



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:56 PM UTC

PDB ID : 7BR8 / pdb_00007br8
EMDB ID : EMD-30159
Title : Epstein-Barr virus, C5 penton vertex, CATC absent.
Authors : Li, Z.; Yu, X.
Deposited on : 2020-03-26
Resolution : 3.80 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:

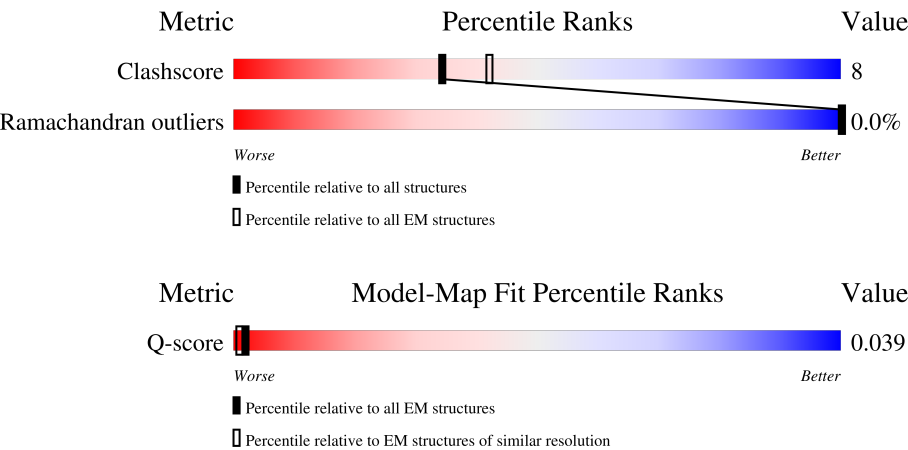
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.80 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	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	2	176	39% 33%9%58%
1	Y	176	35% 40%58%
1	Z	176	37% 39%58%
1	m	176	38% 34%6%60%
1	y	176	36% 32%10%58%

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Mol	Chain	Length	Quality of chain
2	S	1381	
2	T	1381	
2	W	1381	
2	l	1381	
2	x	1381	
3	5	364	
3	e	364	
4	6	301	
4	7	301	
4	f	301	
4	g	301	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 68602 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 Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	71	Total	C	N	O	S	0	0
			600	381	111	107	1		
1	Y	74	Total	C	N	O	S	0	0
			621	394	114	112	1		
1	Z	74	Total	C	N	O	S	0	0
			621	394	114	112	1		
1	2	74	Total	C	N	O	S	0	0
			621	394	114	112	1		
1	y	74	Total	C	N	O	S	0	0
			621	394	114	112	1		

- Molecule 2 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	1333	Total	C	N	O	S	0	0
			10491	6665	1820	1946	60		
2	T	1323	Total	C	N	O	S	0	0
			10398	6600	1808	1929	61		
2	W	1331	Total	C	N	O	S	0	0
			10463	6650	1810	1944	59		
2	x	1325	Total	C	N	O	S	0	0
			10404	6607	1803	1935	59		
2	l	1251	Total	C	N	O	S	0	0
			9883	6283	1717	1824	59		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	e	319	Total	C	N	O	S	0	0
			2505	1608	444	446	7		
3	5	311	Total	C	N	O	S	0	0
			2446	1568	435	436	7		

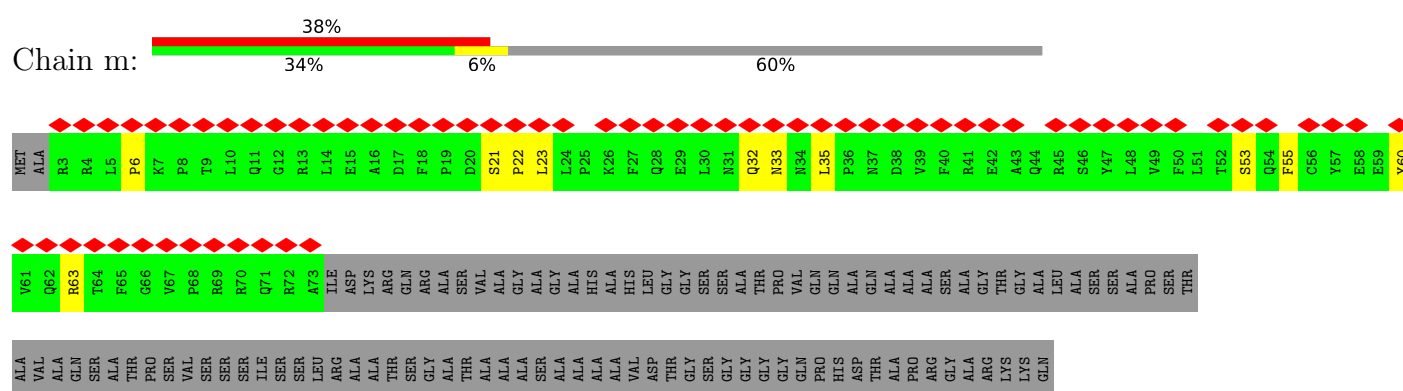
- Molecule 4 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	f	290	Total	C	N	O	S	0	0
			2279	1466	378	419	16		
4	g	281	Total	C	N	O	S	0	0
			2190	1413	358	401	18		
4	6	289	Total	C	N	O	S	0	0
			2272	1461	377	418	16		
4	7	279	Total	C	N	O	S	0	0
			2187	1406	358	405	18		

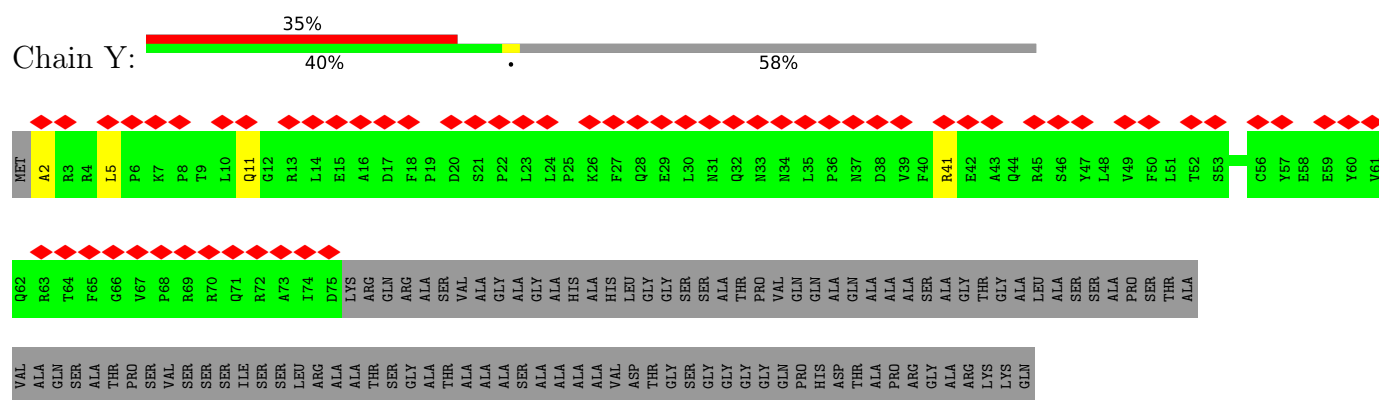
3 Residue-property plots

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.

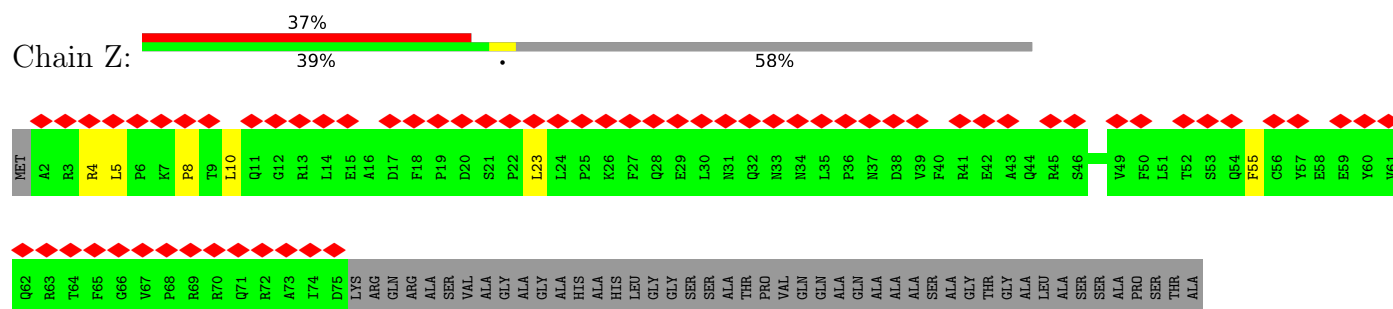
• Molecule 1: Small capsomere-interacting protein



• Molecule 1: Small capsomere-interacting protein



• Molecule 1: Small capsomere-interacting protein



VAL
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SER
VAL
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• Molecule 1: Small capsomere-interacting protein

Chain 2: 

MET
A2
R3
R4
L5
P6
K7
P8
T9
L10
Q11
G12
R13
L14
E15
A16
D17
F18
P19
D20
S21
P22
L23
L24
P25
K26
F27
Q28
E29
L30
N31
Q32
N33
N34
L35
P36
N37
D38
V39
F40
R41
E42
A43
Q44
R45
S46
Y47
L48
V49
F50
L51
T52
S53
C56
Y57
Y60
V61
Q62

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• Molecule 1: Small capsomere-interacting protein

Chain y: 

MET
A2
R3
R4
L5
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K7
P8
T9
L10
Q11
G12
R13
L14
E15
A16
D17
F18
P19
D20
S21
P22
L23
L24
P25
K26
F27
Q28
E29
L30
N31
Q32
N33
N34
L35
P36
N37
D38
V39
F40
R41
E42
A43
Q44
R45
S46
Y47
L48
V49
F50
L51
T52
S53
Q54
F55
C56
Y57
E58
E59
Y60

ALA
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ARG
LYS
LYS
GLN

• Molecule 2: Major capsid protein

Chain S: 

MET
ALA
SER
ASN
E5
G6
V7
E8
P11
F12
P13
Y14
T16
V17
D18
A19
D20
L21
L22
L25
R26
A29
S36
F37
D38
L39
L40
V41
G42
K43
D44
R46
E47
L50
L55
L56
G57
V58
A62
I63
Q64
Y65
V66
R67
F68
L69
E70
T71
A72
L73
A74

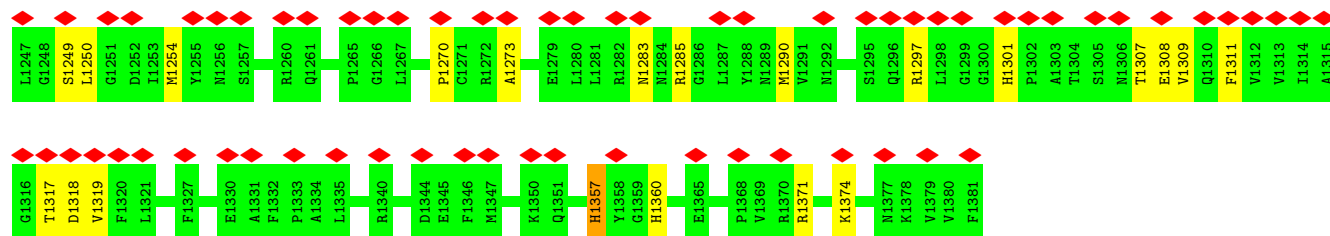
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G91
K92
I93
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F95
R96
I97
S98
I102
A103
H104
G105
R109
P110
S111
A114
T115
F116
K120
N121
K124
I127
S128
T129
S134
M135
L136
D137
L138
E139
I140
L141
E146
V149
E150
Y151
A152

K159
T160
V161
A162
L165
Q166
V169
D170
A171
L172
E173
I177
L181
G182
V183
R186
H187
L189
A198
D199
P200
T201
F202
T203
E204
F207
V211
K212
S213
D214
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F219
E225
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E234
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G239
F240
S241
Q242
L248
S249

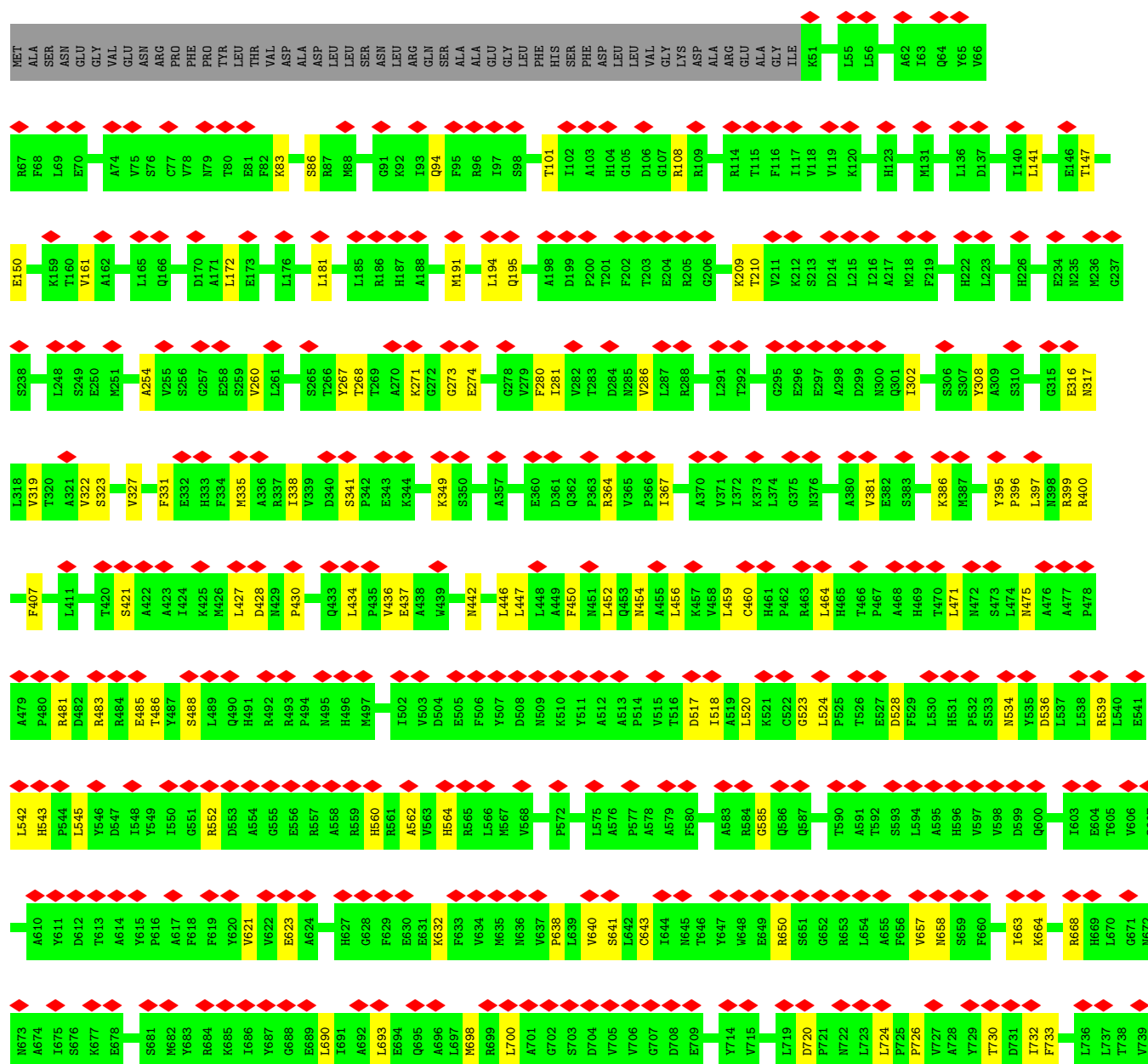
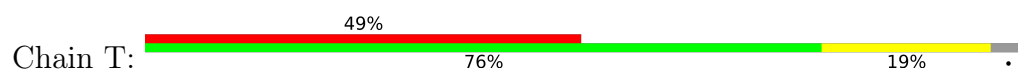
A253
A254
V255
S256
G257
K262
G263
V264
S265
T268
T269
A270
K271
G272
G273
E274
F280
I281
V282
T283
D284
L287
R288
L291
T292
G295
E296
E297
A298
D299
N300
Q301
I302
M303
G304
P305
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G314
G315
E316
N317
T320
S323
Y324
G325
R326

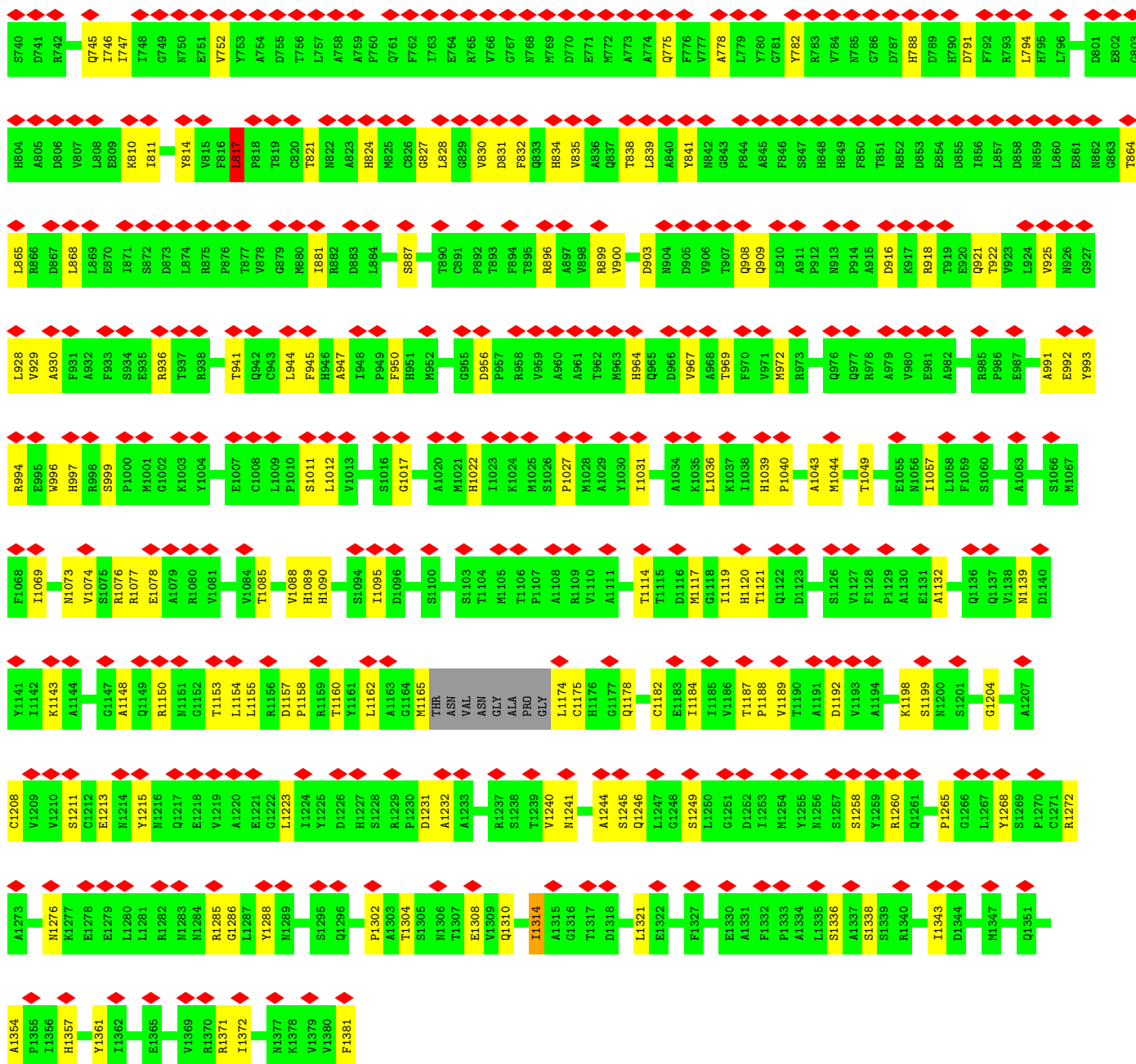
V327
N328
R329
E332
M335
A336
R337
V338
V339
D340
E343
K344
ALA
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SER
THR
LYS
SER
ASP
LEU
PRO
ALA
VAL
ALA
ALA
GLY
VAL
GLU
ASP
GLN
PRO
R364
V365
P366
I367
S368
A369
A370
V371
A378
V379
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Q392
S393
P394
Y395
P396



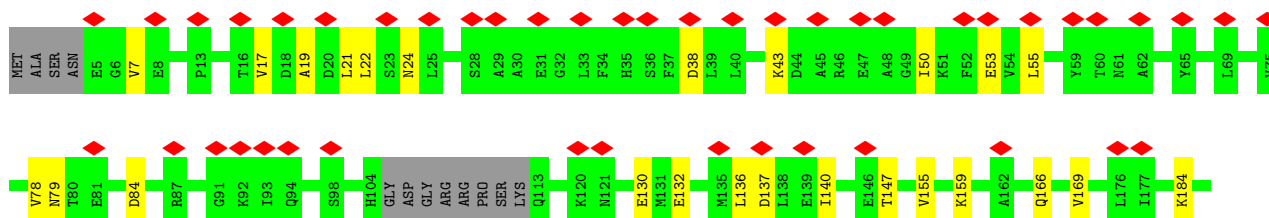
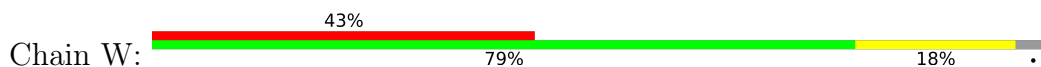


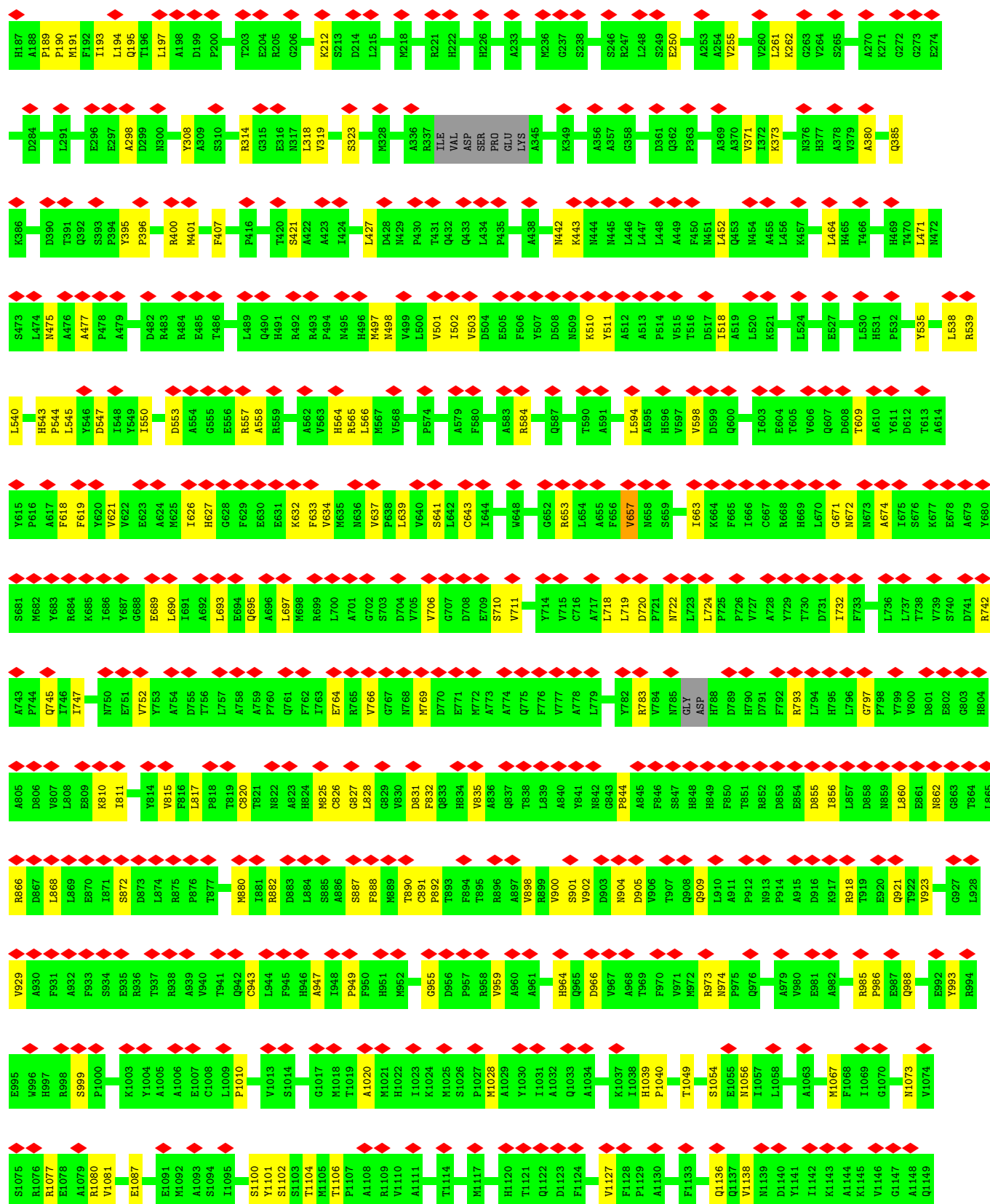
• Molecule 2: Major capsid protein

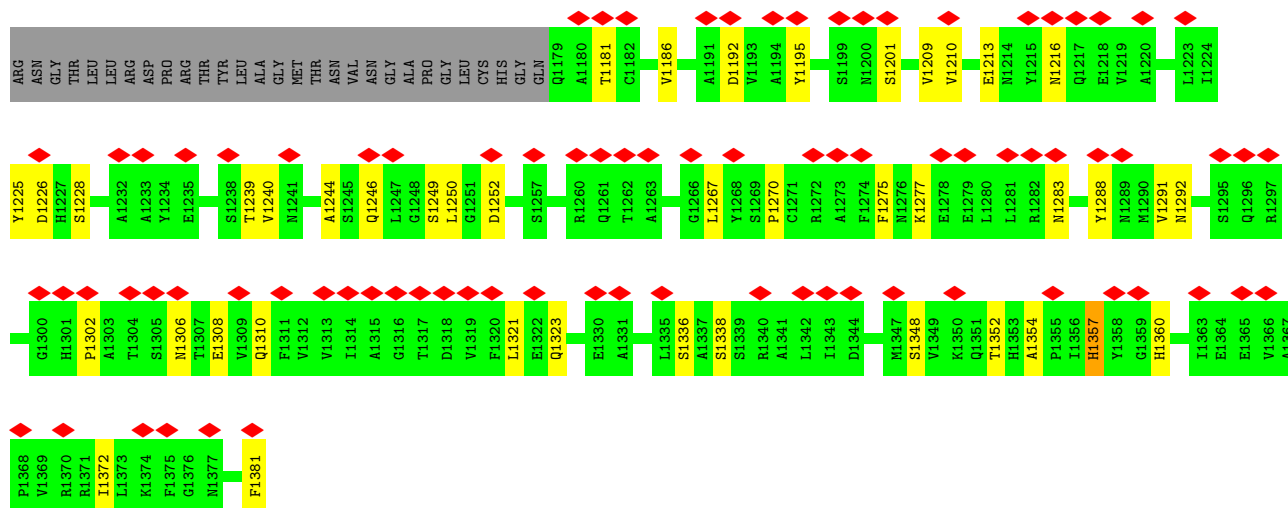




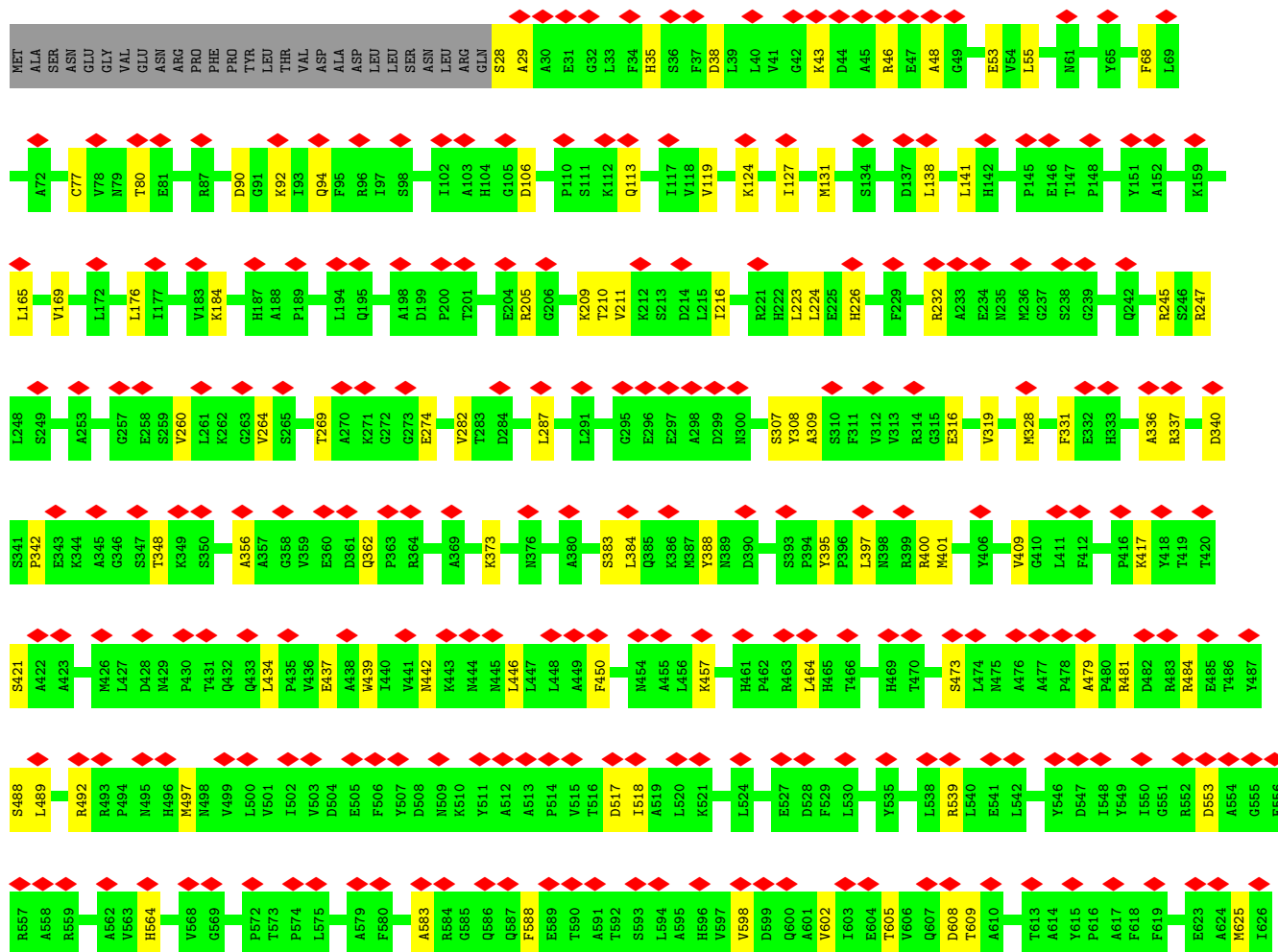
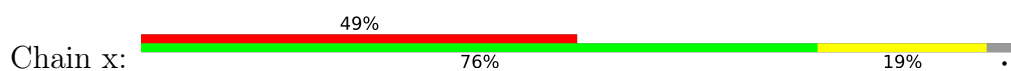
• Molecule 2: Major capsid protein

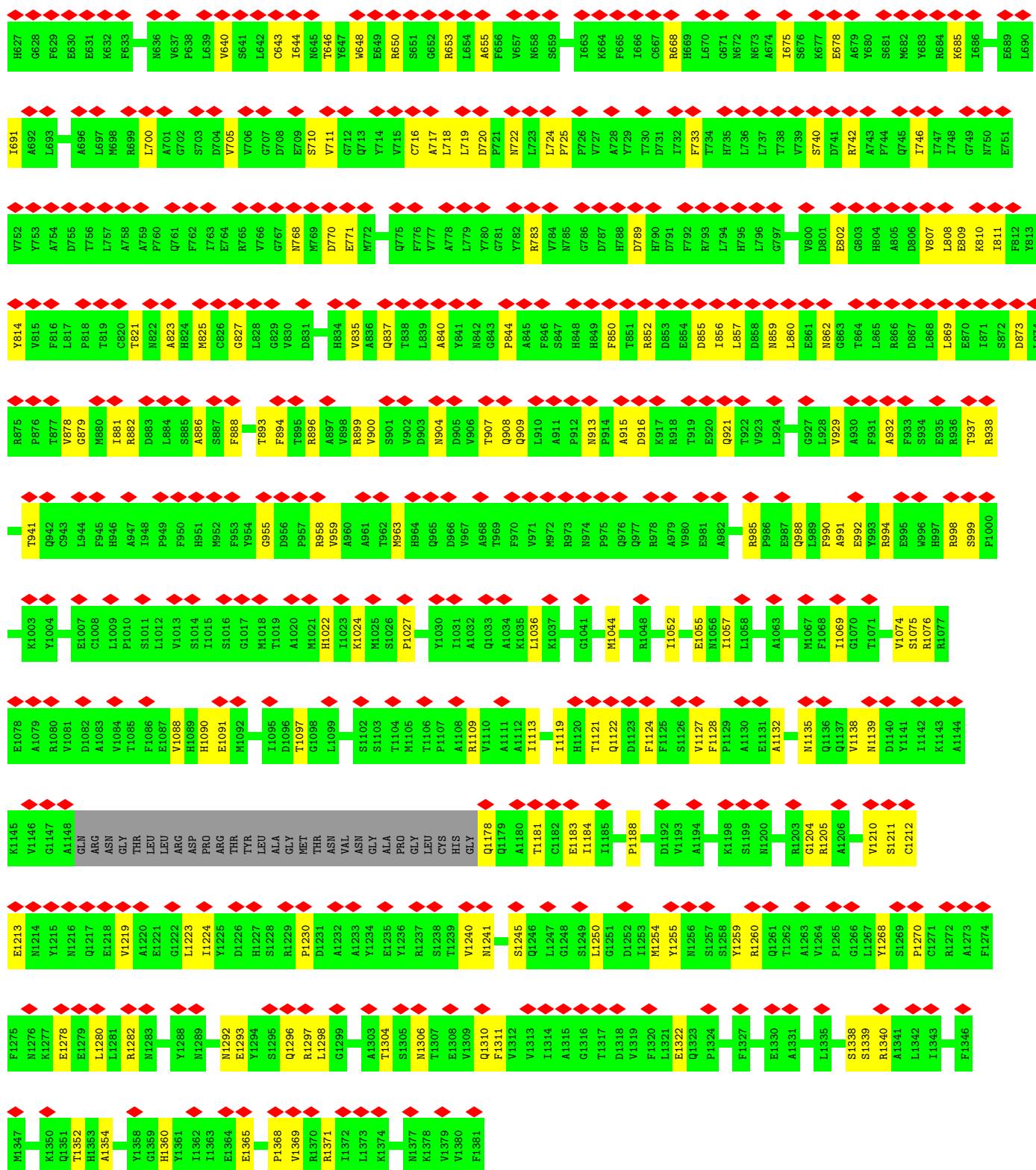




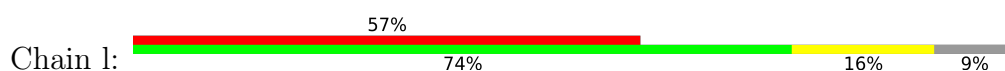


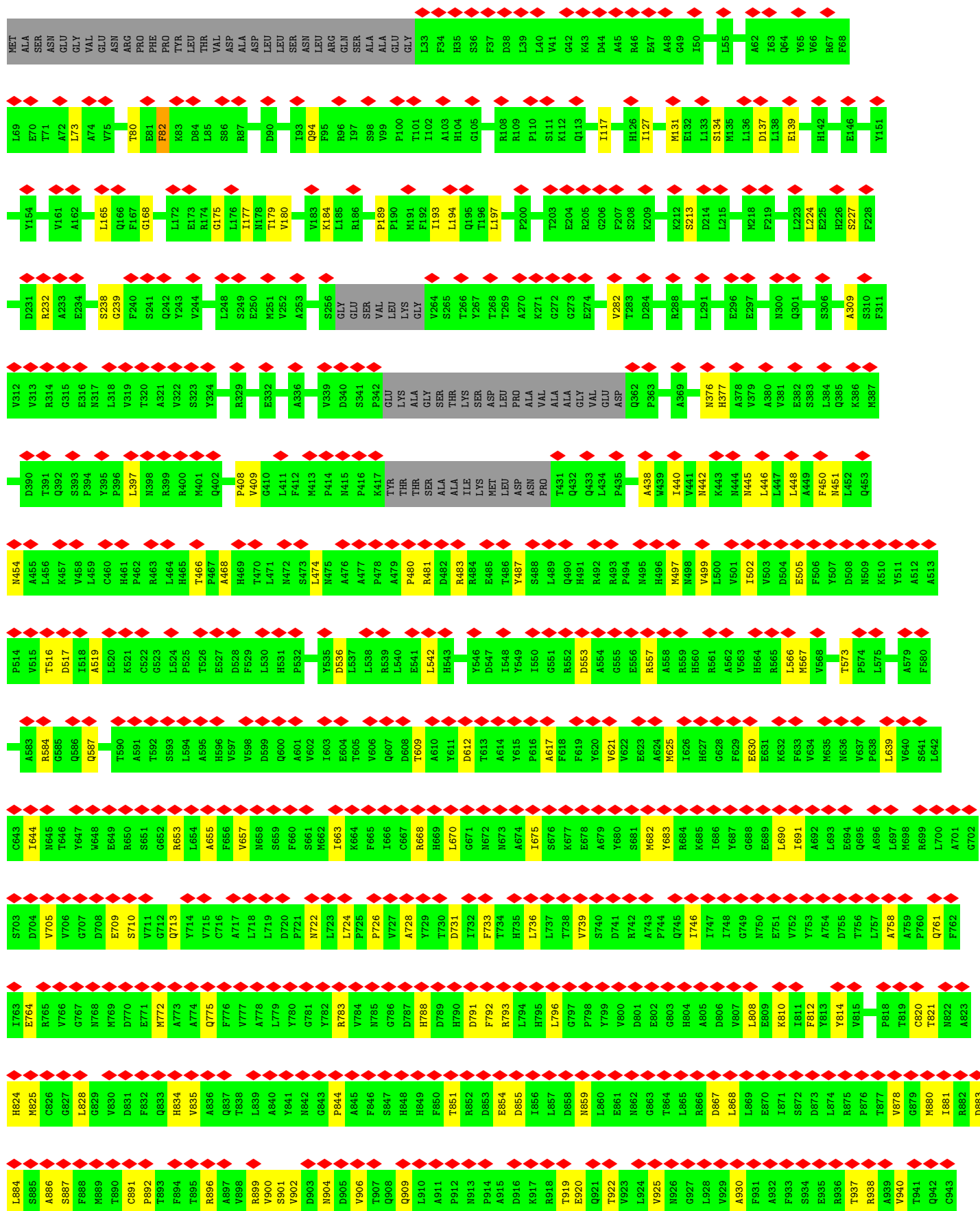
• Molecule 2: Major capsid protein

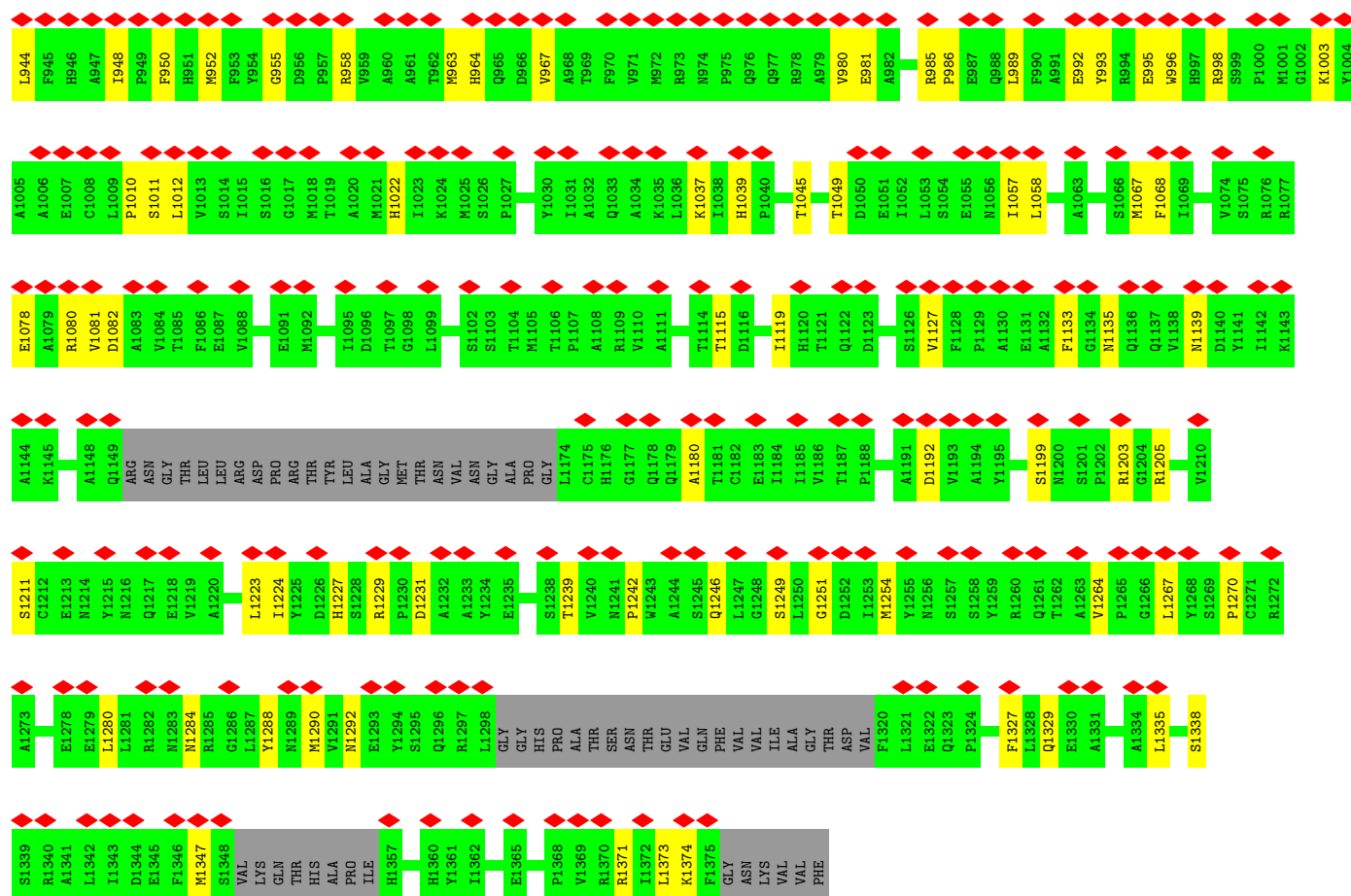




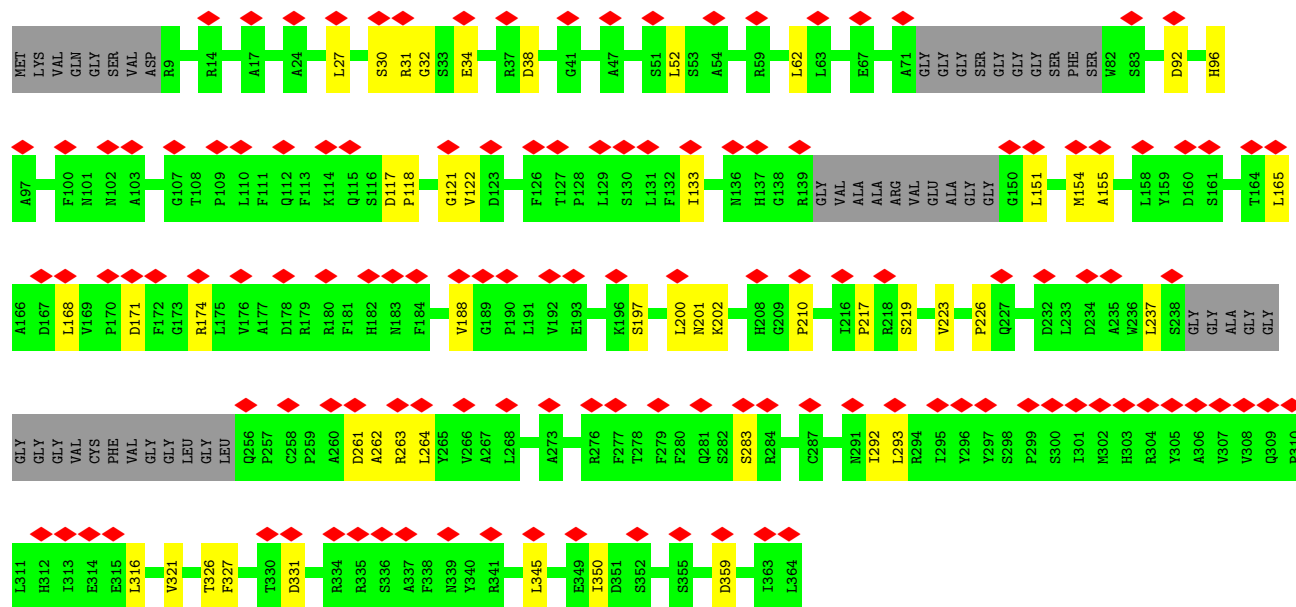
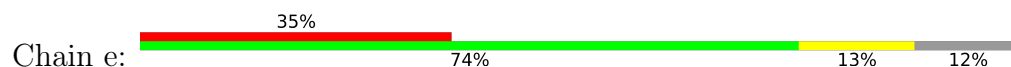
• Molecule 2: Major capsid protein



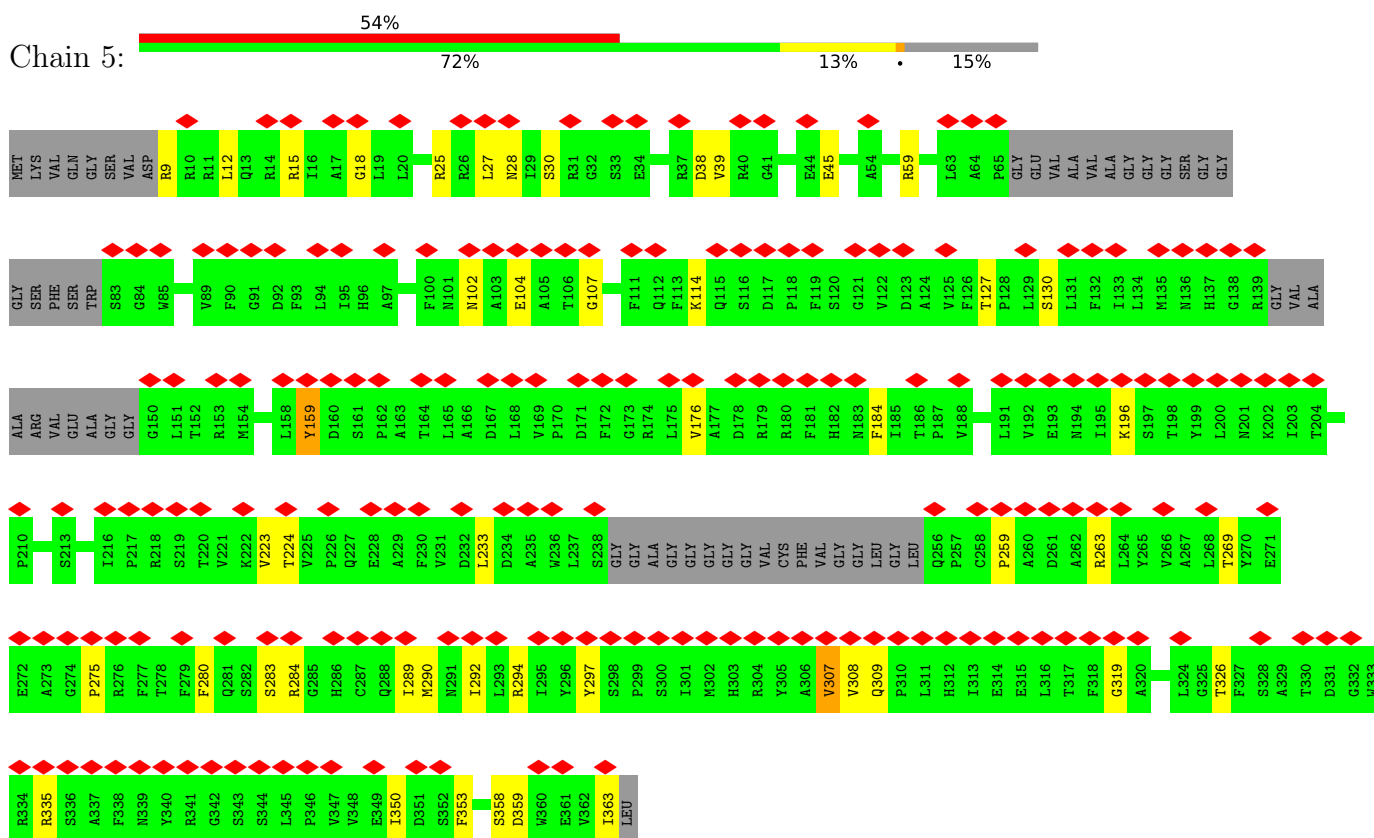




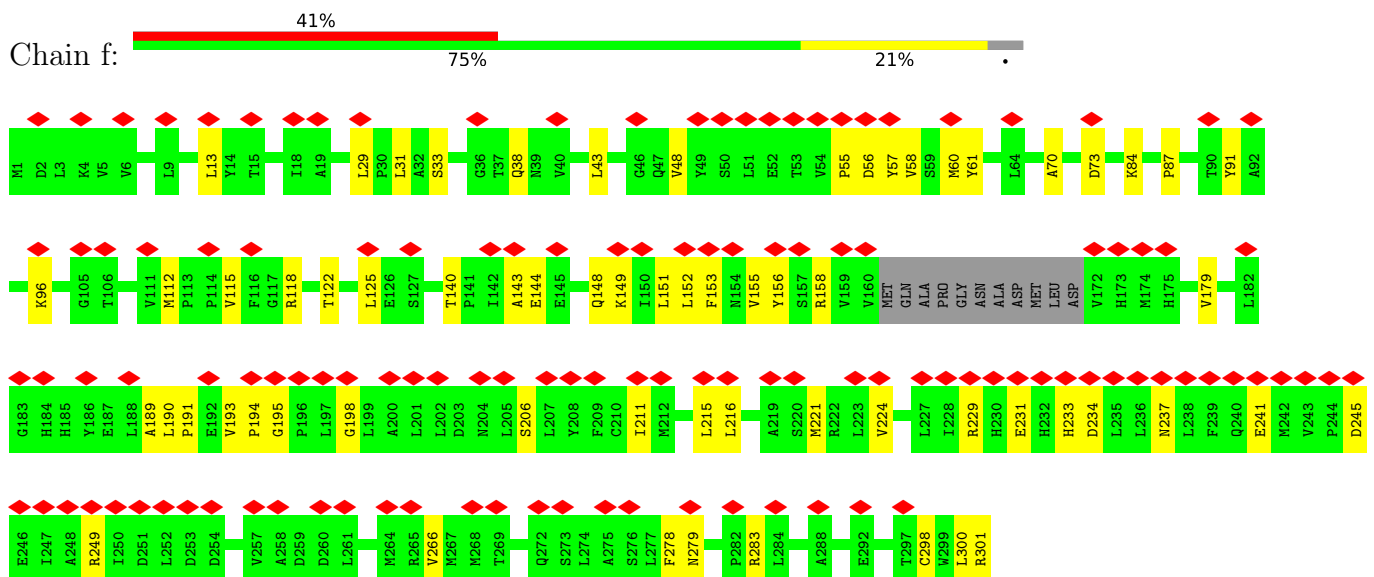
• Molecule 3: Triplex capsid protein 1



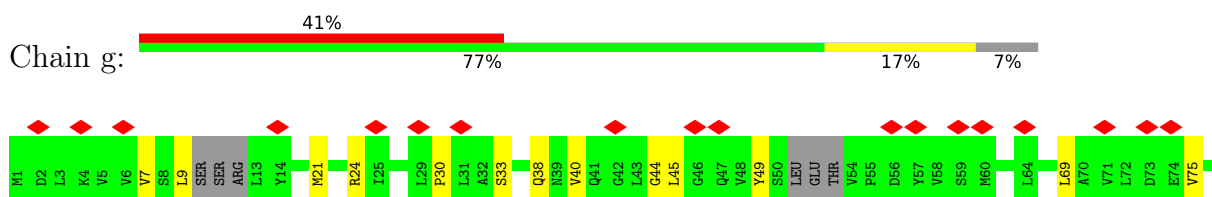
• Molecule 3: Triplex capsid protein 1

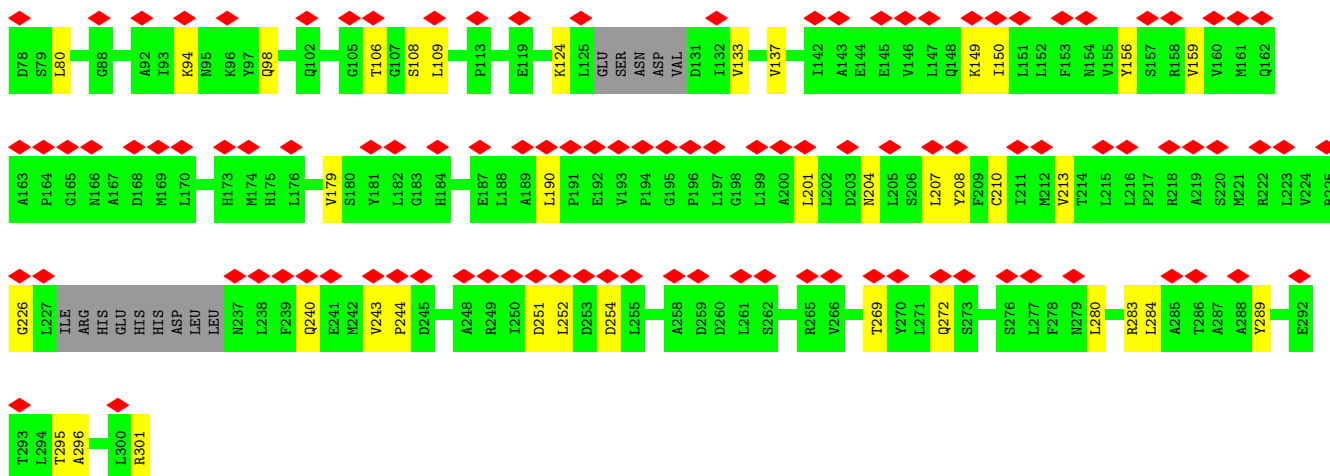


- Molecule 4: Triplex capsid protein 2

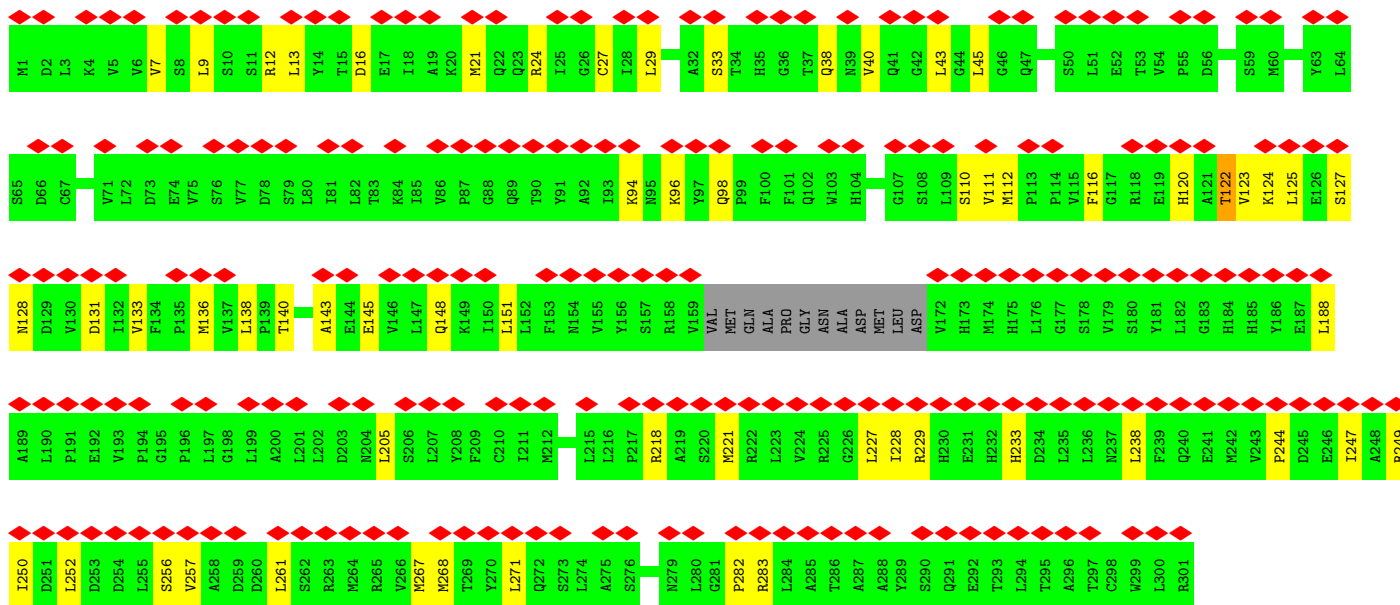
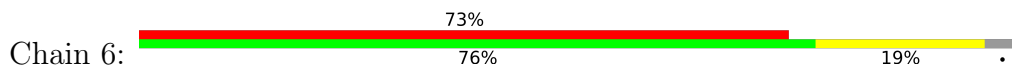


- Molecule 4: Triplex capsid protein 2

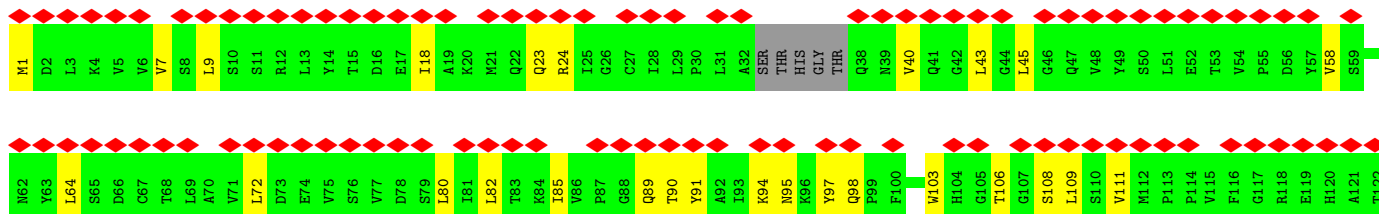
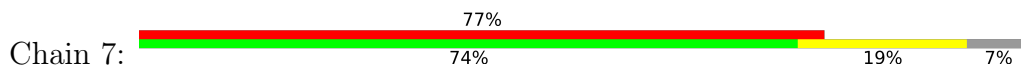




• Molecule 4: Triplex capsid protein 2



• Molecule 4: Triplex capsid protein 2



V123	K124	L125	E126	S127	N128	D129	V130	D131	I132	V133	F134	P135	M136	V137	L138	P139	I142	A143	E144	E145	V146	L147	Q148	K149	I150	L151	L152	F153	N154	V155	Y156	S157	R158	V159	V160	M161	Q162	A163	P164	G165	N166	A167	D168	M169	L170	D171	V172	H173	M174	H175	L176	G177	S178	V179	S180	Y181	L182	G183
H184	H185	Y186	E187	L188	A189	L190	P191	GLU	VAL	PRO	GLY	PRO	LEU	A200	L201	L202	D203	N204	L205	S206	L207	Y208	F209	C210	I211	M212	V213	T214	L215	L216	A219	S220	M221	R222	L223	V224	R225	G226	L227	I228	ARG	HIS	GLU	HIS	HIS	ASP	LEU	N237	L238	F239	Q240	E241	M242	V243	P244			
D245	E246	I247	A248	R249	I250	D251	L252	D253	D254	L255	S256	V257	A258	D259	D260	L261	S262	R263	M264	R265	V266	M267	M268	T269	Y270	L271	Q272	S273	L274	A275	S276	L277	F278	N279	L280	G281	P282	R283	L284	A285	T286	A287	A288	Y289	S290	Q291	E292	T293	L294	T295	A296	T297	C298	W299	L300	R301		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	137356	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.064	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	392.99997, 392.99997, 392.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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	2	0.24	0/636	0.61	1/861 (0.1%)
1	Y	0.20	0/636	0.53	0/861
1	Z	0.21	0/636	0.53	0/861
1	m	0.30	0/615	0.58	0/832
1	y	0.27	0/636	0.54	0/861
2	S	0.32	0/10737	0.55	2/14589 (0.0%)
2	T	0.32	0/10642	0.57	4/14463 (0.0%)
2	W	0.28	0/10706	0.53	1/14549 (0.0%)
2	l	0.25	0/10114	0.57	2/13734 (0.0%)
2	x	0.30	0/10648	0.54	1/14471 (0.0%)
3	5	0.23	0/2511	0.62	2/3418 (0.1%)
3	e	0.30	0/2572	0.61	0/3503
4	6	0.24	0/2320	0.59	0/3159
4	7	0.23	0/2228	0.58	0/3029
4	f	0.24	0/2327	0.59	0/3169
4	g	0.26	0/2233	0.57	0/3037
All	All	0.29	0/70197	0.56	13/95397 (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
2	S	0	1
2	T	0	2
2	W	0	1
3	5	0	1
4	6	0	1
4	7	0	1
All	All	0	7

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	523	GLY	CA-C-N	8.24	133.20	120.68
2	T	523	GLY	C-N-CA	8.24	133.20	120.68
2	T	1314	ILE	N-CA-C	-6.44	107.59	113.71
3	5	159	TYR	CA-C-N	6.41	129.15	120.38
3	5	159	TYR	C-N-CA	6.41	129.15	120.38
2	W	657	VAL	N-CA-C	-6.33	106.34	112.29
2	x	211	VAL	N-CA-C	-5.60	107.36	112.96
2	T	817	LEU	CA-CB-CG	5.47	135.45	116.30
2	S	1179	GLN	CA-C-N	-5.35	114.65	122.78
2	S	1179	GLN	C-N-CA	-5.35	114.65	122.78
2	l	82	PHE	CA-C-N	5.19	131.45	121.54
2	l	82	PHE	C-N-CA	5.19	131.45	121.54
1	2	67	VAL	N-CA-C	5.12	119.94	108.88

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	5	307	VAL	Peptide
4	6	122	THR	Peptide
4	7	278	PHE	Peptide
2	S	1357	HIS	Peptide
2	T	1357	HIS	Peptide
2	T	817	LEU	Peptide
2	W	1357	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	621	0	611	15	0
1	Y	621	0	611	4	0
1	Z	621	0	611	6	0
1	m	600	0	591	10	0
1	y	621	0	611	13	0
2	S	10491	0	10318	194	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	10398	0	10232	227	0
2	W	10463	0	10288	184	0
2	l	9883	0	9710	150	0
2	x	10404	0	10234	183	0
3	5	2446	0	2422	31	0
3	e	2505	0	2479	42	0
4	6	2272	0	2307	41	0
4	7	2187	0	2222	35	0
4	f	2279	0	2316	42	0
4	g	2190	0	2228	33	0
All	All	68602	0	67791	1104	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 8.

All (1104) 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)
2:T:1160:THR:HG21	2:T:1314:ILE:CD1	1.05	1.50
2:T:1160:THR:CG2	2:T:1314:ILE:CD1	1.93	1.47
2:T:1160:THR:CG2	2:T:1314:ILE:HD11	1.47	1.41
2:S:788:HIS:NE2	2:S:893:THR:CG2	1.84	1.38
2:W:518:ILE:HD11	2:W:547:ASP:OD2	1.27	1.31
2:S:788:HIS:NE2	2:S:893:THR:HG21	0.91	1.24
2:T:209:LYS:HE3	2:T:1213:GLU:HA	1.25	1.11
2:S:1175:CYS:HB2	2:T:1223:LEU:HD13	1.27	1.10
2:W:1372:ILE:HG22	2:W:1381:PHE:HD2	1.12	1.10
2:S:788:HIS:CE1	2:S:893:THR:HG21	1.87	1.09
2:S:1120:HIS:CD2	2:S:1179:GLN:OE1	2.07	1.07
2:x:316:GLU:HG2	2:x:331:PHE:CE2	1.90	1.06
2:T:209:LYS:CE	2:T:1213:GLU:HA	1.87	1.05
2:S:1175:CYS:HB2	2:T:1223:LEU:CD1	1.87	1.03
2:T:1160:THR:HG21	2:T:1314:ILE:HD12	1.02	1.02
2:W:518:ILE:CD1	2:W:547:ASP:OD2	2.07	1.02
2:T:1160:THR:HG21	2:T:1314:ILE:CG1	1.90	1.01
2:T:1372:ILE:CD1	2:T:1381:PHE:HD1	1.72	1.01
2:S:788:HIS:CD2	2:S:893:THR:HG21	1.95	1.00
2:T:1155:LEU:O	2:T:1265:PRO:O	1.79	1.00
2:W:1372:ILE:HG22	2:W:1381:PHE:CD2	1.96	0.99
2:x:1132:ALA:HB1	2:x:1139:ASN:ND2	1.78	0.99
2:S:1178:GLN:HG2	2:S:1307:THR:O	1.63	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:385:GLN:HG3	2:W:395:TYR:HD2	1.29	0.98
2:x:316:GLU:HG2	2:x:331:PHE:CD2	1.99	0.97
2:T:1154:LEU:HD13	2:T:1165:MET:HE2	1.45	0.96
2:T:1160:THR:HG21	2:T:1314:ILE:HD11	1.01	0.96
2:T:1160:THR:CG2	2:T:1314:ILE:CG1	2.42	0.96
2:W:385:GLN:HG3	2:W:395:TYR:CD2	2.01	0.95
2:T:1157:ASP:OD1	2:T:1158:PRO:HD2	1.67	0.93
2:T:1132:ALA:HB1	2:T:1139:ASN:HD21	1.34	0.93
2:S:998:ARG:HG2	2:S:998:ARG:HH11	1.33	0.92
2:S:1175:CYS:CB	2:T:1223:LEU:HD13	1.98	0.92
2:S:1120:HIS:CG	2:S:1179:GLN:OE1	2.22	0.92
2:T:1160:THR:O	3:e:121:GLY:HA3	1.70	0.91
2:T:1372:ILE:HD13	2:T:1381:PHE:HD1	1.35	0.90
2:W:518:ILE:CD1	2:W:993:TYR:CE1	2.56	0.88
2:T:1120:HIS:NE2	2:T:1150:ARG:NH1	2.23	0.87
2:T:1178:GLN:HE21	2:T:1310:GLN:HG2	1.38	0.86
2:W:385:GLN:CG	2:W:395:TYR:HD2	1.87	0.86
2:W:395:TYR:HD1	2:W:396:PRO:HD2	1.39	0.85
2:S:706:VAL:HG11	2:S:1138:VAL:HG23	1.59	0.85
2:S:780:TYR:O	2:S:784:VAL:HG22	1.76	0.85
2:T:1160:THR:CG2	2:T:1314:ILE:HG13	2.07	0.85
2:T:1372:ILE:CD1	2:T:1381:PHE:CD1	2.60	0.84
2:W:314:ARG:HG3	2:W:314:ARG:HH11	1.40	0.84
2:T:1178:GLN:NE2	2:T:1310:GLN:HG2	1.92	0.84
2:T:1160:THR:HG23	2:T:1314:ILE:HD11	1.59	0.82
2:T:319:VAL:O	2:T:323:SER:HB3	1.80	0.82
2:S:788:HIS:CD2	2:S:893:THR:OG1	2.32	0.81
2:W:518:ILE:HD12	2:W:993:TYR:CE1	2.15	0.81
2:S:781:GLY:O	2:S:785:ASN:O	1.97	0.81
2:T:1174:LEU:HG	2:T:1308:GLU:HG2	1.60	0.81
2:S:1177:GLY:HA2	2:T:210:THR:HG22	1.61	0.81
2:S:783:ARG:NH1	2:S:888:PHE:O	2.12	0.80
2:T:209:LYS:HE3	2:T:1213:GLU:CA	2.07	0.80
2:S:1175:CYS:HG	2:T:1208:CYS:HG	1.11	0.79
2:S:788:HIS:HD2	2:S:893:THR:OG1	1.65	0.79
2:S:497:MET:HE2	2:S:788:HIS:O	1.81	0.79
1:Y:2:ALA:N	2:S:789:ASP:OD2	2.16	0.79
2:W:1372:ILE:CG2	2:W:1381:PHE:HD2	1.96	0.79
2:W:385:GLN:CG	2:W:395:TYR:CD2	2.63	0.79
2:x:316:GLU:CG	2:x:331:PHE:CE2	2.65	0.79
2:S:1176:HIS:CD2	2:T:1232:ALA:CB	2.67	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:1132:ALA:HB1	2:x:1139:ASN:HD22	1.45	0.78
2:l:772:MET:HE3	2:l:775:GLN:HB2	1.66	0.77
2:T:1372:ILE:HD11	2:T:1381:PHE:CD1	2.19	0.77
2:W:314:ARG:HG3	2:W:314:ARG:NH1	1.98	0.77
2:S:998:ARG:HG2	2:S:998:ARG:NH1	1.99	0.76
2:T:1155:LEU:N	2:T:1155:LEU:HD12	2.01	0.76
2:x:1292:ASN:O	2:x:1296:GLN:HB2	1.84	0.76
2:S:788:HIS:CD2	2:S:893:THR:CG2	2.60	0.75
2:W:1028:MET:CE	2:W:1138:VAL:HG22	2.17	0.75
2:l:127:ILE:HD11	2:l:179:THR:HG23	1.69	0.74
2:l:1288:TYR:CE2	2:l:1292:ASN:ND2	2.56	0.73
2:S:706:VAL:CG1	2:S:1138:VAL:HG23	2.19	0.73
2:W:1136:GLN:HA	2:W:1136:GLN:NE2	2.03	0.73
2:T:1160:THR:CB	2:T:1314:ILE:HD11	2.18	0.73
2:S:1308:GLU:CD	2:S:1308:GLU:H	1.96	0.72
2:T:1132:ALA:HB1	2:T:1139:ASN:ND2	2.03	0.72
2:S:1176:HIS:CD2	2:T:1232:ALA:HB3	2.25	0.71
4:7:172:VAL:O	4:7:176:LEU:HB2	1.91	0.71
2:T:1372:ILE:HD11	2:T:1381:PHE:HD1	1.51	0.70
2:x:316:GLU:CG	2:x:331:PHE:CD2	2.75	0.70
2:T:1174:LEU:HD13	2:T:1174:LEU:N	2.06	0.70
2:S:1116:ASP:HB2	2:S:1178:GLN:O	1.91	0.70
2:W:395:TYR:CD1	2:W:396:PRO:HD2	2.26	0.70
2:T:1154:LEU:N	2:T:1154:LEU:HD22	2.07	0.70
2:T:427:LEU:O	2:T:428:ASP:OD1	2.10	0.70
2:S:788:HIS:NE2	2:S:893:THR:CB	2.55	0.69
1:y:10:LEU:HB3	1:y:45:ARG:HH22	1.58	0.69
2:x:316:GLU:OE2	2:x:316:GLU:N	2.26	0.68
2:W:79:ASN:HB3	2:W:308:TYR:HD1	1.59	0.68
2:x:216:ILE:HG13	2:x:1210:VAL:HG21	1.74	0.68
2:T:1154:LEU:HD11	2:T:1165:MET:HG2	1.75	0.68
2:W:518:ILE:HD11	2:W:993:TYR:CE1	2.29	0.68
2:T:395:TYR:HD1	2:T:396:PRO:HD2	1.58	0.68
2:l:193:ILE:HG22	2:l:197:LEU:HD12	1.74	0.68
2:T:664:LYS:HE2	2:T:668:ARG:HH22	1.60	0.67
2:W:1028:MET:HE1	2:W:1138:VAL:HG22	1.77	0.66
2:S:395:TYR:HD1	2:S:396:PRO:HD2	1.59	0.66
2:x:938:ARG:HG3	2:x:963:MET:HA	1.78	0.65
2:x:916:ASP:HB3	2:x:994:ARG:HH21	1.62	0.65
2:T:1157:ASP:CG	2:T:1304:THR:HG21	2.22	0.65
2:T:1157:ASP:OD1	2:T:1158:PRO:CD	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:395:TYR:CE2	2:x:397:LEU:HB2	2.32	0.65
2:W:905:ASP:O	2:W:909:GLN:HB2	1.98	0.64
2:x:1132:ALA:HB1	2:x:1139:ASN:HD21	1.63	0.64
2:W:79:ASN:HB3	2:W:308:TYR:CD1	2.32	0.64
2:S:817:LEU:HB3	2:S:825:MET:HE1	1.79	0.64
2:T:1153:THR:C	2:T:1154:LEU:HD22	2.22	0.64
2:x:827:GLY:HA2	2:x:929:VAL:HA	1.79	0.64
4:g:252:LEU:HG	4:g:254:ASP:H	1.63	0.64
2:S:1175:CYS:SG	2:T:1223:LEU:HD13	2.38	0.63
2:T:1372:ILE:HD13	2:T:1381:PHE:CD1	2.26	0.63
2:W:518:ILE:CD1	2:W:993:TYR:HE1	2.09	0.63
2:x:400:ARG:HH22	2:x:1306:ASN:HD21	1.47	0.63
2:W:395:TYR:HD1	2:W:396:PRO:CD	2.09	0.63
2:S:1178:GLN:CG	2:S:1307:THR:O	2.43	0.63
2:S:1174:LEU:HD12	2:S:1174:LEU:N	2.14	0.63
3:e:316:LEU:HB3	4:f:211:ILE:HD11	1.80	0.63
2:W:1136:GLN:HA	2:W:1136:GLN:HE21	1.64	0.62
2:x:1338:SER:HG	2:x:1360:HIS:HD1	1.45	0.62
2:S:1176:HIS:CD2	2:T:1232:ALA:HB1	2.33	0.62
2:W:609:THR:HA	2:W:653:ARG:HD3	1.81	0.62
2:S:1309:VAL:HG13	2:S:1311:PHE:CE2	2.35	0.62
2:l:127:ILE:HD11	2:l:179:THR:CG2	2.29	0.62
2:T:209:LYS:HE2	2:T:1213:GLU:HA	1.79	0.62
2:x:316:GLU:CB	2:x:331:PHE:CD2	2.83	0.62
2:S:442:ASN:HD22	2:S:446:LEU:HD12	1.65	0.61
2:l:938:ARG:HG3	2:l:963:MET:HA	1.83	0.61
2:S:1073:ASN:HD22	2:l:1081:VAL:HG13	1.64	0.61
3:5:290:MET:HE3	3:5:294:ARG:HH12	1.66	0.61
2:S:498:ASN:HD22	2:S:501:VAL:HG12	1.65	0.61
2:l:670:LEU:HD23	2:l:675:ILE:HD11	1.82	0.61
3:e:154:MET:HG2	3:e:345:LEU:HD22	1.83	0.61
2:W:518:ILE:HD12	2:W:993:TYR:CD1	2.36	0.61
2:l:828:LEU:HD22	2:l:930:ALA:HB2	1.82	0.60
2:S:780:TYR:O	2:S:784:VAL:CG2	2.48	0.60
2:T:1285:ARG:HH11	2:T:1286:GLY:H	1.48	0.60
2:x:720:ASP:O	2:x:810:LYS:NZ	2.35	0.60
2:x:94:GLN:HG2	2:x:119:VAL:HG12	1.84	0.60
2:W:949:PRO:HB2	2:W:985:ARG:HG2	1.81	0.60
3:5:259:PRO:HG3	3:5:283:SER:HB3	1.84	0.60
2:S:488:SER:HG	2:S:992:GLU:H	1.49	0.60
2:S:791:ASP:O	2:S:896:ARG:NH2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:1212:CYS:HB3	2:x:1223:LEU:HD12	1.83	0.60
2:T:1162:LEU:HD11	3:e:121:GLY:HA2	1.83	0.59
2:T:486:THR:HG21	2:T:552:ARG:HD2	1.82	0.59
2:T:632:LYS:HE3	2:T:887:SER:HB2	1.84	0.59
2:T:747:ILE:HG12	2:T:752:VAL:HG12	1.84	0.59
2:x:35:HIS:HB3	2:x:55:LEU:HD23	1.84	0.59
2:x:1213:GLU:HB3	2:x:1219:VAL:HG11	1.84	0.59
2:S:1039:HIS:ND1	2:S:1040:PRO:O	2.35	0.59
2:W:718:LEU:HD13	2:W:811:ILE:HG13	1.83	0.59
1:2:67:VAL:HG23	1:2:68:PRO:HD3	1.83	0.59
2:x:814:TYR:HB3	2:x:1022:HIS:HE1	1.66	0.59
2:x:894:PHE:HB2	2:x:896:ARG:HE	1.68	0.59
2:S:518:ILE:HD11	2:S:992:GLU:HG3	1.84	0.59
2:W:194:LEU:HD12	2:W:1104:THR:HG22	1.85	0.59
2:x:955:GLY:O	2:x:985:ARG:NH2	2.35	0.59
2:S:1117:MET:SD	2:S:1371:ARG:NH1	2.75	0.59
2:l:497:MET:HE2	2:l:792:PHE:HA	1.85	0.59
2:S:767:GLY:H	2:S:772:MET:HE3	1.67	0.59
2:T:1174:LEU:HB2	2:T:1308:GLU:CD	2.28	0.59
2:W:855:ASP:OD1	2:W:855:ASP:N	2.36	0.59
2:W:1049:THR:HG23	2:W:1270:PRO:HB3	1.85	0.59
2:x:644:ILE:HG22	2:x:655:ALA:HB3	1.85	0.58
2:T:1117:MET:SD	2:T:1371:ARG:NH1	2.76	0.58
2:W:314:ARG:O	2:W:318:LEU:HB2	2.02	0.58
2:x:269:THR:HG22	2:x:274:GLU:O	2.03	0.58
2:T:903:ASP:OD1	2:T:903:ASP:N	2.36	0.58
2:x:904:ASN:O	2:x:909:GLN:NE2	2.37	0.58
2:x:1212:CYS:HB2	2:x:1219:VAL:HG22	1.85	0.58
2:l:772:MET:CE	2:l:775:GLN:HB2	2.33	0.58
2:T:1049:THR:HG21	2:T:1268:TYR:HE2	1.67	0.58
2:l:964:HIS:HB3	2:l:967:VAL:HG22	1.84	0.58
2:W:724:LEU:HD13	2:W:732:ILE:HD12	1.83	0.58
2:T:281:ILE:HG22	2:T:395:TYR:OH	2.02	0.58
3:e:263:ARG:HG2	3:e:326:THR:HG22	1.84	0.58
2:W:724:LEU:O	2:W:921:GLN:NE2	2.36	0.58
2:x:1052:ILE:HG12	2:x:1369:VAL:HG21	1.86	0.58
4:g:243:VAL:HG23	4:g:244:PRO:HD3	1.85	0.58
2:T:1162:LEU:CD1	3:e:121:GLY:HA2	2.33	0.58
2:W:518:ILE:HD11	2:W:993:TYR:HE1	1.68	0.58
2:x:899:ARG:HH22	2:x:991:ALA:H	1.50	0.58
2:x:442:ASN:HD22	2:x:446:LEU:HD12	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:132:GLU:H	2:x:113:GLN:HE21	1.52	0.57
2:x:307:SER:O	2:x:362:GLN:NE2	2.37	0.57
2:S:518:ILE:HD11	2:S:992:GLU:CG	2.33	0.57
2:T:903:ASP:HA	2:T:918:ARG:HA	1.87	0.57
3:e:293:LEU:HD13	3:e:321:VAL:HG11	1.86	0.57
2:T:86:SER:HB2	3:e:217:PRO:HD3	1.86	0.57
2:T:839:LEU:HD22	2:T:881:ILE:HD11	1.86	0.57
2:W:783:ARG:NH1	2:W:891:CYS:O	2.37	0.57
2:l:1251:GLY:HA2	2:l:1254:MET:HE2	1.85	0.57
2:S:1285:ARG:HB2	2:S:1290:MET:HE3	1.87	0.57
2:T:1204:GLY:HA2	2:T:1240:VAL:HG12	1.84	0.57
2:W:538:LEU:O	2:W:1246:GLN:NE2	2.37	0.57
2:W:722:ASN:HB3	2:W:902:VAL:HG11	1.86	0.57
2:S:916:ASP:HB3	2:S:994:ARG:HH21	1.69	0.57
2:x:722:ASN:HD21	2:x:742:ARG:HH11	1.51	0.57
2:l:480:PRO:HG3	2:l:557:ARG:HH22	1.68	0.57
2:S:788:HIS:CD2	2:S:893:THR:CB	2.87	0.57
2:W:766:VAL:HG22	2:W:797:GLY:HA2	1.86	0.57
4:7:144:GLU:OE1	4:7:148:GLN:NE2	2.37	0.57
2:W:477:ALA:O	2:W:557:ARG:NH1	2.36	0.57
2:l:481:ARG:HE	2:l:536:ASP:HB2	1.70	0.57
2:S:392:GLN:NE2	2:W:22:LEU:O	2.38	0.57
4:7:1:MET:HE3	4:7:89:GLN:HE22	1.69	0.57
2:x:716:CYS:SG	2:x:717:ALA:N	2.78	0.57
2:S:21:LEU:HD11	2:x:260:VAL:HG12	1.87	0.56
2:S:1297:ARG:NH1	2:S:1319:VAL:O	2.37	0.56
2:W:1288:TYR:O	2:W:1292:ASN:ND2	2.38	0.56
4:f:33:SER:O	4:f:38:GLN:NE2	2.38	0.56
4:6:238:LEU:HD21	4:7:263:ARG:HA	1.88	0.56
2:S:657:VAL:HA	2:S:663:ILE:HD11	1.88	0.56
2:T:814:TYR:HB3	2:T:1022:HIS:HE1	1.70	0.56
4:f:158:ARG:HD3	4:g:226:GLY:HA2	1.87	0.56
4:g:33:SER:O	4:g:38:GLN:NE2	2.38	0.56
2:l:1049:THR:HG23	2:l:1270:PRO:HB3	1.86	0.56
4:6:24:ARG:NH1	4:6:27:CYS:SG	2.77	0.56
2:l:724:LEU:HD21	2:l:900:VAL:HG11	1.86	0.56
2:l:948:ILE:HG22	2:l:950:PHE:HB3	1.87	0.56
2:l:1280:LEU:O	2:l:1284:ASN:ND2	2.39	0.56
2:T:720:ASP:O	2:T:810:LYS:NZ	2.38	0.56
2:x:932:ALA:HA	2:x:959:VAL:HG23	1.87	0.56
2:l:442:ASN:HD22	2:l:446:LEU:HB2	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:1174:LEU:N	2:T:1174:LEU:HD22	2.21	0.56
2:W:78:VAL:HG11	2:W:261:LEU:HD13	1.87	0.56
2:x:80:THR:HG22	2:x:309:ALA:HB3	1.86	0.56
2:S:1048:ARG:HB3	2:S:1182:CYS:HB3	1.88	0.56
2:S:1175:CYS:CB	2:T:1223:LEU:CD1	2.71	0.56
2:T:941:THR:HG23	2:T:944:LEU:HB2	1.88	0.56
2:l:1078:GLU:HG3	2:l:1080:ARG:HB2	1.88	0.56
2:l:1227:HIS:HD1	2:l:1239:THR:HG1	1.51	0.56
2:S:956:ASP:HB3	2:S:959:VAL:HG12	1.87	0.56
2:l:1242:PRO:O	2:l:1246:GLN:NE2	2.39	0.56
4:6:221:MET:HB3	4:6:247:ILE:HG23	1.86	0.56
2:W:518:ILE:CD1	2:W:993:TYR:CD1	2.89	0.56
2:l:442:ASN:O	2:l:1371:ARG:NH2	2.39	0.56
2:T:623:GLU:HG2	2:T:928:LEU:HD11	1.88	0.55
2:W:817:LEU:HB3	2:W:825:MET:HE1	1.88	0.55
2:T:518:ILE:HG22	2:T:999:SER:OG	2.07	0.55
2:x:176:LEU:HD11	2:x:1069:ILE:HD12	1.88	0.55
2:x:287:LEU:HD22	2:x:383:SER:HB3	1.87	0.55
2:S:172:LEU:HD13	2:S:1090:HIS:HB2	1.89	0.55
2:S:852:ARG:NH1	2:S:883:ASP:OD1	2.38	0.55
2:W:385:GLN:HG2	2:W:395:TYR:CD2	2.40	0.55
2:x:1135:ASN:HB3	2:x:1138:VAL:HB	1.87	0.55
2:W:1209:VAL:HG21	2:W:1283:ASN:HB3	1.88	0.55
2:x:646:THR:O	2:x:650:ARG:HB3	2.06	0.55
4:7:244:PRO:O	4:7:249:ARG:NH2	2.39	0.55
2:T:83:LYS:HD2	2:W:147:THR:HB	1.88	0.55
1:2:69:ARG:HB3	1:2:72:ARG:HB2	1.89	0.55
2:x:625:MET:HE2	2:x:835:VAL:HG23	1.87	0.55
2:x:1224:ILE:HG21	2:x:1280:LEU:HD21	1.87	0.55
4:6:228:ILE:HG22	4:6:229:ARG:HD2	1.89	0.55
2:W:212:LYS:HB3	2:W:1210:VAL:HB	1.88	0.55
2:x:245:ARG:NH1	2:x:373:LYS:O	2.40	0.55
4:f:13:LEU:HD11	4:f:125:LEU:HD22	1.89	0.55
1:Z:5:LEU:HD12	2:T:831:ASP:HB2	1.89	0.55
2:T:1160:THR:HG23	2:T:1314:ILE:CG1	2.31	0.55
2:x:518:ILE:HG22	2:x:999:SER:HB2	1.89	0.55
2:l:445:ASN:ND2	2:l:1347:MET:SD	2.80	0.55
2:l:835:VAL:HG12	2:l:944:LEU:HG	1.89	0.55
1:m:60:TYR:HE2	2:l:883:ASP:HB3	1.71	0.55
2:S:282:VAL:HG12	2:S:1057:ILE:HG12	1.88	0.55
2:l:948:ILE:HG23	2:l:989:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:955:GLY:HA3	2:l:985:ARG:HE	1.71	0.55
2:S:76:SER:HA	2:S:1062:ARG:HA	1.89	0.55
2:W:639:LEU:HB2	2:W:880:MET:HB2	1.89	0.55
2:x:1075:SER:OG	2:x:1076:ARG:N	2.40	0.55
2:S:1175:CYS:HB3	2:T:1232:ALA:HB2	1.89	0.54
2:T:1154:LEU:CD1	2:T:1165:MET:HG2	2.36	0.54
2:W:1372:ILE:CG2	2:W:1381:PHE:CD2	2.79	0.54
2:x:384:LEU:HD12	2:x:395:TYR:HE1	1.72	0.54
2:x:844:PRO:HB2	2:x:878:VAL:HG11	1.89	0.54
2:l:722:ASN:HB3	2:l:902:VAL:HG21	1.88	0.54
2:S:876:PRO:HG2	2:S:881:ILE:HD11	1.89	0.54
2:W:1302:PRO:HB2	2:W:1321:LEU:HD11	1.87	0.54
2:l:705:VAL:HG12	2:l:710:SER:HA	1.89	0.54
2:T:456:LEU:HD13	2:T:1031:ILE:HD13	1.89	0.54
2:T:964:HIS:HB3	2:T:967:VAL:HG22	1.89	0.54
2:T:1154:LEU:HD13	2:T:1165:MET:CE	2.29	0.54
2:x:1055:GLU:OE2	2:x:1109:ARG:NH1	2.41	0.54
2:x:1204:GLY:H	2:x:1245:SER:HB3	1.73	0.54
4:f:231:GLU:OE1	4:f:233:HIS:NE2	2.36	0.54
2:l:617:ALA:HB2	2:l:937:THR:HG23	1.90	0.54
2:l:824:HIS:HE1	2:l:958:ARG:HE	1.54	0.54
4:6:94:LYS:HD2	4:6:96:LYS:HE3	1.88	0.54
2:l:1327:PHE:O	2:l:1329:GLN:NE2	2.40	0.54
4:7:106:THR:HG21	4:7:139:PRO:HB3	1.90	0.54
2:S:658:ASN:HB2	2:S:929:VAL:HG23	1.89	0.54
4:g:108:SER:OG	4:g:301:ARG:NH2	2.40	0.54
2:T:395:TYR:CZ	2:T:397:LEU:HD12	2.42	0.54
2:T:1039:HIS:ND1	2:T:1040:PRO:O	2.35	0.54
2:W:84:ASP:OD1	2:W:84:ASP:N	2.38	0.54
4:g:30:PRO:HG2	4:g:44:GLY:HA3	1.89	0.54
2:S:1176:HIS:CG	2:T:1232:ALA:HB1	2.42	0.54
2:T:623:GLU:OE2	2:T:658:ASN:ND2	2.40	0.54
2:T:828:LEU:HD22	2:T:930:ALA:HB2	1.89	0.54
2:x:124:LYS:NZ	2:x:1091:GLU:OE1	2.41	0.54
2:x:1188:PRO:HD2	2:x:1241:ASN:HB2	1.90	0.54
4:f:279:ASN:OD1	4:f:283:ARG:NH2	2.41	0.54
4:7:24:ARG:NH1	4:7:98:GLN:OE1	2.40	0.54
2:S:1204:GLY:HA2	2:S:1240:VAL:HG12	1.89	0.54
2:W:619:PHE:HE1	2:W:643:CYS:HB3	1.71	0.54
2:W:742:ARG:NH1	2:W:904:ASN:O	2.40	0.54
2:W:1288:TYR:HA	2:W:1291:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:55:PRO:HD2	4:f:191:PRO:HB3	1.89	0.54
2:l:644:ILE:HG22	2:l:655:ALA:HB3	1.88	0.54
2:T:1143:LYS:O	2:T:1148:ALA:HB3	2.08	0.54
2:W:827:GLY:HA2	2:W:929:VAL:HA	1.90	0.54
2:l:1288:TYR:CZ	2:l:1292:ASN:ND2	2.75	0.54
2:T:194:LEU:HB3	2:T:254:ALA:HB1	1.90	0.53
2:T:542:LEU:HB3	2:T:1249:SER:HA	1.89	0.53
2:W:1039:HIS:ND1	2:W:1040:PRO:O	2.41	0.53
2:S:589:GLU:HG2	2:S:594:LEU:HB3	1.89	0.53
3:e:188:VAL:HG12	4:g:106:THR:HG21	1.90	0.53
2:S:56:LEU:HD13	2:T:1095:ILE:HG21	1.91	0.53
2:x:226:HIS:O	2:x:247:ARG:NH1	2.42	0.53
4:f:118:ARG:O	4:f:122:THR:OG1	2.25	0.53
2:l:481:ARG:NH2	2:l:483:ARG:O	2.41	0.53
2:x:336:ALA:HA	2:x:340:ASP:HB2	1.90	0.53
2:S:134:SER:HB2	2:W:43:LYS:HB2	1.91	0.53
2:W:319:VAL:O	2:W:323:SER:HB3	2.08	0.53
2:W:1100:SER:OG	2:W:1101:TYR:N	2.41	0.53
2:l:282:VAL:HG12	2:l:1057:ILE:HG12	1.89	0.53
2:S:747:ILE:HG12	2:S:752:VAL:HG12	1.91	0.53
2:S:1183:GLU:HG2	2:S:1270:PRO:HD2	1.91	0.53
2:T:395:TYR:HD1	2:T:396:PRO:CD	2.22	0.53
2:W:584:ARG:NH1	2:W:1020:ALA:O	2.42	0.53
2:x:668:ARG:NH2	2:x:802:GLU:OE1	2.41	0.53
2:l:553:ASP:OD1	2:l:553:ASP:N	2.40	0.53
2:S:141:LEU:HD11	2:S:161:VAL:HG21	1.91	0.53
2:S:672:ASN:HA	2:T:650:ARG:HH11	1.74	0.53
2:T:1174:LEU:HB2	2:T:1308:GLU:OE2	2.08	0.53
2:W:155:VAL:HG21	2:x:342:PRO:HB2	1.91	0.53
2:W:195:GLN:NE2	2:W:250:GLU:OE1	2.41	0.53
2:W:671:GLY:O	2:x:650:ARG:NH1	2.42	0.53
4:g:9:LEU:HD23	4:g:40:VAL:HG22	1.90	0.53
2:x:1132:ALA:CB	2:x:1139:ASN:ND2	2.63	0.53
2:l:189:PRO:HG2	2:l:194:LEU:HD22	1.91	0.53
1:2:5:LEU:HD13	2:W:831:ASP:HB2	1.91	0.53
2:S:43:LYS:NZ	3:e:331:ASP:OD2	2.41	0.53
2:T:788:HIS:HA	2:T:791:ASP:HB3	1.91	0.53
2:x:401:MET:HG2	2:x:1322:GLU:HB3	1.89	0.53
2:x:907:THR:HB	2:x:1027:PRO:HD2	1.91	0.53
2:l:409:VAL:HG12	2:l:438:ALA:HB3	1.91	0.53
2:S:1080:ARG:HG3	2:S:1082:ASP:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:224:LEU:O	2:x:232:ARG:NH2	2.40	0.53
2:S:1049:THR:HG23	2:S:1270:PRO:HB3	1.91	0.52
2:T:475:ASN:HD21	2:T:560:HIS:H	1.57	0.52
2:T:916:ASP:OD1	2:T:994:ARG:NH2	2.40	0.52
2:x:1304:THR:HG22	2:x:1311:PHE:H	1.74	0.52
4:f:149:LYS:HE3	4:f:179:VAL:HA	1.91	0.52
2:W:618:PHE:HA	2:W:621:VAL:HG22	1.90	0.52
2:W:1239:THR:OG1	2:W:1240:VAL:N	2.42	0.52
2:x:388:TYR:CD1	2:x:395:TYR:HD1	2.26	0.52
3:e:96:HIS:CD2	3:e:122:VAL:HG11	2.44	0.52
4:6:110:SER:OG	4:6:283:ARG:NH1	2.42	0.52
4:6:268:MET:HG3	4:7:148:GLN:HE21	1.73	0.52
2:S:127:ILE:HB	2:S:1090:HIS:HB3	1.91	0.52
2:l:630:GLU:OE2	2:l:668:ARG:NH1	2.42	0.52
2:x:1298:LEU:N	2:x:1298:LEU:HD22	2.24	0.52
2:l:1203:ARG:NH1	2:l:1224:ILE:O	2.43	0.52
3:5:102:ASN:HD21	3:5:196:LYS:HG2	1.74	0.52
2:S:58:VAL:HG23	2:T:94:GLN:HB3	1.91	0.52
2:S:1297:ARG:NH1	2:S:1317:THR:O	2.42	0.52
2:T:996:TRP:HB3	2:T:997:HIS:HD2	1.75	0.52
2:l:134:SER:OG	2:l:137:ASP:OD2	2.27	0.52
2:S:600:GLN:NE2	2:S:1010:PRO:O	2.42	0.52
2:T:817:LEU:HB2	2:T:821:THR:HG23	1.91	0.52
2:x:68:PHE:HB3	2:x:308:TYR:OH	2.09	0.52
2:l:238:SER:OG	2:l:239:GLY:N	2.43	0.52
2:l:904:ASN:O	2:l:909:GLN:NE2	2.39	0.52
1:m:32:GLN:NE2	1:m:35:LEU:O	2.43	0.52
2:T:1154:LEU:N	2:T:1154:LEU:CD2	2.73	0.52
2:W:1054:SER:OG	2:W:1056:ASN:ND2	2.43	0.52
4:6:33:SER:O	4:6:38:GLN:NE2	2.42	0.52
2:S:7:VAL:HG11	2:S:38:ASP:HB2	1.92	0.52
2:S:121:ASN:HD22	4:6:12:ARG:HB2	1.75	0.52
2:T:460:CYS:HB2	2:T:1027:PRO:HB3	1.91	0.52
2:T:726:PRO:HB3	2:T:950:PHE:HE2	1.75	0.52
2:W:672:ASN:HB2	2:x:873:ASP:HB2	1.91	0.52
2:x:710:SER:OG	2:x:711:VAL:N	2.42	0.52
2:S:391:THR:HG23	2:T:101:THR:HA	1.91	0.52
2:S:932:ALA:HA	2:S:959:VAL:HG23	1.92	0.52
2:T:308:TYR:CE1	2:T:1069:ILE:HG13	2.45	0.52
4:7:94:LYS:HG2	4:7:295:THR:HB	1.91	0.52
2:T:1188:PRO:HD2	2:T:1241:ASN:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:289:TYR:HD1	4:g:296:ALA:HB2	1.75	0.52
1:2:3:ARG:O	2:W:498:ASN:ND2	2.43	0.51
2:S:570:ASN:HA	2:S:1000:PRO:HB2	1.91	0.51
2:S:1120:HIS:HB3	2:S:1179:GLN:HB3	1.92	0.51
2:T:1044:MET:HB2	2:T:1184:ILE:HG23	1.92	0.51
4:6:29:LEU:HD13	4:6:43:LEU:HD11	1.90	0.51
2:S:650:ARG:NH2	2:S:872:SER:O	2.43	0.51
2:T:268:THR:OG1	2:T:364:ARG:NH1	2.43	0.51
2:l:567:MET:HE3	2:l:1022:HIS:HA	1.92	0.51
4:7:108:SER:HB2	4:7:301:ARG:HH22	1.76	0.51
2:S:234:GLU:OE1	2:S:1109:ARG:NH1	2.43	0.51
2:S:1174:LEU:N	2:S:1174:LEU:CD1	2.73	0.51
2:T:1192:ASP:N	2:T:1192:ASP:OD1	2.43	0.51
2:W:769:MET:HE2	2:W:890:THR:HG22	1.93	0.51
2:l:180:VAL:HG22	2:l:1067:MET:HE3	1.92	0.51
4:6:244:PRO:HD2	4:6:247:ILE:HD13	1.93	0.51
2:x:705:VAL:HG12	2:x:710:SER:HA	1.93	0.51
2:x:724:LEU:HD12	2:x:900:VAL:HG11	1.93	0.51
3:e:171:ASP:OD1	3:e:171:ASP:N	2.43	0.51
2:l:584:ARG:NH1	2:l:1039:HIS:O	2.41	0.51
1:y:23:LEU:HD12	1:y:51:LEU:HB3	1.93	0.51
3:e:27:LEU:HD11	3:e:38:ASP:HB3	1.91	0.51
2:l:193:ILE:CG2	2:l:197:LEU:HD12	2.41	0.51
1:m:32:GLN:HG2	1:m:35:LEU:HB3	1.92	0.51
2:T:724:LEU:O	2:T:921:GLN:NE2	2.38	0.51
2:l:906:VAL:HG21	2:l:1135:ASN:HB2	1.92	0.51
3:e:359:ASP:OD2	4:g:283:ARG:NH2	2.44	0.51
4:6:45:LEU:HB3	4:6:133:VAL:HG23	1.92	0.51
4:7:24:ARG:HH12	4:7:97:TYR:HA	1.75	0.51
4:7:111:VAL:HG22	4:7:137:VAL:HG22	1.93	0.51
2:W:136:LEU:HD21	3:e:219:SER:HA	1.93	0.51
2:x:43:LYS:HB3	2:x:46:ARG:HB3	1.93	0.51
2:l:573:THR:HG21	2:l:1003:LYS:HD3	1.93	0.51
2:S:567:MET:HE2	2:S:1001:MET:HE1	1.92	0.51
2:S:1175:CYS:O	2:S:1176:HIS:HB2	2.11	0.51
2:T:436:VAL:HG23	2:T:437:GLU:HG3	1.92	0.51
2:W:427:LEU:HD12	2:x:417:LYS:HB2	1.93	0.51
2:x:28:SER:OG	2:x:29:ALA:N	2.40	0.51
4:f:194:PRO:HB2	4:f:198:GLY:HA3	1.93	0.51
2:l:466:THR:HG22	2:l:468:ALA:H	1.76	0.51
3:5:358:SER:OG	3:5:359:ASP:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:474:LEU:HD11	2:S:542:LEU:HD21	1.93	0.50
2:T:700:LEU:HD12	2:T:1036:LEU:HD12	1.93	0.50
2:T:1078:GLU:HB3	2:T:1085:THR:HB	1.93	0.50
4:g:94:LYS:HG2	4:g:295:THR:HG22	1.93	0.50
2:l:127:ILE:CD1	2:l:175:GLY:O	2.59	0.50
2:S:417:LYS:NZ	2:S:431:THR:O	2.41	0.50
2:S:494:PRO:HG3	2:S:988:GLN:HB3	1.93	0.50
2:S:855:ASP:N	2:S:855:ASP:OD1	2.43	0.50
2:T:1155:LEU:N	2:T:1155:LEU:CD1	2.73	0.50
2:W:407:PHE:HB2	2:W:1336:SER:HB2	1.93	0.50
2:W:720:ASP:O	2:W:810:LYS:NZ	2.44	0.50
2:x:450:PHE:HD1	2:x:1119:ILE:HD12	1.76	0.50
2:x:1052:ILE:HG13	2:x:1113:ILE:HG22	1.93	0.50
4:f:234:ASP:O	4:f:237:ASN:ND2	2.43	0.50
4:f:283:ARG:HH11	4:f:301:ARG:HH11	1.58	0.50
4:g:21:MET:HB3	4:g:75:VAL:HG21	1.93	0.50
4:g:49:TYR:HD2	4:g:133:VAL:HG11	1.76	0.50
2:l:517:ASP:OD1	2:l:993:TYR:OH	2.29	0.50
4:6:151:LEU:HD21	4:6:205:LEU:HD22	1.93	0.50
2:x:789:ASP:OD2	1:y:2:ALA:N	2.44	0.50
4:6:111:VAL:HB	4:6:282:PRO:HD2	1.93	0.50
2:W:502:ILE:HD12	2:W:988:GLN:HG3	1.93	0.50
2:x:77:CYS:SG	2:x:184:LYS:NZ	2.82	0.50
2:l:993:TYR:O	2:l:998:ARG:NH1	2.45	0.50
2:T:395:TYR:CD1	2:T:396:PRO:HD2	2.43	0.50
2:T:454:ASN:HD21	2:T:1119:ILE:HB	1.76	0.50
2:W:191:MET:HB2	2:W:1106:THR:HB	1.92	0.50
2:S:8:GLU:OE1	2:x:92:LYS:NZ	2.44	0.50
2:S:109:ARG:HD3	2:S:110:PRO:HD2	1.92	0.50
2:W:511:TYR:O	2:W:974:ASN:ND2	2.45	0.50
4:f:56:ASP:OD1	4:f:56:ASP:N	2.42	0.50
2:l:844:PRO:HB2	2:l:878:VAL:HG11	1.93	0.50
2:l:1011:SER:OG	2:l:1012:LEU:N	2.45	0.50
4:7:95:ASN:ND2	4:7:289:TYR:OH	2.40	0.50
2:W:471:LEU:O	2:W:475:ASN:ND2	2.45	0.50
2:x:609:THR:HG22	2:x:653:ARG:HB3	1.93	0.50
3:e:31:ARG:NH2	3:e:34:GLU:OE1	2.45	0.50
2:l:736:LEU:HA	2:l:739:VAL:HG12	1.93	0.50
2:l:821:THR:HG21	2:l:825:MET:HE3	1.93	0.50
2:l:855:ASP:O	2:l:859:ASN:ND2	2.45	0.50
2:l:919:THR:OG1	2:l:996:TRP:NE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:80:THR:HG22	2:l:309:ALA:HB3	1.93	0.50
2:x:38:ASP:HA	2:x:53:GLU:HA	1.94	0.50
2:x:127:ILE:HB	2:x:1090:HIS:HB3	1.94	0.50
2:x:316:GLU:CB	2:x:331:PHE:CG	2.95	0.50
2:x:1183:GLU:HG3	2:x:1270:PRO:HD2	1.93	0.50
4:7:45:LEU:HD13	4:7:64:LEU:HD13	1.93	0.50
2:W:828:LEU:HA	2:W:947:ALA:HA	1.94	0.49
2:x:886:ALA:HA	1:y:53:SER:HB2	1.94	0.49
2:l:497:MET:HE3	2:l:896:ARG:HH11	1.77	0.49
4:7:138:LEU:HD12	4:7:142:ILE:HG22	1.93	0.49
2:T:273:GLY:O	2:T:274:GLU:HG3	2.12	0.49
2:l:227:SER:O	2:l:232:ARG:NH1	2.46	0.49
2:l:1231:ASP:OD1	2:l:1231:ASP:N	2.45	0.49
2:T:1074:VAL:HA	2:T:1088:VAL:HA	1.93	0.49
2:W:1306:ASN:OD1	2:x:210:THR:OG1	2.31	0.49
3:e:261:ASP:OD1	3:e:261:ASP:N	2.45	0.49
2:l:587:GLN:NE2	2:l:1037:LYS:O	2.39	0.49
2:T:657:VAL:HA	2:T:663:ILE:HD11	1.94	0.49
2:W:19:ALA:HB3	2:W:21:LEU:HD22	1.95	0.49
2:x:1278:GLU:HG3	2:x:1282:ARG:HH21	1.77	0.49
3:e:359:ASP:OD1	3:e:359:ASP:N	2.45	0.49
3:5:114:LYS:HB2	3:5:184:PHE:HD1	1.76	0.49
3:5:233:LEU:HD11	3:5:280:PHE:HB3	1.94	0.49
2:S:269:THR:OG1	2:S:299:ASP:OD2	2.30	0.49
2:S:710:SER:OG	2:S:711:VAL:N	2.46	0.49
2:S:724:LEU:O	2:S:921:GLN:NE2	2.46	0.49
2:S:899:ARG:NH1	2:S:922:THR:OG1	2.40	0.49
2:T:396:PRO:O	2:T:399:ARG:NH1	2.46	0.49
2:T:485:GLU:OE2	2:T:993:TYR:OH	2.24	0.49
2:x:497:MET:HG3	2:x:896:ARG:HD2	1.95	0.49
2:x:1122:GLN:NE2	2:x:1268:TYR:O	2.45	0.49
3:e:165:LEU:HA	3:e:168:LEU:HD12	1.94	0.49
2:l:542:LEU:HB3	2:l:1249:SER:HA	1.94	0.49
4:6:116:PHE:HA	4:6:188:LEU:HA	1.94	0.49
2:S:427:LEU:HD11	2:T:430:PRO:HB2	1.93	0.49
2:S:1142:ILE:HG22	2:S:1143:LYS:N	2.28	0.49
2:T:181:LEU:HD21	2:T:395:TYR:HE1	1.78	0.49
3:e:264:LEU:HB2	3:e:327:PHE:HE1	1.78	0.49
4:g:30:PRO:HA	4:g:69:LEU:HA	1.95	0.49
2:l:165:LEU:HD11	3:5:39:VAL:HG21	1.94	0.49
2:l:980:VAL:O	2:l:985:ARG:NH1	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:98:GLN:HE21	4:6:120:HIS:HD2	1.61	0.49
4:6:267:MET:HE2	4:6:271:LEU:HG	1.95	0.49
2:T:1074:VAL:HB	3:e:52:LEU:HD13	1.93	0.49
2:W:190:PRO:HD2	2:W:193:ILE:HD12	1.95	0.49
2:l:224:LEU:O	2:l:232:ARG:NH2	2.45	0.49
2:S:553:ASP:HA	2:S:558:ALA:HB2	1.95	0.49
2:S:609:THR:HG22	2:S:653:ARG:HB3	1.93	0.49
2:W:544:PRO:HG3	2:W:1186:VAL:HG11	1.95	0.49
2:x:840:ALA:HB3	1:y:49:VAL:HG13	1.95	0.49
2:S:481:ARG:O	2:S:484:ARG:NH1	2.46	0.49
2:T:1246:GLN:HB2	2:T:1249:SER:HB3	1.95	0.49
2:W:695:GLN:OE1	2:x:958:ARG:NH1	2.46	0.49
2:W:955:GLY:HA3	2:W:985:ARG:HE	1.78	0.49
3:e:92:ASP:HB3	3:e:202:LYS:HE3	1.94	0.49
4:f:144:GLU:HG2	4:g:272:GLN:HG2	1.95	0.49
2:l:1335:LEU:HD22	2:l:1373:LEU:HD13	1.95	0.49
4:6:256:SER:OG	4:6:257:VAL:N	2.46	0.49
2:T:280:PHE:HB2	2:T:381:VAL:HG12	1.95	0.48
2:l:451:ASN:OD1	2:l:454:ASN:ND2	2.46	0.48
2:l:821:THR:HG22	2:l:824:HIS:H	1.77	0.48
2:l:899:ARG:NH1	2:l:922:THR:OG1	2.39	0.48
4:6:9:LEU:HD21	4:6:13:LEU:HD13	1.94	0.48
4:6:110:SER:HB2	4:6:140:THR:HG22	1.94	0.48
2:W:130:GLU:HG2	2:W:1087:GLU:HB2	1.96	0.48
2:W:1073:ASN:OD1	2:W:1073:ASN:N	2.44	0.48
2:x:1124:PHE:HA	2:x:1127:VAL:HG12	1.94	0.48
2:S:617:ALA:HA	2:S:620:TYR:HD2	1.79	0.48
2:x:810:LYS:O	2:x:814:TYR:HB2	2.13	0.48
3:5:233:LEU:HD13	3:5:289:ILE:HD11	1.96	0.48
2:T:1174:LEU:CG	2:T:1308:GLU:HG2	2.39	0.48
2:x:733:PHE:HD2	2:x:746:ILE:HD13	1.79	0.48
2:x:857:LEU:HD11	2:x:869:LEU:HB3	1.95	0.48
4:g:204:ASN:HA	4:g:207:LEU:HB3	1.96	0.48
2:S:485:GLU:HG3	2:S:489:LEU:HD21	1.95	0.48
2:x:1205:ARG:NH2	2:x:1230:PRO:O	2.41	0.48
2:l:820:CYS:HA	2:l:1010:PRO:HB3	1.94	0.48
3:5:223:VAL:HB	3:5:350:ILE:HB	1.95	0.48
1:Z:10:LEU:HD22	2:T:841:TYR:HD2	1.77	0.48
2:S:671:GLY:O	2:T:650:ARG:NH1	2.46	0.48
2:W:1252:ASP:OD1	2:W:1252:ASP:N	2.31	0.48
3:5:45:GLU:HG3	3:5:59:ARG:HH22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:176:VAL:HG21	3:5:275:PRO:HG3	1.95	0.48
4:6:227:LEU:HD21	4:6:233:HIS:HD2	1.78	0.48
2:T:824:HIS:ND1	2:T:956:ASP:OD2	2.47	0.48
2:x:724:LEU:O	2:x:921:GLN:NE2	2.41	0.48
4:g:204:ASN:O	4:g:208:TYR:N	2.46	0.48
3:5:104:GLU:OE2	3:5:159:TYR:OH	2.29	0.48
4:7:9:LEU:HD13	4:7:40:VAL:HG21	1.96	0.48
1:2:35:LEU:HD12	1:2:39:VAL:HG23	1.95	0.48
2:S:497:MET:CE	2:S:788:HIS:O	2.57	0.48
2:W:745:GLN:HG3	2:W:752:VAL:HG13	1.96	0.48
2:x:479:ALA:O	2:x:539:ARG:NH2	2.46	0.48
4:f:215:LEU:HD13	4:f:266:VAL:HG13	1.94	0.48
2:T:442:ASN:HD22	2:T:446:LEU:HD12	1.79	0.48
2:W:706:VAL:HG12	2:W:711:VAL:HG12	1.96	0.48
2:x:1128:PHE:HZ	2:x:1260:ARG:HG2	1.78	0.48
2:x:1132:ALA:CB	2:x:1139:ASN:HD21	2.25	0.48
2:T:1338:SER:HB3	2:T:1361:TYR:H	1.78	0.48
2:W:510:LYS:O	2:W:973:ARG:NH2	2.41	0.48
2:S:1246:GLN:HB2	2:S:1249:SER:HB3	1.96	0.47
2:W:1338:SER:HG	2:W:1360:HIS:HD1	1.59	0.47
2:x:719:LEU:HD23	2:x:807:VAL:HG21	1.96	0.47
2:x:131:MET:HE1	2:x:165:LEU:HD22	1.96	0.47
4:f:216:LEU:HD12	4:g:213:VAL:HG13	1.95	0.47
2:l:887:SER:HG	2:l:891:CYS:HG	1.56	0.47
2:T:830:VAL:HG13	2:T:945:PHE:HE1	1.80	0.47
2:T:1160:THR:HB	3:e:122:VAL:HG23	1.95	0.47
2:x:481:ARG:NH1	2:x:517:ASP:OD2	2.48	0.47
3:5:263:ARG:HG2	3:5:326:THR:HG22	1.96	0.47
2:W:783:ARG:NH2	2:W:888:PHE:O	2.48	0.47
2:x:770:ASP:OD1	1:y:57:TYR:OH	2.32	0.47
2:l:408:PRO:HA	2:l:1045:THR:HA	1.96	0.47
1:m:33:ASN:OD1	1:m:33:ASN:N	2.47	0.47
2:S:507:TYR:OH	2:S:984:ASN:O	2.31	0.47
2:S:720:ASP:O	2:S:810:LYS:NZ	2.46	0.47
2:S:783:ARG:NH1	2:S:888:PHE:CE1	2.78	0.47
2:T:1302:PRO:HB3	2:T:1321:LEU:HD11	1.95	0.47
2:x:282:VAL:HG12	2:x:1057:ILE:HG12	1.95	0.47
3:e:30:SER:OG	3:e:34:GLU:OE2	2.32	0.47
2:l:758:ALA:HB1	2:l:761:GLN:HE21	1.78	0.47
2:l:1199:SER:O	2:l:1199:SER:OG	2.33	0.47
2:W:55:LEU:HD23	2:x:328:MET:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:1074:VAL:HG12	2:x:1088:VAL:HG22	1.97	0.47
2:l:733:PHE:HD2	2:l:746:ILE:HD13	1.80	0.47
1:Z:8:PRO:HB2	1:Z:10:LEU:HG	1.97	0.47
2:S:598:VAL:HG12	2:S:685:LYS:HB3	1.97	0.47
2:S:999:SER:N	2:S:1000:PRO:CD	2.78	0.47
2:T:338:ILE:HD11	2:x:319:VAL:HA	1.96	0.47
2:T:528:ASP:OD2	2:T:534:ASN:ND2	2.48	0.47
2:T:1160:THR:CG2	2:T:1314:ILE:HD12	1.95	0.47
2:T:1160:THR:OG1	2:T:1314:ILE:HD11	2.15	0.47
2:W:564:HIS:HD2	2:W:566:LEU:HA	1.79	0.47
2:W:901:SER:O	2:W:918:ARG:NH2	2.48	0.47
2:l:127:ILE:HD13	2:l:175:GLY:C	2.40	0.47
2:l:502:ILE:HA	2:l:505:GLU:HG2	1.95	0.47
2:l:728:ALA:HB3	2:l:925:VAL:HA	1.97	0.47
4:7:90:THR:HG22	4:7:299:TRP:HB3	1.96	0.47
2:T:341:SER:O	2:T:341:SER:OG	2.32	0.47
2:W:53:GLU:HB2	2:x:90:ASP:HB3	1.96	0.47
2:W:137:ASP:HA	2:W:140:ILE:HG22	1.96	0.47
2:W:1226:ASP:OD1	2:W:1228:SER:OG	2.31	0.47
4:6:16:ASP:N	4:6:16:ASP:OD1	2.47	0.47
4:6:112:MET:HB3	4:6:136:MET:HB3	1.95	0.47
2:T:452:LEU:HD22	2:T:1040:PRO:HD3	1.97	0.47
2:W:298:ALA:HB2	2:W:373:LYS:HB2	1.97	0.47
2:x:725:PRO:HG3	2:x:809:GLU:HG3	1.97	0.47
3:e:151:LEU:HD11	3:e:226:PRO:HB2	1.97	0.47
1:Z:4:ARG:HH21	2:T:834:HIS:HE1	1.63	0.47
2:S:839:LEU:HB3	2:S:885:SER:HB3	1.96	0.47
2:S:1080:ARG:NH2	3:5:353:PHE:O	2.48	0.47
2:T:286:VAL:HG11	2:T:1057:ILE:HD11	1.97	0.47
2:T:827:GLY:HA2	2:T:929:VAL:HA	1.97	0.47
2:T:1011:SER:OG	2:T:1012:LEU:N	2.47	0.47
2:x:1293:GLU:O	2:x:1297:ARG:NH1	2.47	0.47
2:l:474:LEU:HD11	2:l:542:LEU:HD13	1.97	0.47
2:S:724:LEU:HD22	2:S:732:ILE:HD12	1.96	0.46
2:T:400:ARG:HH12	2:T:1114:THR:HG21	1.79	0.46
2:W:1348:SER:HB3	2:x:1352:THR:HA	1.96	0.46
2:x:484:ARG:HH22	2:x:553:ASP:HB2	1.80	0.46
2:x:700:LEU:HD12	2:x:1036:LEU:HD22	1.96	0.46
2:x:1365:GLU:OE1	2:x:1371:ARG:NH1	2.48	0.46
4:f:57:TYR:HA	4:f:60:MET:HE3	1.97	0.46
2:l:213:SER:HA	2:l:1211:SER:HB2	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:518:ILE:HD11	2:T:993:TYR:CD1	2.51	0.46
2:T:835:VAL:HG12	2:T:944:LEU:HD23	1.97	0.46
2:T:899:ARG:NH2	2:T:922:THR:OG1	2.40	0.46
2:T:1231:ASP:OD1	2:T:1231:ASP:N	2.48	0.46
2:T:488:SER:OG	2:T:992:GLU:N	2.37	0.46
2:W:518:ILE:HD11	2:W:547:ASP:CG	2.25	0.46
2:x:740:SER:OG	2:x:742:ARG:O	2.30	0.46
4:f:31:LEU:HD13	4:f:38:GLN:HE22	1.81	0.46
2:l:867:ASP:HB3	2:l:940:VAL:HG11	1.98	0.46
1:Z:8:PRO:HB3	2:T:864:THR:HG21	1.97	0.46
2:S:395:TYR:CD1	2:S:396:PRO:HD2	2.46	0.46
2:S:1374:LYS:O	2:T:1198:LYS:NZ	2.49	0.46
2:T:421:SER:HB3	2:T:1354:ALA:HB2	1.97	0.46
2:x:646:THR:O	2:x:650:ARG:CB	2.63	0.46
2:x:691:ILE:HG12	2:x:808:LEU:HD21	1.97	0.46
4:g:24:ARG:NH1	4:g:98:GLN:OE1	2.45	0.46
2:l:1205:ARG:NH1	2:l:1223:LEU:O	2.42	0.46
4:7:243:VAL:HG23	4:7:244:PRO:HD3	1.98	0.46
1:2:70:ARG:HH12	1:y:14:LEU:HA	1.79	0.46
2:S:498:ASN:HD21	2:S:500:LEU:HB3	1.79	0.46
2:T:1175:CYS:O	2:T:1175:CYS:SG	2.73	0.46
2:W:1213:GLU:HB3	2:W:1216:ASN:HD21	1.80	0.46
2:x:768:ASN:HB3	2:x:771:GLU:HG2	1.97	0.46
2:W:697:LEU:HB3	2:W:719:LEU:HD11	1.97	0.46
2:x:457:LYS:HE3	2:x:1121:THR:HB	1.97	0.46
2:x:473:SER:HG	2:x:1259:TYR:HH	1.61	0.46
4:f:193:VAL:HG12	4:f:195:GLY:H	1.81	0.46
4:7:58:VAL:HG22	4:7:277:LEU:HD11	1.98	0.46
2:T:1153:THR:O	2:T:1165:MET:CE	2.64	0.46
2:T:1272:ARG:HG2	2:T:1276:ASN:HD21	1.81	0.46
2:x:464:LEU:HG	2:x:1250:LEU:HD11	1.97	0.46
2:l:609:THR:HG22	2:l:653:ARG:HB3	1.97	0.46
2:l:881:ILE:HA	2:l:884:LEU:HB2	1.97	0.46
2:l:986:PRO:HG2	2:l:989:LEU:HD22	1.96	0.46
2:l:1246:GLN:HB2	2:l:1249:SER:HB2	1.97	0.46
2:S:487:TYR:HB2	2:S:514:PRO:HG2	1.98	0.46
2:S:715:VAL:HG23	2:S:1029:ALA:HA	1.98	0.46
2:T:471:LEU:HD21	2:T:562:ALA:HB2	1.97	0.46
2:W:724:LEU:HD12	2:W:900:VAL:HG21	1.98	0.46
2:x:856:ILE:HG12	2:x:860:LEU:HB2	1.98	0.46
2:l:639:LEU:HB2	2:l:880:MET:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:7:VAL:HG22	4:6:38:GLN:HB2	1.97	0.46
2:T:1043:ALA:HB2	2:T:1189:VAL:HG12	1.97	0.46
2:x:106:ASP:OD1	2:x:106:ASP:N	2.49	0.46
4:6:131:ASP:OD1	4:6:131:ASP:N	2.48	0.46
2:S:521:LYS:HA	2:S:524:LEU:HD12	1.97	0.46
2:S:998:ARG:HH11	2:S:998:ARG:CG	2.12	0.46
2:T:459:LEU:HA	2:T:464:LEU:HD13	1.98	0.46
2:T:782:TYR:OH	2:T:791:ASP:OD2	2.32	0.46
2:T:1073:ASN:O	2:T:1089:HIS:N	2.45	0.46
2:W:844:PRO:O	2:W:882:ARG:NH1	2.49	0.46
2:x:434:LEU:HD22	2:x:583:ALA:HB1	1.97	0.46
2:T:794:LEU:HD13	2:T:925:VAL:HG11	1.98	0.45
2:W:1081:VAL:HB	3:e:210:PRO:HB3	1.97	0.45
2:x:169:VAL:HG21	3:5:9:ARG:HG2	1.97	0.45
2:x:488:SER:HB3	2:x:991:ALA:HA	1.97	0.45
2:x:1178:GLN:HE21	2:x:1310:GLN:HG2	1.81	0.45
2:l:440:ILE:HD11	2:l:1119:ILE:HG23	1.98	0.45
1:2:65:PHE:O	2:x:862:ASN:ND2	2.49	0.45
2:S:639:LEU:HD12	2:S:880:MET:HB2	1.98	0.45
2:S:724:LEU:HD12	2:S:900:VAL:HG21	1.98	0.45
2:x:992:GLU:OE2	2:x:999:SER:OG	2.33	0.45
3:e:197:SER:HB2	3:e:201:ASN:HA	1.98	0.45
2:l:487:TYR:OH	2:l:985:ARG:O	2.34	0.45
1:2:72:ARG:HH22	2:x:859:ASN:HA	1.81	0.45
2:S:138:LEU:HD13	2:S:141:LEU:HD12	1.98	0.45
2:S:488:SER:O	2:S:488:SER:OG	2.35	0.45
2:x:852:ARG:HE	2:x:879:GLY:HA3	1.81	0.45
4:g:7:VAL:HG13	4:g:80:LEU:HB2	1.97	0.45
4:6:267:MET:HG2	4:7:209:PHE:HZ	1.82	0.45
2:S:1357:HIS:O	2:S:1360:HIS:N	2.47	0.45
2:W:898:VAL:HG23	2:W:923:VAL:HG13	1.99	0.45
2:W:1077:ARG:HH21	4:f:84:LYS:HE2	1.80	0.45
2:x:886:ALA:HB1	1:y:57:TYR:HB2	1.97	0.45
2:x:899:ARG:HH12	2:x:990:PHE:HA	1.81	0.45
2:x:1297:ARG:H	2:x:1297:ARG:HD3	1.82	0.45
3:5:28:ASN:OD1	3:5:30:SER:OG	2.34	0.45
4:6:127:SER:OG	4:6:128:ASN:N	2.50	0.45
2:S:280:PHE:HB2	2:S:381:VAL:HG22	1.97	0.45
2:S:594:LEU:HD11	2:S:693:LEU:HD23	1.99	0.45
2:S:791:ASP:C	2:S:793:ARG:H	2.25	0.45
2:T:1288:TYR:OH	2:W:24:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:850:PHE:O	2:x:882:ARG:NH1	2.50	0.45
1:y:35:LEU:HD12	1:y:39:VAL:HG23	1.98	0.45
2:l:1133:PHE:HB2	2:l:1139:ASN:HD21	1.82	0.45
4:6:21:MET:HE1	4:6:123:VAL:HB	1.96	0.45
4:7:85:ILE:HG13	4:7:91:TYR:HE2	1.81	0.45
2:S:998:ARG:NH1	2:S:998:ARG:CG	2.73	0.45
2:T:450:PHE:HZ	2:T:1184:ILE:HD11	1.80	0.45
2:x:223:LEU:HG	2:x:1368:PRO:HG3	1.99	0.45
4:g:149:LYS:HD2	4:g:179:VAL:HG22	1.99	0.45
3:5:12:LEU:HD12	3:5:12:LEU:HA	1.82	0.45
4:6:218:ARG:HH21	4:6:250:ILE:HD12	1.81	0.45
2:W:169:VAL:HG21	3:e:32:GLY:H	1.82	0.45
2:W:1302:PRO:HB3	2:W:1323:GLN:HE22	1.82	0.45
4:f:112:MET:HE3	4:f:143:ALA:HB1	1.98	0.45
2:l:810:LYS:O	2:l:814:TYR:HB2	2.17	0.45
2:l:682:MET:HE3	2:l:682:MET:HB2	1.84	0.45
3:5:289:ILE:HD12	3:5:292:ILE:HB	1.97	0.45
2:S:166:GLN:HE21	2:S:323:SER:HA	1.81	0.45
2:l:184:LYS:HA	2:l:184:LYS:HD3	1.74	0.45
2:S:828:LEU:HD22	2:S:930:ALA:HB2	1.99	0.45
2:S:1195:TYR:OH	2:S:1201:SER:O	2.35	0.45
2:S:1250:LEU:HG	2:S:1254:MET:HE2	1.98	0.45
2:T:260:VAL:HB	2:W:17:VAL:HG11	1.99	0.45
4:f:229:ARG:NH2	4:f:241:GLU:O	2.50	0.45
2:l:952:MET:HE1	2:l:981:GLU:HA	1.99	0.45
1:2:69:ARG:HG3	1:2:71:GLN:H	1.82	0.44
2:S:465:HIS:CE1	2:S:1027:PRO:HD3	2.52	0.44
2:S:1176:HIS:HB2	2:T:1232:ALA:HB1	1.99	0.44
2:W:314:ARG:HH11	2:W:314:ARG:CG	2.14	0.44
2:W:553:ASP:HA	2:W:558:ALA:HB2	1.99	0.44
2:W:1244:ALA:HB1	2:W:1275:PHE:HZ	1.81	0.44
2:x:718:LEU:HD13	2:x:811:ILE:HG12	1.99	0.44
4:g:150:ILE:HG22	4:g:190:LEU:HD21	1.99	0.44
2:l:1115:THR:HB	2:l:1180:ALA:HB2	2.00	0.44
4:7:109:LEU:HD12	4:7:137:VAL:HG12	2.00	0.44
2:S:780:TYR:OH	2:S:784:VAL:HG11	2.16	0.44
2:S:783:ARG:NH1	2:S:888:PHE:CD1	2.85	0.44
2:S:1210:VAL:HG22	2:S:1283:ASN:HB3	1.98	0.44
2:x:316:GLU:HB3	2:x:331:PHE:CD1	2.52	0.44
2:x:316:GLU:HB3	2:x:331:PHE:CG	2.52	0.44
3:e:237:LEU:HD21	3:e:292:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:221:MET:HA	4:f:224:VAL:HG12	1.98	0.44
2:l:851:THR:HG23	2:l:854:GLU:HB2	1.98	0.44
2:l:1192:ASP:OD1	2:l:1192:ASP:N	2.44	0.44
4:7:109:LEU:O	4:7:284:LEU:N	2.48	0.44
1:2:3:ARG:H	2:W:501:VAL:HG11	1.82	0.44
2:S:18:ASP:HB3	2:x:348:THR:HG21	1.99	0.44
2:S:1105:MET:HE2	2:S:1105:MET:HB3	1.82	0.44
2:T:1043:ALA:O	2:T:1187:THR:OG1	2.32	0.44
2:W:1181:THR:H	2:W:1310:GLN:HE21	1.66	0.44
2:l:612:ASP:OD2	2:l:653:ARG:NH2	2.50	0.44
2:l:690:LEU:HD11	2:l:812:PHE:HD1	1.81	0.44
2:l:1267:LEU:HD23	2:l:1267:LEU:HA	1.88	0.44
2:T:775:GLN:HG3	2:T:778:ALA:HB3	1.99	0.44
2:x:46:ARG:HG3	2:x:48:ALA:H	1.83	0.44
2:x:209:LYS:NZ	2:x:1211:SER:O	2.40	0.44
2:x:644:ILE:HD11	2:x:675:ILE:HG12	2.00	0.44
2:x:988:GLN:H	2:x:988:GLN:HG2	1.65	0.44
3:e:151:LEU:O	3:e:155:ALA:N	2.37	0.44
4:g:45:LEU:HB2	4:g:133:VAL:HB	2.00	0.44
2:l:516:THR:HG23	2:l:519:ALA:H	1.82	0.44
2:l:566:LEU:HD11	2:l:919:THR:HG21	1.99	0.44
2:l:992:GLU:HA	2:l:995:GLU:HG3	1.99	0.44
1:Y:11:GLN:NE2	2:S:861:GLU:OE2	2.49	0.44
2:T:1157:ASP:OD1	2:T:1304:THR:HG21	2.18	0.44
2:W:400:ARG:HH22	2:x:205:ARG:HH11	1.65	0.44
2:W:442:ASN:OD1	2:W:443:LYS:N	2.50	0.44
2:W:964:HIS:HD2	2:W:966:ASP:H	1.64	0.44
2:x:821:THR:O	2:x:821:THR:OG1	2.35	0.44
2:x:1184:ILE:O	2:x:1255:TYR:OH	2.34	0.44
2:l:731:ASP:HA	2:l:796:LEU:HD13	2.00	0.44
4:6:250:ILE:HG22	4:7:247:ILE:HD12	2.00	0.44
4:7:7:VAL:HG12	4:7:80:LEU:HB2	2.00	0.44
2:S:860:LEU:HD21	2:S:865:LEU:HD22	2.00	0.44
2:T:564:HIS:CE1	2:T:908:GLN:HG2	2.53	0.44
2:T:1077:ARG:NH1	3:e:92:ASP:OD2	2.50	0.44
2:T:1199:SER:O	2:T:1199:SER:OG	2.31	0.44
4:f:140:THR:HA	4:f:143:ALA:HB3	1.99	0.44
4:g:124:LYS:HB2	4:g:124:LYS:HE2	1.73	0.44
4:g:280:LEU:H	4:g:283:ARG:HH11	1.65	0.44
2:l:82:PHE:HB2	2:l:1068:PHE:HB3	1.99	0.44
4:6:249:ARG:HA	4:6:252:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:262:LYS:HA	2:S:262:LYS:HD2	1.84	0.44
2:S:1071:THR:OG1	2:I:139:GLU:OE2	2.35	0.44
2:T:518:ILE:HD11	2:T:993:TYR:CE1	2.53	0.44
2:T:838:THR:HG22	2:T:865:LEU:HD12	1.98	0.44
2:x:1074:VAL:HG22	3:5:15:ARG:HB3	1.99	0.44
2:S:964:HIS:HB3	2:S:967:VAL:HG22	1.99	0.44
2:S:1120:HIS:CB	2:S:1179:GLN:HB3	2.48	0.44
2:W:764:GLU:HB3	2:W:793:ARG:HH12	1.83	0.44
2:W:1127:VAL:HG22	2:W:1267:LEU:HG	2.00	0.44
2:x:1339:SER:OG	2:x:1340:ARG:N	2.51	0.44
4:6:110:SER:N	4:6:138:LEU:O	2.51	0.44
2:W:79:ASN:CB	2:W:308:TYR:HD1	2.27	0.44
2:I:438:ALA:HA	2:I:1338:SER:HA	1.99	0.44
1:Y:5:LEU:HD12	2:S:831:ASP:HB2	2.00	0.43
2:S:783:ARG:HE	2:S:783:ARG:HB2	1.63	0.43
2:T:730:THR:HG23	2:T:732:ILE:HG23	2.00	0.43
2:T:1160:THR:HG23	2:T:1314:ILE:HG13	1.93	0.43
2:W:401:MET:HE2	2:W:401:MET:HB3	1.93	0.43
2:x:783:ARG:NH2	2:x:888:PHE:O	2.50	0.43
4:f:152:LEU:HA	4:f:155:VAL:HG12	1.99	0.43
1:2:4:ARG:HE	1:2:4:ARG:HB3	1.63	0.43
2:S:68:PHE:HD1	2:S:177:ILE:HG12	1.83	0.43
2:S:410:GLY:O	2:S:1039:HIS:NE2	2.37	0.43
2:S:510:LYS:HA	2:S:510:LYS:HD2	1.80	0.43
2:S:839:LEU:HD21	2:S:884:LEU:HD23	1.99	0.43
2:T:349:LYS:HD3	2:T:349:LYS:HA	1.88	0.43
2:T:1208:CYS:HB2	2:T:1211:SER:HB2	1.99	0.43
2:W:817:LEU:HD23	2:W:817:LEU:HA	1.84	0.43
2:W:1352:THR:O	2:W:1352:THR:OG1	2.36	0.43
1:y:56:CYS:HA	1:y:59:GLU:HG2	2.00	0.43
4:f:224:VAL:HB	4:g:210:CYS:HB3	1.99	0.43
2:S:780:TYR:CE2	2:S:784:VAL:HG21	2.54	0.43
2:S:1175:CYS:HB2	2:T:1223:LEU:HD11	1.90	0.43
2:T:746:ILE:HG23	2:T:900:VAL:HG22	2.00	0.43
2:W:503:VAL:HG12	2:W:986:PRO:HG2	1.99	0.43
2:x:605:THR:HA	2:x:608:ASP:HB2	2.00	0.43
2:I:499:VAL:HG23	2:I:502:ILE:HD11	2.00	0.43
4:6:122:THR:HA	4:6:133:VAL:HG12	2.01	0.43
2:T:407:PHE:HB2	2:T:1336:SER:HB2	2.00	0.43
2:T:1121:THR:HA	2:T:1182:CYS:HB2	2.01	0.43
2:x:908:GLN:HE22	2:x:1024:LYS:HD3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:27:LEU:HD23	3:5:38:ASP:HB3	2.00	0.43
4:6:205:LEU:HD23	4:7:223:LEU:HD21	2.00	0.43
2:S:600:GLN:O	2:S:604:GLU:HB2	2.18	0.43
2:S:783:ARG:NH2	2:S:891:CYS:O	2.52	0.43
2:T:147:THR:HB	2:T:150:GLU:HB2	2.01	0.43
2:x:409:VAL:HB	2:x:1044:MET:HB2	2.01	0.43
3:e:133:ILE:HD11	3:e:165:LEU:HD22	2.00	0.43
4:f:48:VAL:HG23	4:f:60:MET:HG2	2.01	0.43
2:l:184:LYS:HB3	2:l:1058:LEU:HD21	2.01	0.43
2:l:481:ARG:HH22	2:l:483:ARG:HH21	1.66	0.43
1:Y:41:ARG:HD3	1:Y:41:ARG:HA	1.83	0.43
2:T:640:VAL:HA	2:T:643:CYS:HB2	2.01	0.43
2:W:547:ASP:HB2	2:W:565:ARG:HD2	2.00	0.43
4:f:206:SER:OG	4:g:240:GLN:NE2	2.52	0.43
2:l:1290:MET:HE2	2:l:1290:MET:HB3	1.85	0.43
2:S:448:LEU:HD13	2:S:1119:ILE:HB	2.00	0.43
2:S:468:ALA:O	2:S:472:ASN:HB2	2.18	0.43
2:T:483:ARG:HH12	2:T:536:ASP:HB3	1.84	0.43
2:T:1174:LEU:N	2:T:1174:LEU:CD1	2.76	0.43
1:y:30:LEU:HB3	1:y:40:PHE:HE1	1.83	0.43
3:e:122:VAL:CG2	3:e:200:LEU:HD11	2.49	0.43
3:e:171:ASP:HB2	3:e:174:ARG:HB3	1.99	0.43
4:f:58:VAL:HA	4:f:61:TYR:HB2	2.00	0.43
2:T:1258:SER:OG	2:T:1260:ARG:NH2	2.52	0.43
2:W:189:PRO:HG2	2:W:194:LEU:HD11	2.01	0.43
2:W:627:HIS:CE1	2:W:892:PRO:HD3	2.54	0.43
2:W:657:VAL:HA	2:W:663:ILE:HD11	2.00	0.43
2:x:269:THR:HG22	2:x:274:GLU:H	1.84	0.43
2:x:337:ARG:HD3	2:x:337:ARG:HA	1.88	0.43
2:l:448:LEU:HD13	2:l:1119:ILE:HG12	2.00	0.43
1:2:6:PRO:HB2	2:W:943:CYS:HA	2.01	0.43
2:S:870:GLU:OE2	2:S:936:ARG:NH1	2.51	0.43
2:T:1204:GLY:H	2:T:1245:SER:HB3	1.84	0.43
2:x:855:ASP:N	2:x:855:ASP:OD1	2.51	0.43
4:f:115:VAL:O	4:f:189:ALA:N	2.47	0.43
3:5:127:THR:HG23	3:5:130:SER:H	1.83	0.43
2:W:262:LYS:HE3	2:W:262:LYS:HB3	1.88	0.43
2:x:421:SER:HB3	2:x:1354:ALA:HB2	2.01	0.43
2:x:492:ARG:HG3	2:x:988:GLN:HB3	2.00	0.43
2:l:450:PHE:HD2	2:l:1119:ILE:HG22	1.84	0.43
3:5:289:ILE:HD12	3:5:289:ILE:HA	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:69:ARG:HE	1:2:70:ARG:H	1.67	0.42
2:S:632:LYS:HA	2:S:635:MET:HE3	2.01	0.42
2:T:517:ASP:HA	2:T:520:LEU:HB2	2.01	0.42
2:T:698:MET:HE3	2:T:698:MET:HB3	1.90	0.42
2:T:1187:THR:HG22	2:T:1241:ASN:ND2	2.34	0.42
2:W:371:VAL:HA	2:W:380:ALA:HA	2.01	0.42
2:W:832:PHE:HA	2:W:835:VAL:HG22	2.01	0.42
4:f:29:LEU:O	4:f:70:ALA:N	2.51	0.42
2:l:131:MET:HG2	2:l:168:GLY:HA3	2.01	0.42
1:2:38:ASP:OD1	1:2:38:ASP:N	2.47	0.42
2:S:826:CYS:HB3	2:S:963:MET:HE1	2.01	0.42
2:S:857:LEU:HD12	2:S:875:ARG:HD3	2.01	0.42
2:S:1318:ASP:OD2	2:T:108:ARG:NH1	2.52	0.42
2:T:543:HIS:HD2	2:T:545:LEU:H	1.66	0.42
2:W:464:LEU:HG	2:W:1250:LEU:HD21	2.01	0.42
2:W:641:SER:OG	2:W:674:ALA:O	2.31	0.42
2:W:690:LEU:HD22	2:W:811:ILE:HG23	2.00	0.42
2:W:820:CYS:HA	2:W:1010:PRO:HB3	2.02	0.42
2:x:825:MET:HE2	2:x:825:MET:HB3	1.78	0.42
2:x:913:ASN:HD21	2:x:915:ALA:HB3	1.83	0.42
4:f:151:LEU:HD12	4:f:278:PHE:HE1	1.84	0.42
2:l:625:MET:O	2:l:887:SER:OG	2.37	0.42
2:l:764:GLU:HB3	2:l:793:ARG:HD2	2.00	0.42
2:l:788:HIS:HA	2:l:791:ASP:HB3	2.01	0.42
4:6:124:LYS:HD2	4:6:124:LYS:HA	1.83	0.42
2:S:338:ILE:HD12	3:5:18:GLY:HA2	2.01	0.42
2:S:553:ASP:OD1	2:S:553:ASP:N	2.52	0.42
2:S:826:CYS:HB2	2:S:959:VAL:HG13	2.02	0.42
2:S:999:SER:N	2:S:1000:PRO:HD2	2.35	0.42
2:T:317:ASN:HB3	2:T:327:VAL:HG13	2.01	0.42
2:T:335:MET:HE2	2:T:335:MET:HB3	1.94	0.42
2:T:794:LEU:HD22	2:T:896:ARG:HE	1.84	0.42
2:W:826:CYS:HB2	2:W:959:VAL:HG23	2.01	0.42
2:W:1246:GLN:HB2	2:W:1249:SER:HB3	2.02	0.42
2:x:1254:MET:O	2:x:1260:ARG:NH1	2.41	0.42
4:6:7:VAL:HG11	4:6:43:LEU:HD22	2.01	0.42
4:6:13:LEU:HD11	4:6:125:LEU:HD22	2.00	0.42
1:m:23:LEU:HD21	1:m:55:PHE:HB2	2.01	0.42
1:m:53:SER:HB3	2:l:886:ALA:HA	2.00	0.42
2:T:832:PHE:HA	2:T:835:VAL:HG22	2.02	0.42
2:W:634:VAL:HA	2:W:637:VAL:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:251:ASP:OD1	4:g:251:ASP:N	2.48	0.42
3:5:307:VAL:O	3:5:309:GLN:N	2.52	0.42
4:7:147:LEU:O	4:7:151:LEU:HB2	2.19	0.42
2:T:1076:ARG:NH2	3:e:62:LEU:O	2.48	0.42
2:W:421:SER:HB2	2:W:1354:ALA:HB2	2.01	0.42
2:W:497:MET:HE3	2:W:497:MET:HB3	1.90	0.42
2:W:632:LYS:HD3	2:W:887:SER:HB3	2.01	0.42
2:W:1225:TYR:HE2	2:W:1277:LYS:HD3	1.84	0.42
2:W:1357:HIS:O	2:W:1360:HIS:N	2.50	0.42
2:l:73:LEU:HD21	2:l:177:ILE:HG23	2.01	0.42
2:l:408:PRO:HB3	2:l:1045:THR:HG22	2.02	0.42
3:5:284:ARG:HH11	3:5:292:ILE:HD11	1.85	0.42
4:6:9:LEU:HG	4:6:40:VAL:HG21	2.00	0.42
4:6:140:THR:HA	4:6:143:ALA:HB3	2.01	0.42
2:T:172:LEU:HD13	2:T:1090:HIS:HB2	2.00	0.42
2:T:690:LEU:HD22	2:T:811:ILE:HG22	2.02	0.42
2:x:648:TRP:NE1	2:x:678:GLU:OE1	2.48	0.42
2:l:824:HIS:CE1	2:l:958:ARG:HE	2.36	0.42
4:7:23:GLN:HG3	4:7:24:ARG:HG3	2.02	0.42
2:T:810:LYS:O	2:T:814:TYR:HB2	2.19	0.42
2:W:535:TYR:O	2:W:539:ARG:HB2	2.20	0.42
2:W:862:ASN:HA	2:W:866:ARG:HD3	2.02	0.42
2:x:1298:LEU:N	2:x:1298:LEU:CD2	2.82	0.42
2:l:94:GLN:HE21	2:l:117:ILE:HG21	1.84	0.42
2:S:1145:LYS:HA	2:S:1145:LYS:HD2	1.88	0.42
2:T:969:THR:HA	2:T:972:MET:HG2	2.02	0.42
2:W:255:VAL:HG13	2:W:1102:SER:HA	2.02	0.42
2:W:594:LEU:HD11	2:W:693:LEU:HD12	2.01	0.42
2:x:264:VAL:HG22	2:x:356:ALA:HB2	2.00	0.42
2:S:474:LEU:HD13	2:S:548:ILE:HG21	2.02	0.42
2:x:437:GLU:OE1	2:x:439:TRP:NE1	2.52	0.42
3:e:223:VAL:HB	3:e:350:ILE:HB	2.02	0.42
2:l:1205:ARG:HD2	2:l:1227:HIS:CE1	2.54	0.42
3:5:107:GLY:O	3:5:224:THR:N	2.40	0.42
3:5:269:THR:HA	3:5:319:GLY:HA3	2.02	0.42
2:S:853:ASP:OD1	2:S:853:ASP:N	2.47	0.42
2:T:267:TYR:HE2	2:T:367:ILE:HD11	1.84	0.42
2:T:903:ASP:HB2	2:T:909:GLN:HE21	1.85	0.42
2:W:7:VAL:HG11	2:W:38:ASP:HB2	2.02	0.42
2:x:1204:GLY:HA2	2:x:1240:VAL:HG12	2.02	0.42
3:e:122:VAL:HG22	3:e:200:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:297:TYR:HD2	3:5:363:ILE:HG21	1.85	0.42
4:7:153:PHE:O	4:7:157:SER:HB3	2.19	0.42
2:S:1048:ARG:NH1	2:S:1050:ASP:OD2	2.53	0.41
2:S:1089:HIS:HB3	2:l:1081:VAL:HG21	2.02	0.41
2:T:585:GLY:HA3	2:T:1017:GLY:HA2	2.01	0.41
2:T:1120:HIS:CD2	2:T:1150:ARG:NH1	2.87	0.41
2:W:159:LYS:HA	2:W:159:LYS:HD3	1.80	0.41
2:x:260:VAL:HG22	2:x:1097:THR:HB	2.01	0.41
2:x:564:HIS:O	2:x:998:ARG:NH2	2.53	0.41
4:f:245:ASP:OD2	4:f:249:ARG:NH2	2.53	0.41
2:l:621:VAL:HG21	2:l:868:LEU:HD21	2.02	0.41
4:7:222:ARG:HG3	4:7:264:MET:HE3	2.01	0.41
1:m:6:PRO:HB2	2:l:834:HIS:HD2	1.84	0.41
1:2:41:ARG:O	1:2:45:ARG:HG3	2.19	0.41
2:S:149:VAL:HG23	2:W:50:ILE:HD13	2.02	0.41
2:S:316:GLU:O	2:S:320:THR:OG1	2.31	0.41
2:T:191:MET:HE3	2:T:195:GLN:HG3	2.01	0.41
2:T:899:ARG:HH12	2:T:991:ALA:H	1.68	0.41
2:W:518:ILE:O	2:W:999:SER:OG	2.37	0.41
2:W:619:PHE:CE1	2:W:643:CYS:HB3	2.54	0.41
2:x:640:VAL:HA	2:x:643:CYS:HB2	2.00	0.41
4:f:96:LYS:HA	4:f:96:LYS:HD2	1.90	0.41
4:g:201:LEU:HD12	4:g:201:LEU:HA	1.92	0.41
2:S:409:VAL:HG13	2:S:1044:MET:HB2	2.01	0.41
2:T:302:ILE:HG13	2:T:367:ILE:HG13	2.01	0.41
2:l:726:PRO:HD3	2:l:814:TYR:CZ	2.55	0.41
2:W:598:VAL:HB	2:W:689:GLU:HB3	2.01	0.41
2:W:856:ILE:O	2:W:860:LEU:CB	2.68	0.41
2:W:1080:ARG:HH22	3:e:261:ASP:HB3	1.85	0.41
2:W:1338:SER:OG	2:W:1360:HIS:ND1	2.45	0.41
2:x:489:LEU:O	2:x:994:ARG:NH1	2.51	0.41
2:T:733:PHE:HB3	2:T:746:ILE:HD13	2.02	0.41
2:T:1215:TYR:CZ	2:T:1285:ARG:HD3	2.55	0.41
2:W:471:LEU:HD23	2:W:471:LEU:HA	1.93	0.41
2:W:811:ILE:O	2:W:815:VAL:HB	2.20	0.41
2:x:138:LEU:HD12	2:x:141:LEU:HD12	2.01	0.41
2:x:937:THR:O	2:x:941:THR:OG1	2.29	0.41
2:l:657:VAL:HA	2:l:663:ILE:HD11	2.03	0.41
2:l:691:ILE:HG22	2:l:808:LEU:HD21	2.03	0.41
4:6:257:VAL:O	4:6:261:LEU:HB2	2.21	0.41
2:S:722:ASN:HB3	2:S:902:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:693:LEU:HD23	2:T:693:LEU:HA	1.91	0.41
2:T:1241:ASN:HD21	2:T:1244:ALA:HB3	1.84	0.41
4:f:29:LEU:HD13	4:f:43:LEU:HD21	2.02	0.41
4:f:87:PRO:HG3	4:f:300:LEU:HD22	2.01	0.41
2:l:783:ARG:NH1	2:l:892:PRO:O	2.40	0.41
3:5:335:ARG:HE	3:5:335:ARG:HB2	1.69	0.41
2:T:271:LYS:HD2	2:T:271:LYS:HA	1.84	0.41
2:T:936:ARG:HA	2:T:936:ARG:HD2	1.80	0.41
2:W:184:LYS:HD3	2:W:184:LYS:HA	1.76	0.41
4:f:153:PHE:CG	4:f:190:LEU:HD13	2.55	0.41
4:g:109:LEU:HD12	4:g:137:VAL:HG12	2.01	0.41
2:l:376:ASN:OD1	2:l:377:HIS:ND1	2.53	0.41
4:7:18:ILE:HD13	4:7:18:ILE:HA	1.91	0.41
2:T:621:VAL:HG21	2:T:868:LEU:HD21	2.01	0.41
2:W:543:HIS:CE1	2:W:545:LEU:HB2	2.56	0.41
2:W:1067:MET:HE2	2:W:1067:MET:HB3	1.86	0.41
2:x:588:PHE:HE1	2:x:700:LEU:HD22	1.85	0.41
3:e:133:ILE:HD11	3:e:165:LEU:HD13	2.01	0.41
4:g:156:TYR:HA	4:g:159:VAL:HG22	2.03	0.41
2:l:397:LEU:HD21	2:l:1058:LEU:HB2	2.03	0.41
2:l:825:MET:HB3	2:l:825:MET:HE2	1.79	0.41
2:l:884:LEU:HD23	2:l:884:LEU:HA	1.94	0.41
2:l:1127:VAL:HG23	2:l:1264:VAL:HG22	2.02	0.41
2:l:1374:LYS:HA	2:l:1374:LYS:HD3	1.75	0.41
1:m:60:TYR:HA	1:m:63:ARG:HG2	2.01	0.41
2:S:516:THR:HG22	2:S:993:TYR:HE1	1.85	0.41
2:S:549:TYR:OH	2:S:994:ARG:NH1	2.51	0.41
2:S:1273:ALA:HB2	2:S:1301:HIS:CD2	2.55	0.41
2:T:638:PRO:HA	2:T:641:SER:HB2	2.01	0.41
2:W:79:ASN:CB	2:W:308:TYR:CD1	3.03	0.41
2:W:868:LEU:O	2:W:872:SER:HB2	2.21	0.41
2:W:1308:GLU:OE1	2:x:209:LYS:NZ	2.42	0.41
2:x:783:ARG:HG2	2:x:893:THR:HG22	2.03	0.41
2:x:878:VAL:HA	2:x:881:ILE:HG22	2.02	0.41
4:f:91:TYR:O	4:f:298:CYS:N	2.47	0.41
4:f:148:GLN:HE22	4:g:269:THR:HG23	1.86	0.41
4:g:109:LEU:O	4:g:284:LEU:N	2.51	0.41
2:l:655:ALA:O	2:l:683:TYR:OH	2.33	0.41
2:T:447:LEU:HD11	2:T:1343:ILE:HD13	2.02	0.41
2:T:524:LEU:H	2:T:524:LEU:HG	1.73	0.41
2:T:947:ALA:HB3	2:T:964:HIS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:1272:ARG:HG2	2:T:1276:ASN:ND2	2.35	0.41
2:x:598:VAL:HG13	2:x:602:VAL:HB	2.02	0.41
2:x:602:VAL:HG21	2:x:685:LYS:HD3	2.03	0.41
2:x:837:GLN:HA	1:y:49:VAL:HG21	2.03	0.41
2:x:1122:GLN:HE21	2:x:1181:THR:HG21	1.86	0.41
4:f:73:ASP:OD1	4:f:73:ASP:N	2.49	0.41
2:S:552:ARG:HD2	2:S:552:ARG:HA	1.85	0.40
2:T:141:LEU:HD22	2:T:161:VAL:HG21	2.02	0.40
2:T:434:LEU:HD12	2:T:434:LEU:HA	1.89	0.40
2:W:140:ILE:HD12	2:W:140:ILE:HA	1.97	0.40
2:W:452:LEU:HD22	2:W:1040:PRO:HD3	2.03	0.40
2:l:481:ARG:HH12	2:l:483:ARG:HH21	1.69	0.40
1:Z:23:LEU:HD21	1:Z:55:PHE:HB2	2.03	0.40
2:T:745:GLN:HG2	2:T:918:ARG:HH22	1.85	0.40
2:W:540:LEU:HD11	2:W:550:ILE:HG13	2.03	0.40
2:W:1195:TYR:OH	2:W:1201:SER:O	2.36	0.40
2:x:282:VAL:HG23	2:x:383:SER:HB2	2.03	0.40
2:x:821:THR:O	2:x:823:ALA:N	2.51	0.40
2:l:887:SER:OG	2:l:891:CYS:SG	2.69	0.40
2:l:1080:ARG:HG2	2:l:1082:ASP:H	1.87	0.40
2:l:1205:ARG:NH2	2:l:1229:ARG:O	2.54	0.40
3:5:25:ARG:HE	3:5:25:ARG:HB3	1.74	0.40
1:m:60:TYR:CE2	2:l:883:ASP:HB3	2.54	0.40
2:S:11:PRO:HG2	2:T:322:VAL:HG13	2.04	0.40
2:S:857:LEU:HD23	2:S:857:LEU:HA	1.87	0.40
2:S:880:MET:HE2	2:S:880:MET:HB3	1.99	0.40
3:e:96:HIS:NE2	3:e:122:VAL:HG11	2.36	0.40
2:l:901:SER:HB2	2:l:920:GLU:HG3	2.03	0.40
4:7:152:LEU:HD23	4:7:152:LEU:HA	1.95	0.40
1:m:21:SER:HA	1:m:22:PRO:HD3	1.94	0.40
2:S:648:TRP:HH2	2:S:682:MET:HE3	1.86	0.40
2:S:858:ASP:OD1	2:S:859:ASN:ND2	2.55	0.40
2:T:316:GLU:OE1	2:T:331:PHE:HD1	2.04	0.40
2:W:197:LEU:HD23	2:W:197:LEU:HA	1.94	0.40
2:W:319:VAL:O	2:W:323:SER:CB	2.69	0.40
2:W:710:SER:OG	2:W:711:VAL:N	2.54	0.40
2:W:1192:ASP:OD1	2:W:1192:ASP:N	2.49	0.40
3:e:117:ASP:HA	3:e:118:PRO:HD3	1.92	0.40
3:e:262:ALA:HA	3:e:283:SER:HA	2.04	0.40
4:f:152:LEU:O	4:f:156:TYR:HB2	2.22	0.40
2:l:709:GLU:HB3	2:l:713:GLN:HE22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:25:ARG:NH1	3:5:45:GLU:OE2	2.54	0.40
2:S:718:LEU:HD13	2:S:811:ILE:HG12	2.03	0.40
2:S:742:ARG:HB2	2:S:903:ASP:HB2	2.04	0.40
2:S:1141:TYR:CD1	2:S:1141:TYR:C	2.99	0.40
2:T:386:LYS:H	2:T:386:LYS:HG2	1.66	0.40
2:T:481:ARG:HG3	2:T:539:ARG:HD3	2.03	0.40
2:W:166:GLN:HA	2:W:169:VAL:HG22	2.03	0.40
2:W:626:ILE:HD12	2:W:633:PHE:HD1	1.86	0.40
2:W:747:ILE:HG12	2:W:752:VAL:HG22	2.02	0.40
1:y:67:VAL:HG13	1:y:68:PRO:HD3	2.04	0.40
4:f:245:ASP:HB2	4:f:249:ARG:HH21	1.87	0.40
4:6:145:GLU:HA	4:6:148:GLN:HG2	2.02	0.40
4:7:43:LEU:HD21	4:7:132:ILE:HG22	2.03	0.40
4:7:72:LEU:HA	4:7:82:LEU:HA	2.03	0.40
4:7:95:ASN:HB3	4:7:103:TRP:CE2	2.56	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	2	72/176 (41%)	64 (89%)	8 (11%)	0	100	100
1	Y	72/176 (41%)	65 (90%)	7 (10%)	0	100	100
1	Z	72/176 (41%)	67 (93%)	5 (7%)	0	100	100
1	m	69/176 (39%)	64 (93%)	5 (7%)	0	100	100
1	y	72/176 (41%)	65 (90%)	7 (10%)	0	100	100
2	S	1327/1381 (96%)	1246 (94%)	80 (6%)	1 (0%)	48	79
2	T	1319/1381 (96%)	1222 (93%)	97 (7%)	0	100	100
2	W	1321/1381 (96%)	1243 (94%)	78 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	l	1237/1381 (90%)	1164 (94%)	73 (6%)	0	100	100
2	x	1321/1381 (96%)	1243 (94%)	78 (6%)	0	100	100
3	5	303/364 (83%)	285 (94%)	17 (6%)	1 (0%)	36	67
3	e	311/364 (85%)	300 (96%)	11 (4%)	0	100	100
4	6	285/301 (95%)	269 (94%)	16 (6%)	0	100	100
4	7	271/301 (90%)	255 (94%)	16 (6%)	0	100	100
4	f	286/301 (95%)	276 (96%)	10 (4%)	0	100	100
4	g	271/301 (90%)	261 (96%)	10 (4%)	0	100	100
All	All	8609/9717 (89%)	8089 (94%)	518 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S	1176	HIS
3	5	308	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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.

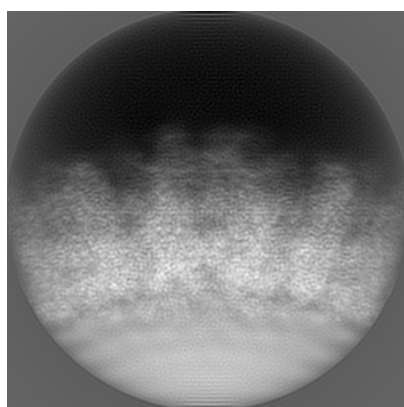
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30159. These allow visual inspection of the internal detail of the map and identification of artifacts.

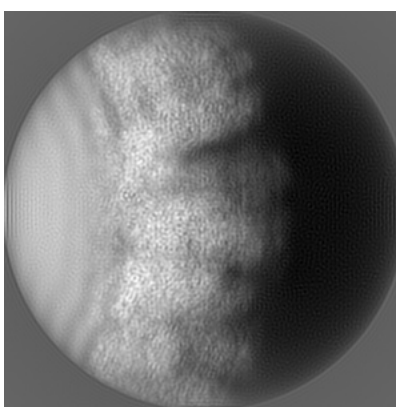
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

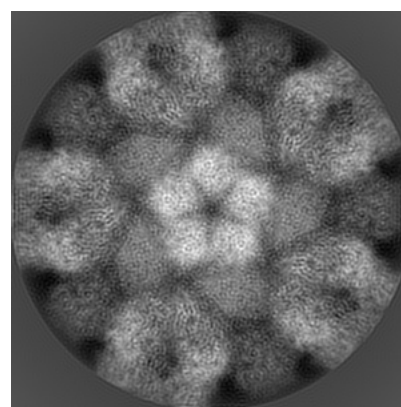
6.1.1 Primary map



X



Y

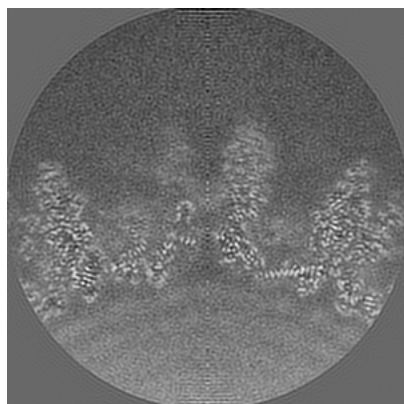


Z

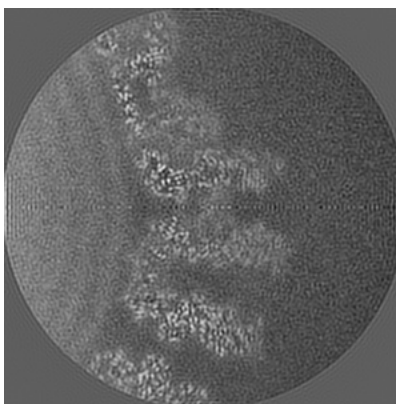
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

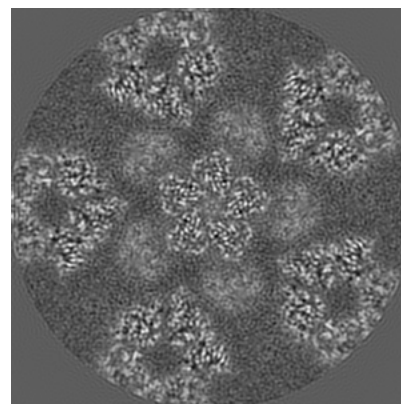
6.2.1 Primary map



X Index: 150



Y Index: 150

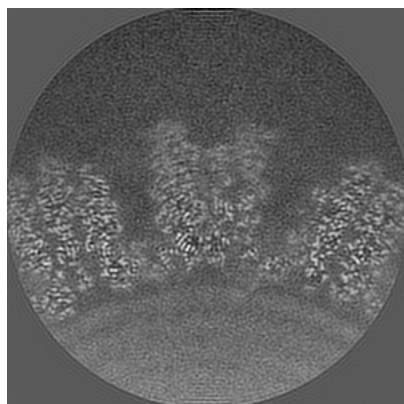


Z Index: 150

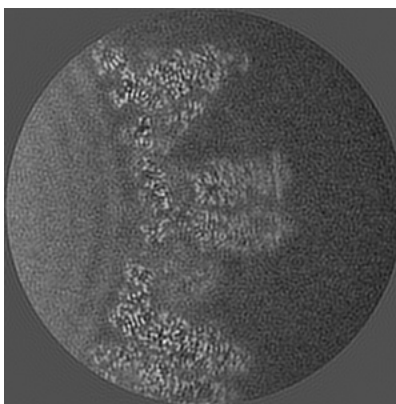
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

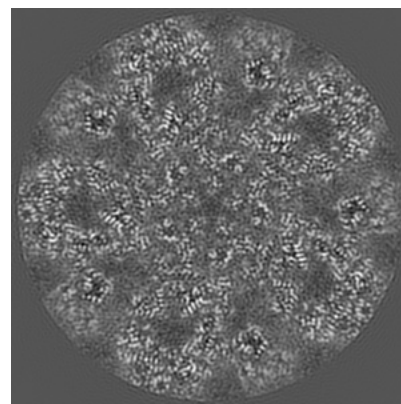
6.3.1 Primary map



X Index: 137



Y Index: 122

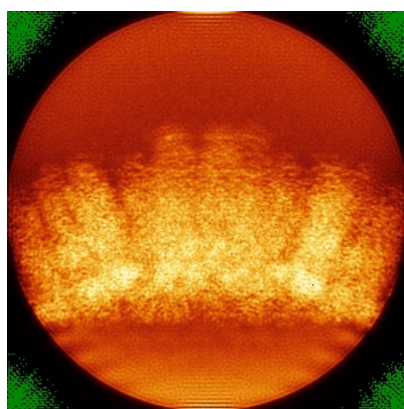


Z Index: 108

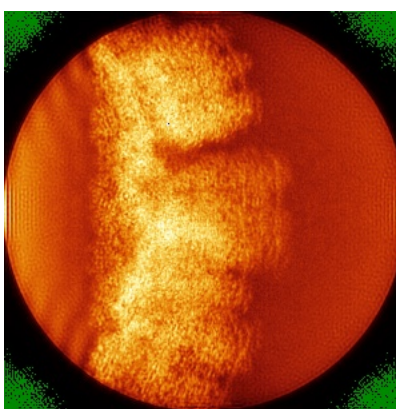
The images above show the largest variance slices of the map in three orthogonal directions.

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

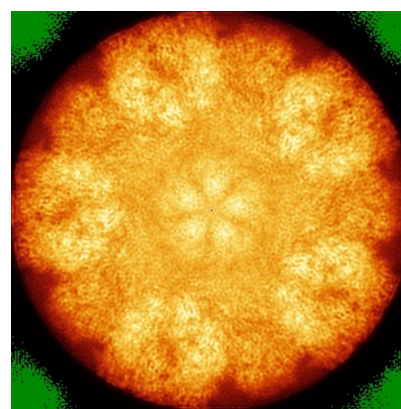
6.4.1 Primary map



X



Y

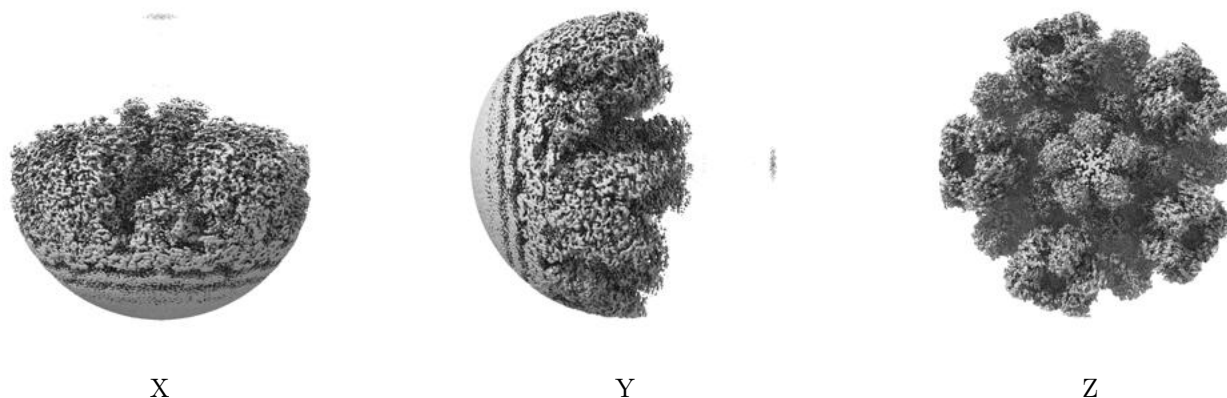


Z

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

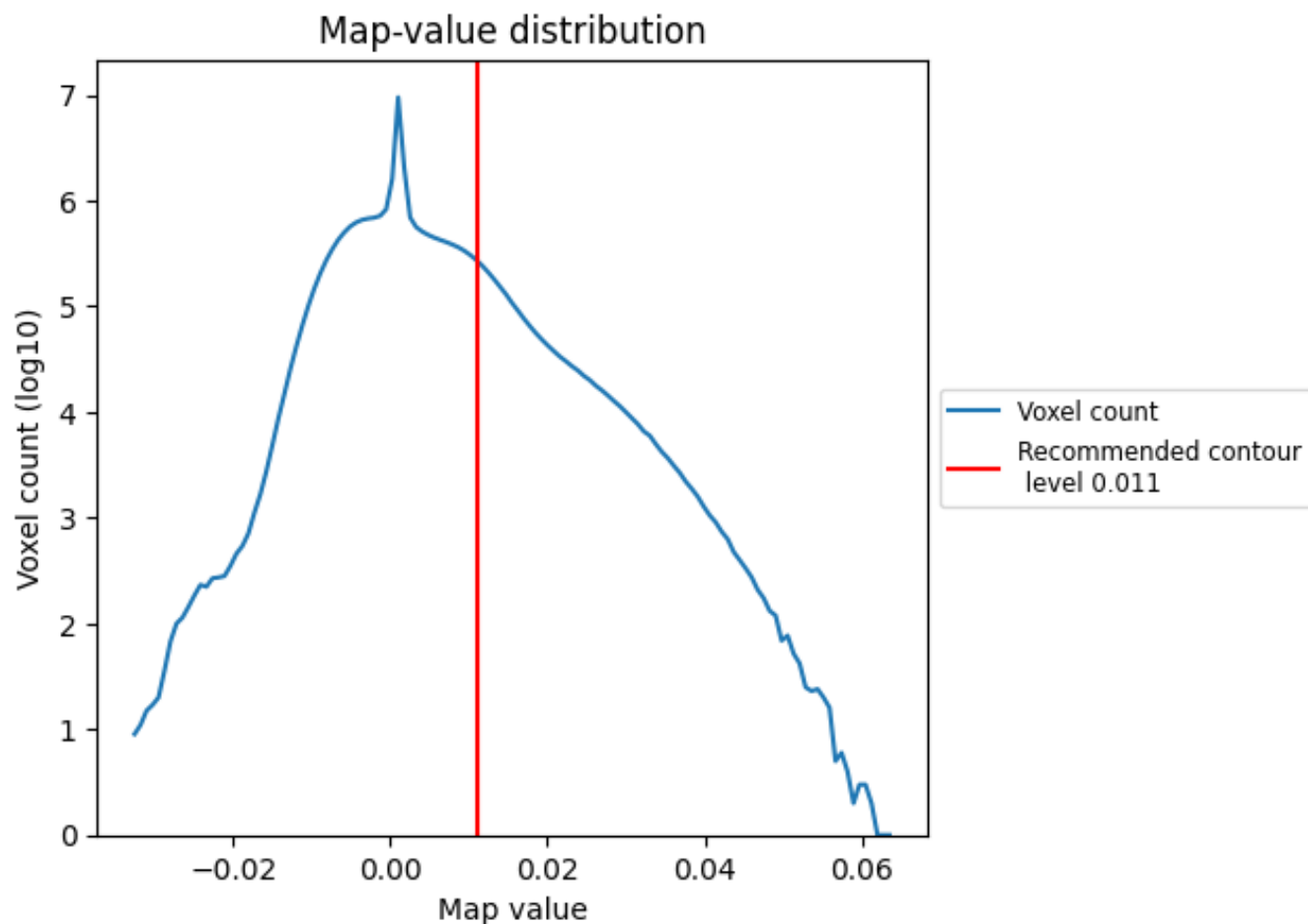
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

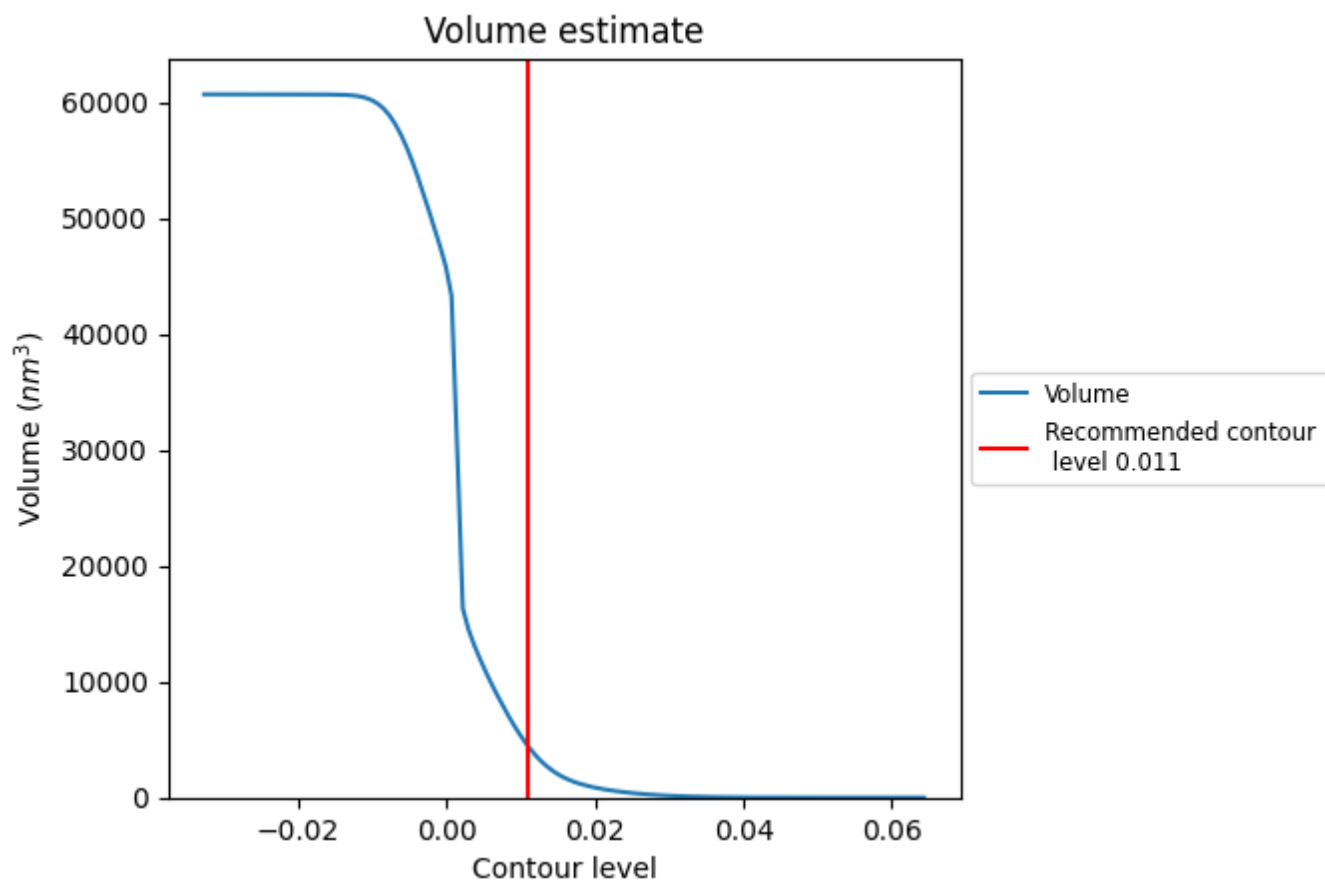
This section contains the results of statistical analysis of the map.

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.

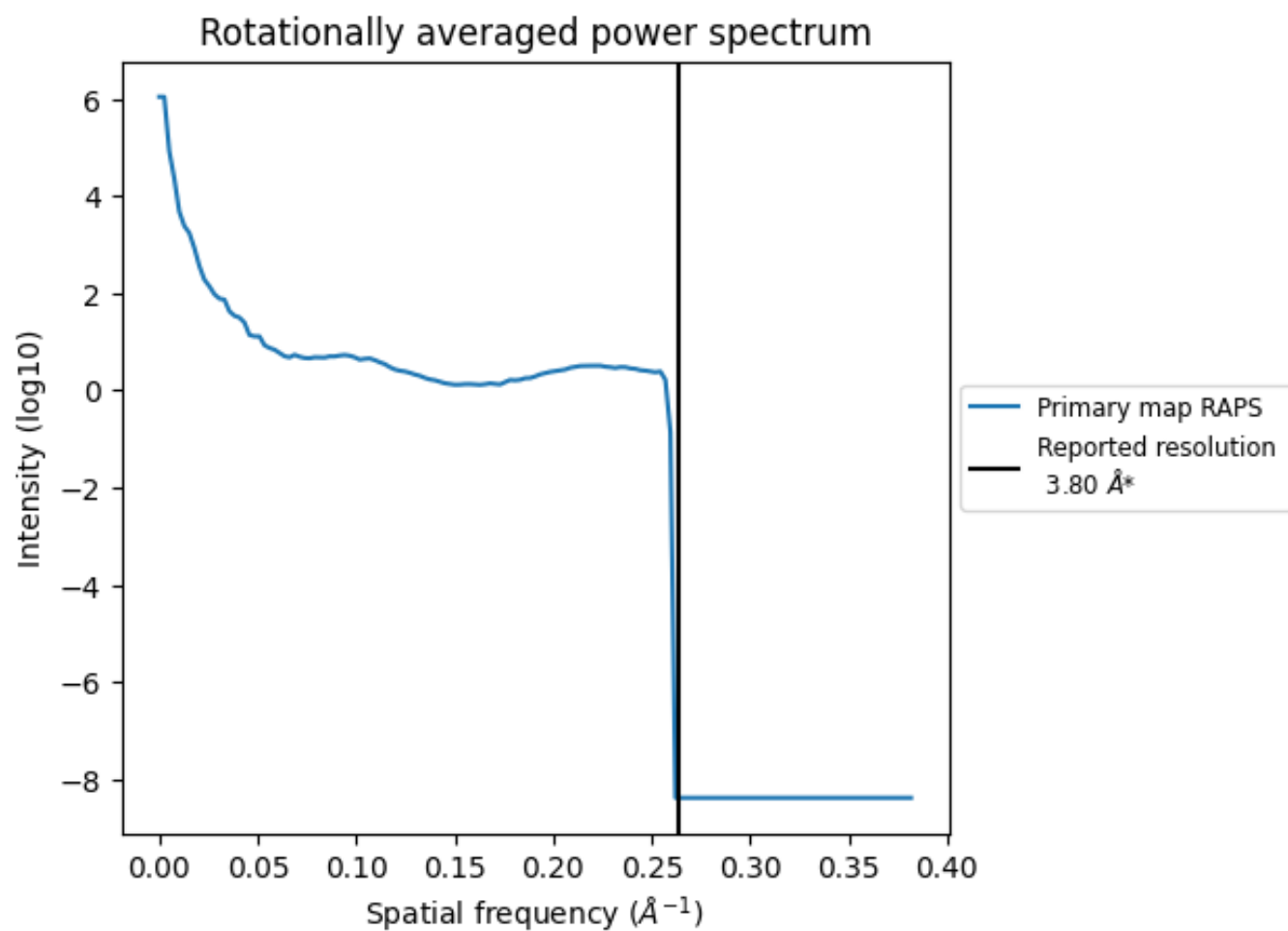
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4476 nm³; this corresponds to an approximate mass of 4043 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 0.263 Å⁻¹

8 Fourier-Shell correlation

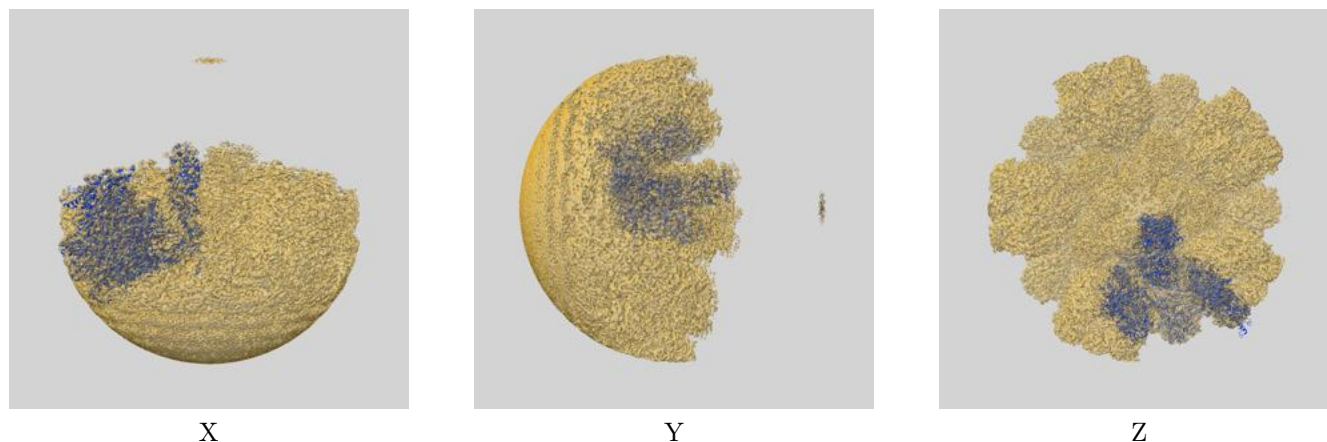
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-30159 and PDB model 7BR8. Per-residue inclusion information can be found in section 3 on page 6.

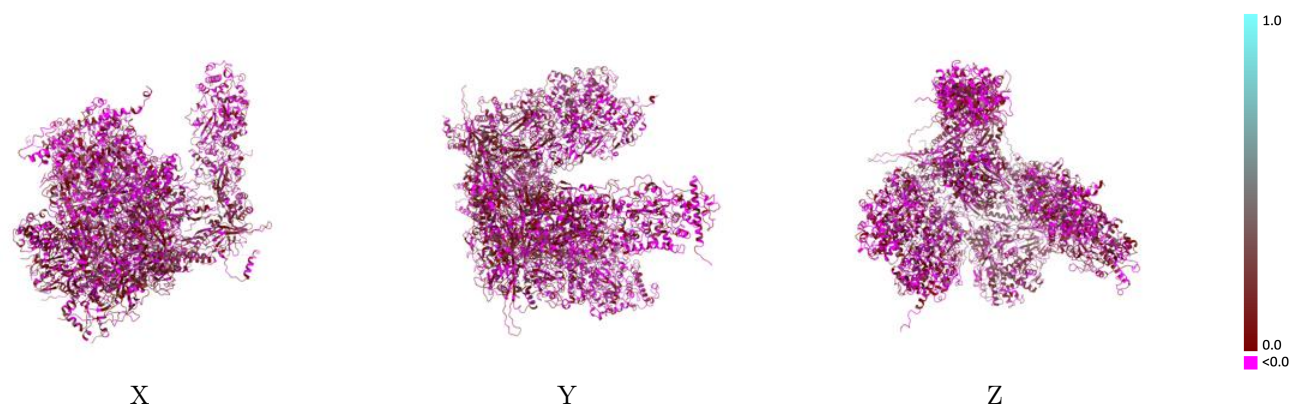
9.1 Map-model overlays

9.1.1 Map-model overlay ⓘ



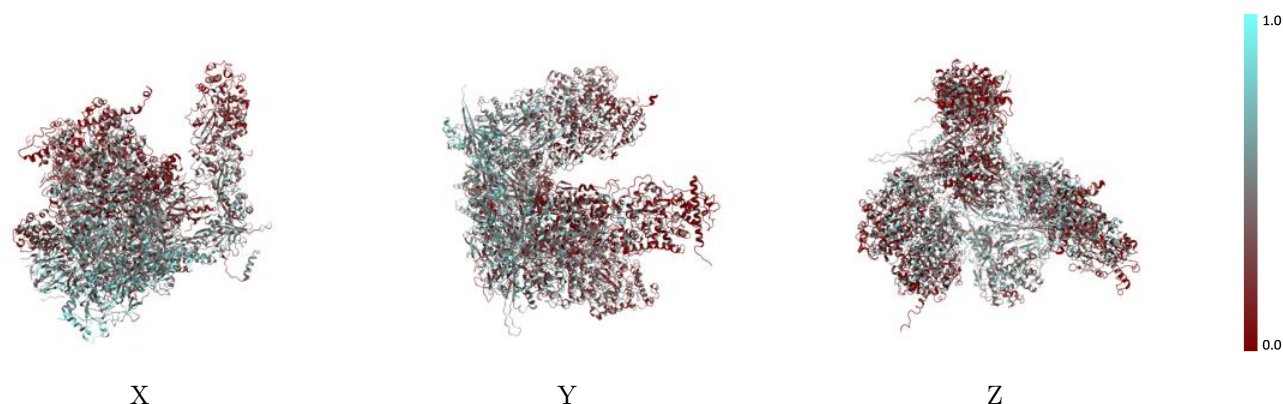
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



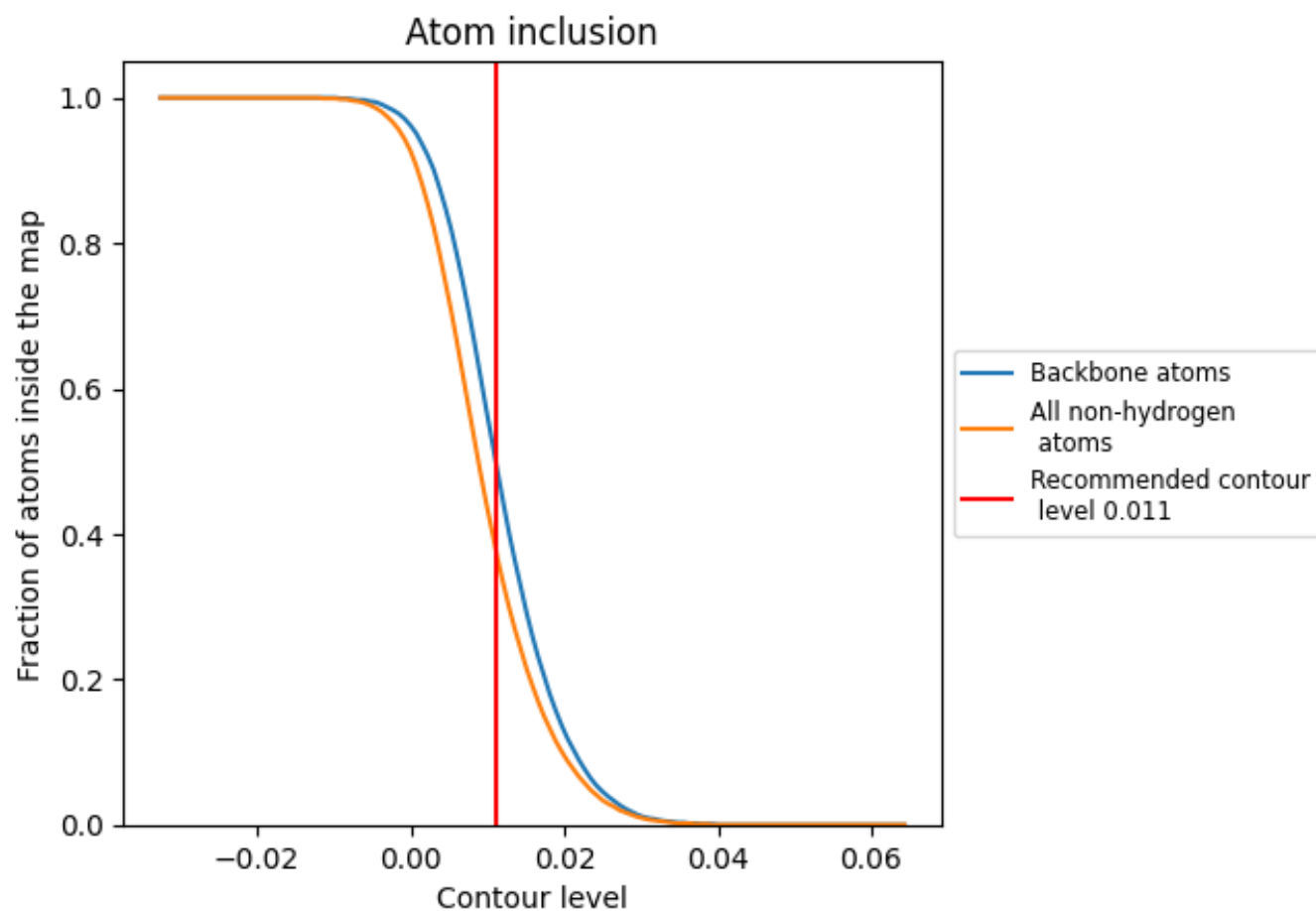
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).

9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 38% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3840	 0.0390
2	 0.0900	 0.0040
5	 0.3400	 0.0580
6	 0.2570	 0.0380
7	 0.2150	 0.0200
S	 0.3920	 0.0270
T	 0.4150	 0.0250
W	 0.4590	 0.0620
Y	 0.1880	 -0.0060
Z	 0.1430	 -0.0060
e	 0.4820	 0.0630
f	 0.4460	 0.0640
g	 0.4600	 0.0620
l	 0.3240	 0.0360
m	 0.0830	 -0.0260
x	 0.4190	 0.0370
y	 0.1570	 0.0320

