molecule 3: Triplex capsid protein 1

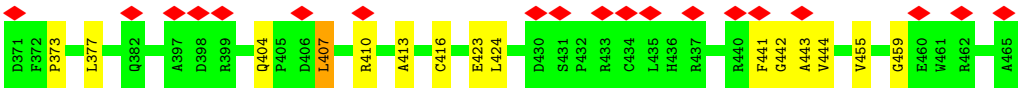
Chain 5:





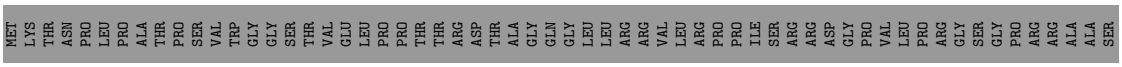


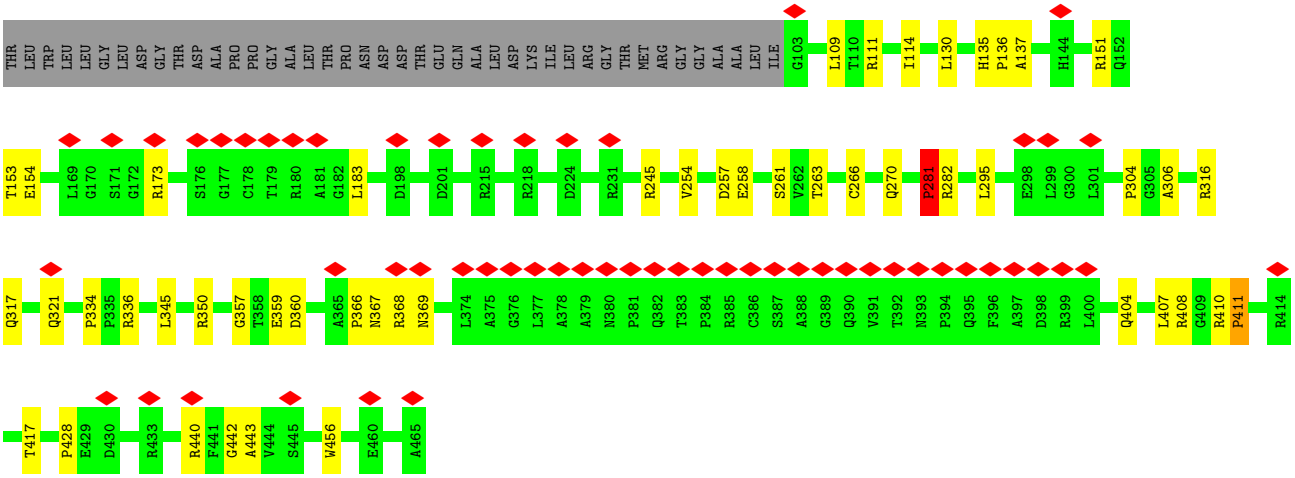




- Molecule 3: Triplex capsid protein 1

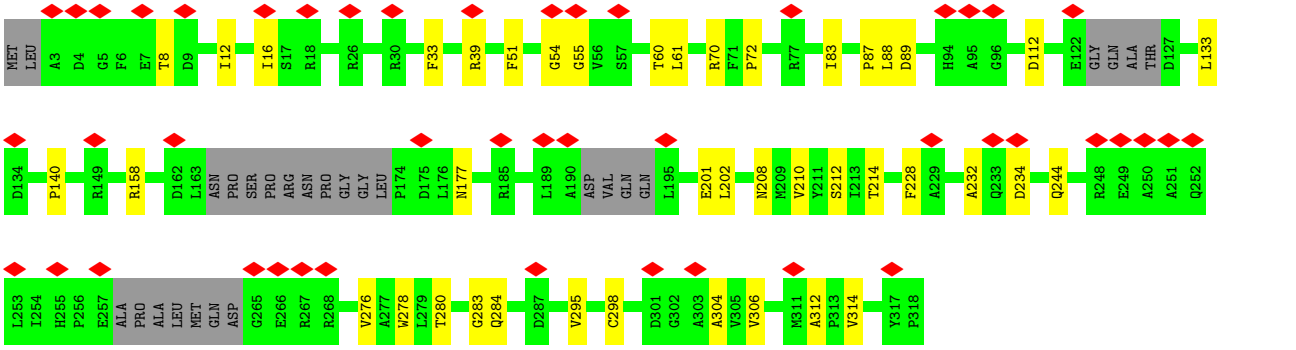
Chain D:





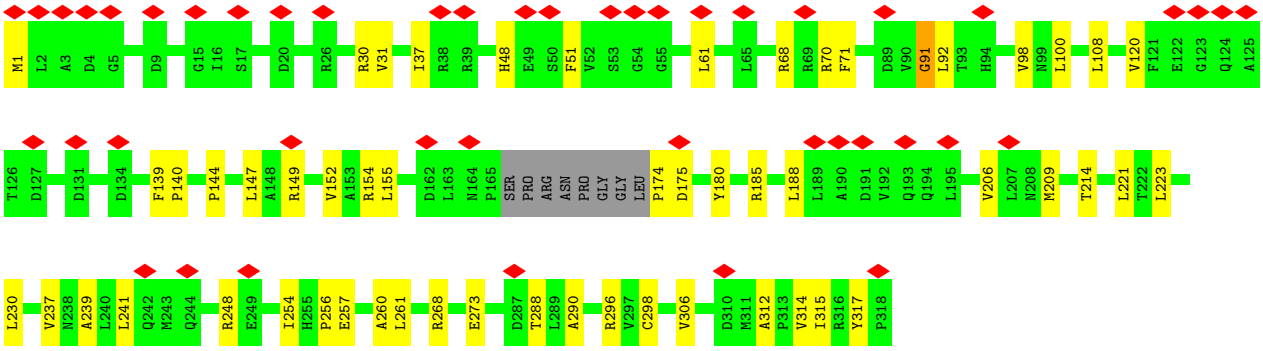
- Molecule 4: Triplex capsid protein 2

Chain 6:



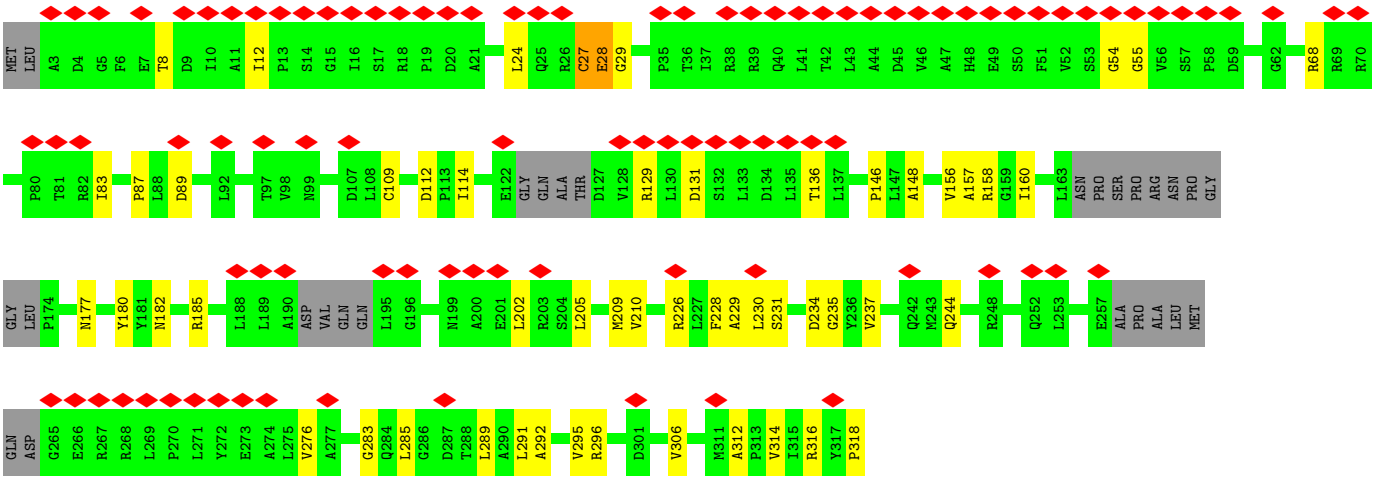
- Molecule 4: Triplex capsid protein 2

Chain 7:



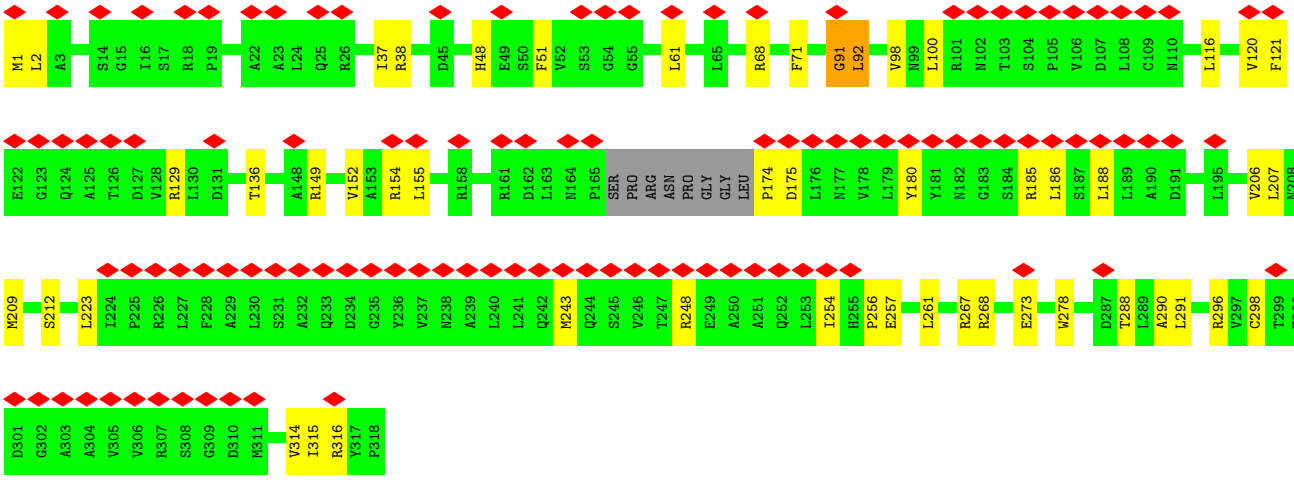
- Molecule 4: Triplex capsid protein 2

Chain H:



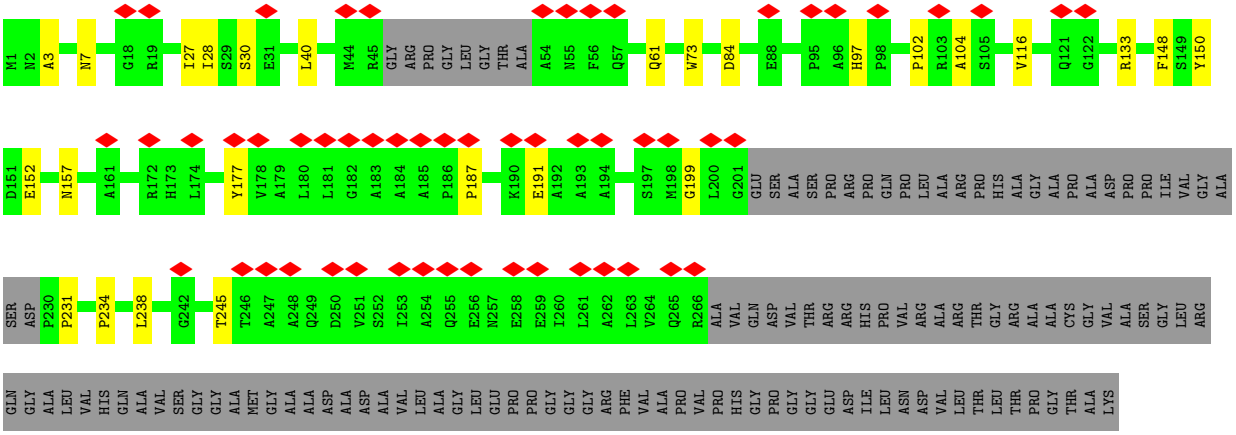
- Molecule 4: Triplex capsid protein 2

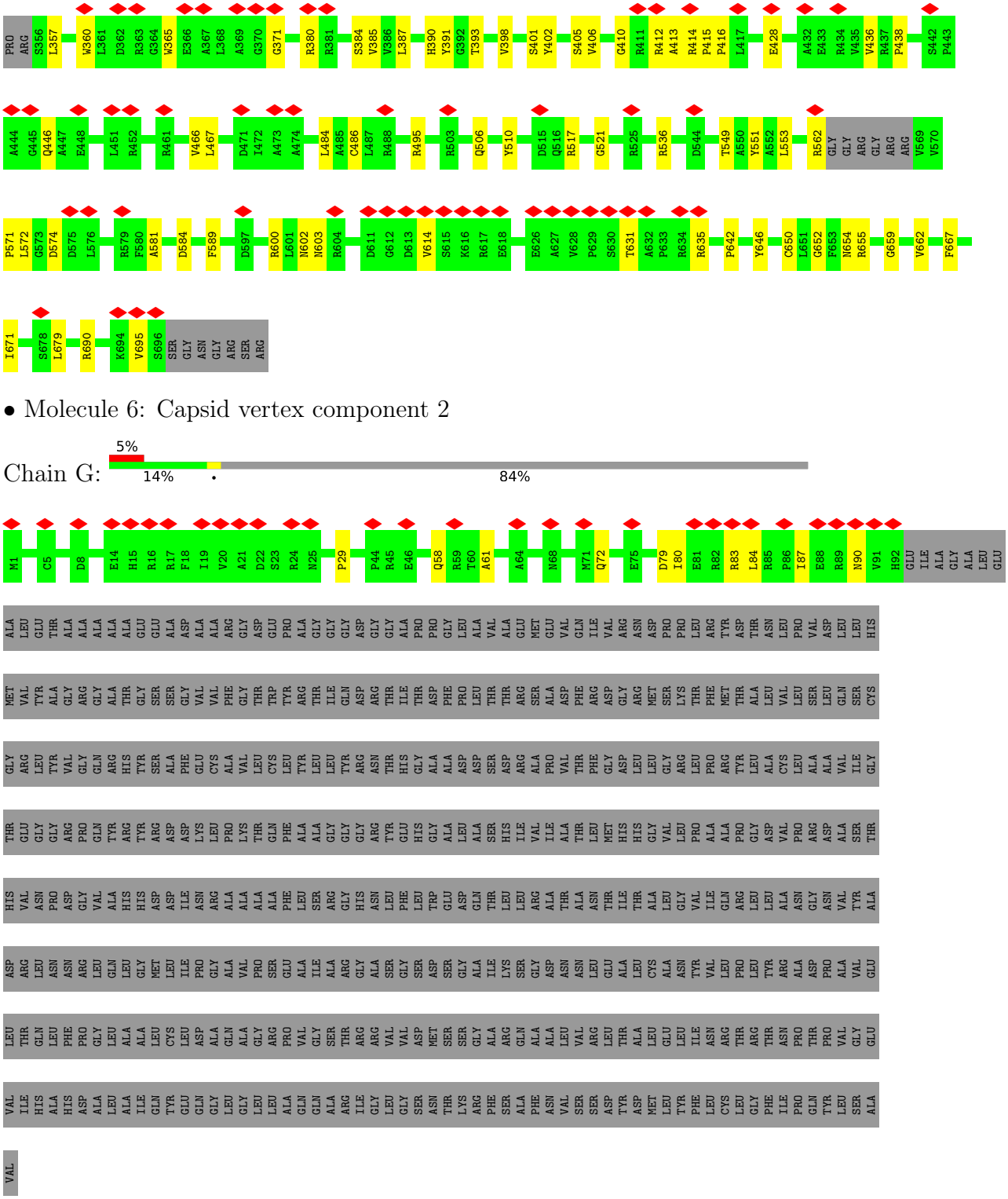
Chain A:



- Molecule 5: Capsid vertex component 1

Chain C:



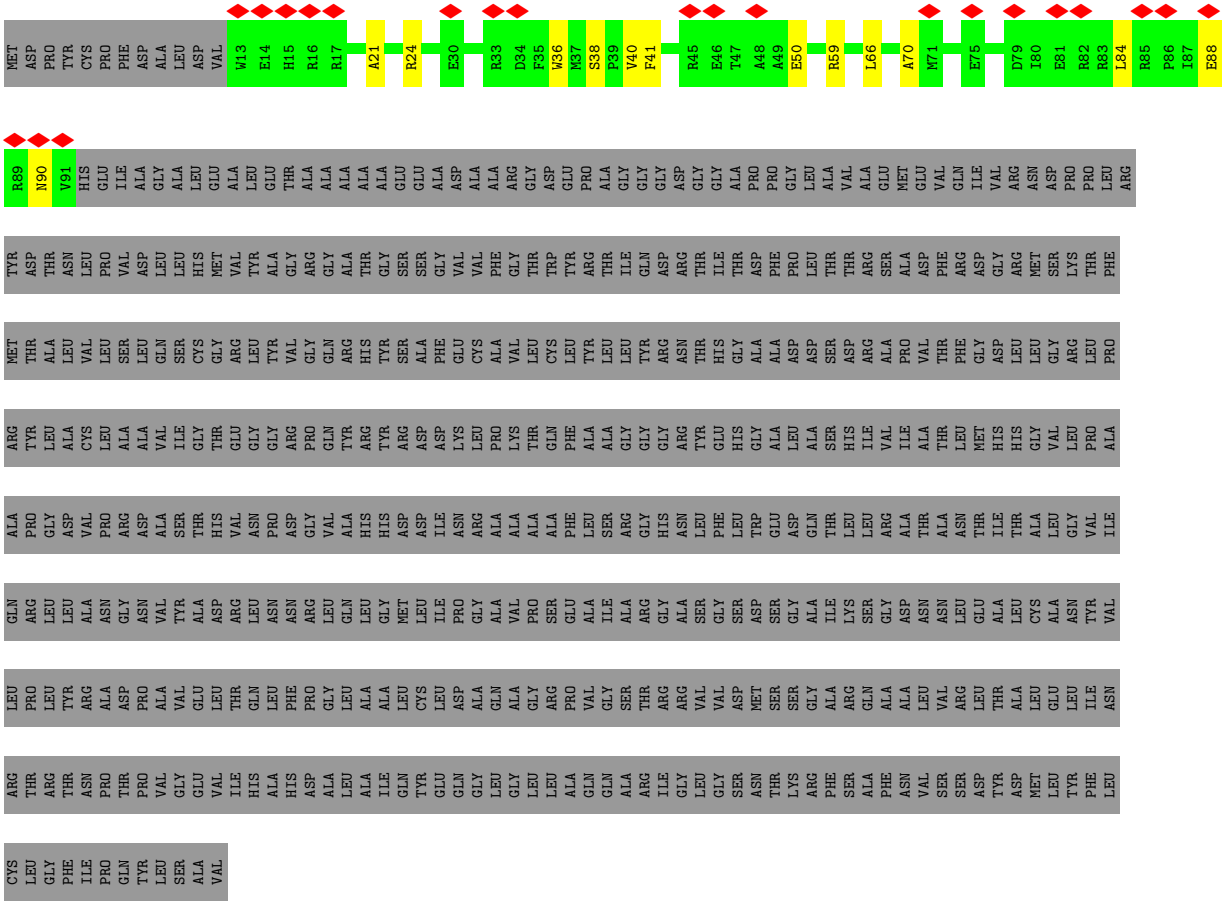


- Molecule 6: Capsid vertex component 2

Chain G:

- Molecule 6: Capsid vertex component 2

Chain K:


MET ASP PRO TYR CYS PRO PHE ASP ALA LEU ASP VAL W13 E14 H15 R16 R17 A21 R24 E30 R33 D34 F35 W36 M37 S38 P39 V40 F41 R45 E46 T47 A48 A49 E50 R59 L66 A70 M71 E75 D79 I80 E81 R82 R83 L84 R85 P86 I87 E88
R89 N90 V91 HIS GLU ILE ALA GLY ALA LEU GLU ALA LEU GLU THR ALA ALA ALA ALA ALA GLU GLU ALA ASP ALA ALA ARG GLY ASP GLU PRO ALA GLY GLY GLY ASP ARG THR ILE THR ASP PHE PRO LEU ALA THR ARG SER ALA ASP PHE ARG ASP GLY ARG MET SER LYS THR PHE
TYR ASP THR ASN LEU PRO VAL ASP LEU LEU HIS MET VAL TYR ALA GLY ARG GLY ALA THR GLY SER SER GLY VAL VAL PHE GLY THR TRP TYR ARG THR ILE ILE GLN ASP ARG THR ILE THR ASP PHE PRO LEU THR THR ARG SER ALA ASP PHE ARG ASP GLY ARG MET THR ALA LEU VAL LEU LEU SER LEU GLN SER SER CYS GLY ARG LEU VAL GLN GLN ARG HIS TYR SER ALA PHE GLU CYS ALA VAL LEU CYS LEU TYR LEU LEU TYR ARG ASN THR HIS GLY ALA ALA ASP SER ASP ARG ALA PRO VAL THR PHE ASP GLY LEU LEU ASP LEU PRO
ARG TYR LEU ALA CYS LEU ALA ALA VAL ILE GLY THR GLU GLY GLY ARG PRO GLN TYR ARG HIS TYR ARG ASP ASP LYS LEU PRO LYS THR GLN PHE ALA ALA GLY GLY GLY ARG TYR GLU HIS GLY ALA LEU ALA SER HIS ILE VAL ILE ALA THR LEU MET HIS HIS GLY VAL LEU PRO ALA
ALA PRO GLY ASP VAL PRO ARG ASP ALA SER THR HIS VAL ASN PRO ASP GLY VAL ALA HIS HIS ASP ASP ILE ASN ARG ALA ALA ALA ALA PHE LEU SER ARG GLY HIS ASN LEU PHE LEU TRP GLU ASP GLN THR LEU LEU ARG ALA THR ALA ASN THR ILE THR ALA LEU GLY VAL ILE
GLN ARG LEU LEU ALA ASN GLY ASN VAL TYR ALA ASP ARG LEU ASN ASN ARG LEU GLN LEU GLY MET LEU ILE PRO GLY ALA VAL PRO SER GLU ALA ILE ALA ARG GLY ALA SER GLY SER ASP SER GLY ASP ALA ALA THR ALA ASN THR ILE LEU GLU CYS VAL
LEU PRO LEU TYR ARG ALA ASP PRO ALA VAL GLU LEU THR GLN LEU PHE PRO GLY LEU ALA ALA ALA LEU CYS LEU ASP ALA GLN ALA GLY ARG PRO VAL GLY SER THR ARG ARG VAL VAL ASP MET SER SER GLY ALA ARG GLN ALA ALA LEU VAL ARG LEU THR ALA LEU CYS ALA ASN TYR VAL
ARG THR ARG THR ASN PRO THR PRO VAL GLY GLU VAL ILE HIS ALA HIS ASP ALA LEU ALA ILE GLN TYR GLU GLN GLY LEU GLY LEU LEU ALA GLY LEU GLY SER ASN THR LYS ARG PHE SER ALA PHE ASN VAL SER SER ASP TYR ASP MET LEU TYR PHE LEU
CYS LEU GLY PHE ILE PRO GLN TYR LEU SER ALA VAL
• Molecule 7: Large tegument protein deneddylase
Chain O:
98%
MET ILE ALA GLY THR PRO PRO HIS SER THR MET GLU ARG GLY GLY ASP ARG ASP ILE VAL VAL THR GLY ALA ARG ASN GLN PHE ALA PRO ASP LEU GLU PRO GLY GLY SER VAL SER CYS MET ARG SER SER LEU SER PHE LEU SER LEU ILE PHE ASP VAL GLY PRO ARG ASP VAL LEU
SER ALA GLU ALA ILE GLU GLY CYS LEU VAL GLU GLY GLY GLU TRP THR ARG ALA THR ALA GLY PRO GLY PRO PRO ARG MET CYS SER ILE VAL GLU LEU PRO ASN PHE LEU GLU TYR PRO GLY ALA ARG GLY GLY LEU ARG CYS VAL PHE SER ARG VAL TYR GLY GLU VAL GLY PHE PHE
GLY GLU PRO ALA ALA GLY LEU LEU GLU THR GLN CYS PRO ALA HIS THR PHE PHE ALA GLY PRO TRP ALA LEU ARG PRO LEU SER TYR THR LEU LEU LEU THR ILE GLY PRO LEU GLY MET GLY LEU PHE ARG ASP GLY ASP THR ALA TYR LEU PHE ASP PRO HIS GLY LEU PRO GLU GLY THR
PRO ALA PHE ILE ALA LYS VAL ARG ALA GLY ASP MET TYR PRO TYR LEU THR TYR TYR ARG ASP ARG PRO ASP VAL ARG TRP ALA GLY ALA MET VAL PHE PHE VAL PRO SER GLY PRO GLU PRO ALA ALA PRO ALA ASP LEU THR ALA ALA ALA ALA LEU LEU GLY GLU SER
THR TYR MET GLN ASP GLU ALA PHE SER GLU ARG ARG VAL ALA ILE THR HIS PRO LEU ARG GLY GLU ILE ALA GLY LEU GLY GLU PRO CYS VAL GLY VAL GLY PRO ARG GLU GLU GLY GLY GLY PRO GLY PRO GLY PRO HIS PRO PRO THR ALA ALA GLN SER PRO PRO PRO THR ARG ALA ARG ARG
ASP ASP ARG ALA SER GLU THR SER ARG GLY THR ALA GLY PRO SER ALA TYR PRO ASN ARG ALA PRO ASP VAL TRP ALA VAL ALA LEU LYS GLY THR PRO PRO THR ASP PRO PRO PRO SER ALA ASP PRO PRO SER ALA ILE PRO PRO PRO PRO PRO PRO ALA
LYS THR PRO ALA ALA GLU ALA ALA GLU GLU ASP ASP MET ARG VAL LEU GLU MET GLY VAL VAL PRO VAL GLY ARG HIS ARG GLY ALA ARG TYR SER ALA ALA GLY LEU PRO LYS ARG ARG ARG PRO VAL THR TRP THR PRO PRO SER SER VAL GLU ASP LEU THR GLY GLU LYS THR LYS
ARG SER ALA PRO PRO ALA LYS THR LYS LYS SER THR PRO LYS GLY LYS THR PRO VAL GLY ALA ALA VAL PRO ALA SER VAL PRO GLU PRO VAL LEU ALA SER ALA PRO PRO ASP PRO ALA GLY PRO PRO VAL ALA GLU ALA GLY GLU ASP ASP GLY PRO MET VAL PRO ALA SER ALA SER SER

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

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

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

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

ALA GLU ASP ARG GLN MET ARG GLU ALA LEU ASP ALA LEU ALA ARG GLY VAL ASP ALA VAL SER GLN HIS ALA GLY PRO LEU GLY VAL MET PRO ALA PRO ALA GLY ALA ALA PRO GLN GLY ALA PRO ARG PRO PRO PRO LEU GLY PRO GLU ALA VAL GLN VAL ARG LEU GLU GLU VAL ARG

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

ARG ASP ILE ALA GLN ARG ALA ALA ILE PRO ALA PRO PRO PRO ILE ALA THR SER PRO THR ALA ILE LEU LEU ARG ASP LEU ILE GLN ARG GLY GLN THR LEU ASP ALA PRO GLU ASP LEU ALA ALA TRP LEU SER VAL LEU THR ASP ALA ALA ASN GLN GLY LEU ILE GLU ARG LYS PRO

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

SER PRO GLU ALA THR ARG MET ALA GLU GLU ALA LEU ARG GLN ALA ARG ALA MET ASP ALA ALA LYS LEU THR ALA GLU LEU ALA PRO ASP ALA ARG ALA ARG LEU ARG GLU ARG ALA ARG SER LEU GLU ALA MET LEU GLU GLY ALA ARG GLU ARG ALA LYS VAL ALA ARG ASP ALA ARG

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

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

VAL SER ASN ALA ILE ASN ALA GLY SER ALA ALA VAL ALA THR ALA ASP PRO ALA SER THR VAL ASP ALA ALA VAL ARG ALA HIS ARG VAL LEU VAL ASP ALA VAL THR ALA LEU GLY ALA ALA ALA SER ASP PRO ALA SER PRO LEU ALA PHE LEU ALA ALA MET ALA ASP SER ALA ALA

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

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

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

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

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

ASP ALA LEU ARG ALA ASP ALA ARG ARG ALA ILE GLY SER VAL ALA LEU ASP LEU ALA ALA ALA ALA GLU GLU ILE SER ALA VAL ARG ASN ASP PRO ALA ALA ALA ALA GLU LEU VAL ARG ALA GLY VAL THR LEU PRO CYS PRO SER GLU ASP ALA LEU VAL ALA CYS VAL ALA ALA LEU

GLU ARG VAL ASP GLN SER PRO VAL LYS ASP THR ALA TYR ALA ASP TYR VAL ALA PHE VAL THR ARG GLN ASP LEU ALA ASP THR LYS ASP ALA VAL VAL ARG ALA LYS GLN GLN ARG ALA GLU ALA THR GLU ARG VAL THR ALA GLY LEU ARG GLU VAL LEU ALA ALA ARG GLU ARG ARG

ALA GLN LEU GLU ALA GLU GLY LEU ALA ASN LEU LYS THR LEU LEU LYS VAL VAL ALA VAL PRO ALA THR VAL ALA LYS THR LEU ASP GLN ALA ARG SER ALA GLU GLU ILE ALA ASP GLN VAL GLU ILE LEU LEU ASP GLN THR GLU LYS ALA ARG GLU LEU ASP VAL GLN ALA VAL ALA

TRP LEU GLU HIS ALA GLN ARG THR PHE GLU THR HIS PRO LEU ASN ALA ALA SER GLY ASP GLY PRO GLY LEU LEU THR ARG GLN GLY ALA ARG LEU GLN ALA LEU PHE ASP THR ARG ARG ARG VAL GLU ALA LEU ARG ARG SER LEU GLU GLU ALA GLU ALA GLU TRP ASP GLU VAL TRP

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

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

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

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

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

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

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

LEU PRO VAL PHE SER THR GLY GLY PRO PRO THR ARG GLY LEU MET PHE GLY THR ARG LEU ALA ASP TRP ARG ARG GLY LYS LEU SER GLU THR ASP PRO LEU ALA PRO TRP ARG SER VAL PRO GLU LEU GLY THR GLU ARG GLY ALA ALA LEU GLY LYS LEU SER PRO ALA GLN ALA LEU

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

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

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

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

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

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

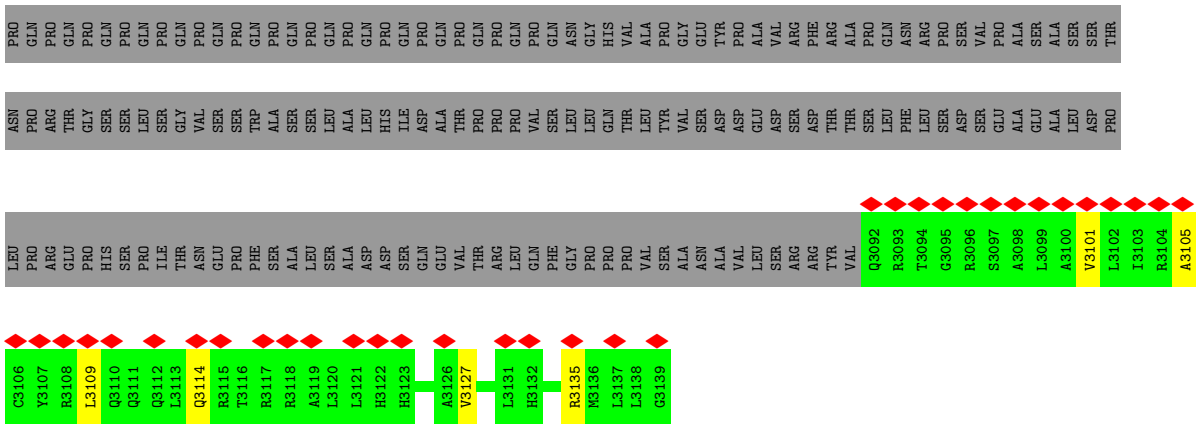
GLN CYS ALA PRO ARG PRO PRO GLY PRO ALA VAL THR ALA ARG GLU ALA ARG PRO GLY VAL PRO ALA GLU SER THR ARG PRO ALA PRO VAL GLY PRO ARG ASP ASP PHE ARG ARG LEU PRO SER PRO GLN SER SER PRO ALA PRO PRO ASP ALA THR ALA PRO ARG PRO PRO ALA SER SER

ARG ALA SER ALA ALA SER SER GLY SER ARG ALA ARG ARG HIS ARG ARG ALA ARG SER LEU ALA ARG ALA THR GLN ALA SER ALA THR THR GLN GLY TRP ARG PRO PRO ALA LEU PRO ASP THR VAL ALA PRO VAL THR ASP PHE ALA ARG PRO PRO ALA PRO PRO LYS PRO PRO GLU

PRO ALA LEU HIS ALA LEU VAL SER GLY VAL PRO LEU PRO LEU GLY PRO GLN PHE ALA GLY GLN ALA SER PRO ALA LEU PRO ILE ASP PRO VAL PRO PRO PRO VAL ALA THR GLY THR VAL LEU PRO GLY GLY GLU ASN ARG ARG PRO PRO LEU THR SER GLY PRO ALA PRO THR PRO PRO

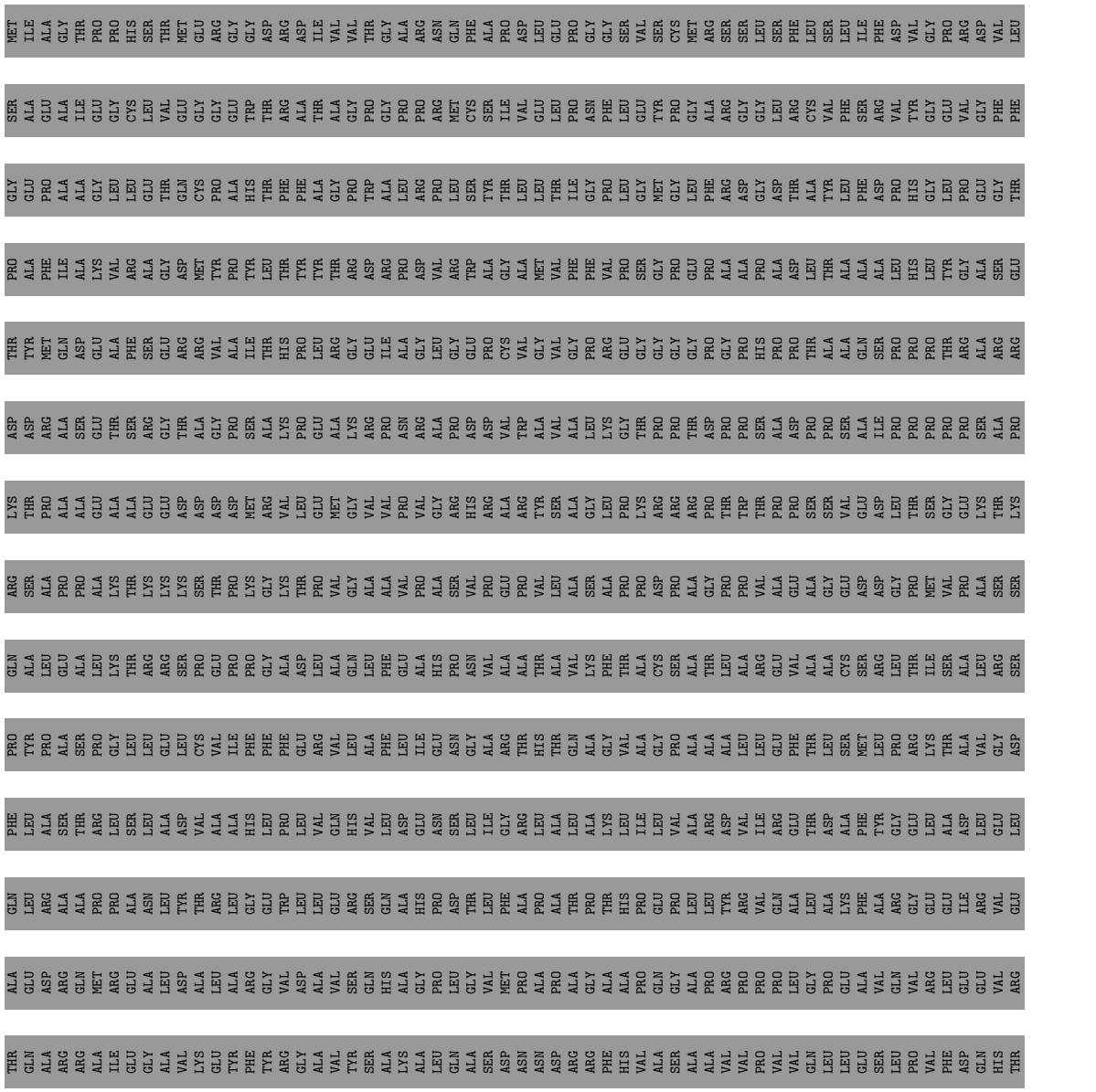
ARG VAL PRO VAL GLY GLY PRO GLN ARG ARG LEU THR ARG PRO ALA VAL ALA SER LEU SER GLU SER ARG GLU SER LEU PRO SER PRO TRP ASP PRO ALA ASP PRO THR ALA PRO VAL LEU GLY ARG ASN PRO ALA GLU PRO THR SER SER SER PRO ALA GLY PRO SER PRO PRO PRO PRO

ALA VAL GLN PRO VAL THR PRO PRO PRO THR SER GLY PRO PRO PRO THR TYR LEU THR LEU GLU GLY GLY VAL THR PRO GLY GLY PRO VAL SER ARG ARG PRO THR THR ARG GLN PRO VAL ALA THR PRO THR THR SER ALA ARG PRO ARG GLY HIS LEU THR VAL ASN ARG LEU SER ALA



- Molecule 7: Large tegument protein deneddylase

Chain B: 98%



ARG ASP ILE ALA GLN ARG ALA ALA ILE PRO ALA PRO PRO PRO ILE ALA THR SER PRO THR ALA ILE LEU LEU ARG ASP LEU ILE GLN ARG GLY GLN THR LEU ASP ALA PRO GLU ASP LEU ALA ALA TRP LEU SER VAL LEU THR ASP ALA ALA ASN GLN GLY LEU ILE GLU ARG LYS PRO

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

SER PRO GLU ALA THR ARG MET ALA GLU GLU ALA LEU ARG GLN ALA ARG ALA MET ASP ALA ALA LYS LEU THR ALA GLU LEU ALA PRO ASP ALA ARG ALA ARG LEU ARG GLU ARG ALA ARG SER LEU GLU ALA MET LEU GLU GLY ALA ARG GLU ARG ALA LYS VAL ALA ARG ASP ALA ARG

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

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

VAL SER ASN ALA ILE ASN ALA GLY SER ALA ALA VAL ALA THR ALA ASP PRO ALA SER THR VAL ASP ALA ALA VAL ARG ALA HIS ARG VAL LEU VAL ASP ALA VAL THR ALA LEU GLY ALA ALA ALA SER ASP PRO ALA SER PRO LEU ALA PHE LEU ALA ALA MET ALA ASP SER ALA ALA

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

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

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

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

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

ASP ALA LEU ARG ALA ASP ALA ARG ARG ALA ILE GLY SER VAL ALA LEU ASP LEU ALA ALA ALA ALA GLU GLU ILE SER ALA VAL ARG ASN ASP PRO ALA ALA ALA ALA GLU LEU VAL ARG ALA GLY VAL THR LEU PRO CYS PRO SER GLU ASP ALA LEU VAL ALA CYS VAL ALA ALA LEU

GLU ARG VAL ASP GLN SER PRO VAL LYS ASP THR ALA TYR ALA ASP TYR VAL ALA PHE VAL THR ARG GLN ASP LEU ALA ASP THR LYS ASP ALA VAL VAL ARG ALA LYS GLN GLN ARG ALA GLU ALA THR GLU ARG VAL THR ALA GLY LEU ARG GLU VAL LEU ALA ALA ARG GLU ARG ARG

ALA GLN LEU GLU ALA GLU GLY LEU ALA ASN LEU LYS THR LEU LEU LYS VAL VAL ALA VAL PRO ALA THR VAL ALA LYS THR LEU ASP GLN ALA ARG SER ALA GLU GLU ILE ALA ASP GLN VAL GLU ILE LEU LEU ASP GLN THR GLU LYS ALA ARG GLU LEU ASP VAL GLN ALA VAL ALA

TRP LEU GLU HIS ALA GLN ARG THR PHE GLU THR HIS PRO LEU ASN ALA ALA SER GLY ASP GLY PRO GLY LEU LEU THR ARG GLN GLY ALA ARG LEU GLN ALA LEU PHE ASP THR ARG ARG ARG VAL GLU ALA LEU ARG ARG SER LEU GLU GLU ALA GLU ALA GLU TRP ASP GLU VAL TRP

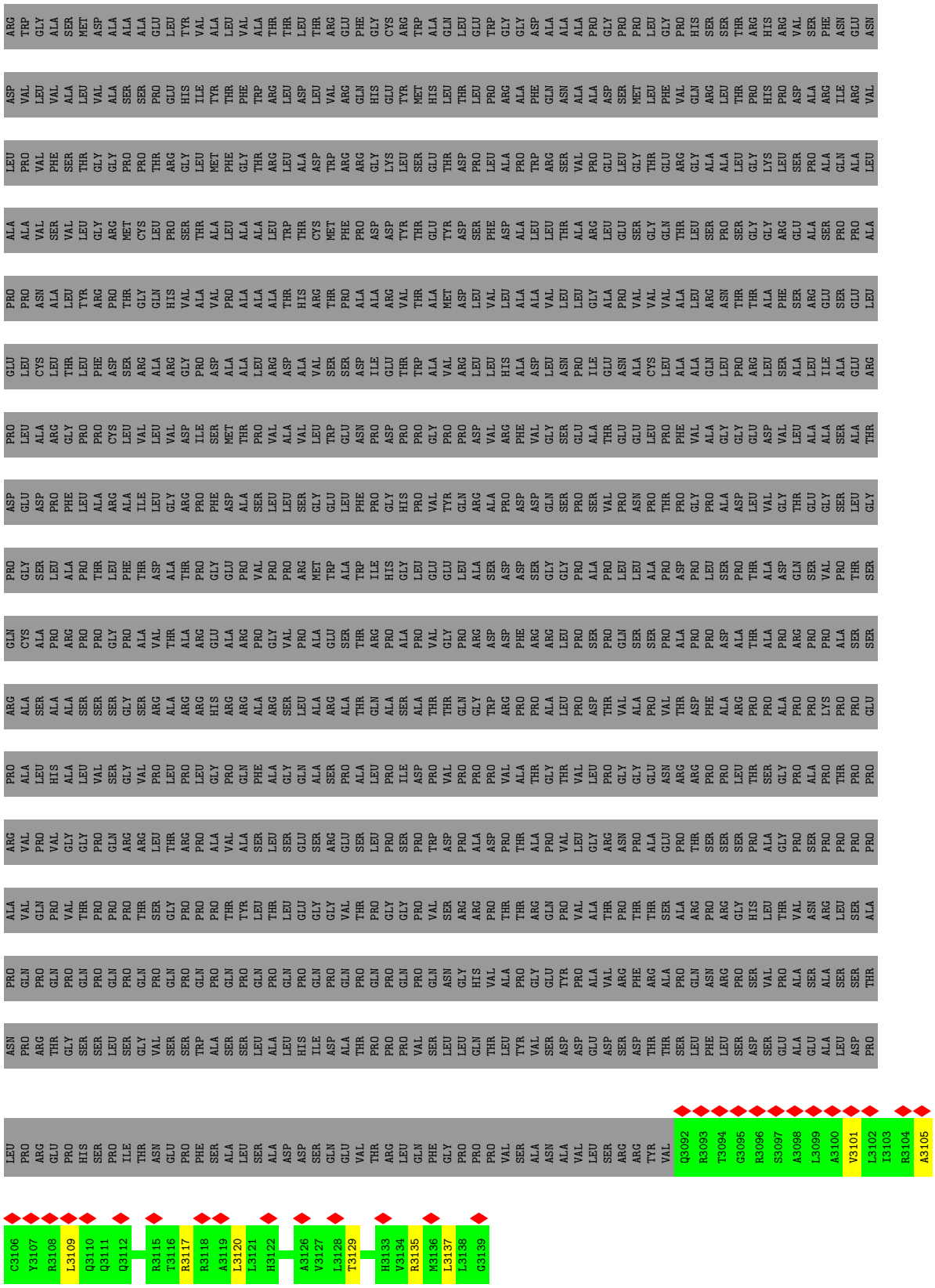
GLY ARG PHE GLY ARG VAL ARG GLY GLY ALA TRP LYS SER PRO GLU GLY PHE ARG ALA ALA CYS GLU GLN LEU ARG ALA LEU GLN ASP THR THR ASN THR VAL SER GLY LEU ARG ALA GLN ARG ASP TYR GLU ARG LEU PRO ALA LYS TYR GLN GLY VAL LEU GLY ALA LYS SER ALA GLU

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

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

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

LEU MET CYS PRO GLU ALA ALA CYS ILE ARG PRO PRO LEU PRO THR ASP THR LEU GLU SER ALA SER THR VAL THR ALA MET TYR VAL ILE THR VAL ILE ASN ARG LEU GLN LEU ALA LEU SER ASP ALA GLN ALA ALA ASN PHE GLN LEU PHE GLY ARG PHE VAL ARG HIS ARG GLN ALA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H3122
A3126
V3127
L3128
T3129
H3133
V3134
R3135
M3136
L3137
L3138
G3139
Q3092
R3093
T3094
G3095
R3096
S3097
A3098
L3099
A3100
V3101
L3102
I3103
R3104
A3105

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	42857	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	24271	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.034	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	395.52, 395.52, 395.52	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	S	0.31	0/10405	0.57	5/14207 (0.0%)
1	T	0.31	0/10728	0.56	1/14645 (0.0%)
1	W	0.30	0/10709	0.56	3/14619 (0.0%)
1	X	0.32	0/10274	0.57	2/14027 (0.0%)
2	E	0.28	0/796	0.45	0/1087
2	F	0.28	0/796	0.45	0/1087
2	L	0.28	0/796	0.45	0/1087
2	P	0.28	0/796	0.45	0/1087
3	5	0.30	0/3036	0.54	0/4134
3	D	0.30	0/2858	0.57	1/3895 (0.0%)
4	6	0.29	0/2255	0.57	1/3080 (0.0%)
4	7	0.29	0/2399	0.57	0/3282
4	A	0.28	0/2399	0.56	0/3282
4	H	0.28	0/2255	0.57	0/3080
5	C	0.30	0/4411	0.54	0/6015
6	G	0.28	0/769	0.53	0/1049
6	K	0.29	0/659	0.50	0/897
7	B	0.24	0/392	0.45	0/526
7	O	0.24	0/392	0.45	0/526
All	All	0.30	0/67125	0.56	13/91612 (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
1	S	0	5
1	T	0	8
1	W	0	8
1	X	0	5
3	D	0	3
4	7	0	1

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Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	1
4	H	0	1
5	C	0	1
All	All	0	33

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	745	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	X	847	ILE	C-N-CA	6.78	138.65	121.70
1	S	466	LEU	CA-CB-CG	6.33	129.85	115.30
1	S	210	LEU	CA-CB-CG	6.09	129.31	115.30
1	T	466	LEU	CA-CB-CG	6.02	129.14	115.30
1	W	635	HIS	N-CA-CB	5.71	120.89	110.60
4	6	202	LEU	CA-CB-CG	5.35	127.61	115.30
1	S	124	ILE	C-N-CA	5.30	134.94	121.70
1	S	779	ASN	C-N-CA	5.17	134.62	121.70
1	W	466	LEU	CA-CB-CG	5.16	127.17	115.30
3	D	440	ARG	C-N-CA	5.11	134.46	121.70
1	W	293	LEU	CA-CB-CG	5.09	127.00	115.30
1	S	983	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	7	91	GLY	Peptide
4	A	91	GLY	Peptide
5	C	631	THR	Peptide
3	D	257	ASP	Peptide
3	D	281	PRO	Peptide
3	D	411	PRO	Peptide
4	H	27	CYS	Peptide
1	S	1357	HIS	Peptide
1	S	419	HIS	Peptide
1	S	43	ARG	Peptide
1	S	779	ASN	Peptide
1	S	780	ASP	Peptide
1	T	110	HIS	Peptide
1	T	1261	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	T	1314	PRO	Peptide
1	T	133	PHE	Peptide
1	T	1357	HIS	Peptide
1	T	419	HIS	Peptide
1	T	800	HIS	Peptide
1	T	913	ALA	Peptide
1	W	110	HIS	Peptide
1	W	1177	MET	Peptide
1	W	1357	HIS	Peptide
1	W	419	HIS	Peptide
1	W	420	ALA	Mainchain
1	W	43	ARG	Peptide
1	W	635	HIS	Peptide
1	W	773	THR	Peptide
1	X	1357	HIS	Peptide
1	X	419	HIS	Peptide
1	X	420	ALA	Mainchain
1	X	773	THR	Peptide
1	X	800	HIS	Peptide

5.2 Too-close contacts (i)

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	S	10151	0	9955	137	0
1	T	10470	0	10279	131	0
1	W	10451	0	10263	109	0
1	X	10027	0	9841	121	0
2	E	774	0	754	11	0
2	F	774	0	754	7	0
2	L	774	0	754	9	0
2	P	774	0	754	9	0
3	5	2963	0	2918	33	0
3	D	2786	0	2737	36	0
4	6	2216	0	2291	31	0
4	7	2355	0	2431	33	0
4	A	2355	0	2431	33	0
4	H	2216	0	2291	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	4305	0	4293	58	0
6	G	749	0	728	9	0
6	K	644	0	635	13	0
7	B	388	0	413	7	0
7	O	388	0	413	5	0
All	All	65560	0	64935	716	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 5.

All (716) 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:X:826:CYS:HG	1:X:969:HIS:HE2	1.31	0.78
1:T:708:THR:HG22	1:T:723:ASN:HD22	1.49	0.76
5:C:603:ASN:HD22	5:C:635:ARG:HH22	1.32	0.75
1:W:1206:ARG:NH1	1:W:1226:MET:SD	2.64	0.70
6:G:72:GLN:HG3	7:O:3127:VAL:HG22	1.73	0.69
1:T:299:GLU:HB3	1:T:362:ARG:HD2	1.76	0.67
1:X:97:PHE:HB2	1:X:120:MET:HB2	1.76	0.67
1:W:708:THR:HG22	1:W:723:ASN:HD22	1.56	0.67
1:X:634:ILE:HG22	1:X:636:GLY:H	1.60	0.66
1:X:626:VAL:HG22	1:X:878:MET:HG3	1.78	0.66
1:S:1206:ARG:NH1	1:S:1226:MET:SD	2.66	0.66
5:C:650:CYS:HB2	5:C:662:VAL:HB	1.77	0.66
4:A:298:CYS:HB2	4:A:315:ILE:HD13	1.77	0.66
1:T:97:PHE:HB2	1:T:120:MET:HB2	1.77	0.66
1:S:626:VAL:HG22	1:S:878:MET:HG3	1.76	0.66
5:C:467:LEU:HD11	5:C:690:ARG:HH22	1.60	0.65
1:W:736:VAL:HG12	1:W:738:ASP:H	1.62	0.65
5:C:506:GLN:HE22	6:K:21:ALA:HB1	1.60	0.65
1:S:622:ASN:ND2	1:X:675:VAL:O	2.31	0.64
2:L:84:PRO:HA	2:P:34:PHE:HB3	1.79	0.64
1:T:634:ILE:HG22	1:T:636:GLY:H	1.63	0.64
1:S:708:THR:HG22	1:S:723:ASN:HD22	1.61	0.64
1:X:1148:ARG:HH22	1:X:1162:PRO:HA	1.63	0.64
3:5:410:ARG:HH22	4:6:228:PHE:HA	1.63	0.63
4:H:210:VAL:HG11	4:A:223:LEU:HD22	1.80	0.63
1:T:1063:VAL:HB	1:T:1111:ALA:HB3	1.81	0.63
1:W:1063:VAL:HB	1:W:1111:ALA:HB3	1.79	0.63
1:S:1160:ALA:HB2	1:S:1172:PRO:HG3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:666:ASN:HD21	1:T:937:ILE:HG23	1.64	0.62
1:T:262:PRO:HG3	1:T:353:GLU:HG2	1.82	0.62
5:C:510:TYR:OH	5:C:642:PRO:O	2.18	0.62
6:K:90:ASN:HD21	7:B:3109:LEU:HD13	1.64	0.62
1:S:700:LEU:HD22	1:S:1025:MET:HG3	1.82	0.62
4:7:298:CYS:HB2	4:7:315:ILE:HD13	1.81	0.62
4:H:24:LEU:HA	4:H:27:CYS:HB3	1.82	0.62
1:X:1072:ALA:HB3	1:X:1100:VAL:HB	1.82	0.61
1:T:826:CYS:SG	1:T:969:HIS:NE2	2.73	0.61
1:T:1000:SER:O	1:T:1003:ARG:NH1	2.33	0.61
1:W:827:THR:HA	1:W:938:LEU:HA	1.81	0.61
1:W:666:ASN:ND2	1:W:938:LEU:O	2.34	0.61
1:T:615:ARG:HH21	1:T:1017:GLU:HG2	1.65	0.61
1:W:826:CYS:HB3	1:W:966:GLY:H	1.66	0.60
1:S:133:PHE:HB3	1:S:1091:PHE:HB2	1.83	0.60
1:W:1000:SER:O	1:W:1003:ARG:NH1	2.35	0.60
5:C:549:THR:HA	5:C:600:ARG:HH12	1.65	0.60
5:C:97:HIS:HD1	5:C:177:TYR:HH	1.46	0.60
1:T:220:VAL:HG11	1:T:1214:TYR:HE1	1.66	0.59
1:T:406:LEU:HB2	1:T:1050:PHE:HB2	1.83	0.59
4:A:243:MET:SD	4:A:248:ARG:NH1	2.74	0.59
1:X:674:VAL:HG13	1:X:678:LEU:HD12	1.84	0.59
1:W:826:CYS:SG	1:W:969:HIS:NE2	2.73	0.59
4:6:12:ILE:HD11	4:6:83:ILE:HG13	1.83	0.59
1:X:1000:SER:O	1:X:1003:ARG:NH1	2.36	0.59
1:T:777:ASN:ND2	2:F:47:GLN:OE1	2.34	0.59
1:T:626:VAL:HG22	1:T:878:MET:HG3	1.85	0.59
1:S:924:THR:O	1:S:927:ARG:NH1	2.35	0.58
1:X:1156:ARG:HE	1:X:1174:ARG:HH12	1.51	0.58
4:H:12:ILE:HD11	4:H:83:ILE:HG13	1.85	0.58
3:5:404:GLN:NE2	4:7:257:GLU:OE2	2.35	0.58
1:T:99:VAL:HB	1:T:118:ASN:HB2	1.84	0.58
1:T:700:LEU:HD22	1:T:1025:MET:HG3	1.86	0.58
4:A:68:ARG:NH1	4:A:288:THR:O	2.36	0.58
4:6:283:GLY:O	4:7:149:ARG:NH1	2.36	0.58
1:T:913:ALA:HB2	1:T:927:ARG:HD3	1.86	0.58
4:7:68:ARG:NH1	4:7:288:THR:O	2.37	0.58
4:H:283:GLY:O	4:A:149:ARG:NH1	2.37	0.58
1:T:225:ARG:NH2	1:S:446:ASP:OD1	2.36	0.57
1:W:1365:ASP:O	1:W:1370:LYS:NZ	2.36	0.57
1:S:272:ARG:HE	1:S:374:LEU:HG	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:232:ALA:O	5:C:412:ARG:NH1	2.36	0.57
4:H:109:CYS:SG	4:H:182:ASN:ND2	2.73	0.57
1:T:213:ARG:HH12	1:T:1216:GLY:HA3	1.70	0.57
1:X:736:VAL:HG12	1:X:738:ASP:H	1.69	0.57
4:7:100:LEU:HD13	4:7:314:VAL:HG21	1.86	0.57
6:G:58:GLN:OE1	6:K:59:ARG:NH1	2.37	0.57
6:G:84:LEU:HA	6:G:87:ILE:HD12	1.86	0.57
1:S:69:ARG:HB2	1:S:72:GLU:HG2	1.85	0.57
1:T:1085:THR:OG1	1:T:1090:ASN:ND2	2.37	0.57
1:S:451:ARG:HE	1:S:453:SER:HG	1.51	0.57
3:5:111:ARG:HG2	3:5:263:THR:HG22	1.86	0.57
1:X:1270:LEU:HD23	1:X:1312:LYS:HD3	1.86	0.57
1:W:133:PHE:HE1	1:W:168:ASN:HB3	1.70	0.57
1:W:445:LYS:HE3	1:W:1118:PRO:HG2	1.87	0.57
1:W:626:VAL:HG22	1:W:878:MET:HG3	1.86	0.57
1:W:1178:ASP:HB2	1:X:1234:PRO:HB2	1.85	0.57
1:T:268:ASP:HB2	1:T:271:GLY:HA3	1.87	0.56
1:X:1051:THR:HG23	1:X:1190:THR:HG21	1.87	0.56
4:H:226:ARG:HA	4:H:229:ALA:HB3	1.86	0.56
1:T:133:PHE:HB3	1:T:1091:PHE:HB2	1.87	0.56
3:5:369:ASN:ND2	4:6:228:PHE:O	2.33	0.56
1:S:251:LEU:HD21	1:S:1111:ALA:HB2	1.88	0.56
1:S:655:TYR:HA	1:S:658:ASN:HB2	1.87	0.56
1:X:519:ARG:NH1	1:X:538:ASN:OD1	2.38	0.56
1:X:822:ARG:HD3	1:X:1010:VAL:HG12	1.87	0.56
5:C:238:LEU:HD21	5:C:385:VAL:HG12	1.87	0.56
6:K:24:ARG:NH1	4:H:234:ASP:OD1	2.38	0.56
1:T:719:GLN:HA	1:T:722:LEU:HD13	1.87	0.56
1:S:577:VAL:H	1:S:581:ASN:HD22	1.53	0.56
1:S:231:SER:O	1:S:1112:THR:OG1	2.23	0.56
1:S:1270:LEU:HD12	1:S:1310:GLN:HB3	1.88	0.56
1:T:748:LEU:HD13	1:T:752:ARG:HH22	1.71	0.56
1:X:99:VAL:HB	1:X:118:ASN:HB2	1.86	0.56
4:6:234:ASP:OD2	5:C:412:ARG:NH2	2.38	0.56
1:S:1063:VAL:HB	1:S:1111:ALA:HB3	1.88	0.56
1:S:1191:PRO:HG2	1:S:1194:THR:HG23	1.87	0.56
3:D:130:LEU:HB3	3:D:183:LEU:HD11	1.86	0.56
1:W:830:VAL:HG21	1:W:937:ILE:HD12	1.88	0.56
1:T:1206:ARG:NH1	1:T:1226:MET:SD	2.79	0.56
4:H:276:VAL:HG11	4:A:154:ARG:HE	1.71	0.56
1:T:310:VAL:HG12	1:T:312:ASN:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:826:CYS:HG	1:W:969:HIS:HE2	1.44	0.56
1:S:544:HIS:HB3	1:S:547:PHE:HB2	1.88	0.56
1:W:69:ARG:HB2	1:W:72:GLU:HG2	1.89	0.55
1:W:711:GLY:HA3	1:W:719:GLN:HE21	1.71	0.55
1:W:1051:THR:HG23	1:W:1190:THR:HG21	1.89	0.55
1:S:262:PRO:HG2	1:S:265:THR:HG22	1.87	0.55
1:X:1365:ASP:O	1:X:1370:LYS:NZ	2.40	0.55
1:T:100:HIS:H	1:S:63:ASN:HD22	1.53	0.55
1:W:895:GLN:NE2	2:L:61:LEU:O	2.39	0.55
1:X:777:ASN:ND2	2:P:47:GLN:OE1	2.32	0.55
3:5:295:LEU:HD21	3:5:345:LEU:HD11	1.89	0.55
1:S:220:VAL:HG11	1:S:1214:TYR:HE1	1.72	0.55
1:S:534:PRO:HD3	1:S:1240:ALA:HB2	1.89	0.55
1:X:1063:VAL:HB	1:X:1111:ALA:HB3	1.88	0.55
1:T:621:ARG:NH2	1:S:698:GLU:OE2	2.38	0.55
5:C:27:ILE:HB	5:C:398:VAL:HB	1.87	0.55
1:W:272:ARG:HE	1:W:374:LEU:HG	1.71	0.55
1:W:299:GLU:HB3	1:W:362:ARG:HD2	1.88	0.55
1:X:531:PHE:O	1:X:536:ASN:ND2	2.40	0.55
5:C:486:CYS:HB3	5:C:551:TYR:HE2	1.71	0.55
3:D:408:ARG:NH2	4:A:261:LEU:O	2.40	0.55
1:W:615:ARG:HH21	1:W:1017:GLU:HG2	1.72	0.55
4:H:158:ARG:NH2	4:H:177:ASN:OD1	2.39	0.55
1:T:827:THR:HA	1:T:938:LEU:HA	1.89	0.55
1:S:1076:GLY:O	1:S:1095:GLN:NE2	2.40	0.55
1:X:1215:ALA:HB1	1:X:1221:ASP:HB3	1.88	0.55
1:S:621:ARG:NH2	1:X:698:GLU:OE2	2.40	0.55
3:D:334:PRO:HB2	3:D:336:ARG:HG2	1.88	0.55
1:W:933:LEU:HD11	1:W:958:LEU:HB2	1.89	0.54
2:E:84:PRO:HA	2:F:34:PHE:HB3	1.89	0.54
4:H:231:SER:OG	4:H:235:GLY:N	2.40	0.54
1:W:678:LEU:O	1:X:622:ASN:ND2	2.40	0.54
1:S:1031:ILE:HG23	1:S:1036:LEU:HD11	1.88	0.54
1:T:193:PRO:HG2	1:T:198:LEU:HD11	1.88	0.54
1:T:622:ASN:ND2	1:S:675:VAL:O	2.40	0.54
3:5:306:ALA:HB3	4:7:37:ILE:HD12	1.88	0.54
1:T:1256:LEU:HA	1:T:1263:LEU:HD12	1.89	0.54
1:T:1298:SER:HB2	1:T:1320:LEU:HD22	1.88	0.54
1:S:406:LEU:HB2	1:S:1050:PHE:HB2	1.88	0.54
1:S:531:PHE:O	1:S:536:ASN:ND2	2.41	0.54
2:P:89:ARG:NH1	2:E:29:THR:OG1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:766:ALA:HB3	1:X:784:LEU:HA	1.90	0.54
1:T:1270:LEU:HD12	1:T:1310:GLN:HB3	1.89	0.54
1:W:261:VAL:HG12	1:W:263:ARG:H	1.73	0.54
1:X:728:ASP:O	1:X:810:LYS:NZ	2.40	0.54
1:W:406:LEU:HB2	1:W:1050:PHE:HB2	1.90	0.54
5:C:152:GLU:OE2	5:C:390:HIS:ND1	2.39	0.54
1:W:133:PHE:HD2	1:W:1091:PHE:HB2	1.72	0.53
1:S:1081:ALA:HB1	4:6:39:ARG:HH12	1.71	0.53
1:T:1173:ARG:NH1	1:T:1174:ARG:O	2.42	0.53
3:5:334:PRO:HG3	4:7:71:PHE:HE1	1.74	0.53
3:D:404:GLN:NE2	4:A:257:GLU:OE2	2.40	0.53
1:W:839:LEU:HD23	1:W:875:VAL:HG21	1.90	0.53
6:G:84:LEU:HB2	7:B:3117:ARG:HE	1.74	0.53
1:W:675:VAL:O	1:X:622:ASN:ND2	2.41	0.53
1:S:728:ASP:O	1:S:810:LYS:NZ	2.42	0.53
4:6:276:VAL:HG11	4:7:154:ARG:HE	1.73	0.53
1:T:895:GLN:NE2	2:F:61:LEU:O	2.41	0.53
1:S:1051:THR:HG23	1:S:1190:THR:HG21	1.88	0.53
1:X:1031:ILE:HG23	1:X:1036:LEU:HD11	1.91	0.53
5:C:199:GLY:HA3	5:C:357:LEU:HD11	1.91	0.53
5:C:157:ASN:ND2	5:C:245:THR:OG1	2.41	0.53
4:H:129:ARG:HG3	4:H:136:THR:HG22	1.91	0.53
1:X:625:ALA:HA	1:X:628:TYR:HD2	1.74	0.53
1:T:275:ASP:OD1	1:T:1068:ARG:NH2	2.40	0.53
1:S:279:VAL:HB	1:S:1064:LEU:HB2	1.90	0.53
1:S:1072:ALA:HB3	1:S:1100:VAL:HB	1.90	0.53
1:X:196:ALA:HB1	1:X:227:PHE:HA	1.91	0.53
1:X:494:PRO:HD3	1:X:909:LEU:HD12	1.91	0.53
1:T:624:PRO:HB3	1:T:882:GLY:HA3	1.91	0.53
1:S:736:VAL:HG12	1:S:738:ASP:H	1.74	0.53
5:C:384:SER:HG	5:C:401:SER:HG	1.57	0.53
1:T:327:ARG:HB2	1:S:58:LEU:HA	1.91	0.52
1:T:1270:LEU:HD11	1:T:1303:ALA:HB2	1.90	0.52
1:W:193:PRO:HG2	1:W:198:LEU:HD11	1.91	0.52
4:6:210:VAL:HG11	4:7:223:LEU:HD22	1.89	0.52
1:W:924:THR:O	1:W:927:ARG:NH1	2.39	0.52
1:S:1152:VAL:O	1:S:1155:ASN:N	2.42	0.52
4:7:120:VAL:HG12	4:7:188:LEU:HB2	1.91	0.52
5:C:438:PRO:O	5:C:446:GLN:NE2	2.42	0.52
4:A:100:LEU:HD13	4:A:314:VAL:HG21	1.91	0.52
1:T:404:LEU:HD21	1:T:1334:LEU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1031:ILE:HG23	1:T:1036:LEU:HD11	1.91	0.52
1:S:1165:VAL:HA	4:7:239:ALA:HB1	1.90	0.52
4:6:89:ASP:OD2	4:7:296:ARG:NH2	2.43	0.52
1:T:1365:ASP:O	1:T:1370:LYS:NZ	2.42	0.52
1:T:196:ALA:HB1	1:T:227:PHE:HA	1.91	0.52
1:S:1000:SER:O	1:S:1003:ARG:NH1	2.43	0.52
1:X:843:VAL:HB	1:X:876:ASN:HD22	1.75	0.52
1:W:1176:GLY:HA3	1:X:1234:PRO:HB3	1.91	0.52
1:T:46:ALA:HB3	1:T:49:LEU:HG	1.91	0.52
1:S:97:PHE:HB2	1:S:120:MET:HB3	1.92	0.52
1:W:1296:THR:HG21	1:W:1327:LEU:HG	1.91	0.52
1:S:219:LEU:O	1:S:223:LEU:N	2.43	0.52
1:S:451:ARG:NE	1:S:453:SER:OG	2.39	0.51
1:T:1054:ARG:NH2	1:T:1056:ASP:OD1	2.43	0.51
1:S:895:GLN:NE2	2:E:61:LEU:O	2.43	0.51
1:X:1270:LEU:HD12	1:X:1310:GLN:HB3	1.91	0.51
6:G:80:ILE:HD13	7:B:3120:LEU:HD21	1.92	0.51
1:T:945:LEU:HD12	1:S:676:THR:HG21	1.91	0.51
4:6:158:ARG:NH2	4:6:177:ASN:OD1	2.44	0.51
4:7:306:VAL:HG11	4:7:312:ALA:HB2	1.93	0.51
1:X:251:LEU:HD21	1:X:1111:ALA:HB2	1.91	0.51
1:X:944:HIS:CE1	1:X:972:ASN:HD22	2.27	0.51
5:C:133:ARG:NH2	5:C:574:ASP:OD1	2.43	0.51
5:C:506:GLN:HA	5:C:667:PHE:HA	1.92	0.51
6:K:84:LEU:O	6:K:88:GLU:N	2.34	0.51
1:T:494:PRO:HD3	1:T:909:LEU:HD12	1.93	0.51
1:S:745:ARG:HH12	1:S:910:CYS:HB2	1.74	0.51
3:D:245:ARG:NH1	4:H:112:ASP:OD1	2.44	0.51
6:K:66:LEU:O	6:K:70:ALA:N	2.44	0.51
3:D:410:ARG:HH22	4:H:228:PHE:HA	1.76	0.51
4:A:129:ARG:HG2	4:A:136:THR:HG22	1.92	0.51
3:5:413:ALA:HA	3:5:416:CYS:HB2	1.91	0.51
3:D:407:LEU:HG	3:D:410:ARG:HG3	1.93	0.51
1:T:397:ALA:HB3	1:T:1321:VAL:HG22	1.91	0.51
5:C:238:LEU:HD22	5:C:387:LEU:HG	1.93	0.51
4:A:61:LEU:HD12	4:A:155:LEU:HB3	1.93	0.51
4:A:120:VAL:HG12	4:A:188:LEU:HB2	1.93	0.51
1:T:620:ASP:OD2	1:T:655:TYR:OH	2.29	0.51
1:X:1207:GLY:HA3	1:X:1243:ASN:H	1.76	0.51
1:W:80:VAL:HB	1:W:1072:ALA:HA	1.92	0.51
1:W:414:GLU:HG2	1:W:1356:THR:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:691:ARG:NH1	1:X:620:ASP:OD1	2.44	0.50
1:W:839:LEU:HA	1:W:875:VAL:HG21	1.92	0.50
1:W:968:ASP:O	1:W:972:ASN:ND2	2.44	0.50
1:T:1051:THR:HG23	1:T:1190:THR:HG21	1.93	0.50
4:A:121:PHE:HE1	4:A:186:LEU:HD13	1.76	0.50
1:S:1365:ASP:O	1:S:1370:LYS:NZ	2.45	0.50
1:X:1152:VAL:O	1:X:1155:ASN:N	2.45	0.50
4:6:33:PHE:HB3	4:6:70:ARG:HB3	1.93	0.50
4:7:180:TYR:OH	4:7:185:ARG:NH1	2.44	0.50
1:S:445:LYS:HD3	1:S:1179:HIS:HB3	1.92	0.50
1:S:1254:ASP:HB3	1:S:1258:ASN:HD21	1.75	0.50
1:W:404:LEU:HB2	1:W:1052:VAL:HB	1.93	0.50
1:S:264:LEU:HD11	1:S:356:SER:HB2	1.93	0.50
3:5:350:ARG:NE	4:6:244:GLN:HE21	2.09	0.50
3:D:130:LEU:HD13	3:D:183:LEU:HD21	1.93	0.50
1:S:95:VAL:HG22	1:X:58:LEU:HB2	1.94	0.50
1:S:204:TYR:HB2	1:S:219:LEU:HD21	1.94	0.50
1:S:1195:ASP:N	1:S:1195:ASP:OD1	2.45	0.50
1:S:1207:GLY:HA3	1:S:1243:ASN:H	1.76	0.50
3:D:317:GLN:NE2	3:D:417:THR:OG1	2.45	0.50
4:H:156:VAL:HG11	4:H:209:MET:HG3	1.93	0.50
1:T:726:MET:HE1	1:T:814:TYR:HB2	1.94	0.50
6:K:84:LEU:HD22	7:O:3114:GLN:HG2	1.93	0.50
1:T:1195:ASP:OD1	1:T:1195:ASP:N	2.45	0.50
1:T:1257:TYR:HB2	1:T:1277:PHE:HD2	1.77	0.50
1:W:1031:ILE:HG23	1:W:1036:LEU:HD11	1.94	0.50
1:X:745:ARG:HH22	1:X:911:SER:C	2.16	0.49
1:X:829:GLY:N	1:X:956:TYR:O	2.43	0.49
5:C:600:ARG:HG2	5:C:602:ASN:H	1.76	0.49
3:D:245:ARG:HH22	4:H:146:PRO:HG3	1.76	0.49
1:W:451:ARG:NH1	1:X:529:GLU:OE2	2.45	0.49
1:W:1054:ARG:NH2	1:W:1056:ASP:OD1	2.44	0.49
1:S:445:LYS:HE3	1:S:1118:PRO:HG2	1.93	0.49
1:X:406:LEU:HB2	1:X:1050:PHE:HB2	1.94	0.49
4:7:92:LEU:HD13	4:7:98:VAL:HG23	1.94	0.49
1:W:63:ASN:HD22	1:X:100:HIS:H	1.60	0.49
1:X:487:TYR:OH	1:X:990:VAL:N	2.41	0.49
1:X:793:ASP:OD1	1:X:798:ARG:NH2	2.40	0.49
4:7:61:LEU:HD12	4:7:155:LEU:HB3	1.93	0.49
6:K:66:LEU:HB2	7:O:3135:ARG:HH11	1.77	0.49
1:T:231:SER:O	1:T:1112:THR:OG1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:1215:ALA:HB1	1:W:1221:ASP:HB3	1.94	0.49
1:S:279:VAL:HG12	1:S:394:LEU:HD22	1.93	0.49
1:X:1296:THR:HG21	1:X:1327:LEU:HG	1.93	0.49
1:X:1258:ASN:HB2	1:X:1261:TYR:HD2	1.78	0.49
1:T:336:LEU:HD22	1:S:156:HIS:HE1	1.78	0.49
1:S:177:GLU:O	1:S:180:THR:OG1	2.28	0.49
1:T:603:ARG:NH1	1:T:706:ASP:OD2	2.46	0.49
1:S:620:ASP:OD1	1:X:691:ARG:NH1	2.46	0.49
1:X:1083:HIS:HB2	1:X:1090:ASN:HB2	1.94	0.49
5:C:390:HIS:HD2	5:C:393:THR:H	1.61	0.49
4:A:152:VAL:HG21	4:A:290:ALA:HB2	1.95	0.49
1:T:644:LEU:HD22	1:T:647:LEU:HD12	1.94	0.49
3:5:129:LEU:HB2	3:5:186:PHE:HB2	1.95	0.49
1:S:1307:SER:HB2	1:S:1311:PHE:HD2	1.78	0.49
3:D:270:GLN:OE1	3:D:456:TRP:NE1	2.44	0.49
1:T:595:ARG:HH21	1:T:1045:HIS:HD2	1.60	0.48
3:D:350:ARG:HE	4:H:244:GLN:HE21	1.61	0.48
1:T:1207:GLY:HA3	1:T:1243:ASN:H	1.77	0.48
1:S:644:LEU:HD22	1:S:647:LEU:HD12	1.95	0.48
4:H:129:ARG:NH1	4:H:131:ASP:OD1	2.46	0.48
1:S:652:ILE:O	1:S:656:TRP:N	2.43	0.48
4:7:152:VAL:HG21	4:7:290:ALA:HB2	1.95	0.48
1:T:445:LYS:HE3	1:T:1118:PRO:HG2	1.95	0.48
1:W:728:ASP:O	1:W:810:LYS:NZ	2.46	0.48
3:5:359:GLU:HA	3:5:360:ASP:HA	1.64	0.48
5:C:391:TYR:HE1	7:B:3137:LEU:HD21	1.78	0.48
1:S:193:PRO:HG2	1:S:198:LEU:HD11	1.95	0.48
1:X:881:ASN:O	2:L:95:ARG:NH1	2.46	0.48
3:D:442:GLY:HA2	3:D:443:ALA:HA	1.59	0.48
1:W:159:LEU:HD11	1:X:340:GLN:HA	1.96	0.48
1:S:732:LEU:HD22	1:S:741:ALA:HB1	1.96	0.48
5:C:406:VAL:HA	5:C:413:ALA:HB3	1.95	0.48
1:W:1191:PRO:HG2	1:W:1194:THR:HG23	1.94	0.48
1:W:1270:LEU:HD12	1:W:1310:GLN:HB3	1.96	0.48
1:S:1054:ARG:HH12	1:S:1122:MET:HG2	1.79	0.48
3:5:373:PRO:HB2	3:5:377:LEU:HG	1.96	0.48
4:6:306:VAL:HG11	4:6:312:ALA:HB2	1.95	0.48
1:S:883:ARG:HG3	1:X:680:GLY:H	1.79	0.48
1:X:771:VAL:HG13	2:P:55:ARG:HG2	1.94	0.48
5:C:517:ARG:O	5:C:521:GLY:N	2.43	0.48
1:X:684:GLU:HA	1:X:687:MET:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:104:ALA:HB3	5:C:234:PRO:HD2	1.95	0.48
5:C:384:SER:OG	5:C:401:SER:OG	2.31	0.48
1:S:83:LYS:HG2	1:S:1075:LEU:HD11	1.95	0.47
1:X:719:GLN:HA	1:X:722:LEU:HD13	1.96	0.47
2:P:89:ARG:NH2	2:E:30:ASN:OD1	2.46	0.47
4:7:144:PRO:HD2	4:7:147:LEU:HD12	1.96	0.47
3:D:304:PRO:HB2	4:A:38:ARG:HG2	1.96	0.47
3:D:316:ARG:NH2	3:D:321:GLN:O	2.47	0.47
1:T:822:ARG:HD3	1:T:1010:VAL:HG12	1.94	0.47
1:W:272:ARG:NH1	1:W:372:GLU:O	2.47	0.47
1:S:554:ALA:HB2	1:S:569:GLY:H	1.79	0.47
1:S:752:ARG:NH1	1:S:915:ASP:OD1	2.47	0.47
1:S:1029:PHE:HB3	1:S:1039:GLN:HE22	1.78	0.47
1:X:974:PRO:HA	1:X:975:ASN:HA	1.58	0.47
1:X:1256:LEU:HA	1:X:1263:LEU:HD12	1.95	0.47
3:5:245:ARG:NH1	4:6:112:ASP:OD1	2.47	0.47
3:5:269:PRO:HA	3:5:455:VAL:HA	1.94	0.47
3:D:306:ALA:HB3	4:A:37:ILE:HD12	1.96	0.47
4:A:116:LEU:HG	4:A:291:LEU:HD11	1.95	0.47
1:W:963:LEU:HD23	1:W:1007:VAL:HG22	1.97	0.47
1:S:102:PRO:HB2	1:X:178:ARG:HH12	1.79	0.47
1:X:631:GLN:HE22	1:X:666:ASN:HD22	1.61	0.47
5:C:84:ASP:N	5:C:84:ASP:OD1	2.47	0.47
4:A:180:TYR:OH	4:A:185:ARG:NH1	2.47	0.47
1:W:97:PHE:HB2	1:W:120:MET:HB2	1.97	0.47
1:X:521:VAL:HG21	1:X:987:VAL:HG12	1.96	0.47
4:6:72:PRO:HB2	4:6:88:LEU:HD12	1.97	0.47
5:C:102:PRO:HB2	5:C:231:PRO:HB3	1.96	0.47
1:T:771:VAL:HG12	2:F:55:ARG:HG2	1.96	0.47
1:T:1083:HIS:CE1	3:D:109:LEU:H	2.33	0.47
1:T:1313:ARG:HG3	1:T:1315:PRO:HA	1.97	0.47
1:X:177:GLU:O	1:X:180:THR:OG1	2.29	0.47
3:5:110:THR:HG22	4:6:298:CYS:HB3	1.97	0.47
4:7:1:MET:HB2	4:7:91:GLY:HA3	1.96	0.47
4:H:306:VAL:HG11	4:H:312:ALA:HB2	1.95	0.47
1:T:1209:ALA:HB3	1:T:1234:PRO:HG2	1.97	0.47
1:S:827:THR:OG1	1:S:958:LEU:O	2.32	0.47
1:S:1231:GLN:NE2	1:X:1173:ARG:O	2.48	0.47
5:C:584:ASP:HA	5:C:654:ASN:HD21	1.79	0.47
6:K:84:LEU:HB3	6:K:88:GLU:HG3	1.97	0.47
4:H:148:ALA:HB1	4:H:291:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:352:ASP:OD1	1:S:352:ASP:N	2.46	0.47
1:X:826:CYS:SG	1:X:969:HIS:NE2	2.69	0.47
3:D:366:PRO:HA	3:D:367:ASN:HA	1.54	0.47
1:S:91:ASN:HD22	1:X:53:GLU:HG3	1.79	0.47
3:D:295:LEU:HD21	3:D:345:LEU:HD11	1.97	0.47
4:H:230:LEU:HA	4:H:231:SER:HA	1.53	0.47
4:A:268:ARG:NH2	4:A:273:GLU:OE1	2.46	0.47
1:W:1195:ASP:OD1	1:W:1195:ASP:N	2.48	0.47
1:S:715:GLY:HA2	1:S:716:GLY:HA2	1.57	0.47
1:X:103:LEU:HD13	1:X:115:PRO:HA	1.97	0.47
1:X:834:ARG:HD3	2:L:90:PRO:HB3	1.97	0.47
4:H:89:ASP:OD2	4:A:296:ARG:NH2	2.47	0.47
1:T:1195:ASP:OD2	1:T:1236:ARG:NH2	2.45	0.46
1:W:236:LYS:HZ2	1:W:1371:GLY:H	1.63	0.46
1:W:1333:PRO:HG2	1:W:1366:ALA:H	1.79	0.46
5:C:549:THR:HB	5:C:600:ARG:HH22	1.79	0.46
1:W:392:TYR:CE2	1:W:394:LEU:HB3	2.50	0.46
1:S:392:TYR:HD2	1:S:395:VAL:HG23	1.80	0.46
1:X:231:SER:O	1:X:1112:THR:OG1	2.33	0.46
3:5:350:ARG:HE	4:6:244:GLN:HE21	1.63	0.46
5:C:402:TYR:HB2	5:C:405:SER:HB3	1.96	0.46
3:D:350:ARG:NE	4:H:244:GLN:HE21	2.13	0.46
1:T:505:PHE:CE1	1:T:992:PRO:HD2	2.51	0.46
1:W:719:GLN:HA	1:W:722:LEU:HD13	1.96	0.46
1:W:1197:ASN:OD1	1:W:1200:ARG:NH1	2.48	0.46
1:X:392:TYR:CE2	1:X:394:LEU:HB3	2.51	0.46
1:X:404:LEU:HD21	1:X:1334:LEU:HB2	1.96	0.46
1:S:617:ALA:HB2	1:S:661:CYS:HB3	1.97	0.46
4:6:8:THR:HG23	4:6:87:PRO:HD3	1.98	0.46
4:6:16:ILE:HG13	4:6:133:LEU:HD11	1.97	0.46
4:7:230:LEU:HG	4:7:237:VAL:HG21	1.96	0.46
4:H:8:THR:HG23	4:H:87:PRO:HD3	1.97	0.46
4:A:254:ILE:HG22	4:A:256:PRO:HD3	1.98	0.46
1:W:521:VAL:HG11	1:W:987:VAL:HG12	1.98	0.46
4:H:68:ARG:HH22	4:H:292:ALA:H	1.64	0.46
4:A:1:MET:HG3	4:A:91:GLY:HA3	1.97	0.46
1:X:440:LEU:N	1:X:452:LEU:O	2.48	0.46
3:5:180:ARG:HE	3:5:182:GLY:HA3	1.81	0.46
3:5:334:PRO:HB2	3:5:336:ARG:HG2	1.98	0.46
4:7:48:HIS:HA	4:7:51:PHE:HB3	1.96	0.46
5:C:589:PHE:HD1	5:C:652:GLY:HA3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:135:HIS:O	3:D:137:ALA:N	2.49	0.46
1:W:346:LEU:HA	1:W:347:ASN:HA	1.69	0.46
1:X:715:GLY:HA2	1:X:716:GLY:HA2	1.62	0.46
1:T:834:ARG:HA	1:T:837:ALA:HB3	1.97	0.46
1:W:527:THR:HG22	1:W:529:GLU:H	1.80	0.46
1:W:713:GLU:HG2	1:W:718:ALA:HB2	1.98	0.46
1:W:726:MET:HE2	1:W:814:TYR:HB2	1.97	0.46
1:S:196:ALA:HB1	1:S:227:PHE:HA	1.98	0.46
1:X:827:THR:OG1	1:X:958:LEU:O	2.32	0.46
3:5:146:ARG:NH1	3:5:242:GLU:OE1	2.48	0.46
4:6:60:THR:HG23	4:6:201:GLU:HG3	1.96	0.46
3:D:411:PRO:HG3	4:H:237:VAL:HG22	1.97	0.46
1:W:777:ASN:ND2	2:L:47:GLN:OE1	2.45	0.46
1:S:1298:SER:HB2	1:S:1320:LEU:HD22	1.98	0.46
1:X:966:GLY:O	1:X:970:VAL:N	2.49	0.46
4:7:241:LEU:HB2	4:7:248:ARG:HH21	1.81	0.46
5:C:466:VAL:HG23	5:C:467:LEU:HG	1.97	0.46
1:T:177:GLU:O	1:T:180:THR:OG1	2.30	0.45
1:T:1208:ARG:NE	1:T:1233:ASP:OD1	2.39	0.45
1:W:73:LEU:HD11	1:W:384:ILE:HD11	1.98	0.45
1:W:644:LEU:HD22	1:W:647:LEU:HD12	1.97	0.45
1:S:77:VAL:HG22	1:S:266:HIS:CG	2.51	0.45
1:S:829:GLY:N	1:S:956:TYR:O	2.48	0.45
1:S:857:PRO:HA	1:S:863:HIS:CD2	2.52	0.45
1:X:856:ASP:N	1:X:860:ASP:OD2	2.48	0.45
3:5:316:ARG:HE	3:5:323:LEU:HG	1.81	0.45
5:C:436:VAL:HB	7:B:3135:ARG:HE	1.80	0.45
1:T:620:ASP:HB3	1:T:623:TYR:HB2	1.98	0.45
1:T:1207:GLY:HA2	1:T:1242:ALA:HB3	1.98	0.45
1:X:615:ARG:HH21	1:X:1017:GLU:HG2	1.80	0.45
5:C:553:LEU:HD22	5:C:572:LEU:HD13	1.98	0.45
1:W:704:VAL:HG11	1:W:727:ARG:HE	1.81	0.45
1:X:77:VAL:HG22	1:X:266:HIS:CG	2.51	0.45
1:X:172:VAL:HG11	1:X:1093:LEU:HD12	1.98	0.45
3:5:442:GLY:HA2	3:5:443:ALA:HA	1.56	0.45
3:D:334:PRO:HG3	4:A:71:PHE:HE1	1.81	0.45
1:T:715:GLY:HA2	1:T:716:GLY:HA2	1.62	0.45
1:T:1082:ARG:HG3	1:T:1091:PHE:HE1	1.82	0.45
1:W:284:ILE:HD11	1:W:1061:GLU:HB3	1.98	0.45
3:5:116:THR:O	3:5:120:GLN:NE2	2.50	0.45
3:5:369:ASN:OD1	3:5:369:ASN:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:187:PRO:O	5:C:191:GLU:N	2.45	0.45
4:A:174:PRO:HA	4:A:175:ASP:HA	1.69	0.45
1:T:192:ALA:HB3	1:T:1110:VAL:HG23	1.98	0.45
1:X:1020:LEU:HA	1:X:1023:ALA:HB3	1.98	0.45
4:7:174:PRO:HA	4:7:175:ASP:HA	1.66	0.45
5:C:116:VAL:HA	5:C:150:TYR:HE1	1.81	0.45
5:C:562:ARG:NH2	5:C:679:LEU:O	2.49	0.45
1:T:103:LEU:HD11	1:T:115:PRO:HA	1.99	0.45
1:T:1034:VAL:HA	1:T:1147:LEU:HD21	1.98	0.45
1:T:1297:GLY:HA2	1:T:1322:GLU:HG2	1.98	0.45
3:5:348:ARG:HG2	5:C:371:GLY:HA3	1.98	0.45
5:C:589:PHE:CD1	5:C:652:GLY:HA3	2.52	0.45
1:W:595:ARG:HH22	1:W:1047:GLY:HA2	1.82	0.45
1:S:1206:ARG:HE	1:S:1247:SER:HA	1.82	0.45
1:X:406:LEU:HD23	1:X:440:LEU:HG	1.99	0.45
5:C:659:GLY:O	5:C:671:ILE:N	2.48	0.45
3:D:266:CYS:SG	4:H:296:ARG:NH1	2.79	0.45
1:T:452:LEU:HD21	1:T:1052:VAL:HG21	1.99	0.45
1:T:1296:THR:HG21	1:T:1327:LEU:HG	1.98	0.45
1:X:442:PHE:HB2	1:X:450:LEU:HB2	1.98	0.45
4:6:295:VAL:HG13	4:6:314:VAL:HG13	1.98	0.45
1:S:950:GLN:HE21	2:P:81:GLY:HA2	1.82	0.45
3:5:190:VAL:HG13	3:5:197:TYR:HE2	1.82	0.45
7:B:3101:VAL:O	7:B:3105:ALA:N	2.50	0.45
1:T:829:GLY:N	1:T:956:TYR:O	2.45	0.45
1:X:518:VAL:HG21	1:X:987:VAL:HG11	1.98	0.45
1:X:648:VAL:HG13	1:X:664:PHE:HE2	1.81	0.45
7:O:3101:VAL:O	7:O:3105:ALA:N	2.50	0.45
1:T:288:LEU:HB3	1:T:293:LEU:HD12	1.99	0.44
1:T:1206:ARG:HH22	1:T:1226:MET:HB3	1.82	0.44
1:S:658:ASN:O	1:S:660:ARG:N	2.49	0.44
1:X:193:PRO:HG2	1:X:198:LEU:HD11	1.99	0.44
5:C:365:TRP:CD1	5:C:380:ARG:HD3	2.52	0.44
4:A:92:LEU:HD13	4:A:98:VAL:HG23	1.98	0.44
1:T:141:ALA:HB1	1:T:146:GLU:HB2	1.99	0.44
1:S:82:THR:HG21	1:S:354:LEU:HD13	1.98	0.44
1:X:491:VAL:HG21	1:X:929:PHE:HD2	1.81	0.44
1:S:777:ASN:ND2	2:E:47:GLN:OE1	2.39	0.44
4:H:295:VAL:HG13	4:H:314:VAL:HG13	1.99	0.44
1:W:487:TYR:HH	1:W:990:VAL:H	1.62	0.44
1:T:491:VAL:HA	1:T:992:PRO:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:713:GLU:HA	1:W:718:ALA:HA	1.98	0.44
1:W:1152:VAL:O	1:W:1155:ASN:N	2.45	0.44
1:S:559:PRO:HA	1:S:560:GLY:HA3	1.74	0.44
1:S:748:LEU:HD13	1:S:752:ARG:HH22	1.83	0.44
1:X:1304:THR:O	1:X:1307:SER:OG	2.35	0.44
4:6:212:SER:O	4:6:278:TRP:NE1	2.45	0.44
3:D:359:GLU:HA	3:D:360:ASP:HA	1.70	0.44
1:T:625:ALA:HA	1:T:628:TYR:HD2	1.83	0.44
5:C:61:GLN:HB3	5:C:73:TRP:CD1	2.53	0.44
1:T:1268:PRO:O	1:T:1312:LYS:N	2.48	0.44
2:L:21:GLY:O	2:L:25:LEU:N	2.51	0.44
4:H:28:GLU:HB3	4:H:29:GLY:H	1.64	0.44
1:T:577:VAL:H	1:T:581:ASN:HD22	1.66	0.44
1:T:1152:VAL:O	1:T:1155:ASN:N	2.44	0.44
1:X:445:LYS:HD3	1:X:1179:HIS:HB3	1.99	0.44
1:X:503:GLN:O	1:X:507:ASN:ND2	2.51	0.44
2:P:21:GLY:O	2:P:25:LEU:N	2.51	0.44
4:7:30:ARG:HH11	4:7:139:PHE:HD2	1.65	0.44
3:D:151:ARG:NH2	3:D:357:GLY:O	2.40	0.44
1:W:491:VAL:HG22	1:W:996:ALA:H	1.83	0.43
1:W:1125:LEU:HB2	1:W:1184:VAL:HA	1.99	0.43
1:S:124:ILE:HG22	1:S:1100:VAL:HG22	1.98	0.43
2:F:22:MET:SD	2:F:22:MET:N	2.90	0.43
3:5:407:LEU:HD12	4:6:228:PHE:HE1	1.82	0.43
5:C:357:LEU:HA	5:C:360:TRP:HD1	1.83	0.43
3:D:428:PRO:HG3	4:A:2:LEU:HD21	2.00	0.43
1:T:578:VAL:H	1:T:581:ASN:ND2	2.16	0.43
1:T:881:ASN:O	2:E:95:ARG:NH1	2.52	0.43
1:S:578:VAL:H	1:S:581:ASN:ND2	2.16	0.43
1:S:631:GLN:NE2	1:S:666:ASN:OD1	2.49	0.43
1:S:1300:VAL:HG21	1:S:1318:ARG:HH21	1.83	0.43
1:X:1195:ASP:N	1:X:1195:ASP:OD1	2.49	0.43
2:L:22:MET:SD	2:L:22:MET:N	2.90	0.43
2:P:84:PRO:HA	2:E:34:PHE:HB3	1.98	0.43
4:6:61:LEU:HD11	4:6:208:ASN:HD22	1.82	0.43
4:7:260:ALA:HA	4:7:261:LEU:HA	1.74	0.43
1:T:266:HIS:HE1	1:T:302:VAL:HG13	1.84	0.43
1:T:488:GLY:HA2	1:T:996:ALA:HB1	1.99	0.43
1:W:392:TYR:HD2	1:W:395:VAL:HG23	1.84	0.43
1:W:1269:VAL:O	1:W:1312:LYS:NZ	2.49	0.43
1:X:1314:PRO:HA	1:X:1315:PRO:HD3	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:112:GLN:HG3	4:6:304:ALA:HB2	2.00	0.43
1:W:1153:ALA:HA	1:W:1154:GLY:HA2	1.65	0.43
4:H:318:PRO:O	4:A:316:ARG:NH1	2.52	0.43
1:T:1054:ARG:NH2	1:T:1122:MET:HA	2.33	0.43
1:T:1211:GLY:HA3	1:T:1212:GLY:HA2	1.83	0.43
1:W:220:VAL:HG11	1:W:1214:TYR:HE1	1.82	0.43
1:W:463:HIS:HA	1:W:464:PRO:HD3	1.91	0.43
2:F:21:GLY:O	2:F:25:LEU:N	2.51	0.43
6:K:38:SER:HB3	6:K:41:PHE:HD2	1.82	0.43
1:W:726:MET:HB3	1:W:726:MET:HE3	1.81	0.43
1:S:815:VAL:HG13	1:S:1024:LEU:HB2	1.99	0.43
4:6:51:PHE:HE1	4:6:70:ARG:HG3	1.83	0.43
5:C:30:SER:HB2	5:C:40:LEU:HD21	2.01	0.43
5:C:428:GLU:OE2	7:B:3129:THR:OG1	2.37	0.43
5:C:484:LEU:HD11	6:K:50:GLU:HB2	2.01	0.43
3:D:254:VAL:HB	3:D:261:SER:HB3	2.00	0.43
4:H:157:ALA:HA	4:H:160:ILE:HD12	1.99	0.43
1:T:1153:ALA:HA	1:T:1154:GLY:HA2	1.64	0.43
1:W:234:LEU:HD12	1:W:1113:ALA:HB1	2.00	0.43
1:W:252:THR:HB	1:W:373:LYS:HE2	2.00	0.43
1:W:727:ARG:HH12	1:X:985:ARG:HH12	1.66	0.43
1:W:866:HIS:CD2	1:W:868:ALA:H	2.36	0.43
1:S:259:VAL:HA	1:S:260:ALA:HA	1.77	0.43
1:S:764:VAL:O	1:S:783:LEU:N	2.40	0.43
1:S:1269:VAL:O	1:S:1312:LYS:NZ	2.51	0.43
1:X:185:LEU:HD11	1:X:380:LEU:HD12	2.00	0.43
1:X:822:ARG:HD2	1:X:1011:ARG:HA	2.00	0.43
4:7:108:LEU:HB2	4:7:306:VAL:HB	2.01	0.43
1:S:192:ALA:HB3	1:S:1110:VAL:HG23	2.01	0.43
1:S:1163:VAL:HG23	1:S:1169:ALA:HB2	2.01	0.43
2:E:21:GLY:O	2:E:25:LEU:N	2.51	0.43
4:7:268:ARG:NH2	4:7:273:GLU:OE1	2.50	0.43
6:G:90:ASN:HD21	7:O:3109:LEU:HB3	1.84	0.43
3:D:153:THR:OG1	3:D:154:GLU:N	2.51	0.43
1:T:346:LEU:HA	1:T:347:ASN:HA	1.60	0.43
1:T:721:GLU:HG3	1:T:727:ARG:HG2	2.00	0.43
1:S:723:ASN:HD21	1:S:1038:HIS:CG	2.37	0.43
1:X:326:VAL:HB	1:X:329:LEU:HB2	2.00	0.43
4:6:33:PHE:HE2	4:6:140:PRO:HG3	1.84	0.43
4:A:206:VAL:HA	4:A:209:MET:HB2	2.01	0.43
1:T:980:LEU:O	1:T:984:SER:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:756:VAL:HG22	1:X:910:CYS:HA	2.00	0.43
3:5:317:GLN:N	3:5:353:ASN:OD1	2.47	0.43
5:C:581:ALA:HA	5:C:655:ARG:HE	1.84	0.43
1:T:898:ALA:HA	1:T:901:MET:HE3	2.00	0.42
1:W:846:GLU:HA	2:L:68:HIS:HE1	1.84	0.42
1:S:1075:LEU:HA	1:S:1097:ARG:HG2	2.01	0.42
1:X:192:ALA:HB3	1:X:1110:VAL:HG23	2.01	0.42
4:6:54:GLY:HA3	4:6:55:GLY:HA3	1.81	0.42
5:C:3:ALA:O	5:C:7:ASN:ND2	2.52	0.42
3:D:368:ARG:HA	3:D:369:ASN:HA	1.79	0.42
4:H:54:GLY:HA3	4:H:55:GLY:HA3	1.78	0.42
1:T:188:LEU:HD23	1:T:191:LYS:HD3	2.01	0.42
1:T:534:PRO:HD3	1:T:1240:ALA:HB2	2.00	0.42
1:S:82:THR:HG22	1:S:307:GLY:HA3	2.00	0.42
1:S:653:THR:HG22	1:S:683:PRO:HD3	2.01	0.42
3:5:441:PHE:O	3:5:444:VAL:N	2.52	0.42
5:C:495:ARG:HA	6:K:36:TRP:HZ2	1.83	0.42
3:D:111:ARG:HG2	3:D:263:THR:HG22	2.00	0.42
4:H:316:ARG:HH12	4:A:316:ARG:HD3	1.84	0.42
1:T:225:ARG:HH12	1:S:447:ARG:NH2	2.18	0.42
1:S:435:PHE:CE1	1:S:598:GLU:HA	2.54	0.42
1:S:724:HIS:ND1	1:S:1028:TYR:O	2.52	0.42
1:W:784:LEU:H	1:W:784:LEU:HG	1.67	0.42
1:W:1257:TYR:HB2	1:W:1277:PHE:HD2	1.83	0.42
1:X:554:ALA:HB2	1:X:569:GLY:H	1.84	0.42
1:T:326:VAL:HB	1:T:329:LEU:HB2	2.01	0.42
1:T:450:LEU:HD13	1:T:1123:GLY:HA2	2.02	0.42
1:S:293:LEU:HD13	1:S:368:VAL:HG11	2.02	0.42
1:S:616:GLY:O	1:S:620:ASP:N	2.53	0.42
1:S:822:ARG:HD2	1:S:1011:ARG:HA	2.01	0.42
1:X:182:ASP:OD1	1:X:385:TYR:OH	2.37	0.42
1:W:677:TYR:HE1	1:X:946:ASP:HA	1.85	0.42
1:S:87:LEU:HD22	1:S:1096:PRO:HB2	2.01	0.42
2:P:22:MET:N	2:P:22:MET:SD	2.90	0.42
4:A:212:SER:HB2	4:A:278:TRP:HD1	1.84	0.42
1:T:466:LEU:O	1:T:544:HIS:NE2	2.53	0.42
1:T:599:LEU:HD13	1:T:703:LEU:HD22	2.01	0.42
1:T:736:VAL:HG12	1:T:738:ASP:H	1.84	0.42
1:S:1103:GLY:HA3	1:S:1107:THR:HG21	2.00	0.42
3:5:191:ALA:HA	3:5:194:ALA:HB2	2.02	0.42
5:C:410:GLY:O	5:C:414:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:589:PHE:CE2	5:C:642:PRO:HG3	2.55	0.42
1:T:440:LEU:N	1:T:452:LEU:O	2.53	0.42
1:T:944:HIS:HE1	1:T:969:HIS:HA	1.85	0.42
1:T:1229:HIS:CE1	1:T:1248:GLN:HG2	2.55	0.42
1:S:289:LEU:HD22	1:S:295:VAL:HG22	2.01	0.42
1:S:487:TYR:OH	1:S:990:VAL:N	2.45	0.42
1:T:959:PRO:HB2	1:T:990:VAL:HG22	2.01	0.42
1:S:404:LEU:HB2	1:S:1052:VAL:HB	2.01	0.42
4:A:48:HIS:HA	4:A:51:PHE:HB3	2.01	0.42
1:W:1211:GLY:HA3	1:W:1212:GLY:HA2	1.88	0.42
1:S:1034:VAL:HA	1:S:1147:LEU:HD21	2.02	0.42
1:X:548:ASP:OD1	1:X:576:ARG:NE	2.41	0.42
1:T:198:LEU:HD23	1:T:198:LEU:HA	1.87	0.41
1:T:223:LEU:O	1:T:227:PHE:N	2.51	0.41
1:T:1191:PRO:HG2	1:T:1194:THR:HG23	2.01	0.41
1:T:1315:PRO:HB2	3:D:173:ARG:HG3	2.00	0.41
1:X:578:VAL:H	1:X:581:ASN:ND2	2.18	0.41
1:X:960:VAL:HG22	1:X:994:LEU:HD13	2.02	0.41
5:C:646:TYR:CD1	6:G:29:PRO:HD3	2.55	0.41
1:T:1138:LEU:HD12	1:T:1140:ASP:H	1.85	0.41
1:W:727:ARG:NH1	1:X:985:ARG:HH12	2.18	0.41
1:S:219:LEU:HD23	1:S:219:LEU:HA	1.90	0.41
1:S:392:TYR:CE2	1:S:394:LEU:HB3	2.56	0.41
1:S:595:ARG:HH22	1:S:1047:GLY:HA2	1.84	0.41
1:X:559:PRO:HA	1:X:560:GLY:HA3	1.69	0.41
1:X:758:ALA:HB2	1:X:908:LEU:HD23	2.02	0.41
1:X:951:ASN:HB3	1:X:974:PRO:HD3	2.02	0.41
4:7:296:ARG:HD3	4:7:317:TYR:HD1	1.85	0.41
5:C:571:PRO:HD3	5:C:695:VAL:HG23	2.02	0.41
6:G:79:ASP:O	6:G:83:ARG:N	2.43	0.41
1:W:1347:ARG:NH1	1:X:1350:GLU:OE2	2.53	0.41
1:X:632:ALA:HB1	1:X:832:PHE:HE1	1.85	0.41
3:5:423:GLU:HB2	3:5:459:GLY:HA3	2.02	0.41
4:H:180:TYR:CE1	4:H:185:ARG:HG2	2.55	0.41
4:H:244:GLN:HA	4:A:207:LEU:HD21	2.01	0.41
1:S:625:ALA:HA	1:S:628:TYR:HD2	1.84	0.41
1:S:643:ALA:HB1	1:S:896:VAL:HG21	2.02	0.41
1:X:1307:SER:HB2	1:X:1311:PHE:HD2	1.85	0.41
2:L:94:LEU:HD23	2:L:94:LEU:HA	1.89	0.41
2:E:22:MET:SD	2:E:22:MET:N	2.90	0.41
4:7:51:PHE:HD1	4:7:70:ARG:NH1	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:863:HIS:CD2	1:T:865:LEU:H	2.39	0.41
1:T:974:PRO:HA	1:T:975:ASN:HA	1.79	0.41
1:T:1130:TYR:HE2	1:T:1151:VAL:HB	1.86	0.41
1:T:1165:VAL:HG21	3:D:154:GLU:HB3	2.01	0.41
1:W:104:ILE:H	1:W:104:ILE:HG13	1.73	0.41
1:W:310:VAL:HG12	1:W:312:ASN:H	1.84	0.41
1:S:745:ARG:NE	1:S:754:CYS:SG	2.92	0.41
5:C:28:ILE:HD11	5:C:148:PHE:HZ	1.86	0.41
5:C:415:PRO:HA	5:C:416:PRO:HA	1.76	0.41
4:H:114:ILE:N	4:H:295:VAL:O	2.51	0.41
1:T:274:VAL:HG11	1:T:376:PHE:HB2	2.02	0.41
1:W:1076:GLY:O	1:W:1095:GLN:NE2	2.51	0.41
1:X:1153:ALA:HA	1:X:1154:GLY:HA2	1.64	0.41
1:T:707:PHE:HA	1:T:1042:THR:HG21	2.02	0.41
1:W:788:GLN:HE22	1:W:794:ALA:HA	1.85	0.41
1:W:124:ILE:HG12	1:W:1100:VAL:HG22	2.02	0.41
1:W:129:LEU:HD11	1:W:1097:ARG:NH1	2.36	0.41
1:W:692:ASP:O	1:W:696:HIS:N	2.47	0.41
1:W:1055:GLN:HB2	1:W:1272:PRO:HB3	2.03	0.41
1:W:1255:LEU:HA	1:W:1261:TYR:HD2	1.84	0.41
1:S:137:THR:OG1	1:S:138:GLU:N	2.53	0.41
1:S:974:PRO:HA	1:S:975:ASN:HA	1.62	0.41
1:S:1270:LEU:HD23	1:S:1312:LYS:HD3	2.02	0.41
4:7:31:VAL:HB	4:7:140:PRO:HG2	2.02	0.41
1:W:857:PRO:HA	1:W:863:HIS:CD2	2.56	0.41
1:W:863:HIS:O	1:W:869:ASN:ND2	2.37	0.41
1:W:1252:TYR:CZ	1:W:1256:LEU:HD11	2.56	0.41
1:S:90:MET:HA	1:X:54:PHE:HB2	2.03	0.41
1:S:476:LEU:HB3	1:S:571:ILE:HD13	2.02	0.41
1:S:828:ALA:HA	1:S:957:PRO:HA	2.02	0.41
1:X:1254:ASP:HB3	1:X:1258:ASN:HD21	1.86	0.41
4:6:214:THR:HG22	4:7:221:LEU:HD23	2.03	0.41
3:D:114:ILE:HD13	3:D:183:LEU:HB2	2.03	0.41
1:T:873:ASN:OD1	2:E:92:PHE:N	2.54	0.41
1:W:827:THR:OG1	1:W:958:LEU:O	2.33	0.41
1:S:668:TYR:HB2	1:S:812:TYR:CD2	2.56	0.41
1:S:1083:HIS:HB3	1:S:1090:ASN:HB2	2.03	0.41
3:5:120:GLN:HG3	3:5:214:TYR:CG	2.56	0.41
4:7:254:ILE:HG22	4:7:256:PRO:HD3	2.03	0.41
1:T:512:ARG:HA	1:T:515:HIS:HD2	1.86	0.40
1:W:178:ARG:HD2	1:W:384:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:584:LEU:HG	1:W:1005:PRO:HB2	2.03	0.40
1:S:822:ARG:HD3	1:S:1010:VAL:HG12	2.02	0.40
1:S:866:HIS:CD2	1:S:868:ALA:H	2.40	0.40
1:X:476:LEU:HG	1:X:1250:PHE:HD2	1.86	0.40
1:X:627:PHE:HE1	1:X:651:CYS:HB3	1.87	0.40
1:X:903:GLU:HG2	1:X:904:ARG:HG2	2.03	0.40
3:5:311:LEU:HG	3:5:424:LEU:HD22	2.03	0.40
6:G:58:GLN:HA	6:G:61:ALA:HB3	2.03	0.40
4:H:285:LEU:HB3	4:H:289:LEU:HD12	2.03	0.40
1:T:69:ARG:HB2	1:T:72:GLU:HG2	2.03	0.40
1:S:674:VAL:HG22	1:S:678:LEU:HD12	2.03	0.40
1:S:698:GLU:HG2	1:S:808:HIS:HE1	1.86	0.40
1:X:392:TYR:HD2	1:X:395:VAL:HG23	1.85	0.40
1:X:577:VAL:H	1:X:581:ASN:HD22	1.67	0.40
1:X:863:HIS:CD2	1:X:865:LEU:H	2.38	0.40
2:E:89:ARG:NH1	2:F:29:THR:OG1	2.51	0.40
3:D:153:THR:HG22	4:A:267:ARG:NH1	2.36	0.40
1:T:204:TYR:HB2	1:T:219:LEU:HD21	2.03	0.40
1:T:1252:TYR:CZ	1:T:1256:LEU:HD11	2.56	0.40
1:W:652:ILE:HG12	1:W:663:ALA:HB3	2.03	0.40
1:W:715:GLY:HA2	1:W:716:GLY:HA2	1.54	0.40
5:C:536:ARG:HE	6:K:40:VAL:HG21	1.86	0.40
1:W:192:ALA:HB3	1:W:1110:VAL:HG23	2.03	0.40
1:S:650:GLN:NE2	1:S:887:ASP:OD2	2.55	0.40
4:7:206:VAL:HA	4:7:209:MET:HB2	2.04	0.40
3:D:281:PRO:HB2	3:D:282:ARG:H	1.78	0.40
4:H:202:LEU:HG	4:H:205:LEU:HD12	2.03	0.40
1:T:828:ALA:N	1:T:937:ILE:O	2.54	0.40
1:T:1314:PRO:HA	1:T:1315:PRO:HD3	1.88	0.40
1:S:104:ILE:HB	1:X:390:VAL:HG21	2.03	0.40
1:X:346:LEU:HA	1:X:347:ASN:HA	1.82	0.40
4:6:280:THR:O	4:6:284:GLN: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	S	1324/1374 (96%)	1237 (93%)	80 (6%)	7 (0%)	29	68
1	T	1367/1374 (100%)	1292 (94%)	74 (5%)	1 (0%)	51	85
1	W	1365/1374 (99%)	1281 (94%)	80 (6%)	4 (0%)	41	76
1	X	1304/1374 (95%)	1237 (95%)	62 (5%)	5 (0%)	34	72
2	E	99/112 (88%)	96 (97%)	3 (3%)	0	100	100
2	F	99/112 (88%)	96 (97%)	3 (3%)	0	100	100
2	L	99/112 (88%)	96 (97%)	3 (3%)	0	100	100
2	P	99/112 (88%)	96 (97%)	3 (3%)	0	100	100
3	5	385/465 (83%)	365 (95%)	20 (5%)	0	100	100
3	D	361/465 (78%)	341 (94%)	17 (5%)	3 (1%)	19	60
4	6	281/318 (88%)	261 (93%)	20 (7%)	0	100	100
4	7	306/318 (96%)	290 (95%)	16 (5%)	0	100	100
4	A	306/318 (96%)	295 (96%)	11 (4%)	0	100	100
4	H	281/318 (88%)	264 (94%)	16 (6%)	1 (0%)	34	72
5	C	555/703 (79%)	526 (95%)	28 (5%)	1 (0%)	47	81
6	G	90/580 (16%)	82 (91%)	8 (9%)	0	100	100
6	K	77/580 (13%)	74 (96%)	3 (4%)	0	100	100
7	B	46/3094 (2%)	45 (98%)	1 (2%)	0	100	100
7	O	46/3094 (2%)	45 (98%)	1 (2%)	0	100	100
All	All	8490/16197 (52%)	8019 (94%)	449 (5%)	22 (0%)	44	76

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	W	420	ALA
1	W	635	HIS
1	S	420	ALA
1	X	420	ALA
1	X	1358	PHE
4	H	28	GLU
1	S	659	THR
1	X	1265	GLY

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Mol	Chain	Res	Type
1	S	124	ILE
3	D	258	GLU
1	T	8	PRO
1	W	801	ARG
1	S	125	ASP
1	S	779	ASN
1	S	780	ASP
1	S	781	GLY
1	X	342	GLU
5	C	614	VAL
3	D	281	PRO
3	D	136	PRO
1	W	634	ILE
1	X	421	GLY

5.3.2 Protein sidechains (i)

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	S	1049/1087 (96%)	1048 (100%)	1 (0%)	93	97
1	T	1084/1087 (100%)	1084 (100%)	0	100	100
1	W	1082/1087 (100%)	1081 (100%)	1 (0%)	93	97
1	X	1039/1087 (96%)	1038 (100%)	1 (0%)	93	97
2	E	80/89 (90%)	80 (100%)	0	100	100
2	F	80/89 (90%)	80 (100%)	0	100	100
2	L	80/89 (90%)	80 (100%)	0	100	100
2	P	80/89 (90%)	80 (100%)	0	100	100
3	5	303/365 (83%)	301 (99%)	2 (1%)	84	90
3	D	285/365 (78%)	285 (100%)	0	100	100
4	6	243/264 (92%)	243 (100%)	0	100	100
4	7	258/264 (98%)	257 (100%)	1 (0%)	91	94
4	A	258/264 (98%)	257 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	243/264 (92%)	243 (100%)	0	100	100
5	C	440/531 (83%)	440 (100%)	0	100	100
6	G	78/449 (17%)	78 (100%)	0	100	100
6	K	66/449 (15%)	66 (100%)	0	100	100
7	B	41/2391 (2%)	41 (100%)	0	100	100
7	O	41/2391 (2%)	41 (100%)	0	100	100
All	All	6830/12701 (54%)	6823 (100%)	7 (0%)	93	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	94	ARG
1	S	216	ARG
1	X	1054	ARG
3	5	367	ASN
3	5	407	LEU
4	7	214	THR
4	A	92	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	266	HIS
1	T	485	ASN
1	T	622	ASN
1	T	658	ASN
1	T	719	GLN
1	T	723	ASN
1	T	863	HIS
1	T	1037	HIS
1	T	1045	HIS
1	T	1083	HIS
1	T	1090	ASN
1	T	1181	GLN
1	T	1204	ASN
1	W	63	ASN
1	W	163	GLN
1	W	164	GLN
1	W	168	ASN

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Mol	Chain	Res	Type
1	W	429	HIS
1	W	485	ASN
1	W	507	ASN
1	W	719	GLN
1	W	723	ASN
1	W	863	HIS
1	W	866	HIS
1	W	895	GLN
1	W	1045	HIS
1	W	1149	ASN
1	W	1179	HIS
1	S	63	ASN
1	S	156	HIS
1	S	266	HIS
1	S	429	HIS
1	S	485	ASN
1	S	622	ASN
1	S	635	HIS
1	S	723	ASN
1	S	808	HIS
1	S	863	HIS
1	S	899	HIS
1	S	944	HIS
1	S	950	GLN
1	S	961	HIS
1	S	1037	HIS
1	S	1039	GLN
1	S	1045	HIS
1	S	1083	HIS
1	S	1179	HIS
1	S	1204	ASN
1	S	1258	ASN
1	X	429	HIS
1	X	507	ASN
1	X	622	ASN
1	X	631	GLN
1	X	658	ASN
1	X	696	HIS
1	X	800	HIS
1	X	863	HIS
1	X	876	ASN
1	X	944	HIS

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Mol	Chain	Res	Type
1	X	972	ASN
1	X	1009	HIS
1	X	1037	HIS
1	X	1204	ASN
1	X	1258	ASN
2	L	5	GLN
2	L	7	HIS
2	L	68	HIS
2	P	5	GLN
2	P	7	HIS
2	E	5	GLN
2	E	7	HIS
2	E	68	HIS
2	F	5	GLN
2	F	7	HIS
2	F	68	HIS
3	5	120	GLN
3	5	235	HIS
3	5	367	ASN
4	6	208	ASN
4	6	281	HIS
4	7	164	ASN
5	C	57	GLN
5	C	157	ASN
5	C	195	HIS
5	C	440	GLN
5	C	483	HIS
5	C	506	GLN
5	C	603	ASN
6	G	15	HIS
6	K	15	HIS
6	K	56	GLN
6	K	90	ASN
3	D	145	GLN
3	D	317	GLN
4	H	208	ASN
4	H	281	HIS
4	A	199	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 monosaccharides 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.

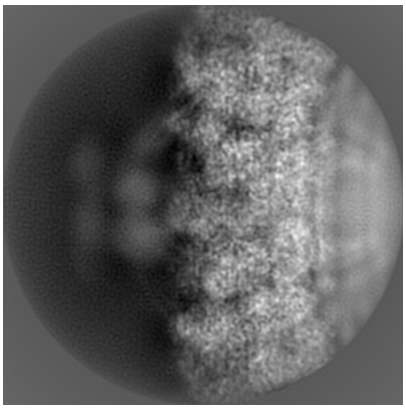
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9860. These allow visual inspection of the internal detail of the map and identification of artifacts.

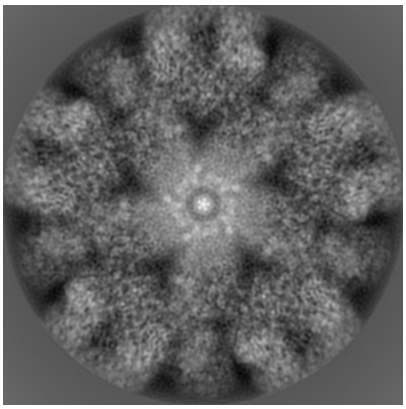
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

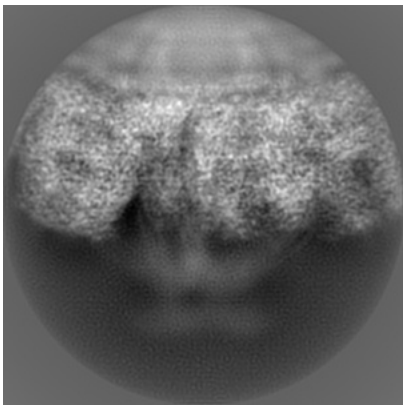
6.1.1 Primary map



X

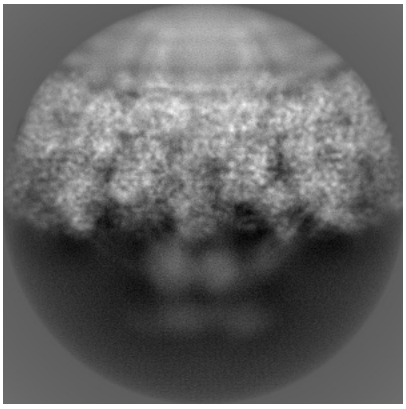


Y

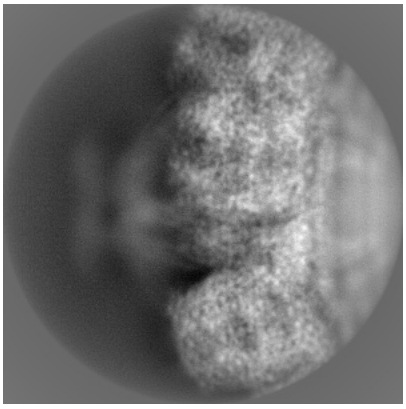


Z

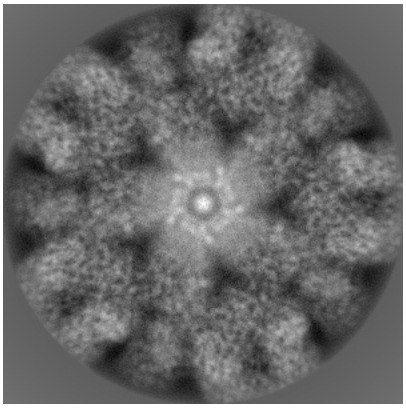
6.1.2 Raw map



X



Y

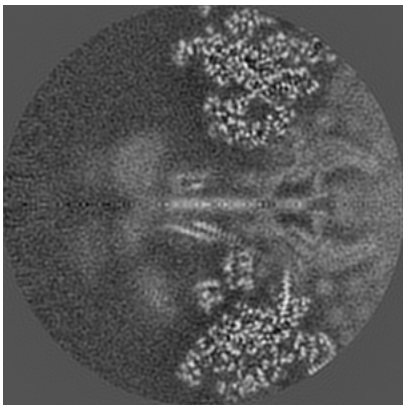


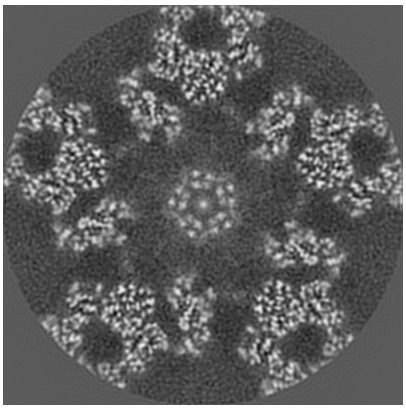
Z

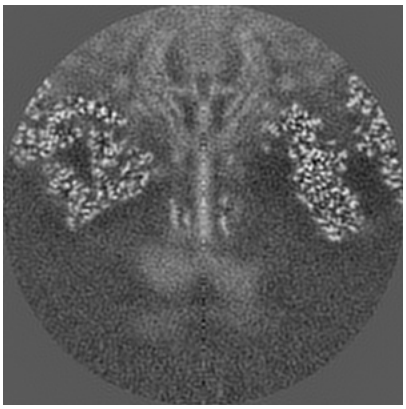
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

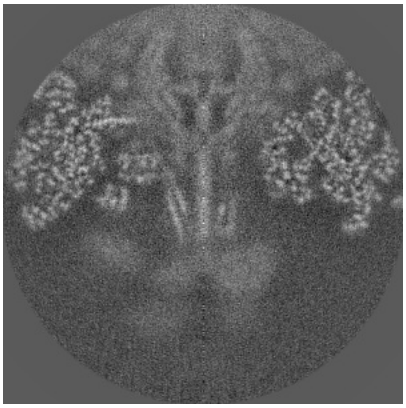
6.2.1 Primary map

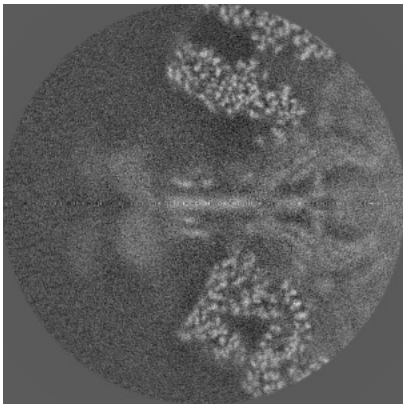

X Index: 192

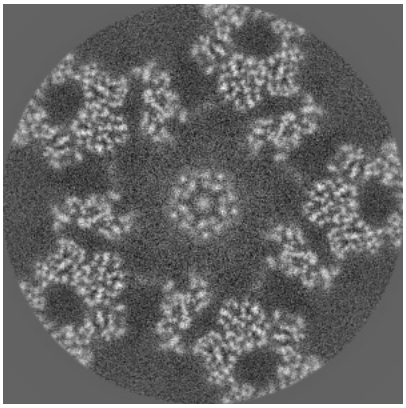

Y Index: 192


Z Index: 192

6.2.2 Raw map


X Index: 192

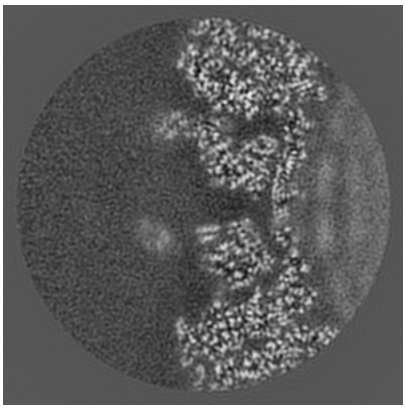

Y Index: 192

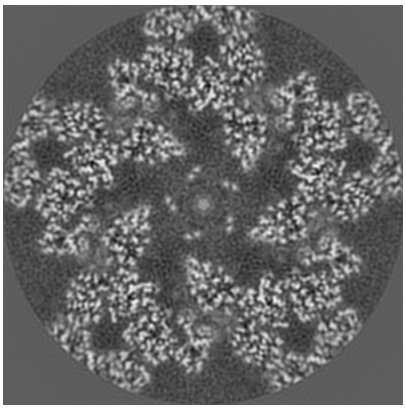

Z Index: 192

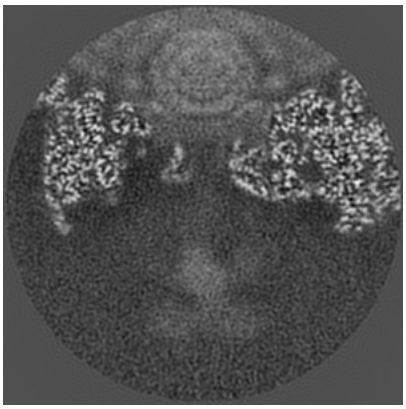
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

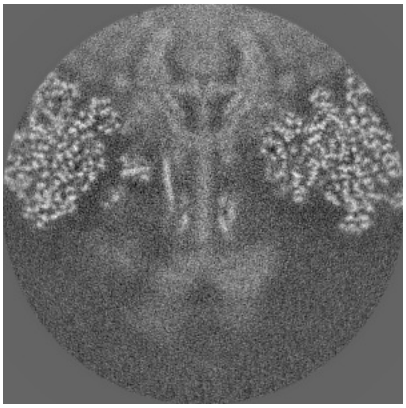
6.3.1 Primary map

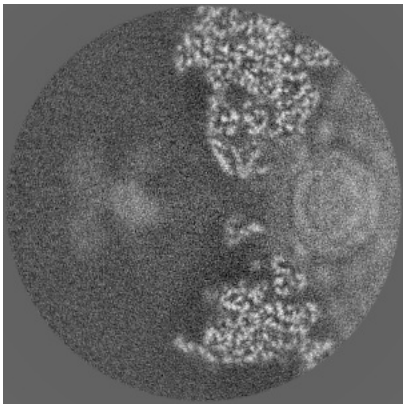

X Index: 265

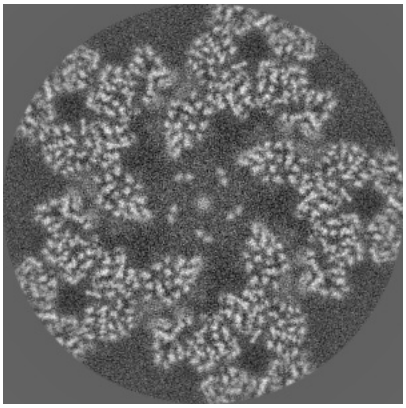

Y Index: 211


Z Index: 231

6.3.2 Raw map


X Index: 197

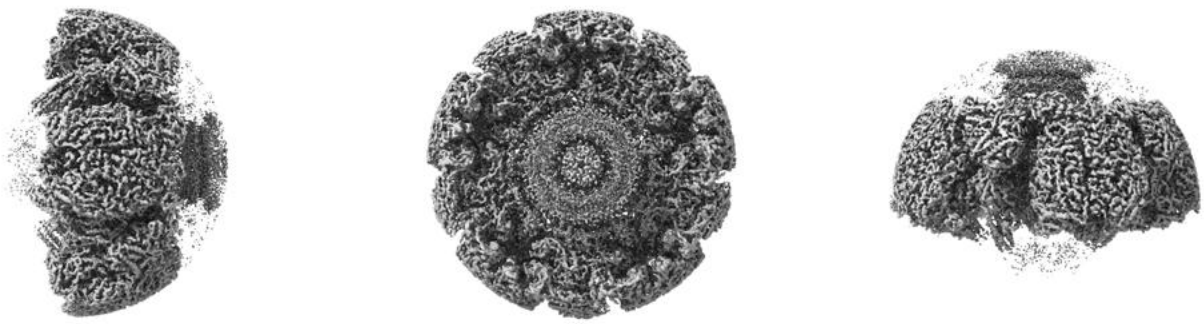

Y Index: 231


Z Index: 211

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

6.4 Orthogonal surface views (i)

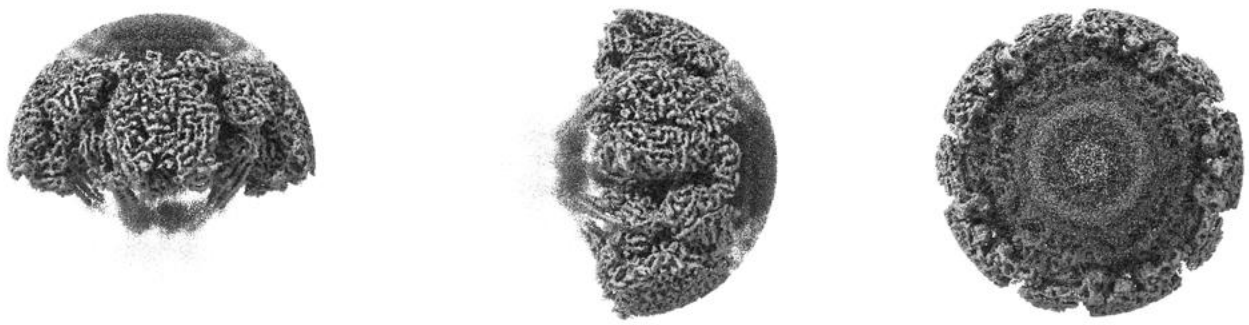
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

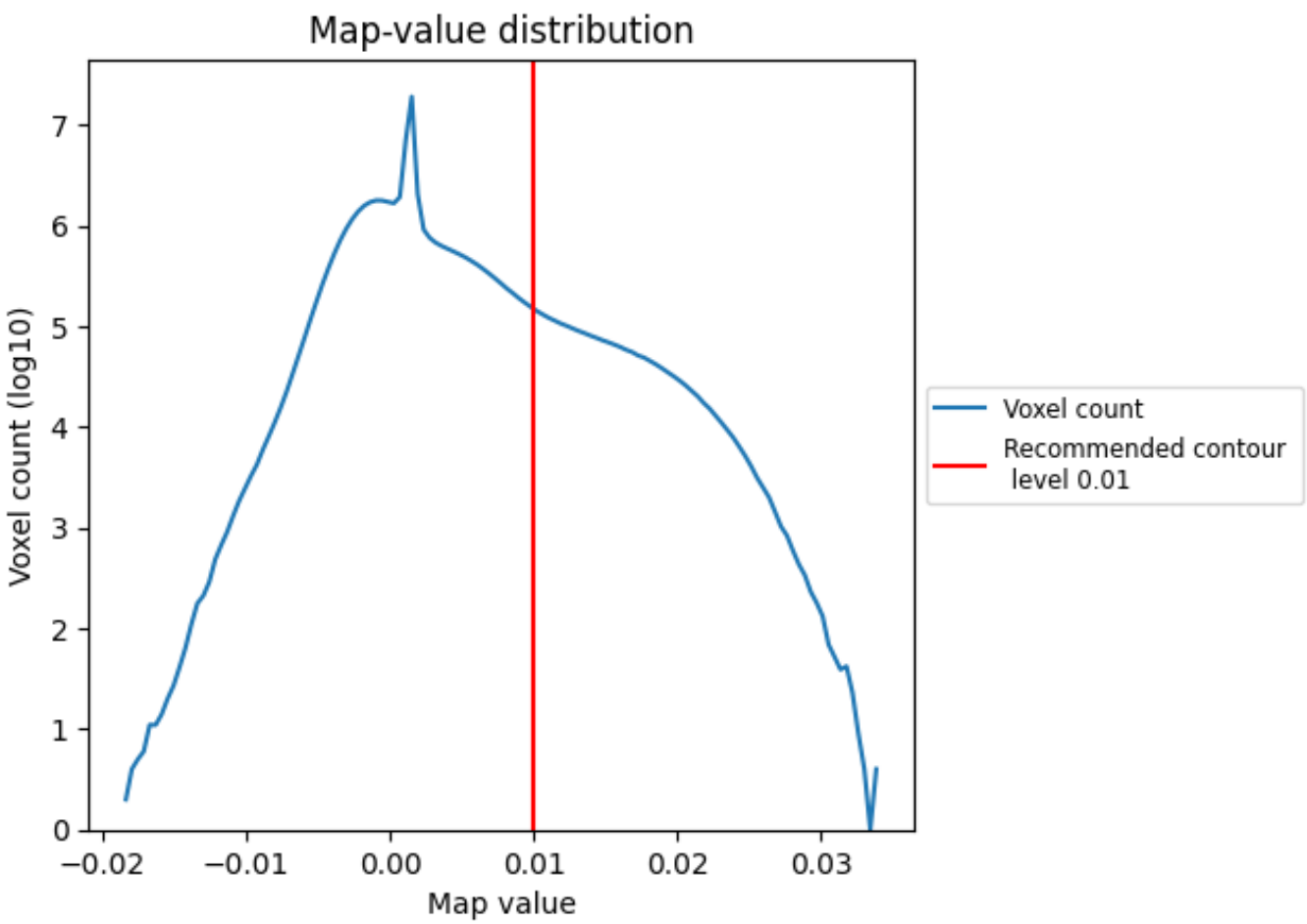
6.5 Mask visualisation (i)

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

7 Map analysis (i)

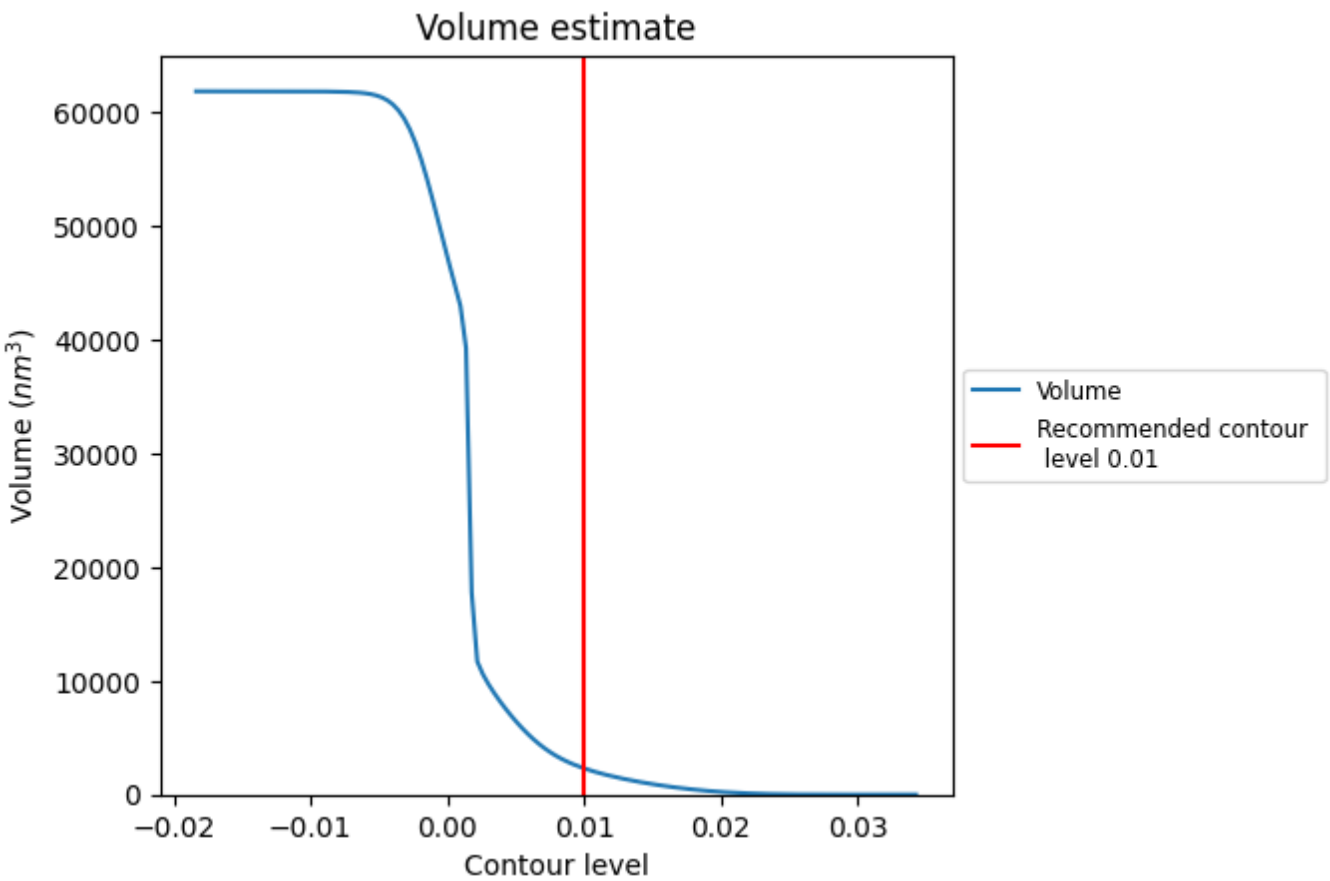
This section contains the results of statistical analysis of the map.

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.

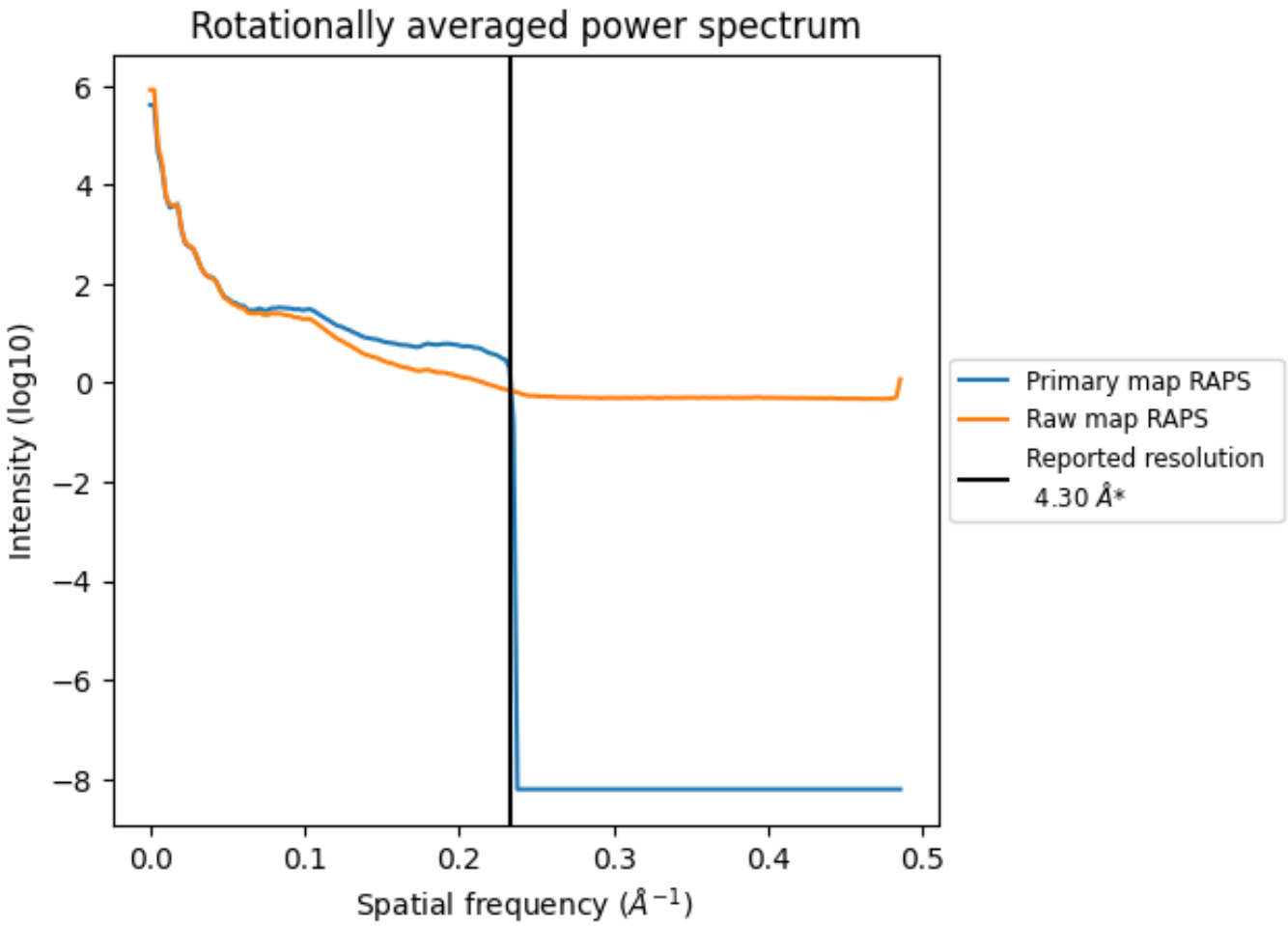
7.2 Volume estimate (i)



The volume at the recommended contour level is 2305 nm^3; this corresponds to an approximate mass of 2082 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)

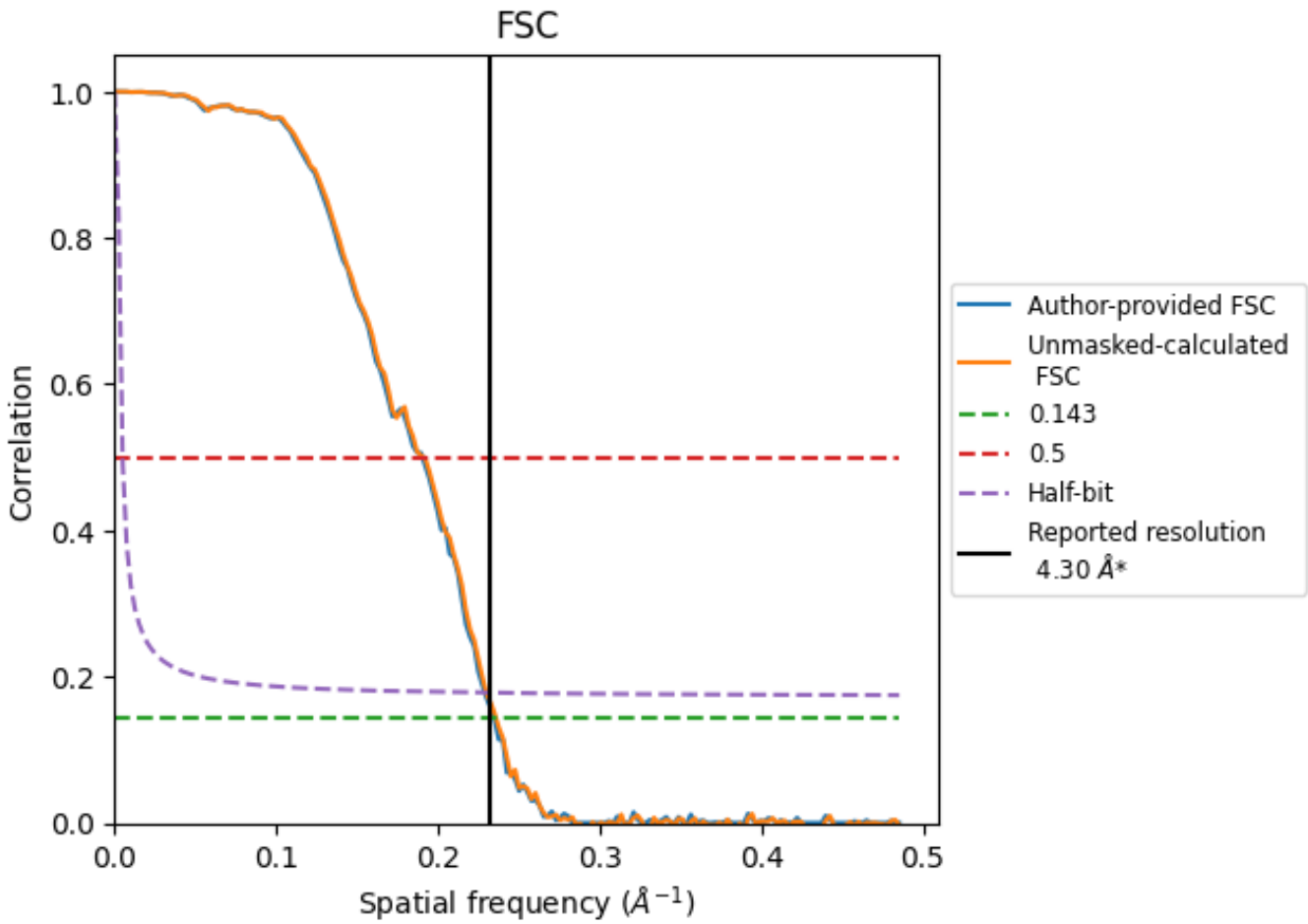


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8.2 Resolution estimates (i)

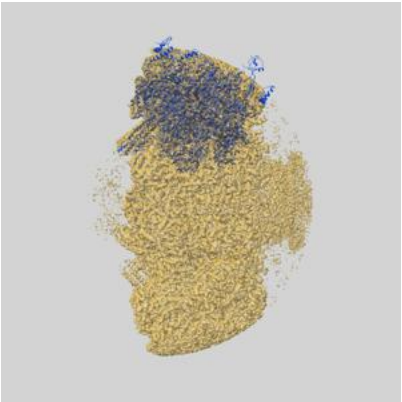
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.26	5.25	4.37
Unmasked-calculated*	4.24	5.23	4.35

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

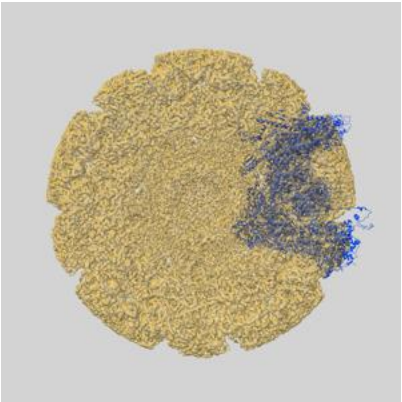
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9860 and PDB model 6ODM. Per-residue inclusion information can be found in section 3 on page 6.

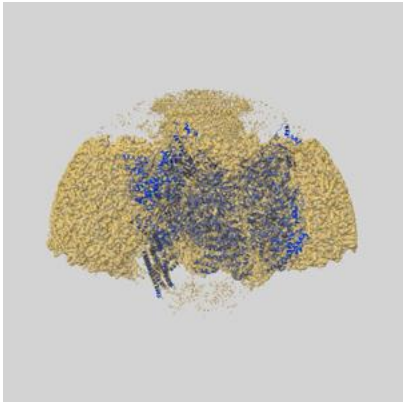
9.1 Map-model overlay (i)



X



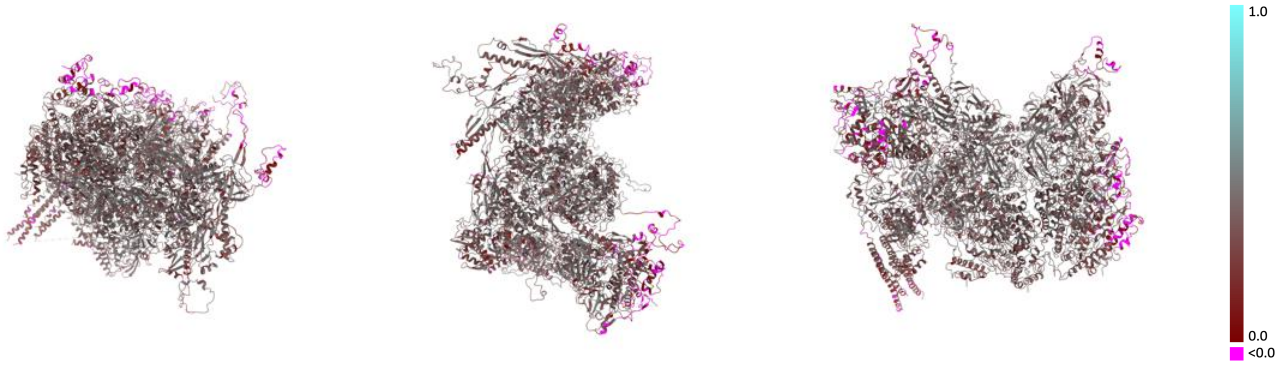
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

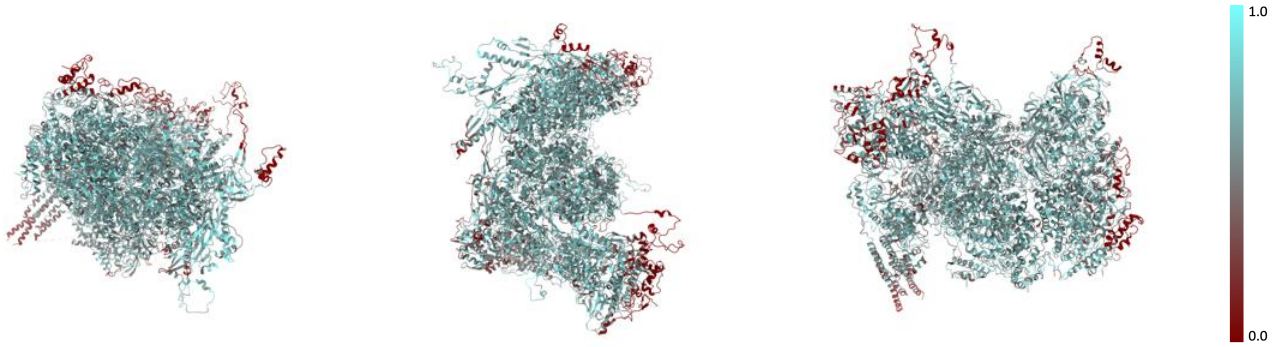
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

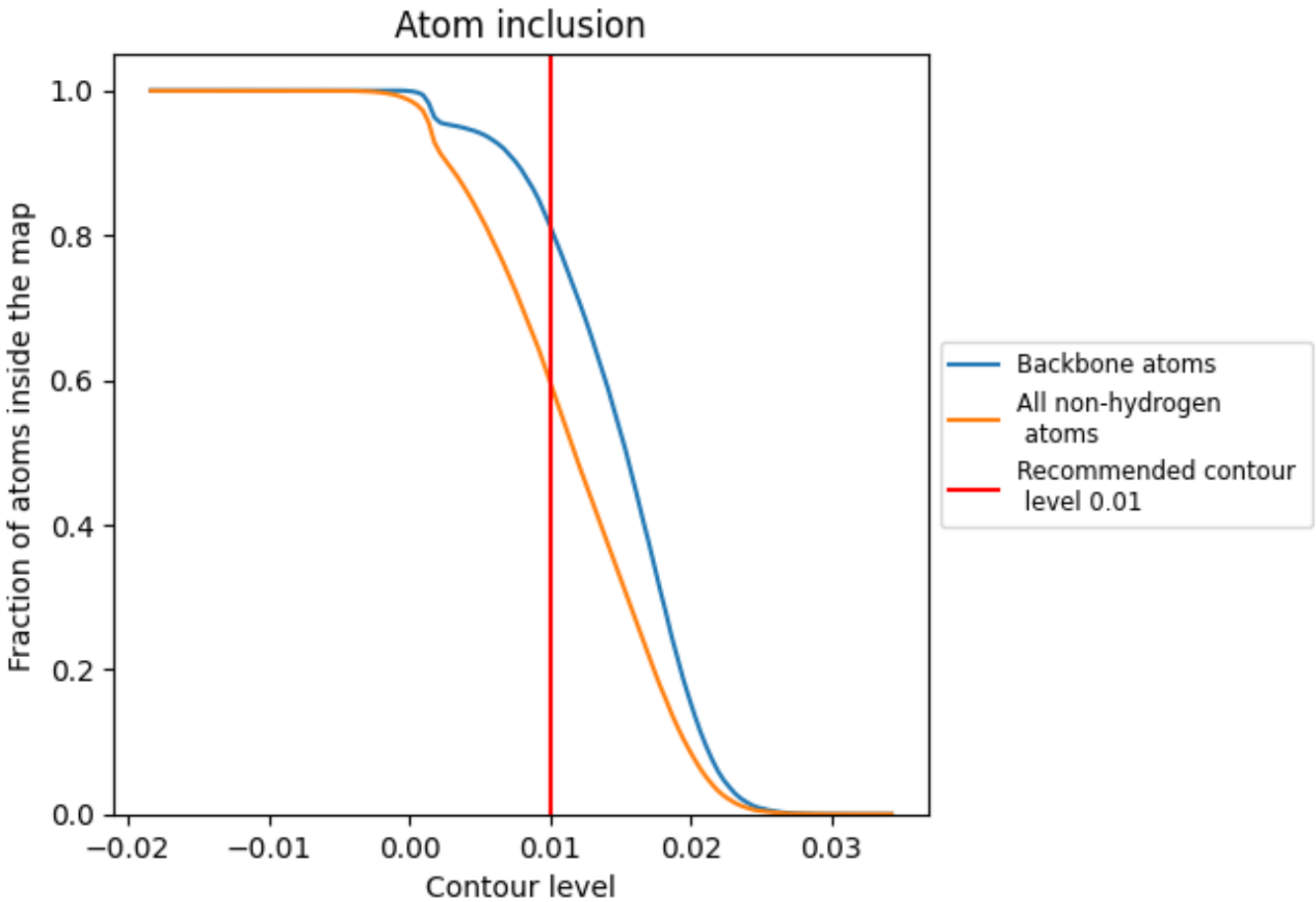
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5970	0.3510
5	0.5604	0.3520
6	0.5904	0.3650
7	0.5956	0.3770
A	0.4497	0.2730
B	0.3639	0.2060
C	0.5896	0.3430
D	0.6049	0.3550
E	0.6495	0.3560
F	0.6243	0.3550
G	0.4904	0.2630
H	0.4773	0.2990
K	0.5482	0.2930
L	0.3003	0.1480
O	0.2965	0.1260
P	0.6389	0.3590
S	0.6482	0.3840
T	0.6282	0.3670
W	0.5769	0.3320
X	0.6524	0.3810