



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 05:54 PM UTC

PDB ID : 6M6G / pdb_00006m6g
EMDB ID : EMD-30123
Title : Structure of HSV2 viron capsid portal vertex
Authors : Wang, X.X.; Wang, N.
Deposited on : 2020-03-14
Resolution : 5.39 Å(reported)

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

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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:

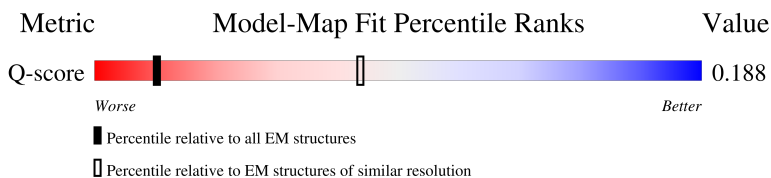
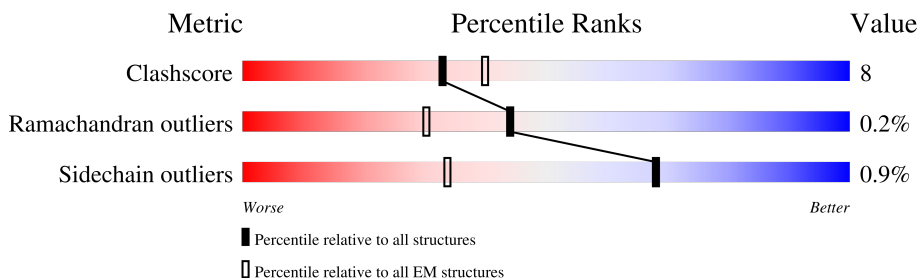
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 5.39 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	498 (4.90 - 5.87)

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	B	1374	25% 77% 21% ..
1	C	1374	31% 80% 18% ..
1	D	1374	26% 79% 19% ..
1	E	1374	20% 79% 19% .

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Mol	Chain	Length	Quality of chain
1	F	1374	
1	I	1374	
2	G	112	
2	M	112	
2	Q	112	
2	T	112	
2	U	112	
2	V	112	
3	K	318	
3	O	318	
4	L	84	
5	P	87	
6	S	466	
7	k	702	
8	l	585	
8	m	585	
9	n	3122	
9	o	3122	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 78731 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1362	Total	C	N	O	S	0	0
			10198	6475	1847	1821	55		
1	C	1362	Total	C	N	O	S	0	0
			10209	6479	1844	1831	55		
1	D	1362	Total	C	N	O	S	0	0
			10221	6485	1848	1833	55		
1	E	1351	Total	C	N	O	S	0	0
			10162	6452	1837	1818	55		
1	F	1351	Total	C	N	O	S	0	0
			9978	6343	1804	1779	52		
1	I	1319	Total	C	N	O	S	0	0
			9831	6234	1785	1758	54		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	MET	ILE	conflict	UNP P89442
B	18	VAL	LEU	conflict	UNP P89442
B	382	LYS	ARG	conflict	UNP P89442
B	986	HIS	ASP	conflict	UNP P89442
C	17	MET	ILE	conflict	UNP P89442
C	18	VAL	LEU	conflict	UNP P89442
C	382	LYS	ARG	conflict	UNP P89442
C	986	HIS	ASP	conflict	UNP P89442
D	17	MET	ILE	conflict	UNP P89442
D	18	VAL	LEU	conflict	UNP P89442
D	382	LYS	ARG	conflict	UNP P89442
D	986	HIS	ASP	conflict	UNP P89442
E	17	MET	ILE	conflict	UNP P89442
E	18	VAL	LEU	conflict	UNP P89442
E	382	LYS	ARG	conflict	UNP P89442
E	986	HIS	ASP	conflict	UNP P89442
F	17	MET	ILE	conflict	UNP P89442
F	18	VAL	LEU	conflict	UNP P89442

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Chain	Residue	Modelled	Actual	Comment	Reference
F	382	LYS	ARG	conflict	UNP P89442
F	986	HIS	ASP	conflict	UNP P89442
I	17	MET	ILE	conflict	UNP P89442
I	18	VAL	LEU	conflict	UNP P89442
I	382	LYS	ARG	conflict	UNP P89442
I	986	HIS	ASP	conflict	UNP P89442

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	101	Total	C	N	O	S	0	0
			772	488	143	139	2		
2	M	101	Total	C	N	O	S	0	0
			772	488	143	139	2		
2	Q	101	Total	C	N	O	S	0	0
			772	488	143	139	2		
2	T	101	Total	C	N	O	S	0	0
			772	488	143	139	2		
2	U	101	Total	C	N	O	S	0	0
			772	488	143	139	2		
2	V	101	Total	C	N	O	S	0	0
			772	488	143	139	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	22	THR	MET	conflict	UNP G9I257
M	22	THR	MET	conflict	UNP G9I257
Q	22	THR	MET	conflict	UNP G9I257
T	22	THR	MET	conflict	UNP G9I257
U	22	THR	MET	conflict	UNP G9I257
V	22	THR	MET	conflict	UNP G9I257

- Molecule 3 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	299	Total	C	N	O	S	0	0
			2078	1341	373	357	7		
3	O	307	Total	C	N	O	S	0	0
			2175	1405	392	370	8		

- Molecule 4 is a protein called coiled coils.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	L	84	Total	C	N	O	0	0
			420	252	84	84		

- Molecule 5 is a protein called Coiled coils.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	P	87	Total	C	N	O	0	0
			435	261	87	87		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	279	Total	C	N	O	S	0	0
			1975	1264	354	341	16		

- Molecule 7 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	553	Total	C	N	O	S	0	0
			4233	2695	773	748	17		

- Molecule 8 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	l	94	Total	C	N	O	S	0	0
			770	493	139	136	2		
8	m	80	Total	C	N	O		0	0
			648	411	123	114			

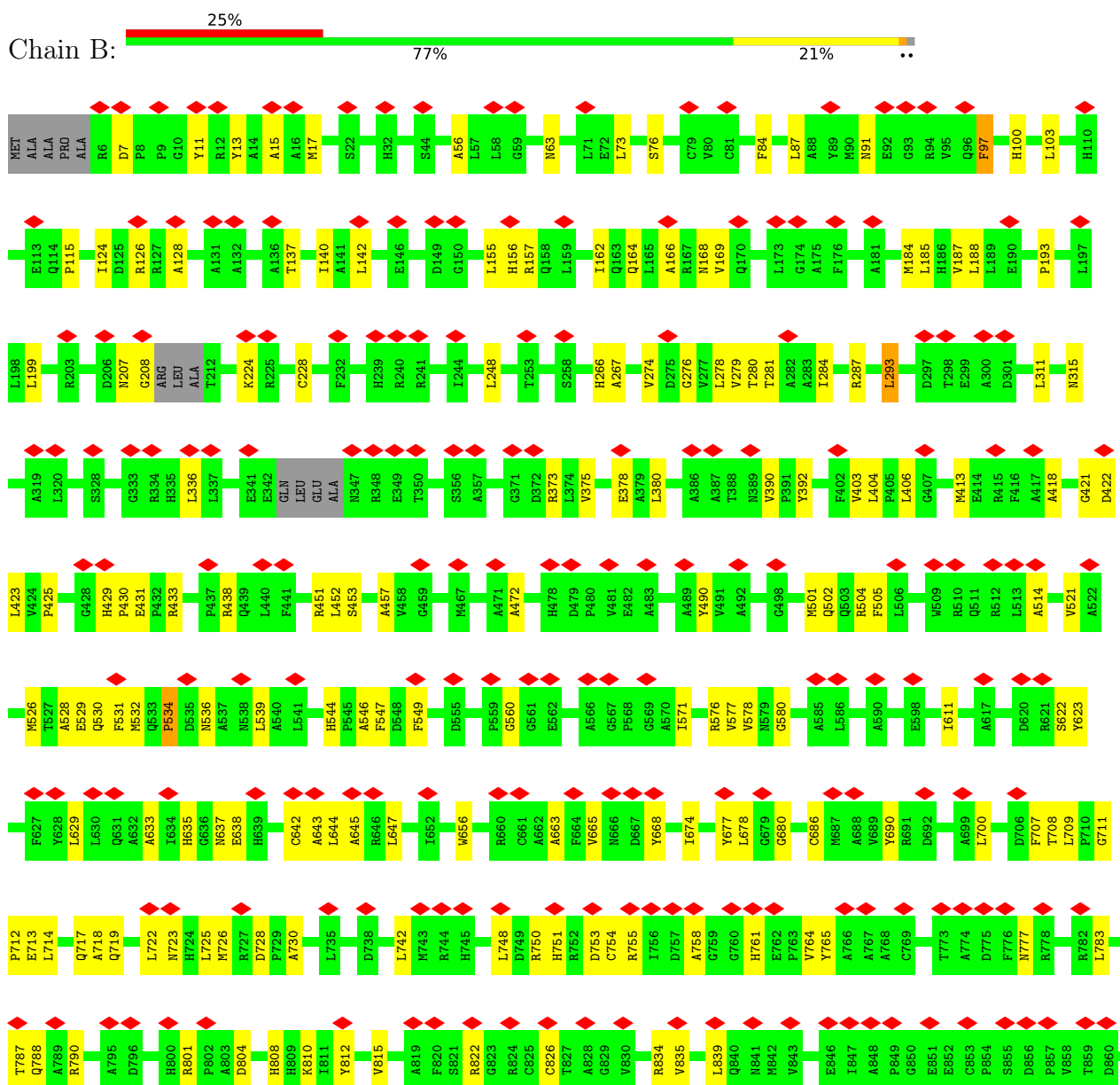
- Molecule 9 is a protein called Large tegument protein deneddylase.

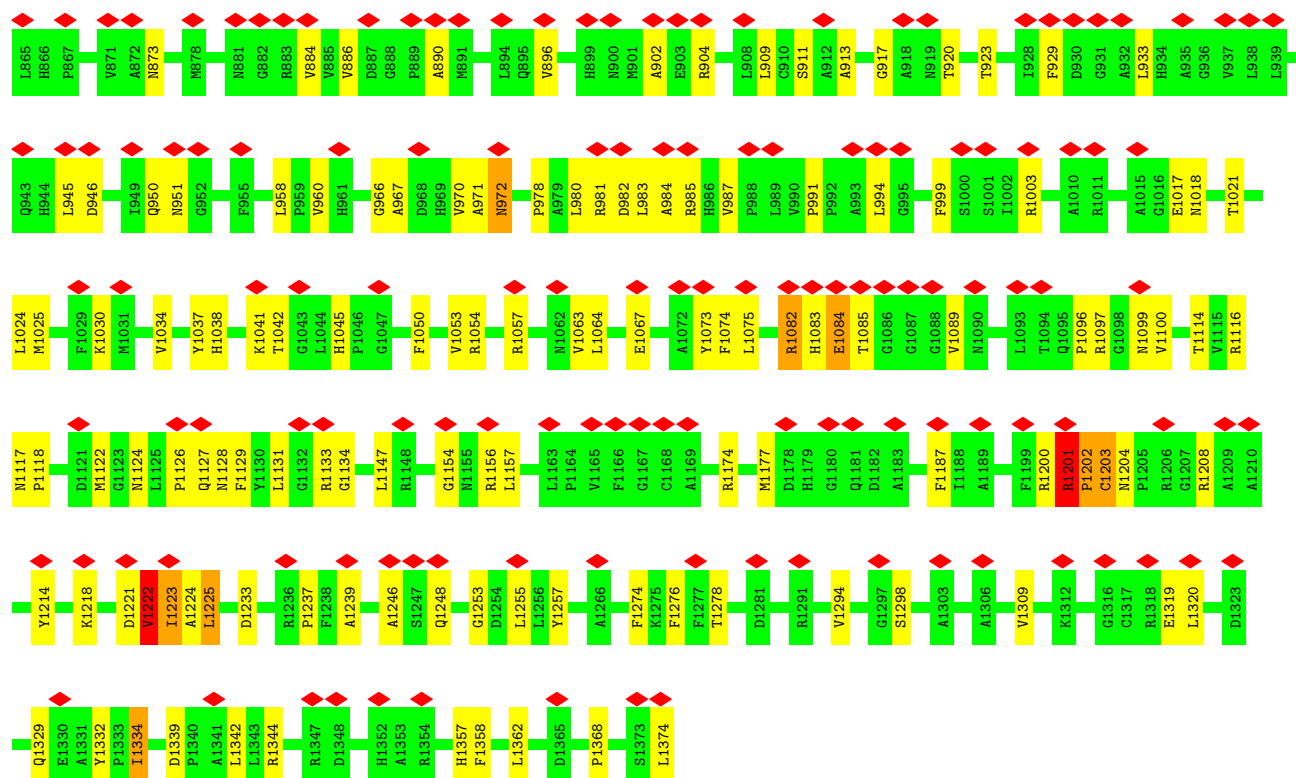
Mol	Chain	Residues	Atoms					AltConf	Trace
9	n	47	Total	C	N	O	S	0	0
			383	234	87	60	2		
9	o	47	Total	C	N	O	S	0	0
			383	234	87	60	2		

3 Residue-property plots

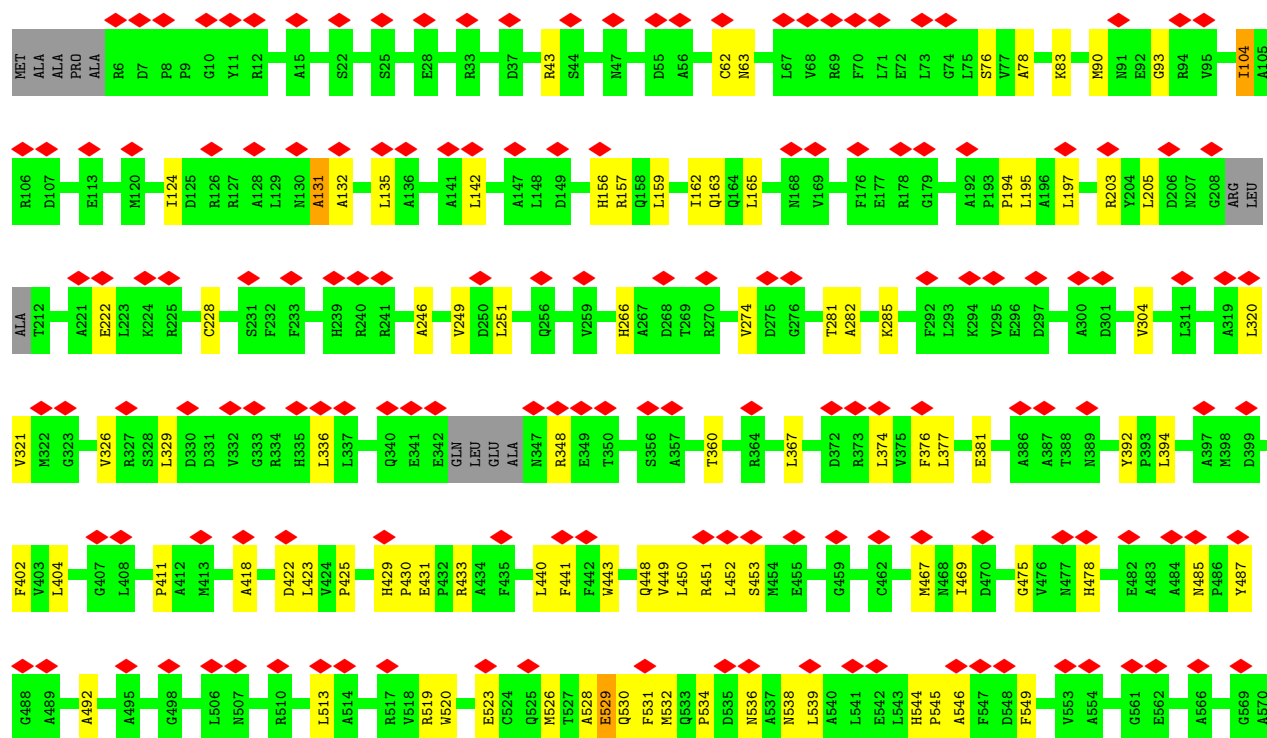
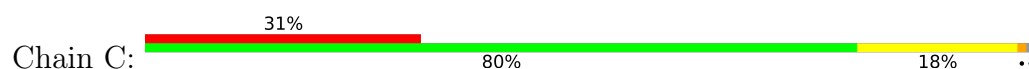
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

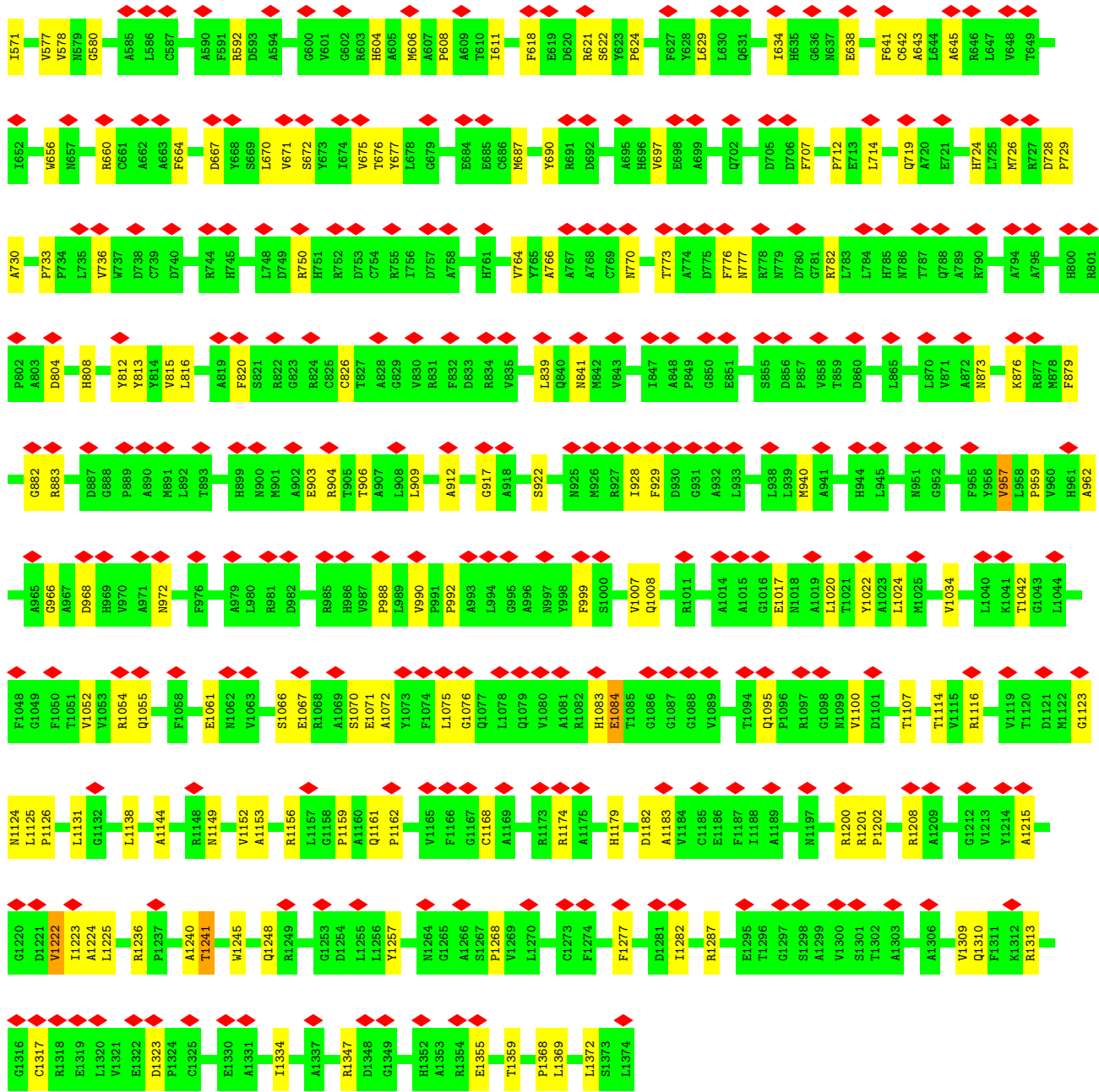
• Molecule 1: Major capsid protein



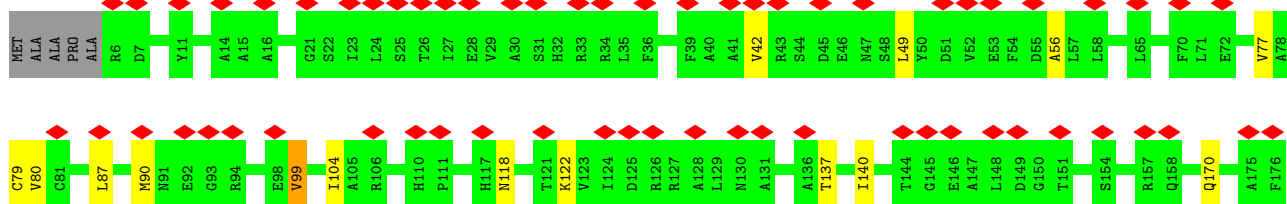
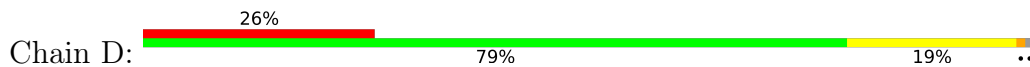


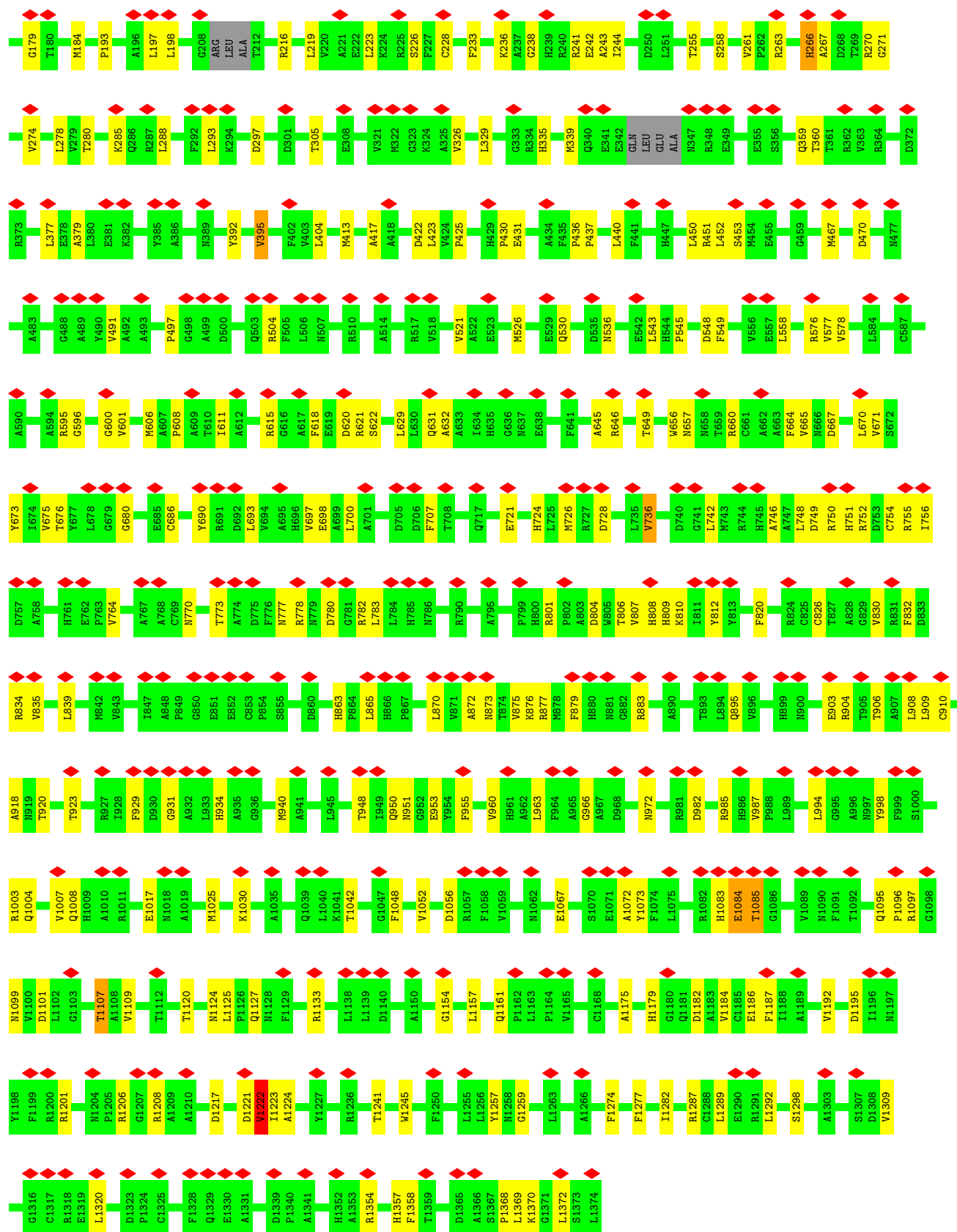
• Molecule 1: Major capsid protein



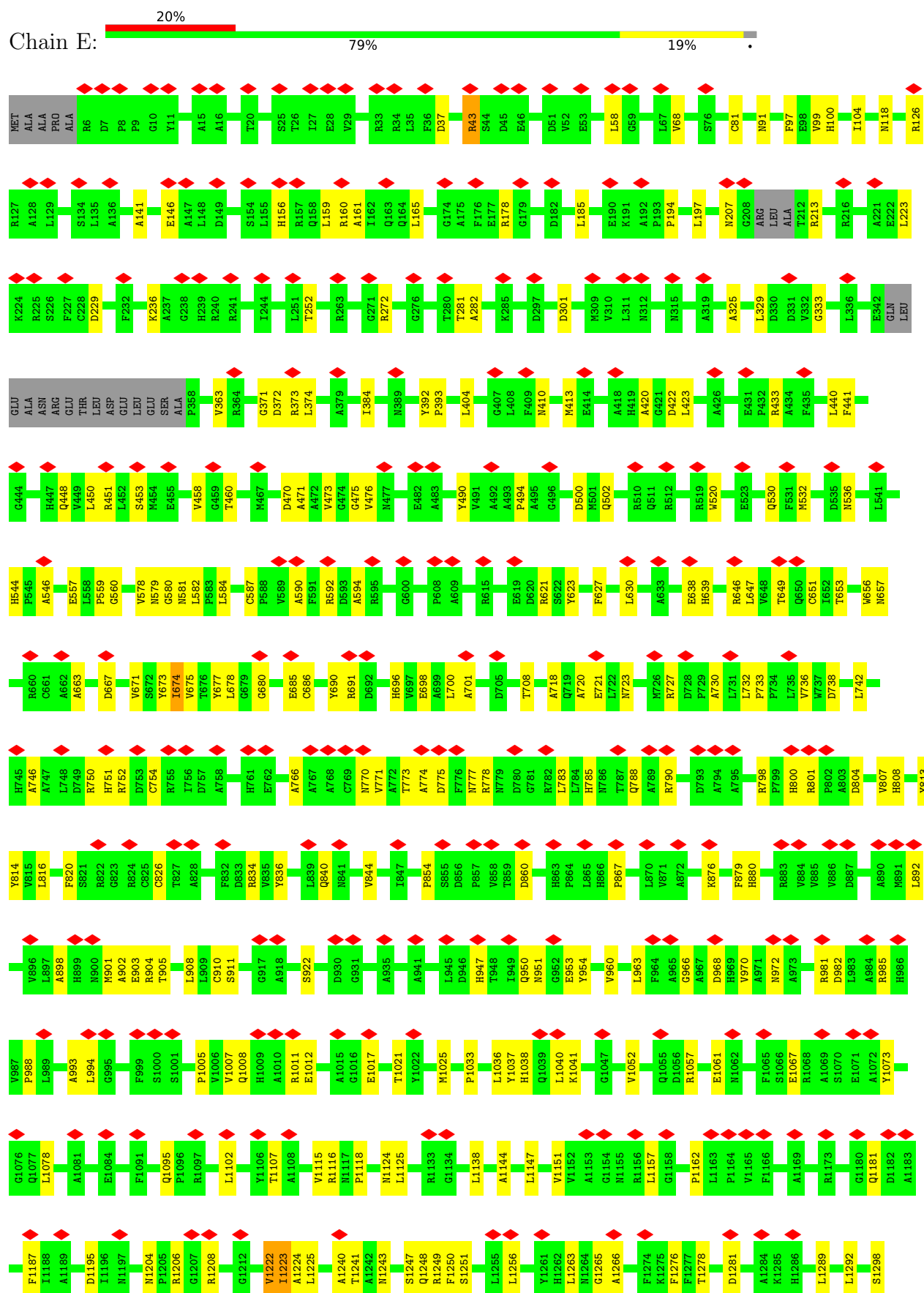


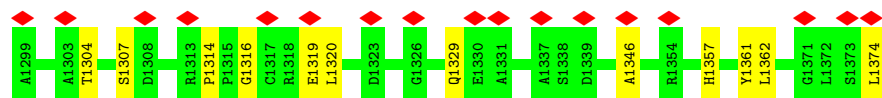
● Molecule 1: Major capsid protein



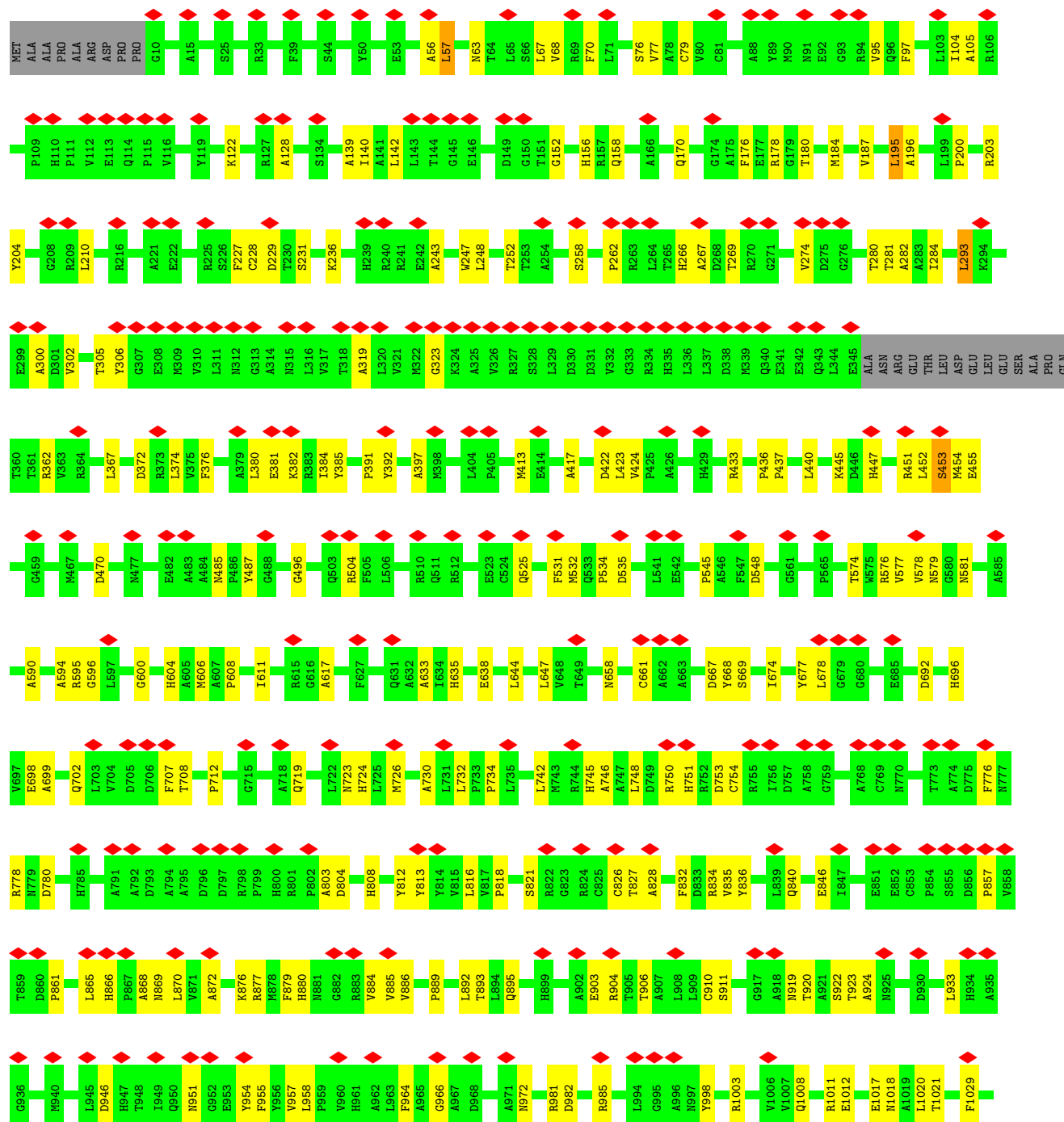
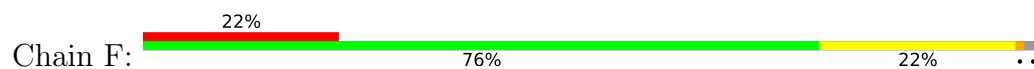


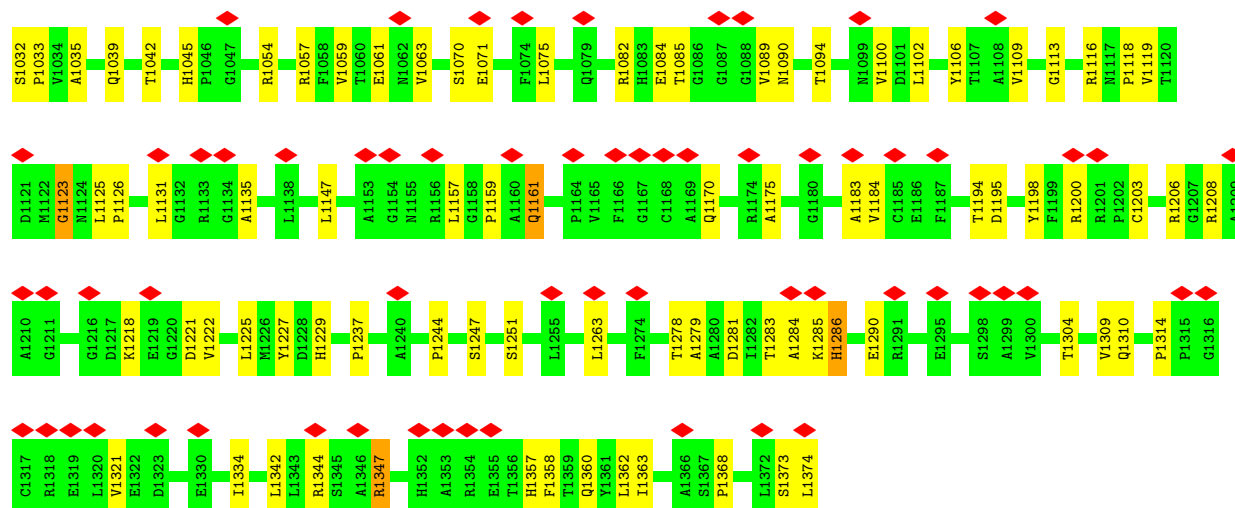
• Molecule 1: Major capsid protein



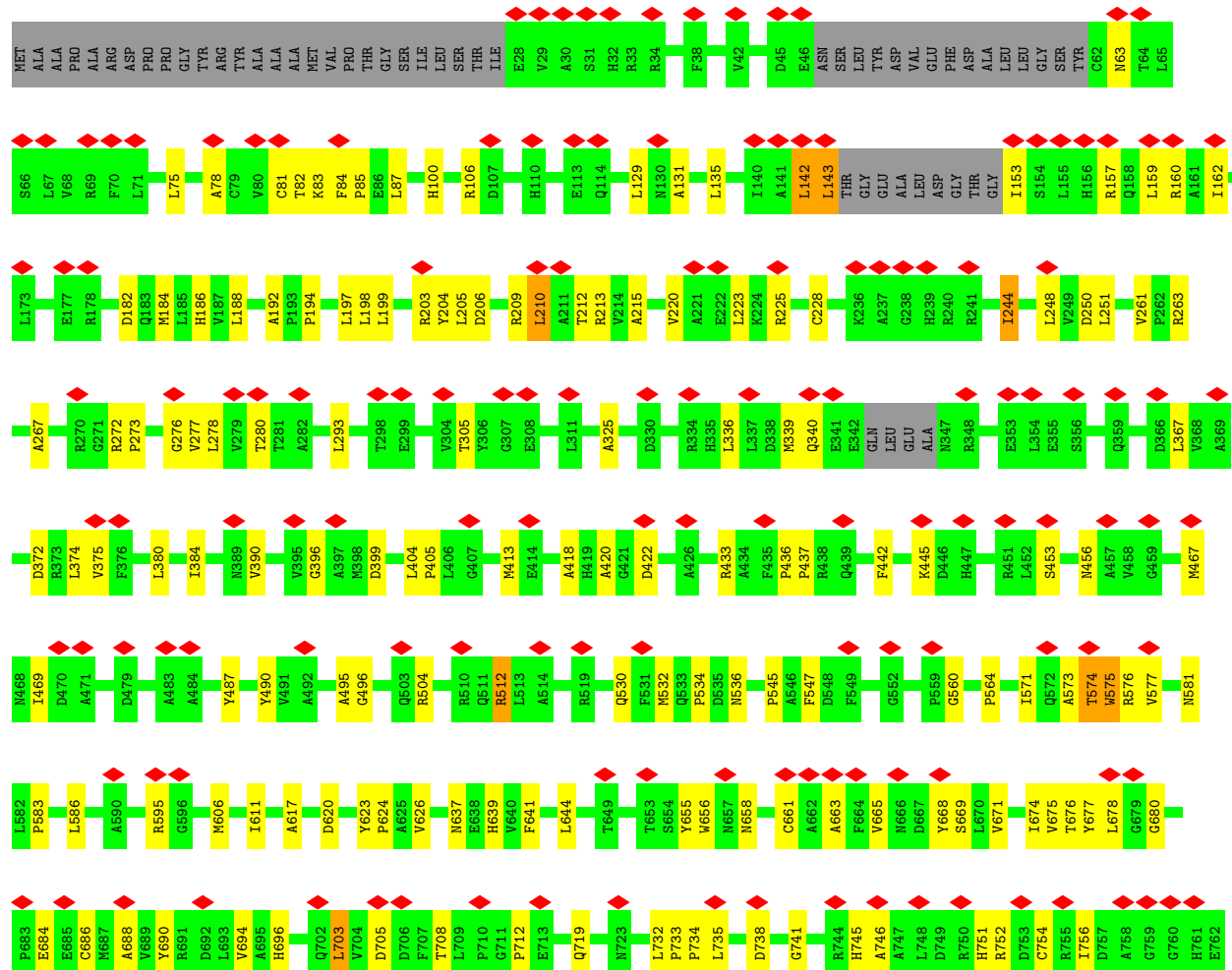


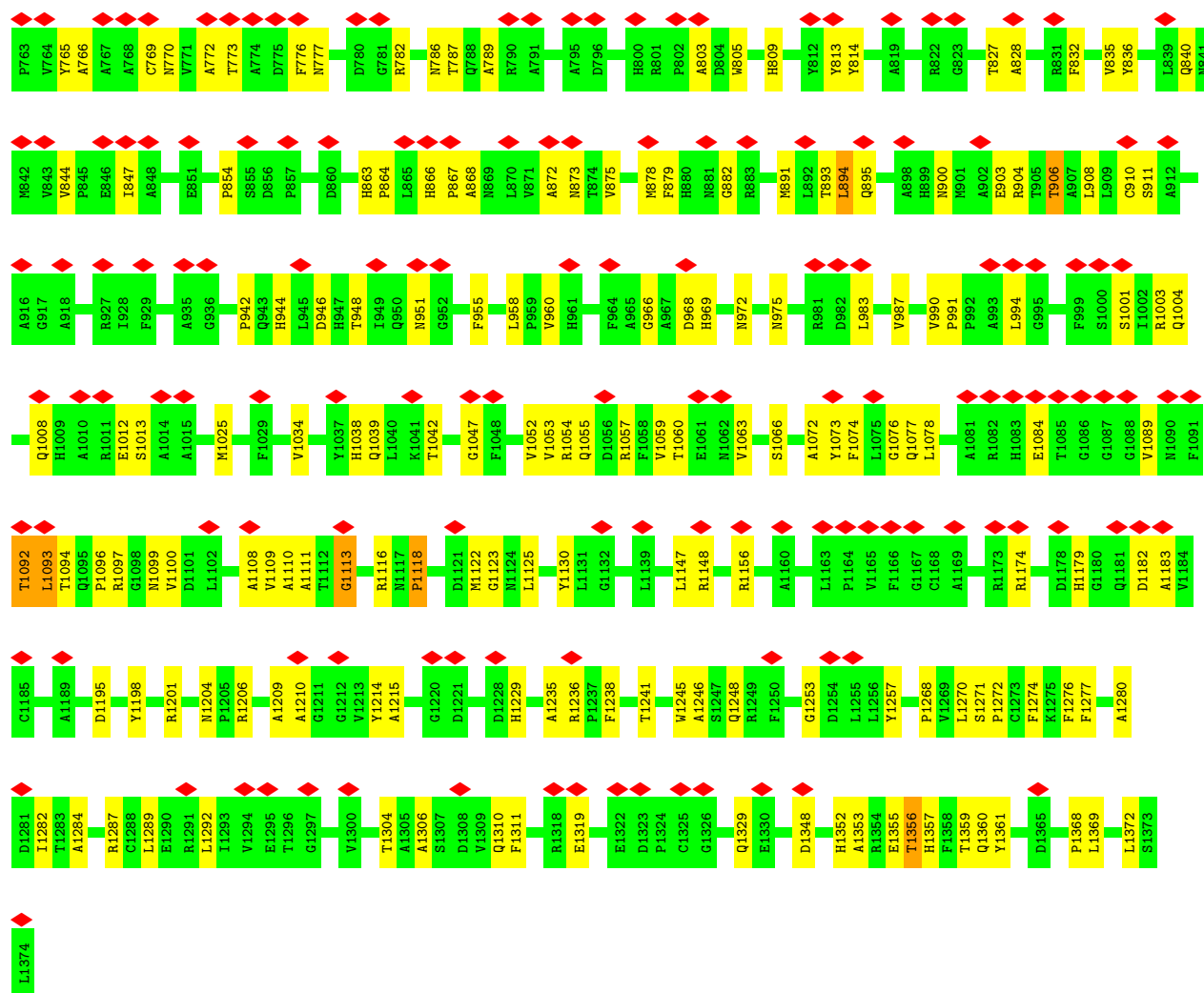
• Molecule 1: Major capsid protein



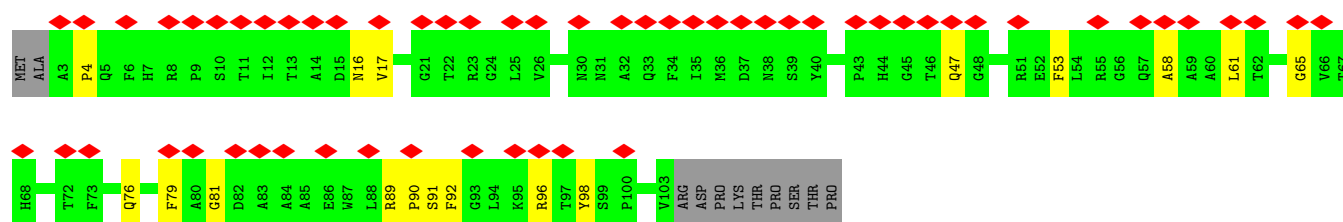
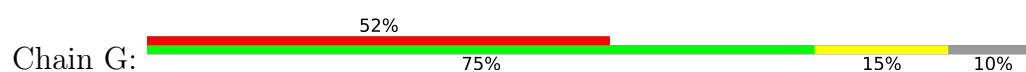


• Molecule 1: Major capsid protein

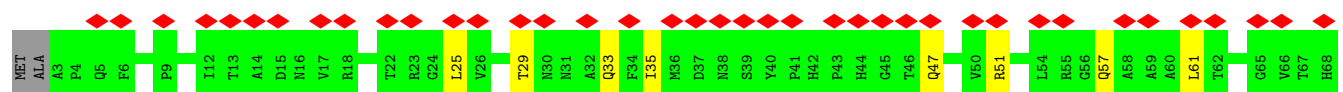
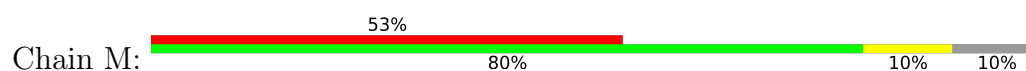




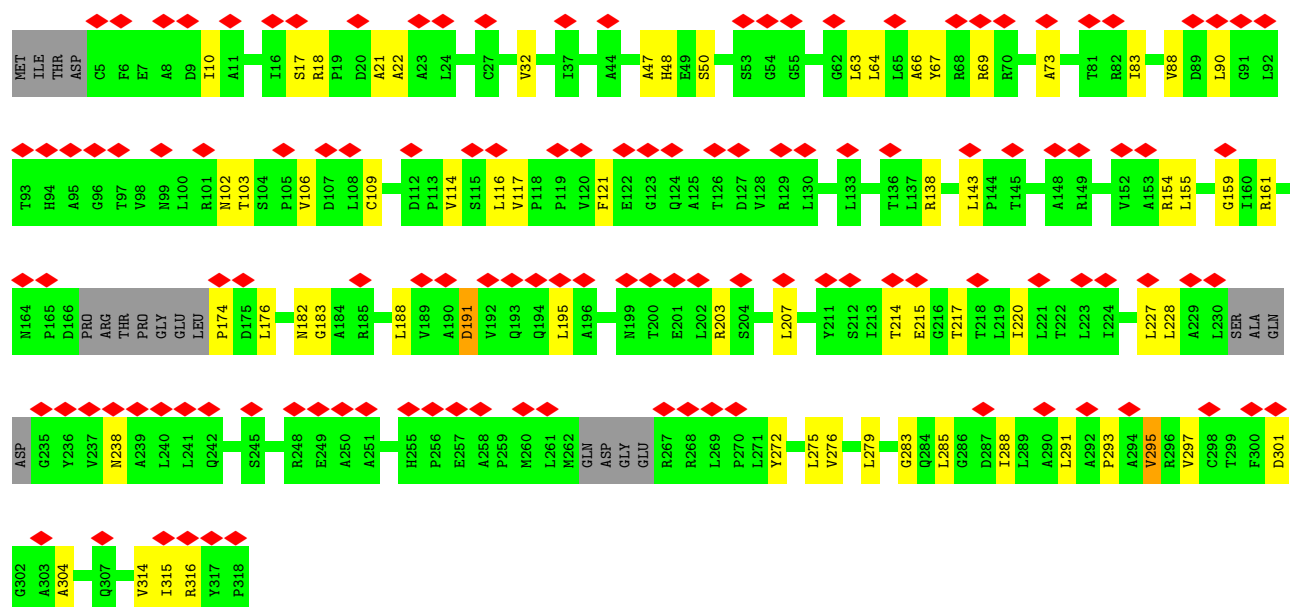
• Molecule 2: Small capsomere-interacting protein



• Molecule 2: Small capsomere-interacting protein

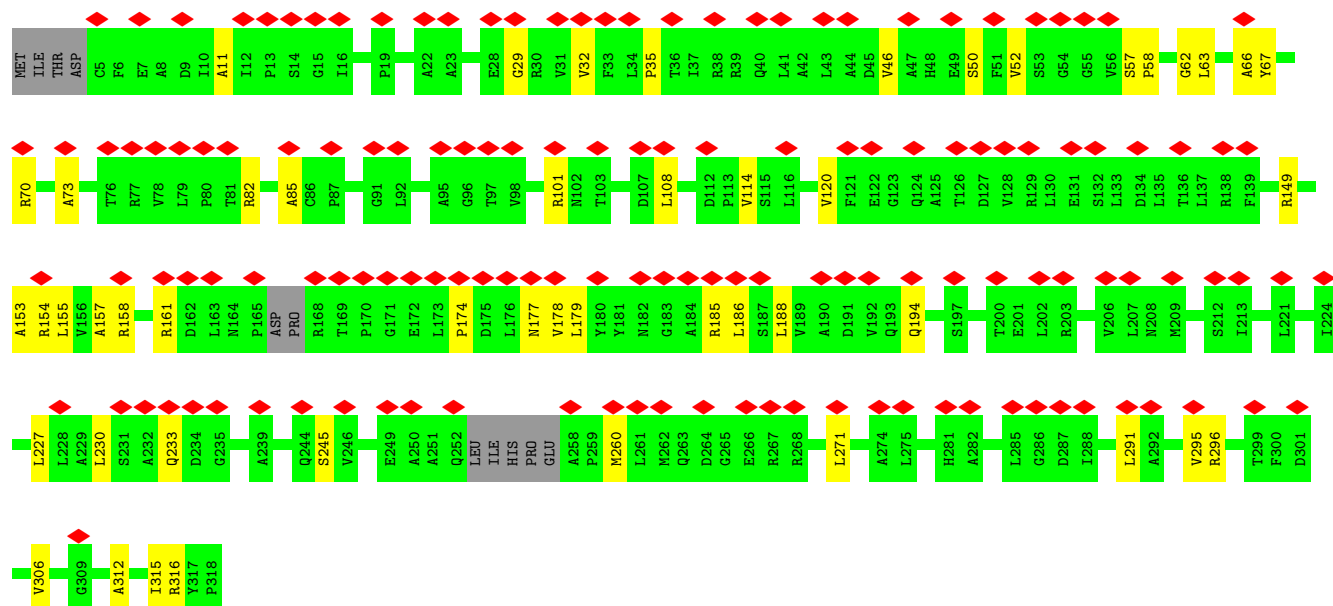


Chain K: 

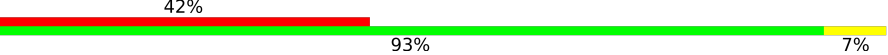


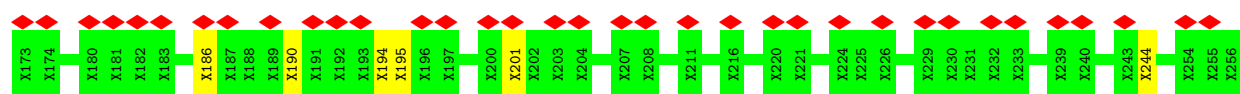
• Molecule 3: Triplex capsid protein 2

Chain O: 

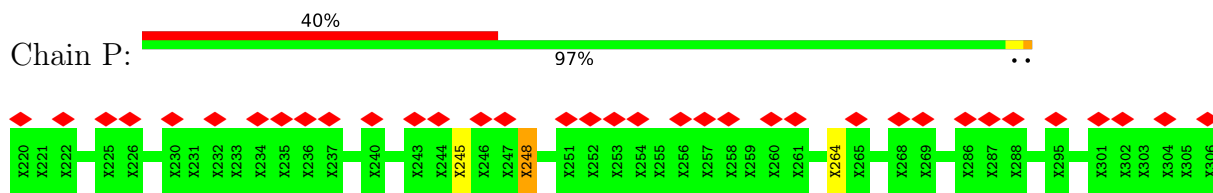


• Molecule 4: coiled coils

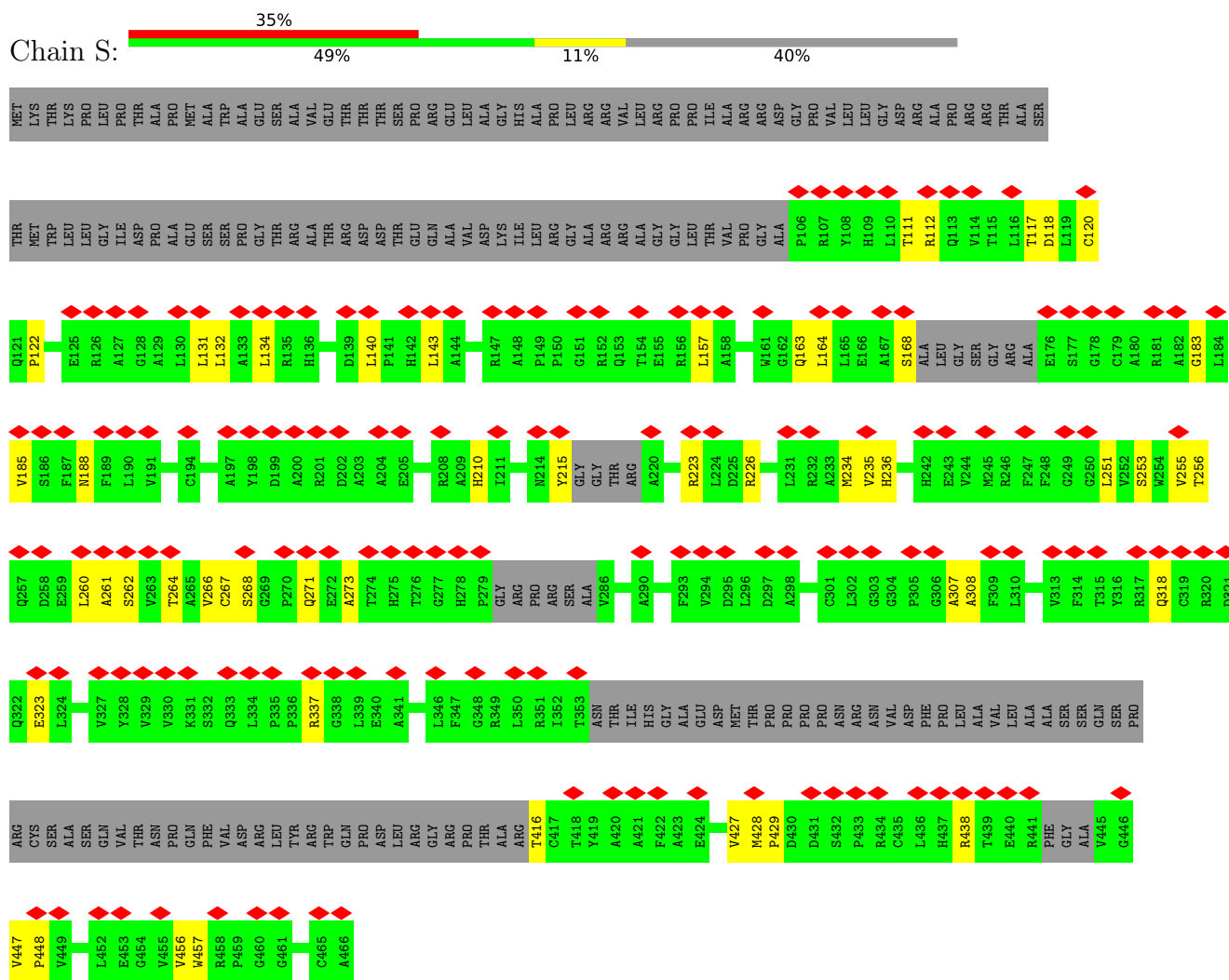
Chain L: 



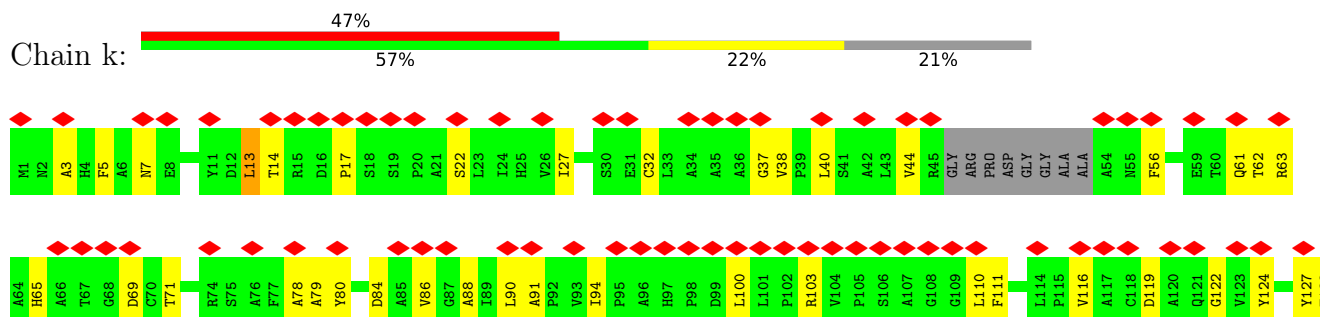
- Molecule 5: Coiled coils

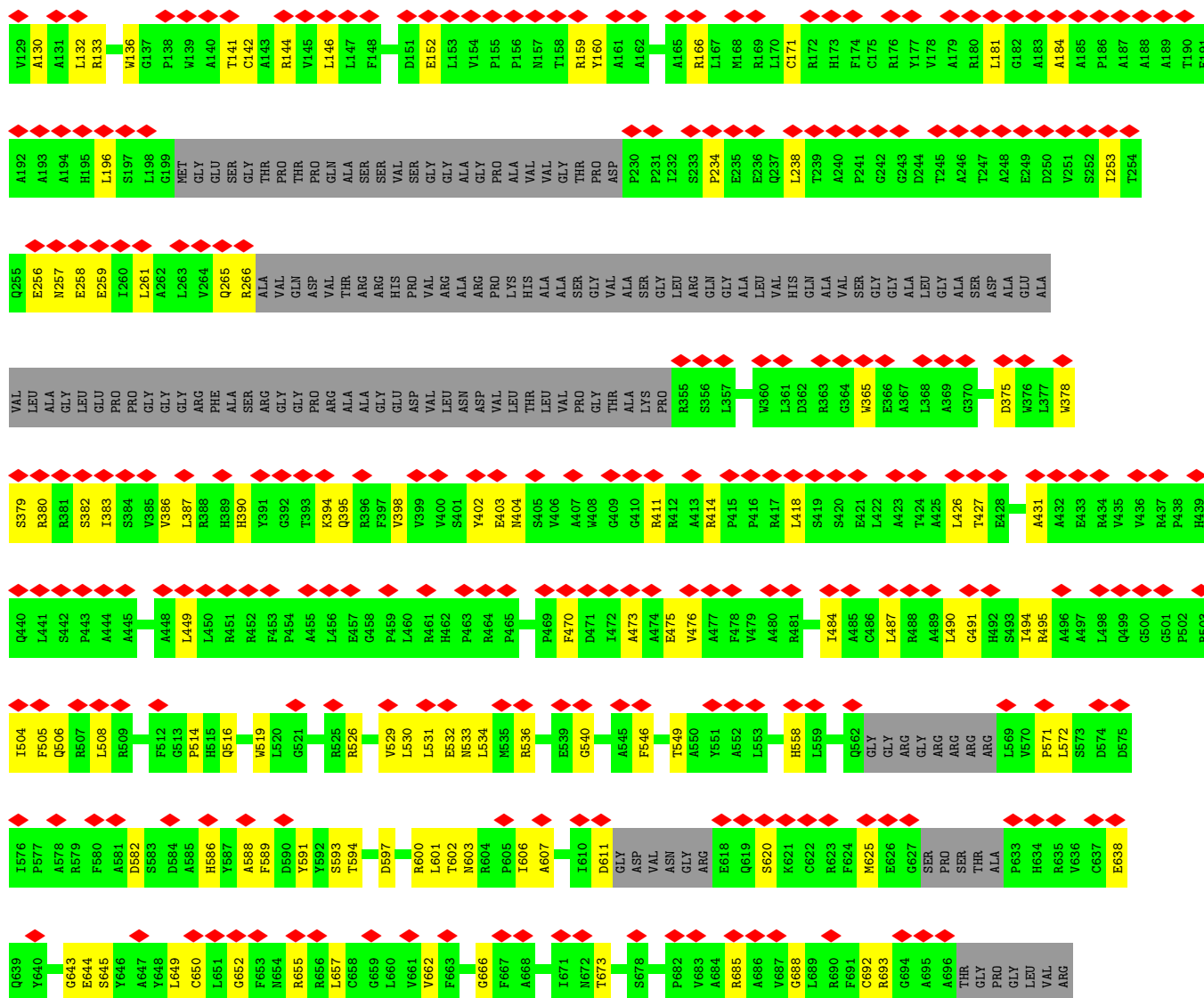


- Molecule 6: Triplex capsid protein 1

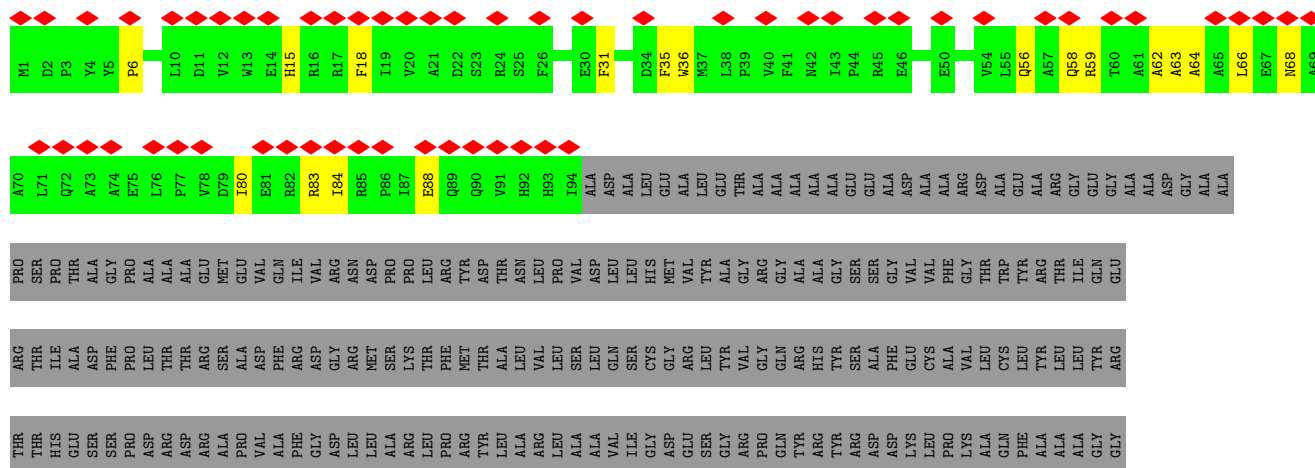


- Molecule 7: Capsid vertex component 1





• Molecule 8: Capsid vertex component 2











LEU	THR	PRO	GLN	ALA	GLY
PRO	LEU	THR	GLN	ALA	ASP
VAL	PRO	THR	PRO	ALA	ARG
GLN	ILE	PRO	PRO	ALA	ARG
ALA	SER	LEU	LEU	VAL	ARG
ASN	SER	PRO	PRO	PRO	GLY
ALA	ASP	PRO	PRO	ARG	ARG
VAL	ASP	VAL	VAL	SER	ARG
LEU	GLU	THR	THR	PRO	GLN
SER	HIS	ARG	THR	GLY	THR
ARG	SER	THR	THR	LEU	THR
TYR	ASP	LEU	THR	ALA	GLY
VAL	ASP	PRO	PRO	PRO	PRO
	R3075				
	S3076				
	T3077				
	G3078				
	R3079				
	S3080				
	A3081				
	L3082				
	A3083				
	V3084				
	L3085				
	I3086				
	R3087				
	A3088				
	C3089				
	R3090				
	R3091				
	I3092				
	Q3093				
	Q3094				
	Q3095				
	L3096				
	Q3097				
	R3098				
	T3099				
	R3100				
	R3101				
	A3102				
	L3103				
	F3104				
	Q3105				
	R3106				
	S3107				
	N3108				
	A3109				
	V3110				
	L3111				
	L3114				
	H3115				
	H3116				
	V3117				
	R3118				
	L3121				
	GLY				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12001	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 ($e^-/\text{\AA}^2$)	30.0, 30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k), FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.035	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size ($\text{\AA}$)	472.5, 472.5, 472.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.35, 1.35, 1.35	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	B	0.37	0/10453	0.75	4/14290 (0.0%)
1	C	0.32	0/10464	0.70	6/14305 (0.0%)
1	D	0.34	0/10475	0.73	8/14317 (0.1%)
1	E	0.36	0/10416	0.72	3/14233 (0.0%)
1	F	0.37	0/10227	0.79	14/13995 (0.1%)
1	I	0.38	0/10071	0.82	13/13769 (0.1%)
2	G	0.25	0/794	0.53	0/1084
2	M	0.15	0/794	0.43	0/1084
2	Q	0.17	0/794	0.45	0/1084
2	T	0.25	0/794	0.57	2/1084 (0.2%)
2	U	0.23	0/794	0.56	0/1084
2	V	0.24	0/794	0.57	0/1084
3	K	0.30	0/2114	0.80	1/2909 (0.0%)
3	O	0.28	0/2215	0.74	5/3047 (0.2%)
6	S	0.32	0/2020	0.82	0/2768
7	k	0.31	0/4342	0.64	0/5924
8	l	0.26	0/792	0.64	0/1081
8	m	0.27	0/664	0.69	0/905
9	n	0.22	0/385	0.60	0/514
9	o	0.24	0/385	0.61	0/514
All	All	0.34	0/79787	0.74	56/109075 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	5
1	C	0	8
1	D	0	6
1	E	0	6
1	F	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	7
3	K	0	2
3	O	0	1
5	P	0	1
6	S	0	1
7	k	0	1
All	All	0	45

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1123	GLY	N-CA-C	10.90	122.57	111.56
1	E	1266	ALA	N-CA-C	-8.46	100.97	114.09
1	F	1285	LYS	CA-C-N	8.28	137.35	121.54
1	F	1285	LYS	C-N-CA	8.28	137.35	121.54
1	D	1084	GLU	CA-C-N	7.79	136.43	121.54
1	D	1084	GLU	C-N-CA	7.79	136.43	121.54
1	F	196	ALA	N-CA-C	-7.23	102.88	114.09
1	C	529	GLU	N-CA-C	-7.05	105.29	114.04
1	D	1083	HIS	CA-C-N	6.92	134.76	121.54
1	D	1083	HIS	C-N-CA	6.92	134.76	121.54
1	F	140	ILE	N-CA-C	-6.91	105.62	111.56
1	F	1347	ARG	CA-C-N	6.82	134.56	121.54
1	F	1347	ARG	C-N-CA	6.82	134.56	121.54
3	O	316	ARG	CA-C-N	6.24	129.75	120.83
3	O	316	ARG	C-N-CA	6.24	129.75	120.83
1	I	1357	HIS	CA-C-N	6.06	129.91	120.82
1	I	1357	HIS	C-N-CA	6.06	129.91	120.82
1	B	917	GLY	CA-C-N	5.91	133.04	123.93
1	B	917	GLY	C-N-CA	5.91	133.04	123.93
1	C	131	ALA	N-CA-C	5.81	117.08	108.60
1	F	293	LEU	CA-C-N	5.79	135.51	122.19
1	F	293	LEU	C-N-CA	5.79	135.51	122.19
3	K	191	ASP	N-CA-C	5.76	118.02	111.11
3	O	120	VAL	N-CA-C	-5.75	107.68	113.20
1	E	43	ARG	CA-C-N	5.68	129.34	120.82
1	E	43	ARG	C-N-CA	5.68	129.34	120.82
1	I	703	LEU	N-CA-C	-5.46	106.98	113.97
3	O	108	LEU	CA-C-N	5.43	131.91	121.54
3	O	108	LEU	C-N-CA	5.43	131.91	121.54
1	I	1118	PRO	CA-C-N	5.42	127.59	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	1118	PRO	C-N-CA	5.42	127.59	120.60
1	I	278	LEU	N-CA-C	5.40	117.77	111.02
1	D	1085	THR	N-CA-C	-5.39	99.32	110.80
1	F	293	LEU	CA-CB-CG	5.37	135.08	116.30
2	T	75	PRO	CA-C-N	5.34	128.77	120.60
2	T	75	PRO	C-N-CA	5.34	128.77	120.60
1	F	816	LEU	CA-C-N	5.34	125.55	120.43
1	F	816	LEU	C-N-CA	5.34	125.55	120.43
1	I	571	ILE	CA-C-N	-5.30	115.22	121.90
1	I	571	ILE	C-N-CA	-5.30	115.22	121.90
1	C	132	ALA	N-CA-C	5.29	122.06	110.80
1	I	1092	THR	CA-CB-CG2	5.25	119.42	110.50
1	C	1084	GLU	CA-C-N	5.24	131.54	121.54
1	C	1084	GLU	C-N-CA	5.24	131.54	121.54
1	D	271	GLY	CA-C-N	-5.24	112.74	122.06
1	D	271	GLY	C-N-CA	-5.24	112.74	122.06
1	F	262	PRO	CA-C-N	5.21	131.49	121.54
1	F	262	PRO	C-N-CA	5.21	131.49	121.54
1	I	574	THR	CA-C-N	5.19	131.45	121.54
1	I	574	THR	C-N-CA	5.19	131.45	121.54
1	I	1113	GLY	CA-C-N	5.13	131.34	121.54
1	I	1113	GLY	C-N-CA	5.13	131.34	121.54
1	D	948	THR	N-CA-C	-5.06	106.24	112.72
1	C	1153	ALA	N-CA-C	5.03	117.14	111.11
1	B	1222	VAL	CA-C-N	5.01	130.98	121.97
1	B	1222	VAL	C-N-CA	5.01	130.98	121.97

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1201	ARG	Peptide
1	B	1222	VAL	Peptide
1	B	534	PRO	Peptide
1	B	764	VAL	Peptide
1	B	972	ASN	Peptide
1	C	1083	HIS	Peptide
1	C	1161	GLN	Peptide
1	C	1162	PRO	Peptide
1	C	1222	VAL	Peptide
1	C	1241	THR	Peptide
1	C	131	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	C	411	PRO	Peptide
1	C	43	ARG	Peptide
1	D	1084	GLU	Peptide
1	D	1161	GLN	Peptide
1	D	1222	VAL	Peptide
1	D	258	SER	Peptide
1	D	266	HIS	Peptide
1	D	755	ARG	Peptide
1	E	1162	PRO	Peptide
1	E	1222	VAL	Peptide
1	E	1265	GLY	Peptide
1	E	1316	GLY	Peptide
1	E	371	GLY	Peptide
1	E	43	ARG	Peptide
1	F	105	ALA	Peptide
1	F	1113	GLY	Peptide
1	F	1161	GLN	Peptide
1	F	1222	VAL	Peptide
1	F	293	LEU	Peptide
1	F	447	HIS	Peptide
1	F	453	SER	Peptide
1	I	1012	GLU	Peptide
1	I	1113	GLY	Peptide
1	I	305	THR	Peptide
1	I	573	ALA	Peptide
1	I	665	VAL	Peptide
1	I	81	CYS	Peptide
1	I	975	ASN	Peptide
3	K	103	THR	Peptide
3	K	315	ILE	Peptide
3	O	260	MET	Peptide
5	P	248	UNK	Peptide
6	S	140	LEU	Peptide
7	k	504	ILE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	10198	0	9937	193	0
1	C	10209	0	9940	154	0
1	D	10221	0	9963	168	0
1	E	10162	0	9939	165	0
1	F	9978	0	9630	191	0
1	I	9831	0	9549	209	0
2	G	772	0	746	15	0
2	M	772	0	746	8	0
2	Q	772	0	746	9	0
2	T	772	0	746	10	0
2	U	772	0	746	18	0
2	V	772	0	746	19	0
3	K	2078	0	2053	40	0
3	O	2175	0	2213	31	0
4	L	420	0	88	6	0
5	P	435	0	89	2	0
6	S	1975	0	1858	31	0
7	k	4233	0	4180	122	0
8	l	770	0	751	16	0
8	m	648	0	636	49	0
9	n	383	0	418	7	0
9	o	383	0	418	12	0
All	All	78731	0	76138	1301	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 (1301) 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)
7:k:495:ARG:HA	8:m:36:TRP:CH2	1.52	1.45
7:k:495:ARG:HB2	8:m:36:TRP:CZ3	1.59	1.38
7:k:495:ARG:CA	8:m:36:TRP:CH2	2.10	1.33
7:k:495:ARG:CB	8:m:36:TRP:CZ3	2.32	1.11
7:k:495:ARG:HA	8:m:36:TRP:CZ2	1.89	1.06
4:L:244:UNK:CB	6:S:260:LEU:HD12	1.87	1.05
7:k:495:ARG:N	8:m:36:TRP:CH2	2.26	1.03
1:F:282:ALA:HB1	1:F:382:LYS:HE3	1.46	0.97
4:L:244:UNK:CB	6:S:260:LEU:CD1	2.42	0.96
7:k:94:ILE:HD12	7:k:100:LEU:CD1	1.96	0.95
7:k:495:ARG:HB2	8:m:36:TRP:CE3	2.02	0.94
5:P:245:UNK:O	5:P:248:UNK:O	1.85	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:k:40:LEU:O	7:k:44:VAL:HG23	1.68	0.93
7:k:495:ARG:CA	8:m:36:TRP:CZ3	2.51	0.92
4:L:201:UNK:CB	5:P:264:UNK:CB	2.49	0.91
2:U:22:THR:OG1	2:U:64:LEU:HD22	1.70	0.91
7:k:494:ILE:C	8:m:36:TRP:HH2	1.80	0.90
7:k:532:GLU:HG2	8:m:38:LEU:HD13	1.51	0.90
8:m:36:TRP:CE3	8:m:41:PHE:CD1	2.61	0.88
8:m:36:TRP:CZ3	8:m:41:PHE:CD1	2.62	0.87
7:k:495:ARG:N	8:m:36:TRP:HH2	1.71	0.86
8:m:36:TRP:CZ3	8:m:41:PHE:CE1	2.68	0.81
4:L:194:UNK:O	4:L:195:UNK:C	2.28	0.79
7:k:94:ILE:HD12	7:k:100:LEU:HD13	1.61	0.79
2:V:22:THR:CG2	2:V:60:ALA:HB1	2.14	0.77
7:k:94:ILE:HD12	7:k:100:LEU:HD12	1.66	0.76
8:m:35:PHE:O	8:m:38:LEU:HG	1.86	0.75
1:B:826:CYS:HB2	1:B:966:GLY:H	1.52	0.74
1:F:895:GLN:HA	2:V:61:LEU:HB3	1.70	0.74
1:I:512:ARG:HH12	1:I:564:PRO:HD2	1.52	0.74
7:k:94:ILE:CD1	7:k:100:LEU:CD1	2.67	0.73
1:I:496:GLY:HA3	1:I:504:ARG:HH22	1.54	0.73
1:B:267:ALA:HB1	1:B:274:VAL:HB	1.71	0.72
4:L:244:UNK:CB	6:S:260:LEU:HD11	2.18	0.72
8:m:35:PHE:O	8:m:38:LEU:CD1	2.38	0.71
7:k:90:LEU:HD22	7:k:166:ARG:HD3	1.70	0.71
7:k:90:LEU:HD22	7:k:166:ARG:CD	2.21	0.71
7:k:94:ILE:CD1	7:k:100:LEU:HD13	2.21	0.70
1:B:63:ASN:HD21	1:I:100:HIS:H	1.40	0.69
1:B:248:LEU:HD23	1:B:293:LEU:HD21	1.73	0.69
1:F:139:ALA:HA	1:F:142:LEU:HB2	1.75	0.69
2:V:22:THR:HG22	2:V:60:ALA:HB1	1.74	0.69
7:k:495:ARG:N	8:m:36:TRP:CZ3	2.62	0.68
1:I:1073:TYR:OH	1:I:1097:ARG:NH1	2.26	0.68
7:k:382:SER:HB2	7:k:403:GLU:HB2	1.76	0.67
6:S:267:CYS:O	6:S:271:GLN:NE2	2.27	0.67
7:k:532:GLU:HG2	8:m:38:LEU:CD1	2.25	0.67
1:I:836:TYR:O	1:I:840:GLN:NE2	2.26	0.67
1:E:530:GLN:O	1:E:536:ASN:ND2	2.26	0.66
3:O:70:ARG:O	6:S:337:ARG:NH2	2.28	0.66
1:D:425:PRO:HG3	1:D:431:GLU:HB2	1.78	0.66
1:D:267:ALA:HB1	1:D:274:VAL:H	1.59	0.66
1:B:281:THR:H	1:B:284:ILE:HD12	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1342:LEU:HB3	1:F:1362:LEU:HD12	1.77	0.65
1:D:450:LEU:HB3	1:D:1124:ASN:HD21	1.60	0.65
1:F:1304:THR:HG21	1:F:1314:PRO:HD2	1.79	0.65
7:k:79:ALA:HB3	7:k:111:PHE:HB2	1.78	0.65
1:B:1117:ASN:ND2	1:I:204:TYR:OH	2.29	0.64
1:B:1124:ASN:O	1:B:1156:ARG:NH2	2.30	0.64
1:C:285:LYS:HE2	1:C:377:LEU:HB3	1.80	0.64
8:m:38:LEU:HD12	8:m:41:PHE:CD2	2.32	0.64
1:F:730:ALA:HB2	1:F:750:ARG:HH12	1.62	0.64
1:I:261:VAL:HG22	1:I:263:ARG:H	1.63	0.64
1:C:228:CYS:HA	1:C:1368:PRO:HG3	1.80	0.64
1:I:1304:THR:HG22	1:I:1306:ALA:H	1.63	0.64
8:l:15:HIS:HB3	8:l:18:PHE:HB2	1.80	0.64
7:k:159:ARG:HG2	7:k:386:VAL:HG22	1.79	0.64
1:D:417:ALA:O	1:D:1354:ARG:NH2	2.31	0.64
6:S:118:ASP:O	6:S:223:ARG:NH1	2.31	0.63
1:B:960:VAL:HA	1:B:994:LEU:HD13	1.80	0.63
1:C:912:ALA:HB3	1:C:928:ILE:HB	1.81	0.63
1:D:193:PRO:HG2	1:D:198:LEU:HD12	1.81	0.63
1:E:252:THR:HG22	1:E:373:ARG:HD3	1.79	0.63
6:S:253:SER:HG	6:S:264:THR:HG1	1.45	0.63
1:E:673:TYR:OH	1:E:801:ARG:NH2	2.32	0.63
1:C:523:GLU:HB3	1:C:1008:GLN:HG2	1.81	0.62
1:E:947:HIS:HB3	2:V:80:ALA:H	1.64	0.62
1:C:485:ASN:HD21	1:C:513:LEU:HA	1.64	0.62
8:m:38:LEU:HD12	8:m:41:PHE:CE2	2.34	0.62
1:B:336:LEU:HD22	1:C:156:HIS:HE1	1.65	0.62
1:B:576:ARG:HA	1:B:1003:ARG:HH12	1.64	0.62
8:m:35:PHE:O	8:m:38:LEU:CG	2.47	0.62
1:D:707:PHE:HA	1:D:1042:THR:HG21	1.82	0.62
1:C:618:PHE:HA	1:C:940:MET:HB3	1.82	0.62
7:k:61:GLN:HE21	7:k:63:ARG:HH21	1.48	0.62
1:D:754:CYS:HA	1:D:910:CYS:HA	1.82	0.61
7:k:90:LEU:HD12	7:k:234:PRO:HB3	1.80	0.61
1:D:620:ASP:OD1	1:E:691:ARG:NH1	2.33	0.61
1:D:873:ASN:HA	2:G:92:PHE:HB2	1.82	0.61
1:B:707:PHE:HA	1:B:1042:THR:HG21	1.83	0.61
1:C:656:TRP:O	1:C:660:ARG:NH1	2.33	0.61
1:E:1276:PHE:HA	1:E:1329:GLN:HE22	1.65	0.61
1:D:982:ASP:OD1	1:D:985:ARG:NH1	2.33	0.61
1:I:182:ASP:O	1:I:186:HIS:ND1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:k:238:LEU:HD22	7:k:387:LEU:HB2	1.81	0.61
1:C:957:VAL:HG22	1:C:959:PRO:HD3	1.82	0.61
1:E:557:GLU:HG3	1:E:559:PRO:HD2	1.80	0.61
1:B:530:GLN:O	1:B:536:ASN:ND2	2.33	0.61
1:D:530:GLN:O	1:D:536:ASN:ND2	2.33	0.61
1:E:982:ASP:OD1	1:E:985:ARG:NH1	2.33	0.61
1:B:1157:LEU:HD21	1:B:1309:VAL:HG11	1.82	0.61
1:D:629:LEU:HB3	1:D:839:LEU:HD21	1.82	0.61
1:D:1182:ASP:HB2	1:D:1309:VAL:HA	1.83	0.61
1:F:1085:THR:OG1	1:F:1090:ASN:ND2	2.34	0.61
1:C:1201:ARG:HH12	1:D:1179:HIS:HE1	1.48	0.60
1:D:236:LYS:NZ	1:D:1370:LYS:O	2.33	0.60
1:I:272:ARG:HE	1:I:374:LEU:HB2	1.65	0.60
1:B:76:SER:OG	1:B:266:HIS:NE2	2.32	0.60
1:D:326:VAL:HB	1:D:329:LEU:HD12	1.84	0.60
8:m:83:ARG:HG3	9:o:3103:LEU:HD11	1.84	0.60
1:I:1130:TYR:HB3	1:I:1148:ARG:HH21	1.66	0.60
3:K:301:ASP:H	6:S:112:ARG:HB3	1.67	0.60
1:B:909:LEU:HD11	1:B:929:PHE:HB3	1.83	0.60
1:D:749:ASP:O	1:D:752:ARG:NH2	2.32	0.60
1:D:1257:TYR:HB2	1:D:1277:PHE:HD2	1.67	0.60
6:S:438:ARG:HA	6:S:448:PRO:HA	1.84	0.60
7:k:132:LEU:HB2	7:k:146:LEU:HB2	1.83	0.60
1:B:490:TYR:OH	1:B:560:GLY:O	2.19	0.60
1:D:834:ARG:HD3	2:G:90:PRO:HB3	1.83	0.60
1:B:712:PRO:O	1:B:719:GLN:NE2	2.35	0.60
1:I:891:MET:O	1:I:895:GLN:NE2	2.34	0.60
1:E:404:LEU:HB2	1:E:1052:VAL:HB	1.84	0.60
1:C:532:MET:HE2	1:C:534:PRO:HG2	1.84	0.59
1:D:664:PHE:HB3	1:D:670:LEU:HD13	1.83	0.59
8:m:80:ILE:HD13	9:n:3103:LEU:HB3	1.84	0.59
1:B:84:PHE:O	1:B:1097:ARG:NH2	2.34	0.59
1:I:674:ILE:HG23	1:I:678:LEU:HD12	1.83	0.59
8:m:35:PHE:O	8:m:38:LEU:HD12	2.01	0.59
1:E:785:HIS:NE2	1:E:798:ARG:O	2.35	0.59
1:I:828:ALA:HB1	1:I:955:PHE:HB3	1.84	0.59
1:B:728:ASP:O	1:B:810:LYS:NZ	2.35	0.59
1:E:674:ILE:HG13	1:E:678:LEU:HD12	1.85	0.59
1:F:826:CYS:SG	1:F:827:THR:N	2.76	0.59
1:I:87:LEU:H	1:I:1076:GLY:HA2	1.67	0.59
1:C:815:VAL:HA	1:C:1024:LEU:HD22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1206:ARG:HB3	1:D:1277:PHE:HE1	1.68	0.59
1:I:769:CYS:O	1:I:900:ASN:ND2	2.35	0.59
6:S:157:LEU:HD11	6:S:234:MET:HA	1.84	0.59
2:V:22:THR:HG22	2:V:60:ALA:CB	2.31	0.59
7:k:650:CYS:HB2	7:k:662:VAL:HB	1.84	0.59
1:F:748:LEU:HD13	1:F:750:ARG:HB2	1.85	0.59
1:I:367:LEU:HD13	1:I:374:LEU:HD21	1.85	0.58
1:I:404:LEU:HB2	1:I:1052:VAL:HB	1.83	0.58
1:D:645:ALA:O	1:D:649:THR:N	2.33	0.58
1:F:707:PHE:HA	1:F:1042:THR:HG21	1.85	0.58
1:C:1236:ARG:NH2	1:C:1241:THR:O	2.36	0.58
1:F:872:ALA:O	2:V:30:ASN:ND2	2.36	0.58
3:K:161:ARG:NH1	3:K:174:PRO:O	2.36	0.58
1:B:276:GLY:HA3	1:B:375:VAL:HG22	1.86	0.58
1:B:406:LEU:HB2	1:B:1050:PHE:HB2	1.85	0.58
1:F:696:HIS:HE1	1:F:1021:THR:HG21	1.67	0.58
1:F:1082:ARG:NH2	1:F:1084:GLU:OE2	2.36	0.58
1:B:629:LEU:HB3	1:B:839:LEU:HD21	1.85	0.58
1:C:777:ASN:O	2:Q:51:ARG:NH2	2.37	0.58
1:B:278:LEU:HD13	1:B:375:VAL:HG11	1.86	0.58
1:B:1237:PRO:HB2	1:C:1156:ARG:HE	1.69	0.58
1:D:99:VAL:O	1:D:118:ASN:ND2	2.36	0.58
1:I:129:LEU:O	1:I:1094:THR:OG1	2.21	0.58
1:I:276:GLY:HA3	1:I:375:VAL:HG13	1.84	0.58
1:I:1004:GLN:O	1:I:1008:GLN:NE2	2.36	0.58
1:B:1118:PRO:HG3	1:B:1374:LEU:HD13	1.85	0.58
1:B:1118:PRO:HD3	1:B:1374:LEU:HD22	1.85	0.58
1:B:1233:ASP:O	1:C:1174:ARG:NH2	2.37	0.58
1:E:460:THR:HG21	1:E:1187:PHE:HB2	1.85	0.58
1:D:870:LEU:HD22	1:D:877:ARG:HA	1.86	0.58
1:D:909:LEU:HA	1:D:931:GLY:HA2	1.85	0.58
1:D:1052:VAL:HG22	1:D:1187:PHE:HE1	1.68	0.58
1:E:413:MET:O	1:F:433:ARG:NH1	2.32	0.58
2:G:76:GLN:O	2:G:96:ARG:NH2	2.30	0.58
1:B:717:GLN:HE21	1:B:748:LEU:HD22	1.69	0.58
1:C:730:ALA:HB2	1:C:750:ARG:HH12	1.69	0.58
1:D:497:PRO:HD2	1:D:504:ARG:HH12	1.69	0.58
1:F:381:GLU:HA	1:F:385:TYR:HB2	1.84	0.58
1:B:677:TYR:HD1	2:T:95:LYS:HG2	1.69	0.57
1:C:826:CYS:HB2	1:C:966:GLY:H	1.68	0.57
1:E:638:GLU:OE1	1:E:801:ARG:NH2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1008:GLN:HE22	1:F:1011:ARG:HH11	1.52	0.57
1:F:413:MET:O	1:I:433:ARG:NH1	2.35	0.57
1:I:960:VAL:HA	1:I:994:LEU:HD13	1.86	0.57
1:B:502:GLN:HA	1:B:505:PHE:HB3	1.86	0.57
1:F:595:ARG:NH1	1:F:1045:HIS:O	2.38	0.57
1:B:425:PRO:HG3	1:B:431:GLU:HB2	1.85	0.57
1:D:137:THR:HA	1:D:140:ILE:HD12	1.86	0.57
1:E:646:ARG:HA	1:E:649:THR:HG22	1.86	0.57
7:k:253:ILE:O	7:k:257:ASN:ND2	2.38	0.57
1:E:544:HIS:CD2	1:E:546:ALA:H	2.22	0.57
1:D:413:MET:O	1:E:433:ARG:NH1	2.38	0.57
1:F:204:TYR:OH	1:F:210:LEU:O	2.22	0.57
1:F:1161:GLN:NE2	1:F:1170:GLN:OE1	2.37	0.57
7:k:91:ALA:O	7:k:103:ARG:NH1	2.38	0.57
1:E:708:THR:HA	1:E:1038:HIS:HB3	1.86	0.57
3:K:275:LEU:HD22	3:O:157:ALA:HB2	1.86	0.57
7:k:124:TYR:HB3	7:k:418:LEU:HD22	1.86	0.57
1:B:373:ARG:NH2	1:B:1067:GLU:OE1	2.38	0.56
1:E:730:ALA:HB2	1:E:750:ARG:HH12	1.70	0.56
1:E:1208:ARG:NH2	1:E:1240:ALA:O	2.38	0.56
1:F:982:ASP:OD1	1:F:985:ARG:NH1	2.38	0.56
3:O:57:SER:O	3:O:194:GLN:NE2	2.37	0.56
1:B:532:MET:HE2	1:B:534:PRO:HG2	1.87	0.56
1:F:67:LEU:HD21	1:F:170:GLN:HB3	1.87	0.56
1:C:1076:GLY:H	1:C:1095:GLN:HE21	1.53	0.56
1:D:42:VAL:HG21	1:D:49:LEU:HD21	1.87	0.56
7:k:256:GLU:OE1	9:o:3098:ARG:NH2	2.39	0.56
1:B:528:ALA:HA	1:B:531:PHE:HB2	1.87	0.56
1:B:1246:ALA:HA	1:B:1253:GLY:HA3	1.86	0.56
1:I:272:ARG:NH2	1:I:372:ASP:O	2.38	0.56
1:D:697:VAL:HG12	1:D:808:HIS:HD2	1.71	0.56
1:F:946:ASP:HB3	1:I:676:THR:HG21	1.88	0.56
1:I:904:ARG:NH1	1:I:906:THR:OG1	2.36	0.56
7:k:600:ARG:NH1	7:k:602:THR:O	2.39	0.56
1:C:159:LEU:O	1:C:163:GLN:NE2	2.38	0.56
1:E:742:LEU:HD21	1:E:908:LEU:HD21	1.87	0.56
3:K:10:ILE:HB	3:K:83:ILE:HB	1.88	0.56
1:C:804:ASP:O	1:C:808:HIS:ND1	2.37	0.56
1:F:95:VAL:HG13	1:I:63:ASN:HB3	1.87	0.56
1:D:875:VAL:O	1:D:879:PHE:N	2.39	0.56
1:E:638:GLU:OE2	1:E:677:TYR:OH	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1074:PHE:HB3	1:B:1097:ARG:HH11	1.71	0.56
1:D:99:VAL:HG13	1:D:118:ASN:HD22	1.70	0.56
1:D:359:GLN:NE2	1:D:360:THR:O	2.39	0.56
1:I:1276:PHE:HA	1:I:1329:GLN:HE22	1.70	0.56
3:K:161:ARG:HE	3:O:271:LEU:HD12	1.71	0.56
1:C:544:HIS:CD2	1:C:546:ALA:H	2.24	0.56
1:D:618:PHE:HA	1:D:940:MET:HB3	1.88	0.56
3:O:179:LEU:HB2	3:O:186:LEU:HB2	1.87	0.56
1:F:981:ARG:HH22	1:I:803:ALA:H	1.53	0.55
1:I:1215:ALA:O	1:I:1287:ARG:NH1	2.39	0.55
7:k:487:LEU:HD23	7:k:490:LEU:HD12	1.88	0.55
1:B:665:VAL:O	1:B:812:TYR:OH	2.22	0.55
1:D:742:LEU:HD12	1:D:908:LEU:HD21	1.87	0.55
1:I:617:ALA:HB2	1:I:661:CYS:HB3	1.86	0.55
1:C:104:ILE:HG23	1:D:179:GLY:HA2	1.88	0.55
1:D:228:CYS:HA	1:D:1368:PRO:HG3	1.88	0.55
1:E:450:LEU:HD22	1:E:1124:ASN:HD22	1.71	0.55
1:F:754:CYS:HA	1:F:910:CYS:HA	1.89	0.55
1:B:1298:SER:HB2	1:B:1320:LEU:HD22	1.89	0.55
1:F:1279:ALA:O	1:F:1283:THR:OG1	2.25	0.55
1:I:951:ASN:ND2	1:I:972:ASN:O	2.37	0.55
8:l:56:GLN:HG3	8:m:55:LEU:HD21	1.88	0.55
1:C:667:ASP:OD1	1:C:813:TYR:OH	2.25	0.55
1:E:590:ALA:O	1:E:594:ALA:N	2.39	0.55
1:E:738:ASP:OD1	1:E:738:ASP:N	2.37	0.55
1:E:1298:SER:HB2	1:E:1320:LEU:HD22	1.88	0.55
1:F:708:THR:OG1	1:F:723:ASN:ND2	2.40	0.55
1:D:255:THR:OG1	1:D:1067:GLU:OE2	2.25	0.55
1:E:951:ASN:ND2	1:E:972:ASN:O	2.39	0.55
1:F:445:LYS:NZ	1:F:1118:PRO:O	2.39	0.55
3:K:276:VAL:HG21	3:O:154:ARG:HD3	1.88	0.55
1:C:968:ASP:O	1:C:972:ASN:ND2	2.36	0.55
3:O:230:LEU:HA	3:O:233:GLN:HE21	1.71	0.55
2:V:51:ARG:HB3	2:V:55:ARG:HH12	1.72	0.55
7:k:44:VAL:HG22	7:k:80:TYR:HE2	1.72	0.55
1:D:1289:LEU:HD13	1:D:1292:LEU:HB2	1.89	0.55
1:E:1181:GLN:NE2	1:E:1307:SER:O	2.40	0.55
1:I:445:LYS:HE2	1:I:1118:PRO:HG2	1.89	0.55
1:B:711:GLY:H	1:B:719:GLN:HG3	1.70	0.55
1:B:1126:PRO:HG2	1:B:1129:PHE:HZ	1.72	0.55
1:C:712:PRO:O	1:C:719:GLN:NE2	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:ARG:NH2	1:D:453:SER:OG	2.40	0.55
1:D:951:ASN:ND2	1:D:972:ASN:O	2.33	0.55
1:F:284:ILE:HD11	1:F:1061:GLU:HB3	1.88	0.55
9:n:3101:ARG:O	9:n:3105:GLN:N	2.40	0.55
1:F:638:GLU:OE2	1:F:677:TYR:OH	2.25	0.54
3:O:306:VAL:HG11	3:O:312:ALA:HB2	1.89	0.54
1:B:1218:LYS:N	1:B:1221:ASP:OD2	2.40	0.54
1:C:1061:GLU:OE1	1:C:1114:THR:OG1	2.25	0.54
1:F:248:LEU:O	1:F:252:THR:N	2.39	0.54
2:G:17:VAL:HG21	2:G:53:PHE:HA	1.89	0.54
1:I:495:ALA:O	1:I:504:ARG:NH1	2.37	0.54
1:I:777:ASN:O	2:U:51:ARG:NH2	2.40	0.54
1:C:281:THR:OG1	1:C:381:GLU:OE2	2.26	0.54
1:I:197:LEU:HA	1:I:223:LEU:HD11	1.89	0.54
6:S:256:THR:HG22	6:S:262:SER:H	1.73	0.54
1:B:1200:ARG:NH2	1:B:1362:LEU:O	2.41	0.54
1:C:62:CYS:SG	1:C:63:ASN:N	2.81	0.54
1:C:76:SER:OG	1:C:266:HIS:NE2	2.40	0.54
3:K:283:GLY:O	3:O:149:ARG:NH1	2.40	0.54
2:U:18:ARG:HA	2:U:60:ALA:HB2	1.89	0.54
1:D:261:VAL:HG12	1:D:263:ARG:H	1.73	0.54
1:D:673:TYR:OH	1:D:801:ARG:NH2	2.40	0.54
1:D:777:ASN:ND2	2:M:47:GLN:OE1	2.40	0.54
1:E:104:ILE:HG12	1:F:178:ARG:HB3	1.88	0.54
1:I:194:PRO:HD2	1:I:197:LEU:HD12	1.90	0.54
1:I:1359:THR:OG1	1:I:1360:GLN:NE2	2.40	0.54
1:C:90:MET:HE3	1:D:56:ALA:HB3	1.89	0.54
1:D:631:GLN:HG3	1:D:670:LEU:HD11	1.90	0.54
1:D:1298:SER:HB2	1:D:1320:LEU:HD22	1.90	0.54
1:F:604:HIS:NE2	1:F:692:ASP:OD1	2.37	0.54
1:B:100:HIS:O	1:C:63:ASN:ND2	2.41	0.54
1:B:451:ARG:NH2	1:B:453:SER:OG	2.40	0.54
1:E:81:CYS:HA	1:E:1073:TYR:HB3	1.89	0.54
1:E:229:ASP:O	1:E:236:LYS:NZ	2.37	0.54
7:k:38:VAL:HG13	7:k:136:TRP:HZ2	1.73	0.54
1:E:700:LEU:HD22	1:E:1025:MET:HG2	1.90	0.54
1:F:545:PRO:O	1:F:576:ARG:NH1	2.41	0.54
7:k:558:HIS:ND1	7:k:655:ARG:O	2.38	0.54
8:m:79:ASP:HB3	9:o:3103:LEU:HD22	1.90	0.54
1:C:1208:ARG:NH2	1:C:1240:ALA:O	2.41	0.53
7:k:65:HIS:H	7:k:128:THR:HG22	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:TYR:HD2	1:D:395:VAL:HG12	1.74	0.53
1:I:777:ASN:ND2	2:U:47:GLN:OE1	2.39	0.53
1:I:944:HIS:HE1	1:I:968:ASP:HB3	1.73	0.53
1:C:621:ARG:NH2	1:D:698:GLU:OE2	2.42	0.53
1:C:1124:ASN:O	1:C:1156:ARG:NH1	2.40	0.53
1:D:906:THR:HB	1:D:934:HIS:HB3	1.90	0.53
1:B:193:PRO:HD3	1:B:1294:VAL:HG12	1.91	0.53
1:B:403:VAL:HG22	1:B:1053:VAL:HG22	1.90	0.53
1:B:1276:PHE:HA	1:B:1329:GLN:HE22	1.74	0.53
1:C:418:ALA:HA	1:D:423:LEU:HD23	1.91	0.53
1:F:440:LEU:HD23	1:F:452:LEU:HD12	1.90	0.53
1:F:577:VAL:HG12	1:F:578:VAL:HG13	1.91	0.53
1:I:1054:ARG:HH22	1:I:1122:MET:HA	1.74	0.53
1:I:1236:ARG:NH2	1:I:1241:THR:O	2.41	0.53
6:S:122:PRO:HB3	6:S:251:LEU:HD11	1.90	0.53
7:k:495:ARG:CB	8:m:36:TRP:CE3	2.79	0.53
1:B:713:GLU:HG2	1:B:718:ALA:HA	1.91	0.53
1:B:777:ASN:O	2:T:51:ARG:NH2	2.37	0.53
1:F:861:PRO:O	1:F:869:ASN:ND2	2.42	0.53
1:C:1123:GLY:H	1:C:1183:ALA:HB3	1.74	0.53
1:C:1200:ARG:NH2	1:C:1355:GLU:OE2	2.41	0.53
1:F:548:ASP:OD1	1:F:576:ARG:NE	2.37	0.53
7:k:473:ALA:HB1	7:k:476:VAL:HB	1.88	0.53
8:m:36:TRP:CZ3	8:m:41:PHE:HD1	2.22	0.53
1:B:623:TYR:OH	1:B:663:ALA:O	2.23	0.53
1:B:663:ALA:N	1:B:690:TYR:OH	2.36	0.53
1:C:530:GLN:HG3	1:C:536:ASN:HD22	1.74	0.53
1:D:122:LYS:NZ	1:D:1101:ASP:O	2.34	0.53
1:E:708:THR:OG1	1:E:723:ASN:ND2	2.39	0.53
1:I:1059:VAL:HG12	1:I:1116:ARG:HD3	1.90	0.53
1:I:1348:ASP:OD2	1:I:1352:HIS:NE2	2.42	0.53
6:S:163:GLN:HB3	6:S:226:ARG:HD2	1.90	0.53
7:k:171:CYS:HB3	7:k:196:LEU:HB3	1.90	0.53
1:B:11:TYR:O	1:B:15:ALA:N	2.40	0.53
1:B:978:PRO:HA	1:B:981:ARG:HG2	1.90	0.53
1:B:982:ASP:OD1	1:B:985:ARG:NH2	2.38	0.53
1:D:80:VAL:HB	1:D:1072:ALA:HA	1.91	0.53
1:D:241:ARG:NH1	1:D:242:GLU:OE2	2.41	0.53
1:I:225:ARG:HH12	1:I:1201:ARG:HH12	1.57	0.53
1:D:198:LEU:HD13	1:D:1109:VAL:HG23	1.91	0.53
1:E:1222:VAL:O	1:E:1224:ALA:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:778:ARG:O	1:F:904:ARG:NE	2.42	0.53
3:K:161:ARG:HH22	3:K:174:PRO:HD2	1.73	0.53
8:l:59:ARG:HG3	9:o:3121:LEU:HD13	1.91	0.53
1:B:709:LEU:H	1:B:1038:HIS:HD2	1.55	0.53
1:B:726:MET:HG3	1:B:1025:MET:HE1	1.90	0.53
1:F:574:THR:OG1	1:F:1003:ARG:NH2	2.41	0.53
1:F:712:PRO:O	1:F:719:GLN:NE2	2.35	0.53
1:I:712:PRO:O	1:I:719:GLN:NE2	2.40	0.53
3:O:11:ALA:HA	3:O:82:ARG:HA	1.91	0.53
6:S:308:ALA:HB3	6:S:428:MET:HB3	1.91	0.53
1:B:873:ASN:ND2	2:T:30:ASN:OD1	2.38	0.52
1:C:203:ARG:NH2	1:C:222:GLU:OE2	2.42	0.52
1:F:832:PHE:HA	1:F:835:VAL:HB	1.90	0.52
1:B:532:MET:HA	1:B:1239:ALA:HA	1.91	0.52
1:B:680:GLY:O	1:I:658:ASN:ND2	2.41	0.52
1:E:1037:TYR:O	1:E:1041:LYS:N	2.37	0.52
1:F:152:GLY:O	1:F:156:HIS:N	2.38	0.52
1:F:267:ALA:HB3	1:F:300:ALA:HB3	1.90	0.52
7:k:256:GLU:HB2	9:o:3095:GLN:HE21	1.74	0.52
1:D:960:VAL:HG12	1:D:994:LEU:HD22	1.91	0.52
1:F:229:ASP:O	1:F:236:LYS:NZ	2.39	0.52
7:k:606:ILE:HD11	7:k:638:GLU:HG2	1.91	0.52
1:C:487:TYR:OH	1:C:990:VAL:N	2.43	0.52
1:C:677:TYR:HD1	2:Q:95:LYS:HG2	1.73	0.52
1:D:288:LEU:HB3	1:D:293:LEU:HD13	1.91	0.52
1:F:865:LEU:HD21	1:F:879:PHE:HB3	1.91	0.52
1:I:445:LYS:HD3	1:I:1179:HIS:HB3	1.92	0.52
6:S:427:VAL:O	6:S:456:VAL:N	2.43	0.52
7:k:508:LEU:HB2	7:k:666:GLY:HA2	1.89	0.52
9:n:3083:ALA:HA	9:n:3086:ILE:HB	1.91	0.52
3:K:215:GLU:OE1	3:O:245:SER:OG	2.27	0.52
1:B:187:VAL:HG11	1:B:1099:ASN:HD21	1.73	0.52
1:B:544:HIS:HD2	1:B:546:ALA:H	1.58	0.52
1:C:1313:ARG:NH1	1:C:1317:CYS:O	2.42	0.52
1:I:1369:LEU:HA	1:I:1372:LEU:HD12	1.91	0.52
1:B:951:ASN:ND2	1:B:972:ASN:O	2.40	0.52
1:D:90:MET:HE1	1:E:58:LEU:HD11	1.91	0.52
1:D:826:CYS:HB2	1:D:966:GLY:H	1.75	0.52
1:E:470:ASP:HB3	1:E:922:SER:HB3	1.92	0.52
1:I:641:PHE:HE2	1:I:677:TYR:HB2	1.75	0.52
1:C:1071:GLU:OE2	1:C:1100:VAL:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:621:ARG:NH2	1:F:698:GLU:OE2	2.43	0.52
1:I:583:PRO:HG2	1:I:586:LEU:HD13	1.91	0.52
1:B:1075:LEU:O	1:B:1097:ARG:NH1	2.42	0.52
1:D:777:ASN:O	2:M:51:ARG:NH2	2.42	0.52
1:D:804:ASP:HA	1:D:807:VAL:HB	1.91	0.52
1:D:903:GLU:HG2	1:D:904:ARG:HG2	1.92	0.52
1:D:1222:VAL:O	1:D:1224:ALA:N	2.43	0.52
1:E:1061:GLU:OE2	1:E:1116:ARG:NH2	2.42	0.52
1:F:1084:GLU:HG3	1:F:1089:VAL:HG12	1.92	0.52
3:O:230:LEU:HD23	3:O:233:GLN:HE21	1.75	0.52
1:D:430:PRO:HB3	1:D:601:VAL:HG11	1.93	0.52
1:E:1225:LEU:HD23	1:F:1175:ALA:HB3	1.92	0.52
1:F:1017:GLU:HA	1:F:1020:LEU:HB3	1.92	0.52
1:I:752:ARG:O	1:I:911:SER:OG	2.28	0.52
3:K:114:VAL:HG11	3:K:291:LEU:HB3	1.92	0.52
8:l:80:ILE:HG22	9:o:3100:ARG:HG2	1.91	0.52
1:B:1037:TYR:OH	1:B:1041:LYS:NZ	2.41	0.51
1:C:124:ILE:HG12	1:C:1100:VAL:HG22	1.92	0.51
1:F:804:ASP:O	1:F:808:HIS:ND1	2.38	0.51
1:F:1118:PRO:HD3	1:F:1374:LEU:HD13	1.92	0.51
1:F:1221:ASP:N	1:F:1221:ASP:OD1	2.41	0.51
8:l:83:ARG:HE	9:n:3099:THR:HG22	1.75	0.51
1:D:491:VAL:HB	1:D:558:LEU:HB3	1.92	0.51
1:D:1195:ASP:OD1	1:D:1195:ASP:N	2.42	0.51
1:D:1217:ASP:N	1:D:1221:ASP:OD2	2.44	0.51
1:E:1256:LEU:HA	1:E:1263:LEU:HD12	1.91	0.51
1:I:754:CYS:HA	1:I:910:CYS:HA	1.92	0.51
7:k:495:ARG:NH2	8:m:42:ASN:OD1	2.38	0.51
1:B:753:ASP:OD1	1:B:911:SER:OG	2.28	0.51
1:C:443:TRP:HH2	1:C:1347:ARG:HB3	1.75	0.51
1:E:1037:TYR:OH	1:E:1147:LEU:O	2.28	0.51
1:F:300:ALA:HA	1:F:362:ARG:HG2	1.92	0.51
1:I:575:TRP:O	1:I:1003:ARG:NH2	2.29	0.51
2:V:22:THR:OG1	2:V:64:LEU:HD13	2.10	0.51
1:B:933:LEU:HD11	1:B:958:LEU:HD23	1.92	0.51
1:F:104:ILE:HD12	1:I:390:VAL:HB	1.93	0.51
1:I:405:PRO:O	1:I:1361:TYR:OH	2.27	0.51
1:I:948:THR:HG21	2:T:95:LYS:HE3	1.93	0.51
1:B:103:LEU:HD11	1:B:115:PRO:HA	1.92	0.51
1:B:164:GLN:O	1:B:168:ASN:N	2.43	0.51
1:B:980:LEU:HD22	1:B:983:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:672:SER:O	1:C:676:THR:OG1	2.22	0.51
1:D:216:ARG:NH2	1:D:1287:ARG:O	2.41	0.51
1:E:141:ALA:HB1	1:E:146:GLU:HB3	1.92	0.51
1:E:372:ASP:OD1	1:E:372:ASP:N	2.43	0.51
1:F:1227:TYR:O	1:F:1229:HIS:ND1	2.44	0.51
1:B:1204:ASN:ND2	1:B:1208:ARG:O	2.44	0.51
1:C:1125:LEU:HD13	1:C:1156:ARG:HD2	1.93	0.51
1:F:451:ARG:NH2	1:F:453:SER:OG	2.44	0.51
6:S:210:HIS:HB2	6:S:447:VAL:HG21	1.93	0.51
8:l:31:PHE:HB2	8:l:35:PHE:HD2	1.75	0.51
1:D:656:TRP:CE2	1:D:686:CYS:HB3	2.46	0.51
1:E:410:ASN:HD21	1:E:1361:TYR:HB3	1.75	0.51
1:E:458:VAL:HG22	1:E:1151:VAL:HG22	1.92	0.51
1:F:104:ILE:HB	1:I:390:VAL:HG21	1.92	0.51
7:k:379:SER:HA	7:k:383:ILE:HD11	1.91	0.51
7:k:506:GLN:NE2	8:m:22:ASP:O	2.44	0.51
7:k:571:PRO:HA	7:k:692:CYS:HA	1.93	0.51
1:B:635:HIS:HB2	1:B:902:ALA:HB2	1.92	0.51
1:B:1201:ARG:HH12	1:C:1179:HIS:HE1	1.58	0.51
1:C:1225:LEU:HD23	1:D:1175:ALA:HB3	1.92	0.51
7:k:473:ALA:HB3	8:m:54:VAL:HG13	1.93	0.51
1:B:422:ASP:OD1	1:B:422:ASP:N	2.42	0.51
1:C:451:ARG:NH2	1:C:453:SER:OG	2.44	0.51
1:C:1149:ASN:HA	1:C:1152:VAL:HB	1.91	0.51
1:D:596:GLY:O	1:D:600:GLY:N	2.44	0.51
1:D:872:ALA:HB2	2:G:76:GLN:HB3	1.92	0.51
7:k:37:GLY:O	7:k:144:ARG:NE	2.44	0.51
7:k:657:LEU:O	7:k:673:THR:OG1	2.29	0.51
1:B:188:LEU:HD23	1:B:1064:LEU:HD21	1.93	0.51
1:B:755:ARG:HG3	1:B:761:HIS:HA	1.93	0.51
1:B:1208:ARG:NE	1:B:1225:LEU:O	2.34	0.51
1:C:804:ASP:HB3	1:C:808:HIS:CE1	2.46	0.51
1:C:1066:SER:OG	1:C:1067:GLU:N	2.43	0.51
1:F:532:MET:HE2	1:F:534:PRO:HG2	1.92	0.51
1:I:244:ILE:O	1:I:248:LEU:N	2.42	0.51
3:K:121:PHE:HE2	3:K:143:LEU:HD11	1.75	0.51
3:O:35:PRO:HB3	3:O:70:ARG:HG2	1.92	0.51
7:k:91:ALA:HB3	7:k:103:ARG:HH11	1.76	0.51
1:D:606:MET:HE1	1:D:820:PHE:HZ	1.76	0.50
1:D:895:GLN:HA	2:M:61:LEU:HD13	1.93	0.50
2:V:22:THR:HG23	2:V:60:ALA:HB1	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1346:ALA:HB2	1:E:1362:LEU:HD11	1.93	0.50
1:F:496:GLY:HA3	1:F:504:ARG:HH22	1.76	0.50
4:L:186:UNK:O	4:L:190:UNK:CB	2.60	0.50
1:D:42:VAL:HG11	1:D:49:LEU:HD11	1.92	0.50
7:k:403:GLU:HG3	7:k:411:ARG:HB2	1.93	0.50
7:k:530:LEU:HD21	7:k:594:THR:HG23	1.94	0.50
1:C:195:LEU:HD22	1:C:251:LEU:HD12	1.94	0.50
1:D:521:VAL:HG21	1:D:987:VAL:HG22	1.94	0.50
1:D:728:ASP:O	1:D:810:LYS:NZ	2.45	0.50
3:K:102:ASN:ND2	3:K:106:VAL:O	2.44	0.50
3:K:114:VAL:HG22	3:K:293:PRO:HA	1.94	0.50
8:m:86:PRO:O	8:m:90:GLN:NE2	2.45	0.50
1:B:228:CYS:HA	1:B:1368:PRO:HG3	1.92	0.50
1:C:608:PRO:HA	1:C:611:ILE:HD12	1.93	0.50
1:I:703:LEU:HB3	1:I:1025:MET:HE1	1.94	0.50
3:O:62:GLY:O	3:O:66:ALA:N	2.44	0.50
1:B:643:ALA:HB1	1:B:896:VAL:HG21	1.93	0.50
1:C:611:ILE:HG23	1:C:820:PHE:HE1	1.75	0.50
1:C:1257:TYR:HB2	1:C:1277:PHE:HD2	1.76	0.50
3:K:279:LEU:HD22	3:O:153:ALA:HB2	1.94	0.50
2:M:76:GLN:O	2:M:96:ARG:NH2	2.41	0.50
6:S:132:LEU:O	6:S:185:VAL:N	2.44	0.50
1:B:758:ALA:HB2	1:B:904:ARG:HH12	1.76	0.50
1:C:959:PRO:HB2	1:C:990:VAL:HG22	1.92	0.50
1:D:467:MET:HG3	1:D:918:ALA:HA	1.93	0.50
1:F:876:LYS:HA	1:F:879:PHE:HB2	1.94	0.50
1:B:433:ARG:NH1	1:I:413:MET:O	2.41	0.50
1:B:980:LEU:O	1:B:984:ALA:N	2.40	0.50
1:C:93:GLY:HA3	1:C:124:ILE:HD12	1.93	0.50
1:C:733:PRO:HG2	1:C:736:VAL:HG22	1.93	0.50
1:D:631:GLN:HE21	1:D:667:ASP:HB2	1.77	0.50
1:D:736:VAL:O	1:D:934:HIS:ND1	2.45	0.50
1:E:963:LEU:HD23	1:E:1007:VAL:HG22	1.94	0.50
1:F:258:SER:OG	1:F:1102:LEU:O	2.29	0.50
1:I:873:ASN:HB2	2:U:30:ASN:HD21	1.76	0.50
1:I:1174:ARG:NH1	1:I:1182:ASP:OD2	2.41	0.50
8:l:59:ARG:NH2	8:m:58:GLN:OE1	2.41	0.50
1:B:730:ALA:HB2	1:B:750:ARG:HH12	1.77	0.50
1:D:883:ARG:HB2	1:E:680:GLY:HA3	1.94	0.50
1:D:1201:ARG:NH1	1:E:448:GLN:OE1	2.45	0.50
2:G:89:ARG:NH2	2:M:29:THR:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:867:PRO:HG3	2:T:98:TYR:HB2	1.93	0.50
7:k:495:ARG:NH2	8:m:36:TRP:O	2.44	0.50
1:B:224:LYS:NZ	1:B:1214:TYR:OH	2.41	0.49
1:C:909:LEU:HD11	1:C:929:PHE:HB3	1.93	0.49
1:I:453:SER:OG	1:I:456:ASN:N	2.41	0.49
1:I:844:VAL:HG22	1:I:864:PRO:HB3	1.93	0.49
1:I:1057:ARG:NH2	1:I:1319:GLU:OE2	2.45	0.49
2:Q:76:GLN:O	2:Q:96:ARG:NH2	2.42	0.49
7:k:44:VAL:CG2	7:k:80:TYR:HE2	2.25	0.49
1:C:804:ASP:HB3	1:C:808:HIS:HE1	1.77	0.49
1:D:876:LYS:HA	1:D:879:PHE:HD2	1.76	0.49
1:I:1280:ALA:O	1:I:1284:ALA:N	2.44	0.49
1:C:664:PHE:HB3	1:C:670:LEU:HD13	1.93	0.49
1:C:1222:VAL:O	1:C:1224:ALA:N	2.44	0.49
1:D:621:ARG:NH2	1:E:698:GLU:OE2	2.45	0.49
1:E:161:ALA:O	1:E:165:LEU:N	2.41	0.49
1:F:453:SER:O	1:F:455:GLU:N	2.45	0.49
1:C:766:ALA:HB2	1:C:782:ARG:HD2	1.94	0.49
1:E:207:ASN:HB2	1:F:391:PRO:HA	1.94	0.49
1:F:231:SER:H	1:F:236:LYS:HZ1	1.60	0.49
1:C:1125:LEU:HD12	1:C:1126:PRO:HD2	1.93	0.49
1:D:436:PRO:HG2	1:D:595:ARG:HB3	1.95	0.49
1:E:1278:THR:HG22	1:E:1281:ASP:H	1.76	0.49
1:F:834:ARG:HD2	1:F:954:TYR:HA	1.94	0.49
1:F:1195:ASP:OD1	1:F:1195:ASP:N	2.45	0.49
1:F:1278:THR:HG22	1:F:1281:ASP:H	1.78	0.49
1:I:159:LEU:HD12	1:I:162:ILE:HB	1.94	0.49
1:I:532:MET:HE2	1:I:534:PRO:HG2	1.95	0.49
1:C:404:LEU:HB2	1:C:1052:VAL:HB	1.95	0.49
1:D:440:LEU:HB3	1:D:452:LEU:HB2	1.95	0.49
1:E:1248:GLN:HB2	1:E:1251:SER:HB3	1.94	0.49
1:F:1206:ARG:NH1	1:F:1247:SER:O	2.46	0.49
7:k:588:ALA:HA	7:k:607:ALA:HA	1.94	0.49
1:C:1182:ASP:HB2	1:C:1309:VAL:HA	1.94	0.49
1:D:285:LYS:HE2	1:D:377:LEU:HB3	1.93	0.49
1:F:1284:ALA:O	1:F:1286:HIS:N	2.43	0.49
1:I:840:GLN:HB2	2:U:61:LEU:HD21	1.94	0.49
1:B:404:LEU:HD21	1:B:1334:ILE:HD11	1.95	0.49
1:C:671:VAL:HG13	1:C:690:TYR:HD1	1.78	0.49
1:C:1017:GLU:HA	1:C:1020:LEU:HB3	1.95	0.49
1:D:724:HIS:CD2	1:D:726:MET:H	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:HIS:H	1:F:63:ASN:HD21	1.61	0.49
1:E:325:ALA:H	1:F:56:ALA:HA	1.77	0.49
1:E:836:TYR:CZ	1:E:901:MET:HB2	2.48	0.49
1:E:867:PRO:HG3	2:V:98:TYR:HB2	1.93	0.49
1:I:827:THR:OG1	1:I:958:LEU:O	2.30	0.49
3:K:64:LEU:HA	3:K:67:TYR:HB2	1.94	0.49
7:k:495:ARG:NE	8:m:36:TRP:CE3	2.74	0.49
7:k:526:ARG:NH2	8:l:36:TRP:O	2.44	0.49
1:D:77:VAL:HG23	1:D:266:HIS:HB3	1.95	0.49
1:D:622:SER:OG	1:E:675:VAL:O	2.25	0.49
1:F:97:PHE:HE1	1:F:122:LYS:HG2	1.78	0.49
1:I:991:PRO:HG2	1:I:994:LEU:HD12	1.95	0.49
3:K:182:ASN:OD1	3:K:183:GLY:N	2.45	0.49
3:O:67:TYR:HB3	3:O:291:LEU:HD21	1.94	0.49
1:D:270:ARG:NH1	1:D:297:ASP:OD1	2.44	0.48
1:E:790:ARG:HH11	2:G:79:PHE:HB2	1.77	0.48
1:F:470:ASP:N	1:F:470:ASP:OD1	2.46	0.48
1:I:396:GLY:N	1:I:1060:THR:O	2.42	0.48
1:B:1124:ASN:HD21	1:I:1238:PHE:HB3	1.77	0.48
1:C:841:ASN:ND2	1:C:873:ASN:O	2.46	0.48
1:E:1195:ASP:N	1:E:1195:ASP:OD1	2.46	0.48
1:F:734:PRO:HD2	1:F:813:TYR:HD2	1.78	0.48
1:I:624:PRO:HB3	1:I:882:GLY:HA3	1.93	0.48
3:K:154:ARG:HD2	3:K:176:LEU:HB3	1.94	0.48
3:O:114:VAL:N	3:O:295:VAL:O	2.41	0.48
1:B:73:LEU:HD21	1:B:380:LEU:HD21	1.94	0.48
1:B:629:LEU:O	1:B:633:ALA:N	2.46	0.48
1:F:1070:SER:OG	1:F:1071:GLU:N	2.46	0.48
1:I:708:THR:HG22	1:I:1038:HIS:HE1	1.79	0.48
1:B:142:LEU:HD21	1:B:157:ARG:HB3	1.95	0.48
1:C:549:PHE:HB3	1:C:571:ILE:HD11	1.95	0.48
1:D:285:LYS:HD3	1:D:379:ALA:HB2	1.95	0.48
1:D:1095:GLN:OE1	1:D:1097:ARG:NH2	2.47	0.48
1:F:658:ASN:ND2	1:I:680:GLY:O	2.47	0.48
1:I:84:PHE:HB2	1:I:1074:PHE:HB3	1.93	0.48
1:I:772:ALA:HA	2:U:55:ARG:HH21	1.78	0.48
1:I:1348:ASP:OD1	1:I:1348:ASP:N	2.45	0.48
3:K:116:LEU:HD21	3:K:143:LEU:HB2	1.95	0.48
1:B:184:MET:O	1:B:1073:TYR:OH	2.31	0.48
1:B:521:VAL:HG11	1:B:987:VAL:HG13	1.95	0.48
1:B:611:ILE:HD11	1:B:1018:ASN:HD21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1222:VAL:O	1:B:1224:ALA:N	2.46	0.48
1:C:135:LEU:HD21	1:C:165:LEU:HD13	1.96	0.48
1:I:228:CYS:HA	1:I:1368:PRO:HG3	1.96	0.48
1:I:832:PHE:HA	1:I:835:VAL:HB	1.95	0.48
1:I:1063:VAL:HB	1:I:1111:ALA:HB3	1.94	0.48
7:k:90:LEU:HD22	7:k:166:ARG:HD2	1.95	0.48
8:l:64:ALA:O	8:l:68:ASN:N	2.42	0.48
1:B:622:SER:OG	1:C:675:VAL:O	2.21	0.48
1:C:776:PHE:HA	1:C:903:GLU:HB2	1.96	0.48
1:F:846:GLU:HA	2:V:68:HIS:CE1	2.48	0.48
7:k:62:THR:OG1	7:k:71:THR:OG1	2.27	0.48
8:m:91:VAL:HG11	9:n:3092:ILE:HB	1.96	0.48
1:B:128:ALA:HA	1:B:1096:PRO:HA	1.95	0.48
1:C:78:ALA:O	1:C:1070:SER:OG	2.28	0.48
1:C:326:VAL:HB	1:C:329:LEU:HB2	1.95	0.48
1:E:981:ARG:HH22	1:F:803:ALA:H	1.61	0.48
1:F:1218:LYS:HB3	1:F:1221:ASP:HB3	1.96	0.48
1:B:544:HIS:CD2	1:B:546:ALA:H	2.31	0.48
1:C:724:HIS:CD2	1:C:726:MET:H	2.32	0.48
1:C:812:TYR:HA	1:C:816:LEU:HD13	1.95	0.48
1:F:753:ASP:OD1	1:F:911:SER:OG	2.25	0.48
1:F:857:PRO:HG3	1:F:885:VAL:HG22	1.96	0.48
3:K:297:VAL:HG22	3:K:314:VAL:HG22	1.96	0.48
1:D:963:LEU:HG	1:D:1007:VAL:HG22	1.94	0.48
1:I:766:ALA:HB2	1:I:782:ARG:HD3	1.96	0.48
2:V:71:ASN:HA	2:V:102:VAL:HB	1.96	0.48
7:k:27:ILE:HB	7:k:398:VAL:HB	1.96	0.48
1:B:390:VAL:HG22	1:I:106:ARG:HH21	1.79	0.48
1:B:421:GLY:HA3	1:I:420:ALA:HB2	1.95	0.48
1:B:438:ARG:HD3	1:B:1045:HIS:HB2	1.94	0.48
1:B:539:LEU:O	1:B:1248:GLN:NE2	2.43	0.48
1:D:79:CYS:HB3	1:D:184:MET:HE2	1.95	0.48
1:D:1099:ASN:OD1	1:D:1099:ASN:N	2.47	0.48
1:E:854:PRO:HB3	1:E:860:ASP:HB3	1.95	0.48
1:E:1008:GLN:HE21	1:E:1012:GLU:HB2	1.79	0.48
1:F:281:THR:HG22	1:F:392:TYR:HE2	1.79	0.48
1:E:667:ASP:OD1	1:E:813:TYR:OH	2.32	0.47
1:E:1017:GLU:O	1:E:1021:THR:OG1	2.24	0.47
1:I:192:ALA:HB1	1:I:1110:ALA:HB2	1.96	0.47
7:k:65:HIS:HE1	7:k:470:PHE:H	1.62	0.47
7:k:365:TRP:CD1	7:k:380:ARG:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:LEU:HD22	1:B:1097:ARG:HA	1.96	0.47
1:F:1106:TYR:OH	1:F:1290:GLU:O	2.32	0.47
1:B:87:LEU:HD22	1:B:1097:ARG:HE	1.79	0.47
1:D:632:ALA:HB1	1:D:832:PHE:HE1	1.79	0.47
1:E:301:ASP:N	1:E:363:VAL:O	2.42	0.47
1:E:754:CYS:HA	1:E:910:CYS:HA	1.95	0.47
1:E:1057:ARG:NH2	1:E:1319:GLU:OE2	2.47	0.47
1:I:225:ARG:NH1	1:I:1201:ARG:HH12	2.13	0.47
1:I:442:PHE:HE2	1:I:1122:MET:HB3	1.79	0.47
1:I:577:VAL:HG21	1:I:1001:SER:HA	1.95	0.47
1:I:746:ALA:HA	1:I:751:HIS:CG	2.49	0.47
1:I:894:LEU:HB2	2:U:61:LEU:HB3	1.95	0.47
2:V:18:ARG:NH2	2:V:63:ASP:OD2	2.36	0.47
1:C:1138:LEU:HB2	1:C:1144:ALA:HB2	1.94	0.47
1:D:548:ASP:OD1	1:D:576:ARG:NE	2.39	0.47
1:F:422:ASP:N	1:F:422:ASP:OD1	2.45	0.47
1:F:919:ASN:HD21	1:F:924:ALA:HA	1.79	0.47
1:I:966:GLY:HA3	1:I:969:HIS:HB2	1.96	0.47
1:I:1078:LEU:HD12	1:I:1093:LEU:HD13	1.95	0.47
3:O:296:ARG:HB3	3:O:315:ILE:HG13	1.96	0.47
1:B:311:LEU:HD12	1:B:315:ASN:HB3	1.96	0.47
1:C:304:VAL:HG12	1:C:360:THR:HG22	1.95	0.47
1:C:526:MET:N	1:C:529:GLU:OE1	2.48	0.47
1:C:622:SER:OG	1:D:675:VAL:O	2.25	0.47
1:C:777:ASN:ND2	2:Q:47:GLN:OE1	2.47	0.47
1:D:646:ARG:HA	1:D:649:THR:HG22	1.97	0.47
1:E:840:GLN:HE22	2:G:58:ALA:HB2	1.80	0.47
1:I:1198:TYR:OH	1:I:1204:ASN:O	2.31	0.47
7:k:591:TYR:HB2	7:k:602:THR:HG23	1.96	0.47
1:B:1274:PHE:O	1:B:1278:THR:OG1	2.32	0.47
1:E:156:HIS:CE1	1:E:160:ARG:HE	2.33	0.47
1:E:653:THR:O	1:E:657:ASN:ND2	2.48	0.47
1:E:1033:PRO:HA	1:E:1036:LEU:HB2	1.96	0.47
1:F:667:ASP:OD2	1:F:669:SER:OG	2.31	0.47
1:F:836:TYR:O	1:F:840:GLN:NE2	2.46	0.47
1:F:889:PRO:HA	1:F:892:LEU:HB3	1.97	0.47
1:B:1344:ARG:NH2	1:I:1353:ALA:O	2.43	0.47
1:D:526:MET:O	1:D:530:GLN:N	2.45	0.47
1:D:909:LEU:HD11	1:D:929:PHE:HB3	1.97	0.47
1:E:329:LEU:O	1:E:333:GLY:N	2.44	0.47
1:F:184:MET:HA	1:F:187:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:280:THR:HG23	1:F:1063:VAL:HG22	1.96	0.47
1:F:372:ASP:OD1	1:F:372:ASP:N	2.44	0.47
1:F:674:ILE:HG23	1:F:678:LEU:HD12	1.97	0.47
1:F:699:ALA:HA	1:F:702:GLN:HE21	1.79	0.47
1:F:828:ALA:HB1	1:F:955:PHE:HB3	1.95	0.47
1:I:277:VAL:HB	1:I:1066:SER:HB3	1.96	0.47
1:I:671:VAL:HG13	1:I:690:TYR:HD1	1.79	0.47
1:I:1077:GLN:H	1:I:1096:PRO:HD2	1.80	0.47
3:K:214:THR:HG21	3:O:227:LEU:HD11	1.96	0.47
7:k:494:ILE:C	8:m:36:TRP:CH2	2.68	0.47
1:B:642:CYS:HA	1:B:645:ALA:HB2	1.96	0.47
1:E:450:LEU:HD13	1:E:1124:ASN:HB2	1.96	0.47
1:E:579:ASN:N	1:E:579:ASN:OD1	2.47	0.47
1:I:639:HIS:HA	2:U:79:PHE:HE2	1.79	0.47
1:I:770:ASN:H	1:I:773:THR:HB	1.79	0.47
1:I:854:PRO:HB3	1:I:863:HIS:HA	1.97	0.47
1:I:1289:LEU:HA	1:I:1292:LEU:HD12	1.95	0.47
6:S:131:LEU:HD21	6:S:251:LEU:HD12	1.96	0.47
6:S:134:LEU:HB3	6:S:183:GLY:HA2	1.97	0.47
1:E:281:THR:OG1	1:E:282:ALA:N	2.43	0.47
1:F:305:THR:OG1	1:F:306:TYR:N	2.48	0.47
1:F:525:GLN:NE2	1:F:535:ASP:O	2.48	0.47
1:F:826:CYS:HA	1:F:964:PHE:HB3	1.97	0.47
1:F:1344:ARG:HG2	1:F:1347:ARG:HH12	1.79	0.47
1:I:83:LYS:HE3	1:I:85:PRO:HD3	1.97	0.47
1:I:1099:ASN:OD1	1:I:1099:ASN:N	2.47	0.47
2:U:13:THR:OG1	2:U:16:ASN:ND2	2.48	0.47
1:C:1055:GLN:HB3	1:C:1310:GLN:HE22	1.80	0.47
1:E:778:ARG:O	1:E:904:ARG:NE	2.48	0.47
1:I:248:LEU:HD12	1:I:251:LEU:HD13	1.96	0.47
1:I:267:ALA:HA	1:I:273:PRO:HA	1.97	0.47
1:B:452:LEU:HD21	1:B:1124:ASN:HA	1.97	0.46
1:I:248:LEU:HA	1:I:251:LEU:HD13	1.97	0.46
1:I:1257:TYR:HB2	1:I:1277:PHE:HD2	1.80	0.46
1:B:577:VAL:HG12	1:B:578:VAL:HG13	1.97	0.46
1:B:884:VAL:HG12	1:B:886:VAL:HG23	1.98	0.46
1:I:1066:SER:HA	1:I:1108:ALA:HA	1.97	0.46
1:I:1270:LEU:HB3	1:I:1310:GLN:HB3	1.97	0.46
6:S:273:ALA:HB2	6:S:457:TRP:HE1	1.79	0.46
7:k:5:PHE:HE2	7:k:375:ASP:HA	1.80	0.46
7:k:534:LEU:HD21	7:k:649:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:929:PHE:N	1:C:999:PHE:O	2.48	0.46
1:F:70:PHE:O	1:F:76:SER:OG	2.33	0.46
1:F:742:LEU:HA	1:F:745:HIS:HB3	1.98	0.46
2:G:81:GLY:N	2:G:91:SER:OG	2.42	0.46
1:I:1125:LEU:HD11	1:I:1156:ARG:HB3	1.96	0.46
8:m:83:ARG:HD2	9:o:3099:THR:HG22	1.97	0.46
1:F:677:TYR:HD1	2:V:95:LYS:HG2	1.79	0.46
2:G:4:PRO:HB3	2:G:16:ASN:HB3	1.97	0.46
1:I:75:LEU:HD12	1:I:78:ALA:HB3	1.97	0.46
1:I:467:MET:HE1	1:I:575:TRP:HE1	1.79	0.46
3:K:48:HIS:CD2	3:K:138:ARG:HD3	2.51	0.46
3:K:155:LEU:O	3:K:159:GLY:N	2.48	0.46
7:k:22:SER:HB2	7:k:116:VAL:HB	1.97	0.46
9:n:3111:LEU:HD23	9:n:3114:LEU:HD12	1.97	0.46
1:B:578:VAL:HG23	1:B:580:GLY:H	1.81	0.46
1:C:425:PRO:HG3	1:C:431:GLU:HB2	1.98	0.46
1:C:467:MET:O	1:C:922:SER:OG	2.33	0.46
1:F:668:TYR:HB2	1:F:812:TYR:CG	2.51	0.46
1:E:520:TRP:HH2	1:E:988:PRO:HD2	1.80	0.46
1:E:578:VAL:N	1:E:581:ASN:OD1	2.38	0.46
1:E:766:ALA:N	1:E:783:LEU:O	2.39	0.46
1:E:1243:ASN:O	1:E:1247:SER:OG	2.29	0.46
1:F:79:CYS:HB3	1:F:184:MET:HE2	1.97	0.46
1:I:626:VAL:HG13	1:I:878:MET:HG3	1.97	0.46
1:I:675:VAL:HG21	1:I:694:VAL:HG21	1.96	0.46
7:k:69:ASP:OD1	7:k:685:ARG:NH1	2.47	0.46
1:B:822:ARG:NH2	1:B:1017:GLU:OE2	2.47	0.46
1:E:451:ARG:NH2	1:E:453:SER:OG	2.49	0.46
1:F:606:MET:HB2	1:F:1018:ASN:HD21	1.80	0.46
1:I:248:LEU:HD23	1:I:293:LEU:HD21	1.97	0.46
1:I:873:ASN:ND2	2:U:30:ASN:OD1	2.38	0.46
3:O:155:LEU:HD22	3:O:158:ARG:HH11	1.80	0.46
1:C:764:VAL:HG13	1:C:782:ARG:HE	1.81	0.46
1:D:335:HIS:O	1:D:339:MET:N	2.48	0.46
1:D:697:VAL:HG12	1:D:808:HIS:CD2	2.51	0.46
1:F:866:HIS:CD2	1:F:868:ALA:H	2.34	0.46
1:F:870:LEU:HD22	1:F:877:ARG:HA	1.98	0.46
3:K:285:LEU:HD23	3:K:288:ILE:HD12	1.97	0.46
6:S:307:ALA:HB1	6:S:429:PRO:HA	1.96	0.46
7:k:593:SER:HB3	7:k:601:LEU:HD21	1.98	0.46
1:B:644:LEU:HD23	1:B:647:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:873:ASN:ND2	2:Q:30:ASN:OD1	2.43	0.46
1:E:422:ASP:OD1	1:E:422:ASP:N	2.48	0.46
1:E:494:PRO:HG3	1:E:993:ALA:HB1	1.98	0.46
1:E:844:VAL:HG11	1:E:892:LEU:HD12	1.96	0.46
1:E:950:GLN:HB3	1:E:953:GLU:HB2	1.97	0.46
1:E:968:ASP:O	1:E:972:ASN:ND2	2.38	0.46
1:F:274:VAL:HG11	1:F:376:PHE:CD2	2.51	0.46
1:F:724:HIS:CD2	1:F:726:MET:H	2.33	0.46
1:F:1237:PRO:HB3	1:I:1156:ARG:HH12	1.81	0.46
1:I:220:VAL:HG11	1:I:1214:TYR:HE1	1.80	0.46
1:I:1206:ARG:HD3	1:I:1210:ALA:HB2	1.97	0.46
3:K:109:CYS:HB2	3:K:304:ALA:HB1	1.97	0.46
3:K:272:TYR:HD2	3:O:161:ARG:HE	1.64	0.46
7:k:611:ASP:HB2	7:k:620:SER:HB2	1.98	0.46
1:B:423:LEU:H	1:I:418:ALA:HA	1.81	0.46
1:B:717:GLN:HE22	1:B:750:ARG:HD3	1.81	0.46
1:D:417:ALA:HB2	1:D:1358:PHE:HE1	1.81	0.46
1:F:247:TRP:HE3	1:F:248:LEU:HD12	1.80	0.46
1:I:487:TYR:OH	1:I:990:VAL:N	2.49	0.46
2:V:21:GLY:O	2:V:25:LEU:N	2.49	0.46
7:k:495:ARG:HE	8:m:36:TRP:HE3	1.53	0.46
1:B:1156:ARG:HD2	1:B:1174:ARG:HH22	1.81	0.45
1:B:1174:ARG:HD2	1:B:1177:MET:HB3	1.98	0.45
1:D:87:LEU:HD22	1:D:1096:PRO:HB2	1.98	0.45
1:E:584:LEU:HG	1:E:1005:PRO:HB3	1.99	0.45
3:K:155:LEU:HD11	3:K:188:LEU:HD11	1.97	0.45
7:k:426:LEU:HD23	7:k:449:LEU:HD13	1.97	0.45
1:B:7:ASP:O	1:B:11:TYR:N	2.37	0.45
1:B:637:ASN:HA	1:B:787:THR:HA	1.98	0.45
1:C:1369:LEU:HA	1:C:1372:LEU:HD12	1.97	0.45
1:D:422:ASP:N	1:D:422:ASP:OD1	2.48	0.45
1:D:1073:TYR:HD1	1:D:1099:ASN:HB3	1.82	0.45
1:E:775:ASP:HB3	1:E:778:ARG:HD2	1.99	0.45
1:E:788:GLN:HB3	1:E:800:HIS:CG	2.51	0.45
1:F:892:LEU:HD11	2:V:68:HIS:CG	2.51	0.45
1:F:1008:GLN:NE2	1:F:1012:GLU:OE1	2.41	0.45
1:F:1054:ARG:HH11	1:F:1123:GLY:HA3	1.81	0.45
1:I:199:LEU:HD21	1:I:250:ASP:HB3	1.97	0.45
1:I:620:ASP:OD2	1:I:655:TYR:OH	2.32	0.45
1:I:1054:ARG:HH12	1:I:1123:GLY:H	1.64	0.45
1:I:1182:ASP:O	1:I:1310:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:k:427:THR:O	7:k:431:ALA:N	2.49	0.45
1:B:155:LEU:HB2	1:I:340:GLN:HE22	1.81	0.45
1:E:532:MET:HA	1:E:1240:ALA:H	1.81	0.45
1:E:656:TRP:CD2	1:E:686:CYS:HB3	2.51	0.45
1:E:834:ARG:HD2	1:E:954:TYR:HA	1.98	0.45
6:S:188:ASN:ND2	6:S:215:TYR:OH	2.38	0.45
7:k:133:ARG:HH12	7:k:572:LEU:HB3	1.82	0.45
1:B:1116:ARG:HH21	1:I:203:ARG:HD3	1.80	0.45
1:C:539:LEU:O	1:C:1248:GLN:NE2	2.48	0.45
1:D:832:PHE:HA	1:D:835:VAL:HB	1.97	0.45
1:I:280:THR:HG22	1:I:1063:VAL:HG13	1.98	0.45
7:k:80:TYR:HA	7:k:110:LEU:HA	1.98	0.45
7:k:136:TRP:HB2	7:k:142:CYS:HB3	1.98	0.45
7:k:238:LEU:HD13	7:k:387:LEU:HD13	1.97	0.45
1:B:804:ASP:O	1:B:808:HIS:ND1	2.43	0.45
1:C:1215:ALA:O	1:C:1287:ARG:NH1	2.35	0.45
1:D:665:VAL:O	1:D:812:TYR:OH	2.28	0.45
1:E:213:ARG:NH1	1:F:1175:ALA:O	2.50	0.45
1:F:195:LEU:HB2	1:F:1109:VAL:HB	1.99	0.45
1:F:1208:ARG:NE	1:F:1225:LEU:O	2.47	0.45
1:I:576:ARG:NH1	1:I:581:ASN:O	2.49	0.45
1:I:741:GLY:O	1:I:745:HIS:N	2.39	0.45
1:B:166:ALA:HA	1:B:169:VAL:HG12	1.99	0.45
1:D:1127:GLN:HB2	1:D:1186:GLU:HG2	1.99	0.45
1:E:647:LEU:O	1:E:651:CYS:N	2.47	0.45
1:I:623:TYR:OH	1:I:663:ALA:O	2.31	0.45
8:l:58:GLN:HB3	8:m:59:ARG:HE	1.82	0.45
1:B:834:ARG:NH1	2:Q:86:GLU:O	2.47	0.45
1:C:580:GLY:HA2	1:C:592:ARG:HH12	1.81	0.45
1:E:777:ASN:ND2	2:G:47:GLN:OE1	2.49	0.45
1:F:176:PHE:O	1:F:180:THR:N	2.49	0.45
1:F:753:ASP:OD1	1:F:753:ASP:N	2.50	0.45
1:F:998:TYR:O	1:F:1003:ARG:NH2	2.48	0.45
2:G:61:LEU:O	2:G:65:GLY:N	2.50	0.45
1:I:1355:GLU:HB3	1:I:1356:THR:HG22	1.99	0.45
3:O:52:VAL:HA	3:O:58:PRO:HD3	1.98	0.45
7:k:572:LEU:HD23	7:k:693:ARG:HB2	1.99	0.45
1:C:392:TYR:CZ	1:C:394:LEU:HB2	2.51	0.45
1:D:764:VAL:HG13	1:D:782:ARG:HE	1.81	0.45
1:E:502:GLN:HE22	1:E:970:VAL:HG22	1.82	0.45
1:E:1304:THR:HG21	1:E:1314:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:243:ALA:O	1:F:247:TRP:N	2.50	0.45
1:F:644:LEU:HD23	1:F:647:LEU:HD23	1.98	0.45
1:F:1184:VAL:HG23	1:F:1310:GLN:HE21	1.82	0.45
1:I:184:MET:O	1:I:188:LEU:N	2.45	0.45
1:I:805:TRP:CE2	1:I:809:HIS:HE1	2.35	0.45
3:K:88:VAL:HG11	3:K:295:VAL:HG22	1.98	0.45
6:S:271:GLN:H	6:S:271:GLN:HG3	1.58	0.45
7:k:86:VAL:HG12	7:k:234:PRO:HB2	1.99	0.45
7:k:644:GLU:OE1	7:k:645:SER:OG	2.34	0.45
1:B:647:LEU:HA	1:B:890:ALA:HB1	1.98	0.45
1:B:1131:LEU:HD12	1:B:1131:LEU:HA	1.82	0.45
1:C:142:LEU:HD21	1:C:157:ARG:HG3	1.98	0.45
1:D:778:ARG:NH2	1:D:780:ASP:OD2	2.42	0.45
1:D:873:ASN:OD1	2:G:92:PHE:N	2.48	0.45
1:F:590:ALA:O	1:F:594:ALA:N	2.49	0.45
1:F:633:ALA:O	1:F:635:HIS:ND1	2.39	0.45
1:F:751:HIS:NE2	1:F:754:CYS:HB2	2.32	0.45
1:F:1200:ARG:HG2	1:F:1363:ILE:HG23	1.98	0.45
1:I:422:ASP:N	1:I:422:ASP:OD1	2.50	0.45
7:k:533:ASN:HA	7:k:536:ARG:HB2	1.98	0.45
1:C:642:CYS:HA	1:C:645:ALA:HB2	1.98	0.44
1:D:783:LEU:HD21	1:D:908:LEU:HD13	1.99	0.44
1:F:1157:LEU:HD21	1:F:1309:VAL:HG11	1.99	0.44
3:O:29:GLY:O	3:O:101:ARG:N	2.40	0.44
6:S:164:LEU:O	6:S:168:SER:N	2.43	0.44
2:V:25:LEU:HD21	2:V:57:GLN:HG2	1.98	0.44
1:B:287:ARG:HH12	1:B:1114:THR:HG21	1.82	0.44
1:D:404:LEU:HB2	1:D:1052:VAL:HB	1.99	0.44
1:D:1004:GLN:HE21	1:D:1008:GLN:HB2	1.82	0.44
1:E:804:ASP:HA	1:E:807:VAL:HB	1.99	0.44
1:F:200:PRO:HA	1:F:203:ARG:HG2	1.99	0.44
1:I:336:LEU:HA	1:I:339:MET:HG3	1.99	0.44
1:I:1183:ALA:HA	1:I:1310:GLN:HE22	1.82	0.44
3:K:66:ALA:HA	3:K:69:ARG:HB3	2.00	0.44
3:O:161:ARG:HH12	3:O:174:PRO:HG2	1.81	0.44
7:k:84:ASP:O	7:k:88:ALA:N	2.50	0.44
1:B:501:MET:HA	1:B:504:ARG:HG2	1.99	0.44
1:C:281:THR:OG1	1:C:282:ALA:N	2.51	0.44
1:D:238:GLY:HA2	1:D:244:ILE:HD11	2.00	0.44
1:E:156:HIS:HE1	1:E:160:ARG:HE	1.65	0.44
1:E:904:ARG:NH1	1:E:905:THR:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:CYS:HA	1:F:1368:PRO:HG3	1.99	0.44
1:I:131:ALA:HB3	1:I:1092:THR:HG23	1.97	0.44
7:k:141:THR:HG21	7:k:603:ASN:HB3	1.99	0.44
1:D:280:THR:O	1:D:392:TYR:OH	2.25	0.44
1:D:748:LEU:HD13	1:D:750:ARG:HB2	1.99	0.44
1:D:770:ASN:H	1:D:773:THR:HB	1.83	0.44
1:D:1125:LEU:HD11	1:D:1157:LEU:HG	1.99	0.44
1:E:1078:LEU:HD23	1:E:1095:GLN:HB2	2.00	0.44
1:F:269:THR:HG22	1:F:362:ARG:HH12	1.83	0.44
1:F:893:THR:HA	1:F:895:GLN:HG2	2.00	0.44
1:I:545:PRO:HG3	1:I:1245:TRP:CD2	2.52	0.44
1:B:472:ALA:HB2	1:B:1255:LEU:HD11	2.00	0.44
1:B:549:PHE:HB3	1:B:571:ILE:HD11	1.99	0.44
1:C:697:VAL:HG12	1:C:808:HIS:HD2	1.82	0.44
1:D:1208:ARG:HB2	1:D:1241:THR:HG22	1.98	0.44
1:E:99:VAL:HG23	1:E:118:ASN:HD22	1.83	0.44
1:F:1059:VAL:HG11	1:F:1116:ARG:HD2	2.00	0.44
1:I:210:LEU:HD23	1:I:210:LEU:HA	1.83	0.44
1:I:891:MET:HA	1:I:894:LEU:HD21	1.98	0.44
7:k:589:PHE:HA	7:k:652:GLY:HA2	1.99	0.44
8:m:65:ALA:HA	8:m:68:ASN:HB2	2.00	0.44
1:B:750:ARG:HA	1:B:913:ALA:HB3	1.99	0.44
1:B:1034:VAL:HG22	1:B:1147:LEU:HD13	1.99	0.44
1:C:904:ARG:NH1	1:C:906:THR:OG1	2.50	0.44
1:D:676:THR:O	2:M:95:LYS:NZ	2.38	0.44
1:D:1259:GLY:HA3	1:D:1274:PHE:HE1	1.83	0.44
1:F:203:ARG:HB2	1:I:1116:ARG:HH12	1.83	0.44
1:I:576:ARG:HA	1:I:1003:ARG:HH12	1.82	0.44
7:k:65:HIS:CD2	7:k:127:TYR:HB3	2.53	0.44
7:k:378:TRP:CE2	7:k:404:ASN:HB3	2.52	0.44
1:B:280:THR:HG22	1:B:1063:VAL:HG12	1.99	0.44
1:C:320:LEU:HD12	1:C:321:VAL:HG23	2.00	0.44
1:C:440:LEU:HB3	1:C:452:LEU:HB2	2.00	0.44
1:C:634:ILE:HD13	1:C:641:PHE:HD1	1.83	0.44
1:D:577:VAL:HG12	1:D:578:VAL:HG13	1.99	0.44
1:E:701:ALA:O	1:E:727:ARG:NH2	2.50	0.44
1:F:128:ALA:O	1:F:1094:THR:OG1	2.35	0.44
1:F:319:ALA:O	1:F:323:GLY:N	2.50	0.44
1:F:436:PRO:HA	1:F:437:PRO:HD3	1.77	0.44
1:I:946:ASP:OD1	1:I:946:ASP:N	2.50	0.44
1:I:1054:ARG:NH2	1:I:1122:MET:HA	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:k:32:CYS:HA	7:k:395:GLN:HG3	2.00	0.44
7:k:484:ILE:HD11	8:m:50:GLU:HB2	1.99	0.44
1:C:429:HIS:HA	1:C:430:PRO:HD3	1.73	0.44
1:E:804:ASP:HB3	1:E:808:HIS:CE1	2.52	0.44
1:F:724:HIS:HD2	1:F:726:MET:H	1.64	0.44
1:F:1033:PRO:HB2	1:F:1147:LEU:HD21	1.99	0.44
1:I:751:HIS:NE2	1:I:754:CYS:HB2	2.33	0.44
6:S:111:THR:HG23	6:S:266:VAL:HG23	1.99	0.44
1:B:418:ALA:HA	1:C:423:LEU:H	1.82	0.44
1:D:1206:ARG:NH2	1:D:1208:ARG:O	2.50	0.44
1:E:718:ALA:H	1:E:721:GLU:HB2	1.82	0.44
1:E:1208:ARG:HB2	1:E:1241:THR:HG22	2.00	0.44
1:F:397:ALA:HB3	1:F:1321:VAL:HG13	1.99	0.44
1:F:608:PRO:HA	1:F:611:ILE:HD12	2.00	0.44
1:I:82:THR:OG1	1:I:83:LYS:N	2.51	0.44
1:I:738:ASP:OD1	1:I:738:ASP:N	2.47	0.44
1:I:875:VAL:O	1:I:879:PHE:N	2.48	0.44
1:I:1034:VAL:HG22	1:I:1147:LEU:HD22	2.00	0.44
8:l:84:ILE:HB	9:o:3100:ARG:HD2	2.00	0.44
1:C:883:ARG:HG3	1:D:680:GLY:HA3	2.00	0.43
1:E:582:LEU:HD11	1:E:587:CYS:HB2	2.00	0.43
1:F:1029:PHE:HB3	1:F:1039:GLN:NE2	2.33	0.43
6:S:117:THR:HG23	6:S:261:ALA:HB2	2.00	0.43
8:l:84:ILE:O	8:l:88:GLU:N	2.47	0.43
1:D:197:LEU:HA	1:D:223:LEU:HD11	2.01	0.43
1:I:1004:GLN:NE2	1:I:1008:GLN:OE1	2.51	0.43
7:k:643:GLY:N	7:k:650:CYS:SG	2.83	0.43
1:B:645:ALA:HB1	1:B:678:LEU:HD21	1.99	0.43
1:C:876:LYS:HA	1:C:879:PHE:HD2	1.82	0.43
1:C:1131:LEU:HD23	1:C:1159:PRO:HG3	2.00	0.43
1:C:1168:CYS:HB2	1:C:1268:PRO:HD3	2.00	0.43
1:D:629:LEU:HG	1:D:835:VAL:HG13	2.00	0.43
1:D:1369:LEU:HA	1:D:1372:LEU:HD12	2.00	0.43
1:E:752:ARG:O	1:E:911:SER:OG	2.30	0.43
1:F:904:ARG:NH1	1:F:906:THR:OG1	2.51	0.43
1:F:1198:TYR:CZ	1:F:1203:CYS:HB2	2.53	0.43
1:I:1195:ASP:OD1	1:I:1195:ASP:N	2.46	0.43
7:k:531:LEU:HD23	7:k:534:LEU:HD12	2.00	0.43
1:B:56:ALA:HA	1:I:325:ALA:HB3	2.01	0.43
1:B:668:TYR:HB2	1:B:812:TYR:CG	2.54	0.43
1:B:765:TYR:HE1	1:B:783:LEU:HD13	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:967:ALA:O	1:B:971:ALA:N	2.48	0.43
1:B:1344:ARG:CZ	1:I:1355:GLU:HB2	2.48	0.43
1:C:492:ALA:H	1:C:992:PRO:HB2	1.82	0.43
1:C:1323:ASP:OD1	1:C:1323:ASP:N	2.51	0.43
1:D:233:PHE:HZ	1:D:243:ALA:HB1	1.84	0.43
1:D:950:GLN:HB3	1:D:953:GLU:HG3	2.01	0.43
1:E:272:ARG:HH11	1:E:374:LEU:HD12	1.83	0.43
1:E:392:TYR:HA	1:E:393:PRO:HD3	1.88	0.43
1:F:1032:SER:OG	1:F:1035:ALA:N	2.43	0.43
1:F:1131:LEU:HD23	1:F:1159:PRO:HG3	2.01	0.43
1:F:1135:ALA:HA	1:F:1263:LEU:HD22	1.98	0.43
1:I:1054:ARG:HH22	1:I:1123:GLY:H	1.66	0.43
3:K:228:LEU:HG	3:K:238:ASN:HA	2.00	0.43
2:U:33:GLN:HE21	2:U:35:ILE:HD13	1.83	0.43
7:k:56:PHE:HB3	7:k:78:ALA:HB3	2.00	0.43
1:D:219:LEU:O	1:D:223:LEU:N	2.50	0.43
1:D:305:THR:OG1	1:D:359:GLN:OE1	2.34	0.43
1:D:423:LEU:HD12	1:D:1357:HIS:NE2	2.34	0.43
1:D:615:ARG:NH1	1:D:1017:GLU:OE2	2.51	0.43
1:D:806:THR:HA	1:D:809:HIS:HB2	2.00	0.43
1:E:732:LEU:O	1:E:814:TYR:OH	2.30	0.43
1:F:857:PRO:HD3	1:F:885:VAL:HG13	2.00	0.43
1:I:733:PRO:HA	1:I:814:TYR:HE2	1.84	0.43
1:I:1209:ALA:HB2	1:I:1235:ALA:HB2	2.01	0.43
7:k:3:ALA:O	7:k:7:ASN:ND2	2.51	0.43
7:k:160:TYR:OH	7:k:402:TYR:O	2.35	0.43
1:B:886:VAL:HG13	1:B:890:ALA:HB3	2.00	0.43
1:D:721:GLU:O	1:D:1030:LYS:NZ	2.41	0.43
1:D:830:VAL:HG22	1:D:955:PHE:HD1	1.84	0.43
1:D:1048:PHE:HA	1:D:1192:VAL:HG13	1.99	0.43
1:E:420:ALA:HB2	1:F:424:VAL:HG21	1.99	0.43
1:E:696:HIS:HE1	1:E:1021:THR:HG21	1.84	0.43
1:E:751:HIS:CE1	1:E:754:CYS:HB2	2.53	0.43
1:F:440:LEU:HA	1:F:440:LEU:HD12	1.86	0.43
1:F:1125:LEU:HD12	1:F:1126:PRO:HD2	1.99	0.43
3:O:50:SER:O	3:O:70:ARG:NH2	2.50	0.43
1:C:629:LEU:HB3	1:C:839:LEU:HD21	2.00	0.43
1:C:675:VAL:HA	1:C:687:MET:HE1	2.01	0.43
1:D:1369:LEU:HD13	1:D:1372:LEU:HD12	1.99	0.43
1:E:99:VAL:O	1:E:118:ASN:ND2	2.46	0.43
1:E:490:TYR:OH	1:E:560:GLY:O	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:774:ALA:HA	1:E:903:GLU:HB3	2.01	0.43
1:I:639:HIS:HA	2:U:79:PHE:CE2	2.53	0.43
3:K:217:THR:HA	3:K:220:ILE:HG22	2.01	0.43
1:B:1339:ASP:HB2	1:B:1342:LEU:HG	2.01	0.43
1:C:83:LYS:HE2	1:C:1075:LEU:HD22	1.99	0.43
1:C:402:PHE:HB2	1:C:1054:ARG:HG2	2.01	0.43
1:E:816:LEU:HD23	1:E:820:PHE:HE2	1.83	0.43
2:G:76:GLN:OE1	2:G:98:TYR:OH	2.25	0.43
1:I:436:PRO:HA	1:I:437:PRO:HD3	1.80	0.43
1:I:611:ILE:H	1:I:611:ILE:HG13	1.65	0.43
1:I:637:ASN:HA	1:I:787:THR:HA	2.00	0.43
1:I:1246:ALA:HA	1:I:1253:GLY:HA3	2.00	0.43
7:k:516:GLN:HA	7:k:519:TRP:HD1	1.84	0.43
7:k:586:HIS:HD2	7:k:625:MET:HE2	1.83	0.43
1:B:457:ALA:HA	1:B:1187:PHE:CE2	2.54	0.43
1:B:1154:GLY:H	1:I:534:PRO:HB3	1.83	0.43
1:D:223:LEU:O	1:D:226:SER:OG	2.34	0.43
1:E:771:VAL:HG13	1:E:898:ALA:HA	2.00	0.43
1:F:920:THR:N	1:F:923:THR:OG1	2.39	0.43
1:F:933:LEU:HD11	1:F:958:LEU:HD23	2.00	0.43
1:F:1373:SER:OG	1:F:1374:LEU:N	2.52	0.43
6:S:318:GLN:OE1	6:S:416:THR:N	2.51	0.43
1:B:97:PHE:HD1	1:B:97:PHE:HA	1.72	0.43
1:B:629:LEU:HG	1:B:835:VAL:HG13	2.01	0.43
1:B:929:PHE:N	1:B:999:PHE:O	2.48	0.43
1:D:804:ASP:O	1:D:808:HIS:ND1	2.42	0.43
1:I:157:ARG:HA	1:I:160:ARG:HE	1.84	0.43
2:T:17:VAL:HB	2:T:56:GLY:HA3	2.01	0.43
7:k:427:THR:HG22	9:o:3116:HIS:CE1	2.53	0.43
1:B:13:TYR:O	1:B:17:MET:HG2	2.18	0.42
1:B:629:LEU:HD23	1:B:839:LEU:HG	2.01	0.42
1:B:1187:PHE:O	1:B:1257:TYR:OH	2.29	0.42
1:C:1072:ALA:HB3	1:C:1100:VAL:HB	2.01	0.42
1:E:37:ASP:OD1	1:E:37:ASP:N	2.51	0.42
1:E:876:LYS:HA	1:E:879:PHE:HB2	2.00	0.42
1:F:380:LEU:HD13	1:F:384:ILE:HD11	2.01	0.42
1:F:1357:HIS:O	1:F:1360:GLN:N	2.52	0.42
3:K:203:ARG:HH22	3:K:207:LEU:HD11	1.84	0.42
6:S:267:CYS:SG	6:S:268:SER:N	2.92	0.42
8:l:83:ARG:HB3	9:n:3099:THR:HG22	2.00	0.42
1:B:725:LEU:HA	1:B:1030:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:GLN:NE2	1:C:449:VAL:O	2.48	0.42
1:C:450:LEU:HD13	1:C:1124:ASN:HB2	2.01	0.42
1:D:863:HIS:CE1	1:D:865:LEU:HB2	2.54	0.42
1:E:441:PHE:HE1	1:E:451:ARG:HG3	1.84	0.42
1:F:77:VAL:HG22	1:F:266:HIS:CD2	2.54	0.42
1:F:485:ASN:O	1:F:487:TYR:N	2.48	0.42
3:K:272:TYR:HB2	3:O:161:ARG:HH21	1.83	0.42
7:k:253:ILE:O	9:o:3095:GLN:NE2	2.52	0.42
1:B:137:THR:HA	1:B:140:ILE:HD12	2.01	0.42
1:B:708:THR:OG1	1:B:723:ASN:ND2	2.50	0.42
1:C:157:ARG:HD2	1:C:157:ARG:HA	1.84	0.42
1:C:433:ARG:O	1:C:1359:THR:OG1	2.34	0.42
1:D:543:LEU:HB2	1:D:549:PHE:CE2	2.55	0.42
1:E:471:ALA:O	1:E:475:GLY:N	2.53	0.42
1:E:500:ASP:OD1	1:E:500:ASP:N	2.51	0.42
1:E:1115:VAL:HG11	1:E:1374:LEU:HD11	2.01	0.42
1:F:142:LEU:HD23	1:F:158:GLN:HA	2.01	0.42
1:F:578:VAL:N	1:F:581:ASN:OD1	2.42	0.42
1:F:1100:VAL:HG13	1:F:1102:LEU:HB2	2.01	0.42
1:I:756:ILE:HB	1:I:908:LEU:HD12	2.00	0.42
1:I:789:ALA:HB1	2:U:79:PHE:CG	2.54	0.42
3:K:63:LEU:O	3:K:67:TYR:N	2.44	0.42
2:M:33:GLN:HG2	2:M:35:ILE:H	1.84	0.42
7:k:487:LEU:O	7:k:491:GLY:N	2.43	0.42
7:k:688:GLY:O	7:k:692:CYS:N	2.52	0.42
1:B:946:ASP:HB3	1:C:676:THR:HG22	2.01	0.42
1:E:627:PHE:HD1	1:E:630:LEU:HD12	1.84	0.42
1:E:1138:LEU:HD12	1:E:1144:ALA:HA	2.00	0.42
1:F:470:ASP:HB3	1:F:922:SER:HB3	2.00	0.42
1:I:669:SER:OG	1:I:809:HIS:NE2	2.36	0.42
2:V:45:GLY:O	2:V:49:ALA:N	2.52	0.42
1:B:751:HIS:CE1	1:B:754:CYS:HB2	2.54	0.42
1:E:880:HIS:NE2	2:V:98:TYR:HB3	2.33	0.42
1:E:1040:LEU:HD23	1:E:1040:LEU:HA	1.84	0.42
1:F:840:GLN:H	1:F:840:GLN:HG2	1.51	0.42
1:F:1123:GLY:HA2	1:F:1183:ALA:HB3	2.02	0.42
1:I:198:LEU:HD22	1:I:1109:VAL:HG21	2.01	0.42
1:I:668:TYR:HB3	1:I:809:HIS:CD2	2.54	0.42
1:I:983:LEU:HD12	1:I:987:VAL:HG11	2.01	0.42
1:B:815:VAL:HA	1:B:1024:LEU:HD22	2.01	0.42
1:C:714:LEU:HD13	1:C:719:GLN:HE22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:804:ASP:HB3	1:D:808:HIS:CE1	2.54	0.42
1:E:68:VAL:HG21	1:E:384:ILE:HG22	2.02	0.42
1:E:656:TRP:HZ2	1:E:685:GLU:HG2	1.85	0.42
1:F:880:HIS:HE1	2:U:98:TYR:HB3	1.84	0.42
1:I:143:LEU:HD21	1:I:153:ILE:CG2	2.50	0.42
1:I:547:PHE:O	1:I:576:ARG:NE	2.53	0.42
1:I:595:ARG:HH22	1:I:1047:GLY:HA2	1.84	0.42
3:K:17:SER:O	3:K:21:ALA:N	2.49	0.42
3:K:67:TYR:HE2	3:K:117:VAL:HA	1.83	0.42
6:S:235:VAL:HB	6:S:323:GLU:HB3	2.02	0.42
7:k:119:ASP:H	7:k:122:GLY:HA2	1.83	0.42
9:o:3095:GLN:HA	9:o:3098:ARG:HE	1.85	0.42
1:B:124:ILE:HB	1:B:1100:VAL:HG22	2.01	0.42
1:B:185:LEU:HD21	1:B:279:VAL:HG11	2.01	0.42
1:B:1054:ARG:HH11	1:B:1122:MET:HB3	1.83	0.42
1:C:367:LEU:HD23	1:C:376:PHE:HA	2.00	0.42
1:E:623:TYR:OH	1:E:663:ALA:O	2.25	0.42
1:F:282:ALA:CB	1:F:382:LYS:HE3	2.34	0.42
1:F:884:VAL:HG12	1:F:886:VAL:HG23	2.01	0.42
1:F:1057:ARG:HB3	1:F:1119:VAL:HB	2.01	0.42
1:I:530:GLN:HG3	1:I:536:ASN:ND2	2.34	0.42
1:I:769:CYS:HB3	1:I:786:ASN:HD22	1.85	0.42
1:B:544:HIS:CD2	1:B:547:PHE:HD2	2.38	0.42
1:B:1082:ARG:HE	1:B:1082:ARG:HB3	1.49	0.42
1:C:622:SER:OG	1:D:676:THR:O	2.38	0.42
1:D:700:LEU:HD22	1:D:1025:MET:HG2	2.01	0.42
1:D:1206:ARG:HH12	1:D:1208:ARG:HD3	1.83	0.42
1:E:1067:GLU:HB2	1:E:1107:THR:HG23	2.02	0.42
7:k:90:LEU:HD12	7:k:234:PRO:CB	2.49	0.42
1:C:475:GLY:O	1:C:478:HIS:NE2	2.53	0.42
1:E:751:HIS:NE2	1:E:754:CYS:HB2	2.35	0.42
1:E:836:TYR:OH	1:E:902:ALA:N	2.51	0.42
1:F:367:LEU:HB3	1:F:374:LEU:HD11	2.02	0.42
1:F:417:ALA:HB2	1:F:1358:PHE:CE1	2.55	0.42
1:I:684:GLU:O	1:I:688:ALA:N	2.48	0.42
1:I:708:THR:HA	1:I:1038:HIS:CE1	2.55	0.42
2:T:89:ARG:HE	2:U:29:THR:HB	1.85	0.42
2:U:81:GLY:N	2:U:91:SER:OG	2.39	0.42
7:k:529:VAL:HG12	7:k:533:ASN:HD21	1.84	0.42
7:k:593:SER:OG	7:k:597:ASP:O	2.34	0.42
1:B:514:ALA:HB2	1:B:980:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:945:LEU:HD23	1:B:945:LEU:HA	1.83	0.42
1:B:950:GLN:HB2	2:Q:80:ALA:HB1	2.02	0.42
1:B:1057:ARG:HH22	1:B:1319:GLU:HB3	1.84	0.42
1:B:1201:ARG:O	1:B:1203:CYS:N	2.38	0.42
1:C:643:ALA:HB2	2:Q:78:MET:HE1	2.01	0.42
1:C:728:ASP:HA	1:C:729:PRO:HD3	1.88	0.42
1:C:962:ALA:HB3	1:C:1007:VAL:HG21	2.02	0.42
1:D:671:VAL:HG13	1:D:690:TYR:HD1	1.85	0.42
1:E:1289:LEU:HD13	1:E:1292:LEU:HB2	2.02	0.42
1:I:272:ARG:HA	1:I:273:PRO:HD3	1.92	0.42
1:I:1072:ALA:HB3	1:I:1100:VAL:H	1.84	0.42
7:k:394:LYS:HE2	8:m:63:ALA:HB1	2.02	0.42
1:B:156:HIS:NE2	1:I:340:GLN:HB2	2.34	0.41
1:B:750:ARG:HD3	1:B:750:ARG:HH11	1.73	0.41
1:C:917:GLY:HA3	1:C:1034:VAL:HG23	2.02	0.41
1:E:1118:PRO:HG3	1:E:1374:LEU:HD13	2.02	0.41
3:K:18:ARG:O	3:K:22:ALA:N	2.45	0.41
7:k:582:ASP:O	7:k:655:ARG:NH2	2.53	0.41
1:B:293:LEU:H	1:B:293:LEU:HG	1.48	0.41
1:B:530:GLN:HG3	1:B:536:ASN:HD21	1.84	0.41
1:C:83:LYS:HG2	1:C:1075:LEU:HB2	2.03	0.41
1:C:528:ALA:HA	1:C:531:PHE:HB2	2.03	0.41
1:C:604:HIS:O	1:C:1022:TYR:OH	2.36	0.41
1:E:272:ARG:NH1	1:E:374:LEU:HB2	2.35	0.41
1:E:1125:LEU:HD11	1:E:1157:LEU:HG	2.02	0.41
1:F:1075:LEU:HD13	1:F:1075:LEU:HA	1.92	0.41
1:B:87:LEU:HB2	1:B:1097:ARG:HH21	1.84	0.41
1:B:429:HIS:HA	1:B:430:PRO:HD3	1.77	0.41
1:B:920:THR:N	1:B:923:THR:OG1	2.42	0.41
1:B:991:PRO:HG2	1:B:994:LEU:HD12	2.01	0.41
1:B:1054:ARG:NH1	1:B:1122:MET:HB3	2.36	0.41
1:D:657:ASN:HA	1:D:660:ARG:HH12	1.85	0.41
3:O:178:VAL:HG13	3:O:185:ARG:HG2	2.00	0.41
7:k:62:THR:H	7:k:71:THR:HB	1.84	0.41
1:B:1221:ASP:O	1:B:1225:LEU:HB2	2.20	0.41
1:C:606:MET:HB2	1:C:611:ILE:HD11	2.02	0.41
1:C:638:GLU:OE2	1:C:677:TYR:OH	2.32	0.41
1:C:1125:LEU:HD13	1:C:1156:ARG:HH11	1.85	0.41
1:D:278:LEU:HD23	1:D:278:LEU:HA	1.90	0.41
1:E:733:PRO:HG2	1:E:736:VAL:HG22	2.02	0.41
1:F:531:PHE:HE2	1:F:1194:THR:HG22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:596:GLY:O	1:F:600:GLY:N	2.54	0.41
1:F:1244:PRO:O	1:F:1251:SER:OG	2.31	0.41
1:I:212:THR:O	1:I:215:ALA:N	2.36	0.41
1:I:606:MET:HG3	1:I:696:HIS:CG	2.56	0.41
1:B:638:GLU:OE1	1:B:801:ARG:NH2	2.53	0.41
1:B:873:ASN:HA	2:Q:92:PHE:CD2	2.56	0.41
1:B:1202:PRO:HB3	1:B:1332:TYR:HA	2.02	0.41
1:C:274:VAL:HG22	1:C:374:LEU:HD22	2.02	0.41
1:C:422:ASP:OD1	1:C:422:ASP:N	2.52	0.41
1:C:534:PRO:HB3	1:D:1154:GLY:HA3	2.02	0.41
1:C:770:ASN:H	1:C:773:THR:HB	1.85	0.41
1:D:470:ASP:OD1	1:D:470:ASP:N	2.51	0.41
1:D:918:ALA:O	1:D:923:THR:OG1	2.24	0.41
1:D:1056:ASP:HA	1:D:1120:THR:HG21	2.03	0.41
1:E:423:LEU:HD12	1:E:1357:HIS:CE1	2.55	0.41
1:E:770:ASN:H	1:E:773:THR:HB	1.84	0.41
1:E:1223:ILE:H	1:E:1223:ILE:HG13	1.63	0.41
1:F:826:CYS:HB2	1:F:966:GLY:H	1.85	0.41
1:F:946:ASP:N	1:F:946:ASP:OD1	2.53	0.41
1:F:951:ASN:ND2	1:F:972:ASN:O	2.54	0.41
1:I:872:ALA:H	2:T:76:GLN:HG2	1.85	0.41
1:I:1039:GLN:O	1:I:1042:THR:OG1	2.39	0.41
3:K:47:ALA:O	3:K:50:SER:OG	2.29	0.41
6:S:268:SER:C	6:S:271:GLN:HE21	2.29	0.41
7:k:65:HIS:HE1	7:k:470:PHE:N	2.19	0.41
1:B:278:LEU:O	1:B:378:GLU:N	2.53	0.41
1:C:450:LEU:HD23	1:C:450:LEU:HA	1.90	0.41
1:C:624:PRO:HB3	1:C:882:GLY:HA3	2.01	0.41
1:E:1008:GLN:HA	1:E:1011:ARG:HG2	2.03	0.41
1:I:143:LEU:H	1:I:143:LEU:HG	1.61	0.41
1:I:866:HIS:CD2	1:I:868:ALA:H	2.39	0.41
1:I:903:GLU:HG2	1:I:904:ARG:H	1.85	0.41
1:I:1084:GLU:HA	1:I:1089:VAL:HB	2.03	0.41
3:K:32:VAL:O	3:K:73:ALA:N	2.51	0.41
7:k:536:ARG:O	7:k:540:GLY:N	2.51	0.41
1:B:413:MET:O	1:C:433:ARG:NH1	2.45	0.41
1:B:1357:HIS:HD1	1:B:1358:PHE:H	1.69	0.41
1:E:404:LEU:HD23	1:E:440:LEU:HD23	2.03	0.41
1:F:780:ASP:OD1	1:F:780:ASP:N	2.53	0.41
1:F:1374:LEU:H	1:F:1374:LEU:HG	1.68	0.41
1:I:656:TRP:CG	1:I:686:CYS:HG	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:191:ASP:HA	3:K:195:LEU:HD13	2.02	0.41
7:k:514:PRO:HD3	8:m:17:ARG:HB2	2.02	0.41
1:B:526:MET:N	1:B:529:GLU:OE1	2.50	0.41
1:B:788:GLN:HG2	1:B:790:ARG:H	1.86	0.41
1:B:1083:HIS:HB2	1:B:1084:GLU:H	1.72	0.41
1:C:336:LEU:HD23	1:C:336:LEU:HA	1.90	0.41
1:C:441:PHE:HE1	1:C:451:ARG:HG3	1.85	0.41
1:D:436:PRO:HA	1:D:437:PRO:HD3	1.92	0.41
1:D:746:ALA:HA	1:D:751:HIS:CD2	2.56	0.41
1:E:185:LEU:HD12	1:E:185:LEU:HA	1.90	0.41
1:F:269:THR:HG22	1:F:300:ALA:HB2	2.01	0.41
1:I:142:LEU:HD13	1:I:142:LEU:HA	1.74	0.41
1:I:735:LEU:HD12	1:I:813:TYR:CZ	2.56	0.41
8:l:62:ALA:O	8:l:66:LEU:N	2.47	0.41
1:B:91:ASN:H	1:B:126:ARG:HH22	1.69	0.41
1:C:348:ARG:NE	1:D:170:GLN:OE1	2.54	0.41
1:C:519:ARG:HG3	1:C:538:ASN:ND2	2.36	0.41
1:C:520:TRP:HZ3	1:C:988:PRO:HD2	1.85	0.41
1:C:545:PRO:HG3	1:C:1245:TRP:CD2	2.56	0.41
1:D:104:ILE:HG12	1:E:178:ARG:HB3	2.03	0.41
1:E:91:ASN:O	1:E:126:ARG:NH2	2.54	0.41
1:E:197:LEU:HA	1:E:223:LEU:HD11	2.02	0.41
1:E:720:ALA:HB1	1:E:727:ARG:HG3	2.02	0.41
1:E:746:ALA:HA	1:E:751:HIS:CD2	2.56	0.41
1:E:826:CYS:HB2	1:E:966:GLY:H	1.86	0.41
1:E:960:VAL:HA	1:E:994:LEU:HD13	2.03	0.41
1:F:579:ASN:OD1	1:F:579:ASN:N	2.52	0.41
1:F:776:PHE:HD1	1:F:903:GLU:HA	1.85	0.41
1:I:893:THR:OG1	1:I:894:LEU:N	2.52	0.41
1:I:942:PRO:HB3	1:I:969:HIS:CD2	2.56	0.41
1:I:1271:SER:HB3	1:I:1274:PHE:HB2	2.03	0.41
2:M:25:LEU:HD21	2:M:57:GLN:HG2	2.03	0.41
2:U:54:LEU:HD23	2:U:54:LEU:HA	1.94	0.41
1:B:280:THR:O	1:B:392:TYR:OH	2.34	0.41
1:B:656:TRP:CD2	1:B:686:CYS:HB3	2.56	0.41
1:B:714:LEU:HB2	1:B:722:LEU:HD11	2.02	0.41
1:B:1223:ILE:H	1:B:1223:ILE:HG13	1.50	0.41
1:D:608:PRO:HA	1:D:611:ILE:HD12	2.03	0.41
1:D:1125:LEU:HD23	1:D:1184:VAL:HG22	2.03	0.41
1:E:639:HIS:HA	2:G:79:PHE:HE2	1.86	0.41
1:E:1204:ASN:HB3	1:E:1206:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:617:ALA:HB2	1:F:661:CYS:HB3	2.01	0.41
1:F:985:ARG:NH1	1:I:705:ASP:OD2	2.54	0.41
1:I:776:PHE:HD1	1:I:903:GLU:HA	1.85	0.41
3:K:90:LEU:O	3:K:316:ARG:NE	2.54	0.41
2:T:76:GLN:O	2:T:96:ARG:NH2	2.43	0.41
7:k:63:ARG:NH1	7:k:475:GLU:OE2	2.54	0.41
7:k:152:GLU:OE2	7:k:390:HIS:ND1	2.33	0.41
7:k:473:ALA:HB2	8:m:57:ALA:HB3	2.02	0.41
1:C:577:VAL:HG12	1:C:578:VAL:HG13	2.03	0.40
1:D:339:MET:HE3	1:E:159:LEU:HD23	2.03	0.40
1:F:742:LEU:O	1:F:746:ALA:N	2.47	0.40
1:I:644:LEU:HG	1:I:893:THR:HG22	2.03	0.40
1:I:746:ALA:HA	1:I:751:HIS:CD2	2.56	0.40
3:O:58:PRO:HB2	3:O:63:LEU:HG	2.04	0.40
7:k:546:PHE:O	7:k:549:THR:OG1	2.36	0.40
1:D:998:TYR:O	1:D:1003:ARG:NH2	2.49	0.40
1:E:473:VAL:HA	1:E:476:VAL:HG12	2.03	0.40
1:E:580:GLY:HA2	1:E:592:ARG:HH12	1.86	0.40
1:E:1249:ARG:HG2	1:E:1250:PHE:CD2	2.56	0.40
1:F:57:LEU:HD22	1:F:57:LEU:HA	1.95	0.40
1:F:818:PRO:HA	1:F:821:SER:HB3	2.02	0.40
1:F:1017:GLU:O	1:F:1021:THR:OG1	2.30	0.40
1:I:490:TYR:OH	1:I:560:GLY:O	2.35	0.40
1:I:734:PRO:HB3	1:I:960:VAL:HG21	2.02	0.40
1:I:1053:VAL:HG12	1:I:1272:PRO:HB2	2.03	0.40
3:O:32:VAL:HG13	3:O:46:VAL:HG13	2.03	0.40
3:O:177:ASN:OD1	3:O:188:LEU:N	2.37	0.40
7:k:62:THR:HA	7:k:130:ALA:HA	2.04	0.40
1:B:207:ASN:OD1	1:B:208:GLY:N	2.53	0.40
1:B:700:LEU:HD11	1:B:1021:THR:HG22	2.03	0.40
1:B:751:HIS:NE2	1:B:754:CYS:HB2	2.36	0.40
1:E:194:PRO:HD2	1:E:197:LEU:HD12	2.02	0.40
1:I:847:ILE:HD12	1:I:847:ILE:HA	1.98	0.40
1:I:1268:PRO:HB2	1:I:1311:PHE:HD1	1.86	0.40
7:k:13:LEU:HB3	7:k:14:THR:H	1.71	0.40
1:B:502:GLN:HE22	1:B:970:VAL:HG22	1.85	0.40
1:C:194:PRO:HG2	1:C:197:LEU:HB2	2.04	0.40
1:C:246:ALA:HA	1:C:249:VAL:HG12	2.04	0.40
1:C:707:PHE:HA	1:C:1042:THR:HG21	2.04	0.40
1:C:1061:GLU:OE2	1:C:1116:ARG:NH1	2.54	0.40
1:F:227:PHE:O	1:F:231:SER:OG	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:423:LEU:HD12	1:F:1357:HIS:CD2	2.56	0.40
1:I:399:ASP:OD2	1:I:1055:GLN:NE2	2.52	0.40
1:I:765:TYR:HA	1:I:782:ARG:HG3	2.04	0.40
6:S:236:HIS:HA	6:S:323:GLU:HG2	2.03	0.40
7:k:505:PHE:CD1	8:m:26:PHE:HB2	2.57	0.40
7:k:514:PRO:HG3	8:m:17:ARG:HG3	2.03	0.40
7:k:532:GLU:OE2	8:m:38:LEU:HD21	2.22	0.40
1:B:188:LEU:HD12	1:B:188:LEU:HA	1.90	0.40
1:D:545:PRO:HG3	1:D:1245:TRP:CD2	2.57	0.40
1:D:693:LEU:HD21	1:D:812:TYR:HE1	1.87	0.40
1:E:97:PHE:HZ	1:E:1102:LEU:HD12	1.86	0.40
1:E:671:VAL:HG13	1:E:690:TYR:HD1	1.87	0.40
1:I:1229:HIS:HE1	1:I:1248:GLN:HA	1.86	0.40
3:O:73:ALA:HB1	3:O:85:ALA:HB1	2.02	0.40
2:T:83:ALA:HB2	2:T:91:SER:HB3	2.04	0.40
7:k:181:LEU:HG	7:k:184:ALA:HB3	2.03	0.40
8:l:6:PRO:HB3	8:m:24:ARG:HB2	2.03	0.40
8:l:63:ALA:HB1	9:o:3118:ARG:NE	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1356/1374 (99%)	1200 (88%)	150 (11%)	6 (0%)	30	67
1	C	1356/1374 (99%)	1223 (90%)	130 (10%)	3 (0%)	43	77
1	D	1356/1374 (99%)	1205 (89%)	146 (11%)	5 (0%)	30	67
1	E	1345/1374 (98%)	1193 (89%)	151 (11%)	1 (0%)	48	82
1	F	1347/1374 (98%)	1162 (86%)	183 (14%)	2 (0%)	48	82
1	I	1311/1374 (95%)	1114 (85%)	193 (15%)	4 (0%)	36	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	99/112 (88%)	91 (92%)	8 (8%)	0	100	100
2	M	99/112 (88%)	93 (94%)	6 (6%)	0	100	100
2	Q	99/112 (88%)	96 (97%)	3 (3%)	0	100	100
2	T	99/112 (88%)	92 (93%)	7 (7%)	0	100	100
2	U	99/112 (88%)	89 (90%)	10 (10%)	0	100	100
2	V	99/112 (88%)	90 (91%)	9 (9%)	0	100	100
3	K	291/318 (92%)	253 (87%)	38 (13%)	0	100	100
3	O	301/318 (95%)	274 (91%)	27 (9%)	0	100	100
6	S	267/466 (57%)	216 (81%)	50 (19%)	1 (0%)	30	67
7	k	539/702 (77%)	506 (94%)	32 (6%)	1 (0%)	43	77
8	l	92/585 (16%)	84 (91%)	8 (9%)	0	100	100
8	m	78/585 (13%)	72 (92%)	6 (8%)	0	100	100
9	n	45/3122 (1%)	44 (98%)	1 (2%)	0	100	100
9	o	45/3122 (1%)	45 (100%)	0	0	100	100
All	All	10323/18134 (57%)	9142 (89%)	1158 (11%)	23 (0%)	44	77

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1223	ILE
1	C	1223	ILE
1	D	1085	THR
1	D	1223	ILE
1	E	1223	ILE
1	I	206	ASP
1	C	1084	GLU
1	F	454	MET
6	S	120	CYS
1	B	1202	PRO
1	D	1107	THR
1	B	1203	CYS
1	F	1286	HIS
1	I	213	ARG
1	I	1013	SER
1	B	1201	ARG
1	B	1222	VAL
1	C	1202	PRO

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Mol	Chain	Res	Type
1	D	920	THR
1	I	575	TRP
1	D	1222	VAL
7	k	17	PRO
1	B	1134	GLY

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	B	1014/1080 (94%)	998 (98%)	16 (2%)	55	69
1	C	1018/1080 (94%)	1010 (99%)	8 (1%)	73	78
1	D	1020/1080 (94%)	1012 (99%)	8 (1%)	73	78
1	E	1018/1080 (94%)	1017 (100%)	1 (0%)	88	88
1	F	968/1080 (90%)	961 (99%)	7 (1%)	76	80
1	I	970/1080 (90%)	952 (98%)	18 (2%)	50	66
2	G	78/88 (89%)	78 (100%)	0	100	100
2	M	78/88 (89%)	78 (100%)	0	100	100
2	Q	78/88 (89%)	78 (100%)	0	100	100
2	T	78/88 (89%)	78 (100%)	0	100	100
2	U	78/88 (89%)	78 (100%)	0	100	100
2	V	78/88 (89%)	78 (100%)	0	100	100
3	K	195/264 (74%)	193 (99%)	2 (1%)	68	76
3	O	214/264 (81%)	214 (100%)	0	100	100
6	S	181/365 (50%)	179 (99%)	2 (1%)	65	74
7	k	426/529 (80%)	419 (98%)	7 (2%)	55	69
8	l	78/451 (17%)	78 (100%)	0	100	100
8	m	64/451 (14%)	64 (100%)	0	100	100
9	n	41/2370 (2%)	41 (100%)	0	100	100
9	o	41/2370 (2%)	41 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7716/14072 (55%)	7647 (99%)	69 (1%)	68 77

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	97	PHE
1	B	162	ILE
1	B	199	LEU
1	B	293	LEU
1	B	674	ILE
1	B	742	LEU
1	B	1082	ARG
1	B	1084	GLU
1	B	1085	THR
1	B	1089	VAL
1	B	1127	GLN
1	B	1128	ASN
1	B	1133	ARG
1	B	1222	VAL
1	B	1225	LEU
1	B	1334	ILE
1	C	104	ILE
1	C	162	ILE
1	C	205	LEU
1	C	469	ILE
1	C	957	VAL
1	C	1107	THR
1	C	1282	ILE
1	C	1334	ILE
1	D	99	VAL
1	D	395	VAL
1	D	736	VAL
1	D	756	ILE
1	D	1107	THR
1	D	1133	ARG
1	D	1222	VAL
1	D	1282	ILE
1	E	674	ILE
1	F	57	LEU
1	F	68	VAL
1	F	195	LEU
1	F	302	VAL

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Mol	Chain	Res	Type
1	F	732	LEU
1	F	957	VAL
1	F	1334	ILE
1	I	135	LEU
1	I	142	LEU
1	I	143	LEU
1	I	205	LEU
1	I	209	ARG
1	I	210	LEU
1	I	244	ILE
1	I	380	LEU
1	I	384	ILE
1	I	469	ILE
1	I	512	ARG
1	I	574	THR
1	I	732	LEU
1	I	894	LEU
1	I	906	THR
1	I	1093	LEU
1	I	1282	ILE
1	I	1356	THR
3	K	227	LEU
3	K	295	VAL
6	S	143	LEU
6	S	255	VAL
7	k	13	LEU
7	k	258	GLU
7	k	259	GLU
7	k	261	LEU
7	k	265	GLN
7	k	266	ARG
7	k	414	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (187) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	63	ASN
1	B	168	ASN
1	B	256	GLN
1	B	347	ASN
1	B	389	ASN
1	B	507	ASN

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Mol	Chain	Res	Type
1	B	511	GLN
1	B	544	HIS
1	B	658	ASN
1	B	717	GLN
1	B	723	ASN
1	B	724	HIS
1	B	866	HIS
1	B	950	GLN
1	B	972	ASN
1	B	1008	GLN
1	B	1018	ASN
1	B	1038	HIS
1	B	1039	GLN
1	B	1045	HIS
1	B	1079	GLN
1	B	1083	HIS
1	B	1090	ASN
1	B	1095	GLN
1	B	1124	ASN
1	B	1128	ASN
1	B	1149	ASN
1	B	1161	GLN
1	B	1170	GLN
1	B	1329	GLN
1	B	1360	GLN
1	C	63	ASN
1	C	164	GLN
1	C	168	ASN
1	C	485	ASN
1	C	544	HIS
1	C	639	HIS
1	C	658	ASN
1	C	717	GLN
1	C	751	HIS
1	C	777	ASN
1	C	866	HIS
1	C	950	GLN
1	C	1127	GLN
1	C	1155	ASN
1	C	1179	HIS
1	C	1204	ASN
1	C	1286	HIS

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Mol	Chain	Res	Type
1	C	1310	GLN
1	C	1360	GLN
1	D	32	HIS
1	D	110	HIS
1	D	118	ASN
1	D	156	HIS
1	D	164	GLN
1	D	202	GLN
1	D	340	GLN
1	D	439	GLN
1	D	507	ASN
1	D	536	ASN
1	D	544	HIS
1	D	657	ASN
1	D	696	HIS
1	D	702	GLN
1	D	717	GLN
1	D	880	HIS
1	D	895	GLN
1	D	1004	GLN
1	D	1018	ASN
1	D	1124	ASN
1	D	1127	GLN
1	D	1141	ASN
1	E	32	HIS
1	E	110	HIS
1	E	130	ASN
1	E	156	HIS
1	E	183	GLN
1	E	202	GLN
1	E	410	ASN
1	E	463	HIS
1	E	502	GLN
1	E	511	GLN
1	E	544	HIS
1	E	657	ASN
1	E	658	ASN
1	E	696	HIS
1	E	723	ASN
1	E	751	HIS
1	E	770	ASN
1	E	777	ASN

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Mol	Chain	Res	Type
1	E	869	ASN
1	E	975	ASN
1	E	997	ASN
1	E	1018	ASN
1	E	1045	HIS
1	E	1124	ASN
1	E	1128	ASN
1	E	1170	GLN
1	E	1197	ASN
1	E	1329	GLN
1	F	100	HIS
1	F	164	GLN
1	F	256	GLN
1	F	266	HIS
1	F	658	ASN
1	F	696	HIS
1	F	702	GLN
1	F	717	GLN
1	F	723	ASN
1	F	880	HIS
1	F	919	ASN
1	F	1004	GLN
1	F	1008	GLN
1	F	1018	ASN
1	F	1039	GLN
1	F	1062	ASN
1	F	1090	ASN
1	F	1155	ASN
1	F	1286	HIS
1	F	1310	GLN
2	G	7	HIS
2	G	16	ASN
2	G	33	GLN
2	G	38	ASN
2	G	42	HIS
1	I	207	ASN
1	I	286	GLN
1	I	315	ASN
1	I	419	HIS
1	I	448	GLN
1	I	502	GLN
1	I	544	HIS

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Mol	Chain	Res	Type
1	I	581	ASN
1	I	604	HIS
1	I	631	GLN
1	I	658	ASN
1	I	696	HIS
1	I	723	ASN
1	I	724	HIS
1	I	777	ASN
1	I	880	HIS
1	I	900	ASN
1	I	950	GLN
1	I	972	ASN
1	I	1004	GLN
1	I	1008	GLN
1	I	1141	ASN
1	I	1179	HIS
1	I	1204	ASN
1	I	1264	ASN
1	I	1310	GLN
1	I	1329	GLN
3	K	25	GLN
3	K	48	HIS
3	K	110	ASN
3	K	281	HIS
2	M	5	GLN
2	M	7	HIS
2	M	16	ASN
2	M	44	HIS
3	O	233	GLN
3	O	307	GLN
2	Q	7	HIS
2	Q	16	ASN
2	Q	47	GLN
6	S	109	HIS
6	S	188	ASN
6	S	210	HIS
6	S	242	HIS
6	S	271	GLN
6	S	275	HIS
2	T	5	GLN
2	T	16	ASN
2	T	38	ASN

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Mol	Chain	Res	Type
2	U	16	ASN
2	U	33	GLN
2	U	68	HIS
2	V	33	GLN
2	V	42	HIS
7	k	61	GLN
7	k	65	HIS
7	k	506	GLN
7	k	533	ASN
8	l	72	GLN
8	l	93	HIS
8	m	68	ASN
9	o	3097	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.

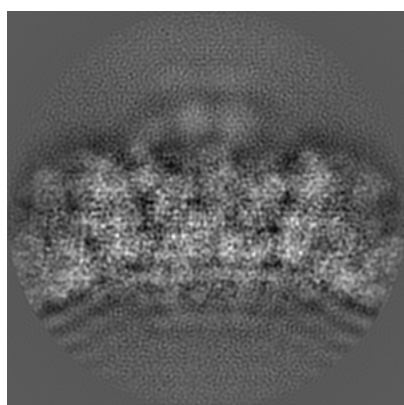
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30123. These allow visual inspection of the internal detail of the map and identification of artifacts.

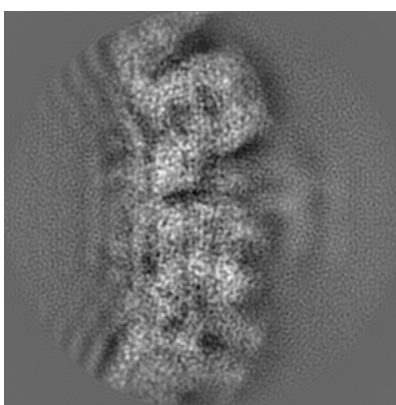
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

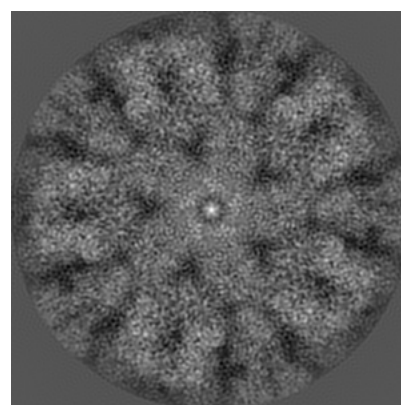
6.1.1 Primary map



X



Y

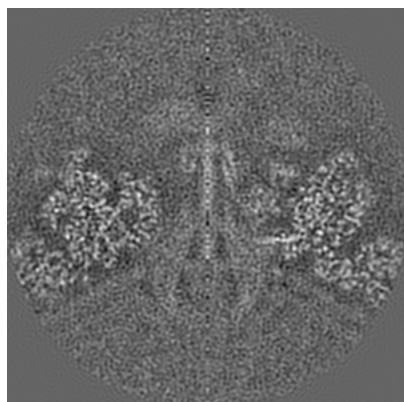


Z

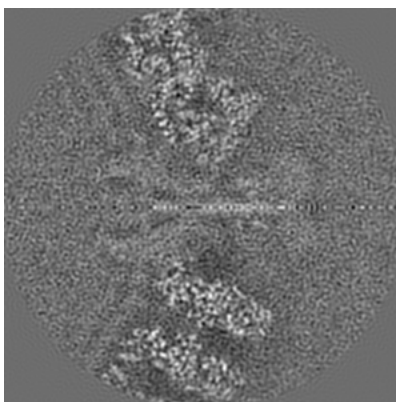
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

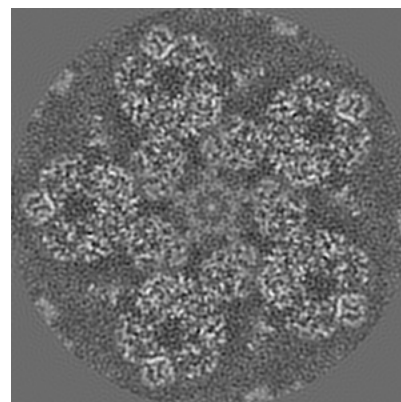
6.2.1 Primary map



X Index: 175



Y Index: 175

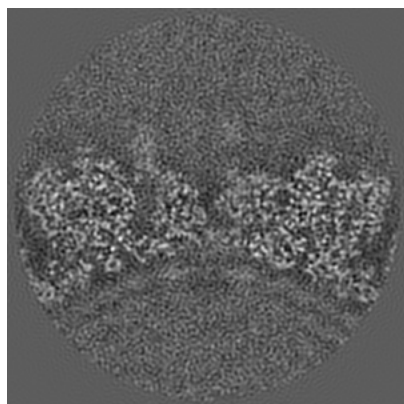


Z Index: 175

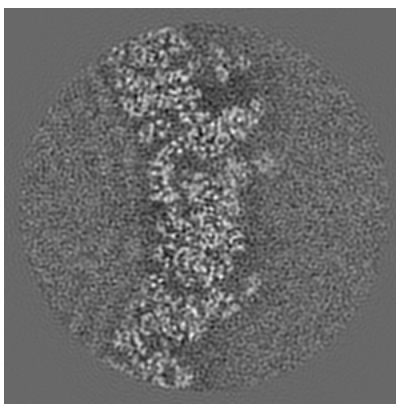
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

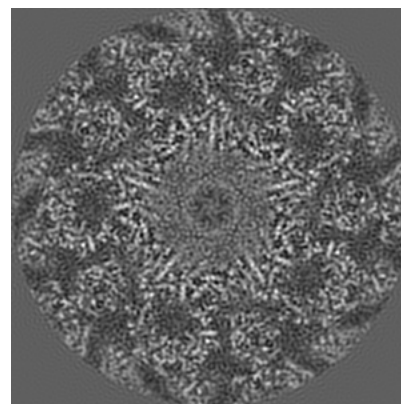
6.3.1 Primary map



X Index: 123



Y Index: 103

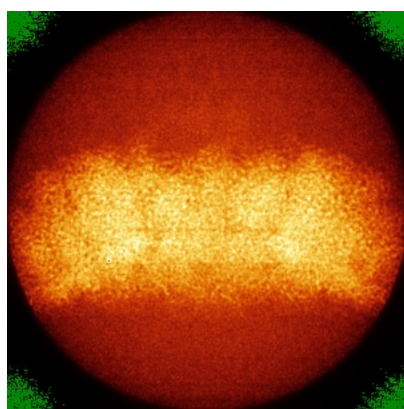


Z Index: 147

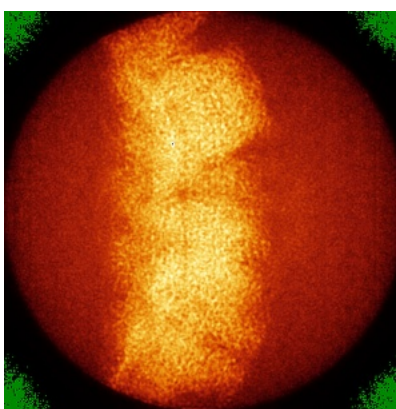
The images above show the largest variance slices of the map in three orthogonal directions.

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

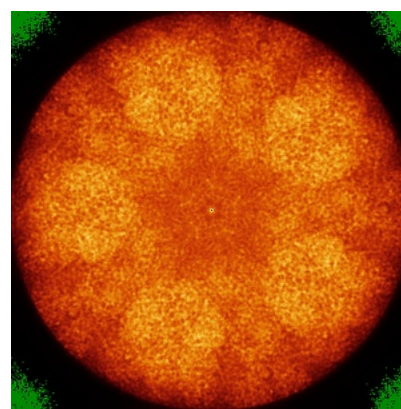
6.4.1 Primary map



X



Y

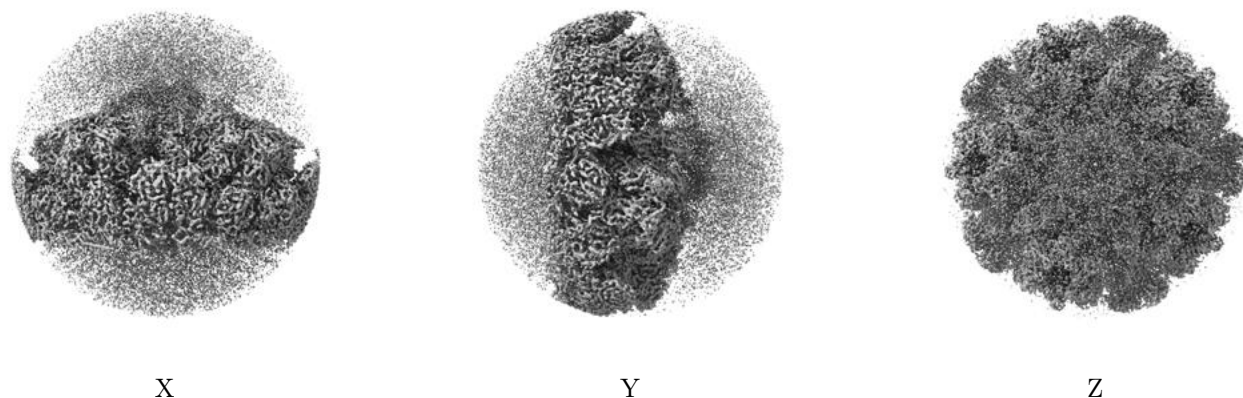


Z

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

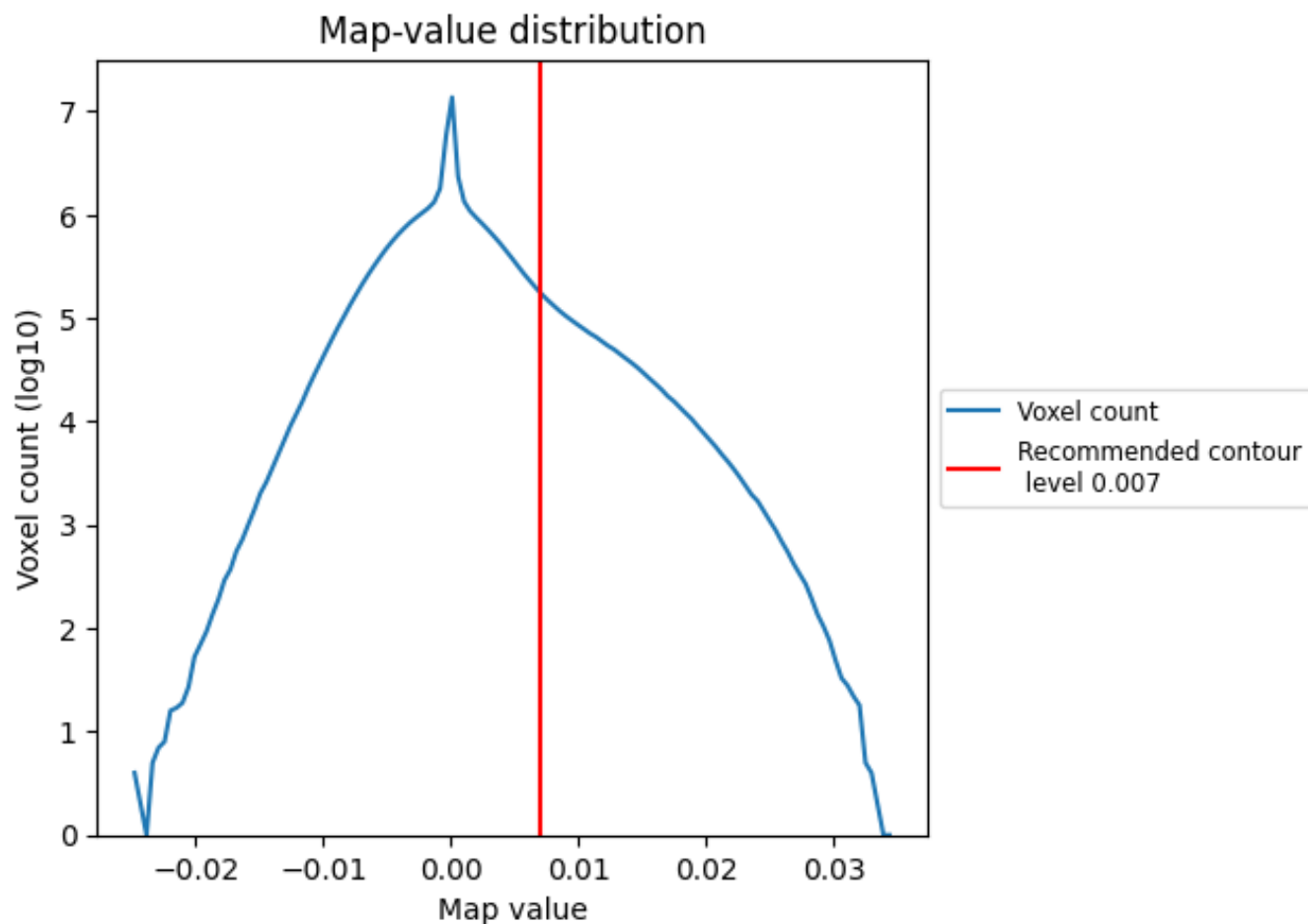
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

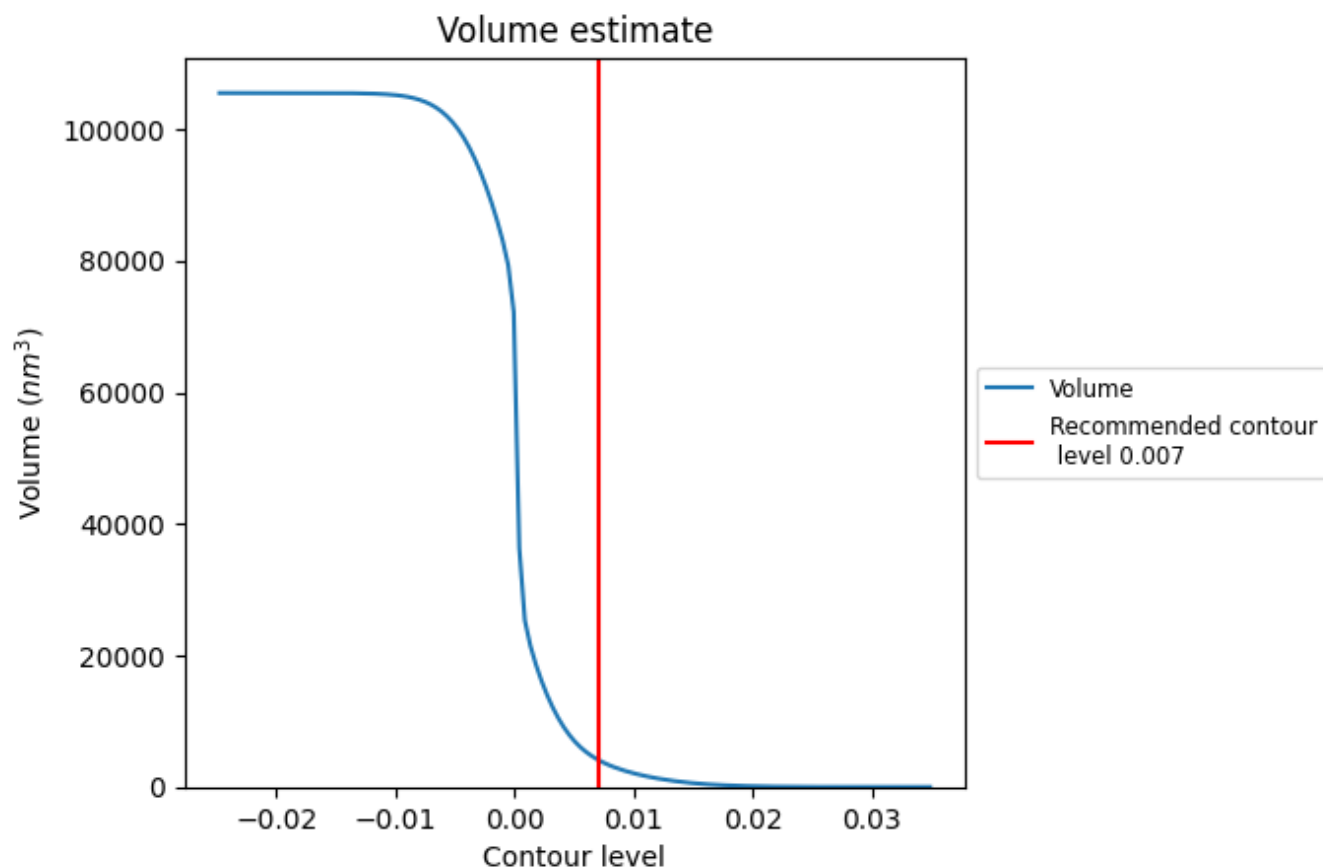
This section contains the results of statistical analysis of the map.

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.

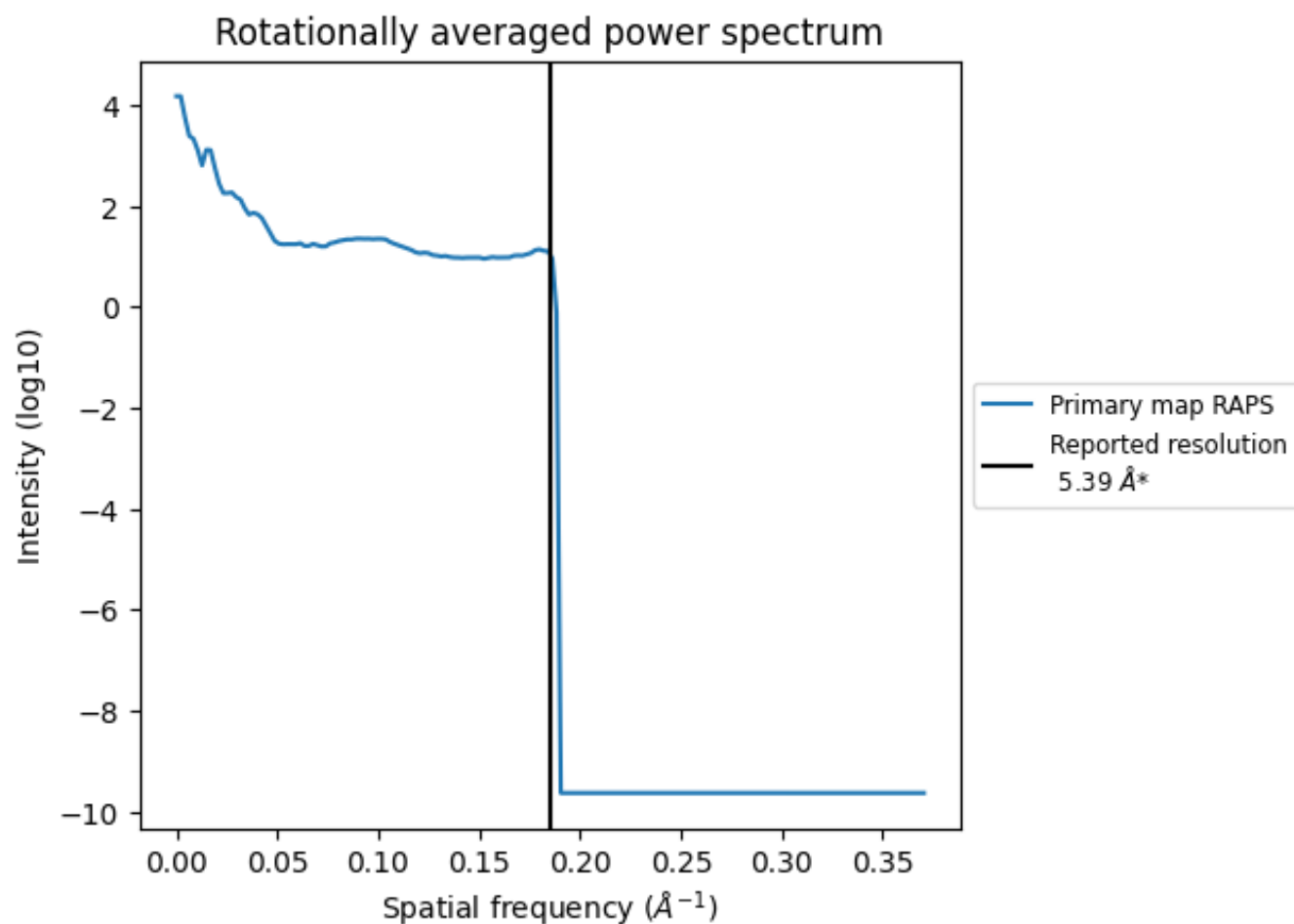
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4131 nm³; this corresponds to an approximate mass of 3731 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 0.186 Å⁻¹

8 Fourier-Shell correlation ⓘ

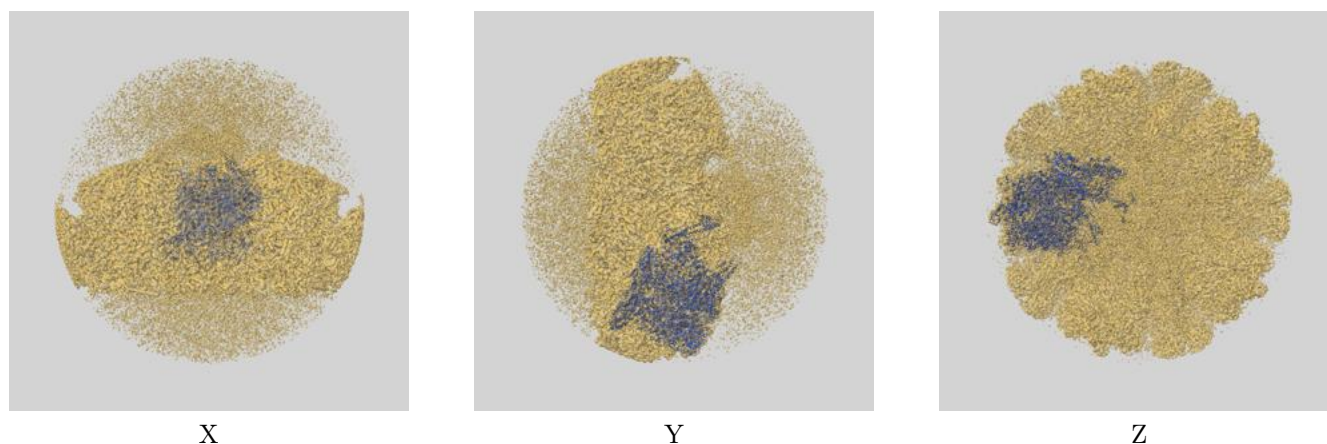
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

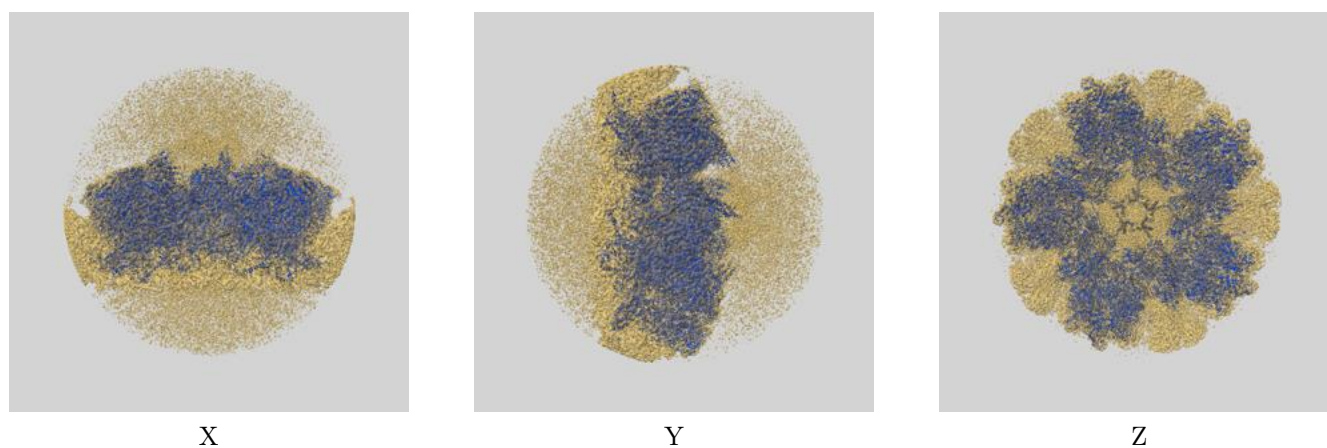
This section contains information regarding the fit between EMDB map EMD-30123 and PDB model 6M6G. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

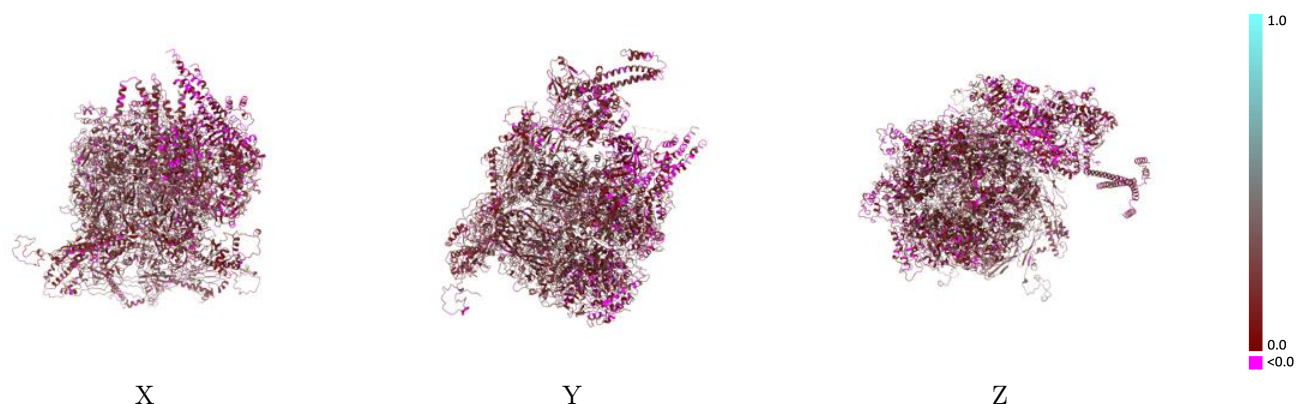


9.1.2 Map-model assembly overlay [i](#)



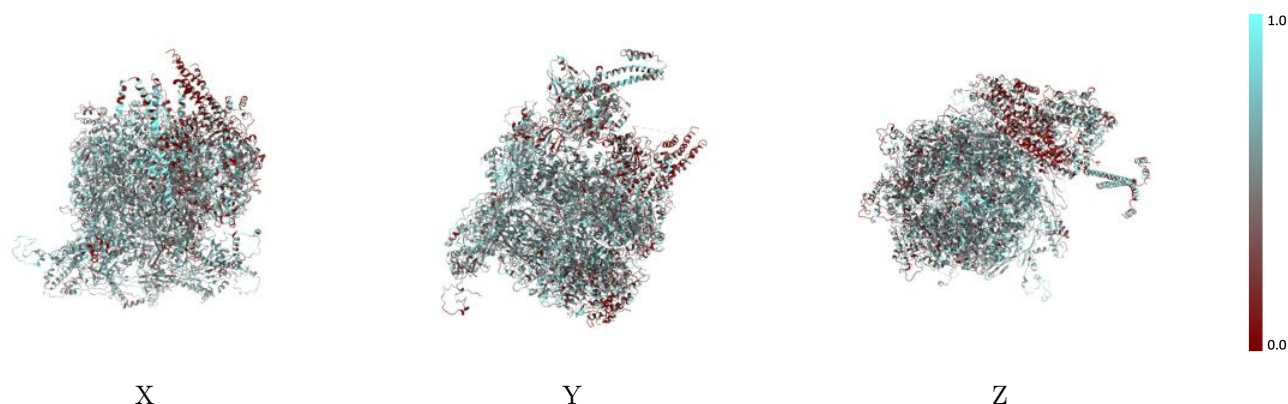
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



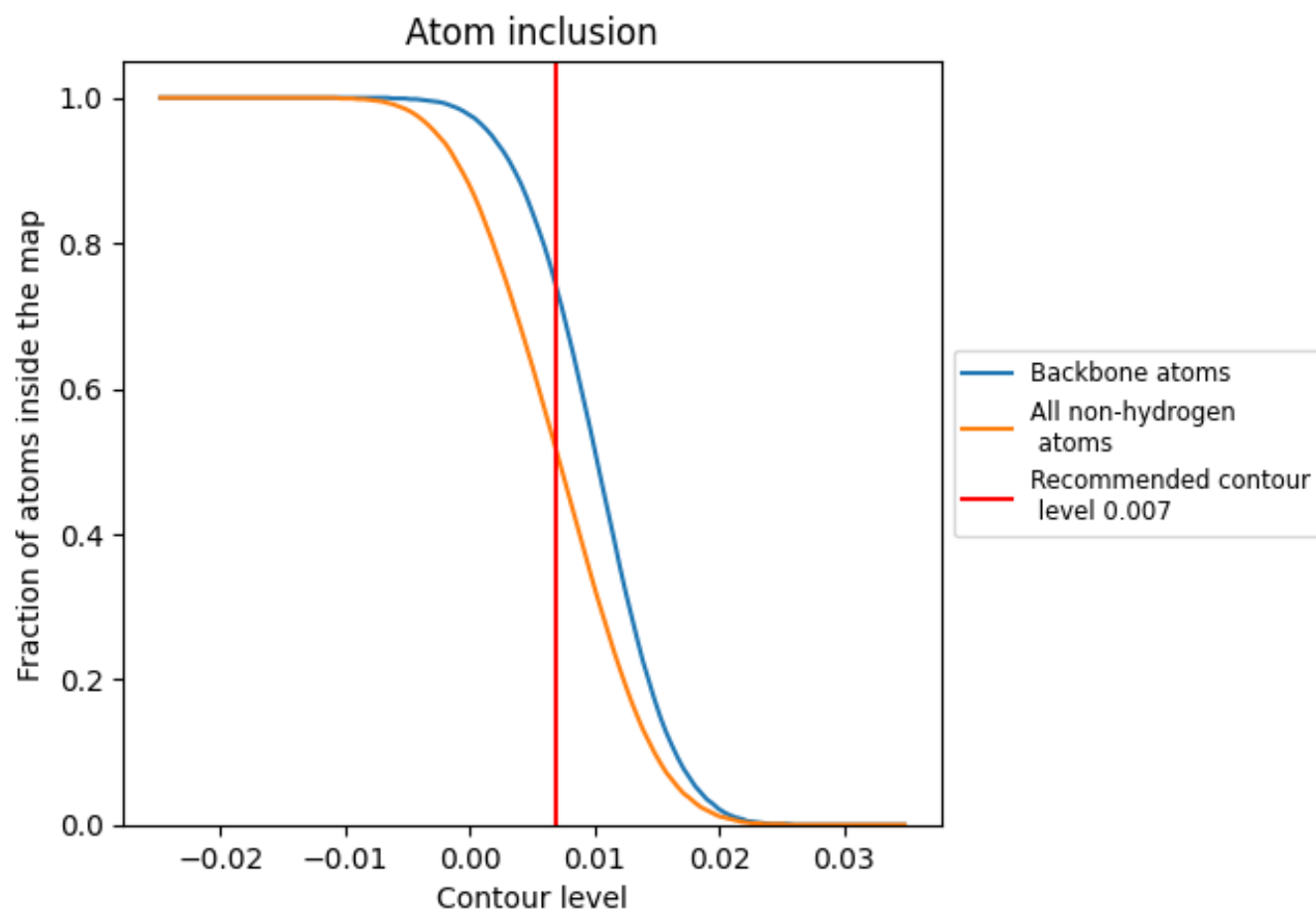
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 51% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5120	 0.1880
B	 0.5500	 0.2060
C	 0.5180	 0.2010
D	 0.5360	 0.2040
E	 0.5700	 0.2130
F	 0.5680	 0.2140
G	 0.3720	 0.1420
I	 0.5580	 0.2110
K	 0.4620	 0.1560
L	 0.5480	 0.1710
M	 0.3460	 0.1140
O	 0.4340	 0.1720
P	 0.5380	 0.1790
Q	 0.2810	 0.0660
S	 0.3840	 0.1140
T	 0.3210	 0.0940
U	 0.3780	 0.1160
V	 0.4520	 0.1580
k	 0.3670	 0.0930
l	 0.3540	 0.1190
m	 0.3510	 0.1150
n	 0.1300	 0.0470
o	 0.2070	 0.0270

