



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 11:40 PM UTC

PDB ID : 7RD1 / pdb_00007rd1
EMDB ID : EMD-24408
Title : The Capsid Structure of the ChAdOx1 viral vector/chimpanzee adenovirus Y25
Authors : Baker, A.T.; Boyd, R.J.; Sarkar, D.; Vermaas, J.V.; Williams, D.; Singharoy, A.
Deposited on : 2021-07-08
Resolution : 3.07 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

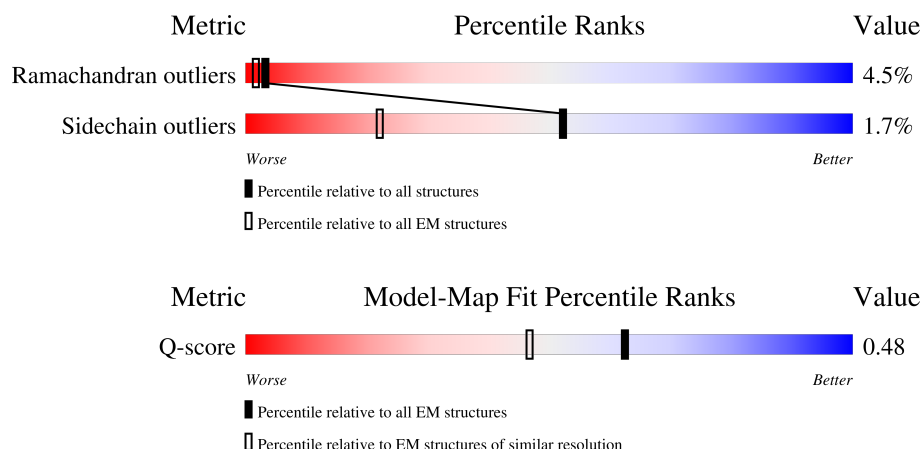
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.07 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.



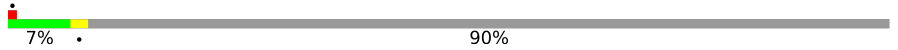
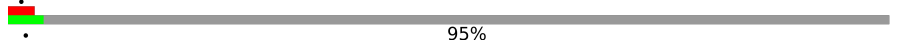
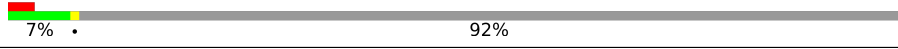
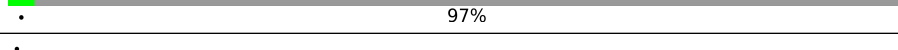
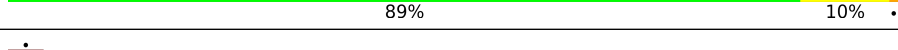
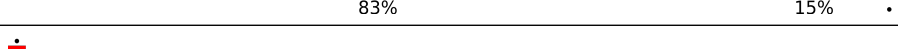
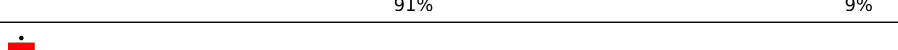
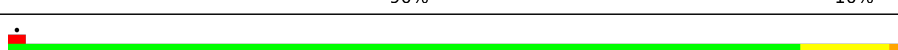
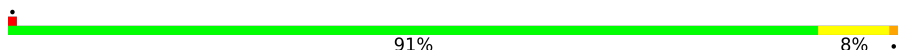
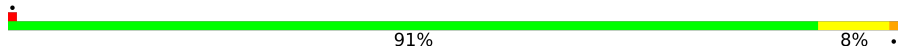
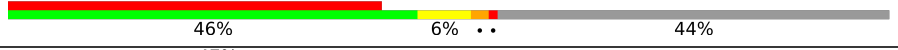
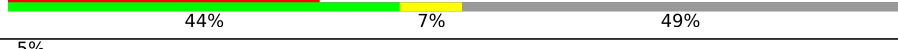
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13977 (2.57 - 3.57)

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	0	243	97%
1	1	243	6% 93%
1	2	243	8% 91%
1	3	243	8% 89%
1	4	243	8% 91%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	8	243	
1	U	243	
1	V	243	
1	W	243	
1	X	243	
1	Y	243	
1	Z	243	
2	A	942	
2	B	942	
2	C	942	
2	D	942	
2	E	942	
2	F	942	
2	G	942	
2	H	942	
2	I	942	
2	J	942	
2	K	942	
2	L	942	
3	M	532	
4	N	142	
4	O	142	
4	P	142	
4	Q	142	
5	R	589	

Continued on next page...

Mol	Chain	Length	Quality of chain
6	S	227	5% 69% 7% 23%
6	T	227	5% 67% 11% 22%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 197782 atoms, of which 96589 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 Pre-protein VI.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	7	Total	C	H	N	O		0	0
			106	35	51	8	12			
1	U	11	Total	C	H	N	O		0	0
			171	55	83	17	16			
1	1	17	Total	C	H	N	O		0	0
			245	77	118	23	27			
1	V	20	Total	C	H	N	O	S	0	0
			286	96	136	22	31	1		
1	2	21	Total	C	H	N	O	S	0	0
			323	106	156	31	29	1		
1	W	24	Total	C	H	N	O	S	0	0
			361	118	174	34	34	1		
1	3	26	Total	C	H	N	O	S	0	0
			386	125	186	36	38	1		
1	X	26	Total	C	H	N	O	S	0	0
			386	125	186	36	38	1		
1	4	22	Total	C	H	N	O	S	0	0
			335	110	160	32	32	1		
1	Y	26	Total	C	H	N	O	S	0	0
			386	125	186	36	38	1		
1	8	24	Total	C	H	N	O	S	0	0
			363	118	177	34	33	1		
1	Z	7	Total	C	H	N	O		0	0
			106	35	51	8	12			

- Molecule 2 is a protein called Hexon protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		
2	B	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		
2	C	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		
2	E	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		
2	F	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		
2	G	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		
2	H	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		
2	I	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		
2	J	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		
2	K	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		
2	L	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		

- Molecule 3 is a protein called Penton protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	M	435	Total	C	H	N	O	S	0	0
			6923	2219	3423	596	672	13		

- Molecule 4 is a protein called Hexon-interlacing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	N	89	Total	C	H	N	O	S	0	0
			1328	412	664	114	135	3		
4	O	79	Total	C	H	N	O	S	0	0
			1187	368	595	102	119	3		
4	P	96	Total	C	H	N	O	S	0	0
			1435	443	720	125	144	3		
4	Q	73	Total	C	H	N	O	S	0	0
			1108	342	560	99	104	3		

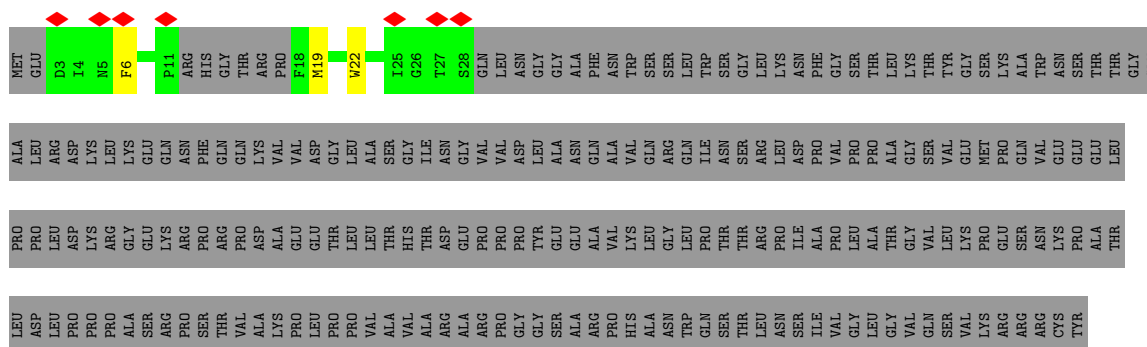
- Molecule 5 is a protein called Pre-hexon-linking protein IIIa.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	R	114	Total	C	H	N	O	S	0	0
			1767	539	885	167	173	3		

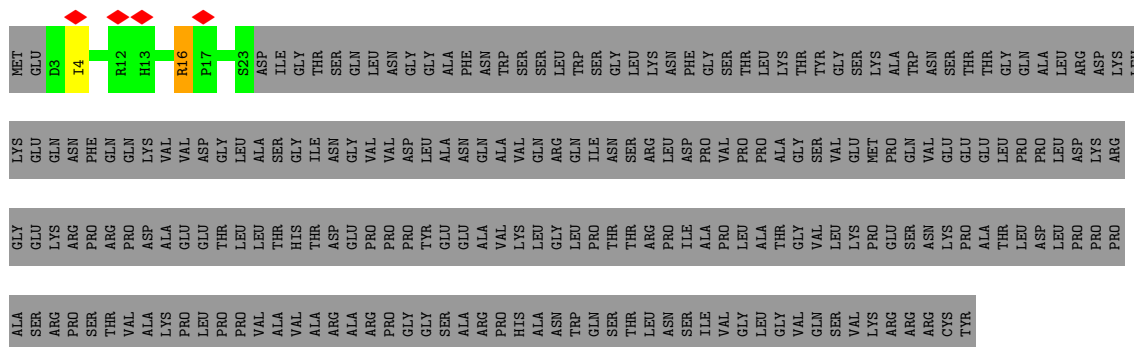
- Molecule 6 is a protein called Pre-hexon-linking protein VIII.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	S	175	Total	C	H	N	O	S	0	0
			2673	861	1308	234	265	5		
6	T	177	Total	C	H	N	O	S	0	0
			2695	867	1318	236	269	5		

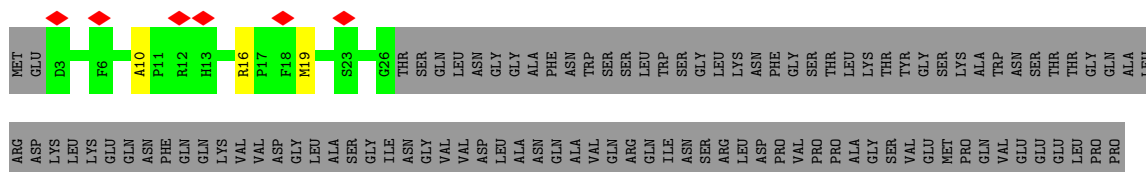
- Molecule 1: Pre-protein VI



- Molecule 1: Pre-protein VI

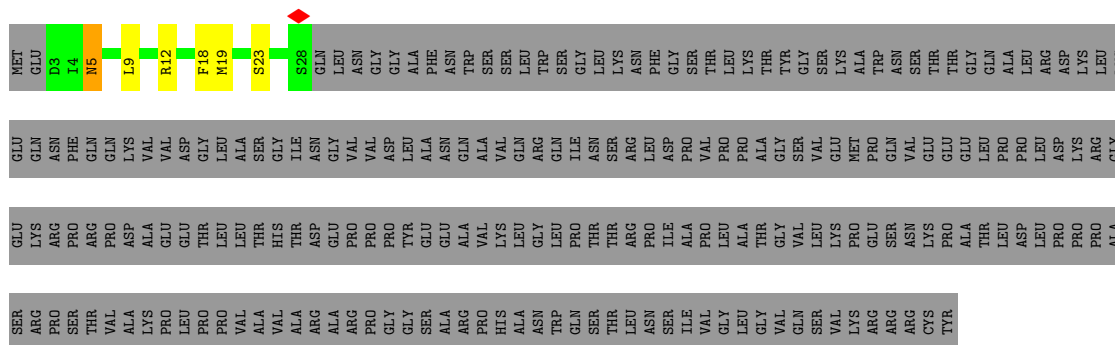


- Molecule 1: Pre-protein VI

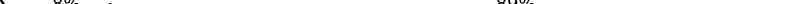


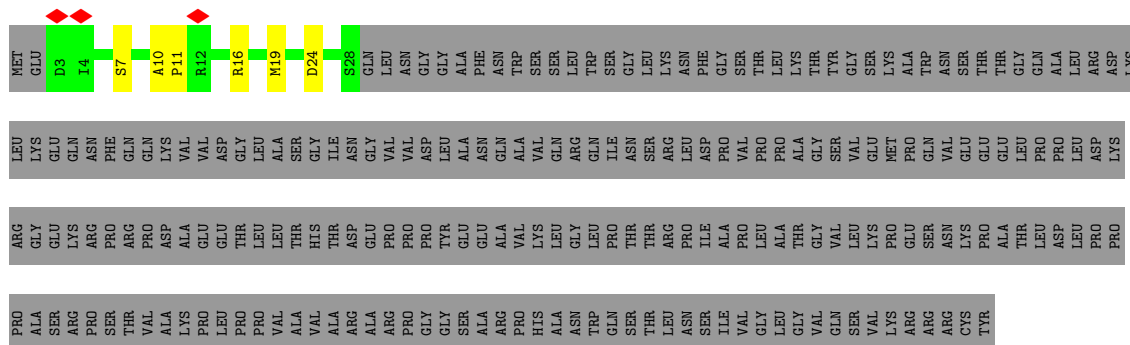
- Molecule 1: Pre-protein VI

Chain 3: 8% 89%



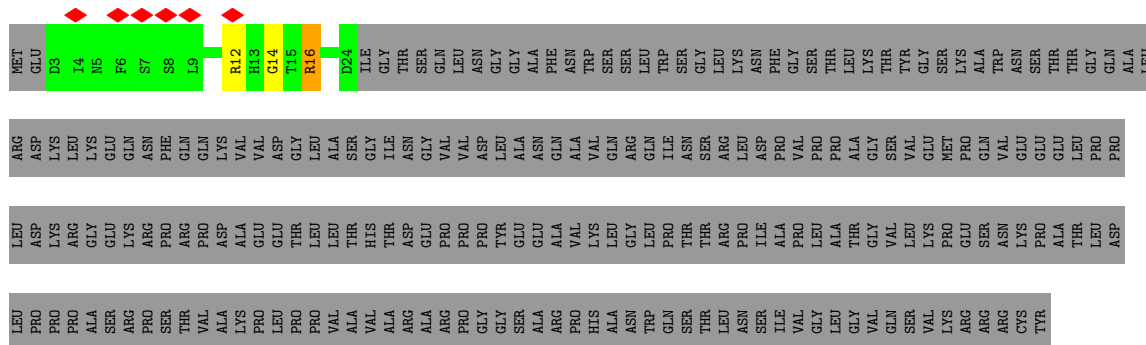
- Molecule 1: Pre-protein VI

Chain X:  8% 89%

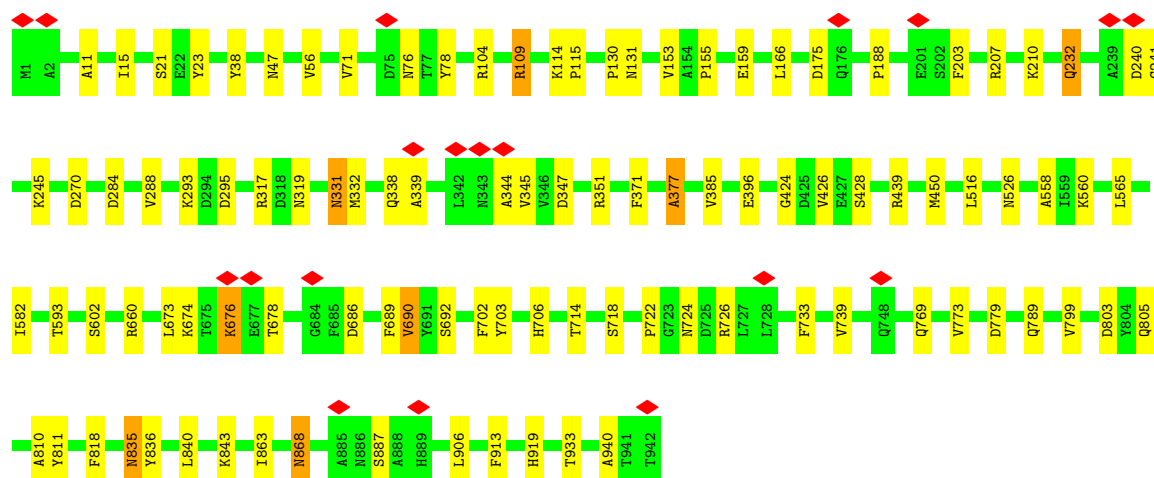


- Molecule 1: Pre-protein VI

Chain 4: 8% 91%

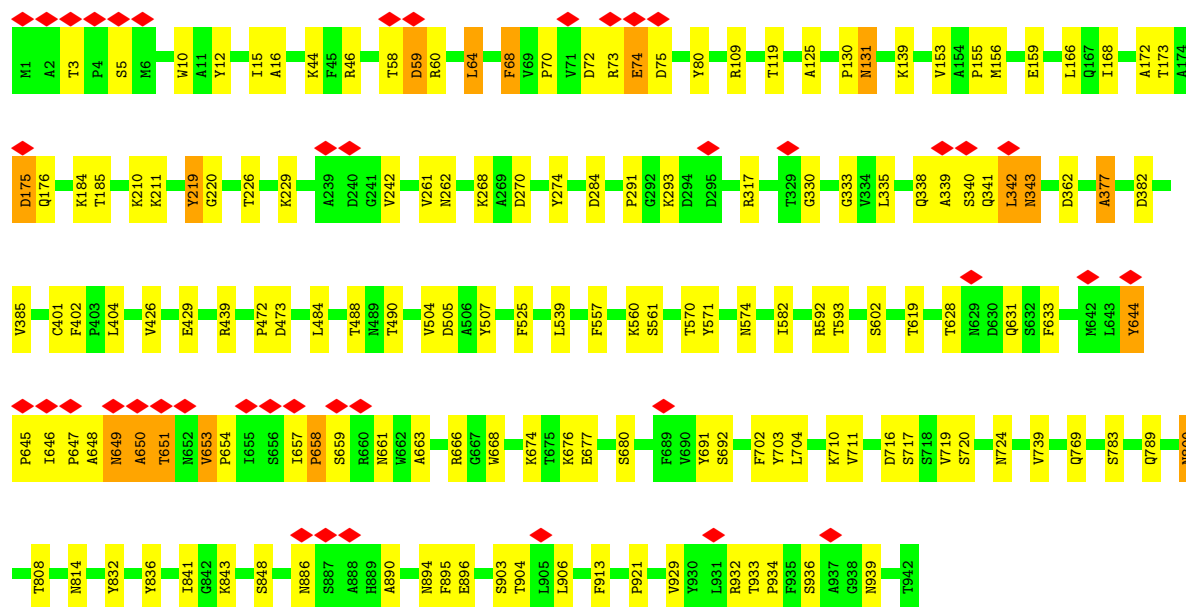


- Molecule 1: Pre-protein VI



• Molecule 2: Hexon protein

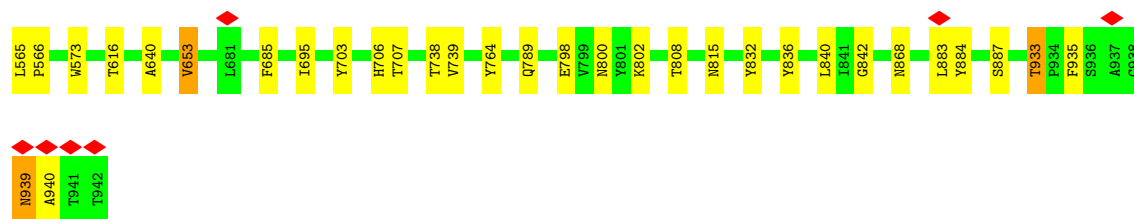
Chain B: 83% 15%



• Molecule 2: Hexon protein

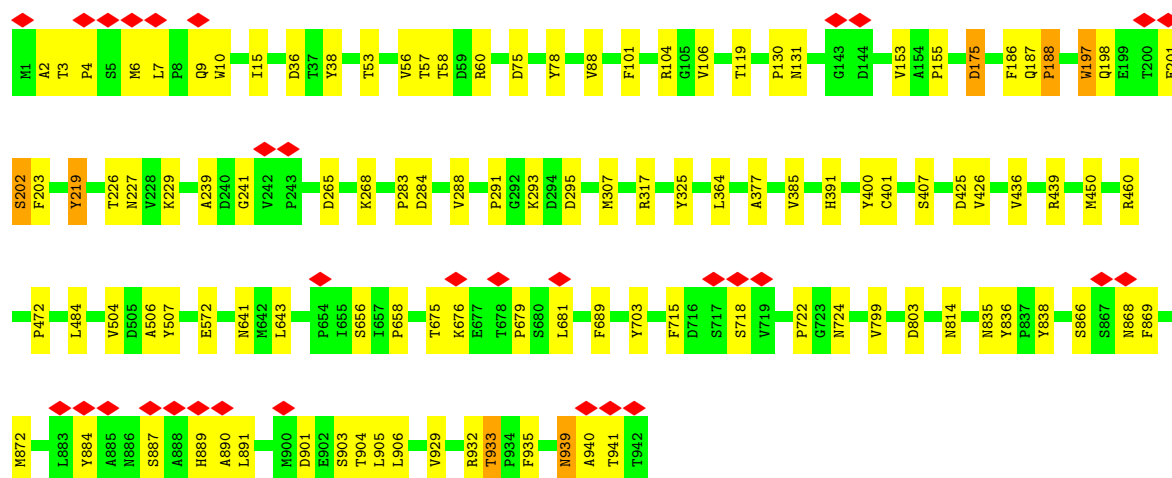
Chain C: 91% 9%





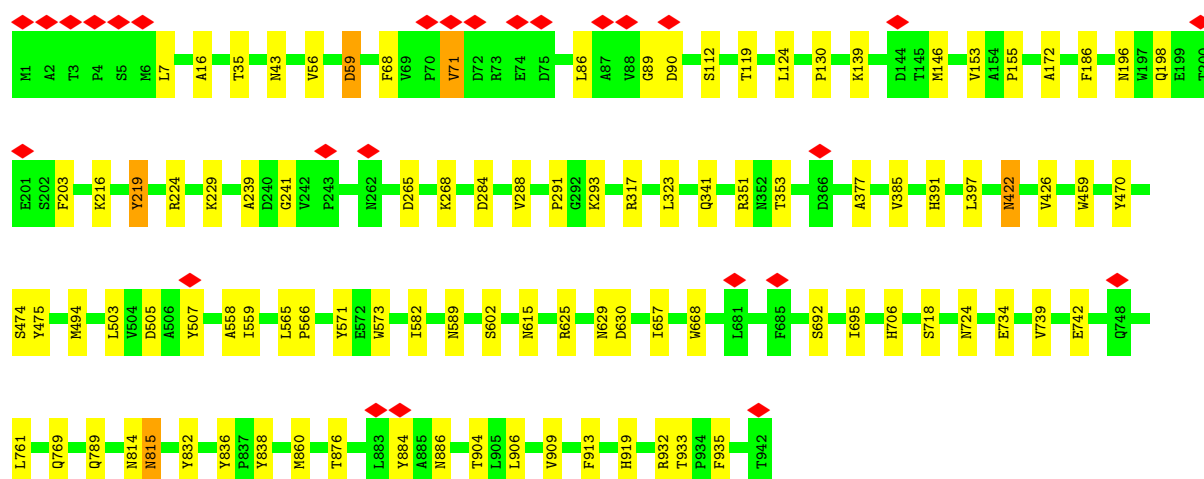
• Molecule 2: Hexon protein

Chain D: 88% 11%



• Molecule 2: Hexon protein

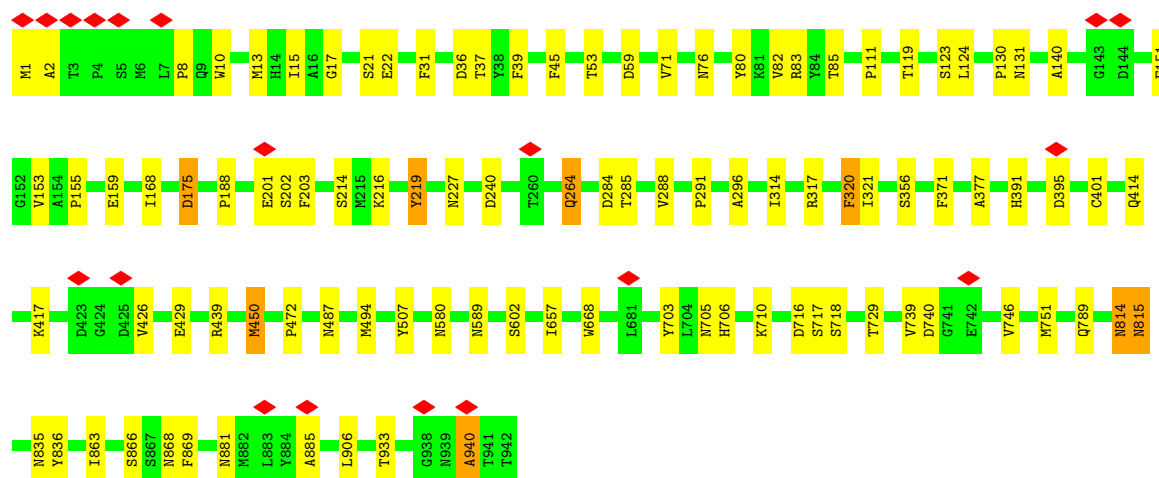
Chain E: 90% 10%



• Molecule 2: Hexon protein

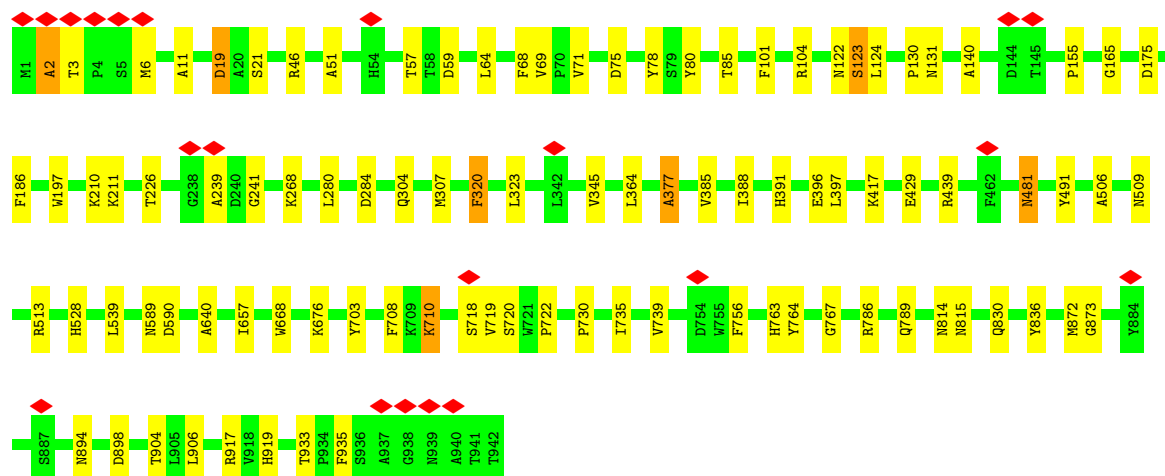
Chain F: 89% 10%





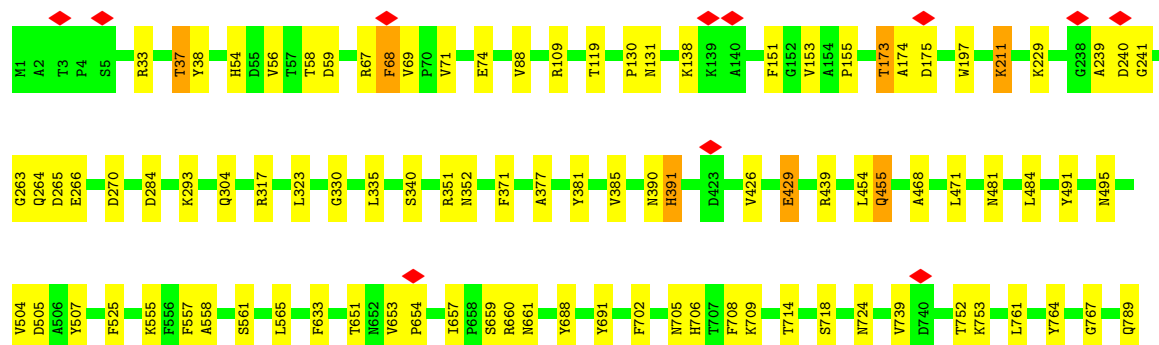
• Molecule 2: Hexon protein

Chain G: 90% 10%



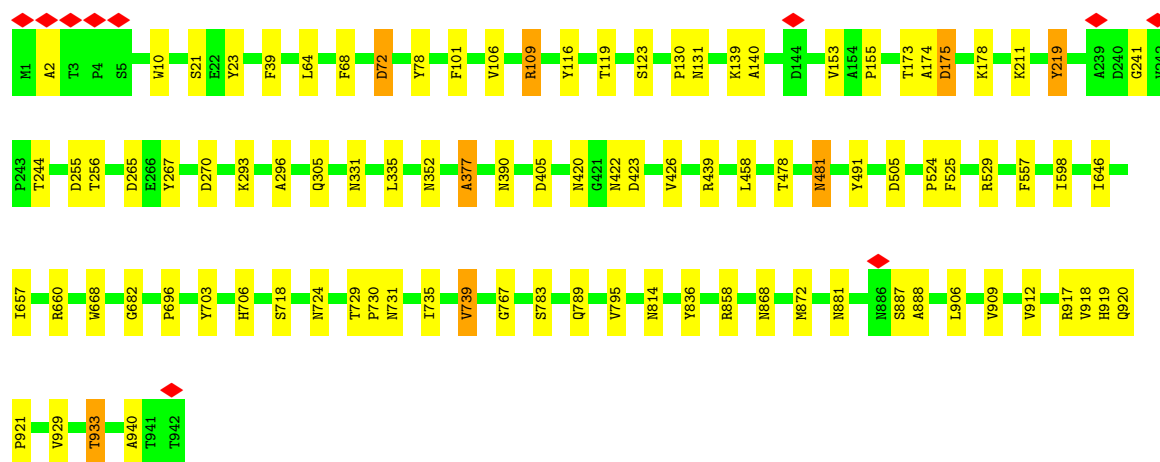
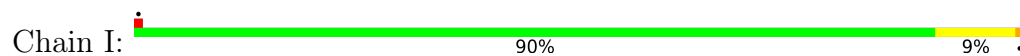
• Molecule 2: Hexon protein

Chain H: 88% 11%

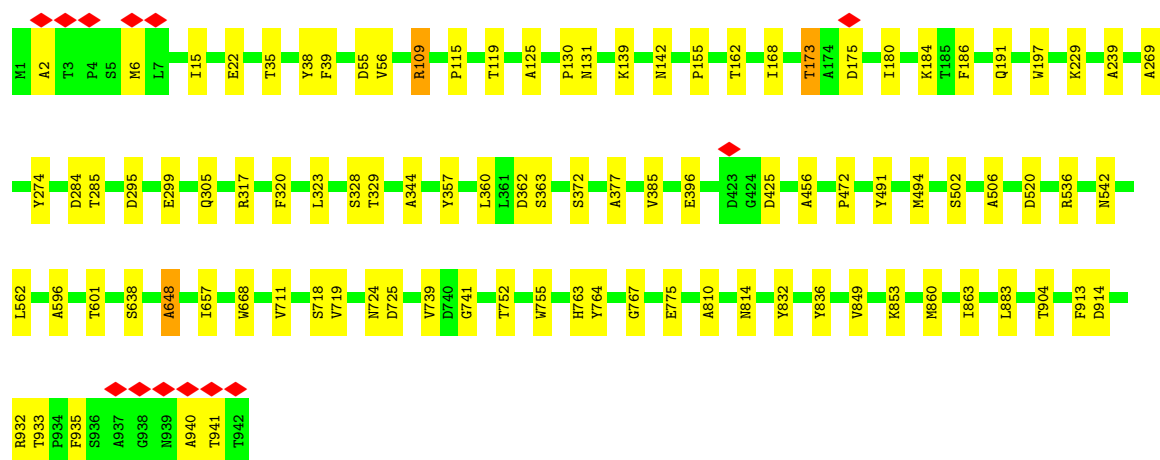
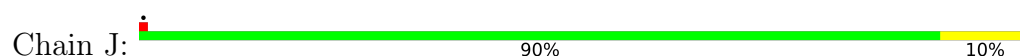




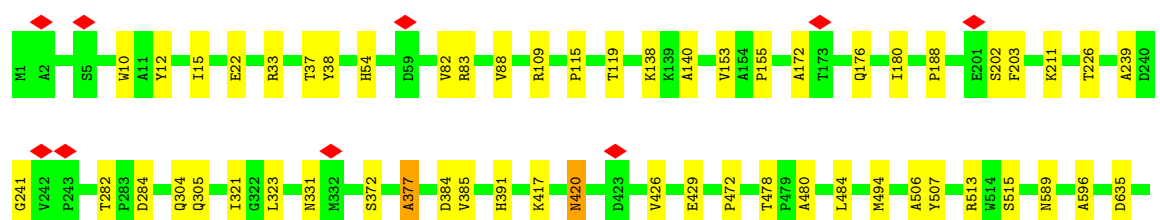
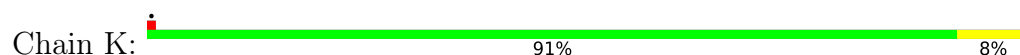
• Molecule 2: Hexon protein

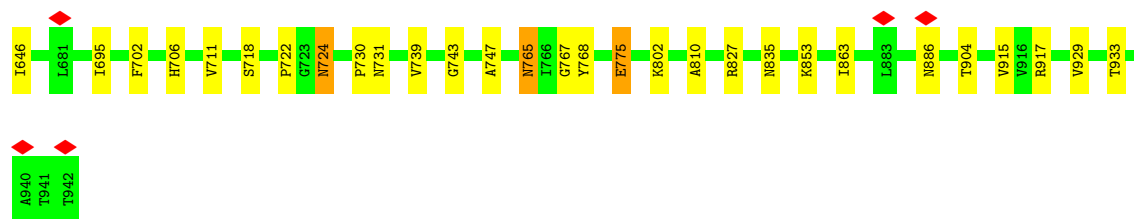


• Molecule 2: Hexon protein



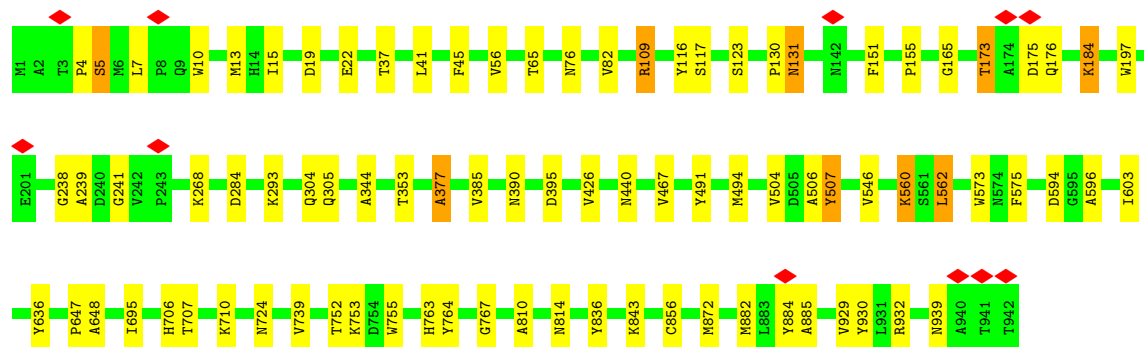
• Molecule 2: Hexon protein





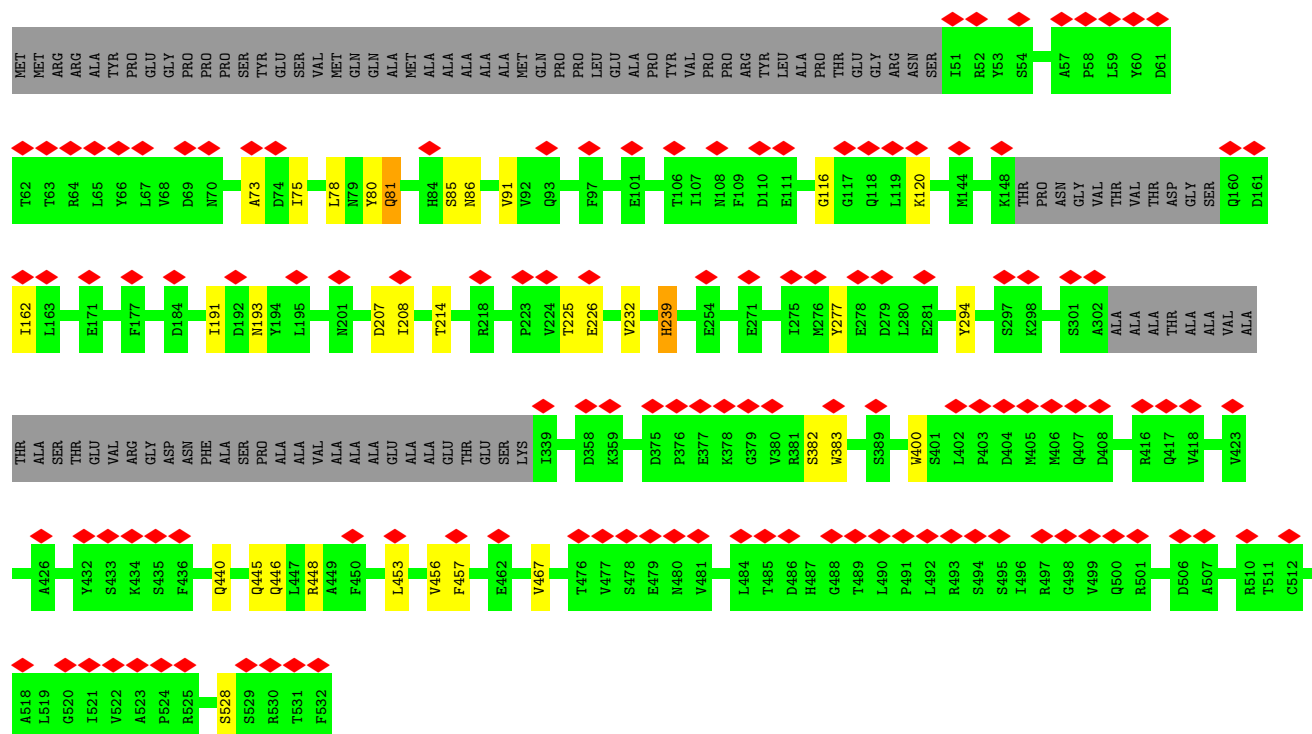
• Molecule 2: Hexon protein

Chain L: 91% 8%

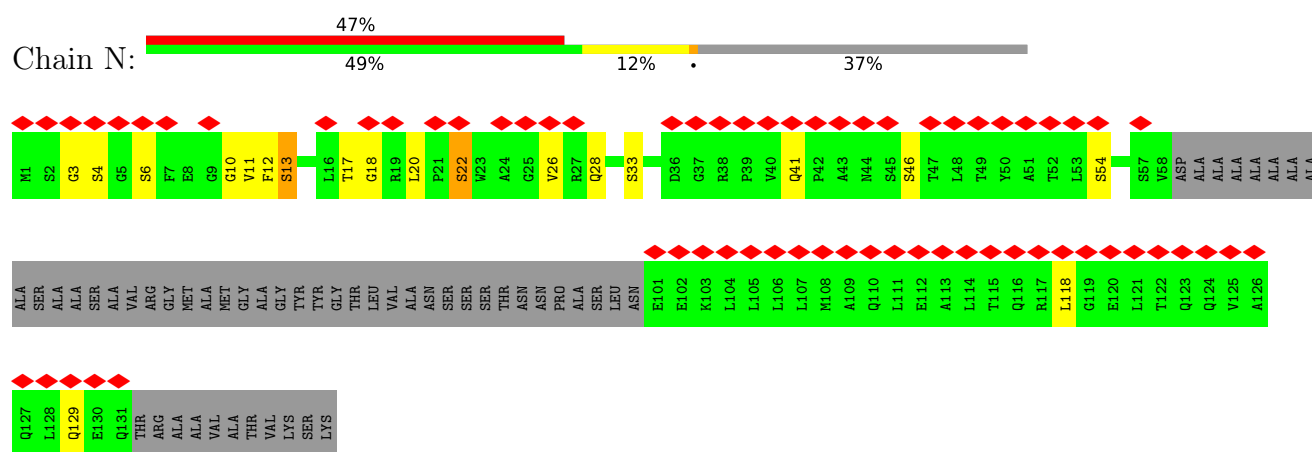


• Molecule 3: Penton protein

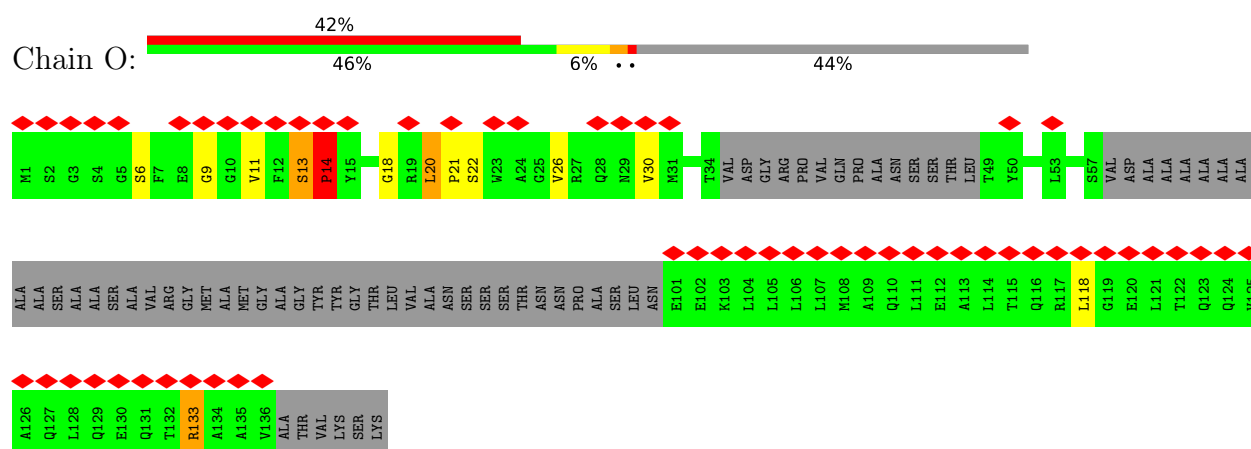
Chain M: 24% 75% 6% 18%



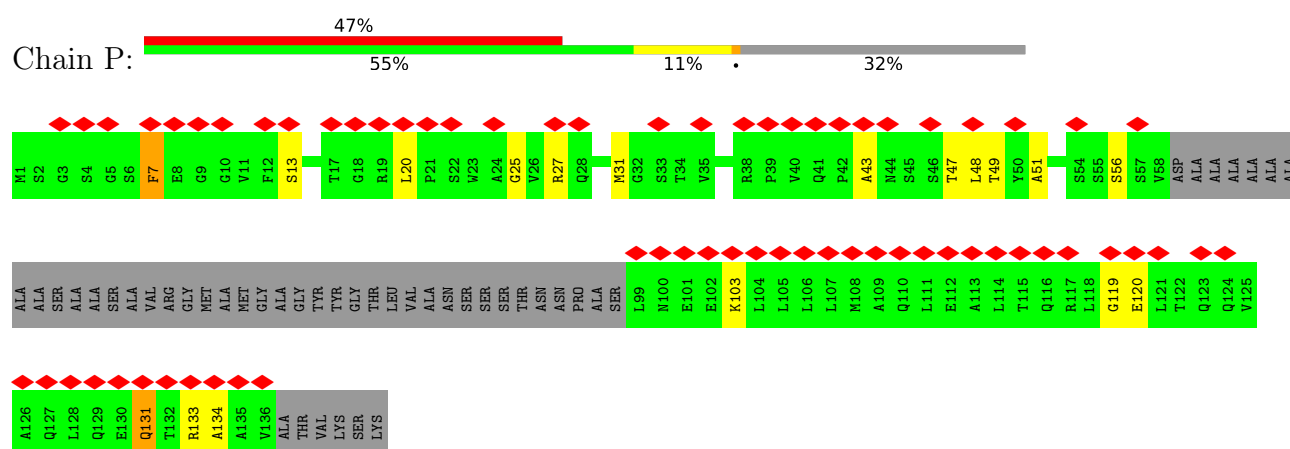
• Molecule 4: Hexon-interlacing protein



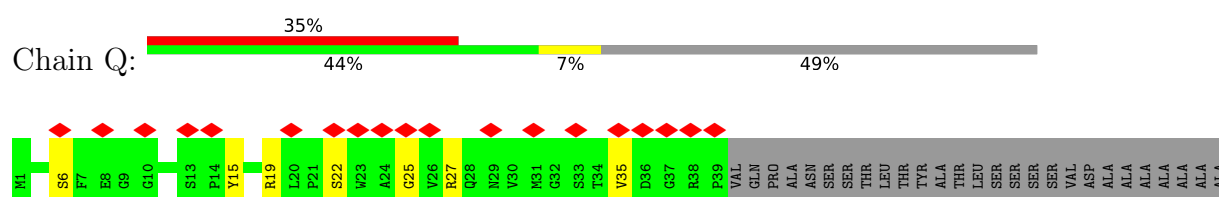
• Molecule 4: Hexon-interlacing protein

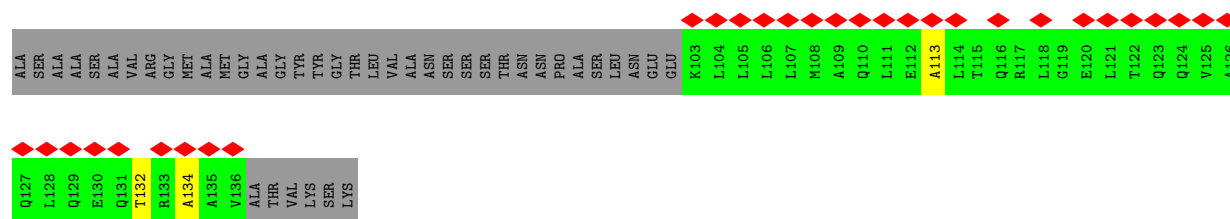


• Molecule 4: Hexon-interlacing protein

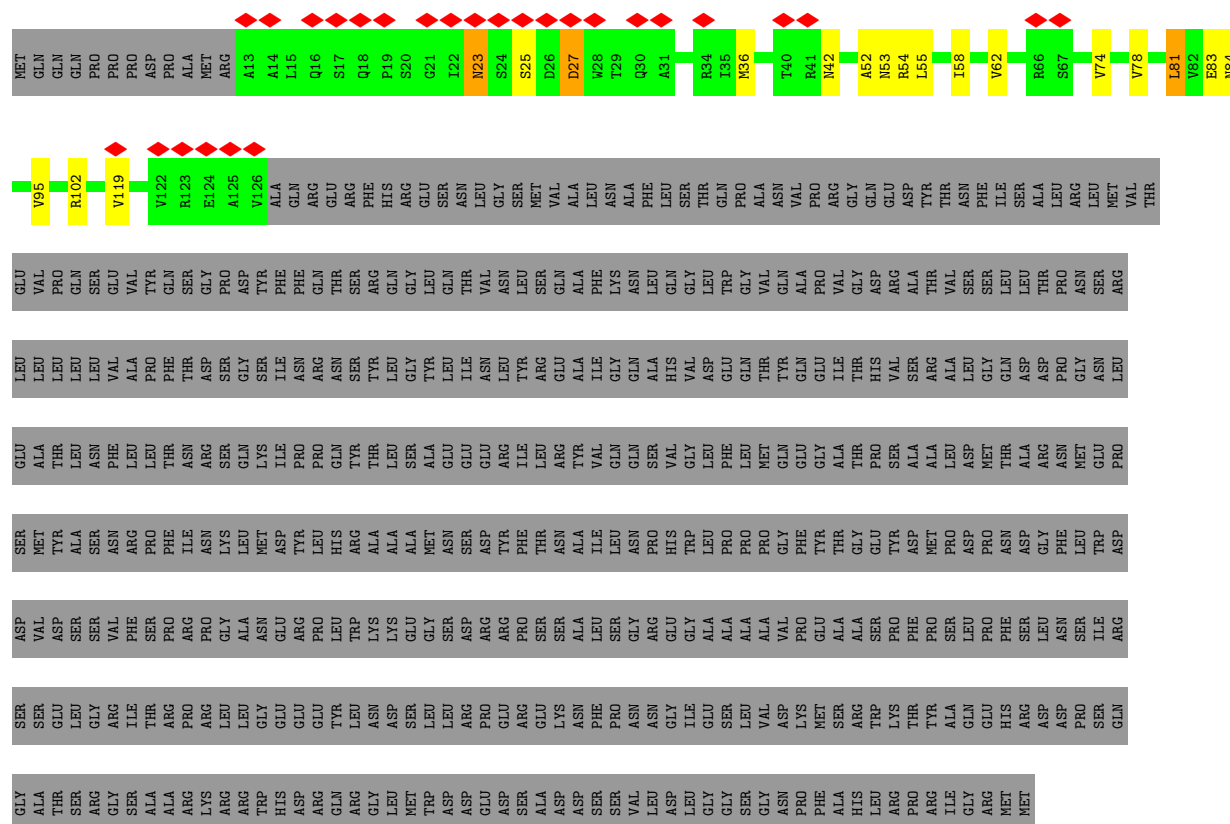


• Molecule 4: Hexon-interlacing protein

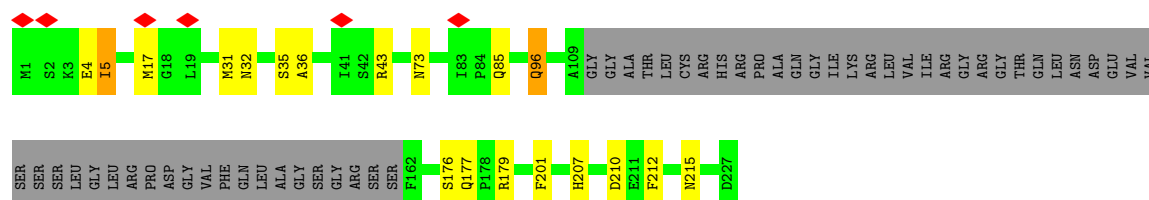




• Molecule 5: Pre-hexon-linking protein IIIa

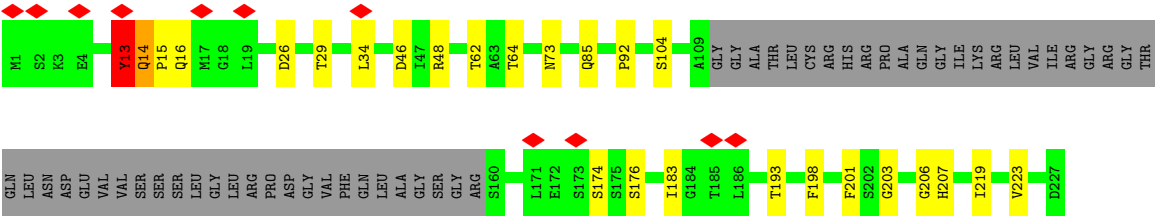


• Molecule 6: Pre-hexon-linking protein VIII



• Molecule 6: Pre-hexon-linking protein VIII





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5748	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.1802	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	0.095	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	1929.6006, 1929.6006, 1929.6006	wwPDB
Map dimensions	1260, 1260, 1260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.531429, 1.531429, 1.531429	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	0	1.10	0/55	1.26	0/73
1	1	1.07	0/128	1.65	1/171 (0.6%)
1	2	1.04	0/173	1.51	0/234
1	3	0.98	0/206	1.72	4/279 (1.4%)
1	4	0.93	0/181	1.57	0/245
1	8	1.20	0/192	1.68	2/260 (0.8%)
1	U	1.09	0/90	1.44	0/121
1	V	1.05	0/153	1.54	0/206
1	W	1.02	0/193	1.53	0/261
1	X	1.20	0/206	1.63	2/279 (0.7%)
1	Y	0.96	0/206	1.64	0/279
1	Z	1.08	0/55	0.90	0/73
2	A	1.21	1/7683 (0.0%)	1.51	66/10460 (0.6%)
2	B	1.23	0/7683	1.53	97/10460 (0.9%)
2	C	1.22	0/7683	1.49	58/10460 (0.6%)
2	D	1.19	0/7683	1.51	63/10460 (0.6%)
2	E	1.21	0/7683	1.48	63/10460 (0.6%)
2	F	1.23	0/7683	1.48	69/10460 (0.7%)
2	G	1.23	0/7683	1.49	78/10460 (0.7%)
2	H	1.23	0/7683	1.51	81/10460 (0.8%)
2	I	1.22	0/7683	1.49	59/10460 (0.6%)
2	J	1.22	0/7683	1.48	70/10460 (0.7%)
2	K	1.23	0/7683	1.46	53/10460 (0.5%)
2	L	1.23	0/7683	1.47	53/10460 (0.5%)
3	M	1.15	0/3580	1.45	24/4872 (0.5%)
4	N	1.14	0/672	1.63	12/909 (1.3%)
4	O	1.05	0/597	1.60	8/803 (1.0%)
4	P	1.15	0/723	1.56	8/979 (0.8%)
4	Q	1.12	0/554	1.52	6/746 (0.8%)
5	R	1.23	0/892	1.56	14/1213 (1.2%)
6	S	1.16	0/1403	1.54	10/1917 (0.5%)
6	T	1.20	0/1415	1.60	16/1933 (0.8%)
All	All	1.21	1/103870 (0.0%)	1.50	917/141373 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	2
2	B	0	5
2	D	0	6
2	E	0	4
2	F	0	2
2	G	0	1
2	H	0	3
2	I	0	6
2	J	0	2
2	K	0	1
2	L	0	5
3	M	0	1
4	O	0	1
4	Q	0	1
5	R	0	1
6	T	0	2
All	All	0	43

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	673	LEU	CA-C	-5.45	1.50	1.53

All (917) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	15	ILE	N-CA-C	-11.37	102.57	112.12
2	E	385	VAL	N-CA-C	-11.17	102.85	111.90
2	K	385	VAL	N-CA-C	-10.88	103.02	111.62
2	I	72	ASP	CA-CB-CG	10.15	122.75	112.60
2	G	756	PHE	N-CA-C	-9.98	100.98	113.55
2	D	385	VAL	N-CA-C	-9.62	104.11	111.90
2	H	385	VAL	N-CA-C	-9.48	104.13	111.62
2	A	385	VAL	N-CA-C	-9.39	104.20	111.62
2	J	175	ASP	N-CA-C	-8.96	102.92	114.04
2	E	884	TYR	N-CA-C	-8.76	100.92	111.69
2	D	241	GLY	CA-C-N	8.68	125.71	120.24
2	D	241	GLY	C-N-CA	8.68	125.71	120.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	4	ILE	N-CA-C	-8.64	104.80	111.62
2	B	848	SER	CA-C-N	8.50	133.34	122.37
2	B	848	SER	C-N-CA	8.50	133.34	122.37
2	G	19	ASP	CA-CB-CG	8.42	121.02	112.60
2	A	241	GLY	CA-C-N	8.32	125.48	120.24
2	A	241	GLY	C-N-CA	8.32	125.48	120.24
2	B	385	VAL	N-CA-C	-8.26	105.21	111.90
2	E	288	VAL	N-CA-C	-8.21	105.91	113.71
5	R	62	VAL	N-CA-C	-8.18	105.25	112.12
2	F	22	GLU	N-CA-C	-8.12	105.36	114.62
2	A	159	GLU	N-CA-C	-7.99	105.51	114.62
2	B	653	VAL	CB-CA-C	7.96	118.49	109.89
2	G	71	VAL	N-CA-C	-7.94	104.78	113.43
2	I	241	GLY	CA-C-N	7.93	125.24	120.24
2	I	241	GLY	C-N-CA	7.93	125.24	120.24
2	F	8	PRO	N-CA-C	-7.93	106.44	114.68
2	J	385	VAL	N-CA-C	-7.89	105.49	112.12
2	B	592	ARG	N-CA-C	-7.85	102.67	112.72
5	R	74	VAL	N-CA-C	-7.80	104.92	113.43
2	G	241	GLY	CA-C-N	7.80	125.15	120.24
2	G	241	GLY	C-N-CA	7.80	125.15	120.24
3	M	457	PHE	N-CA-C	-7.79	102.75	112.72
2	B	789	GLN	CA-C-N	7.76	127.77	119.78
2	B	789	GLN	C-N-CA	7.76	127.77	119.78
2	J	520	ASP	N-CA-C	-7.74	104.73	114.56
2	H	241	GLY	CA-C-N	7.74	125.11	120.24
2	H	241	GLY	C-N-CA	7.74	125.11	120.24
2	A	15	ILE	N-CA-C	-7.65	105.31	112.96
4	P	25	GLY	CA-C-N	7.63	130.96	120.35
4	P	25	GLY	C-N-CA	7.63	130.96	120.35
2	H	507	TYR	N-CA-C	-7.59	102.08	112.03
2	I	270	ASP	N-CA-C	-7.58	105.19	114.75
2	E	724	ASN	N-CA-C	-7.54	104.04	112.57
2	A	47	ASN	CA-CB-CG	7.51	120.11	112.60
6	S	17	MET	N-CA-C	-7.50	104.16	113.38
2	I	557	PHE	CA-CB-CG	-7.47	106.33	113.80
3	M	456	VAL	N-CA-C	-7.47	106.03	113.20
2	F	124	LEU	N-CA-C	-7.42	103.80	114.12
2	A	293	LYS	N-CA-C	-7.41	105.15	114.56
2	A	799	VAL	N-CA-C	-7.40	105.91	111.90
2	J	755	TRP	N-CA-C	-7.40	104.87	114.04
2	G	735	ILE	N-CA-C	-7.38	105.92	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	929	VAL	N-CA-C	-7.38	97.85	108.48
2	G	2	ALA	CA-C-N	7.37	129.31	120.09
2	G	2	ALA	C-N-CA	7.37	129.31	120.09
2	H	33	ARG	N-CA-C	-7.35	104.17	113.43
2	A	789	GLN	CA-C-N	7.33	127.33	119.78
2	A	789	GLN	C-N-CA	7.33	127.33	119.78
2	J	832	TYR	N-CA-C	-7.32	101.63	108.22
2	I	101	PHE	CA-CB-CG	-7.30	106.50	113.80
6	S	5	ILE	N-CA-C	-7.28	99.81	107.60
2	A	371	PHE	CA-CB-CG	-7.24	106.56	113.80
2	L	755	TRP	N-CA-C	-7.23	105.38	114.56
4	P	31	MET	N-CA-C	-7.21	103.94	114.39
2	K	12	TYR	N-CA-C	-7.16	106.45	114.62
2	D	88	VAL	N-CA-C	-7.16	97.30	107.75
2	A	288	VAL	N-CA-C	-7.15	106.92	113.71
2	G	140	ALA	N-CA-C	-7.13	104.85	113.97
2	B	80	TYR	N-CA-C	-7.10	98.24	108.60
2	A	835	ASN	CA-CB-CG	7.00	119.60	112.60
2	D	391	HIS	N-CA-C	-6.98	103.43	113.21
2	D	835	ASN	CA-CB-CG	6.96	119.56	112.60
2	A	351	ARG	N-CA-C	-6.94	98.77	109.24
2	D	724	ASN	CA-CB-CG	6.94	119.54	112.60
2	D	288	VAL	N-CA-C	-6.93	107.12	113.71
6	T	46	ASP	N-CA-C	-6.91	105.79	114.56
2	D	799	VAL	N-CA-C	-6.89	106.33	112.12
2	C	362	ASP	CA-CB-CG	6.88	119.47	112.60
2	D	681	LEU	N-CA-C	-6.85	104.53	113.17
2	L	385	VAL	N-CA-C	-6.84	105.17	111.67
2	C	467	VAL	N-CA-C	-6.82	106.24	111.62
2	E	323	LEU	N-CA-C	-6.74	105.62	114.31
2	F	391	HIS	N-CA-C	-6.73	103.66	112.41
2	H	832	TYR	N-CA-C	-6.73	102.16	108.22
2	H	789	GLN	CA-C-N	6.73	126.75	119.89
2	H	789	GLN	C-N-CA	6.73	126.75	119.89
2	K	731	ASN	N-CA-C	-6.73	106.02	114.56
2	K	863	ILE	N-CA-C	-6.73	101.49	108.15
2	E	505	ASP	CA-CB-CG	6.71	119.31	112.60
5	R	95	VAL	N-CA-C	-6.71	106.12	113.43
2	G	385	VAL	N-CA-C	-6.70	105.30	111.67
2	C	789	GLN	CA-C-N	6.70	126.68	119.78
2	C	789	GLN	C-N-CA	6.70	126.68	119.78
6	T	14	GLN	N-CA-C	-6.69	98.67	109.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	507	TYR	N-CA-C	-6.66	102.28	110.61
2	F	71	VAL	N-CA-C	-6.66	106.17	113.43
2	H	270	ASP	N-CA-C	-6.64	105.06	113.43
4	O	13	SER	CA-C-N	6.64	128.14	119.84
4	O	13	SER	C-N-CA	6.64	128.14	119.84
6	T	219	ILE	N-CA-C	-6.64	106.26	112.83
2	E	90	ASP	CA-CB-CG	-6.64	105.96	112.60
2	E	265	ASP	N-CA-C	-6.63	105.19	113.28
6	T	13	TYR	N-CA-C	-6.63	98.42	108.96
2	K	15	ILE	N-CA-C	-6.62	106.34	112.43
4	N	28	GLN	N-CA-C	-6.62	105.12	113.72
2	B	270	ASP	N-CA-C	-6.61	105.85	114.04
2	H	330	GLY	N-CA-C	-6.60	106.05	114.37
2	A	919	HIS	CA-CB-CG	6.60	120.40	113.80
2	C	884	TYR	N-CA-C	-6.59	104.55	112.59
2	C	935	PHE	CA-CB-CG	-6.59	107.21	113.80
2	I	881	ASN	N-CA-C	-6.59	104.47	113.30
2	B	362	ASP	N-CA-C	-6.58	105.27	113.55
2	I	735	ILE	N-CA-C	-6.57	105.43	111.67
2	G	720	SER	CA-C-N	6.57	129.06	120.26
2	G	720	SER	C-N-CA	6.57	129.06	120.26
2	F	10	TRP	N-CA-C	-6.56	104.90	113.17
2	E	351	ARG	N-CA-C	-6.56	98.71	109.40
2	H	865	PHE	N-CA-C	-6.55	100.56	109.54
2	C	45	PHE	CA-CB-CG	-6.55	107.25	113.80
2	K	765	ASN	N-CA-CB	6.54	121.54	110.49
2	C	317	ARG	CA-C-N	6.52	129.31	120.38
2	C	317	ARG	C-N-CA	6.52	129.31	120.38
2	C	883	LEU	N-CA-C	-6.50	105.08	114.12
2	A	23	TYR	N-CA-C	-6.49	105.01	113.12
2	E	203	PHE	CA-CB-CG	-6.49	107.31	113.80
2	B	913	PHE	CA-CB-CG	-6.48	107.32	113.80
2	A	779	ASP	CA-CB-CG	6.47	119.07	112.60
2	B	119	THR	N-CA-C	-6.47	99.49	109.52
2	J	299	GLU	CA-C-N	6.47	129.32	120.46
2	J	299	GLU	C-N-CA	6.47	129.32	120.46
2	F	868	ASN	N-CA-C	-6.46	99.20	109.59
2	L	390	ASN	N-CA-C	-6.46	98.08	109.06
2	G	68	PHE	CA-CB-CG	-6.46	107.34	113.80
2	J	15	ILE	N-CA-C	-6.45	106.71	112.90
2	A	109	ARG	N-CA-C	-6.44	98.90	109.40
2	I	458	LEU	N-CA-C	-6.43	105.59	113.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	707	THR	N-CA-C	-6.42	105.98	113.88
5	R	102	ARG	N-CA-C	-6.41	106.09	114.04
2	J	6	MET	CA-C-N	6.39	128.08	120.09
2	J	6	MET	C-N-CA	6.39	128.08	120.09
2	L	353	THR	N-CA-C	-6.39	106.45	114.56
2	C	159	GLU	N-CA-C	-6.38	107.35	114.62
3	M	91	VAL	N-CA-C	-6.37	106.49	113.43
2	A	702	PHE	N-CA-C	-6.35	99.32	108.60
2	L	15	ILE	N-CA-C	-6.34	106.61	112.96
2	B	488	THR	N-CA-C	-6.33	105.59	113.38
2	F	140	ALA	N-CA-C	-6.32	104.36	113.21
2	D	504	VAL	CA-C-N	6.32	129.04	120.38
2	D	504	VAL	C-N-CA	6.32	129.04	120.38
2	G	122	ASN	CA-CB-CG	-6.32	106.28	112.60
2	H	504	VAL	CA-C-N	6.31	128.74	120.28
2	H	504	VAL	C-N-CA	6.31	128.74	120.28
3	M	448	ARG	N-CA-C	-6.31	105.74	113.50
2	A	526	ASN	N-CA-C	-6.30	102.70	110.65
4	O	14	PRO	N-CA-C	6.30	125.45	112.47
2	F	881	ASN	CA-CB-CG	6.29	118.89	112.60
2	H	304	GLN	N-CA-C	-6.28	100.08	108.74
2	C	840	LEU	N-CA-C	-6.27	103.81	112.03
2	G	388	ILE	CA-C-N	6.26	131.02	122.19
2	G	388	ILE	C-N-CA	6.26	131.02	122.19
2	E	629	ASN	CA-CB-CG	-6.25	106.35	112.60
2	F	706	HIS	N-CA-C	-6.25	105.30	113.17
2	H	381	TYR	N-CA-C	-6.25	98.81	109.24
2	F	401	CYS	N-CA-C	-6.24	99.56	109.23
2	G	80	TYR	N-CA-C	-6.22	98.10	108.75
2	H	109	ARG	N-CA-C	-6.21	99.58	109.59
2	B	229	LYS	N-CA-C	-6.20	104.19	112.94
2	A	593	THR	N-CA-C	-6.20	104.20	112.94
2	B	488	THR	CA-C-N	6.18	129.07	120.29
2	B	488	THR	C-N-CA	6.18	129.07	120.29
2	B	472	PRO	CA-C-N	6.18	128.56	120.28
2	B	472	PRO	C-N-CA	6.18	128.56	120.28
2	H	705	ASN	CA-CB-CG	-6.17	106.43	112.60
2	B	131	ASN	N-CA-CB	6.16	120.89	110.49
2	K	180	ILE	N-CA-C	-6.16	99.49	108.11
2	C	344	ALA	N-CA-C	-6.15	104.94	112.88
2	I	293	LYS	N-CA-C	-6.15	106.75	114.56
2	F	940	ALA	CA-C-N	6.15	130.03	120.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	940	ALA	C-N-CA	6.15	130.03	120.75
2	L	4	PRO	CA-C-N	6.14	133.28	121.54
2	L	4	PRO	C-N-CA	6.14	133.28	121.54
2	E	59	ASP	CA-C-N	6.14	128.51	120.28
2	E	59	ASP	C-N-CA	6.14	128.51	120.28
2	K	88	VAL	N-CA-C	-6.14	98.79	107.75
2	E	216	LYS	N-CA-C	-6.14	98.74	109.48
2	B	68	PHE	CA-CB-CG	-6.13	107.67	113.80
2	F	835	ASN	CA-CB-CG	6.12	118.72	112.60
2	K	420	ASN	N-CA-CB	6.12	120.83	110.49
5	R	84	ASN	N-CA-C	-6.12	106.46	114.04
2	B	570	THR	N-CA-C	-6.11	100.04	109.52
2	L	41	LEU	N-CA-C	-6.11	104.02	112.03
2	H	71	VAL	N-CA-C	-6.11	105.71	113.22
2	F	131	ASN	N-CA-CB	6.10	120.80	110.49
2	G	131	ASN	N-CA-CB	6.09	120.78	110.49
1	3	5	ASN	CA-CB-CG	6.08	118.69	112.60
2	K	304	GLN	N-CA-C	-6.08	99.90	108.96
2	L	238	GLY	N-CA-C	-6.06	104.69	110.21
2	A	906	LEU	N-CA-C	-6.06	99.52	109.40
2	F	450	MET	N-CA-C	-6.06	99.84	109.23
2	I	868	ASN	N-CA-C	-6.05	99.79	109.96
2	I	335	LEU	N-CA-C	-6.05	97.98	108.69
2	G	917	ARG	N-CA-C	-6.05	99.86	109.59
2	C	119	THR	N-CA-C	-6.04	100.30	109.85
2	E	475	TYR	N-CA-C	-6.04	106.23	113.97
2	K	775	GLU	N-CA-CB	6.04	120.69	110.49
2	H	197	TRP	N-CA-C	-6.03	105.92	113.28
2	D	929	VAL	N-CA-C	-6.03	99.80	108.48
2	E	615	ASN	N-CA-C	-6.03	105.95	113.55
2	C	241	GLY	CA-C-N	6.03	125.15	120.33
2	C	241	GLY	C-N-CA	6.03	125.15	120.33
2	L	440	ASN	CA-CB-CG	-6.03	106.57	112.60
3	M	80	TYR	N-CA-C	-6.02	104.78	113.21
2	I	390	ASN	N-CA-C	-6.00	99.57	108.99
2	G	304	GLN	N-CA-C	-5.99	100.90	108.45
6	S	201	PHE	CA-CB-CG	-5.99	107.81	113.80
6	T	201	PHE	CA-CB-CG	-5.98	107.82	113.80
2	L	197	TRP	N-CA-C	-5.98	105.56	112.92
2	A	660	ARG	N-CA-C	-5.98	100.23	109.14
2	L	467	VAL	N-CA-C	5.98	116.72	110.62
2	L	843	LYS	N-CA-C	-5.97	105.65	113.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	18	PHE	N-CA-C	5.96	120.02	112.87
2	C	76	ASN	N-CA-C	-5.96	100.24	109.24
2	H	557	PHE	CA-CB-CG	-5.96	107.84	113.80
3	M	116	GLY	CA-C-N	5.95	127.26	120.53
3	M	116	GLY	C-N-CA	5.95	127.26	120.53
2	B	890	ALA	N-CA-C	-5.95	100.52	108.19
2	C	616	THR	N-CA-C	-5.95	105.99	113.72
2	A	339	ALA	N-CA-C	-5.95	106.07	113.38
2	D	6	MET	CA-C-N	5.94	128.22	120.26
2	D	6	MET	C-N-CA	5.94	128.22	120.26
2	H	119	THR	N-CA-C	-5.93	100.33	109.52
2	J	472	PRO	CA-C-N	5.93	128.22	120.28
2	J	472	PRO	C-N-CA	5.93	128.22	120.28
3	M	453	LEU	CA-C-N	5.93	128.22	120.28
3	M	453	LEU	C-N-CA	5.93	128.22	120.28
2	B	12	TYR	N-CA-C	-5.92	106.08	113.55
2	A	203	PHE	CA-CB-CG	-5.92	107.88	113.80
2	K	507	TYR	N-CA-C	-5.91	103.47	112.99
2	F	371	PHE	N-CA-C	-5.91	100.37	109.52
2	D	715	PHE	N-CA-C	-5.90	97.52	108.02
2	J	168	ILE	N-CA-C	-5.90	106.99	112.83
5	R	78	VAL	N-CA-C	-5.90	106.99	112.83
2	F	175	ASP	CA-CB-CG	5.90	118.50	112.60
2	L	131	ASN	N-CA-CB	5.89	120.45	110.49
2	B	668	TRP	N-CA-C	-5.89	99.05	109.06
2	L	932	ARG	N-CA-C	-5.89	99.05	109.06
6	T	223	VAL	N-CA-C	-5.89	99.87	108.11
2	K	10	TRP	N-CA-C	-5.88	106.14	113.38
2	B	628	THR	N-CA-C	-5.88	105.29	112.88
2	H	651	THR	N-CA-C	-5.88	105.42	112.59
2	A	843	LYS	N-CA-C	-5.88	105.77	113.17
2	F	395	ASP	N-CA-C	-5.88	103.39	110.44
2	L	344	ALA	N-CA-C	-5.88	104.77	112.41
2	G	101	PHE	CA-CB-CG	-5.87	107.93	113.80
2	L	241	GLY	CA-C-N	5.86	125.02	120.33
2	L	241	GLY	C-N-CA	5.86	125.02	120.33
2	A	724	ASN	N-CA-C	-5.85	104.69	112.94
2	I	789	GLN	CA-C-N	5.85	125.86	119.89
2	I	789	GLN	C-N-CA	5.85	125.86	119.89
4	N	13	SER	O-C-N	-5.85	114.59	121.32
4	P	120	GLU	N-CA-C	-5.84	106.12	113.72
2	G	657	ILE	CA-C-N	5.84	127.14	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	657	ILE	C-N-CA	5.84	127.14	119.84
2	E	695	ILE	N-CA-C	-5.84	101.77	107.55
2	I	682	GLY	N-CA-C	-5.84	106.44	116.01
2	F	203	PHE	CA-CB-CG	-5.83	107.97	113.80
2	G	668	TRP	N-CA-C	-5.83	100.43	109.24
2	K	305	GLN	N-CA-C	-5.83	98.78	108.75
2	A	913	PHE	CA-CB-CG	-5.83	107.97	113.80
2	J	711	VAL	N-CA-C	-5.82	100.66	108.35
2	D	58	THR	N-CA-C	-5.82	105.27	112.72
5	R	119	VAL	N-CA-C	-5.82	104.83	113.39
2	B	557	PHE	CA-CB-CG	-5.82	107.98	113.80
2	B	666	ARG	N-CA-C	-5.82	98.41	110.80
2	E	815	ASN	N-CA-CB	5.81	120.31	110.49
2	J	536	ARG	CA-C-N	5.81	128.07	120.28
2	J	536	ARG	C-N-CA	5.81	128.07	120.28
2	C	800	ASN	N-CA-C	-5.81	108.00	114.62
2	B	674	LYS	N-CA-C	-5.80	99.20	109.06
2	K	706	HIS	N-CA-C	-5.79	106.21	113.28
2	D	15	ILE	N-CA-C	-5.78	107.49	113.10
3	M	162	ILE	N-CA-C	-5.78	100.02	108.11
2	I	525	PHE	N-CA-C	-5.78	104.45	112.30
2	F	317	ARG	CA-C-N	5.77	129.48	120.82
2	F	317	ARG	C-N-CA	5.77	129.48	120.82
2	C	131	ASN	N-CA-CB	5.77	120.24	110.49
2	D	229	LYS	N-CA-C	-5.77	105.44	112.88
2	F	111	PRO	N-CA-C	-5.76	108.69	114.68
2	F	15	ILE	N-CA-C	-5.76	107.67	113.20
2	D	226	THR	N-CA-C	-5.76	104.93	112.41
2	G	906	LEU	N-CA-C	-5.75	100.33	109.59
2	K	226	THR	N-CA-C	-5.75	104.98	113.61
2	F	657	ILE	CA-C-N	5.75	125.76	119.89
2	F	657	ILE	C-N-CA	5.75	125.76	119.89
3	M	191	ILE	N-CA-C	-5.75	106.14	113.22
2	C	92	ARG	N-CA-C	-5.75	100.56	109.24
2	H	265	ASP	N-CA-C	-5.75	106.90	114.31
2	H	69	VAL	CA-C-N	5.75	125.75	119.89
2	H	69	VAL	C-N-CA	5.75	125.75	119.89
2	F	751	MET	N-CA-C	-5.74	99.69	108.76
2	H	335	LEU	N-CA-C	-5.74	99.31	109.06
2	D	295	ASP	N-CA-C	-5.74	106.63	113.97
2	C	460	ARG	CA-C-N	5.73	128.43	120.29
2	C	460	ARG	C-N-CA	5.73	128.43	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	752	THR	CA-C-N	5.73	127.96	120.28
2	L	752	THR	C-N-CA	5.73	127.96	120.28
2	D	131	ASN	N-CA-CB	5.73	120.17	110.49
2	A	396	GLU	N-CA-C	-5.73	104.05	113.50
2	G	51	ALA	CA-C-N	5.72	125.73	119.89
2	G	51	ALA	C-N-CA	5.72	125.73	119.89
2	G	894	ASN	N-CA-C	-5.72	100.65	109.52
2	A	450	MET	CA-C-N	5.72	128.99	120.87
2	A	450	MET	C-N-CA	5.72	128.99	120.87
2	H	752	THR	CA-C-N	5.72	127.94	120.28
2	H	752	THR	C-N-CA	5.72	127.94	120.28
2	H	352	ASN	CA-C-N	5.72	127.94	120.28
2	H	352	ASN	C-N-CA	5.72	127.94	120.28
2	B	702	PHE	N-CA-C	-5.71	100.05	108.79
2	B	168	ILE	N-CA-C	-5.71	107.42	112.90
2	H	390	ASN	N-CA-C	-5.71	100.39	109.07
4	N	18	GLY	N-CA-C	-5.71	99.65	113.18
2	E	657	ILE	CA-C-N	5.70	126.97	119.84
2	E	657	ILE	C-N-CA	5.70	126.97	119.84
2	H	555	LYS	N-CA-C	-5.70	107.57	114.75
4	N	3	GLY	CA-C-N	5.70	132.43	121.54
4	N	3	GLY	C-N-CA	5.70	132.43	121.54
4	O	118	LEU	N-CA-C	-5.70	106.31	113.72
2	C	109	ARG	N-CA-C	-5.70	100.12	109.40
2	J	119	THR	N-CA-C	-5.69	100.69	109.52
2	A	424	GLY	N-CA-C	-5.69	106.33	112.08
2	G	64	LEU	N-CA-C	-5.69	103.85	112.04
2	L	707	THR	N-CA-C	-5.69	107.33	114.56
2	E	932	ARG	N-CA-C	-5.68	98.63	108.69
2	C	832	TYR	N-CA-C	-5.68	103.11	108.22
2	K	241	GLY	CA-C-N	5.68	124.87	120.33
2	K	241	GLY	C-N-CA	5.68	124.87	120.33
2	J	657	ILE	CA-C-N	5.68	126.94	119.84
2	J	657	ILE	C-N-CA	5.68	126.94	119.84
6	T	193	THR	CA-C-N	5.68	125.69	119.90
6	T	193	THR	C-N-CA	5.68	125.69	119.90
2	A	582	ILE	N-CA-C	-5.67	107.60	113.10
2	A	811	TYR	N-CA-C	-5.67	106.02	114.64
2	C	101	PHE	CA-CB-CG	-5.67	108.13	113.80
2	H	351	ARG	N-CA-C	-5.67	100.44	109.23
2	I	909	VAL	N-CA-C	-5.67	100.17	108.11
2	B	657	ILE	N-CA-C	-5.67	104.54	109.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	229	LYS	N-CA-C	-5.67	105.68	112.59
2	K	929	VAL	N-CA-C	-5.66	99.96	108.12
2	B	832	TYR	N-CA-C	-5.66	103.13	108.22
2	J	502	SER	N-CA-C	-5.66	106.54	113.50
2	B	59	ASP	CA-CB-CG	5.65	118.25	112.60
2	L	304	GLN	N-CA-C	-5.65	100.12	108.99
2	I	352	ASN	CA-C-N	5.64	127.84	120.28
2	I	352	ASN	C-N-CA	5.64	127.84	120.28
2	K	484	LEU	CA-C-N	5.64	125.65	119.90
2	K	484	LEU	C-N-CA	5.64	125.65	119.90
2	D	906	LEU	N-CA-C	-5.64	100.70	109.72
2	E	565	LEU	CA-C-N	5.63	126.88	119.84
2	E	565	LEU	C-N-CA	5.63	126.88	119.84
4	O	26	VAL	CA-C-N	5.63	129.10	121.05
4	O	26	VAL	C-N-CA	5.63	129.10	121.05
2	C	653	VAL	CA-C-N	5.63	125.58	119.78
2	C	653	VAL	C-N-CA	5.63	125.58	119.78
2	L	305	GLN	N-CA-C	-5.63	100.71	109.72
2	H	471	LEU	CA-C-N	5.63	125.63	119.89
2	H	471	LEU	C-N-CA	5.63	125.63	119.89
2	E	89	GLY	N-CA-C	-5.62	99.85	113.18
2	G	528	HIS	CA-CB-CG	5.62	119.42	113.80
2	D	941	THR	N-CA-C	-5.62	106.41	113.72
2	F	227	ASN	CA-C-N	5.62	128.16	120.46
2	F	227	ASN	C-N-CA	5.62	128.16	120.46
2	D	932	ARG	N-CA-C	-5.62	99.14	108.75
2	E	241	GLY	CA-C-N	5.61	123.77	120.24
2	E	241	GLY	C-N-CA	5.61	123.77	120.24
2	G	919	HIS	CA-CB-CG	5.61	119.41	113.80
2	H	58	THR	N-CA-C	-5.61	100.19	108.99
2	B	156	MET	CA-C-N	5.60	125.30	119.92
2	B	156	MET	C-N-CA	5.60	125.30	119.92
2	B	226	THR	N-CA-C	-5.60	105.04	113.89
2	B	783	SER	CA-C-N	5.60	130.10	121.19
2	B	783	SER	C-N-CA	5.60	130.10	121.19
2	J	935	PHE	CA-CB-CG	-5.60	108.20	113.80
2	A	887	SER	N-CA-C	-5.60	104.70	112.03
2	C	425	ASP	CA-CB-CG	5.60	118.20	112.60
2	L	151	PHE	N-CA-C	-5.59	100.79	109.24
2	J	932	ARG	N-CA-C	-5.59	98.79	108.69
2	D	718	SER	CA-C-N	5.59	132.04	121.97
2	D	718	SER	C-N-CA	5.59	132.04	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	172	ALA	N-CA-C	-5.59	103.63	110.61
2	A	818	PHE	N-CA-C	-5.58	107.47	114.56
2	L	239	ALA	N-CA-C	-5.58	105.25	112.68
2	B	932	ARG	N-CA-C	-5.58	101.08	109.95
2	D	119	THR	N-CA-C	-5.58	100.87	109.52
2	D	101	PHE	CA-CB-CG	-5.58	108.22	113.80
2	F	188	PRO	CA-C-N	5.57	128.14	120.39
2	F	188	PRO	C-N-CA	5.57	128.14	120.39
2	E	559	ILE	N-CA-C	-5.57	107.85	113.20
2	J	131	ASN	CA-CB-CG	5.57	118.17	112.60
2	I	296	ALA	N-CA-C	-5.57	102.08	108.49
2	C	695	ILE	N-CA-C	-5.57	102.04	107.55
2	E	909	VAL	N-CA-C	-5.56	100.38	108.17
2	F	906	LEU	N-CA-C	-5.56	100.34	109.40
2	D	203	PHE	CA-CB-CG	-5.55	108.25	113.80
5	R	55	LEU	N-CA-C	-5.55	105.20	112.41
2	E	769	GLN	N-CA-C	-5.54	105.83	112.59
2	H	454	LEU	CA-C-N	5.54	127.71	120.28
2	H	454	LEU	C-N-CA	5.54	127.71	120.28
2	E	602	SER	N-CA-CB	5.54	119.85	110.49
2	H	565	LEU	N-CA-C	-5.54	103.67	110.31
2	A	11	ALA	CA-C-N	5.53	127.69	120.28
2	A	11	ALA	C-N-CA	5.53	127.69	120.28
2	B	539	LEU	N-CA-C	-5.53	106.30	113.16
2	F	83	ARG	N-CA-C	-5.53	101.16	109.95
2	C	175	ASP	N-CA-C	-5.52	99.03	110.80
2	J	913	PHE	CA-CB-CG	-5.52	108.28	113.80
2	K	478	THR	CA-C-N	5.52	125.52	119.89
2	K	478	THR	C-N-CA	5.52	125.52	119.89
2	D	307	MET	CA-C-N	5.51	125.82	119.92
2	D	307	MET	C-N-CA	5.51	125.82	119.92
2	I	219	TYR	N-CA-C	-5.51	99.06	110.80
2	L	603	ILE	N-CA-C	-5.51	100.40	108.11
3	M	440	GLN	N-CA-C	-5.51	105.87	112.59
2	D	106	VAL	CA-C-N	5.50	130.24	122.09
2	D	106	VAL	C-N-CA	5.50	130.24	122.09
4	O	13	SER	CA-C-O	-5.50	112.62	120.16
2	F	320	PHE	N-CA-CB	5.50	119.79	110.49
2	F	789	GLN	CA-C-N	5.50	125.50	119.89
2	F	789	GLN	C-N-CA	5.50	125.50	119.89
2	F	815	ASN	N-CA-CB	5.50	119.78	110.49
2	I	529	ARG	N-CA-C	-5.50	105.93	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	906	LEU	N-CA-C	-5.49	100.44	109.40
6	S	85	GLN	CA-C-N	5.49	126.71	119.84
6	S	85	GLN	C-N-CA	5.49	126.71	119.84
2	I	109	ARG	N-CA-C	-5.49	100.93	109.72
2	F	216	LYS	N-CA-C	-5.49	100.63	109.58
2	J	648	ALA	N-CA-CB	5.49	119.77	110.49
3	M	445	GLN	N-CA-C	-5.49	106.25	113.17
2	D	57	THR	N-CA-C	-5.49	103.24	110.43
2	J	883	LEU	N-CA-C	-5.48	106.75	113.50
2	I	255	ASP	CA-CB-CG	5.48	118.08	112.60
2	J	162	THR	CA-C-N	5.48	127.97	120.46
2	J	162	THR	C-N-CA	5.48	127.97	120.46
2	K	695	ILE	N-CA-C	-5.48	102.12	107.55
2	C	399	ASN	N-CA-C	-5.48	101.19	109.85
2	J	180	ILE	N-CA-C	-5.48	100.44	108.11
2	K	702	PHE	N-CA-C	-5.48	100.60	108.60
6	T	64	THR	CA-C-N	5.48	125.49	119.90
6	T	64	THR	C-N-CA	5.48	125.49	119.90
2	H	495	ASN	N-CA-C	-5.47	106.73	113.41
2	I	478	THR	CA-C-N	5.47	125.47	119.89
2	I	478	THR	C-N-CA	5.47	125.47	119.89
2	D	7	LEU	CA-C-O	-5.47	113.37	118.73
2	C	565	LEU	CA-C-N	5.47	126.67	119.84
2	C	565	LEU	C-N-CA	5.47	126.67	119.84
2	J	323	LEU	N-CA-C	-5.47	107.26	114.31
2	G	590	ASP	N-CA-C	-5.46	98.29	108.02
2	L	575	PHE	CA-CB-CG	-5.46	108.33	113.80
2	B	895	PHE	N-CA-C	-5.46	101.00	109.24
4	N	129	GLN	N-CA-C	-5.46	105.84	112.88
2	B	377	ALA	N-CA-C	-5.45	99.18	110.80
2	B	658	PRO	CA-C-N	5.45	131.96	121.54
2	B	658	PRO	C-N-CA	5.45	131.96	121.54
2	E	913	PHE	CA-CB-CG	-5.45	108.35	113.80
2	I	256	THR	CA-C-N	5.45	125.75	119.92
2	I	256	THR	C-N-CA	5.45	125.75	119.92
2	I	668	TRP	N-CA-C	-5.45	101.01	109.24
2	L	377	ALA	N-CA-C	-5.45	99.20	110.80
2	K	203	PHE	CA-CB-CG	-5.45	108.35	113.80
2	B	582	ILE	N-CA-C	-5.44	107.49	111.90
2	H	59	ASP	N-CA-C	-5.44	105.59	113.21
3	M	120	LYS	N-CA-C	-5.44	99.45	108.75
4	N	10	GLY	CA-C-N	5.44	131.76	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	10	GLY	C-N-CA	5.44	131.76	121.97
2	B	402	PHE	CA-C-N	5.44	126.64	119.84
2	B	402	PHE	C-N-CA	5.44	126.64	119.84
2	C	738	THR	N-CA-C	-5.43	99.55	108.41
6	S	207	HIS	N-CA-C	-5.43	105.67	114.09
2	G	123	SER	N-CA-CB	5.43	119.67	110.49
2	I	505	ASP	CA-CB-CG	5.43	118.03	112.60
2	G	323	LEU	N-CA-C	-5.43	106.82	113.50
2	J	360	LEU	N-CA-C	-5.43	107.02	113.97
2	H	211	LYS	CA-C-N	5.43	127.56	120.28
2	H	211	LYS	C-N-CA	5.43	127.56	120.28
2	J	456	ALA	CA-C-N	5.43	127.56	120.28
2	J	456	ALA	C-N-CA	5.43	127.56	120.28
2	B	184	LYS	N-CA-C	-5.43	106.52	114.39
2	H	455	GLN	CA-C-N	5.43	127.55	120.28
2	H	455	GLN	C-N-CA	5.43	127.55	120.28
2	B	490	THR	CA-C-N	5.42	127.55	120.28
2	B	490	THR	C-N-CA	5.42	127.55	120.28
2	K	722	PRO	CA-C-N	5.42	126.66	120.53
2	K	722	PRO	C-N-CA	5.42	126.66	120.53
2	G	104	ARG	N-CA-C	-5.42	101.05	109.24
2	E	838	TYR	N-CA-C	-5.42	102.14	110.32
2	H	323	LEU	N-CA-C	-5.42	106.71	113.38
2	J	494	MET	CA-C-N	5.42	127.54	120.28
2	J	494	MET	C-N-CA	5.42	127.54	120.28
2	I	64	LEU	N-CA-C	-5.42	106.04	113.30
2	B	109	ARG	N-CA-C	-5.42	101.06	109.72
2	L	173	THR	N-CA-CB	5.42	119.64	110.49
2	H	525	PHE	CA-CB-CG	-5.41	108.39	113.80
2	H	708	PHE	CA-CB-CG	-5.41	108.39	113.80
2	H	753	LYS	CA-C-N	5.41	127.53	120.28
2	H	753	LYS	C-N-CA	5.41	127.53	120.28
2	J	229	LYS	N-CA-C	-5.41	105.99	112.59
2	F	866	SER	CA-C-N	5.41	127.53	120.28
2	F	866	SER	C-N-CA	5.41	127.53	120.28
2	J	396	GLU	N-CA-C	-5.40	105.32	112.94
2	B	505	ASP	CA-CB-CG	5.40	118.00	112.60
2	C	472	PRO	CA-C-N	5.40	128.05	120.28
2	C	472	PRO	C-N-CA	5.40	128.05	120.28
2	F	657	ILE	N-CA-C	-5.39	102.01	107.89
2	I	739	VAL	N-CA-CB	5.39	120.13	111.23
2	J	425	ASP	CA-CB-CG	5.39	118.00	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	198	PHE	N-CA-C	5.39	116.84	111.07
2	C	640	ALA	N-CA-C	-5.39	99.62	108.41
6	T	203	GLY	N-CA-C	-5.39	104.46	111.52
2	B	720	SER	N-CA-C	-5.39	99.62	108.41
2	G	898	ASP	CA-C-N	5.39	125.40	119.90
2	G	898	ASP	C-N-CA	5.39	125.40	119.90
2	E	571	TYR	N-CA-C	-5.39	99.49	108.32
2	H	484	LEU	CA-C-N	5.38	125.38	119.89
2	H	484	LEU	C-N-CA	5.38	125.38	119.89
2	I	724	ASN	N-CA-C	-5.38	106.58	112.72
1	8	10	ALA	CA-C-N	5.38	126.56	119.84
1	8	10	ALA	C-N-CA	5.38	126.56	119.84
2	E	906	LEU	N-CA-C	-5.38	100.13	108.90
2	L	5	SER	N-CA-C	5.38	122.26	110.80
2	B	719	VAL	N-CA-C	-5.38	100.73	108.48
2	L	109	ARG	N-CA-C	-5.38	101.40	109.95
2	A	676	LYS	N-CA-CB	5.37	119.57	110.49
4	Q	6	SER	N-CA-C	5.37	119.32	112.87
2	B	933	THR	CB-CA-C	5.37	115.67	111.00
2	G	935	PHE	CA-CB-CG	-5.37	108.43	113.80
2	F	13	MET	N-CA-C	-5.36	100.56	109.46
2	I	119	THR	N-CA-C	-5.36	100.92	109.23
2	I	657	ILE	CA-C-N	5.36	126.54	119.84
2	I	657	ILE	C-N-CA	5.36	126.54	119.84
2	F	17	GLY	CA-C-N	5.36	128.84	120.75
2	F	17	GLY	C-N-CA	5.36	128.84	120.75
2	I	646	ILE	CA-C-O	-5.36	117.15	119.94
2	I	175	ASP	N-CA-C	-5.36	99.39	110.80
2	J	362	ASP	CA-C-N	5.36	131.77	121.54
2	J	362	ASP	C-N-CA	5.36	131.77	121.54
2	E	582	ILE	N-CA-C	-5.36	107.62	112.12
2	J	197	TRP	N-CA-C	-5.36	105.43	113.89
6	T	85	GLN	CA-C-N	5.36	125.35	119.89
6	T	85	GLN	C-N-CA	5.36	125.35	119.89
2	G	69	VAL	CA-C-N	5.35	125.35	119.89
2	G	69	VAL	C-N-CA	5.35	125.35	119.89
2	H	131	ASN	N-CA-CB	5.35	119.54	110.49
2	G	211	LYS	CA-C-N	5.35	127.71	120.38
2	G	211	LYS	C-N-CA	5.35	127.71	120.38
2	A	724	ASN	CA-CB-CG	-5.35	107.25	112.60
4	Q	132	THR	N-CA-C	-5.35	106.77	113.72
2	G	417	LYS	CA-C-N	5.35	127.78	120.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	417	LYS	C-N-CA	5.35	127.78	120.35
2	B	274	TYR	CA-C-N	5.34	128.46	120.87
2	B	274	TYR	C-N-CA	5.34	128.46	120.87
2	G	789	GLN	CA-C-N	5.34	125.34	119.89
2	G	789	GLN	C-N-CA	5.34	125.34	119.89
2	C	808	THR	CA-C-N	5.34	127.44	120.28
2	C	808	THR	C-N-CA	5.34	127.44	120.28
2	J	357	TYR	N-CA-C	-5.34	106.14	113.30
2	L	165	GLY	CA-C-N	5.34	128.29	120.71
2	L	165	GLY	C-N-CA	5.34	128.29	120.71
2	L	184	LYS	CA-C-N	5.34	127.44	120.28
2	L	184	LYS	C-N-CA	5.34	127.44	120.28
2	H	151	PHE	N-CA-C	-5.34	100.70	109.40
3	M	78	LEU	N-CA-C	-5.34	106.78	113.72
2	E	459	TRP	CA-C-N	5.33	127.38	120.44
2	E	459	TRP	C-N-CA	5.33	127.38	120.44
2	D	838	TYR	N-CA-C	-5.33	101.89	109.62
2	F	863	ILE	CA-C-N	5.33	125.27	119.78
2	F	863	ILE	C-N-CA	5.33	125.27	119.78
3	M	239	HIS	CA-C-N	5.33	126.51	119.84
3	M	239	HIS	C-N-CA	5.33	126.51	119.84
6	T	206	GLY	N-CA-C	-5.33	107.67	115.72
2	J	668	TRP	N-CA-C	-5.33	101.19	109.24
2	B	808	THR	CA-C-N	5.33	127.42	120.28
2	B	808	THR	C-N-CA	5.33	127.42	120.28
2	A	706	HIS	N-CA-C	-5.33	106.65	112.72
2	D	401	CYS	N-CA-C	-5.33	100.63	108.99
2	I	405	ASP	CA-CB-CG	5.33	117.93	112.60
2	G	815	ASN	N-CA-CB	5.32	119.49	110.49
2	G	307	MET	CA-C-N	5.32	125.32	119.89
2	G	307	MET	C-N-CA	5.32	125.32	119.89
2	E	860	MET	N-CA-C	-5.32	100.23	108.90
4	P	49	THR	N-CA-C	5.32	117.80	110.35
2	B	650	ALA	N-CA-C	5.32	122.12	110.80
2	C	3	THR	CA-C-N	5.32	126.49	119.84
2	C	3	THR	C-N-CA	5.32	126.49	119.84
2	C	351	ARG	N-CA-C	-5.32	101.50	109.95
2	E	119	THR	N-CA-C	-5.32	101.28	109.52
2	F	288	VAL	N-CA-C	-5.32	107.20	113.42
2	K	494	MET	CA-C-N	5.32	127.40	120.28
2	K	494	MET	C-N-CA	5.32	127.40	120.28
2	C	530	ASN	N-CA-C	-5.31	101.78	109.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	317	ARG	CA-C-N	5.31	129.10	120.60
2	A	317	ARG	C-N-CA	5.31	129.10	120.60
6	S	210	ASP	N-CA-C	-5.31	106.18	113.30
2	B	561	SER	N-CA-C	-5.31	106.30	114.16
2	D	188	PRO	N-CA-C	-5.31	101.54	112.47
2	J	38	TYR	N-CA-C	-5.31	107.82	114.56
2	J	752	THR	CA-C-N	5.31	127.39	120.28
2	J	752	THR	C-N-CA	5.31	127.39	120.28
2	C	381	TYR	N-CA-C	-5.30	101.30	109.52
2	G	377	ALA	N-CA-C	-5.30	99.50	110.80
2	J	719	VAL	N-CA-C	-5.30	100.84	108.48
2	J	344	ALA	N-CA-C	-5.30	105.47	112.94
2	K	323	LEU	N-CA-C	-5.30	106.70	114.39
2	L	45	PHE	CA-CB-CG	-5.30	108.50	113.80
2	E	293	LYS	N-CA-C	-5.30	104.82	113.19
2	A	428	SER	N-CA-C	-5.30	106.50	113.17
2	F	668	TRP	N-CA-C	-5.30	101.24	109.24
2	K	513	ARG	N-CA-C	-5.30	99.89	108.52
2	E	196	ASN	CA-CB-CG	5.29	117.89	112.60
2	E	789	GLN	CA-C-N	5.29	125.29	119.89
2	E	789	GLN	C-N-CA	5.29	125.29	119.89
2	B	317	ARG	CA-C-N	5.29	128.11	120.38
2	B	317	ARG	C-N-CA	5.29	128.11	120.38
2	K	83	ARG	N-CA-C	-5.29	101.25	109.72
2	A	733	PHE	N-CA-C	-5.29	99.70	108.75
2	F	31	PHE	CA-C-N	5.28	127.36	120.28
2	F	31	PHE	C-N-CA	5.28	127.36	120.28
2	G	513	ARG	N-CA-C	-5.28	100.29	108.90
2	K	377	ALA	N-CA-C	-5.28	99.55	110.80
2	J	849	VAL	CA-C-N	5.28	128.37	120.87
2	J	849	VAL	C-N-CA	5.28	128.37	120.87
2	D	887	SER	N-CA-C	-5.28	99.56	110.80
2	I	783	SER	CA-C-N	5.28	127.35	120.28
2	I	783	SER	C-N-CA	5.28	127.35	120.28
6	S	177	GLN	CA-C-N	5.28	125.28	119.90
6	S	177	GLN	C-N-CA	5.28	125.28	119.90
2	B	404	LEU	CA-C-N	5.28	127.35	120.28
2	B	404	LEU	C-N-CA	5.28	127.35	120.28
2	G	210	LYS	CA-C-N	5.27	127.87	120.28
2	G	210	LYS	C-N-CA	5.27	127.87	120.28
2	G	75	ASP	N-CA-C	-5.27	101.29	109.72
2	A	805	GLN	N-CA-C	-5.27	101.98	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	710	LYS	N-CA-CB	5.27	119.39	110.49
2	B	343	ASN	CA-CB-CG	5.27	117.87	112.60
2	H	173	THR	N-CA-CB	5.27	119.39	110.49
2	A	270	ASP	N-CA-C	-5.26	107.51	114.04
2	B	525	PHE	CA-CB-CG	-5.26	108.54	113.80
2	J	372	SER	N-CA-C	-5.26	107.51	114.04
2	H	468	ALA	CA-C-N	5.26	127.33	120.28
2	H	468	ALA	C-N-CA	5.26	127.33	120.28
2	J	173	THR	N-CA-CB	5.26	119.38	110.49
2	K	743	GLY	N-CA-C	-5.26	106.46	115.08
2	L	560	LYS	N-CA-C	-5.26	99.60	110.80
2	I	929	VAL	N-CA-C	-5.25	101.07	108.27
2	C	939	ASN	N-CA-CB	5.25	119.37	110.49
3	M	446	GLN	N-CA-C	-5.25	106.92	113.38
4	Q	25	GLY	N-CA-C	-5.25	107.40	116.01
2	H	709	LYS	N-CA-C	-5.25	106.81	113.43
2	D	202	SER	N-CA-C	-5.25	99.63	110.80
3	M	400	TRP	N-CA-C	-5.24	101.33	109.72
2	G	124	LEU	N-CA-C	-5.24	106.12	112.88
2	A	175	ASP	N-CA-C	-5.24	99.64	110.80
2	F	85	THR	N-CA-C	-5.24	99.87	108.41
2	J	305	GLN	N-CA-C	-5.24	101.34	109.72
2	K	140	ALA	CA-C-N	5.24	124.95	119.92
2	K	140	ALA	C-N-CA	5.24	124.95	119.92
2	F	356	SER	CA-C-N	5.24	127.30	120.28
2	F	356	SER	C-N-CA	5.24	127.30	120.28
2	C	268	LYS	N-CA-C	-5.23	99.65	110.80
2	I	131	ASN	N-CA-CB	5.23	119.33	110.49
2	A	347	ASP	N-CA-C	-5.23	101.35	109.72
2	I	178	LYS	N-CA-C	-5.23	103.48	110.07
6	T	193	THR	N-CA-C	-5.23	103.48	110.07
2	D	656	SER	N-CA-C	-5.22	100.79	108.99
2	D	675	THR	CA-C-N	5.22	131.52	121.54
2	D	675	THR	C-N-CA	5.22	131.52	121.54
2	B	382	ASP	N-CA-C	-5.22	103.19	109.72
2	E	494	MET	CA-C-N	5.22	127.28	120.28
2	E	494	MET	C-N-CA	5.22	127.28	120.28
3	M	193	ASN	N-CA-C	-5.22	106.96	113.38
3	M	277	TYR	CA-C-N	5.22	127.28	120.28
3	M	277	TYR	C-N-CA	5.22	127.28	120.28
2	G	197	TRP	N-CA-C	-5.22	106.06	112.90
2	K	109	ARG	N-CA-C	-5.22	101.19	109.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	13	MET	N-CA-C	-5.22	106.30	113.30
2	A	773	VAL	CA-C-N	5.22	125.21	119.89
2	A	773	VAL	C-N-CA	5.22	125.21	119.89
2	F	494	MET	CA-C-N	5.22	127.28	120.28
2	F	494	MET	C-N-CA	5.22	127.28	120.28
2	H	68	PHE	CA-C-N	5.22	131.79	122.13
2	H	68	PHE	C-N-CA	5.22	131.79	122.13
2	E	832	TYR	CA-C-N	5.22	125.22	119.90
2	E	832	TYR	C-N-CA	5.22	125.22	119.90
2	F	2	ALA	N-CA-C	-5.22	108.18	114.75
2	G	226	THR	N-CA-C	-5.21	105.59	112.94
2	J	269	ALA	N-CA-C	-5.21	99.16	108.13
2	H	88	VAL	N-CA-C	-5.21	100.62	108.12
2	E	668	TRP	N-CA-C	-5.20	101.38	109.24
4	N	118	LEU	CA-C-N	5.20	125.72	120.00
4	N	118	LEU	C-N-CA	5.20	125.72	120.00
2	B	619	THR	N-CA-C	-5.20	107.00	113.55
2	E	139	LYS	N-CA-C	-5.20	106.33	113.30
2	B	484	LEU	CA-C-N	5.20	126.33	119.84
2	B	484	LEU	C-N-CA	5.20	126.33	119.84
2	A	722	PRO	N-CA-C	-5.19	105.92	114.75
2	B	677	GLU	N-CA-C	5.19	117.34	111.11
2	C	22	GLU	N-CA-C	-5.19	108.21	114.75
2	L	5	SER	CA-C-N	5.19	129.99	122.36
2	L	5	SER	C-N-CA	5.19	129.99	122.36
2	E	734	GLU	N-CA-C	-5.19	100.45	108.90
2	F	414	GLN	CA-C-N	5.19	124.90	119.92
2	F	414	GLN	C-N-CA	5.19	124.90	119.92
2	I	267	TYR	N-CA-C	-5.19	99.44	109.24
2	A	868	ASN	N-CA-C	-5.18	100.07	108.52
2	H	702	PHE	N-CA-C	-5.18	100.86	108.79
2	B	401	CYS	N-CA-C	-5.18	100.95	109.40
4	N	22	SER	CA-C-N	5.18	128.13	120.82
4	N	22	SER	C-N-CA	5.18	128.13	120.82
2	J	317	ARG	CA-C-N	5.18	127.94	120.38
2	J	317	ARG	C-N-CA	5.18	127.94	120.38
5	R	36	MET	N-CA-C	-5.18	107.01	113.38
2	F	580	ASN	N-CA-C	-5.18	107.01	113.38
2	G	320	PHE	N-CA-CB	5.18	119.24	110.49
2	D	641	ASN	CA-CB-CG	-5.18	107.42	112.60
2	D	484	LEU	CA-C-N	5.17	125.17	119.89
2	D	484	LEU	C-N-CA	5.17	125.17	119.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	371	PHE	N-CA-C	-5.17	99.53	108.69
2	B	68	PHE	CA-C-N	5.17	131.70	122.13
2	B	68	PHE	C-N-CA	5.17	131.70	122.13
2	C	184	LYS	N-CA-C	-5.17	107.03	113.38
2	I	68	PHE	CA-CB-CG	-5.17	108.63	113.80
2	L	546	VAL	CA-C-N	5.17	125.46	119.93
2	L	546	VAL	C-N-CA	5.17	125.46	119.93
2	D	3	THR	CA-C-O	-5.17	113.08	120.16
2	E	422	ASN	N-CA-CB	5.17	119.22	110.49
2	H	882	MET	CA-C-N	5.17	127.20	120.28
2	H	882	MET	C-N-CA	5.17	127.20	120.28
2	G	873	GLY	N-CA-C	-5.16	103.36	111.00
2	L	695	ILE	N-CA-C	-5.16	102.44	107.55
2	E	112	SER	CA-C-N	5.16	128.04	120.71
2	E	112	SER	C-N-CA	5.16	128.04	120.71
2	I	10	TRP	N-CA-C	-5.16	107.03	113.38
2	J	860	MET	N-CA-C	-5.16	100.99	109.40
4	Q	113	ALA	N-CA-C	-5.16	107.37	113.97
2	B	10	TRP	N-CA-C	-5.16	107.04	113.38
2	H	932	ARG	N-CA-C	-5.16	99.93	108.75
2	K	22	GLU	N-CA-C	-5.15	108.26	114.75
2	J	914	ASP	CA-C-N	5.15	127.40	120.50
2	J	914	ASP	C-N-CA	5.15	127.40	120.50
2	B	3	THR	CA-C-N	5.15	126.27	119.84
2	B	3	THR	C-N-CA	5.15	126.27	119.84
2	C	868	ASN	N-CA-C	-5.15	100.06	108.76
2	I	265	ASP	N-CA-C	-5.15	106.97	114.12
2	F	151	PHE	N-CA-C	-5.14	99.91	108.34
2	L	395	ASP	CA-CB-CG	5.14	117.74	112.60
2	C	362	ASP	N-CA-C	-5.14	107.06	113.38
5	R	81	LEU	N-CA-C	-5.14	107.04	113.72
2	F	729	THR	N-CA-C	-5.14	102.10	109.24
2	F	76	ASN	N-CA-C	-5.14	101.48	109.24
2	I	696	PRO	CA-C-N	5.13	127.16	120.28
2	I	696	PRO	C-N-CA	5.13	127.16	120.28
2	J	22	GLU	N-CA-C	-5.13	108.04	114.56
2	A	131	ASN	N-CA-CB	5.13	119.15	110.49
2	F	80	TYR	N-CA-C	-5.13	101.28	109.07
2	G	165	GLY	CA-C-N	5.13	127.99	120.71
2	G	165	GLY	C-N-CA	5.13	127.99	120.71
2	D	104	ARG	N-CA-C	-5.12	101.58	109.52
2	I	657	ILE	N-CA-C	-5.12	101.52	107.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	119	THR	N-CA-C	-5.12	99.63	108.69
2	H	426	VAL	N-CA-C	-5.12	106.91	112.80
2	K	372	SER	N-CA-C	-5.12	108.06	114.56
2	B	159	GLU	N-CA-C	-5.12	106.98	113.43
2	C	73	ARG	N-CA-C	-5.12	100.95	108.99
2	D	9	GLN	N-CA-C	-5.12	106.55	112.89
2	L	22	GLU	N-CA-C	-5.12	108.06	114.56
2	B	814	ASN	N-CA-C	-5.11	100.01	108.75
2	G	539	LEU	N-CA-C	-5.11	106.82	113.16
2	G	708	PHE	CA-CB-CG	-5.11	108.69	113.80
2	K	472	PRO	CA-C-N	5.11	127.13	120.28
2	K	472	PRO	C-N-CA	5.11	127.13	120.28
2	B	473	ASP	CA-C-N	5.11	127.13	120.28
2	B	473	ASP	C-N-CA	5.11	127.13	120.28
2	B	649	ASN	CA-C-N	5.11	131.29	121.54
2	B	649	ASN	C-N-CA	5.11	131.29	121.54
2	D	504	VAL	N-CA-C	-5.11	98.72	109.34
2	F	264	GLN	N-CA-C	-5.11	106.74	113.17
5	R	27	ASP	CA-C-N	5.11	127.12	120.28
5	R	27	ASP	C-N-CA	5.11	127.12	120.28
2	A	803	ASP	N-CA-C	-5.10	106.36	112.59
2	I	139	LYS	N-CA-C	-5.10	106.46	113.30
2	A	565	LEU	CA-C-N	5.10	126.22	119.84
2	A	565	LEU	C-N-CA	5.10	126.22	119.84
2	G	872	MET	N-CA-C	-5.10	104.78	112.99
2	I	305	GLN	N-CA-C	-5.10	101.53	109.24
2	I	377	ALA	N-CA-C	-5.10	99.93	110.80
2	I	331	ASN	N-CA-C	-5.10	104.78	112.99
5	R	83	GLU	N-CA-C	-5.10	106.37	112.59
2	A	769	GLN	N-CA-C	-5.10	105.78	112.41
2	J	184	LYS	CA-C-N	5.10	127.11	120.28
2	J	184	LYS	C-N-CA	5.10	127.11	120.28
2	H	293	LYS	N-CA-C	-5.10	106.31	112.88
2	B	125	ALA	CA-C-N	5.10	125.09	119.89
2	B	125	ALA	C-N-CA	5.10	125.09	119.89
2	A	71	VAL	N-CA-C	-5.09	108.16	113.10
2	A	104	ARG	N-CA-C	-5.09	101.55	109.24
2	E	391	HIS	N-CA-C	-5.09	104.79	112.99
2	J	863	ILE	CA-C-N	5.09	125.81	120.11
2	J	863	ILE	C-N-CA	5.09	125.81	120.11
2	G	6	MET	CA-C-N	5.09	126.45	120.09
2	G	6	MET	C-N-CA	5.09	126.45	120.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	769	GLN	N-CA-C	-5.09	105.76	112.94
2	K	515	SER	N-CA-C	-5.09	100.88	109.07
2	B	644	TYR	CA-C-O	-5.09	115.43	120.26
2	L	882	MET	N-CA-C	-5.09	104.89	111.71
2	K	188	PRO	CA-C-N	5.09	127.46	120.39
2	K	188	PRO	C-N-CA	5.09	127.46	120.39
6	S	212	PHE	N-CA-C	-5.08	106.32	112.88
2	K	635	ASP	N-CA-CB	5.08	117.49	110.17
2	D	436	VAL	N-CA-C	-5.08	107.51	112.29
2	I	244	THR	N-CA-C	-5.08	101.52	108.38
2	E	935	PHE	CA-CB-CG	-5.08	108.72	113.80
2	I	919	HIS	CA-CB-CG	5.08	118.88	113.80
2	J	328	SER	N-CA-C	-5.08	99.71	108.69
2	C	71	VAL	N-CA-C	-5.07	107.81	112.83
2	D	265	ASP	N-CA-C	-5.07	100.63	108.90
2	E	317	ARG	CA-C-N	5.07	127.08	120.28
2	E	317	ARG	C-N-CA	5.07	127.08	120.28
2	H	819	VAL	CA-C-N	5.07	125.97	120.44
2	H	819	VAL	C-N-CA	5.07	125.97	120.44
2	A	840	LEU	N-CA-C	-5.07	106.94	114.64
2	K	176	GLN	N-CA-C	-5.07	100.20	108.76
4	P	7	PHE	N-CA-CB	5.07	119.05	110.49
4	P	48	LEU	CA-C-N	5.07	128.86	121.31
4	P	48	LEU	C-N-CA	5.07	128.86	121.31
4	Q	22	SER	CA-C-N	5.07	131.22	121.54
4	Q	22	SER	C-N-CA	5.07	131.22	121.54
2	D	60	ARG	N-CA-C	-5.07	101.04	108.99
2	E	224	ARG	CA-C-N	5.07	125.06	119.89
2	E	224	ARG	C-N-CA	5.07	125.06	119.89
2	H	429	GLU	N-CA-CB	5.07	119.05	110.49
2	K	646	ILE	N-CA-C	-5.06	99.71	107.71
2	K	119	THR	N-CA-C	-5.06	101.85	109.85
2	F	45	PHE	CA-CB-CG	-5.06	108.74	113.80
2	D	227	ASN	CA-CB-CG	5.06	117.66	112.60
2	A	338	GLN	N-CA-C	-5.06	107.16	113.38
2	B	175	ASP	CA-CB-CG	5.06	117.66	112.60
2	K	711	VAL	N-CA-C	-5.05	101.19	108.42
2	H	56	VAL	N-CA-C	-5.05	108.20	113.10
2	L	594	ASP	N-CA-C	-5.05	107.29	113.50
2	D	175	ASP	N-CA-CB	5.05	119.02	110.49
2	B	333	GLY	N-CA-C	-5.05	101.22	113.18
2	C	484	LEU	CA-C-N	5.05	125.04	119.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	484	LEU	C-N-CA	5.05	125.04	119.89
2	B	15	ILE	N-CA-C	-5.04	105.97	113.39
2	G	85	THR	N-CA-C	-5.04	100.95	109.07
2	B	896	GLU	N-CA-C	-5.04	101.07	108.99
2	G	397	LEU	CA-C-N	5.04	124.95	119.76
2	G	397	LEU	C-N-CA	5.04	124.95	119.76
2	G	391	HIS	N-CA-C	-5.04	104.88	112.99
2	K	724	ASN	N-CA-CB	5.04	119.01	110.49
5	R	53	ASN	N-CA-C	-5.04	107.12	114.12
1	X	16	ARG	CA-C-N	5.04	125.03	119.89
1	X	16	ARG	C-N-CA	5.04	125.03	119.89
2	L	494	MET	CA-C-N	5.03	126.98	120.44
2	L	494	MET	C-N-CA	5.03	126.98	120.44
2	B	704	LEU	N-CA-C	-5.03	105.87	112.41
2	H	659	SER	CA-C-N	5.03	131.15	121.54
2	H	659	SER	C-N-CA	5.03	131.15	121.54
2	K	384	ASP	CA-CB-CG	5.03	117.63	112.60
2	D	317	ARG	N-CA-C	5.03	116.82	110.33
2	G	640	ALA	N-CA-C	-5.03	100.21	108.41
1	3	19	MET	CA-C-N	5.03	128.46	122.03
1	3	19	MET	C-N-CA	5.03	128.46	122.03
2	E	630	ASP	CA-CB-CG	5.03	117.63	112.60
2	F	37	THR	N-CA-C	-5.03	106.83	113.17
2	G	59	ASP	CA-CB-CG	5.03	117.63	112.60
2	H	266	GLU	N-CA-C	-5.03	101.26	108.60
2	H	505	ASP	CA-CB-CG	5.03	117.63	112.60
2	J	295	ASP	N-CA-C	-5.03	107.18	113.72
2	A	295	ASP	N-CA-C	-5.03	107.19	113.72
2	D	935	PHE	CA-CB-CG	-5.03	108.78	113.80
2	A	377	ALA	N-CA-C	-5.02	100.10	110.80
2	C	244	THR	N-CA-C	-5.02	101.44	109.07
3	M	207	ASP	CA-CB-CG	5.02	117.62	112.60
2	A	863	ILE	N-CA-C	-5.02	98.04	108.88
2	B	46	ARG	NE-CZ-NH2	5.02	123.72	119.20
2	E	507	TYR	N-CA-C	-5.02	102.88	110.06
2	E	761	LEU	CA-C-N	5.02	127.01	120.28
2	E	761	LEU	C-N-CA	5.02	127.01	120.28
2	F	814	ASN	N-CA-C	-5.02	100.11	110.80
2	H	761	LEU	N-CA-C	-5.02	105.64	112.26
2	H	830	GLN	CA-C-N	5.02	125.30	119.93
2	H	830	GLN	C-N-CA	5.02	125.30	119.93
2	J	35	THR	N-CA-C	-5.02	105.89	112.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	480	ALA	N-CA-C	5.02	116.75	111.28
2	L	76	ASN	N-CA-C	-5.02	101.44	109.07
2	L	562	LEU	N-CA-C	-5.02	100.11	110.80
2	J	274	TYR	CA-C-N	5.02	127.83	120.71
2	J	274	TYR	C-N-CA	5.02	127.83	120.71
2	D	803	ASP	N-CA-C	-5.02	106.41	112.88
2	B	335	LEU	N-CA-C	-5.01	99.82	108.69
3	M	214	THR	N-CA-C	-5.01	107.02	114.64
2	A	331	ASN	N-CA-CB	5.01	118.95	110.49
2	D	460	ARG	CA-C-N	5.01	126.99	120.28
2	D	460	ARG	C-N-CA	5.01	126.99	120.28
2	J	109	ARG	N-CA-C	-5.01	101.23	109.40
4	O	133	ARG	NE-CZ-NH2	5.01	123.71	119.20
2	D	75	ASP	CA-CB-CG	5.01	117.61	112.60
2	F	869	PHE	CA-CB-CG	-5.01	108.79	113.80
2	B	293	LYS	N-CA-C	-5.01	106.59	113.30
2	D	939	ASN	N-CA-CB	5.01	118.95	110.49
2	G	345	VAL	N-CA-C	-5.01	100.86	108.17
2	H	661	ASN	N-CA-C	-5.01	101.01	109.07
2	G	11	ALA	CA-C-N	5.00	126.98	120.28
2	G	11	ALA	C-N-CA	5.00	126.98	120.28
2	G	830	GLN	CA-C-N	5.00	126.09	119.84
2	G	830	GLN	C-N-CA	5.00	126.09	119.84

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	109	ARG	Sidechain
2	A	207	ARG	Sidechain
2	B	219	TYR	Sidechain
2	B	507	TYR	Sidechain
2	B	571	TYR	Sidechain
2	B	654	PRO	Peptide
2	B	676	LYS	Peptide
2	D	187	GLN	Peptide
2	D	219	TYR	Sidechain
2	D	325	TYR	Sidechain
2	D	400	TYR	Sidechain
2	D	507	TYR	Sidechain
2	D	722	PRO	Peptide
2	E	219	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	E	470	TYR	Sidechain
2	E	625	ARG	Sidechain
2	E	68	PHE	Peptide
2	F	219	TYR	Sidechain
2	F	507	TYR	Sidechain
2	G	491	TYR	Sidechain
2	H	491	TYR	Sidechain
2	H	653	VAL	Peptide
2	H	691	TYR	Sidechain
2	I	109	ARG	Sidechain
2	I	116	TYR	Sidechain
2	I	23	TYR	Sidechain
2	I	491	TYR	Sidechain
2	I	729	THR	Peptide
2	I	917	ARG	Sidechain
2	J	109	ARG	Sidechain
2	J	491	TYR	Sidechain
2	K	768	TYR	Sidechain
2	L	109	ARG	Sidechain
2	L	491	TYR	Sidechain
2	L	507	TYR	Sidechain
2	L	636	TYR	Sidechain
2	L	930	TYR	Sidechain
3	M	294	TYR	Sidechain
4	O	20	LEU	Peptide
4	Q	27	ARG	Sidechain
5	R	54	ARG	Sidechain
6	T	13	TYR	Sidechain
6	T	14	GLN	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	0	55	51	50	0	0
1	1	127	118	116	0	0
1	2	167	156	155	0	0
1	3	200	186	185	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4	175	160	159	0	0
1	8	186	177	176	0	0
1	U	88	83	82	0	0
1	V	150	136	134	0	0
1	W	187	174	173	0	0
1	X	200	186	185	0	0
1	Y	200	186	185	0	0
1	Z	55	51	50	0	0
2	A	7480	7121	7121	0	0
2	B	7480	7121	7121	0	0
2	C	7480	7121	7121	0	0
2	D	7480	7121	7121	0	0
2	E	7480	7121	7121	0	0
2	F	7480	7121	7121	0	0
2	G	7480	7121	7121	0	0
2	H	7480	7121	7121	0	0
2	I	7480	7121	7121	0	0
2	J	7480	7121	7121	0	0
2	K	7480	7121	7121	0	0
2	L	7480	7121	7121	0	0
3	M	3500	3423	3420	0	0
4	N	664	664	663	0	0
4	O	592	595	593	0	0
4	P	715	720	719	0	0
4	Q	548	560	559	0	0
5	R	882	885	884	0	0
6	S	1365	1308	1307	0	0
6	T	1377	1318	1317	0	0
All	All	101193	96589	96564	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	0	5/243 (2%)	4 (80%)	0	1 (20%)	0	0
1	1	13/243 (5%)	9 (69%)	3 (23%)	1 (8%)	1	4
1	2	19/243 (8%)	15 (79%)	2 (10%)	2 (10%)	0	2
1	3	24/243 (10%)	16 (67%)	7 (29%)	1 (4%)	2	11
1	4	20/243 (8%)	14 (70%)	3 (15%)	3 (15%)	0	0
1	8	22/243 (9%)	13 (59%)	5 (23%)	4 (18%)	0	0
1	U	9/243 (4%)	7 (78%)	2 (22%)	0	100	100
1	V	16/243 (7%)	13 (81%)	2 (12%)	1 (6%)	1	6
1	W	22/243 (9%)	12 (54%)	8 (36%)	2 (9%)	0	3
1	X	24/243 (10%)	16 (67%)	3 (12%)	5 (21%)	0	0
1	Y	24/243 (10%)	18 (75%)	5 (21%)	1 (4%)	2	11
1	Z	5/243 (2%)	5 (100%)	0	0	100	100
2	A	940/942 (100%)	822 (87%)	80 (8%)	38 (4%)	2	12
2	B	940/942 (100%)	771 (82%)	99 (10%)	70 (7%)	1	4
2	C	940/942 (100%)	824 (88%)	85 (9%)	31 (3%)	3	15
2	D	940/942 (100%)	819 (87%)	75 (8%)	46 (5%)	1	9
2	E	940/942 (100%)	826 (88%)	79 (8%)	35 (4%)	2	13
2	F	940/942 (100%)	834 (89%)	67 (7%)	39 (4%)	2	12
2	G	940/942 (100%)	824 (88%)	82 (9%)	34 (4%)	2	14
2	H	940/942 (100%)	811 (86%)	89 (10%)	40 (4%)	2	11
2	I	940/942 (100%)	827 (88%)	79 (8%)	34 (4%)	2	14
2	J	940/942 (100%)	829 (88%)	75 (8%)	36 (4%)	2	13
2	K	940/942 (100%)	816 (87%)	95 (10%)	29 (3%)	3	16
2	L	940/942 (100%)	827 (88%)	75 (8%)	38 (4%)	2	12
3	M	429/532 (81%)	390 (91%)	28 (6%)	11 (3%)	4	19
4	N	85/142 (60%)	65 (76%)	9 (11%)	11 (13%)	0	1
4	O	73/142 (51%)	54 (74%)	9 (12%)	10 (14%)	0	1
4	P	92/142 (65%)	69 (75%)	11 (12%)	12 (13%)	0	1
4	Q	69/142 (49%)	57 (83%)	9 (13%)	3 (4%)	2	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	R	112/589 (19%)	94 (84%)	13 (12%)	5 (4%)	2	10
6	S	171/227 (75%)	141 (82%)	20 (12%)	10 (6%)	1	7
6	T	173/227 (76%)	143 (83%)	18 (10%)	12 (7%)	1	5
All	All	12687/16363 (78%)	10985 (87%)	1137 (9%)	565 (4%)	3	10

All (565) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	V	6	PHE
1	W	10	ALA
1	8	25	ILE
2	A	21	SER
2	A	76	ASN
2	A	232	GLN
2	A	344	ALA
2	A	377	ALA
2	A	676	LYS
2	A	686	ASP
2	A	810	ALA
2	B	59	ASP
2	B	70	PRO
2	B	219	TYR
2	B	342	LEU
2	B	645	PRO
2	B	650	ALA
2	B	651	THR
2	B	661	ASN
2	B	663	ALA
2	B	717	SER
2	B	724	ASN
2	B	836	TYR
2	B	936	SER
2	C	5	SER
2	C	11	ALA
2	C	187	GLN
2	C	339	ALA
2	C	377	ALA
2	C	558	ALA
2	C	706	HIS
2	C	836	TYR
2	D	2	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	4	PRO
2	D	175	ASP
2	D	197	TRP
2	D	198	GLN
2	D	377	ALA
2	D	425	ASP
2	D	689	PHE
2	D	866	SER
2	D	889	HIS
2	D	890	ALA
2	D	891	LEU
2	D	903	SER
2	E	7	LEU
2	E	172	ALA
2	E	239	ALA
2	E	377	ALA
2	E	558	ALA
2	E	886	ASN
2	F	21	SER
2	F	175	ASP
2	F	202	SER
2	F	284	ASP
2	F	377	ALA
2	F	716	ASP
2	F	836	TYR
2	F	885	ALA
2	F	933	THR
2	F	940	ALA
2	G	46	ARG
2	G	123	SER
2	G	506	ALA
2	G	718	SER
2	G	786	ARG
2	G	836	TYR
2	G	933	THR
2	H	174	ALA
2	H	175	ASP
2	H	239	ALA
2	H	377	ALA
2	H	391	HIS
2	H	558	ALA
2	H	654	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	657	ILE
2	H	660	ARG
2	H	724	ASN
2	H	937	ALA
2	I	2	ALA
2	I	21	SER
2	I	140	ALA
2	I	175	ASP
2	I	219	TYR
2	I	706	HIS
2	I	836	TYR
2	J	125	ALA
2	J	506	ALA
2	J	596	ALA
2	J	648	ALA
2	J	810	ALA
2	J	836	TYR
2	K	377	ALA
2	K	420	ASN
2	K	724	ASN
2	K	765	ASN
2	K	775	GLU
2	K	810	ALA
2	K	933	THR
2	L	5	SER
2	L	123	SER
2	L	175	ASP
2	L	560	LYS
2	L	648	ALA
2	L	706	HIS
2	L	724	ASN
2	L	810	ALA
2	L	939	ASN
3	M	75	ILE
3	M	85	SER
3	M	239	HIS
3	M	382	SER
4	N	4	SER
4	N	6	SER
4	N	11	VAL
4	N	12	PHE
4	N	13	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	N	26	VAL
4	O	13	SER
4	P	7	PHE
4	P	43	ALA
6	S	36	ALA
1	1	6	PHE
1	2	4	ILE
1	X	7	SER
1	X	19	MET
1	Y	8	SER
2	A	331	ASN
2	A	426	VAL
2	A	516	LEU
2	B	68	PHE
2	B	73	ARG
2	B	155	PRO
2	B	173	THR
2	B	176	GLN
2	B	338	GLN
2	B	339	ALA
2	B	377	ALA
2	B	631	GLN
2	B	647	PRO
2	B	649	ASN
2	B	680	SER
2	B	711	VAL
2	C	155	PRO
2	C	175	ASP
2	C	506	ALA
2	C	933	THR
2	D	130	PRO
2	D	188	PRO
2	D	202	SER
2	D	268	LYS
2	D	284	ASP
2	D	426	VAL
2	D	676	LYS
2	D	836	TYR
2	D	884	TYR
2	D	939	ASN
2	D	940	ALA
2	E	56	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	59	ASP
2	E	130	PRO
2	E	155	PRO
2	E	268	LYS
2	E	426	VAL
2	E	474	SER
2	E	742	GLU
2	E	836	TYR
2	E	933	THR
2	F	155	PRO
2	F	214	SER
2	F	296	ALA
2	F	426	VAL
2	F	815	ASN
2	G	239	ALA
2	G	320	PHE
2	G	364	LEU
2	G	377	ALA
2	G	481	ASN
2	G	589	ASN
2	G	764	TYR
2	H	130	PRO
2	H	240	ASP
2	H	340	SER
2	H	439	ARG
2	H	481	ASN
2	H	706	HIS
2	H	718	SER
2	H	739	VAL
2	I	123	SER
2	I	377	ALA
2	I	420	ASN
2	I	426	VAL
2	I	739	VAL
2	I	888	ALA
2	I	933	THR
2	J	2	ALA
2	J	173	THR
2	J	191	GLN
2	J	363	SER
2	J	377	ALA
2	J	718	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	940	ALA
2	K	155	PRO
2	K	202	SER
2	K	426	VAL
2	L	10	TRP
2	L	19	ASP
2	L	56	VAL
2	L	155	PRO
2	L	173	THR
2	L	377	ALA
2	L	426	VAL
2	L	562	LEU
2	L	596	ALA
2	L	764	TYR
2	L	836	TYR
2	L	872	MET
2	L	884	TYR
2	L	885	ALA
3	M	81	GLN
3	M	208	ILE
4	N	22	SER
4	N	46	SER
4	N	54	SER
4	O	6	SER
4	O	11	VAL
4	O	30	VAL
4	P	27	ARG
4	P	47	THR
4	Q	19	ARG
4	Q	134	ALA
5	R	23	ASN
5	R	27	ASP
5	R	52	ALA
6	T	176	SER
1	X	10	ALA
1	4	12	ARG
1	8	12	ARG
1	8	20	GLY
2	A	78	TYR
2	A	155	PRO
2	A	210	LYS
2	A	240	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	439	ARG
2	A	558	ALA
2	A	692	SER
2	A	718	SER
2	A	836	TYR
2	B	5	SER
2	B	16	ALA
2	B	210	LYS
2	B	220	GLY
2	B	262	ASN
2	B	330	GLY
2	B	560	LYS
2	B	659	SER
2	B	691	TYR
2	B	800	ASN
2	B	906	LEU
2	B	939	ASN
2	C	130	PRO
2	C	210	LYS
2	C	240	ASP
2	C	815	ASN
2	C	842	GLY
2	C	887	SER
2	C	939	ASN
2	D	36	ASP
2	D	78	TYR
2	D	291	PRO
2	D	364	LEU
2	D	506	ALA
2	D	703	TYR
2	D	814	ASN
2	D	901	ASP
2	E	16	ALA
2	E	43	ASN
2	E	71	VAL
2	E	198	GLN
2	E	341	GLN
2	E	422	ASN
2	E	718	SER
2	E	815	ASN
2	F	36	ASP
2	F	59	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	219	TYR
2	F	718	SER
2	G	2	ALA
2	G	175	ASP
2	G	186	PHE
2	G	710	LYS
2	G	767	GLY
2	H	37	THR
2	H	173	THR
2	H	263	GLY
2	H	264	GLN
2	H	688	TYR
2	H	764	TYR
2	H	767	GLY
2	H	814	ASN
2	H	836	TYR
2	H	887	SER
2	H	936	SER
2	I	39	PHE
2	I	130	PRO
2	I	174	ALA
2	I	422	ASN
2	I	481	ASN
2	I	767	GLY
2	I	887	SER
2	I	940	ALA
2	J	55	ASP
2	J	142	ASN
2	J	239	ALA
2	J	284	ASP
2	J	562	LEU
2	J	724	ASN
2	J	741	GLY
2	J	763	HIS
2	J	764	TYR
2	J	767	GLY
2	K	33	ARG
2	K	54	HIS
2	K	391	HIS
2	K	718	SER
2	K	767	GLY
2	L	7	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	117	SER
2	L	268	LYS
2	L	284	ASP
2	L	767	GLY
2	L	814	ASN
3	M	73	ALA
3	M	86	ASN
4	O	9	GLY
4	O	22	SER
4	O	133	ARG
4	P	119	GLY
4	P	131	GLN
6	S	43	ARG
6	S	73	ASN
6	S	176	SER
6	T	15	PRO
6	T	29	THR
6	T	34	LEU
6	T	73	ASN
6	T	174	SER
1	0	4	ILE
1	2	16	ARG
2	A	38	TYR
2	A	188	PRO
2	A	345	VAL
2	A	674	LYS
2	A	689	PHE
2	A	690	VAL
2	A	703	TYR
2	B	74	GLU
2	B	130	PRO
2	B	175	ASP
2	B	340	SER
2	B	426	VAL
2	B	648	ALA
2	B	692	SER
2	B	716	ASP
2	B	843	LYS
2	B	886	ASN
2	C	37	THR
2	C	202	SER
2	C	439	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	764	TYR
2	C	798	GLU
2	D	155	PRO
2	D	186	PHE
2	D	219	TYR
2	D	239	ALA
2	D	439	ARG
2	D	472	PRO
2	D	868	ASN
2	E	86	LEU
2	E	124	LEU
2	E	219	TYR
2	E	284	ASP
2	E	692	SER
2	E	739	VAL
2	F	159	GLU
2	F	168	ILE
2	F	201	GLU
2	F	240	ASP
2	F	291	PRO
2	F	320	PHE
2	F	739	VAL
2	F	814	ASN
2	G	78	TYR
2	G	155	PRO
2	G	268	LYS
2	G	429	GLU
2	G	439	ARG
2	G	730	PRO
2	G	739	VAL
2	G	763	HIS
2	H	38	TYR
2	H	67	ARG
2	H	317	ARG
2	I	78	TYR
2	I	703	TYR
2	I	718	SER
2	I	814	ASN
2	J	39	PHE
2	J	155	PRO
2	J	320	PHE
2	J	941	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	37	THR
2	K	38	TYR
2	K	239	ALA
2	K	331	ASN
2	K	506	ALA
2	K	835	ASN
2	L	130	PRO
2	L	176	GLN
2	L	293	LYS
2	L	763	HIS
3	M	226	GLU
3	M	528	SER
4	N	33	SER
4	O	18	GLY
4	O	21	PRO
4	P	13	SER
4	P	51	ALA
4	P	56	SER
4	P	133	ARG
4	Q	35	VAL
5	R	25	SER
5	R	42	ASN
6	S	4	GLU
6	S	32	ASN
6	S	35	SER
6	S	96	GLN
6	S	215	ASN
6	T	16	GLN
6	T	26	ASP
6	T	183	ILE
6	T	207	HIS
1	3	23	SER
1	X	24	ASP
1	4	16	ARG
2	A	130	PRO
2	A	166	LEU
2	A	284	ASP
2	A	602	SER
2	A	726	ARG
2	A	739	VAL
2	A	940	ALA
2	B	60	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	64	LEU
2	B	72	ASP
2	B	131	ASN
2	B	166	LEU
2	B	284	ASP
2	B	291	PRO
2	B	602	SER
2	B	739	VAL
2	B	903	SER
2	C	185	THR
2	C	331	ASN
2	C	685	PHE
2	C	703	TYR
2	C	739	VAL
2	C	940	ALA
2	D	38	TYR
2	D	407	SER
2	E	186	PHE
2	E	291	PRO
2	E	706	HIS
2	E	814	ASN
2	F	123	SER
2	F	130	PRO
2	F	429	GLU
2	F	439	ARG
2	F	602	SER
2	F	717	SER
2	F	740	ASP
2	G	130	PRO
2	G	284	ASP
2	G	814	ASN
2	H	155	PRO
2	H	429	GLU
2	H	561	SER
2	I	155	PRO
2	I	423	ASP
2	I	439	ARG
2	I	730	PRO
2	I	731	ASN
2	I	858	ARG
2	J	130	PRO
2	J	139	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	186	PHE
2	J	739	VAL
2	J	775	GLU
2	J	814	ASN
2	K	172	ALA
2	K	284	ASP
2	K	429	GLU
2	K	596	ALA
2	K	739	VAL
2	K	747	ALA
2	L	131	ASN
2	L	506	ALA
2	L	739	VAL
3	M	383	TRP
4	O	14	PRO
4	P	20	LEU
4	P	134	ALA
6	S	31	MET
1	W	19	MET
2	A	678	THR
2	B	75	ASP
2	B	242	VAL
2	B	268	LYS
2	B	341	GLN
2	B	429	GLU
2	B	439	ARG
2	B	658	PRO
2	B	703	TYR
2	B	921	PRO
2	D	201	GLU
2	D	658	PRO
2	D	679	PRO
2	D	933	THR
2	E	876	THR
2	F	39	PHE
2	F	314	ILE
2	F	703	TYR
2	F	705	ASN
2	G	396	GLU
2	G	703	TYR
2	G	719	VAL
2	G	722	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	54	HIS
2	H	284	ASP
2	J	115	PRO
2	J	725	ASP
2	K	115	PRO
6	T	104	SER
2	A	933	THR
2	B	261	VAL
2	C	56	VAL
2	I	524	PRO
2	J	56	VAL
2	L	504	VAL
1	X	11	PRO
1	8	11	PRO
2	A	115	PRO
2	B	504	VAL
2	H	864	PRO
2	H	921	PRO
2	K	730	PRO
6	T	92	PRO
2	A	114	LYS
2	B	934	PRO
2	D	283	PRO
2	I	921	PRO
4	N	20	LEU
2	F	472	PRO
2	L	647	PRO
1	4	14	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	0	7/203 (3%)	7 (100%)	0	100	100
1	1	15/203 (7%)	14 (93%)	1 (7%)	15	41
1	2	18/203 (9%)	17 (94%)	1 (6%)	19	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	22/203 (11%)	19 (86%)	3 (14%)	3	14
1	4	19/203 (9%)	18 (95%)	1 (5%)	20	48
1	8	20/203 (10%)	19 (95%)	1 (5%)	22	50
1	U	10/203 (5%)	9 (90%)	1 (10%)	7	26
1	V	17/203 (8%)	15 (88%)	2 (12%)	5	20
1	W	20/203 (10%)	19 (95%)	1 (5%)	22	50
1	X	22/203 (11%)	22 (100%)	0	100	100
1	Y	22/203 (11%)	21 (96%)	1 (4%)	24	53
1	Z	7/203 (3%)	7 (100%)	0	100	100
2	A	810/810 (100%)	799 (99%)	11 (1%)	59	73
2	B	810/810 (100%)	787 (97%)	23 (3%)	38	63
2	C	810/810 (100%)	794 (98%)	16 (2%)	48	69
2	D	810/810 (100%)	796 (98%)	14 (2%)	53	71
2	E	810/810 (100%)	797 (98%)	13 (2%)	55	72
2	F	810/810 (100%)	797 (98%)	13 (2%)	55	72
2	G	810/810 (100%)	801 (99%)	9 (1%)	65	76
2	H	810/810 (100%)	799 (99%)	11 (1%)	59	73
2	I	810/810 (100%)	796 (98%)	14 (2%)	53	71
2	J	810/810 (100%)	802 (99%)	8 (1%)	68	77
2	K	810/810 (100%)	795 (98%)	15 (2%)	50	70
2	L	810/810 (100%)	801 (99%)	9 (1%)	65	76
3	M	393/461 (85%)	389 (99%)	4 (1%)	68	77
4	N	74/105 (70%)	72 (97%)	2 (3%)	39	64
4	O	64/105 (61%)	62 (97%)	2 (3%)	35	61
4	P	79/105 (75%)	77 (98%)	2 (2%)	42	66
4	Q	58/105 (55%)	57 (98%)	1 (2%)	53	71
5	R	96/502 (19%)	93 (97%)	3 (3%)	35	61
6	S	149/189 (79%)	146 (98%)	3 (2%)	48	69
6	T	151/189 (80%)	148 (98%)	3 (2%)	48	69
All	All	10983/13917 (79%)	10795 (98%)	188 (2%)	52	71

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	12	ARG
1	1	12	ARG
1	V	19	MET
1	V	22	TRP
1	2	16	ARG
1	W	16	ARG
1	3	5	ASN
1	3	9	LEU
1	3	12	ARG
1	4	16	ARG
1	Y	25	ILE
1	8	4	ILE
2	A	56	VAL
2	A	153	VAL
2	A	232	GLN
2	A	245	LYS
2	A	319	ASN
2	A	332	MET
2	A	560	LYS
2	A	690	VAL
2	A	714	THR
2	A	835	ASN
2	A	868	ASN
2	B	44	LYS
2	B	58	THR
2	B	64	LEU
2	B	74	GLU
2	B	139	LYS
2	B	153	VAL
2	B	185	THR
2	B	211	LYS
2	B	342	LEU
2	B	343	ASN
2	B	574	ASN
2	B	593	THR
2	B	633	PHE
2	B	644	TYR
2	B	646	ILE
2	B	651	THR
2	B	653	VAL
2	B	710	LYS
2	B	800	ASN
2	B	841	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	894	ASN
2	B	904	THR
2	B	929	VAL
2	C	37	THR
2	C	53	THR
2	C	65	THR
2	C	138	LYS
2	C	153	VAL
2	C	185	THR
2	C	211	LYS
2	C	281	GLU
2	C	319	ASN
2	C	404	LEU
2	C	560	LYS
2	C	566	PRO
2	C	573	TRP
2	C	653	VAL
2	C	802	LYS
2	C	933	THR
2	D	10	TRP
2	D	53	THR
2	D	56	VAL
2	D	153	VAL
2	D	197	TRP
2	D	293	LYS
2	D	450	MET
2	D	572	GLU
2	D	643	LEU
2	D	869	PHE
2	D	872	MET
2	D	904	THR
2	D	905	LEU
2	D	933	THR
2	E	35	THR
2	E	71	VAL
2	E	146	MET
2	E	153	VAL
2	E	229	LYS
2	E	353	THR
2	E	397	LEU
2	E	503	LEU
2	E	566	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	573	TRP
2	E	589	ASN
2	E	904	THR
2	E	919	HIS
2	F	1	MET
2	F	53	THR
2	F	82	VAL
2	F	153	VAL
2	F	264	GLN
2	F	285	THR
2	F	321	ILE
2	F	417	LYS
2	F	450	MET
2	F	487	ASN
2	F	589	ASN
2	F	710	LYS
2	F	746	VAL
2	G	3	THR
2	G	19	ASP
2	G	21	SER
2	G	57	THR
2	G	280	LEU
2	G	481	ASN
2	G	509	ASN
2	G	676	LYS
2	G	904	THR
2	H	37	THR
2	H	68	PHE
2	H	74	GLU
2	H	138	LYS
2	H	153	VAL
2	H	211	LYS
2	H	391	HIS
2	H	455	GLN
2	H	633	PHE
2	H	714	THR
2	H	918	VAL
2	I	72	ASP
2	I	106	VAL
2	I	153	VAL
2	I	173	THR
2	I	211	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	481	ASN
2	I	598	ILE
2	I	660	ARG
2	I	795	VAL
2	I	872	MET
2	I	912	VAL
2	I	918	VAL
2	I	920	GLN
2	I	933	THR
2	J	285	THR
2	J	329	THR
2	J	542	ASN
2	J	601	THR
2	J	638	SER
2	J	853	LYS
2	J	904	THR
2	J	933	THR
2	K	82	VAL
2	K	138	LYS
2	K	153	VAL
2	K	211	LYS
2	K	282	THR
2	K	321	ILE
2	K	417	LYS
2	K	589	ASN
2	K	802	LYS
2	K	827	ARG
2	K	853	LYS
2	K	886	ASN
2	K	904	THR
2	K	915	VAL
2	K	917	ARG
2	L	37	THR
2	L	65	THR
2	L	82	VAL
2	L	116	TYR
2	L	184	LYS
2	L	573	TRP
2	L	710	LYS
2	L	753	LYS
2	L	856	CYS
3	M	81	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	M	225	THR
3	M	232	VAL
3	M	467	VAL
4	N	17	THR
4	N	41	GLN
4	O	14	PRO
4	O	20	LEU
4	P	103	LYS
4	P	131	GLN
4	Q	15	TYR
5	R	23	ASN
5	R	58	ILE
5	R	81	LEU
6	S	5	ILE
6	S	96	GLN
6	S	179	ARG
6	T	13	TYR
6	T	48	ARG
6	T	62	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

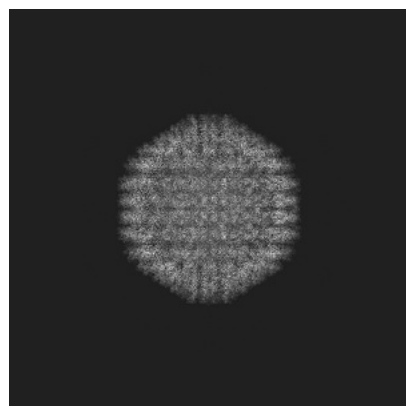
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24408. These allow visual inspection of the internal detail of the map and identification of artifacts.

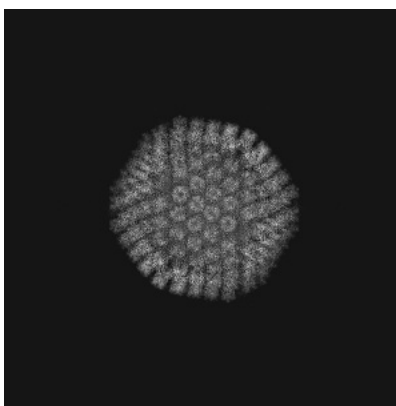
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

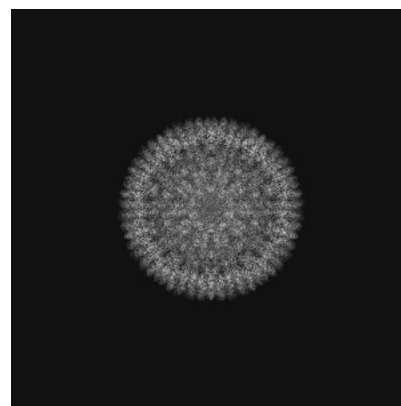
6.1.1 Primary map



X

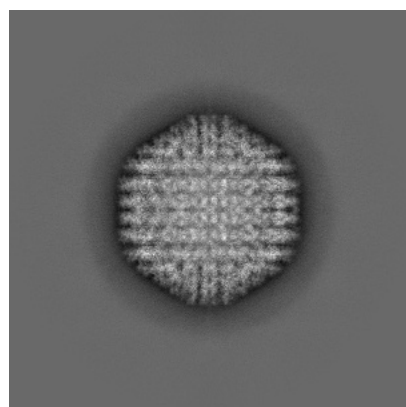


Y

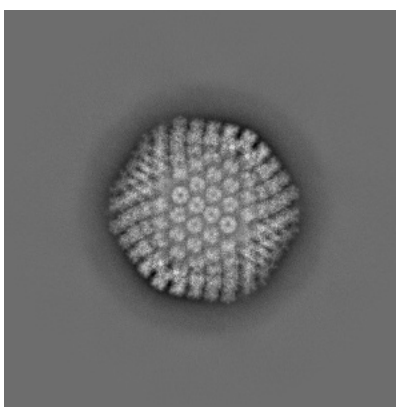


Z

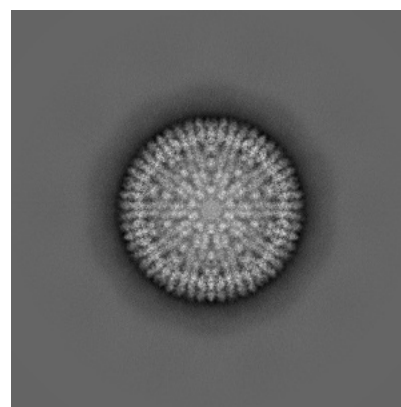
6.1.2 Raw map



X



Y

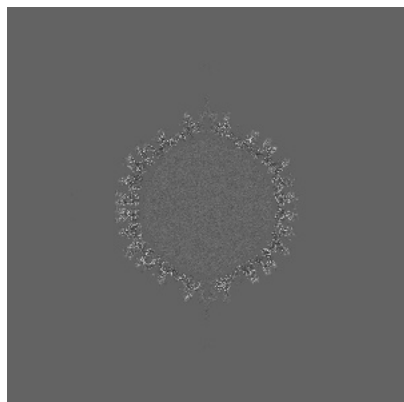


Z

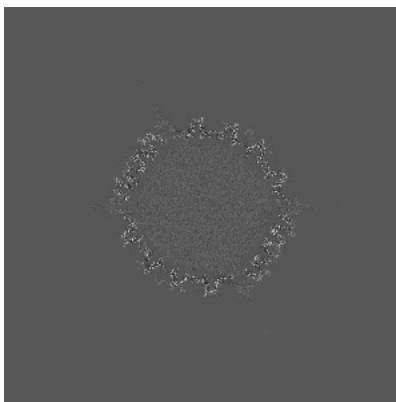
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

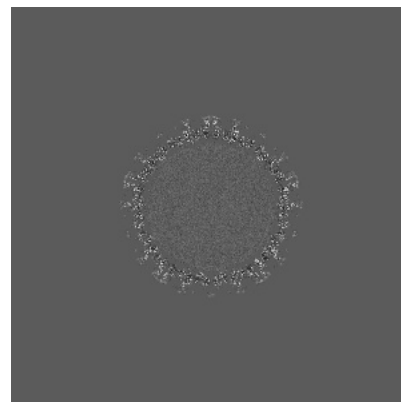
6.2.1 Primary map



X Index: 630

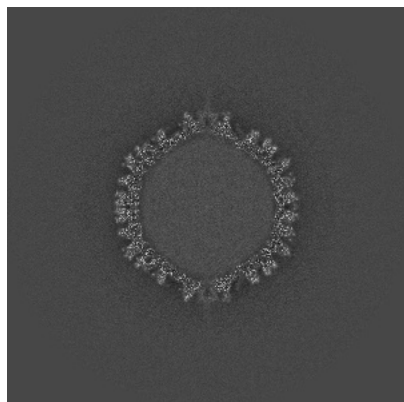


Y Index: 630

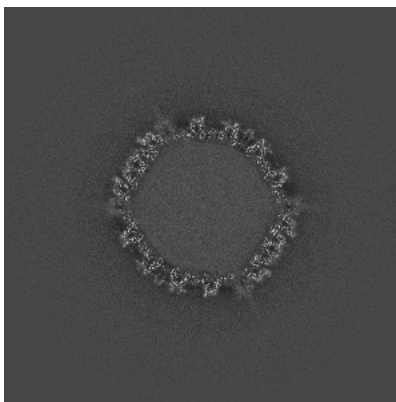


Z Index: 630

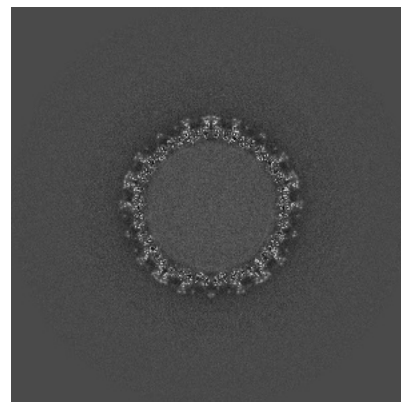
6.2.2 Raw map



X Index: 630



Y Index: 630

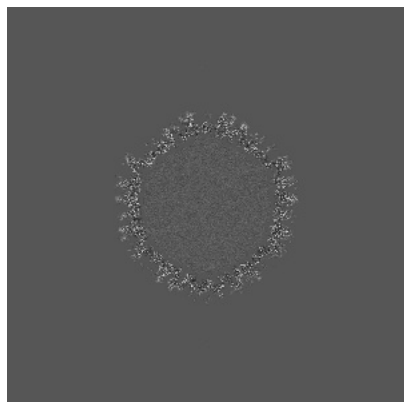


Z Index: 630

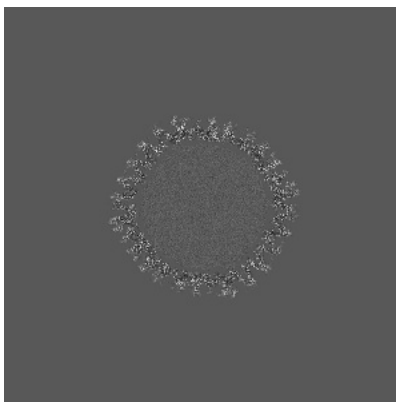
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

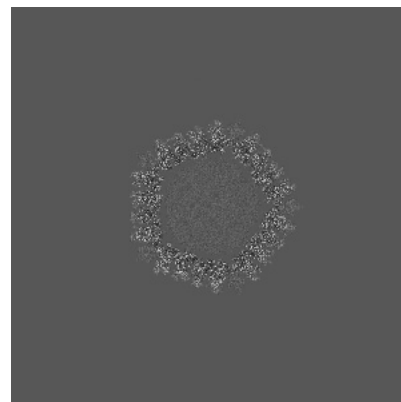
6.3.1 Primary map



X Index: 601

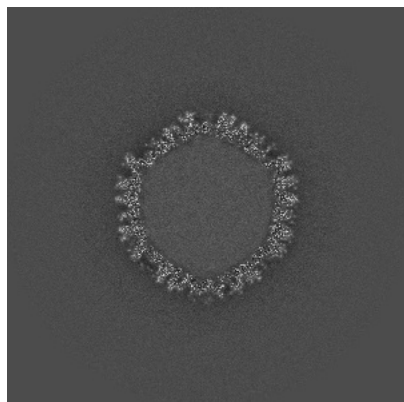


Y Index: 583

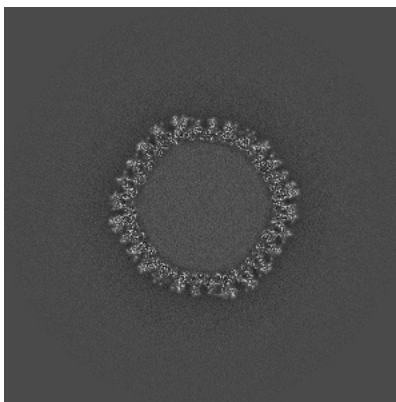


Z Index: 492

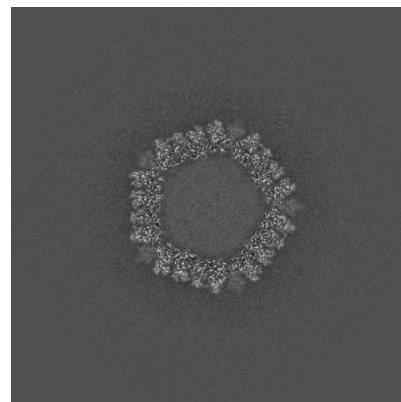
6.3.2 Raw map



X Index: 601



Y Index: 581

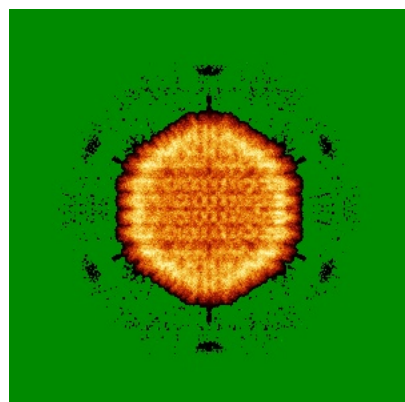


Z Index: 492

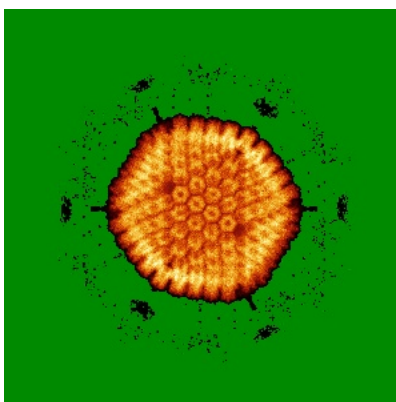
The images above show the largest variance slices of the map in three orthogonal directions.

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

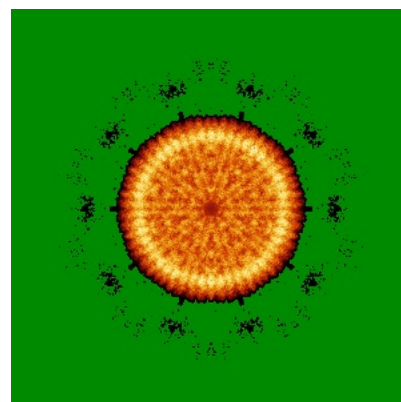
6.4.1 Primary map



X

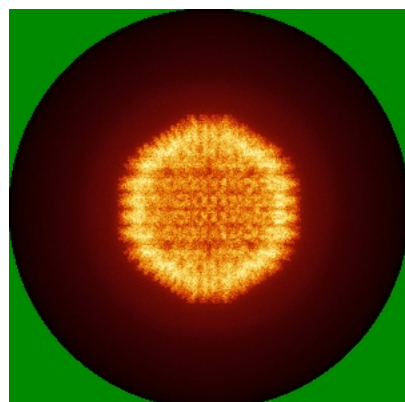


Y

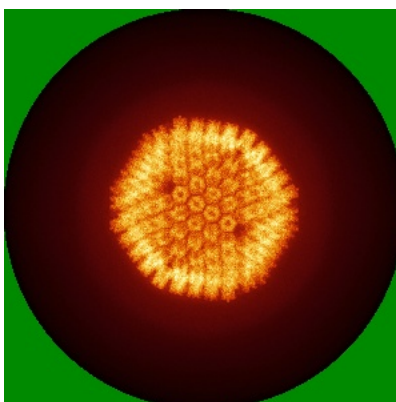


Z

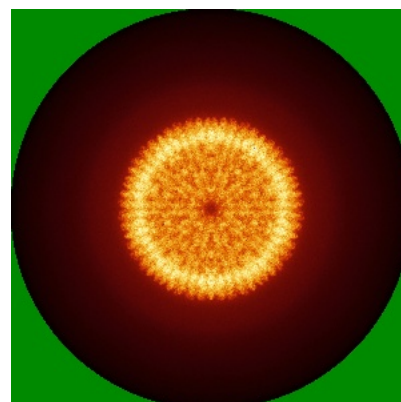
6.4.2 Raw map



X



Y

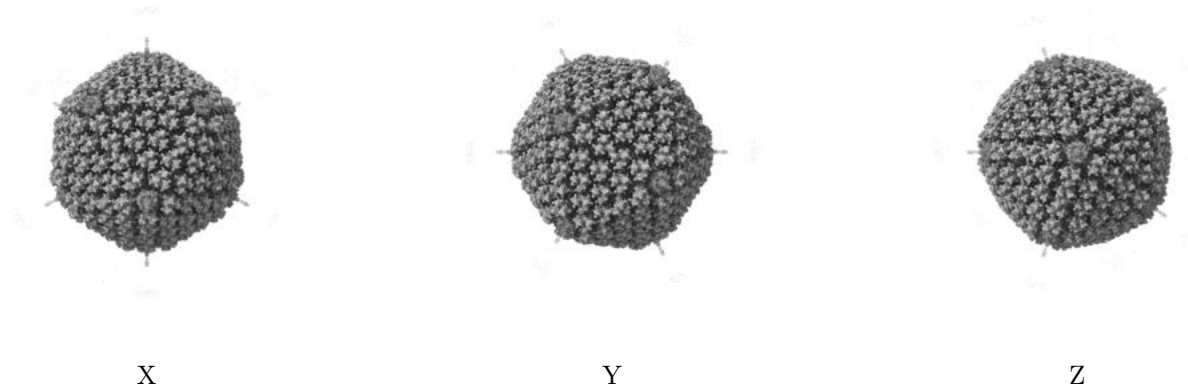


Z

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

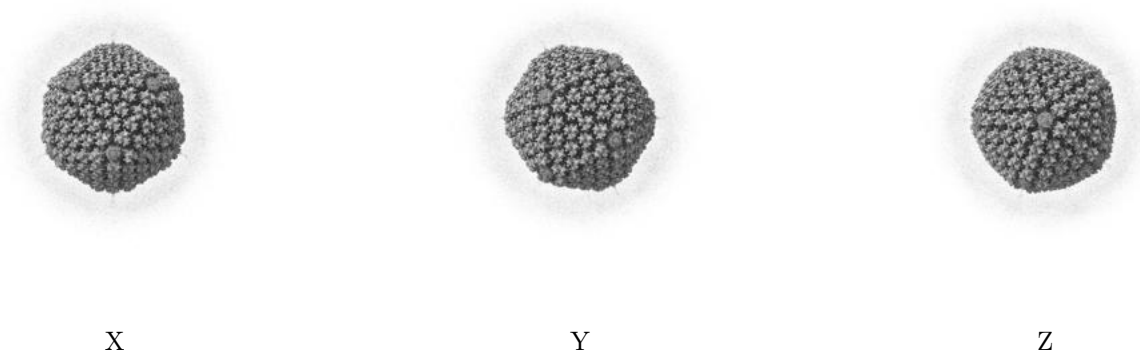
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

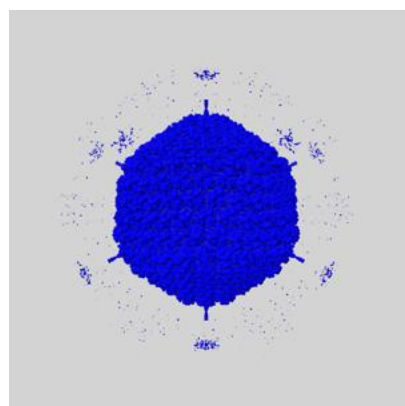
6.6 Mask visualisation [i](#)

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

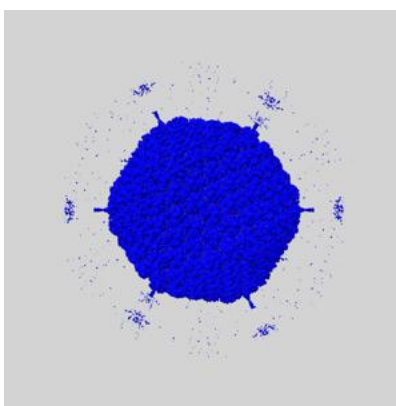
A mask typically either:

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

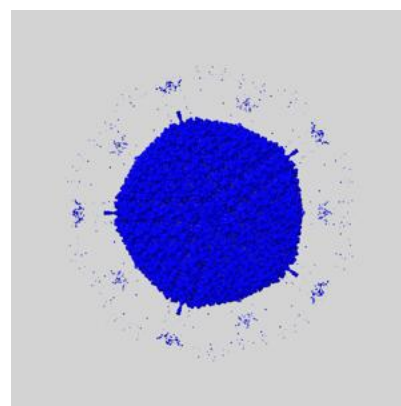
6.6.1 emd_24408_msk_1.map [i](#)



X



Y

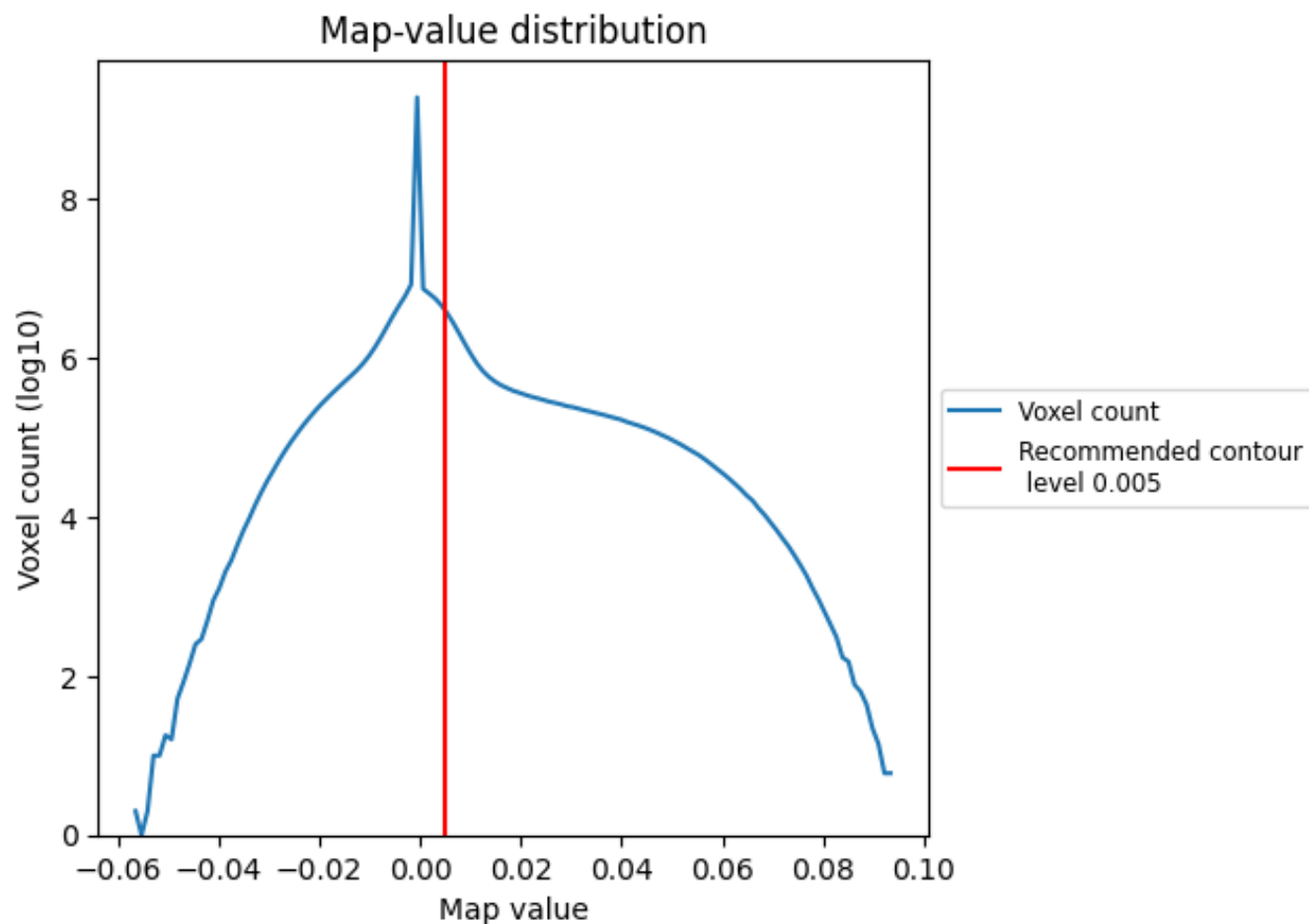


Z

7 Map analysis [i](#)

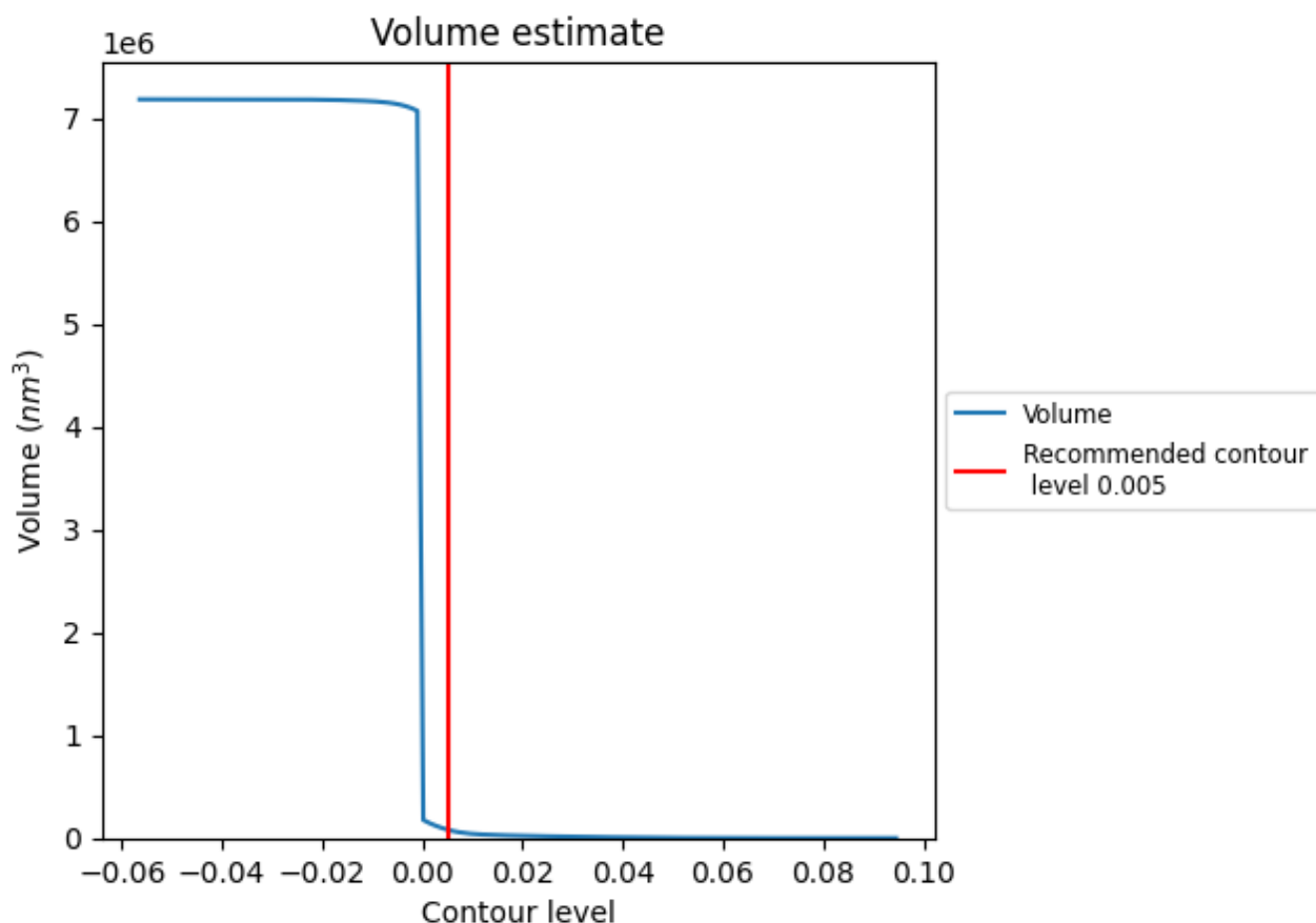
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

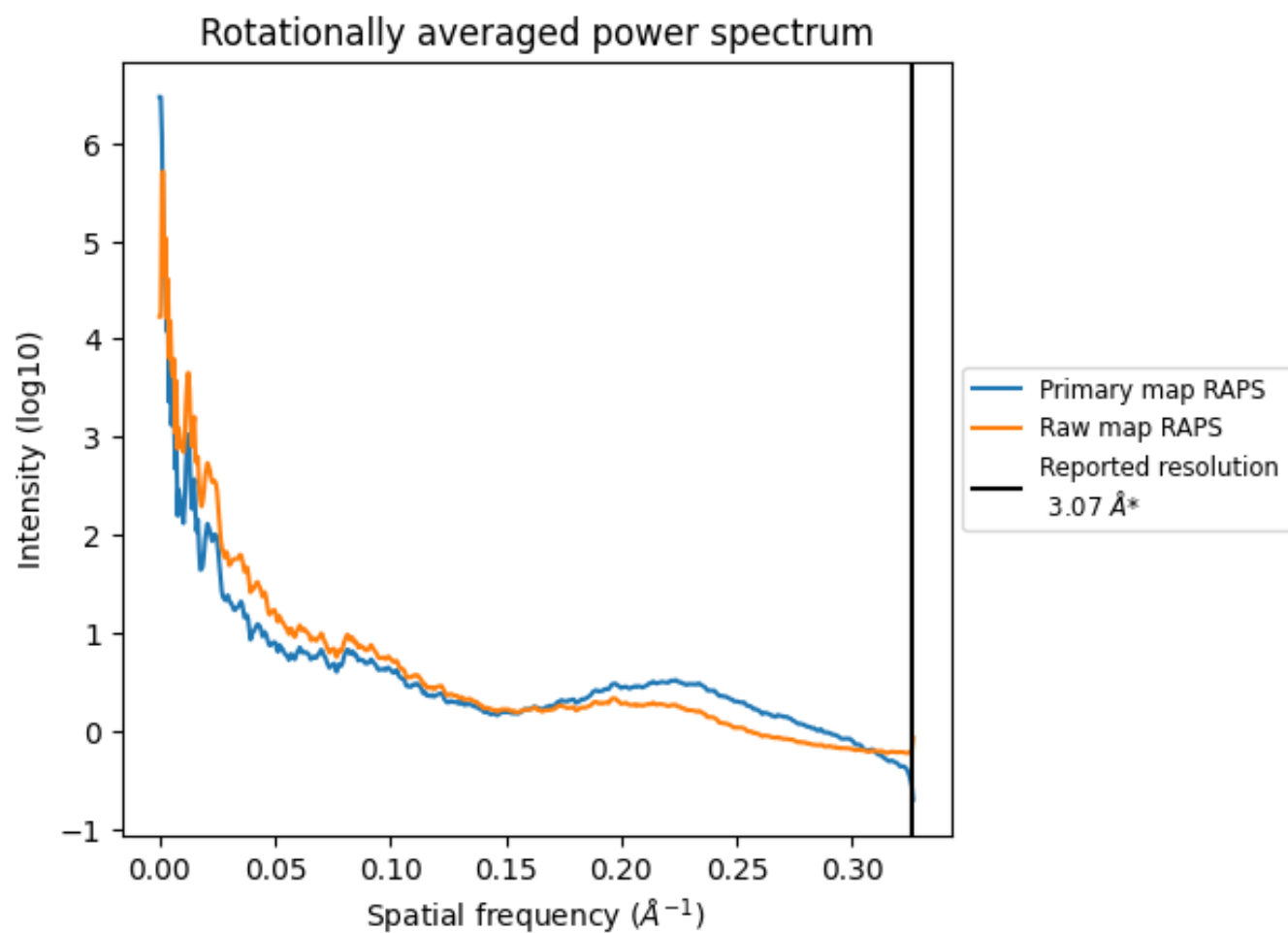
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 82016 nm³; this corresponds to an approximate mass of 74087 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 ⓘ

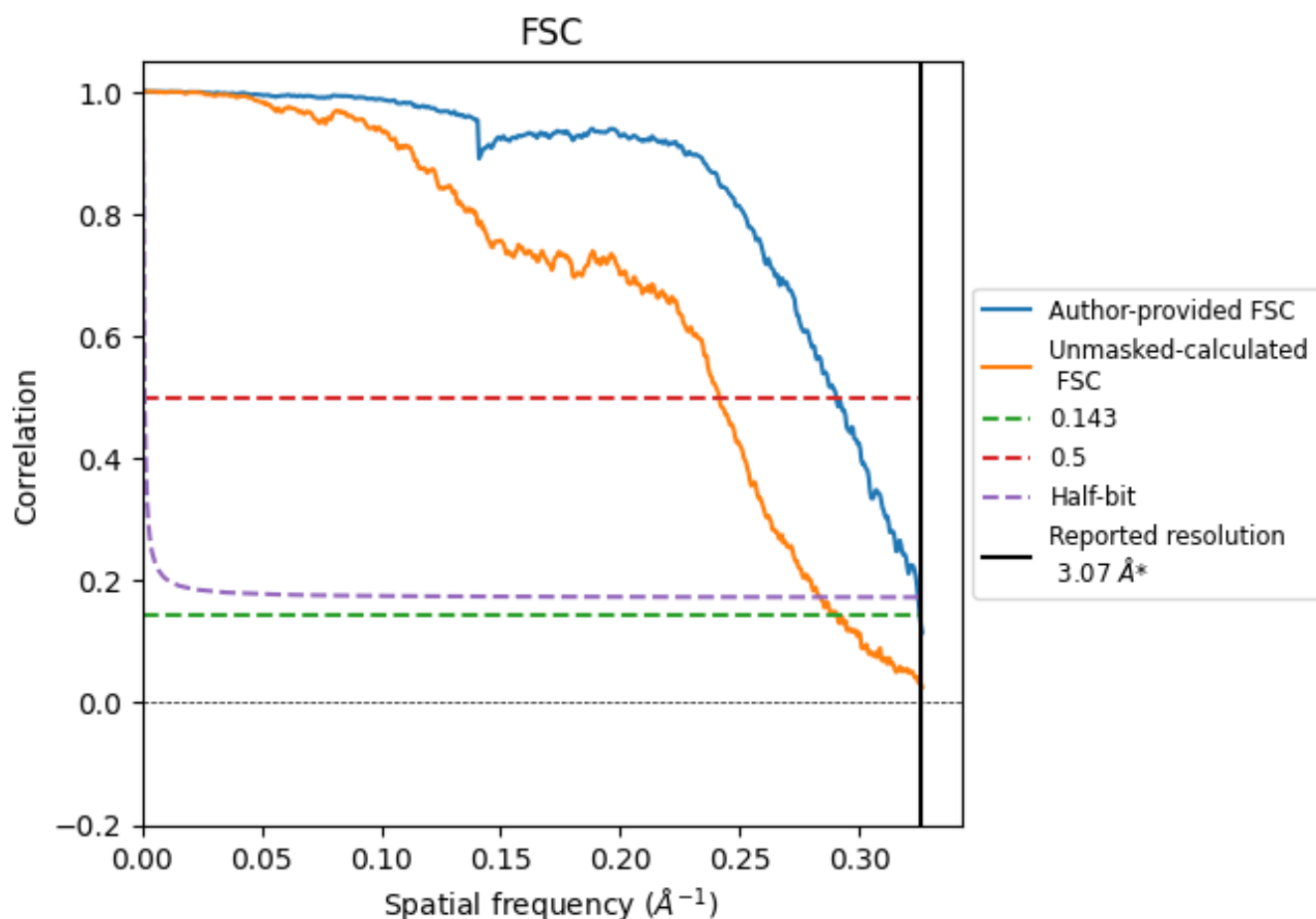


*Reported resolution corresponds to spatial frequency of 0.326 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.326 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	3.07	3.44	3.08
Unmasked-calculated*	3.44	4.14	3.52

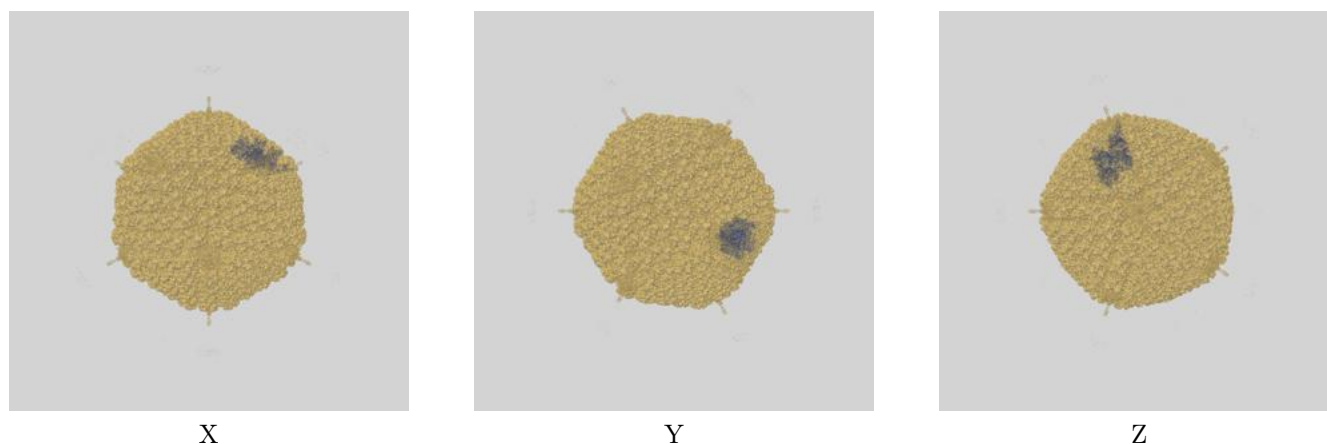
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.44 differs from the reported value 3.07 by more than 10 %

9 Map-model fit [i](#)

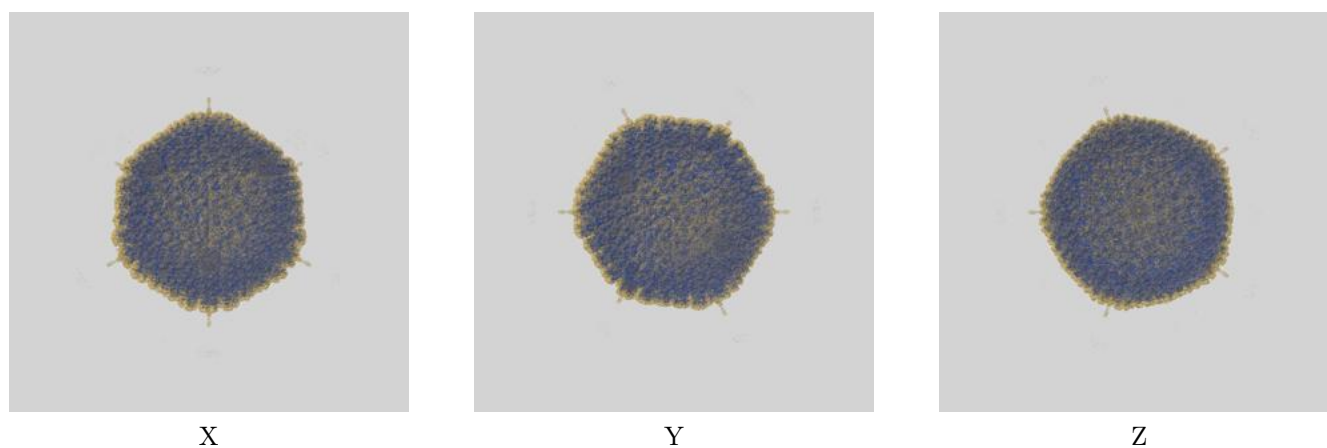
This section contains information regarding the fit between EMDB map EMD-24408 and PDB model 7RD1. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

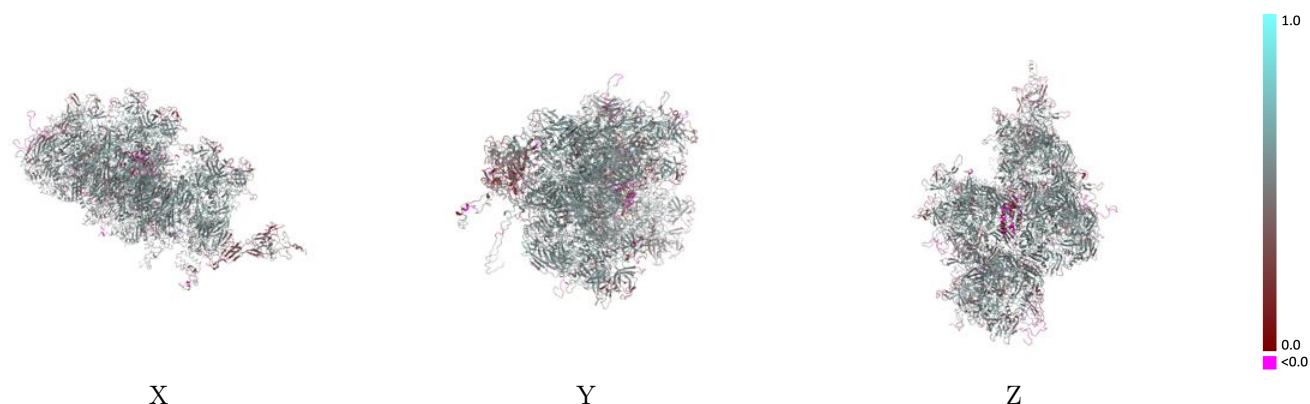


9.1.2 Map-model assembly overlay [i](#)



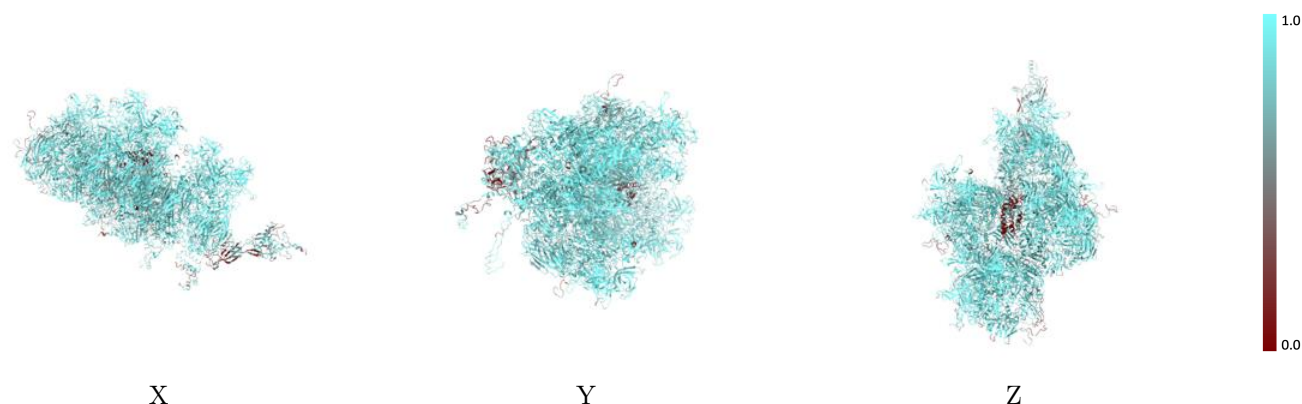
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



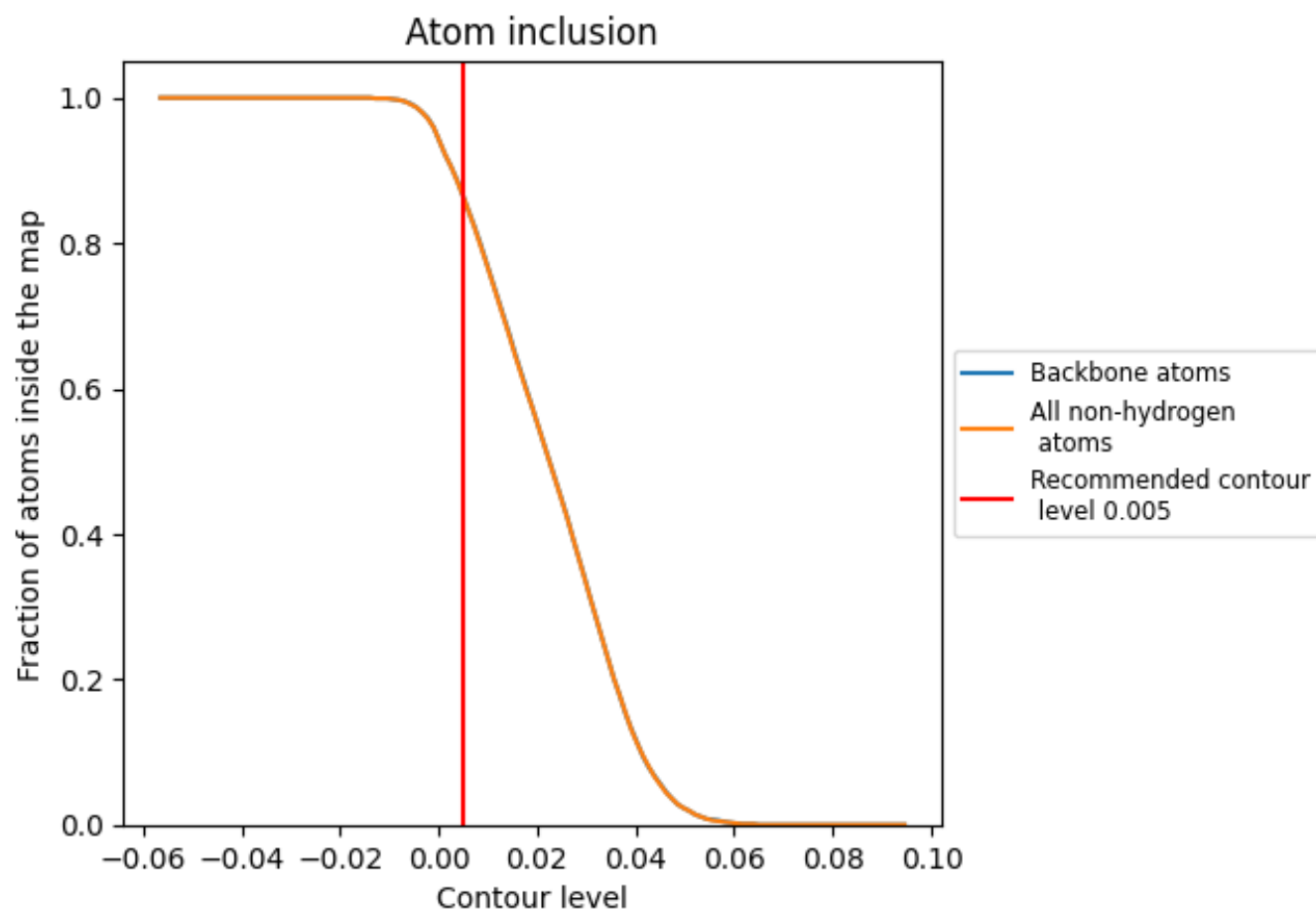
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8640	 0.4800
0	 0.2550	 0.1320
1	 0.5040	 0.2770
2	 0.6850	 0.3000
3	 0.7790	 0.4030
4	 0.5880	 0.3410
8	 0.7680	 0.3730
A	 0.9030	 0.4950
B	 0.8720	 0.4690
C	 0.9010	 0.5030
D	 0.8990	 0.5020
E	 0.9060	 0.5030
F	 0.9130	 0.5090
G	 0.9080	 0.5070
H	 0.9040	 0.5030
I	 0.9140	 0.5120
J	 0.9180	 0.5090
K	 0.9200	 0.5100
L	 0.9220	 0.5070
M	 0.5530	 0.3240
N	 0.2530	 0.1310
O	 0.1960	 0.0970
P	 0.2490	 0.0980
Q	 0.3000	 0.1510
R	 0.6450	 0.3480
S	 0.8390	 0.4490
T	 0.7980	 0.4300
U	 0.3370	 0.1390
V	 0.4830	 0.2980
W	 0.6210	 0.3490
X	 0.7030	 0.3460
Y	 0.5080	 0.2970
Z	 0.4360	 0.2690

