



Full wwPDB EM Validation Report ⓘ

Jul 21, 2025 – 05:21 PM EDT

PDB ID : 9NO1 / pdb_00009no1
EMDB ID : EMD-49591
Title : Cryo-ET map of the VZV capsid vertex (5-fold axis).
Authors : Oliver, S.L.; Chen, M.
Deposited on : 2025-03-07
Resolution : 8.30 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:

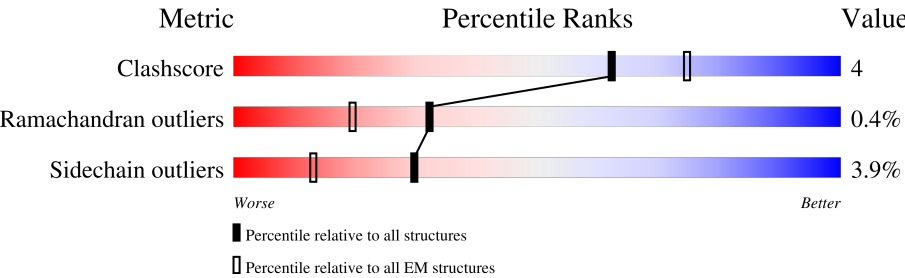
EMDB validation analysis : 0.0.1.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

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 8.30 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1396	<div> <div>40%</div> <div>70%</div> <div>13%</div> <div>16%</div> </div>
1	B	1396	<div> <div>45%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
1	D	1396	<div> <div>42%</div> <div>83%</div> <div>12%</div> <div>• •</div> </div>
1	F	1396	<div> <div>43%</div> <div>85%</div> <div>10%</div> <div>• •</div> </div>
1	H	1396	<div> <div>39%</div> <div>80%</div> <div>11%</div> <div>8%</div> </div>
1	J	1396	<div> <div>46%</div> <div>78%</div> <div>13%</div> <div>• 8%</div> </div>
1	L	1396	<div> <div>46%</div> <div>80%</div> <div>13%</div> <div>• 6%</div> </div>
2	C	235	<div> <div>10%</div> <div>40%</div> <div>•</div> <div>57%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	235	
2	G	235	
2	I	235	
2	K	235	
2	M	235	
3	N	483	
3	Q	483	
4	O	316	
4	P	316	
4	R	316	
4	S	316	
5	T	676	
6	U	579	
6	V	579	
7	W	2763	
7	X	2763	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 102113 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 ORF40.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1166	Total	C	N	O	S	0	0
			9043	5744	1576	1664	59		
1	B	1332	Total	C	N	O	S	0	0
			10283	6529	1786	1900	68		
1	D	1337	Total	C	N	O	S	0	0
			10245	6510	1760	1909	66		
1	F	1337	Total	C	N	O	S	0	0
			10328	6558	1786	1916	68		
1	H	1281	Total	C	N	O	S	0	0
			9821	6246	1690	1819	66		
1	J	1279	Total	C	N	O	S	0	0
			9850	6242	1714	1829	65		
1	L	1314	Total	C	N	O	S	0	0
			10181	6461	1766	1888	66		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	101	Total	C	N	O	S	0	0
			724	461	123	138	2		
2	E	97	Total	C	N	O	S	0	0
			712	452	126	132	2		
2	G	101	Total	C	N	O	S	0	0
			736	467	129	138	2		
2	I	101	Total	C	N	O	S	0	0
			742	470	132	138	2		
2	K	101	Total	C	N	O	S	0	0
			742	470	132	138	2		
2	M	101	Total	C	N	O	S	0	0
			721	459	122	138	2		

- Molecule 3 is a protein called ORF20.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	357	Total	C	N	O	S	0	0
			2767	1753	483	515	16		
3	Q	357	Total	C	N	O	S	0	0
			2770	1754	484	516	16		

- Molecule 4 is a protein called ORF41.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	298	Total	C	N	O	S	0	0
			2288	1458	397	422	11		
4	P	275	Total	C	N	O	S	0	0
			2080	1333	354	384	9		
4	R	298	Total	C	N	O	S	0	0
			2288	1458	397	422	11		
4	S	275	Total	C	N	O	S	0	0
			2083	1334	354	386	9		

- Molecule 5 is a protein called ORF43.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	593	Total	C	N	O	S	0	0
			4593	2943	782	843	25		

- Molecule 6 is a protein called ORF34.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	531	Total	C	N	O	S	0	0
			4200	2636	745	799	20		
6	V	531	Total	C	N	O	S	0	0
			4200	2636	745	799	20		

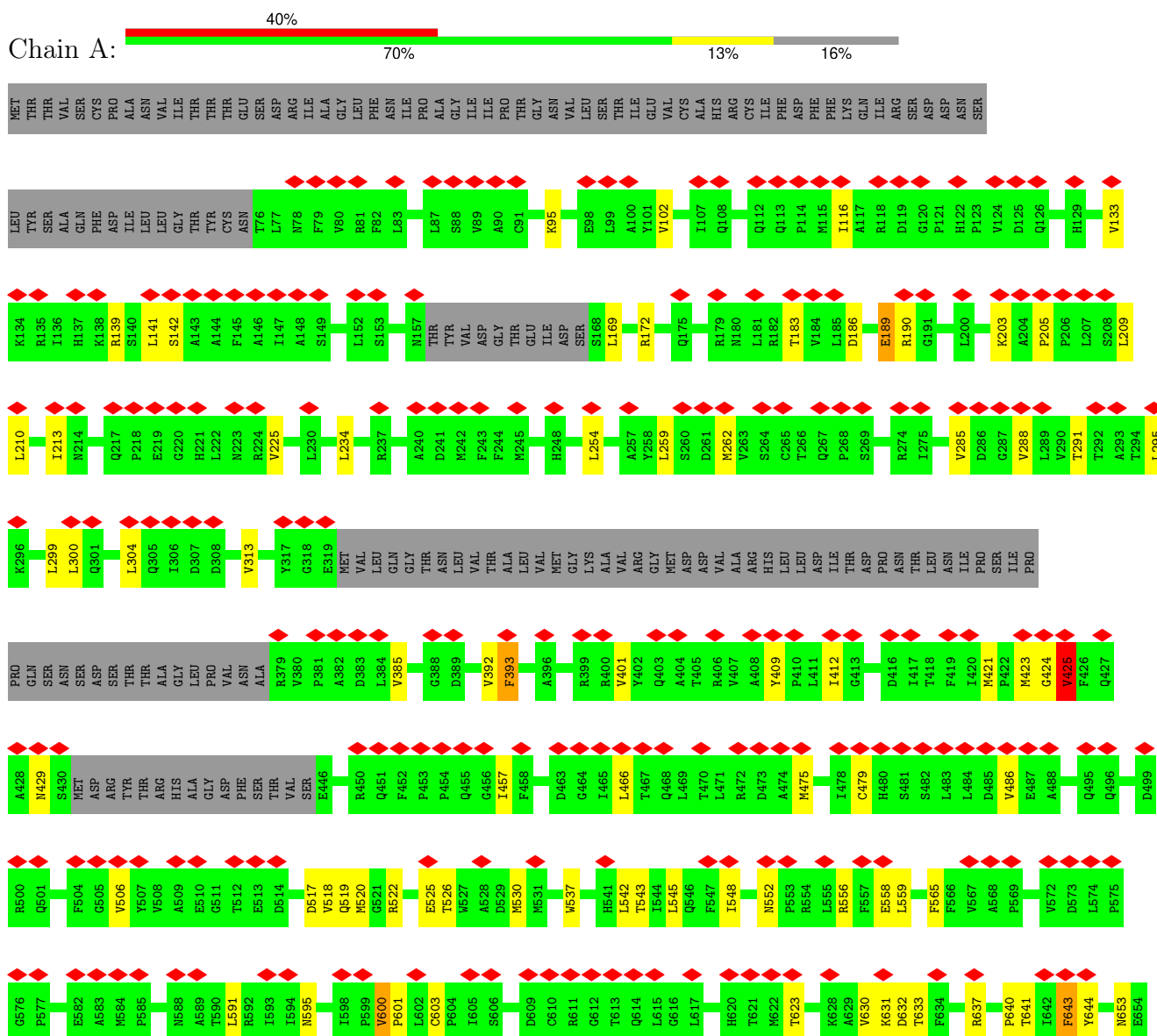
- Molecule 7 is a protein called Large tegument protein deneddylase.

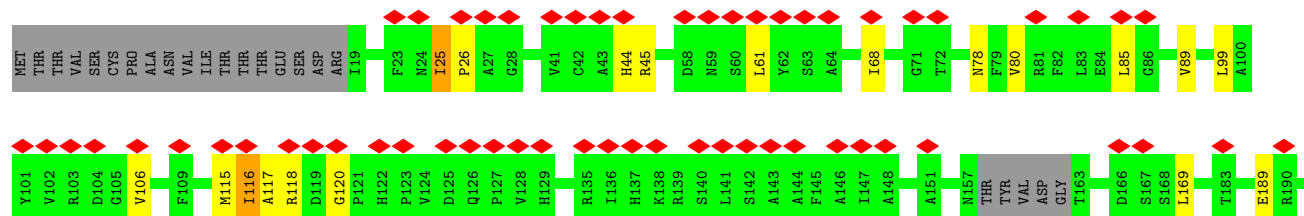
Mol	Chain	Residues	Atoms					AltConf	Trace
7	W	45	Total	C	N	O	S	0	0
			358	228	64	63	3		
7	X	45	Total	C	N	O	S	0	0
			358	228	64	63	3		

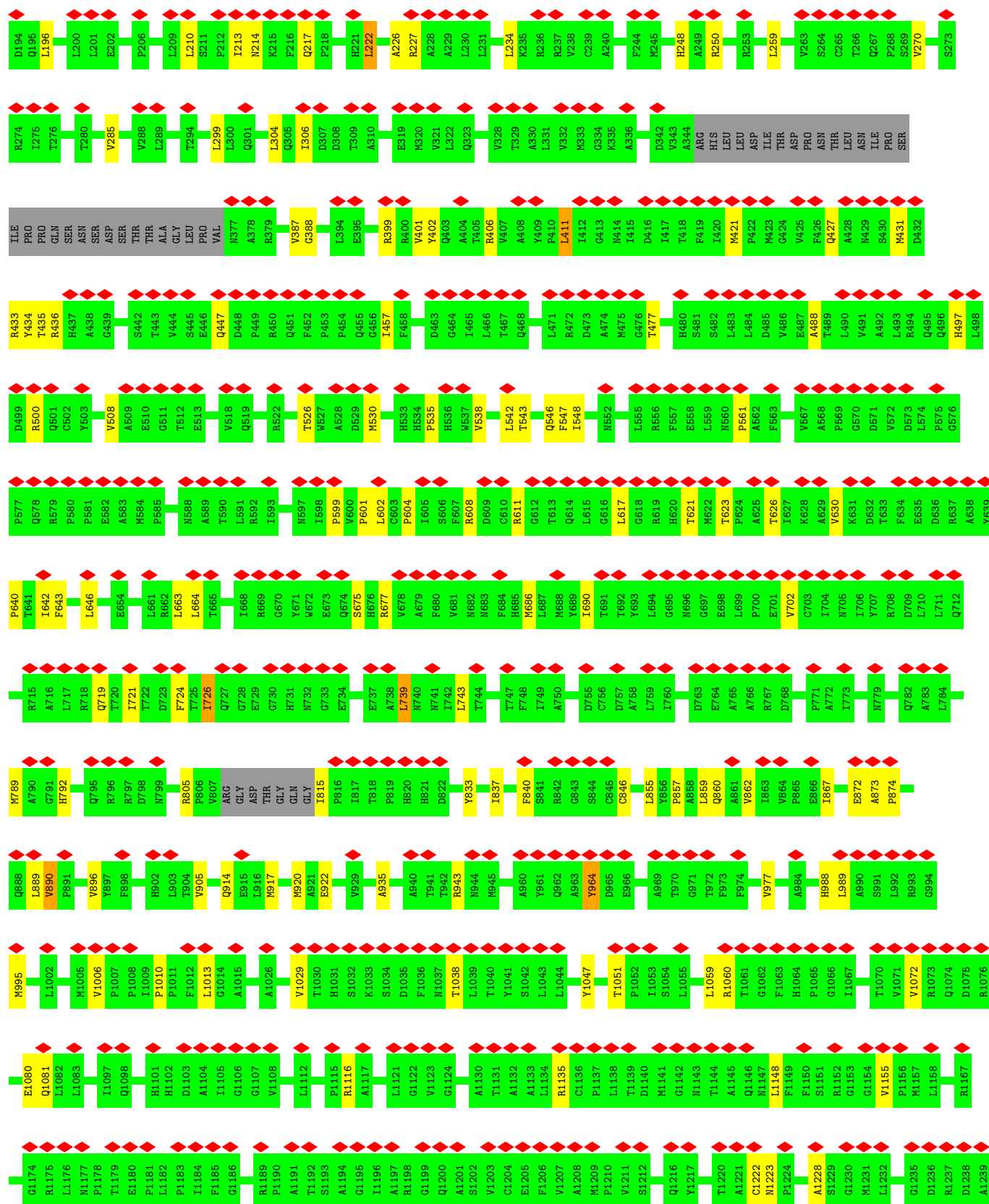
3 Residue-property plots

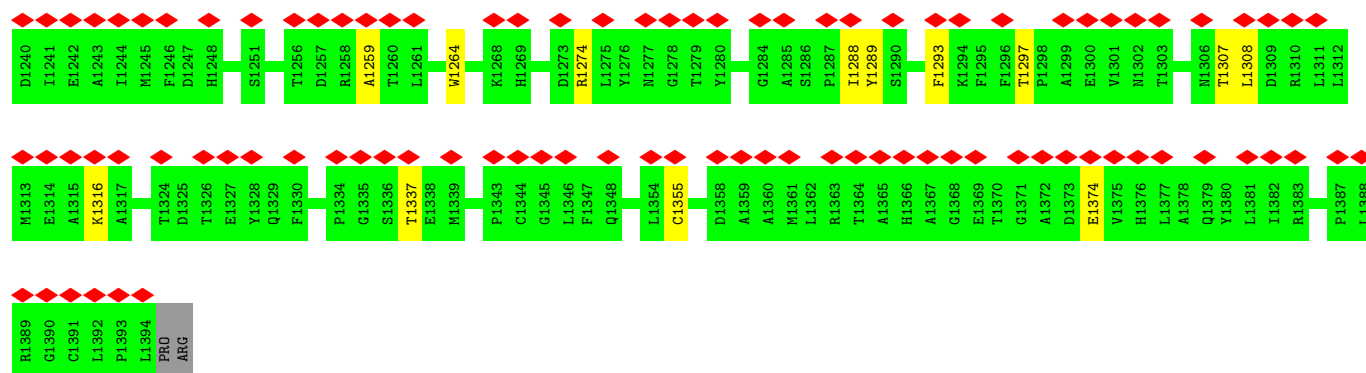
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: ORF40

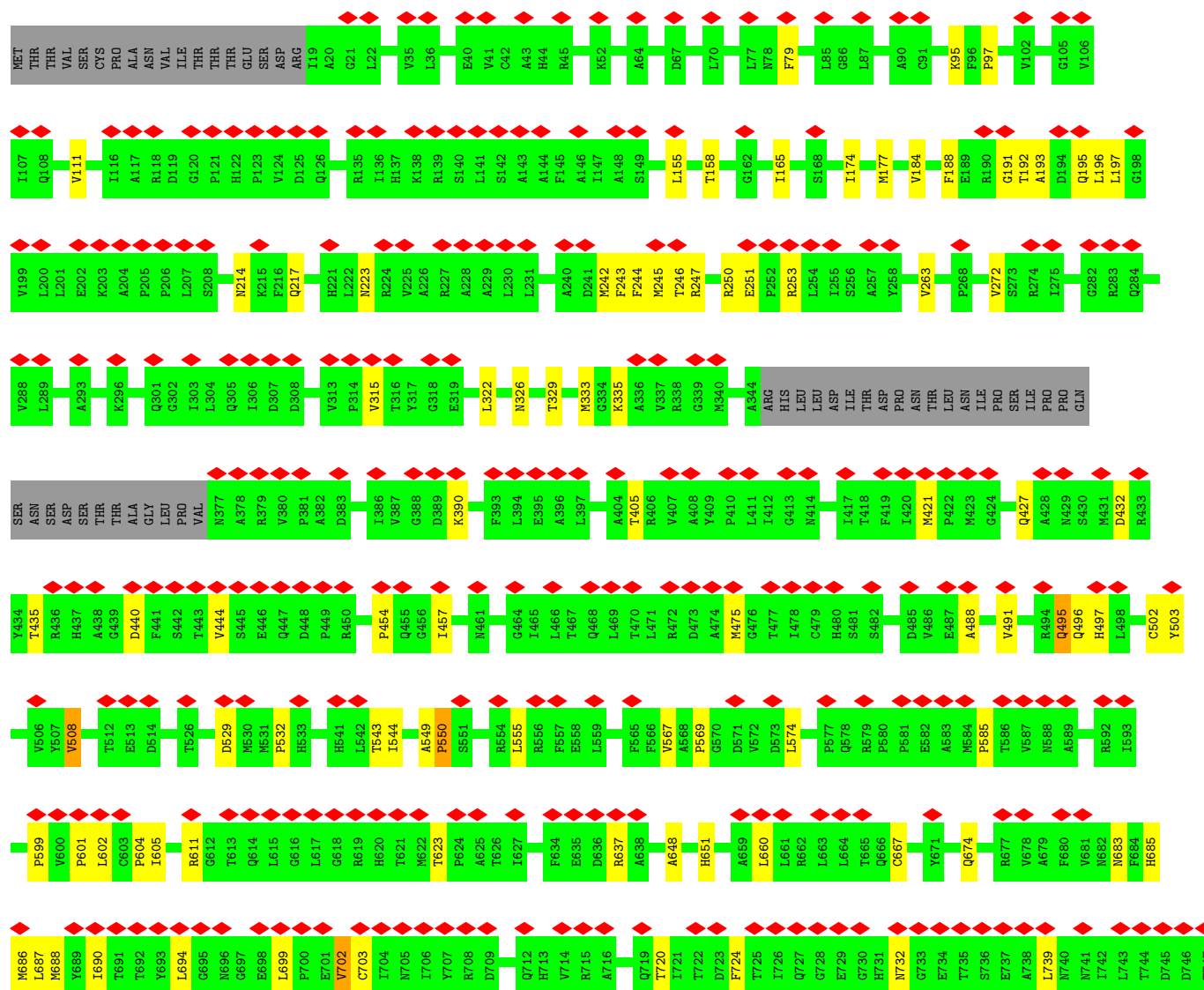
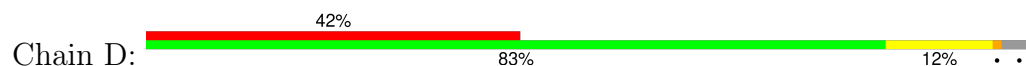


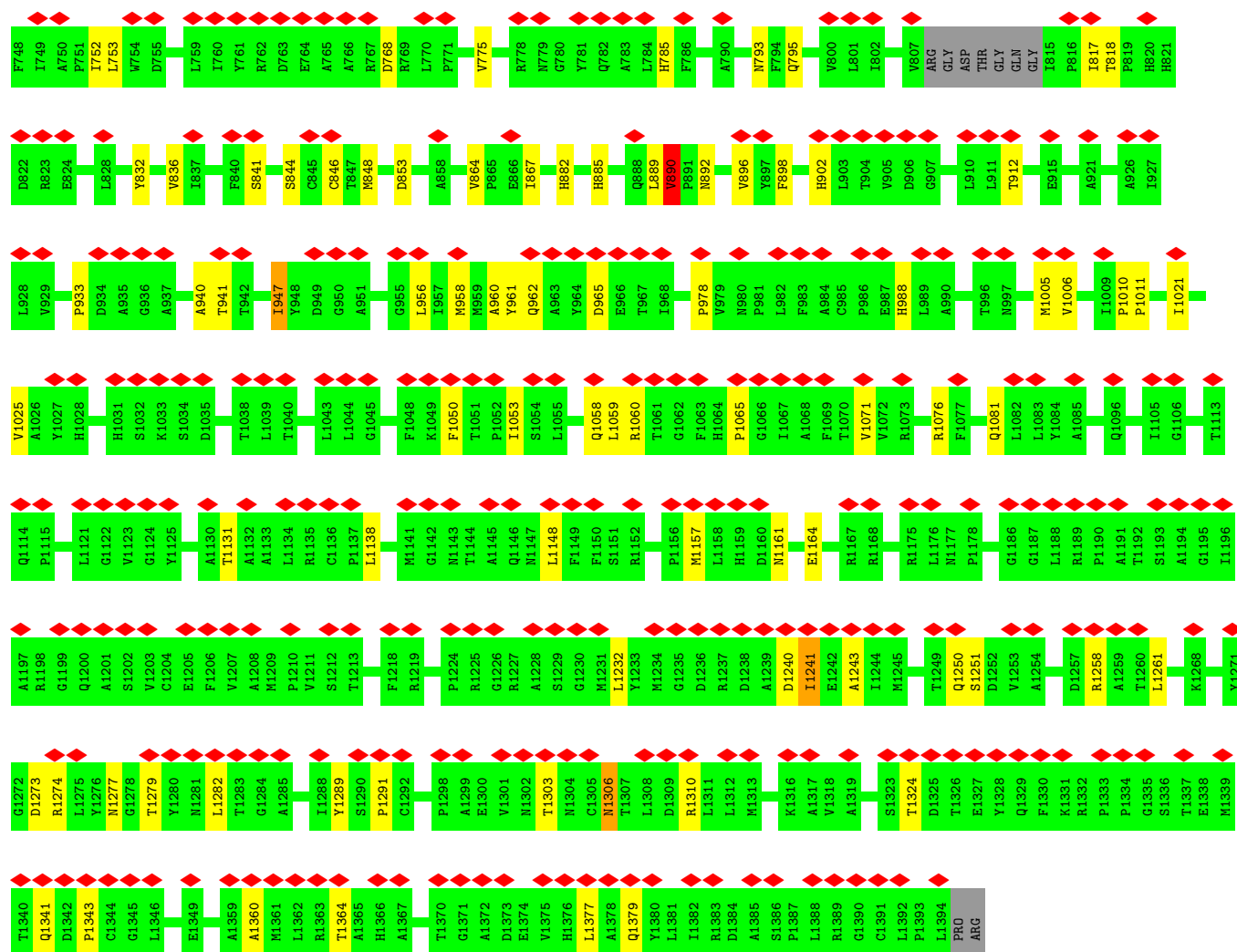




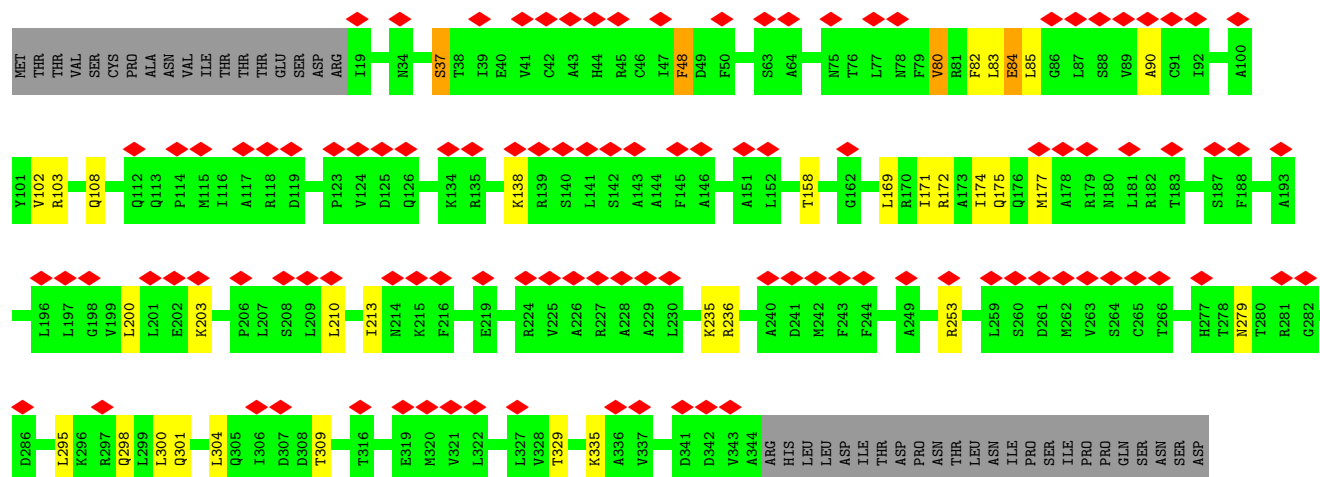
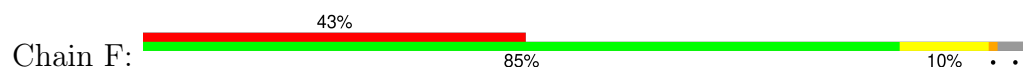


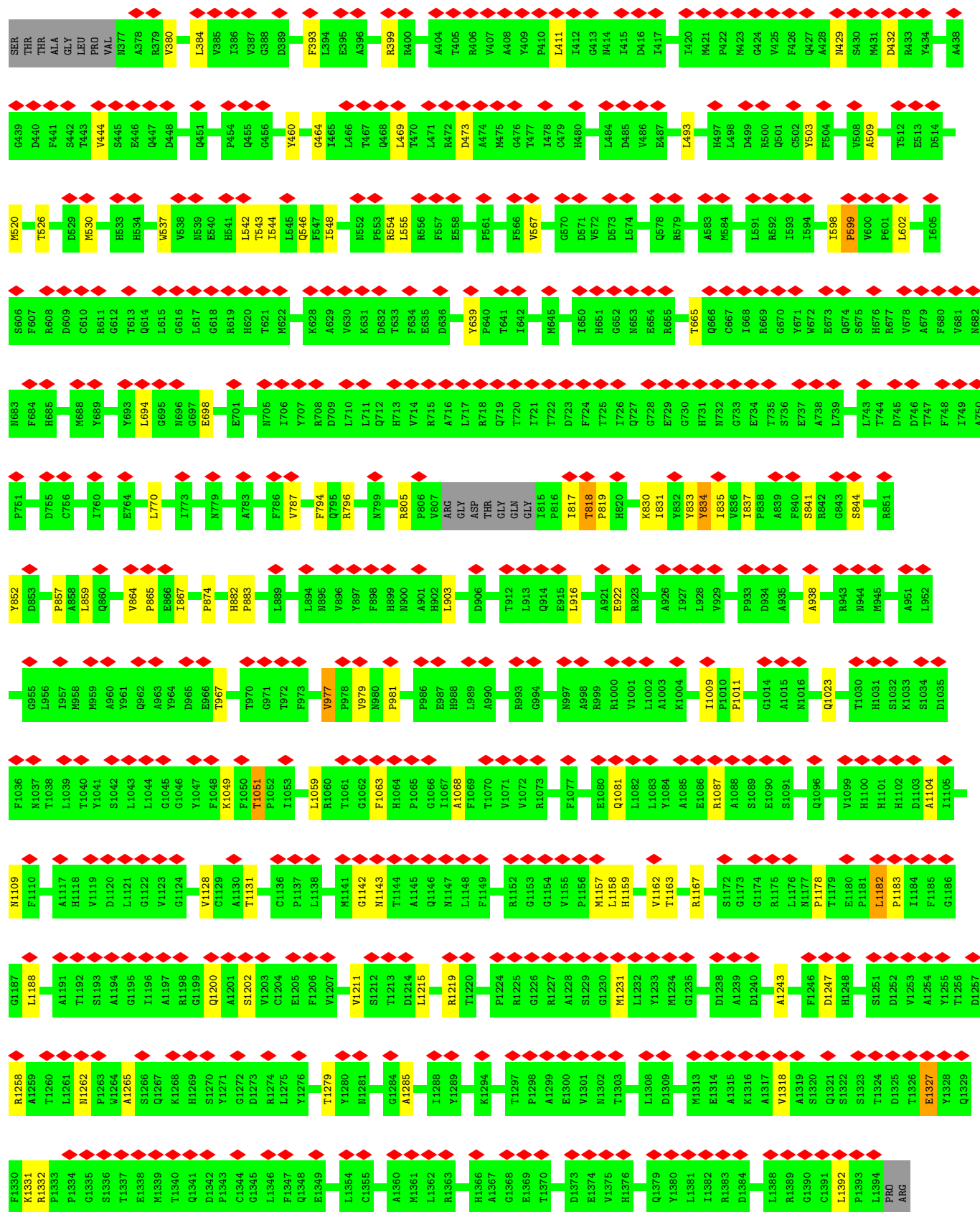
● Molecule 1: ORF40

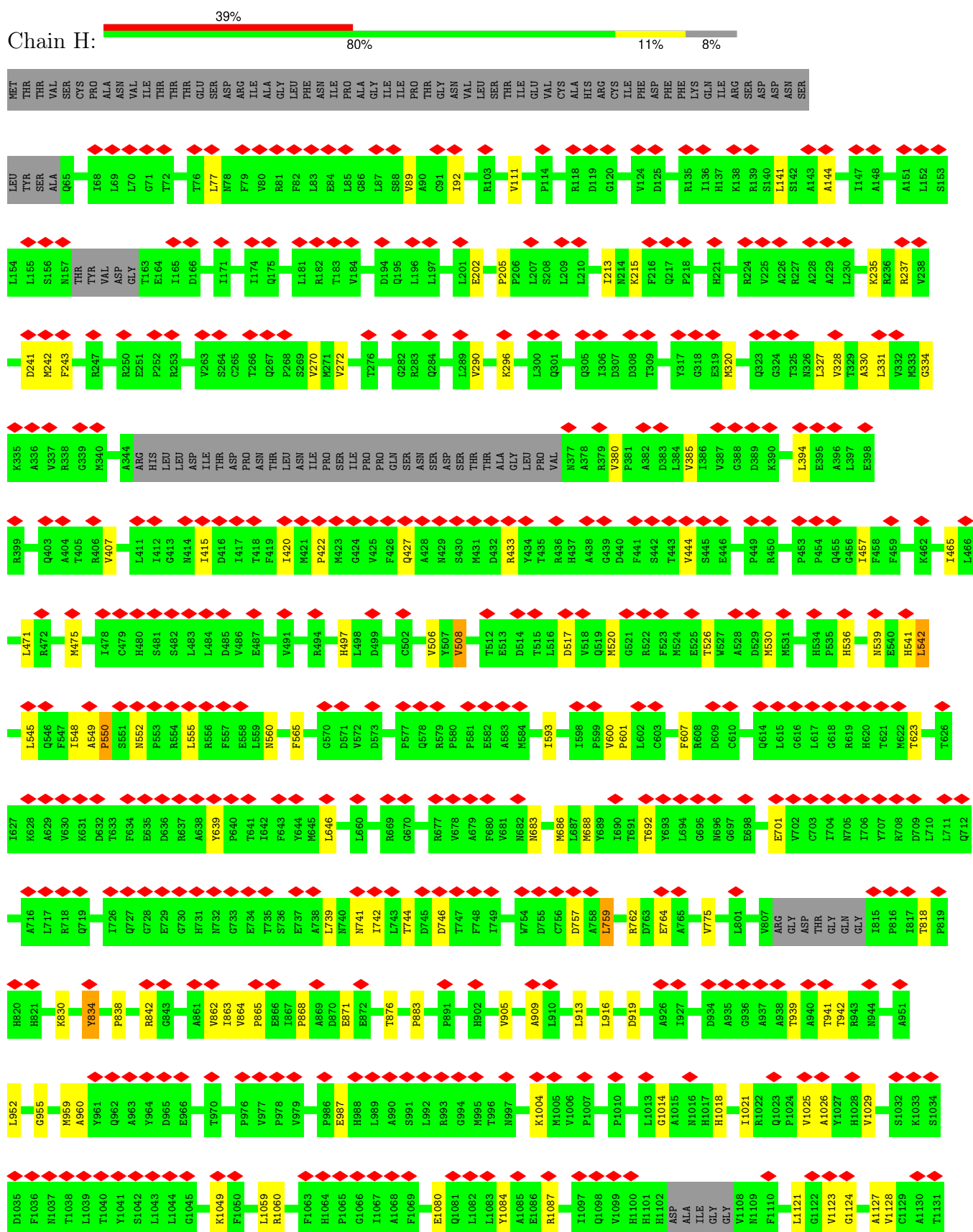


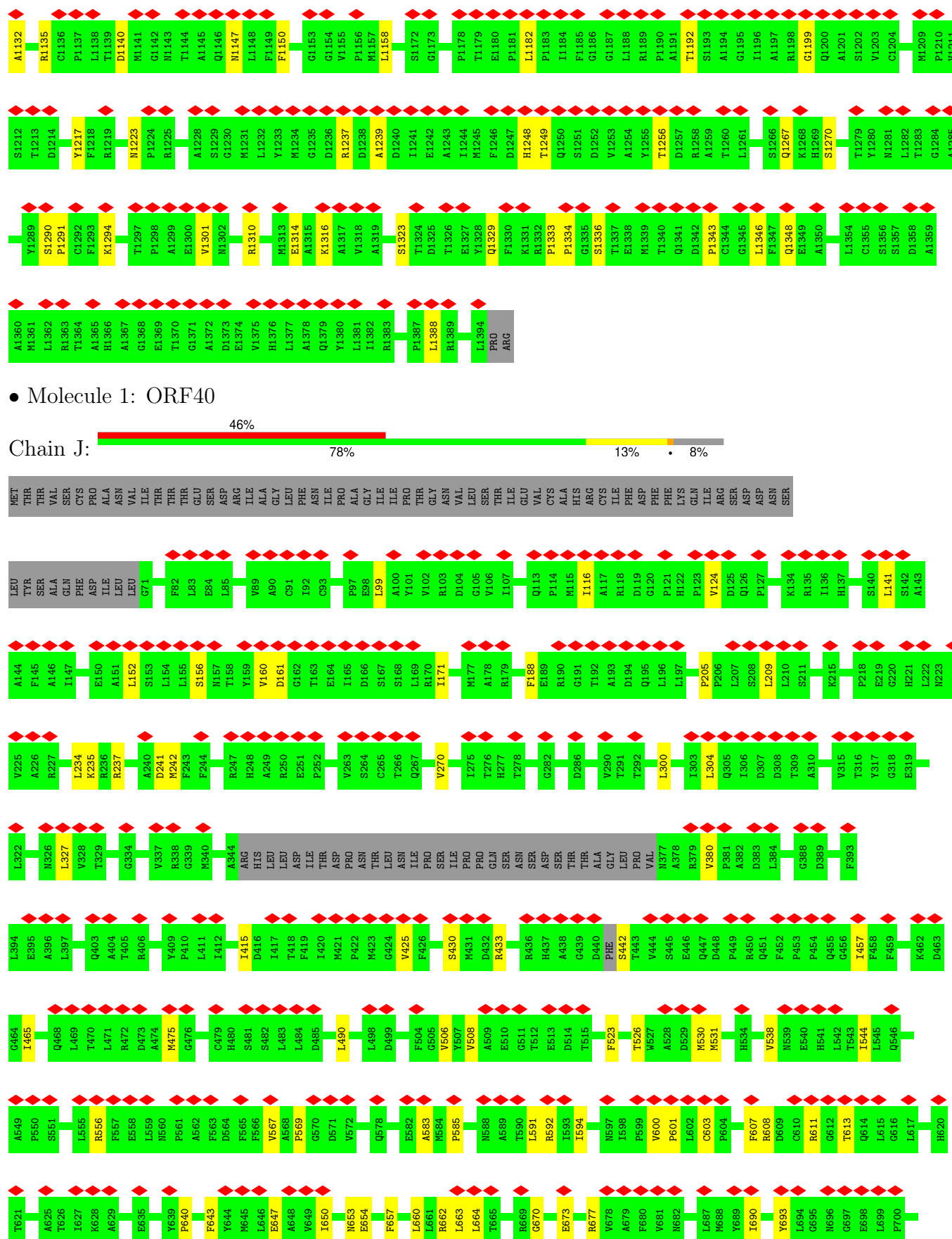


● Molecule 1: ORF40



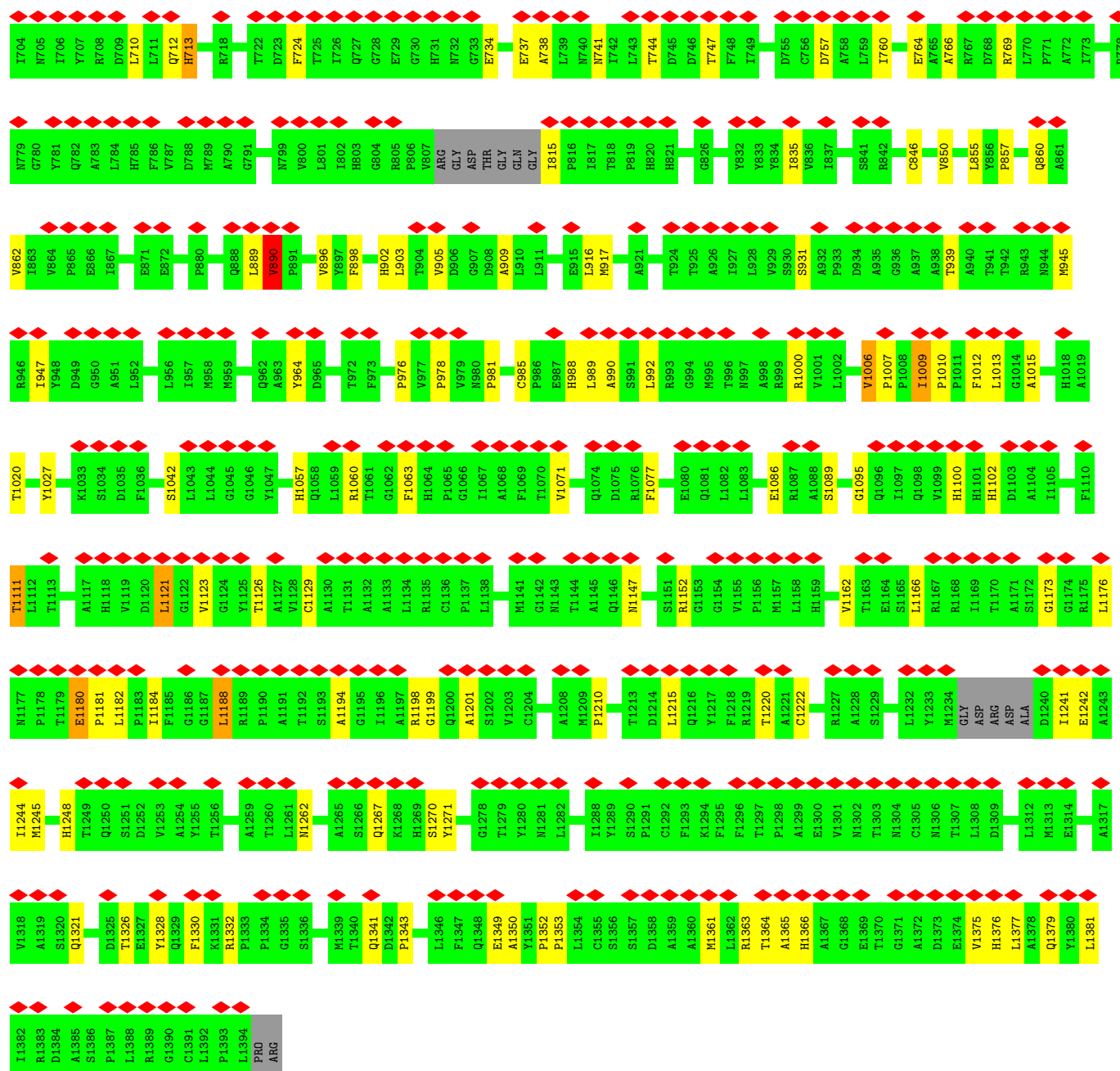




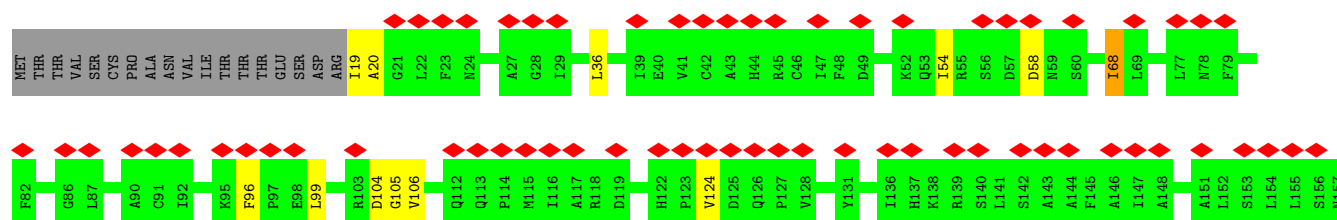
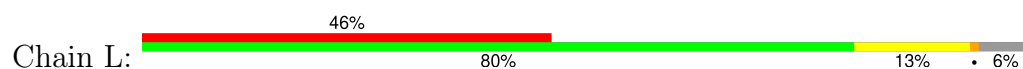


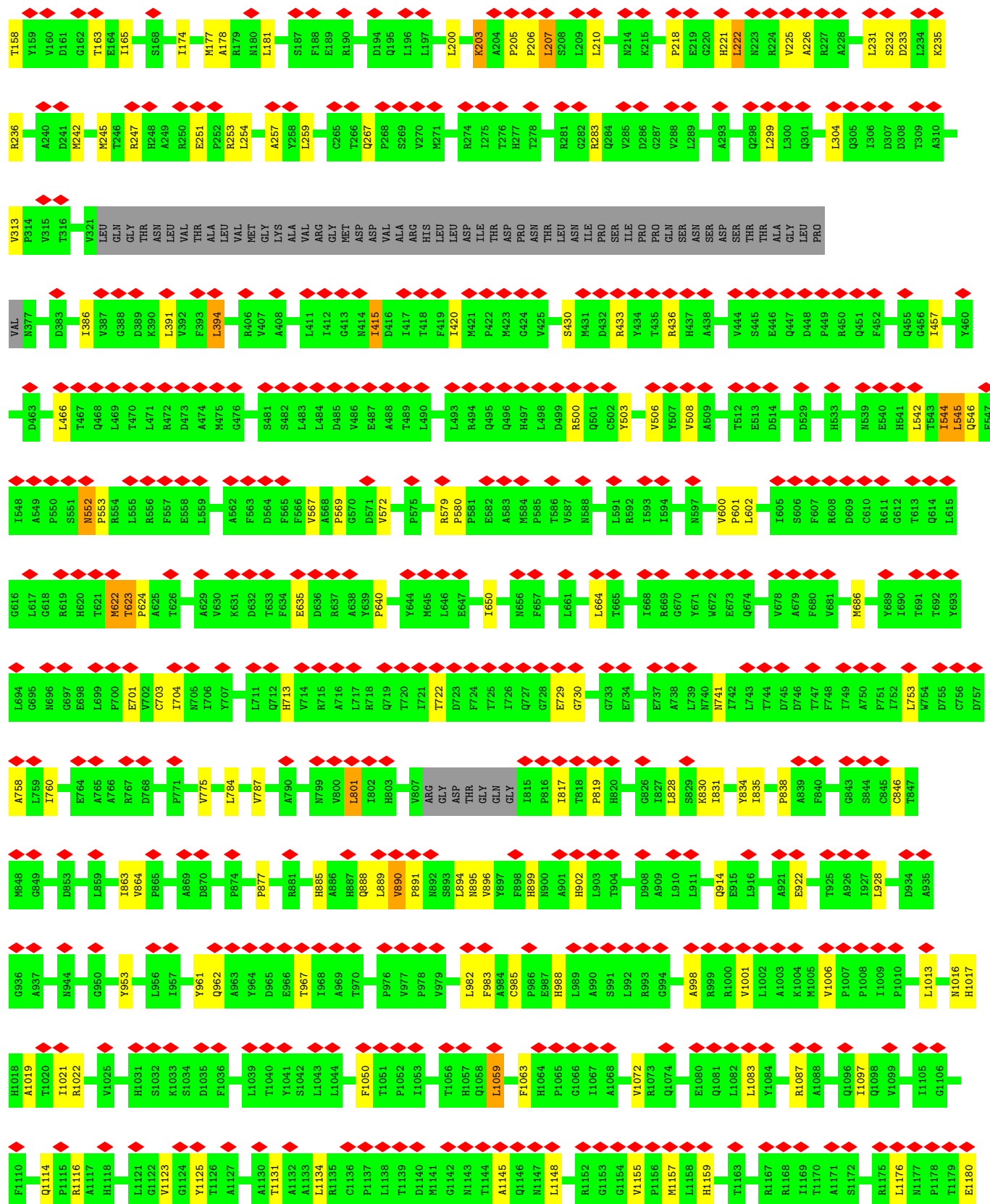
• Molecule 1: ORF40



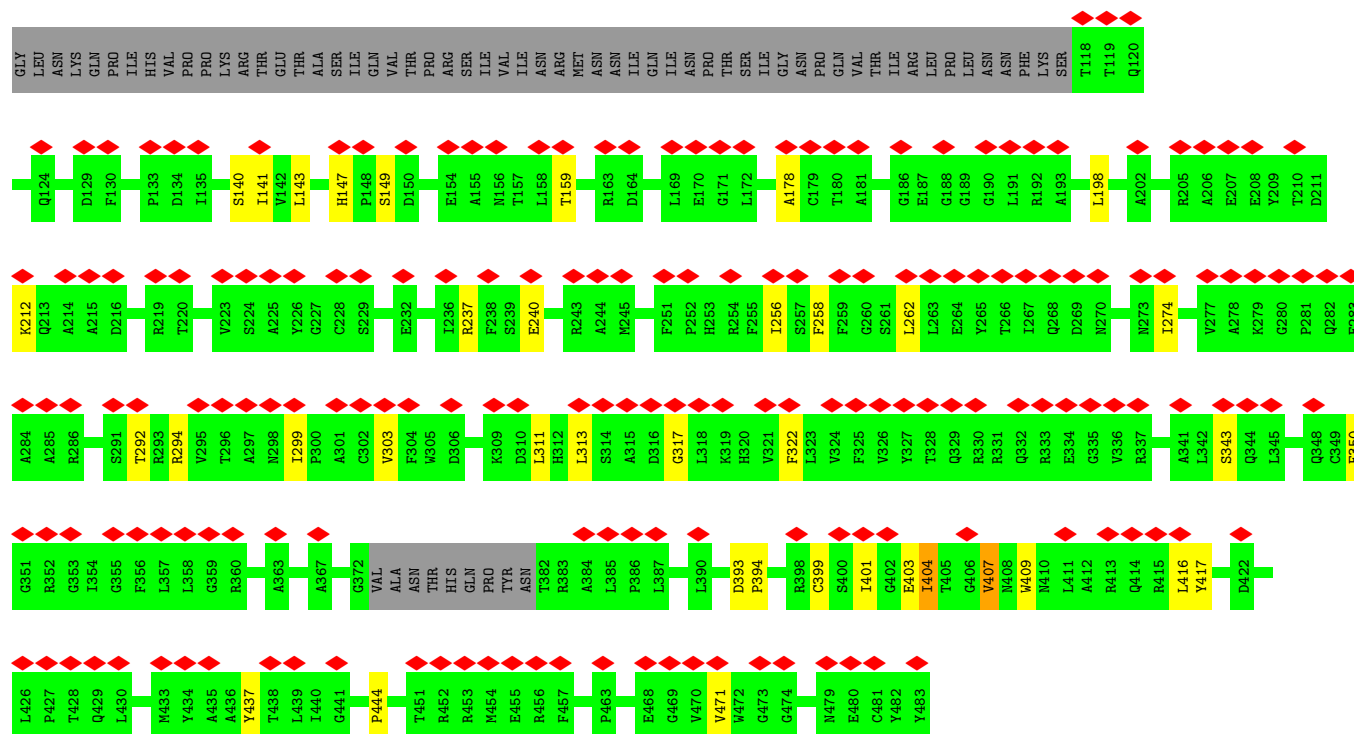


• Molecule 1: ORF40

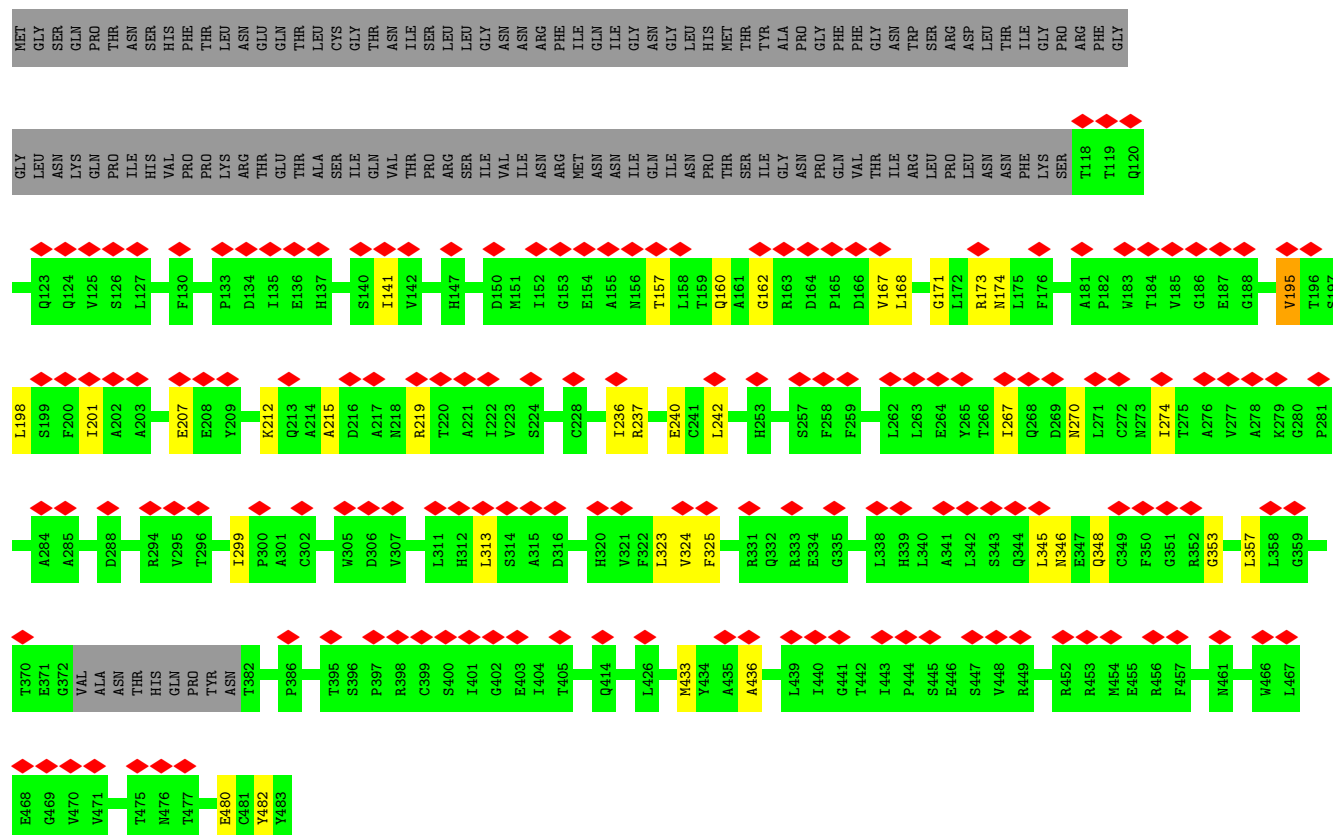




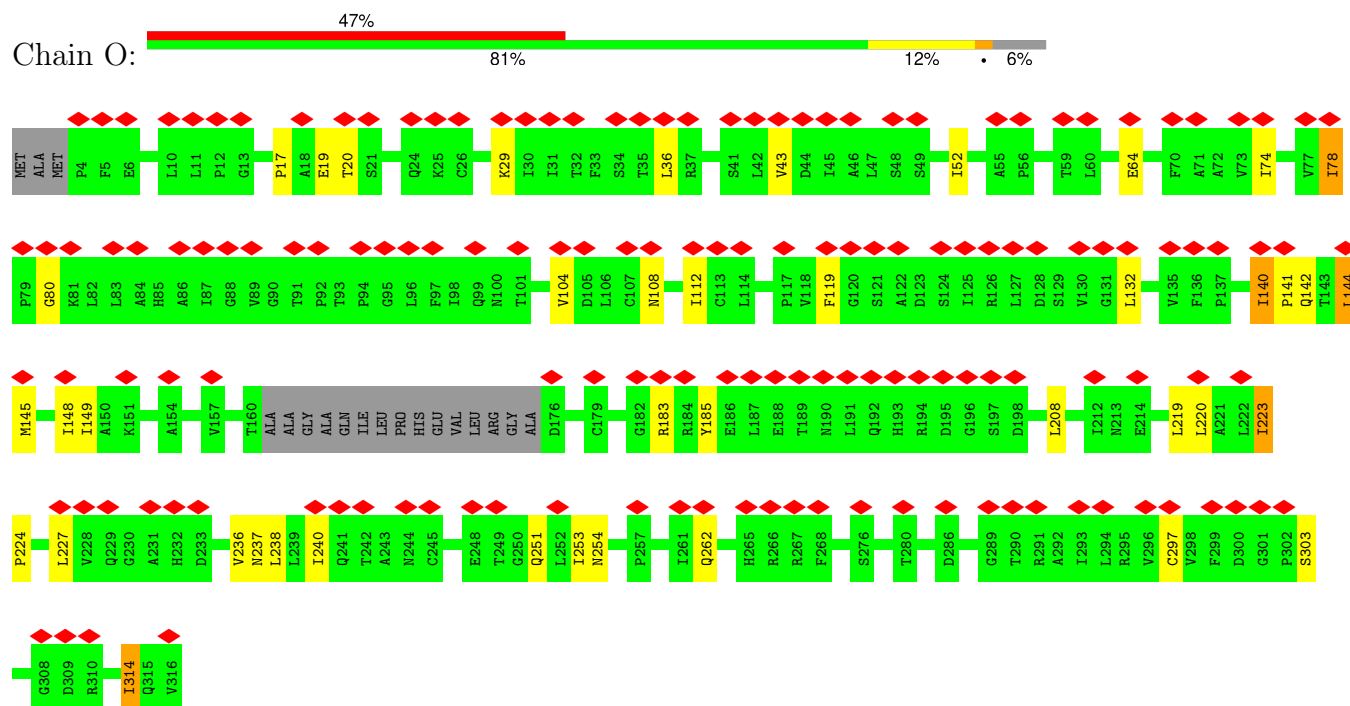
MET	GLY	SER	GLN	PRO	THR	ASN	SER	HIS	PHE	THR	LEU	ASN	GLN	THR	LEU	CYS	GLY	THR	ASN	SER	LEU	LEU	GLY	ASN	ASN	ARG	PHE	ILE	GLN	ILE	GLY	ASN	GLY	ALA	PRO	GLY	PHE	PHE	ASN	TRP	SER	ARG	ASP	LEU	THR	ILE	PRO	ARG	PHE	TYR
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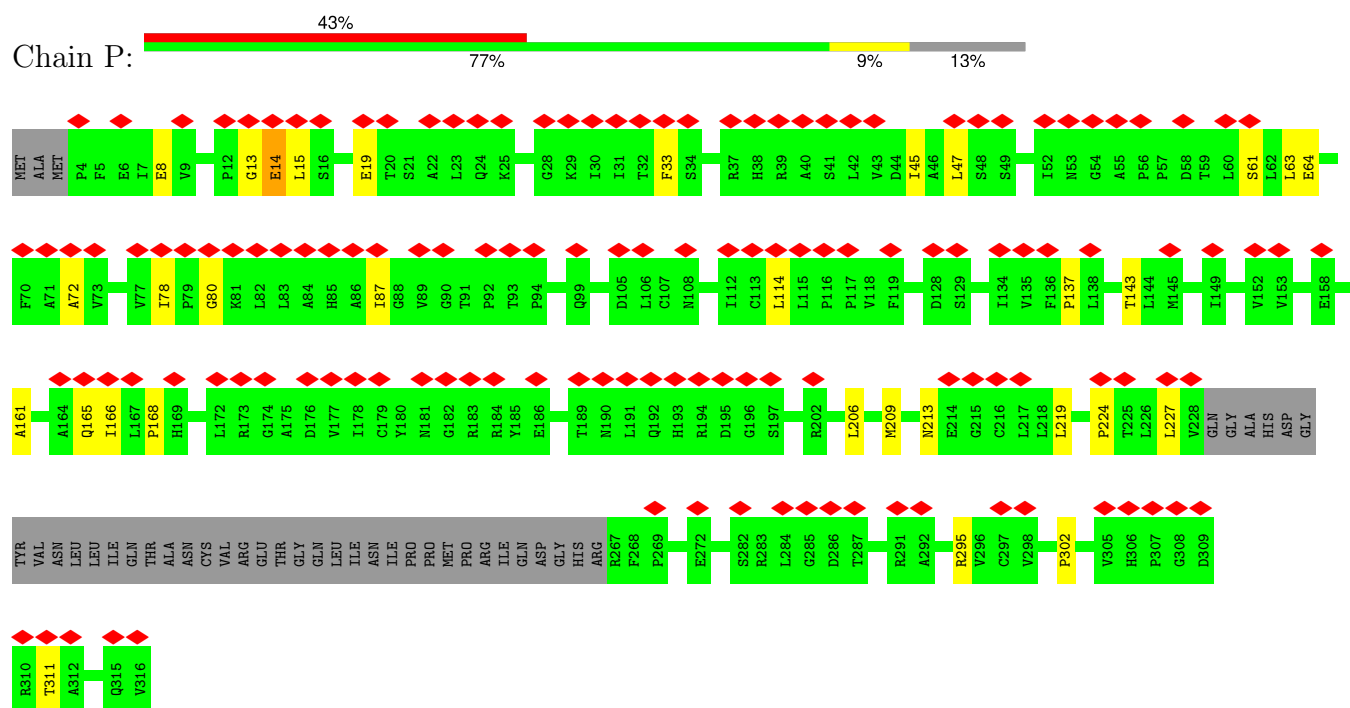
• Molecule 3: ORF20



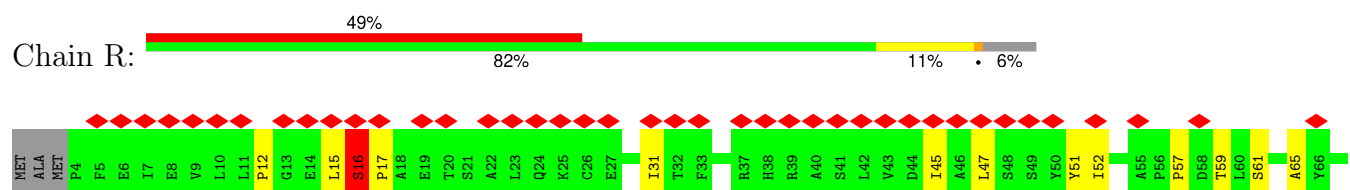
- Molecule 4: ORF41

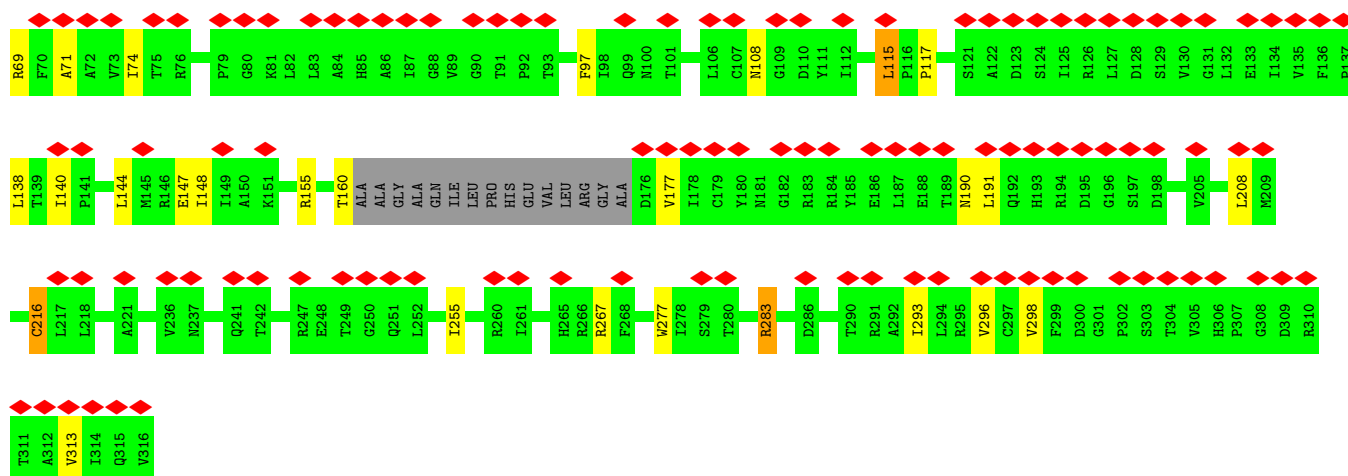


- Molecule 4: ORF41

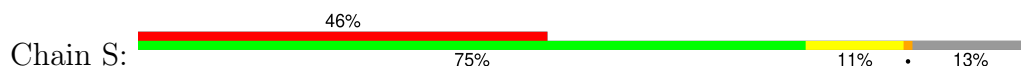


- Molecule 4: ORF41

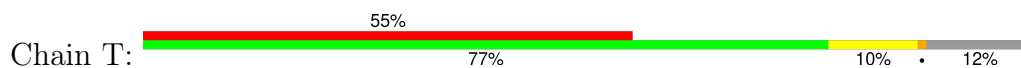




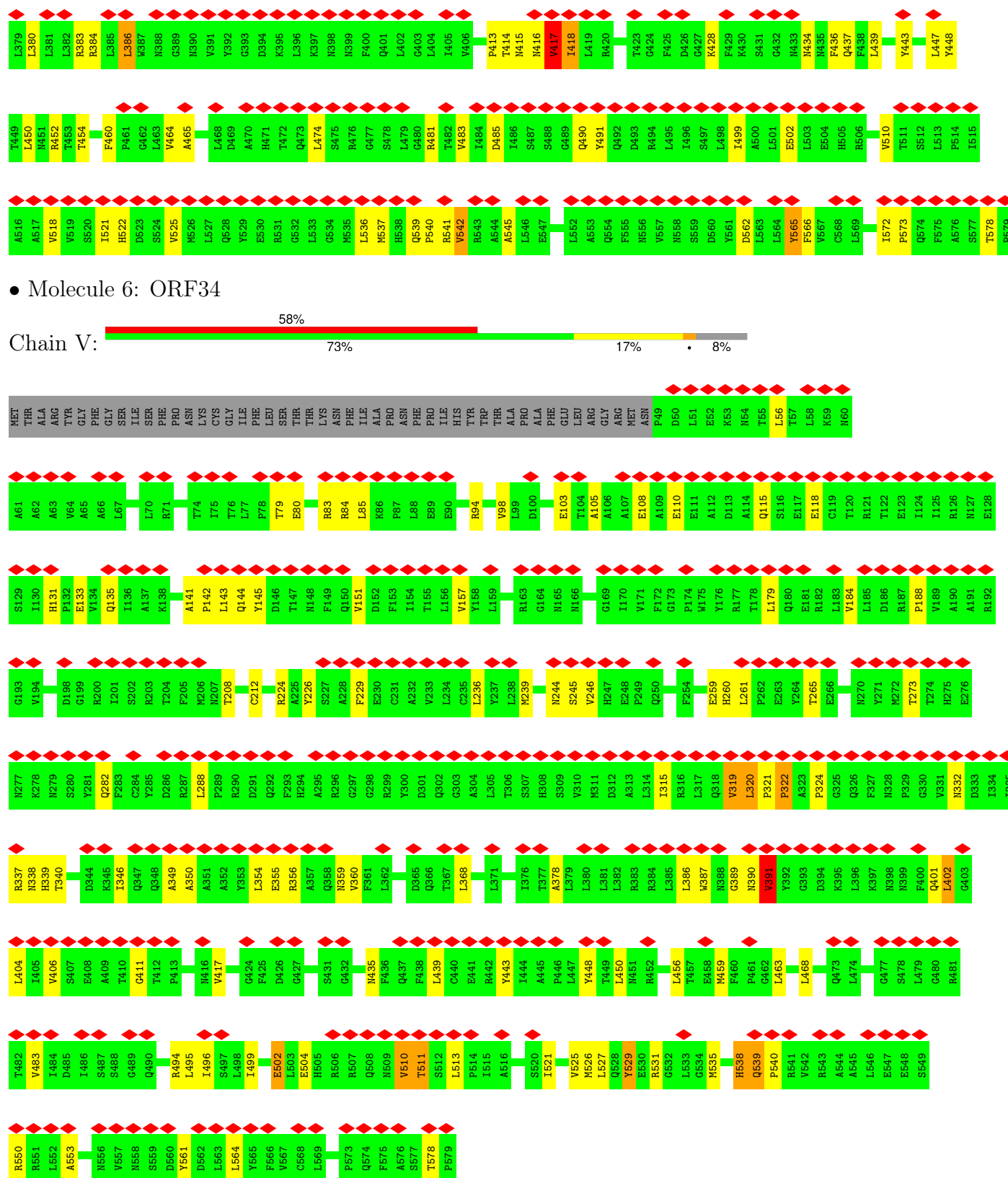
• Molecule 4: ORF41



• Molecule 5: ORF43







• Molecule 7: Large tegument protein deneddylase

Chain W: 98%









4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of subtomograms used	3804	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	82.3	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	14.690	Depositor
Minimum map value	-7.382	Depositor
Average map value	0.033	Depositor
Map value standard deviation	0.423	Depositor
Recommended contour level	1.05	Depositor
Map size (Å)	660.48, 660.48, 660.48	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.4399998, 3.4399998, 3.4399998	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.09	0/9259	0.23	0/12619
1	B	0.08	0/10530	0.22	0/14358
1	D	0.15	0/10493	0.25	0/14326
1	F	0.08	0/10575	0.21	0/14419
1	H	0.08	0/10059	0.21	0/13730
1	J	0.09	0/10085	0.24	0/13758
1	L	0.13	0/10430	0.26	2/14225 (0.0%)
2	C	0.09	0/741	0.23	0/1022
2	E	0.10	0/727	0.25	0/997
2	G	0.09	0/753	0.22	0/1036
2	I	0.09	0/759	0.23	0/1043
2	K	0.09	0/759	0.20	0/1043
2	M	0.10	0/738	0.25	0/1019
3	N	0.07	0/2829	0.20	0/3850
3	Q	0.08	0/2832	0.21	0/3854
4	O	0.08	0/2331	0.23	0/3178
4	P	0.09	0/2119	0.21	0/2892
4	R	0.08	0/2331	0.22	0/3178
4	S	0.08	0/2122	0.22	0/2896
5	T	0.08	0/4700	0.23	0/6406
6	U	0.11	0/4277	0.30	0/5806
6	V	0.15	0/4277	0.32	0/5806
7	W	0.06	0/361	0.12	0/484
7	X	0.07	0/361	0.15	0/484
All	All	0.10	0/104448	0.24	2/142429 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	1377	LEU	CA-C-N	-5.41	115.13	123.14
1	L	1377	LEU	C-N-CA	-5.41	115.13	123.14

There are no chirality outliers.

There are no planarity outliers.

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	9043	0	8818	81	0
1	B	10283	0	10047	73	0
1	D	10245	0	9938	83	0
1	F	10328	0	10090	71	0
1	H	9821	0	9535	71	0
1	J	9850	0	9593	101	0
1	L	10181	0	9923	103	0
2	C	724	0	696	2	0
2	E	712	0	706	7	0
2	G	736	0	718	5	0
2	I	742	0	729	4	0
2	K	742	0	729	10	0
2	M	721	0	687	4	0
3	N	2767	0	2675	22	0
3	Q	2770	0	2679	21	0
4	O	2288	0	2352	25	0
4	P	2080	0	2136	16	0
4	R	2288	0	2352	21	0
4	S	2083	0	2138	18	0
5	T	4593	0	4609	39	0
6	U	4200	0	4166	64	0
6	V	4200	0	4166	61	0
7	W	358	0	379	3	0
7	X	358	0	379	9	0
All	All	102113	0	100240	834	0

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

All (834) 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:J:898:PHE:O	1:J:902:HIS:HB3	1.66	0.96
1:J:737:GLU:O	1:J:741:ASN:HB2	1.69	0.93
1:B:25:ILE:HG13	1:B:26:PRO:HD3	1.59	0.85
1:D:602:LEU:HG	1:D:605:ILE:HD12	1.64	0.80
6:U:248:GLU:H	6:U:249:PRO:HD2	1.50	0.77
1:F:1243:ALA:O	1:F:1247:ASP:HB2	1.85	0.76
3:Q:353:GLY:O	3:Q:357:LEU:HB2	1.88	0.74
1:J:1006:VAL:HG23	1:J:1007:PRO:HD3	1.69	0.73
6:V:439:LEU:O	6:V:443:TYR:HB2	1.90	0.71
1:B:120:GLY:HA2	1:D:195:GLN:HB2	1.73	0.70
1:A:291:THR:HG21	1:A:295:LEU:HB2	1.74	0.69
1:H:1310:ARG:O	1:H:1314:GLU:HB2	1.92	0.69
1:J:640:PRO:HB2	1:J:643:PHE:HB2	1.74	0.69
1:B:543:THR:HA	1:B:546:GLN:HG2	1.76	0.68
6:V:389:GLY:HA3	6:V:435:ASN:HD22	1.58	0.68
5:T:557:ASN:H	5:T:629:GLN:HB3	1.58	0.68
1:A:299:LEU:HD12	1:A:304:LEU:HG	1.75	0.68
1:J:526:THR:O	1:J:530:MET:HB2	1.93	0.67
1:L:1123:VAL:HG13	1:L:1125:TYR:H	1.59	0.67
1:D:599:PRO:HB2	1:D:604:PRO:HD3	1.77	0.66
5:T:207:VAL:HG13	5:T:208:SER:H	1.61	0.66
3:N:292:THR:HG23	3:N:294:ARG:H	1.61	0.65
1:D:1241:ILE:HG23	1:D:1243:ALA:H	1.62	0.65
1:L:760:ILE:HG21	1:L:819:PRO:HG3	1.79	0.65
3:Q:160:GLN:HG2	3:Q:162:GLY:H	1.61	0.65
1:J:747:THR:HG21	1:J:931:SER:HB3	1.79	0.64
4:P:161:ALA:O	4:P:165:GLN:HB2	1.96	0.64
4:O:237:ASN:HA	4:O:240:ILE:HG12	1.80	0.64
1:J:237:ARG:O	1:J:241:ASP:HB3	1.98	0.63
6:V:495:LEU:HD12	6:V:525:VAL:HG22	1.80	0.63
5:T:41:LEU:HD23	5:T:45:LYS:HB3	1.80	0.63
1:J:712:GLN:HG3	1:L:635:GLU:HG2	1.81	0.63
2:K:96:VAL:HB	1:L:895:ASN:HB2	1.79	0.62
6:U:144:GLN:HE21	6:U:149:PHE:H	1.47	0.62
1:H:868:PRO:HB2	1:H:871:GLU:HB2	1.80	0.62
1:F:817:ILE:HG12	1:F:819:PRO:HD2	1.81	0.62
1:J:300:LEU:HA	1:J:304:LEU:HB2	1.80	0.62
1:J:710:LEU:HA	1:J:713:HIS:HD2	1.65	0.62
1:H:420:ILE:HG23	1:H:422:PRO:HD3	1.82	0.62
1:D:193:ALA:HA	1:D:196:LEU:HB3	1.81	0.62
6:U:183:LEU:HA	6:U:186:ASP:HB2	1.81	0.62
1:L:579:ARG:HH11	1:L:580:PRO:HD2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:663:LEU:HD12	1:J:909:ALA:HB1	1.81	0.61
1:D:611:ARG:HH12	1:D:1065:PRO:HA	1.63	0.61
6:U:413:PRO:HB3	6:U:417:VAL:HB	1.81	0.61
6:V:340:THR:HB	6:V:368:LEU:HB3	1.82	0.61
1:A:660:LEU:HD23	1:A:663:LEU:HD21	1.82	0.61
1:L:552:ASN:H	1:L:553:PRO:HD2	1.66	0.61
6:V:143:LEU:HB3	6:V:406:VAL:HG22	1.82	0.61
1:D:694:LEU:HD21	1:D:699:LEU:HD23	1.83	0.61
1:F:1142:GLY:HA3	1:F:1202:SER:H	1.66	0.61
1:A:139:ARG:HH22	1:A:141:LEU:HD12	1.66	0.60
1:B:526:THR:O	1:B:530:MET:HB2	2.01	0.60
1:D:898:PHE:O	1:D:902:HIS:HB3	2.01	0.60
6:U:277:ASN:HB2	6:U:386:LEU:HB2	1.83	0.60
3:N:299:ILE:HB	3:N:303:VAL:HG11	1.81	0.60
1:F:1104:ALA:HB2	1:F:1109:ASN:HB2	1.83	0.60
1:D:785:HIS:HD2	1:D:817:ILE:HG13	1.66	0.60
1:F:429:ASN:HD21	1:F:432:ASP:HB3	1.67	0.60
1:L:885:HIS:HA	1:L:888:GLN:HG3	1.83	0.60
1:D:846:CYS:HB2	1:D:988:HIS:HD2	1.66	0.60
4:R:31:ILE:HG12	4:R:74:ILE:HD11	1.84	0.59
1:H:1084:TYR:HB3	1:H:1128:VAL:HG23	1.83	0.59
6:U:125:ILE:HG23	6:U:224:ARG:HD3	1.85	0.59
1:H:415:ILE:HG22	1:H:1343:PRO:HG3	1.83	0.59
1:D:933:PRO:HG3	1:D:947:ILE:HG12	1.85	0.59
1:J:1086:GLU:HB2	1:J:1089:SER:HB2	1.84	0.59
6:U:172:PHE:HB2	6:U:176:TYR:HB2	1.84	0.59
1:L:760:ILE:HD11	1:L:817:ILE:HG23	1.85	0.59
1:L:1224:PRO:HG3	1:L:1348:GLN:HB3	1.85	0.59
1:J:205:PRO:HG2	1:J:1129:CYS:H	1.67	0.58
1:J:976:PRO:HD2	1:J:992:LEU:HD13	1.85	0.58
2:K:99:LYS:HE3	1:L:891:PRO:HB3	1.85	0.58
2:I:98:LEU:HD13	1:J:896:VAL:HG12	1.85	0.58
1:J:415:ILE:HG22	1:J:1077:PHE:H	1.68	0.58
3:Q:215:ALA:HB1	3:Q:219:ARG:HH21	1.67	0.58
6:V:332:ASN:HA	6:V:336:ASP:HB2	1.85	0.58
1:D:739:LEU:HD22	1:D:1050:PHE:HB2	1.86	0.58
1:L:299:LEU:HD13	1:L:394:LEU:HD11	1.86	0.58
1:H:471:LEU:HD21	1:H:1059:LEU:HB3	1.86	0.58
1:J:611:ARG:HH12	1:J:1042:SER:HA	1.69	0.58
4:O:220:LEU:HD13	4:O:253:ILE:HG12	1.86	0.58
1:A:423:MET:HE2	1:A:457:ILE:HG21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:VAL:HG13	1:A:601:PRO:HD3	1.86	0.58
6:U:173:GLY:HA2	6:U:573:PRO:HA	1.85	0.58
1:A:558:GLU:HA	1:A:565:PHE:HB2	1.86	0.58
1:B:640:PRO:HD2	1:B:643:PHE:HB2	1.85	0.58
1:J:1267:GLN:HE22	1:J:1270:SER:HB2	1.68	0.57
4:O:208:LEU:HB3	4:P:219:LEU:HD12	1.85	0.57
6:U:183:LEU:HD22	6:U:192:ARG:HB2	1.86	0.57
3:Q:207:GLU:HA	3:Q:212:LYS:HD3	1.86	0.57
1:D:882:HIS:HB3	1:D:885:HIS:HB2	1.87	0.57
4:S:35:THR:HB	4:S:40:ALA:HB2	1.85	0.57
1:D:1341:GLN:HG3	1:D:1343:PRO:HD3	1.86	0.57
1:J:99:LEU:HD13	1:J:1095:GLY:HA3	1.87	0.57
1:H:213:ILE:HD11	1:H:237:ARG:HG3	1.87	0.57
1:L:415:ILE:HG23	1:L:1343:PRO:HG3	1.87	0.57
1:B:115:MET:HG2	1:D:184:VAL:HG13	1.87	0.56
1:J:1152:ARG:HH12	1:J:1184:ILE:HD13	1.70	0.56
1:A:1374:GLU:HA	1:A:1381:LEU:HB2	1.86	0.56
1:B:601:PRO:HA	1:B:604:PRO:HG3	1.88	0.56
1:D:253:ARG:HH12	1:F:298:GLN:HG2	1.71	0.56
1:D:637:ARG:HA	1:D:960:ALA:HB1	1.86	0.56
1:J:1121:LEU:HD13	1:J:1123:VAL:HG12	1.87	0.56
1:J:734:GLU:HG2	1:J:738:ALA:H	1.71	0.56
4:R:115:LEU:HD21	4:R:140:ILE:HB	1.88	0.56
3:Q:433:MET:HA	3:Q:482:TYR:HB3	1.87	0.56
6:U:183:LEU:HB3	6:U:192:ARG:HD3	1.86	0.56
1:B:889:LEU:HD23	2:E:98:LEU:HB2	1.87	0.56
1:A:537:TRP:CD1	1:A:1022:ARG:HH21	2.23	0.56
1:J:1010:PRO:HG2	1:J:1013:LEU:HB2	1.88	0.56
4:R:65:ALA:HB1	4:R:69:ARG:HE	1.71	0.56
4:R:57:PRO:HG2	4:R:61:SER:HB3	1.87	0.56
6:U:98:VAL:HG11	7:X:7:LEU:HD22	1.87	0.56
1:B:431:MET:HB3	1:D:1360:ALA:HB2	1.88	0.55
1:D:1050:PHE:HB3	1:D:1053:ILE:HG22	1.88	0.55
1:D:1306:ASN:O	1:D:1310:ARG:HB2	2.05	0.55
4:O:145:MET:HA	4:O:148:ILE:HG12	1.87	0.55
1:D:720:THR:O	1:D:724:PHE:HB2	2.05	0.55
1:J:664:LEU:HD23	1:J:690:ILE:HD11	1.88	0.55
6:V:208:THR:HA	6:V:212:CYS:HB2	1.87	0.55
1:J:1180:GLU:H	1:J:1181:PRO:HD2	1.70	0.55
1:L:163:THR:HG23	1:L:165:ILE:H	1.71	0.55
3:Q:157:THR:HG23	4:R:267:ARG:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:494:ARG:HB3	6:V:521:ILE:HG23	1.88	0.55
5:T:409:ASP:HB2	7:W:42:LEU:HD13	1.88	0.55
1:H:560:ASN:H	1:H:565:PHE:HZ	1.54	0.55
4:R:59:THR:HG21	4:R:190:ASN:HD21	1.71	0.55
1:B:427:GLN:HE21	1:B:433:ARG:HE	1.55	0.55
1:B:210:LEU:HA	1:B:213:ILE:HG22	1.89	0.55
1:J:670:GLY:HA3	1:J:903:LEU:HD21	1.89	0.55
1:L:623:THR:HG23	1:L:624:PRO:HD3	1.88	0.55
1:H:1267:GLN:HB2	1:H:1270:SER:HB3	1.89	0.54
6:V:504:GLU:HG3	6:V:513:LEU:HD12	1.89	0.54
1:A:518:VAL:HG21	6:U:521:ILE:HG22	1.89	0.54
1:D:848:MET:HE3	1:D:988:HIS:HB3	1.87	0.54
6:V:103:GLU:HG3	7:X:5:LEU:HD13	1.88	0.54
1:J:662:ARG:HB2	2:K:101:THR:HG23	1.88	0.54
1:J:860:GLN:HE22	2:K:62:ALA:HB2	1.71	0.54
6:U:383:ARG:HH11	6:U:540:PRO:HD2	1.72	0.54
1:L:775:VAL:HG11	1:L:928:LEU:H	1.73	0.54
1:D:244:PHE:HA	1:D:247:ARG:HG2	1.88	0.54
1:F:469:LEU:HD21	1:F:1143:ASN:HD22	1.72	0.54
6:V:320:LEU:HB2	6:V:324:PRO:HG3	1.89	0.54
1:B:1223:ASN:HD21	1:B:1228:ALA:H	1.54	0.54
1:F:1178:PRO:HB2	1:F:1183:PRO:HD2	1.89	0.54
1:J:1198:ARG:H	1:L:218:PRO:HG3	1.73	0.54
1:J:1201:ALA:HB3	1:L:225:VAL:HB	1.90	0.54
1:A:203:LYS:HE2	1:A:1124:GLY:HA2	1.89	0.54
1:F:818:THR:HG23	1:F:819:PRO:HD3	1.90	0.54
1:B:599:PRO:HB2	1:B:602:LEU:HD23	1.90	0.53
1:F:90:ALA:HB1	1:F:1087:ARG:HA	1.89	0.53
1:H:1291:PRO:HA	1:H:1294:LYS:HG2	1.89	0.53
4:O:78:ILE:HG23	4:O:80:GLY:H	1.73	0.53
5:T:146:GLU:HG3	5:T:361:ARG:HH21	1.73	0.53
1:D:793:ASN:HD21	1:D:795:GLN:HB2	1.74	0.53
1:L:500:ARG:HB3	1:L:567:VAL:HG11	1.90	0.53
6:V:439:LEU:O	6:V:443:TYR:CB	2.55	0.53
6:U:450:LEU:HB3	6:V:417:VAL:HA	1.90	0.53
1:B:726:ILE:HG21	1:B:1060:ARG:HE	1.73	0.53
1:D:475:MET:HA	1:D:1059:LEU:HG	1.90	0.53
1:A:519:GLN:HE22	1:A:1012:PHE:HD2	1.54	0.53
1:H:330:ALA:HA	1:H:334:GLY:H	1.74	0.53
2:I:93:ARG:HB3	1:J:857:PRO:HG2	1.91	0.53
1:H:427:GLN:HE21	1:H:433:ARG:HE	1.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:251:GLU:HB3	1:L:254:LEU:HB2	1.91	0.53
1:B:872:GLU:HG2	1:B:874:PRO:HD3	1.91	0.53
1:H:916:LEU:HD11	1:H:919:ASP:HB2	1.90	0.53
1:J:152:LEU:O	1:J:156:SER:HB2	2.09	0.53
6:V:321:PRO:HB2	6:V:322:PRO:HD3	1.90	0.53
1:A:637:ARG:HA	1:A:959:MET:HE1	1.90	0.53
4:O:29:LYS:HB3	4:O:74:ILE:HD12	1.90	0.53
1:F:833:TYR:HA	1:F:837:ILE:HD12	1.91	0.52
1:L:982:LEU:HD21	1:L:1022:ARG:HB2	1.89	0.52
6:U:248:GLU:H	6:U:249:PRO:CD	2.18	0.52
2:E:85:GLU:HA	2:E:90:THR:HG21	1.91	0.52
1:L:205:PRO:HD2	1:L:207:LEU:HD23	1.90	0.52
1:L:1157:MET:H	1:L:1159:HIS:HD2	1.56	0.52
6:U:63:ALA:HB2	7:X:44:LEU:HD21	1.91	0.52
1:D:892:ASN:H	2:G:98:LEU:HD13	1.74	0.52
1:F:1285:ALA:HB1	1:F:1331:LYS:HG3	1.92	0.52
4:O:140:ILE:HD11	4:O:144:LEU:HB2	1.90	0.52
5:T:478:GLN:HA	5:T:640:GLY:HA3	1.90	0.52
1:J:1241:ILE:HD12	1:J:1244:ILE:HD12	1.91	0.52
1:J:506:VAL:HA	1:J:1015:ALA:HB2	1.90	0.52
1:L:1301:VAL:HG23	1:L:1310:ARG:HH12	1.74	0.52
6:U:316:ARG:HG3	6:U:317:LEU:HD12	1.91	0.52
1:L:729:GLU:HG2	1:L:730:GLY:H	1.73	0.52
3:N:404:ILE:HG21	4:O:227:LEU:HD21	1.91	0.52
1:J:425:VAL:HG13	1:J:1215:LEU:HD21	1.92	0.52
4:S:75:THR:HG22	4:S:76:ARG:H	1.74	0.52
1:L:245:MET:HE2	1:L:259:LEU:HD22	1.91	0.52
1:D:427:GLN:HB3	1:D:432:ASP:HB3	1.92	0.52
1:H:1323:SER:HB2	1:H:1329:GLN:HA	1.91	0.52
5:T:358:ILE:HG22	5:T:360:PRO:HD3	1.92	0.52
1:D:508:VAL:HA	1:D:1011:PRO:HB2	1.92	0.52
1:J:1194:ALA:HB3	1:J:1198:ARG:HD2	1.90	0.52
2:K:10:VAL:HG11	2:K:36:LEU:HB3	1.92	0.52
4:R:208:LEU:HD22	4:S:219:LEU:HB3	1.91	0.51
1:H:905:VAL:HG11	1:H:909:ALA:H	1.75	0.51
5:T:467:ILE:HG13	5:T:503:ILE:HD12	1.92	0.51
6:U:384:ARG:HH21	6:U:540:PRO:HG2	1.74	0.51
6:V:244:ASN:HD22	6:V:245:SER:H	1.58	0.51
1:D:683:ASN:HB2	1:D:686:MET:HB2	1.92	0.51
1:D:687:LEU:HD23	1:D:690:ILE:HD11	1.92	0.51
1:L:1013:LEU:HD23	1:L:1022:ARG:HH12	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:224:PRO:HB2	4:P:227:LEU:HB2	1.92	0.51
1:L:1184:ILE:HG22	1:L:1185:PHE:H	1.76	0.51
1:J:766:ALA:HB1	1:J:769:ARG:HB2	1.92	0.51
1:L:542:LEU:HD22	1:L:546:GLN:HB3	1.93	0.51
4:P:72:ALA:HB1	4:P:87:ILE:HD13	1.91	0.51
6:V:401:GLN:HG3	6:V:404:LEU:HG	1.92	0.51
1:H:237:ARG:O	1:H:241:ASP:CB	2.59	0.51
6:V:282:GLN:HG2	6:V:539:GLN:HE21	1.76	0.51
1:B:538:VAL:HG21	1:B:1006:VAL:HG12	1.92	0.51
5:T:153:ARG:HB2	5:T:358:ILE:HB	1.91	0.51
6:U:292:GLN:HB2	6:U:354:LEU:HB3	1.92	0.51
1:D:978:PRO:HB3	1:D:1010:PRO:HG3	1.93	0.51
1:J:1341:GLN:HG3	1:J:1343:PRO:HD3	1.93	0.51
6:V:229:PHE:HB3	6:V:448:TYR:HB2	1.92	0.51
1:A:833:TYR:HA	1:A:837:ILE:HD13	1.92	0.51
4:O:297:CYS:HB3	4:O:314:ILE:HG21	1.92	0.51
4:R:155:ARG:HB3	4:R:191:LEU:HD11	1.92	0.51
1:H:1333:PRO:HG2	1:H:1336:SER:HB3	1.93	0.50
1:F:210:LEU:HD12	1:F:213:ILE:HD12	1.93	0.50
2:G:22:GLU:HG3	2:G:67:ARG:HH11	1.77	0.50
1:L:899:HIS:HA	1:L:902:HIS:HD2	1.76	0.50
4:O:262:GLN:HB3	5:T:6:ALA:HA	1.94	0.50
4:S:11:LEU:HD13	4:S:82:LEU:HD13	1.93	0.50
1:D:1021:ILE:HG22	1:D:1025:VAL:HG23	1.93	0.50
1:H:1147:ASN:HB3	1:H:1150:PHE:HB3	1.93	0.50
1:J:1210:PRO:HG3	1:J:1262:ASN:HB3	1.92	0.50
1:B:299:LEU:HD12	1:B:304:LEU:HD23	1.93	0.50
4:S:211:SER:HG	4:S:277:TRP:CD1	2.27	0.50
1:B:80:VAL:HG11	1:B:401:VAL:HA	1.92	0.50
1:B:561:PRO:HG3	1:B:1264:TRP:HD1	1.76	0.50
1:F:235:LYS:HG3	1:F:236:ARG:N	2.26	0.50
3:Q:433:MET:HG3	3:Q:480:GLU:HB3	1.93	0.50
6:U:378:ALA:HA	6:U:474:LEU:HD12	1.92	0.50
1:B:535:PRO:HB2	1:B:538:VAL:HG22	1.94	0.50
2:C:50:ILE:HB	2:C:54:ARG:HB2	1.92	0.50
1:H:683:ASN:HB3	1:H:686:MET:HG2	1.93	0.50
1:J:1012:PHE:HD1	1:J:1013:LEU:HD23	1.75	0.50
1:A:186:ASP:HA	1:A:189:GLU:CD	2.37	0.50
1:B:890:VAL:HG23	2:E:97:GLY:HA3	1.93	0.50
1:F:874:PRO:HB2	1:F:882:HIS:HD2	1.76	0.50
1:J:603:CYS:HB2	1:J:607:PHE:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:223:ILE:HG13	4:O:224:PRO:HD3	1.94	0.50
3:N:322:PHE:HD2	3:N:437:TYR:HB2	1.77	0.50
4:O:219:LEU:HB3	4:P:213:ASN:HD21	1.76	0.50
3:Q:480:GLU:H	4:R:283:ARG:HH22	1.60	0.50
6:V:224:ARG:HH22	6:V:350:ALA:HB1	1.76	0.50
1:A:190:ARG:HD2	1:A:401:VAL:HA	1.93	0.49
1:A:421:MET:HE3	1:A:1355:CYS:HB3	1.94	0.49
1:D:491:VAL:HG22	1:D:495:GLN:HE22	1.76	0.49
1:H:526:THR:O	1:H:530:MET:HB3	2.12	0.49
1:H:746:ASP:HB3	1:H:762:ARG:HE	1.76	0.49
1:A:859:LEU:HG	1:A:917:MET:HE1	1.94	0.49
1:F:841:SER:HB2	1:F:844:SER:HB3	1.94	0.49
1:L:242:MET:HE1	1:L:1388:LEU:HB2	1.94	0.49
1:L:1013:LEU:HG	1:L:1016:ASN:HB2	1.93	0.49
6:V:236:LEU:HA	6:V:239:MET:HG2	1.94	0.49
1:A:842:ARG:HG3	1:A:1039:LEU:HD11	1.94	0.49
1:B:867:ILE:HD12	1:B:873:ALA:HB2	1.93	0.49
1:H:1223:ASN:HD21	1:H:1348:GLN:HB3	1.77	0.49
1:L:877:PRO:HG3	1:L:899:HIS:HB3	1.95	0.49
6:V:105:ALA:O	6:V:108:GLU:HG3	2.13	0.49
1:D:674:GLN:HG2	1:F:698:GLU:HG3	1.94	0.49
1:L:701:GLU:HA	1:L:704:ILE:HG12	1.94	0.49
6:V:94:ARG:HH11	6:V:98:VAL:HG21	1.77	0.49
3:Q:346:ASN:HD21	3:Q:348:GLN:HB3	1.78	0.49
4:R:144:LEU:O	4:R:147:GLU:HG3	2.13	0.49
4:S:42:LEU:HD13	4:S:45:ILE:HD13	1.94	0.49
6:V:80:GLU:HA	6:V:83:ARG:HD3	1.93	0.49
1:A:526:THR:O	1:A:530:MET:HB2	2.13	0.49
1:B:542:LEU:HD12	1:D:1060:ARG:HE	1.76	0.49
1:F:1068:ALA:HB2	1:F:1211:VAL:HA	1.94	0.49
1:H:555:LEU:HD23	1:H:1248:HIS:HB3	1.95	0.49
3:N:393:ASP:HB2	3:N:394:PRO:HD3	1.94	0.49
6:V:526:MET:HA	6:V:529:TYR:HD1	1.78	0.49
1:F:665:THR:HG21	1:F:694:LEU:HD13	1.95	0.49
3:Q:195:VAL:HG11	3:Q:274:ILE:HG21	1.94	0.49
5:T:482:TYR:HE2	5:T:640:GLY:H	1.59	0.49
6:V:338:ASN:HB2	6:V:456:LEU:HD23	1.94	0.49
1:H:960:ALA:HA	1:H:987:GLU:HG3	1.95	0.49
1:L:569:PRO:HG2	1:L:572:VAL:HG21	1.93	0.49
3:N:317:GLY:HA2	4:O:36:LEU:HB3	1.95	0.49
1:D:454:PRO:HG3	1:D:1379:GLN:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:488:ALA:HB3	1:D:1274:ARG:HH22	1.77	0.49
1:J:741:ASN:HD22	1:J:744:THR:HB	1.78	0.49
4:O:17:PRO:HA	4:O:20:THR:HB	1.95	0.49
5:T:358:ILE:HG23	5:T:371:ILE:HG13	1.94	0.49
1:H:270:VAL:HG12	1:H:1123:VAL:HG13	1.95	0.48
1:L:801:LEU:HD13	1:L:922:GLU:HG3	1.95	0.48
4:R:71:ALA:HB2	4:R:293:ILE:HD12	1.94	0.48
1:A:990:ALA:HB1	1:A:1000:ARG:HE	1.78	0.48
1:D:333:MET:HE2	1:D:335:LYS:HD2	1.95	0.48
5:T:81:LEU:HD23	5:T:84:LEU:HD21	1.96	0.48
6:U:450:LEU:H	6:V:417:VAL:HG12	1.78	0.48
1:A:938:ALA:HA	1:A:943:ARG:HH21	1.78	0.48
1:H:536:HIS:HA	1:H:539:ASN:HD21	1.78	0.48
1:B:477:THR:HG21	1:B:1148:LEU:HB3	1.94	0.48
1:F:981:PRO:HB3	1:F:1009:ILE:HG22	1.95	0.48
1:H:465:ILE:HG22	1:J:1220:THR:HB	1.95	0.48
1:L:1214:ASP:HB3	1:L:1217:TYR:HB3	1.94	0.48
3:N:399:CYS:HB3	3:N:403:GLU:HB2	1.95	0.48
6:U:229:PHE:HD2	6:U:464:VAL:HG13	1.77	0.48
6:V:378:ALA:HB2	6:V:463:LEU:HD22	1.94	0.48
1:A:210:LEU:HD12	1:A:213:ILE:HD13	1.94	0.48
1:A:409:TYR:HB3	1:A:412:ILE:HG13	1.96	0.48
1:D:1289:TYR:HB3	1:D:1291:PRO:HD2	1.95	0.48
1:D:1081:GLN:HG2	1:D:1131:THR:HB	1.96	0.48
1:J:141:LEU:HD21	1:J:188:PHE:HZ	1.78	0.48
1:J:1361:MET:HE3	1:J:1379:GLN:HB3	1.95	0.48
4:O:142:GLN:HA	4:O:145:MET:HB3	1.96	0.48
4:S:11:LEU:HB2	4:S:82:LEU:HD22	1.95	0.48
1:H:541:HIS:HD2	1:H:542:LEU:HD23	1.79	0.48
1:L:962:GLN:HE21	1:L:967:THR:HB	1.78	0.48
3:N:147:HIS:HD2	3:N:149:SER:HB2	1.78	0.48
5:T:190:VAL:HA	5:T:193:MET:HE2	1.96	0.48
6:U:447:LEU:HD12	6:U:448:TYR:HB2	1.96	0.48
1:F:460:TYR:HB3	1:F:464:GLY:HA2	1.95	0.48
6:U:452:ARG:HE	6:V:141:ALA:HB2	1.79	0.48
1:D:174:ILE:O	1:D:177:MET:HG3	2.14	0.48
1:L:889:LEU:HG	1:L:890:VAL:H	1.79	0.48
3:N:258:PHE:HB3	4:P:295:ARG:HH22	1.79	0.48
4:R:108:ASN:HD21	4:R:298:VAL:HG22	1.79	0.48
6:U:56:LEU:HD13	6:V:56:LEU:HD11	1.95	0.48
1:B:675:SER:HB2	1:B:677:ARG:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:648:ALA:HB2	1:D:956:LEU:HD21	1.96	0.48
1:J:556:ARG:HD2	1:J:1248:HIS:HD2	1.79	0.48
4:S:100:ASN:HB3	4:S:307:PRO:HA	1.95	0.48
5:T:182:ILE:HA	5:T:185:TYR:HD1	1.78	0.48
1:A:205:PRO:HD2	1:A:1127:ALA:HB3	1.95	0.47
4:O:104:VAL:HG12	4:O:183:ARG:HH12	1.79	0.47
1:F:1049:LYS:HB3	1:F:1051:THR:HG22	1.95	0.47
3:N:143:LEU:HD23	3:N:256:ILE:HG21	1.96	0.47
1:A:1094:VAL:HG23	1:A:1116:ARG:HE	1.80	0.47
1:H:741:ASN:HD22	1:H:744:THR:HG23	1.79	0.47
1:J:650:ILE:HA	1:J:653:ASN:HB2	1.96	0.47
2:M:87:ASP:HB3	2:M:90:THR:HG22	1.96	0.47
4:O:29:LYS:HD2	4:O:29:LYS:HA	1.71	0.47
1:D:155:LEU:HD13	1:D:158:THR:HG21	1.95	0.47
1:D:702:VAL:HG23	1:D:703:CYS:H	1.80	0.47
1:F:174:ILE:HA	1:F:177:MET:HG2	1.97	0.47
1:H:144:ALA:HB3	1:J:124:VAL:HG21	1.96	0.47
1:J:889:LEU:O	1:J:890:VAL:HG22	2.15	0.47
1:J:1182:LEU:HD13	1:J:1188:LEU:HD13	1.95	0.47
6:V:320:LEU:HD22	6:V:320:LEU:HA	1.75	0.47
1:A:1051:THR:O	1:A:1055:LEU:HB2	2.15	0.47
1:A:1218:PHE:HA	1:A:1222:CYS:HB3	1.96	0.47
1:B:664:LEU:HD22	1:B:690:ILE:HD11	1.96	0.47
1:L:200:LEU:HD11	1:L:1083:LEU:HB2	1.96	0.47
1:A:747:THR:HA	1:A:762:ARG:HG3	1.96	0.47
1:B:117:ALA:HB3	1:D:188:PHE:HA	1.95	0.47
1:L:1145:ALA:HB3	1:L:1176:LEU:HD21	1.97	0.47
6:V:115:GLN:O	6:V:118:GLU:HG3	2.15	0.47
1:B:630:VAL:HG13	1:B:840:PHE:HE1	1.79	0.47
1:F:857:PRO:HB2	2:G:54:ARG:HD2	1.97	0.47
1:F:865:PRO:HG3	1:F:883:PRO:HG3	1.95	0.47
1:H:952:LEU:HD21	1:H:955:GLY:HA3	1.96	0.47
1:J:442:SER:HB3	1:L:436:ARG:HB2	1.97	0.47
1:J:1147:ASN:HD21	1:J:1330:PHE:HE1	1.63	0.47
3:N:262:LEU:H	3:N:262:LEU:HD23	1.80	0.47
3:N:407:VAL:HG13	3:N:409:TRP:H	1.78	0.47
3:Q:141:ILE:H	3:Q:299:ILE:HD11	1.80	0.47
3:Q:173:ARG:HA	3:Q:173:ARG:HD2	1.71	0.47
4:R:216:CYS:SG	4:S:213:ASN:HA	2.55	0.47
6:U:415:ASN:HB3	6:U:436:PHE:HE1	1.80	0.47
6:U:439:LEU:O	6:U:443:TYR:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:499:ILE:O	6:U:502:GLU:HG3	2.14	0.47
6:V:226:TYR:HB2	6:V:337:ARG:HB3	1.96	0.47
6:V:456:LEU:HA	6:V:459:MET:HB2	1.97	0.47
6:V:550:ARG:HG2	6:V:553:ALA:HB2	1.96	0.47
1:B:457:ILE:HD11	1:B:1355:CYS:HB2	1.95	0.47
4:O:112:ILE:HA	4:O:141:PRO:HB3	1.97	0.47
6:V:531:ARG:HB3	6:V:535:MET:HE2	1.97	0.47
1:A:630:VAL:HA	1:A:633:THR:HG22	1.95	0.47
1:B:890:VAL:HG21	2:E:95:THR:HG22	1.95	0.47
1:L:283:ARG:HD2	1:L:391:LEU:HD22	1.96	0.47
6:U:51:LEU:HA	6:U:54:ASN:HD21	1.80	0.47
6:U:562:ASP:HA	6:U:565:TYR:HD1	1.80	0.47
1:A:545:LEU:HD13	1:A:548:ILE:HD11	1.96	0.47
1:B:421:MET:HE3	1:B:457:ILE:HG12	1.95	0.47
1:D:497:HIS:HE1	1:D:585:PRO:HG2	1.78	0.47
1:H:508:VAL:HG13	1:H:1014:GLY:HA3	1.97	0.47
4:R:97:PHE:HD1	4:R:313:VAL:H	1.63	0.47
1:B:227:ARG:HD3	1:B:1307:THR:HG21	1.96	0.46
1:H:863:ILE:HD11	2:I:30:VAL:HG11	1.97	0.46
6:U:239:MET:HG3	6:U:286:ASP:HB3	1.98	0.46
6:V:468:LEU:HD22	6:V:495:LEU:HD11	1.97	0.46
1:A:939:THR:HB	1:A:1157:MET:HE1	1.96	0.46
1:J:209:LEU:HB3	1:J:234:LEU:HD22	1.96	0.46
1:J:978:PRO:HD3	1:J:989:LEU:HD21	1.95	0.46
1:F:831:ILE:HG23	1:F:835:ILE:HD12	1.97	0.46
4:P:15:LEU:O	4:P:19:GLU:HB2	2.16	0.46
6:U:416:ASN:C	6:U:418:ILE:H	2.23	0.46
1:J:862:VAL:HB	1:J:917:MET:HE1	1.97	0.46
1:L:500:ARG:HH12	1:L:553:PRO:HB3	1.80	0.46
1:A:1036:PHE:HA	1:A:1039:LEU:HB2	1.97	0.46
1:D:961:TYR:HB2	1:D:988:HIS:CE1	2.50	0.46
1:F:526:THR:O	1:F:530:MET:CB	2.64	0.46
1:F:1159:HIS:HB3	1:F:1162:VAL:HG22	1.96	0.46
1:J:1366:HIS:HB2	1:L:1373:ASP:HB2	1.97	0.46
3:N:262:LEU:HD12	3:N:274:ILE:HG21	1.96	0.46
5:T:230:ARG:O	5:T:233:GLU:HG3	2.15	0.46
1:D:889:LEU:O	1:D:890:VAL:HG22	2.16	0.46
1:L:650:ILE:HG12	1:L:686:MET:HE3	1.97	0.46
3:Q:195:VAL:HG21	3:Q:274:ILE:HG13	1.97	0.46
1:A:1300:GLU:HA	1:A:1303:THR:HG22	1.98	0.46
1:B:411:LEU:HD21	1:B:1081:GLN:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:917:MET:HA	1:B:920:MET:HE3	1.97	0.46
1:F:503:TYR:HE1	1:F:567:VAL:HB	1.80	0.46
1:F:1081:GLN:HA	1:F:1131:THR:HG21	1.98	0.46
6:U:147:THR:HG21	6:U:166:ASN:HB3	1.97	0.46
6:V:386:LEU:HD22	6:V:443:TYR:HE2	1.81	0.46
1:B:434:TYR:HE2	1:D:1377:LEU:HD13	1.81	0.46
1:F:830:LYS:O	1:F:834:TYR:HB2	2.15	0.46
1:H:202:GLU:HB2	1:H:1316:LYS:HA	1.97	0.46
1:H:600:VAL:N	1:H:601:PRO:HD3	2.31	0.46
1:J:1199:GLY:H	1:L:226:ALA:HB1	1.80	0.46
1:L:267:GLN:HE21	1:L:1125:TYR:HB3	1.79	0.46
4:P:13:GLY:O	4:P:14:GLU:HG3	2.16	0.46
6:V:261:LEU:O	6:V:265:THR:HB	2.16	0.46
1:D:846:CYS:HB2	1:D:988:HIS:CD2	2.50	0.46
1:F:80:VAL:HA	1:F:84:GLU:HG2	1.98	0.46
1:F:1167:ARG:HE	1:F:1182:LEU:HD21	1.79	0.46
1:J:757:ASP:HA	1:J:760:ILE:HD12	1.98	0.46
1:L:174:ILE:HA	1:L:177:MET:HG2	1.98	0.46
1:L:1180:GLU:HG3	1:L:1181:PRO:HD3	1.98	0.46
1:A:972:THR:HG23	6:U:536:LEU:HD11	1.98	0.46
1:D:1161:ASN:O	1:D:1164:GLU:HG3	2.16	0.46
1:L:753:LEU:HB2	1:L:953:TYR:HE1	1.81	0.46
1:B:548:ILE:HA	1:B:1259:ALA:HB2	1.98	0.45
1:B:989:LEU:HB3	1:B:995:MET:HE1	1.97	0.45
5:T:80:ALA:HA	5:T:83:ASN:HD21	1.81	0.45
1:F:787:VAL:HG11	1:F:796:ARG:HH12	1.81	0.45
1:F:805:ARG:HA	1:F:818:THR:HG21	1.97	0.45
1:H:692:THR:HG21	1:J:964:TYR:HB2	1.98	0.45
6:U:170:ILE:HG23	6:U:465:ALA:HB1	1.99	0.45
6:U:177:ARG:HH21	6:U:578:THR:HB	1.81	0.45
6:V:83:ARG:HE	6:V:84:ARG:HH12	1.64	0.45
1:A:799:ASN:H	1:A:925:THR:HG21	1.81	0.45
1:B:248:HIS:CD2	1:B:250:ARG:H	2.34	0.45
1:D:1250:GLN:CD	1:D:1251:SER:H	2.24	0.45
1:F:1332:ARG:HH21	3:Q:270:ASN:HD21	1.63	0.45
1:H:865:PRO:HB3	1:H:883:PRO:HG3	1.99	0.45
1:J:583:ALA:HB2	5:T:575:LEU:HD22	1.99	0.45
1:J:846:CYS:HB2	1:J:985:CYS:HB3	1.74	0.45
3:N:140:SER:HA	3:N:198:LEU:HD22	1.99	0.45
4:P:295:ARG:HA	4:P:295:ARG:HD2	1.74	0.45
4:S:10:LEU:HD23	4:S:39:ARG:HH21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:85:LEU:HD13	7:X:23:ARG:HG2	1.99	0.45
1:H:1140:ASP:HB2	1:H:1199:GLY:HA3	1.98	0.45
6:U:234:LEU:HA	6:U:237:TYR:HD1	1.82	0.45
1:D:503:TYR:HB3	1:D:569:PRO:HG3	1.97	0.45
1:H:407:VAL:HG13	1:J:116:ILE:HD13	1.99	0.45
1:J:465:ILE:HG12	1:L:1216:GLN:HE22	1.80	0.45
1:A:183:THR:HA	1:A:186:ASP:OD2	2.17	0.45
1:A:475:MET:O	1:A:479:CYS:HB2	2.16	0.45
1:A:1086:GLU:CD	1:A:1087:ARG:H	2.25	0.45
1:H:701:GLU:HG3	1:J:677:ARG:HH22	1.82	0.45
1:L:457:ILE:HG23	1:L:1356:SER:H	1.82	0.45
6:U:226:TYR:HB2	6:V:411:GLY:HA2	1.98	0.45
1:D:421:MET:HG2	1:D:457:ILE:HG21	1.99	0.45
1:H:838:PRO:O	1:H:842:ARG:HB3	2.16	0.45
4:S:207:ASN:HA	4:S:210:PHE:HD1	1.82	0.45
5:T:476:LEU:O	5:T:477:GLN:HG3	2.16	0.45
6:U:239:MET:HE3	6:U:239:MET:HB3	1.82	0.45
1:L:1114:GLN:HB3	1:L:1116:ARG:HE	1.82	0.45
6:U:278:LYS:HD3	6:U:428:LYS:HB3	1.97	0.45
6:U:481:ARG:HB3	6:U:483:VAL:HG22	1.99	0.45
6:V:315:ILE:HG22	6:V:319:VAL:HG12	1.99	0.45
1:A:595:ASN:HD21	1:A:1049:LYS:HA	1.81	0.45
1:A:1140:ASP:HB2	1:A:1202:SER:HB2	1.99	0.45
1:H:939:THR:HG23	1:H:942:THR:H	1.82	0.45
3:N:444:PRO:HD3	3:N:471:VAL:HG22	1.99	0.45
4:P:61:SER:O	4:P:64:GLU:HG3	2.16	0.45
4:P:78:ILE:HG22	4:P:80:GLY:H	1.82	0.45
6:U:380:LEU:HD11	6:U:537:MET:HG3	1.99	0.45
1:B:833:TYR:HD1	1:B:837:ILE:HD12	1.82	0.45
1:F:411:LEU:HB3	1:F:1081:GLN:HB3	1.99	0.45
6:U:51:LEU:HA	6:U:54:ASN:ND2	2.32	0.45
1:A:1101:HIS:HB3	1:A:1110:PHE:HB3	1.99	0.44
1:D:1240:ASP:O	1:D:1241:ILE:HG22	2.18	0.44
1:F:171:ILE:HA	1:F:174:ILE:HG12	1.99	0.44
1:H:1087:ARG:HH21	1:H:1124:GLY:HA3	1.83	0.44
1:J:1173:GLY:HA3	1:L:1251:SER:HB2	1.99	0.44
1:J:1321:GLN:HA	1:J:1332:ARG:HB2	1.98	0.44
4:S:59:THR:HG23	4:S:118:VAL:HG11	1.98	0.44
5:T:26:VAL:HB	5:T:371:ILE:HG23	1.98	0.44
6:U:138:LYS:HE3	6:U:414:THR:HA	1.99	0.44
1:A:517:ASP:O	1:A:520:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:LEU:HD12	1:B:1116:ARG:HH12	1.82	0.44
1:H:549:ALA:N	1:H:550:PRO:HD2	2.32	0.44
1:J:594:ILE:HD12	1:J:1020:THR:H	1.81	0.44
1:L:914:GLN:HG2	2:M:65:ALA:HB1	1.99	0.44
1:L:1364:THR:HB	1:L:1368:GLY:HA2	1.99	0.44
1:A:725:THR:HG21	1:A:740:ASN:HA	1.98	0.44
2:E:92:LEU:HD23	2:E:92:LEU:HA	1.88	0.44
1:J:608:ARG:O	1:J:611:ARG:HG3	2.17	0.44
1:L:1180:GLU:N	1:L:1181:PRO:HD2	2.33	0.44
1:F:537:TRP:HB2	1:F:554:ARG:HH21	1.83	0.44
1:J:1057:HIS:HA	1:J:1060:ARG:HG2	1.99	0.44
1:J:1176:LEU:HD13	1:L:1244:ILE:HA	1.99	0.44
2:K:98:LEU:HD13	1:L:896:VAL:HG21	1.98	0.44
3:Q:237:ARG:O	3:Q:240:GLU:HG3	2.17	0.44
7:X:11:ALA:O	7:X:14:ARG:HG3	2.18	0.44
2:C:9:VAL:HG12	2:C:11:PHE:H	1.83	0.44
1:F:598:ILE:N	1:F:599:PRO:HD2	2.33	0.44
5:T:242:ILE:HD12	6:V:94:ARG:HE	1.82	0.44
6:U:522:HIS:HA	6:U:525:VAL:HB	1.99	0.44
1:A:653:ASN:HB3	1:A:656:ASN:HB2	2.00	0.44
4:P:33:PHE:HD1	4:P:45:ILE:HG21	1.81	0.44
1:A:850:VAL:HG12	1:A:956:LEU:HD22	1.99	0.44
1:D:502:CYS:HA	1:D:532:PRO:HG2	1.99	0.44
1:H:471:LEU:HD23	1:H:475:MET:HG2	2.00	0.44
4:R:138:LEU:HD23	4:R:140:ILE:HD11	1.99	0.44
1:A:424:GLY:O	1:A:425:VAL:HG12	2.18	0.44
1:B:846:CYS:HB3	1:B:988:HIS:CE1	2.53	0.44
1:D:555:LEU:HD23	1:D:555:LEU:H	1.82	0.44
1:D:660:LEU:HD22	1:D:912:THR:HB	2.00	0.44
1:D:732:ASN:HD21	1:D:768:ASP:HB3	1.82	0.44
1:F:48:PHE:HD1	1:F:48:PHE:HA	1.72	0.44
1:F:520:MET:HE1	1:F:977:VAL:HG12	1.99	0.44
1:F:526:THR:O	1:F:530:MET:HB2	2.18	0.44
1:H:688:MET:HE2	1:H:688:MET:HB2	1.92	0.44
1:L:247:ARG:HD3	1:L:1134:LEU:HD13	1.99	0.44
1:L:831:ILE:HA	1:L:835:ILE:HD12	2.00	0.44
6:U:167:SER:O	6:U:168:PRO:C	2.60	0.44
1:H:759:LEU:O	1:H:762:ARG:HG3	2.18	0.44
1:J:1349:GLU:H	1:J:1349:GLU:HG3	1.59	0.44
3:N:343:SER:HB3	3:N:350:PHE:HE1	1.83	0.44
4:O:145:MET:O	4:O:149:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:47:LEU:O	4:R:51:TYR:HB2	2.18	0.44
4:S:106:LEU:H	4:S:305:VAL:HG21	1.82	0.44
1:A:640:PRO:HB2	1:A:643:PHE:HB2	2.00	0.43
1:F:82:PHE:HB3	1:F:83:LEU:H	1.70	0.43
1:F:335:LYS:HA	1:F:335:LYS:HD2	1.89	0.43
1:H:475:MET:HE1	1:H:1060:ARG:HB2	2.00	0.43
1:H:506:VAL:HA	1:H:1018:HIS:NE2	2.33	0.43
1:J:1361:MET:HA	1:J:1376:HIS:HE1	1.82	0.43
5:T:446:ALA:HA	5:T:449:PHE:CE2	2.53	0.43
6:V:510:VAL:O	6:V:511:THR:HG22	2.18	0.43
1:A:209:LEU:HB2	1:A:234:LEU:HD11	2.00	0.43
2:G:17:THR:HG23	2:G:18:THR:H	1.82	0.43
1:J:1326:THR:HG23	1:J:1328:TYR:H	1.83	0.43
1:J:1363:ARG:HB3	1:L:1374:GLU:HG2	2.00	0.43
6:V:184:VAL:HA	6:V:188:PRO:HB3	2.00	0.43
1:A:637:ARG:HH21	1:A:962:GLN:HB3	1.82	0.43
1:D:1076:ARG:HE	1:D:1138:LEU:HD22	1.84	0.43
1:D:1258:ARG:HH12	1:D:1261:LEU:HD12	1.82	0.43
4:R:148:ILE:HD13	4:R:148:ILE:HA	1.90	0.43
5:T:586:LYS:H	5:T:586:LYS:HG3	1.75	0.43
6:U:313:ALA:HA	6:U:316:ARG:HG2	2.00	0.43
1:A:1156:PRO:HG3	4:O:236:VAL:HB	2.00	0.43
1:B:721:ILE:HA	1:B:724:PHE:HD2	1.84	0.43
1:B:889:LEU:HD12	1:B:889:LEU:HA	1.79	0.43
1:F:542:LEU:HA	1:F:546:GLN:HB2	2.00	0.43
1:L:430:SER:HA	1:L:433:ARG:HH22	1.83	0.43
1:L:961:TYR:HB2	1:L:988:HIS:NE2	2.33	0.43
6:U:566:PHE:HA	6:U:572:ILE:HD11	2.00	0.43
6:V:390:ASN:O	6:V:391:VAL:HG12	2.18	0.43
1:B:118:ARG:HA	1:D:193:ALA:H	1.84	0.43
1:H:205:PRO:HD2	1:H:1127:ALA:HB1	1.99	0.43
1:L:863:ILE:HD12	2:M:27:TYR:HB2	1.99	0.43
4:O:253:ILE:HG13	4:O:254:ASN:H	1.84	0.43
5:T:166:LYS:HD2	5:T:204:ILE:HG23	2.00	0.43
5:T:546:TYR:HD2	5:T:547:LEU:HG	1.83	0.43
1:B:118:ARG:N	1:D:192:THR:H	2.16	0.43
1:F:169:LEU:O	1:F:172:ARG:HG2	2.18	0.43
1:F:1200:GLN:HG3	1:F:1327:GLU:HA	2.01	0.43
1:H:242:MET:HG2	1:H:243:PHE:HD1	1.83	0.43
1:H:296:LYS:HD3	1:H:394:LEU:HD21	2.00	0.43
1:H:1080:GLU:HG2	1:H:1135:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1102:HIS:HB2	1:J:1111:THR:HG22	2.00	0.43
1:B:935:ALA:HB2	1:B:943:ARG:HD2	2.01	0.43
1:L:233:ASP:HA	1:L:236:ARG:HE	1.84	0.43
1:L:251:GLU:HG2	1:L:254:LEU:HD12	2.00	0.43
1:L:664:LEU:HD23	1:L:664:LEU:HA	1.90	0.43
1:A:1210:PRO:HG3	1:A:1264:TRP:HB2	2.01	0.43
1:B:399:ARG:HG3	1:B:401:VAL:HG22	2.00	0.43
1:F:253:ARG:HD2	1:F:253:ARG:HA	1.83	0.43
1:F:1262:ASN:HB2	1:F:1265:ALA:HB3	2.00	0.43
1:H:237:ARG:O	1:H:241:ASP:HB3	2.19	0.43
1:H:517:ASP:HA	1:H:520:MET:HE3	2.01	0.43
1:J:523:PHE:HB2	1:J:1012:PHE:HE2	1.83	0.43
1:J:647:GLU:HA	1:J:650:ILE:HG22	1.99	0.43
4:P:206:LEU:O	4:P:209:MET:HG3	2.18	0.43
6:U:108:GLU:HA	6:U:111:GLU:CD	2.44	0.43
6:V:103:GLU:HB2	7:X:5:LEU:HB3	2.01	0.43
1:A:631:LYS:HD3	1:A:631:LYS:HA	1.77	0.43
1:A:1214:ASP:HB2	1:A:1261:LEU:HG	1.99	0.43
1:B:611:ARG:HH12	1:B:1038:THR:HG22	1.84	0.43
1:B:805:ARG:HA	1:B:805:ARG:HD2	1.85	0.43
1:B:964:TYR:HD1	1:B:964:TYR:HA	1.76	0.43
1:J:160:VAL:HG23	1:J:161:ASP:H	1.83	0.43
1:J:985:CYS:HB2	1:J:988:HIS:HB2	2.00	0.43
1:J:1100:HIS:HB3	1:J:1111:THR:HG23	2.00	0.43
1:J:1121:LEU:HD12	1:J:1123:VAL:H	1.84	0.43
1:L:457:ILE:HD12	1:L:1355:CYS:HB2	2.00	0.43
1:L:1328:TYR:O	1:L:1329:GLN:HG3	2.19	0.43
1:A:95:LYS:HD2	1:A:95:LYS:HA	1.86	0.43
1:A:169:LEU:HD12	1:A:172:ARG:HE	1.84	0.43
1:A:641:THR:HG23	1:A:956:LEU:HD21	2.01	0.43
1:A:1166:LEU:HD23	1:A:1169:ILE:HD11	2.01	0.43
1:B:623:THR:HG23	1:B:626:THR:H	1.84	0.43
1:D:549:ALA:N	1:D:550:PRO:HD2	2.34	0.43
1:H:1237:ARG:HG2	1:H:1239:ALA:H	1.84	0.43
2:I:82:MET:H	2:I:82:MET:HG2	1.65	0.43
4:P:168:PRO:HG3	5:T:336:ILE:HG12	2.01	0.43
4:R:16:SER:H	4:R:17:PRO:HD2	1.84	0.43
5:T:66:GLU:HG3	5:T:67:PRO:HD2	2.01	0.43
6:U:274:THR:HG22	6:U:276:GLU:H	1.84	0.43
6:V:135:GLN:HE21	6:V:402:LEU:HB3	1.83	0.43
6:V:179:LEU:HD11	6:V:495:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LEU:O	1:A:262:MET:HG2	2.19	0.42
1:B:789:MET:HA	1:B:792:HIS:HD2	1.83	0.42
1:H:939:THR:HG23	1:H:941:THR:H	1.84	0.42
1:H:1290:SER:N	1:H:1291:PRO:HD2	2.34	0.42
1:J:235:LYS:HE2	1:J:1349:GLU:HB3	2.01	0.42
1:J:591:LEU:HD23	1:J:591:LEU:HA	1.88	0.42
1:J:1222:CYS:HB2	1:J:1350:ALA:HB3	2.00	0.42
1:L:205:PRO:HB2	1:L:206:PRO:HD2	2.01	0.42
1:L:1059:LEU:HG	1:L:1063:PHE:HE2	1.83	0.42
1:L:1097:ILE:HD12	1:L:1114:GLN:HB2	2.01	0.42
3:N:416:LEU:HB3	3:N:417:TYR:H	1.55	0.42
5:T:57:THR:HG22	5:T:66:GLU:H	1.83	0.42
6:U:542:VAL:HG12	6:U:545:ALA:HB3	2.01	0.42
1:A:429:ASN:HD21	1:A:603:CYS:HA	1.84	0.42
1:B:500:ARG:HD2	1:B:500:ARG:HA	1.88	0.42
1:B:1080:GLU:H	1:B:1135:ARG:HG3	1.83	0.42
1:D:95:LYS:HG3	1:D:97:PRO:HD3	2.00	0.42
1:D:245:MET:HG2	1:D:246:THR:HG23	2.00	0.42
2:E:22:GLU:HG2	2:E:67:ARG:HD2	2.01	0.42
1:J:1365:ALA:HB2	1:L:1376:HIS:HB2	2.01	0.42
1:L:210:LEU:HD11	1:L:1308:LEU:HD22	2.00	0.42
1:L:245:MET:HE3	1:L:245:MET:HB3	1.82	0.42
4:O:119:PHE:HE1	4:O:185:TYR:HB3	1.83	0.42
3:Q:171:GLY:HA2	3:Q:174:ASN:HD21	1.83	0.42
3:Q:171:GLY:HA2	3:Q:174:ASN:ND2	2.34	0.42
4:S:51:TYR:HB3	4:S:56:PRO:HG3	2.01	0.42
4:S:219:LEU:O	4:S:223:ILE:HB	2.19	0.42
5:T:4:HIS:O	5:T:8:GLU:HG2	2.18	0.42
1:A:522:ARG:O	1:A:525:GLU:HG3	2.19	0.42
1:B:116:ILE:HA	1:D:191:GLY:HA3	2.01	0.42
1:D:326:ASN:HA	1:D:329:THR:HG22	1.99	0.42
1:H:739:LEU:HD13	1:H:1049:LYS:HZ1	1.83	0.42
1:L:222:LEU:HD12	1:L:226:ALA:HB2	2.01	0.42
1:L:600:VAL:N	1:L:601:PRO:HD2	2.34	0.42
1:L:998:ALA:HA	1:L:1001:VAL:HG22	1.99	0.42
3:N:178:ALA:HB2	3:N:237:ARG:HD2	2.02	0.42
1:A:304:LEU:HD13	1:A:385:VAL:HG21	2.01	0.42
1:A:707:TYR:HA	1:A:710:LEU:HD23	2.01	0.42
1:B:214:ASN:HA	1:B:217:GLN:HE22	1.84	0.42
1:J:1176:LEU:O	1:L:1250:GLN:HB3	2.19	0.42
1:L:466:LEU:HD13	1:L:1359:ALA:HB1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:12:PRO:HB2	4:R:15:LEU:HD21	2.01	0.42
6:U:129:SER:O	6:U:130:ILE:HG22	2.20	0.42
6:U:434:ASN:HA	6:U:437:GLN:HE21	1.83	0.42
6:V:346:ILE:HD12	6:V:349:ALA:HB3	2.01	0.42
6:V:527:LEU:HD13	6:V:531:ARG:HH22	1.84	0.42
1:D:685:HIS:HA	1:D:688:MET:HE3	2.02	0.42
1:D:832:TYR:O	1:D:836:VAL:HG22	2.19	0.42
1:L:253:ARG:HA	1:L:257:ALA:HB2	2.01	0.42
6:V:133:GLU:HB3	6:V:142:PRO:HB2	2.01	0.42
1:B:1010:PRO:HG2	1:B:1013:LEU:HD12	2.00	0.42
3:N:141:ILE:HB	3:N:198:LEU:HD13	2.01	0.42
6:U:192:ARG:HD2	6:U:192:ARG:HA	1.86	0.42
6:V:135:GLN:HG2	6:V:402:LEU:HD12	2.01	0.42
1:A:907:GLY:HA2	1:A:910:LEU:HD12	2.01	0.42
1:B:406:ARG:HD2	1:B:406:ARG:HA	1.88	0.42
1:B:857:PRO:HA	1:B:860:GLN:HE22	1.85	0.42
2:K:32:LEU:O	2:K:36:LEU:HB2	2.20	0.42
5:T:165:CYS:HA	5:T:168:LEU:HD23	2.01	0.42
1:A:729:GLU:HB2	1:A:739:LEU:HD11	2.01	0.42
1:A:959:MET:HG3	1:A:960:ALA:H	1.83	0.42
1:B:44:HIS:O	1:B:45:ARG:HG2	2.20	0.42
1:J:430:SER:HB3	1:J:433:ARG:HH22	1.85	0.42
1:J:981:PRO:HB3	1:J:1009:ILE:HG23	2.01	0.42
5:T:400:ASP:HB3	7:W:35:GLN:NE2	2.34	0.42
6:V:103:GLU:HA	7:X:5:LEU:HD22	2.00	0.42
1:A:288:VAL:HG23	1:A:1085:ALA:HB3	2.01	0.42
1:J:990:ALA:HA	1:J:1000:ARG:HD3	2.02	0.42
3:N:311:LEU:HD12	3:N:311:LEU:HA	1.87	0.42
4:R:277:TRP:CE2	4:S:212:ILE:HG12	2.55	0.42
5:T:384:ARG:HG2	5:T:389:PRO:HG3	2.02	0.42
5:T:637:LEU:HD12	5:T:638:PRO:HD2	2.02	0.42
1:A:559:LEU:HD23	1:A:559:LEU:HA	1.84	0.42
1:D:962:GLN:HB2	1:D:965:ASP:HB2	2.02	0.42
1:F:509:ALA:HB3	1:F:1011:PRO:HB2	2.01	0.42
1:F:922:GLU:H	1:F:922:GLU:HG3	1.58	0.42
1:H:1333:PRO:HA	1:H:1334:PRO:HD3	1.94	0.42
1:J:654:GLU:HA	1:J:657:PHE:HB3	2.02	0.42
1:J:1352:PRO:HA	1:J:1353:PRO:HD3	1.89	0.42
1:L:1017:HIS:CD2	1:L:1022:ARG:HH21	2.38	0.42
1:L:1087:ARG:H	1:L:1087:ARG:HG2	1.67	0.42
6:V:131:HIS:HB3	6:V:144:GLN:HE22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:538:HIS:ND1	6:V:540:PRO:HD2	2.35	0.42
1:A:726:ILE:H	1:A:1057:HIS:CD2	2.38	0.41
1:A:874:PRO:HB2	1:A:876:THR:HG22	2.02	0.41
1:A:1092:TYR:HD1	1:A:1118:HIS:HB3	1.85	0.41
1:B:1010:PRO:HB2	1:B:1013:LEU:HB2	2.02	0.41
1:L:19:ILE:HB	1:L:20:ALA:H	1.73	0.41
1:L:838:PRO:HG3	1:L:983:PHE:HZ	1.84	0.41
4:S:87:ILE:HG22	4:S:92:PRO:HA	2.02	0.41
6:U:91:GLN:HB3	7:X:14:ARG:CZ	2.50	0.41
1:A:285:VAL:HG21	1:A:393:PHE:HD1	1.85	0.41
1:A:1356:SER:HB3	1:A:1362:LEU:HD12	2.02	0.41
1:D:611:ARG:HH22	1:D:1058:GLN:HE22	1.68	0.41
1:L:232:SER:HA	1:L:235:LYS:HG2	2.03	0.41
4:O:108:ASN:HB2	4:O:303:SER:HB2	2.02	0.41
6:U:289:PRO:HD2	6:U:376:ILE:HD11	2.02	0.41
6:V:339:HIS:CD2	6:V:359:ASN:HD21	2.38	0.41
6:V:496:ILE:O	6:V:499:ILE:HG13	2.20	0.41
1:B:608:ARG:HA	1:B:611:ARG:HG2	2.00	0.41
1:B:1316:LYS:HD3	1:B:1316:LYS:HA	1.68	0.41
1:F:174:ILE:HG13	1:F:175:GLN:N	2.35	0.41
1:F:1157:MET:HG3	1:F:1163:THR:HG21	2.03	0.41
1:F:1182:LEU:HD13	1:F:1182:LEU:HA	1.96	0.41
2:K:28:THR:HB	2:K:29:PRO:HD3	2.02	0.41
1:L:1361:MET:HG3	1:L:1362:LEU:HD12	2.01	0.41
4:O:251:GLN:H	4:O:251:GLN:HG2	1.64	0.41
3:Q:198:LEU:HD12	3:Q:201:ILE:HD11	2.02	0.41
4:R:117:PRO:HG3	4:R:138:LEU:HD13	2.02	0.41
6:U:454:THR:HB	6:U:460:PHE:HB3	2.03	0.41
6:U:490:GLN:H	6:U:490:GLN:HG3	1.65	0.41
1:B:116:ILE:CA	1:D:191:GLY:HA3	2.51	0.41
1:D:940:ALA:H	1:D:1157:MET:HE2	1.85	0.41
2:K:26:ALA:C	2:K:29:PRO:HD2	2.45	0.41
6:U:136:ILE:HA	6:U:142:PRO:HB3	2.02	0.41
1:A:142:SER:HB3	1:A:1113:THR:HG22	2.01	0.41
1:D:79:PHE:HD1	1:D:79:PHE:HA	1.78	0.41
1:D:841:SER:HB2	1:D:844:SER:HB3	2.02	0.41
1:D:1273:ASP:O	1:D:1277:ASN:HB2	2.21	0.41
1:F:279:ASN:HD22	1:F:384:LEU:HD13	1.85	0.41
1:J:611:ARG:HD3	1:J:1063:PHE:HE1	1.85	0.41
4:P:114:LEU:HD22	4:P:137:PRO:HG2	2.03	0.41
5:T:354:ARG:HB3	5:T:376:ASN:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:GLN:HG3	1:B:617:LEU:HD12	2.02	0.41
1:D:549:ALA:O	1:D:550:PRO:C	2.63	0.41
1:F:200:LEU:HD22	1:F:203:LYS:HE3	2.03	0.41
1:F:1059:LEU:HA	1:F:1063:PHE:HA	2.02	0.41
1:H:545:LEU:HD13	1:H:548:ILE:HD11	2.01	0.41
1:J:569:PRO:HG3	1:J:585:PRO:HA	2.03	0.41
1:J:592:ARG:HH21	1:J:594:ILE:HB	1.86	0.41
1:J:1376:HIS:HD2	1:J:1377:LEU:HG	1.85	0.41
1:L:304:LEU:HD12	1:L:304:LEU:HA	1.81	0.41
4:S:97:PHE:HE1	4:S:310:ARG:HE	1.68	0.41
1:F:384:LEU:HD23	1:F:393:PHE:HB3	2.03	0.41
1:L:96:PHE:HB2	1:L:99:LEU:HD12	2.03	0.41
3:Q:325:PHE:HB2	3:Q:436:ALA:HB3	2.02	0.41
5:T:88:LYS:HE2	5:T:90:GLU:HG2	2.03	0.41
1:D:214:ASN:HA	1:D:217:GLN:HE21	1.86	0.41
2:G:41:PRO:HB2	2:G:44:PRO:HD2	2.03	0.41
1:H:1004:LYS:HD3	1:H:1004:LYS:HA	1.63	0.41
1:L:544:ILE:HG23	1:L:545:LEU:H	1.86	0.41
3:N:178:ALA:HB2	3:N:237:ARG:HH11	1.85	0.41
4:O:223:ILE:HG13	4:O:224:PRO:CD	2.51	0.41
1:A:116:ILE:HD12	1:A:116:ILE:HA	1.92	0.41
1:A:552:ASN:O	1:A:556:ARG:HB3	2.21	0.41
1:B:117:ALA:O	1:D:193:ALA:HB3	2.21	0.41
1:B:222:LEU:HB2	1:B:226:ALA:HB3	2.02	0.41
1:B:402:TYR:HD1	1:B:402:TYR:HA	1.79	0.41
1:B:739:LEU:HD11	1:B:1051:THR:HG21	2.03	0.41
1:B:855:LEU:HG	2:E:93:ARG:HD2	2.03	0.41
1:D:263:VAL:HG21	1:D:390:LYS:HD2	2.02	0.41
1:F:300:LEU:HA	1:F:304:LEU:HB2	2.03	0.41
1:F:1215:LEU:HG	1:F:1219:ARG:HE	1.86	0.41
1:H:552:ASN:HD21	1:H:1249:THR:HG22	1.85	0.41
1:H:1021:ILE:HG21	1:H:1025:VAL:HG13	2.03	0.41
1:H:1080:GLU:HB2	1:H:1132:ALA:HB1	2.01	0.41
2:K:96:VAL:HG11	1:L:894:LEU:HB3	2.03	0.41
1:L:203:LYS:HD2	1:L:203:LYS:HA	1.59	0.41
1:L:758:ALA:HB1	1:L:830:LYS:HZ1	1.85	0.41
3:Q:345:LEU:HD12	3:Q:345:LEU:HA	1.88	0.41
7:X:12:CYS:O	7:X:15:MET:HG2	2.21	0.41
1:D:250:ARG:HG3	1:D:251:GLU:HG2	2.02	0.41
1:H:639:TYR:HB2	1:H:959:MET:HB3	2.03	0.41
1:H:1026:ALA:HA	1:H:1029:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:600:VAL:HB	1:J:601:PRO:HD3	2.02	0.41
1:L:1245:MET:HE2	1:L:1245:MET:HB2	1.91	0.41
3:Q:168:LEU:HD23	3:Q:168:LEU:HA	1.95	0.41
1:A:674:GLN:HG3	1:A:675:SER:N	2.36	0.40
1:B:99:LEU:HD12	1:B:99:LEU:HA	1.93	0.40
1:D:242:MET:HG3	1:D:243:PHE:H	1.85	0.40
1:J:1176:LEU:HA	1:L:1247:ASP:HB3	2.03	0.40
1:L:54:ILE:HG12	1:L:58:ASP:HB2	2.02	0.40
5:T:598:LYS:HB2	5:T:598:LYS:HE3	1.85	0.40
1:A:995:MET:HG3	1:A:1000:ARG:HG3	2.03	0.40
1:F:138:LYS:HE2	1:F:138:LYS:HB3	1.90	0.40
1:F:295:LEU:HD23	1:F:295:LEU:HA	1.94	0.40
1:F:399:ARG:HD2	1:F:399:ARG:HA	1.84	0.40
1:F:794:PHE:HZ	1:F:852:TYR:HB2	1.87	0.40
1:F:834:TYR:HD1	1:F:834:TYR:HA	1.76	0.40
1:J:660:LEU:HD23	1:J:660:LEU:HA	1.86	0.40
1:L:386:ILE:HG23	1:L:391:LEU:HG	2.03	0.40
6:U:266:GLU:HA	6:U:269:VAL:HG22	2.03	0.40
6:U:491:TYR:HD1	6:U:491:TYR:HA	1.78	0.40
6:V:499:ILE:O	6:V:502:GLU:HG3	2.20	0.40
6:V:539:GLN:H	6:V:539:GLN:HG3	1.66	0.40
1:B:488:ALA:HB3	1:B:1274:ARG:NH2	2.36	0.40
1:F:103:ARG:HH12	1:F:335:LYS:HA	1.86	0.40
1:F:108:GLN:H	1:F:108:GLN:HG3	1.73	0.40
1:F:548:ILE:HD13	1:F:1258:ARG:HE	1.86	0.40
1:F:938:ALA:HB2	1:F:1158:LEU:HD22	2.04	0.40
1:J:171:ILE:HD13	1:J:171:ILE:HA	1.94	0.40
1:J:766:ALA:HA	1:J:769:ARG:HE	1.86	0.40
1:L:622:MET:HE3	1:L:713:HIS:CE1	2.56	0.40
6:U:87:PRO:O	6:U:90:GLU:HG3	2.21	0.40
6:U:539:GLN:HB3	6:U:541:ARG:HH21	1.85	0.40
1:A:304:LEU:HD22	1:A:385:VAL:HG21	2.04	0.40
1:A:1166:LEU:HA	1:A:1169:ILE:HG12	2.03	0.40
1:H:237:ARG:O	1:H:241:ASP:HB2	2.21	0.40
1:H:243:PHE:HE2	1:H:1388:LEU:HB2	1.86	0.40
1:H:830:LYS:O	1:H:834:TYR:HB2	2.21	0.40
1:H:862:VAL:HG22	1:H:913:LEU:HD21	2.03	0.40
1:J:945:MET:H	1:J:945:MET:HG3	1.62	0.40
1:L:1019:ALA:HB3	1:L:1021:ILE:HD11	2.03	0.40
2:M:56:ILE:HA	2:M:59:VAL:HG22	2.02	0.40
3:N:212:LYS:H	3:N:212:LYS:HG3	1.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:302:PRO:HG3	4:P:311:THR:HG23	2.04	0.40
5:T:359:VAL:HB	5:T:372:VAL:HB	2.04	0.40
5:T:431:ASN:HA	5:T:434:ASN:HD21	1.86	0.40
6:U:321:PRO:HA	6:U:322:PRO:HD3	1.98	0.40
6:V:356:ARG:HD2	6:V:356:ARG:HA	1.84	0.40
7:W:12:CYS:O	7:W:15:MET:HG2	2.21	0.40
1:A:880:PRO:HA	1:A:887:HIS:HB3	2.03	0.40
1:B:259:LEU:HD13	1:B:388:GLY:HA2	2.02	0.40
1:F:1231:MET:H	1:F:1231:MET:HG3	1.69	0.40
1:L:104:ASP:HB3	1:L:105:GLY:H	1.67	0.40
1:L:178:ALA:O	1:L:181:LEU:HG	2.21	0.40
1:L:846:CYS:HB2	1:L:985:CYS:HB3	1.82	0.40
5:T:422:LEU:HD12	5:T:422:LEU:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1148/1396 (82%)	1081 (94%)	63 (6%)	4 (0%)	37	73
1	B	1324/1396 (95%)	1252 (95%)	70 (5%)	2 (0%)	44	78
1	D	1331/1396 (95%)	1238 (93%)	87 (6%)	6 (0%)	25	64
1	F	1331/1396 (95%)	1268 (95%)	58 (4%)	5 (0%)	30	68
1	H	1271/1396 (91%)	1213 (95%)	55 (4%)	3 (0%)	44	78
1	J	1269/1396 (91%)	1189 (94%)	76 (6%)	4 (0%)	37	73
1	L	1308/1396 (94%)	1231 (94%)	72 (6%)	5 (0%)	30	68
2	C	99/235 (42%)	93 (94%)	5 (5%)	1 (1%)	13	49
2	E	93/235 (40%)	90 (97%)	3 (3%)	0	100	100
2	G	99/235 (42%)	93 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	99/235 (42%)	95 (96%)	4 (4%)	0	100	100
2	K	99/235 (42%)	94 (95%)	5 (5%)	0	100	100
2	M	99/235 (42%)	90 (91%)	9 (9%)	0	100	100
3	N	353/483 (73%)	337 (96%)	16 (4%)	0	100	100
3	Q	353/483 (73%)	341 (97%)	12 (3%)	0	100	100
4	O	294/316 (93%)	283 (96%)	9 (3%)	2 (1%)	19	57
4	P	271/316 (86%)	261 (96%)	9 (3%)	1 (0%)	30	68
4	R	294/316 (93%)	283 (96%)	9 (3%)	2 (1%)	19	57
4	S	271/316 (86%)	263 (97%)	8 (3%)	0	100	100
5	T	589/676 (87%)	558 (95%)	29 (5%)	2 (0%)	37	73
6	U	529/579 (91%)	466 (88%)	55 (10%)	8 (2%)	8	40
6	V	529/579 (91%)	464 (88%)	60 (11%)	5 (1%)	14	52
7	W	43/2763 (2%)	43 (100%)	0	0	100	100
7	X	43/2763 (2%)	43 (100%)	0	0	100	100
All	All	13139/20772 (63%)	12369 (94%)	720 (6%)	50 (0%)	32	68

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	392	VAL
1	A	425	VAL
1	D	550	PRO
1	D	1241	ILE
1	F	599	PRO
1	H	550	PRO
1	L	68	ILE
1	L	640	PRO
5	T	207	VAL
6	U	130	ILE
6	U	168	PRO
6	U	248	GLU
6	U	417	VAL
6	V	391	VAL
1	A	506	VAL
1	F	1023	GLN
1	H	593	ILE
1	J	1180	GLU

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Mol	Chain	Res	Type
4	O	43	VAL
4	O	52	ILE
6	U	194	VAL
6	U	418	ILE
6	U	510	VAL
6	V	510	VAL
2	C	15	ASN
1	L	552	ASN
4	R	16	SER
5	T	482	TYR
1	D	440	ASP
6	V	322	PRO
6	V	360	VAL
1	B	436	ARG
1	D	508	VAL
1	F	1392	LEU
1	J	890	VAL
1	L	508	VAL
6	U	136	ILE
6	V	246	VAL
1	A	1096	GLN
1	F	37	SER
1	J	508	VAL
1	J	1364	THR
1	B	508	VAL
1	H	508	VAL
1	D	601	PRO
4	P	166	ILE
4	R	52	ILE
1	D	890	VAL
1	L	890	VAL
1	F	639	TYR

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	964/1182 (82%)	918 (95%)	46 (5%)	21	43
1	B	1097/1182 (93%)	1044 (95%)	53 (5%)	21	43
1	D	1087/1182 (92%)	1043 (96%)	44 (4%)	27	47
1	F	1102/1182 (93%)	1066 (97%)	36 (3%)	33	52
1	H	1040/1182 (88%)	1001 (96%)	39 (4%)	28	49
1	J	1050/1182 (89%)	1009 (96%)	41 (4%)	27	48
1	L	1089/1182 (92%)	1048 (96%)	41 (4%)	28	49
2	C	72/189 (38%)	71 (99%)	1 (1%)	62	75
2	E	72/189 (38%)	67 (93%)	5 (7%)	13	33
2	G	74/189 (39%)	73 (99%)	1 (1%)	62	75
2	I	75/189 (40%)	74 (99%)	1 (1%)	65	77
2	K	75/189 (40%)	71 (95%)	4 (5%)	19	40
2	M	71/189 (38%)	71 (100%)	0	100	100
3	N	288/410 (70%)	282 (98%)	6 (2%)	48	66
3	Q	289/410 (70%)	281 (97%)	8 (3%)	38	57
4	O	256/267 (96%)	247 (96%)	9 (4%)	31	51
4	P	229/267 (86%)	224 (98%)	5 (2%)	47	65
4	R	256/267 (96%)	247 (96%)	9 (4%)	31	51
4	S	230/267 (86%)	217 (94%)	13 (6%)	17	38
5	T	503/573 (88%)	487 (97%)	16 (3%)	34	53
6	U	457/497 (92%)	440 (96%)	17 (4%)	29	49
6	V	457/497 (92%)	431 (94%)	26 (6%)	17	38
7	W	38/2413 (2%)	37 (97%)	1 (3%)	41	59
7	X	38/2413 (2%)	37 (97%)	1 (3%)	41	59
All	All	10909/17689 (62%)	10486 (96%)	423 (4%)	30	48

All (423) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	VAL
1	A	133	VAL
1	A	189	GLU
1	A	225	VAL
1	A	254	LEU
1	A	300	LEU

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Mol	Chain	Res	Type
1	A	313	VAL
1	A	393	PHE
1	A	425	VAL
1	A	466	LEU
1	A	486	VAL
1	A	542	LEU
1	A	543	THR
1	A	591	LEU
1	A	600	VAL
1	A	623	THR
1	A	632	ASP
1	A	643	PHE
1	A	644	TYR
1	A	673	GLU
1	A	681	VAL
1	A	706	ILE
1	A	710	LEU
1	A	721	ILE
1	A	764	GLU
1	A	834	TYR
1	A	852	TYR
1	A	856	TYR
1	A	867	ILE
1	A	875	THR
1	A	890	VAL
1	A	903	LEU
1	A	905	VAL
1	A	954	HIS
1	A	977	VAL
1	A	1006	VAL
1	A	1029	VAL
1	A	1099	VAL
1	A	1114	GLN
1	A	1146	GLN
1	A	1164	GLU
1	A	1172	SER
1	A	1313	MET
1	A	1340	THR
1	A	1346	LEU
1	A	1388	LEU
1	B	25	ILE
1	B	61	LEU

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Mol	Chain	Res	Type
1	B	68	ILE
1	B	78	ASN
1	B	85	LEU
1	B	89	VAL
1	B	106	VAL
1	B	116	ILE
1	B	169	LEU
1	B	189	GLU
1	B	222	LEU
1	B	234	LEU
1	B	270	VAL
1	B	285	VAL
1	B	306	ILE
1	B	387	VAL
1	B	411	LEU
1	B	435	THR
1	B	497	HIS
1	B	547	PHE
1	B	621	THR
1	B	642	ILE
1	B	646	LEU
1	B	663	LEU
1	B	686	MET
1	B	702	VAL
1	B	719	GLN
1	B	726	ILE
1	B	739	LEU
1	B	743	LEU
1	B	815	ILE
1	B	859	LEU
1	B	862	VAL
1	B	890	VAL
1	B	896	VAL
1	B	905	VAL
1	B	914	GLN
1	B	922	GLU
1	B	964	TYR
1	B	977	VAL
1	B	1029	VAL
1	B	1047	TYR
1	B	1059	LEU
1	B	1072	VAL

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Mol	Chain	Res	Type
1	B	1155	VAL
1	B	1222	CYS
1	B	1288	ILE
1	B	1289	TYR
1	B	1293	PHE
1	B	1297	THR
1	B	1308	LEU
1	B	1337	THR
1	B	1374	GLU
2	C	42	LEU
1	D	111	VAL
1	D	165	ILE
1	D	197	LEU
1	D	223	ASN
1	D	272	VAL
1	D	315	VAL
1	D	322	LEU
1	D	405	THR
1	D	435	THR
1	D	444	VAL
1	D	495	GLN
1	D	496	GLN
1	D	529	ASP
1	D	543	THR
1	D	544	ILE
1	D	567	VAL
1	D	574	LEU
1	D	623	THR
1	D	651	HIS
1	D	667	CYS
1	D	702	VAL
1	D	752	ILE
1	D	753	LEU
1	D	775	VAL
1	D	818	THR
1	D	853	ASP
1	D	864	VAL
1	D	867	ILE
1	D	890	VAL
1	D	896	VAL
1	D	941	THR
1	D	947	ILE

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Mol	Chain	Res	Type
1	D	958	MET
1	D	1005	MET
1	D	1006	VAL
1	D	1071	VAL
1	D	1148	LEU
1	D	1232	LEU
1	D	1279	THR
1	D	1282	LEU
1	D	1303	THR
1	D	1306	ASN
1	D	1324	THR
1	D	1364	THR
2	E	90	THR
2	E	95	THR
2	E	96	VAL
2	E	98	LEU
2	E	100	ARG
1	F	37	SER
1	F	48	PHE
1	F	80	VAL
1	F	84	GLU
1	F	85	LEU
1	F	102	VAL
1	F	158	THR
1	F	301	GLN
1	F	309	THR
1	F	329	THR
1	F	380	VAL
1	F	444	VAL
1	F	473	ASP
1	F	493	LEU
1	F	543	THR
1	F	544	ILE
1	F	555	LEU
1	F	602	LEU
1	F	770	LEU
1	F	818	THR
1	F	834	TYR
1	F	859	LEU
1	F	864	VAL
1	F	867	ILE
1	F	903	LEU

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Mol	Chain	Res	Type
1	F	916	LEU
1	F	967	THR
1	F	977	VAL
1	F	979	VAL
1	F	1051	THR
1	F	1128	VAL
1	F	1182	LEU
1	F	1188	LEU
1	F	1279	THR
1	F	1318	VAL
1	F	1327	GLU
2	G	17	THR
1	H	77	LEU
1	H	89	VAL
1	H	92	ILE
1	H	111	VAL
1	H	141	LEU
1	H	215	LYS
1	H	235	LYS
1	H	272	VAL
1	H	290	VAL
1	H	320	MET
1	H	327	LEU
1	H	328	VAL
1	H	331	LEU
1	H	380	VAL
1	H	385	VAL
1	H	444	VAL
1	H	457	ILE
1	H	497	HIS
1	H	542	LEU
1	H	607	PHE
1	H	623	THR
1	H	646	LEU
1	H	742	ILE
1	H	757	ASP
1	H	759	LEU
1	H	764	GLU
1	H	775	VAL
1	H	818	THR
1	H	834	TYR
1	H	864	VAL

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Mol	Chain	Res	Type
1	H	876	THR
1	H	1121	LEU
1	H	1158	LEU
1	H	1182	LEU
1	H	1192	THR
1	H	1217	TYR
1	H	1256	THR
1	H	1301	VAL
1	H	1346	LEU
2	I	17	THR
1	J	242	MET
1	J	270	VAL
1	J	327	LEU
1	J	380	VAL
1	J	457	ILE
1	J	475	MET
1	J	490	LEU
1	J	531	MET
1	J	538	VAL
1	J	544	ILE
1	J	567	VAL
1	J	613	THR
1	J	673	GLU
1	J	693	TYR
1	J	713	HIS
1	J	724	PHE
1	J	764	GLU
1	J	815	ILE
1	J	835	ILE
1	J	850	VAL
1	J	855	LEU
1	J	890	VAL
1	J	905	VAL
1	J	916	LEU
1	J	939	THR
1	J	947	ILE
1	J	1006	VAL
1	J	1009	ILE
1	J	1027	TYR
1	J	1071	VAL
1	J	1111	THR
1	J	1121	LEU

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Mol	Chain	Res	Type
1	J	1126	THR
1	J	1162	VAL
1	J	1166	LEU
1	J	1188	LEU
1	J	1242	GLU
1	J	1245	MET
1	J	1271	TYR
1	J	1375	VAL
1	J	1381	LEU
2	K	36	LEU
2	K	42	LEU
2	K	80	THR
2	K	98	LEU
1	L	36	LEU
1	L	68	ILE
1	L	106	VAL
1	L	124	VAL
1	L	158	THR
1	L	203	LYS
1	L	207	LEU
1	L	221	HIS
1	L	222	LEU
1	L	231	LEU
1	L	313	VAL
1	L	394	LEU
1	L	415	ILE
1	L	420	ILE
1	L	503	TYR
1	L	506	VAL
1	L	544	ILE
1	L	545	LEU
1	L	602	LEU
1	L	622	MET
1	L	623	THR
1	L	703	CYS
1	L	722	THR
1	L	741	ASN
1	L	784	LEU
1	L	787	VAL
1	L	801	LEU
1	L	828	LEU
1	L	834	TYR

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Mol	Chain	Res	Type
1	L	864	VAL
1	L	1006	VAL
1	L	1050	PHE
1	L	1059	LEU
1	L	1072	VAL
1	L	1131	THR
1	L	1148	LEU
1	L	1155	VAL
1	L	1182	LEU
1	L	1203	VAL
1	L	1290	SER
1	L	1379	GLN
3	N	159	THR
3	N	240	GLU
3	N	313	LEU
3	N	401	ILE
3	N	404	ILE
3	N	407	VAL
4	O	19	GLU
4	O	64	GLU
4	O	78	ILE
4	O	132	LEU
4	O	140	ILE
4	O	144	LEU
4	O	223	ILE
4	O	238	LEU
4	O	314	ILE
4	P	8	GLU
4	P	14	GLU
4	P	47	LEU
4	P	63	LEU
4	P	143	THR
3	Q	167	VAL
3	Q	195	VAL
3	Q	236	ILE
3	Q	242	LEU
3	Q	267	ILE
3	Q	313	LEU
3	Q	323	LEU
3	Q	324	VAL
4	R	16	SER
4	R	45	ILE

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Mol	Chain	Res	Type
4	R	115	LEU
4	R	160	THR
4	R	177	VAL
4	R	216	CYS
4	R	255	ILE
4	R	283	ARG
4	R	296	VAL
4	S	10	LEU
4	S	35	THR
4	S	60	LEU
4	S	75	THR
4	S	91	THR
4	S	112	ILE
4	S	125	ILE
4	S	140	ILE
4	S	167	LEU
4	S	204	LEU
4	S	210	PHE
4	S	218	LEU
4	S	220	LEU
5	T	22	LEU
5	T	23	LEU
5	T	84	LEU
5	T	90	GLU
5	T	159	GLN
5	T	168	LEU
5	T	175	THR
5	T	185	TYR
5	T	241	LEU
5	T	439	LEU
5	T	469	GLU
5	T	482	TYR
5	T	499	THR
5	T	509	VAL
5	T	580	VAL
5	T	651	LEU
6	U	51	LEU
6	U	111	GLU
6	U	123	GLU
6	U	130	ILE
6	U	146	ASP
6	U	235	CYS

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Mol	Chain	Res	Type
6	U	237	TYR
6	U	278	LYS
6	U	310	VAL
6	U	354	LEU
6	U	358	GLN
6	U	386	LEU
6	U	417	VAL
6	U	485	ASP
6	U	518	VAL
6	U	542	VAL
6	U	565	TYR
6	V	79	THR
6	V	110	GLU
6	V	145	TYR
6	V	151	VAL
6	V	157	VAL
6	V	259	GLU
6	V	260	HIS
6	V	273	THR
6	V	288	LEU
6	V	319	VAL
6	V	320	LEU
6	V	354	LEU
6	V	355	GLU
6	V	387	TRP
6	V	391	VAL
6	V	402	LEU
6	V	450	LEU
6	V	483	VAL
6	V	502	GLU
6	V	511	THR
6	V	529	TYR
6	V	538	HIS
6	V	539	GLN
6	V	561	TYR
6	V	564	LEU
6	V	578	THR
7	W	5	LEU
7	X	5	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (219) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	403	GLN
1	A	429	ASN
1	A	495	GLN
1	A	519	GLN
1	A	533	HIS
1	A	536	HIS
1	A	546	GLN
1	A	552	ASN
1	A	595	ASN
1	A	799	ASN
1	A	899	HIS
1	A	1057	HIS
1	A	1058	GLN
1	A	1118	HIS
1	A	1267	GLN
1	A	1269	HIS
1	B	122	HIS
1	B	129	HIS
1	B	180	ASN
1	B	214	ASN
1	B	217	GLN
1	B	427	GLN
1	B	468	GLN
1	B	560	ASN
1	B	620	HIS
1	B	666	GLN
1	B	727	GLN
1	B	731	HIS
1	B	732	ASN
1	B	740	ASN
1	B	782	GLN
1	B	792	HIS
1	B	820	HIS
1	B	821	HIS
1	B	1057	HIS
1	B	1058	GLN
1	B	1074	GLN
1	B	1143	ASN
1	B	1147	ASN
1	B	1223	ASN
1	B	1277	ASN
1	B	1302	ASN
1	B	1348	GLN

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Mol	Chain	Res	Type
1	B	1376	HIS
1	D	53	GLN
1	D	108	GLN
1	D	122	HIS
1	D	176	GLN
1	D	195	GLN
1	D	217	GLN
1	D	495	GLN
1	D	497	HIS
1	D	793	ASN
1	D	795	GLN
1	D	885	HIS
1	D	895	ASN
1	D	899	HIS
1	D	900	ASN
1	D	954	HIS
1	D	988	HIS
1	D	1058	GLN
1	D	1101	HIS
1	D	1114	GLN
1	D	1118	HIS
1	D	1177	ASN
1	D	1269	HIS
1	D	1304	ASN
1	F	65	GLN
1	F	112	GLN
1	F	126	GLN
1	F	129	HIS
1	F	267	GLN
1	F	277	HIS
1	F	284	GLN
1	F	429	ASN
1	F	447	GLN
1	F	468	GLN
1	F	656	ASN
1	F	713	HIS
1	F	740	ASN
1	F	882	HIS
1	F	895	ASN
1	F	1058	GLN
1	F	1118	HIS
1	F	1143	ASN

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Mol	Chain	Res	Type
1	F	1159	HIS
1	F	1262	ASN
1	F	1306	ASN
1	F	1341	GLN
1	H	75	ASN
1	H	157	ASN
1	H	175	GLN
1	H	427	GLN
1	H	437	HIS
1	H	468	GLN
1	H	533	HIS
1	H	539	ASN
1	H	552	ASN
1	H	560	ASN
1	H	614	GLN
1	H	651	HIS
1	H	685	HIS
1	H	696	ASN
1	H	727	GLN
1	H	741	ASN
1	H	793	ASN
1	H	944	ASN
1	H	1017	HIS
1	H	1031	HIS
1	H	1102	HIS
1	H	1304	ASN
2	I	15	ASN
2	I	72	HIS
1	J	122	HIS
1	J	137	HIS
1	J	468	GLN
1	J	533	HIS
1	J	546	GLN
1	J	597	ASN
1	J	653	ASN
1	J	656	ASN
1	J	713	HIS
1	J	727	GLN
1	J	741	ASN
1	J	860	GLN
1	J	885	HIS
1	J	887	HIS

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Mol	Chain	Res	Type
1	J	914	GLN
1	J	944	ASN
1	J	988	HIS
1	J	1074	GLN
1	J	1100	HIS
1	J	1114	GLN
1	J	1159	HIS
1	J	1248	HIS
1	J	1267	GLN
1	J	1329	GLN
1	J	1366	HIS
1	J	1376	HIS
1	L	129	HIS
1	L	195	GLN
1	L	214	ASN
1	L	267	GLN
1	L	414	ASN
1	L	429	ASN
1	L	461	ASN
1	L	480	HIS
1	L	560	ASN
1	L	578	GLN
1	L	683	ASN
1	L	712	GLN
1	L	713	HIS
1	L	741	ASN
1	L	782	GLN
1	L	820	HIS
1	L	885	HIS
1	L	944	ASN
1	L	997	ASN
1	L	1017	HIS
1	L	1058	GLN
1	L	1081	GLN
1	L	1096	GLN
1	L	1098	GLN
1	L	1118	HIS
1	L	1159	HIS
1	L	1216	GLN
1	L	1366	HIS
2	M	15	ASN
3	N	124	GLN

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Mol	Chain	Res	Type
3	N	137	HIS
3	N	147	HIS
3	N	282	GLN
3	N	461	ASN
4	O	38	HIS
4	O	207	ASN
4	O	232	HIS
4	P	85	HIS
3	Q	124	GLN
3	Q	137	HIS
3	Q	365	ASN
3	Q	479	ASN
4	R	24	GLN
4	R	38	HIS
4	R	108	ASN
4	R	193	HIS
4	R	229	GLN
4	R	315	GLN
4	S	108	ASN
5	T	18	HIS
5	T	83	ASN
5	T	95	HIS
5	T	101	HIS
5	T	197	HIS
5	T	234	ASN
5	T	235	ASN
5	T	250	ASN
5	T	376	ASN
5	T	410	ASN
5	T	412	GLN
5	T	434	ASN
5	T	451	ASN
5	T	628	ASN
5	T	632	GLN
6	U	144	GLN
6	U	207	ASN
6	U	302	GLN
6	U	328	ASN
6	U	332	ASN
6	U	401	GLN
6	U	451	ASN
6	U	473	GLN

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Mol	Chain	Res	Type
6	U	528	GLN
6	U	539	GLN
6	V	244	ASN
6	V	359	ASN
6	V	433	ASN
6	V	435	ASN
6	V	492	GLN
7	W	35	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

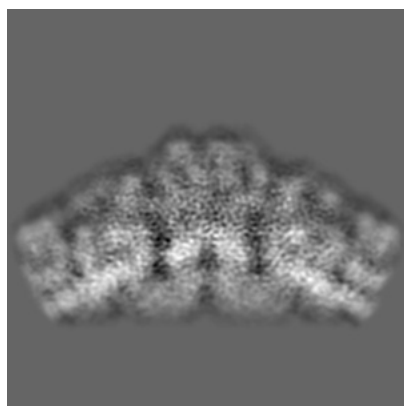
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49591. These allow visual inspection of the internal detail of the map and identification of artifacts.

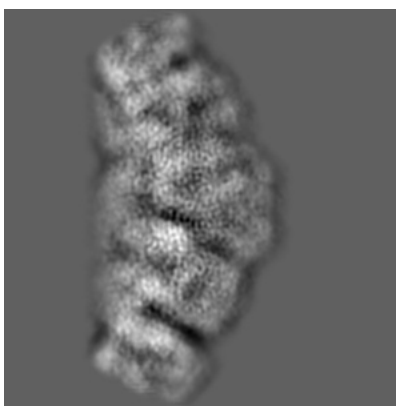
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

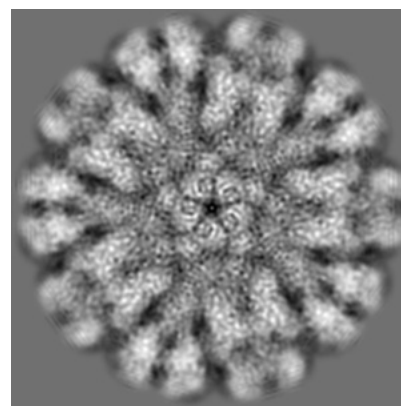
6.1.1 Primary map



X

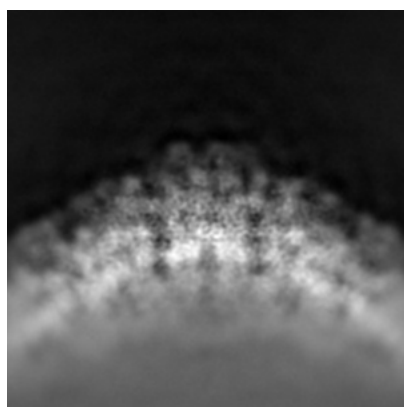


Y

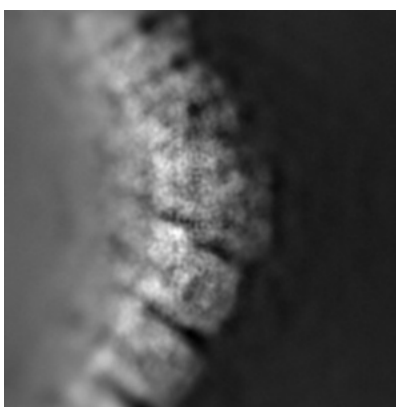


Z

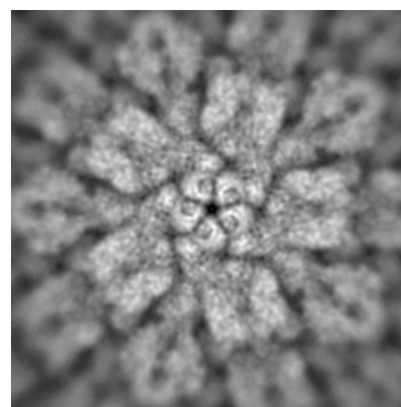
6.1.2 Raw map



X



Y

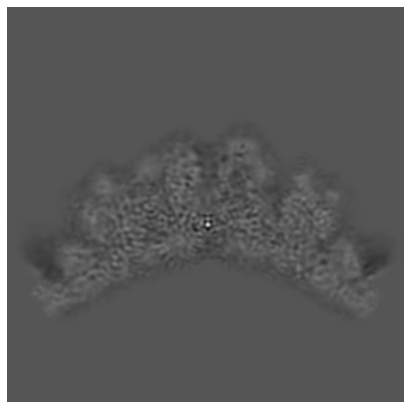


Z

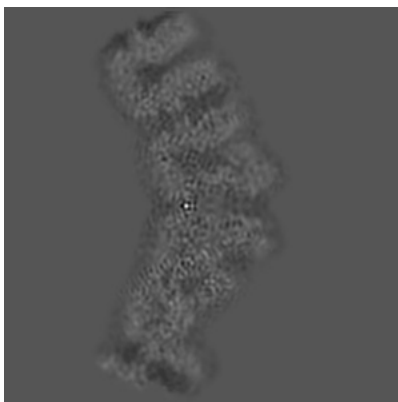
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

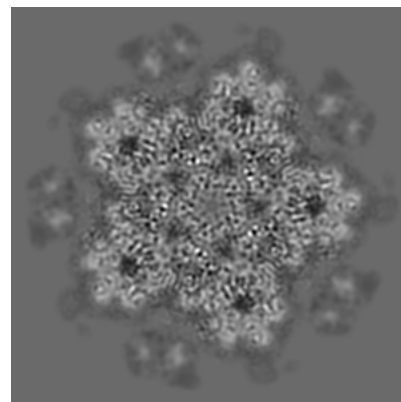
6.2.1 Primary map



X Index: 96

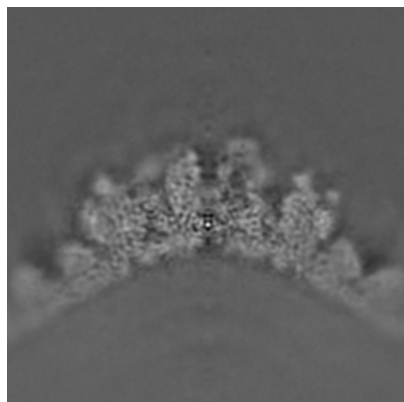


Y Index: 96

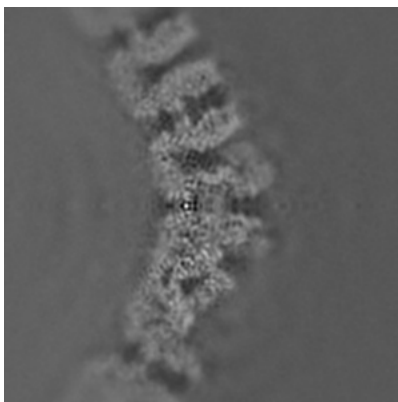


Z Index: 96

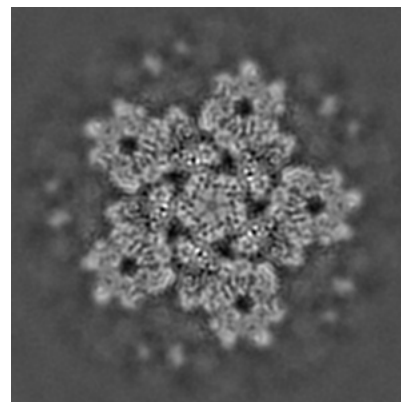
6.2.2 Raw map



X Index: 96



Y Index: 96

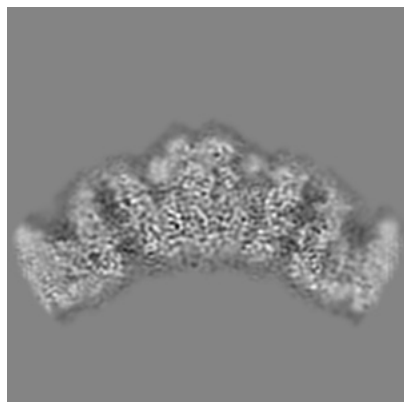


Z Index: 96

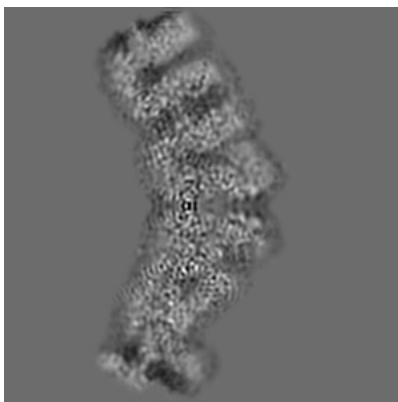
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

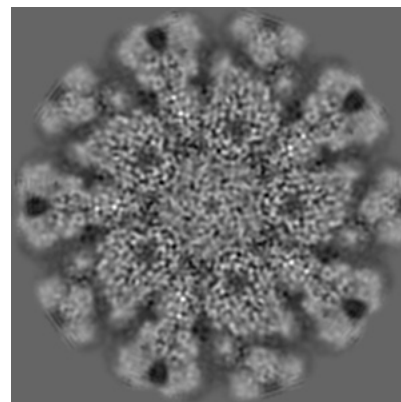
6.3.1 Primary map



X Index: 110

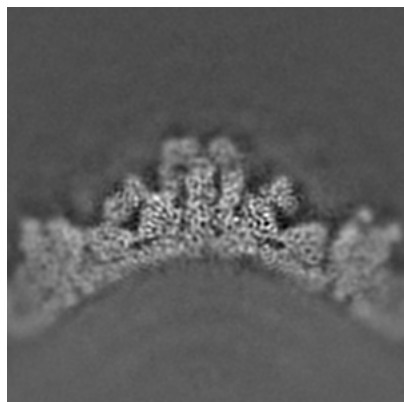


Y Index: 95

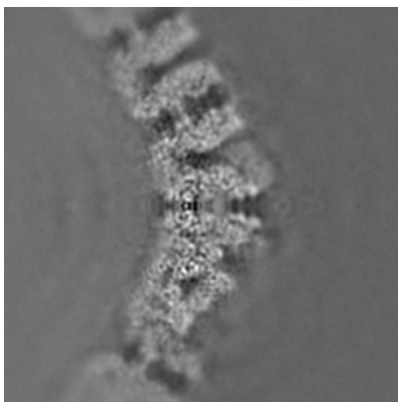


Z Index: 80

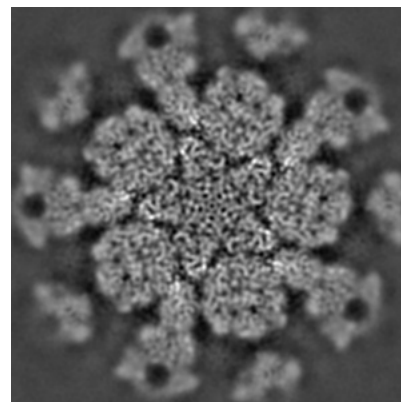
6.3.2 Raw map



X Index: 85



Y Index: 95

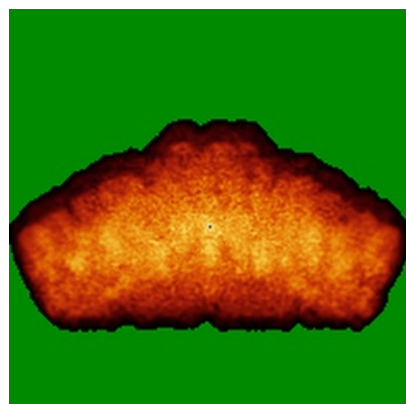


Z Index: 84

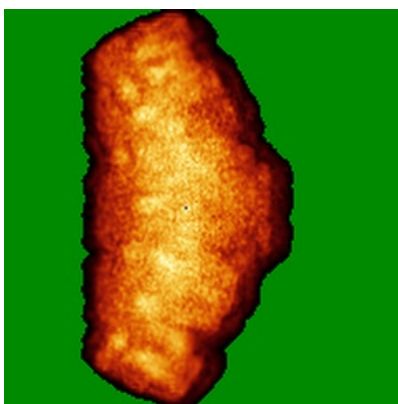
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

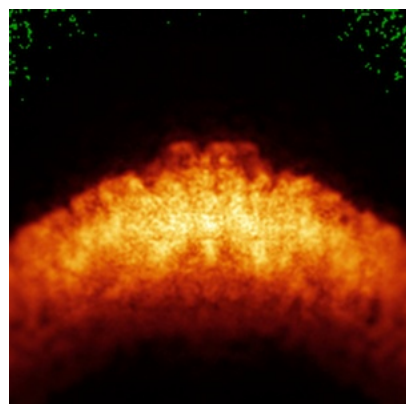


Y

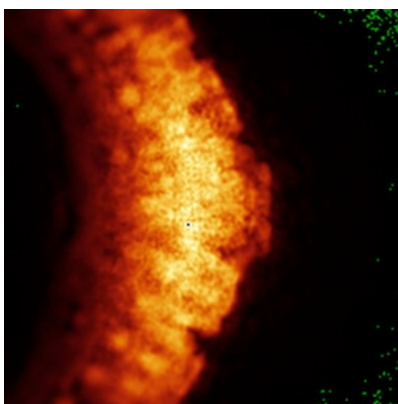


Z

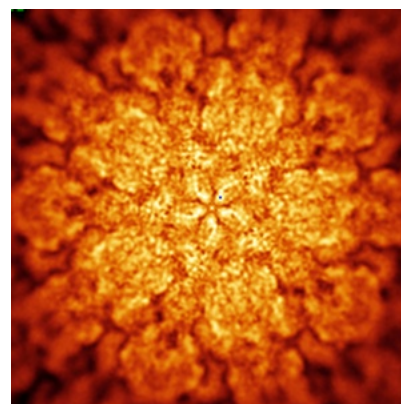
6.4.2 Raw map



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 1.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

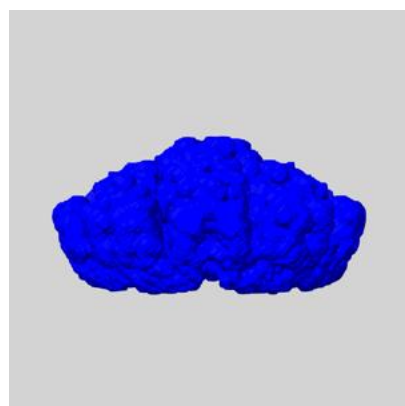
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

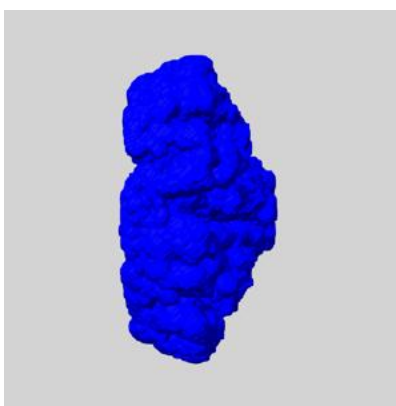
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

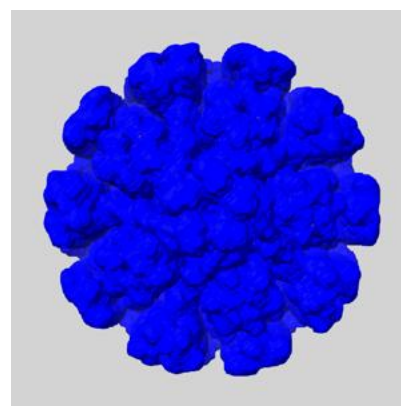
6.6.1 emd_49591_msk_1.map [i](#)



X



Y

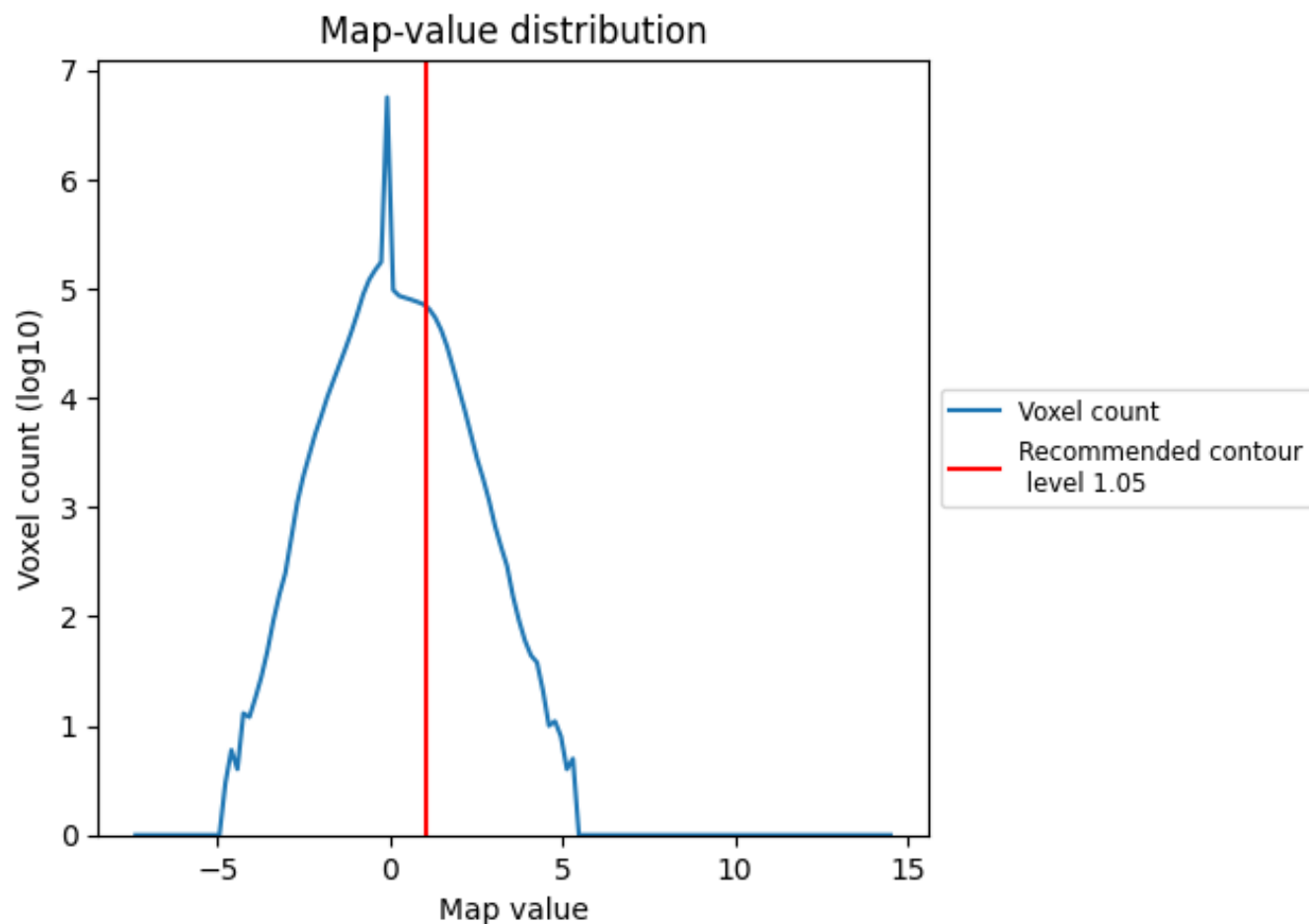


Z

7 Map analysis [i](#)

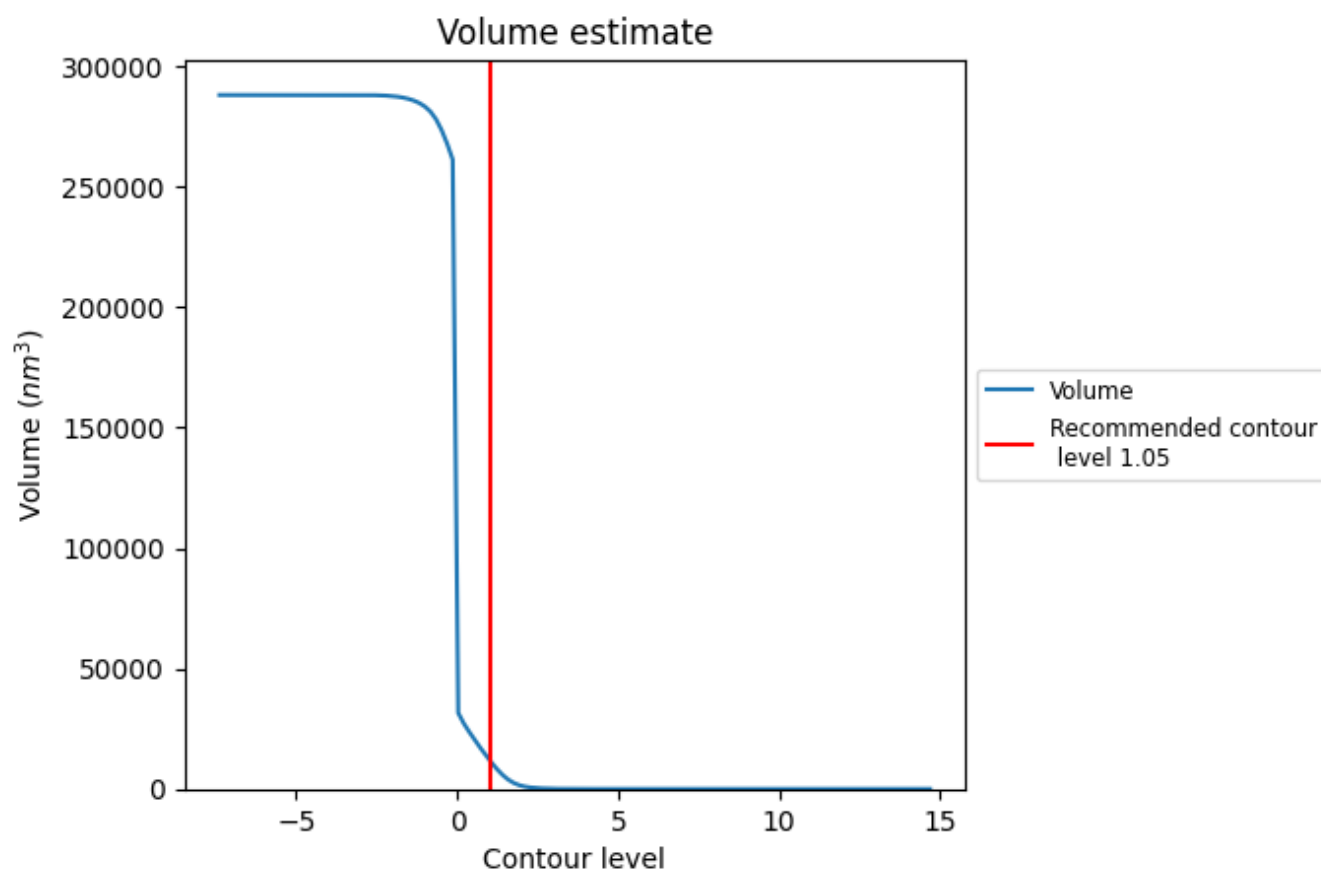
This section contains the results of statistical analysis of the map.

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.

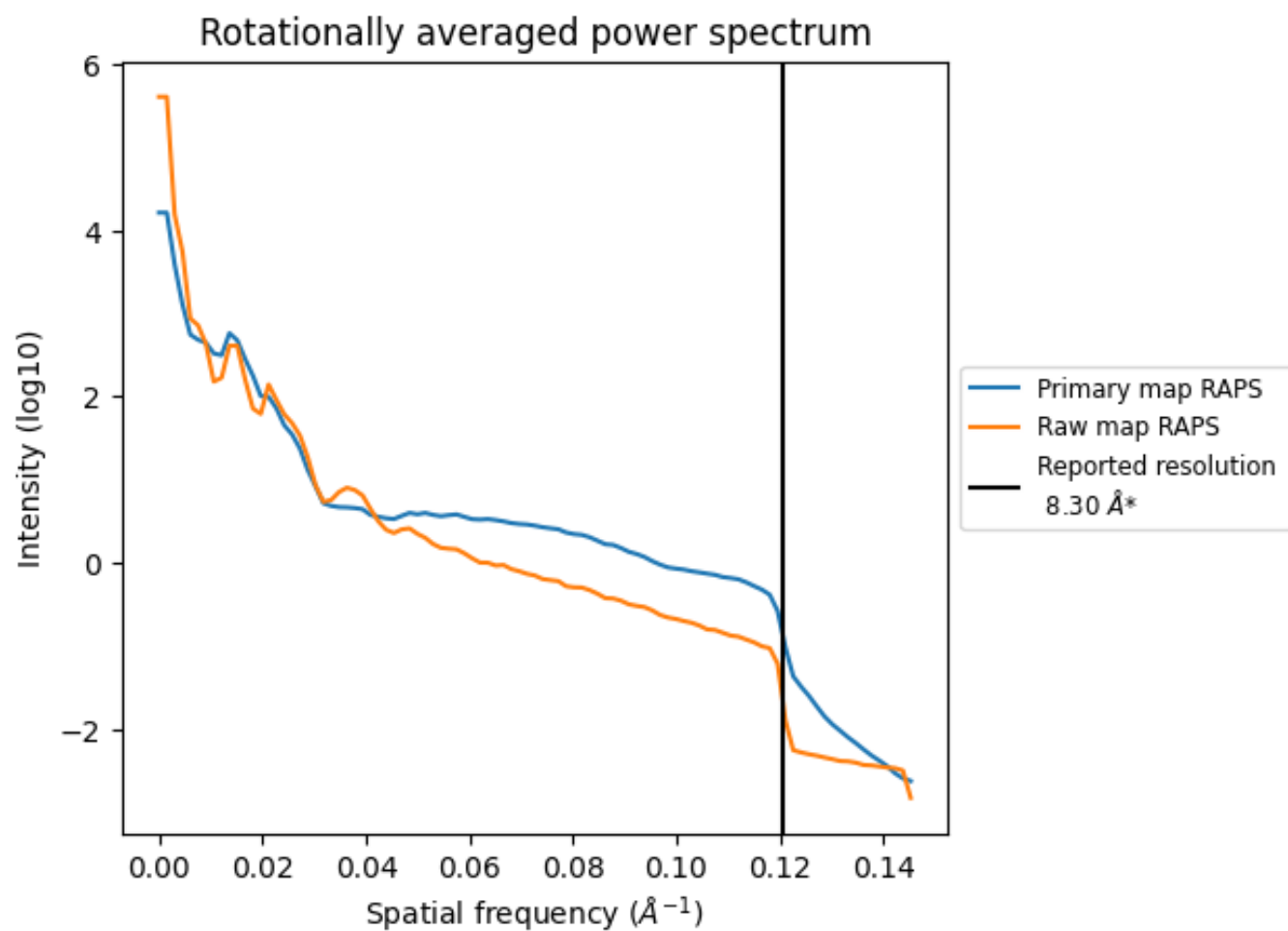
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 11235 nm^3 ; this corresponds to an approximate mass of 10149 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 ⓘ

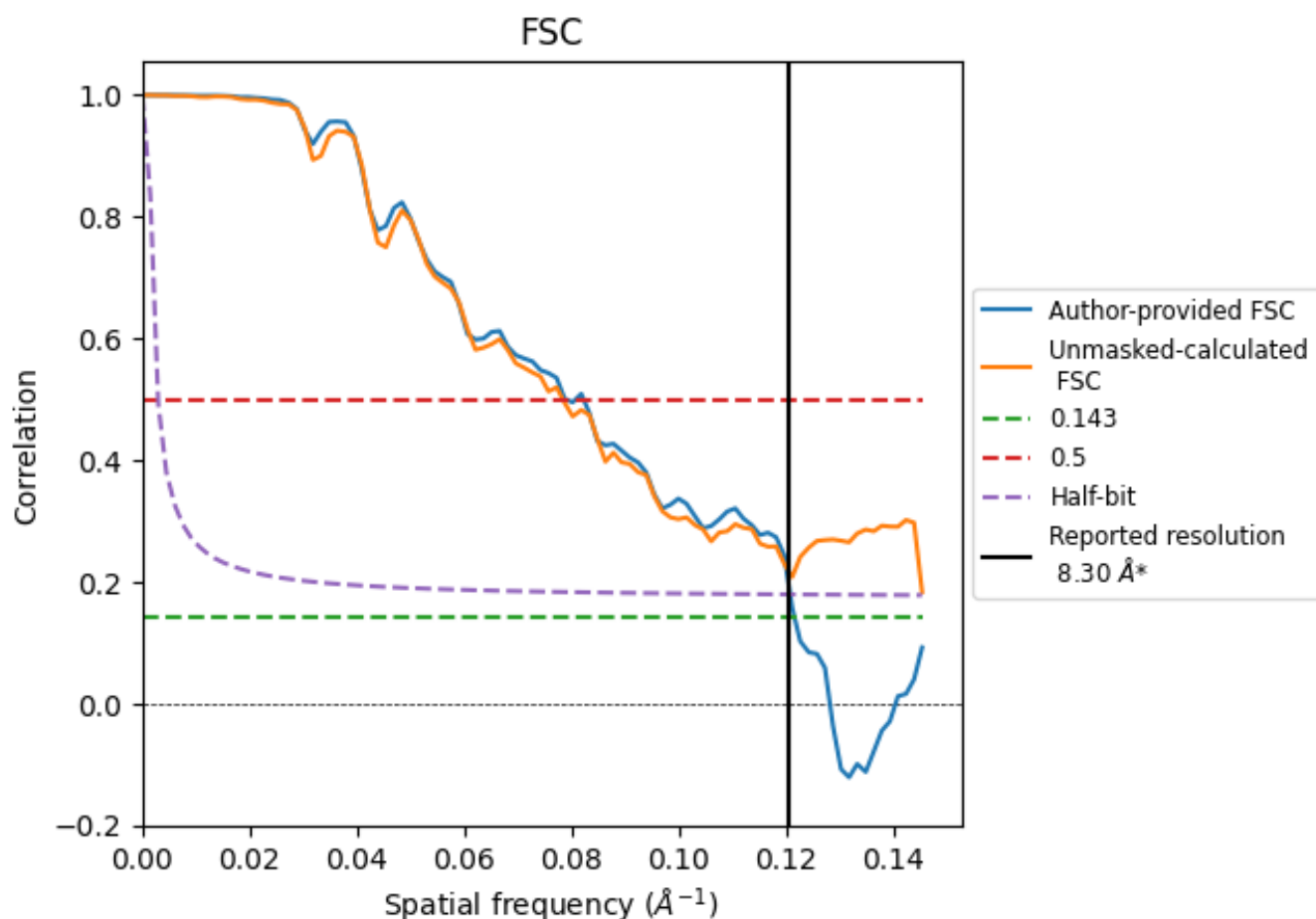


*Reported resolution corresponds to spatial frequency of 0.120 Å⁻¹

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 0.120 \AA^{-1}

8.2 Resolution estimates [i](#)

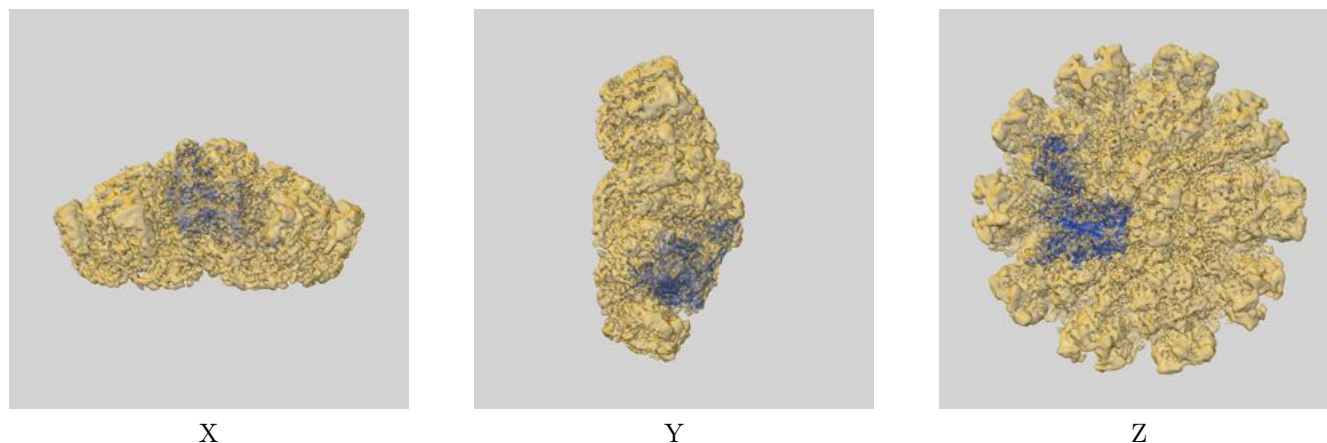
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.30	-	-
Author-provided FSC curve	8.23	12.67	8.29
Unmasked-calculated*	-	12.76	-

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

9 Map-model fit [i](#)

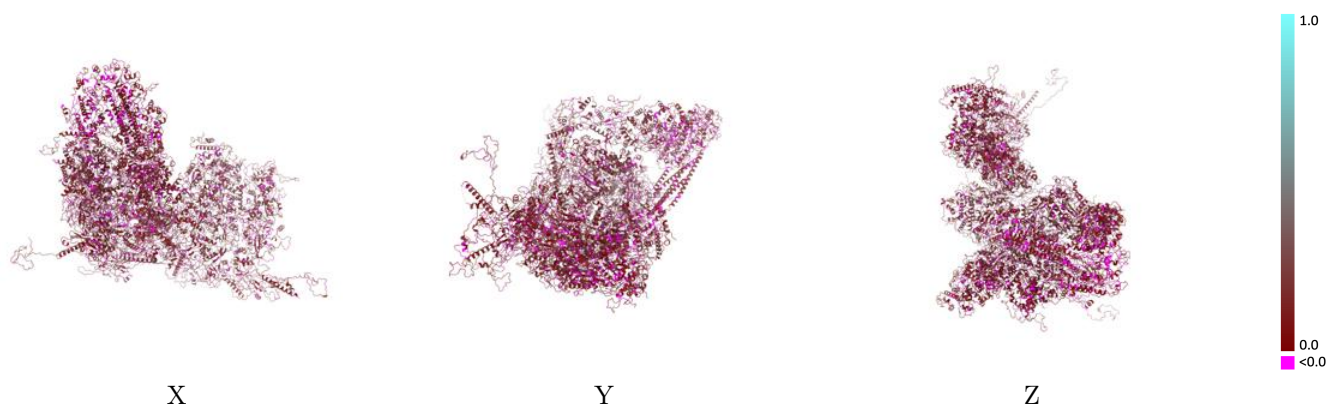
This section contains information regarding the fit between EMDB map EMD-49591 and PDB model 9NO1. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



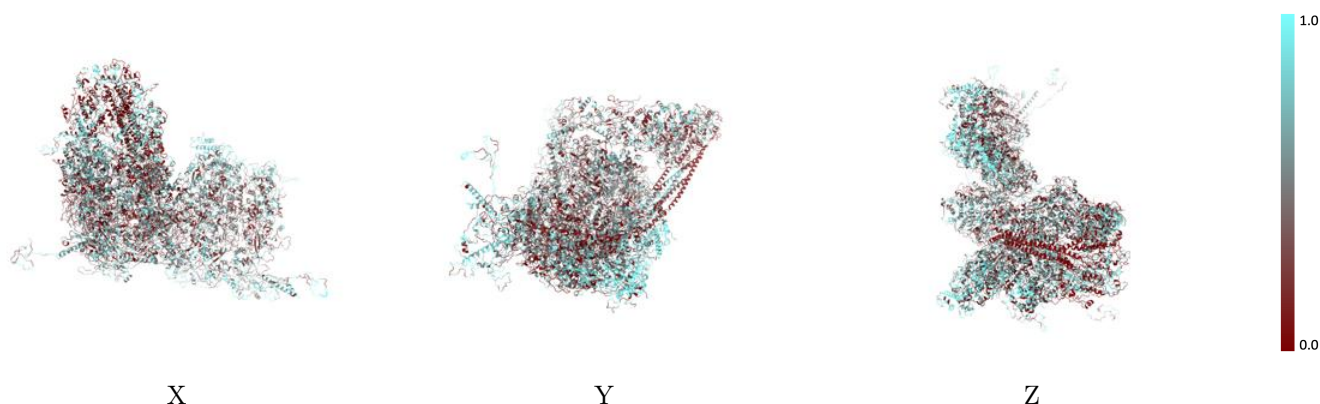
The images above show the 3D surface view of the map at the recommended contour level 1.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



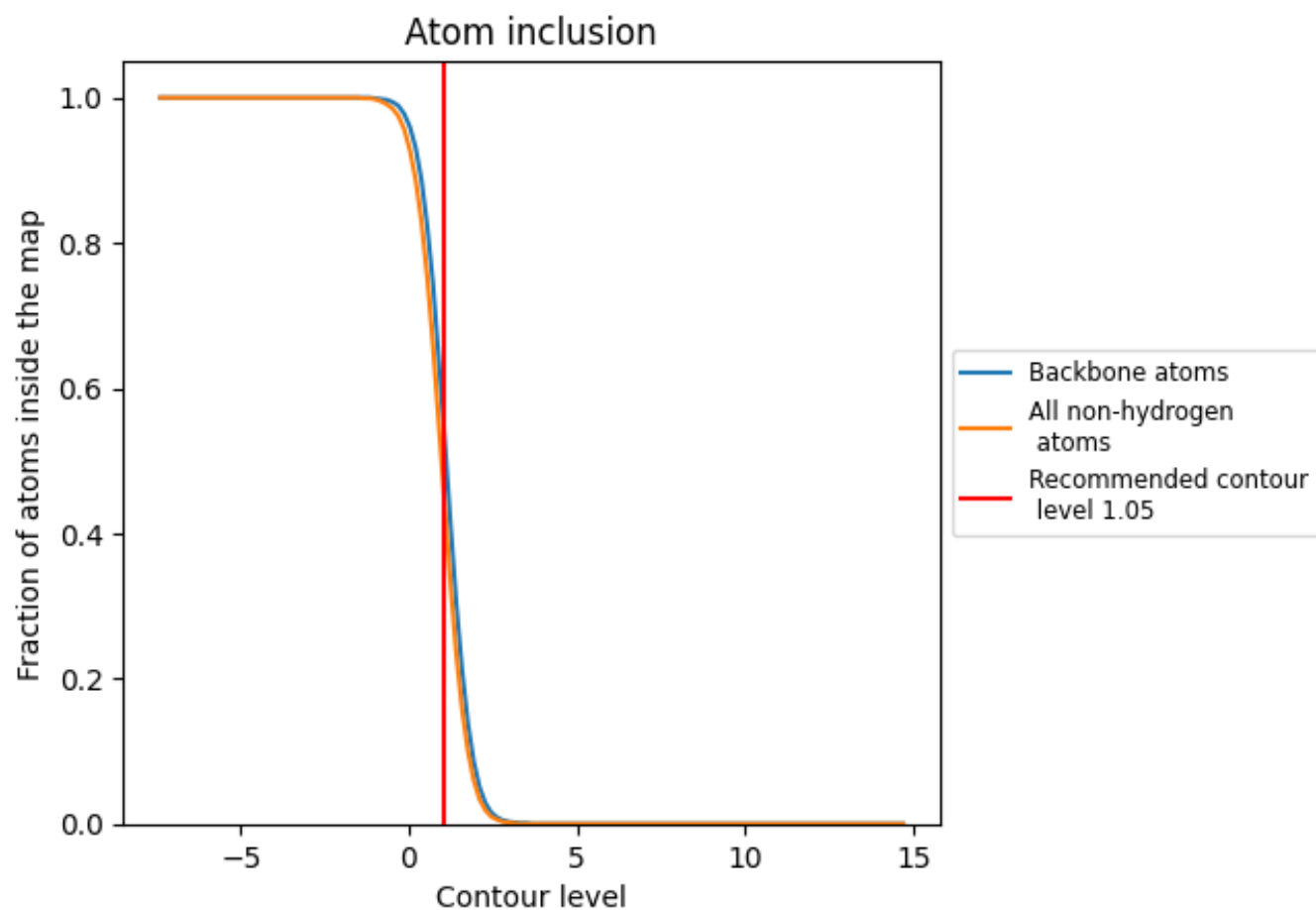
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.05).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 45% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4500	 0.1170
A	 0.4480	 0.1270
B	 0.4660	 0.1120
C	 0.6990	 0.1060
D	 0.4970	 0.1200
E	 0.7370	 0.1210
F	 0.4660	 0.1290
G	 0.7680	 0.1510
H	 0.5030	 0.1200
I	 0.7670	 0.1270
J	 0.4240	 0.1150
K	 0.6740	 0.1120
L	 0.4480	 0.1240
M	 0.7050	 0.1240
N	 0.4170	 0.1370
O	 0.4160	 0.1400
P	 0.4080	 0.1430
Q	 0.4900	 0.1210
R	 0.4150	 0.1290
S	 0.4190	 0.1410
T	 0.3260	 0.1100
U	 0.2520	 0.0660
V	 0.3440	 0.0490
W	 0.5400	 0.1040
X	 0.0920	 0.0440

