



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 06:54 PM EST

PDB ID : 6W2E
EMDB ID : EMD-21526
Title : Structures of Capsid and Capsid-Associated Tegument Complex inside the Epstein-Barr Virus
Authors : Liu, W.; Cui, Y.X.; Wang, C.Y.; Li, Z.H.; Gong, D.Y.; Dai, X.H.; Bi, G.Q.; Sun, R.; Zhou, Z.H.
Deposited on : 2020-03-05
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

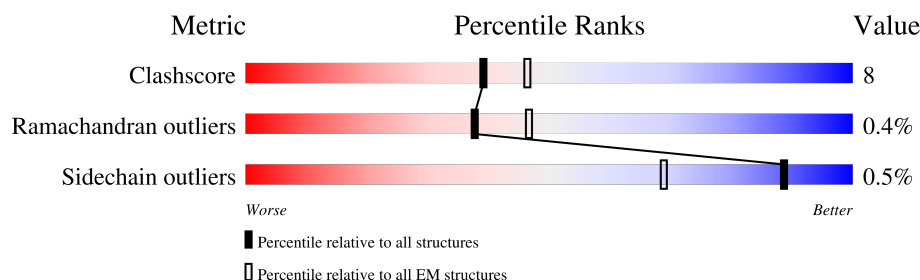
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	J	1381	
1	K	1381	
1	N	1381	
1	O	1381	
2	v	507	
3	w	570	
3	x	570	
4	y	3149	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	z	3149	
5	Z	176	
5	a	176	
5	d	176	
5	e	176	
6	f	364	
6	h	364	
7	k	301	
7	m	301	
7	p	301	
7	r	301	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 62525 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	J	1305	Total	C	N	O	S	0	0
			10252	6507	1779	1908	58		
1	K	1381	Total	C	N	O	S	0	0
			10832	6868	1884	2018	62		
1	N	1362	Total	C	N	O	S	0	0
			10683	6777	1854	1991	61		
1	O	1299	Total	C	N	O	S	0	0
			10194	6468	1771	1895	60		

- Molecule 2 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	v	293	Total	C	N	O	S	0	0
			2288	1472	398	407	11		

- Molecule 3 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	w	68	Total	C	N	O	S	0	0
			549	332	106	108	3		
3	x	68	Total	C	N	O	S	0	0
			549	332	106	108	3		

- Molecule 4 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	y	37	Total	C	N	O	0	0
			317	200	64	53		
4	z	37	Total	C	N	O	0	0
			317	200	64	53		

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

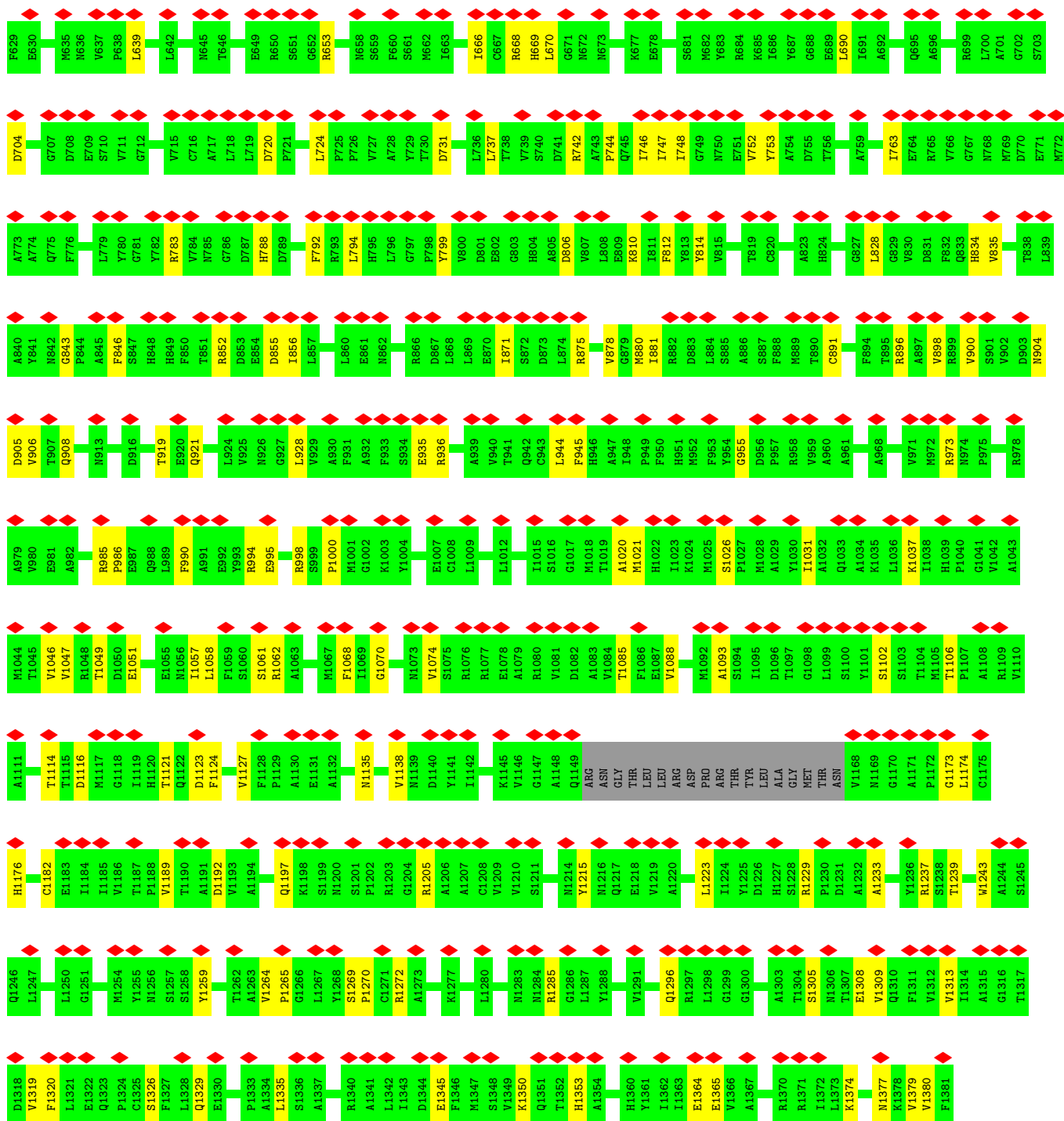
Mol	Chain	Residues	Atoms					AltConf	Trace
5	Z	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
5	a	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
5	d	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
5	e	77	Total	C	N	O	S	0	0
			649	411	121	115	2		

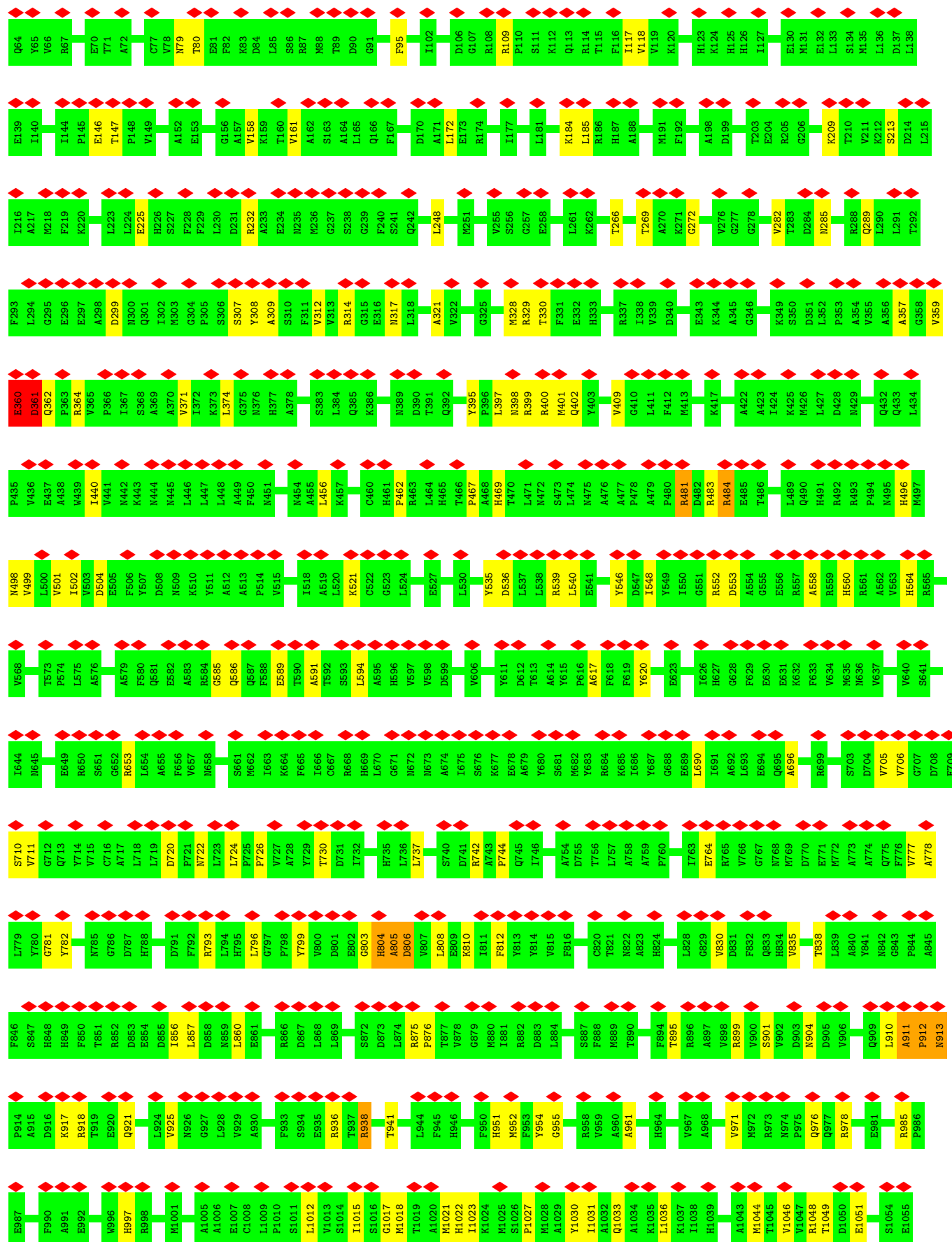
- Molecule 6 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	253	Total	C	N	O	S	0	0
			1992	1291	333	361	7		
6	h	336	Total	C	N	O	S	0	0
			2604	1667	458	471	8		

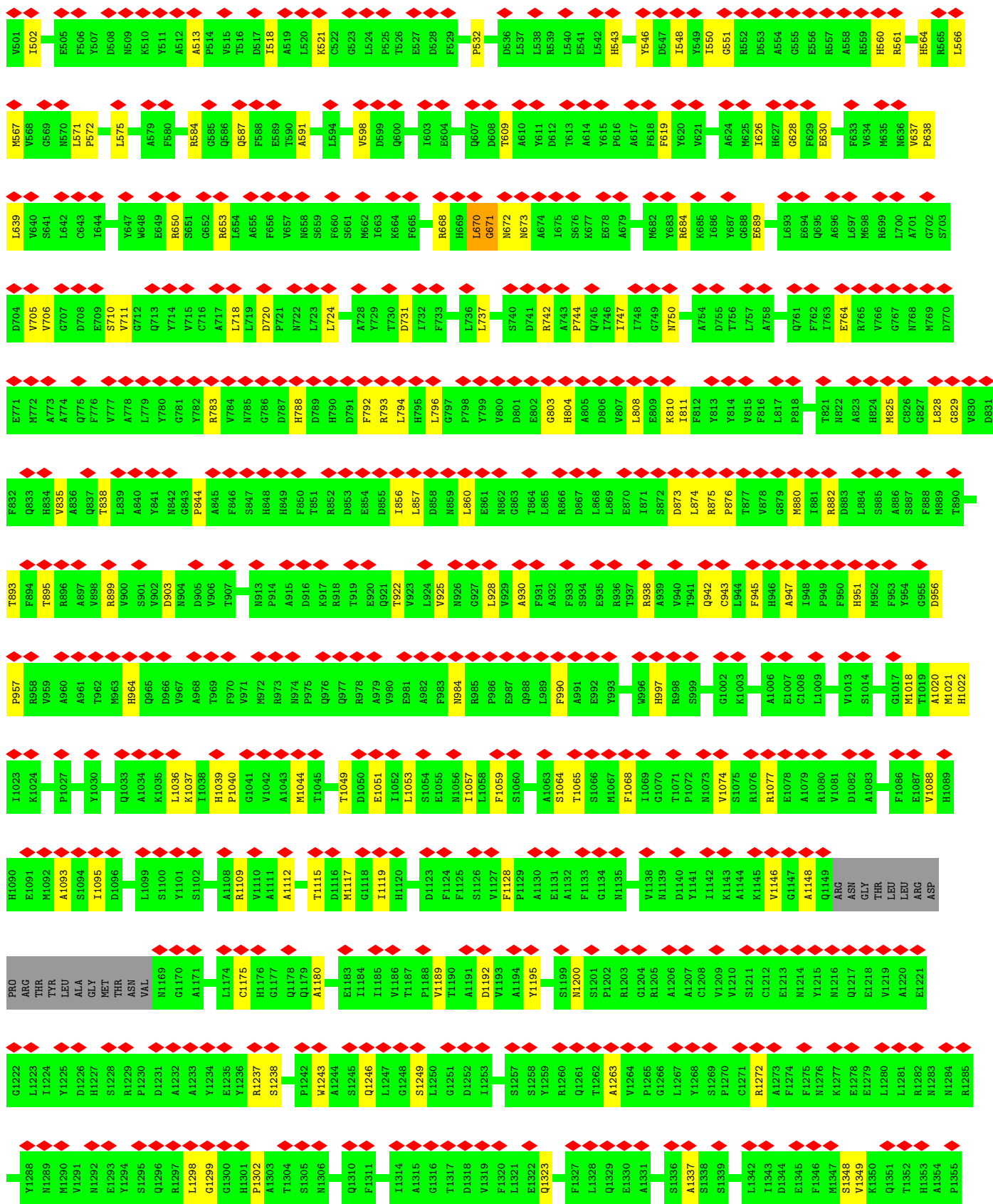
- Molecule 7 is a protein called Triplex capsid protein 2.

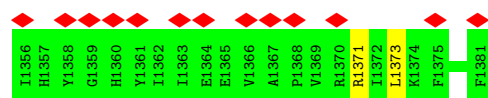
Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
7	m	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
7	p	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
7	r	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		



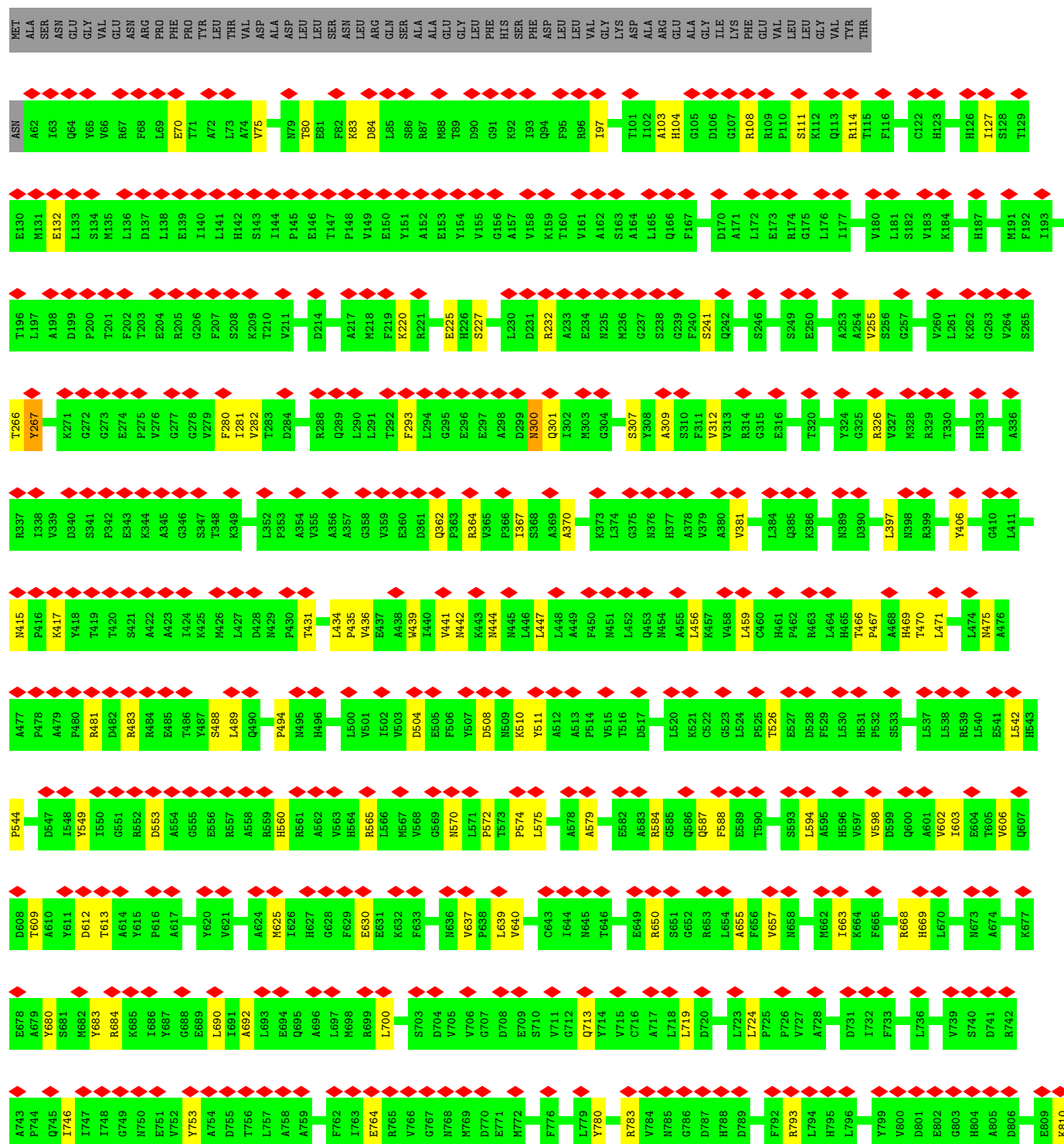
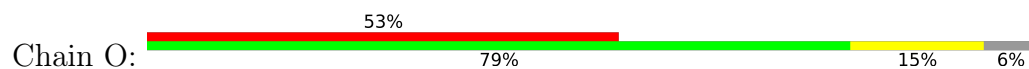


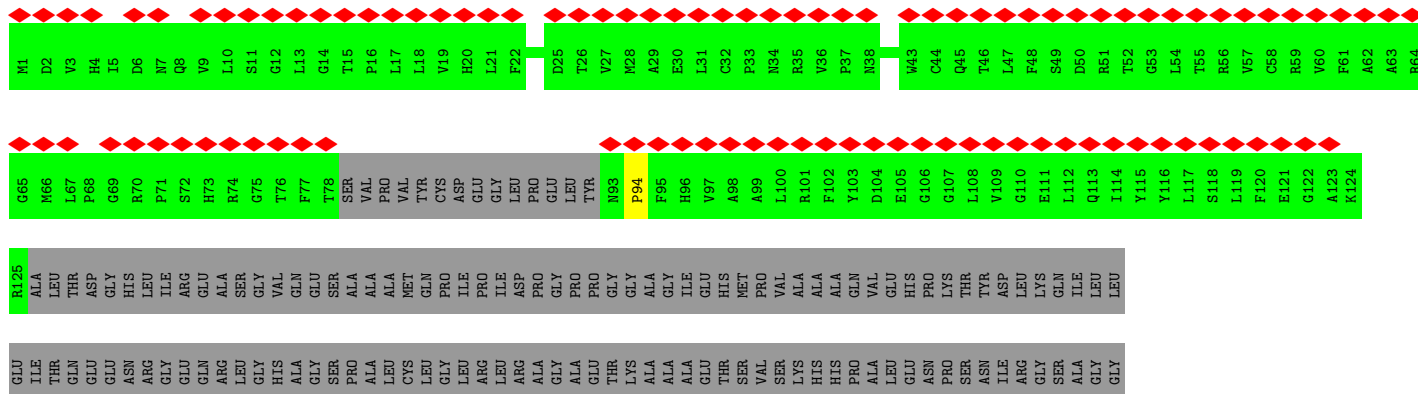
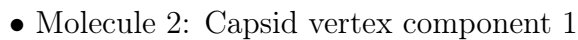


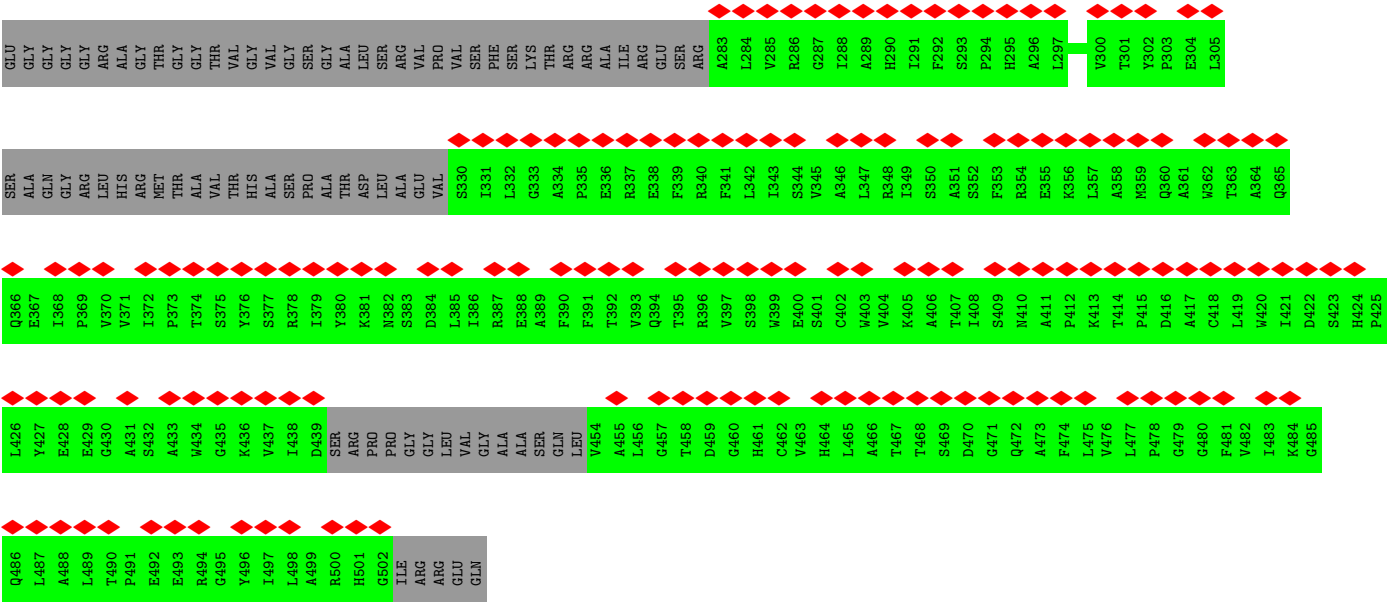




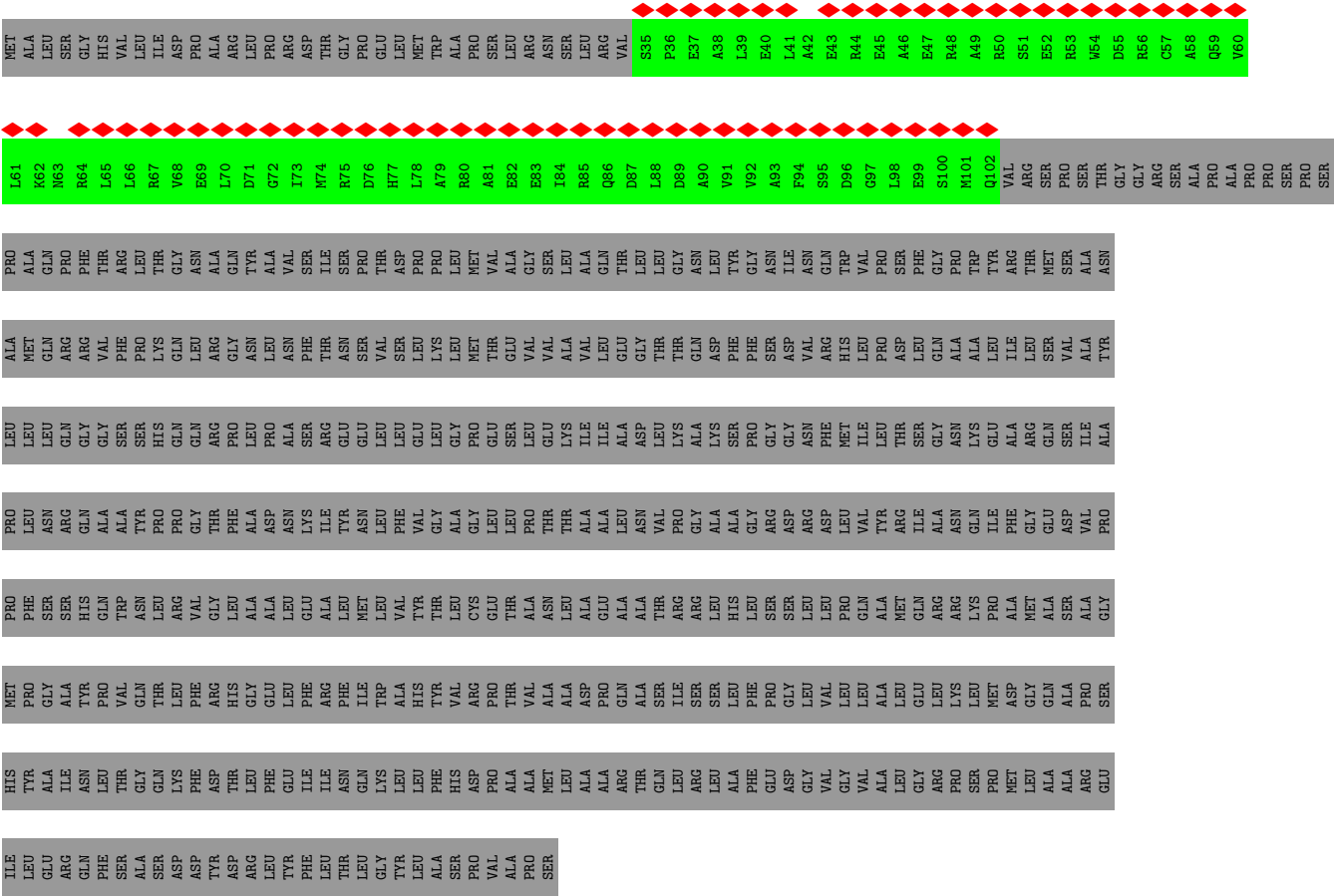
• Molecule 1: Major capsid protein







• Molecule 3: Capsid vertex component 2



• Molecule 3: Capsid vertex component 2





R3121	PRO	LYS	THR	LEU	GLY
F3122	SER	GLU	ALA	ALA	ARG
V3123	VAL	ALA	ALA	ALA	GLU
S3124	VAL	PRO	PRO	PRO	GLU
Q3125	THR	PRO	SER	HIS	GLU
R3126	GLN	SER	ALA	THR	ALA
R3127	PHE	ALA	ALA	PRO	ILE
R3128	ILE	SER	SER	VAL	ARG
K3129	ILE	GLN	PRO	GLY	PRO
L3130	ASP	LEU	PRO	SER	ALA
E3131	ILE	PRO	VAL	LEU	THR
R3132	ILE	MET	SER	PRO	ARG
S3133	ARG	PRO	LEU	ARG	LEU
T3134	GLU	LYS	VAL	GLN	THR
H3135	VAL	CYS	VAL	LYS	ALA
H3136	VAL	ASP	SER	THR	VAL
R3136	THR	SER	ARG	GLN	GLY
L3137	GLY	MET	GLN	ALA	LEU
I3138	SER	TYR	GLN	GLN	ARG
A3139	THR	TYR	SER	PRO	PRO
D3140	SER	PRO	PRO	GLN	ALA
L3141	ASP	SER	ALA	ASP	PRO
E3142	LEU	GLY	ILE	ALA	VAL
R3143	VAL	SER	PRO	ALA	VAL
L3144	VAL	ALA	LEU	ALA	ALA
K3145	PRO	ARG	PRO	LEU	GLY
F3146	SER	TYR	PRO	PRO	ALA
L3147	GLY	PRO	MET	THR	ALA
Y3148	ALA	ALA	HIS	PRO	ALA
L3149	PRO	PRO	SER	THR	ALA
	SER	PHE	GLY	ALA	PHE
	LEU	SER	ALA	ALA	ASP
	ALA	SER	ARG	ARG	ASP
	PRO	GLN	PRO	PRO	PRO
	GLU	SER	GLU	VAL	GLY
	GLN	VAL	VAL	PRO	GLU
	ASP	ALA	ARG	LYS	ALA
	LEU	SER	LEU	ALA	PRO
	ARG	PRO	SER	THR	SER
	TYR	ALA	GLN	GLY	GLY
	SER	PRO	TYR	ALA	PHE
	LEU	SER	ARG	LEU	PRO
	THR	SER	HIS	ALA	ILE
	LEU	ASP	ALA	ALA	PRO
	S3113	GLN	GLY	GLY	GLN
Q3114	THR	THR	PRO	ALA	ALA
A3115	THR	THR	GLN	ARG	PRO
S3116	LEU	LEU	THR	PRO	ALA
R3117	LEU	LEU	TYR	ARG	LEU
V3118	ASP	ASN	THR	VAL	GLY
L3119	THR	THR	ARG	PRO	SER
S3120					GLY

- Molecule 4: Large tegument protein deneddylase

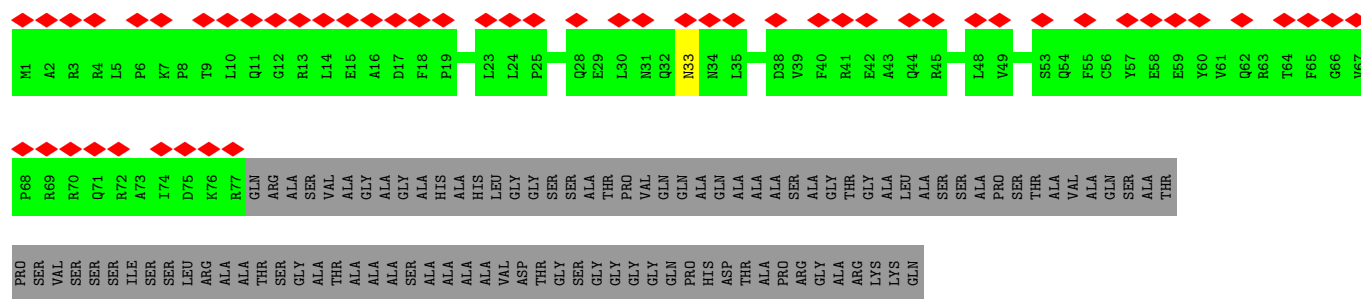
Chain z:  99%

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

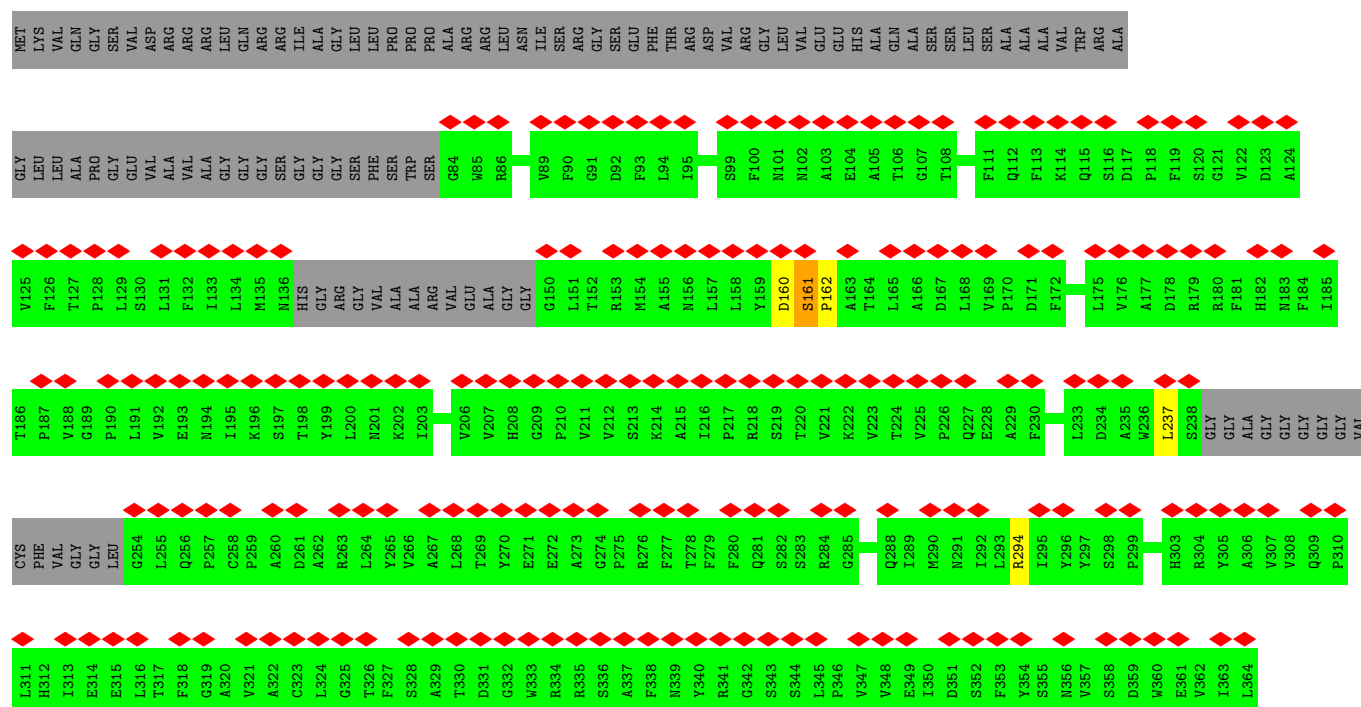




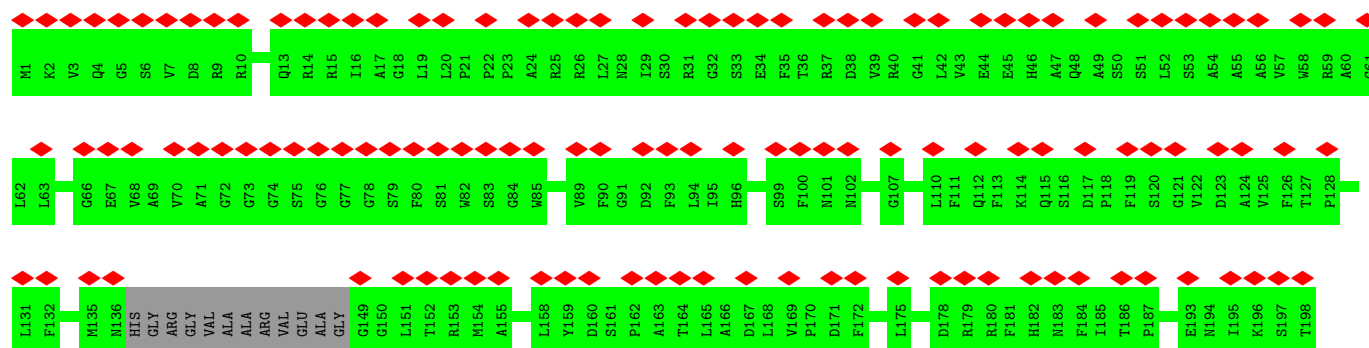
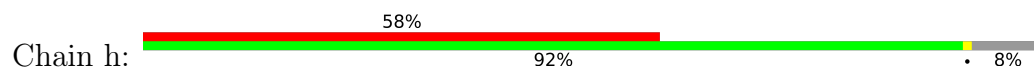


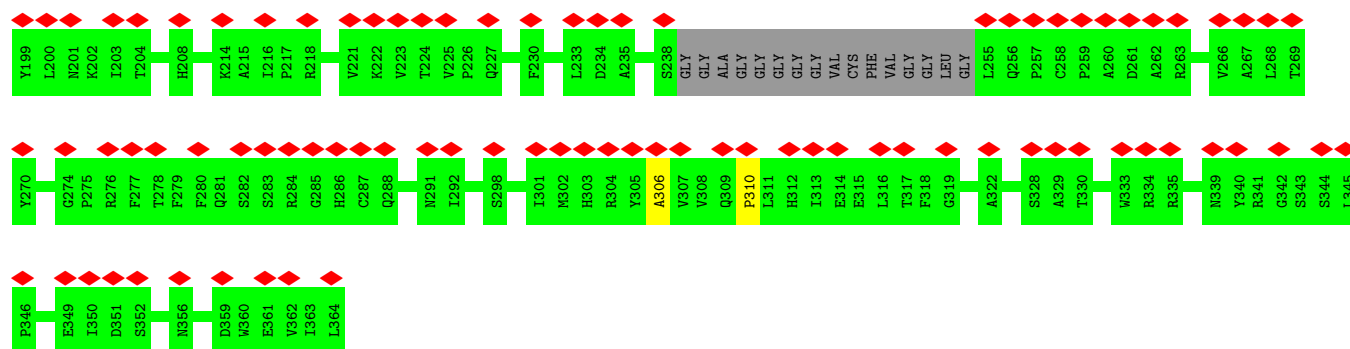


• Molecule 6: Triplex capsid protein 1

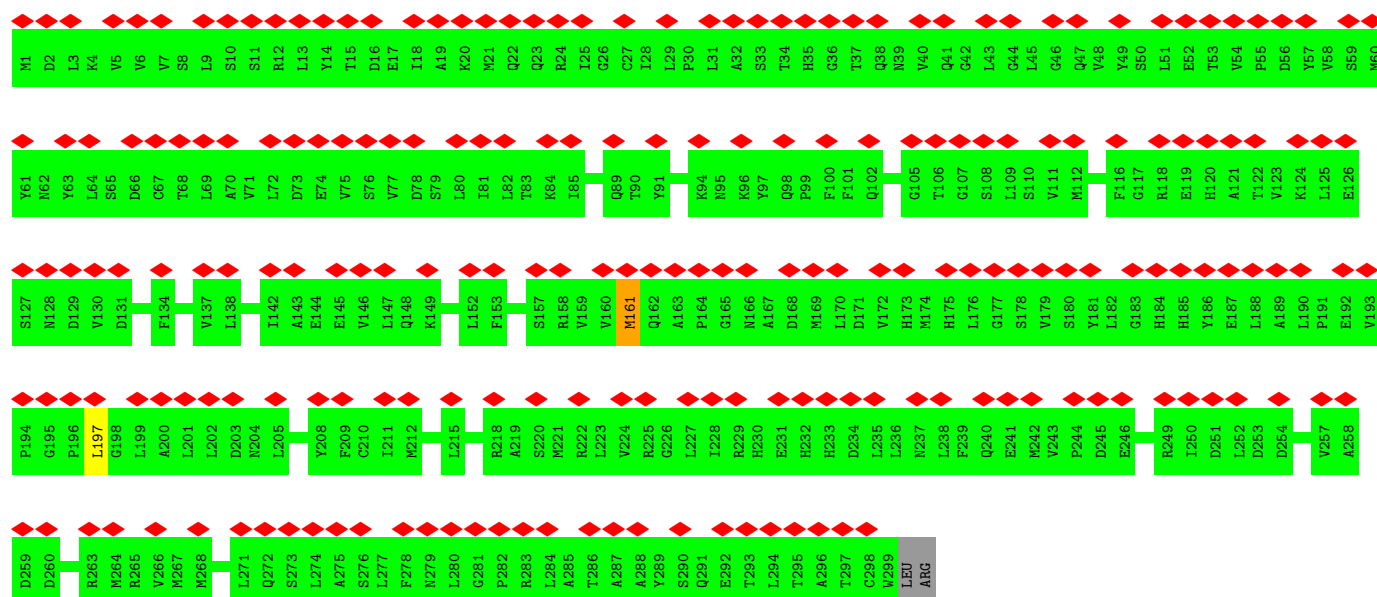


• Molecule 6: Triplex capsid protein 1

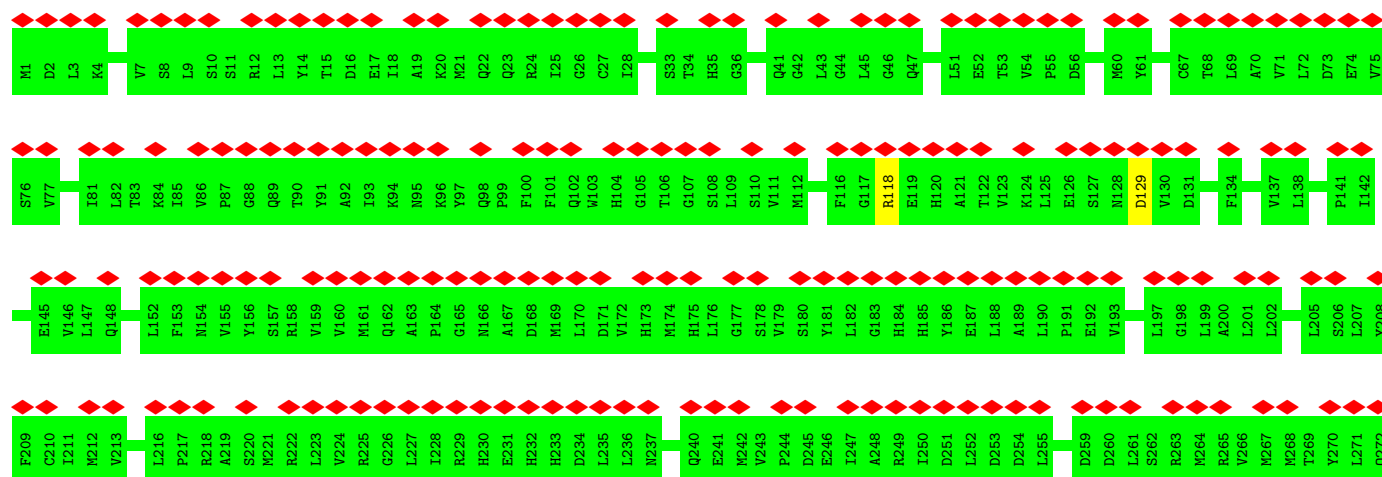


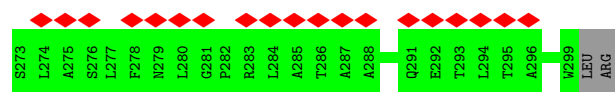


• Molecule 7: Triplex capsid protein 2

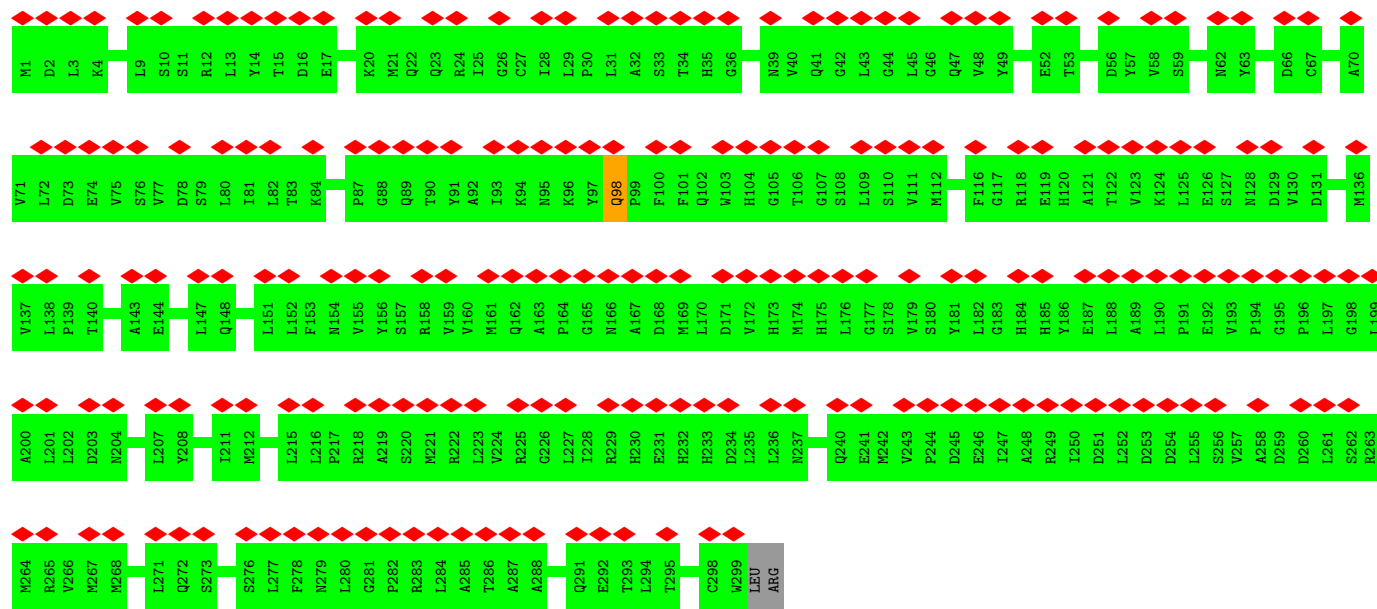


• Molecule 7: Triplex capsid protein 2





• Molecule 7: Triplex capsid protein 2



• Molecule 7: Triplex capsid protein 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2305	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 ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.040	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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	J	0.34	0/10492	0.57	0/14259
1	K	0.34	0/11085	0.58	0/15066
1	N	0.34	0/10933	0.57	0/14858
1	O	0.35	0/10435	0.57	0/14183
2	v	0.36	0/2346	0.61	0/3190
3	w	0.32	0/553	0.58	0/741
3	x	0.32	0/553	0.50	0/741
4	y	0.31	0/320	0.58	0/424
4	z	0.30	0/320	0.57	0/424
5	Z	0.35	0/664	0.58	0/896
5	a	0.34	0/664	0.60	1/896 (0.1%)
5	d	0.34	0/664	0.57	0/896
5	e	0.31	0/664	0.51	0/896
6	f	0.34	0/2049	0.63	2/2795 (0.1%)
6	h	0.34	0/2672	0.60	0/3635
7	k	0.34	0/2388	0.61	0/3254
7	m	0.35	0/2388	0.62	0/3254
7	p	0.32	0/2388	0.61	0/3254
7	r	0.33	0/2388	0.65	2/3254 (0.1%)
All	All	0.34	0/63966	0.59	5/86916 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	r	203	ASP	CB-CG-OD1	9.93	127.24	118.30
6	f	161	SER	C-N-CA	-7.42	90.86	122.00
7	r	203	ASP	CB-CG-OD2	-5.82	113.07	118.30
5	a	18	PHE	C-N-CA	-5.42	99.25	122.00
6	f	160	ASP	CB-CG-OD2	5.23	123.00	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	10252	0	10074	154	0
1	K	10832	0	10655	174	0
1	N	10683	0	10500	144	0
1	O	10194	0	10022	135	0
2	v	2288	0	2273	0	0
3	w	549	0	540	0	0
3	x	549	0	540	0	0
4	y	317	0	341	0	0
4	z	317	0	341	0	0
5	Z	649	0	649	5	0
5	a	649	0	649	0	0
5	d	649	0	649	0	0
5	e	649	0	649	0	0
6	f	1992	0	1953	0	0
6	h	2604	0	2577	0	0
7	k	2338	0	2364	0	0
7	m	2338	0	2364	0	0
7	p	2338	0	2364	0	0
7	r	2338	0	2364	0	0
All	All	62525	0	61868	587	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 (587) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:857:LEU:HD12	1:K:875:ARG:CD	1.20	1.58
1:J:1264:VAL:CG1	1:J:1265:PRO:HD2	1.34	1.52
1:K:1264:VAL:HB	1:K:1265:PRO:CD	1.09	1.44
1:K:1264:VAL:CB	1:K:1265:PRO:HD2	1.45	1.42
1:K:467:PRO:CG	1:K:912:PRO:HG3	1.59	1.33

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:483:ARG:NH2	1:O:553:ASP:OD2	1.62	1.32
1:K:857:LEU:CD1	1:K:875:ARG:CD	2.08	1.29
1:K:1264:VAL:CB	1:K:1265:PRO:CD	2.02	1.28
1:K:803:GLY:O	1:K:804:HIS:CD2	1.86	1.27
1:K:857:LEU:CD1	1:K:875:ARG:HD3	1.65	1.27
1:K:484:ARG:CD	1:K:552:ARG:HA	1.68	1.23
1:K:803:GLY:C	1:K:804:HIS:CD2	2.16	1.19
1:J:1264:VAL:CG1	1:J:1265:PRO:CD	2.20	1.18
1:J:1264:VAL:HG13	1:J:1265:PRO:CD	1.74	1.18
1:N:670:LEU:CG	1:N:671:GLY:H	1.54	1.18
1:J:871:ILE:HD13	1:J:936:ARG:NH2	1.57	1.17
1:K:1264:VAL:HB	1:K:1265:PRO:HD3	1.16	1.15
1:K:803:GLY:O	1:K:804:HIS:CG	1.98	1.15
1:N:670:LEU:HG	1:N:671:GLY:N	1.30	1.14
1:J:85:LEU:HD11	1:J:1070:GLY:HA2	1.29	1.12
1:K:857:LEU:HD12	1:K:875:ARG:HD2	1.29	1.07
1:J:85:LEU:CD1	1:J:1070:GLY:HA2	1.84	1.07
1:J:1264:VAL:HG12	1:J:1265:PRO:HD2	1.35	1.05
1:K:484:ARG:HD3	1:K:552:ARG:CA	1.88	1.02
1:K:857:LEU:HD11	1:K:875:ARG:HG2	1.37	1.02
1:K:1252:ASP:OD1	1:K:1256:ASN:ND2	1.92	1.02
1:K:467:PRO:HG2	1:K:912:PRO:CG	1.92	1.00
1:K:1264:VAL:CG2	1:K:1265:PRO:HD2	1.90	0.99
1:K:467:PRO:CG	1:K:912:PRO:CG	2.40	0.99
1:J:556:GLU:HG2	1:J:557:ARG:H	1.27	0.97
1:K:467:PRO:HG2	1:K:912:PRO:HG3	0.96	0.95
1:K:484:ARG:HD3	1:K:552:ARG:HA	0.95	0.94
1:N:731:ASP:HA	1:N:796:LEU:HD21	1.45	0.94
1:J:72:ALA:HB2	1:J:369:ALA:HB2	1.50	0.93
1:K:857:LEU:CD1	1:K:875:ARG:CG	2.46	0.92
1:J:556:GLU:HG2	1:J:557:ARG:N	1.87	0.90
1:O:483:ARG:CZ	1:O:553:ASP:OD2	2.20	0.89
1:K:857:LEU:CD1	1:K:875:ARG:HG2	2.03	0.88
1:J:1264:VAL:HG12	1:J:1265:PRO:CD	1.98	0.87
1:O:1010:PRO:O	1:O:1011:SER:O	1.92	0.86
1:J:1264:VAL:HG13	1:J:1265:PRO:HD2	0.87	0.86
1:O:483:ARG:HE	1:O:553:ASP:CG	1.80	0.85
1:N:265:SER:O	1:N:266:THR:O	1.93	0.85
1:J:871:ILE:HD13	1:J:936:ARG:HH21	1.37	0.84
1:J:556:GLU:CG	1:J:557:ARG:N	2.41	0.84
1:K:857:LEU:HD11	1:K:875:ARG:CG	2.07	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:484:ARG:HH11	1:N:484:ARG:HG2	1.41	0.83
1:N:619:PHE:HE1	1:N:874:LEU:HD23	1.41	0.83
1:N:670:LEU:CG	1:N:671:GLY:N	2.20	0.81
1:K:857:LEU:HD12	1:K:875:ARG:HD3	0.82	0.81
1:K:1256:ASN:OD1	1:K:1275:PHE:O	2.00	0.80
1:K:1264:VAL:HB	1:K:1265:PRO:HD2	0.80	0.80
1:J:482:ASP:HB2	1:J:484:ARG:NH1	1.97	0.78
1:N:825:MET:HA	1:N:930:ALA:O	1.84	0.77
1:K:1252:ASP:CG	1:K:1256:ASN:ND2	2.38	0.77
1:N:899:ARG:NH1	1:N:922:THR:HG23	1.99	0.76
1:J:828:LEU:HB3	1:J:928:LEU:O	1.87	0.74
1:K:467:PRO:HG3	1:K:912:PRO:HG3	1.67	0.72
1:K:1252:ASP:CG	1:K:1256:ASN:HD21	1.89	0.72
1:J:936:ARG:HD3	1:O:669:HIS:CD2	2.25	0.72
1:J:85:LEU:HD11	1:J:1070:GLY:CA	2.16	0.72
1:K:617:ALA:O	1:K:620:TYR:HB2	1.90	0.72
1:N:543:HIS:HD2	1:N:546:TYR:H	1.36	0.71
1:N:619:PHE:CE1	1:N:874:LEU:HD23	2.25	0.71
1:K:360:GLU:O	1:K:362:GLN:N	2.23	0.71
1:N:484:ARG:HD3	1:N:550:ILE:HG22	1.72	0.71
1:O:860:LEU:HD22	1:O:866:ARG:HG2	1.72	0.71
1:K:803:GLY:C	1:K:804:HIS:CG	2.52	0.70
1:K:456:LEU:HD11	1:K:1031:ILE:HG13	1.74	0.70
1:K:1252:ASP:CB	1:K:1256:ASN:ND2	2.54	0.70
1:N:899:ARG:HH11	1:N:922:THR:CG2	2.05	0.70
1:J:871:ILE:HD13	1:J:936:ARG:HH22	1.54	0.70
1:O:483:ARG:NE	1:O:553:ASP:CG	2.44	0.70
1:K:804:HIS:HE1	1:K:808:LEU:HD11	1.57	0.69
1:J:96:ARG:HG2	1:J:117:ILE:HG12	1.75	0.68
1:K:805:ALA:O	1:K:806:ASP:OD1	2.11	0.68
1:K:722:ASN:HD22	1:K:742:ARG:HH21	1.40	0.68
1:K:912:PRO:O	1:K:913:ASN:HB3	1.93	0.68
1:K:1252:ASP:CB	1:K:1256:ASN:HD22	2.07	0.67
1:K:1256:ASN:OD1	1:K:1275:PHE:HB3	1.95	0.67
1:O:241:SER:HA	1:O:293:PHE:HZ	1.58	0.67
1:J:856:ILE:HG13	1:J:881:ILE:HD12	1.76	0.67
1:O:639:LEU:HD12	1:O:880:MET:HB3	1.76	0.66
1:N:1068:PHE:HB2	1:N:1093:ALA:HB3	1.78	0.66
1:J:436:VAL:HG11	1:J:587:GLN:HE22	1.59	0.66
1:J:456:LEU:HD21	1:J:1031:ILE:HG13	1.77	0.66
1:K:912:PRO:O	1:K:913:ASN:CB	2.44	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:401:MET:O	1:J:1051:GLU:HA	1.96	0.65
1:O:565:ARG:O	1:O:570:ASN:ND2	2.27	0.65
1:N:650:ARG:NE	1:N:873:ASP:OD2	2.29	0.65
1:O:1117:MET:SD	1:O:1371:ARG:NH1	2.70	0.65
1:O:1068:PHE:HB2	1:O:1093:ALA:HB3	1.77	0.65
1:N:899:ARG:HH11	1:N:922:THR:HG23	1.60	0.65
1:K:467:PRO:HG3	1:K:912:PRO:CG	2.22	0.65
1:K:901:SER:HB3	1:K:918:ARG:HD2	1.80	0.64
1:K:911:ALA:HB3	1:K:912:PRO:CD	2.28	0.64
1:N:129:THR:HG22	1:O:103:ALA:HB2	1.80	0.64
1:O:104:HIS:HE1	1:O:108:ARG:HB2	1.62	0.64
1:J:1192:ASP:OD2	1:J:1237:ARG:NH2	2.31	0.64
1:J:828:LEU:HD11	1:J:945:PHE:HB3	1.80	0.64
1:O:594:LEU:HD11	1:O:692:ALA:HB1	1.79	0.64
1:K:857:LEU:CD1	1:K:875:ARG:HD2	2.06	0.64
1:J:72:ALA:CB	1:J:369:ALA:HB2	2.26	0.64
1:K:803:GLY:C	1:K:804:HIS:HD2	1.96	0.63
1:N:409:VAL:HG13	1:N:1044:MET:HG3	1.80	0.63
1:N:718:LEU:HD13	1:N:811:ILE:HG12	1.81	0.63
1:O:764:GLU:OE1	1:O:793:ARG:NH1	2.32	0.63
1:N:1192:ASP:OD2	1:N:1237:ARG:NH2	2.31	0.63
1:K:764:GLU:HG3	1:K:793:ARG:HH11	1.64	0.62
1:K:1252:ASP:HB3	1:K:1256:ASN:HD22	1.63	0.62
1:J:1264:VAL:HG12	1:J:1265:PRO:N	2.15	0.62
1:K:804:HIS:CE1	1:K:808:LEU:HD11	2.35	0.62
1:K:1195:TYR:O	1:K:1200:ASN:ND2	2.31	0.62
1:N:804:HIS:CD2	1:N:808:LEU:HD11	2.35	0.62
1:O:436:VAL:HG11	1:O:587:GLN:HE22	1.65	0.62
1:J:783:ARG:NH2	1:J:891:CYS:O	2.33	0.61
1:J:72:ALA:HB2	1:J:369:ALA:CB	2.27	0.61
1:J:225:GLU:O	1:J:232:ARG:NH2	2.33	0.61
1:K:400:ARG:NE	1:K:1051:GLU:OE2	2.30	0.61
1:N:747:ILE:HB	1:N:899:ARG:HB2	1.81	0.61
1:N:1246:GLN:HB2	1:N:1249:SER:HB3	1.82	0.61
1:N:362:GLN:O	1:N:364:ARG:NH1	2.34	0.61
1:K:285:ASN:O	1:K:289:GLN:NE2	2.32	0.61
1:K:1252:ASP:HA	1:K:1256:ASN:ND2	2.15	0.61
1:N:53:GLU:OE2	1:O:326:ARG:NH1	2.33	0.61
1:O:225:GLU:O	1:O:232:ARG:NH1	2.34	0.61
1:K:184:LYS:NZ	1:K:1064:SER:OG	2.34	0.61
1:N:93:ILE:HD12	1:N:1095:ILE:HG21	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:439:TRP:HB2	1:N:1337:ALA:HB3	1.83	0.60
1:J:10:ARG:NH1	1:K:321:ALA:O	2.32	0.60
1:N:484:ARG:HG2	1:N:484:ARG:NH1	2.14	0.60
1:N:737:LEU:HD23	1:N:744:PRO:HG2	1.82	0.60
1:N:619:PHE:CE1	1:N:874:LEU:CD2	2.84	0.60
1:K:1068:PHE:HB2	1:K:1093:ALA:HB3	1.83	0.60
1:J:431:THR:HG23	1:J:432:GLN:HG3	1.84	0.59
1:N:783:ARG:HA	1:N:788:HIS:HE1	1.66	0.59
1:K:484:ARG:CD	1:K:552:ARG:CA	2.63	0.59
1:N:184:LYS:NZ	1:N:1064:SER:OG	2.36	0.59
1:O:783:ARG:NH2	1:O:891:CYS:O	2.34	0.59
1:J:1374:LYS:HG2	1:J:1379:VAL:HG22	1.83	0.59
1:K:484:ARG:HD2	1:K:552:ARG:HA	1.76	0.59
1:O:301:GLN:HA	1:O:367:ILE:O	2.01	0.59
1:N:484:ARG:HD2	1:N:551:GLY:O	2.02	0.59
1:K:409:VAL:HG13	1:K:1044:MET:HG3	1.85	0.59
1:K:548:ILE:HD11	1:K:560:HIS:HB3	1.85	0.59
1:N:1074:VAL:HG22	1:N:1088:VAL:HG22	1.84	0.59
1:N:803:GLY:O	1:N:804:HIS:HB2	2.03	0.58
1:O:850:PHE:HE2	1:O:878:VAL:HG21	1.68	0.58
1:J:936:ARG:HD3	1:O:669:HIS:HD2	1.68	0.58
1:N:942:GLN:NE2	1:N:943:CYS:SG	2.76	0.58
1:K:317:ASN:ND2	1:K:328:MET:O	2.36	0.58
1:J:551:GLY:HA3	1:J:559:ARG:HH11	1.67	0.58
1:K:724:LEU:O	1:K:921:GLN:NE2	2.36	0.58
1:N:185:LEU:HD13	1:N:399:ARG:HH21	1.69	0.58
1:J:463:ARG:HH22	1:J:1259:TYR:HB3	1.68	0.58
1:J:720:ASP:OD1	1:J:742:ARG:NH2	2.37	0.58
1:K:496:HIS:HE1	1:K:502:ILE:HG13	1.68	0.58
1:N:1195:TYR:O	1:N:1200:ASN:ND2	2.37	0.58
1:K:185:LEU:HD13	1:K:399:ARG:HH21	1.68	0.58
1:N:997:HIS:HE1	1:N:1022:HIS:HE1	1.52	0.58
1:O:406:TYR:HA	1:O:1046:VAL:O	2.03	0.58
1:O:549:TYR:OH	1:O:994:ARG:NH2	2.36	0.57
1:N:80:THR:HG22	1:N:309:ALA:HB3	1.87	0.57
1:O:904:ASN:ND2	1:O:908:GLN:O	2.37	0.57
1:K:359:VAL:O	1:K:360:GLU:O	2.22	0.57
1:K:496:HIS:ND1	1:K:498:ASN:OD1	2.37	0.57
1:N:401:MET:O	1:N:1051:GLU:HA	2.04	0.57
1:N:441:VAL:HG11	1:N:1373:LEU:HD22	1.85	0.57
1:K:586:GLN:NE2	1:K:589:GLU:OE2	2.36	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:439:TRP:HB3	1:O:447:LEU:HD11	1.87	0.57
1:J:406:TYR:HA	1:J:1046:VAL:O	2.05	0.57
1:N:742:ARG:HB3	1:N:903:ASP:HB2	1.85	0.57
1:K:594:LEU:HD13	1:K:696:ALA:HB2	1.87	0.57
1:O:282:VAL:HG12	1:O:1057:ILE:HG12	1.86	0.56
1:J:995:GLU:O	1:J:998:ARG:NH2	2.38	0.56
1:J:85:LEU:CD1	1:J:1070:GLY:CA	2.74	0.56
1:O:584:ARG:NH1	1:O:1020:ALA:O	2.35	0.56
1:O:650:ARG:NH1	1:O:873:ASP:O	2.39	0.56
1:K:585:GLY:HA3	1:K:1017:GLY:HA2	1.88	0.56
1:N:133:LEU:HD13	1:N:138:LEU:HD21	1.87	0.56
1:N:731:ASP:CA	1:N:796:LEU:HD21	2.26	0.56
1:J:443:LYS:HD3	1:J:1116:ASP:HA	1.88	0.56
1:N:673:ASN:HB3	1:O:650:ARG:HH22	1.71	0.56
1:N:567:MET:SD	1:N:1022:HIS:ND1	2.77	0.56
1:O:483:ARG:NE	1:O:553:ASP:OD2	2.39	0.56
1:J:584:ARG:NH1	1:J:1020:ALA:O	2.38	0.56
1:K:1246:GLN:HB2	1:K:1249:SER:HB3	1.88	0.56
1:O:111:SER:OG	1:O:114:ARG:NH2	2.39	0.56
1:J:555:GLY:O	1:J:557:ARG:N	2.39	0.56
1:J:666:ILE:HA	1:J:670:LEU:HD12	1.87	0.56
1:N:230:LEU:HD21	1:N:289:GLN:HG2	1.86	0.56
1:N:670:LEU:HG	1:N:671:GLY:H	0.62	0.56
1:J:400:ARG:NH2	1:J:1051:GLU:OE1	2.38	0.55
1:K:266:THR:O	1:K:364:ARG:NH1	2.34	0.55
1:O:127:ILE:HB	1:O:1090:HIS:O	2.06	0.55
1:O:1080:ARG:HE	1:O:1082:ASP:HB2	1.71	0.55
1:K:307:SER:OG	1:K:362:GLN:NE2	2.39	0.55
1:K:938:ARG:HA	1:K:941:THR:HB	1.88	0.55
1:N:783:ARG:HE	1:N:893:THR:HG22	1.71	0.55
1:K:911:ALA:N	1:K:912:PRO:HD2	2.22	0.55
1:N:269:THR:HG22	1:N:271:LYS:H	1.72	0.55
1:J:746:ILE:HB	1:J:753:TYR:HB3	1.87	0.55
1:J:763:ILE:HG12	1:J:794:LEU:HD11	1.89	0.55
1:K:269:THR:OG1	1:K:272:GLY:O	2.23	0.55
1:N:856:ILE:HD12	1:N:876:PRO:HG2	1.89	0.55
1:N:857:LEU:HD12	1:N:875:ARG:HG2	1.88	0.55
1:J:935:GLU:OE1	1:O:668:ARG:NH1	2.38	0.55
1:J:955:GLY:HA3	1:J:985:ARG:HE	1.72	0.55
1:O:814:TYR:OH	1:O:921:GLN:NE2	2.40	0.55
1:J:1135:ASN:HB3	1:J:1138:VAL:HG12	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:630:GLU:OE2	1:O:669:HIS:NE2	2.36	0.55
1:N:267:TYR:HD1	1:N:267:TYR:N	2.05	0.54
1:J:1174:LEU:O	1:K:213:SER:OG	2.21	0.54
1:J:1308:GLU:HG3	1:J:1309:VAL:HG13	1.88	0.54
1:K:40:LEU:HD22	1:K:44:ASP:HB3	1.88	0.54
1:K:1117:MET:SD	1:K:1371:ARG:NH2	2.80	0.54
1:J:195:GLN:NE2	1:J:250:GLU:OE2	2.40	0.54
1:J:871:ILE:CD1	1:J:936:ARG:HH21	2.14	0.54
1:K:591:ALA:HB1	1:K:1036:LEU:HD12	1.88	0.54
1:K:952:MET:HA	1:K:985:ARG:HH22	1.71	0.54
1:J:303:MET:O	1:J:364:ARG:N	2.41	0.54
1:K:95:PHE:HB2	1:K:118:VAL:HB	1.90	0.54
1:N:287:LEU:HD13	1:N:383:SER:HB3	1.90	0.54
1:N:844:PRO:O	1:N:882:ARG:NH2	2.36	0.54
1:K:720:ASP:O	1:K:810:LYS:NZ	2.40	0.54
1:K:997:HIS:HE1	1:K:1022:HIS:HE1	1.54	0.54
1:N:1119:ILE:HD11	1:O:1235:GLU:HB3	1.90	0.54
1:N:1298:LEU:HD21	1:N:1302:PRO:HG3	1.90	0.54
1:N:572:PRO:HG2	1:N:575:LEU:HD12	1.90	0.54
1:N:1053:LEU:HD12	1:N:1112:ALA:HB3	1.90	0.54
1:O:1299:GLY:O	1:O:1323:GLN:NE2	2.41	0.54
1:J:400:ARG:HH22	1:J:1114:THR:HG21	1.72	0.53
1:K:911:ALA:CB	1:K:912:PRO:CD	2.86	0.53
1:K:910:LEU:C	1:K:912:PRO:HD2	2.29	0.53
1:J:617:ALA:HA	1:J:620:TYR:HD2	1.73	0.53
1:K:329:ARG:HG2	1:K:330:THR:HG23	1.90	0.53
1:J:565:ARG:O	1:J:570:ASN:ND2	2.35	0.53
1:J:589:GLU:HG2	1:J:594:LEU:HD12	1.90	0.53
1:K:312:VAL:HG12	1:K:314:ARG:H	1.73	0.53
1:K:1264:VAL:HG23	1:K:1265:PRO:HD2	1.88	0.53
1:N:282:VAL:HG12	1:N:1057:ILE:HG12	1.90	0.53
1:N:532:PRO:HB3	1:N:1238:SER:HB2	1.90	0.53
1:O:598:VAL:HG13	1:O:602:VAL:HG13	1.89	0.53
1:J:399:ARG:HD3	1:J:1320:PHE:HB3	1.90	0.53
1:J:1326:SER:O	1:J:1329:GLN:NE2	2.42	0.53
1:J:85:LEU:HD13	1:J:1070:GLY:HA2	1.85	0.53
1:K:690:LEU:HD11	1:K:812:PHE:HB2	1.91	0.53
1:K:803:GLY:O	1:K:804:HIS:NE2	2.40	0.53
1:K:804:HIS:HE1	1:K:808:LEU:CD1	2.20	0.53
1:O:307:SER:OG	1:O:362:GLN:OE1	2.27	0.53
1:J:427:LEU:O	1:J:427:LEU:HD23	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:535:TYR:HE2	1:K:539:ARG:HH21	1.57	0.53
1:J:281:ILE:HD12	1:J:1058:LEU:HD23	1.90	0.53
1:K:225:GLU:O	1:K:232:ARG:NH2	2.38	0.53
1:O:417:LYS:NZ	1:O:431:THR:O	2.40	0.53
1:O:625:MET:SD	1:O:887:SER:OG	2.61	0.52
1:O:504:ASP:O	1:O:508:ASP:HB2	2.09	0.52
1:N:484:ARG:HH11	1:N:484:ARG:CG	2.16	0.52
1:O:510:LYS:O	1:O:973:ARG:NH2	2.42	0.52
1:J:904:ASN:ND2	1:J:919:THR:OG1	2.33	0.52
1:O:921:GLN:HB2	1:O:996:TRP:CD1	2.44	0.52
1:J:367:ILE:O	1:J:368:SER:OG	2.21	0.52
1:O:835:VAL:O	1:O:838:THR:OG1	2.26	0.52
1:O:902:VAL:O	1:O:918:ARG:HA	2.09	0.52
1:N:267:TYR:N	1:N:267:TYR:CD1	2.76	0.52
1:N:835:VAL:O	1:N:838:THR:OG1	2.25	0.52
1:O:1128:PHE:HZ	1:O:1260:ARG:HD2	1.75	0.52
1:K:803:GLY:CA	1:K:804:HIS:CD2	2.92	0.52
1:N:513:ALA:HB1	1:N:984:ASN:HD22	1.75	0.52
1:N:1115:THR:HG22	1:N:1180:ALA:HB2	1.92	0.52
1:N:1299:GLY:HA3	1:N:1323:GLN:HE21	1.74	0.52
1:K:553:ASP:HB3	1:K:558:ALA:HB2	1.91	0.51
1:O:266:THR:O	1:O:364:ARG:NH1	2.41	0.51
1:J:731:ASP:HB3	1:J:799:TYR:HB2	1.92	0.51
1:K:401:MET:O	1:K:1051:GLU:HA	2.11	0.51
1:K:1203:ARG:HE	1:K:1245:SER:HA	1.75	0.51
1:J:855:ASP:OD2	1:J:875:ARG:NH2	2.39	0.51
1:K:1205:ARG:HG2	1:K:1231:ASP:HB3	1.93	0.51
1:N:587:GLN:NE2	1:N:1037:LYS:O	2.44	0.51
1:O:603:ILE:HD13	1:O:1011:SER:O	2.11	0.51
1:J:1176:HIS:HE1	1:K:1233:ALA:HA	1.76	0.51
1:O:406:TYR:HE2	1:O:1196:PHE:HD1	1.58	0.51
1:J:1123:ASP:N	1:J:1123:ASP:OD1	2.43	0.51
1:K:1252:ASP:CA	1:K:1256:ASN:ND2	2.74	0.51
1:N:637:VAL:HG23	1:N:638:PRO:HD3	1.92	0.51
1:O:456:LEU:HA	1:O:459:LEU:HB2	1.91	0.51
1:J:587:GLN:NE2	1:J:1037:LYS:O	2.44	0.51
1:K:521:LYS:NZ	1:K:540:LEU:O	2.44	0.51
1:K:1027:PRO:HA	1:K:1030:TYR:HD2	1.74	0.51
1:O:1315:ALA:HB1	1:O:1317:THR:HG23	1.92	0.51
1:K:1159:ARG:NH2	1:K:1317:THR:OG1	2.44	0.51
1:J:581:GLN:HE21	1:J:1021:MET:HG2	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:434:LEU:HD12	1:O:435:PRO:HD2	1.93	0.50
1:J:564:HIS:HD2	1:J:566:LEU:HD23	1.76	0.50
1:K:971:VAL:HG13	1:K:978:ARG:HE	1.77	0.50
1:J:482:ASP:HB2	1:J:484:ARG:HH12	1.75	0.50
1:K:777:VAL:O	1:K:781:GLY:N	2.42	0.50
1:N:673:ASN:ND2	1:O:873:ASP:OD2	2.44	0.50
1:O:655:ALA:O	1:O:683:TYR:OH	2.28	0.50
1:J:72:ALA:CB	1:J:369:ALA:CB	2.89	0.50
1:K:440:ILE:HG21	1:K:1048:ARG:HH22	1.77	0.50
1:O:470:THR:HG22	1:O:1253:ILE:HG13	1.94	0.50
1:K:1350:LYS:O	1:K:1353:HIS:ND1	2.45	0.50
1:N:230:LEU:HD22	1:N:1109:ARG:HD2	1.94	0.50
1:N:484:ARG:CD	1:N:551:GLY:O	2.60	0.50
1:O:1350:LYS:O	1:O:1353:HIS:ND1	2.36	0.50
1:J:75:VAL:HG22	1:J:267:TYR:HD2	1.75	0.50
1:J:131:MET:O	1:J:1085:THR:HA	2.12	0.50
1:J:1197:GLN:NE2	1:J:1364:GLU:OE1	2.44	0.50
1:O:70:GLU:HA	1:O:367:ILE:HD12	1.95	0.49
1:J:908:GLN:NE2	1:J:1026:SER:OG	2.45	0.49
1:N:518:ILE:HA	1:N:521:LYS:HB2	1.94	0.49
1:N:548:ILE:HA	1:N:561:ARG:O	2.12	0.49
1:K:361:ASP:O	1:K:362:GLN:C	2.49	0.49
5:Z:61:VAL:O	5:Z:64:THR:OG1	2.27	0.49
1:N:829:GLY:HA2	1:N:895:THR:HG21	1.95	0.49
1:O:780:TYR:O	1:O:783:ARG:HB2	2.12	0.49
1:O:825:MET:N	1:O:956:ASP:OD2	2.43	0.49
1:J:123:HIS:O	1:J:1093:ALA:HA	2.12	0.49
1:J:213:SER:OG	1:O:1174:LEU:O	2.22	0.49
1:N:481:ARG:O	1:N:484:ARG:NH1	2.45	0.49
1:O:657:VAL:HA	1:O:663:ILE:HD11	1.94	0.49
1:J:571:LEU:HB3	1:J:575:LEU:HD23	1.95	0.49
1:J:1350:LYS:O	1:J:1353:HIS:ND1	2.45	0.49
1:N:804:HIS:CG	1:N:808:LEU:HD11	2.48	0.49
1:K:911:ALA:HB3	1:K:912:PRO:HD3	1.95	0.49
1:O:526:THR:HG22	1:O:574:PRO:HA	1.94	0.49
1:K:1264:VAL:CB	1:K:1265:PRO:HD3	2.04	0.48
1:N:951:HIS:HA	1:N:990:PHE:HE1	1.77	0.48
1:N:312:VAL:HG11	1:N:314:ARG:HH11	1.79	0.48
1:O:724:LEU:O	1:O:921:GLN:NE2	2.33	0.48
1:N:73:LEU:HD13	1:N:177:ILE:HD11	1.95	0.48
1:N:403:TYR:O	1:N:1049:THR:HA	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:518:ILE:HG22	1:N:521:LYS:HD2	1.95	0.48
1:J:549:TYR:OH	1:J:994:ARG:NH1	2.35	0.48
1:K:440:ILE:HD12	1:K:1119:ILE:HG22	1.95	0.48
1:O:475:ASN:HB3	1:O:560:HIS:HD2	1.78	0.48
1:O:1121:THR:HA	1:O:1182:CYS:HB2	1.96	0.48
1:J:1049:THR:HG23	1:J:1270:PRO:HB3	1.96	0.48
1:N:1039:HIS:ND1	1:N:1040:PRO:O	2.45	0.48
1:O:80:THR:HG22	1:O:309:ALA:HB3	1.96	0.48
1:O:467:PRO:HB2	1:O:471:LEU:HD23	1.94	0.48
1:O:985:ARG:HH21	1:O:990:PHE:HZ	1.61	0.48
1:J:186:ARG:NH2	1:J:1296:GLN:O	2.46	0.48
1:J:1205:ARG:HG3	1:J:1239:THR:HG23	1.95	0.48
1:N:731:ASP:HA	1:N:796:LEU:CD2	2.32	0.48
1:J:1173:GLY:HA2	1:K:209:LYS:HD3	1.96	0.48
1:J:205:ARG:NH1	1:O:1318:ASP:O	2.46	0.48
1:J:424:ILE:HD11	1:J:1345:GLU:HG2	1.96	0.48
1:J:1121:THR:HA	1:J:1182:CYS:HB2	1.96	0.47
1:K:360:GLU:OE1	1:K:360:GLU:HA	2.11	0.47
1:O:690:LEU:HD21	1:O:812:PHE:HB2	1.96	0.47
1:J:522:CYS:HB3	1:J:1000:PRO:HG3	1.97	0.47
1:J:1068:PHE:HB2	1:J:1093:ALA:HB3	1.95	0.47
1:O:300:ASN:HA	1:O:370:ALA:HA	1.96	0.47
1:J:511:TYR:HD1	1:J:973:ARG:HH12	1.61	0.47
1:K:804:HIS:CE1	1:K:808:LEU:CD1	2.97	0.47
1:N:794:LEU:HD11	1:N:925:VAL:HG21	1.97	0.47
1:N:947:ALA:H	1:N:964:HIS:HE1	1.62	0.47
1:O:588:PHE:HE1	1:O:700:LEU:HG	1.79	0.47
1:J:834:HIS:HD2	5:Z:8:PRO:HD3	1.79	0.47
1:N:484:ARG:NH1	1:N:484:ARG:CG	2.74	0.47
1:N:684:ARG:HH22	1:O:613:THR:H	1.63	0.47
1:O:724:LEU:O	1:O:814:TYR:OH	2.29	0.47
1:J:1233:ALA:HA	1:O:1176:HIS:HE1	1.80	0.47
1:K:730:THR:HB	1:K:799:TYR:HA	1.97	0.47
1:K:835:VAL:O	1:K:838:THR:OG1	2.30	0.47
1:K:857:LEU:CG	1:K:875:ARG:HD2	2.44	0.47
1:N:395:TYR:CE2	1:N:397:LEU:HB2	2.49	0.47
1:N:705:VAL:HG12	1:N:710:SER:HA	1.96	0.47
1:O:1316:GLY:HA2	1:O:1319:VAL:HB	1.97	0.47
5:Z:20:ASP:HA	5:Z:24:LEU:HD11	1.96	0.47
1:J:747:ILE:HG12	1:J:752:VAL:HG12	1.97	0.47
1:N:128:SER:HA	1:N:1088:VAL:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:442:ASN:O	1:O:1371:ARG:NH2	2.45	0.47
1:O:281:ILE:HD12	1:O:1058:LEU:HD23	1.96	0.46
1:K:359:VAL:C	1:K:360:GLU:O	2.53	0.46
1:N:874:LEU:O	1:N:876:PRO:HD3	2.15	0.46
1:N:456:LEU:HD23	1:N:1146:VAL:HG23	1.97	0.46
1:O:957:PRO:O	1:O:961:ALA:HB2	2.15	0.46
1:K:961:ALA:HB2	1:K:971:VAL:HG21	1.98	0.46
1:K:1195:TYR:OH	1:K:1203:ARG:O	2.33	0.46
1:J:282:VAL:HG12	1:J:1057:ILE:HG12	1.96	0.46
1:J:1074:VAL:HG22	1:J:1088:VAL:HG22	1.97	0.46
1:K:1204:GLY:HA3	1:K:1240:VAL:H	1.81	0.46
1:N:440:ILE:HD12	1:N:1119:ILE:HG22	1.97	0.46
1:J:412:PHE:HB2	1:J:1189:VAL:HG12	1.98	0.46
1:J:434:LEU:HD12	1:J:435:PRO:HD2	1.98	0.46
1:J:1215:TYR:HE1	1:J:1285:ARG:HG2	1.80	0.46
1:N:298:ALA:HB3	1:N:371:VAL:HG23	1.97	0.46
1:N:670:LEU:O	1:N:671:GLY:C	2.54	0.46
1:J:806:ASP:HB3	1:J:810:LYS:HE3	1.98	0.46
1:K:706:VAL:HG23	1:K:711:VAL:HG12	1.98	0.46
1:N:499:VAL:HA	1:N:502:ILE:HD12	1.98	0.46
1:N:584:ARG:NH1	1:N:1020:ALA:O	2.44	0.46
1:K:79:ASN:HB3	1:K:308:TYR:CD1	2.51	0.46
1:N:619:PHE:HE1	1:N:874:LEU:CD2	2.15	0.46
1:J:544:PRO:HG3	1:J:1243:TRP:CD2	2.51	0.46
1:K:1263:ALA:O	1:K:1264:VAL:O	2.33	0.46
1:O:544:PRO:HG3	1:O:1243:TRP:CD2	2.51	0.46
1:O:985:ARG:HD2	1:O:990:PHE:CE1	2.51	0.46
1:J:280:PHE:HB2	1:J:381:VAL:HG22	1.97	0.46
1:N:279:VAL:O	1:N:1059:PHE:HA	2.15	0.46
1:K:80:THR:HG22	1:K:309:ALA:HB3	1.98	0.45
1:N:302:ILE:HG13	1:N:367:ILE:HB	1.98	0.45
1:O:281:ILE:HG22	1:O:397:LEU:HD11	1.97	0.45
1:J:486:THR:HG21	1:J:552:ARG:HB2	1.99	0.45
1:K:805:ALA:O	1:K:806:ASP:CG	2.55	0.45
1:O:84:ASP:N	1:O:84:ASP:OD1	2.49	0.45
1:O:860:LEU:HD11	1:O:865:LEU:HB3	1.97	0.45
1:J:190:PRO:HD2	1:J:193:ILE:HD12	1.98	0.45
1:J:255:VAL:HG13	1:J:1102:SER:HA	1.99	0.45
1:J:1350:LYS:HD3	1:J:1380:VAL:HG13	1.98	0.45
1:K:804:HIS:CD2	1:K:804:HIS:N	2.81	0.45
1:N:267:TYR:HD1	1:N:267:TYR:H	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1146:VAL:HG13	1:N:1148:ALA:H	1.80	0.45
1:O:951:HIS:O	1:O:955:GLY:N	2.49	0.45
1:O:1187:THR:HG23	1:O:1241:ASN:HB3	1.99	0.45
1:J:155:VAL:HA	1:J:158:VAL:HG22	1.98	0.45
1:J:814:TYR:OH	1:J:921:GLN:NE2	2.49	0.45
1:K:402:GLN:HB2	1:K:1323:GLN:HB3	1.99	0.45
1:N:61:ASN:HD22	1:O:97:ILE:HG23	1.82	0.45
1:N:947:ALA:H	1:N:964:HIS:CE1	2.34	0.45
1:O:441:VAL:HG11	1:O:1373:LEU:HD22	1.97	0.45
1:N:630:GLU:OE2	1:N:668:ARG:NH2	2.50	0.45
1:J:1377:ASN:N	1:K:1364:GLU:OE1	2.40	0.45
1:K:955:GLY:O	1:K:985:ARG:NH2	2.49	0.45
1:K:1023:ILE:HG21	1:K:1033:GLN:HE21	1.81	0.45
1:J:497:MET:HE3	1:J:792:PHE:HA	1.98	0.45
1:N:591:ALA:HB1	1:N:1036:LEU:HD12	1.99	0.45
1:N:828:LEU:HD11	1:N:945:PHE:HB3	1.97	0.45
1:J:986:PRO:O	1:J:990:PHE:N	2.48	0.45
1:K:499:VAL:HA	1:K:502:ILE:HD12	1.99	0.45
1:K:1276:ASN:HB3	1:K:1279:GLU:HB2	1.98	0.45
1:K:481:ARG:NH1	1:K:536:ASP:OD2	2.51	0.44
1:K:796:LEU:HD21	1:K:925:VAL:HG13	1.99	0.44
1:K:951:HIS:O	1:K:955:GLY:N	2.50	0.44
1:O:132:GLU:HG2	1:O:1085:THR:HG22	1.98	0.44
1:O:572:PRO:HD2	1:O:575:LEU:HD12	1.99	0.44
1:O:637:VAL:HA	1:O:640:VAL:HG22	1.99	0.44
1:J:94:GLN:HG2	1:J:119:VAL:HG22	1.99	0.44
1:N:619:PHE:CZ	1:N:874:LEU:HD22	2.52	0.44
1:K:1051:GLU:N	1:K:1115:THR:OG1	2.50	0.44
1:O:680:TYR:OH	1:O:684:ARG:NH1	2.50	0.44
1:N:609:THR:HG22	1:N:653:ARG:HB3	1.98	0.44
1:N:1348:SER:OG	1:N:1349:VAL:N	2.51	0.44
1:N:564:HIS:HD2	1:N:566:LEU:HD23	1.82	0.44
1:N:571:LEU:HD12	1:N:572:PRO:HD2	2.00	0.44
1:N:1018:MET:HA	1:N:1021:MET:HE2	1.99	0.44
1:N:598:VAL:HB	1:N:689:GLU:HB2	2.00	0.44
1:K:395:TYR:CE2	1:K:397:LEU:HB2	2.53	0.44
1:K:856:ILE:HD12	1:K:876:PRO:HG2	2.00	0.44
1:N:706:VAL:HG23	1:N:711:VAL:HG12	1.99	0.44
1:O:469:HIS:HB2	1:O:1259:TYR:HE2	1.82	0.44
1:O:1010:PRO:O	1:O:1011:SER:C	2.55	0.44
1:J:1223:LEU:HD11	1:O:1173:GLY:HA3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:483:ARG:O	1:K:483:ARG:HG2	2.16	0.44
1:N:720:ASP:O	1:N:810:LYS:NZ	2.51	0.44
1:J:544:PRO:O	1:J:565:ARG:NH1	2.51	0.44
1:N:639:LEU:HD12	1:N:880:MET:HB3	2.00	0.44
1:O:746:ILE:HB	1:O:753:TYR:HB3	1.98	0.44
1:O:663:ILE:HG23	1:O:683:TYR:HD1	1.83	0.43
1:J:307:SER:OG	1:J:364:ARG:NH1	2.50	0.43
1:J:485:GLU:HB3	1:J:517:ASP:HB2	2.00	0.43
1:N:158:VAL:HA	1:N:161:VAL:HG12	2.00	0.43
1:N:956:ASP:HA	1:N:957:PRO:HD3	1.86	0.43
1:J:668:ARG:HH11	1:J:669:HIS:CE1	2.37	0.43
1:N:857:LEU:HD23	1:N:860:LEU:HD12	1.98	0.43
1:O:227:SER:O	1:O:232:ARG:NH2	2.49	0.43
1:O:866:ARG:O	1:O:870:GLU:HB2	2.18	0.43
1:J:737:LEU:HG	1:J:744:PRO:HG2	2.01	0.43
1:N:412:PHE:HD1	1:N:1189:VAL:HG12	1.83	0.43
1:J:704:ASP:O	1:K:976:GLN:NE2	2.47	0.43
1:K:1255:TYR:HB2	1:K:1275:PHE:HD2	1.83	0.43
1:N:474:LEU:HG	1:N:560:HIS:CE1	2.53	0.43
1:K:282:VAL:HG12	1:K:1057:ILE:HG12	2.00	0.43
1:O:75:VAL:HG23	1:O:267:TYR:CG	2.54	0.43
1:O:83:LYS:HG3	1:O:312:VAL:HG23	1.99	0.43
1:J:1335:LEU:HG	1:J:1365:GLU:HB2	2.00	0.43
1:K:904:ASN:ND2	1:K:917:LYS:O	2.52	0.43
1:N:1117:MET:SD	1:N:1371:ARG:NH1	2.91	0.43
1:O:587:GLN:NE2	1:O:1037:LYS:O	2.52	0.43
1:K:95:PHE:O	1:K:117:ILE:HA	2.19	0.43
1:N:317:ASN:HD21	1:N:331:PHE:HB2	1.82	0.43
1:K:546:TYR:HA	1:K:564:HIS:HA	2.01	0.43
1:K:1049:THR:HG23	1:K:1270:PRO:HB3	2.01	0.43
1:O:280:PHE:HB2	1:O:381:VAL:HG22	2.00	0.43
1:O:444:ASN:HD22	1:O:1176:HIS:CD2	2.36	0.43
1:J:668:ARG:HH11	1:J:669:HIS:HE1	1.67	0.43
1:K:856:ILE:HG22	1:K:860:LEU:HB2	2.01	0.43
1:K:1217:GLN:HE22	1:K:1281:LEU:HD23	1.84	0.43
1:J:639:LEU:HD12	1:J:880:MET:HB3	2.00	0.42
1:J:1313:VAL:HG21	1:J:1319:VAL:HG21	2.01	0.42
1:O:810:LYS:O	1:O:814:TYR:HB2	2.19	0.42
1:J:400:ARG:NE	1:J:1305:SER:OG	2.52	0.42
1:J:547:ASP:O	1:J:562:ALA:HA	2.20	0.42
1:K:172:LEU:HD11	1:K:1090:HIS:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:705:VAL:HA	1:N:711:VAL:HG13	2.00	0.42
1:J:285:ASN:HD22	1:J:288:ARG:HH22	1.68	0.42
1:K:501:VAL:HA	1:K:504:ASP:HB2	2.00	0.42
1:N:77:CYS:SG	1:N:1065:THR:OG1	2.72	0.42
1:N:764:GLU:HB2	1:N:793:ARG:HD3	2.02	0.42
1:N:856:ILE:HG22	1:N:860:LEU:HG	2.01	0.42
1:O:415:ASN:HD21	1:O:579:ALA:HB2	1.85	0.42
1:O:1039:HIS:ND1	1:O:1040:PRO:O	2.53	0.42
1:J:1124:PHE:HA	1:J:1127:VAL:HG12	2.01	0.42
1:O:606:VAL:O	1:O:609:THR:OG1	2.31	0.42
1:K:467:PRO:HG3	1:K:912:PRO:HG2	2.01	0.42
1:K:737:LEU:HD23	1:K:744:PRO:HG2	2.01	0.42
1:J:385:GLN:HG2	1:J:389:ASN:HD21	1.83	0.42
1:J:405:TYR:O	1:J:1047:VAL:HA	2.20	0.42
1:J:690:LEU:HD21	1:J:812:PHE:HB2	2.01	0.42
1:J:724:LEU:HD12	1:J:900:VAL:HG21	2.01	0.42
1:J:905:ASP:OD1	1:J:906:VAL:N	2.51	0.42
1:K:778:ALA:O	1:K:782:TYR:N	2.51	0.42
1:K:1012:LEU:HA	1:K:1015:ILE:HD12	2.01	0.42
1:J:415:ASN:OD1	1:J:417:LYS:NZ	2.39	0.42
1:J:621:VAL:O	1:J:625:MET:HG2	2.20	0.42
1:J:788:HIS:O	1:J:896:ARG:NH1	2.53	0.42
1:N:155:VAL:HA	1:N:158:VAL:HG22	2.02	0.42
1:O:814:TYR:HH	1:O:921:GLN:HE22	1.68	0.42
1:O:1049:THR:HG23	1:O:1270:PRO:HB3	2.02	0.42
1:J:748:ILE:HG13	1:J:898:VAL:HG13	2.02	0.42
1:J:1269:SER:HB2	1:J:1272:ARG:HB2	2.01	0.42
1:K:1146:VAL:HG13	1:K:1148:ALA:H	1.85	0.42
1:K:1225:TYR:CE2	1:K:1277:LYS:HE2	2.55	0.42
1:N:312:VAL:HG12	1:N:314:ARG:H	1.84	0.42
1:O:828:LEU:HD11	1:O:945:PHE:HB3	2.01	0.42
1:J:521:LYS:NZ	1:J:541:GLU:OE2	2.40	0.42
1:K:158:VAL:HA	1:K:161:VAL:HG12	2.01	0.42
1:O:494:PRO:HB3	1:O:988:GLN:HG2	2.01	0.42
1:J:843:GLY:HA2	1:J:846:PHE:HB3	2.02	0.42
1:J:856:ILE:HD11	1:J:878:VAL:HA	2.02	0.42
1:K:726:PRO:HG3	1:K:954:TYR:HE2	1.85	0.42
1:N:638:PRO:HG2	1:N:880:MET:SD	2.59	0.42
1:N:828:LEU:HB3	1:N:928:LEU:O	2.20	0.42
1:N:1175:CYS:H	1:O:1232:ALA:HB1	1.85	0.41
1:O:906:VAL:HA	1:O:909:GLN:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:705:VAL:HG12	1:K:710:SER:HA	2.00	0.41
1:N:626:ILE:HG22	1:N:628:GLY:H	1.85	0.41
1:N:684:ARG:NH2	1:O:612:ASP:HA	2.35	0.41
1:O:909:GLN:HE21	1:O:917:LYS:HD3	1.85	0.41
1:O:977:GLN:HE21	1:O:983:PHE:HA	1.85	0.41
1:K:830:VAL:H	1:K:895:THR:HG21	1.86	0.41
1:O:466:THR:HB	1:O:910:LEU:HD13	2.02	0.41
1:J:80:THR:HG21	1:J:1068:PHE:HE1	1.85	0.41
1:O:713:GLN:NE2	1:O:719:LEU:O	2.44	0.41
1:K:299:ASP:HB2	1:K:371:VAL:HG21	2.03	0.41
1:O:955:GLY:HA3	1:O:985:ARG:NE	2.36	0.41
1:J:444:ASN:HD22	1:J:1176:HIS:HD2	1.69	0.41
1:J:852:ARG:NH2	5:Z:63:ARG:HD3	2.35	0.41
1:N:724:LEU:HD23	1:N:724:LEU:HA	1.85	0.41
1:K:1285:ARG:NH2	1:K:1293:GLU:OE1	2.54	0.41
1:O:220:LYS:HZ3	1:O:1328:LEU:HB3	1.86	0.41
1:O:989:LEU:HD23	1:O:989:LEU:HA	1.75	0.41
1:J:147:THR:HA	1:J:148:PRO:HD3	1.96	0.41
1:J:871:ILE:HD12	1:J:871:ILE:HA	1.89	0.41
1:K:1157:ASP:HA	1:K:1158:PRO:HD3	1.95	0.41
1:K:1046:VAL:HG22	1:K:1184:ILE:HG13	2.02	0.41
1:N:268:THR:HG22	1:N:275:PRO:HB3	2.03	0.41
1:N:336:ALA:HA	1:N:340:ASP:HB2	2.03	0.41
1:O:255:VAL:HG13	1:O:1102:SER:HA	2.02	0.41
1:O:1201:SER:OG	1:O:1205:ARG:O	2.36	0.41
1:N:1128:PHE:CE1	1:N:1263:ALA:HB2	2.56	0.41
1:J:255:VAL:HG11	1:J:1061:SER:HB3	2.03	0.40
1:J:835:VAL:HG22	1:J:944:LEU:HD22	2.02	0.40
1:J:1057:ILE:HB	1:J:1106:THR:HG22	2.03	0.40
1:K:899:ARG:HA	1:K:899:ARG:HD2	1.83	0.40
1:K:1018:MET:HA	1:K:1021:MET:HG3	2.04	0.40
1:N:575:LEU:HD13	1:N:1243:TRP:HH2	1.87	0.40
1:N:750:ASN:H	1:N:792:PHE:HE1	1.68	0.40
1:O:511:TYR:HA	1:O:973:ARG:HH12	1.86	0.40
1:O:542:LEU:HB3	1:O:1249:SER:HA	2.03	0.40
1:J:580:PHE:CE1	1:J:1189:VAL:HG11	2.57	0.40
1:K:469:HIS:HB2	1:K:1253:ILE:HD12	2.03	0.40
1:O:255:VAL:HG21	1:O:1059:PHE:HD2	1.86	0.40
1:K:146:GLU:HG3	1:K:147:THR:HG23	2.02	0.40
1:K:248:LEU:HB3	1:K:374:LEU:HD21	2.02	0.40
1:K:462:PRO:HG2	1:K:1131:GLU:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1229:ARG:HD3	1:O:1172:PRO:HD3	2.04	0.40
1:K:395:TYR:HB3	1:K:398:ASN:ND2	2.36	0.40
1:K:1174:LEU:HD23	1:K:1174:LEU:HA	1.97	0.40
1:N:269:THR:HG22	1:N:271:LYS:N	2.35	0.40
1:O:877:THR:OG1	1:O:880:MET:SD	2.67	0.40
1:O:938:ARG:HA	1:O:941:THR:HG22	2.03	0.40
1:O:1247:LEU:HD23	1:O:1247:LEU:HA	1.91	0.40
5:Z:68:PRO:HG2	5:Z:71:GLN:HB3	2.02	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	J	1299/1381 (94%)	1225 (94%)	73 (6%)	1 (0%)	51	85
1	K	1379/1381 (100%)	1313 (95%)	56 (4%)	10 (1%)	22	62
1	N	1358/1381 (98%)	1305 (96%)	49 (4%)	4 (0%)	41	76
1	O	1295/1381 (94%)	1239 (96%)	52 (4%)	4 (0%)	41	76
2	v	283/507 (56%)	260 (92%)	22 (8%)	1 (0%)	34	72
3	w	66/570 (12%)	65 (98%)	1 (2%)	0	100	100
3	x	66/570 (12%)	66 (100%)	0	0	100	100
4	y	35/3149 (1%)	35 (100%)	0	0	100	100
4	z	35/3149 (1%)	34 (97%)	1 (3%)	0	100	100
5	Z	75/176 (43%)	71 (95%)	4 (5%)	0	100	100
5	a	75/176 (43%)	71 (95%)	3 (4%)	1 (1%)	12	48
5	d	75/176 (43%)	73 (97%)	2 (3%)	0	100	100
5	e	75/176 (43%)	73 (97%)	1 (1%)	1 (1%)	12	48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	f	247/364 (68%)	224 (91%)	21 (8%)	2 (1%)	19	60
6	h	330/364 (91%)	308 (93%)	20 (6%)	2 (1%)	25	65
7	k	297/301 (99%)	282 (95%)	14 (5%)	1 (0%)	41	76
7	m	297/301 (99%)	281 (95%)	15 (5%)	1 (0%)	41	76
7	p	297/301 (99%)	285 (96%)	11 (4%)	1 (0%)	41	76
7	r	297/301 (99%)	282 (95%)	10 (3%)	5 (2%)	9	43
All	All	7881/16105 (49%)	7492 (95%)	355 (4%)	34 (0%)	38	72

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	556	GLU
1	K	360	GLU
1	K	911	ALA
1	K	912	PRO
1	K	1264	VAL
1	K	1265	PRO
1	N	266	THR
1	O	488	SER
1	O	1011	SER
5	a	19	PRO
6	h	306	ALA
7	p	98	GLN
7	r	192	GLU
7	r	193	VAL
7	r	203	ASP
1	K	361	ASP
5	e	33	ASN
7	r	255	LEU
1	K	805	ALA
1	O	300	ASN
7	k	161	MET
7	m	129	ASP
1	K	806	ASP
1	K	913	ASN
1	O	489	LEU
6	f	161	SER
6	h	310	PRO
1	N	484	ARG
1	N	671	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	672	ASN
7	r	194	PRO
1	K	357	ALA
6	f	162	PRO
2	v	94	PRO

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	J	1110/1171 (95%)	1107 (100%)	3 (0%)	92	95
1	K	1171/1171 (100%)	1160 (99%)	11 (1%)	78	88
1	N	1155/1171 (99%)	1148 (99%)	7 (1%)	86	92
1	O	1103/1171 (94%)	1098 (100%)	5 (0%)	88	93
2	v	243/400 (61%)	243 (100%)	0	100	100
3	w	57/465 (12%)	57 (100%)	0	100	100
3	x	57/465 (12%)	57 (100%)	0	100	100
4	y	35/2539 (1%)	35 (100%)	0	100	100
4	z	35/2539 (1%)	35 (100%)	0	100	100
5	Z	71/128 (56%)	71 (100%)	0	100	100
5	a	71/128 (56%)	70 (99%)	1 (1%)	67	81
5	d	71/128 (56%)	71 (100%)	0	100	100
5	e	71/128 (56%)	71 (100%)	0	100	100
6	f	218/289 (75%)	216 (99%)	2 (1%)	78	88
6	h	278/289 (96%)	278 (100%)	0	100	100
7	k	265/267 (99%)	263 (99%)	2 (1%)	81	89
7	m	265/267 (99%)	264 (100%)	1 (0%)	91	94
7	p	265/267 (99%)	264 (100%)	1 (0%)	91	94
7	r	265/267 (99%)	261 (98%)	4 (2%)	65	80
All	All	6806/13250 (51%)	6769 (100%)	37 (0%)	89	93

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	556	GLU
1	J	653	ARG
1	J	1062	ARG
1	K	109	ARG
1	K	360	GLU
1	K	361	ASP
1	K	481	ARG
1	K	484	ARG
1	K	653	ARG
1	K	804	HIS
1	K	936	ARG
1	K	938	ARG
1	K	1150	ARG
1	K	1264	VAL
1	N	266	THR
1	N	267	TYR
1	N	484	ARG
1	N	670	LEU
1	N	938	ARG
1	N	1077	ARG
1	N	1272	ARG
1	O	267	TYR
1	O	481	ARG
1	O	889	MET
1	O	1109	ARG
1	O	1139	ASN
5	a	20	ASP
6	f	237	LEU
6	f	294	ARG
7	k	161	MET
7	k	197	LEU
7	m	118	ARG
7	p	98	GLN
7	r	193	VAL
7	r	201	LEU
7	r	202	LEU
7	r	265	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	126	HIS
1	J	285	ASN
1	J	300	ASN
1	J	389	ASN
1	J	444	ASN
1	J	581	GLN
1	J	587	GLN
1	J	596	HIS
1	J	636	ASN
1	J	669	HIS
1	J	834	HIS
1	J	859	ASN
1	J	904	ASN
1	J	908	GLN
1	J	921	GLN
1	J	1176	HIS
1	J	1241	ASN
1	J	1360	HIS
1	K	123	HIS
1	K	289	GLN
1	K	317	ASN
1	K	362	GLN
1	K	385	GLN
1	K	389	ASN
1	K	543	HIS
1	K	795	HIS
1	K	804	HIS
1	K	822	ASN
1	K	824	HIS
1	K	997	HIS
1	K	1197	GLN
1	K	1217	GLN
1	N	123	HIS
1	N	125	HIS
1	N	317	ASN
1	N	362	GLN
1	N	444	ASN
1	N	496	HIS
1	N	543	HIS
1	N	564	HIS
1	N	587	GLN
1	N	788	HIS
1	N	804	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	942	GLN
1	N	964	HIS
1	N	997	HIS
1	N	1179	GLN
1	N	1284	ASN
1	N	1323	GLN
1	O	121	ASN
1	O	226	HIS
1	O	415	ASN
1	O	432	GLN
1	O	491	HIS
1	O	496	HIS
1	O	531	HIS
1	O	581	GLN
1	O	587	GLN
1	O	824	HIS
1	O	977	GLN
1	O	1090	HIS
1	O	1176	HIS
2	v	7	ASN
2	v	45	GLN
2	v	290	HIS
3	w	77	HIS
6	h	291	ASN
6	h	309	GLN
7	k	120	HIS
7	k	128	ASN
7	k	204	ASN
7	m	128	ASN
7	m	148	GLN
7	m	175	HIS
7	m	204	ASN
7	m	291	GLN
7	p	95	ASN
7	p	102	GLN
7	p	148	GLN
7	r	120	HIS
7	r	154	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

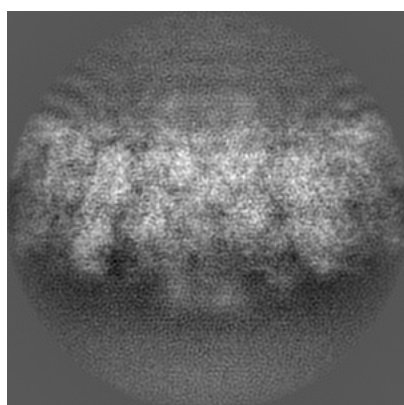
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21526. These allow visual inspection of the internal detail of the map and identification of artifacts.

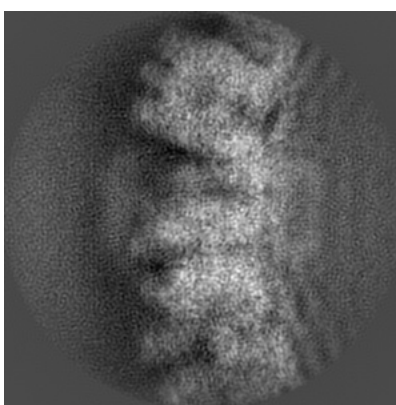
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

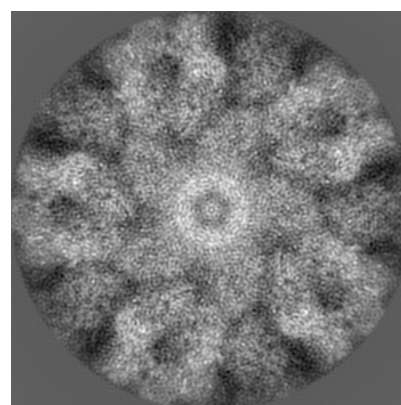
6.1.1 Primary map



X



Y

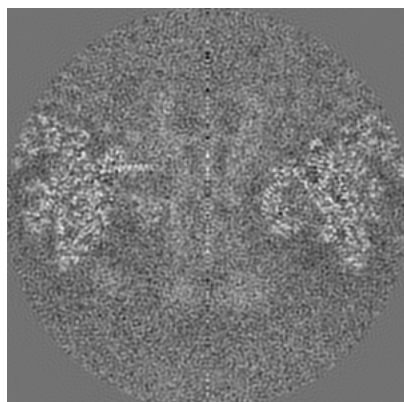


Z

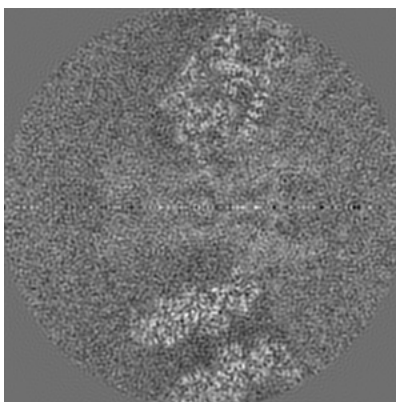
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

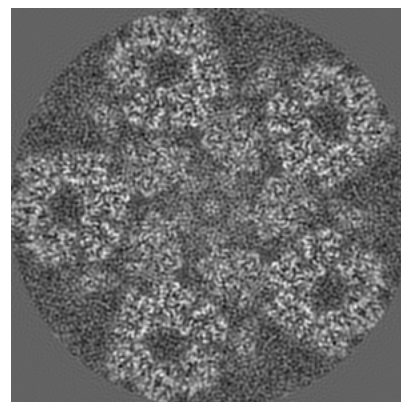
6.2.1 Primary map



X Index: 160



Y Index: 160

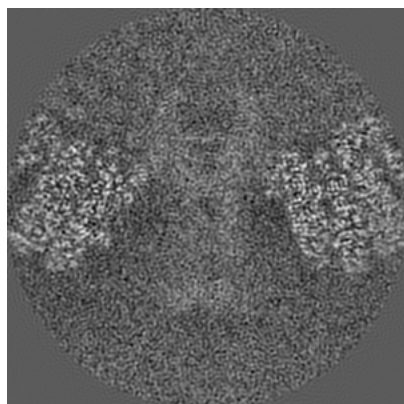


Z Index: 160

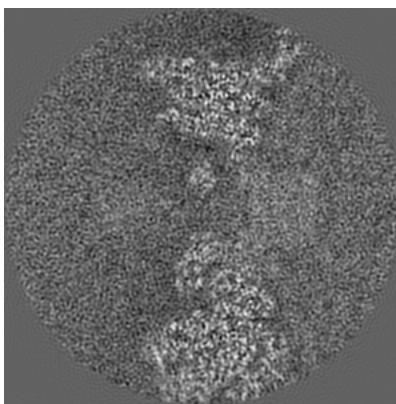
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

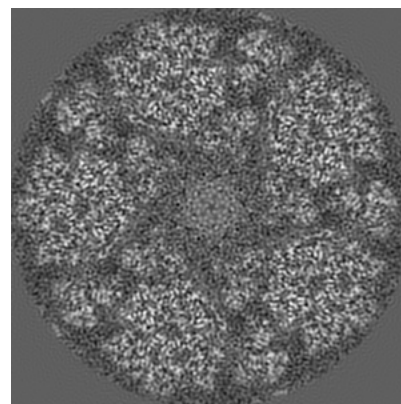
6.3.1 Primary map



X Index: 147



Y Index: 193

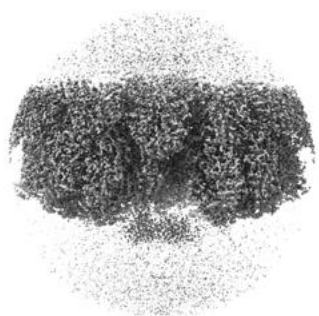


Z Index: 175

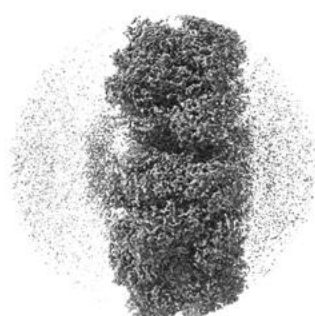
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

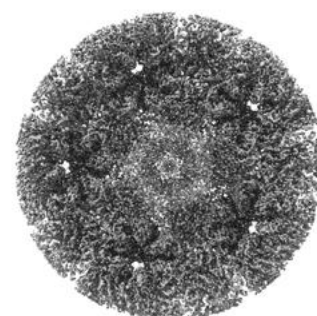
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

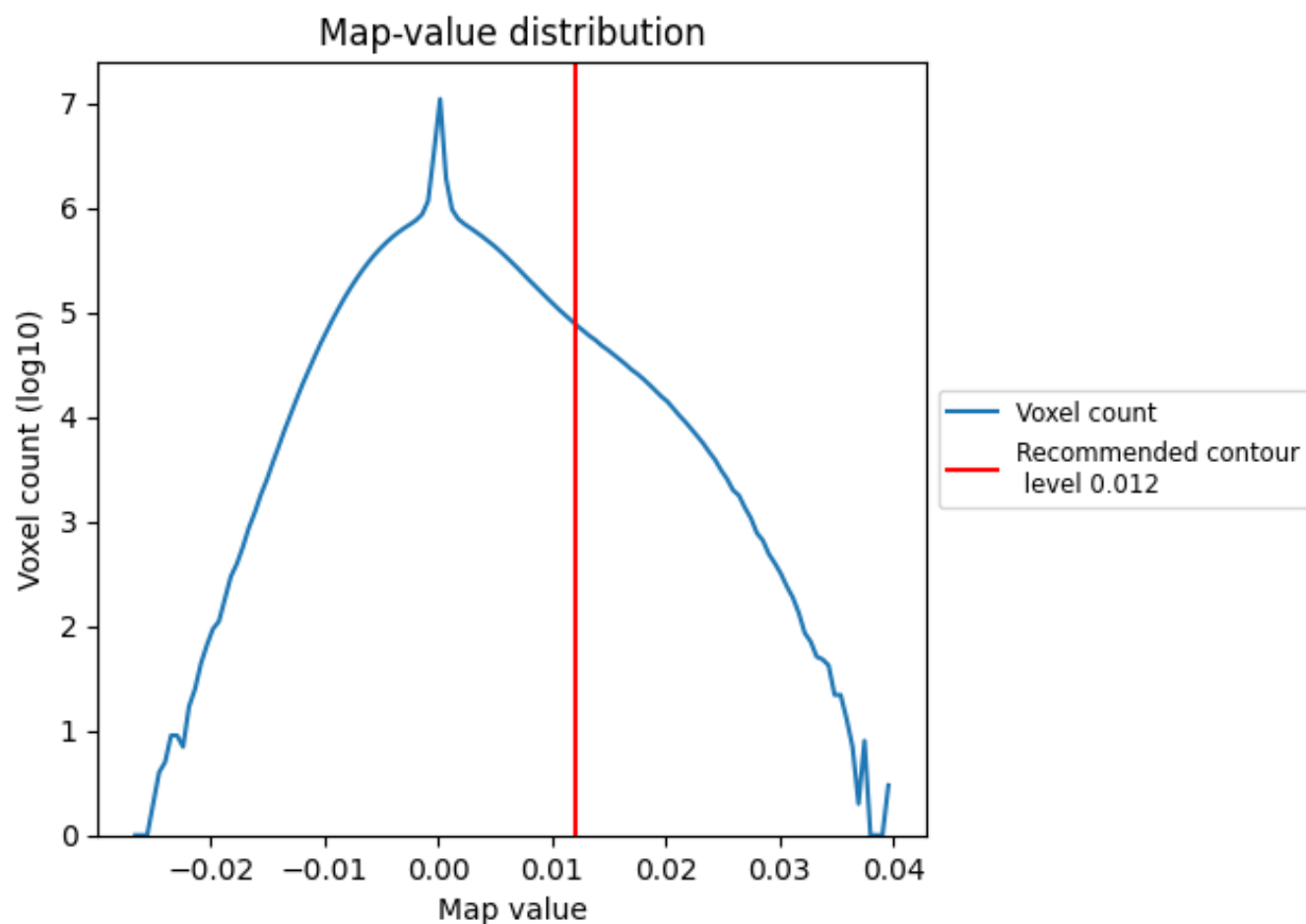
6.5 Mask visualisation

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

7 Map analysis [i](#)

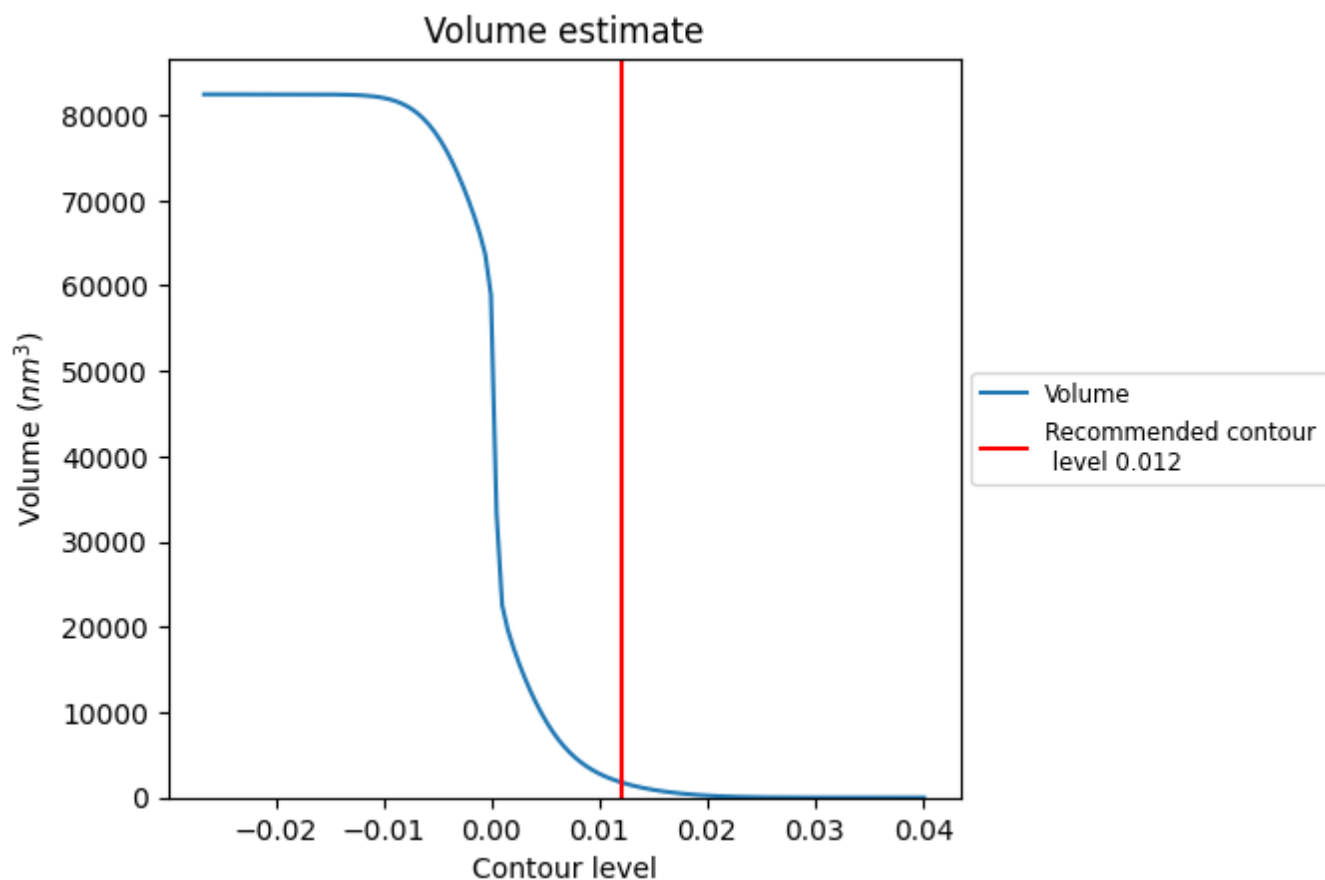
This section contains the results of statistical analysis of the map.

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.

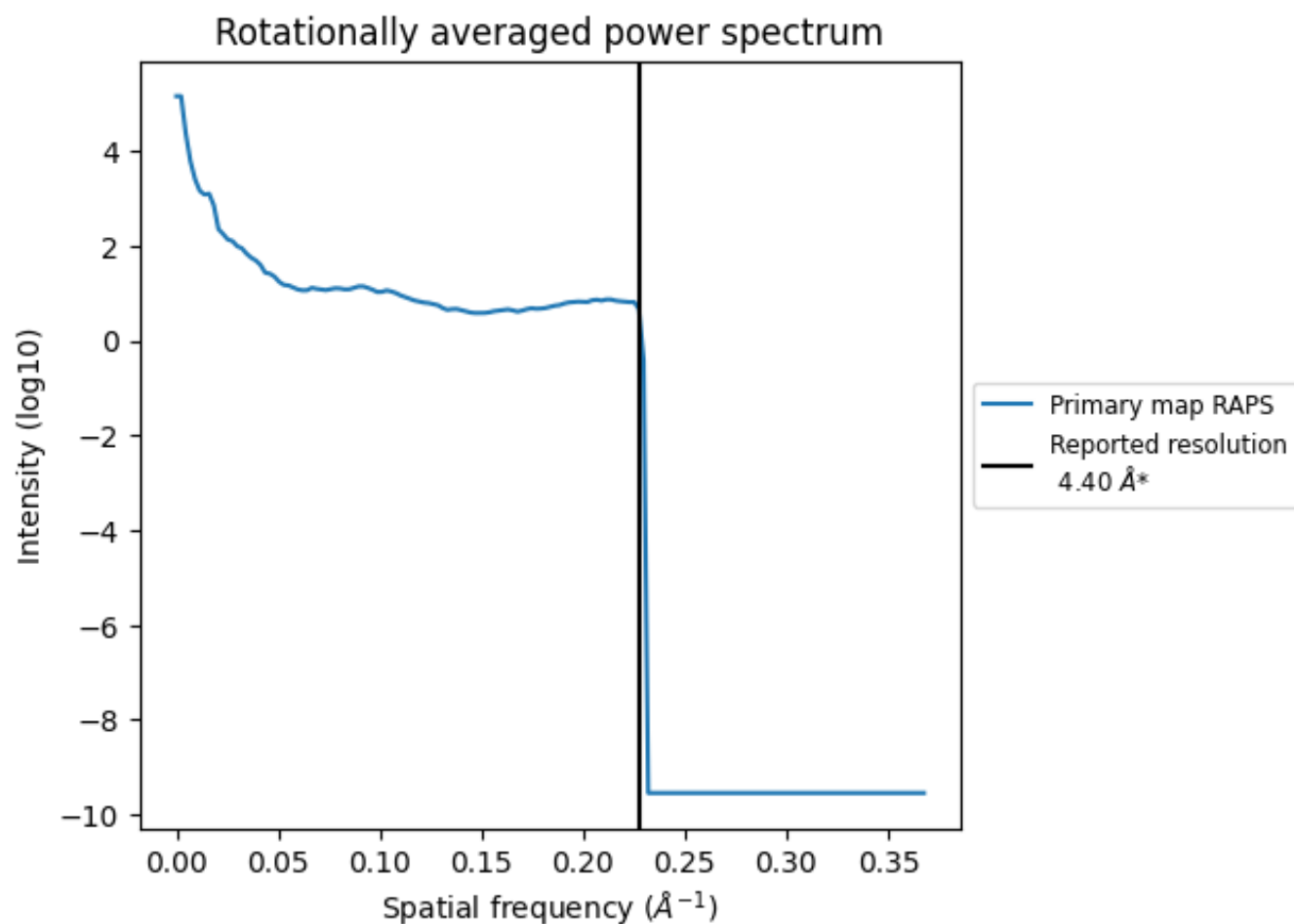
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1798 nm³; this corresponds to an approximate mass of 1624 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 0.227 \AA^{-1}

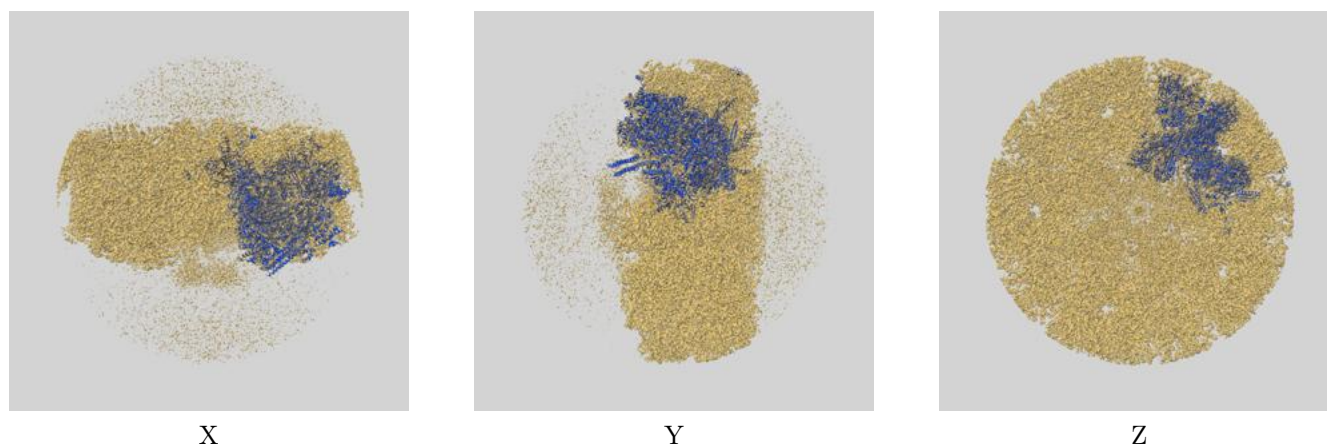
8 Fourier-Shell correlation ⓘ

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-21526 and PDB model 6W2E. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



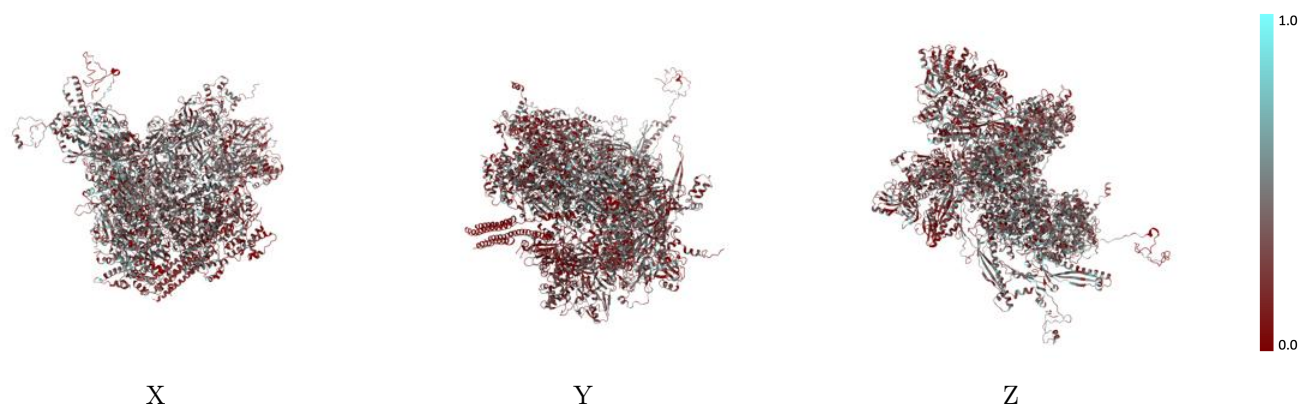
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



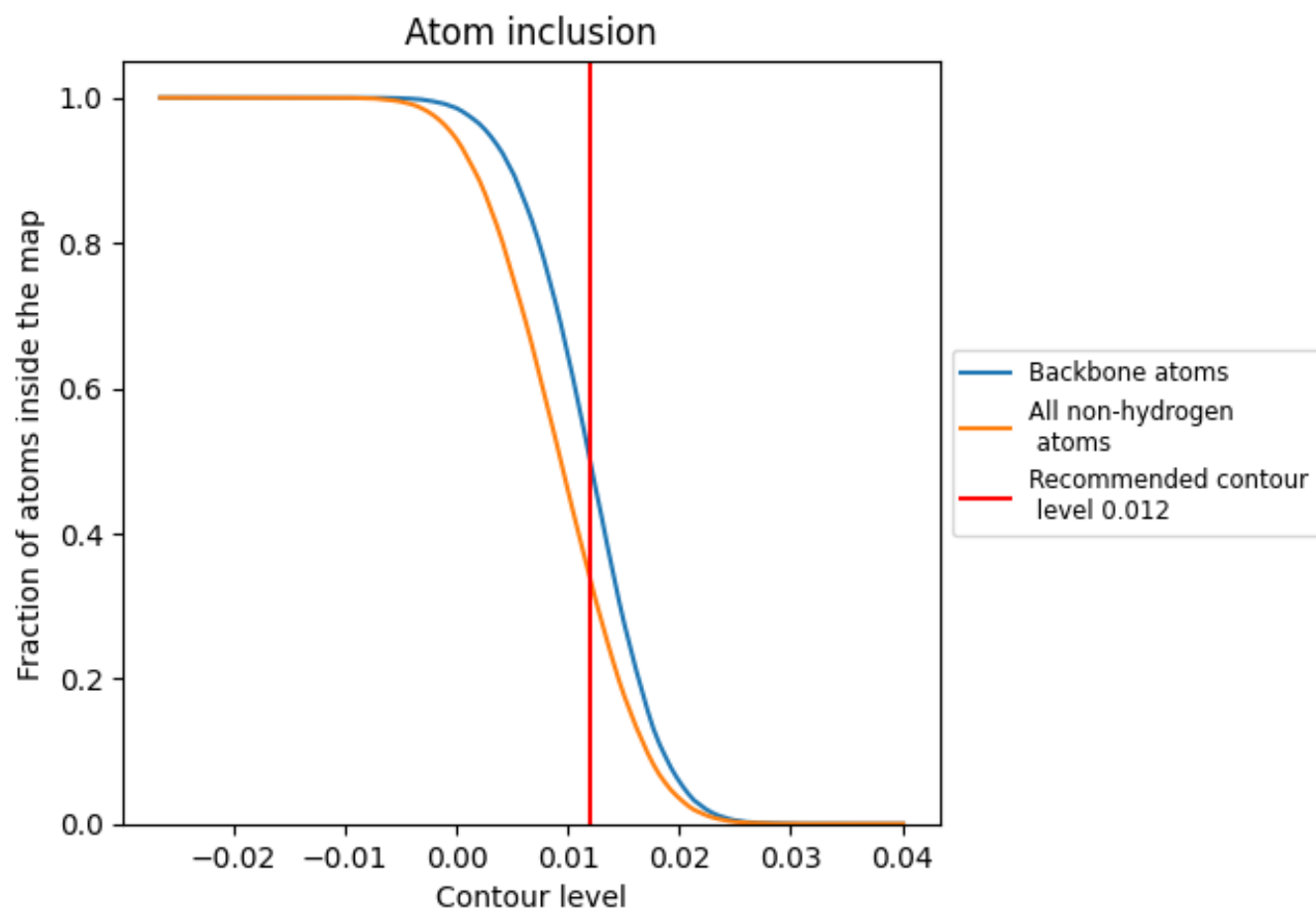
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 34% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3364	 0.2450
J	 0.3909	 0.2500
K	 0.3873	 0.2640
N	 0.3498	 0.2590
O	 0.3698	 0.2460
Z	 0.3003	 0.2310
a	 0.3099	 0.2180
d	 0.1725	 0.1880
e	 0.2859	 0.2230
f	 0.2491	 0.2260
h	 0.3450	 0.2610
k	 0.2775	 0.2310
m	 0.2858	 0.2490
p	 0.2914	 0.2330
r	 0.2993	 0.2550
v	 0.1691	 0.1870
w	 0.0720	 0.1710
x	 0.1174	 0.1700
y	 0.0629	 0.1150
z	 0.0497	 0.1040

