Full wwPDB EM Validation Report ⓘ

Jan 1, 2025 – 10:35 AM EST

PDB ID	:	8TEW
EMDB ID	:	EMD-41204
Title	:	Human cytomegalovirus penton vertex, CVSC-bound configuration
Authors	:	Jih, J.; Liu, Y.T.; Liu, W.; Zhou, H.
Deposited on	:	2023-07-07
Resolution	:	3.02 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

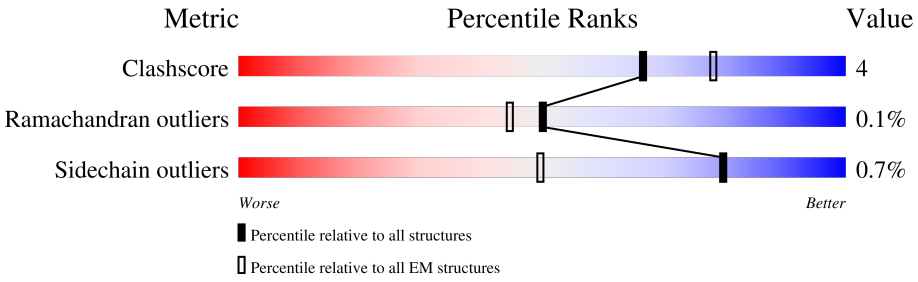
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.02 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1	1370	88% 7% 5%
1	H	1370	90% 7%
1	I	1370	89% 9%
1	J	1370	86% 10%
1	K	1370	90% 8%
1	L	1370	89% 9%
1	M	1370	88% 10%
2	2	75	77% 7% 16%

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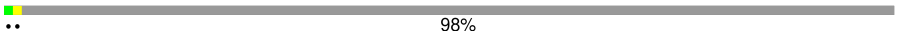
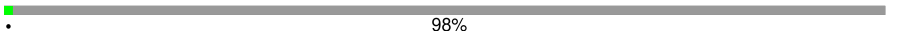
Mol	Chain	Length	Quality of chain
2	N	75	
2	O	75	
2	P	75	
2	Q	75	
2	R	75	
2	S	75	
3	3	1048	
3	Z	1048	
4	A	2241	
4	C	2241	
5	E	642	
5	F	642	
6	G	594	
7	T	290	
7	W	290	
8	U	306	
8	V	306	
8	X	306	
8	Y	306	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 104261 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
1	1	1306	Total	C	N	O	S	0	0
			10362	6608	1796	1899	59		
1	H	1335	Total	C	N	O	S	0	0
			10574	6733	1830	1950	61		
1	I	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		
1	J	1317	Total	C	N	O	S	0	0
			10433	6641	1814	1919	59		
1	K	1351	Total	C	N	O	S	0	0
			10705	6816	1854	1974	61		
1	L	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		
1	M	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
2	N	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
2	O	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
2	P	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
2	Q	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
2	R	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
2	S	63	Total	C	N	O	S	0	0
			513	321	97	91	4		

- Molecule 3 is a protein called Large structural phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
3	Z	284	Total	C	N	O	S	0	0
			2320	1463	425	420	12		

- Molecule 4 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	43	Total	C	N	O	S	0	0
			354	228	63	62	1		
4	C	36	Total	C	N	O	S	0	0
			301	193	55	52	1		

- Molecule 5 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	82	Total	C	N	O	S	0	0
			681	419	133	125	4		
5	F	478	Total	C	N	O	S	0	0
			3893	2508	686	688	11		

- Molecule 6 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	472	Total	C	N	O	S	0	0
			3873	2422	744	693	14		

- Molecule 7 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	129	Total	C	N	O	S	0	0
			1067	691	185	186	5		
7	W	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

- Molecule 8 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	303	Total	C	N	O	S	0	0
			2406	1541	419	428	18		
8	V	298	Total	C	N	O	S	0	0
			2369	1517	414	421	17		

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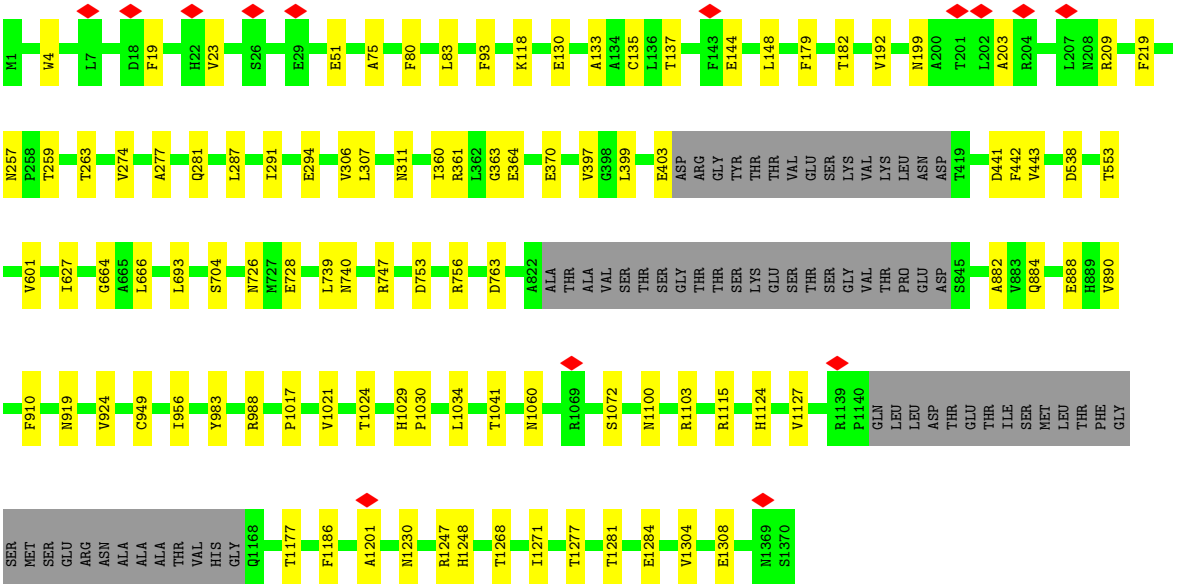
Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	295	Total	C	N	O	S	0	0
			2334	1501	402	412	19		
8	Y	285	Total	C	N	O	S	0	0
			2266	1456	387	405	18		

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.

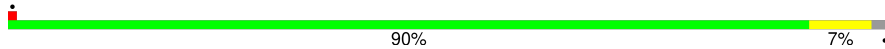
• Molecule 1: Major capsid protein

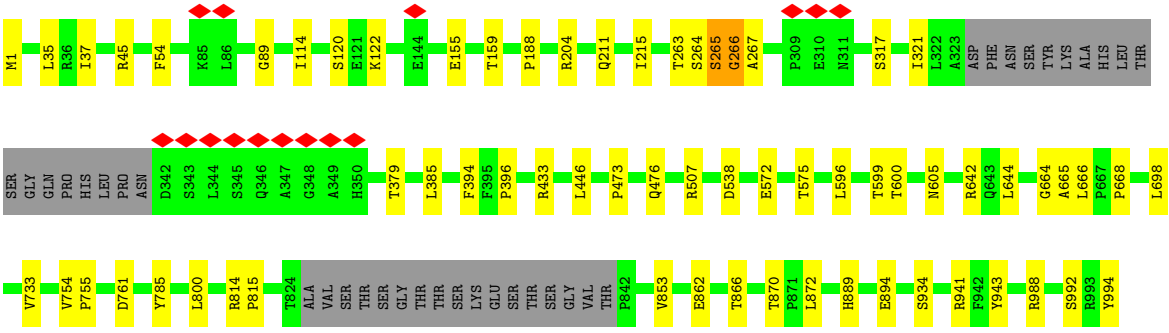
Chain 1:

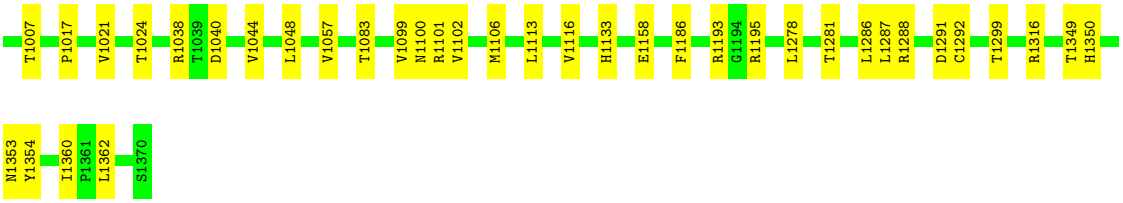


• Molecule 1: Major capsid protein

Chain H:

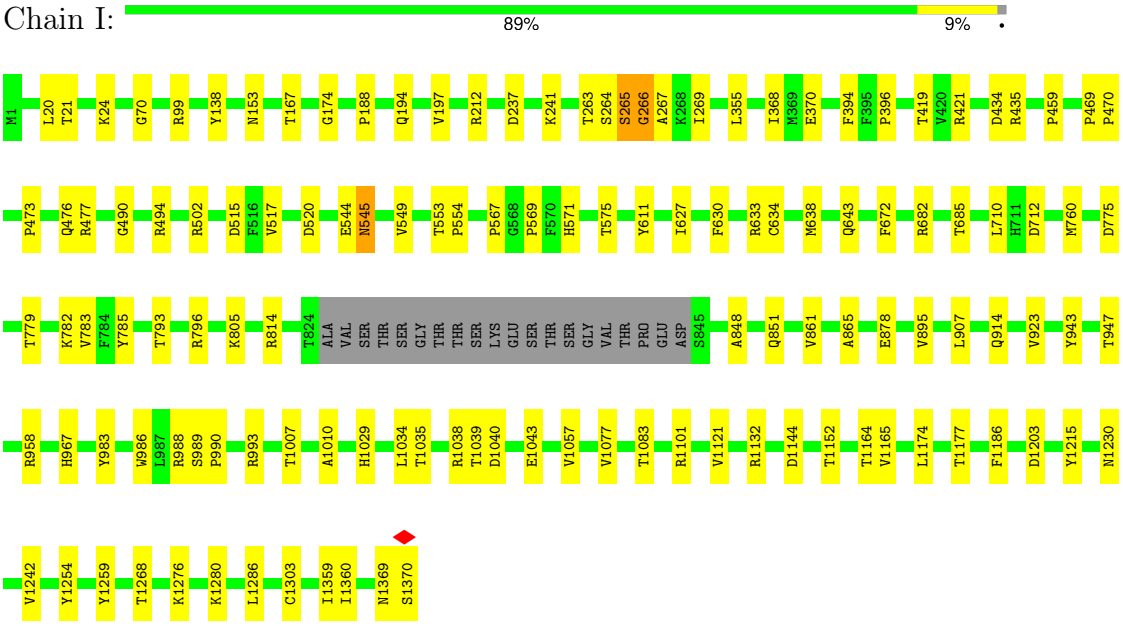






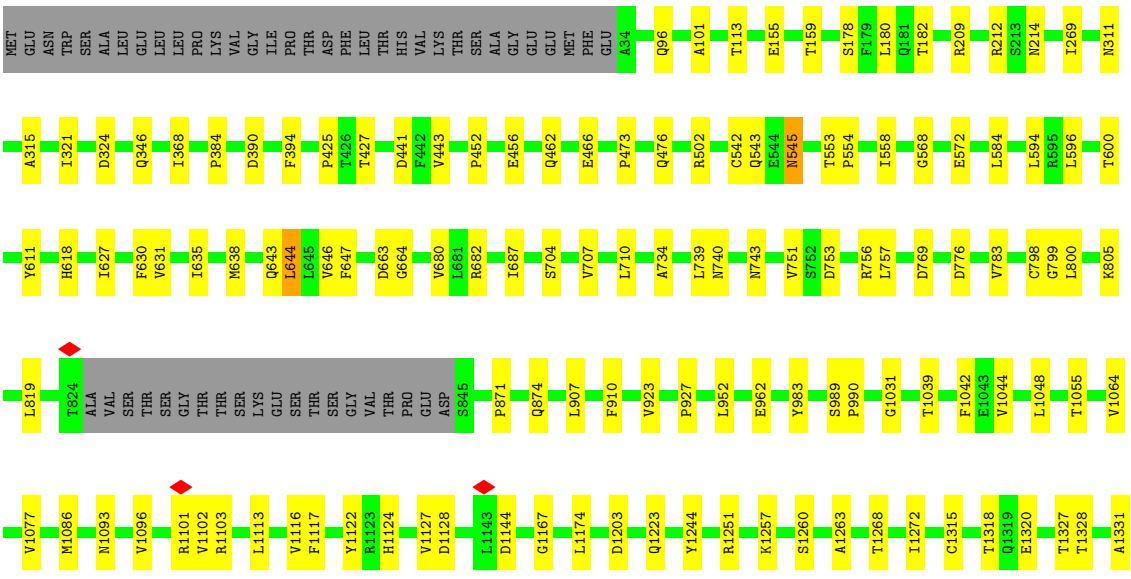
• Molecule 1: Major capsid protein

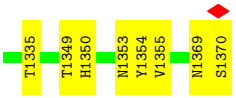
Chain I:



• Molecule 1: Major capsid protein

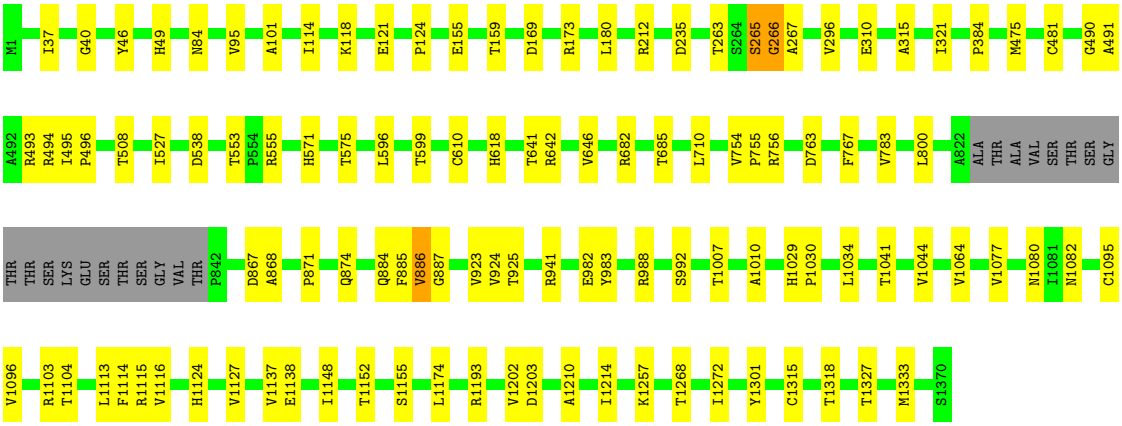
Chain J:





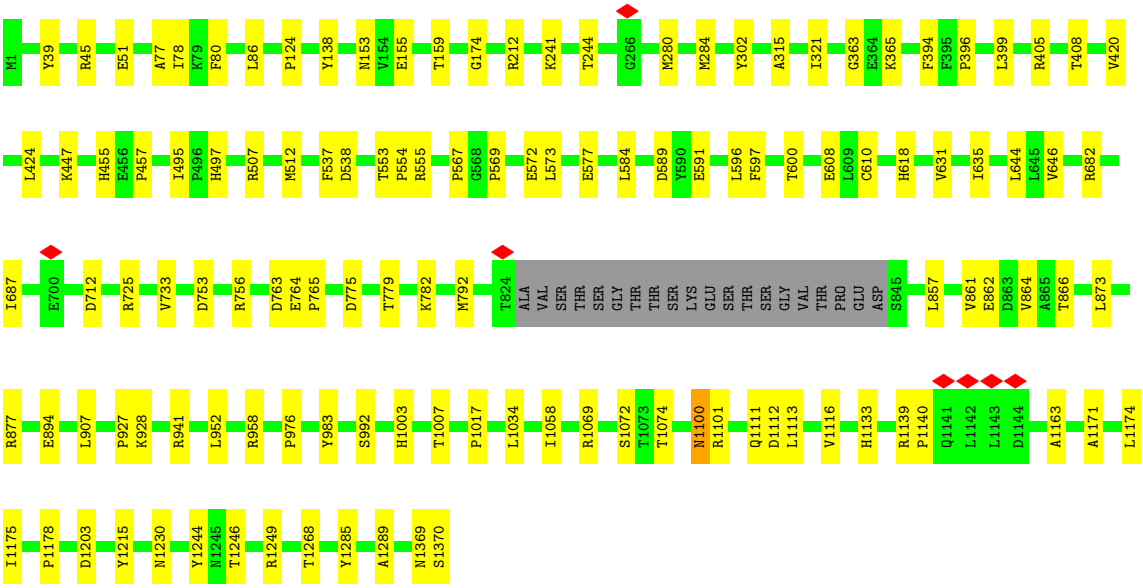
• Molecule 1: Major capsid protein

Chain K:



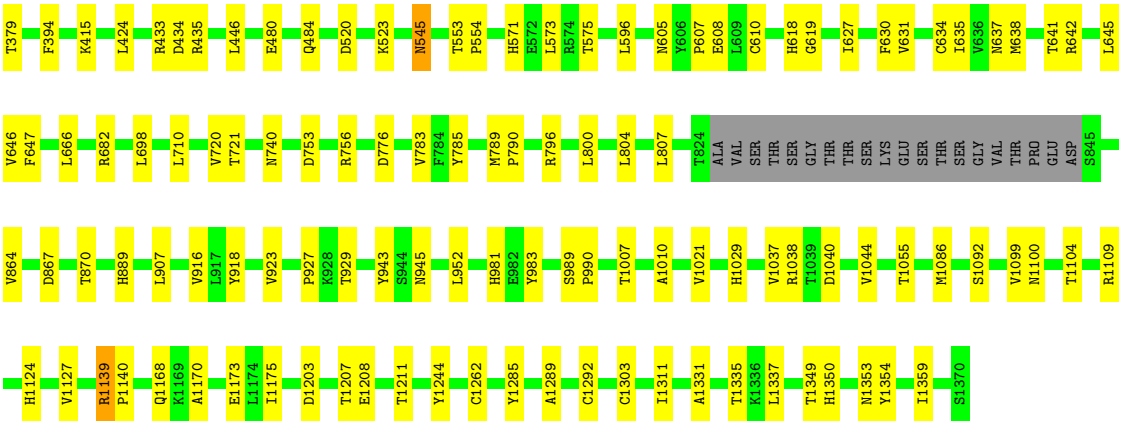
• Molecule 1: Major capsid protein

Chain L:



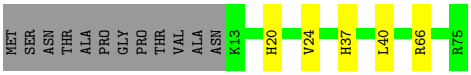
• Molecule 1: Major capsid protein

Chain M:



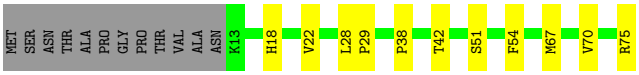
- Molecule 2: Small capsomere-interacting protein

Chain 2:



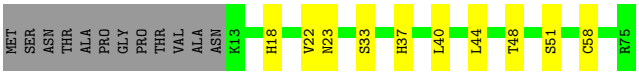
- Molecule 2: Small capsomere-interacting protein

Chain N:



- Molecule 2: Small capsomere-interacting protein

Chain O:

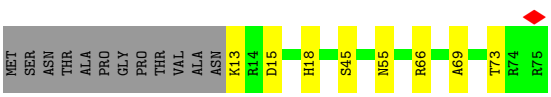


- Molecule 2: Small capsomere-interacting protein

Chain P:

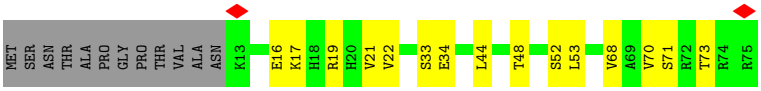
- Molecule 2: Small capsomere-interacting protein

Chain Q:



- Molecule 2: Small capsomere-interacting protein

Chain R:

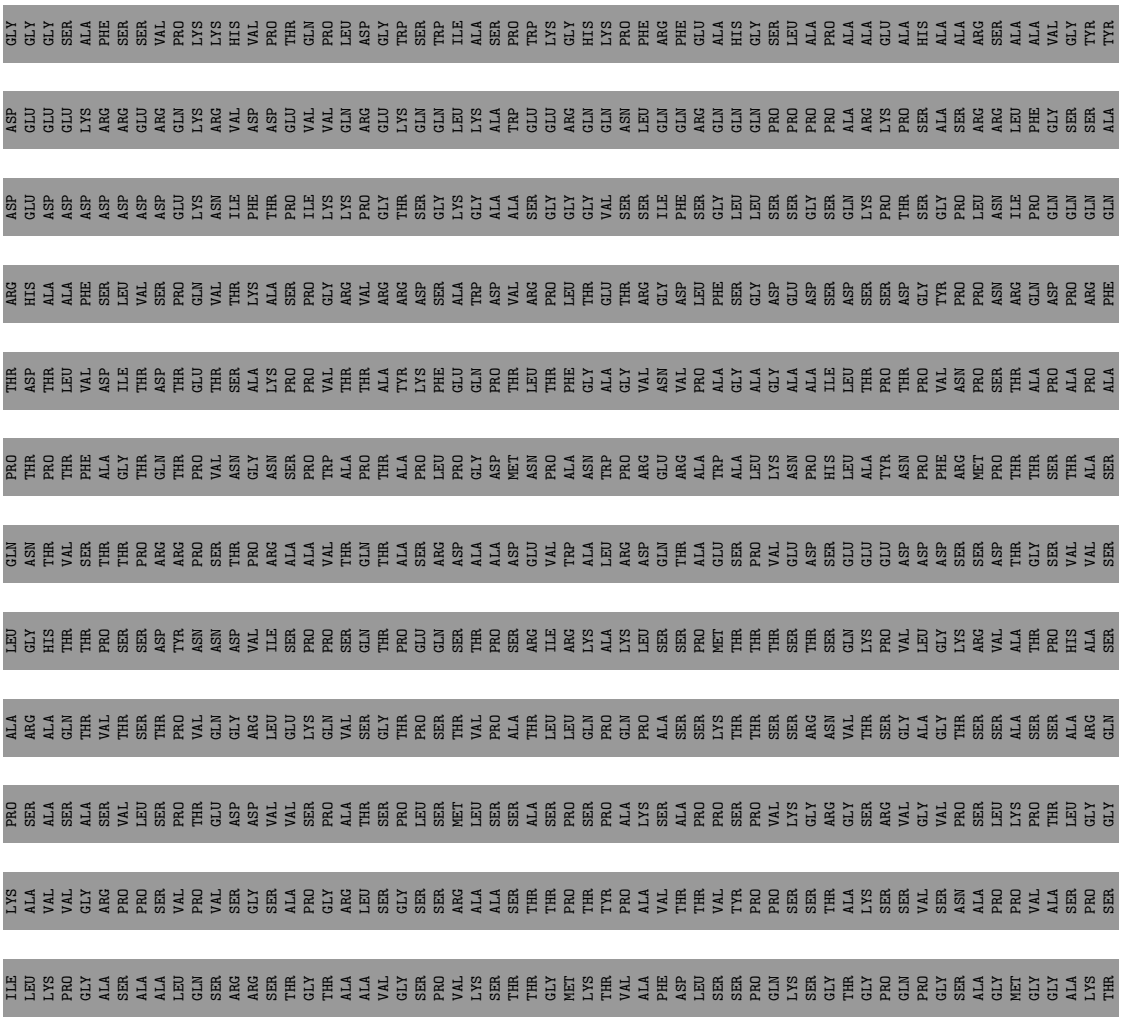


• Molecule 2: Small capsomere-interacting protein

Chain S:

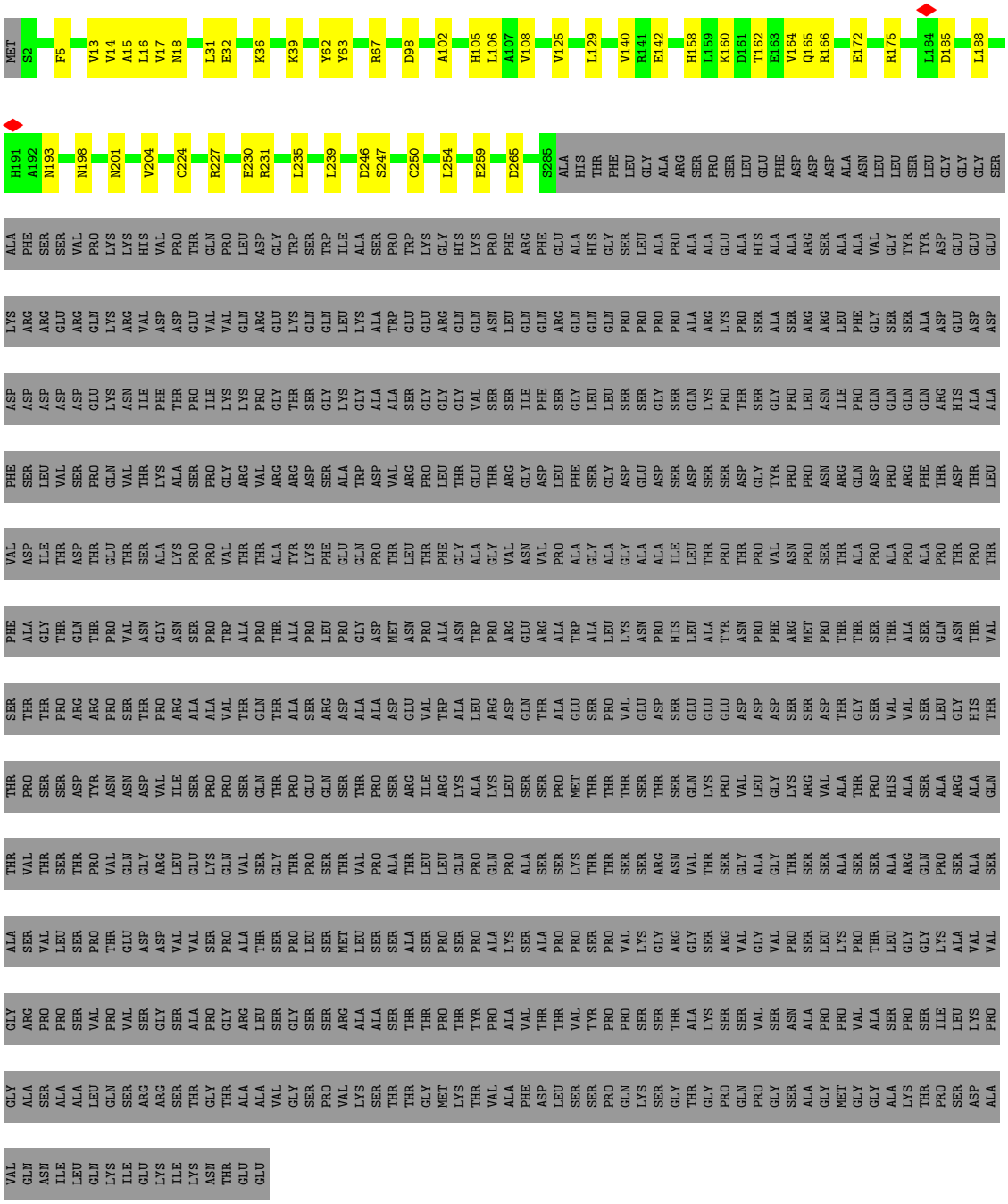
• Molecule 3: Large structural phosphoprotein

Chain 3:



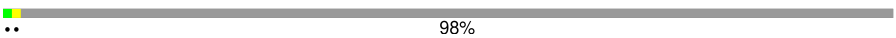
• Molecule 3: Large structural phosphoprotein

Chain Z:



• Molecule 4: Large tegument protein deneddylase

Chain A:



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

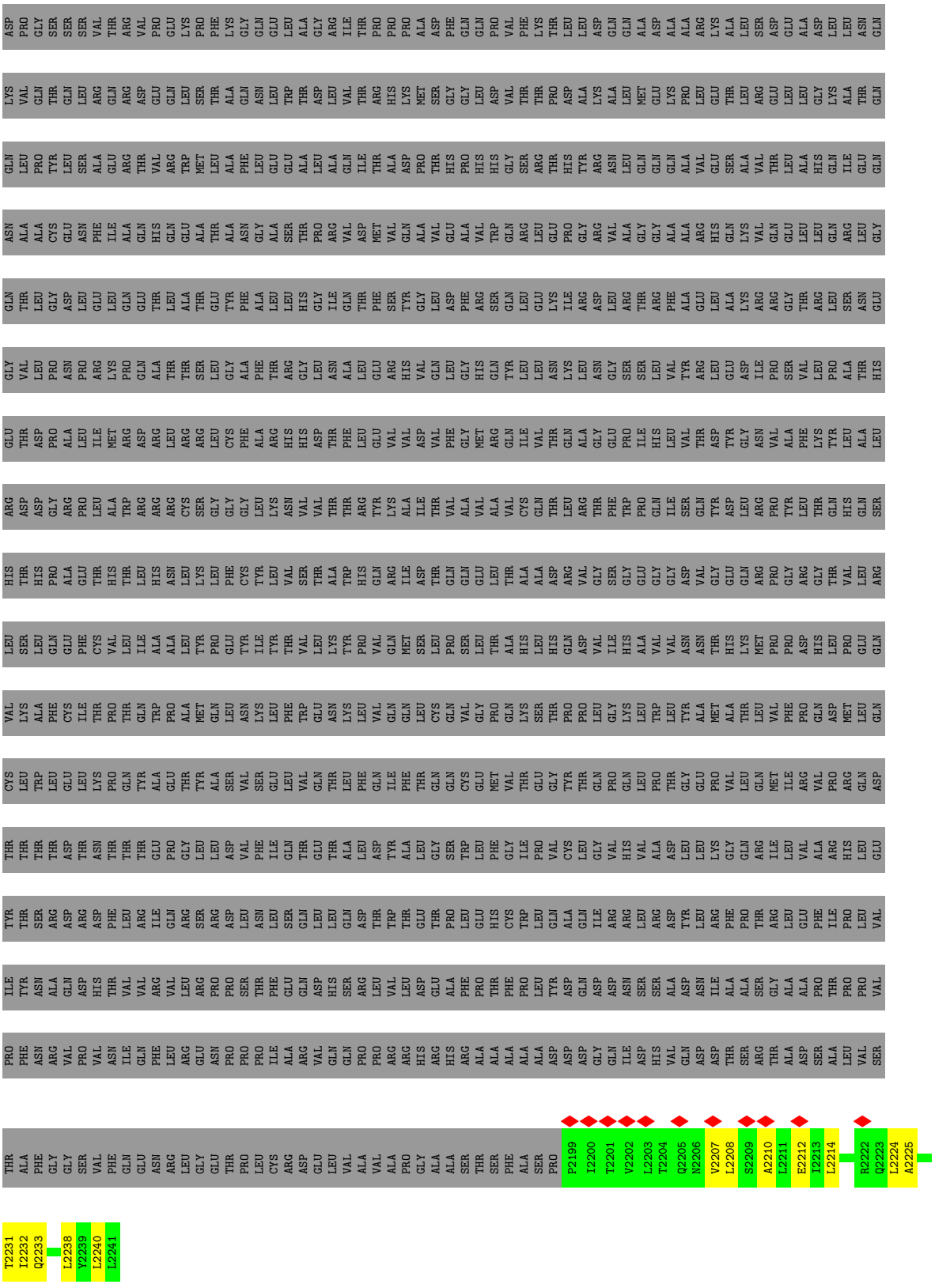
LYS ARG PHE GLN ALA LEU ARG GLU LEU VAL TYR PHE PHE ARG ASN HIS GLU TYR PHE PHE GLN HIS MET VAL GLY ARG LEU GLY VAL GLY PRO GLN VAL THR GLU LEU TYR GLU ARG TYR GLN HIS GLU MET GLU GLN HIS LEU GLU ARG LEU GLU ARG GLU TRP GLN GLU ALA

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

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

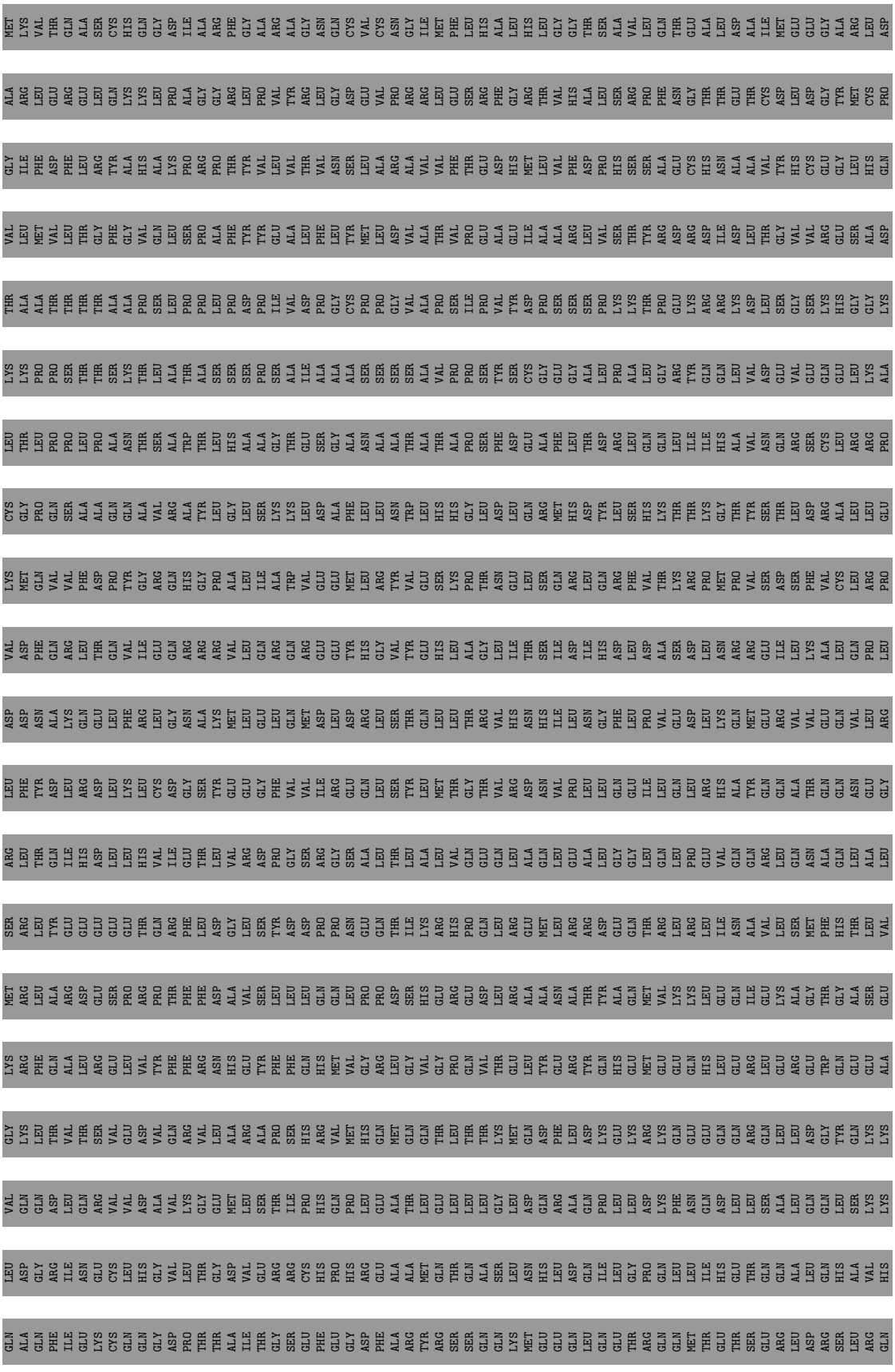
LEU ASP GLY ARG ILE ASN GLU CYS LEU HIS GLY VAL LEU THR GLY ASP VAL GLU ARG ARG CYS HIS PRO HIS ARG GLU ALA ALA MET GLN THR GLN ALA SER LEU ASN HIS LEU ASP GLN ILE LEU GLY PRO GLN LEU LEU ILE HIS GLU THR GLN GLN ALA LEU GLN HIS ALA VAL HIS

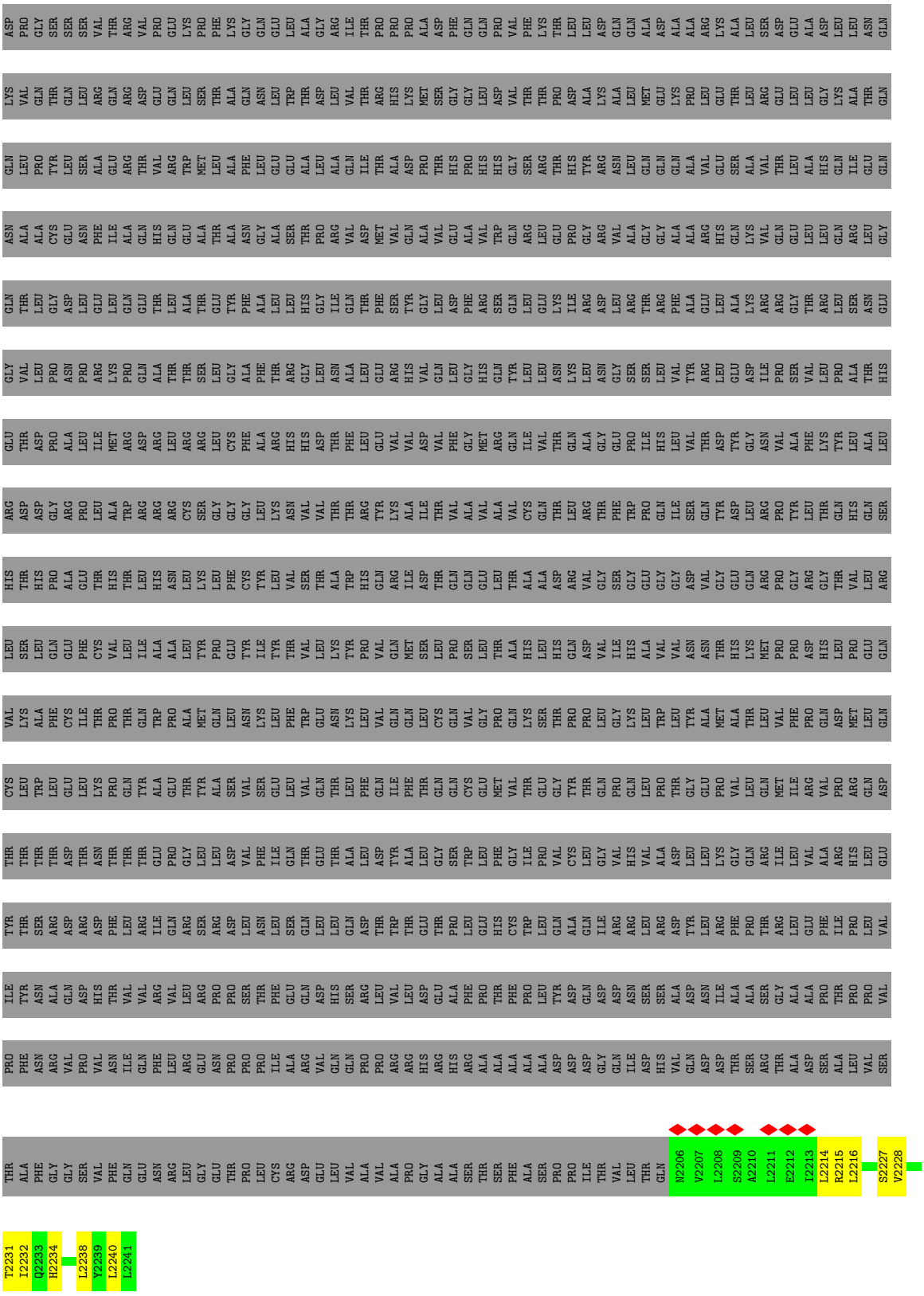
GLN ALA GLN PHE ILE GLU LYS CYS GLN GLN GLY ASP PRO THR THR ALA ILE THR GLY SER GLU PHE GLU GLY ASP PHE ALA ARG TYR ARG SER SER GLN GLN LYS MET GLU GLU GLN LEU GLN GLU THR ARG GLN GLN MET THR GLU THR SER GLU ARG LEU ASP ARG SER LEU ARG GLN



• Molecule 4: Large tegument protein deneddylase

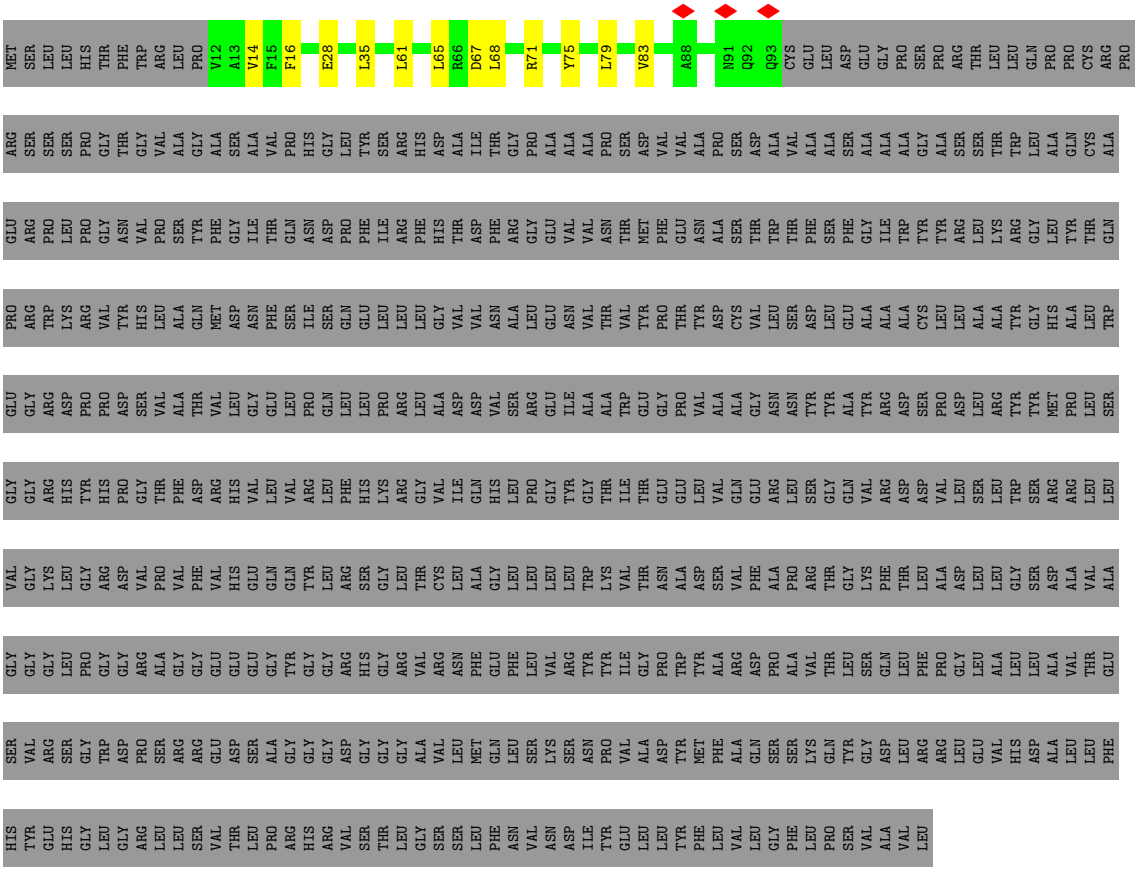
Chain C:





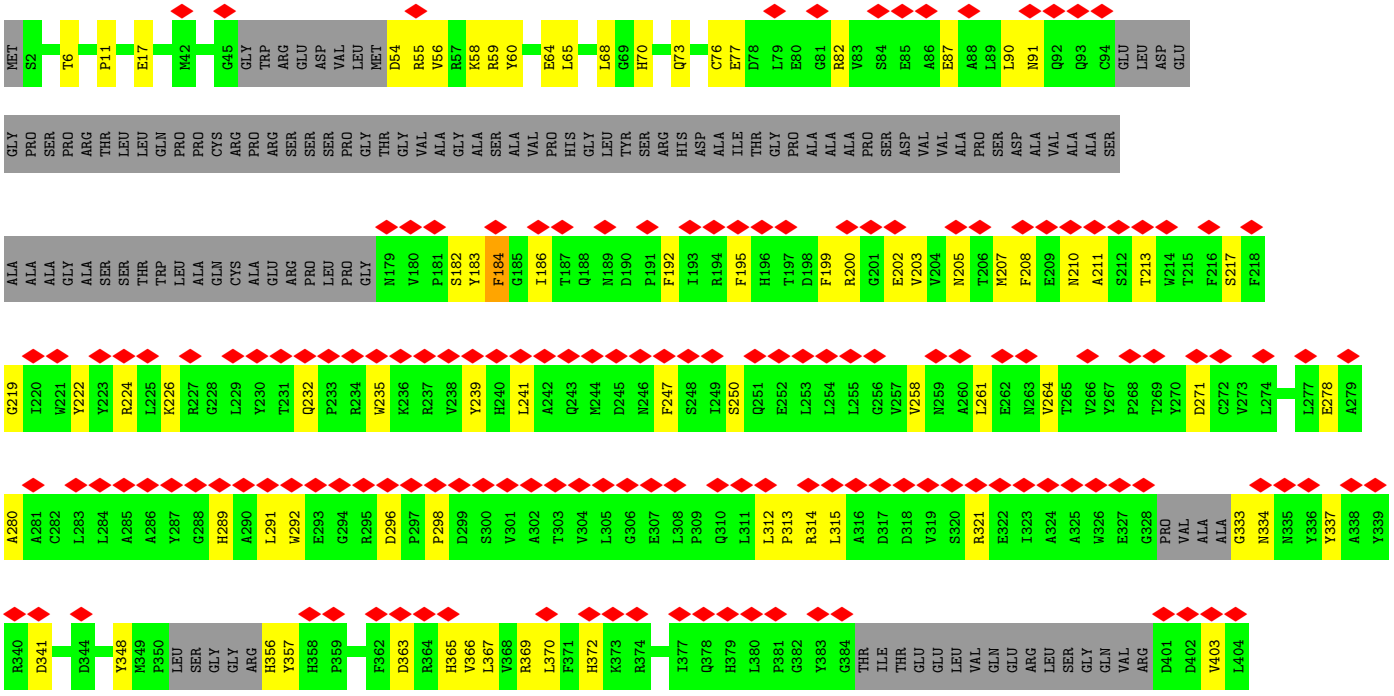
• Molecule 5: Capsid vertex component 2

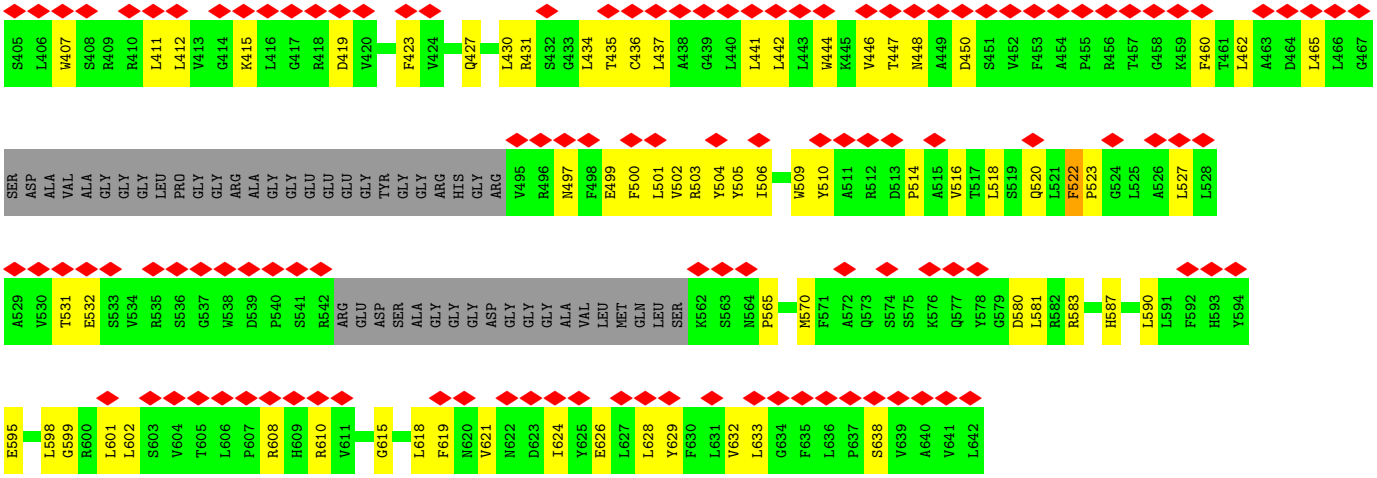
Chain E: 11% 87%



• Molecule 5: Capsid vertex component 2

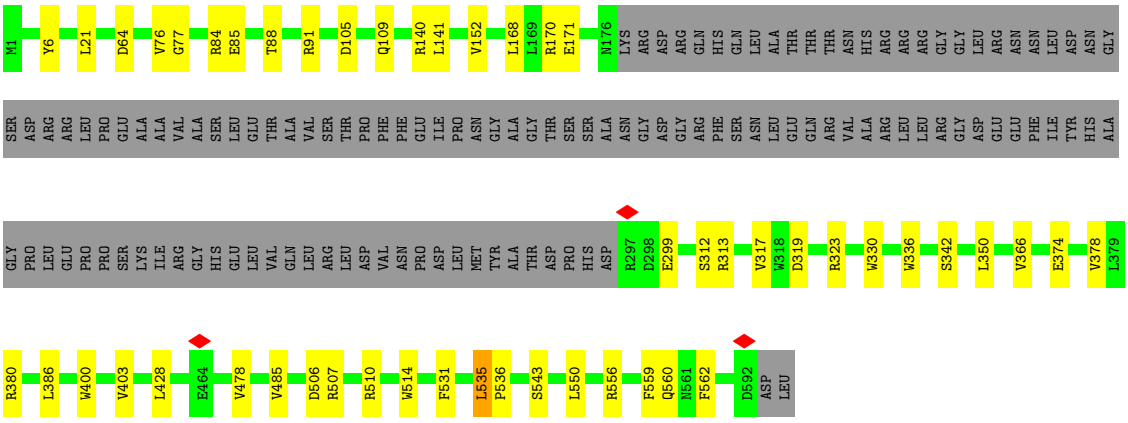
Chain F:





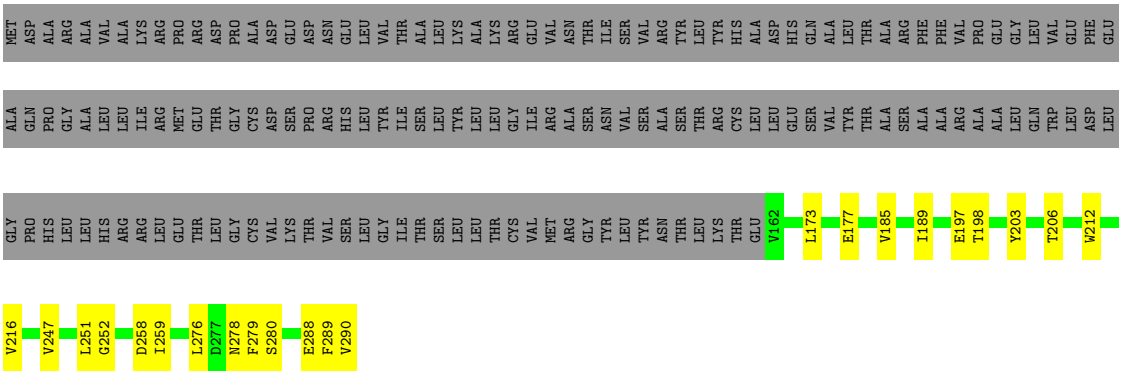
• Molecule 6: Capsid vertex component 1

Chain G:



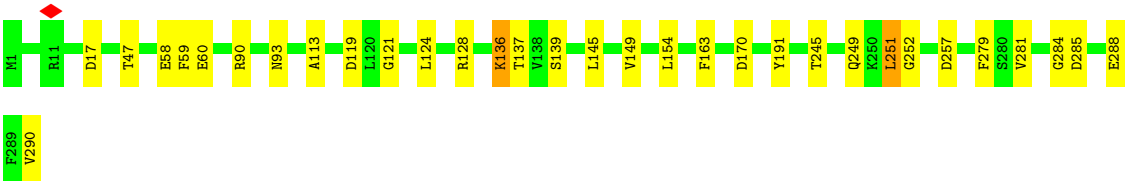
• Molecule 7: Triplex capsid protein 1

Chain T:



• Molecule 7: Triplex capsid protein 1

Chain W:

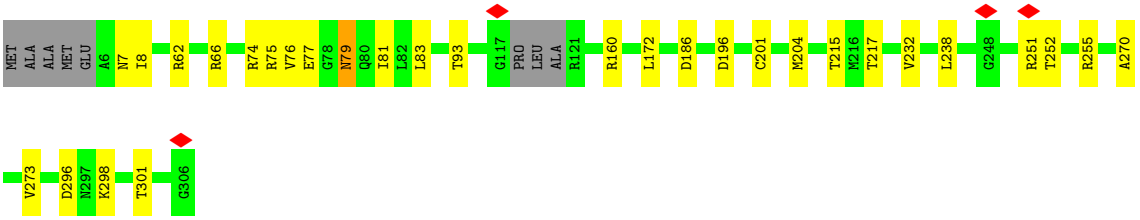


• Molecule 8: Triplex capsid protein 2

Chain U:

• Molecule 8: Triplex capsid protein 2

Chain V:

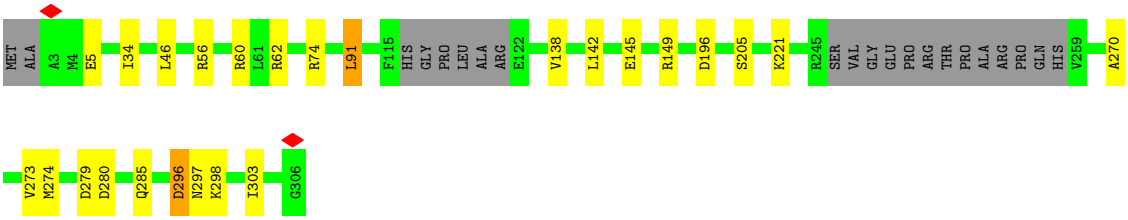


• Molecule 8: Triplex capsid protein 2

Chain X:

• Molecule 8: Triplex capsid protein 2

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	355778	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 ($e^-/Å^2$)	47.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0045	Depositor
Map size (Å)	489.6, 489.6, 489.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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	1	0.30	0/10613	0.51	0/14458
1	H	0.30	0/10824	0.52	0/14743
1	I	0.30	0/10949	0.51	0/14916
1	J	0.29	0/10682	0.51	0/14553
1	K	0.31	0/10962	0.51	0/14933
1	L	0.30	0/10949	0.51	0/14916
1	M	0.29	0/10949	0.51	0/14916
2	2	0.27	0/520	0.57	0/697
2	N	0.26	0/520	0.52	0/697
2	O	0.26	0/520	0.51	0/697
2	P	0.27	0/520	0.55	0/697
2	Q	0.26	0/520	0.56	0/697
2	R	0.26	0/520	0.53	0/697
2	S	0.25	0/520	0.52	0/697
3	3	0.27	0/2366	0.51	0/3192
3	Z	0.28	0/2358	0.53	0/3182
4	A	0.26	0/357	0.49	0/482
4	C	0.25	0/303	0.50	0/407
5	E	0.27	0/690	0.54	0/927
5	F	0.25	0/3995	0.52	0/5426
6	G	0.30	0/3962	0.59	0/5371
7	T	0.30	0/1093	0.53	0/1481
7	W	0.32	0/2374	0.56	1/3221 (0.0%)
8	U	0.29	0/2453	0.53	0/3332
8	V	0.28	0/2414	0.53	0/3277
8	X	0.28	0/2379	0.52	1/3230 (0.0%)
8	Y	0.28	0/2305	0.52	0/3126
All	All	0.29	0/106617	0.52	2/144968 (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	1	0	1
1	H	0	2
1	I	0	1
1	K	0	1
1	L	0	1
1	M	0	1
6	G	0	1
8	Y	0	1
All	All	0	9

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	W	251	LEU	CA-CB-CG	5.38	127.69	115.30
8	X	159	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	1100	ASN	Peptide
6	G	77	GLY	Peptide
1	H	1100	ASN	Peptide
1	H	265	SER	Peptide
1	I	265	SER	Peptide
1	K	265	SER	Peptide
1	L	1100	ASN	Peptide
1	M	1100	ASN	Peptide
8	Y	296	ASP	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	1	10362	0	10310	51	0
1	H	10574	0	10522	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	10693	0	10635	70	0
1	J	10433	0	10379	81	0
1	K	10705	0	10641	67	0
1	L	10693	0	10635	72	0
1	M	10693	0	10635	82	0
2	2	513	0	539	3	0
2	N	513	0	539	5	0
2	O	513	0	539	5	0
2	P	513	0	539	15	0
2	Q	513	0	539	4	0
2	R	513	0	539	9	0
2	S	513	0	539	6	0
3	3	2328	0	2363	10	0
3	Z	2320	0	2351	27	0
4	A	354	0	384	11	0
4	C	301	0	323	8	0
5	E	681	0	674	11	0
5	F	3893	0	3823	101	0
6	G	3873	0	3792	28	0
7	T	1067	0	1076	15	0
7	W	2325	0	2363	20	0
8	U	2406	0	2495	16	0
8	V	2369	0	2456	18	0
8	X	2334	0	2431	13	0
8	Y	2266	0	2355	14	0
All	All	104261	0	104416	766	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 (766) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:575:THR:HG21	1:K:1007:THR:HA	1.58	0.85
5:F:450:ASP:HB2	5:F:624:ILE:HG13	1.62	0.80
3:Z:230:GLU:OE2	3:Z:231:ARG:NH1	2.16	0.79
1:K:1193:ARG:NH2	1:K:1214:ILE:O	2.15	0.79
1:I:1152:THR:HG21	7:W:113:ALA:HB2	1.65	0.79
1:I:575:THR:HG21	1:I:1007:THR:HA	1.67	0.76
1:M:575:THR:HG21	1:M:1007:THR:HA	1.67	0.75
5:F:369:ARG:HA	5:F:372:HIS:CE1	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:296:ASP:O	8:Y:298:LYS:N	2.20	0.73
6:G:76:VAL:O	6:G:556:ARG:NH2	2.21	0.73
1:H:600:THR:HG22	1:H:644:LEU:HB2	1.69	0.72
5:F:565:PRO:HB2	5:F:590:LEU:HD13	1.71	0.72
1:H:866:THR:OG1	1:H:870:THR:O	2.08	0.72
5:F:442:LEU:HD12	5:F:602:LEU:HD13	1.71	0.71
7:T:258:ASP:OD2	7:T:278:ASN:N	2.22	0.71
4:A:2233:GLN:HB3	5:F:581:LEU:HB2	1.71	0.71
7:T:185:VAL:HG12	7:T:206:THR:HG22	1.72	0.71
7:T:290:VAL:HG22	8:U:277:GLN:HG2	1.72	0.71
5:F:291:LEU:HD13	5:F:314:ARG:HH11	1.56	0.70
1:J:390:ASP:OD1	1:J:1039:THR:OG1	2.09	0.70
5:F:200:ARG:NH2	5:F:520:GLN:O	2.25	0.70
1:M:1044:VAL:HG23	1:M:1099:VAL:HB	1.74	0.70
5:F:369:ARG:HD3	5:F:372:HIS:HE1	1.56	0.69
5:F:505:TYR:HA	5:F:509:TRP:HD1	1.57	0.69
1:J:600:THR:HG22	1:J:644:LEU:HB2	1.75	0.69
1:K:169:ASP:OD2	1:K:173:ARG:NH1	2.26	0.68
4:C:2228:VAL:HG23	5:F:68:LEU:HD11	1.77	0.67
1:H:159:THR:HG21	1:L:45:ARG:HH21	1.60	0.66
5:F:365:HIS:HE1	5:F:367:LEU:HB2	1.59	0.66
6:G:506:ASP:OD1	6:G:507:ARG:N	2.28	0.66
3:Z:32:GLU:OE2	3:Z:227:ARG:NH1	2.29	0.66
5:F:365:HIS:CE1	5:F:367:LEU:HB2	2.31	0.66
1:L:763:ASP:O	1:L:765:PRO:HD2	1.95	0.65
1:H:1044:VAL:HG12	1:H:1099:VAL:HG22	1.79	0.65
1:L:596:LEU:O	1:L:600:THR:HG23	1.97	0.65
1:K:1029:HIS:ND1	1:K:1030:PRO:O	2.28	0.65
1:K:263:THR:HG22	1:K:296:VAL:HG12	1.76	0.64
1:K:101:ALA:HB3	1:L:174:GLY:HA3	1.79	0.64
5:F:239:TYR:OH	5:F:570:MET:SD	2.56	0.64
1:J:212:ARG:NH2	1:J:1203:ASP:OD1	2.26	0.63
1:M:804:LEU:HA	1:M:807:LEU:HB3	1.80	0.63
1:1:51:GLU:N	1:1:51:GLU:OE1	2.31	0.63
1:K:1327:THR:HG21	1:K:1333:MET:HB2	1.80	0.63
1:I:212:ARG:NH2	1:I:1203:ASP:OD1	2.30	0.63
8:U:290:VAL:HG12	8:U:302:CYS:SG	2.39	0.63
1:1:83:LEU:HD13	1:1:1060:ASN:HB3	1.80	0.63
4:A:2231:THR:HG21	5:E:68:LEU:HD13	1.81	0.62
1:H:265:SER:O	1:H:267:ALA:N	2.33	0.62
5:F:366:VAL:HG23	5:F:367:LEU:HD12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:369:ARG:HD3	5:F:372:HIS:CE1	2.34	0.62
1:1:441:ASP:OD1	1:1:442:PHE:N	2.33	0.62
5:F:460:PHE:HD2	5:F:626:GLU:HG2	1.65	0.62
1:J:757:LEU:HD22	2:P:62:LEU:HD23	1.82	0.62
1:H:1057:VAL:HG12	1:H:1083:THR:HG22	1.81	0.62
1:K:315:ALA:HB2	1:K:321:ILE:HD11	1.80	0.62
1:K:1041:THR:HG23	1:K:1103:ARG:HB3	1.83	0.61
1:1:443:VAL:HG22	1:1:1024:THR:HG22	1.82	0.61
8:X:212:SER:HB3	8:X:267:ARG:HD2	1.82	0.61
1:M:638:MET:SD	1:M:864:VAL:HG23	2.41	0.60
1:I:265:SER:O	1:I:267:ALA:N	2.34	0.60
1:K:571:HIS:O	1:K:575:THR:HG23	2.01	0.60
1:M:138:TYR:O	1:M:153:ASN:ND2	2.34	0.60
1:M:710:LEU:HD21	1:M:783:VAL:HG22	1.82	0.60
5:E:28:GLU:N	5:E:28:GLU:OE1	2.34	0.60
3:Z:13:VAL:O	3:Z:17:VAL:HG12	2.01	0.60
5:F:446:VAL:HG22	5:F:608:ARG:HH11	1.67	0.60
1:K:1124:HIS:HB3	1:K:1127:VAL:HG12	1.83	0.60
7:W:257:ASP:HB2	8:X:1:MET:HB2	1.84	0.59
1:I:571:HIS:O	1:I:575:THR:HG23	2.02	0.59
5:F:431:ARG:NH2	5:F:595:GLU:OE2	2.35	0.59
1:L:138:TYR:O	1:L:153:ASN:ND2	2.35	0.59
1:I:1038:ARG:NH1	1:I:1040:ASP:OD2	2.36	0.59
7:W:58:GLU:N	7:W:60:GLU:OE1	2.32	0.58
1:1:538:ASP:OD2	1:1:988:ARG:NH1	2.36	0.58
1:I:627:ILE:HG22	1:I:630:PHE:HB3	1.84	0.58
1:H:188:PRO:HA	1:H:1286:LEU:HD21	1.86	0.58
1:J:819:LEU:HD11	2:P:32:ILE:HD13	1.84	0.58
1:M:575:THR:HG22	1:M:1010:ALA:HB3	1.85	0.58
5:F:73:GLN:O	5:F:77:GLU:HG2	2.04	0.58
1:K:124:PRO:HA	1:K:1080:ASN:HA	1.85	0.58
1:L:631:VAL:O	1:L:635:ILE:HG23	2.03	0.58
1:I:1121:VAL:HG12	1:I:1132:ARG:HH21	1.68	0.58
1:K:885:PHE:O	1:K:887:GLY:N	2.35	0.58
1:M:571:HIS:O	1:M:575:THR:HG23	2.02	0.58
7:T:173:LEU:HD22	7:T:203:TYR:HB3	1.85	0.58
1:1:890:VAL:HA	1:1:919:ASN:HB2	1.86	0.58
5:F:518:LEU:HG	5:F:522:PHE:HD2	1.68	0.57
1:L:572:GLU:HG2	1:L:1007:THR:HG21	1.86	0.57
1:I:947:THR:HG22	1:I:967:HIS:CE1	2.38	0.57
1:M:1175:ILE:HG22	1:M:1244:TYR:HE2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:212:ARG:NH2	1:M:1203:ASP:OD1	2.36	0.57
1:H:433:ARG:NH2	1:H:1102:VAL:O	2.36	0.57
2:P:44:LEU:O	2:P:48:THR:OG1	2.16	0.57
7:W:121:GLY:H	7:W:128:ARG:HH12	1.52	0.57
1:M:1124:HIS:HB3	1:M:1127:VAL:HG22	1.86	0.57
1:1:263:THR:OG1	1:1:294:GLU:OE1	2.18	0.57
1:J:315:ALA:HB2	1:J:321:ILE:HD11	1.87	0.57
7:W:93:ASN:ND2	7:W:170:ASP:O	2.38	0.57
8:Y:91:LEU:HA	8:Y:303:ILE:HA	1.87	0.57
4:A:2210:ALA:O	4:A:2214:LEU:HG	2.04	0.57
5:F:441:LEU:HD11	5:F:602:LEU:HD21	1.86	0.57
6:G:386:LEU:HD11	6:G:535:LEU:HD21	1.86	0.57
5:F:580:ASP:HA	5:F:583:ARG:HE	1.69	0.56
3:Z:67:ARG:NH2	3:Z:265:ASP:OD1	2.37	0.56
3:Z:5:PHE:HZ	3:Z:16:LEU:HD21	1.71	0.56
4:A:2224:LEU:HD21	5:E:75:TYR:HB3	1.86	0.56
1:K:265:SER:O	1:K:267:ALA:N	2.37	0.56
1:1:753:ASP:OD2	1:1:756:ARG:NH1	2.38	0.56
1:I:1164:THR:HG23	1:J:209:ARG:HH21	1.70	0.56
1:H:862:GLU:O	1:H:866:THR:HG22	2.06	0.56
1:I:575:THR:HG22	1:I:1010:ALA:HB3	1.86	0.56
5:F:435:THR:HG23	5:F:598:LEU:HD21	1.87	0.56
1:I:545:ASN:ND2	1:I:545:ASN:O	2.37	0.56
8:V:296:ASP:OD2	8:V:298:LYS:NZ	2.27	0.56
1:I:1165:VAL:HG21	1:J:1223:GLN:HB2	1.87	0.56
1:L:447:LYS:HD2	1:L:1112:ASP:HB3	1.88	0.56
1:J:631:VAL:O	1:J:635:ILE:HG23	2.06	0.55
1:L:1111:GLN:HB3	1:L:1171:ALA:HB1	1.88	0.55
8:Y:285:GLN:N	8:Y:285:GLN:OE1	2.39	0.55
3:Z:5:PHE:CZ	3:Z:16:LEU:HD21	2.41	0.55
1:J:96:GLN:HG2	1:J:113:THR:HG22	1.88	0.55
1:J:710:LEU:HD21	1:J:783:VAL:HG22	1.88	0.55
1:J:805:LYS:HE3	2:P:58:CYS:HB2	1.87	0.55
8:X:163:GLU:N	8:X:163:GLU:OE1	2.38	0.55
1:L:420:VAL:HG11	1:L:577:GLU:HA	1.88	0.55
2:S:15:ASP:O	2:S:19:ARG:HG2	2.05	0.55
6:G:366:VAL:HG11	6:G:550:LEU:HD21	1.89	0.55
1:J:425:PRO:HB3	1:J:1328:THR:OG1	2.07	0.55
1:L:600:THR:HG22	1:L:644:LEU:HB2	1.88	0.55
1:M:627:ILE:HG22	1:M:630:PHE:HB3	1.88	0.55
1:1:277:ALA:O	1:1:281:GLN:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1041:THR:HG23	1:1:1103:ARG:HB3	1.88	0.55
1:H:89:GLY:HA2	1:H:120:SER:H	1.72	0.55
1:M:1139:ARG:HD2	1:M:1140:PRO:HD2	1.89	0.55
5:F:505:TYR:HA	5:F:509:TRP:CD1	2.41	0.55
1:M:753:ASP:OD2	1:M:756:ARG:NE	2.29	0.55
1:J:751:VAL:O	2:P:66:ARG:NH1	2.34	0.55
7:T:189:ILE:HG12	7:T:247:VAL:HG22	1.89	0.54
1:H:1287:LEU:HD23	1:H:1288:ARG:HB2	1.89	0.54
1:I:861:VAL:HG13	1:I:865:ALA:HB3	1.89	0.54
1:J:753:ASP:OD2	1:J:756:ARG:NE	2.31	0.54
1:M:682:ARG:NH2	1:M:776:ASP:OD2	2.38	0.54
3:Z:166:ARG:NH2	3:Z:185:ASP:O	2.39	0.54
5:F:460:PHE:CD2	5:F:626:GLU:HG2	2.43	0.54
1:J:1350:HIS:N	1:J:1353:ASN:O	2.40	0.54
1:J:1044:VAL:HG11	1:J:1096:VAL:HG13	1.90	0.54
8:V:93:THR:HG22	8:V:301:THR:HG22	1.89	0.54
1:J:462:GLN:O	1:J:466:GLU:HG2	2.08	0.54
1:1:148:LEU:HD23	1:1:148:LEU:H	1.70	0.53
5:E:35:LEU:HD11	6:G:380:ARG:HD3	1.90	0.53
5:F:183:TYR:HB2	5:F:192:PHE:HB3	1.91	0.53
5:F:312:LEU:HD11	5:F:444:TRP:CD2	2.43	0.53
2:R:34:GLU:HG3	2:R:44:LEU:HD12	1.90	0.53
1:1:209:ARG:HD3	1:1:1201:ALA:HB2	1.90	0.53
1:K:1044:VAL:HG11	1:K:1096:VAL:HG13	1.91	0.53
5:F:207:MET:HE1	5:F:465:LEU:HD22	1.90	0.53
2:R:44:LEU:O	2:R:48:THR:OG1	2.26	0.53
3:3:163:GLU:HB3	3:3:186:LEU:HD11	1.90	0.53
1:H:45:ARG:HH21	1:L:159:THR:HG21	1.72	0.53
1:H:1113:LEU:HA	1:H:1116:VAL:HG22	1.89	0.53
7:W:136:LYS:O	7:W:137:THR:HG23	2.08	0.53
3:3:276:ASP:OD1	3:3:276:ASP:N	2.41	0.53
1:H:379:THR:HG23	1:I:99:ARG:HA	1.89	0.53
1:L:1034:LEU:HD12	1:L:1174:LEU:HB3	1.89	0.53
2:P:18:HIS:CE1	2:P:44:LEU:HD13	2.43	0.53
1:J:596:LEU:O	1:J:600:THR:HG23	2.09	0.53
7:W:252:GLY:HA3	7:W:279:PHE:CE1	2.43	0.53
1:I:1039:THR:HG21	1:I:1259:TYR:HE2	1.74	0.53
1:L:447:LYS:HB3	1:L:1112:ASP:HB3	1.91	0.53
1:L:1139:ARG:HD3	1:L:1140:PRO:HD2	1.91	0.53
1:K:941:ARG:HD3	1:K:992:SER:HB2	1.91	0.53
8:X:71:THR:HG22	8:X:85:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:5:GLU:OE2	8:Y:74:ARG:NH1	2.41	0.53
5:F:337:TYR:CZ	5:F:367:LEU:HD11	2.43	0.53
7:T:252:GLY:HA3	7:T:279:PHE:CZ	2.44	0.53
1:H:596:LEU:O	1:H:600:THR:HG23	2.09	0.53
1:H:761:ASP:OD1	1:H:889:HIS:ND1	2.30	0.53
1:H:1193:ARG:NH2	1:H:1195:ARG:HB3	2.24	0.53
1:1:1177:THR:HG22	1:1:1230:ASN:ND2	2.24	0.52
3:3:178:MET:HE1	3:3:217:TRP:HB2	1.91	0.52
5:F:312:LEU:HG	5:F:313:PRO:HD3	1.89	0.52
1:I:517:VAL:HG12	1:I:520:ASP:HB2	1.90	0.52
6:G:140:ARG:HG2	6:G:342:SER:HB3	1.91	0.52
7:W:279:PHE:CE2	7:W:281:VAL:HG12	2.44	0.52
3:3:284:GLN:N	3:3:284:GLN:OE1	2.43	0.52
5:F:356:HIS:HA	5:F:427:GLN:HE21	1.74	0.52
5:F:217:SER:N	5:F:638:SER:O	2.42	0.52
1:J:1327:THR:HB	1:J:1355:VAL:HG13	1.91	0.52
1:M:446:LEU:HD22	1:M:1021:VAL:HG12	1.91	0.52
8:V:217:THR:HG22	8:V:255:ARG:HH21	1.74	0.52
3:Z:259:GLU:N	3:Z:259:GLU:OE1	2.42	0.52
6:G:428:LEU:HD11	6:G:559:PHE:HE1	1.75	0.52
1:K:710:LEU:HD21	1:K:783:VAL:HG22	1.91	0.52
1:M:1037:VAL:HG21	1:M:1262:CYS:HB3	1.91	0.52
8:X:145:GLU:O	8:X:149:ARG:HG2	2.10	0.52
5:F:499:GLU:OE2	5:F:503:ARG:NH1	2.42	0.52
1:1:397:VAL:HG13	1:1:1034:LEU:HB2	1.92	0.52
1:I:682:ARG:O	1:I:685:THR:HG22	2.09	0.52
1:L:1285:TYR:HA	1:L:1289:ALA:HB3	1.92	0.52
3:Z:36:LYS:HA	3:Z:39:LYS:HE2	1.91	0.52
1:I:1043:GLU:OE2	1:I:1101:ARG:NH1	2.37	0.51
1:J:1318:THR:HG23	1:J:1320:GLU:HG2	1.91	0.51
1:K:1064:VAL:HG22	1:K:1077:VAL:HG12	1.91	0.51
1:L:941:ARG:HG2	1:L:992:SER:HB3	1.91	0.51
3:Z:15:ALA:HA	3:Z:18:ASN:ND2	2.25	0.51
1:1:274:VAL:HG12	1:1:370:GLU:HB3	1.92	0.51
1:K:95:VAL:HG13	1:K:114:ILE:HB	1.92	0.51
8:U:88:HIS:CD2	8:U:306:GLY:H	2.28	0.51
7:W:245:THR:HG22	7:W:290:VAL:HA	1.91	0.51
3:3:259:GLU:N	3:3:259:GLU:OE1	2.43	0.51
4:C:2228:VAL:O	4:C:2232:ILE:HG12	2.09	0.51
5:F:411:LEU:HD12	5:F:412:LEU:HG	1.93	0.51
6:G:313:ARG:HB2	6:G:330:TRP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:627:ILE:HG22	1:J:630:PHE:HB3	1.92	0.51
1:K:155:GLU:O	1:K:159:THR:HG23	2.10	0.51
2:R:19:ARG:HA	2:R:22:VAL:HG12	1.92	0.51
1:K:121:GLU:O	1:K:1082:ASN:ND2	2.43	0.51
1:M:646:VAL:HG12	1:M:647:PHE:CD2	2.45	0.51
1:M:77:ALA:HB1	1:M:302:TYR:HD1	1.75	0.51
1:L:584:LEU:HD12	1:L:687:ILE:HD11	1.92	0.51
1:M:800:LEU:HD23	1:M:923:VAL:HG21	1.91	0.51
1:M:1104:THR:HG22	1:M:1168:GLN:HB3	1.92	0.51
2:S:19:ARG:HA	2:S:22:VAL:HG12	1.93	0.51
8:X:114:LEU:HD13	8:X:182:PHE:HB3	1.93	0.51
8:Y:34:ILE:HD11	8:Y:46:LEU:HD23	1.93	0.51
1:I:138:TYR:O	1:I:153:ASN:ND2	2.40	0.51
1:I:553:THR:HG21	1:I:983:TYR:O	2.11	0.51
1:J:553:THR:HG21	1:J:983:TYR:O	2.11	0.51
1:J:618:HIS:HE1	1:J:769:ASP:OD2	1.93	0.51
1:L:1069:ARG:HH22	1:L:1074:THR:HG22	1.76	0.51
1:1:75:ALA:HB2	1:1:179:PHE:CZ	2.46	0.51
6:G:374:GLU:O	6:G:378:VAL:HG12	2.11	0.51
1:J:611:TYR:CZ	1:J:923:VAL:HG23	2.45	0.50
3:Z:102:ALA:O	3:Z:106:LEU:HD23	2.10	0.50
5:F:531:THR:HG21	5:F:618:LEU:HD13	1.94	0.50
1:H:785:TYR:O	1:H:943:TYR:OH	2.25	0.50
1:H:664:GLY:O	1:H:666:LEU:N	2.44	0.50
2:R:17:LYS:O	2:R:21:VAL:HG12	2.11	0.50
2:S:16:GLU:OE1	2:S:16:GLU:N	2.34	0.50
6:G:535:LEU:HB2	6:G:536:PRO:HD2	1.94	0.50
1:L:1178:PRO:HD2	1:L:1230:ASN:OD1	2.12	0.50
2:2:20:HIS:O	2:2:24:VAL:HG12	2.12	0.50
1:I:1369:ASN:OD1	1:I:1370:SER:N	2.44	0.50
1:L:725:ARG:NH1	1:L:775:ASP:OD1	2.44	0.50
8:Y:145:GLU:HG3	8:Y:149:ARG:HD2	1.93	0.50
1:M:610:CYS:SG	1:M:646:VAL:HG13	2.52	0.50
1:1:739:LEU:O	1:1:740:ASN:ND2	2.45	0.50
1:I:793:THR:HG22	1:I:796:ARG:HB2	1.94	0.50
1:J:682:ARG:NH2	1:J:776:ASP:OD2	2.27	0.50
1:L:212:ARG:NH2	1:L:1203:ASP:OD1	2.44	0.50
5:F:219:GLY:HA3	5:F:619:PHE:HA	1.93	0.49
1:I:1177:THR:HG22	1:I:1230:ASN:ND2	2.27	0.49
1:I:1359:ILE:HG23	1:I:1360:ILE:HG23	1.94	0.49
5:F:615:GLY:HA3	5:F:621:VAL:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:180:LEU:HD23	1:K:384:PRO:HG2	1.94	0.49
1:L:1113:LEU:HA	1:L:1116:VAL:HG12	1.94	0.49
3:Z:105:HIS:HA	3:Z:108:VAL:HG12	1.94	0.49
1:H:1360:ILE:O	1:H:1362:LEU:N	2.43	0.49
1:L:753:ASP:OD2	1:L:756:ARG:HD3	2.13	0.49
8:U:65:LEU:HD21	8:U:110:VAL:HG22	1.93	0.49
3:Z:31:LEU:HD12	3:Z:62:TYR:CG	2.47	0.49
1:L:39:TYR:CZ	8:U:295:PRO:HG2	2.47	0.49
8:Y:56:ARG:HG2	8:Y:60:ARG:HD2	1.94	0.49
1:1:199:ASN:O	1:1:203:ALA:N	2.45	0.49
1:I:785:TYR:O	1:I:943:TYR:OH	2.25	0.49
5:F:232:GLN:HB3	5:F:235:TRP:HD1	1.76	0.49
5:F:235:TRP:HB3	5:F:239:TYR:CE2	2.47	0.49
1:I:805:LYS:HE2	2:O:58:CYS:HB2	1.95	0.49
1:J:311:ASN:HB3	1:J:321:ILE:HD12	1.95	0.49
2:P:55:ASN:OD1	2:P:55:ASN:N	2.44	0.49
6:G:85:GLU:O	6:G:88:THR:HG22	2.12	0.49
1:H:668:PRO:HB2	1:I:643:GLN:HG2	1.93	0.49
1:L:280:MET:O	1:L:284:MET:HG2	2.13	0.49
1:M:634:CYS:O	1:M:638:MET:HG2	2.12	0.49
8:X:219:VAL:HG23	8:Y:205:SER:HB3	1.92	0.49
1:I:167:THR:HG21	1:I:1077:VAL:HG21	1.94	0.49
2:P:18:HIS:HE1	2:P:44:LEU:HD13	1.77	0.49
1:1:257:ASN:OD1	1:1:259:THR:HG22	2.13	0.49
1:J:441:ASP:OD1	1:J:443:VAL:HG12	2.12	0.49
1:L:124:PRO:HG2	8:X:40:LEU:HD21	1.95	0.49
7:W:251:LEU:HD12	7:W:251:LEU:O	2.13	0.49
5:F:366:VAL:O	5:F:369:ARG:HB2	2.13	0.49
1:J:554:PRO:HD3	1:J:907:LEU:HD12	1.95	0.49
1:J:1113:LEU:HA	1:J:1116:VAL:HG12	1.94	0.48
2:N:38:PRO:O	2:N:42:THR:HG23	2.13	0.48
2:Q:55:ASN:OD1	2:Q:55:ASN:N	2.46	0.48
6:G:168:LEU:HD23	6:G:317:VAL:HG11	1.95	0.48
1:H:317:SER:O	1:H:321:ILE:HG12	2.13	0.48
1:J:1144:ASP:OD1	1:J:1144:ASP:N	2.45	0.48
1:L:608:GLU:CD	1:L:928:LYS:H	2.17	0.48
1:M:618:HIS:O	1:M:618:HIS:ND1	2.47	0.48
1:M:1349:THR:HA	1:M:1354:TYR:HA	1.94	0.48
4:A:2225:ALA:HB2	5:F:76:CYS:SG	2.53	0.48
6:G:400:TRP:HA	6:G:403:VAL:HG12	1.95	0.48
1:H:642:ARG:HB2	1:H:644:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1038:ARG:NH1	1:H:1040:ASP:OD2	2.43	0.48
1:L:862:GLU:O	1:L:866:THR:OG1	2.21	0.48
1:M:789:MET:HB3	1:M:790:PRO:HD3	1.95	0.48
2:P:18:HIS:CE1	2:P:44:LEU:HB2	2.48	0.48
2:P:32:ILE:HD11	2:P:37:HIS:HB2	1.94	0.48
3:3:162:THR:O	3:3:165:GLN:HG3	2.14	0.48
1:K:475:MET:HG2	1:K:527:ILE:HG23	1.96	0.48
1:M:1175:ILE:HG22	1:M:1244:TYR:CE2	2.47	0.48
1:1:1247:ARG:HH12	1:1:1248:HIS:CE1	2.31	0.48
5:F:182:SER:HB3	5:F:195:PHE:O	2.14	0.48
6:G:6:TYR:HB2	8:V:232:VAL:HG22	1.96	0.48
1:J:927:PRO:HD2	1:J:952:LEU:HD11	1.96	0.48
1:L:495:ILE:HD12	1:L:976:PRO:HG2	1.94	0.48
1:L:610:CYS:SG	1:L:646:VAL:HB	2.52	0.48
1:1:19:PHE:O	1:1:23:VAL:HG22	2.14	0.48
5:F:17:GLU:N	5:F:17:GLU:OE1	2.47	0.48
5:F:333:GLY:O	5:F:334:ASN:ND2	2.46	0.48
1:I:502:ARG:NH2	1:I:958:ARG:HD2	2.29	0.48
1:K:575:THR:HG22	1:K:1010:ALA:HB3	1.95	0.48
1:1:726:ASN:OD1	1:1:728:GLU:HG2	2.14	0.48
5:F:366:VAL:O	5:F:370:LEU:HD12	2.13	0.48
5:F:369:ARG:HH11	5:F:372:HIS:HE1	1.60	0.48
5:F:444:TRP:O	5:F:448:ASN:ND2	2.46	0.48
4:C:2215:ARG:HD2	4:C:2215:ARG:HA	1.67	0.48
5:F:224:ARG:HH22	5:F:618:LEU:HD22	1.78	0.48
1:H:155:GLU:O	1:H:159:THR:HG23	2.14	0.48
1:H:800:LEU:HD11	1:H:934:SER:HB2	1.94	0.48
7:W:279:PHE:HE2	7:W:281:VAL:HG12	1.79	0.48
8:Y:270:ALA:HA	8:Y:273:VAL:HG12	1.96	0.48
1:I:473:PRO:HA	1:I:476:GLN:HG2	1.96	0.48
1:J:502:ARG:NE	1:J:962:GLU:OE2	2.47	0.48
6:G:64:ASP:OD1	6:G:84:ARG:NH1	2.47	0.47
1:H:1291:ASP:OD1	1:H:1316:ARG:NH1	2.44	0.47
1:K:618:HIS:ND1	1:K:618:HIS:O	2.47	0.47
1:L:554:PRO:HD3	1:L:907:LEU:HD12	1.96	0.47
2:R:16:GLU:OE1	2:R:16:GLU:N	2.45	0.47
1:J:594:LEU:HD21	1:J:680:VAL:HG21	1.95	0.47
1:H:538:ASP:OD2	1:H:988:ARG:NH1	2.46	0.47
1:M:147:ILE:O	1:M:151:ILE:HG12	2.15	0.47
5:F:184:PHE:HB3	5:F:504:TYR:CD2	2.49	0.47
5:F:430:LEU:O	5:F:434:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:607:PRO:HG2	1:M:610:CYS:SG	2.55	0.47
2:P:16:GLU:HA	2:P:19:ARG:NH1	2.28	0.47
3:Z:63:TYR:HB2	3:Z:224:CYS:SG	2.54	0.47
5:F:55:ARG:HH12	5:F:59:ARG:HH11	1.63	0.47
1:K:1115:ARG:NH1	1:K:1138:GLU:OE2	2.35	0.47
1:1:306:VAL:HG23	1:K:49:HIS:HA	1.96	0.47
1:1:363:GLY:O	1:1:364:GLU:HG3	2.14	0.47
1:J:1044:VAL:CG1	1:J:1096:VAL:HG13	2.45	0.47
1:L:155:GLU:O	1:L:159:THR:HG23	2.14	0.47
1:M:635:ILE:HD11	1:M:666:LEU:HD21	1.95	0.47
1:1:553:THR:HG21	1:1:983:TYR:O	2.15	0.47
6:G:105:ASP:O	6:G:109:GLN:HG2	2.14	0.47
1:I:712:ASP:O	1:I:782:LYS:NZ	2.48	0.47
1:J:1369:ASN:OD1	1:J:1370:SER:N	2.48	0.47
1:L:1215:TYR:CE2	1:L:1268:THR:HG21	2.50	0.47
1:M:180:LEU:HD22	1:M:372:LEU:HD12	1.96	0.47
1:M:927:PRO:HD2	1:M:952:LEU:HD21	1.97	0.47
8:V:270:ALA:HA	8:V:273:VAL:HG12	1.97	0.47
7:W:154:LEU:HB3	7:W:163:PHE:HB2	1.96	0.47
7:W:285:ASP:OD1	7:W:285:ASP:N	2.44	0.47
3:Z:98:ASP:N	3:Z:98:ASP:OD1	2.45	0.47
1:1:627:ILE:HD11	1:1:882:ALA:HB2	1.95	0.47
3:3:194:THR:HG22	3:3:196:LEU:H	1.79	0.47
1:M:605:ASN:ND2	1:M:642:ARG:HD3	2.30	0.47
7:T:251:LEU:HD12	7:T:251:LEU:O	2.15	0.47
3:Z:188:LEU:HD11	3:Z:198:ASN:HA	1.97	0.47
5:F:363:ASP:HA	5:F:369:ARG:NH2	2.30	0.47
1:J:734:ALA:HB2	1:J:739:LEU:HD11	1.97	0.47
1:L:1003:HIS:O	1:L:1007:THR:HG23	2.15	0.47
5:F:278:GLU:OE2	5:F:415:LYS:NZ	2.44	0.47
1:K:1114:PHE:CD1	1:K:1137:VAL:HG11	2.49	0.47
6:G:312:SER:O	6:G:313:ARG:HG2	2.15	0.46
1:J:646:VAL:HG23	1:J:647:PHE:CD2	2.51	0.46
1:K:263:THR:O	1:K:266:GLY:HA2	2.15	0.46
1:M:698:LEU:HD13	1:M:1127:VAL:HG12	1.98	0.46
4:A:2214:LEU:HD13	5:F:87:GLU:HG3	1.96	0.46
1:J:553:THR:HG23	1:J:910:PHE:CE1	2.51	0.46
1:J:1122:TYR:HB2	1:J:1128:ASP:HB2	1.97	0.46
1:K:212:ARG:NH2	1:K:1203:ASP:OD1	2.48	0.46
1:K:1315:CYS:HA	1:K:1318:THR:HG22	1.96	0.46
1:L:873:LEU:O	1:L:877:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1112:ASP:OD1	1:L:1112:ASP:N	2.39	0.46
6:G:478:VAL:HG23	6:G:485:VAL:HG22	1.97	0.46
1:H:853:VAL:HG21	1:H:872:LEU:HD21	1.97	0.46
1:I:20:LEU:HG	1:I:21:THR:HG23	1.96	0.46
1:I:1276:LYS:HD2	1:I:1280:LYS:HE2	1.95	0.46
1:K:1113:LEU:HA	1:K:1116:VAL:HG22	1.96	0.46
1:L:877:ARG:HH11	1:L:877:ARG:HG2	1.80	0.46
1:1:601:VAL:HG13	1:1:924:VAL:HG11	1.97	0.46
1:I:1121:VAL:HG12	1:I:1132:ARG:NH2	2.31	0.46
1:M:172:GLU:O	1:M:176:ILE:HG12	2.16	0.46
1:M:619:GLY:HA3	1:M:721:THR:HG21	1.97	0.46
3:Z:172:GLU:OE2	3:Z:175:ARG:NH2	2.39	0.46
5:F:55:ARG:NH2	5:F:56:VAL:HG22	2.30	0.46
6:G:319:ASP:OD1	6:G:323:ARG:N	2.47	0.46
1:J:452:PRO:O	1:J:456:GLU:HG2	2.15	0.46
1:K:641:THR:HG23	1:K:642:ARG:HG3	1.96	0.46
5:F:239:TYR:O	5:F:250:SER:OG	2.26	0.46
5:F:289:HIS:HB2	5:F:407:TRP:HE1	1.80	0.46
1:K:491:ALA:O	1:K:495:ILE:HG13	2.16	0.46
2:R:70:VAL:O	2:R:73:THR:HG22	2.14	0.46
8:V:79:ASN:O	8:V:79:ASN:ND2	2.47	0.46
1:J:740:ASN:ND2	1:J:743:ASN:OD1	2.49	0.46
8:U:71:THR:HG22	8:U:85:VAL:HG22	1.98	0.46
7:W:47:THR:HG22	7:W:149:VAL:HG12	1.97	0.46
4:A:2240:LEU:HD23	4:A:2240:LEU:HA	1.83	0.46
5:F:226:LYS:HG3	5:F:241:LEU:HD22	1.97	0.46
1:J:1055:THR:HA	1:J:1086:MET:HG2	1.98	0.46
1:K:37:ILE:O	1:K:46:TYR:HE1	1.99	0.46
1:M:484:GLN:O	1:M:981:HIS:NE2	2.38	0.46
2:S:21:VAL:O	2:S:25:VAL:HB	2.15	0.46
1:1:291:ILE:HD13	1:1:360:ILE:HD13	1.98	0.46
5:F:184:PHE:HB3	5:F:504:TYR:CE2	2.51	0.46
1:I:634:CYS:O	1:I:638:MET:HG2	2.16	0.46
1:I:1034:LEU:HD13	1:I:1174:LEU:HD22	1.97	0.46
1:J:704:SER:HA	1:J:707:VAL:HG12	1.97	0.46
1:M:434:ASP:OD1	1:M:435:ARG:N	2.44	0.46
1:M:1350:HIS:N	1:M:1353:ASN:O	2.47	0.46
2:N:67:MET:HA	2:N:70:VAL:HG12	1.97	0.46
1:J:584:LEU:HD12	1:J:687:ILE:HD11	1.97	0.46
1:L:315:ALA:HB2	1:L:321:ILE:HD11	1.98	0.46
1:M:608:GLU:CD	1:M:929:THR:H	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:2216:LEU:HB3	5:F:82:ARG:HH22	1.81	0.45
1:K:84:ASN:OD1	1:K:1080:ASN:ND2	2.47	0.45
5:F:312:LEU:HD11	5:F:444:TRP:CG	2.51	0.45
1:L:1369:ASN:OD1	1:L:1370:SER:N	2.49	0.45
1:K:867:ASP:OD1	1:K:868:ALA:N	2.48	0.45
1:L:424:LEU:HB2	1:L:573:LEU:HD22	1.99	0.45
1:M:1104:THR:HB	1:M:1170:ALA:HB2	1.97	0.45
8:V:62:ARG:O	8:V:66:ARG:HG2	2.16	0.45
7:W:249:GLN:NE2	7:W:284:GLY:O	2.41	0.45
4:C:2234:HIS:NE2	4:C:2238:LEU:HD12	2.30	0.45
6:G:556:ARG:HD2	6:G:560:GLN:OE1	2.16	0.45
1:J:663:ASP:OD1	1:J:664:GLY:N	2.49	0.45
5:F:348:TYR:O	5:F:357:TYR:OH	2.16	0.45
1:K:538:ASP:OD2	1:K:988:ARG:NH1	2.49	0.45
1:L:1246:THR:HA	1:L:1249:ARG:HB3	1.99	0.45
1:L:861:VAL:HA	1:L:864:VAL:HG22	1.97	0.45
4:C:2227:SER:O	4:C:2231:THR:OG1	2.28	0.45
6:G:170:ARG:HG3	6:G:171:GLU:OE1	2.17	0.45
2:R:52:SER:OG	2:R:53:LEU:N	2.49	0.45
7:T:252:GLY:HA2	7:T:280:SER:O	2.17	0.45
4:C:2214:LEU:HD22	5:E:83:VAL:HG13	1.99	0.45
5:F:54:ASP:OD1	5:F:58:LYS:NZ	2.50	0.45
1:J:178:SER:O	1:J:182:THR:HG23	2.16	0.45
1:L:78:ILE:O	1:L:1058:ILE:HA	2.17	0.45
1:L:927:PRO:HD2	1:L:952:LEU:HD11	1.98	0.45
1:1:130:GLU:OE2	1:1:1072:SER:OG	2.26	0.45
1:I:263:THR:O	1:I:266:GLY:HA2	2.16	0.45
1:J:1042:PHE:CD2	1:J:1102:VAL:HG12	2.52	0.45
1:J:1315:CYS:HA	1:J:1318:THR:HG22	1.99	0.45
8:Y:62:ARG:NH1	8:Y:280:ASP:O	2.50	0.45
3:3:91:GLY:HA3	3:3:106:LEU:HD21	1.98	0.44
4:A:2208:LEU:O	4:A:2212:GLU:HG2	2.16	0.44
5:F:532:GLU:OE2	5:F:601:LEU:HD13	2.17	0.44
1:H:122:LYS:NZ	8:V:77:GLU:OE2	2.50	0.44
1:H:263:THR:OG1	1:H:264:SER:N	2.50	0.44
1:J:558:ILE:HD11	1:J:1031:GLY:HA3	1.98	0.44
1:L:589:ASP:OD1	1:L:591:GLU:HG2	2.16	0.44
8:V:251:ARG:HG3	8:V:252:THR:H	1.81	0.44
5:F:403:VAL:HG12	5:F:407:TRP:CD1	2.51	0.44
5:F:580:ASP:O	5:F:583:ARG:HG2	2.17	0.44
1:I:983:TYR:O	1:I:988:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:40:GLY:HA2	1:K:46:TYR:CE1	2.53	0.44
1:L:80:PHE:HE2	1:L:86:LEU:HD23	1.81	0.44
1:L:396:PRO:HB2	1:L:399:LEU:CD2	2.47	0.44
1:L:553:THR:HG21	1:L:983:TYR:O	2.17	0.44
1:M:311:ASN:HA	1:M:314:THR:HG22	1.99	0.44
8:U:120:ALA:O	8:U:122:GLU:N	2.49	0.44
3:Z:140:VAL:HG13	3:Z:142:GLU:H	1.82	0.44
1:I:194:GLN:HA	1:I:197:VAL:HG12	1.99	0.44
5:E:79:LEU:HD12	5:E:79:LEU:HA	1.84	0.44
1:J:638:MET:HG3	1:J:646:VAL:HG11	2.00	0.44
1:J:1349:THR:HA	1:J:1354:TYR:HA	1.99	0.44
1:K:310:GLU:OE2	1:K:310:GLU:N	2.47	0.44
1:M:4:TRP:CD1	1:M:36:ARG:HG3	2.52	0.44
1:1:307:LEU:HG	1:1:311:ASN:HD21	1.83	0.44
4:A:2238:LEU:HD21	6:G:350:LEU:HD23	2.00	0.44
6:G:152:VAL:HG11	6:G:562:PHE:CE2	2.53	0.44
1:M:545:ASN:O	1:M:545:ASN:ND2	2.46	0.44
4:A:2232:ILE:CD1	5:F:65:LEU:HD22	2.48	0.44
5:E:16:PHE:CD1	5:F:6:THR:HG21	2.52	0.44
5:E:67:ASP:O	5:E:71:ARG:HG3	2.18	0.44
5:F:403:VAL:HG12	5:F:407:TRP:HD1	1.83	0.44
1:H:385:LEU:HD21	1:H:1048:LEU:HD23	1.99	0.44
1:I:434:ASP:OD1	1:I:435:ARG:N	2.50	0.44
8:U:115:PHE:HZ	8:U:119:LEU:HD23	1.83	0.44
1:1:287:LEU:O	1:1:291:ILE:HG12	2.18	0.44
5:F:321:ARG:NH1	2:O:51:SER:OG	2.51	0.44
1:H:941:ARG:HD3	1:H:992:SER:HB2	2.00	0.44
1:I:544:GLU:HG3	1:I:549:VAL:HG21	1.99	0.44
1:I:1215:TYR:CE2	1:I:1268:THR:HG21	2.52	0.44
1:L:712:ASP:O	1:L:782:LYS:NZ	2.51	0.44
1:L:857:LEU:O	1:L:861:VAL:HG12	2.17	0.44
1:M:1285:TYR:HA	1:M:1289:ALA:HB3	2.00	0.44
3:Z:246:ASP:OD1	3:Z:247:SER:N	2.51	0.44
5:F:200:ARG:HH22	5:F:523:PRO:HD3	1.83	0.44
5:F:292:TRP:CZ3	5:F:298:PRO:HG3	2.53	0.44
5:F:580:ASP:HA	5:F:583:ARG:NE	2.33	0.44
6:G:91:ARG:NH1	8:U:159:ASP:OD1	2.44	0.44
1:L:1139:ARG:HD3	1:L:1140:PRO:CD	2.48	0.44
1:M:155:GLU:O	1:M:159:THR:HG23	2.17	0.44
1:M:720:VAL:HG13	1:M:916:VAL:HG21	2.00	0.44
2:N:18:HIS:O	2:N:22:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:44:LEU:O	2:O:48:THR:HG23	2.17	0.44
5:F:337:TYR:CE2	5:F:602:LEU:HD23	2.53	0.44
6:G:170:ARG:HG3	6:G:171:GLU:H	1.82	0.44
1:H:1040:ASP:OD1	1:H:1106:MET:HG2	2.18	0.44
8:V:160:ARG:NH1	8:V:186:ASP:OD2	2.49	0.44
5:F:203:VAL:HG21	5:F:633:LEU:HD21	2.00	0.43
1:H:572:GLU:O	1:H:575:THR:HG22	2.18	0.43
1:J:542:CYS:SG	1:J:543:GLN:N	2.91	0.43
1:J:989:SER:N	1:J:990:PRO:HD2	2.33	0.43
1:K:1210:ALA:O	1:K:1214:ILE:HG23	2.18	0.43
1:M:376:TYR:O	1:M:379:THR:HG23	2.17	0.43
1:M:1292:CYS:HA	1:M:1311:ILE:HG12	1.99	0.43
2:P:21:VAL:HA	2:P:25:VAL:HG23	1.99	0.43
2:S:33:SER:OG	2:S:34:GLU:N	2.51	0.43
1:1:1284:GLU:HB3	1:1:1304:VAL:HG11	2.01	0.43
1:1:1308:GLU:CD	1:1:1308:GLU:H	2.20	0.43
5:F:423:PHE:HB3	5:F:430:LEU:CD1	2.48	0.43
1:I:237:ASP:O	1:I:241:LYS:HG2	2.18	0.43
1:J:155:GLU:O	1:J:159:THR:HG23	2.18	0.43
1:J:452:PRO:HG3	1:J:1122:TYR:CE1	2.53	0.43
1:L:1100:ASN:OD1	1:L:1100:ASN:N	2.51	0.43
1:M:1173:GLU:HG2	1:M:1262:CYS:SG	2.58	0.43
2:N:51:SER:HA	2:N:54:PHE:HE2	1.83	0.43
8:Y:138:VAL:HG13	8:Y:142:LEU:HD23	2.00	0.43
8:Y:270:ALA:O	8:Y:274:MET:HG2	2.18	0.43
1:1:1277:THR:O	1:1:1281:THR:HG23	2.19	0.43
1:K:481:CYS:SG	1:K:508:THR:HA	2.59	0.43
2:N:28:LEU:HG	2:N:29:PRO:HD2	2.01	0.43
1:1:179:PHE:O	1:1:182:THR:HG22	2.19	0.43
5:F:460:PHE:CE1	5:F:465:LEU:HD21	2.53	0.43
1:1:361:ARG:NH2	1:1:364:GLU:HA	2.34	0.43
1:1:949:CYS:HB3	1:1:956:ILE:HD13	2.00	0.43
1:L:1069:ARG:HG2	1:L:1072:SER:O	2.18	0.43
8:U:61:LEU:HD22	8:U:112:PRO:HB3	2.00	0.43
7:W:58:GLU:O	7:W:59:PHE:HB2	2.19	0.43
3:Z:162:THR:O	3:Z:165:GLN:HG3	2.17	0.43
1:H:814:ARG:HG2	1:H:815:PRO:HD2	2.01	0.43
1:H:994:TYR:OH	1:H:1007:THR:HG21	2.17	0.43
1:K:610:CYS:SG	1:K:646:VAL:HG22	2.58	0.43
1:M:159:THR:HG22	1:M:162:ARG:NH2	2.33	0.43
1:M:554:PRO:HD3	1:M:907:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1038:ARG:NH1	1:M:1040:ASP:OD2	2.51	0.43
8:V:215:THR:HG22	8:V:238:LEU:HD11	2.00	0.43
1:H:1133:HIS:CE1	1:I:477:ARG:HE	2.36	0.43
1:K:941:ARG:NH2	1:K:982:GLU:OE1	2.34	0.43
1:L:321:ILE:HD13	1:L:321:ILE:HA	1.83	0.43
1:M:796:ARG:O	1:M:945:ASN:ND2	2.51	0.43
2:Q:69:ALA:O	2:Q:73:THR:HG23	2.19	0.43
8:Y:196:ASP:OD1	8:Y:196:ASP:N	2.52	0.43
5:F:280:ALA:HB2	5:F:436:CYS:HB3	2.00	0.43
5:F:337:TYR:HB2	5:F:599:GLY:HA2	2.01	0.43
1:I:263:THR:OG1	1:I:264:SER:N	2.52	0.43
1:I:775:ASP:O	1:I:779:THR:HG23	2.19	0.43
1:1:553:THR:HG23	1:1:910:PHE:CE1	2.53	0.43
1:1:1029:HIS:ND1	1:1:1030:PRO:O	2.38	0.43
2:2:37:HIS:HB3	2:2:40:LEU:HB3	2.00	0.43
5:F:315:LEU:HD21	5:F:437:LEU:HD21	2.00	0.43
1:I:611:TYR:CZ	1:I:923:VAL:HG23	2.54	0.43
1:K:321:ILE:N	1:L:51:GLU:O	2.51	0.43
1:K:538:ASP:OD1	1:K:555:ARG:NE	2.50	0.43
1:K:756:ARG:HG3	1:K:767:PHE:CE1	2.53	0.43
1:M:229:LEU:HD11	1:M:242:PHE:CE1	2.54	0.43
7:T:212:TRP:CH2	7:T:216:VAL:HG21	2.54	0.43
3:3:1:MET:SD	3:3:2:SER:N	2.92	0.43
5:F:510:TYR:HE1	5:F:514:PRO:HB3	1.84	0.43
1:I:554:PRO:HD3	1:I:907:LEU:HD12	2.01	0.43
1:K:1041:THR:HG22	1:K:1104:THR:HG23	2.01	0.43
1:K:1155:SER:OG	7:T:177:GLU:OE2	2.23	0.43
1:L:408:THR:HG23	1:M:415:LYS:HB3	2.00	0.43
1:L:1175:ILE:HG22	1:L:1244:TYR:CE2	2.54	0.43
7:T:197:GLU:HG3	7:T:198:THR:H	1.84	0.43
7:T:258:ASP:OD1	7:T:278:ASN:ND2	2.48	0.43
1:L:567:PRO:HB2	1:L:569:PRO:HD2	2.01	0.42
1:M:1207:THR:O	1:M:1211:THR:HG23	2.19	0.42
3:3:127:ARG:O	3:3:130:VAL:HG12	2.19	0.42
1:H:473:PRO:HA	1:H:476:GLN:HG2	2.00	0.42
1:H:1158:GLU:HG2	1:H:1299:THR:HG21	2.00	0.42
1:J:871:PRO:HD2	1:J:874:GLN:OE1	2.20	0.42
1:K:1202:VAL:HG22	1:L:1163:ALA:HB2	2.00	0.42
1:K:1268:THR:O	1:K:1272:ILE:HG12	2.19	0.42
1:M:720:VAL:HG23	1:M:918:TYR:HD1	1.85	0.42
1:M:1207:THR:OG1	1:M:1208:GLU:OE1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:17:LYS:O	2:P:21:VAL:HG12	2.19	0.42
6:G:428:LEU:HD11	6:G:559:PHE:CE1	2.54	0.42
1:H:1017:PRO:O	1:H:1021:VAL:HG12	2.19	0.42
1:I:396:PRO:HB3	1:I:1186:PHE:CZ	2.54	0.42
2:S:15:ASP:OD1	2:S:15:ASP:N	2.52	0.42
7:W:90:ARG:CZ	7:W:119:ASP:HB3	2.50	0.42
1:I:1144:ASP:OD1	1:I:1144:ASP:N	2.51	0.42
1:J:473:PRO:HA	1:J:476:GLN:HG2	2.01	0.42
1:K:754:VAL:N	1:K:755:PRO:HD2	2.35	0.42
1:K:1257:LYS:HG3	1:K:1301:TYR:CD1	2.55	0.42
1:M:39:TYR:CZ	8:X:295:PRO:HG2	2.54	0.42
1:M:631:VAL:O	1:M:635:ILE:HG23	2.19	0.42
1:M:1109:ARG:HB2	1:M:1109:ARG:HH11	1.84	0.42
1:1:133:ALA:O	1:1:137:THR:HG23	2.20	0.42
1:1:693:LEU:HD21	1:1:704:SER:HA	2.02	0.42
6:G:21:LEU:HD22	6:G:336:TRP:NE1	2.34	0.42
1:H:1278:LEU:O	1:H:1281:THR:HG22	2.20	0.42
1:I:848:ALA:O	1:I:851:GLN:HG3	2.19	0.42
1:J:1103:ARG:O	1:J:1167:GLY:HA3	2.19	0.42
1:M:596:LEU:HD23	1:M:645:LEU:HD23	2.01	0.42
1:1:1268:THR:HA	1:1:1271:ILE:HD12	2.01	0.42
1:H:35:LEU:HD11	1:H:37:ILE:HD11	2.01	0.42
1:J:1048:LEU:HD12	1:J:1093:ASN:O	2.19	0.42
1:J:1174:LEU:O	1:J:1244:TYR:OH	2.28	0.42
1:K:575:THR:HG22	1:K:1010:ALA:CB	2.50	0.42
1:M:637:ASN:O	1:M:641:THR:HG22	2.19	0.42
3:Z:235:LEU:HD23	3:Z:254:LEU:HD21	2.02	0.42
5:F:264:VAL:C	5:F:587:HIS:HE2	2.21	0.42
1:H:446:LEU:HD21	1:H:1024:THR:HG21	2.01	0.42
1:H:1349:THR:HA	1:H:1354:TYR:HA	2.02	0.42
1:I:710:LEU:HD21	1:I:783:VAL:HG22	2.01	0.42
1:J:798:CYS:SG	1:J:799:GLY:N	2.93	0.42
1:K:871:PRO:HD2	1:K:874:GLN:CD	2.40	0.42
1:L:618:HIS:O	1:L:618:HIS:ND1	2.53	0.42
1:L:635:ILE:HG22	1:L:646:VAL:HG23	2.00	0.42
1:M:424:LEU:HD13	1:M:573:LEU:HD23	2.02	0.42
8:U:64:LEU:O	8:U:68:MET:HG3	2.19	0.42
5:F:516:VAL:HG13	5:F:520:GLN:HB3	2.02	0.42
6:G:531:PHE:CE2	6:G:543:SER:HB3	2.55	0.42
1:I:515:ASP:HB3	1:I:993:ARG:HH22	1.85	0.42
1:I:1035:THR:HG23	1:I:1177:THR:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:269:ILE:HD13	1:J:368:ILE:HD11	2.01	0.42
1:K:493:ARG:O	1:K:496:PRO:HD2	2.19	0.42
1:M:188:PRO:HD2	1:M:1092:SER:O	2.19	0.42
1:M:520:ASP:HA	1:M:523:LYS:HD3	2.02	0.42
1:M:698:LEU:CD1	1:M:1127:VAL:HG12	2.49	0.42
2:O:22:VAL:HG23	2:O:23:ASN:OD1	2.19	0.42
1:K:553:THR:HG21	1:K:983:TYR:O	2.19	0.42
1:L:597:PHE:HD1	1:L:792:MET:HG2	1.85	0.42
1:M:785:TYR:O	1:M:943:TYR:OH	2.32	0.42
1:M:1055:THR:HA	1:M:1086:MET:HG2	2.02	0.42
8:X:159:ASP:HB3	8:Y:221:LYS:HE2	2.02	0.42
5:F:70:HIS:O	5:F:73:GLN:HG3	2.18	0.42
1:H:446:LEU:HD23	1:H:446:LEU:HA	1.94	0.42
1:I:419:THR:HG22	1:I:421:ARG:H	1.85	0.42
1:K:1034:LEU:HD12	1:K:1174:LEU:HD13	2.01	0.42
1:L:538:ASP:OD1	1:L:555:ARG:NE	2.45	0.42
7:W:139:SER:OG	7:W:145:LEU:HB3	2.20	0.42
1:1:144:GLU:N	1:1:144:GLU:OE1	2.52	0.41
5:F:296:ASP:OD1	5:F:296:ASP:N	2.53	0.41
5:F:447:THR:HG22	5:F:628:LEU:HD21	2.00	0.41
5:F:502:VAL:HA	5:F:506:ILE:HG12	2.00	0.41
5:F:610:ARG:HD2	5:F:610:ARG:HA	1.85	0.41
1:H:698:LEU:HD23	1:H:698:LEU:HA	1.81	0.41
1:I:269:ILE:HD13	1:I:368:ILE:HD11	2.02	0.41
1:J:1064:VAL:HG22	1:J:1077:VAL:HG12	2.02	0.41
1:M:295:THR:HA	1:M:356:SER:HA	2.03	0.41
1:M:1331:ALA:O	1:M:1335:THR:HG23	2.20	0.41
8:U:222:LEU:HD23	8:U:222:LEU:HA	1.92	0.41
3:Z:140:VAL:HG21	3:Z:158:HIS:NE2	2.35	0.41
5:F:60:TYR:O	5:F:64:GLU:HG3	2.20	0.41
1:J:1331:ALA:O	1:J:1335:THR:HG23	2.19	0.41
7:T:289:PHE:HA	8:U:277:GLN:OE1	2.20	0.41
8:U:96:ASN:HB3	8:U:102:TRP:CH2	2.54	0.41
8:X:281:LEU:HD12	8:X:282:ILE:HG23	2.01	0.41
1:H:211:GLN:O	1:H:215:ILE:HG12	2.20	0.41
1:H:733:VAL:HG13	1:H:894:GLU:HB3	2.02	0.41
1:K:886:VAL:HG13	1:K:887:GLY:N	2.35	0.41
7:W:17:ASP:N	7:W:17:ASP:OD1	2.53	0.41
8:X:115:PHE:CE2	8:X:185:PRO:HB3	2.55	0.41
4:C:2240:LEU:HD21	5:E:61:LEU:HD23	2.02	0.41
5:F:202:GLU:HA	5:F:205:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:672:PHE:CZ	1:J:643:GLN:HB2	2.55	0.41
1:M:66:PHE:HA	1:M:176:ILE:HD11	2.01	0.41
1:M:229:LEU:HD11	1:M:242:PHE:CZ	2.55	0.41
1:M:1124:HIS:O	1:M:1127:VAL:HG22	2.20	0.41
1:1:93:PHE:HE2	1:1:118:LYS:HG3	1.86	0.41
1:1:192:VAL:HG23	1:1:219:PHE:CZ	2.55	0.41
1:I:989:SER:N	1:I:990:PRO:HD2	2.35	0.41
1:J:1124:HIS:ND1	1:J:1127:VAL:HG23	2.35	0.41
1:J:1223:GLN:O	1:J:1223:GLN:HG2	2.20	0.41
1:K:1148:ILE:O	1:K:1152:THR:HG22	2.20	0.41
1:L:457:PRO:HG3	1:L:537:PHE:CE2	2.56	0.41
1:L:733:VAL:HG13	1:L:894:GLU:HB3	2.02	0.41
1:M:867:ASP:HB3	1:M:870:THR:HG22	2.02	0.41
2:O:37:HIS:HB3	2:O:40:LEU:HB3	2.02	0.41
7:T:259:ILE:HG12	7:T:276:LEU:HD22	2.03	0.41
7:T:288:GLU:OE1	7:T:288:GLU:N	2.46	0.41
8:V:217:THR:HG22	8:V:255:ARG:NH2	2.35	0.41
1:1:1017:PRO:O	1:1:1021:VAL:HG13	2.20	0.41
5:F:208:PHE:CE1	5:F:213:THR:HG21	2.55	0.41
5:F:527:LEU:HD23	5:F:527:LEU:HA	1.89	0.41
1:H:114:ILE:HD13	1:H:204:ARG:HD3	2.02	0.41
1:H:596:LEU:O	1:H:599:THR:HG22	2.21	0.41
1:I:174:GLY:HA3	1:J:101:ALA:HB3	2.02	0.41
1:J:568:GLY:O	1:J:572:GLU:HG2	2.20	0.41
1:J:1268:THR:O	1:J:1272:ILE:HG12	2.20	0.41
5:F:501:LEU:O	5:F:505:TYR:HB2	2.20	0.41
1:L:775:ASP:O	1:L:779:THR:HG23	2.20	0.41
2:P:16:GLU:CD	2:P:19:ARG:HH22	2.23	0.41
5:F:186:ILE:HG23	5:F:632:VAL:HG21	2.02	0.41
1:H:396:PRO:HB3	1:H:1186:PHE:CZ	2.56	0.41
1:I:895:VAL:HB	1:I:914:GLN:HB2	2.01	0.41
1:J:324:ASP:OD2	1:J:346:GLN:NE2	2.54	0.41
1:J:427:THR:HG22	1:J:441:ASP:HB3	2.02	0.41
1:J:687:ILE:HD13	1:J:687:ILE:HA	1.94	0.41
1:J:1116:VAL:HG13	1:J:1117:PHE:CD2	2.56	0.41
1:J:1257:LYS:HE3	1:J:1257:LYS:HB3	1.88	0.41
1:J:1260:SER:OG	1:J:1263:ALA:HB2	2.21	0.41
1:K:924:VAL:HG23	1:K:925:THR:HG23	2.02	0.41
2:R:44:LEU:HD23	2:R:44:LEU:HA	1.88	0.41
1:1:884:GLN:HA	2:2:66:ARG:HB2	2.02	0.41
1:1:1124:HIS:HB3	1:1:1127:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:210:ASN:OD1	5:F:211:ALA:N	2.54	0.41
5:F:497:ASN:HA	5:F:500:PHE:CE2	2.55	0.41
1:I:1101:ARG:HD3	1:J:214:ASN:HB3	2.02	0.41
1:L:241:LYS:HA	1:L:244:THR:HG22	2.03	0.41
1:M:1359:ILE:HD12	1:M:1359:ILE:HA	1.99	0.41
2:R:68:VAL:O	2:R:71:SER:OG	2.29	0.41
8:U:261:PRO:HB3	8:V:172:LEU:HD13	2.03	0.41
8:V:8:ILE:HB	8:V:83:LEU:HB2	2.03	0.41
7:W:124:LEU:HD23	7:W:191:TYR:CE2	2.56	0.41
3:Z:14:VAL:HA	3:Z:17:VAL:CG1	2.51	0.41
3:Z:239:LEU:HD21	3:Z:250:CYS:HB3	2.03	0.41
5:E:14:VAL:HG22	5:F:11:PRO:HB2	2.03	0.41
5:E:65:LEU:HA	5:E:65:LEU:HD23	1.74	0.41
5:F:258:VAL:HA	5:F:261:LEU:HG	2.02	0.41
5:F:341:ASP:OD1	5:F:341:ASP:N	2.50	0.41
1:H:1350:HIS:N	1:H:1353:ASN:O	2.52	0.41
1:I:469:PRO:HA	1:I:470:PRO:HD3	1.99	0.41
1:I:633:ARG:NH2	1:I:878:GLU:OE2	2.43	0.41
1:L:455:HIS:CD2	1:L:1017:PRO:HG3	2.56	0.41
1:M:989:SER:N	1:M:990:PRO:HD2	2.36	0.41
8:X:151:LEU:HD22	8:X:281:LEU:HD13	2.03	0.41
1:I:490:GLY:O	1:I:494:ARG:HG3	2.21	0.40
1:I:1057:VAL:HG12	1:I:1083:THR:HG22	2.03	0.40
1:J:800:LEU:HD23	1:J:923:VAL:HG11	2.03	0.40
1:K:800:LEU:HD23	1:K:923:VAL:HG21	2.03	0.40
1:L:507:ARG:HH21	1:L:512:MET:HG2	1.85	0.40
1:M:804:LEU:HD23	1:M:889:HIS:HD2	1.86	0.40
8:U:194:LEU:HD23	8:U:197:MET:HE3	2.03	0.40
8:V:201:CYS:O	8:V:204:MET:HG2	2.21	0.40
1:1:664:GLY:C	1:1:666:LEU:H	2.24	0.40
1:1:747:ARG:NH1	1:1:888:GLU:OE1	2.44	0.40
1:K:596:LEU:O	1:K:599:THR:HG22	2.21	0.40
1:M:553:THR:HG21	1:M:983:TYR:O	2.20	0.40
2:Q:13:LYS:HG3	2:Q:15:ASP:H	1.87	0.40
3:Z:125:VAL:O	3:Z:129:LEU:HG	2.22	0.40
3:Z:201:ASN:O	3:Z:204:VAL:HG12	2.21	0.40
1:H:754:VAL:N	1:H:755:PRO:HD2	2.36	0.40
1:I:70:GLY:N	1:I:370:GLU:OE1	2.54	0.40
1:I:567:PRO:HB2	1:I:569:PRO:HD2	2.04	0.40
1:J:545:ASN:O	1:J:545:ASN:ND2	2.49	0.40
1:K:884:GLN:HA	2:Q:66:ARG:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:363:GLY:C	1:L:365:LYS:H	2.25	0.40
1:M:575:THR:HG22	1:M:1010:ALA:CB	2.50	0.40
8:V:76:VAL:HG12	8:V:81:ILE:HD13	2.04	0.40
4:A:2207:VAL:HG22	5:F:90:LEU:HD21	2.03	0.40
5:F:199:PHE:O	5:F:203:VAL:HG22	2.21	0.40
1:H:605:ASN:ND2	1:H:642:ARG:HD3	2.37	0.40
1:K:118:LYS:HB3	1:K:118:LYS:HE2	1.89	0.40
1:K:682:ARG:HA	1:K:685:THR:HG22	2.02	0.40
1:1:399:LEU:HD11	1:1:1186:PHE:CE2	2.56	0.40
1:H:263:THR:O	1:H:266:GLY:HA2	2.22	0.40
1:I:188:PRO:HA	1:I:1286:LEU:HD21	2.03	0.40
1:I:459:PRO:HB2	1:I:1242:VAL:HG21	2.04	0.40
1:J:180:LEU:HD23	1:J:384:PRO:HG2	2.04	0.40
1:K:490:GLY:O	1:K:494:ARG:HG3	2.21	0.40
1:L:77:ALA:HB1	1:L:302:TYR:HD1	1.87	0.40
1:M:1337:LEU:HD13	1:M:1337:LEU:HA	1.96	0.40
2:P:44:LEU:HD12	2:P:45:SER:N	2.37	0.40
8:V:7:ASN:OD1	8:V:74:ARG:NH2	2.54	0.40
8:V:196:ASP:OD1	8:V:196:ASP:N	2.53	0.40
3:Z:160:LYS:O	3:Z:164:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	1298/1370 (95%)	1238 (95%)	60 (5%)	0	100	100
1	H	1329/1370 (97%)	1264 (95%)	62 (5%)	3 (0%)	44	76
1	I	1346/1370 (98%)	1297 (96%)	48 (4%)	1 (0%)	48	80
1	J	1313/1370 (96%)	1263 (96%)	50 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	K	1347/1370 (98%)	1300 (96%)	45 (3%)	2 (0%)	48 80
1	L	1346/1370 (98%)	1293 (96%)	51 (4%)	2 (0%)	48 80
1	M	1346/1370 (98%)	1291 (96%)	54 (4%)	1 (0%)	48 80
2	2	61/75 (81%)	61 (100%)	0	0	100 100
2	N	61/75 (81%)	59 (97%)	2 (3%)	0	100 100
2	O	61/75 (81%)	59 (97%)	2 (3%)	0	100 100
2	P	61/75 (81%)	59 (97%)	2 (3%)	0	100 100
2	Q	61/75 (81%)	57 (93%)	4 (7%)	0	100 100
2	R	61/75 (81%)	59 (97%)	2 (3%)	0	100 100
2	S	61/75 (81%)	60 (98%)	1 (2%)	0	100 100
3	3	283/1048 (27%)	276 (98%)	7 (2%)	0	100 100
3	Z	282/1048 (27%)	272 (96%)	9 (3%)	1 (0%)	30 64
4	A	41/2241 (2%)	40 (98%)	1 (2%)	0	100 100
4	C	34/2241 (2%)	34 (100%)	0	0	100 100
5	E	80/642 (12%)	79 (99%)	1 (1%)	0	100 100
5	F	462/642 (72%)	454 (98%)	8 (2%)	0	100 100
6	G	468/594 (79%)	452 (97%)	16 (3%)	0	100 100
7	T	127/290 (44%)	120 (94%)	7 (6%)	0	100 100
7	W	288/290 (99%)	272 (94%)	16 (6%)	0	100 100
8	U	301/306 (98%)	285 (95%)	15 (5%)	1 (0%)	37 69
8	V	294/306 (96%)	283 (96%)	11 (4%)	0	100 100
8	X	291/306 (95%)	281 (97%)	10 (3%)	0	100 100
8	Y	279/306 (91%)	265 (95%)	13 (5%)	1 (0%)	30 64
All	All	12982/20375 (64%)	12473 (96%)	497 (4%)	12 (0%)	50 80

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	266	GLY
1	I	266	GLY
1	K	266	GLY
1	K	886	VAL
1	L	764	GLU
8	Y	297	ASN

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Mol	Chain	Res	Type
1	M	377	LYS
1	H	665	ALA
8	U	122	GLU
1	H	1101	ARG
3	Z	193	ASN
1	L	1101	ARG

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	1	1138/1192 (96%)	1132 (100%)	6 (0%)	86 94
1	H	1162/1192 (98%)	1157 (100%)	5 (0%)	89 95
1	I	1175/1192 (99%)	1165 (99%)	10 (1%)	75 89
1	J	1146/1192 (96%)	1141 (100%)	5 (0%)	89 95
1	K	1177/1192 (99%)	1174 (100%)	3 (0%)	91 96
1	L	1175/1192 (99%)	1169 (100%)	6 (0%)	86 94
1	M	1175/1192 (99%)	1164 (99%)	11 (1%)	75 89
2	2	59/68 (87%)	59 (100%)	0	100 100
2	N	59/68 (87%)	58 (98%)	1 (2%)	56 80
2	O	59/68 (87%)	57 (97%)	2 (3%)	32 65
2	P	59/68 (87%)	58 (98%)	1 (2%)	56 80
2	Q	59/68 (87%)	57 (97%)	2 (3%)	32 65
2	R	59/68 (87%)	58 (98%)	1 (2%)	56 80
2	S	59/68 (87%)	58 (98%)	1 (2%)	56 80
3	3	256/883 (29%)	254 (99%)	2 (1%)	79 90
3	Z	255/883 (29%)	255 (100%)	0	100 100
4	A	41/1941 (2%)	41 (100%)	0	100 100
4	C	34/1941 (2%)	34 (100%)	0	100 100
5	E	72/526 (14%)	72 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	F	415/526 (79%)	406 (98%)	9 (2%)	47 75
6	G	398/500 (80%)	393 (99%)	5 (1%)	65 84
7	T	117/252 (46%)	117 (100%)	0	100 100
7	W	252/252 (100%)	250 (99%)	2 (1%)	79 90
8	U	272/273 (100%)	272 (100%)	0	100 100
8	V	268/273 (98%)	266 (99%)	2 (1%)	81 91
8	X	263/273 (96%)	261 (99%)	2 (1%)	79 90
8	Y	257/273 (94%)	255 (99%)	2 (1%)	79 90
All	All	11461/17616 (65%)	11383 (99%)	78 (1%)	80 91

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	4	TRP
1	1	80	PHE
1	1	135	CYS
1	1	403	GLU
1	1	763	ASP
1	1	1115	ARG
3	3	165	GLN
3	3	246	ASP
5	F	91	ASN
5	F	184	PHE
5	F	222	TYR
5	F	247	PHE
5	F	271	ASP
5	F	419	ASP
5	F	462	LEU
5	F	522	PHE
5	F	629	TYR
6	G	141	LEU
6	G	299	GLU
6	G	510	ARG
6	G	514	TRP
6	G	535	LEU
1	H	1	MET
1	H	54	PHE
1	H	394	PHE
1	H	507	ARG

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Mol	Chain	Res	Type
1	H	1292	CYS
1	I	24	LYS
1	I	355	LEU
1	I	394	PHE
1	I	545	ASN
1	I	760	MET
1	I	814	ARG
1	I	986	TRP
1	I	1029	HIS
1	I	1254	TYR
1	I	1303	CYS
1	J	394	PHE
1	J	545	ASN
1	J	644	LEU
1	J	1101	ARG
1	J	1251	ARG
1	K	235	ASP
1	K	763	ASP
1	K	1095	CYS
1	L	394	PHE
1	L	405	ARG
1	L	497	HIS
1	L	682	ARG
1	L	958	ARG
1	L	1133	HIS
1	M	209	ARG
1	M	241	LYS
1	M	364	GLU
1	M	394	PHE
1	M	433	ARG
1	M	480	GLU
1	M	545	ASN
1	M	740	ASN
1	M	1029	HIS
1	M	1139	ARG
1	M	1303	CYS
2	N	75	ARG
2	O	18	HIS
2	O	33	SER
2	P	50	MET
2	Q	18	HIS
2	Q	45	SER

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Mol	Chain	Res	Type
2	R	33	SER
2	S	20	HIS
8	V	75	ARG
8	V	79	ASN
7	W	136	LYS
7	W	288	GLU
8	X	114	LEU
8	X	220	ARG
8	Y	91	LEU
8	Y	279	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	49	HIS
1	1	451	HIS
5	F	365	HIS
5	F	372	HIS
5	F	427	GLN
5	F	448	ASN
1	H	1363	GLN
1	J	618	HIS
1	K	1230	ASN
1	L	432	ASN
2	P	18	HIS
7	W	156	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.

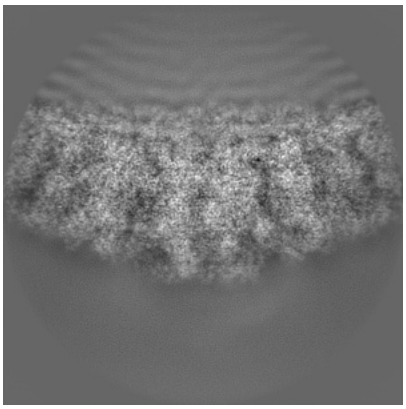
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41204. These allow visual inspection of the internal detail of the map and identification of artifacts.

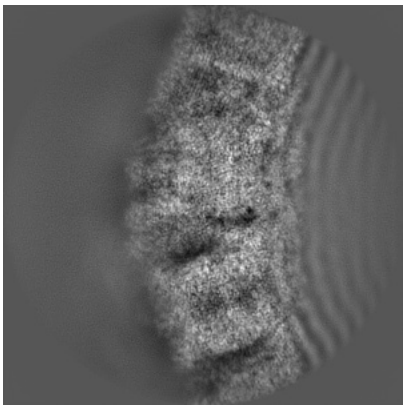
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

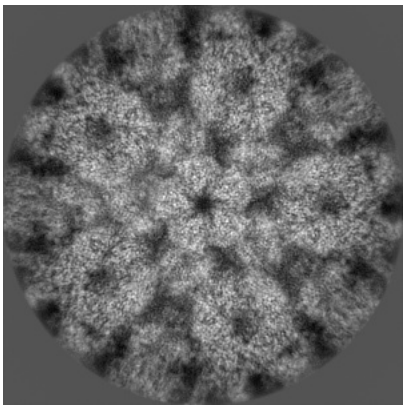
6.1.1 Primary map



X

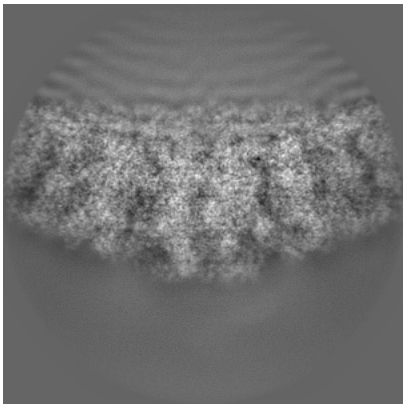


Y

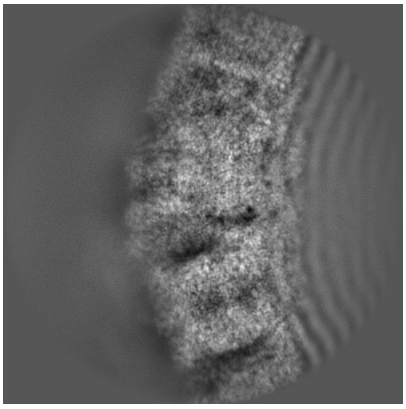


Z

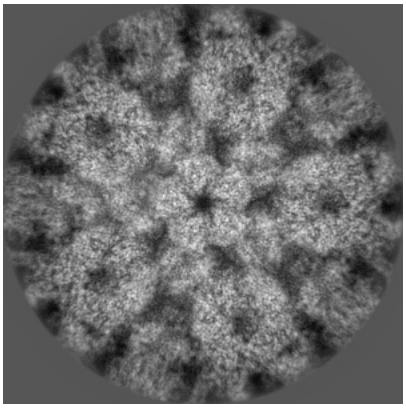
6.1.2 Raw map



X



Y

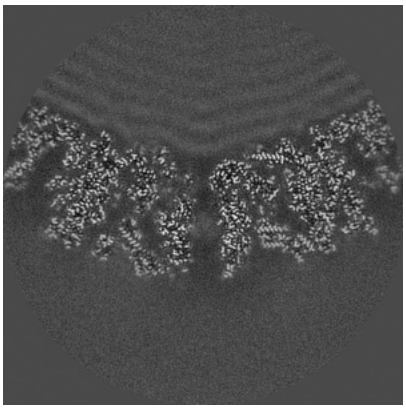


Z

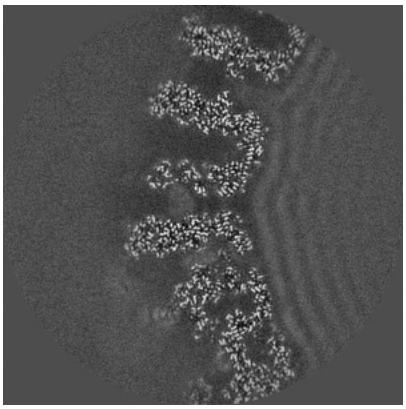
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

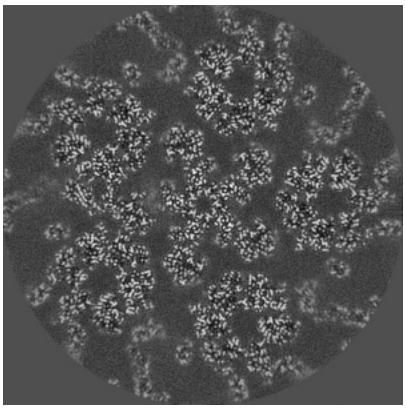
6.2.1 Primary map



X Index: 180

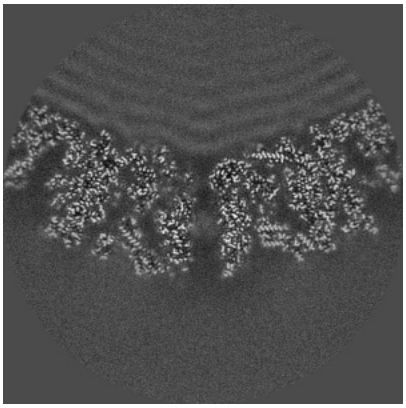


Y Index: 180

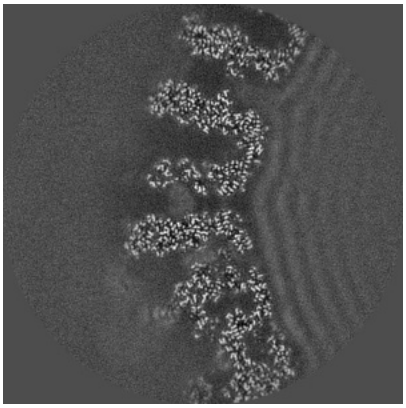


Z Index: 180

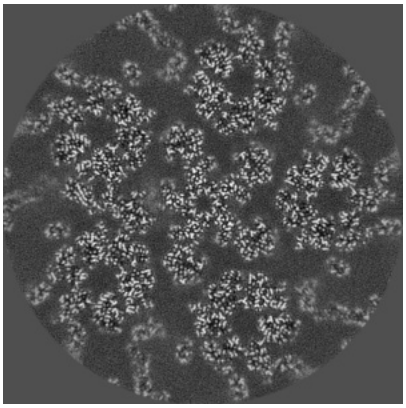
6.2.2 Raw map



X Index: 180



Y Index: 180

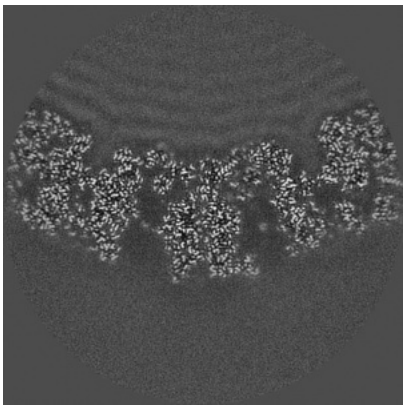


Z Index: 180

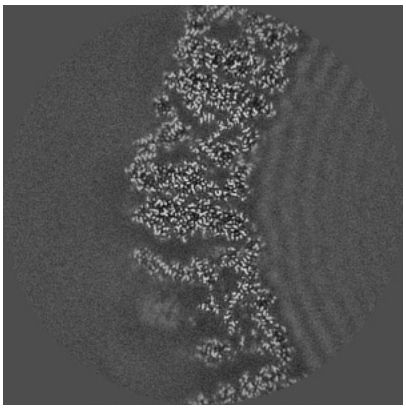
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

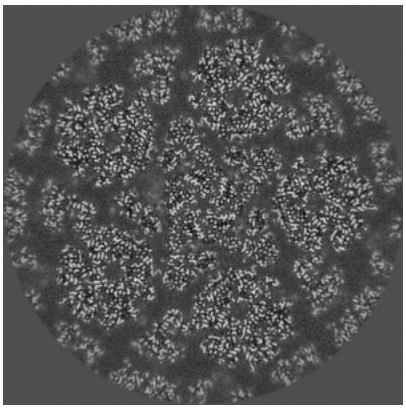
6.3.1 Primary map



X Index: 204

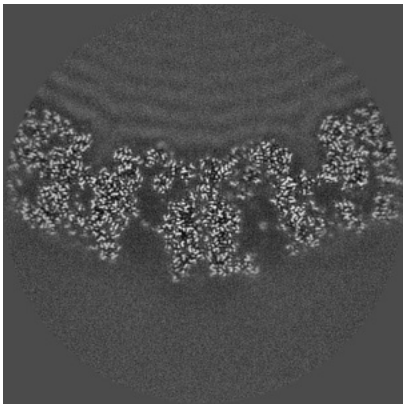


Y Index: 159

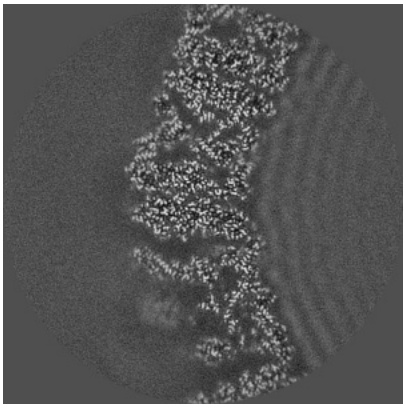


Z Index: 205

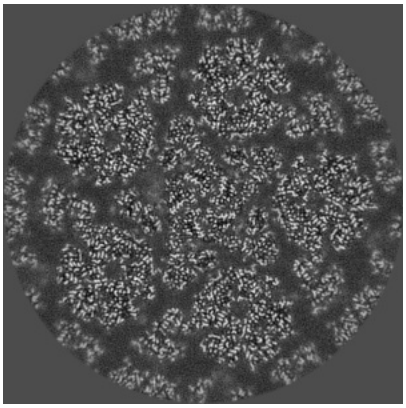
6.3.2 Raw map



X Index: 204



Y Index: 159

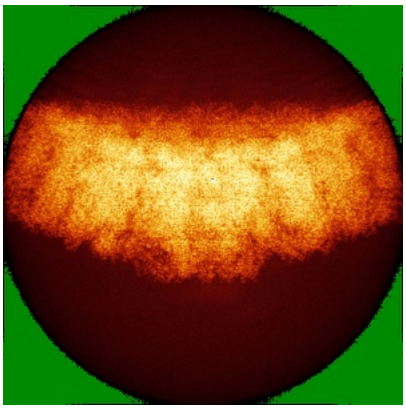


Z Index: 205

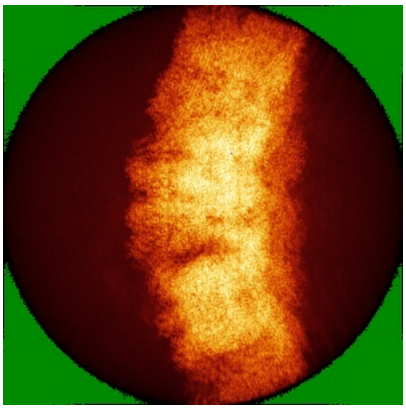
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

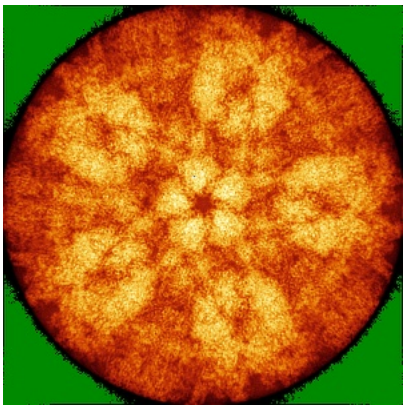
6.4.1 Primary map



X

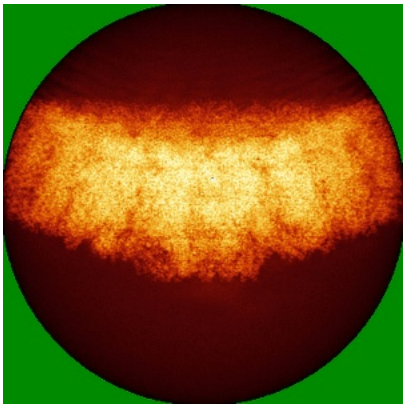


Y

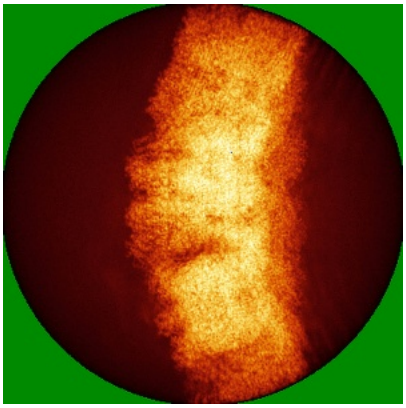


Z

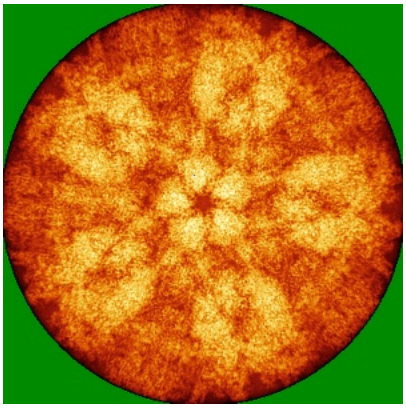
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0045. 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

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.

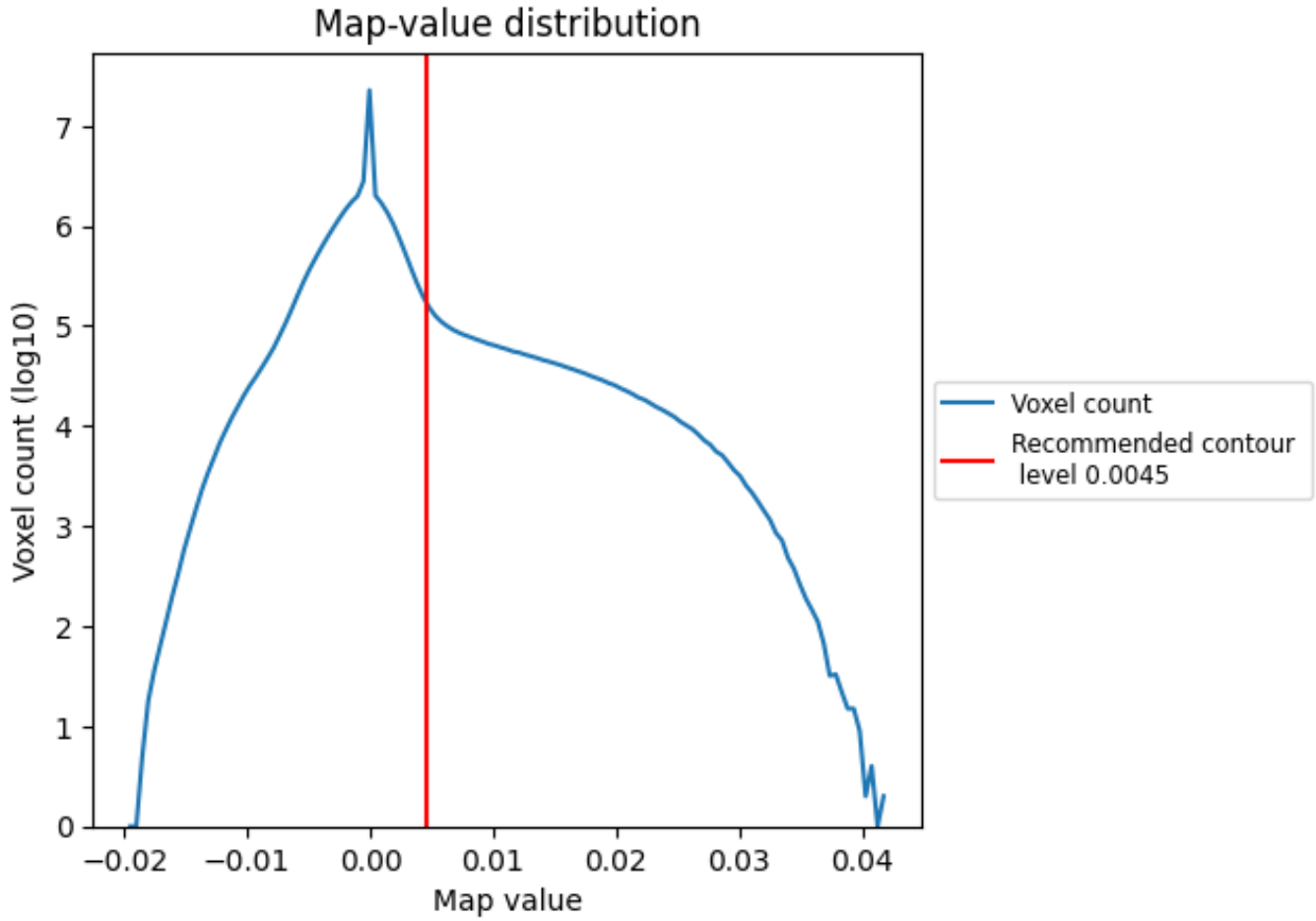
6.6 Mask visualisation (i)

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

7 Map analysis

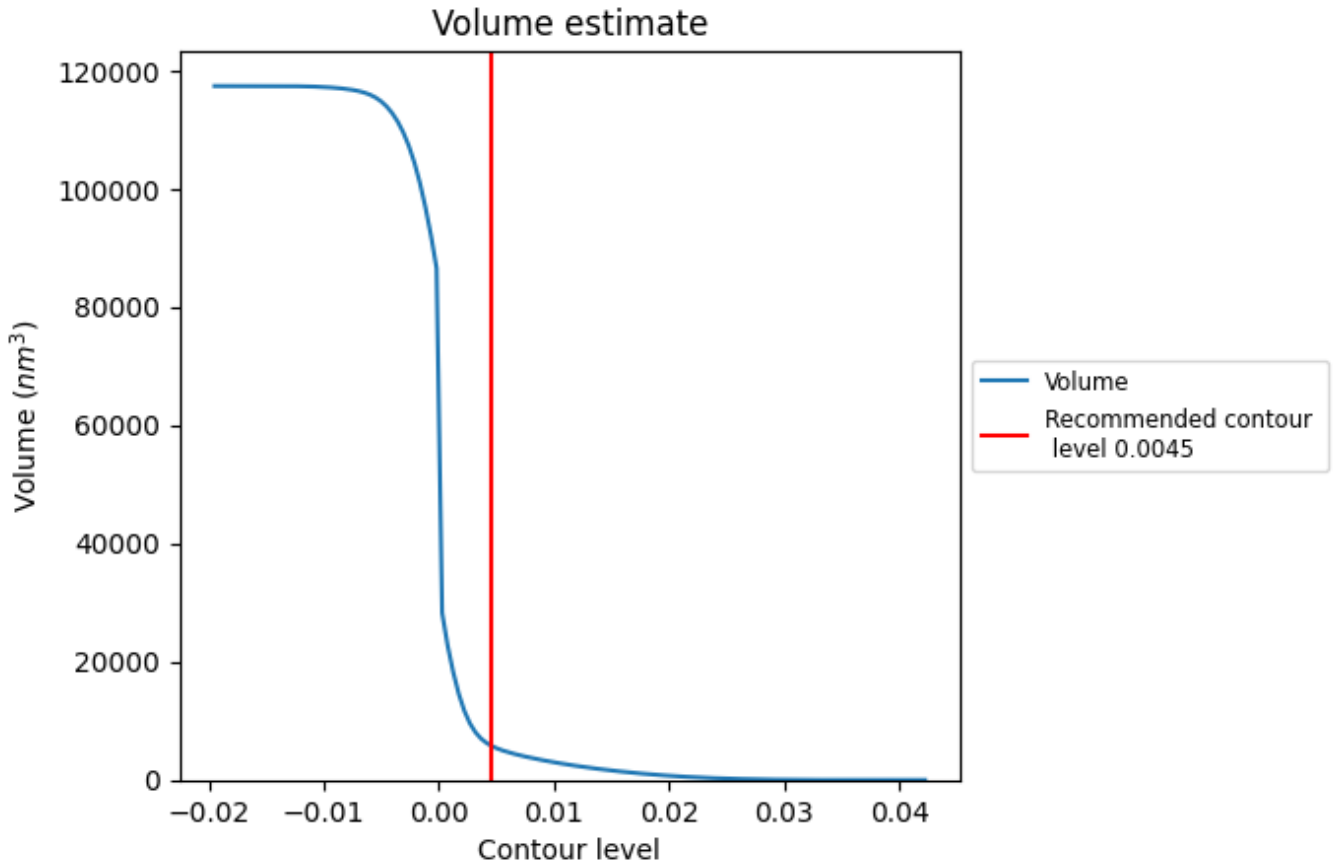
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

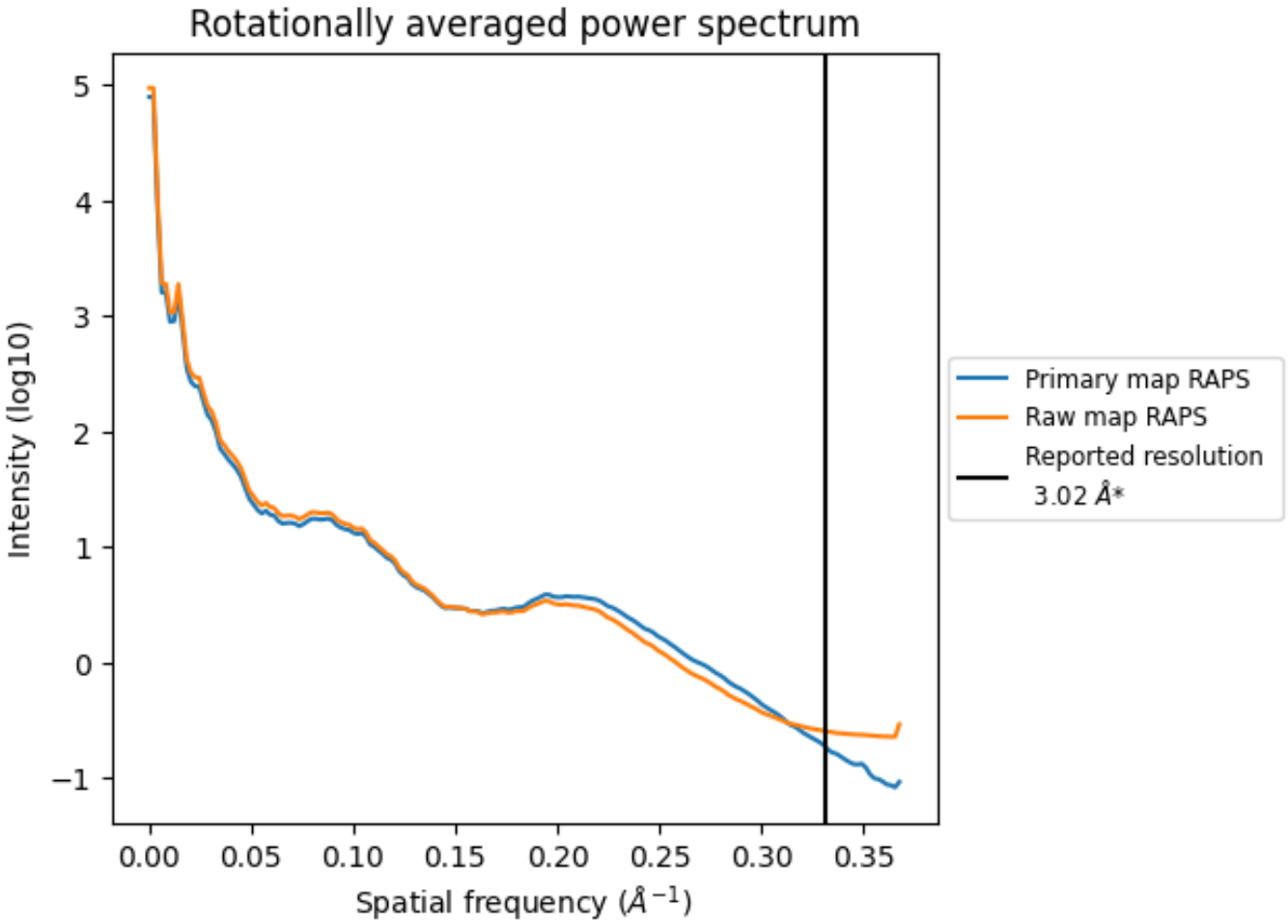
7.2 Volume estimate



The volume at the recommended contour level is 5844 nm^3; this corresponds to an approximate mass of 5279 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)

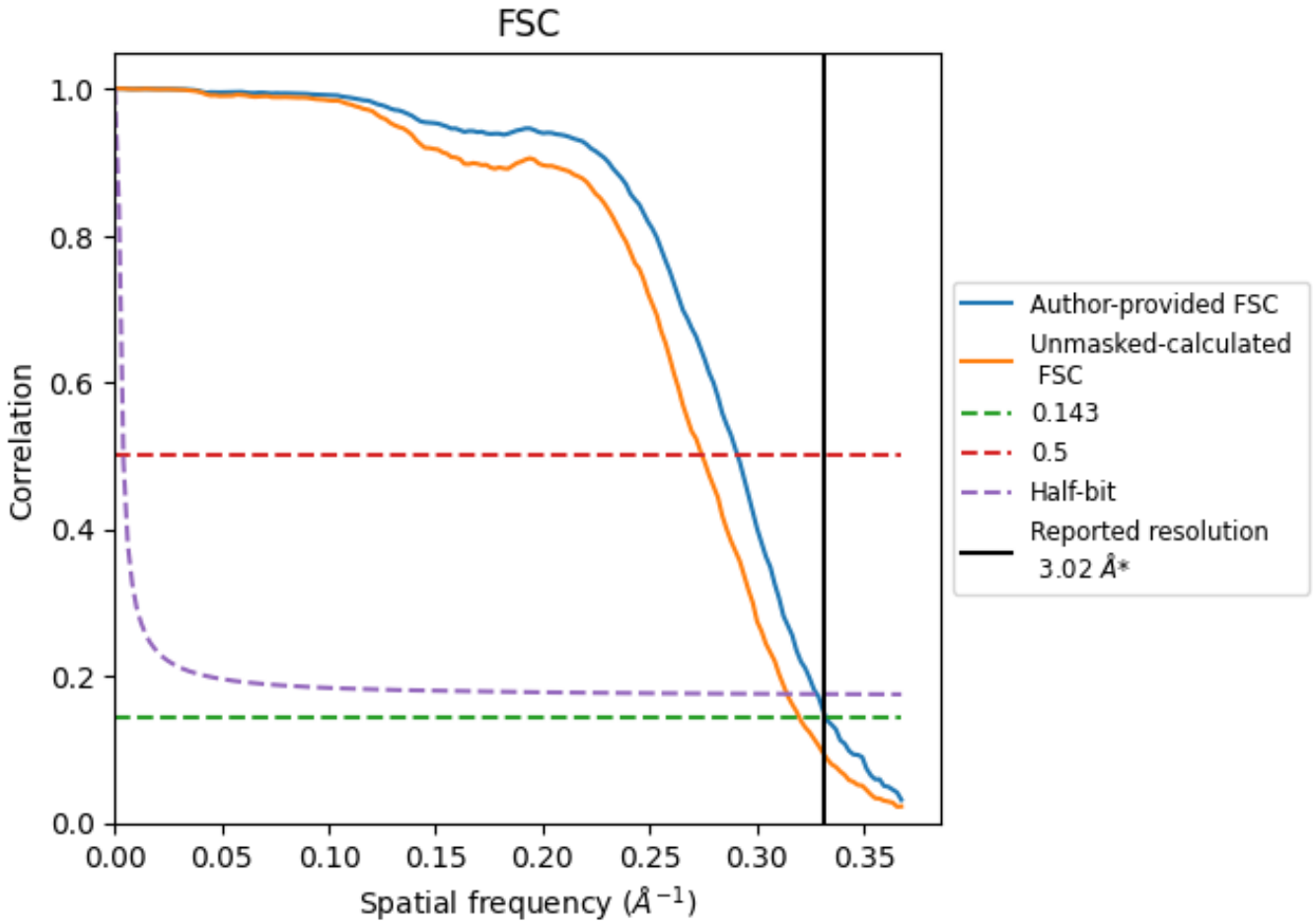


*Reported resolution corresponds to spatial frequency of 0.331 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.331 Å^{-1}

8.2 Resolution estimates (i)

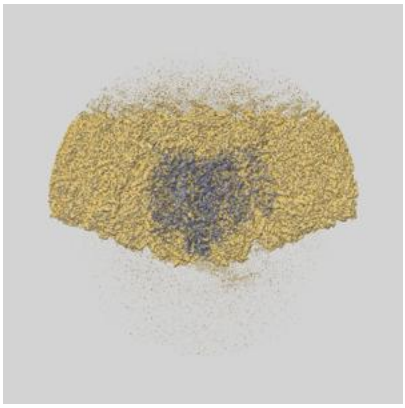
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.01	3.44	3.05
Unmasked-calculated*	3.12	3.64	3.18

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

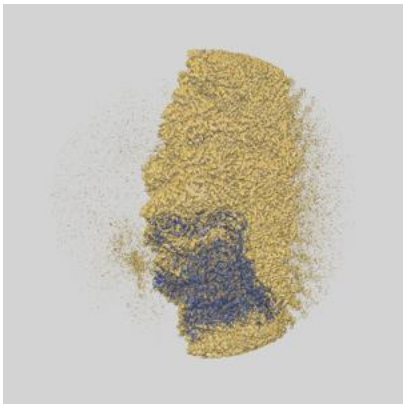
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41204 and PDB model 8TEW. Per-residue inclusion information can be found in section 3 on page 7.

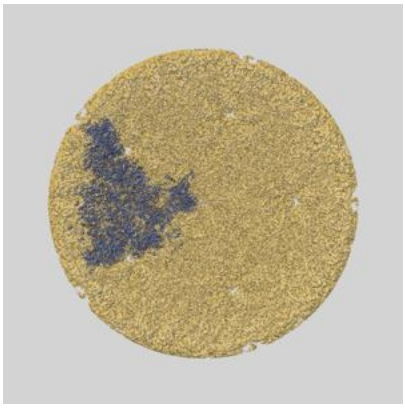
9.1 Map-model overlay



X



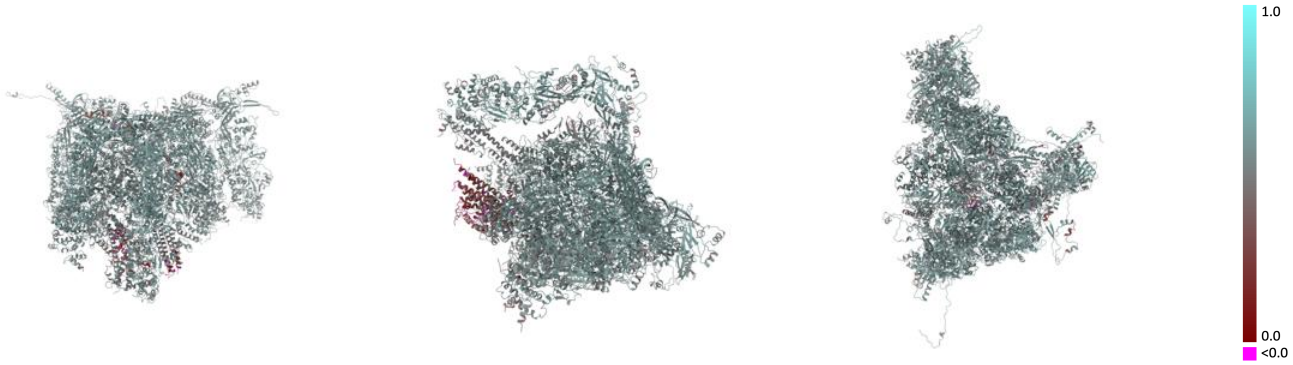
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0045 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.

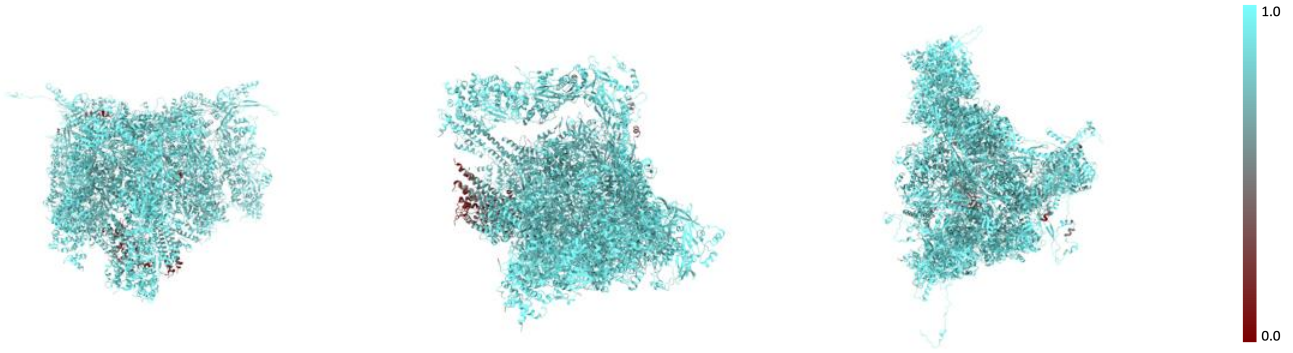
9.2 Q-score mapped to coordinate model



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.

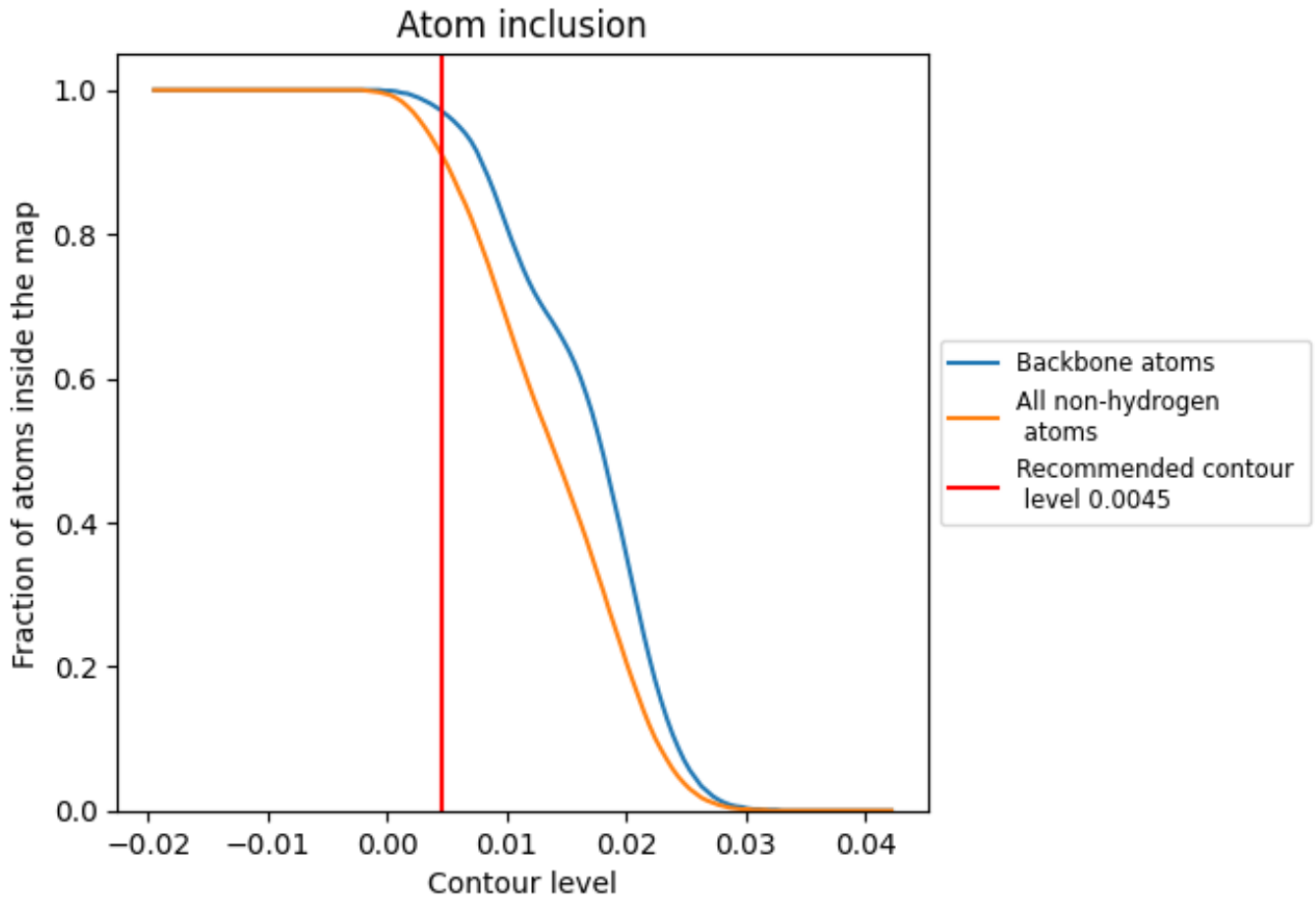
9.3 Atom inclusion mapped to coordinate model



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 (0.0045).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9120	0.5440
1	0.9340	0.5620
2	0.9360	0.5110
3	0.8970	0.5020
A	0.6900	0.3290
C	0.6920	0.3360
E	0.8220	0.4600
F	0.3900	0.2390
G	0.9380	0.5540
H	0.9460	0.5760
I	0.9540	0.5750
J	0.9370	0.5590
K	0.9510	0.5770
L	0.9400	0.5660
M	0.9310	0.5560
N	0.9240	0.4970
O	0.9080	0.5060
P	0.8750	0.4790
Q	0.8980	0.4990
R	0.8900	0.4920
S	0.9000	0.5010
T	0.9030	0.5300
U	0.9140	0.5570
V	0.9060	0.5430
W	0.9290	0.5610
X	0.9000	0.5420
Y	0.9140	0.5440
Z	0.8930	0.4980