



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:08 AM UTC

PDB ID : 8TES / pdb_00008tes
EMDB ID : EMD-41200
Title : Human cytomegalovirus portal vertex, virion configuration 2 (VC2)
Authors : Jih, J.; Liu, Y.T.; Liu, W.; Zhou, H.
Deposited on : 2023-07-06
Resolution : 3.27 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

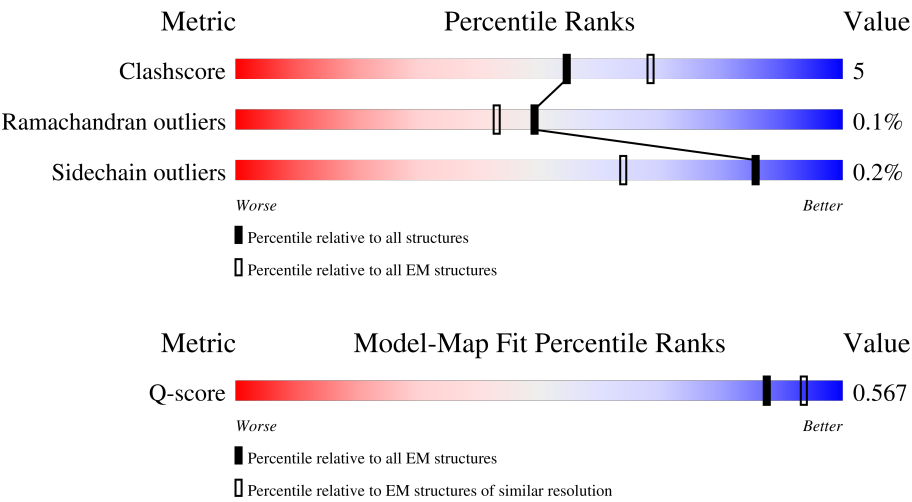
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.27 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14508 (2.77 - 3.77)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2241	98%
1	C	2241	98%
2	E	642	10% 12% 87%
2	F	642	12% 11% 87%

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Mol	Chain	Length	Quality of chain
3	G	594	
4	H	1370	
4	I	1370	
4	J	1370	
4	K	1370	
4	L	1370	
4	M	1370	
5	N	75	
5	O	75	
5	P	75	
5	Q	75	
5	R	75	
5	S	75	
6	T	290	
6	W	290	
7	U	306	
7	V	306	
7	X	306	
7	Y	306	
8	Z	1048	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 88005 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 Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	40	Total	C	N	O	S	0	0
			332	213	60	58	1		
1	C	43	Total	C	N	O	S	0	0
			354	228	63	62	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	84	Total	C	N	O	S	0	0
			696	427	135	129	5		
2	F	85	Total	C	N	O	S	0	0
			710	442	138	126	4		

- Molecule 3 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	471	Total	C	N	O	S	0	0
			3862	2416	740	692	14		

- Molecule 4 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	1311	Total	C	N	O	S	0	0
			10406	6630	1802	1913	61		
4	I	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		
4	J	1317	Total	C	N	O	S	0	0
			10433	6641	1814	1919	59		
4	K	1298	Total	C	N	O	S	0	0
			10282	6544	1792	1887	59		
4	L	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		

- Molecule 5 is a protein called Small capsomere-interacting protein.

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

- Molecule 6 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	240	Total	C	N	O	S	0	0
			1919	1235	335	338	11		
6	W	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

- Molecule 7 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	292	Total	C	N	O	S	0	0
			2317	1489	399	411	18		
7	V	288	Total	C	N	O	S	0	0
			2292	1471	397	407	17		
7	X	295	Total	C	N	O	S	0	0
			2334	1501	402	412	19		
7	Y	285	Total	C	N	O	S	0	0
			2266	1456	387	405	18		

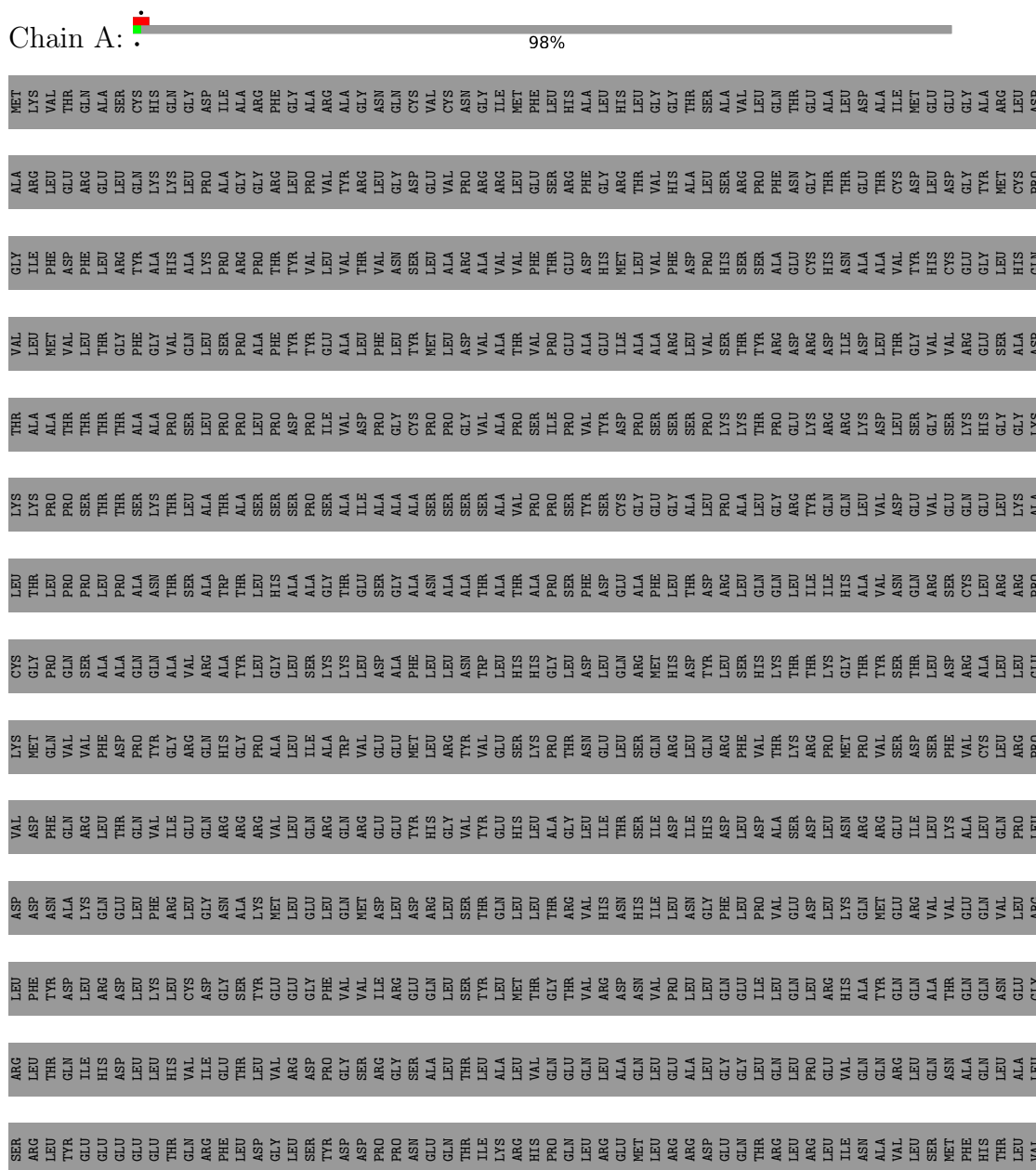
- Molecule 8 is a protein called Large structural phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	284	Total	C	N	O	S	0	0
			2320	1463	425	420	12		

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.

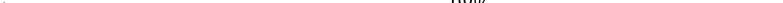
- Molecule 1: Large tegument protein deneddylase



WORLDWIDE
PDB
PROTEIN DATA BANK

[illegible]

- Molecule 1: Large tegument protein deneddylase

Chain C: 

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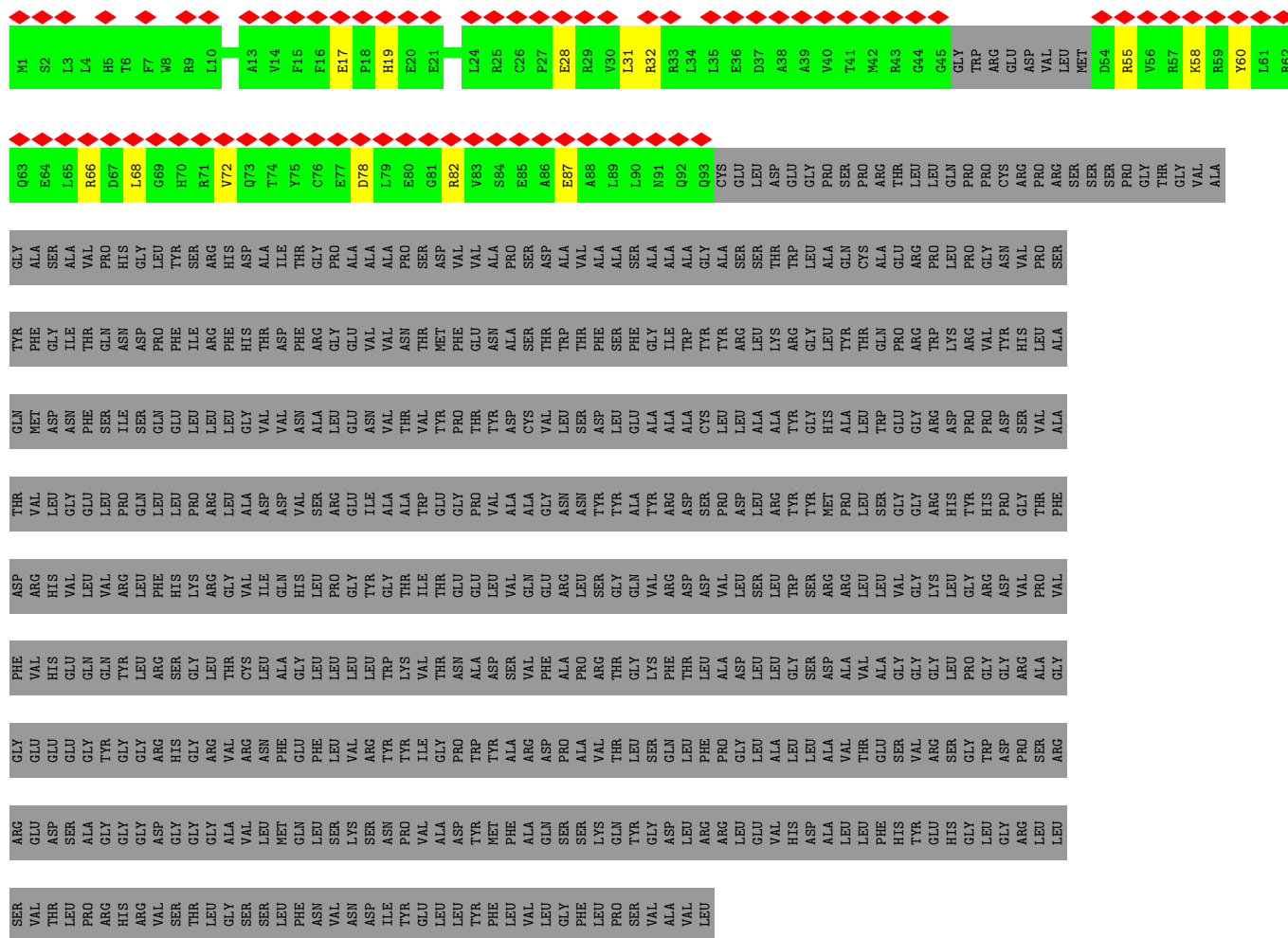


- Molecule 2: Capsid vertex component 2

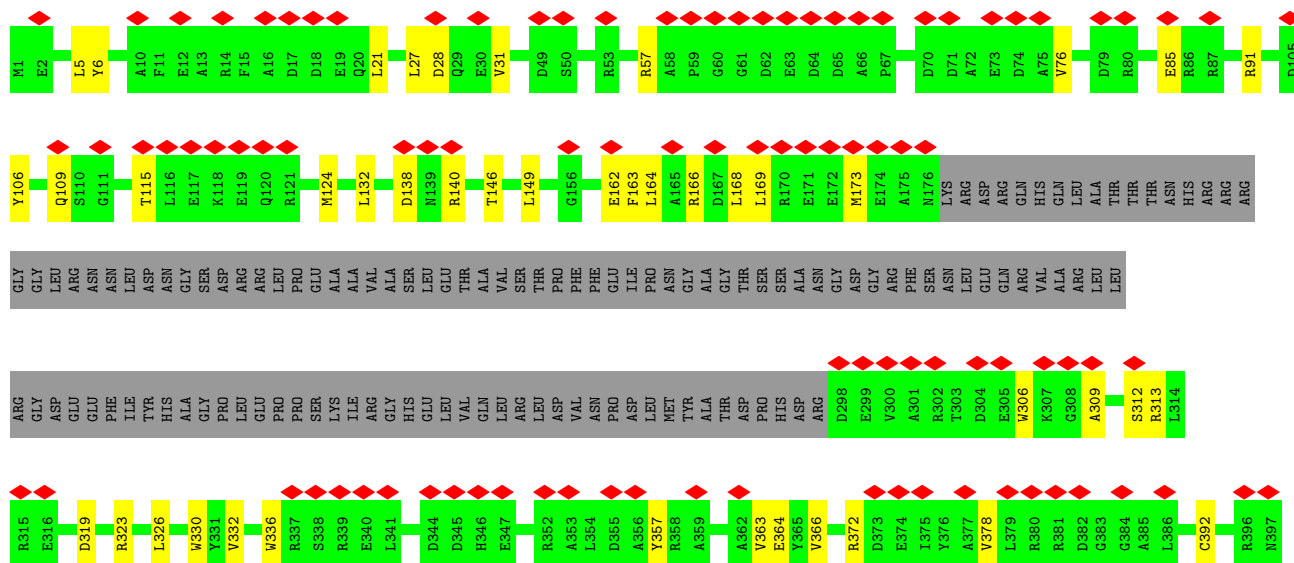
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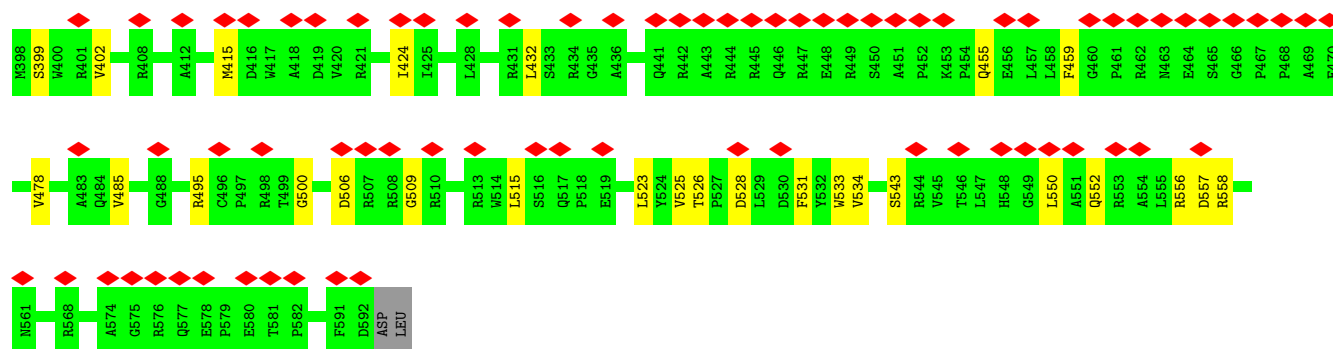
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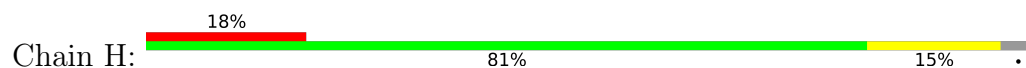


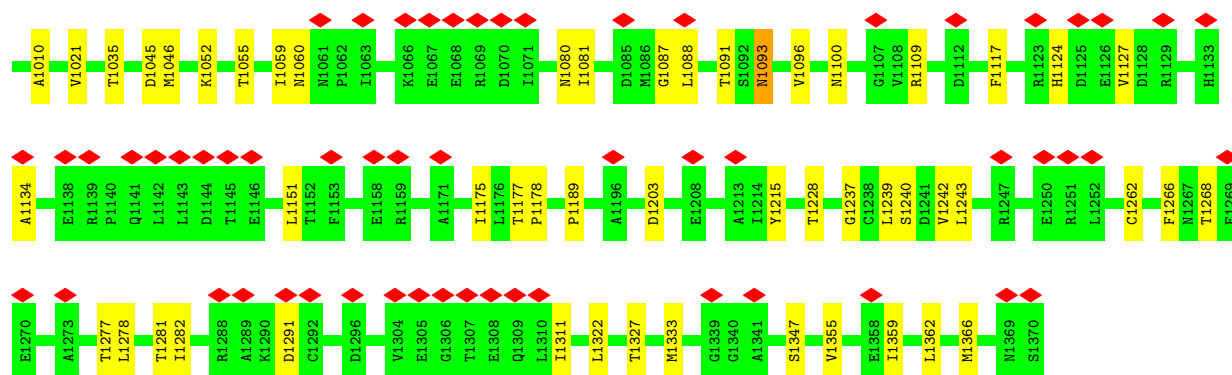
• Molecule 3: Capsid vertex component 1



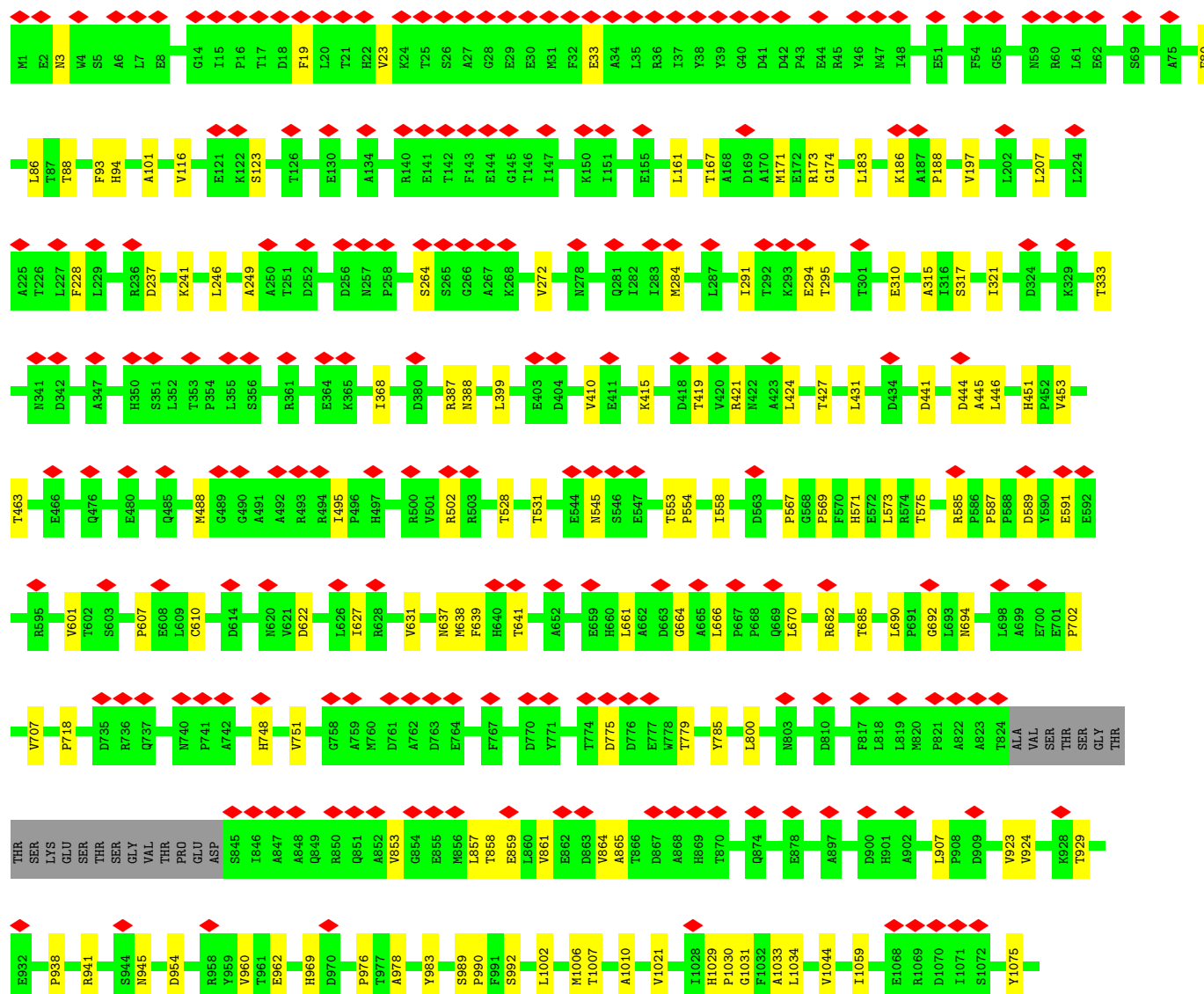
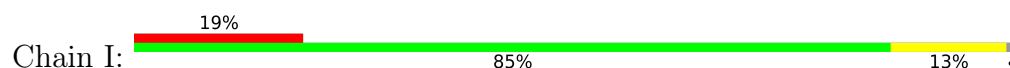


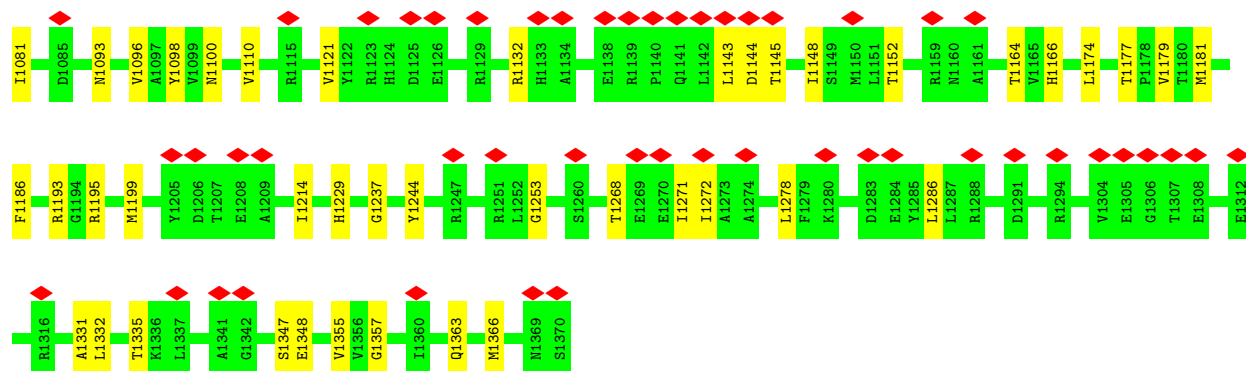
• Molecule 4: Major capsid protein



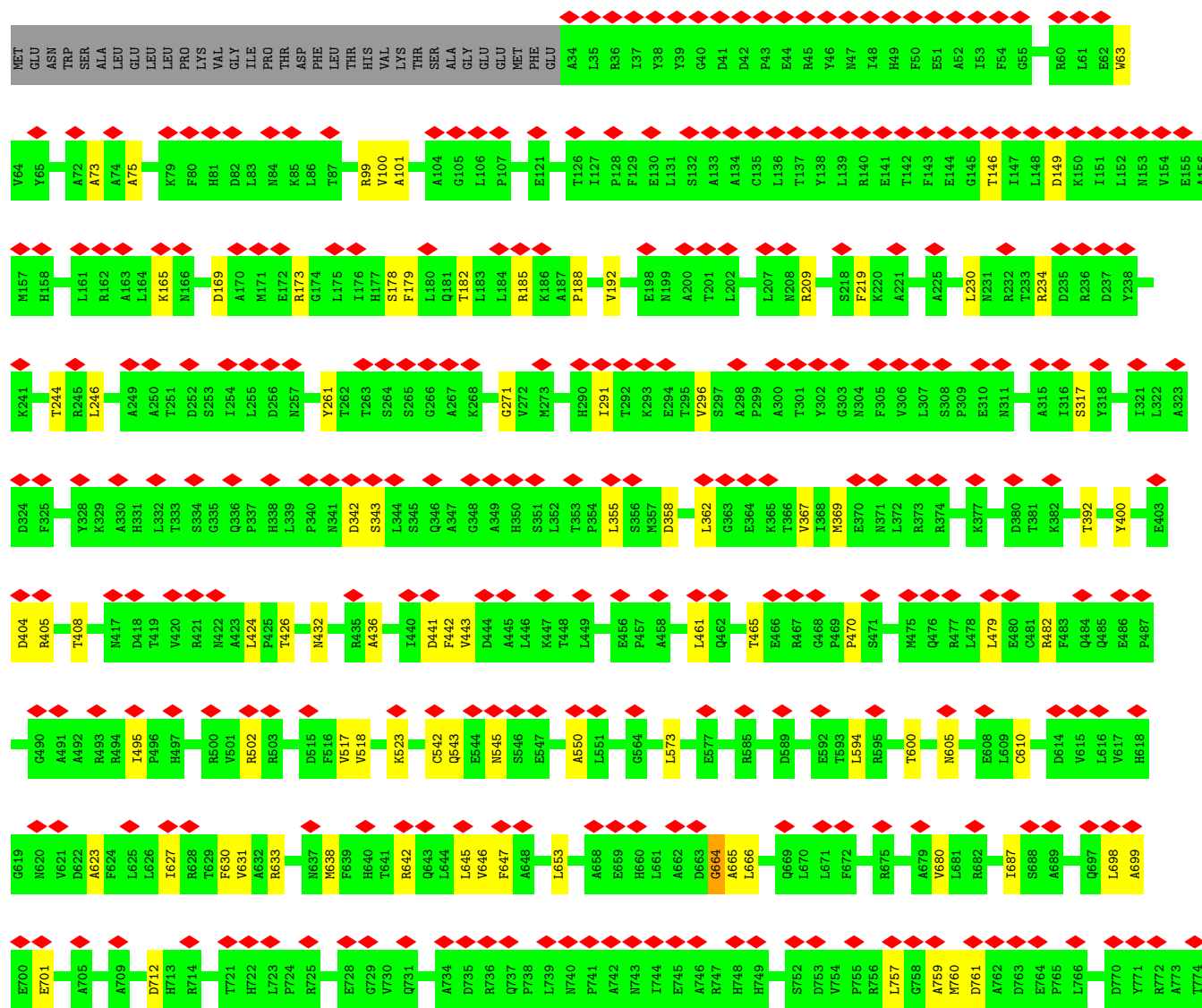
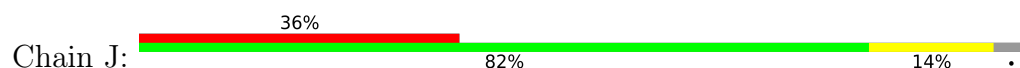


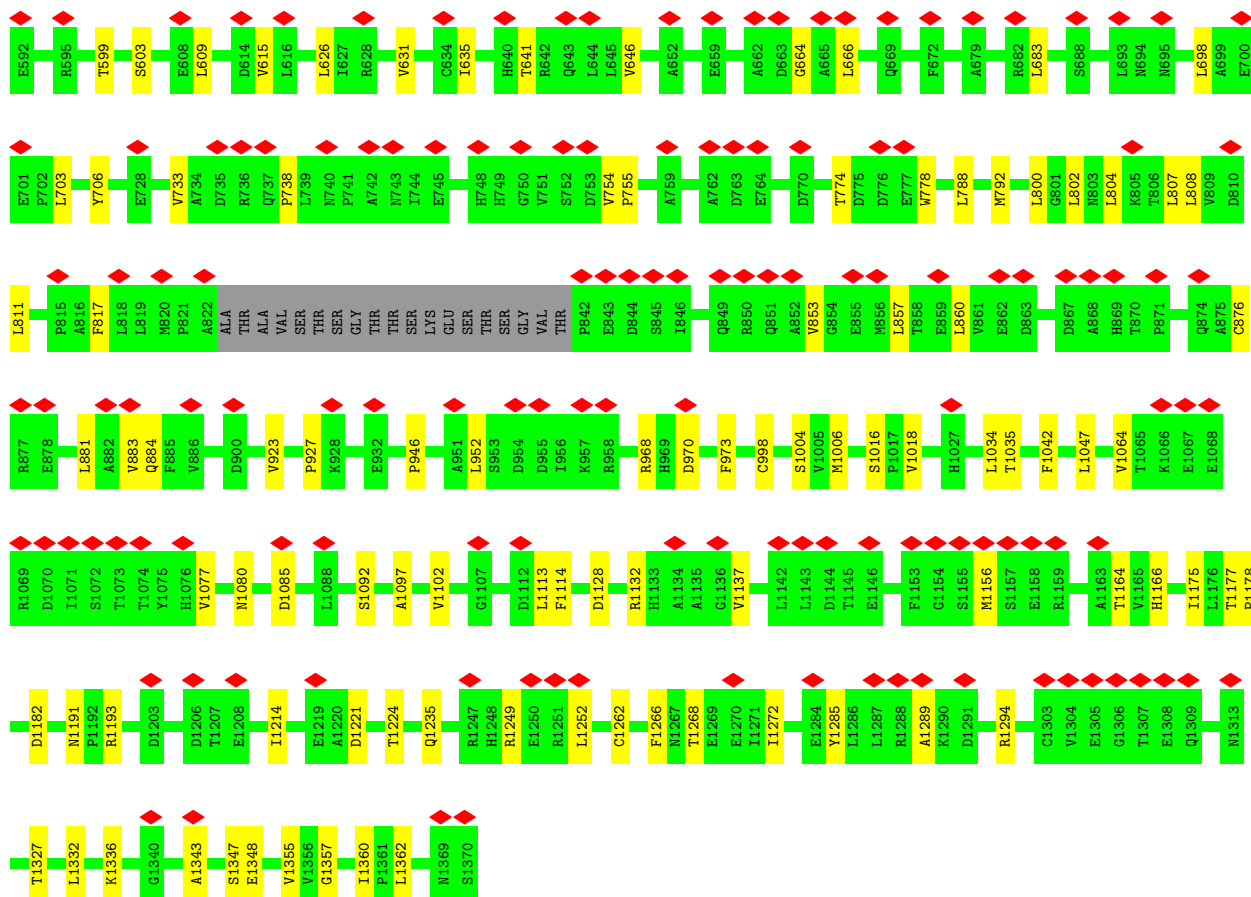
• Molecule 4: Major capsid protein



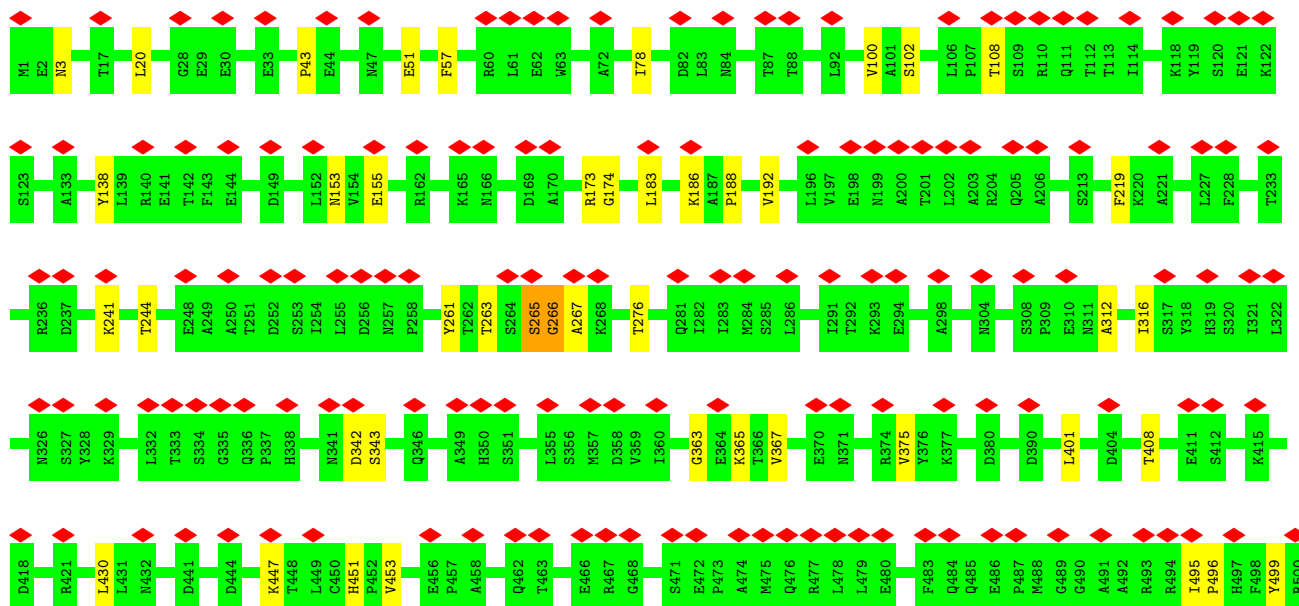
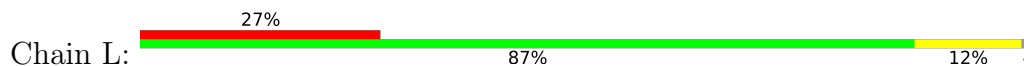


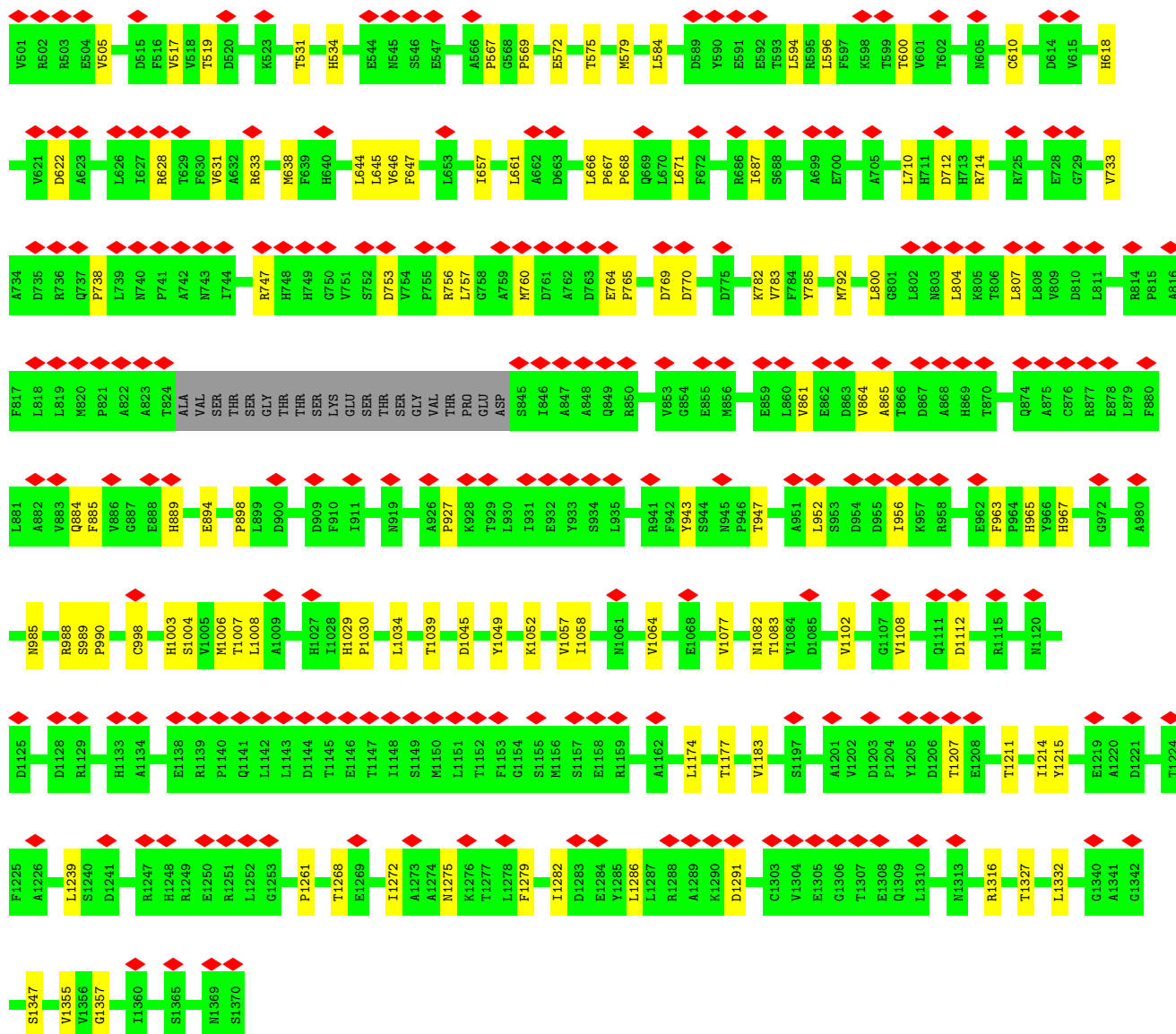
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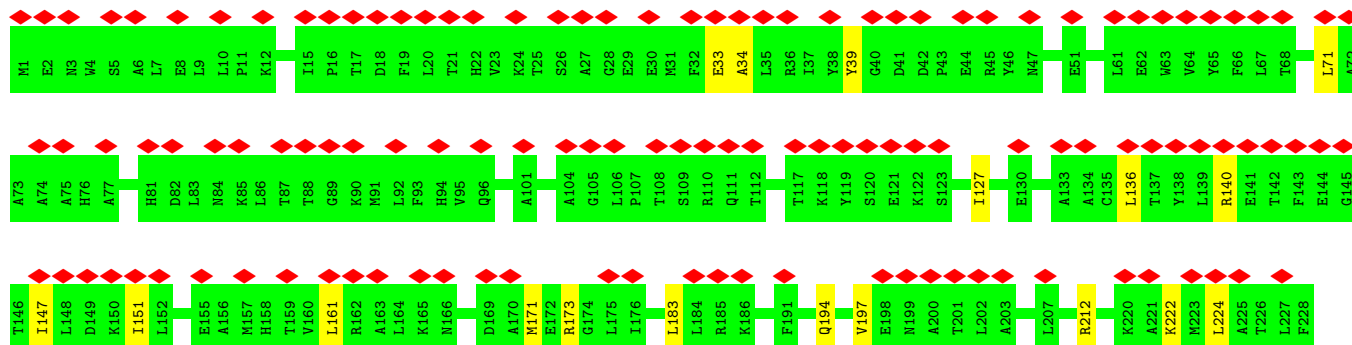
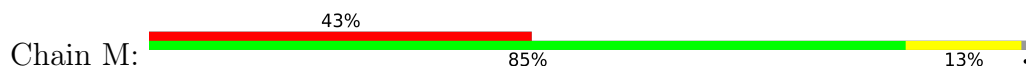


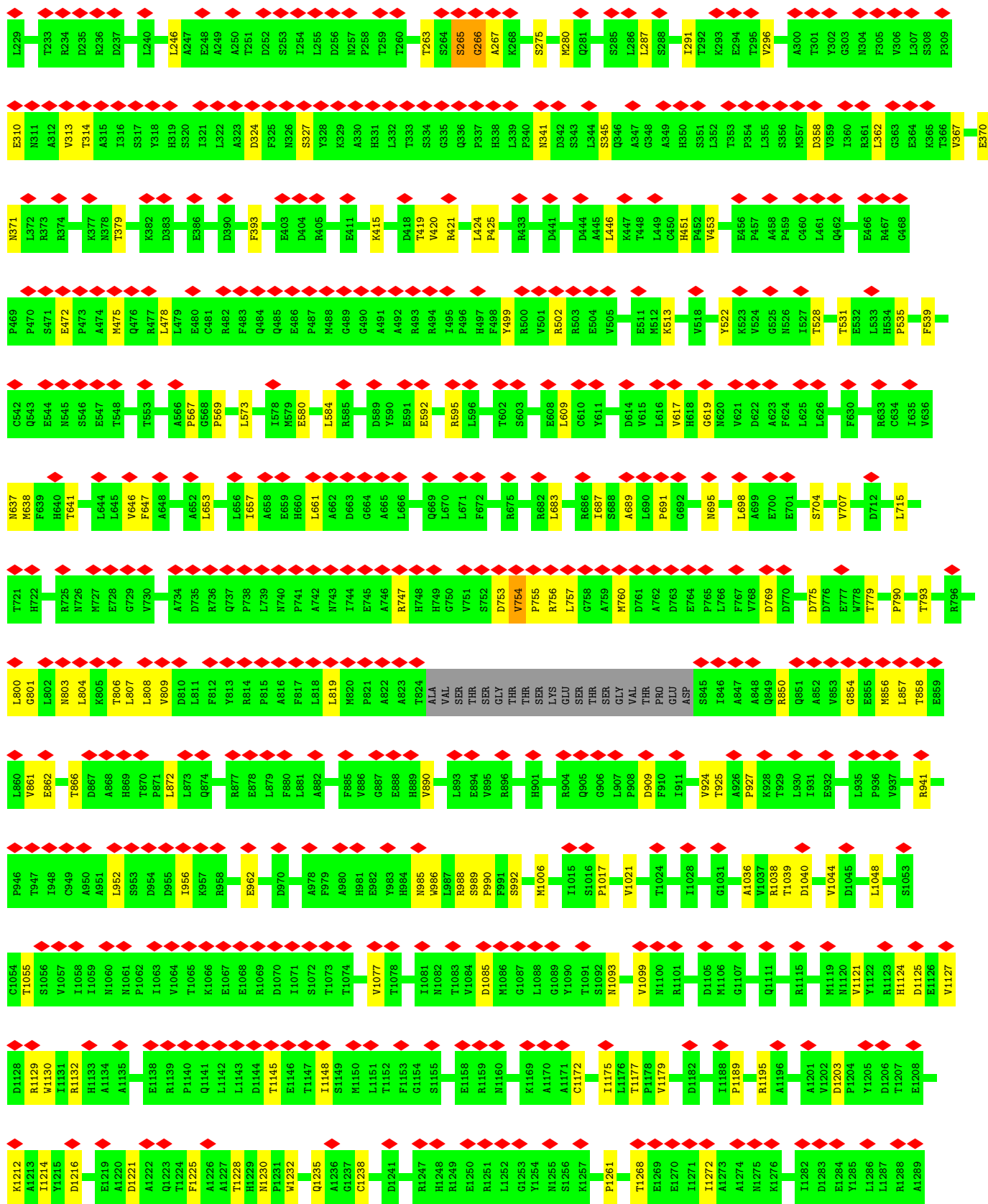
• Molecule 4: Major capsid protein





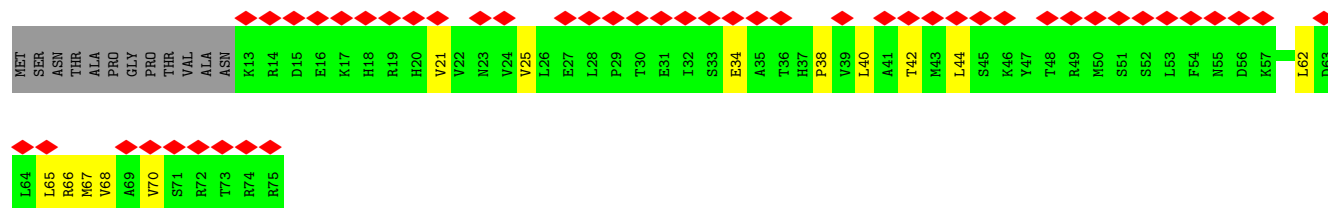
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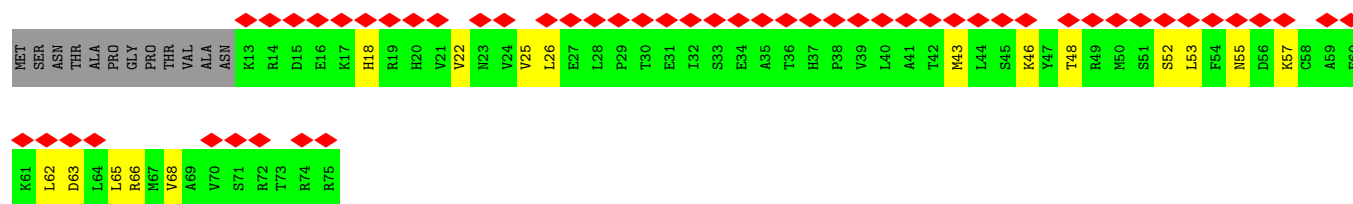
• Molecule 5: Small capsomere-interacting protein



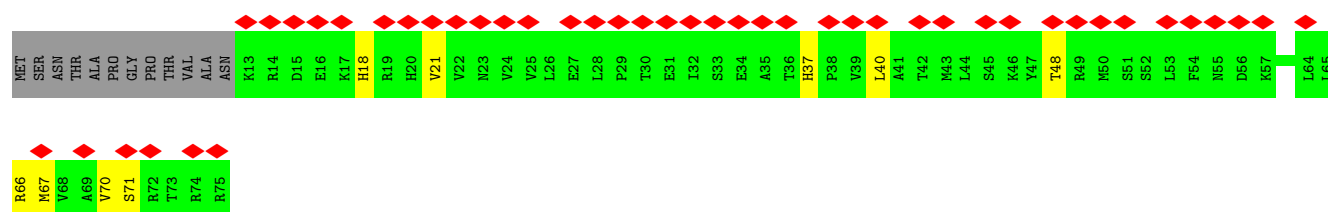
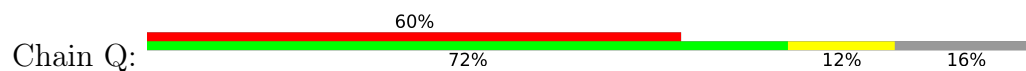
• Molecule 5: Small capsomere-interacting protein



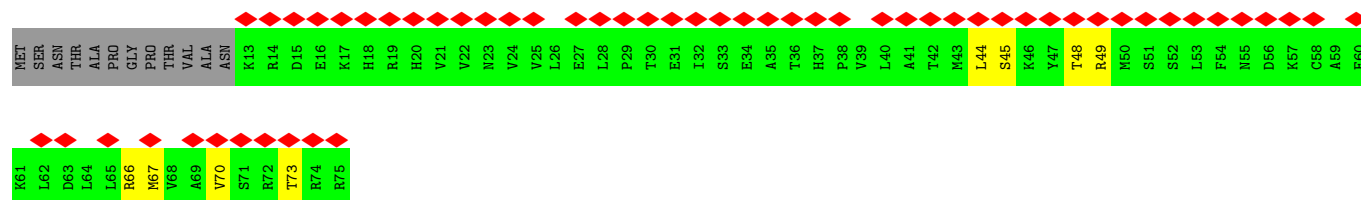
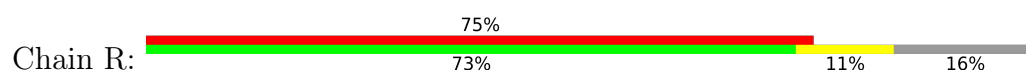
• Molecule 5: Small capsomere-interacting protein



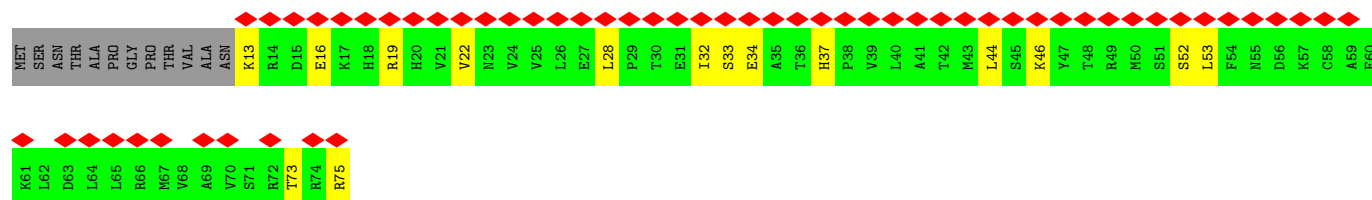
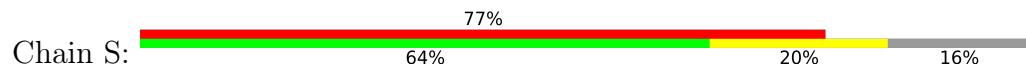
• Molecule 5: Small capsomere-interacting protein



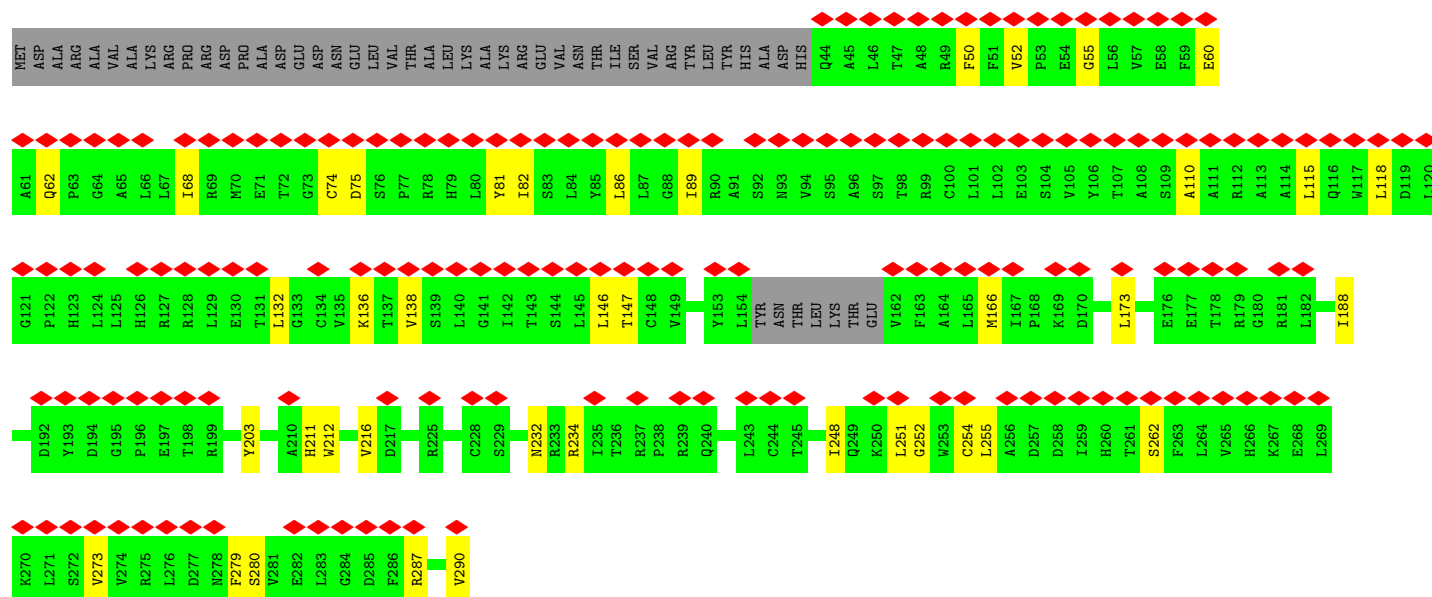
• Molecule 5: Small capsomere-interacting protein



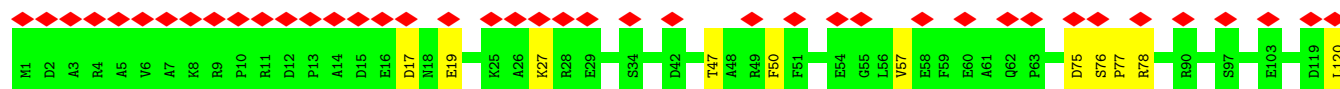
- Molecule 5: Small capsomere-interacting protein

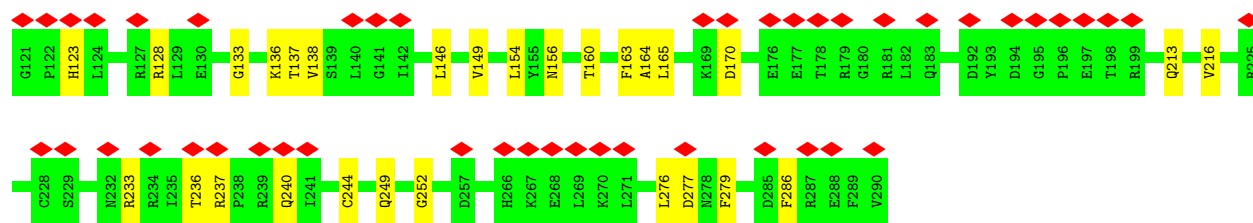


- Molecule 6: Triplex capsid protein 1



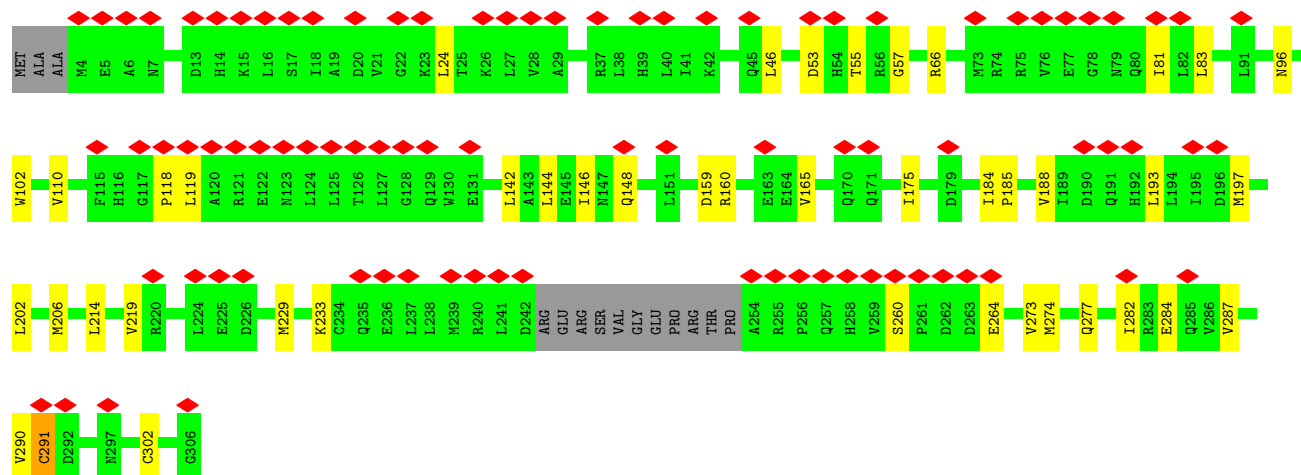
- Molecule 6: Triplex capsid protein 1





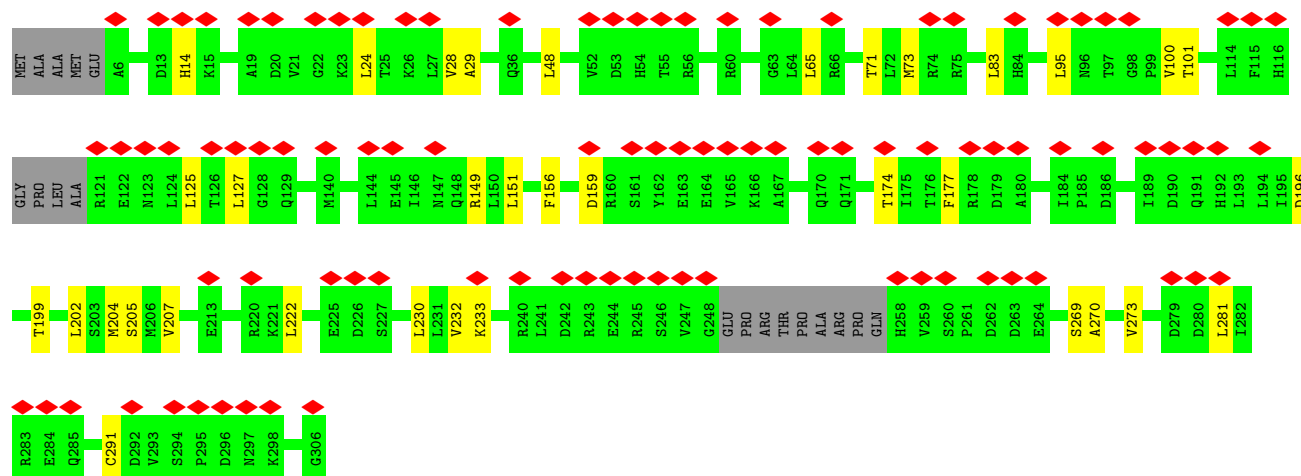
• Molecule 7: Triplex capsid protein 2

Chain U:



• Molecule 7: Triplex capsid protein 2

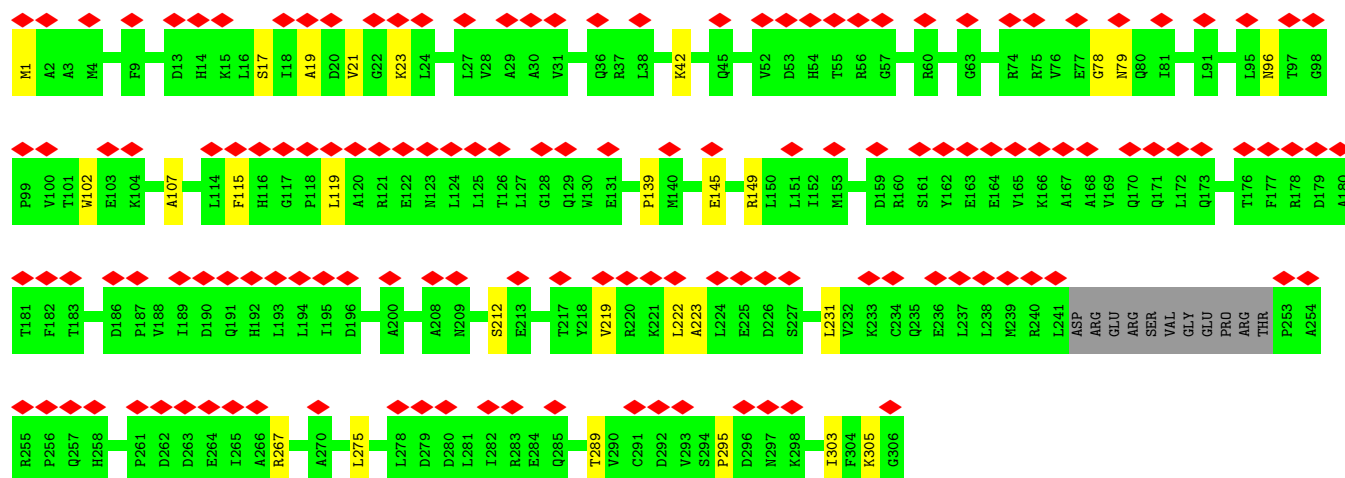
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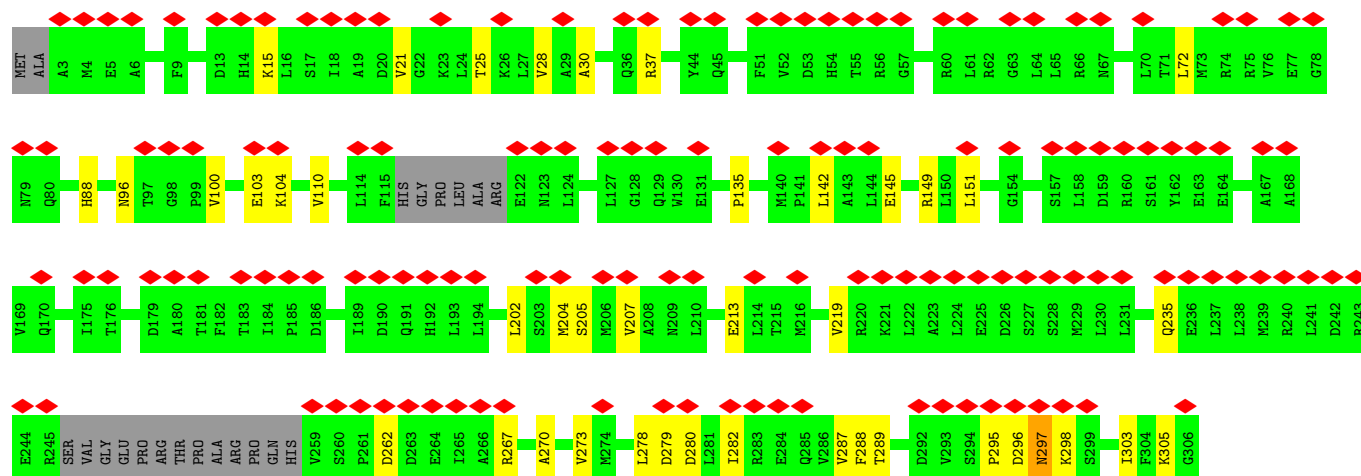
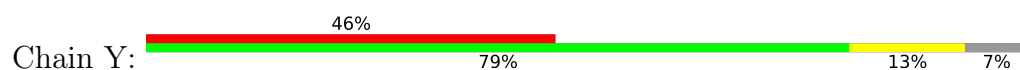
• Molecule 7: Triplex capsid protein 2

Chain X:

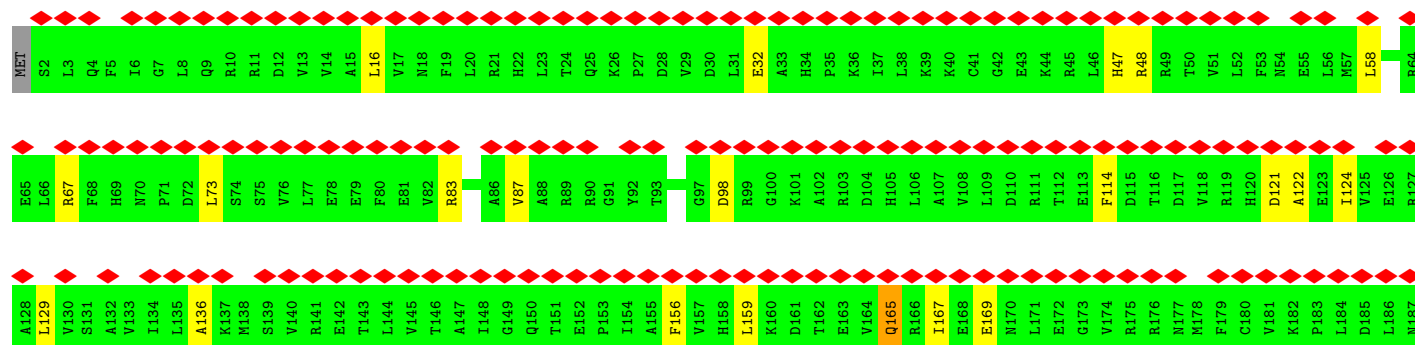




• Molecule 7: Triplex capsid protein 2



• Molecule 8: Large structural phosphoprotein



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	69628	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 ($e^-/\text{\AA}^2$)	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	0.066	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.016	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 [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	A	0.18	0/334	0.45	0/450
1	C	0.17	0/357	0.34	0/482
2	E	0.19	0/705	0.34	0/947
2	F	0.17	0/721	0.37	0/969
3	G	0.27	0/3951	0.48	2/5357 (0.0%)
4	H	0.29	0/10653	0.46	0/14508
4	I	0.29	0/10949	0.47	0/14916
4	J	0.27	0/10682	0.46	3/14553 (0.0%)
4	K	0.29	0/10527	0.46	0/14339
4	L	0.27	0/10949	0.46	0/14916
4	M	0.26	0/10949	0.45	0/14916
5	N	0.21	0/520	0.39	0/697
5	O	0.21	0/520	0.37	0/697
5	P	0.20	0/520	0.39	0/697
5	Q	0.24	0/520	0.37	0/697
5	R	0.19	0/520	0.31	0/697
5	S	0.17	0/520	0.36	0/697
6	T	0.23	0/1960	0.44	0/2658
6	W	0.27	0/2374	0.48	0/3221
7	U	0.28	0/2361	0.51	2/3206 (0.1%)
7	V	0.27	0/2333	0.50	0/3164
7	X	0.25	0/2379	0.45	0/3230
7	Y	0.25	0/2305	0.46	0/3126
8	Z	0.21	0/2358	0.39	0/3182
All	All	0.27	0/89967	0.46	7/122322 (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
4	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	I	0	1
4	J	0	1
4	L	0	1
4	M	0	1
7	U	0	1
7	V	0	1
All	All	0	7

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	665	ALA	CA-C-N	6.70	137.35	122.67
4	J	665	ALA	C-N-CA	6.70	137.35	122.67
4	J	664	GLY	N-CA-C	-6.59	104.35	111.21
7	U	291	CYS	CA-C-N	5.24	131.55	121.54
7	U	291	CYS	C-N-CA	5.24	131.55	121.54
3	G	534	VAL	CA-C-N	5.02	130.61	122.48
3	G	534	VAL	C-N-CA	5.02	130.61	122.48

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	265	SER	Peptide
4	I	1143	LEU	Peptide
4	J	853	VAL	Peptide
4	L	265	SER	Peptide
4	M	265	SER	Peptide
7	U	291	CYS	Peptide
7	V	291	CYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	332	0	358	11	0
1	C	354	0	384	8	0
2	E	696	0	685	5	0
2	F	710	0	711	10	0
3	G	3862	0	3779	47	0
4	H	10406	0	10362	122	0
4	I	10693	0	10635	111	0
4	J	10433	0	10379	120	0
4	K	10282	0	10238	90	0
4	L	10693	0	10635	102	0
4	M	10693	0	10635	112	0
5	N	513	0	539	9	0
5	O	513	0	539	8	0
5	P	513	0	539	10	0
5	Q	513	0	539	6	0
5	R	513	0	539	5	0
5	S	513	0	539	10	0
6	T	1919	0	1957	26	0
6	W	2325	0	2363	28	0
7	U	2317	0	2405	28	0
7	V	2292	0	2379	22	0
7	X	2334	0	2431	19	0
7	Y	2266	0	2355	28	0
8	Z	2320	0	2351	28	0
All	All	88005	0	88276	892	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 (892) 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)
4:I:463:THR:HG21	4:I:1237:GLY:HA3	1.53	0.89
4:M:1322:LEU:HD12	4:M:1359:ILE:HG21	1.55	0.88
4:J:1043:GLU:OE1	4:J:1101:ARG:NH1	2.08	0.85
4:H:575:THR:HG21	4:H:1007:THR:HA	1.60	0.83
4:H:689:ALA:HB1	4:H:694:ASN:HD21	1.46	0.81
4:L:1272:ILE:O	4:L:1275:ASN:ND2	2.15	0.79
3:G:146:THR:HA	3:G:164:LEU:HA	1.65	0.79
4:L:985:ASN:O	4:L:988:ARG:NH1	2.17	0.77
5:Q:21:VAL:HG11	5:Q:48:THR:HG22	1.66	0.76
4:M:1214:ILE:HD13	4:M:1268:THR:HG23	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:315:ALA:HB2	4:K:321:ILE:HD11	1.67	0.75
4:J:1038:ARG:NH1	4:J:1040:ASP:OD2	2.20	0.74
4:J:759:ALA:O	4:J:761:ASP:N	2.21	0.74
4:I:427:THR:HG22	4:I:441:ASP:HB3	1.71	0.73
4:M:754:VAL:HG23	4:M:755:PRO:HD3	1.72	0.72
6:T:252:GLY:HA3	6:T:280:SER:O	1.90	0.72
1:A:2236:ARG:HH21	2:F:66:ARG:HB2	1.55	0.70
4:J:244:THR:HA	4:J:362:LEU:HD13	1.73	0.70
4:J:594:LEU:HD21	4:J:680:VAL:HG21	1.74	0.69
4:J:862:GLU:O	4:J:866:THR:OG1	2.10	0.69
4:K:87:THR:HG22	4:K:88:THR:HG23	1.76	0.68
4:I:1002:LEU:HG	4:I:1006:MET:HE2	1.75	0.68
4:K:626:LEU:HD21	4:K:881:LEU:HB3	1.76	0.68
5:S:73:THR:HG22	5:S:75:ARG:H	1.58	0.68
1:C:2218:ARG:HA	1:C:2221:LEU:HD12	1.76	0.68
4:I:575:THR:HG21	4:I:1007:THR:HA	1.76	0.68
4:L:572:GLU:HG2	4:L:1007:THR:HG21	1.76	0.68
4:M:502:ARG:NH1	4:M:962:GLU:OE2	2.27	0.67
7:U:202:LEU:HD22	7:V:230:LEU:HD21	1.77	0.67
4:I:488:MET:HE1	4:I:978:ALA:HB1	1.77	0.66
4:J:542:CYS:SG	4:J:543:GLN:N	2.69	0.66
4:K:232:ARG:HH22	4:K:1360:ILE:HG22	1.60	0.65
4:H:93:PHE:HB2	4:H:116:VAL:HG13	1.79	0.65
4:I:1193:ARG:NH1	4:I:1195:ARG:O	2.29	0.65
3:G:28:ASP:HB3	3:G:124:MET:HE3	1.78	0.65
4:J:610:CYS:SG	4:J:646:VAL:HG13	2.36	0.65
4:H:601:VAL:HG22	4:H:924:VAL:HG11	1.78	0.65
4:M:617:VAL:HG13	4:M:619:GLY:H	1.62	0.65
4:H:51:GLU:HB2	4:I:88:THR:HB	1.78	0.64
4:K:683:LEU:HG	4:K:1006:MET:HE1	1.79	0.64
4:I:601:VAL:HG13	4:I:924:VAL:HG11	1.78	0.64
1:A:2236:ARG:HD2	1:A:2240:LEU:HD12	1.79	0.64
4:M:753:ASP:OD2	4:M:756:ARG:NE	2.25	0.64
3:G:432:LEU:O	3:G:556:ARG:NH1	2.29	0.64
4:L:733:VAL:HG12	4:L:738:PRO:HA	1.79	0.64
4:I:571:HIS:O	4:I:575:THR:HG23	1.98	0.64
4:M:212:ARG:NH2	4:M:1203:ASP:OD1	2.28	0.64
4:H:571:HIS:O	4:H:575:THR:HG23	1.99	0.63
4:K:532:GLU:O	4:K:1235:GLN:NE2	2.32	0.63
4:L:78:ILE:HB	4:L:1058:ILE:HG22	1.79	0.63
8:Z:165:GLN:O	8:Z:169:GLU:HG2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:463:THR:O	4:H:467:ARG:HG3	1.99	0.63
4:I:1029:HIS:ND1	4:I:1030:PRO:O	2.25	0.63
4:H:1362:LEU:HA	4:H:1366:MET:HG2	1.79	0.63
4:M:194:GLN:HA	4:M:197:VAL:HG12	1.80	0.63
4:I:575:THR:HG22	4:I:1010:ALA:HB3	1.80	0.63
6:T:166:MET:HG3	6:T:273:VAL:HG11	1.81	0.63
3:G:163:PHE:HB3	3:G:319:ASP:HA	1.80	0.62
4:I:1145:THR:HB	6:W:120:LEU:HD21	1.81	0.62
7:X:303:ILE:HD11	7:Y:37:ARG:HH22	1.62	0.62
4:H:941:ARG:HG3	4:H:992:SER:HB3	1.80	0.62
4:M:1039:THR:HG23	4:M:1261:PRO:HB3	1.82	0.62
7:U:144:LEU:HB2	7:U:282:ILE:HG22	1.80	0.62
4:H:35:LEU:HD11	4:H:37:ILE:HD11	1.82	0.62
4:K:1327:THR:HG22	4:K:1355:VAL:HG13	1.81	0.62
4:L:1064:VAL:HG22	4:L:1077:VAL:HG12	1.81	0.62
7:X:78:GLY:O	7:X:79:ASN:ND2	2.33	0.62
4:K:1336:LYS:NZ	4:K:1348:GLU:OE2	2.33	0.61
8:Z:16:LEU:HD11	8:Z:58:LEU:HD13	1.82	0.61
4:H:1189:PRO:HG3	4:H:1359:ILE:HD13	1.82	0.61
3:G:132:LEU:HD11	3:G:149:LEU:HD13	1.83	0.61
4:H:265:SER:O	4:H:267:ALA:N	2.32	0.61
4:H:420:VAL:HG11	4:H:576:TRP:HB3	1.81	0.61
4:H:538:ASP:OD2	4:H:988:ARG:NH1	2.33	0.61
4:J:470:PRO:HD2	4:J:479:LEU:HD21	1.82	0.61
3:G:57:ARG:NH1	3:G:85:GLU:OE2	2.30	0.61
4:I:1033:ALA:HB2	4:I:1179:VAL:HG23	1.83	0.60
4:H:1021:VAL:HG21	4:H:1134:ALA:HB1	1.82	0.60
7:Y:296:ASP:O	7:Y:298:LYS:N	2.34	0.60
4:J:1150:MET:O	4:J:1154:GLY:N	2.35	0.60
4:H:873:LEU:O	4:H:877:ARG:HG2	2.02	0.60
4:M:1327:THR:HG22	4:M:1355:VAL:HG13	1.84	0.60
4:M:280:MET:HG3	4:M:371:ASN:HB3	1.84	0.60
4:J:800:LEU:HD23	4:J:923:VAL:HG21	1.84	0.60
6:T:254:CYS:SG	6:T:255:LEU:N	2.75	0.59
4:K:1156:MET:HE1	4:K:1294:ARG:HH11	1.67	0.59
4:H:274:VAL:HG22	4:H:370:GLU:HB3	1.85	0.59
4:M:927:PRO:HD2	4:M:952:LEU:HD11	1.84	0.59
4:L:1029:HIS:ND1	4:L:1030:PRO:O	2.36	0.59
4:M:804:LEU:HA	4:M:807:LEU:HB3	1.85	0.59
4:K:434:ASP:O	4:K:436:ALA:N	2.35	0.59
3:G:146:THR:HG22	3:G:164:LEU:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:312:SER:O	3:G:313:ARG:HG2	2.03	0.58
4:M:265:SER:O	4:M:267:ALA:N	2.35	0.58
3:G:557:ASP:OD1	3:G:558:ARG:N	2.36	0.58
4:K:110:ARG:NH1	7:X:1:MET:SD	2.72	0.58
5:R:44:LEU:O	5:R:48:THR:OG1	2.17	0.58
6:W:76:SER:HB3	6:W:77:PRO:HD3	1.84	0.58
4:J:785:TYR:O	4:J:943:TYR:OH	2.17	0.58
4:H:575:THR:HG22	4:H:1010:ALA:HB3	1.86	0.58
4:I:333:THR:HG21	4:K:309:PRO:HB3	1.84	0.58
4:J:502:ARG:NH1	4:J:962:GLU:OE2	2.35	0.58
7:Y:289:THR:HG22	7:Y:303:ILE:HG12	1.83	0.58
4:L:342:ASP:OD1	4:L:343:SER:N	2.37	0.58
3:G:162:GLU:OE2	3:G:323:ARG:NH2	2.36	0.58
8:Z:67:ARG:HA	8:Z:217:TRP:HH2	1.69	0.58
4:I:80:PHE:HE2	4:I:86:LEU:HD23	1.68	0.57
6:T:188:ILE:HG22	6:T:248:ILE:HG23	1.85	0.57
4:H:1124:HIS:HB3	4:H:1127:VAL:HG22	1.87	0.57
4:J:1113:LEU:HA	4:J:1116:VAL:HG12	1.87	0.57
4:L:747:ARG:NH1	4:L:769:ASP:OD1	2.35	0.57
4:J:1033:ALA:O	4:J:1177:THR:HB	2.04	0.57
4:J:1109:ARG:HG3	4:J:1109:ARG:HH11	1.69	0.57
7:U:290:VAL:HG12	7:U:302:CYS:SG	2.45	0.57
4:L:1058:ILE:HG13	4:L:1082:ASN:HB3	1.86	0.57
6:W:133:GLY:HA3	6:W:149:VAL:O	2.03	0.57
4:J:1035:THR:HB	4:J:1175:ILE:HG13	1.86	0.57
4:J:664:GLY:C	4:J:666:LEU:H	2.11	0.56
4:K:664:GLY:O	4:K:666:LEU:N	2.38	0.56
4:H:508:THR:HG23	4:H:511:GLU:H	1.70	0.56
4:I:197:VAL:HG23	4:L:20:LEU:HD11	1.86	0.56
6:W:136:LYS:O	6:W:137:THR:OG1	2.22	0.56
7:X:275:LEU:HD13	7:Y:278:LEU:HD23	1.88	0.56
4:L:265:SER:O	4:L:267:ALA:N	2.37	0.56
4:M:1177:THR:HG22	4:M:1230:ASN:ND2	2.20	0.56
4:L:764:GLU:HB3	4:L:765:PRO:HD3	1.87	0.56
3:G:313:ARG:HB2	3:G:330:TRP:HB2	1.87	0.56
4:H:1322:LEU:HG	4:H:1359:ILE:HD11	1.88	0.56
4:J:178:SER:O	4:J:182:THR:HG23	2.06	0.56
4:L:800:LEU:HD22	4:L:952:LEU:HD21	1.87	0.56
6:T:52:VAL:HG12	6:T:81:TYR:HB2	1.87	0.56
6:T:55:GLY:HA3	6:T:110:ALA:HB3	1.87	0.56
4:L:1207:THR:O	4:L:1211:THR:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:173:LEU:HD22	6:T:203:TYR:HB3	1.86	0.56
6:W:75:ASP:OD1	6:W:78:ARG:NH2	2.36	0.56
7:Y:213:GLU:OE2	7:Y:267:ARG:NH1	2.38	0.56
4:I:315:ALA:HB2	4:I:321:ILE:HD11	1.87	0.56
5:N:62:LEU:O	5:N:66:ARG:HG2	2.05	0.56
4:H:662:ALA:HA	4:H:671:LEU:HD11	1.88	0.55
4:J:1003:HIS:O	4:J:1007:THR:HG23	2.07	0.55
4:L:1003:HIS:O	4:L:1007:THR:HG23	2.06	0.55
4:M:806:THR:HA	4:M:809:VAL:HG12	1.88	0.55
4:H:419:THR:HG22	4:H:421:ARG:H	1.71	0.55
4:J:850:ARG:NH1	4:J:862:GLU:OE2	2.33	0.55
8:Z:260:ASN:OD1	8:Z:261:GLY:N	2.39	0.55
5:O:43:MET:HE1	8:Z:277:ILE:HD13	1.88	0.55
3:G:76:VAL:HG12	3:G:552:GLN:HG3	1.87	0.55
4:I:188:PRO:HA	4:I:1286:LEU:HD21	1.88	0.55
4:I:861:VAL:HG13	4:I:865:ALA:HB3	1.88	0.55
3:G:27:LEU:HB3	3:G:31:VAL:HG11	1.89	0.55
4:H:446:LEU:HD21	4:H:1021:VAL:HG23	1.88	0.55
4:H:712:ASP:O	4:H:782:LYS:NZ	2.40	0.55
4:H:9:LEU:HD23	4:L:155:GLU:HG3	1.89	0.55
7:V:29:ALA:HB3	7:V:95:LEU:HG	1.89	0.55
7:Y:96:ASN:N	7:Y:298:LYS:O	2.33	0.55
4:M:1332:LEU:HD13	4:M:1355:VAL:HG23	1.89	0.55
4:K:355:LEU:HD13	4:K:357:MET:HE2	1.89	0.54
3:G:85:GLU:HG3	3:G:556:ARG:HG3	1.89	0.54
4:H:188:PRO:HB3	4:H:1282:ILE:HD11	1.89	0.54
1:C:2217:VAL:HG11	2:E:83:VAL:HG11	1.90	0.54
4:M:183:LEU:HB3	4:M:1048:LEU:HD21	1.90	0.54
4:I:1144:ASP:O	4:I:1148:ILE:HB	2.08	0.54
4:M:446:LEU:HD22	4:M:1021:VAL:HG12	1.89	0.54
7:Y:145:GLU:O	7:Y:149:ARG:HG2	2.08	0.54
4:M:609:LEU:HD22	4:M:861:VAL:HG23	1.89	0.54
7:Y:219:VAL:HG12	7:Y:235:GLN:HB2	1.88	0.54
4:I:1059:ILE:HG22	4:I:1081:ILE:HG22	1.88	0.54
4:M:425:PRO:HB3	4:M:1328:THR:OG1	2.07	0.54
6:T:290:VAL:HG21	7:U:274:MET:HE1	1.88	0.54
7:U:175:ILE:HD11	7:U:184:ILE:HD11	1.89	0.54
4:H:287:LEU:O	4:H:291:ILE:HG12	2.08	0.54
4:I:1033:ALA:O	4:I:1177:THR:HB	2.07	0.54
4:J:1122:TYR:HB2	4:J:1128:ASP:HB2	1.90	0.54
4:H:65:TYR:HA	4:H:172:GLU:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:246:LEU:O	4:I:1093:ASN:ND2	2.41	0.54
4:I:800:LEU:HD23	4:I:923:VAL:HG21	1.89	0.54
4:K:804:LEU:HA	4:K:807:LEU:HB3	1.89	0.54
4:L:183:LEU:HD12	4:L:186:LYS:HE3	1.90	0.54
4:M:1235:GLN:HB2	4:M:1238:CYS:HB3	1.90	0.54
6:W:138:VAL:HG22	6:W:146:LEU:HD22	1.90	0.54
7:Y:110:VAL:HG13	7:Y:135:PRO:HB2	1.90	0.54
3:G:366:VAL:HG13	3:G:550:LEU:HD21	1.90	0.54
4:H:1215:TYR:CE2	4:H:1268:THR:HG21	2.42	0.54
4:L:100:VAL:HG23	4:M:379:THR:HG21	1.90	0.54
7:U:142:LEU:O	7:U:146:ILE:HG22	2.07	0.54
4:H:261:TYR:HB2	4:H:1052:LYS:HE3	1.90	0.53
4:J:465:THR:HG22	4:J:550:ALA:HB3	1.91	0.53
4:H:144:GLU:HG2	4:H:145:GLY:H	1.72	0.53
4:I:1166:HIS:NE2	4:J:1223:GLN:HA	2.23	0.53
4:L:998:CYS:SG	4:L:1004:SER:HB2	2.47	0.53
4:M:263:THR:O	4:M:266:GLY:HA2	2.06	0.53
4:I:941:ARG:HG2	4:I:992:SER:HB3	1.90	0.53
7:V:151:LEU:HD21	7:V:281:LEU:HD13	1.89	0.53
4:I:638:MET:HE3	4:I:864:VAL:HA	1.89	0.53
4:L:733:VAL:HG22	4:L:894:GLU:HB3	1.89	0.53
4:M:657:ILE:HG23	4:M:661:LEU:HD12	1.90	0.53
1:A:2217:VAL:HG22	2:E:82:ARG:HD3	1.90	0.53
4:H:664:GLY:O	4:H:666:LEU:N	2.42	0.53
4:I:424:LEU:HD13	4:I:573:LEU:HD23	1.90	0.53
4:M:1349:THR:HA	4:M:1354:TYR:HA	1.89	0.53
7:Y:279:ASP:OD1	7:Y:280:ASP:N	2.42	0.53
8:Z:114:PHE:CD1	8:Z:124:ILE:HD11	2.44	0.53
4:L:1291:ASP:OD1	4:L:1316:ARG:NH2	2.36	0.53
4:I:183:LEU:HD12	4:I:186:LYS:HE3	1.91	0.53
4:L:1327:THR:HG22	4:L:1355:VAL:HG13	1.90	0.53
4:M:862:GLU:O	4:M:866:THR:OG1	2.14	0.53
4:I:1268:THR:O	4:I:1272:ILE:HG12	2.09	0.53
4:K:579:MET:SD	4:K:1006:MET:HE3	2.49	0.53
7:X:219:VAL:HG23	7:Y:205:SER:HB3	1.91	0.53
4:I:558:ILE:HD11	4:I:1031:GLY:HA3	1.91	0.52
4:H:96:GLN:HG3	4:H:113:THR:HG22	1.90	0.52
4:H:83:LEU:HB2	4:H:1060:ASN:HB3	1.91	0.52
4:H:800:LEU:HD23	4:H:923:VAL:HG21	1.91	0.52
4:K:698:LEU:O	4:K:706:TYR:OH	2.21	0.52
4:L:638:MET:HE3	4:L:864:VAL:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:478:VAL:HG23	3:G:485:VAL:HG22	1.90	0.52
4:H:1291:ASP:O	4:H:1311:ILE:N	2.40	0.52
4:J:291:ILE:HD12	4:J:369:MET:SD	2.49	0.52
4:J:1178:PRO:HD2	4:J:1230:ASN:OD1	2.09	0.52
4:L:610:CYS:SG	4:L:646:VAL:HG22	2.49	0.52
4:H:459:PRO:O	4:H:463:THR:HG22	2.09	0.52
4:H:1045:ASP:OD1	4:H:1100:ASN:ND2	2.41	0.52
4:J:182:THR:HG22	4:J:185:ARG:HH21	1.75	0.52
4:J:638:MET:HE1	4:J:642:ARG:CZ	2.40	0.52
4:H:7:LEU:HD13	4:K:92:LEU:HG	1.91	0.52
4:K:432:ASN:HD21	4:K:1166:HIS:CD2	2.28	0.52
5:Q:18:HIS:HA	5:Q:21:VAL:HG22	1.91	0.52
7:U:219:VAL:HG23	7:V:205:SER:OG	2.09	0.52
6:W:78:ARG:HD2	7:Y:103:GLU:OE2	2.09	0.52
8:Z:263:SER:HA	8:Z:266:THR:HG22	1.92	0.52
4:I:495:ILE:HG21	4:I:938:PRO:HD2	1.92	0.52
4:I:664:GLY:C	4:I:666:LEU:H	2.18	0.52
4:J:1142:LEU:HD21	4:J:1148:ILE:HD11	1.92	0.52
5:S:33:SER:OG	5:S:34:GLU:N	2.43	0.52
4:L:600:THR:HG21	4:L:645:LEU:HD23	1.92	0.52
4:L:1214:ILE:HD12	4:L:1272:ILE:HD11	1.92	0.52
4:M:528:THR:O	4:M:531:THR:HG22	2.09	0.52
4:K:1047:LEU:HD22	4:K:1097:ALA:HB2	1.92	0.52
4:I:528:THR:O	4:I:531:THR:HG22	2.10	0.51
6:T:74:CYS:SG	6:T:75:ASP:N	2.83	0.51
4:J:646:VAL:HG12	4:J:647:PHE:CD2	2.45	0.51
4:J:981:HIS:O	4:J:985:ASN:ND2	2.38	0.51
4:M:800:LEU:HD22	4:M:952:LEU:HD21	1.92	0.51
4:J:1323:PRO:HG2	4:J:1359:ILE:HB	1.92	0.51
4:K:808:LEU:HD13	4:K:883:VAL:HG13	1.91	0.51
6:W:249:GLN:HB3	6:W:286:PHE:HA	1.92	0.51
1:A:2221:LEU:HD23	1:A:2224:LEU:HD21	1.92	0.51
4:J:1195:ARG:NH2	4:J:1216:ASP:O	2.43	0.51
4:M:324:ASP:HB3	4:M:327:SER:HB3	1.91	0.51
4:M:803:ASN:HD22	4:M:806:THR:HG22	1.75	0.51
6:T:212:TRP:CZ2	6:T:216:VAL:HG21	2.45	0.51
4:J:1230:ASN:HB3	4:J:1233:ALA:HB3	1.92	0.51
4:K:807:LEU:O	4:K:811:LEU:HB2	2.09	0.51
4:L:1034:LEU:HD12	4:L:1174:LEU:HB3	1.92	0.51
4:M:341:ASN:OD1	4:M:345:SER:OG	2.28	0.51
4:J:342:ASP:OD1	4:J:343:SER:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:93:PHE:HB2	4:I:116:VAL:HG22	1.91	0.51
6:T:115:LEU:HA	6:T:118:LEU:HD12	1.93	0.51
7:V:48:LEU:HD21	7:V:65:LEU:HD13	1.92	0.51
4:K:501:VAL:HG12	4:K:503:ARG:HG2	1.93	0.51
5:N:21:VAL:O	5:N:25:VAL:HG22	2.11	0.51
8:Z:32:GLU:HG3	8:Z:223:LYS:HZ3	1.76	0.51
4:K:470:PRO:HD2	4:K:479:LEU:HD21	1.93	0.51
5:P:18:HIS:HA	5:P:48:THR:HG21	1.93	0.51
5:S:52:SER:OG	5:S:53:LEU:N	2.43	0.51
7:X:145:GLU:HG3	7:X:149:ARG:HD2	1.93	0.50
4:H:246:LEU:HG	4:H:1093:ASN:ND2	2.25	0.50
4:I:431:LEU:HB2	4:I:1363:GLN:HE22	1.77	0.50
4:I:495:ILE:HD12	4:I:976:PRO:HG2	1.93	0.50
5:N:38:PRO:O	5:N:42:THR:HG23	2.12	0.50
4:H:61:LEU:HD23	4:H:61:LEU:H	1.77	0.50
4:I:1164:THR:HG23	4:J:209:ARG:NH2	2.26	0.50
4:H:724:PRO:HG2	4:H:727:MET:HG2	1.94	0.50
4:H:756:ARG:NH2	4:H:886:VAL:O	2.44	0.50
4:K:186:LYS:HE2	4:K:1085:ASP:HB2	1.93	0.50
4:L:263:THR:O	4:L:266:GLY:HA2	2.11	0.50
4:L:710:LEU:HD21	4:L:783:VAL:HG22	1.93	0.50
5:P:43:MET:HE1	5:P:46:LYS:HD3	1.94	0.50
4:I:387:ARG:C	4:I:388:ASN:HD22	2.20	0.50
4:J:775:ASP:O	4:J:779:THR:HG23	2.10	0.50
4:K:1114:PHE:CD1	4:K:1137:VAL:HG11	2.47	0.50
4:L:78:ILE:O	4:L:1058:ILE:HA	2.12	0.50
4:M:801:GLY:HA3	4:M:890:VAL:HB	1.94	0.50
7:X:223:ALA:HA	7:X:231:LEU:HD21	1.93	0.50
3:G:364:GLU:OE1	3:G:558:ARG:NH1	2.44	0.50
4:H:794:ASN:ND2	4:H:995:SER:O	2.41	0.50
4:H:1109:ARG:HG3	4:H:1109:ARG:HH11	1.77	0.50
6:T:138:VAL:HG13	6:T:146:LEU:HB3	1.94	0.50
4:H:262:THR:OG1	4:H:266:GLY:O	2.30	0.50
4:I:410:VAL:HG11	4:I:1348:GLU:HG3	1.94	0.50
4:I:1347:SER:HB3	4:I:1357:GLY:H	1.77	0.50
4:J:698:LEU:HD13	4:J:1127:VAL:HG22	1.94	0.50
4:K:317:SER:O	4:L:3:ASN:ND2	2.45	0.50
4:K:432:ASN:ND2	4:K:434:ASP:OD1	2.44	0.50
4:M:775:ASP:O	4:M:779:THR:HG23	2.12	0.50
7:U:24:LEU:HD21	7:U:81:ILE:HD11	1.94	0.50
3:G:495:ARG:NH1	3:G:500:GLY:O	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:506:ASP:O	3:G:509:GLY:N	2.38	0.49
4:K:138:TYR:CE2	4:K:152:LEU:HB2	2.47	0.49
4:K:1035:THR:HG23	4:K:1175:ILE:HG12	1.93	0.49
4:I:1332:LEU:HD13	4:I:1355:VAL:HG23	1.94	0.49
4:L:753:ASP:OD2	4:L:756:ARG:NE	2.37	0.49
7:V:196:ASP:HA	7:V:199:THR:HG22	1.93	0.49
3:G:363:VAL:HG11	3:G:558:ARG:HG2	1.94	0.49
4:H:236:ARG:HA	4:H:286:LEU:HD21	1.93	0.49
6:W:156:ASN:HD22	6:W:160:THR:HG23	1.77	0.49
4:H:470:PRO:HD2	4:H:479:LEU:HD11	1.93	0.49
4:H:565:LEU:HG	4:H:1178:PRO:HB3	1.93	0.49
4:I:945:ASN:HD22	4:I:969:HIS:CD2	2.31	0.49
6:T:60:GLU:O	6:T:62:GLN:N	2.46	0.49
8:Z:32:GLU:HG3	8:Z:223:LYS:NZ	2.27	0.49
3:G:424:ILE:HG22	3:G:525:VAL:HG21	1.94	0.49
4:J:757:LEU:HD23	5:P:62:LEU:HD13	1.95	0.49
4:K:631:VAL:O	4:K:635:ILE:HG12	2.13	0.49
4:K:1042:PHE:CZ	4:K:1362:LEU:HD21	2.48	0.49
4:L:517:VAL:HG12	4:L:519:THR:H	1.78	0.49
4:M:280:MET:HE2	4:M:280:MET:HA	1.94	0.49
4:M:790:PRO:HA	4:M:793:THR:HG22	1.95	0.49
4:M:1124:HIS:CD2	4:M:1127:VAL:HG23	2.47	0.49
4:K:448:THR:HG23	4:K:1113:LEU:HD22	1.95	0.49
4:K:1064:VAL:HG12	4:K:1077:VAL:HB	1.94	0.49
8:Z:121:ASP:HA	8:Z:124:ILE:HG12	1.95	0.49
4:H:1088:LEU:HD23	4:H:1088:LEU:H	1.78	0.49
4:I:1164:THR:HG23	4:J:209:ARG:HH21	1.77	0.49
4:L:757:LEU:HA	4:L:760:MET:HG3	1.95	0.49
7:V:100:VAL:HG22	7:V:101:THR:H	1.78	0.49
4:H:816:ALA:O	4:H:877:ARG:NH1	2.46	0.49
4:I:3:ASN:ND2	4:J:317:SER:O	2.45	0.49
4:I:123:SER:O	4:I:1081:ILE:HG12	2.12	0.49
4:I:249:ALA:HB3	4:I:1093:ASN:HD21	1.78	0.49
4:K:171:MET:HE3	4:K:1077:VAL:HG13	1.95	0.49
4:K:599:THR:O	4:K:603:SER:HB2	2.12	0.49
4:K:1214:ILE:HD11	4:K:1268:THR:HG23	1.95	0.49
7:V:24:LEU:HD13	7:V:125:LEU:HD13	1.94	0.49
7:V:199:THR:HA	7:V:202:LEU:HG	1.95	0.49
1:A:2204:THR:O	1:A:2207:VAL:HG22	2.13	0.48
4:I:502:ARG:HD3	4:I:962:GLU:OE1	2.14	0.48
4:J:230:LEU:O	4:J:234:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:1042:PHE:CZ	4:J:1362:LEU:HD21	2.47	0.48
4:M:358:ASP:OD1	4:M:358:ASP:N	2.38	0.48
4:M:451:HIS:ND1	4:M:453:VAL:HG22	2.28	0.48
4:H:1278:LEU:O	4:H:1282:ILE:HG22	2.14	0.48
4:I:954:ASP:N	4:I:954:ASP:OD1	2.40	0.48
4:L:596:LEU:HG	4:L:645:LEU:HD22	1.94	0.48
4:M:531:THR:OG1	4:M:539:PHE:O	2.30	0.48
4:I:161:LEU:HD11	6:W:27:LYS:HG3	1.95	0.48
4:M:1145:THR:HA	4:M:1148:ILE:HG22	1.95	0.48
7:X:115:PHE:HB2	7:X:119:LEU:HD13	1.95	0.48
3:G:366:VAL:HG11	3:G:550:LEU:HD11	1.95	0.48
4:J:424:LEU:HD13	4:J:573:LEU:HD23	1.94	0.48
4:K:110:ARG:NH1	7:X:1:MET:HA	2.29	0.48
4:L:579:MET:SD	4:L:1006:MET:HE3	2.53	0.48
4:M:224:LEU:HD21	4:M:1322:LEU:HD11	1.95	0.48
4:M:638:MET:HG3	4:M:646:VAL:HG21	1.94	0.48
4:H:1035:THR:OG1	4:H:1177:THR:HG21	2.14	0.48
4:I:173:ARG:HD2	4:J:99:ARG:O	2.13	0.48
4:J:188:PRO:HA	4:J:1286:LEU:HD21	1.95	0.48
4:J:820:MET:HE2	4:J:877:ARG:HG2	1.95	0.48
4:J:1342:GLY:H	4:J:1364:GLN:NE2	2.11	0.48
4:M:39:TYR:CZ	7:X:295:PRO:HG2	2.49	0.48
7:U:57:GLY:HA3	7:U:188:VAL:HG22	1.96	0.48
4:H:3:ASN:ND2	4:I:317:SER:O	2.46	0.48
4:H:144:GLU:HG2	4:H:145:GLY:N	2.28	0.48
4:M:1125:ASP:OD2	4:M:1129:ARG:NH1	2.36	0.48
5:Q:67:MET:O	5:Q:71:SER:OG	2.28	0.48
3:G:5:LEU:HD13	3:G:306:TRP:CG	2.49	0.48
4:H:627:ILE:O	4:H:630:PHE:N	2.47	0.48
4:L:401:LEU:HD11	4:L:1183:VAL:HG11	1.94	0.48
4:M:862:GLU:HA	4:M:872:LEU:HD13	1.95	0.48
7:U:193:LEU:HG	7:U:197:MET:HE2	1.95	0.48
3:G:399:SER:O	3:G:402:VAL:HG22	2.14	0.48
4:I:702:PRO:HG3	4:J:964:PRO:HB2	1.96	0.48
4:K:1285:TYR:HA	4:K:1289:ALA:HB3	1.95	0.48
4:M:647:PHE:CD1	4:M:653:LEU:HD13	2.49	0.48
7:U:273:VAL:O	7:U:277:GLN:HG2	2.14	0.48
4:H:84:ASN:OD1	4:H:1080:ASN:ND2	2.46	0.48
3:G:378:VAL:HG21	3:G:543:SER:HB2	1.94	0.47
4:H:1277:THR:O	4:H:1281:THR:HG23	2.14	0.47
4:M:1021:VAL:HG21	4:M:1130:TRP:CZ3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:17:GLU:HG2	2:F:19:HIS:H	1.78	0.47
4:H:279:VAL:O	4:H:283:ILE:HG12	2.14	0.47
4:I:718:PRO:HD2	4:I:785:TYR:HB3	1.97	0.47
4:H:144:GLU:OE1	4:H:144:GLU:N	2.41	0.47
4:H:173:ARG:NH1	4:H:375:VAL:O	2.46	0.47
4:J:461:LEU:O	4:J:465:THR:HG23	2.14	0.47
4:J:627:ILE:HG22	4:J:630:PHE:HB3	1.96	0.47
4:J:945:ASN:OD1	4:J:947:THR:HG22	2.14	0.47
4:L:102:SER:HB3	4:L:108:THR:HG22	1.96	0.47
4:L:622:ASP:OD1	4:L:622:ASP:N	2.46	0.47
4:H:192:VAL:HA	4:H:219:PHE:CE1	2.49	0.47
7:V:270:ALA:HA	7:V:273:VAL:HG22	1.96	0.47
6:W:17:ASP:N	6:W:17:ASP:OD1	2.44	0.47
2:F:31:LEU:HB3	3:G:402:VAL:HG21	1.95	0.47
3:G:164:LEU:CD1	3:G:166:ARG:HB3	2.45	0.47
4:I:690:LEU:HD12	4:I:707:VAL:HG21	1.95	0.47
4:K:1182:ASP:OD1	4:K:1182:ASP:N	2.44	0.47
6:W:252:GLY:HA3	6:W:279:PHE:CZ	2.49	0.47
4:J:1342:GLY:H	4:J:1364:GLN:HE22	1.63	0.47
4:K:287:LEU:O	4:K:291:ILE:HD12	2.14	0.47
4:M:637:ASN:O	4:M:641:THR:HG22	2.14	0.47
5:S:13:LYS:HB2	5:S:16:GLU:HB2	1.96	0.47
2:F:78:ASP:O	2:F:82:ARG:HG2	2.15	0.47
3:G:164:LEU:HD13	3:G:166:ARG:HB3	1.97	0.47
3:G:459:PHE:HE2	4:I:1152:THR:HG22	1.79	0.47
4:H:186:LYS:HB2	4:H:186:LYS:HE3	1.72	0.47
4:H:461:LEU:HD13	4:H:552:CYS:HB2	1.97	0.47
4:I:692:GLY:O	4:J:993:ARG:NH2	2.48	0.47
4:I:1098:TYR:CE2	4:I:1100:ASN:HB3	2.50	0.47
4:K:800:LEU:HD23	4:K:923:VAL:HG21	1.96	0.47
4:L:584:LEU:HD12	4:L:687:ILE:HD11	1.96	0.47
4:L:804:LEU:HA	4:L:807:LEU:HB3	1.97	0.47
4:M:584:LEU:HD12	4:M:687:ILE:HD11	1.96	0.47
5:N:40:LEU:O	5:N:44:LEU:HG	2.15	0.47
4:I:415:LYS:HB3	4:J:408:THR:HG22	1.97	0.47
6:W:237:ARG:HH21	6:W:240:GLN:HG3	1.80	0.47
7:Y:100:VAL:HG21	7:Y:142:LEU:HD22	1.96	0.47
4:H:639:PHE:CG	4:H:670:LEU:HD21	2.50	0.47
4:I:553:THR:HG21	4:I:983:TYR:O	2.15	0.47
4:M:136:LEU:O	4:M:140:ARG:HG2	2.15	0.47
4:M:275:SER:HB2	4:M:280:MET:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:195:THR:HG21	4:H:215:ILE:HG23	1.97	0.47
4:H:212:ARG:NH2	4:H:1203:ASP:OD1	2.42	0.47
4:L:963:PHE:HB3	4:L:965:HIS:CE1	2.50	0.47
4:M:757:LEU:HA	4:M:760:MET:HG2	1.96	0.47
2:E:28:GLU:CD	2:E:28:GLU:H	2.22	0.46
3:G:455:GLN:HG2	4:I:1253:GLY:HA2	1.97	0.46
4:H:761:ASP:CG	4:H:889:HIS:HD1	2.23	0.46
4:K:1128:ASP:O	4:K:1132:ARG:HG2	2.16	0.46
6:T:232:ASN:HB2	7:V:233:LYS:HE2	1.97	0.46
4:L:714:ARG:NH1	4:L:898:PRO:O	2.49	0.46
7:U:53:ASP:OD1	7:U:55:THR:HG22	2.15	0.46
8:Z:83:ARG:HE	8:Z:202:LYS:HB3	1.81	0.46
4:H:463:THR:HG21	4:H:1237:GLY:HA3	1.96	0.46
4:I:682:ARG:O	4:I:685:THR:HG22	2.14	0.46
4:I:1121:VAL:HG12	4:I:1132:ARG:HH21	1.79	0.46
4:J:1037:VAL:HG11	4:J:1262:CYS:SG	2.55	0.46
6:T:212:TRP:CZ2	6:T:287:ARG:HG2	2.51	0.46
4:H:522:TYR:HB3	4:H:1228:THR:O	2.16	0.46
4:J:664:GLY:O	4:J:666:LEU:N	2.49	0.46
4:K:311:ASN:HB3	4:K:321:ILE:HD12	1.97	0.46
4:H:642:ARG:HB2	4:H:644:LEU:HD22	1.98	0.46
4:I:502:ARG:NH1	4:I:962:GLU:OE1	2.37	0.46
4:M:287:LEU:O	4:M:291:ILE:HG12	2.16	0.46
4:M:857:LEU:O	4:M:861:VAL:HG12	2.15	0.46
5:P:25:VAL:HA	5:P:57:LYS:HG2	1.96	0.46
4:K:853:VAL:HG21	4:K:876:CYS:SG	2.55	0.46
6:W:156:ASN:HD22	6:W:160:THR:CG2	2.29	0.46
4:I:272:VAL:HG23	4:I:368:ILE:HB	1.97	0.46
4:M:424:LEU:HD13	4:M:573:LEU:HD23	1.97	0.46
7:U:96:ASN:HB3	7:U:102:TRP:CH2	2.51	0.46
3:G:6:TYR:HB2	7:V:232:VAL:HG22	1.98	0.46
4:H:1347:SER:OG	4:H:1355:VAL:O	2.29	0.46
4:I:622:ASP:OD1	4:I:622:ASP:N	2.49	0.46
4:K:83:LEU:HB3	4:K:1080:ASN:HD22	1.81	0.46
4:K:284:MET:HA	4:K:291:ILE:HD13	1.98	0.46
4:H:257:ASN:OD1	4:H:259:THR:HG22	2.15	0.46
4:H:579:MET:HE3	4:H:1006:MET:HE2	1.98	0.46
4:I:775:ASP:O	4:I:779:THR:HG23	2.16	0.46
4:I:1174:LEU:O	4:I:1244:TYR:OH	2.28	0.46
4:M:1323:PRO:HG2	4:M:1359:ILE:HB	1.98	0.46
7:Y:278:LEU:O	7:Y:282:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:871:PRO:HD2	4:J:874:GLN:OE1	2.16	0.45
4:K:71:LEU:HD13	4:K:274:VAL:HG21	1.98	0.45
4:M:127:ILE:HG22	4:M:171:MET:HE2	1.98	0.45
4:M:698:LEU:CD1	4:M:1127:VAL:HG22	2.46	0.45
7:X:212:SER:HB3	7:X:267:ARG:HD2	1.97	0.45
7:X:219:VAL:HG22	7:Y:202:LEU:HD12	1.97	0.45
1:C:2235:MET:HE1	2:F:68:LEU:HD22	1.99	0.45
3:G:163:PHE:CD2	3:G:168:LEU:HD21	2.52	0.45
4:H:628:ARG:NH1	4:H:660:HIS:O	2.50	0.45
4:H:1059:ILE:HG22	4:H:1081:ILE:HG12	1.97	0.45
4:I:853:VAL:HB	4:I:857:LEU:HB2	1.99	0.45
4:K:218:SER:OG	4:K:222:LYS:HE2	2.16	0.45
3:G:115:THR:HG23	3:G:312:SER:HB3	1.97	0.45
4:H:451:HIS:CE1	4:H:1117:PHE:HB2	2.51	0.45
4:K:788:LEU:O	4:K:792:MET:HG2	2.17	0.45
4:L:495:ILE:HB	4:L:496:PRO:HD3	1.98	0.45
7:U:66:ARG:NH2	7:U:284:GLU:OE2	2.40	0.45
4:H:650:SER:OG	4:H:653:LEU:HB2	2.15	0.45
4:H:1240:SER:HA	4:H:1243:LEU:HB2	1.99	0.45
4:I:173:ARG:HB3	4:J:100:VAL:HG22	1.99	0.45
4:J:73:ALA:HA	4:J:261:TYR:CZ	2.52	0.45
4:J:712:ASP:O	4:J:782:LYS:NZ	2.46	0.45
4:K:946:PRO:HG3	4:K:973:PHE:CG	2.52	0.45
4:K:1164:THR:HG22	4:K:1166:HIS:O	2.17	0.45
5:Q:37:HIS:ND1	5:Q:40:LEU:HB2	2.32	0.45
7:V:204:MET:O	7:V:207:VAL:HG12	2.17	0.45
1:C:2203:LEU:HD23	1:C:2203:LEU:HA	1.88	0.45
4:J:623:ALA:O	4:J:627:ILE:HG12	2.16	0.45
4:J:1249:ARG:HG2	4:J:1254:TYR:CG	2.52	0.45
4:K:192:VAL:HA	4:K:219:PHE:CE1	2.52	0.45
4:L:785:TYR:O	4:L:943:TYR:OH	2.33	0.45
5:O:52:SER:OG	5:O:53:LEU:N	2.50	0.45
7:U:260:SER:O	7:U:264:GLU:HG2	2.17	0.45
8:Z:240:ARG:NH1	8:Z:240:ARG:HB3	2.32	0.45
4:H:257:ASN:O	4:H:1052:LYS:NZ	2.47	0.45
4:H:502:ARG:HD3	4:H:962:GLU:OE1	2.17	0.45
4:J:633:ARG:NH2	4:J:878:GLU:OE2	2.41	0.45
4:K:998:CYS:SG	4:K:1004:SER:OG	2.71	0.45
4:L:1215:TYR:CE2	4:L:1268:THR:HG21	2.52	0.45
4:M:263:THR:HG22	4:M:296:VAL:HG12	1.99	0.45
4:M:941:ARG:HG2	4:M:992:SER:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:392:CYS:HB2	3:G:515:LEU:HD23	1.98	0.45
3:G:523:LEU:HB2	3:G:533:TRP:CE3	2.51	0.45
4:H:194:GLN:HA	4:H:197:VAL:HG12	1.98	0.45
4:K:1035:THR:HG22	4:K:1177:THR:OG1	2.16	0.45
4:I:207:LEU:HD11	4:I:1278:LEU:HD22	1.99	0.45
4:L:594:LEU:HD22	4:L:792:MET:HE3	1.98	0.45
4:M:420:VAL:HG12	4:M:580:GLU:CD	2.42	0.45
5:N:67:MET:O	5:N:70:VAL:HG22	2.17	0.45
7:U:96:ASN:HB3	7:U:102:TRP:CZ2	2.52	0.45
7:U:110:VAL:HG23	7:U:287:VAL:HG21	1.99	0.45
7:X:19:ALA:O	7:X:23:LYS:HG2	2.17	0.45
4:I:1034:LEU:HD13	4:I:1174:LEU:HD22	1.99	0.45
1:C:2228:VAL:O	1:C:2232:ILE:HG23	2.17	0.44
4:J:699:ALA:C	4:J:701:GLU:H	2.25	0.44
4:K:1268:THR:O	4:K:1272:ILE:HG12	2.17	0.44
4:L:138:TYR:O	4:L:153:ASN:ND2	2.51	0.44
4:M:194:GLN:HG3	4:M:222:LYS:HE2	1.99	0.44
4:M:1044:VAL:HG23	4:M:1099:VAL:HB	1.99	0.44
6:W:233:ARG:HA	6:W:236:THR:HG22	1.99	0.44
8:Z:156:PHE:CZ	8:Z:167:ILE:HG21	2.52	0.44
4:H:757:LEU:HD11	5:N:66:ARG:HD3	1.99	0.44
4:I:1193:ARG:NH2	4:I:1214:ILE:O	2.51	0.44
4:K:635:ILE:HG22	4:K:646:VAL:HG23	1.98	0.44
4:M:715:LEU:HD13	4:M:986:TRP:CG	2.52	0.44
4:M:985:ASN:O	4:M:988:ARG:NH1	2.51	0.44
8:Z:73:LEU:HD11	8:Z:213:VAL:HG11	2.00	0.44
1:A:2214:LEU:HB3	2:F:87:GLU:OE1	2.17	0.44
4:M:246:LEU:O	4:M:1093:ASN:ND2	2.49	0.44
4:M:819:LEU:HD21	5:S:32:ILE:HD13	1.99	0.44
5:O:75:ARG:O	8:Z:251:ARG:NH2	2.50	0.44
6:T:68:ILE:N	6:T:82:ILE:O	2.45	0.44
8:Z:274:ASP:HB2	8:Z:277:ILE:HD12	1.99	0.44
3:G:162:GLU:HG3	3:G:357:TYR:HE1	1.83	0.44
4:H:1035:THR:HB	4:H:1175:ILE:HG12	1.99	0.44
4:H:1327:THR:HG21	4:H:1333:MET:HB2	1.99	0.44
4:I:228:PHE:HD2	4:I:1366:MET:HE1	1.81	0.44
4:L:927:PRO:HD2	4:L:952:LEU:HD11	1.99	0.44
4:M:472:GLU:HB2	4:M:475:MET:HG2	1.98	0.44
4:M:850:ARG:NE	4:M:862:GLU:OE2	2.48	0.44
6:T:262:SER:O	6:T:273:VAL:N	2.35	0.44
1:C:2214:LEU:HD22	2:E:87:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:426:THR:HG23	4:J:442:PHE:HD1	1.83	0.44
4:J:1039:THR:HG23	4:J:1261:PRO:HB3	1.98	0.44
4:J:1221:ASP:O	4:J:1225:PHE:HA	2.17	0.44
4:K:188:PRO:HD2	4:K:1092:SER:O	2.16	0.44
4:K:968:ARG:NH1	4:K:970:ASP:OD2	2.37	0.44
4:K:1336:LYS:HE3	4:K:1343:ALA:O	2.18	0.44
4:L:534:HIS:CE1	4:L:1239:LEU:HD12	2.52	0.44
4:L:804:LEU:HD23	4:L:889:HIS:HD2	1.82	0.44
3:G:106:TYR:O	3:G:109:GLN:HG2	2.17	0.44
4:H:704:SER:HA	4:H:707:VAL:HG12	2.00	0.44
4:H:1046:MET:HE1	4:H:1096:VAL:HG22	2.00	0.44
4:I:1075:TYR:OH	6:W:19:GLU:OE2	2.32	0.44
4:J:271:GLY:C	4:J:367:VAL:HG23	2.42	0.44
4:M:689:ALA:O	4:M:691:PRO:HD3	2.18	0.44
4:M:804:LEU:O	4:M:808:LEU:HD23	2.18	0.44
3:G:309:ALA:HB1	3:G:332:VAL:CG1	2.47	0.44
4:I:554:PRO:HD3	4:I:907:LEU:HD12	1.99	0.44
4:K:101:ALA:HB3	4:L:174:GLY:HA3	2.00	0.44
4:K:461:LEU:HD13	4:K:552:CYS:HB2	2.00	0.44
4:K:1347:SER:HB3	4:K:1357:GLY:H	1.82	0.44
5:O:47:TYR:OH	5:O:63:ASP:OD2	2.19	0.44
6:T:82:ILE:HG23	6:T:86:LEU:HD23	1.99	0.44
6:W:236:THR:HG23	6:W:237:ARG:HG2	1.99	0.44
4:H:246:LEU:HG	4:H:1093:ASN:HD22	1.83	0.44
4:H:793:THR:HG22	4:H:796:ARG:HB2	1.99	0.44
4:I:1214:ILE:HD12	4:I:1272:ILE:HD11	1.99	0.44
4:J:362:LEU:HD12	4:J:362:LEU:O	2.18	0.44
4:L:408:THR:CG2	4:M:415:LYS:HB3	2.48	0.44
4:L:1039:THR:HG23	4:L:1261:PRO:HB3	1.99	0.44
4:M:854:GLY:O	4:M:858:THR:HB	2.18	0.44
5:S:28:LEU:HB3	5:S:32:ILE:HG23	2.00	0.44
7:U:214:LEU:HD11	7:V:156:PHE:CE1	2.52	0.44
7:X:17:SER:O	7:X:21:VAL:HG23	2.17	0.44
4:H:139:LEU:HD22	4:H:160:VAL:HG21	2.00	0.44
4:K:884:GLN:HA	5:Q:66:ARG:HB2	2.00	0.44
8:Z:83:ARG:O	8:Z:87:VAL:HG23	2.18	0.44
4:H:188:PRO:HB2	4:H:192:VAL:HG21	1.99	0.43
4:I:1199:MET:HG3	4:I:1271:ILE:O	2.18	0.43
4:K:469:PRO:HB3	4:K:548:THR:HG21	2.00	0.43
5:O:28:LEU:HD23	5:O:29:PRO:HD2	2.00	0.43
5:O:34:GLU:HB2	5:O:44:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:63:ASP:HA	5:P:66:ARG:HG2	2.00	0.43
6:W:213:GLN:O	6:W:216:VAL:HG12	2.18	0.43
8:Z:121:ASP:OD1	8:Z:122:ALA:N	2.51	0.43
4:H:188:PRO:HB2	4:H:192:VAL:CG2	2.47	0.43
4:I:419:THR:HG22	4:I:421:ARG:H	1.82	0.43
4:I:637:ASN:O	4:I:641:THR:HG22	2.17	0.43
4:M:1195:ARG:NH2	4:M:1216:ASP:O	2.51	0.43
5:N:34:GLU:OE1	5:N:34:GLU:N	2.47	0.43
6:T:86:LEU:HD12	6:T:89:ILE:HD12	2.00	0.43
4:K:733:VAL:HG22	4:K:738:PRO:HA	2.01	0.43
4:L:276:THR:HG21	4:L:1045:ASP:OD2	2.18	0.43
4:L:600:THR:HB	4:L:644:LEU:HB2	1.99	0.43
4:L:657:ILE:HG23	4:L:661:LEU:HD12	1.99	0.43
4:M:393:PHE:HA	4:M:1322:LEU:O	2.18	0.43
4:M:1038:ARG:NH1	4:M:1040:ASP:OD2	2.52	0.43
5:S:32:ILE:HD11	5:S:37:HIS:HB2	2.00	0.43
3:G:91:ARG:NH1	7:U:159:ASP:OD1	2.40	0.43
4:H:499:TYR:CD2	4:H:956:ILE:HG12	2.53	0.43
4:I:853:VAL:HG23	4:I:858:THR:OG1	2.19	0.43
4:K:1332:LEU:HD13	4:K:1355:VAL:HG23	1.99	0.43
4:L:633:ARG:HD2	4:L:865:ALA:O	2.18	0.43
4:H:174:GLY:HA3	4:I:101:ALA:HB3	1.99	0.43
4:J:482:ARG:HD3	4:J:543:GLN:HB3	2.00	0.43
4:J:884:GLN:HA	5:P:66:ARG:HB2	2.01	0.43
4:L:861:VAL:HG13	4:L:865:ALA:HB3	2.00	0.43
4:M:924:VAL:HG23	4:M:925:THR:HG23	2.00	0.43
7:V:100:VAL:HG21	7:V:177:PHE:CD1	2.54	0.43
8:Z:188:LEU:HD23	8:Z:202:LYS:HE3	1.99	0.43
1:A:2213:ILE:O	1:A:2217:VAL:HG23	2.18	0.43
3:G:85:GLU:CG	3:G:556:ARG:HG3	2.48	0.43
4:I:415:LYS:HB3	4:J:408:THR:CG2	2.49	0.43
4:J:192:VAL:HA	4:J:219:PHE:CE1	2.53	0.43
4:K:754:VAL:N	4:K:755:PRO:HD2	2.33	0.43
5:P:65:LEU:O	5:P:68:VAL:HG12	2.19	0.43
4:H:66:PHE:O	4:H:72:ALA:HB2	2.18	0.43
4:H:857:LEU:O	4:H:861:VAL:HG22	2.19	0.43
4:J:75:ALA:HB2	4:J:179:PHE:CZ	2.53	0.43
4:K:169:ASP:OD2	4:K:173:ARG:NH1	2.44	0.43
4:L:1332:LEU:HD13	4:L:1355:VAL:HG23	2.01	0.43
4:M:33:GLU:HG3	4:M:34:ALA:N	2.34	0.43
4:H:222:LYS:O	4:H:226:THR:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:946:PRO:HD2	4:J:969:HIS:CD2	2.54	0.43
4:K:1249:ARG:HA	4:K:1252:LEU:HD23	2.01	0.43
4:M:1189:PRO:HB3	4:M:1322:LEU:HD13	2.01	0.43
6:W:123:HIS:O	6:W:128:ARG:NH2	2.46	0.43
8:Z:129:LEU:HD11	8:Z:207:GLY:HA3	2.00	0.43
3:G:372:ARG:HD3	3:G:415:MET:HE3	2.01	0.43
4:J:400:TYR:HB3	4:J:1179:VAL:CG1	2.49	0.43
4:J:698:LEU:CD1	4:J:1127:VAL:HG22	2.49	0.43
4:L:451:HIS:ND1	4:L:453:VAL:HG22	2.34	0.43
4:M:33:GLU:HG3	4:M:34:ALA:H	1.84	0.43
4:M:592:GLU:OE1	4:M:595:ARG:NH2	2.48	0.43
5:N:66:ARG:O	5:N:70:VAL:HG13	2.18	0.43
3:G:138:ASP:C	3:G:140:ARG:H	2.27	0.43
4:I:567:PRO:HB2	4:I:569:PRO:HD2	2.00	0.43
4:L:631:VAL:HG23	4:L:661:LEU:HD11	2.01	0.43
5:R:67:MET:HA	5:R:70:VAL:HG12	2.01	0.43
8:Z:136:ALA:HB2	8:Z:200:VAL:HG21	2.01	0.43
4:H:132:SER:HB2	4:L:43:PRO:HG3	2.00	0.42
4:I:627:ILE:HG22	4:I:631:VAL:HG23	2.00	0.42
4:J:1101:ARG:HD3	4:J:1101:ARG:N	2.34	0.42
4:L:646:VAL:HG13	4:L:647:PHE:CD2	2.53	0.42
4:L:712:ASP:O	4:L:782:LYS:NZ	2.52	0.42
7:Y:295:PRO:C	7:Y:297:ASN:H	2.27	0.42
4:J:1032:PHE:HA	4:J:1179:VAL:HG23	2.00	0.42
4:K:1191:ASN:OD1	4:K:1193:ARG:HG2	2.19	0.42
4:L:499:TYR:CD2	4:L:956:ILE:HG12	2.54	0.42
4:L:1057:VAL:HG12	4:L:1083:THR:HG22	2.01	0.42
4:M:147:ILE:O	4:M:151:ILE:HG12	2.19	0.42
4:M:1036:ALA:HB1	4:M:1172:CYS:HB3	2.01	0.42
6:T:50:PHE:CZ	6:T:132:LEU:HD13	2.54	0.42
7:Y:289:THR:CG2	7:Y:303:ILE:HG12	2.50	0.42
4:H:82:ASP:OD1	4:H:82:ASP:N	2.52	0.42
4:I:1331:ALA:O	4:I:1335:THR:HG23	2.19	0.42
4:L:600:THR:CB	4:L:644:LEU:HB2	2.49	0.42
4:M:1021:VAL:HG21	4:M:1130:TRP:HZ3	1.84	0.42
7:V:71:THR:HG21	7:V:83:LEU:HB3	2.00	0.42
4:I:33:GLU:OE2	7:Y:15:LYS:HE3	2.19	0.42
4:I:167:THR:O	4:I:171:MET:HG2	2.18	0.42
4:I:174:GLY:HA3	4:J:101:ALA:HB3	2.00	0.42
4:J:169:ASP:OD2	4:J:173:ARG:NE	2.35	0.42
4:J:296:VAL:O	4:J:355:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:241:LYS:HA	4:L:244:THR:HG22	2.01	0.42
4:H:754:VAL:N	4:H:755:PRO:HD2	2.34	0.42
4:H:1362:LEU:HA	4:H:1366:MET:CG	2.49	0.42
4:I:1044:VAL:CG1	4:I:1096:VAL:HG13	2.49	0.42
6:T:212:TRP:CE2	6:T:216:VAL:HG21	2.54	0.42
6:T:290:VAL:HG22	7:U:277:GLN:HG3	2.00	0.42
7:V:28:VAL:HG23	7:V:73:MET:HE2	2.00	0.42
6:W:50:PHE:CE1	7:Y:104:LYS:HE2	2.54	0.42
4:H:13:VAL:HG13	4:L:57:PHE:CD1	2.54	0.42
4:I:19:PHE:CD1	4:I:23:VAL:HG22	2.54	0.42
4:I:694:ASN:OD1	4:J:968:ARG:NH2	2.52	0.42
4:I:989:SER:N	4:I:990:PRO:HD2	2.34	0.42
4:J:1350:HIS:O	4:J:1351:PHE:C	2.63	0.42
4:K:1221:ASP:HB3	4:K:1224:THR:O	2.19	0.42
4:L:567:PRO:HB2	4:L:569:PRO:HD2	2.01	0.42
4:M:310:GLU:HA	4:M:313:VAL:HG12	2.01	0.42
6:T:136:LYS:HB3	6:T:147:THR:HG23	2.01	0.42
4:I:284:MET:HG2	4:I:291:ILE:HD13	2.02	0.42
4:I:585:ARG:O	4:I:587:PRO:HD3	2.19	0.42
4:I:639:PHE:CG	4:I:670:LEU:HD11	2.55	0.42
4:J:441:ASP:HB2	4:J:443:VAL:HG22	2.01	0.42
4:J:517:VAL:HG22	4:J:518:VAL:H	1.85	0.42
4:J:1360:ILE:O	4:J:1362:LEU:N	2.47	0.42
4:K:122:LYS:HE2	4:K:122:LYS:HB2	1.85	0.42
4:K:1332:LEU:HB3	4:K:1355:VAL:CG2	2.49	0.42
4:L:628:ARG:HG2	4:L:661:LEU:CD2	2.50	0.42
4:L:1034:LEU:CD1	4:L:1174:LEU:HD13	2.50	0.42
4:M:909:ASP:OD1	4:M:909:ASP:N	2.49	0.42
4:M:1055:THR:HG22	4:M:1085:ASP:HA	2.02	0.42
5:P:22:VAL:HA	5:P:26:LEU:HB2	2.02	0.42
7:V:149:ARG:NH2	7:V:174:THR:O	2.48	0.42
6:W:213:GLN:HA	6:W:216:VAL:HG12	2.01	0.42
1:C:2232:ILE:HG13	1:C:2233:GLN:N	2.34	0.42
4:I:444:ASP:OD1	4:J:523:LYS:NZ	2.44	0.42
4:J:600:THR:HG21	4:J:645:LEU:O	2.20	0.42
4:J:782:LYS:O	4:J:786:LEU:HB2	2.20	0.42
4:J:800:LEU:HD22	4:J:952:LEU:HD11	2.02	0.42
4:J:1142:LEU:H	4:J:1142:LEU:HD23	1.85	0.42
4:M:1268:THR:O	4:M:1272:ILE:HG12	2.19	0.42
5:P:52:SER:OG	5:P:53:LEU:N	2.53	0.42
6:T:211:HIS:CD2	7:U:66:ARG:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:287:VAL:HG23	7:Y:288:PHE:CD2	2.55	0.42
8:Z:73:LEU:HD11	8:Z:213:VAL:CG1	2.49	0.42
4:H:478:LEU:HD23	4:H:527:ILE:HD12	2.01	0.42
4:I:661:LEU:HD23	4:I:666:LEU:HD22	2.00	0.42
4:K:433:ARG:HD2	4:K:1102:VAL:HG13	2.01	0.42
4:M:704:SER:HA	4:M:707:VAL:HG12	2.02	0.42
4:M:747:ARG:HH21	4:M:769:ASP:CG	2.27	0.42
4:M:1221:ASP:O	4:M:1225:PHE:HA	2.19	0.42
8:Z:159:LEU:HD23	8:Z:159:LEU:HA	1.90	0.42
4:H:233:THR:HG21	4:H:238:TYR:CD2	2.55	0.42
4:L:733:VAL:CG2	4:L:894:GLU:HB3	2.50	0.42
4:L:1347:SER:HB3	4:L:1357:GLY:N	2.35	0.42
4:M:161:LEU:HD12	4:M:161:LEU:HA	1.94	0.42
4:M:499:TYR:CD2	4:M:956:ILE:HG12	2.55	0.42
4:M:513:LYS:HB2	4:M:513:LYS:HE2	1.89	0.42
5:N:65:LEU:O	5:N:68:VAL:HG12	2.20	0.42
5:R:70:VAL:O	5:R:73:THR:HG22	2.19	0.42
5:S:44:LEU:HD23	5:S:44:LEU:HA	1.92	0.42
6:W:164:ALA:HB2	6:W:277:ASP:HA	2.01	0.42
7:X:212:SER:HB3	7:X:267:ARG:CD	2.50	0.42
3:G:523:LEU:HB2	3:G:533:TRP:HE3	1.85	0.41
4:H:1087:GLY:HA3	4:H:1091:THR:HG21	2.01	0.41
4:I:264:SER:HB3	4:I:295:THR:HG23	2.01	0.41
4:J:1039:THR:HG21	4:J:1259:TYR:OH	2.20	0.41
4:J:1104:THR:HG22	4:J:1168:GLN:HB3	2.00	0.41
4:K:927:PRO:HD2	4:K:952:LEU:HD21	2.01	0.41
4:L:451:HIS:CE1	4:L:453:VAL:HG13	2.55	0.41
4:L:770:ASP:OD1	4:L:770:ASP:N	2.49	0.41
7:Y:28:VAL:O	7:Y:28:VAL:HG12	2.20	0.41
1:A:2221:LEU:HA	1:A:2224:LEU:HD23	2.02	0.41
3:G:21:LEU:HB3	3:G:336:TRP:CE3	2.55	0.41
4:H:753:ASP:OD2	4:H:756:ARG:HD3	2.20	0.41
4:I:237:ASP:O	4:I:241:LYS:HG2	2.21	0.41
4:J:940:HIS:HB3	4:J:942:PHE:O	2.20	0.41
4:J:1099:VAL:HG22	4:J:1100:ASN:O	2.19	0.41
4:J:1267:ASN:O	4:J:1271:ILE:HG12	2.20	0.41
4:K:641:THR:O	4:L:668:PRO:HG3	2.20	0.41
4:M:171:MET:HE3	4:M:1077:VAL:HG13	2.02	0.41
4:M:989:SER:N	4:M:990:PRO:HD2	2.35	0.41
5:P:55:ASN:OD1	5:P:55:ASN:N	2.53	0.41
6:T:251:LEU:HB3	6:T:279:PHE:HZ	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:136:LYS:HE3	6:W:149:VAL:CG2	2.50	0.41
6:W:154:LEU:HB2	6:W:163:PHE:HB2	2.02	0.41
8:Z:67:ARG:HA	8:Z:217:TRP:CH2	2.52	0.41
8:Z:188:LEU:HD21	8:Z:198:ASN:HA	2.02	0.41
1:C:2239:TYR:OH	2:F:60:TYR:HB3	2.21	0.41
4:H:87:THR:O	4:H:122:LYS:HE2	2.21	0.41
4:I:399:LEU:HD11	4:I:1186:PHE:CE2	2.55	0.41
4:J:291:ILE:HD11	4:J:358:ASP:HB3	2.02	0.41
4:J:861:VAL:O	4:J:861:VAL:HG12	2.21	0.41
4:K:774:THR:O	4:K:778:TRP:HB2	2.19	0.41
4:K:1177:THR:HG22	4:K:1178:PRO:O	2.20	0.41
4:L:947:THR:HG22	4:L:967:HIS:NE2	2.36	0.41
4:M:310:GLU:O	4:M:314:THR:HG22	2.20	0.41
5:O:62:LEU:O	5:O:66:ARG:HG2	2.21	0.41
7:U:160:ARG:HB2	7:U:165:VAL:HG23	2.02	0.41
2:F:55:ARG:HA	2:F:58:LYS:NZ	2.36	0.41
4:H:682:ARG:NH2	4:H:776:ASP:OD2	2.44	0.41
4:J:432:ASN:HD22	4:J:436:ALA:HB3	1.85	0.41
4:K:273:MET:HB2	4:K:369:MET:HE2	2.03	0.41
4:K:284:MET:HG2	4:K:291:ILE:HD13	2.02	0.41
4:K:615:VAL:HG21	4:K:802:LEU:HD12	2.02	0.41
4:M:535:PRO:HG3	4:M:1232:TRP:CE3	2.55	0.41
4:M:856:MET:HE3	4:M:856:MET:HB2	1.91	0.41
4:M:1212:LYS:HE2	4:M:1212:LYS:HB3	1.85	0.41
6:T:234:ARG:HG2	7:U:206:MET:HE1	2.01	0.41
1:A:2205:GLN:H	1:A:2205:GLN:HG3	1.67	0.41
4:J:495:ILE:HG21	4:J:938:PRO:HD2	2.03	0.41
4:J:545:ASN:O	4:J:545:ASN:ND2	2.52	0.41
4:J:1144:ASP:N	4:J:1144:ASP:OD1	2.51	0.41
4:J:1279:PHE:HA	4:J:1282:ILE:HG12	2.02	0.41
4:J:1327:THR:HB	4:J:1355:VAL:HG13	2.02	0.41
4:M:522:TYR:HB3	4:M:1228:THR:O	2.21	0.41
7:X:222:LEU:HD23	7:X:231:LEU:HD13	2.01	0.41
7:Y:21:VAL:O	7:Y:25:THR:HG23	2.20	0.41
4:H:861:VAL:HG21	4:H:876:CYS:SG	2.60	0.41
4:I:859:GLU:OE2	4:I:929:THR:OG1	2.31	0.41
4:I:1181:MET:HG3	4:I:1229:HIS:O	2.21	0.41
4:J:647:PHE:CD1	4:J:653:LEU:HD13	2.56	0.41
4:J:779:THR:O	4:J:783:VAL:HG23	2.20	0.41
4:K:609:LEU:HD23	4:K:860:LEU:O	2.20	0.41
4:L:312:ALA:O	4:L:316:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:666:LEU:HD23	4:L:671:LEU:HB2	2.02	0.41
7:U:118:PRO:O	7:U:119:LEU:HB3	2.20	0.41
7:U:148:GLN:HA	7:U:282:ILE:HD12	2.03	0.41
7:V:71:THR:CG2	7:V:83:LEU:HB3	2.51	0.41
6:W:47:THR:HG22	6:W:149:VAL:HG22	2.01	0.41
7:Y:270:ALA:O	7:Y:273:VAL:HG12	2.21	0.41
4:H:892:VAL:HG11	4:H:979:PHE:CE1	2.56	0.41
4:H:1239:LEU:O	4:H:1242:VAL:HG22	2.20	0.41
4:K:817:PHE:CZ	4:K:853:VAL:HG23	2.56	0.41
4:L:192:VAL:HA	4:L:219:PHE:CE1	2.56	0.41
4:L:363:GLY:C	4:L:365:LYS:H	2.28	0.41
4:L:367:VAL:HG11	4:L:1049:TYR:HE1	1.85	0.41
4:L:1058:ILE:HD11	4:L:1082:ASN:HD22	1.86	0.41
7:V:159:ASP:OD1	7:V:159:ASP:N	2.52	0.41
1:A:2207:VAL:HG11	2:E:90:LEU:HD13	2.03	0.41
3:G:526:THR:OG1	3:G:528:ASP:OD1	2.30	0.41
4:H:597:PHE:HD1	4:H:792:MET:HG2	1.85	0.41
4:H:638:MET:HE3	4:H:864:VAL:HA	2.03	0.41
4:H:1262:CYS:O	4:H:1266:PHE:HD2	2.04	0.41
4:I:589:ASP:OD1	4:I:591:GLU:HG2	2.21	0.41
4:J:246:LEU:O	4:J:1093:ASN:ND2	2.52	0.41
4:K:397:VAL:HB	4:K:1034:LEU:HD23	2.01	0.41
4:M:683:LEU:HG	4:M:1006:MET:HE1	2.02	0.41
4:M:687:ILE:HD13	4:M:687:ILE:HA	1.84	0.41
7:U:229:MET:O	7:U:233:LYS:HG2	2.21	0.41
3:G:169:LEU:HD13	3:G:173:MET:HG3	2.03	0.41
4:I:445:ALA:HA	4:I:1110:VAL:HG11	2.03	0.41
4:I:748:HIS:HB3	4:I:751:VAL:HB	2.02	0.41
4:J:400:TYR:HB3	4:J:1179:VAL:HG12	2.03	0.41
4:K:811:LEU:HG	4:K:857:LEU:HG	2.03	0.41
4:L:100:VAL:HG22	4:M:173:ARG:HB3	2.02	0.41
4:L:430:LEU:HD13	4:L:1108:VAL:HG11	2.03	0.41
4:L:947:THR:HG22	4:L:967:HIS:CE1	2.55	0.41
4:M:567:PRO:HB2	4:M:569:PRO:HD2	2.01	0.41
5:S:19:ARG:HA	5:S:22:VAL:HG22	2.02	0.41
5:S:46:LYS:HE3	5:S:46:LYS:HB2	1.76	0.41
7:U:46:LEU:HD13	7:U:83:LEU:HD11	2.03	0.41
7:X:107:ALA:O	7:X:139:PRO:HA	2.20	0.41
7:Y:151:LEU:HD23	7:Y:151:LEU:HA	1.90	0.41
7:Y:262:ASP:OD1	7:Y:262:ASP:N	2.54	0.41
1:A:2228:VAL:HG11	2:F:72:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:58:CYS:HA	4:I:94:HIS:O	2.21	0.41
4:J:63:TRP:CZ2	4:J:165:LYS:HE2	2.56	0.41
4:J:146:THR:HG23	4:J:149:ASP:H	1.86	0.41
4:J:392:THR:HG23	4:J:1039:THR:HG22	2.02	0.41
4:J:605:ASN:O	4:J:642:ARG:NH1	2.54	0.41
4:J:687:ILE:HD13	4:J:687:ILE:HA	1.85	0.41
4:J:777:GLU:O	4:J:781:GLN:HG3	2.21	0.41
4:K:1262:CYS:O	4:K:1266:PHE:HD1	2.04	0.41
4:L:188:PRO:HA	4:L:1286:LEU:HD21	2.03	0.41
4:L:884:GLN:O	5:R:66:ARG:NH1	2.53	0.41
4:L:1279:PHE:HA	4:L:1282:ILE:HG12	2.03	0.41
5:Q:67:MET:O	5:Q:70:VAL:HG12	2.21	0.41
8:Z:272:ILE:HA	8:Z:272:ILE:HD13	1.85	0.41
4:J:631:VAL:HG13	4:J:647:PHE:CE2	2.56	0.40
5:O:19:ARG:HB2	5:O:19:ARG:CZ	2.50	0.40
7:Y:30:ALA:O	7:Y:72:LEU:HA	2.21	0.40
7:Y:88:HIS:ND1	7:Y:305:LYS:HA	2.36	0.40
4:H:231:ASN:HB3	4:H:1366:MET:HB2	2.02	0.40
4:H:883:VAL:O	4:H:886:VAL:HG23	2.22	0.40
4:J:404:ASP:OD1	4:J:405:ARG:N	2.54	0.40
4:K:1016:SER:OG	4:K:1018:VAL:HG22	2.22	0.40
4:L:173:ARG:NH1	4:L:375:VAL:O	2.54	0.40
4:L:447:LYS:HB3	4:L:1112:ASP:HA	2.04	0.40
4:L:1004:SER:O	4:L:1008:LEU:HD23	2.20	0.40
4:L:1034:LEU:HD11	4:L:1174:LEU:HD13	2.03	0.40
4:M:478:LEU:HD11	4:M:528:THR:HG22	2.02	0.40
4:M:1017:PRO:O	4:M:1021:VAL:HG13	2.21	0.40
4:M:1121:VAL:HG12	4:M:1132:ARG:HH21	1.86	0.40
7:U:184:ILE:HA	7:U:185:PRO:HD3	1.95	0.40
7:V:269:SER:O	7:V:273:VAL:HG13	2.21	0.40
6:W:57:VAL:HG12	6:W:57:VAL:O	2.21	0.40
6:W:165:LEU:HD23	6:W:276:LEU:HD12	2.02	0.40
2:F:28:GLU:O	2:F:32:ARG:HG2	2.20	0.40
4:H:542:CYS:N	4:H:549:VAL:O	2.41	0.40
4:H:611:TYR:OH	4:H:925:THR:HG22	2.22	0.40
4:I:310:GLU:H	4:I:310:GLU:CD	2.29	0.40
4:J:594:LEU:HD12	4:J:792:MET:HE3	2.03	0.40
4:K:262:THR:HG22	4:K:263:THR:O	2.22	0.40
4:L:667:PRO:HA	4:L:668:PRO:HD3	1.96	0.40
7:V:14:HIS:HB3	7:V:127:LEU:HD13	2.02	0.40
7:X:289:THR:OG1	7:X:305:LYS:HD2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:204:MET:O	7:Y:207:VAL:HG12	2.22	0.40
8:Z:98:ASP:OD1	8:Z:98:ASP:N	2.42	0.40
4:H:388:ASN:HB3	4:H:1311:ILE:HG23	2.04	0.40
4:H:690:LEU:HD12	4:H:707:VAL:HG21	2.03	0.40
4:I:451:HIS:CE1	4:I:453:VAL:HG13	2.57	0.40
4:J:1034:LEU:HD13	4:J:1174:LEU:HD22	2.02	0.40
4:K:321:ILE:N	4:L:51:GLU:O	2.52	0.40
4:L:261:TYR:HB2	4:L:1052:LYS:HD2	2.03	0.40
4:L:989:SER:N	4:L:990:PRO:HD2	2.37	0.40
4:M:71:LEU:N	4:M:370:GLU:OE1	2.55	0.40
4:M:419:THR:HG22	4:M:421:ARG:H	1.87	0.40
7:X:96:ASN:HB3	7:X:102:TRP:CH2	2.56	0.40
3:G:531:PHE:CE2	3:G:543:SER:HB3	2.57	0.40
4:I:446:LEU:HD22	4:I:1021:VAL:HG12	2.02	0.40
4:I:607:PRO:HG2	4:I:610:CYS:SG	2.62	0.40
4:L:575:THR:O	4:L:579:MET:HG3	2.22	0.40
4:L:618:HIS:NE2	4:L:885:PHE:O	2.37	0.40
4:M:362:LEU:HD12	4:M:367:VAL:HG21	2.03	0.40
5:R:45:SER:OG	5:R:49:ARG:NH1	2.55	0.40
6:W:170:ASP:OD1	6:W:170:ASP:N	2.55	0.40
8:Z:47:HIS:CG	8:Z:48:ARG:N	2.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	38/2241 (2%)	37 (97%)	1 (3%)	0	100	100
1	C	41/2241 (2%)	40 (98%)	1 (2%)	0	100	100
2	E	82/642 (13%)	82 (100%)	0	0	100	100
2	F	81/642 (13%)	78 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	467/594 (79%)	452 (97%)	15 (3%)	0	100	100
4	H	1305/1370 (95%)	1247 (96%)	57 (4%)	1 (0%)	48	76
4	I	1346/1370 (98%)	1272 (94%)	74 (6%)	0	100	100
4	J	1313/1370 (96%)	1247 (95%)	65 (5%)	1 (0%)	48	76
4	K	1292/1370 (94%)	1244 (96%)	48 (4%)	0	100	100
4	L	1346/1370 (98%)	1289 (96%)	56 (4%)	1 (0%)	48	76
4	M	1346/1370 (98%)	1281 (95%)	64 (5%)	1 (0%)	48	76
5	N	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
5	O	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
5	P	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
5	Q	61/75 (81%)	57 (93%)	4 (7%)	0	100	100
5	R	61/75 (81%)	61 (100%)	0	0	100	100
5	S	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
6	T	236/290 (81%)	228 (97%)	8 (3%)	0	100	100
6	W	288/290 (99%)	271 (94%)	16 (6%)	1 (0%)	36	66
7	U	288/306 (94%)	271 (94%)	17 (6%)	0	100	100
7	V	282/306 (92%)	270 (96%)	12 (4%)	0	100	100
7	X	291/306 (95%)	281 (97%)	10 (3%)	0	100	100
7	Y	279/306 (91%)	264 (95%)	14 (5%)	1 (0%)	30	60
8	Z	282/1048 (27%)	273 (97%)	9 (3%)	0	100	100
All	All	10969/17882 (61%)	10480 (96%)	483 (4%)	6 (0%)	49	76

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	266	GLY
4	J	760	MET
4	L	266	GLY
4	M	266	GLY
7	Y	297	ASN
6	W	244	CYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	38/1941 (2%)	38 (100%)	0	100	100
1	C	41/1941 (2%)	41 (100%)	0	100	100
2	E	74/526 (14%)	74 (100%)	0	100	100
2	F	76/526 (14%)	76 (100%)	0	100	100
3	G	397/500 (79%)	396 (100%)	1 (0%)	86	86
4	H	1144/1192 (96%)	1140 (100%)	4 (0%)	86	86
4	I	1175/1192 (99%)	1172 (100%)	3 (0%)	86	86
4	J	1146/1192 (96%)	1146 (100%)	0	100	100
4	K	1131/1192 (95%)	1130 (100%)	1 (0%)	88	91
4	L	1175/1192 (99%)	1171 (100%)	4 (0%)	86	86
4	M	1175/1192 (99%)	1170 (100%)	5 (0%)	84	85
5	N	59/68 (87%)	59 (100%)	0	100	100
5	O	59/68 (87%)	59 (100%)	0	100	100
5	P	59/68 (87%)	59 (100%)	0	100	100
5	Q	59/68 (87%)	59 (100%)	0	100	100
5	R	59/68 (87%)	59 (100%)	0	100	100
5	S	59/68 (87%)	59 (100%)	0	100	100
6	T	209/252 (83%)	209 (100%)	0	100	100
6	W	252/252 (100%)	252 (100%)	0	100	100
7	U	262/273 (96%)	262 (100%)	0	100	100
7	V	260/273 (95%)	259 (100%)	1 (0%)	84	85
7	X	263/273 (96%)	262 (100%)	1 (0%)	84	85
7	Y	257/273 (94%)	257 (100%)	0	100	100
8	Z	255/883 (29%)	254 (100%)	1 (0%)	84	85
All	All	9684/15473 (63%)	9663 (100%)	21 (0%)	85	88

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	326	LEU
4	H	13	VAL
4	H	1055	THR
4	H	1093	ASN
4	H	1151	LEU
4	I	294	GLU
4	I	545	ASN
4	I	960	VAL
4	K	703	LEU
4	L	505	VAL
4	L	531	THR
4	L	1102	VAL
4	L	1177	THR
4	M	695	ASN
4	M	754	VAL
4	M	1175	ILE
4	M	1179	VAL
4	M	1367	LEU
7	V	222	LEU
7	X	42	LYS
8	Z	165	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	34	ASN
3	G	321	GLN
3	G	322	HIS
3	G	446	GLN
4	H	49	HIS
4	H	153	ASN
4	H	290	HIS
4	H	451	HIS
4	H	455	HIS
4	H	510	ASN
4	H	581	HIS
4	H	618	HIS
4	H	694	ASN
4	H	749	HIS
4	H	884	GLN
4	H	903	GLN
4	H	967	HIS
4	H	1076	HIS

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Mol	Chain	Res	Type
4	H	1080	ASN
4	H	1124	HIS
4	H	1166	HIS
4	H	1248	HIS
4	H	1275	ASN
4	H	1364	GLN
4	I	304	ASN
4	I	455	HIS
4	I	514	GLN
4	I	581	HIS
4	I	620	ASN
4	I	722	HIS
4	I	869	HIS
4	I	945	ASN
4	I	965	HIS
4	I	984	HIS
4	I	1027	HIS
4	I	1076	HIS
4	I	1093	ASN
4	I	1319	GLN
4	J	81	HIS
4	J	94	HIS
4	J	111	GLN
4	J	181	GLN
4	J	211	GLN
4	J	278	ASN
4	J	304	ASN
4	J	350	HIS
4	J	432	ASN
4	J	731	GLN
4	J	740	ASN
4	J	743	ASN
4	J	914	GLN
4	J	915	HIS
4	J	981	HIS
4	J	1027	HIS
4	J	1076	HIS
4	J	1111	GLN
4	J	1364	GLN
4	K	153	ASN
4	K	158	HIS
4	K	311	ASN

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Mol	Chain	Res	Type
4	K	338	HIS
4	K	432	ASN
4	K	514	GLN
4	K	660	HIS
4	K	694	ASN
4	K	713	HIS
4	K	740	ASN
4	K	874	GLN
4	K	915	HIS
4	K	967	HIS
4	K	1000	ASN
4	K	1023	GLN
4	K	1027	HIS
4	K	1061	ASN
4	K	1363	GLN
4	L	94	HIS
4	L	153	ASN
4	L	331	HIS
4	L	455	HIS
4	L	510	ASN
4	L	514	GLN
4	L	640	HIS
4	L	803	ASN
4	L	1184	ASN
4	M	47	ASN
4	M	153	ASN
4	M	290	HIS
4	M	304	ASN
4	M	371	ASN
4	M	388	ASN
4	M	432	ASN
4	M	510	ASN
4	M	541	HIS
4	M	581	HIS
4	M	726	ASN
4	M	781	GLN
4	M	803	ASN
4	M	869	HIS
4	M	1027	HIS
4	M	1100	ASN
4	M	1230	ASN
4	M	1313	ASN

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Mol	Chain	Res	Type
5	P	37	HIS
6	T	260	HIS
7	U	39	HIS
7	U	116	HIS
7	U	173	GLN
7	V	50	GLN
7	V	191	GLN
6	W	156	ASN
6	W	232	ASN
6	W	260	HIS
7	X	50	GLN
7	X	79	ASN
7	X	235	GLN
7	Y	39	HIS
7	Y	45	GLN
7	Y	50	GLN
7	Y	129	GLN
7	Y	171	GLN
8	Z	170	ASN
8	Z	229	GLN

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

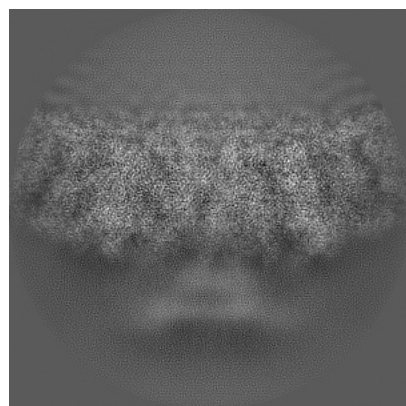
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41200. These allow visual inspection of the internal detail of the map and identification of artifacts.

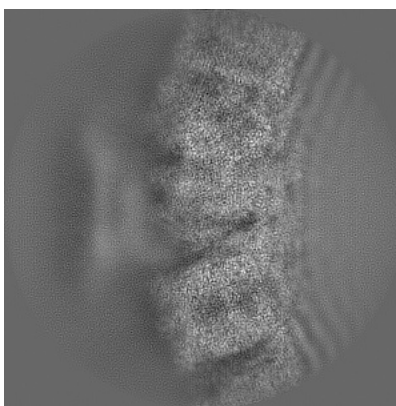
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

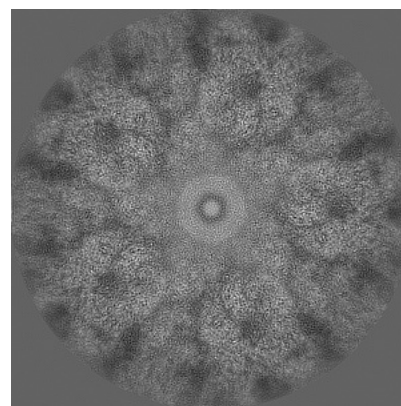
6.1.1 Primary map



X

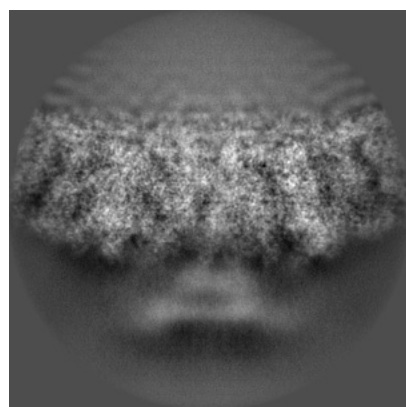


Y

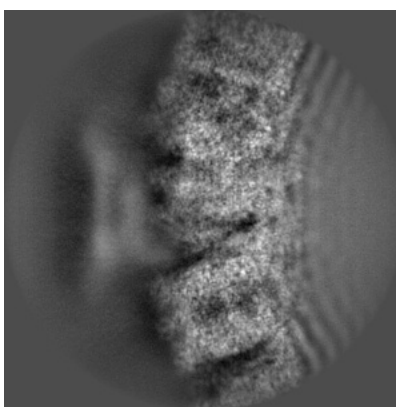


Z

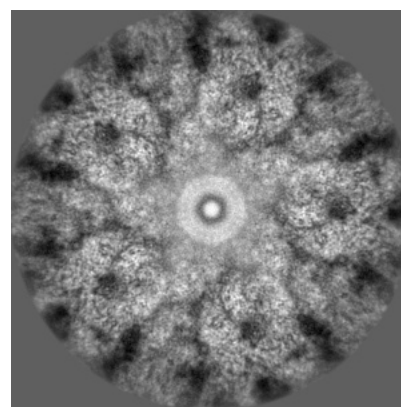
6.1.2 Raw map



X



Y

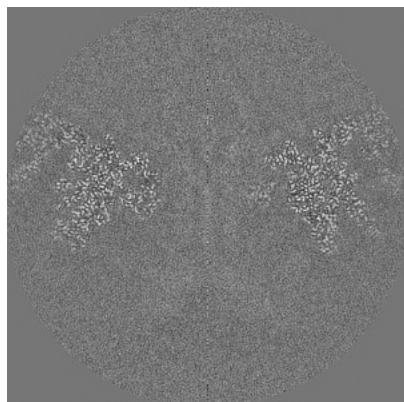


Z

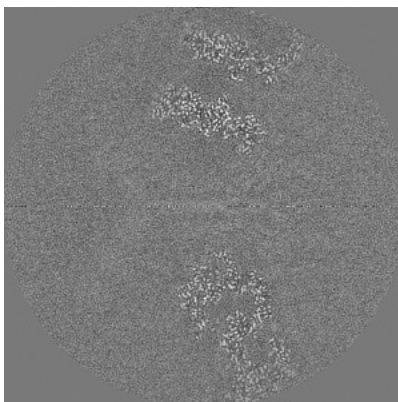
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

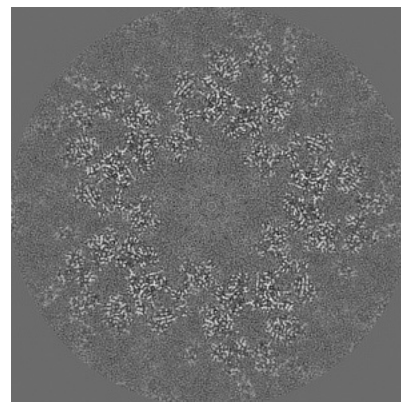
6.2.1 Primary map



X Index: 180

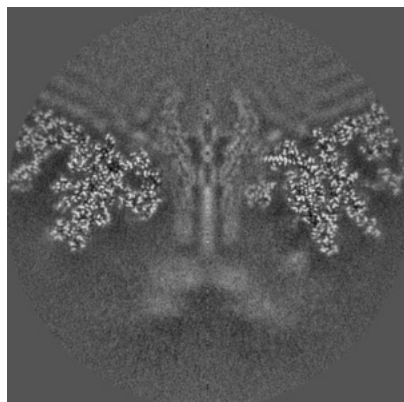


Y Index: 180

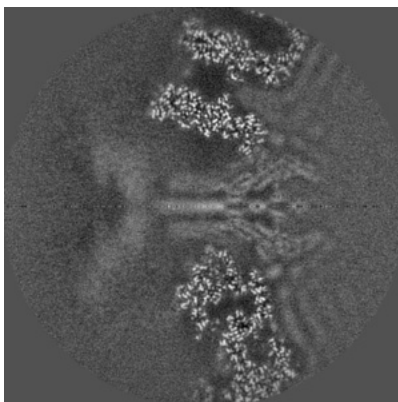


Z Index: 180

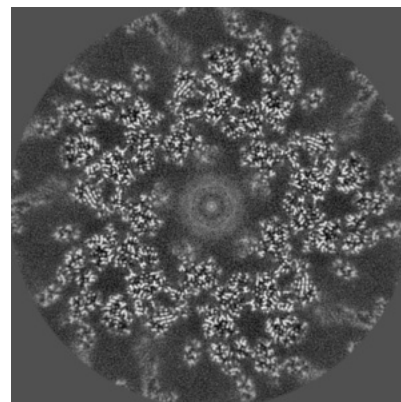
6.2.2 Raw map



X Index: 180



Y Index: 180

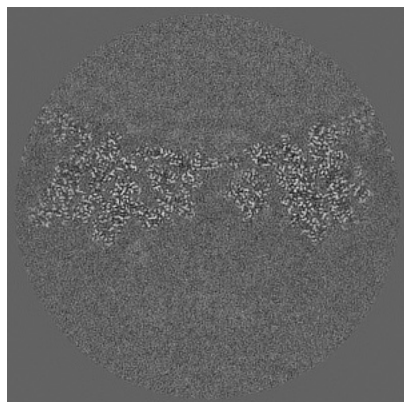


Z Index: 180

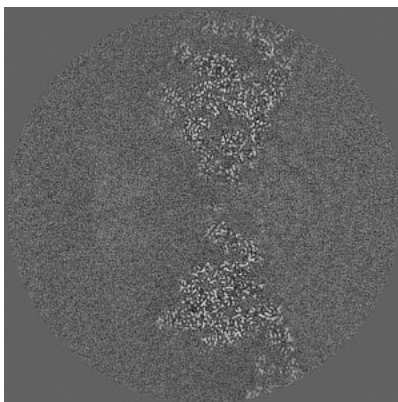
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

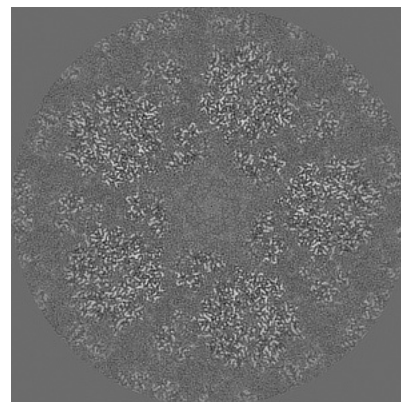
6.3.1 Primary map



X Index: 234

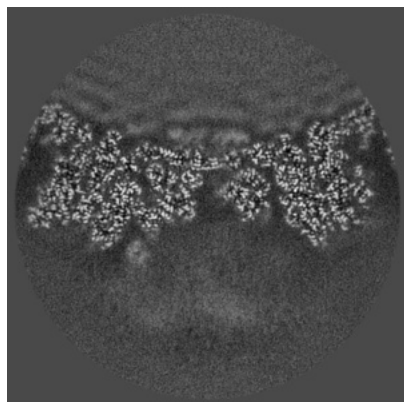


Y Index: 217

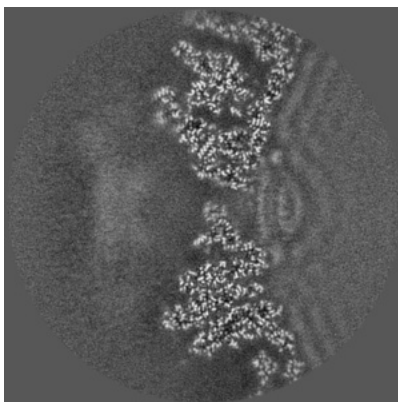


Z Index: 202

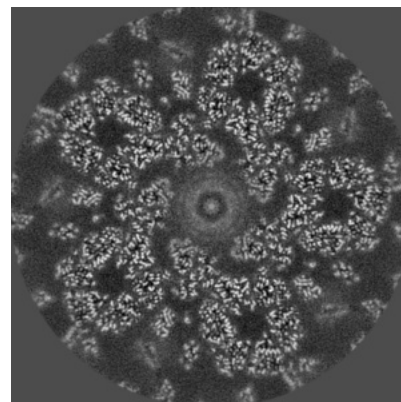
6.3.2 Raw map



X Index: 234



Y Index: 220

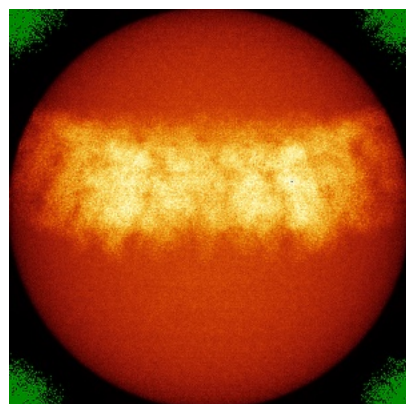


Z Index: 189

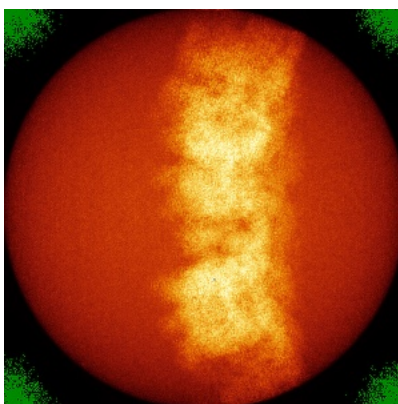
The images above show the largest variance slices of the map in three orthogonal directions.

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

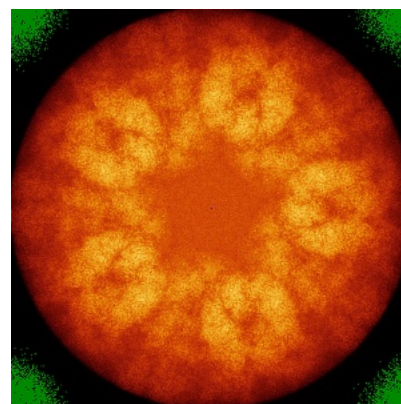
6.4.1 Primary map



X

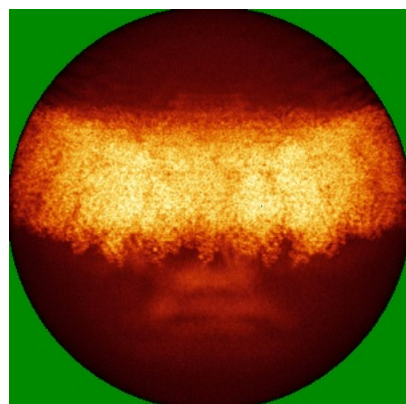


Y

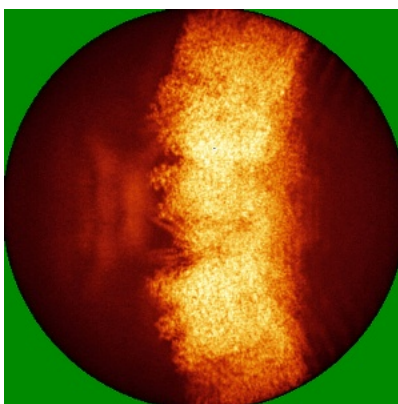


Z

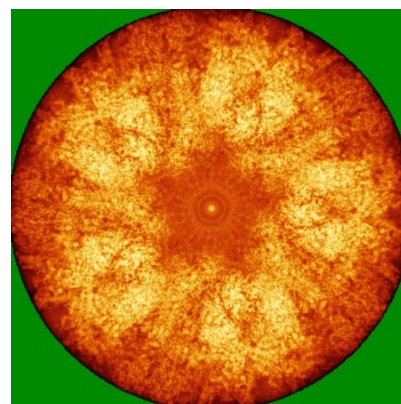
6.4.2 Raw map



X



Y

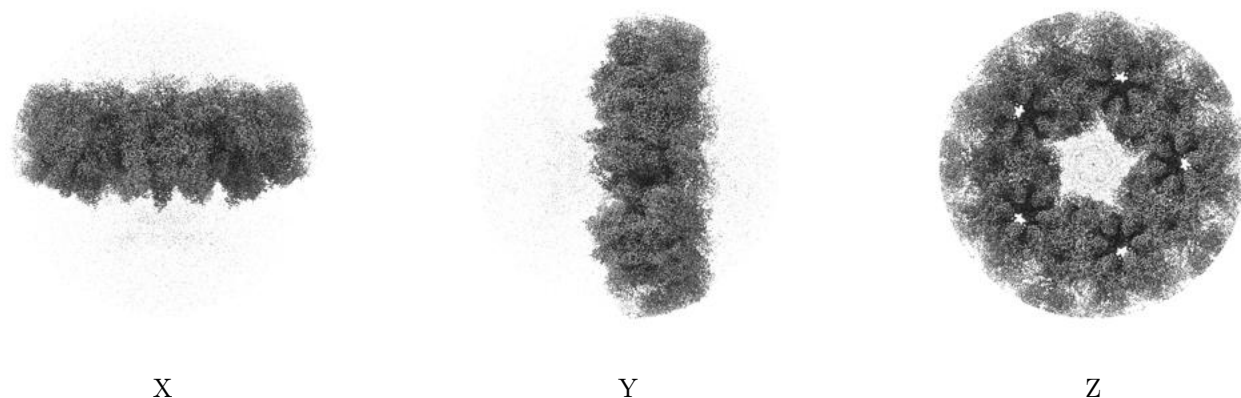


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

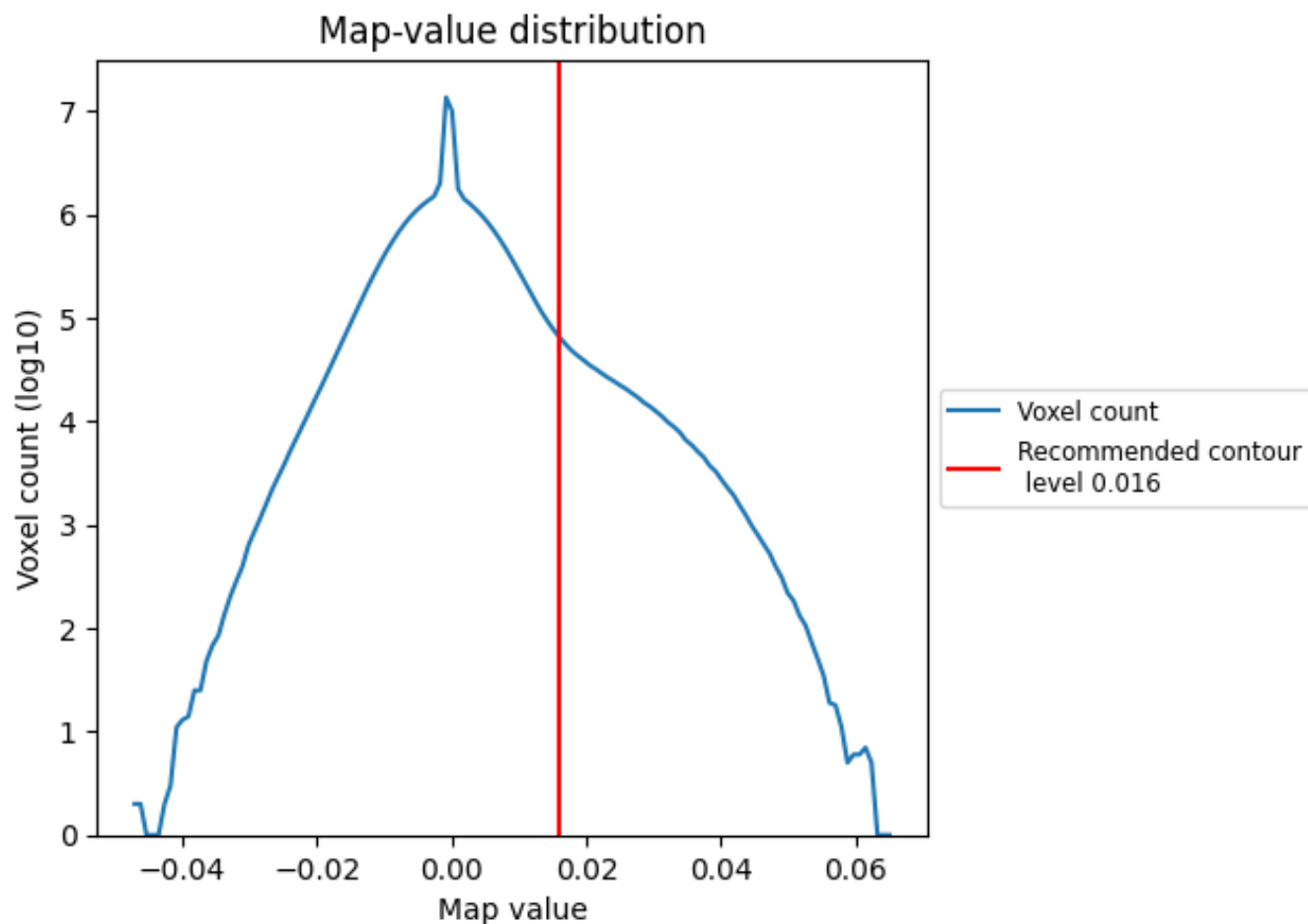
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

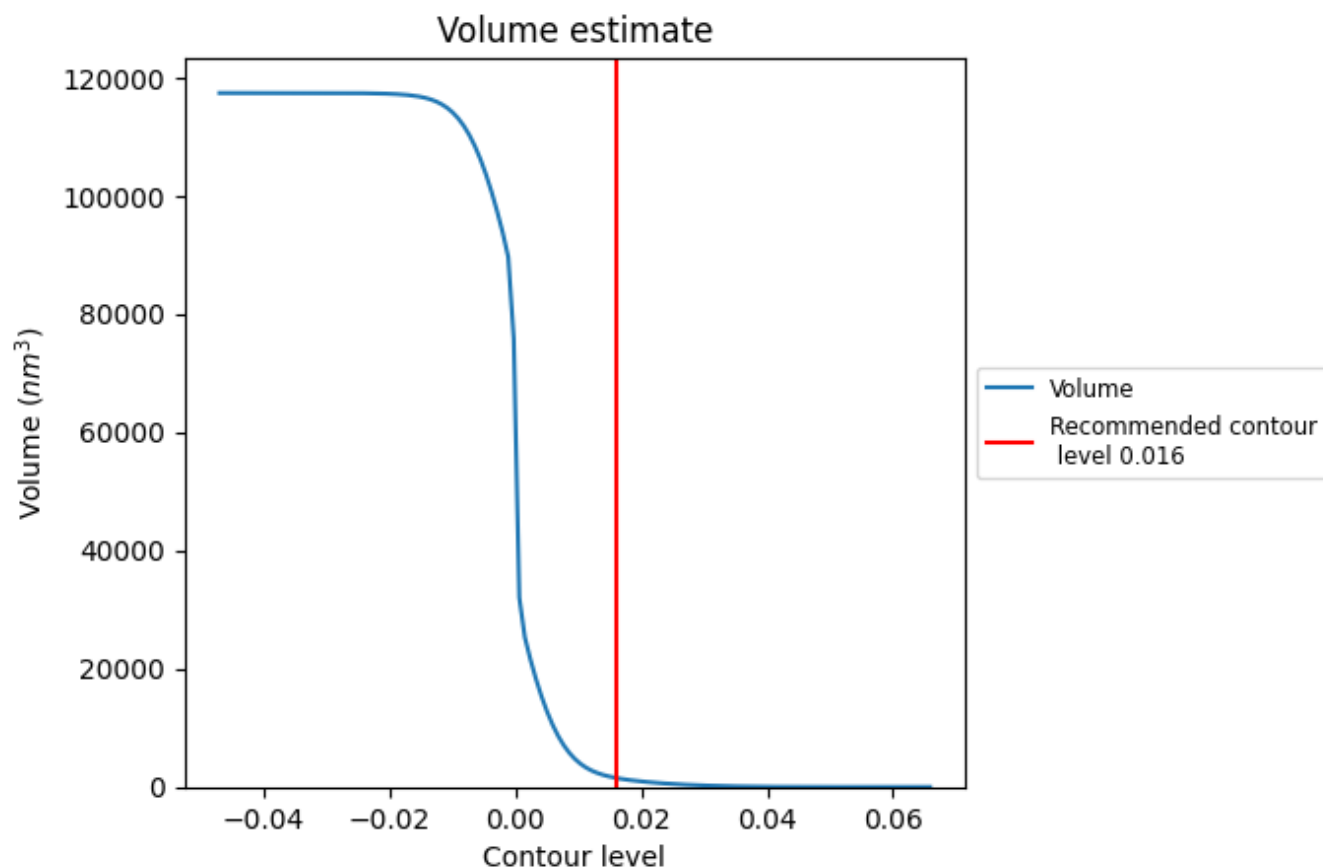
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

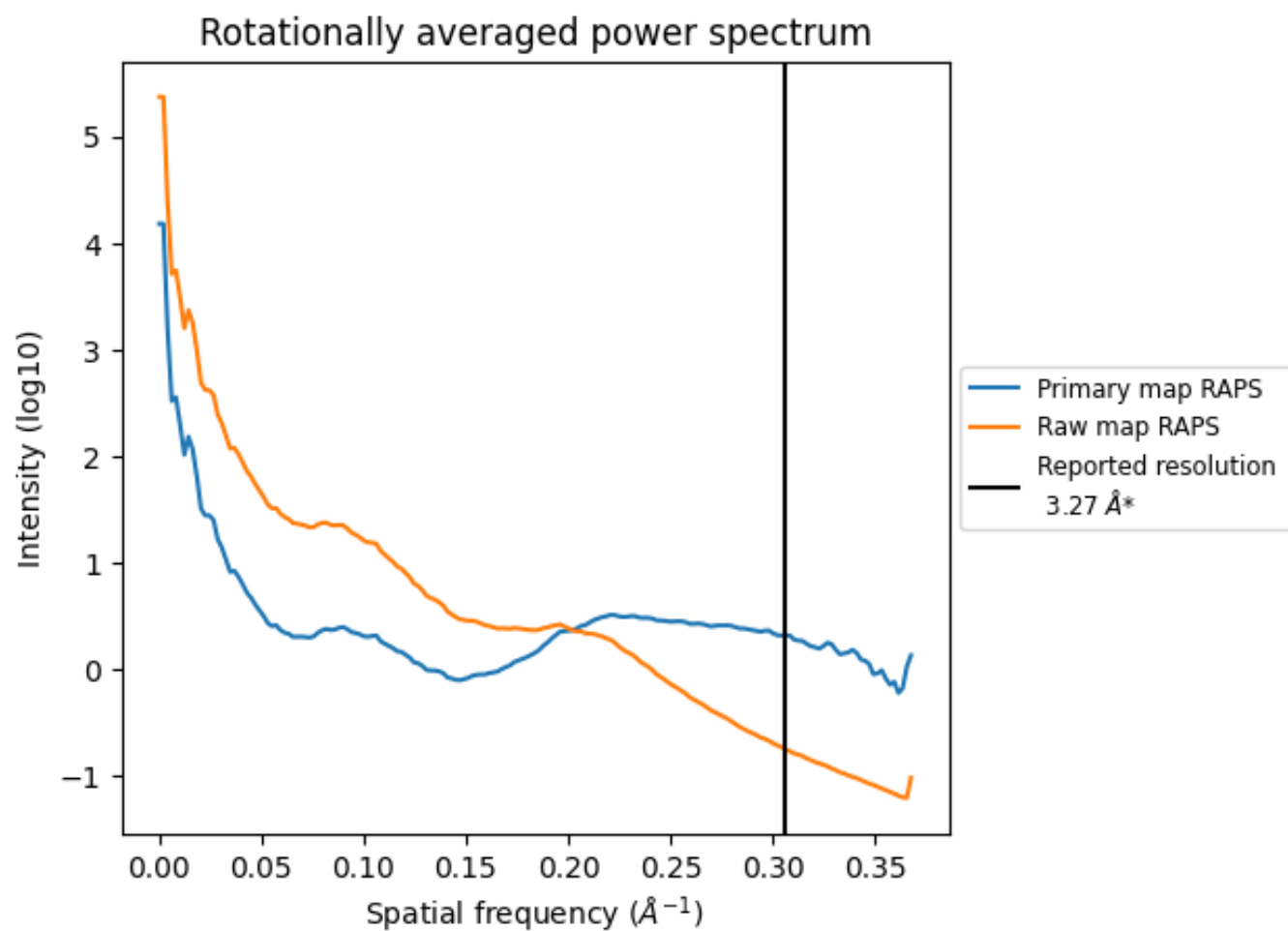
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1522 nm³; this corresponds to an approximate mass of 1375 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

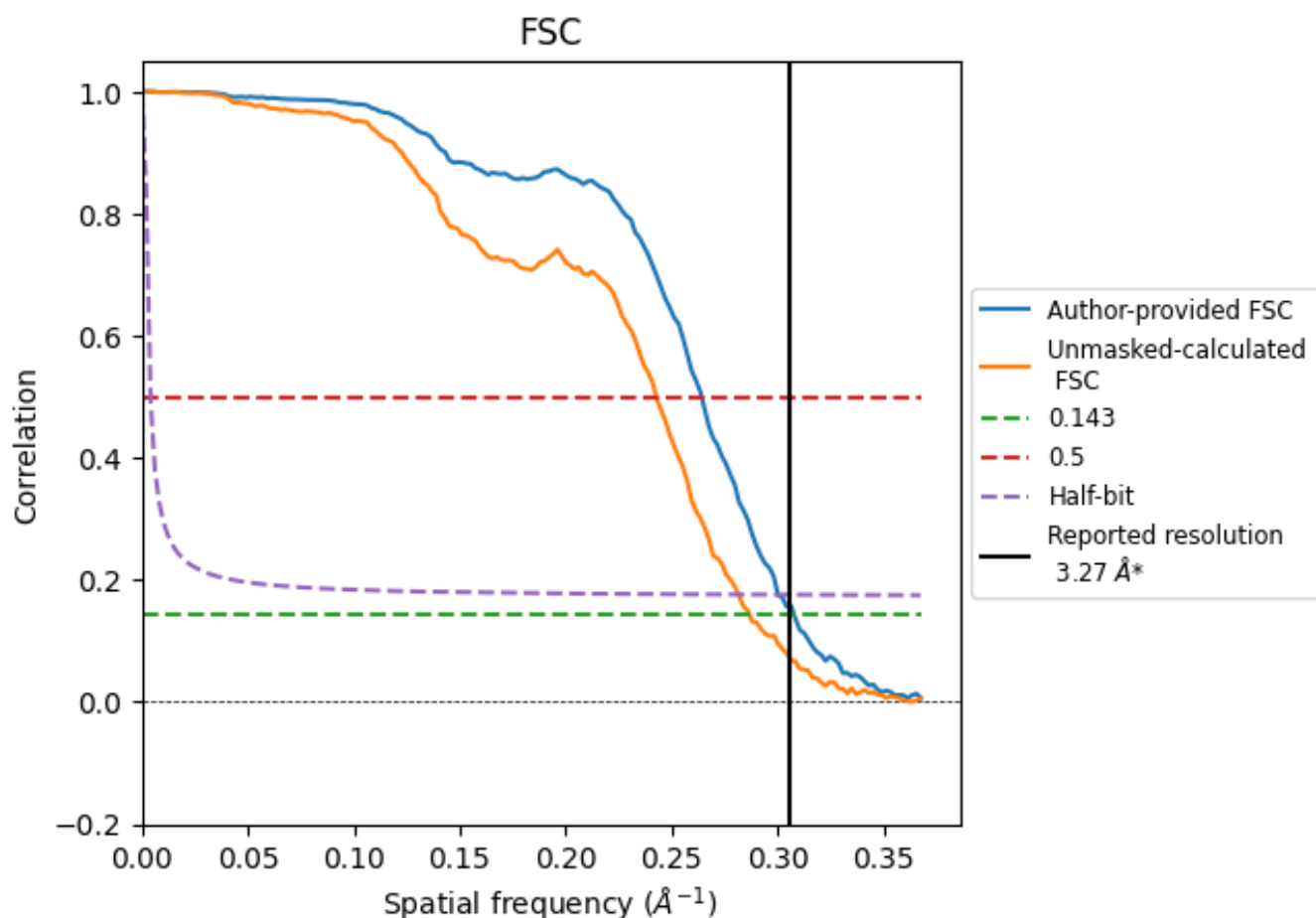


*Reported resolution corresponds to spatial frequency of 0.306 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.306 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

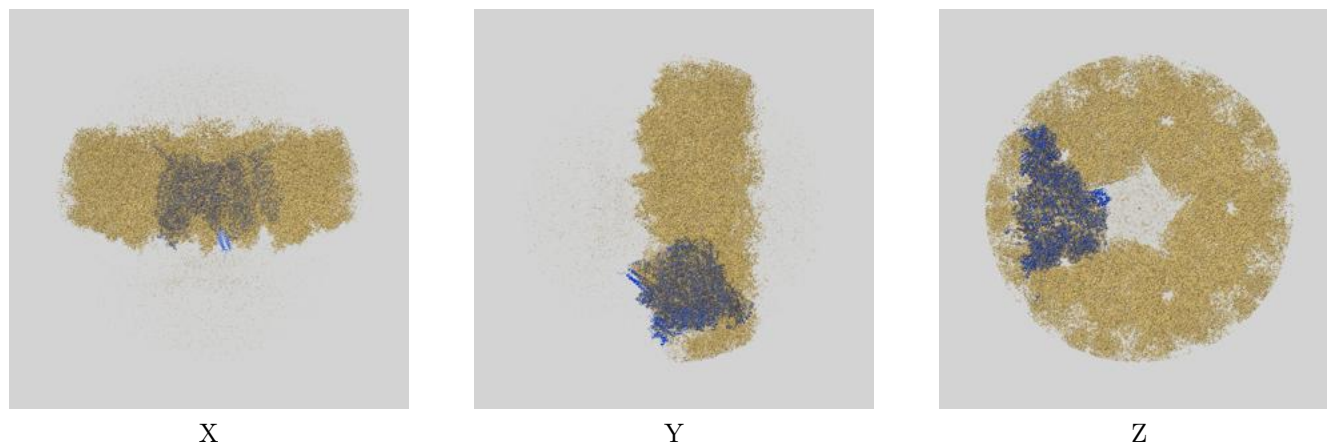
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.27	-	-
Author-provided FSC curve	3.25	3.79	3.33
Unmasked-calculated*	3.49	4.12	3.55

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

9 Map-model fit [i](#)

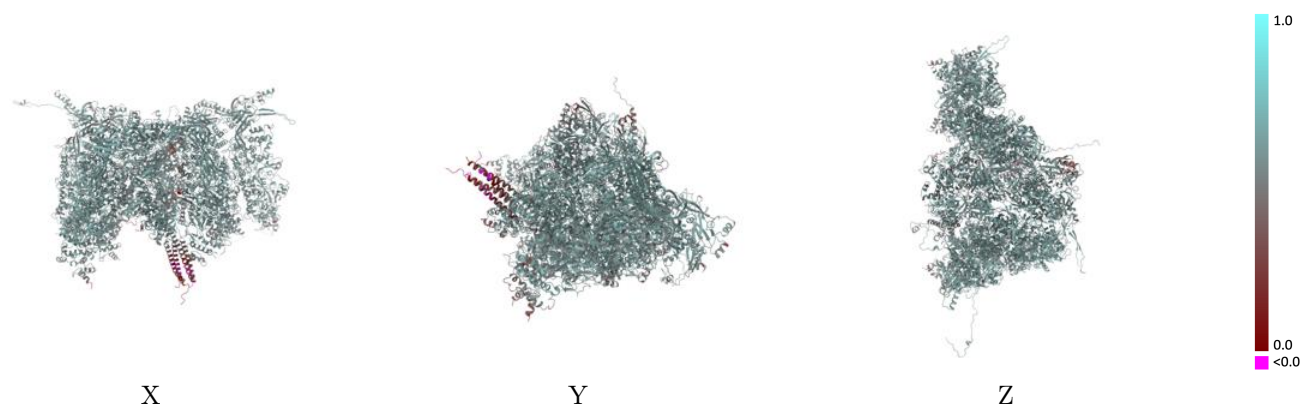
This section contains information regarding the fit between EMDB map EMD-41200 and PDB model 8TES. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



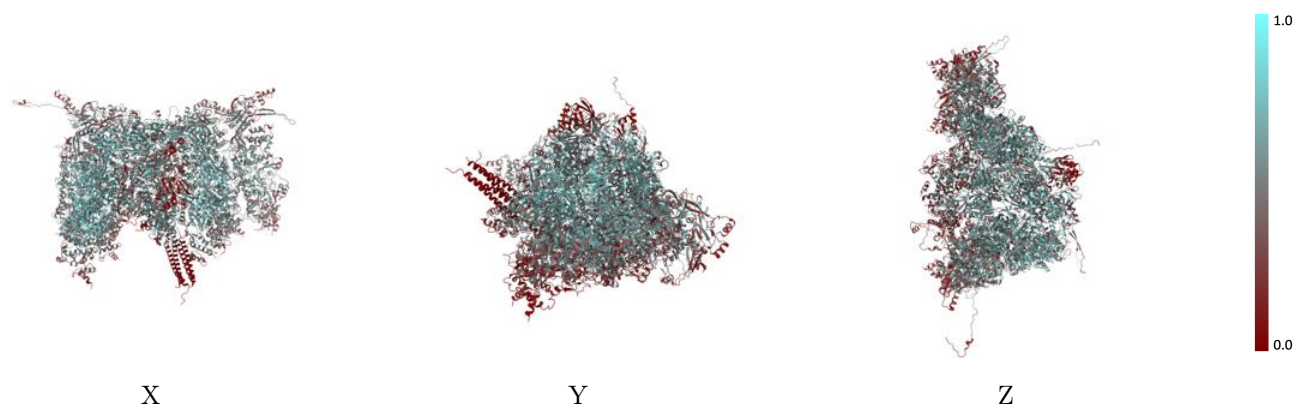
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



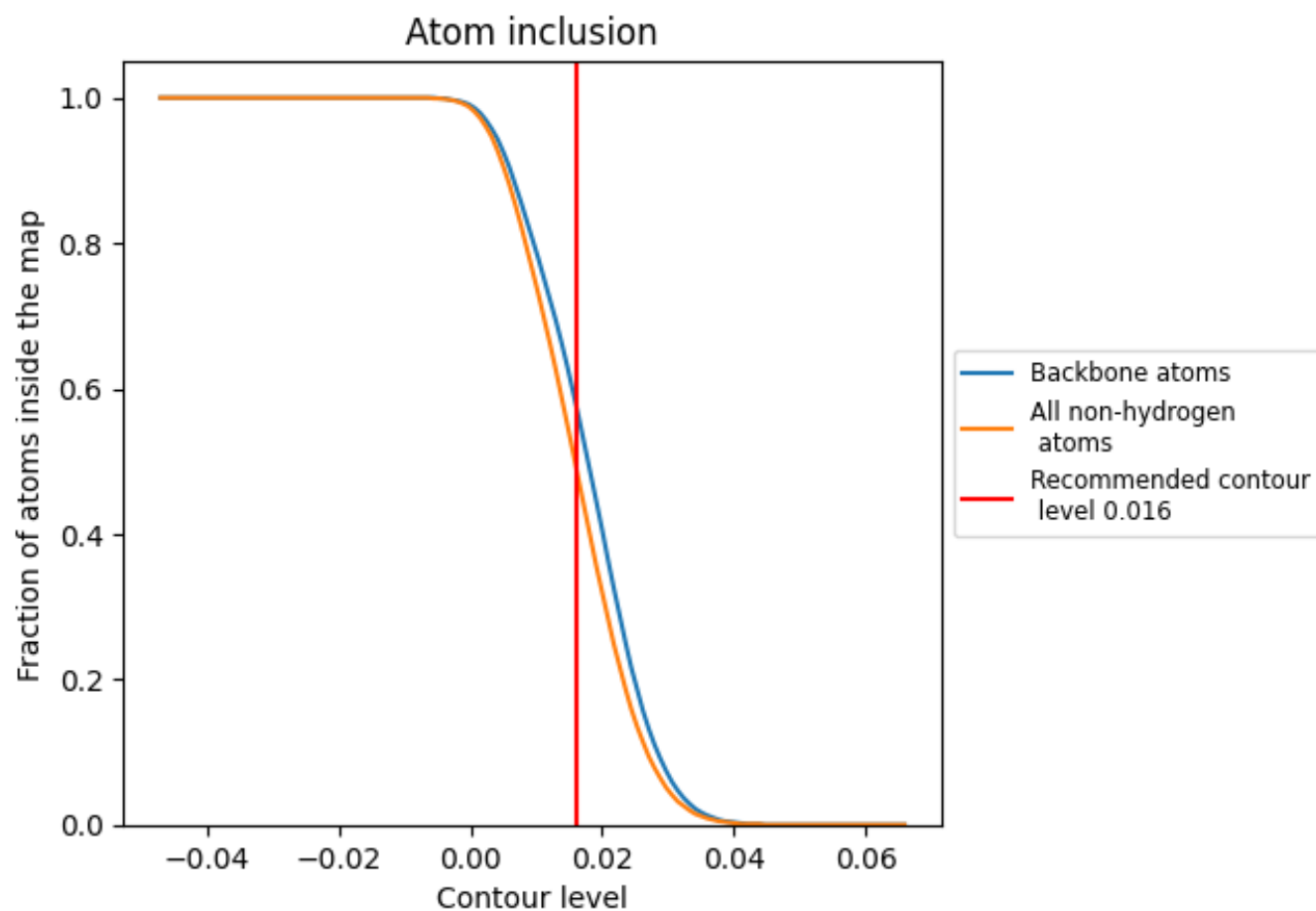
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 49% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4930	 0.5670
A	 0.0770	 0.2550
C	 0.0170	 0.2810
E	 0.2220	 0.4310
F	 0.1260	 0.3560
G	 0.5070	 0.5720
H	 0.6110	 0.5940
I	 0.5890	 0.5900
J	 0.4810	 0.5760
K	 0.5950	 0.5870
L	 0.5330	 0.5830
M	 0.4360	 0.5690
N	 0.2670	 0.4780
O	 0.3090	 0.5190
P	 0.1790	 0.4660
Q	 0.2730	 0.4670
R	 0.1630	 0.4590
S	 0.1370	 0.4890
T	 0.2700	 0.5140
U	 0.5050	 0.5690
V	 0.4870	 0.5620
W	 0.5070	 0.5750
X	 0.3920	 0.5560
Y	 0.4040	 0.5610
Z	 0.2190	 0.5050

