



Full wwPDB EM Validation Report ⓘ

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 ⓘ 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.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

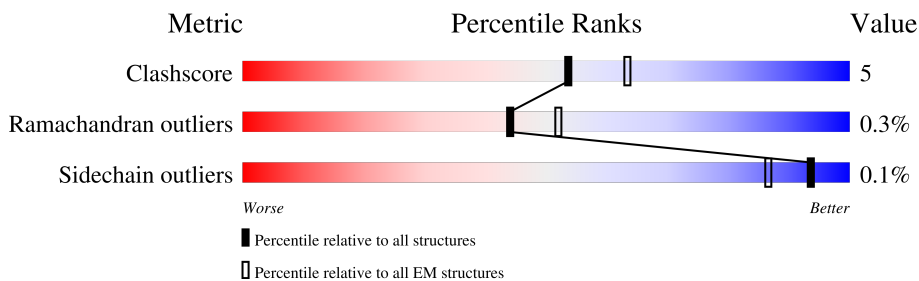
1 Overall quality at a glance

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	S	1374	
1	T	1374	
1	W	1374	
1	X	1374	
2	E	112	
2	F	112	
2	L	112	
2	P	112	

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Mol	Chain	Length	Quality of chain
3	5	465	
3	D	465	
4	6	318	
4	7	318	
4	A	318	
4	H	318	
5	C	703	
6	G	580	
6	K	580	
7	B	3094	
7	O	3094	

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
4	6	291	Total	C	N	O	S	0	0
			2216	1413	393	403	7		
4	7	310	Total	C	N	O	S	0	0
			2355	1497	417	432	9		
4	H	291	Total	C	N	O	S	0	0
			2216	1413	393	403	7		
4	A	310	Total	C	N	O	S	0	0
			2355	1497	417	432	9		

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

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

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

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

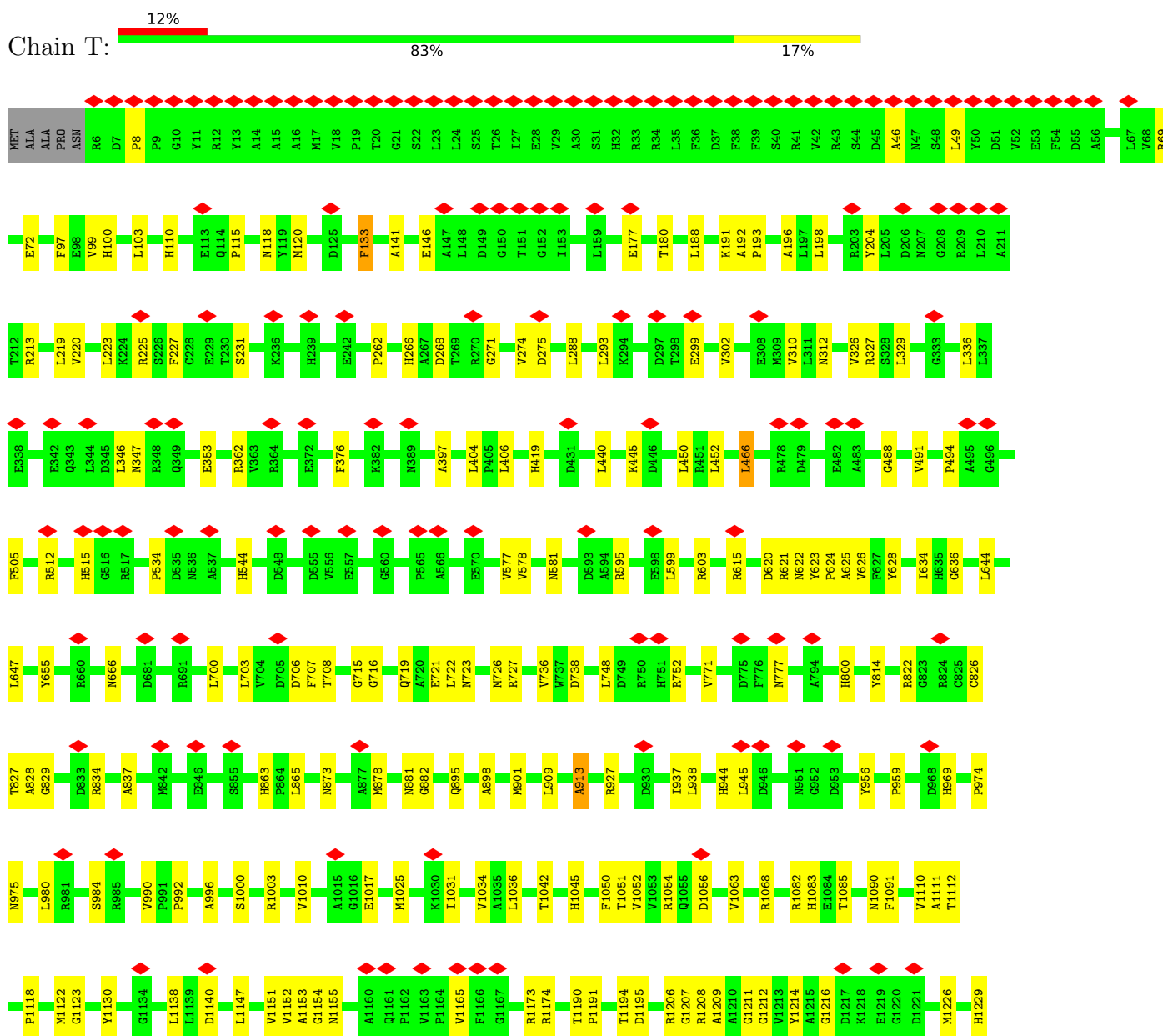
- Molecule 7 is a protein called Large tegument protein deneddylase.

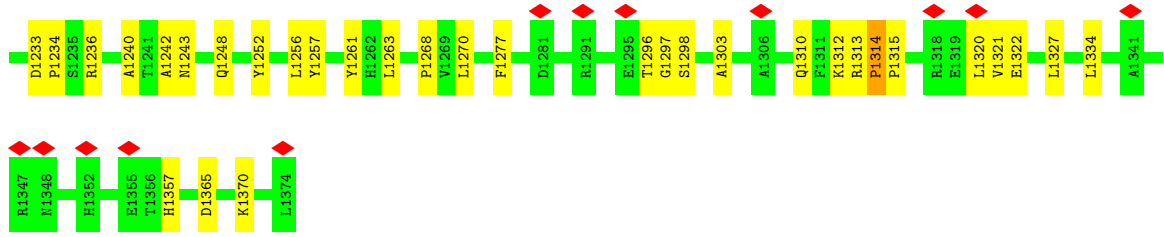
Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	48	Total	C	N	O	S	0	0
			388	239	85	62	2		
7	B	48	Total	C	N	O	S	0	0
			388	239	85	62	2		

3 Residue-property plots

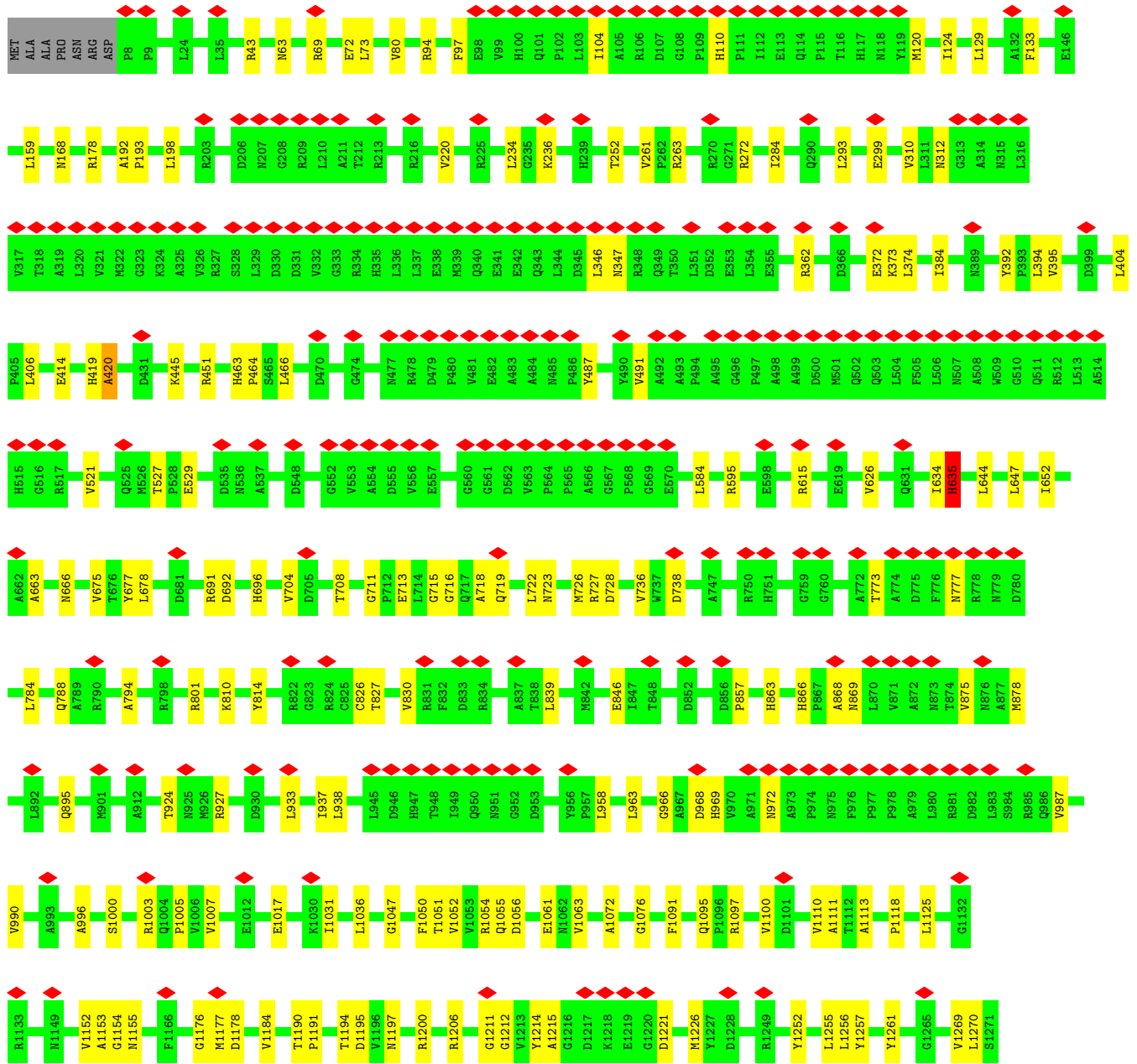
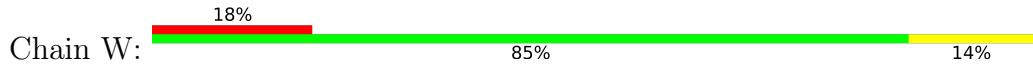
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

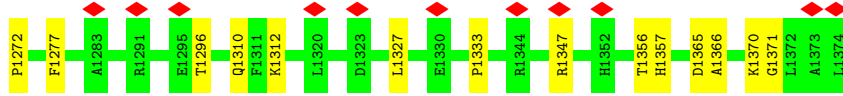
- Molecule 1: Major capsid protein



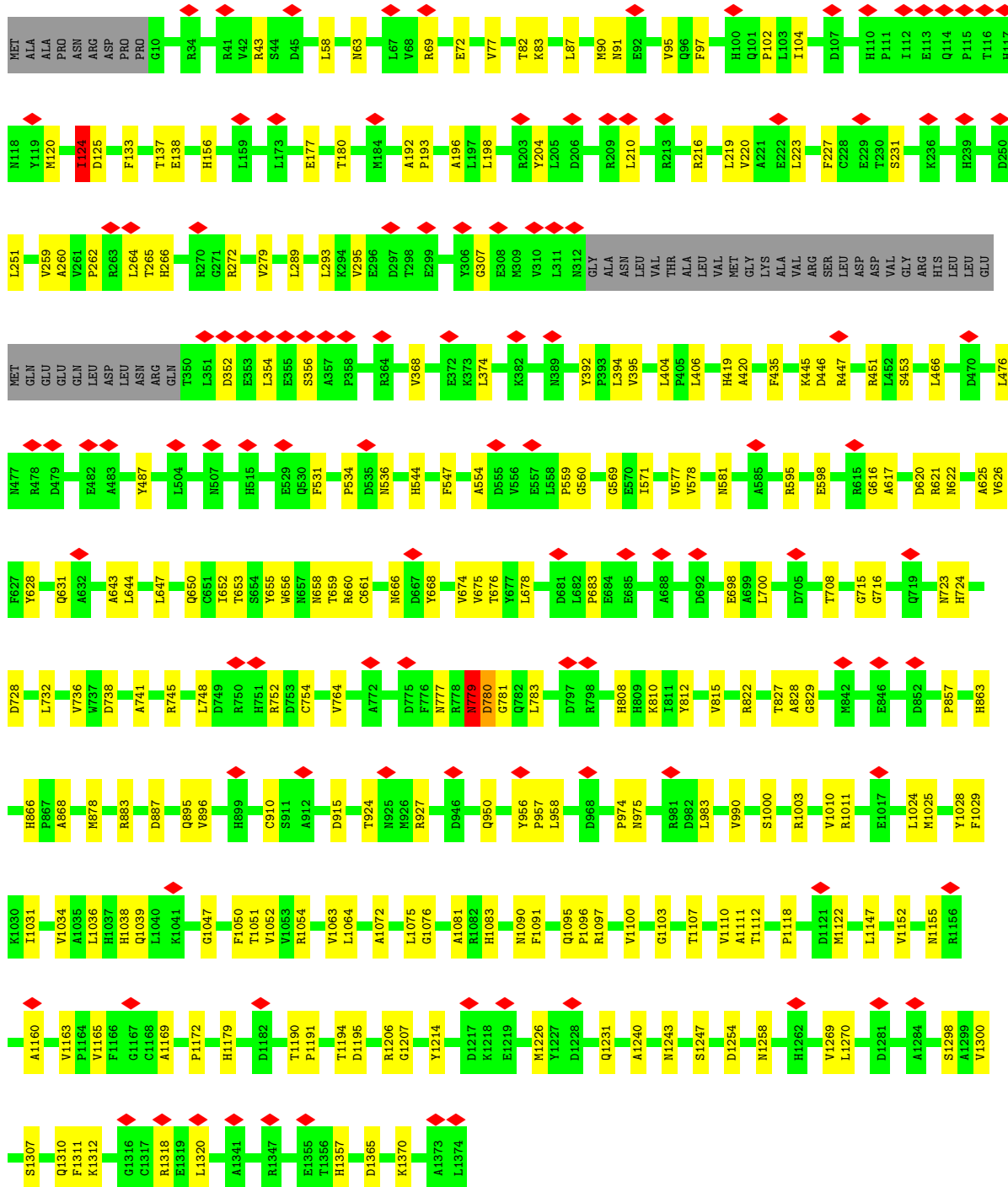
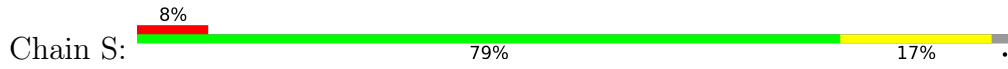


• Molecule 1: Major capsid protein

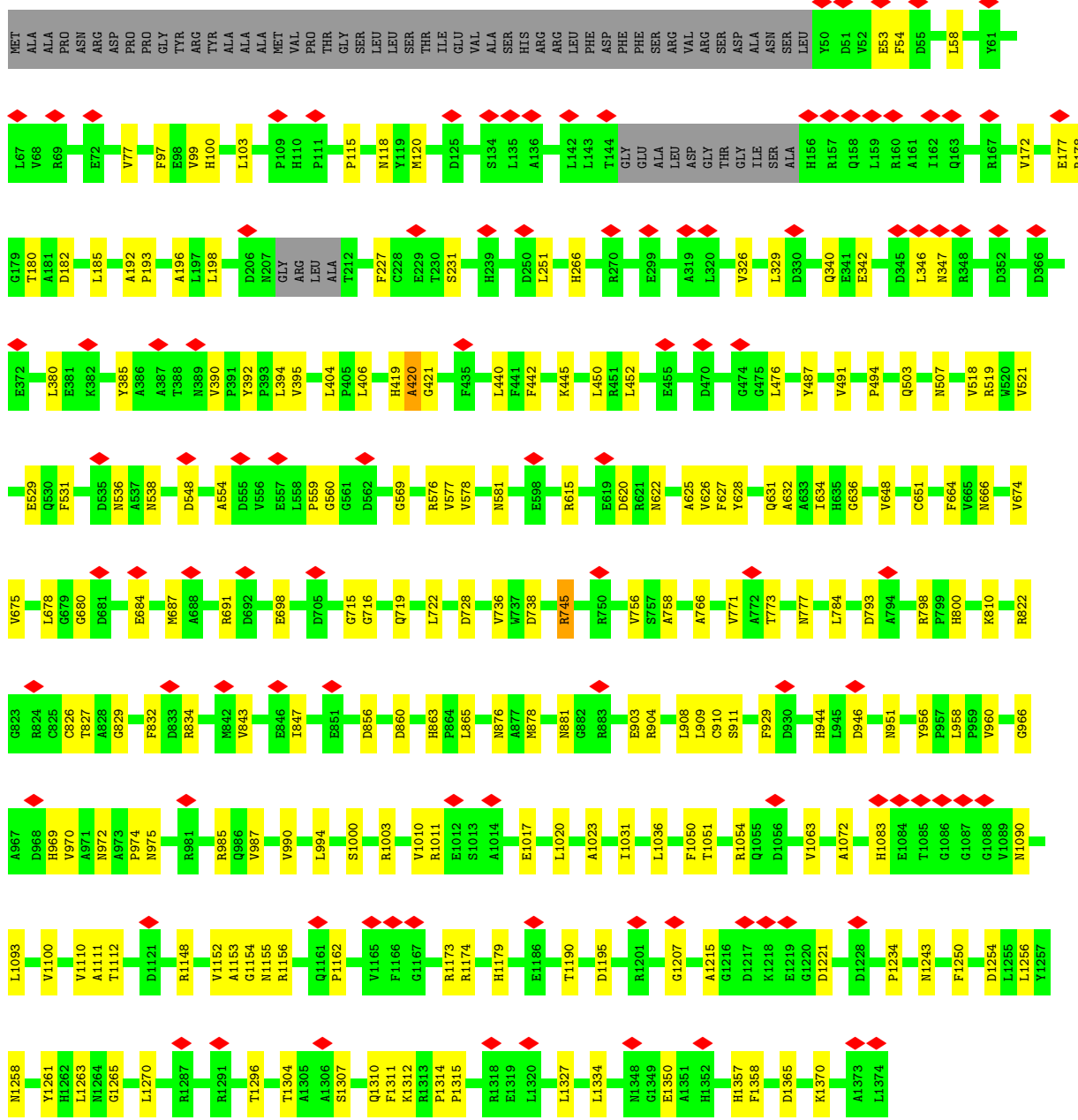
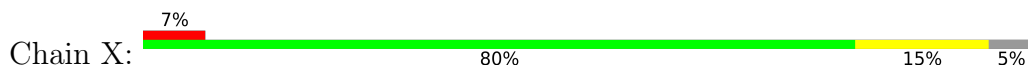




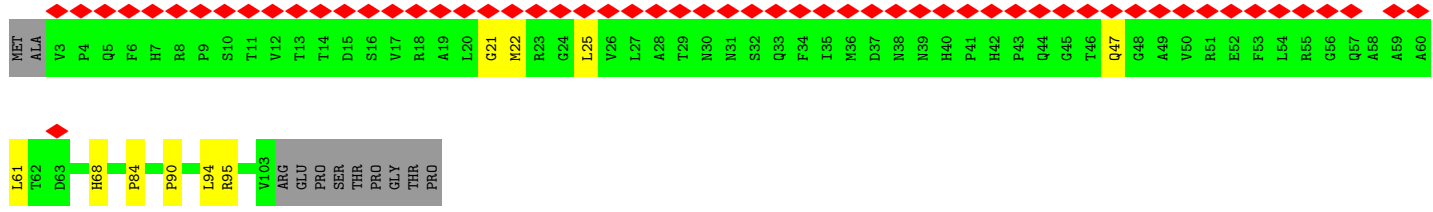
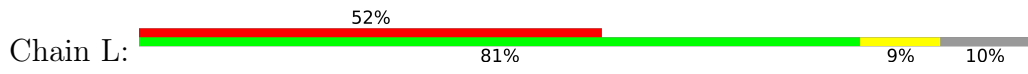
• Molecule 1: Major capsid protein



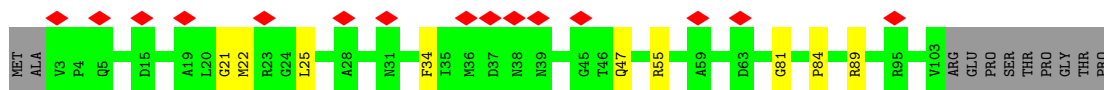
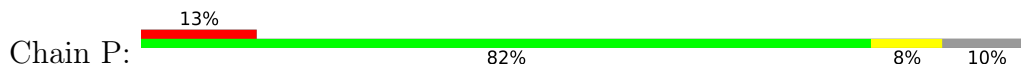
• Molecule 1: Major capsid protein



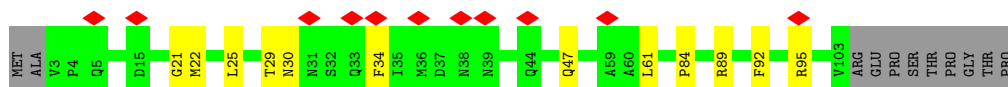
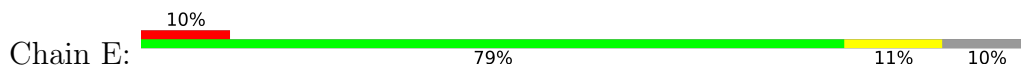
● Molecule 2: Small capsomere-interacting protein



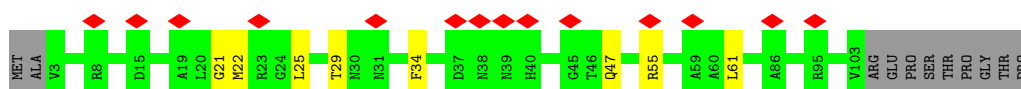
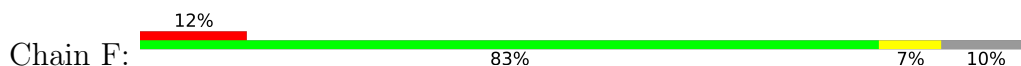
• Molecule 2: Small capsomere-interacting protein



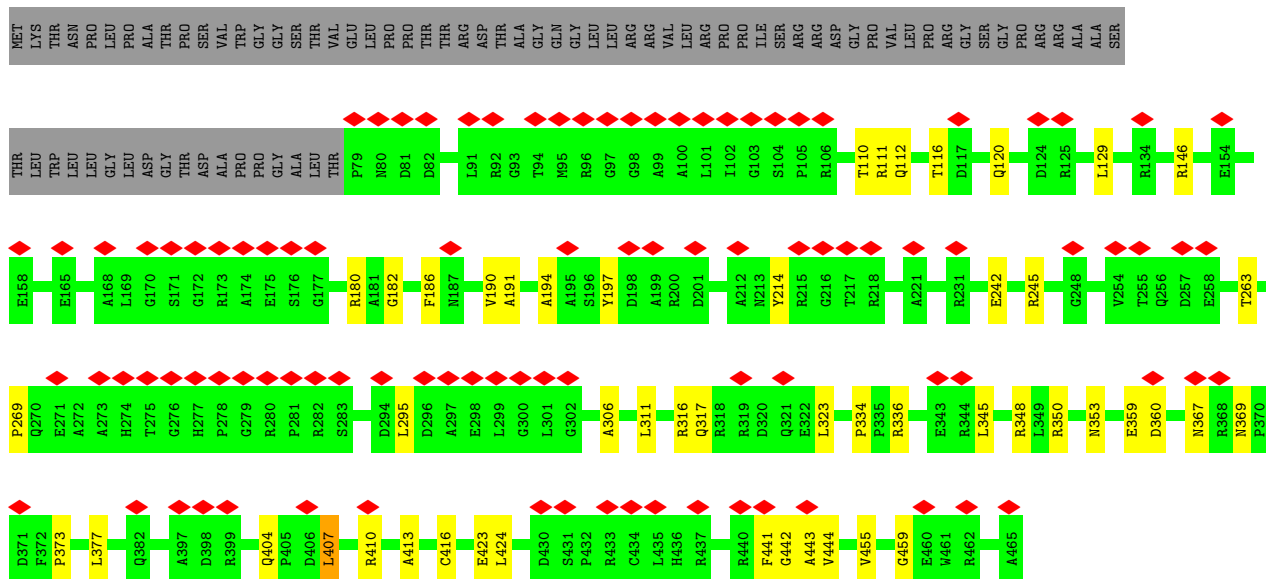
• Molecule 2: Small capsomere-interacting protein



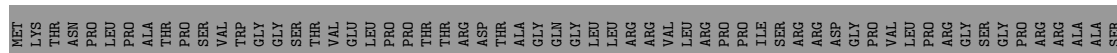
• Molecule 2: Small capsomere-interacting protein

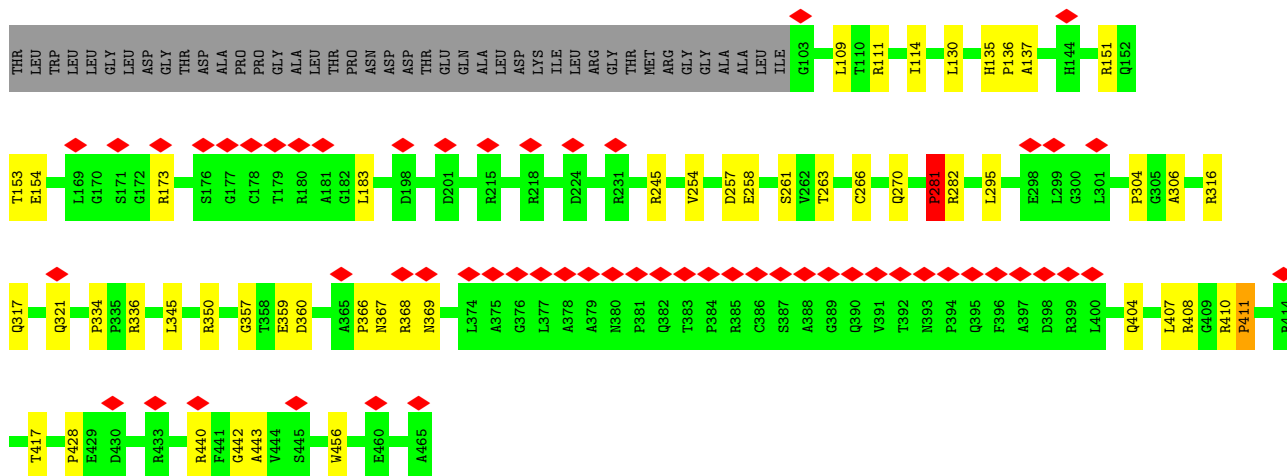


• Molecule 3: Triplex capsid protein 1

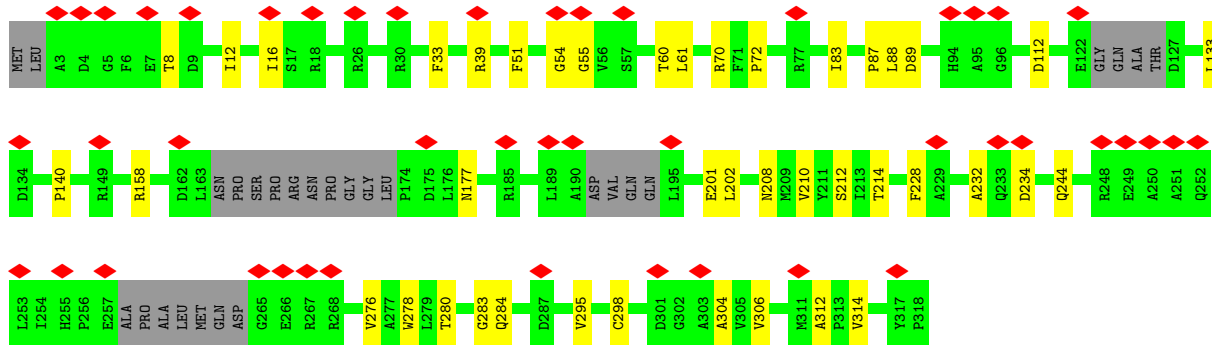
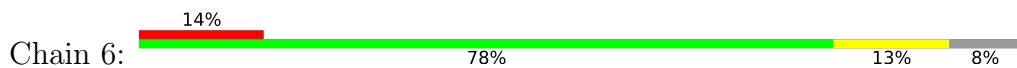


• Molecule 3: Triplex capsid protein 1

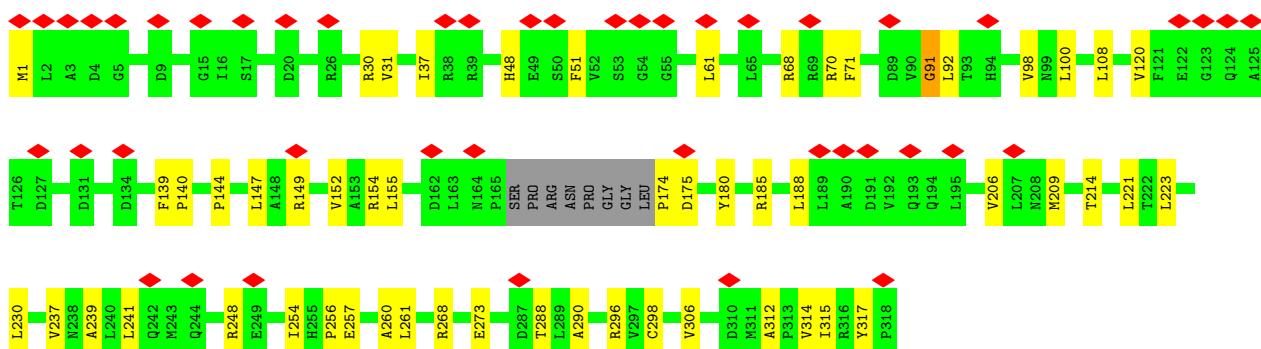
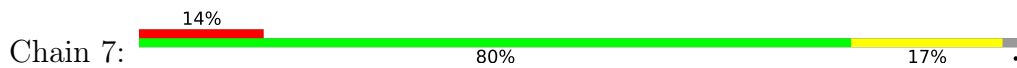




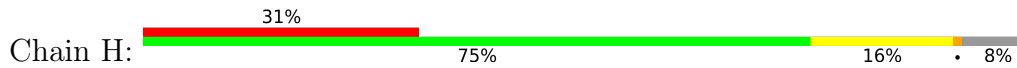
• Molecule 4: Triplex capsid protein 2

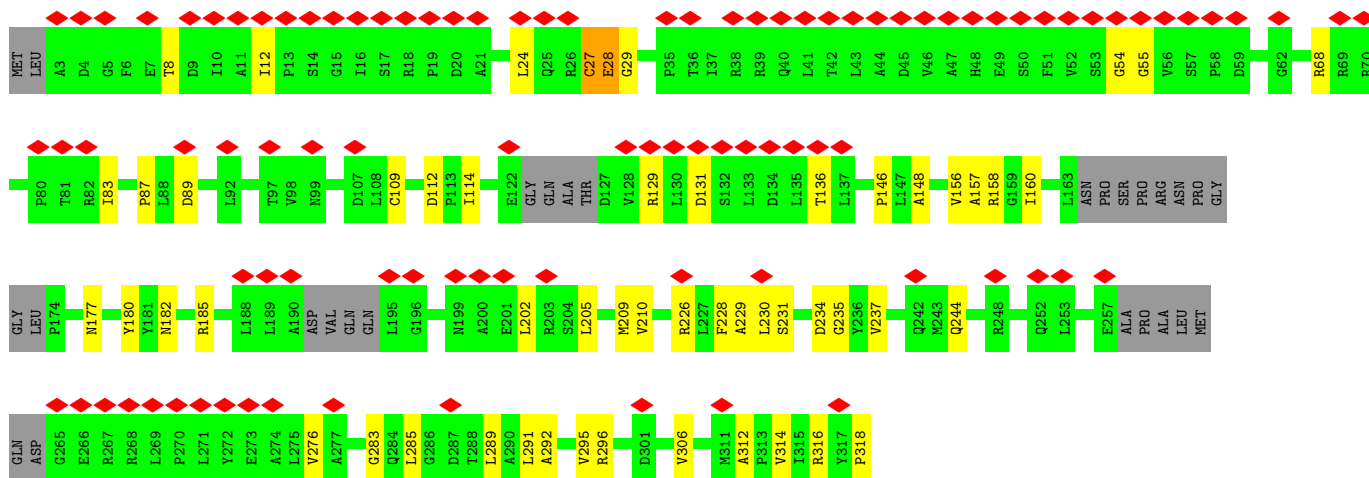


• Molecule 4: Triplex capsid protein 2

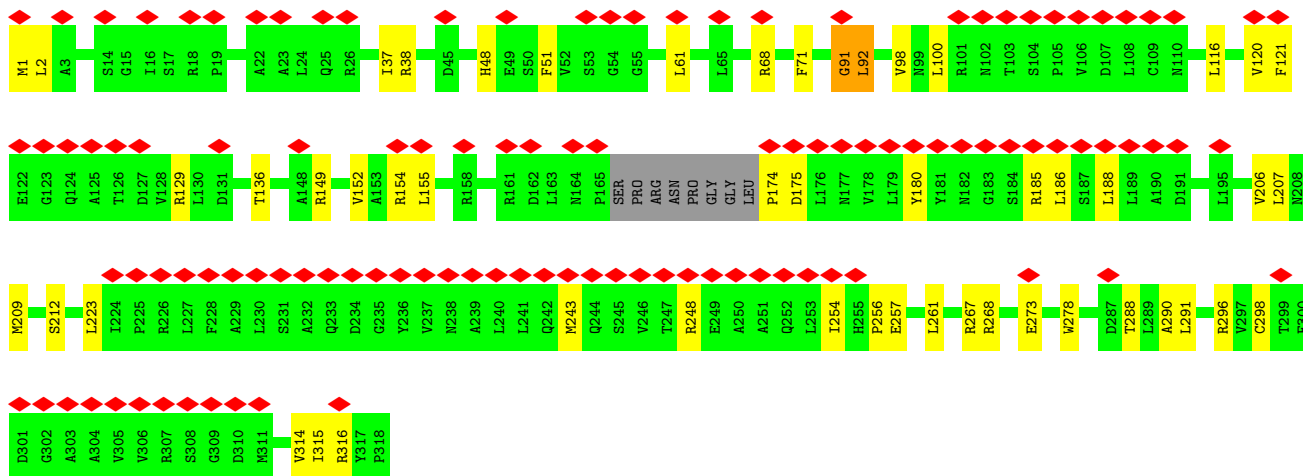
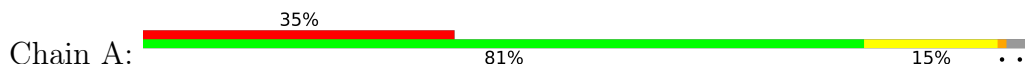


• Molecule 4: Triplex capsid protein 2

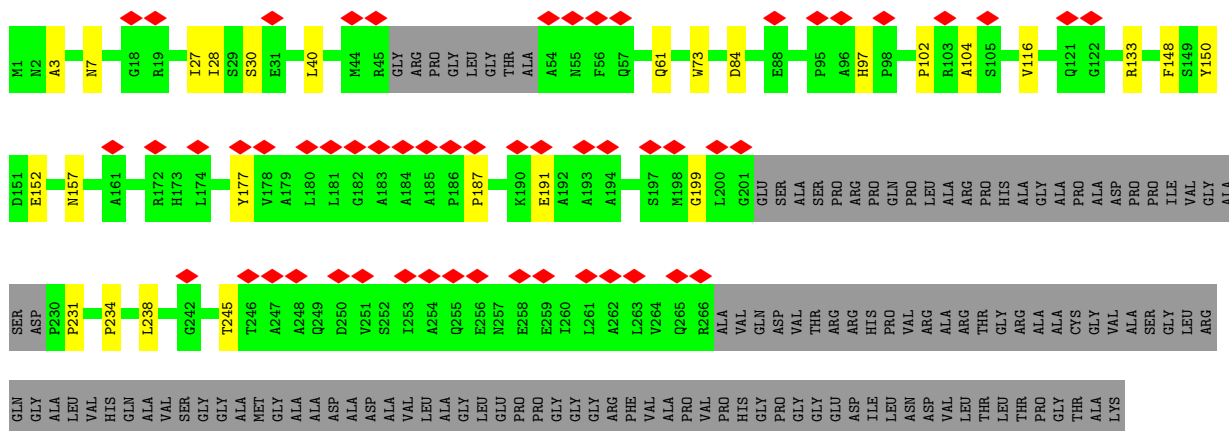


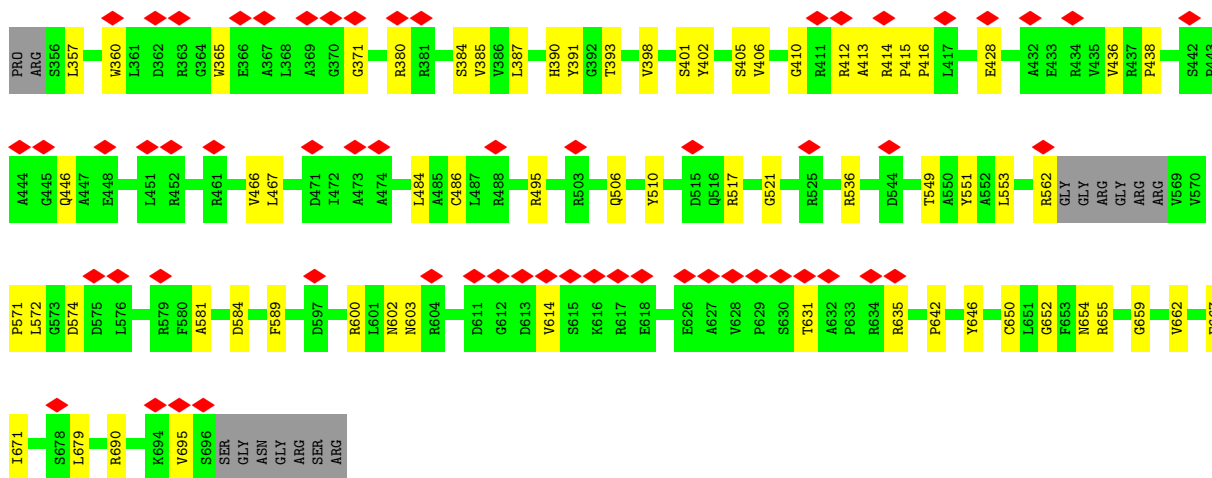


• Molecule 4: Triplex capsid protein 2

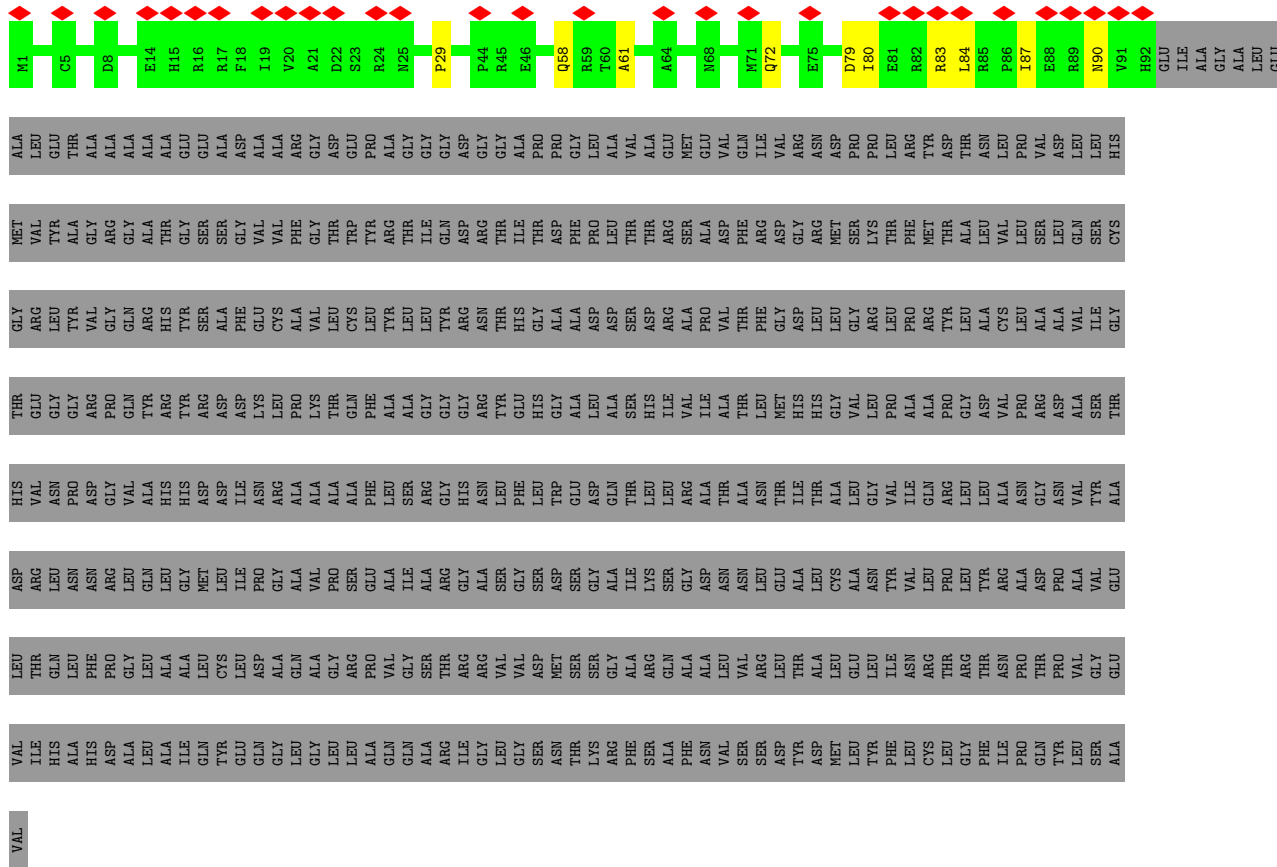


• Molecule 5: Capsid vertex component 1





• Molecule 6: Capsid vertex component 2



• Molecule 6: Capsid vertex component 2



MET	ASP	PRO	TYR	ASN	CYS	PRO	PHE	ASP	ALA	LEU	ASP	VAL	W13	E14	H15	R16	R17	A21	R24	E30	R33	D34	F35	W36	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	
GLY	R89	I90	Y91	HIS	GLU	ILE	ALA	GLY	ALA	LEU	ALA	ALA	LEU	GLU	THR	GLY	ALA	ALA	ALA	GLY	GLU	SER	GLY	GLY	GLY	ALA	GLY	GLY	ASP	GLY	GLY	GLY	ALA	PRO	PRO	ALA	GLY	LEU	ALA	VAL	GLN	ILE	GLY	VAL	ARG	GLY	LEU	ARG		
TYR	ASP	THR	ASN	LEU	PRO	VAL	ASP	GLY	LEU	LEU	LEU	VAL	MET	TYR	ALA	GLY	ARG	ALA	ALA	THR	GLY	SER	SER	GLY	VAL	VAL	ALA	GLY	ILE	ARG	ASP	THR	ILE	THR	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	PHE	
MET	THR	ALA	ASP	VAL	LEU	SER	LEU	ALA	LEU	GLN	SER	GLY	GLY	ARG	LEU	TYR	VAL	VAL	TYR	TYR	GLY	SER	ASP	ALA	PHE	GLY	ASP	ILE	ASP	THR	HIS	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	PRO		
ARG	TYR	LEU	ALA	CYS	VAL	ALA	ALA	ALA	VAL	VAL	ILE	THR	THR	GLY	GLY	GLY	GLN	TYR	ARG	HIS	ARG	TYR	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ALA
ALA	PRO	GLY	ASP	VAL	PRO	ARG	ASP	ASP	ALA	VAL	ALA	THR	THR	GLY	ALA	ASN	PRO	PRO	ASP	GLY	PRO	GLY	PRO	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	ILE
GLN	ARG	LEU	LEU	ALA	ASN	GLY	ASN	ASN	VAL	VAL	VAL	ASP	ASP	TYR	ALA	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	VAL
LEU	PRO	TYR	THR	ASN	ALA	ASP	PRO	THR	VAL	VAL	VAL	THR	GLN	LEU	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ASN		
ARG	THR	ARG	THR	ASN	ILE	PRO	PRO	THR	VAL	VAL	VAL	THR	HIS	ILE	ALA	HIS	ALA	ILE	GLN	TYR	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LEU			
CYS	LEU	GLY	PHE	ILE	PRO	GLM	TYR	VAL	LEU	LEU	LEU	VAL	VAL	VAL	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA		

● Molecule 7: Large tegument protein deneedylase

Chain O:  98%

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

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 (\AA)	395.52, 395.52, 395.52	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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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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(°)	Ideal(°)
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 ⓘ

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.

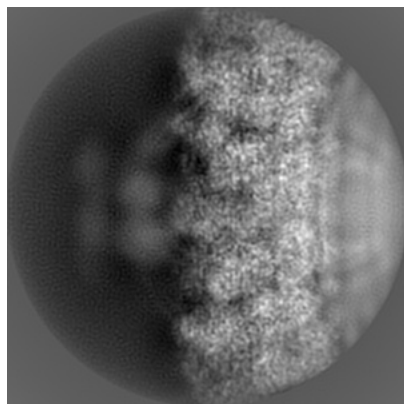
6 Map visualisation [i](#)

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.

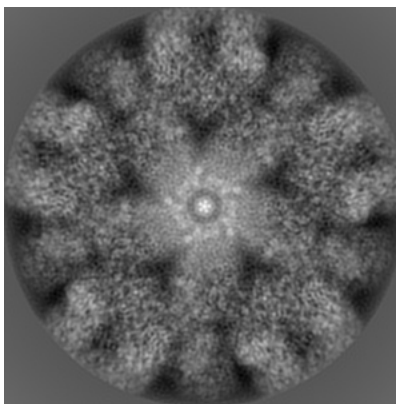
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

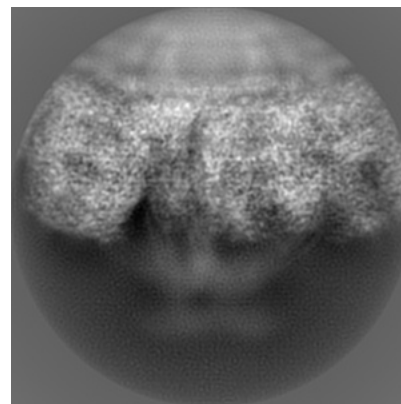
6.1.1 Primary map



X

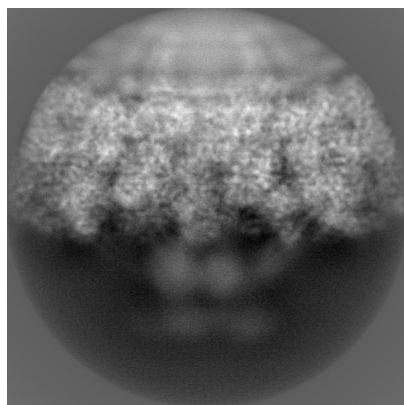


Y

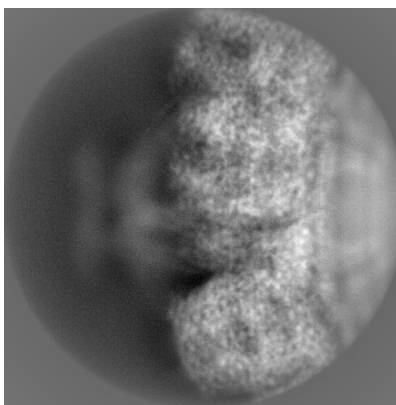


Z

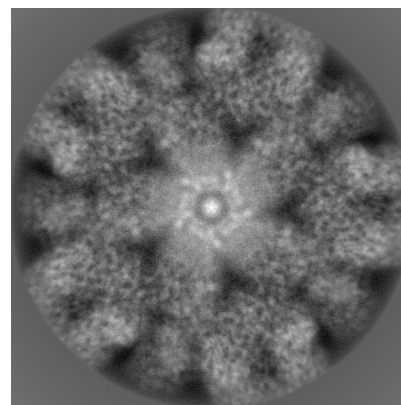
6.1.2 Raw map



X



Y

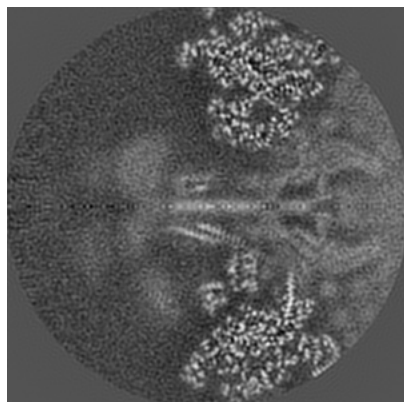


Z

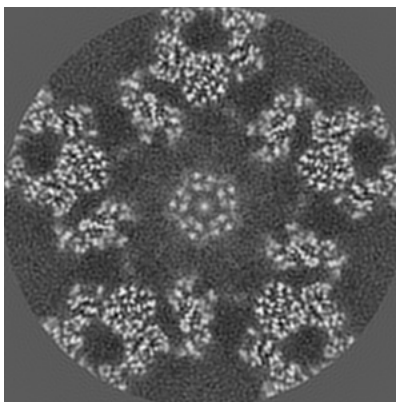
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

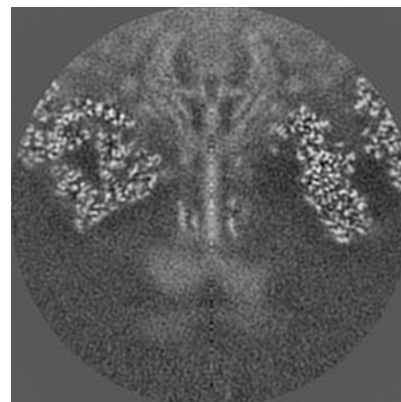
6.2.1 Primary map



X Index: 192

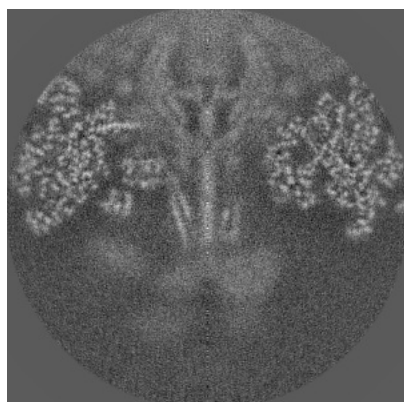


Y Index: 192

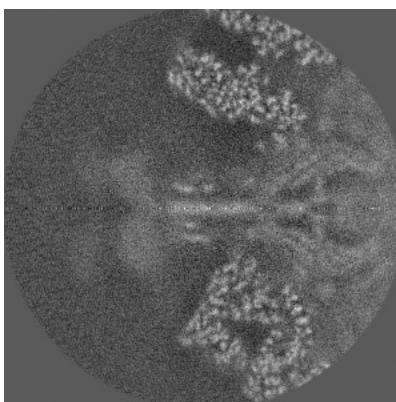


Z Index: 192

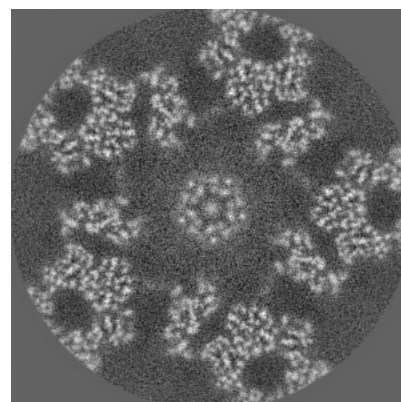
6.2.2 Raw map



X Index: 192



Y Index: 192

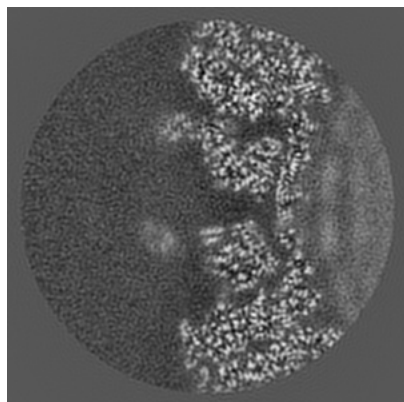


Z Index: 192

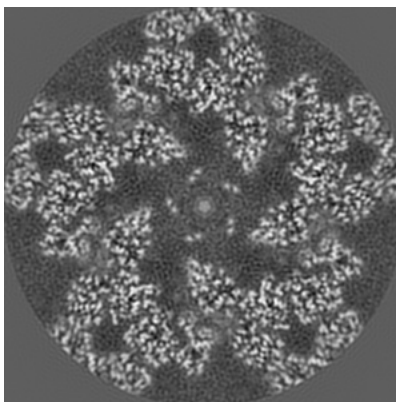
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

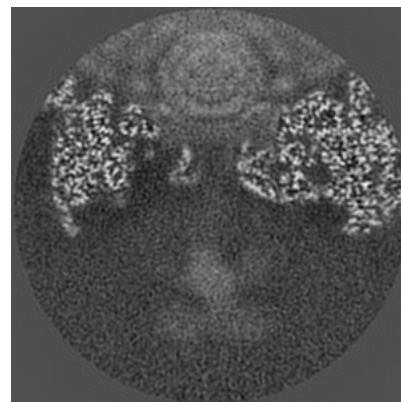
6.3.1 Primary map



X Index: 265

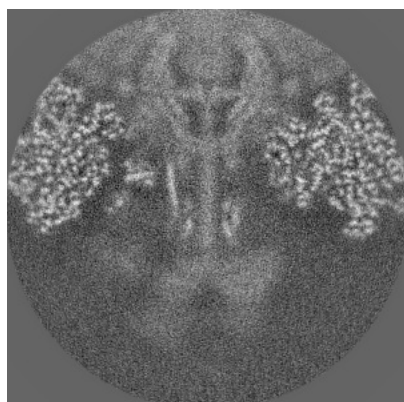


Y Index: 211

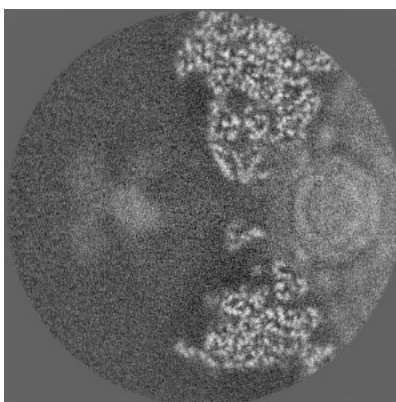


Z Index: 231

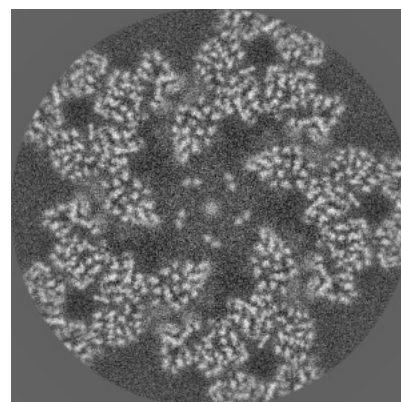
6.3.2 Raw map



X Index: 197



Y Index: 231

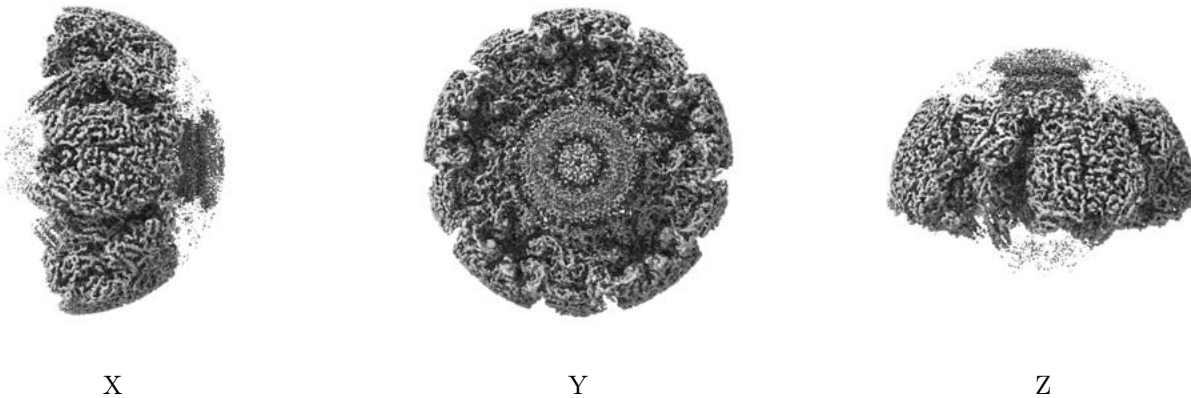


Z Index: 211

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

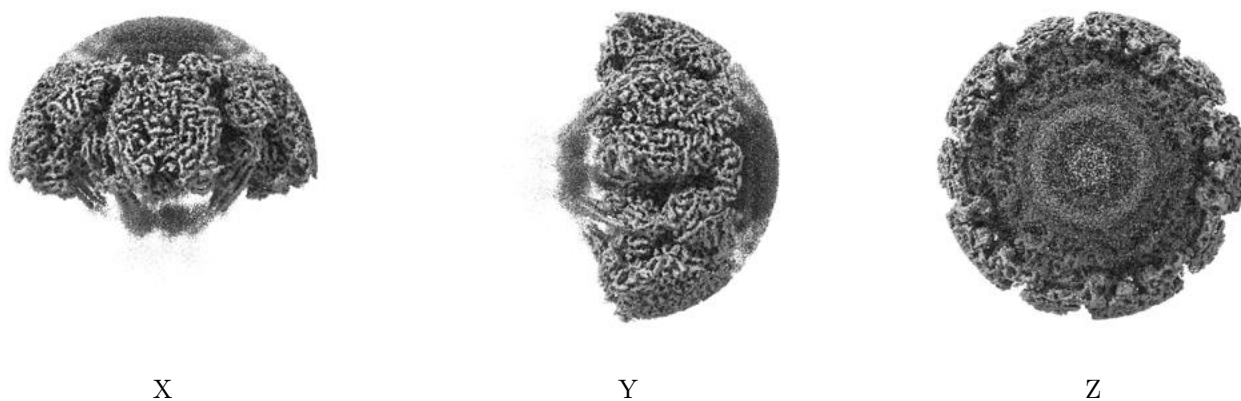
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



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



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.

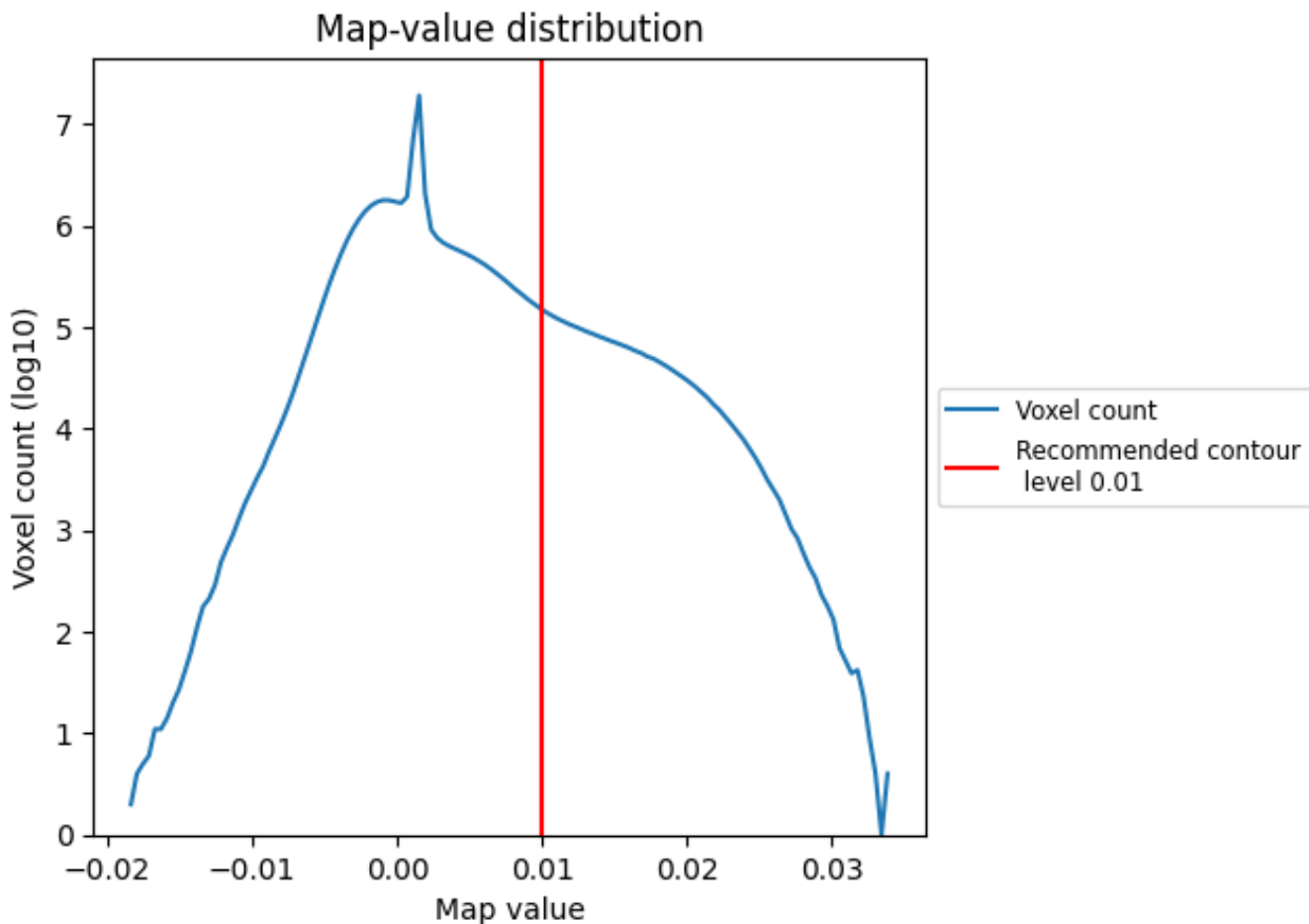
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

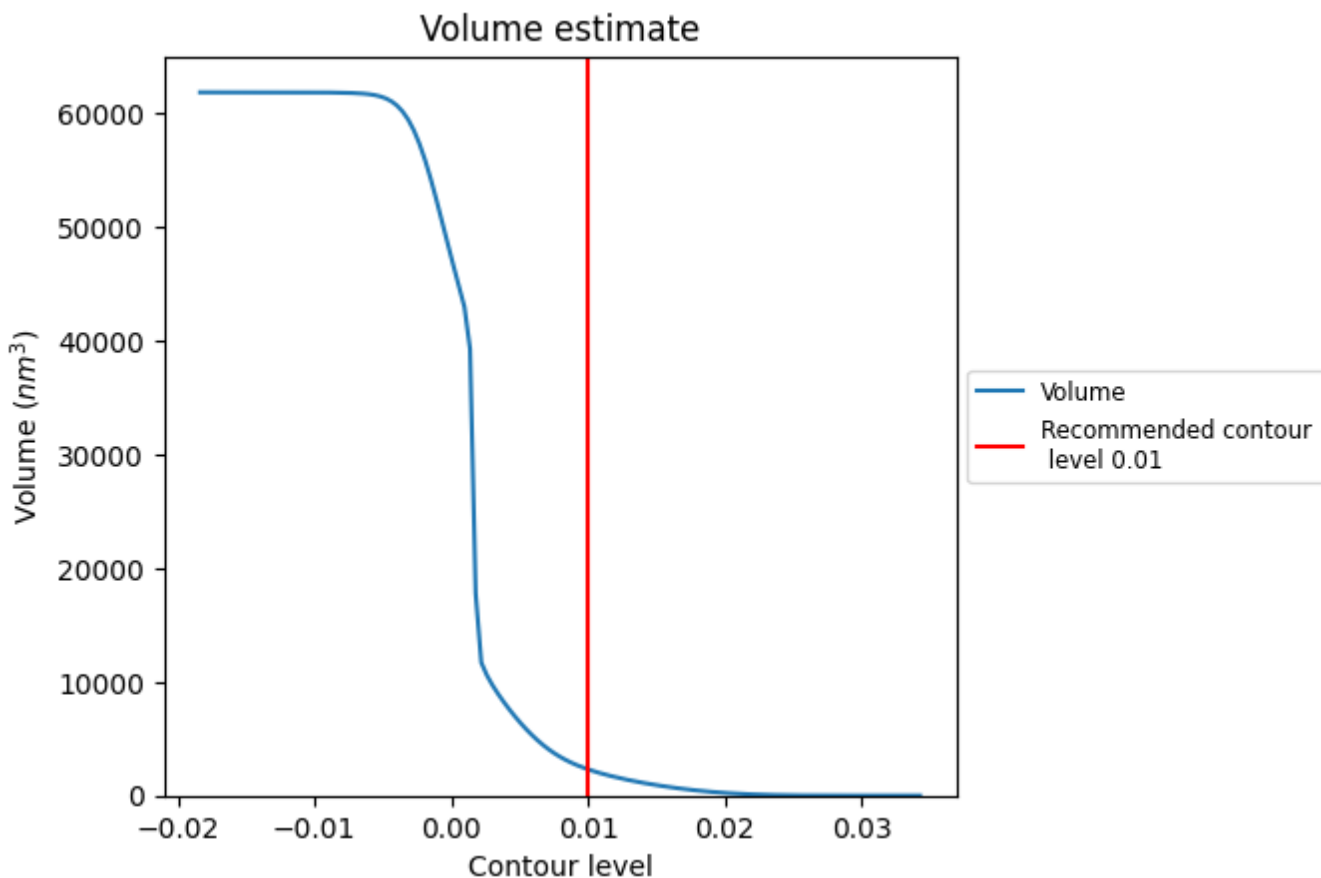
This section contains the results of statistical analysis of the map.

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.

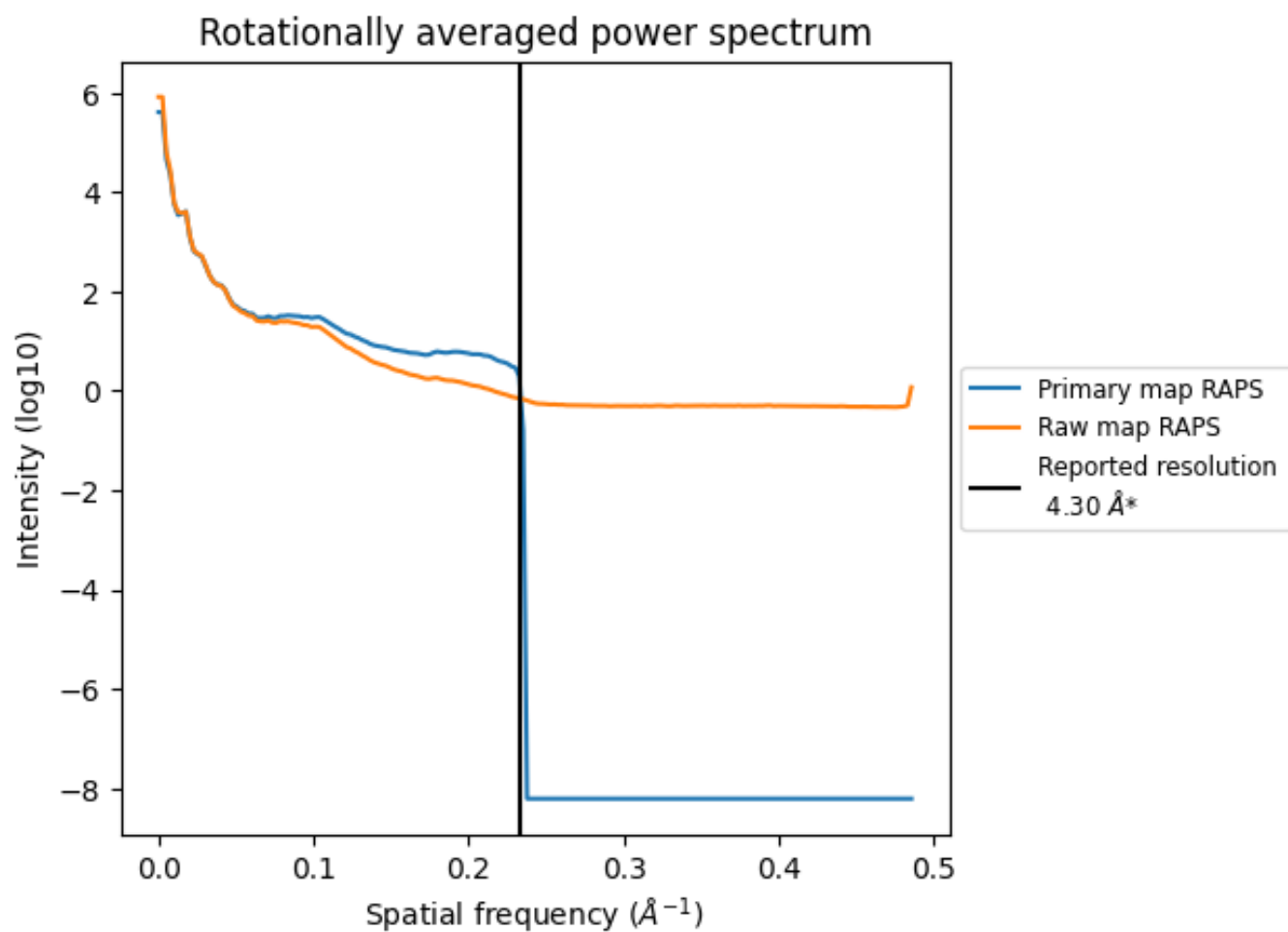
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2305 nm³; 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](#)

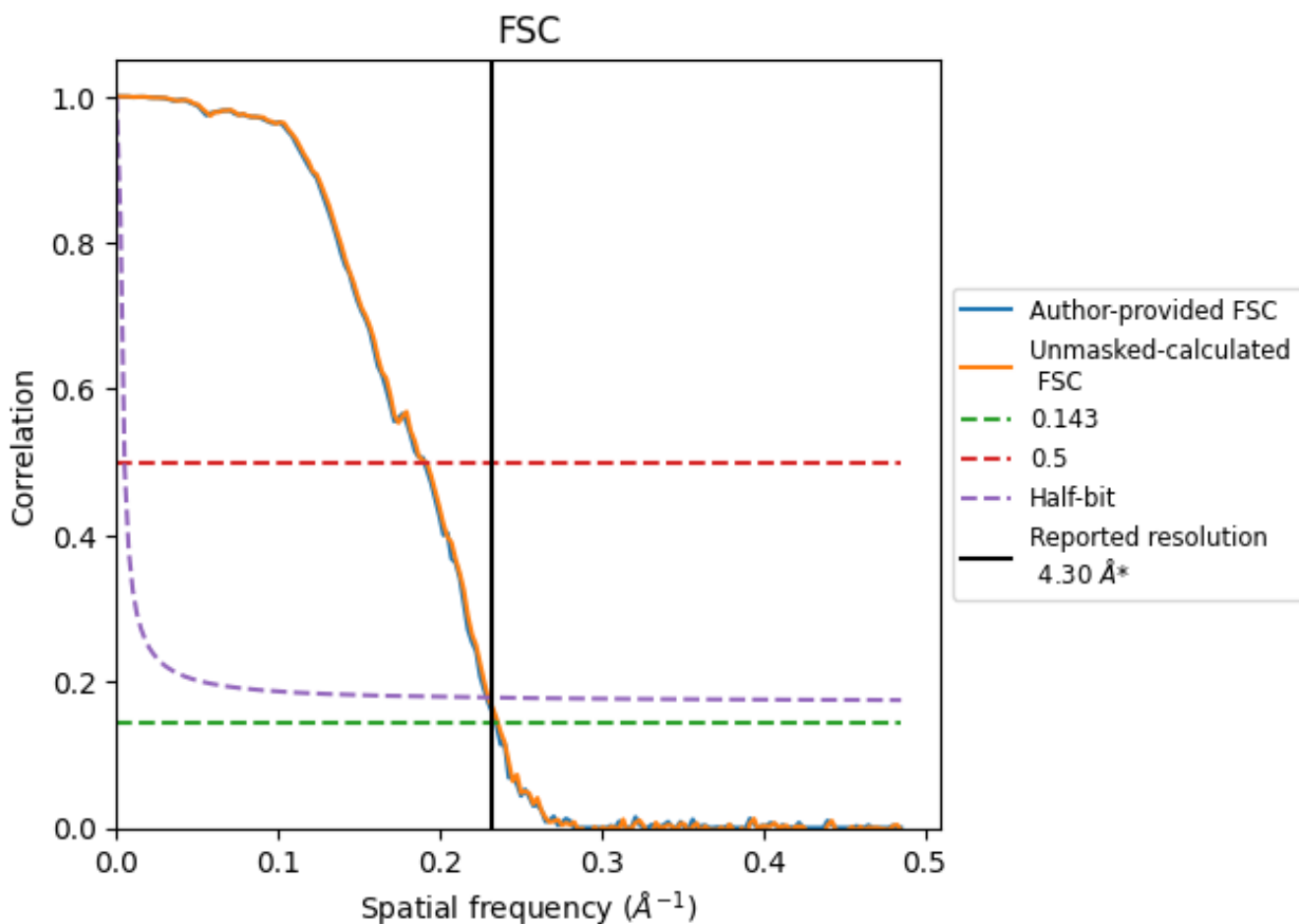


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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](#)

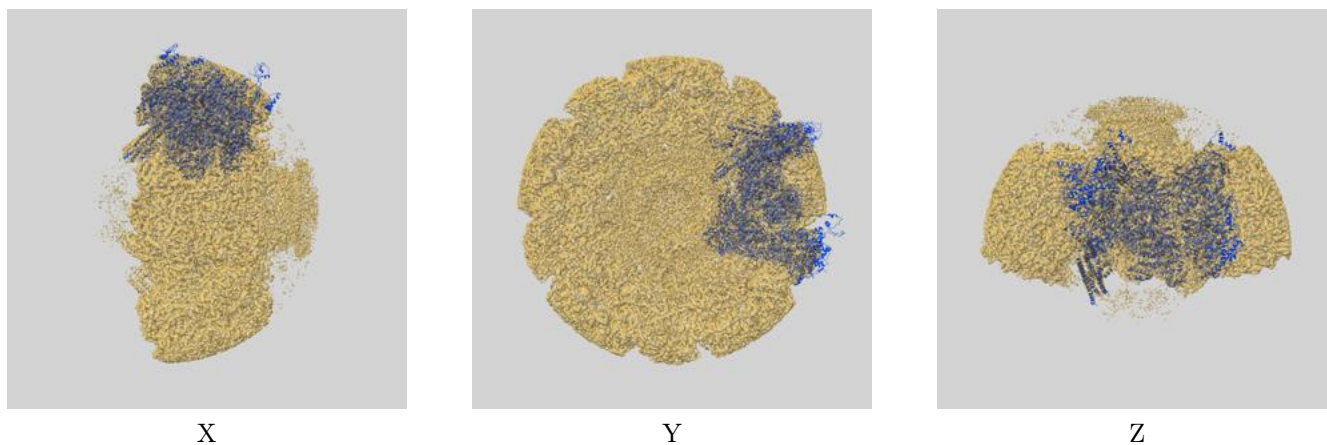
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.26	5.25	4.37
Unmasked-calculated*	4.24	5.23	4.35

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

9 Map-model fit [i](#)

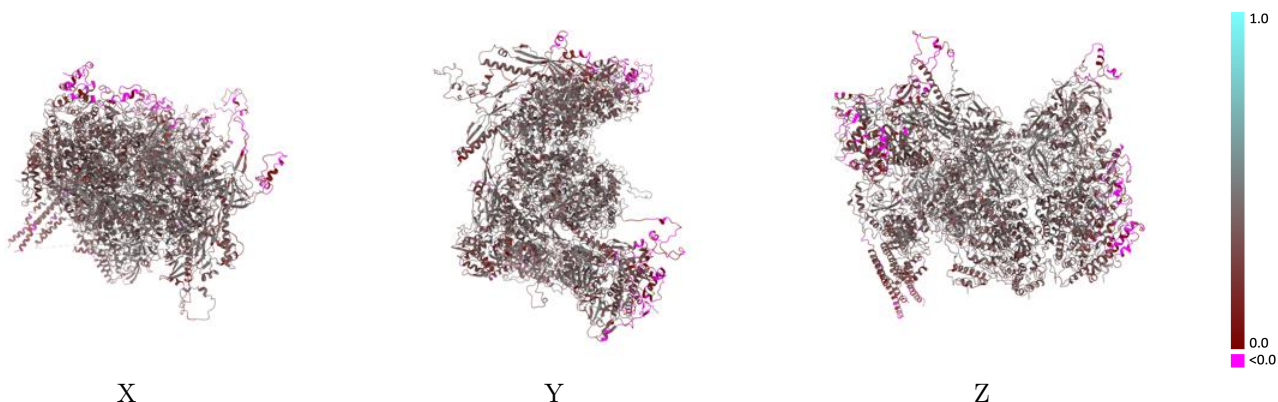
This section contains information regarding the fit between EMDB map EMD-9860 and PDB model 6ODM. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



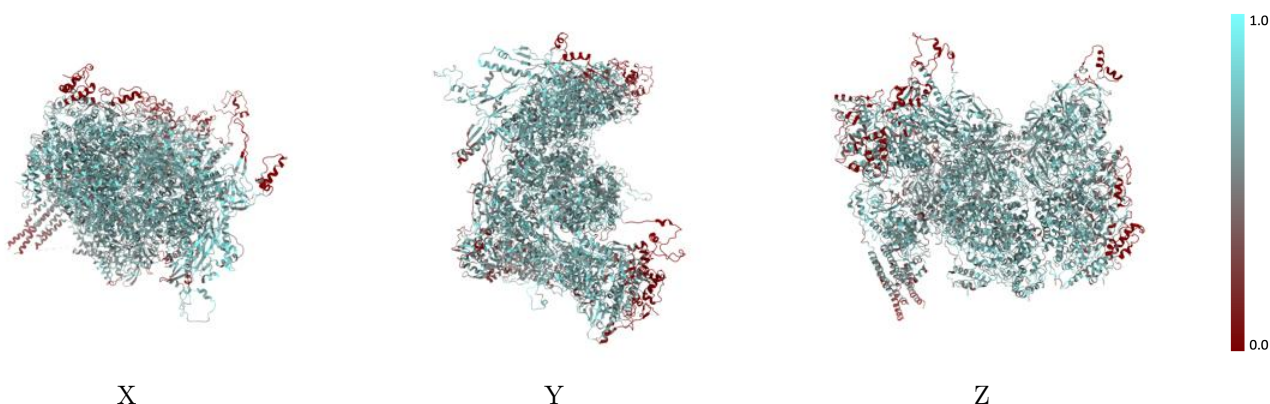
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



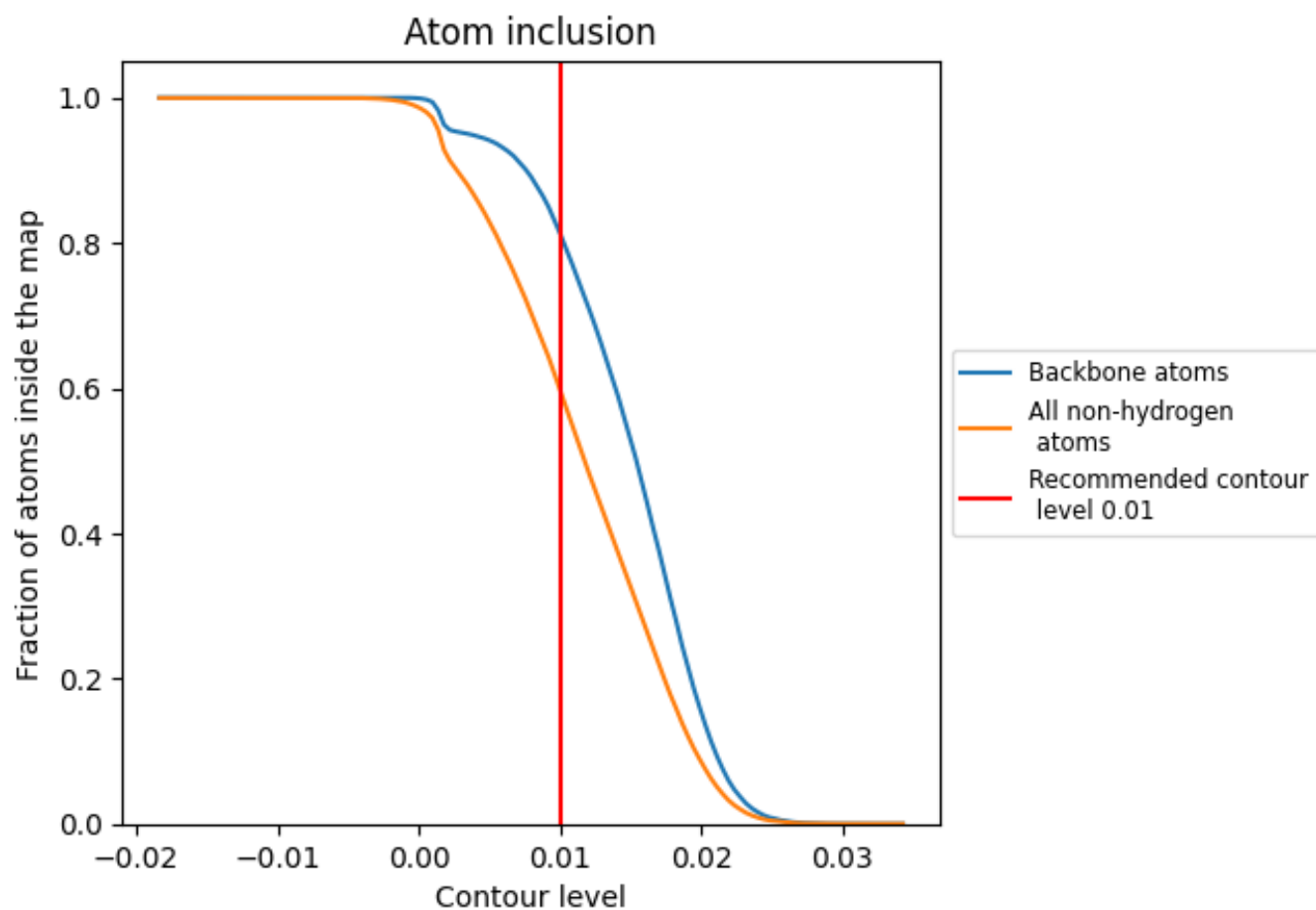
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).









































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

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

