



Full wwPDB EM Validation Report ⓘ

Dec 9, 2025 – 12:59 am GMT

PDB ID : 9R78 / pdb_00009r78
EMDB ID : EMD-53736
Title : Human Adenovirus D 10 Capsid Structure
Authors : Waraich, K.; Mundy, R.M.; Bates, E.A.; da Fonseca, P.; Morris, E.; Rizkallah, P.J.; Baker, A.T.; Young, M.T.; Parker, A.L.; Bhella, D.
Deposited on : 2025-05-14
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.47

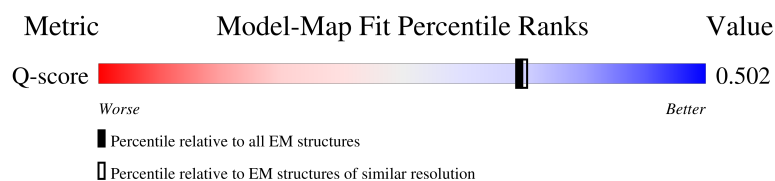
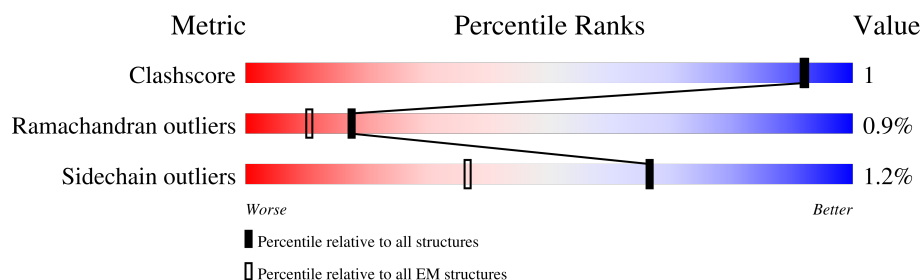
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



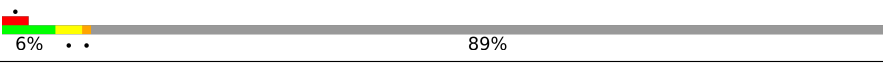
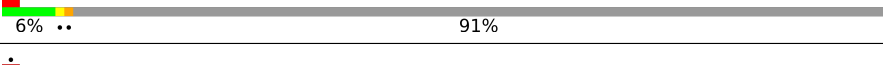

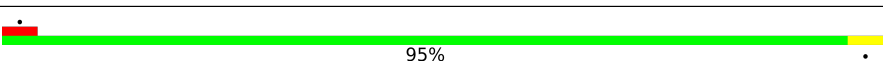
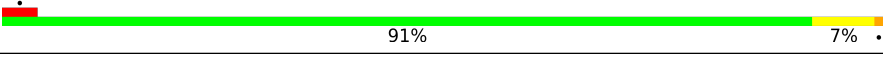
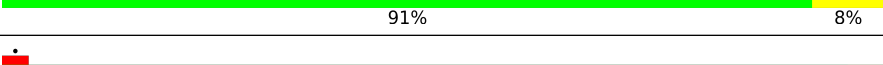
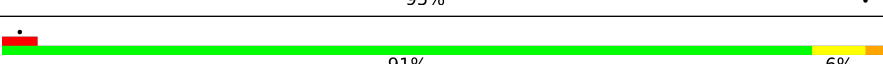
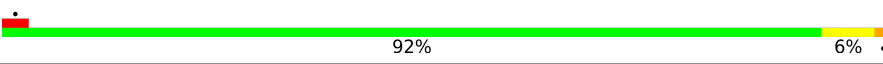
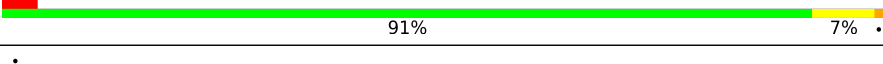
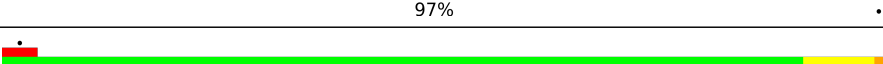
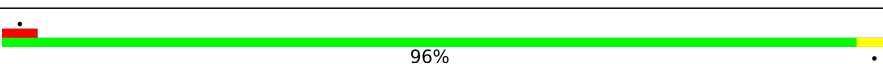
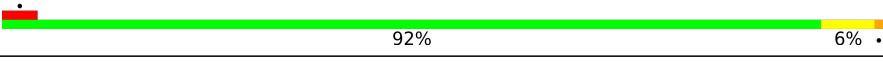
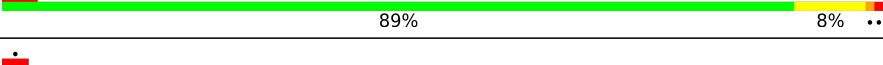


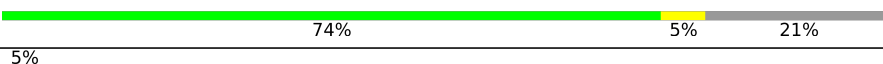

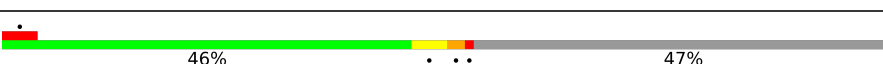





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	1	234	 6% • 91%
1	2	234	 6% • 93%
1	3	234	 • 5% • 91%
1	4	234	 • • 95%

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Mol	Chain	Length	Quality of chain
1	5	234	 6% 89%
1	6	234	 6% 91%
1	7	234	 7% 88%
1	8	234	 6% 93%
2	A	941	 95%
2	B	941	 91% 7%
2	C	941	 91% 8%
2	D	941	 95%
2	E	941	 91% 6%
2	F	941	 92% 6%
2	G	941	 91% 7%
2	H	941	 97%
2	I	941	 90% 8%
2	J	941	 96%
2	K	941	 92% 6%
2	L	941	 89% 8%
3	M	519	 87% 9%
4	N	559	 5% 48% 50%
5	O	227	 72% 6% 22%
5	P	227	 74% 5% 21%
6	Q	134	 5% 29% 71%
6	R	134	 26% 73%
6	S	134	 46% 47%
6	T	134	7% 22% 76%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 198096 atoms, of which 96875 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	1	22	Total	C	H	N	O	S	0	0
			340	112	163	33	31	1		
1	2	16	Total	C	H	N	O	S	0	0
			216	68	103	20	24	1		
1	3	21	Total	C	H	N	O	S	0	0
			325	107	157	32	28	1		
1	4	11	Total	C	H	N	O	S	0	0
			172	58	81	18	14	1		
1	5	25	Total	C	H	N	O	S	0	0
			393	128	191	36	36	2		
1	6	20	Total	C	H	N	O	S	0	0
			309	102	148	31	27	1		
1	7	27	Total	C	H	N	O	S	0	0
			415	134	204	39	37	1		
1	8	17	Total	C	H	N	O	S	0	0
			271	90	131	26	23	1		

- Molecule 2 is a protein called Hexon protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	941	Total	C	H	N	O	S	0	0
			14639	4751	7148	1264	1441	35		
2	B	941	Total	C	H	N	O	S	0	0
			14639	4751	7148	1264	1441	35		
2	C	941	Total	C	H	N	O	S	0	0
			14640	4751	7149	1264	1441	35		
2	D	941	Total	C	H	N	O	S	0	0
			14640	4751	7149	1264	1441	35		
2	E	941	Total	C	H	N	O	S	0	0
			14639	4751	7148	1264	1441	35		
2	F	941	Total	C	H	N	O	S	0	0
			14639	4751	7148	1264	1441	35		
2	G	941	Total	C	H	N	O	S	0	0
			14640	4751	7149	1264	1441	35		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	941	Total	C	H	N	O	S	0	0
			14639	4751	7148	1264	1441	35		
2	I	941	Total	C	H	N	O	S	0	0
			14639	4751	7148	1264	1441	35		
2	J	941	Total	C	H	N	O	S	0	0
			14639	4751	7148	1264	1441	35		
2	K	941	Total	C	H	N	O	S	0	0
			14639	4751	7148	1264	1441	35		
2	L	939	Total	C	H	N	O	S	0	0
			14604	4741	7129	1262	1439	33		

- Molecule 3 is a protein called Penton protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	M	472	Total	C	H	N	O	S	0	0
			7509	2410	3715	642	728	14		

- Molecule 4 is a protein called Pre-hexon-linking protein IIIa.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	N	281	Total	C	H	N	O	S	0	0
			4346	1354	2170	397	422	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	O	177	Total	C	H	N	O	S	0	0
			2706	868	1329	237	267	5		
5	P	180	Total	C	H	N	O	S	0	0
			2727	874	1338	240	270	5		

- Molecule 6 is a protein called Hexon-interlacing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	Q	39	Total	C	H	N	O		0	0
			619	188	317	52	62			
6	R	36	Total	C	H	N	O		0	0
			579	175	294	51	59			
6	S	71	Total	C	H	N	O	S	0	0
			1017	305	513	88	109	2		
6	T	32	Total	C	H	N	O		0	0
			516	154	261	48	53			

ALA	PRO	PRO	LYS	ALA	THR	PRO	VAL	VAL	GLN	ALA	ALA	PRO	PRO	VAL	ALA	ALA	THR	ALA	VAL	ARG	ARG	VAL	VAL	PRO	ALA	ALA	ARG	ARG	GLN	GLN	ASN	TRP	TRP	GLN	SER	SER	THR	HIS	LEU	LEU	GLY	VAL	VAL	LYS	VAL	SER	SER	LEU	LEU	LYS	ARG	ARG	ARG	CYS	TYR
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Chain 4:  95%

THR	LEU	PRO	PRO	PRO	LYS	GLU	LYS	ARG	PRO	ARG	PRO	ASP	ALA	GLU	GLU	THR	ILE	LEU	GLN	VAL	ASP	GLU	PRO	PRO	SER	TYR	GLU	GLU	ALA	ALA	VAL	LYS	ALA	GLY	MET	PRO	THR	THR	ARG	ILE	ILE	ALA	PRO	LEU	ALA	ALA	THR	GLY	VAL	MET	LYS	PRO	PRO	PRO	PRO
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PRO	ALA	PRO	ALA	ALA	PRO	PRO	PRO	LYS	ALA	THR	VAL	VAL	GLN	ALA	ALA	PRO	PRO	VAL	ALA	ALA	THR	ALA	VAL	ARG	ARG	VAL	PRO	PRO	ALA	ALA	ARG	ARG	GLN	GLN	GLN	ASN	TRP	TRP	GLN	SER	SER	THR	THR	LEU	LEU	LEU	GLY	GLY	VAL	VAL	LYS	LYS	SER	SER	LYS	LYS	LEU	LEU	LEU	GLY	GLY	VAL	VAL	THR	THR	ARG	ARG	ARG	ARG	CYS	CYS	TYR	TYR
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Chain 5:  6% 89%

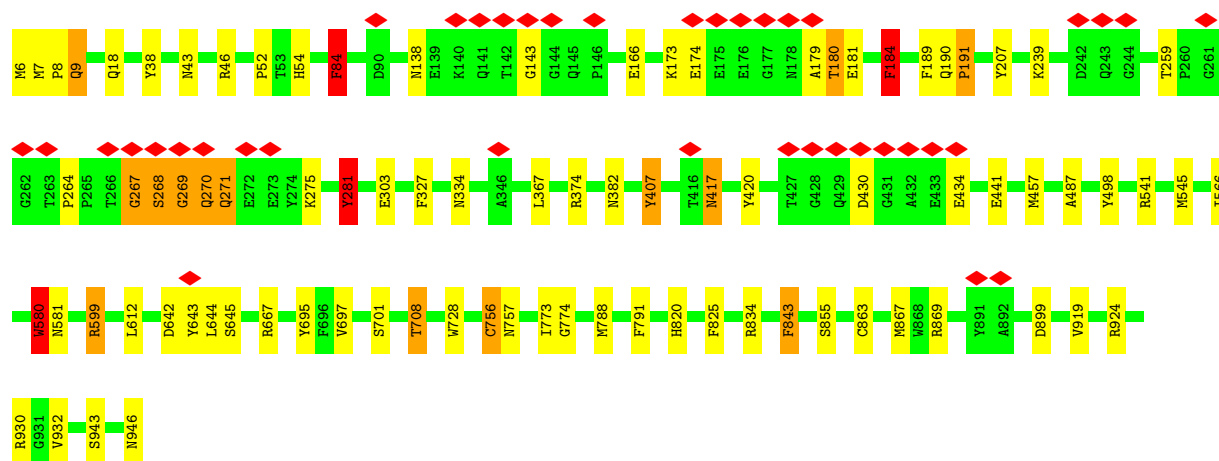
lys	gly	lys	arg	pro	arg	pro	pro	asp	ala	glu	glu	thr	ile	leu	glu	asp	glu	pro	pro	ser	tyr	glu	glu	ala	val	lys	ala	ala	gly	met	thr	thr	arg	ile	ile	ala	pro	leu	leu	thr	ala	thr	ala	pro	pro	pro	ala	ala	pro
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PRO LYS ALA THR PRO PRO VAL VAL GLN ALA ALA PRO PRO VAL VAL THR THR VAL VAL ARG ARG ARG ARG ARG GLN ALA ALA ASN TRP TRP SER SER HIS SER SER ILE ILE VAL VAL GLY LEU LEU LEU GLY GLY VAL LYS LYS SER SER LEU LEU LYS ARG ARG ARG ARG CYS TYR

Chain 6: 6% 91%

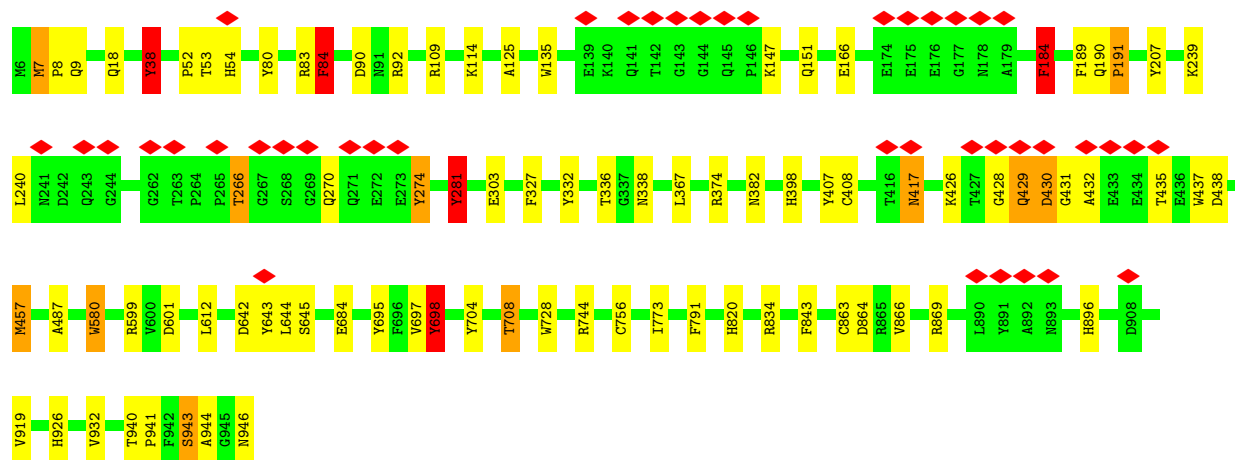
LYS	GLY	GLU	GLY	LYS	ARG	PRO	ARG	PRO	ASP	ALA	GLU	THR	ILE	LEU	GLN	VAL	ASP	GLU	PRO	PRO	SER	TYR	GLU	GLY	ALA	ALA	GLY	MET	PRO	THR	THR	ARG	ILE	ILE	ALA	PRO	PRO	LEU	LEU	LEU	LEU	PRO	PRO	PRO	ALA	ALA	PRO	PRO
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Chain B:  91% 7%



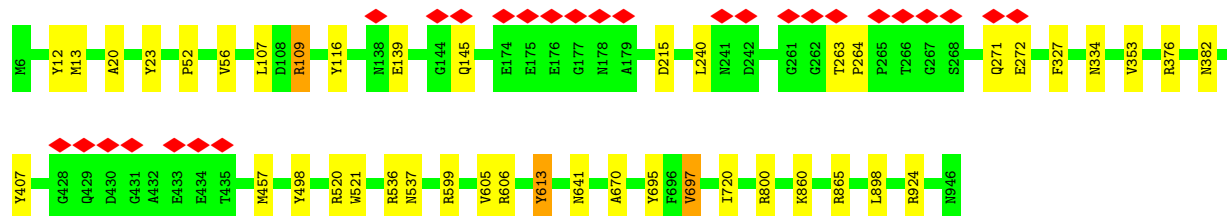
• Molecule 2: Hexon protein

Chain C: 91% 8% ..



• Molecule 2: Hexon protein

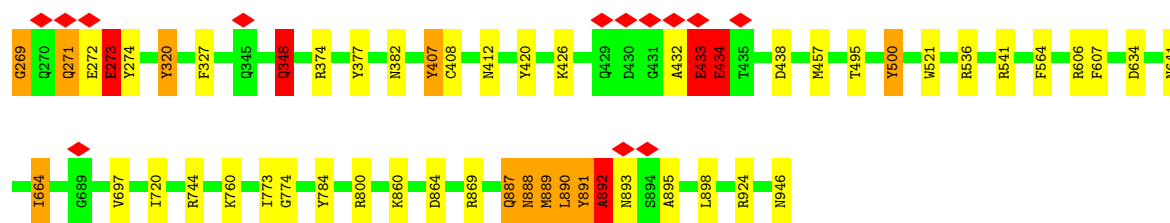
Chain D: 95% 5% .



• Molecule 2: Hexon protein

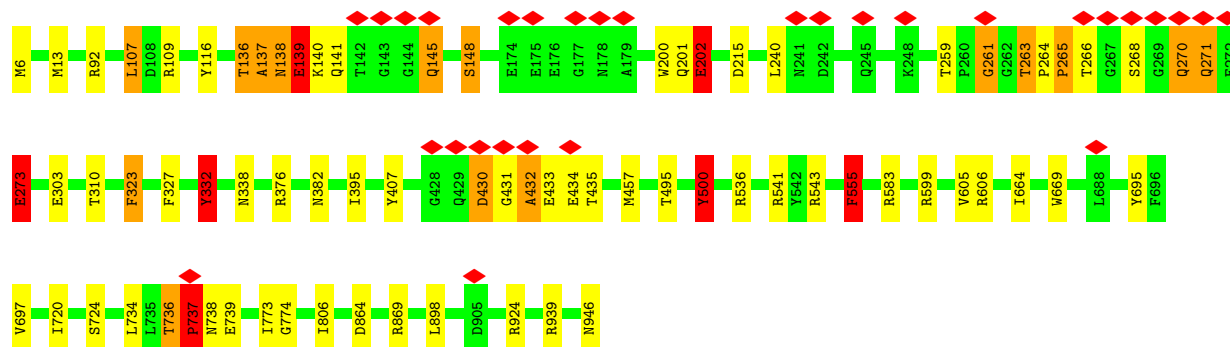
Chain E: 91% 6% ..





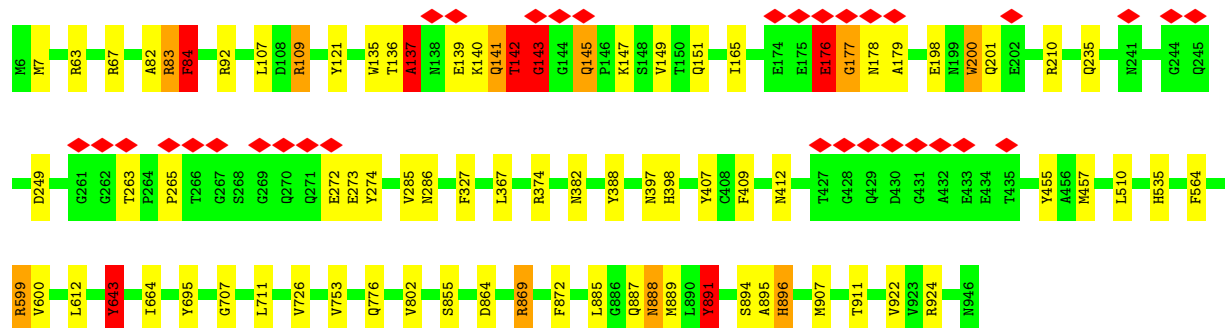
• Molecule 2: Hexon protein

Chain F: 92% 6% ..



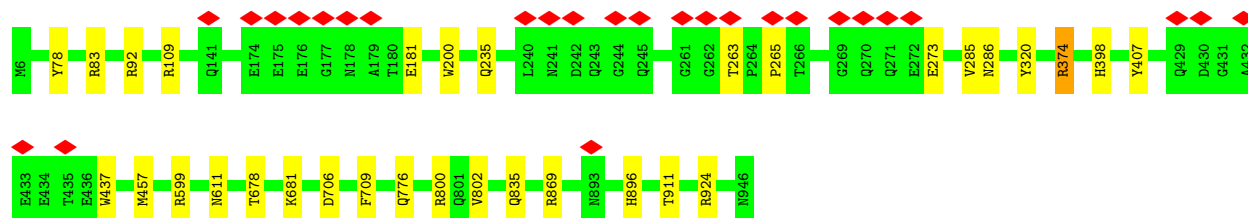
• Molecule 2: Hexon protein

Chain G: 91% 7% ..

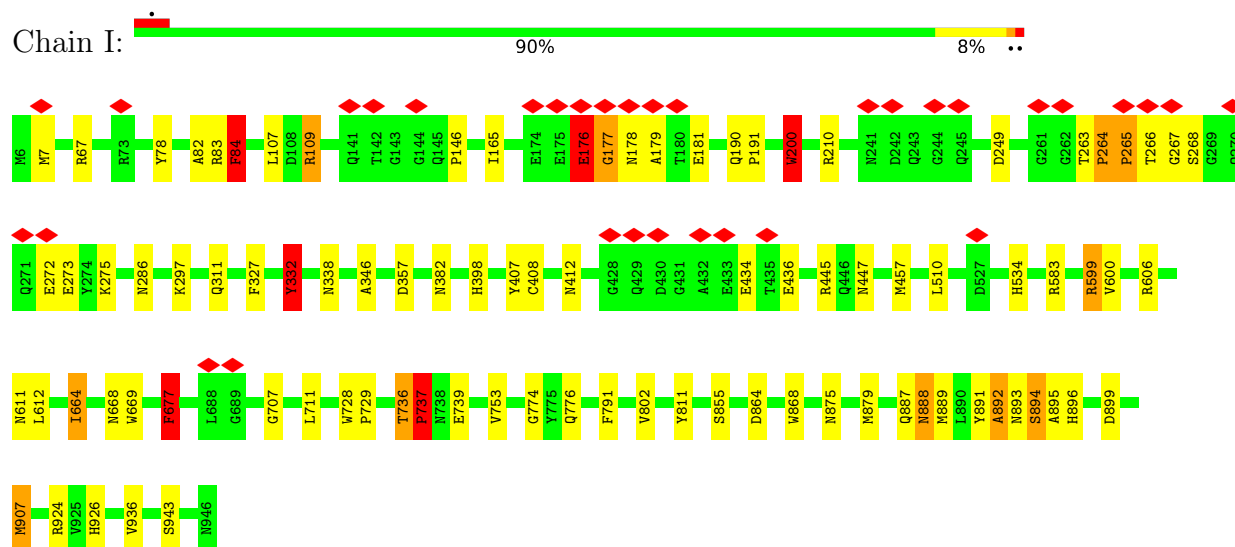


• Molecule 2: Hexon protein

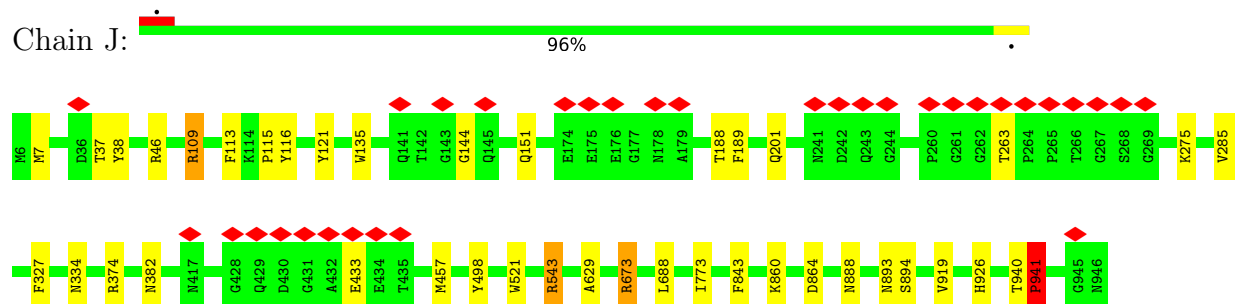
Chain H: 97%



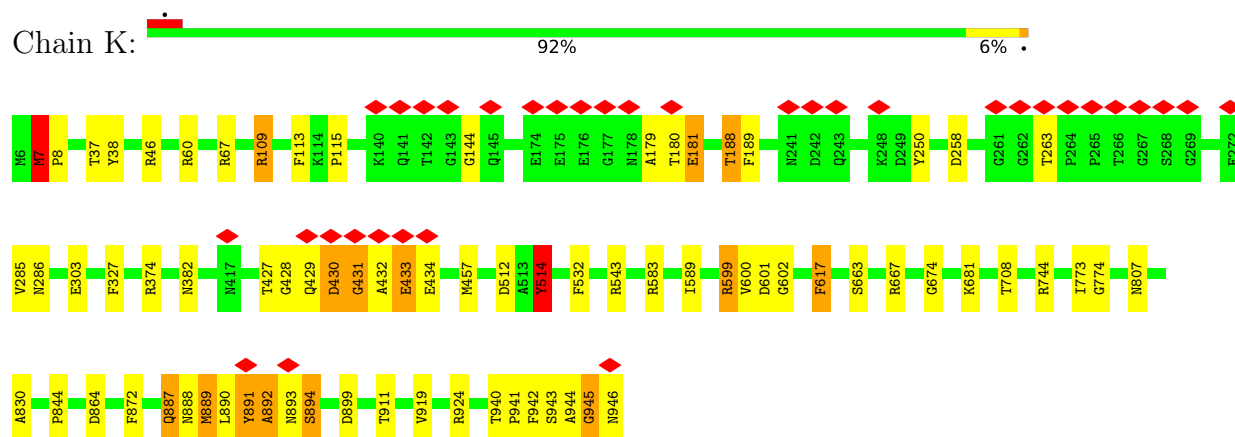
• Molecule 2: Hexon protein



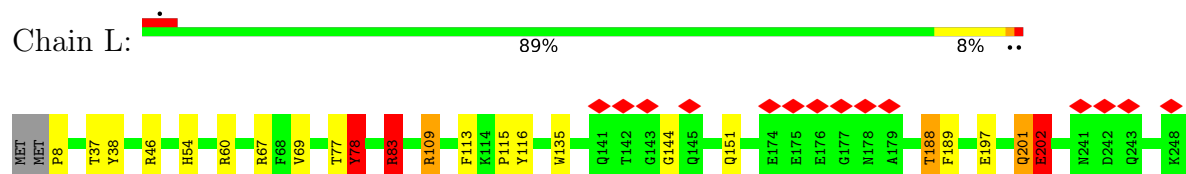
• Molecule 2: Hexon protein

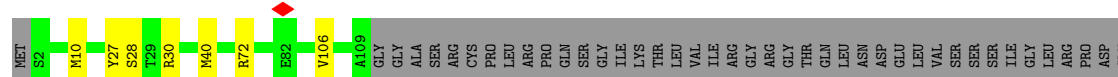


• Molecule 2: Hexon protein



• Molecule 2: Hexon protein





MET	ASN	GLY	THR	GLY	GLY	ALA	PHE	GLU	GLY	GLY	LEU	PHE	SER	PRO	TYR	LEU	THR	THR	ARG	LEU	PRO	PRO	GLY	TRP	ALA	GLY	VAL	ARG	GLN	ASN	VAL	MET	GLY	SER	SER	THR	THR	ASP	GLY	ARG	PRO	VAL	LEU	PRO	ALA	ASN	SER	SER	SER	THR	MET	THR	TYR	ALA	THR	VAL	GLY	SER	SER	SER	LEU	ASP
SER	THR	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	MET	THR	ALA	THR	ARG	LEU	ALA	SER	SER	TYR	PRO	MET	PRO	SER	SER	GLY	SER	SER	PRO	SER	VAL	PRO	SER	SER	ILE	ILE	ALA	GLU	GLU	LYS	LEU	LEU	A103	L104	L105	A106	E107	R113	Q114	L115	Q121	L125	R126	Q132	N133	K134						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	5524	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0216	Depositor
Map size (Å)	1193.76, 1193.76, 1193.76	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.658, 1.658, 1.658	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	1	1.07	0/183	1.86	2/248 (0.8%)
1	2	1.21	0/114	1.66	0/153
1	3	1.08	0/174	2.10	6/236 (2.5%)
1	4	0.97	0/95	2.10	3/128 (2.3%)
1	5	0.90	0/208	1.64	1/281 (0.4%)
1	6	1.15	0/167	1.70	1/226 (0.4%)
1	7	1.04	0/217	1.71	3/294 (1.0%)
1	8	1.04	0/144	1.65	2/193 (1.0%)
2	A	0.73	0/7696	1.31	20/10469 (0.2%)
2	B	0.85	12/7696 (0.2%)	1.51	72/10469 (0.7%)
2	C	0.75	0/7696	1.48	76/10469 (0.7%)
2	D	0.72	0/7696	1.29	12/10469 (0.1%)
2	E	0.78	2/7696 (0.0%)	1.55	89/10469 (0.9%)
2	F	0.75	0/7696	1.46	58/10469 (0.6%)
2	G	0.74	0/7696	1.51	74/10469 (0.7%)
2	H	0.72	0/7696	1.30	15/10469 (0.1%)
2	I	0.74	0/7696	1.49	69/10469 (0.7%)
2	J	0.73	0/7696	1.32	21/10469 (0.2%)
2	K	0.75	0/7696	1.49	62/10469 (0.6%)
2	L	0.75	0/7680	1.49	72/10448 (0.7%)
3	M	0.74	0/3887	1.35	9/5290 (0.2%)
4	N	0.75	0/2212	1.38	1/3011 (0.0%)
5	O	0.77	0/1414	1.37	4/1929 (0.2%)
5	P	0.77	0/1426	1.40	4/1944 (0.2%)
6	Q	0.64	0/302	1.29	0/406
6	R	0.60	0/284	1.27	0/381
6	S	0.91	0/505	1.63	5/683 (0.7%)
6	T	0.67	0/254	1.34	0/339
All	All	0.76	14/103922 (0.0%)	1.44	681/141349 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	3	0	1
2	A	0	4
2	B	0	13
2	C	0	14
2	D	0	9
2	E	0	14
2	F	0	17
2	G	0	16
2	H	0	8
2	I	0	8
2	J	0	9
2	K	0	11
2	L	0	17
3	M	0	4
4	N	0	1
5	O	0	3
All	All	0	149

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	180	THR	CA-CB	-17.48	1.23	1.53
2	B	180	THR	CB-OG1	-16.99	1.16	1.43
2	E	200	TRP	NE1-CE2	-13.87	1.22	1.37
2	B	180	THR	C-O	-11.58	1.09	1.23
2	B	181	GLU	CD-OE2	-9.87	1.06	1.25
2	B	179	ALA	C-O	-9.33	1.12	1.24
2	B	173	LYS	C-O	-9.20	1.12	1.24
2	B	180	THR	CB-CG2	-9.14	1.22	1.52
2	B	180	THR	CA-C	-6.92	1.44	1.52
2	B	179	ALA	C-N	-6.37	1.25	1.33
2	B	181	GLU	CG-CD	-6.25	1.36	1.52
2	B	181	GLU	CD-OE1	-6.22	1.13	1.25
2	B	181	GLU	CA-CB	-5.31	1.43	1.54
2	E	178	ASN	CA-C	5.29	1.59	1.52

All (681) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	179	ALA	N-CA-C	22.79	137.12	112.97
2	G	177	GLY	CA-C-N	12.95	139.25	122.16
2	G	177	GLY	C-N-CA	12.95	139.25	122.16
2	K	431	GLY	CA-C-N	12.90	144.53	123.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	431	GLY	C-N-CA	12.90	144.53	123.37
2	E	268	SER	N-CA-C	12.62	131.70	107.98
2	I	895	ALA	N-CA-C	12.57	129.15	110.30
2	E	408	CYS	CA-CB-SG	12.27	142.61	114.40
2	K	285	VAL	N-CA-C	11.86	124.97	113.71
2	C	54	HIS	N-CA-C	11.63	123.95	111.28
2	B	54	HIS	N-CA-C	11.45	123.77	111.28
2	L	431	GLY	CA-C-N	11.28	137.90	122.79
2	L	431	GLY	C-N-CA	11.28	137.90	122.79
2	E	200	TRP	NE1-CE2-CD2	-11.12	92.95	107.40
2	G	895	ALA	N-CA-C	10.79	126.49	110.30
2	B	268	SER	CA-C-N	10.74	142.47	121.41
2	B	268	SER	C-N-CA	10.74	142.47	121.41
2	F	737	PRO	CA-N-CD	-10.54	97.25	112.00
2	B	270	GLN	CA-C-N	10.53	141.66	121.54
2	B	270	GLN	C-N-CA	10.53	141.66	121.54
2	L	891	TYR	CB-CA-C	10.53	129.52	110.88
2	F	737	PRO	CA-CB-CG	-10.53	84.50	104.50
2	G	142	THR	CA-CB-CG2	10.50	128.35	110.50
2	L	943	SER	N-CA-C	10.42	123.23	108.54
2	E	273	GLU	CB-CG-CD	10.39	130.25	112.60
2	F	266	THR	N-CA-C	-10.37	92.47	108.96
2	L	201	GLN	CA-C-N	10.34	136.72	121.31
2	L	201	GLN	C-N-CA	10.34	136.72	121.31
2	B	184	PHE	CB-CG-CD2	-10.33	103.14	120.70
2	G	643	TYR	CB-CG-CD2	-10.30	105.35	120.80
2	E	200	TRP	CD1-CG-CD2	-10.29	89.84	106.30
2	E	434	GLU	CA-CB-CG	10.26	134.62	114.10
2	B	773	ILE	N-CA-C	10.13	122.31	111.58
2	F	201	GLN	CA-C-N	10.13	139.49	121.97
2	F	201	GLN	C-N-CA	10.13	139.49	121.97
2	C	698	TYR	CB-CG-CD2	-10.09	105.66	120.80
2	C	430	ASP	CA-C-N	9.82	140.66	121.41
2	C	430	ASP	C-N-CA	9.82	140.66	121.41
2	E	272	GLU	CA-C-N	9.79	140.23	121.54
2	E	272	GLU	C-N-CA	9.79	140.23	121.54
2	B	84	PHE	CB-CG-CD2	-9.74	104.14	120.70
2	E	267	GLY	CA-C-N	9.64	137.76	122.34
2	E	267	GLY	C-N-CA	9.64	137.76	122.34
2	I	737	PRO	CA-C-N	9.58	137.12	122.37
2	I	737	PRO	C-N-CA	9.58	137.12	122.37
2	E	201	GLN	CA-C-N	9.57	139.82	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	201	GLN	C-N-CA	9.57	139.82	121.54
2	G	891	TYR	CA-C-N	9.44	139.57	121.54
2	G	891	TYR	C-N-CA	9.44	139.57	121.54
2	C	84	PHE	CB-CG-CD2	-9.38	104.75	120.70
2	G	142	THR	N-CA-CB	-9.34	94.71	110.49
4	N	202	PHE	CA-CB-CG	9.31	123.11	113.80
2	E	773	ILE	N-CA-C	9.26	121.10	111.00
2	K	427	THR	CA-C-N	9.22	133.99	122.83
2	K	427	THR	C-N-CA	9.22	133.99	122.83
2	I	177	GLY	CA-C-N	9.10	138.93	121.54
2	I	177	GLY	C-N-CA	9.10	138.93	121.54
2	B	774	GLY	N-CA-C	8.99	125.02	113.24
2	C	184	PHE	CB-CG-CD2	-8.99	105.42	120.70
2	C	580	TRP	CB-CG-CD1	-8.98	113.43	126.90
2	G	891	TYR	CB-CA-C	8.89	125.52	111.73
2	K	432	ALA	CA-C-N	8.89	138.52	121.54
2	K	432	ALA	C-N-CA	8.89	138.52	121.54
2	L	617	PHE	CA-CB-CG	8.84	122.64	113.80
2	E	202	GLU	CA-CB-CG	8.83	131.76	114.10
2	L	430	ASP	N-CA-C	8.82	122.54	112.57
2	B	580	TRP	CB-CG-CD1	-8.79	113.71	126.90
2	I	176	GLU	CA-C-N	8.77	138.60	121.41
2	I	176	GLU	C-N-CA	8.77	138.60	121.41
2	F	431	GLY	CA-C-N	8.75	139.66	123.13
2	F	431	GLY	C-N-CA	8.75	139.66	123.13
2	K	617	PHE	CA-CB-CG	8.74	122.54	113.80
2	K	428	GLY	CA-C-N	8.74	138.23	121.54
2	K	428	GLY	C-N-CA	8.74	138.23	121.54
2	G	891	TYR	CA-CB-CG	8.70	129.55	113.90
2	G	176	GLU	CA-C-N	8.66	138.38	121.41
2	G	176	GLU	C-N-CA	8.66	138.38	121.41
2	L	432	ALA	CA-C-N	8.54	137.86	121.54
2	L	432	ALA	C-N-CA	8.54	137.86	121.54
2	C	580	TRP	CB-CG-CD2	8.53	138.74	126.80
2	E	176	GLU	N-CA-C	8.50	123.22	113.02
2	F	202	GLU	CA-CB-CG	8.47	131.04	114.10
2	G	141	GLN	CA-C-N	8.34	137.46	121.54
2	G	141	GLN	C-N-CA	8.34	137.46	121.54
2	L	285	VAL	N-CA-C	8.32	121.62	113.71
2	L	890	LEU	CA-C-N	8.31	135.30	122.42
2	L	890	LEU	C-N-CA	8.31	135.30	122.42
2	I	776	GLN	CA-C-N	8.31	136.65	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	776	GLN	C-N-CA	8.31	136.65	121.70
2	F	500	TYR	CB-CG-CD2	-8.28	108.38	120.80
2	L	710	TYR	CB-CG-CD2	-8.27	108.39	120.80
2	I	664	ILE	CB-CA-C	8.23	118.11	110.13
2	K	774	GLY	N-CA-C	8.22	122.86	112.83
2	G	142	THR	N-CA-C	8.15	128.17	110.80
2	F	737	PRO	CA-C-N	-8.12	105.10	121.18
2	F	737	PRO	C-N-CA	-8.12	105.10	121.18
2	B	180	THR	OG1-CB-CG2	-8.09	93.12	109.30
2	F	864	ASP	N-CA-C	8.06	123.15	113.16
2	C	274	TYR	CA-CB-CG	8.01	128.31	113.90
2	K	181	GLU	CA-CB-CG	7.97	130.04	114.10
2	E	888	ASN	CA-C-N	7.94	136.71	121.54
2	E	888	ASN	C-N-CA	7.94	136.71	121.54
2	C	644	LEU	CA-C-N	7.93	132.01	120.82
2	C	644	LEU	C-N-CA	7.93	132.01	120.82
2	C	429	GLN	CA-C-N	7.92	136.67	121.54
2	C	429	GLN	C-N-CA	7.92	136.67	121.54
2	B	8	PRO	N-CA-C	7.91	123.94	113.57
2	L	430	ASP	CA-CB-CG	7.91	120.51	112.60
2	I	895	ALA	CA-C-N	7.88	132.70	121.42
2	I	895	ALA	C-N-CA	7.88	132.70	121.42
2	G	895	ALA	CA-C-N	7.84	132.63	121.42
2	G	895	ALA	C-N-CA	7.84	132.63	121.42
2	E	143	GLY	N-CA-C	-7.80	94.69	113.18
2	H	776	GLN	CA-C-N	7.79	135.73	121.70
2	H	776	GLN	C-N-CA	7.79	135.73	121.70
3	M	70	ASN	CA-CB-CG	7.78	120.38	112.60
2	E	434	GLU	CB-CA-C	-7.77	94.97	110.42
2	C	728	TRP	N-CA-C	7.74	122.73	112.35
2	C	274	TYR	CB-CA-C	-7.73	97.07	110.45
2	L	698	TYR	CB-CG-CD2	-7.68	109.28	120.80
2	G	200	TRP	CD1-CG-CD2	-7.67	94.02	106.30
2	L	332	TYR	CB-CG-CD2	-7.67	109.30	120.80
2	G	776	GLN	CA-C-N	7.66	135.50	121.70
2	G	776	GLN	C-N-CA	7.66	135.50	121.70
2	B	834	ARG	NE-CZ-NH2	7.65	126.08	119.20
2	E	180	THR	CA-CB-CG2	7.61	123.44	110.50
2	G	140	LYS	CA-C-N	7.61	136.08	121.54
2	G	140	LYS	C-N-CA	7.61	136.08	121.54
2	F	332	TYR	CB-CG-CD2	-7.59	109.41	120.80
2	A	834	ARG	NE-CZ-NH2	7.56	126.00	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	580	TRP	CB-CG-CD2	7.52	137.33	126.80
2	B	728	TRP	N-CA-C	7.52	122.43	112.35
2	A	644	LEU	CA-C-N	7.52	131.80	121.05
2	A	644	LEU	C-N-CA	7.52	131.80	121.05
2	E	864	ASP	N-CA-C	7.52	122.64	113.17
2	K	773	ILE	N-CA-C	7.51	118.43	112.12
2	E	268	SER	CA-C-O	-7.48	113.20	121.58
2	F	430	ASP	N-CA-C	7.42	126.61	110.80
2	F	773	ILE	N-CA-C	7.39	119.05	111.00
2	E	145	GLN	N-CA-C	7.38	122.39	109.48
2	I	896	HIS	N-CA-C	7.37	121.84	110.20
2	K	943	SER	N-CA-C	7.34	126.44	110.80
2	B	791	PHE	N-CA-C	7.33	118.96	110.97
2	C	834	ARG	NE-CZ-NH2	7.27	125.74	119.20
2	C	191	PRO	N-CA-CB	7.26	107.59	102.65
2	L	617	PHE	CB-CA-C	7.25	121.77	109.82
2	K	181	GLU	N-CA-CB	-7.24	100.50	110.42
2	C	84	PHE	CA-CB-CG	7.23	121.03	113.80
2	L	78	TYR	CB-CG-CD2	-7.22	109.97	120.80
2	I	200	TRP	CD1-CG-CD2	-7.21	94.77	106.30
2	B	191	PRO	N-CA-CB	7.21	107.47	102.35
2	K	60	ARG	CB-CG-CD	7.15	127.75	111.30
2	J	285	VAL	N-CA-C	7.11	120.46	113.71
2	G	137	ALA	O-C-N	-7.06	113.20	122.59
2	I	707	GLY	N-CA-C	-7.05	98.97	110.95
2	I	263	THR	CA-C-N	7.05	127.64	120.38
2	I	263	THR	C-N-CA	7.05	127.64	120.38
2	L	428	GLY	CA-C-N	7.01	134.00	121.66
2	L	428	GLY	C-N-CA	7.01	134.00	121.66
2	D	264	PRO	N-CA-CB	7.00	107.11	103.19
2	G	274	TYR	N-CA-C	6.97	120.42	109.96
2	I	677	PHE	CB-CG-CD2	-6.97	108.85	120.70
2	B	6	MET	CA-C-N	6.97	128.80	120.09
2	B	6	MET	C-N-CA	6.97	128.80	120.09
2	K	945	GLY	CA-C-N	6.97	134.24	121.70
2	K	945	GLY	C-N-CA	6.97	134.24	121.70
2	E	142	THR	CB-CA-C	6.93	124.21	110.42
2	K	617	PHE	CB-CA-C	6.92	121.25	109.82
2	B	84	PHE	CA-CB-CG	6.92	120.72	113.80
2	G	200	TRP	N-CA-C	6.89	120.78	112.38
2	K	892	ALA	CA-C-O	-6.87	113.42	120.84
2	E	408	CYS	N-CA-CB	-6.86	98.94	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	144	GLY	CA-C-N	6.85	127.43	119.83
2	L	144	GLY	C-N-CA	6.85	127.43	119.83
5	O	227	ASP	CA-CB-CG	6.85	119.45	112.60
2	B	946	ASN	CA-CB-CG	6.83	119.43	112.60
2	K	188	THR	CA-C-N	6.82	133.97	121.70
2	K	188	THR	C-N-CA	6.82	133.97	121.70
2	J	37	THR	N-CA-C	-6.80	96.56	108.20
2	K	434	GLU	N-CA-CB	-6.80	100.11	110.45
2	E	774	GLY	N-CA-C	6.79	120.86	112.64
2	E	144	GLY	N-CA-C	6.77	132.94	113.30
1	4	19	MET	CA-C-N	6.77	130.97	121.22
1	4	19	MET	C-N-CA	6.77	130.97	121.22
2	E	142	THR	CA-CB-CG2	6.77	122.01	110.50
2	E	426	LYS	N-CA-C	6.76	118.34	110.97
2	E	176	GLU	CA-CB-CG	6.76	127.61	114.10
2	E	606	ARG	NE-CZ-NH2	6.75	125.28	119.20
2	L	664	ILE	CB-CA-C	6.75	116.68	110.13
2	L	188	THR	CA-C-N	6.74	133.84	121.70
2	L	188	THR	C-N-CA	6.74	133.84	121.70
2	E	179	ALA	N-CA-CB	-6.72	101.11	110.65
2	E	174	GLU	CA-C-O	-6.72	113.95	121.00
2	E	145	GLN	OE1-CD-NE2	-6.69	115.91	122.60
2	I	855	SER	N-CA-C	6.68	120.42	109.06
2	G	707	GLY	N-CA-C	-6.68	99.60	110.95
2	D	272	GLU	CA-C-N	6.66	131.25	120.60
2	D	272	GLU	C-N-CA	6.66	131.25	120.60
2	F	555	PHE	CA-CB-CG	6.66	120.46	113.80
2	C	7	MET	N-CA-C	6.65	122.75	113.57
2	B	52	PRO	N-CA-C	6.65	122.56	113.98
2	K	144	GLY	CA-C-N	6.65	127.21	119.83
2	K	144	GLY	C-N-CA	6.65	127.21	119.83
2	I	332	TYR	CB-CG-CD2	-6.65	110.83	120.80
2	L	83	ARG	CB-CG-CD	6.65	126.59	111.30
2	B	599	ARG	NE-CZ-NH2	6.62	125.16	119.20
2	I	264	PRO	CA-C-N	6.62	128.11	119.84
2	I	264	PRO	C-N-CA	6.62	128.11	119.84
2	C	428	GLY	CA-C-N	6.61	132.39	122.67
2	C	428	GLY	C-N-CA	6.61	132.39	122.67
2	I	891	TYR	N-CA-C	-6.59	96.30	108.24
2	K	887	GLN	CA-C-N	6.59	132.22	122.86
2	K	887	GLN	C-N-CA	6.59	132.22	122.86
2	B	644	LEU	CA-C-N	6.59	130.47	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	644	LEU	C-N-CA	6.59	130.47	121.05
2	F	737	PRO	N-CA-C	6.56	125.99	112.47
2	J	188	THR	CA-C-N	6.56	133.51	121.70
2	J	188	THR	C-N-CA	6.56	133.51	121.70
2	F	271	GLN	CA-C-N	6.56	135.06	121.94
2	F	271	GLN	C-N-CA	6.56	135.06	121.94
2	L	698	TYR	CA-CB-CG	6.55	125.68	113.90
2	K	7	MET	CA-CB-CG	6.54	127.19	114.10
2	A	599	ARG	NE-CZ-NH2	6.54	125.09	119.20
2	B	756	CYS	N-CA-CB	-6.53	101.40	111.46
2	K	430	ASP	CA-CB-CG	6.53	119.13	112.60
2	A	52	PRO	N-CA-C	6.53	122.03	114.20
2	C	240	LEU	N-CA-C	6.53	120.92	113.15
2	G	896	HIS	N-CA-C	6.52	120.51	110.20
2	L	202	GLU	CA-CB-CG	6.52	127.14	114.10
2	I	408	CYS	CA-CB-SG	6.51	129.38	114.40
2	I	600	VAL	N-CA-C	-6.51	101.14	109.80
2	C	281	TYR	CB-CG-CD2	-6.50	111.05	120.80
2	I	774	GLY	N-CA-C	6.49	122.07	113.37
2	C	599	ARG	NE-CZ-NH2	6.48	125.03	119.20
2	F	500	TYR	CD1-CG-CD2	-6.48	108.38	118.10
2	G	149	VAL	CB-CA-C	-6.47	104.20	111.45
2	E	433	GLU	CA-C-N	-6.47	109.19	121.54
2	E	433	GLU	C-N-CA	-6.47	109.19	121.54
2	B	788	MET	N-CA-C	6.46	118.32	111.28
2	C	698	TYR	N-CA-C	6.44	119.10	108.99
2	C	773	ILE	N-CA-C	6.44	118.02	111.00
2	I	753	VAL	CB-CA-C	-6.44	100.41	110.52
2	E	200	TRP	CG-CD2-CE3	-6.42	127.48	133.90
2	B	180	THR	N-CA-C	6.41	119.07	110.35
2	K	602	GLY	N-CA-C	6.41	124.53	115.30
2	E	434	GLU	CA-C-N	6.41	134.87	123.34
2	E	434	GLU	C-N-CA	6.41	134.87	123.34
2	G	143	GLY	O-C-N	-6.40	114.37	122.70
2	F	136	THR	O-C-N	-6.39	113.80	122.94
2	I	445	ARG	NE-CZ-NH2	6.39	124.95	119.20
2	G	145	GLN	N-CA-C	6.38	118.57	108.23
2	F	136	THR	CA-C-N	-6.37	109.37	121.54
2	F	136	THR	C-N-CA	-6.37	109.37	121.54
2	C	53	THR	CA-CB-CG2	6.36	121.32	110.50
2	F	738	ASN	N-CA-C	-6.36	105.38	113.01
2	G	600	VAL	N-CA-C	-6.35	101.35	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	843	PHE	N-CA-C	6.35	123.83	109.81
2	E	18	GLN	N-CA-C	6.34	119.80	109.59
2	B	7	MET	N-CA-C	6.34	122.16	113.16
2	E	269	GLY	CA-C-N	6.33	133.63	121.54
2	E	269	GLY	C-N-CA	6.33	133.63	121.54
3	M	496	ARG	NE-CZ-NH2	6.33	124.90	119.20
2	K	109	ARG	NE-CZ-NH2	6.33	124.89	119.20
2	E	54	HIS	N-CA-C	6.32	120.84	111.04
2	F	137	ALA	CA-C-N	6.32	133.61	121.54
2	F	137	ALA	C-N-CA	6.32	133.61	121.54
2	B	281	TYR	CB-CG-CD2	-6.32	111.33	120.80
2	L	896	HIS	CB-CG-CD2	-6.31	123.00	131.20
2	C	728	TRP	CB-CA-C	-6.31	102.76	113.04
2	K	430	ASP	N-CA-C	6.30	122.06	113.37
1	3	18	PHE	CA-C-N	6.30	133.56	121.54
1	3	18	PHE	C-N-CA	6.30	133.56	121.54
2	J	773	ILE	N-CA-C	6.29	117.40	112.12
2	E	887	GLN	CA-C-N	6.29	133.55	121.54
2	E	887	GLN	C-N-CA	6.29	133.55	121.54
2	B	487	ALA	N-CA-C	6.29	118.94	111.71
2	E	200	TRP	CE2-CD2-CE3	-6.29	112.51	118.80
2	F	432	ALA	CA-C-N	6.27	133.52	121.54
2	F	432	ALA	C-N-CA	6.27	133.52	121.54
2	G	84	PHE	CD1-CG-CD2	-6.27	109.19	118.60
2	C	18	GLN	N-CA-C	6.27	118.87	110.35
2	L	888	ASN	CA-C-N	6.26	133.50	121.54
2	L	888	ASN	C-N-CA	6.26	133.50	121.54
2	B	264	PRO	N-CA-C	-6.26	103.88	110.58
2	F	136	THR	N-CA-C	-6.24	100.26	109.81
2	G	139	GLU	N-CA-C	6.24	119.57	109.40
2	G	147	LYS	N-CA-C	6.23	120.96	113.23
2	E	109	ARG	NE-CZ-NH2	6.22	124.80	119.20
2	G	643	TYR	CD1-CG-CD2	-6.21	108.78	118.10
2	F	264	PRO	N-CA-CB	6.20	109.09	103.08
2	C	791	PHE	N-CA-C	6.19	117.72	110.97
2	B	932	VAL	N-CA-C	6.19	119.18	108.90
2	B	190	GLN	N-CA-C	6.17	122.09	113.57
2	L	37	THR	N-CA-C	-6.17	98.67	108.73
2	C	698	TYR	CA-CB-CG	6.15	124.98	113.90
2	L	602	GLY	N-CA-C	6.15	124.15	115.30
2	F	395	ILE	N-CA-C	6.14	117.62	110.62
2	E	272	GLU	CA-CB-CG	6.13	126.35	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	147	LYS	N-CA-C	6.12	118.75	111.71
2	G	145	GLN	CA-C-N	6.11	126.02	119.85
2	G	145	GLN	C-N-CA	6.11	126.02	119.85
2	E	892	ALA	CA-C-N	6.11	129.30	120.38
2	E	892	ALA	C-N-CA	6.11	129.30	120.38
2	I	599	ARG	N-CA-C	-6.10	104.55	111.14
2	D	109	ARG	NE-CZ-NH2	6.09	124.68	119.20
3	M	352	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	1	5	ASN	CA-CB-CG	6.07	118.67	112.60
2	L	698	TYR	CB-CG-CD1	6.07	129.91	120.80
2	I	249	ASP	N-CA-C	6.06	118.63	109.41
2	E	176	GLU	O-C-N	-6.05	114.58	122.39
2	F	924	ARG	NE-CZ-NH2	6.05	124.64	119.20
2	B	834	ARG	CD-NE-CZ	6.04	132.86	124.40
2	D	924	ARG	NE-CZ-NH2	6.04	124.63	119.20
2	L	109	ARG	NE-CZ-NH2	6.04	124.63	119.20
2	L	37	THR	CA-C-N	6.03	132.56	121.70
2	L	37	THR	C-N-CA	6.03	132.56	121.70
2	J	144	GLY	CA-C-N	6.02	126.52	119.83
2	J	144	GLY	C-N-CA	6.02	126.52	119.83
2	F	273	GLU	N-CA-C	6.02	123.62	110.80
2	C	834	ARG	CD-NE-CZ	6.01	132.82	124.40
2	F	555	PHE	CB-CG-CD2	-6.01	110.48	120.70
2	G	753	VAL	CB-CA-C	-6.01	101.08	110.52
2	I	200	TRP	N-CA-C	6.01	120.08	112.87
2	E	19	ASP	CA-CB-CG	5.99	118.59	112.60
2	J	109	ARG	NE-CZ-NH2	5.99	124.59	119.20
2	E	664	ILE	CB-CA-C	5.99	115.94	110.13
3	M	270	ASP	CA-CB-CG	5.97	118.58	112.60
2	J	37	THR	CA-C-N	5.97	132.45	121.70
2	J	37	THR	C-N-CA	5.97	132.45	121.70
2	B	374	ARG	NE-CZ-NH2	5.97	124.57	119.20
2	C	932	VAL	N-CA-C	5.96	118.80	108.90
2	G	285	VAL	N-CA-C	5.96	118.88	113.10
2	K	434	GLU	N-CA-C	5.95	118.59	110.55
1	6	6	PHE	N-CA-C	5.95	118.11	109.07
2	L	891	TYR	N-CA-CB	-5.95	99.62	110.27
2	F	435	THR	N-CA-C	5.94	119.40	108.58
2	E	895	ALA	CA-C-N	-5.94	112.44	120.87
2	E	895	ALA	C-N-CA	-5.94	112.44	120.87
1	3	10	ALA	N-CA-C	5.93	122.92	109.81
2	E	180	THR	N-CA-C	5.93	119.41	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	866	VAL	CB-CA-C	-5.93	104.81	111.45
2	A	54	HIS	N-CA-C	5.92	117.81	111.36
2	C	698	TYR	CB-CG-CD1	5.92	129.68	120.80
2	E	438	ASP	CA-CB-CG	5.92	118.52	112.60
2	H	92	ARG	NE-CZ-NH2	5.91	124.52	119.20
2	L	286	ASN	CA-CB-CG	5.91	118.51	112.60
2	L	710	TYR	N-CA-CB	-5.90	100.51	110.49
2	L	943	SER	CA-C-N	5.90	132.32	121.70
2	L	943	SER	C-N-CA	5.90	132.32	121.70
2	B	580	TRP	CB-CA-C	5.90	121.36	109.38
2	A	834	ARG	CD-NE-CZ	5.89	132.64	124.40
2	E	200	TRP	CB-CG-CD2	5.88	135.04	126.80
2	L	543	ARG	NE-CZ-NH2	5.88	124.50	119.20
2	L	690	SER	N-CA-C	-5.88	101.13	109.96
2	A	46	ARG	NE-CZ-NH2	5.88	124.49	119.20
2	C	109	ARG	NE-CZ-NH2	5.87	124.48	119.20
2	C	207	TYR	CA-C-N	5.87	126.23	122.18
2	C	207	TYR	C-N-CA	5.87	126.23	122.18
2	E	180	THR	CB-CA-C	-5.87	102.58	109.80
2	B	930	ARG	CB-CG-CD	-5.86	97.81	111.30
2	C	642	ASP	N-CA-C	-5.86	101.37	110.10
2	F	140	LYS	N-CA-C	5.85	119.67	111.30
2	I	677	PHE	CA-CB-CG	5.85	119.65	113.80
2	E	271	GLN	CA-C-N	5.84	133.95	122.61
2	E	271	GLN	C-N-CA	5.84	133.95	122.61
2	B	9	GLN	OE1-CD-NE2	-5.84	116.76	122.60
2	L	428	GLY	N-CA-C	5.84	120.55	112.37
2	G	397	ASN	N-CA-C	5.84	118.67	109.39
2	L	188	THR	N-CA-C	-5.83	99.68	109.07
2	F	145	GLN	N-CA-C	5.83	119.69	109.48
2	L	891	TYR	CD1-CG-CD2	-5.83	109.35	118.10
2	G	887	GLN	CA-C-N	5.82	132.66	121.54
2	G	887	GLN	C-N-CA	5.82	132.66	121.54
2	G	235	GLN	OE1-CD-NE2	-5.82	116.78	122.60
2	E	145	GLN	CG-CD-NE2	5.82	125.12	116.40
2	E	200	TRP	NE1-CE2-CZ2	-5.80	121.40	130.10
2	K	37	THR	N-CA-C	-5.79	98.31	108.20
2	C	190	GLN	N-CA-C	5.78	121.55	113.57
2	I	272	GLU	N-CA-C	5.78	117.92	108.55
2	I	776	GLN	O-C-N	-5.78	115.38	122.55
3	M	397	VAL	N-CA-C	5.76	120.08	112.76
2	F	946	ASN	CA-CB-CG	5.75	118.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	894	SER	CA-C-N	5.74	130.39	121.26
2	G	894	SER	C-N-CA	5.74	130.39	121.26
2	K	286	ASN	CA-CB-CG	5.74	118.34	112.60
2	L	54	HIS	CB-CG-CD2	-5.74	123.74	131.20
2	E	374	ARG	NE-CZ-NH2	5.74	124.36	119.20
2	F	939	ARG	NE-CZ-NH2	5.74	124.36	119.20
2	G	726	VAL	N-CA-C	5.74	112.35	106.21
2	I	611	ASN	CA-CB-CG	5.73	118.33	112.60
2	E	107	LEU	CB-CA-C	-5.73	99.81	109.50
2	F	500	TYR	CB-CA-C	5.73	119.95	110.90
2	H	924	ARG	NE-CZ-NH2	5.72	124.35	119.20
2	E	178	ASN	CA-C-N	5.72	131.99	122.66
2	E	178	ASN	C-N-CA	5.72	131.99	122.66
2	G	888	ASN	N-CA-CB	5.72	120.16	110.49
2	B	645	SER	N-CA-C	5.72	118.64	110.24
2	C	84	PHE	CD1-CG-CD2	-5.72	110.03	118.60
2	F	270	GLN	O-C-N	-5.71	117.50	123.56
6	S	110	ALA	CA-C-N	5.71	127.86	120.44
6	S	110	ALA	C-N-CA	5.71	127.86	120.44
2	B	267	GLY	CA-C-N	5.70	132.43	121.54
2	B	267	GLY	C-N-CA	5.70	132.43	121.54
2	G	285	VAL	CA-CB-CG1	5.69	120.07	110.40
2	B	259	THR	CA-C-N	5.69	126.15	120.52
2	B	259	THR	C-N-CA	5.69	126.15	120.52
2	A	774	GLY	N-CA-C	5.68	121.26	113.99
2	K	943	SER	N-CA-CB	-5.68	100.89	110.49
2	F	259	THR	CA-C-N	5.67	126.93	119.84
2	F	259	THR	C-N-CA	5.67	126.93	119.84
2	I	84	PHE	CD1-CG-CD2	-5.67	110.10	118.60
2	L	710	TYR	CA-CB-CG	5.66	124.09	113.90
2	E	433	GLU	O-C-N	-5.66	115.83	123.19
2	K	830	ALA	N-CA-C	5.66	113.31	108.22
2	G	92	ARG	NE-CZ-NH2	5.66	124.29	119.20
2	K	543	ARG	NE-CZ-NH2	5.66	124.29	119.20
2	F	774	GLY	N-CA-C	5.65	119.06	112.50
2	G	198	GLU	N-CA-C	5.65	119.35	112.23
2	A	374	ARG	NE-CZ-NH2	5.64	124.27	119.20
2	C	820	HIS	CB-CG-CD2	-5.63	123.89	131.20
2	C	239	LYS	CB-CA-C	5.62	119.03	109.53
2	K	514	TYR	N-CA-CB	-5.62	102.17	110.49
2	L	83	ARG	NE-CZ-NH2	5.62	124.26	119.20
2	G	210	ARG	NE-CZ-NH2	5.62	124.26	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	855	SER	N-CA-C	5.62	117.81	108.99
2	L	435	THR	CA-C-N	5.61	131.01	122.65
2	L	435	THR	C-N-CA	5.61	131.01	122.65
2	I	894	SER	CA-C-N	5.61	130.17	121.26
2	I	894	SER	C-N-CA	5.61	130.17	121.26
2	L	844	PRO	N-CA-CB	5.60	106.06	102.92
2	C	863	CYS	N-CA-C	-5.60	98.69	107.93
2	B	184	PHE	N-CA-CB	-5.59	101.69	110.69
2	I	899	ASP	CA-CB-CG	5.59	118.19	112.60
2	J	543	ARG	NE-CZ-NH2	5.59	124.23	119.20
2	L	543	ARG	NH1-CZ-NH2	-5.59	112.04	119.30
2	I	888	ASN	N-CA-CB	5.57	119.91	110.49
2	I	907	MET	N-CA-C	5.56	120.22	113.38
2	G	107	LEU	CB-CA-C	-5.56	100.11	109.50
2	J	286	ASN	CA-CB-CG	5.55	118.15	112.60
2	C	708	THR	CA-CB-CG2	5.54	119.92	110.50
2	I	737	PRO	N-CA-C	5.54	123.88	112.47
2	K	667	ARG	N-CA-CB	-5.54	101.70	111.39
2	B	863	CYS	N-CA-C	-5.53	98.81	107.93
2	G	142	THR	CA-C-O	-5.53	112.61	120.51
2	E	177	GLY	CA-C-N	5.52	132.09	121.54
2	E	177	GLY	C-N-CA	5.52	132.09	121.54
2	F	148	SER	CA-C-N	5.52	131.91	121.97
2	F	148	SER	C-N-CA	5.52	131.91	121.97
2	I	109	ARG	NE-CZ-NH2	5.52	124.17	119.20
2	E	890	LEU	CA-C-N	5.52	132.09	121.54
2	E	890	LEU	C-N-CA	5.52	132.09	121.54
2	L	599	ARG	N-CA-C	-5.52	105.35	111.36
2	I	447	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	7	10	ALA	N-CA-C	5.51	121.99	109.81
2	C	38	TYR	CB-CG-CD2	-5.51	112.54	120.80
2	J	543	ARG	NH1-CZ-NH2	-5.51	112.14	119.30
2	E	149	VAL	CB-CA-C	-5.50	105.29	111.45
2	C	431	GLY	CA-C-N	5.49	132.03	121.54
2	C	431	GLY	C-N-CA	5.49	132.03	121.54
2	C	864	ASP	CA-CB-CG	5.49	118.09	112.60
2	F	376	ARG	NE-CZ-NH2	5.49	124.14	119.20
2	F	606	ARG	NE-CZ-NH2	5.48	124.13	119.20
2	K	899	ASP	CA-CB-CG	5.48	118.08	112.60
2	H	235	GLN	OE1-CD-NE2	-5.47	117.13	122.60
2	B	138	ASN	N-CA-C	5.47	117.66	108.96
2	I	668	ASN	OD1-CG-ND2	-5.47	117.13	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	297	LYS	CB-CA-C	5.47	117.40	109.20
2	F	92	ARG	NE-CZ-NH2	5.46	124.12	119.20
2	E	607	PHE	CA-CB-CG	5.46	119.26	113.80
2	B	84	PHE	CD1-CG-CD2	-5.46	110.41	118.60
2	B	728	TRP	CB-CA-C	-5.46	104.15	113.04
2	F	107	LEU	CB-CA-C	-5.45	100.29	109.50
2	I	267	GLY	CA-C-N	5.45	131.94	121.54
2	I	267	GLY	C-N-CA	5.45	131.94	121.54
6	S	76	ARG	NE-CZ-NH2	5.45	124.10	119.20
2	C	946	ASN	CA-CB-CG	5.44	118.04	112.60
2	H	800	ARG	NE-CZ-NH2	5.44	124.10	119.20
2	C	943	SER	CB-CA-C	-5.44	101.69	110.77
2	E	198	GLU	N-CA-C	5.44	118.13	111.82
2	C	417	ASN	N-CA-C	5.43	119.19	112.24
5	O	192	PHE	N-CA-C	5.43	119.07	111.90
2	A	708	THR	CA-CB-CG2	5.43	119.72	110.50
2	K	807	ASN	N-CA-CB	-5.43	104.00	112.41
2	B	434	GLU	N-CA-C	-5.42	100.77	109.39
2	A	235	GLN	OE1-CD-NE2	-5.42	117.18	122.60
2	K	543	ARG	NH1-CZ-NH2	-5.42	112.26	119.30
2	L	773	ILE	N-CA-C	5.41	116.67	112.12
2	G	109	ARG	NE-CZ-NH2	5.41	124.07	119.20
2	I	357	ASP	N-CA-CB	-5.41	102.97	110.65
2	K	179	ALA	CA-C-N	-5.41	115.26	122.72
2	K	179	ALA	C-N-CA	-5.41	115.26	122.72
2	E	634	ASP	CA-CB-CG	5.40	118.00	112.60
1	4	16	ARG	NE-CZ-NH2	5.40	124.06	119.20
2	C	438	ASP	CA-CB-CG	5.39	117.99	112.60
1	8	18	PHE	N-CA-CB	-5.39	104.15	110.35
1	7	18	PHE	CA-CB-CG	5.39	119.19	113.80
2	A	773	ILE	N-CA-C	5.38	116.04	110.82
2	A	273	GLU	N-CA-C	5.38	122.26	110.80
2	B	303	GLU	N-CA-C	5.38	117.81	110.55
2	I	534	HIS	CB-CG-CD2	-5.38	124.21	131.20
2	J	374	ARG	NE-CZ-NH2	5.38	124.04	119.20
2	B	820	HIS	CB-CG-CD2	-5.37	124.22	131.20
2	B	184	PHE	CD1-CG-CD2	-5.37	110.55	118.60
2	C	184	PHE	CD1-CG-CD2	-5.36	110.57	118.60
2	I	811	TYR	N-CA-C	5.36	117.94	109.96
2	B	239	LYS	CB-CA-C	5.35	118.58	109.53
2	E	924	ARG	NE-CZ-NH2	5.35	124.02	119.20
2	G	137	ALA	CA-C-N	-5.35	113.21	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	137	ALA	C-N-CA	-5.35	113.21	122.14
2	E	146	PRO	N-CA-C	-5.34	101.47	112.47
2	F	139	GLU	CA-C-O	5.34	127.00	120.92
2	G	855	SER	N-CA-C	5.33	118.13	109.06
3	M	281	ASP	CA-CB-CG	5.33	117.93	112.60
2	K	285	VAL	N-CA-CB	-5.33	103.36	111.57
2	L	432	ALA	N-CA-C	-5.33	101.55	109.11
2	J	188	THR	O-C-N	-5.32	117.26	123.27
2	G	136	THR	N-CA-C	5.32	117.21	109.71
2	D	376	ARG	NE-CZ-NH2	5.31	123.98	119.20
2	E	433	GLU	N-CA-C	-5.31	101.22	109.72
2	C	435	THR	N-CA-C	5.31	118.25	108.58
2	B	642	ASP	N-CA-C	-5.31	102.19	110.10
2	K	180	THR	N-CA-C	5.31	117.89	109.24
2	C	338	ASN	N-CA-CB	-5.31	103.65	111.51
5	P	48	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	J	334	ASN	OD1-CG-ND2	-5.29	117.31	122.60
2	B	417	ASN	N-CA-C	5.29	119.02	112.24
2	K	374	ARG	NE-CZ-NH2	5.29	123.96	119.20
2	K	924	ARG	NE-CZ-NH2	5.29	123.96	119.20
2	G	409	PHE	CA-C-N	5.29	125.22	119.78
2	G	409	PHE	C-N-CA	5.29	125.22	119.78
2	I	510	LEU	N-CA-C	-5.28	102.47	110.28
2	H	285	VAL	CA-CB-CG1	5.28	119.38	110.40
2	I	7	MET	N-CA-C	5.28	120.85	113.57
2	L	514	TYR	N-CA-CB	-5.28	102.68	110.49
1	7	6	PHE	CA-CB-CG	5.28	119.08	113.80
2	I	924	ARG	NE-CZ-NH2	5.27	123.95	119.20
2	K	599	ARG	N-CA-C	-5.27	105.20	111.69
2	G	776	GLN	N-CA-C	5.27	118.66	111.39
2	I	107	LEU	CB-CA-C	-5.27	100.60	109.50
3	M	105	ARG	NE-CZ-NH2	5.27	123.94	119.20
2	G	7	MET	N-CA-C	5.27	120.84	113.57
2	C	303	GLU	N-CA-C	5.26	117.66	110.55
2	G	599	ARG	N-CA-C	-5.26	104.98	111.40
2	G	922	VAL	N-CA-C	5.26	116.16	108.53
6	S	60	ASP	CA-CB-CG	5.26	117.86	112.60
2	F	303	GLU	N-CA-C	5.25	116.87	110.41
2	L	260	PRO	CA-C-N	5.25	136.49	122.78
2	L	260	PRO	C-N-CA	5.25	136.49	122.78
2	F	140	LYS	CA-CB-CG	5.25	124.59	114.10
2	B	407	TYR	N-CA-C	5.24	117.62	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	645	SER	N-CA-C	5.24	117.91	110.10
2	I	273	GLU	N-CA-C	5.24	119.64	112.88
2	D	697	VAL	CA-CB-CG1	5.24	119.31	110.40
2	L	332	TYR	CD1-CG-CD2	-5.24	110.25	118.10
2	K	37	THR	CA-C-N	5.24	131.12	121.70
2	K	37	THR	C-N-CA	5.24	131.12	121.70
2	G	564	PHE	N-CA-C	5.23	116.98	111.28
2	C	52	PRO	N-CA-C	5.22	120.47	114.20
2	G	510	LEU	N-CA-C	-5.22	102.55	110.28
2	L	616	PHE	CA-CB-CG	5.22	119.02	113.80
2	G	249	ASP	N-CA-C	5.22	117.61	109.52
2	L	374	ARG	NE-CZ-NH2	5.22	123.90	119.20
2	I	146	PRO	CB-CA-C	5.22	118.15	111.21
2	A	520	ARG	NE-CZ-NH2	5.20	123.88	119.20
2	B	930	ARG	CB-CA-C	5.20	120.25	110.63
3	M	449	ASP	CA-CB-CG	5.20	117.80	112.60
2	B	43	ASN	CA-CB-CG	5.20	117.80	112.60
2	B	855	SER	N-CA-CB	-5.20	101.86	111.52
2	C	896	HIS	CB-CG-CD2	-5.20	124.44	131.20
2	J	888	ASN	CA-C-N	5.19	131.21	123.05
2	J	888	ASN	C-N-CA	5.19	131.21	123.05
2	D	606	ARG	NE-CZ-NH2	5.19	123.87	119.20
2	B	899	ASP	CA-CB-CG	5.19	117.79	112.60
2	C	429	GLN	OE1-CD-NE2	-5.19	117.41	122.60
2	G	924	ARG	NE-CZ-NH2	5.19	123.87	119.20
2	H	374	ARG	NE-CZ-NH2	5.18	123.87	119.20
2	B	143	GLY	CA-C-N	5.18	125.73	119.98
2	B	143	GLY	C-N-CA	5.18	125.73	119.98
2	D	334	ASN	OD1-CG-ND2	-5.18	117.42	122.60
2	G	263	THR	CA-C-N	5.18	125.71	120.38
2	G	263	THR	C-N-CA	5.18	125.71	120.38
2	J	926	HIS	CB-CG-CD2	-5.18	124.47	131.20
2	K	617	PHE	CB-CG-CD2	-5.18	111.90	120.70
2	A	744	ARG	NE-CZ-NH2	5.17	123.86	119.20
5	P	168	TYR	CA-CB-CG	5.17	123.21	113.90
2	K	942	PHE	N-CA-C	-5.17	104.30	111.28
2	A	756	CYS	N-CA-CB	-5.17	103.50	111.46
2	F	140	LYS	CA-C-N	-5.17	111.67	121.54
2	F	140	LYS	C-N-CA	-5.17	111.67	121.54
3	M	101	ASP	CA-CB-CG	-5.17	107.43	112.60
2	B	271	GLN	N-CA-CB	-5.16	101.77	110.49
2	I	67	ARG	NE-CZ-NH2	5.15	123.84	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	564	PHE	N-CA-C	5.15	116.90	111.28
2	F	543	ARG	NE-CZ-NH2	5.15	123.84	119.20
2	I	887	GLN	CA-C-N	5.15	131.38	121.54
2	I	887	GLN	C-N-CA	5.15	131.38	121.54
2	L	202	GLU	CB-CA-C	-5.15	101.47	109.61
2	J	673	ARG	NE-CZ-NH2	5.15	123.84	119.20
2	K	188	THR	N-CA-C	-5.15	100.12	108.52
2	B	18	GLN	N-CA-C	5.14	117.34	110.35
2	K	258	ASP	CA-CB-CG	5.14	117.74	112.60
2	C	374	ARG	NE-CZ-NH2	5.14	123.83	119.20
2	C	941	PRO	N-CA-CB	5.14	108.22	103.39
2	K	830	ALA	N-CA-CB	-5.14	105.71	111.10
2	C	487	ALA	N-CA-C	5.13	117.61	111.71
2	C	274	TYR	N-CA-C	-5.13	102.86	110.46
2	G	374	ARG	NE-CZ-NH2	5.13	123.82	119.20
2	I	791	PHE	N-CA-C	5.13	116.56	110.97
1	8	22	TRP	N-CA-C	5.13	117.55	109.39
2	A	645	SER	N-CA-C	5.13	117.78	110.24
2	I	943	SER	CB-CA-C	-5.13	101.68	109.89
2	K	434	GLU	CA-C-N	5.13	131.33	121.54
2	K	434	GLU	C-N-CA	5.13	131.33	121.54
2	B	207	TYR	CA-C-N	5.12	125.72	122.18
2	B	207	TYR	C-N-CA	5.12	125.72	122.18
2	B	943	SER	N-CA-C	5.12	117.14	110.43
2	C	744	ARG	NE-CZ-NH2	5.12	123.80	119.20
2	L	663	SER	CA-C-N	5.11	127.78	123.33
2	L	663	SER	C-N-CA	5.11	127.78	123.33
1	3	17	PRO	CA-C-N	5.11	131.30	121.54
1	3	17	PRO	C-N-CA	5.11	131.30	121.54
2	L	891	TYR	CA-C-N	5.11	128.80	121.50
2	L	891	TYR	C-N-CA	5.11	128.80	121.50
2	D	520	ARG	NE-CZ-NH2	5.10	123.79	119.20
2	G	201	GLN	CB-CA-C	-5.10	103.15	111.06
2	D	800	ARG	NE-CZ-NH2	5.10	123.79	119.20
6	S	101	LEU	N-CA-C	5.10	118.43	110.32
2	C	926	HIS	CB-CG-CD2	-5.09	124.58	131.20
2	G	83	ARG	NE-CZ-NH2	5.09	123.78	119.20
2	L	667	ARG	N-CA-CB	-5.09	102.47	111.39
2	K	303	GLU	N-CA-C	5.09	116.67	110.41
2	L	943	SER	O-C-N	-5.09	115.96	122.83
2	E	348	GLN	OE1-CD-NE2	-5.09	117.51	122.60
2	H	263	THR	CA-C-N	5.09	125.62	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	263	THR	C-N-CA	5.09	125.62	120.38
2	H	611	ASN	CA-CB-CG	5.08	117.68	112.60
2	E	432	ALA	CA-C-N	5.07	130.78	122.81
2	E	432	ALA	C-N-CA	5.07	130.78	122.81
2	H	835	GLN	OE1-CD-NE2	-5.07	117.53	122.60
2	I	926	HIS	CB-CG-CD2	-5.07	124.61	131.20
5	O	212	PHE	CA-CB-CG	5.07	118.87	113.80
1	5	22	TRP	N-CA-C	5.07	116.31	107.49
2	L	78	TYR	CA-CB-CG	5.07	123.02	113.90
2	K	663	SER	CA-C-N	5.07	127.74	123.33
2	K	663	SER	C-N-CA	5.07	127.74	123.33
1	3	19	MET	N-CA-C	5.06	121.58	110.80
2	C	90	ASP	N-CA-C	5.06	118.23	111.75
2	A	924	ARG	NE-CZ-NH2	5.06	123.75	119.20
2	A	632	ARG	NE-CZ-NH2	5.06	123.75	119.20
2	C	866	VAL	CA-CB-CG1	5.05	118.99	110.40
2	B	924	ARG	NE-CZ-NH2	5.05	123.75	119.20
2	C	457	MET	CB-CA-C	5.05	118.48	109.65
2	H	896	HIS	N-CA-C	5.04	117.54	110.23
2	D	537	ASN	CA-CB-CG	5.04	117.64	112.60
5	P	30	ARG	NE-CZ-NH2	5.04	123.73	119.20
2	G	535	HIS	CB-CG-CD2	-5.03	124.66	131.20
2	I	892	ALA	CA-C-N	5.03	131.16	121.54
2	I	892	ALA	C-N-CA	5.03	131.16	121.54
5	O	224	ASP	CA-CB-CG	5.03	117.63	112.60
2	C	336	THR	N-CA-C	5.03	116.45	111.07
2	I	311	GLN	OE1-CD-NE2	-5.03	117.57	122.60
5	P	212	PHE	CA-CB-CG	5.03	118.83	113.80
2	E	800	ARG	NE-CZ-NH2	5.03	123.72	119.20
2	C	114	LYS	CA-C-N	5.02	126.12	119.84
2	C	114	LYS	C-N-CA	5.02	126.12	119.84
2	E	744	ARG	NE-CZ-NH2	5.02	123.72	119.20
2	I	893	ASN	CA-CB-CG	5.02	117.62	112.60
2	I	200	TRP	CB-CG-CD2	-5.02	119.77	126.80
2	C	9	GLN	OE1-CD-NE2	-5.02	117.58	122.60
2	C	266	THR	CB-CA-C	5.02	117.86	110.14
2	C	756	CYS	N-CA-CB	-5.01	103.74	111.46
2	I	210	ARG	NE-CZ-NH2	5.01	123.71	119.20
2	J	941	PRO	N-CA-CB	5.01	108.52	103.25
2	B	708	THR	CA-CB-CG2	5.01	119.02	110.50
1	1	22	TRP	N-CA-C	5.01	118.93	111.87
2	H	83	ARG	NE-CZ-NH2	5.01	123.71	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	407	TYR	CA-C-N	5.01	130.45	122.74
2	E	407	TYR	C-N-CA	5.01	130.45	122.74
2	F	738	ASN	CA-C-N	5.01	130.74	122.33
2	F	738	ASN	C-N-CA	5.01	130.74	122.33
2	H	776	GLN	OE1-CD-NE2	-5.01	117.59	122.60

There are no chirality outliers.

All (149) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	3	19	MET	Peptide
2	A	140	LYS	Peptide
2	A	407	TYR	Sidechain
2	A	433	GLU	Peptide
2	A	80	TYR	Sidechain
2	B	184	PHE	Sidechain
2	B	281	TYR	Sidechain
2	B	38	TYR	Sidechain
2	B	407	TYR	Sidechain
2	B	420	TYR	Sidechain
2	B	46	ARG	Sidechain
2	B	498	TYR	Sidechain
2	B	541	ARG	Sidechain
2	B	599	ARG	Sidechain
2	B	667	ARG	Sidechain
2	B	695	TYR	Sidechain
2	B	84	PHE	Sidechain
2	B	869	ARG	Sidechain
2	C	184	PHE	Sidechain
2	C	274	TYR	Sidechain
2	C	281	TYR	Sidechain
2	C	332	TYR	Sidechain
2	C	38	TYR	Sidechain
2	C	407	TYR	Sidechain
2	C	695	TYR	Sidechain
2	C	698	TYR	Sidechain
2	C	704	TYR	Sidechain
2	C	8	PRO	Mainchain
2	C	80	TYR	Sidechain
2	C	83	ARG	Sidechain
2	C	84	PHE	Sidechain
2	C	869	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	D	109	ARG	Sidechain
2	D	116	TYR	Sidechain
2	D	12	TYR	Sidechain
2	D	407	TYR	Sidechain
2	D	498	TYR	Sidechain
2	D	599	ARG	Sidechain
2	D	613	TYR	Sidechain
2	D	695	TYR	Sidechain
2	D	865	ARG	Sidechain
2	E	109	ARG	Sidechain
2	E	175	GLU	Peptide
2	E	176	GLU	Mainchain,Peptide
2	E	202	GLU	Peptide
2	E	274	TYR	Sidechain
2	E	320	TYR	Sidechain
2	E	377	TYR	Sidechain
2	E	407	TYR	Sidechain
2	E	420	TYR	Sidechain
2	E	433	GLU	Mainchain
2	E	500	TYR	Sidechain
2	E	784	TYR	Sidechain
2	E	869	ARG	Sidechain
2	F	109	ARG	Sidechain
2	F	116	TYR	Sidechain
2	F	136	THR	Mainchain,Peptide
2	F	139	GLU	Peptide
2	F	265	PRO	Peptide
2	F	268	SER	Peptide
2	F	323	PHE	Sidechain
2	F	332	TYR	Sidechain
2	F	407	TYR	Sidechain
2	F	500	TYR	Sidechain
2	F	541	ARG	Sidechain
2	F	555	PHE	Sidechain
2	F	599	ARG	Sidechain
2	F	695	TYR	Sidechain
2	F	737	PRO	Peptide
2	F	869	ARG	Sidechain
2	G	109	ARG	Sidechain
2	G	121	TYR	Sidechain
2	G	137	ALA	Mainchain
2	G	141	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	G	388	TYR	Sidechain
2	G	407	TYR	Sidechain
2	G	455	TYR	Sidechain
2	G	599	ARG	Sidechain
2	G	63	ARG	Sidechain
2	G	643	TYR	Sidechain
2	G	67	ARG	Sidechain
2	G	695	TYR	Sidechain
2	G	84	PHE	Sidechain
2	G	869	ARG	Sidechain
2	G	891	TYR	Sidechain
2	G	896	HIS	Sidechain
2	H	109	ARG	Sidechain
2	H	320	TYR	Sidechain
2	H	374	ARG	Sidechain
2	H	407	TYR	Sidechain
2	H	599	ARG	Sidechain
2	H	706	ASP	Peptide
2	H	78	TYR	Sidechain
2	H	869	ARG	Sidechain
2	I	109	ARG	Sidechain
2	I	332	TYR	Sidechain
2	I	407	TYR	Sidechain
2	I	599	ARG	Sidechain
2	I	606	ARG	Sidechain
2	I	677	PHE	Sidechain
2	I	78	TYR	Sidechain
2	I	84	PHE	Sidechain
2	J	109	ARG	Sidechain
2	J	116	TYR	Sidechain
2	J	121	TYR	Sidechain
2	J	38	TYR	Sidechain
2	J	46	ARG	Sidechain
2	J	498	TYR	Sidechain
2	J	543	ARG	Sidechain
2	J	673	ARG	Sidechain
2	J	688	LEU	Peptide
2	K	109	ARG	Sidechain
2	K	38	TYR	Sidechain
2	K	430	ASP	Peptide
2	K	46	ARG	Sidechain
2	K	514	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	K	599	ARG	Sidechain
2	K	617	PHE	Sidechain
2	K	67	ARG	Sidechain
2	K	7	MET	Peptide
2	K	744	ARG	Sidechain
2	K	891	TYR	Sidechain
2	L	109	ARG	Sidechain
2	L	116	TYR	Sidechain
2	L	320	TYR	Sidechain
2	L	332	TYR	Sidechain
2	L	38	TYR	Sidechain
2	L	46	ARG	Sidechain
2	L	514	TYR	Sidechain
2	L	599	ARG	Sidechain
2	L	60	ARG	Sidechain
2	L	617	PHE	Sidechain
2	L	67	ARG	Sidechain
2	L	698	TYR	Sidechain
2	L	710	TYR	Sidechain
2	L	78	TYR	Sidechain
2	L	792	PHE	Sidechain
2	L	83	ARG	Sidechain
2	L	891	TYR	Sidechain
3	M	386	TYR	Sidechain
3	M	396	PRO	Peptide
3	M	484	ARG	Sidechain
3	M	497	ARG	Sidechain
4	N	93	TYR	Sidechain
5	O	27	TYR	Sidechain
5	O	30	ARG	Sidechain
5	O	72	ARG	Sidechain

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	1	177	163	162	2	0
1	2	113	103	102	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	168	157	156	2	0
1	4	91	81	80	2	0
1	5	202	191	191	3	0
1	6	161	148	147	1	0
1	7	211	204	203	1	0
1	8	140	131	129	1	0
2	A	7491	7148	7145	11	0
2	B	7491	7148	7145	22	0
2	C	7491	7149	7146	21	0
2	D	7491	7149	7146	12	0
2	E	7491	7148	7145	33	0
2	F	7491	7148	7145	37	0
2	G	7491	7149	7146	26	0
2	H	7491	7148	7145	4	0
2	I	7491	7148	7145	39	0
2	J	7491	7148	7145	12	0
2	K	7491	7148	7145	26	0
2	L	7475	7129	7129	50	0
3	M	3794	3715	3712	2	0
4	N	2176	2170	2169	2	0
5	O	1377	1329	1327	4	0
5	P	1389	1338	1336	4	0
6	Q	302	317	317	0	0
6	R	285	294	293	0	0
6	S	504	513	511	3	0
6	T	255	261	260	0	0
All	All	101221	96875	96822	281	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 1.

All (281) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:734:LEU:HB2	2:F:737:PRO:CG	2.12	0.79
2:F:495:THR:HA	2:F:500:TYR:CD2	2.20	0.77
2:B:191:PRO:HG3	2:B:281:TYR:CD2	2.22	0.73
2:F:495:THR:HG22	2:F:500:TYR:CE2	2.26	0.71
2:I:736:THR:H	2:I:737:PRO:CD	2.06	0.69
2:G:142:THR:HG23	2:G:145:GLN:C	2.18	0.69
2:G:142:THR:HG22	2:G:143:GLY:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:734:LEU:HB2	2:F:737:PRO:CD	2.26	0.65
2:C:191:PRO:HG3	2:C:281:TYR:CD2	2.30	0.64
2:E:200:TRP:HE1	2:E:412:ASN:HA	1.61	0.64
2:C:166:GLU:HB3	2:C:184:PHE:CD2	2.32	0.64
2:I:84:PHE:CD2	2:I:612:LEU:HB2	2.33	0.64
2:F:724:SER:HB2	2:L:69:VAL:HG22	1.78	0.64
2:I:736:THR:H	2:I:737:PRO:HD3	1.62	0.64
2:F:734:LEU:HB2	2:F:737:PRO:HG2	1.78	0.63
2:G:84:PHE:CD2	2:G:612:LEU:HB2	2.33	0.63
2:I:936:VAL:HG23	5:P:40:MET:HE3	1.79	0.63
2:B:267:GLY:C	2:B:269:GLY:H	2.07	0.62
2:G:84:PHE:CE2	2:G:612:LEU:HB2	2.34	0.62
2:C:684:GLU:HG2	2:C:698:TYR:CE2	2.35	0.62
2:E:495:THR:HA	2:E:500:TYR:CD2	2.34	0.62
2:J:113:PHE:CZ	2:J:115:PRO:HG3	2.35	0.61
2:F:734:LEU:HB2	2:F:737:PRO:HD2	1.81	0.61
4:N:188:THR:HA	4:N:196:VAL:HG22	1.82	0.60
2:L:83:ARG:HD2	2:L:577:THR:HG23	1.84	0.60
2:K:512:ASP:HB3	2:K:514:TYR:CD1	2.37	0.59
2:L:512:ASP:HB3	2:L:514:TYR:CD1	2.38	0.59
2:L:332:TYR:CE1	2:L:583:ARG:HG2	2.38	0.59
2:F:734:LEU:CB	2:F:737:PRO:HG2	2.33	0.59
2:G:367:LEU:HA	2:G:643:TYR:CD2	2.38	0.59
2:C:191:PRO:HG3	2:C:281:TYR:CE2	2.37	0.58
2:I:84:PHE:CE2	2:I:612:LEU:HB2	2.38	0.58
2:I:264:PRO:HG2	2:I:266:THR:HG22	1.86	0.57
2:F:107:LEU:HD23	2:F:605:VAL:HG22	1.86	0.57
2:F:734:LEU:CD1	2:F:737:PRO:HG2	2.34	0.57
2:E:320:TYR:CE2	2:E:541:ARG:HG2	2.39	0.57
2:G:142:THR:HG22	2:G:143:GLY:N	2.20	0.57
2:L:320:TYR:CE2	2:L:541:ARG:HG2	2.40	0.57
2:D:457:MET:HE1	2:E:457:MET:HG3	1.84	0.57
2:C:426:LYS:HG2	2:C:429:GLN:HB2	1.86	0.56
2:E:893:ASN:HA	2:I:346:ALA:HB1	1.85	0.56
2:L:261:GLY:HA3	2:L:270:GLN:HB2	1.87	0.56
2:E:200:TRP:CZ3	2:F:310:THR:HA	2.41	0.56
2:L:885:LEU:O	2:L:891:TYR:CD2	2.58	0.56
2:E:176:GLU:O	2:E:177:GLY:C	2.49	0.56
2:K:514:TYR:CD2	2:K:844:PRO:HG3	2.41	0.55
2:F:734:LEU:HD12	2:F:737:PRO:HG2	1.88	0.55
2:K:457:MET:HE2	2:L:457:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:15:THR:HG22	1:4:16:ARG:H	1.71	0.55
2:L:113:PHE:CZ	2:L:115:PRO:HG3	2.41	0.55
4:N:193:LEU:O	4:N:196:VAL:HG23	2.06	0.55
2:L:710:TYR:CD1	2:L:711:LEU:HG	2.42	0.55
1:5:10:ALA:HB1	1:5:11:PRO:HD2	1.88	0.55
2:B:166:GLU:HB3	2:B:184:PHE:CD2	2.42	0.55
2:B:174:GLU:HA	2:B:180:THR:HG22	1.89	0.55
2:L:512:ASP:HB3	2:L:514:TYR:CE1	2.41	0.55
2:L:780:VAL:HG13	2:L:792:PHE:HE2	1.72	0.55
2:L:77:THR:HB	2:L:78:TYR:CD1	2.42	0.54
2:C:191:PRO:CG	2:C:281:TYR:CD2	2.90	0.54
2:B:166:GLU:CB	2:B:184:PHE:CD2	2.90	0.54
2:L:514:TYR:CD2	2:L:844:PRO:HG3	2.42	0.54
2:L:890:LEU:C	2:L:891:TYR:CD1	2.85	0.54
2:D:670:ALA:HB1	2:F:6:MET:HE1	1.89	0.53
2:E:457:MET:HE2	2:F:457:MET:HE2	1.89	0.53
2:G:457:MET:HE3	2:I:457:MET:HE1	1.91	0.53
2:B:545:MET:HE1	2:C:398:HIS:ND1	2.23	0.53
2:F:332:TYR:CE1	2:F:583:ARG:HG2	2.43	0.53
2:G:872:PHE:CZ	2:G:891:TYR:CE2	2.97	0.53
2:E:433:GLU:C	2:E:434:GLU:HG3	2.34	0.53
2:E:176:GLU:HG2	2:E:180:THR:HG23	1.91	0.53
2:D:457:MET:HE2	2:F:457:MET:HE2	1.91	0.52
2:E:142:THR:HG23	2:E:145:GLN:O	2.09	0.52
2:G:84:PHE:CD2	2:G:612:LEU:CB	2.92	0.52
2:L:430:ASP:C	2:L:432:ALA:H	2.16	0.52
2:I:332:TYR:CE1	2:I:583:ARG:HG2	2.44	0.52
2:D:613:TYR:CZ	2:E:760:LYS:HE2	2.45	0.52
2:I:711:LEU:HD22	2:I:907:MET:HE1	1.92	0.52
2:C:166:GLU:CB	2:C:184:PHE:CD2	2.93	0.52
2:E:200:TRP:C	2:E:202:GLU:H	2.17	0.51
2:D:20:ALA:HA	2:D:23:TYR:CE2	2.46	0.51
2:A:825:PHE:CE2	2:C:125:ALA:HB2	2.45	0.51
2:G:457:MET:CE	2:I:457:MET:HE1	2.41	0.51
2:K:944:ALA:C	2:K:946:ASN:H	2.19	0.51
2:A:327:PHE:CZ	2:A:382:ASN:HB2	2.46	0.51
1:6:9:LEU:HG	1:6:10:ALA:H	1.75	0.51
2:I:200:TRP:CE3	2:I:412:ASN:HB3	2.46	0.51
2:A:890:LEU:HD21	2:C:7:MET:HE3	1.93	0.50
2:F:270:GLN:H	2:F:273:GLU:HG3	1.76	0.50
2:K:512:ASP:HB3	2:K:514:TYR:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:77:THR:HB	2:L:78:TYR:HD1	1.75	0.50
2:D:457:MET:HE2	2:E:457:MET:HE2	1.93	0.50
2:F:332:TYR:CD2	2:F:338:ASN:HB3	2.46	0.50
2:I:664:ILE:HD11	2:I:669:TRP:CH2	2.47	0.50
2:A:437:TRP:CD1	2:B:275:LYS:HA	2.46	0.50
2:A:275:LYS:HA	2:C:437:TRP:CD1	2.47	0.49
2:G:367:LEU:HA	2:G:643:TYR:CE2	2.46	0.49
2:F:430:ASP:HB3	2:F:432:ALA:HB3	1.93	0.49
2:I:84:PHE:CD2	2:I:612:LEU:CB	2.95	0.49
2:I:327:PHE:CZ	2:I:382:ASN:HB2	2.48	0.49
2:L:83:ARG:CD	2:L:577:THR:HG23	2.41	0.49
2:G:83:ARG:C	2:G:84:PHE:HD1	2.21	0.49
6:S:88:SER:H	6:S:89:PRO:HD2	1.77	0.49
2:L:940:THR:HG23	2:L:941:PRO:HD3	1.93	0.49
2:F:664:ILE:HD11	2:F:669:TRP:CH2	2.48	0.49
2:L:710:TYR:CE1	2:L:711:LEU:HG	2.48	0.49
2:D:457:MET:HG3	2:F:457:MET:HE1	1.94	0.48
2:F:327:PHE:CZ	2:F:382:ASN:HB2	2.47	0.48
2:K:940:THR:HG23	2:K:941:PRO:HD3	1.94	0.48
2:E:200:TRP:CH2	2:F:310:THR:HA	2.49	0.48
2:K:113:PHE:CZ	2:K:115:PRO:HG3	2.48	0.48
2:K:583:ARG:O	2:K:589:ILE:HD11	2.13	0.48
2:K:940:THR:HG23	2:K:941:PRO:CD	2.43	0.48
2:L:940:THR:HG23	2:L:941:PRO:CD	2.43	0.48
2:D:327:PHE:CZ	2:D:382:ASN:HB2	2.48	0.48
2:K:327:PHE:CZ	2:K:382:ASN:HB2	2.48	0.48
2:E:200:TRP:HE1	2:E:412:ASN:CA	2.25	0.48
2:A:890:LEU:CD2	2:C:7:MET:HE3	2.43	0.48
2:C:327:PHE:CZ	2:C:382:ASN:HB2	2.48	0.48
2:L:113:PHE:CZ	2:L:115:PRO:CG	2.97	0.48
2:L:327:PHE:CZ	2:L:382:ASN:HB2	2.49	0.48
2:F:734:LEU:CB	2:F:737:PRO:HD2	2.44	0.48
2:K:891:TYR:CD1	2:K:892:ALA:N	2.81	0.48
2:F:332:TYR:CD2	2:F:338:ASN:CB	2.97	0.48
2:L:698:TYR:CD1	2:L:699:SER:N	2.82	0.48
1:5:10:ALA:HB1	1:5:11:PRO:CD	2.44	0.47
2:B:327:PHE:CZ	2:B:382:ASN:HB2	2.50	0.47
2:C:266:THR:H	2:C:270:GLN:HB2	1.79	0.47
2:E:327:PHE:CZ	2:E:382:ASN:HB2	2.49	0.47
2:B:441:GLU:HG3	2:C:147:LYS:HE2	1.96	0.47
2:I:83:ARG:C	2:I:84:PHE:HD1	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:332:TYR:CD2	2:I:338:ASN:CB	2.98	0.47
2:J:113:PHE:CZ	2:J:115:PRO:CG	2.98	0.47
2:J:940:THR:HG23	2:J:941:PRO:CD	2.45	0.47
2:K:188:THR:HG21	2:K:250:TYR:CD2	2.50	0.47
2:L:936:VAL:HG23	5:O:40:MET:HE3	1.96	0.47
2:L:188:THR:HG21	2:L:250:TYR:CD2	2.50	0.47
2:G:176:GLU:C	2:G:178:ASN:H	2.22	0.47
1:7:22:TRP:CG	1:7:23:ASN:H	2.33	0.47
2:L:78:TYR:CD2	2:L:692:PHE:CG	3.02	0.47
2:L:781:PRO:HD2	2:L:792:PHE:CD2	2.50	0.46
2:F:138:ASN:HA	2:F:148:SER:HA	1.97	0.46
2:J:457:MET:HG3	2:L:457:MET:HE1	1.97	0.46
5:O:10:MET:HE2	5:O:194:PRO:HB3	1.97	0.46
2:L:919:VAL:HG12	2:L:941:PRO:HG2	1.96	0.46
2:B:84:PHE:CD2	2:B:612:LEU:HB3	2.51	0.46
2:K:919:VAL:HG12	2:K:941:PRO:HG2	1.97	0.46
1:1:13:HIS:CG	1:1:14:GLY:N	2.82	0.46
2:J:940:THR:HG23	2:J:941:PRO:HD3	1.98	0.46
2:E:176:GLU:CG	2:E:180:THR:HG23	2.46	0.46
2:G:872:PHE:HZ	2:G:891:TYR:CE2	2.34	0.45
2:K:113:PHE:CZ	2:K:115:PRO:CG	2.99	0.45
2:B:166:GLU:HB2	2:B:184:PHE:CD2	2.51	0.45
2:F:265:PRO:HG3	2:F:270:GLN:C	2.41	0.45
2:K:600:VAL:HG12	2:K:601:ASP:H	1.81	0.45
2:K:887:GLN:HA	2:K:890:LEU:HD12	1.98	0.45
2:B:84:PHE:CE2	2:B:612:LEU:CB	2.99	0.45
2:E:889:MET:C	2:E:891:TYR:N	2.75	0.45
2:I:737:PRO:HB2	2:I:739:GLU:H	1.80	0.45
2:L:698:TYR:CE1	2:L:700:GLY:N	2.85	0.45
2:B:701:SER:HB3	2:B:708:THR:CG2	2.47	0.45
3:M:64:ALA:HA	3:M:67:ALA:HB3	1.98	0.45
2:E:892:ALA:O	2:I:346:ALA:HB1	2.17	0.45
2:K:189:PHE:CD1	2:K:189:PHE:N	2.83	0.45
1:3:12:ARG:H	1:3:13:HIS:CD2	2.35	0.45
1:8:8:SER:C	1:8:9:LEU:HD22	2.42	0.45
2:L:698:TYR:CD1	2:L:698:TYR:C	2.95	0.44
2:D:107:LEU:HD23	2:D:605:VAL:HG22	1.98	0.44
2:F:734:LEU:HB2	2:F:737:PRO:CB	2.46	0.44
2:I:736:THR:N	2:I:737:PRO:HD3	2.28	0.44
2:B:84:PHE:CD2	2:B:612:LEU:CB	3.00	0.44
2:E:176:GLU:C	2:E:178:ASN:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:323:PHE:CZ	2:F:555:PHE:CE2	3.06	0.44
2:L:684:GLU:HG2	2:L:698:TYR:CE2	2.52	0.44
2:E:320:TYR:HE2	2:E:541:ARG:HG2	1.82	0.44
2:F:200:TRP:C	2:F:202:GLU:H	2.25	0.44
2:L:681:LYS:HA	2:L:911:THR:HG22	2.00	0.44
2:E:269:GLY:H	2:E:273:GLU:HB3	1.83	0.44
2:A:895:ALA:HB2	2:L:346:ALA:HB2	2.00	0.44
2:L:332:TYR:CD2	2:L:338:ASN:CB	3.01	0.44
2:C:84:PHE:CD2	2:C:612:LEU:CB	3.01	0.43
2:I:332:TYR:CD2	2:I:338:ASN:HB3	2.53	0.43
1:5:1:MET:SD	2:G:869:ARG:HD3	2.58	0.43
2:B:84:PHE:CE2	2:B:612:LEU:HB3	2.54	0.43
2:E:887:GLN:HA	2:E:890:LEU:CD1	2.48	0.43
2:E:202:GLU:O	2:E:203:THR:HB	2.18	0.43
2:G:84:PHE:HD2	2:G:612:LEU:HB2	1.82	0.43
2:G:327:PHE:CZ	2:G:382:ASN:HB2	2.54	0.43
2:I:82:ALA:HB1	2:I:84:PHE:HE1	1.83	0.43
2:E:52:PRO:HG2	2:E:56:VAL:HG21	1.99	0.43
2:G:711:LEU:HD22	2:G:907:MET:HE1	2.01	0.43
2:L:583:ARG:O	2:L:589:ILE:HD11	2.19	0.43
2:L:890:LEU:HB2	2:L:891:TYR:CZ	2.53	0.43
2:G:135:TRP:CZ2	2:G:151:GLN:HG3	2.54	0.43
2:I:84:PHE:HD2	2:I:612:LEU:HB2	1.81	0.43
2:K:681:LYS:HA	2:K:911:THR:HG22	2.00	0.43
2:L:189:PHE:CD1	2:L:189:PHE:N	2.86	0.43
2:C:166:GLU:CB	2:C:184:PHE:CE2	3.02	0.43
2:E:320:TYR:CD1	2:E:320:TYR:N	2.87	0.43
2:E:521:TRP:CE2	2:E:860:LYS:HE2	2.53	0.43
2:I:894:SER:HB2	5:P:188:PHE:CE2	2.53	0.43
2:C:84:PHE:CD2	2:C:612:LEU:HB3	2.53	0.43
2:G:142:THR:CG2	2:G:143:GLY:N	2.82	0.43
2:L:944:ALA:C	2:L:946:ASN:H	2.27	0.43
2:A:457:MET:SD	2:B:457:MET:HE3	2.59	0.43
2:B:566:ILE:HD11	2:B:580:TRP:CH2	2.53	0.43
2:J:629:ALA:HB2	5:P:89:VAL:HG11	2.01	0.43
2:K:889:MET:N	2:K:891:TYR:CE2	2.87	0.43
2:F:737:PRO:HA	2:F:739:GLU:H	1.83	0.42
2:I:176:GLU:C	2:I:178:ASN:H	2.26	0.42
2:I:677:PHE:CD1	2:I:868:TRP:HB2	2.54	0.42
2:I:728:TRP:CG	2:I:729:PRO:HA	2.54	0.42
2:J:919:VAL:HG12	2:J:941:PRO:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:720:ILE:HG23	2:F:898:LEU:HD11	2.00	0.42
2:G:82:ALA:HB1	2:G:84:PHE:HE1	1.85	0.42
1:4:15:THR:HG22	1:4:16:ARG:N	2.32	0.42
2:E:433:GLU:C	2:E:434:GLU:CG	2.91	0.42
2:J:189:PHE:CD1	2:J:189:PHE:N	2.86	0.42
2:B:457:MET:HE1	2:C:457:MET:SD	2.59	0.42
2:A:125:ALA:HB2	2:B:825:PHE:CE2	2.55	0.42
6:S:76:ARG:C	6:S:76:ARG:HD2	2.44	0.42
2:D:720:ILE:HG23	2:D:898:LEU:HD11	2.02	0.42
2:G:907:MET:HG2	2:G:911:THR:HG21	2.02	0.42
2:K:889:MET:HA	2:K:891:TYR:CE2	2.55	0.42
2:C:135:TRP:CZ2	2:C:151:GLN:HG3	2.55	0.42
2:F:806:ILE:HD13	6:S:111:LEU:HB3	2.02	0.42
2:H:457:MET:SD	2:I:457:MET:HE2	2.60	0.42
2:B:756:CYS:SG	2:B:757:ASN:N	2.93	0.42
2:F:107:LEU:CD2	2:F:605:VAL:HG22	2.48	0.42
2:F:737:PRO:HA	2:F:739:GLU:N	2.34	0.42
2:L:8:PRO:HD3	5:P:18:GLY:HA2	2.02	0.42
2:L:943:SER:OG	5:O:28:SER:C	2.63	0.42
2:G:200:TRP:CE3	2:G:412:ASN:HB3	2.55	0.42
2:H:681:LYS:HA	2:H:911:THR:HG22	2.02	0.42
2:L:891:TYR:CD1	2:L:891:TYR:N	2.78	0.42
2:A:366:LEU:HB3	2:A:644:LEU:HD13	2.01	0.42
1:1:13:HIS:CG	1:1:14:GLY:H	2.38	0.41
2:F:736:THR:H	2:F:737:PRO:HD2	1.85	0.41
2:K:887:GLN:HA	2:K:890:LEU:CD1	2.50	0.41
2:B:166:GLU:CB	2:B:184:PHE:CE2	3.03	0.41
2:I:190:GLN:HA	2:I:191:PRO:C	2.45	0.41
2:K:532:PHE:CD2	2:K:708:THR:HB	2.54	0.41
2:L:263:THR:H	2:L:264:PRO:CD	2.32	0.41
2:C:84:PHE:CE2	2:C:612:LEU:CB	3.03	0.41
2:H:437:TRP:CD1	2:I:275:LYS:HA	2.55	0.41
2:J:135:TRP:CZ2	2:J:151:GLN:HG3	2.55	0.41
2:B:566:ILE:HD11	2:B:580:TRP:CZ3	2.55	0.41
2:I:82:ALA:HB1	2:I:84:PHE:CE1	2.55	0.41
2:L:135:TRP:CZ2	2:L:151:GLN:HG3	2.54	0.41
2:I:264:PRO:HB2	2:I:265:PRO:HD2	2.01	0.41
2:I:875:ASN:HD21	2:I:879:MET:HE2	1.84	0.41
2:L:600:VAL:HG12	2:L:601:ASP:H	1.85	0.41
1:3:8:SER:C	1:3:9:LEU:HD12	2.45	0.41
2:D:521:TRP:CE2	2:D:860:LYS:HE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:893:ASN:HA	2:I:346:ALA:CB	2.50	0.41
2:G:165:ILE:HD12	2:G:165:ILE:H	1.86	0.41
2:G:178:ASN:CG	2:G:179:ALA:H	2.28	0.41
2:J:843:PHE:CD1	2:J:843:PHE:C	2.99	0.41
2:K:674:GLY:HA2	2:K:872:PHE:HB2	2.03	0.41
2:L:320:TYR:HE2	2:L:541:ARG:HG2	1.82	0.41
2:A:135:TRP:CZ2	2:A:151:GLN:HG3	2.56	0.41
2:E:142:THR:HG21	2:E:145:GLN:HE21	1.85	0.41
2:I:165:ILE:HD12	2:I:165:ILE:H	1.85	0.41
2:I:332:TYR:HD2	2:I:338:ASN:HB3	1.85	0.41
2:K:113:PHE:CE1	2:K:115:PRO:HG3	2.55	0.41
2:K:888:ASN:O	2:K:889:MET:HG2	2.21	0.41
2:K:892:ALA:O	2:K:894:SER:N	2.54	0.41
2:L:893:ASN:HA	5:O:10:MET:SD	2.61	0.41
2:E:720:ILE:HG23	2:E:898:LEU:HD11	2.02	0.41
2:H:678:THR:HG21	2:H:709:PHE:CE1	2.56	0.41
2:I:200:TRP:CD2	2:I:412:ASN:HB3	2.55	0.41
2:L:521:TRP:CZ2	2:L:860:LYS:HE2	2.56	0.41
2:D:52:PRO:HG2	2:D:56:VAL:HG21	2.03	0.40
2:I:178:ASN:CG	2:I:179:ALA:H	2.30	0.40
2:L:197:GLU:HB2	2:L:202:GLU:CD	2.46	0.40
2:G:872:PHE:CZ	2:G:885:LEU:HB3	2.55	0.40
2:I:434:GLU:HG3	2:I:436:GLU:H	1.87	0.40
2:E:20:ALA:HA	2:E:23:TYR:CE2	2.57	0.40
2:J:327:PHE:CZ	2:J:382:ASN:HB2	2.57	0.40
2:J:521:TRP:CZ2	2:J:860:LYS:HE2	2.56	0.40
2:F:261:GLY:C	2:F:263:THR:H	2.30	0.40
3:M:237:PRO:HA	3:M:268:TYR:CG	2.57	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	1	20/234 (8%)	16 (80%)	4 (20%)	0	100	100
1	2	14/234 (6%)	9 (64%)	4 (29%)	1 (7%)	1	7
1	3	19/234 (8%)	9 (47%)	7 (37%)	3 (16%)	0	1
1	4	9/234 (4%)	4 (44%)	4 (44%)	1 (11%)	0	2
1	5	23/234 (10%)	14 (61%)	5 (22%)	4 (17%)	0	1
1	6	18/234 (8%)	10 (56%)	5 (28%)	3 (17%)	0	1
1	7	25/234 (11%)	17 (68%)	5 (20%)	3 (12%)	0	1
1	8	13/234 (6%)	8 (62%)	5 (38%)	0	100	100
2	A	939/941 (100%)	883 (94%)	53 (6%)	3 (0%)	37	66
2	B	939/941 (100%)	881 (94%)	49 (5%)	9 (1%)	13	42
2	C	939/941 (100%)	886 (94%)	45 (5%)	8 (1%)	14	44
2	D	939/941 (100%)	877 (93%)	59 (6%)	3 (0%)	37	66
2	E	939/941 (100%)	866 (92%)	59 (6%)	14 (2%)	8	33
2	F	939/941 (100%)	875 (93%)	53 (6%)	11 (1%)	11	38
2	G	939/941 (100%)	881 (94%)	49 (5%)	9 (1%)	13	42
2	H	939/941 (100%)	888 (95%)	50 (5%)	1 (0%)	48	76
2	I	939/941 (100%)	879 (94%)	50 (5%)	10 (1%)	12	40
2	J	939/941 (100%)	880 (94%)	54 (6%)	5 (0%)	25	56
2	K	939/941 (100%)	879 (94%)	50 (5%)	10 (1%)	12	40
2	L	937/941 (100%)	881 (94%)	48 (5%)	8 (1%)	14	44
3	M	468/519 (90%)	438 (94%)	30 (6%)	0	100	100
4	N	279/559 (50%)	254 (91%)	23 (8%)	2 (1%)	19	50
5	O	173/227 (76%)	163 (94%)	10 (6%)	0	100	100
5	P	176/227 (78%)	162 (92%)	14 (8%)	0	100	100
6	Q	37/134 (28%)	37 (100%)	0	0	100	100
6	R	34/134 (25%)	33 (97%)	1 (3%)	0	100	100
6	S	67/134 (50%)	53 (79%)	10 (15%)	4 (6%)	1	9
6	T	30/134 (22%)	30 (100%)	0	0	100	100
All	All	12671/15232 (83%)	11813 (93%)	746 (6%)	112 (1%)	17	44

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3	16	ARG
1	5	6	PHE
1	6	10	ALA
2	B	268	SER
2	B	269	GLY
2	B	270	GLN
2	B	271	GLN
2	C	430	ASP
2	C	432	ALA
2	C	944	ALA
2	E	177	GLY
2	E	271	GLN
2	E	273	GLU
2	E	434	GLU
2	E	889	MET
2	F	137	ALA
2	F	138	ASN
2	F	261	GLY
2	F	271	GLN
2	F	434	GLU
2	G	142	THR
2	G	143	GLY
2	G	888	ASN
2	G	889	MET
2	I	268	SER
2	I	736	THR
2	I	888	ASN
2	K	431	GLY
2	K	433	GLU
2	K	893	ASN
2	L	433	GLU
1	2	29	GLN
1	7	18	PHE
2	E	203	THR
2	E	888	ASN
2	E	892	ALA
2	F	273	GLU
2	F	433	GLU
2	G	176	GLU
2	G	177	GLY
2	I	176	GLU
2	I	889	MET
2	K	429	GLN

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Mol	Chain	Res	Type
2	L	889	MET
2	L	894	SER
6	S	74	ALA
6	S	83	PRO
6	S	88	SER
1	3	5	ASN
1	5	15	THR
1	6	9	LEU
2	D	271	GLN
2	E	891	TYR
2	I	177	GLY
2	I	892	ALA
2	J	893	ASN
2	J	894	SER
2	K	8	PRO
2	K	864	ASP
2	K	889	MET
2	L	864	ASP
4	N	148	PRO
1	5	19	MET
2	A	9	GLN
2	A	843	PHE
2	B	9	GLN
2	B	843	PHE
2	C	189	PHE
2	C	843	PHE
2	D	263	THR
2	E	175	GLU
2	E	202	GLU
2	F	141	GLN
2	J	864	ASP
1	3	4	ILE
1	4	17	PRO
1	6	14	GLY
2	A	697	VAL
2	B	430	ASP
2	C	697	VAL
2	E	263	THR
2	E	348	GLN
2	F	736	THR
2	G	137	ALA
2	G	864	ASP

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Mol	Chain	Res	Type
2	I	265	PRO
2	I	864	ASP
2	J	263	THR
2	L	263	THR
1	5	10	ALA
2	B	189	PHE
2	B	697	VAL
2	C	601	ASP
2	K	894	SER
2	L	893	ASN
2	L	945	GLY
4	N	152	PRO
6	S	91	VAL
1	7	10	ALA
1	7	17	PRO
2	K	945	GLY
2	C	940	THR
2	E	697	VAL
2	J	941	PRO
2	D	697	VAL
2	F	697	VAL
2	L	843	PHE
2	G	265	PRO
2	H	265	PRO
2	I	737	PRO
2	K	263	THR
2	F	263	THR

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	1	18/195 (9%)	14 (78%)	4 (22%)	1	3
1	2	11/195 (6%)	10 (91%)	1 (9%)	7	27
1	3	17/195 (9%)	15 (88%)	2 (12%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4	9/195 (5%)	7 (78%)	2 (22%)	1	3
1	5	21/195 (11%)	17 (81%)	4 (19%)	1	5
1	6	16/195 (8%)	15 (94%)	1 (6%)	15	41
1	7	22/195 (11%)	18 (82%)	4 (18%)	1	6
1	8	14/195 (7%)	14 (100%)	0	100	100
2	A	813/813 (100%)	805 (99%)	8 (1%)	73	84
2	B	813/813 (100%)	804 (99%)	9 (1%)	70	82
2	C	813/813 (100%)	801 (98%)	12 (2%)	60	77
2	D	813/813 (100%)	805 (99%)	8 (1%)	73	84
2	E	813/813 (100%)	802 (99%)	11 (1%)	62	78
2	F	813/813 (100%)	804 (99%)	9 (1%)	70	82
2	G	813/813 (100%)	807 (99%)	6 (1%)	81	88
2	H	813/813 (100%)	807 (99%)	6 (1%)	81	88
2	I	813/813 (100%)	807 (99%)	6 (1%)	81	88
2	J	813/813 (100%)	809 (100%)	4 (0%)	86	91
2	K	813/813 (100%)	809 (100%)	4 (0%)	86	91
2	L	811/813 (100%)	798 (98%)	13 (2%)	58	76
3	M	426/461 (92%)	420 (99%)	6 (1%)	62	78
4	N	236/473 (50%)	233 (99%)	3 (1%)	65	79
5	O	152/190 (80%)	150 (99%)	2 (1%)	65	79
5	P	152/190 (80%)	147 (97%)	5 (3%)	33	60
6	Q	33/102 (32%)	33 (100%)	0	100	100
6	R	30/102 (29%)	29 (97%)	1 (3%)	33	60
6	S	54/102 (53%)	51 (94%)	3 (6%)	17	45
6	T	27/102 (26%)	25 (93%)	2 (7%)	11	34
All	All	10992/13038 (84%)	10856 (99%)	136 (1%)	66	80

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	9	LEU
1	1	16	ARG
1	1	19	MET

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Mol	Chain	Res	Type
1	1	23	ASN
1	2	29	GLN
1	3	6	PHE
1	3	19	MET
1	4	16	ARG
1	4	22	TRP
1	5	1	MET
1	5	4	ILE
1	5	12	ARG
1	5	25	ILE
1	6	18	PHE
1	7	5	ASN
1	7	16	ARG
1	7	19	MET
1	7	29	GLN
2	A	334	ASN
2	A	367	LEU
2	A	417	ASN
2	A	643	TYR
2	A	708	THR
2	A	738	ASN
2	A	848	ILE
2	A	919	VAL
2	B	84	PHE
2	B	334	ASN
2	B	367	LEU
2	B	417	ASN
2	B	580	TRP
2	B	581	ASN
2	B	643	TYR
2	B	867	MET
2	B	919	VAL
2	C	38	TYR
2	C	84	PHE
2	C	92	ARG
2	C	367	LEU
2	C	408	CYS
2	C	417	ASN
2	C	580	TRP
2	C	643	TYR
2	C	698	TYR
2	C	708	THR

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Mol	Chain	Res	Type
2	C	919	VAL
2	C	943	SER
2	D	13	MET
2	D	139	GLU
2	D	145	GLN
2	D	215	ASP
2	D	240	LEU
2	D	353	VAL
2	D	536	ARG
2	D	641	ASN
2	E	139	GLU
2	E	145	GLN
2	E	200	TRP
2	E	202	GLU
2	E	215	ASP
2	E	240	LEU
2	E	348	GLN
2	E	536	ARG
2	E	641	ASN
2	E	664	ILE
2	E	946	ASN
2	F	13	MET
2	F	139	GLU
2	F	145	GLN
2	F	202	GLU
2	F	215	ASP
2	F	240	LEU
2	F	536	ARG
2	F	555	PHE
2	F	737	PRO
2	G	272	GLU
2	G	273	GLU
2	G	286	ASN
2	G	398	HIS
2	G	664	ILE
2	G	802	VAL
2	H	181	GLU
2	H	200	TRP
2	H	273	GLU
2	H	286	ASN
2	H	398	HIS
2	H	802	VAL

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Mol	Chain	Res	Type
2	I	181	GLU
2	I	200	TRP
2	I	286	ASN
2	I	398	HIS
2	I	677	PHE
2	I	802	VAL
2	J	7	MET
2	J	201	GLN
2	J	275	LYS
2	J	433	GLU
2	K	7	MET
2	K	181	GLU
2	K	433	GLU
2	K	514	TYR
2	L	78	TYR
2	L	201	GLN
2	L	202	GLU
2	L	275	LYS
2	L	408	CYS
2	L	430	ASP
2	L	433	GLU
2	L	514	TYR
2	L	570	LEU
2	L	580	TRP
2	L	698	TYR
2	L	710	TYR
2	L	890	LEU
3	M	52	ASP
3	M	341	ASN
3	M	383	GLU
3	M	385	VAL
3	M	401	SER
3	M	441	THR
4	N	91	LEU
4	N	178	TYR
4	N	195	THR
5	O	106	VAL
5	O	211	GLU
5	P	4	GLU
5	P	34	LEU
5	P	69	LEU
5	P	106	VAL

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Mol	Chain	Res	Type
5	P	168	TYR
6	R	114	GLN
6	S	60	ASP
6	S	76	ARG
6	S	91	VAL
6	T	107	GLU
6	T	121	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (175) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	13	HIS
1	8	5	ASN
2	A	14	HIS
2	A	18	GLN
2	A	54	HIS
2	A	131	ASN
2	A	235	GLN
2	A	284	ASN
2	A	286	ASN
2	A	311	GLN
2	A	338	ASN
2	A	345	GLN
2	A	365	GLN
2	A	417	ASN
2	A	448	GLN
2	A	464	ASN
2	A	581	ASN
2	A	648	ASN
2	A	659	ASN
2	A	757	ASN
2	A	794	ASN
2	A	893	ASN
2	A	896	HIS
2	A	926	HIS
2	B	9	GLN
2	B	14	HIS
2	B	131	ASN
2	B	235	GLN
2	B	286	ASN
2	B	326	ASN
2	B	338	ASN

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Mol	Chain	Res	Type
2	B	365	GLN
2	B	406	ASN
2	B	464	ASN
2	B	581	ASN
2	B	648	ASN
2	B	757	ASN
2	B	770	HIS
2	B	794	ASN
2	C	18	GLN
2	C	134	GLN
2	C	235	GLN
2	C	270	GLN
2	C	284	ASN
2	C	286	ASN
2	C	311	GLN
2	C	326	ASN
2	C	338	ASN
2	C	365	GLN
2	C	406	ASN
2	C	417	ASN
2	C	448	GLN
2	C	581	ASN
2	C	587	ASN
2	C	757	ASN
2	C	794	ASN
2	C	893	ASN
2	D	14	HIS
2	D	345	GLN
2	D	447	ASN
2	D	528	ASN
2	E	134	GLN
2	E	145	GLN
2	E	284	ASN
2	E	326	ASN
2	E	365	GLN
2	E	417	ASN
2	E	558	GLN
2	E	581	ASN
2	E	641	ASN
2	E	807	ASN
2	E	819	GLN
2	E	946	ASN

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Mol	Chain	Res	Type
2	F	134	GLN
2	F	178	ASN
2	F	326	ASN
2	F	345	GLN
2	F	348	GLN
2	F	417	ASN
2	F	447	ASN
2	F	528	ASN
2	F	558	GLN
2	F	581	ASN
2	F	819	GLN
2	F	946	ASN
2	G	131	ASN
2	G	134	GLN
2	G	190	GLN
2	G	241	ASN
2	G	271	GLN
2	G	286	ASN
2	G	338	ASN
2	G	398	HIS
2	G	406	ASN
2	G	464	ASN
2	G	581	ASN
2	G	611	ASN
2	G	794	ASN
2	G	835	GLN
2	H	14	HIS
2	H	131	ASN
2	H	134	GLN
2	H	190	GLN
2	H	201	GLN
2	H	338	ASN
2	H	382	ASN
2	H	406	ASN
2	H	464	ASN
2	H	496	ASN
2	H	794	ASN
2	I	131	ASN
2	I	134	GLN
2	I	235	GLN
2	I	241	ASN
2	I	406	ASN

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Mol	Chain	Res	Type
2	I	464	ASN
2	I	581	ASN
2	I	766	GLN
2	I	835	GLN
2	I	893	ASN
2	J	14	HIS
2	J	18	GLN
2	J	62	GLN
2	J	134	GLN
2	J	178	ASN
2	J	201	GLN
2	J	326	ASN
2	J	338	ASN
2	J	365	GLN
2	J	488	ASN
2	J	558	GLN
2	J	633	ASN
2	J	926	HIS
2	K	134	GLN
2	K	286	ASN
2	K	338	ASN
2	K	348	GLN
2	K	365	GLN
2	K	488	ASN
2	K	558	GLN
2	K	611	ASN
2	K	926	HIS
2	L	131	ASN
2	L	134	GLN
2	L	178	ASN
2	L	201	GLN
2	L	286	ASN
2	L	326	ASN
2	L	338	ASN
2	L	348	GLN
2	L	365	GLN
2	L	464	ASN
2	L	488	ASN
2	L	659	ASN
2	L	926	HIS
3	M	117	ASN
3	M	120	ASN

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Mol	Chain	Res	Type
3	M	179	ASN
3	M	191	GLN
3	M	347	HIS
4	N	46	GLN
4	N	68	HIS
5	O	14	GLN
5	O	53	GLN
5	O	166	GLN
5	O	199	ASN
5	P	103	ASN
5	P	172	GLN
6	Q	114	GLN
6	R	121	GLN
6	R	128	GLN
6	S	128	GLN
6	S	129	GLN
6	T	114	GLN
6	T	133	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

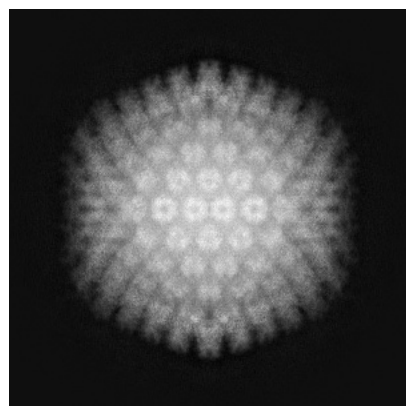
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53736. These allow visual inspection of the internal detail of the map and identification of artifacts.

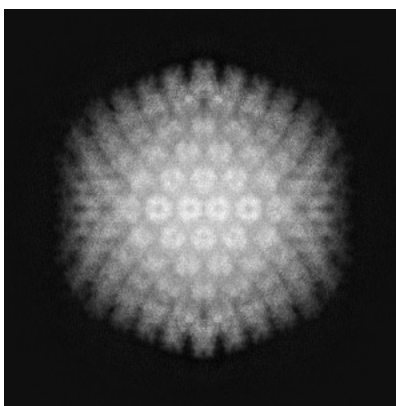
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

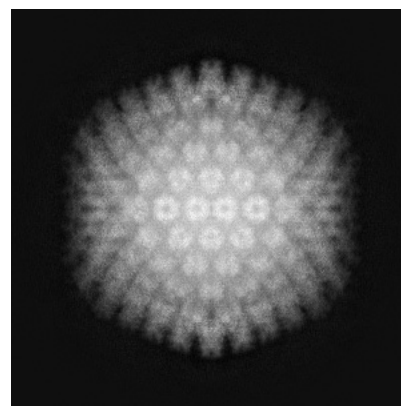
6.1.1 Primary map



X

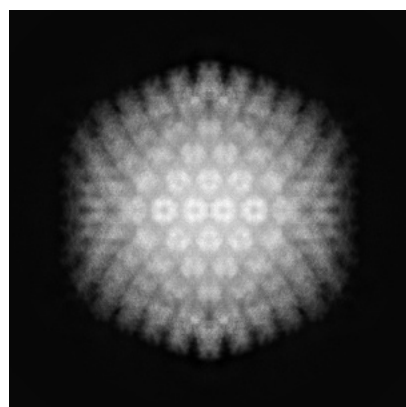


Y

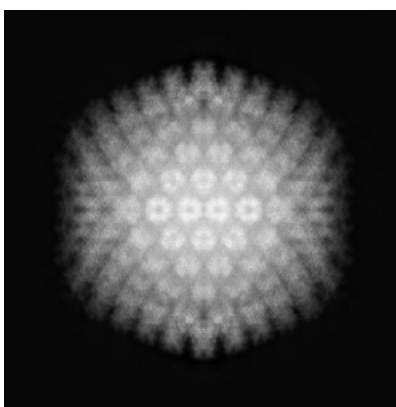


Z

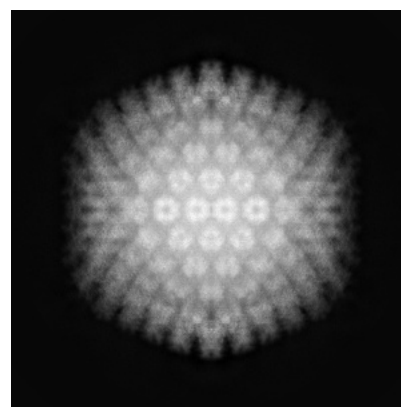
6.1.2 Raw map



X



Y

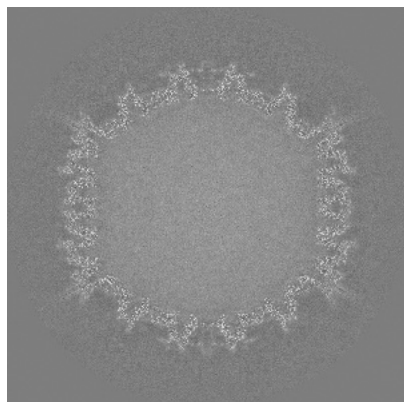


Z

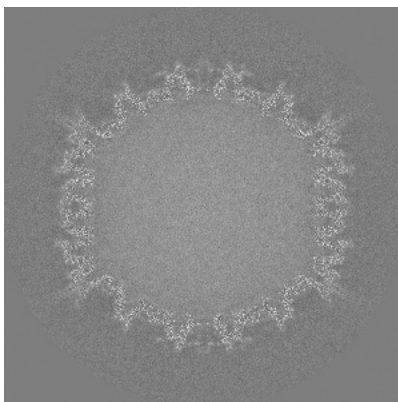
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

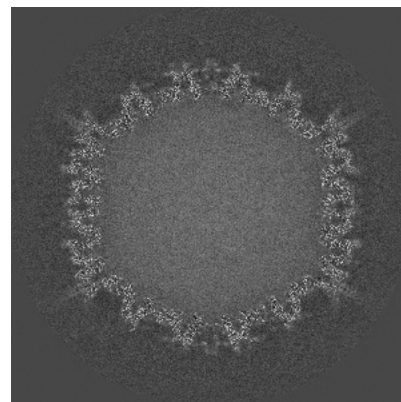
6.2.1 Primary map



X Index: 360

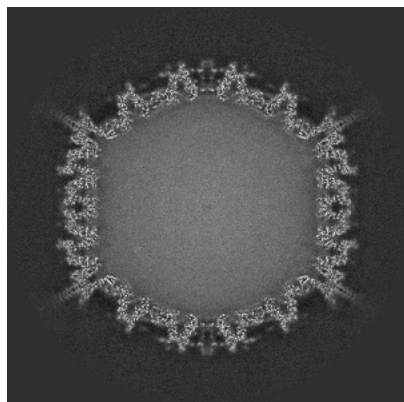


Y Index: 360

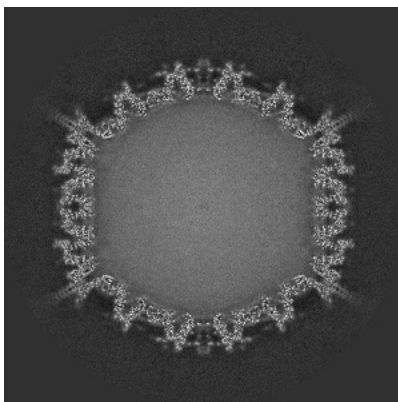


Z Index: 360

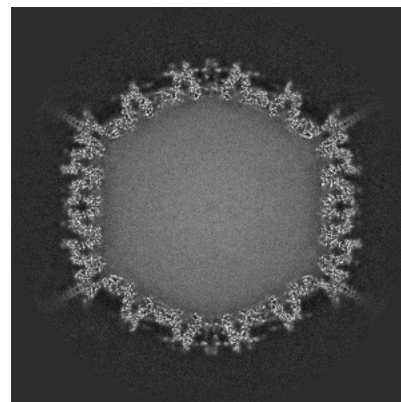
6.2.2 Raw map



X Index: 360



Y Index: 360

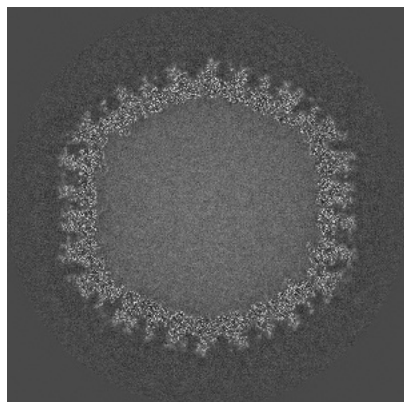


Z Index: 360

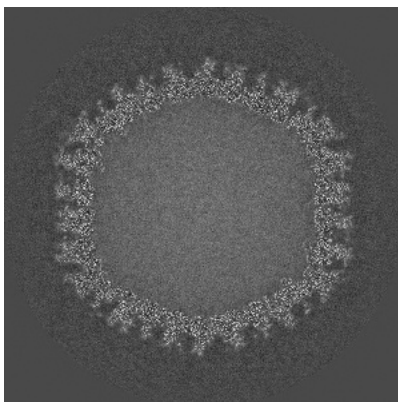
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

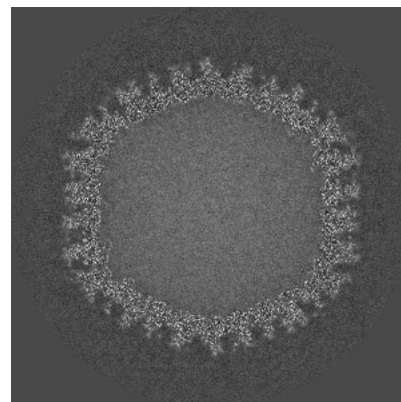
6.3.1 Primary map



X Index: 348

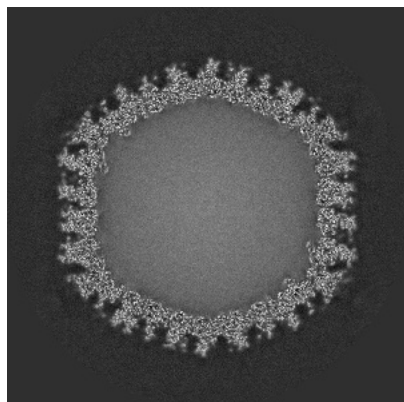


Y Index: 348

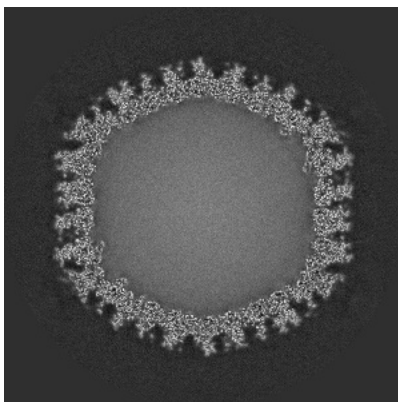


Z Index: 371

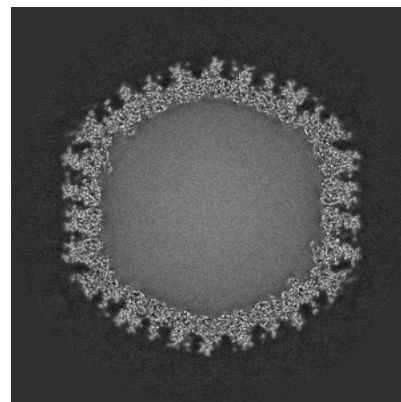
6.3.2 Raw map



X Index: 348



Y Index: 372

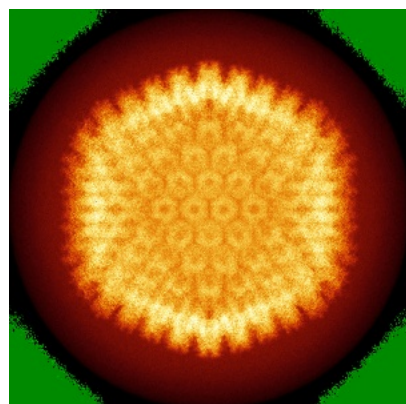


Z Index: 347

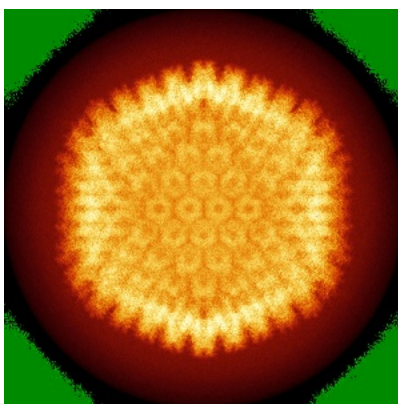
The images above show the largest variance slices of the map in three orthogonal directions.

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

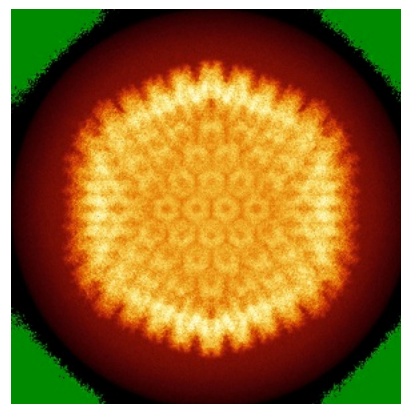
6.4.1 Primary map



X

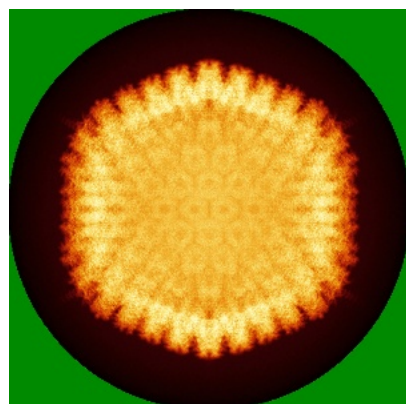


Y

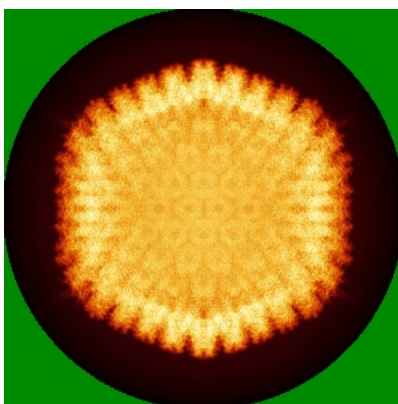


Z

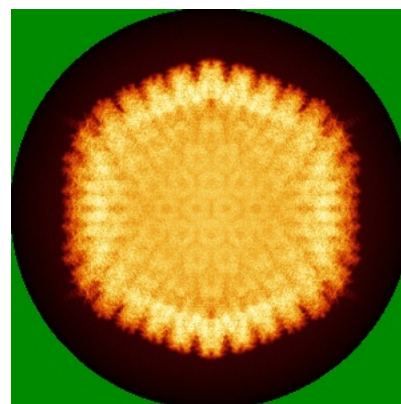
6.4.2 Raw map



X



Y

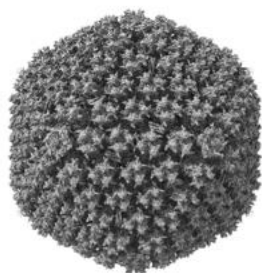


Z

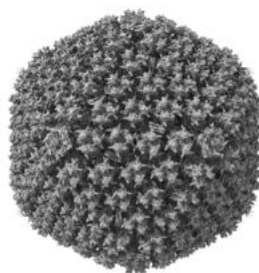
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

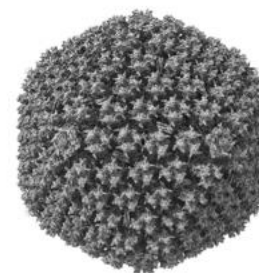
6.5.1 Primary map



X



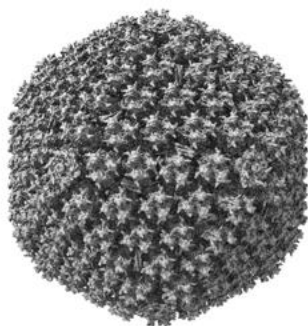
Y



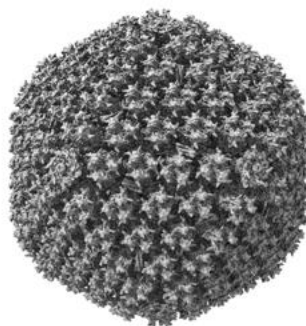
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0216. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

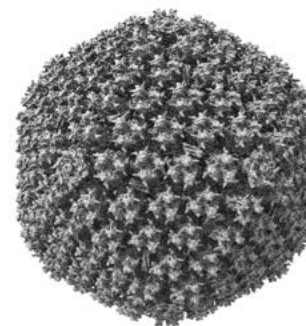
6.5.2 Raw map



X



Y



Z

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.

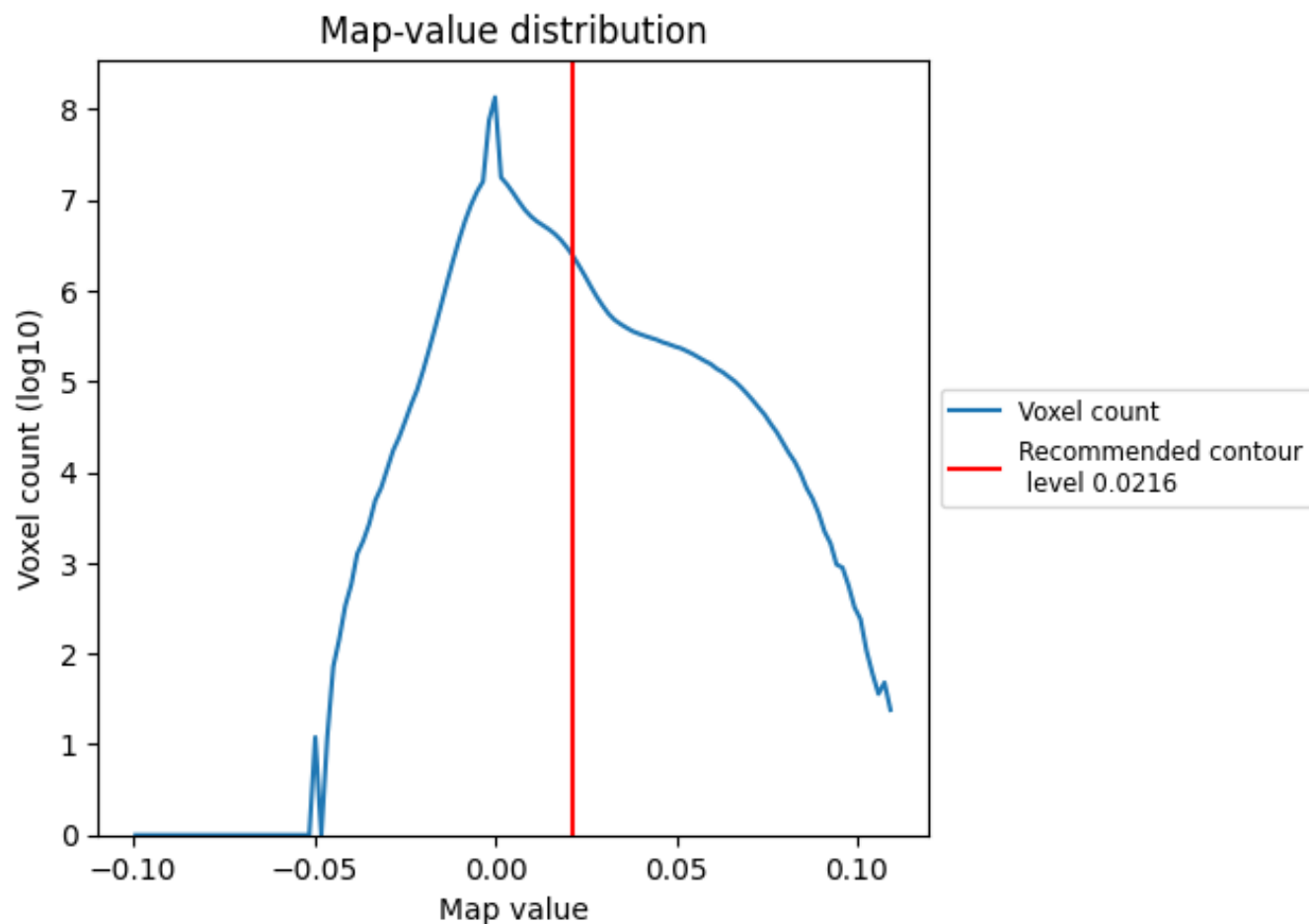
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

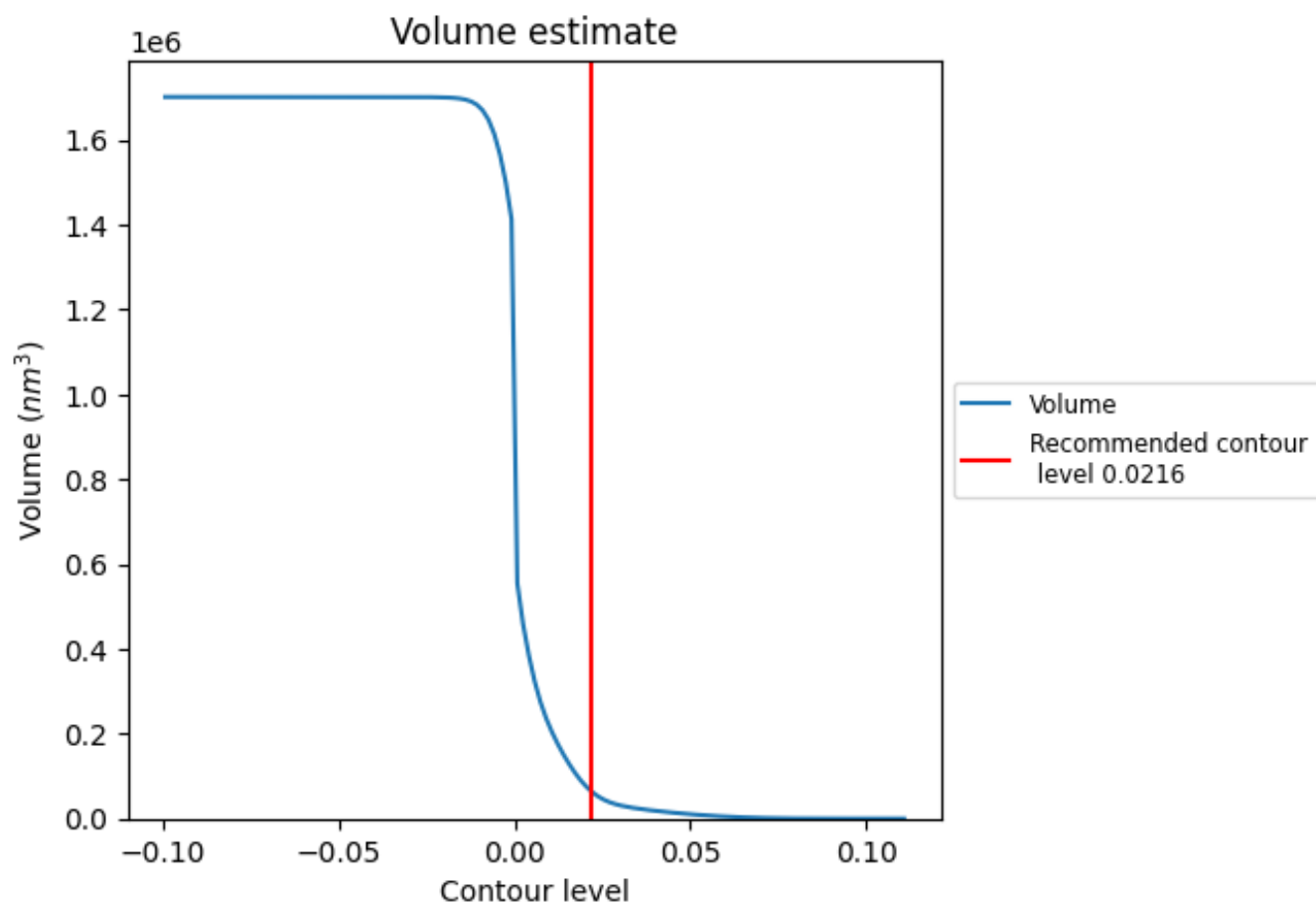
This section contains the results of statistical analysis of the map.

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.

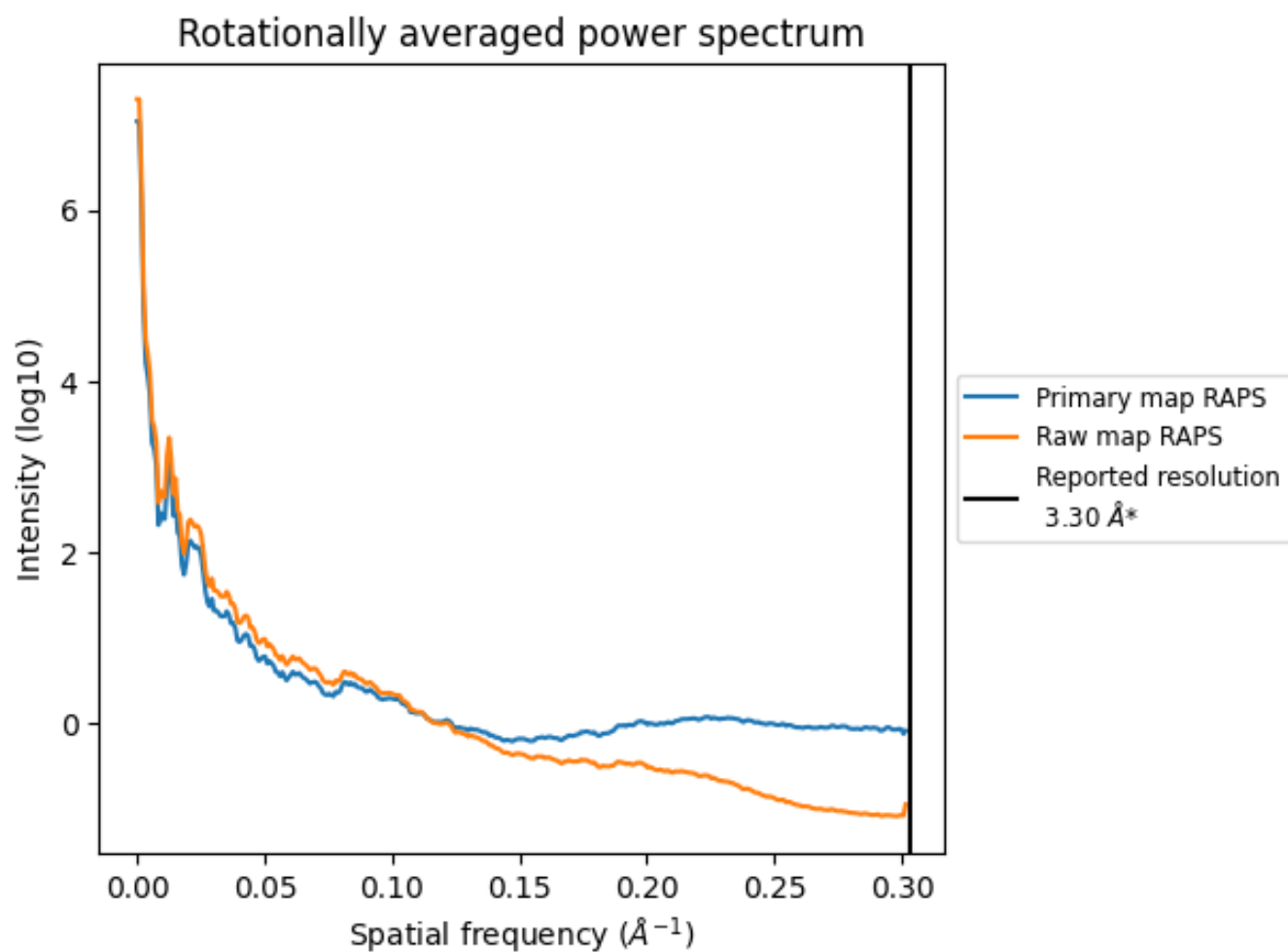
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66526 nm³; this corresponds to an approximate mass of 60095 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 ⓘ

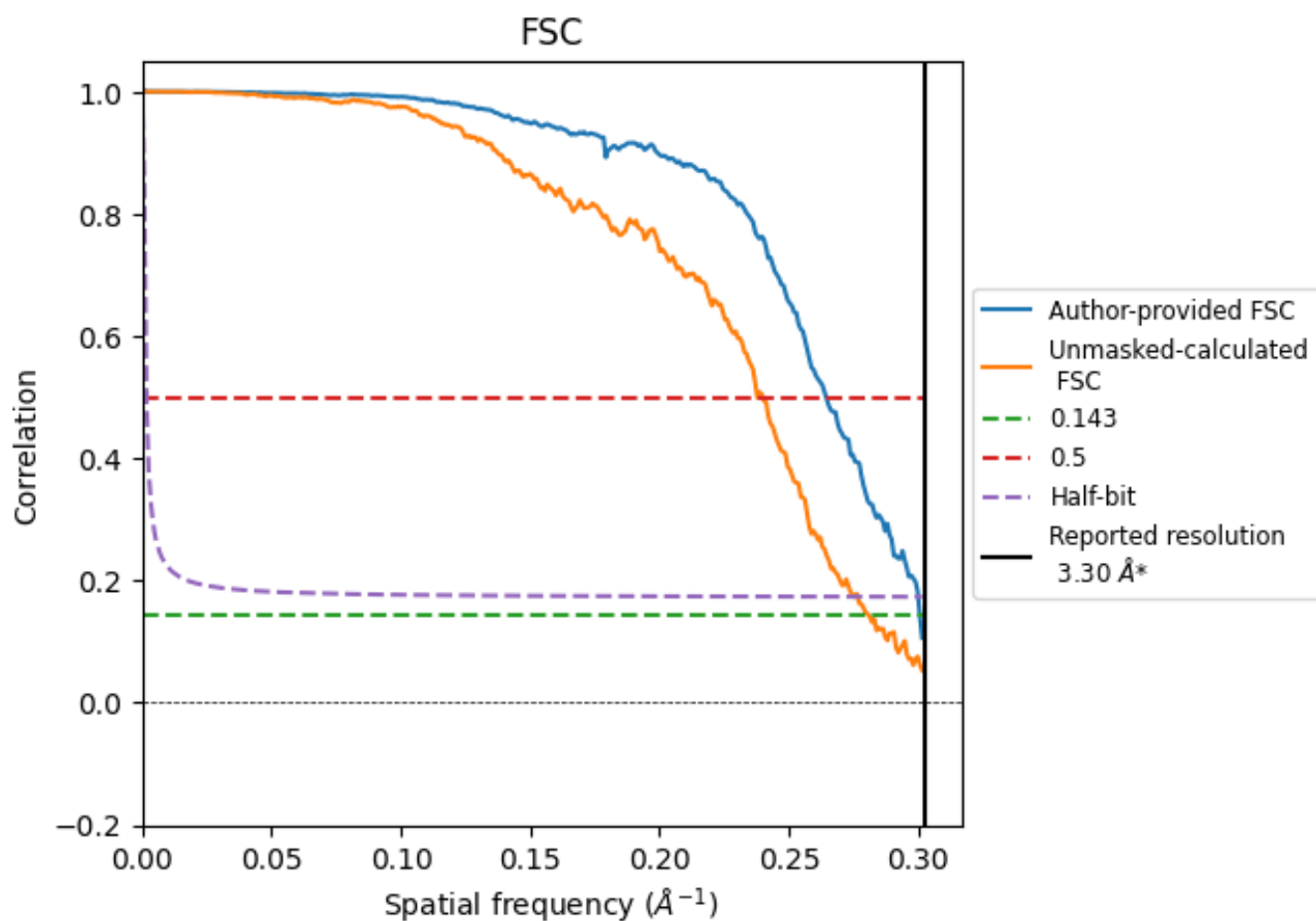


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.33	3.78	3.33
Unmasked-calculated*	3.56	4.20	3.63

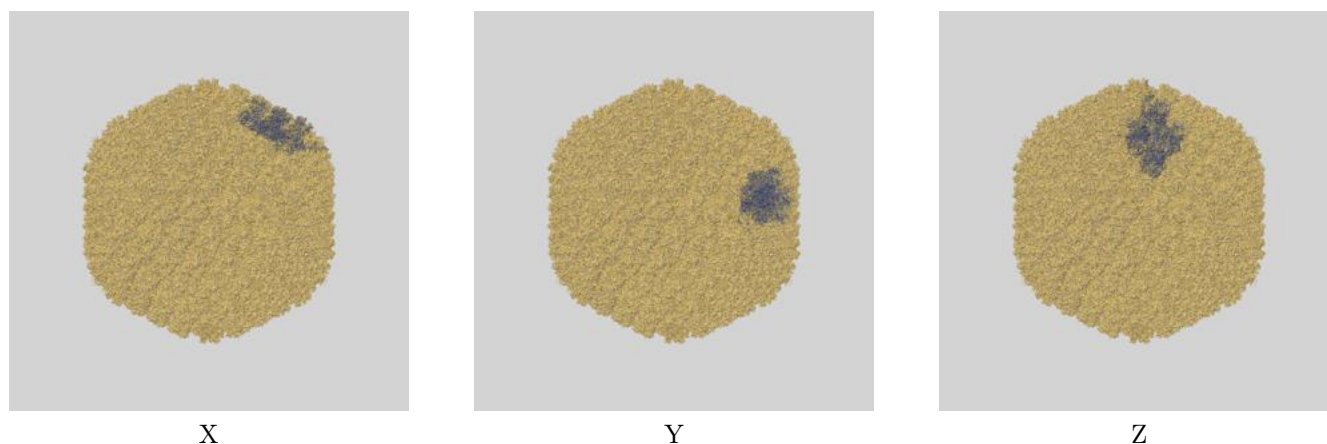
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

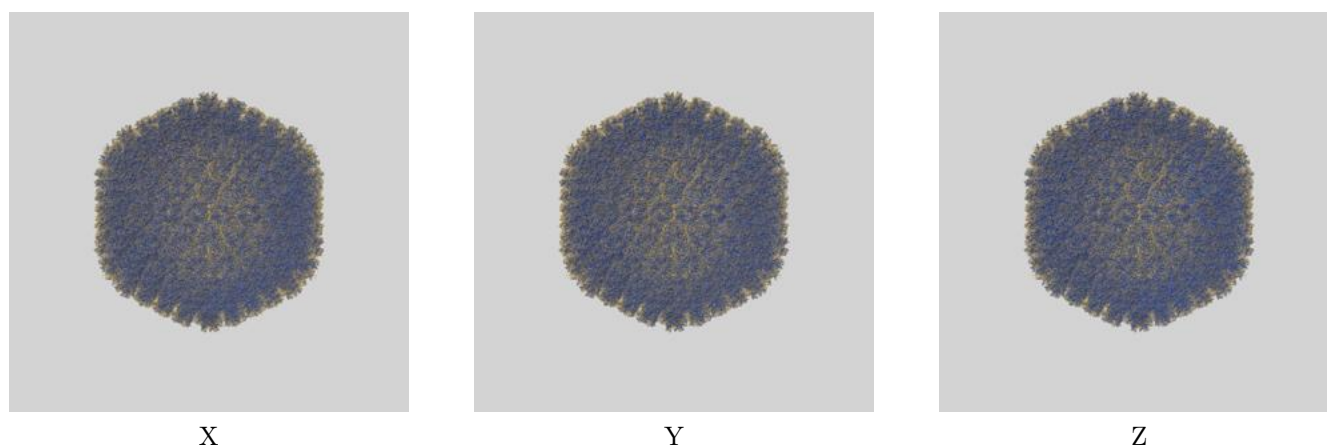
This section contains information regarding the fit between EMDB map EMD-53736 and PDB model 9R78. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

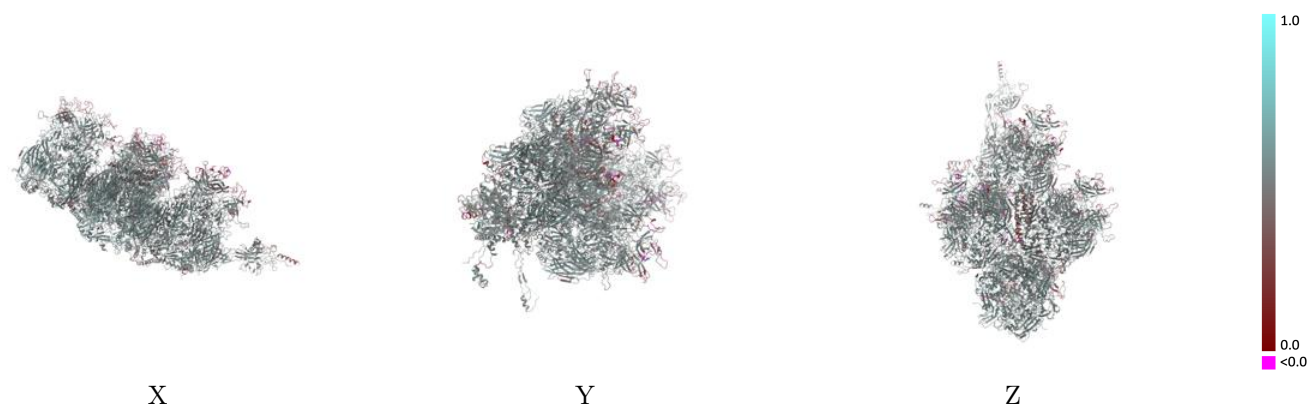


9.1.2 Map-model assembly overlay [i](#)



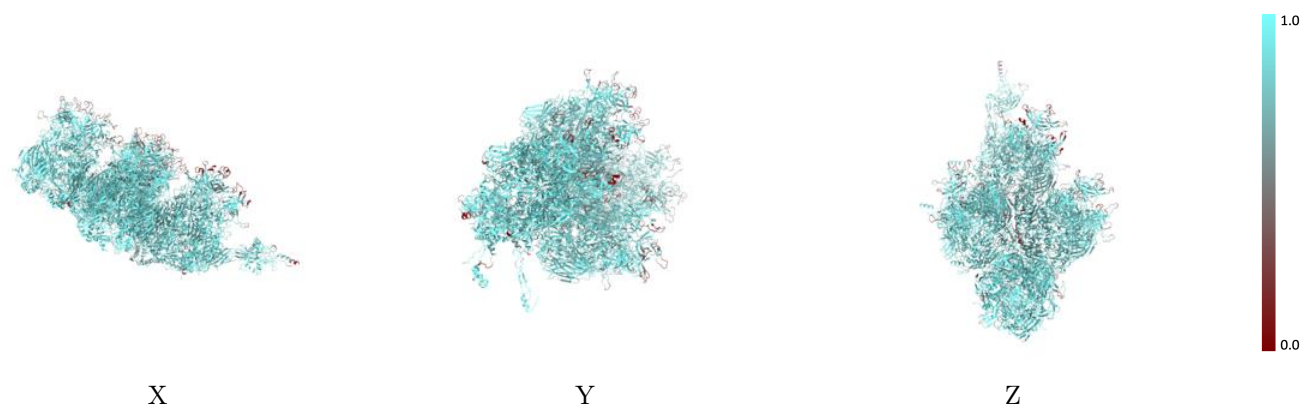
The images above show the 3D surface view of the map at the recommended contour level 0.0216 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



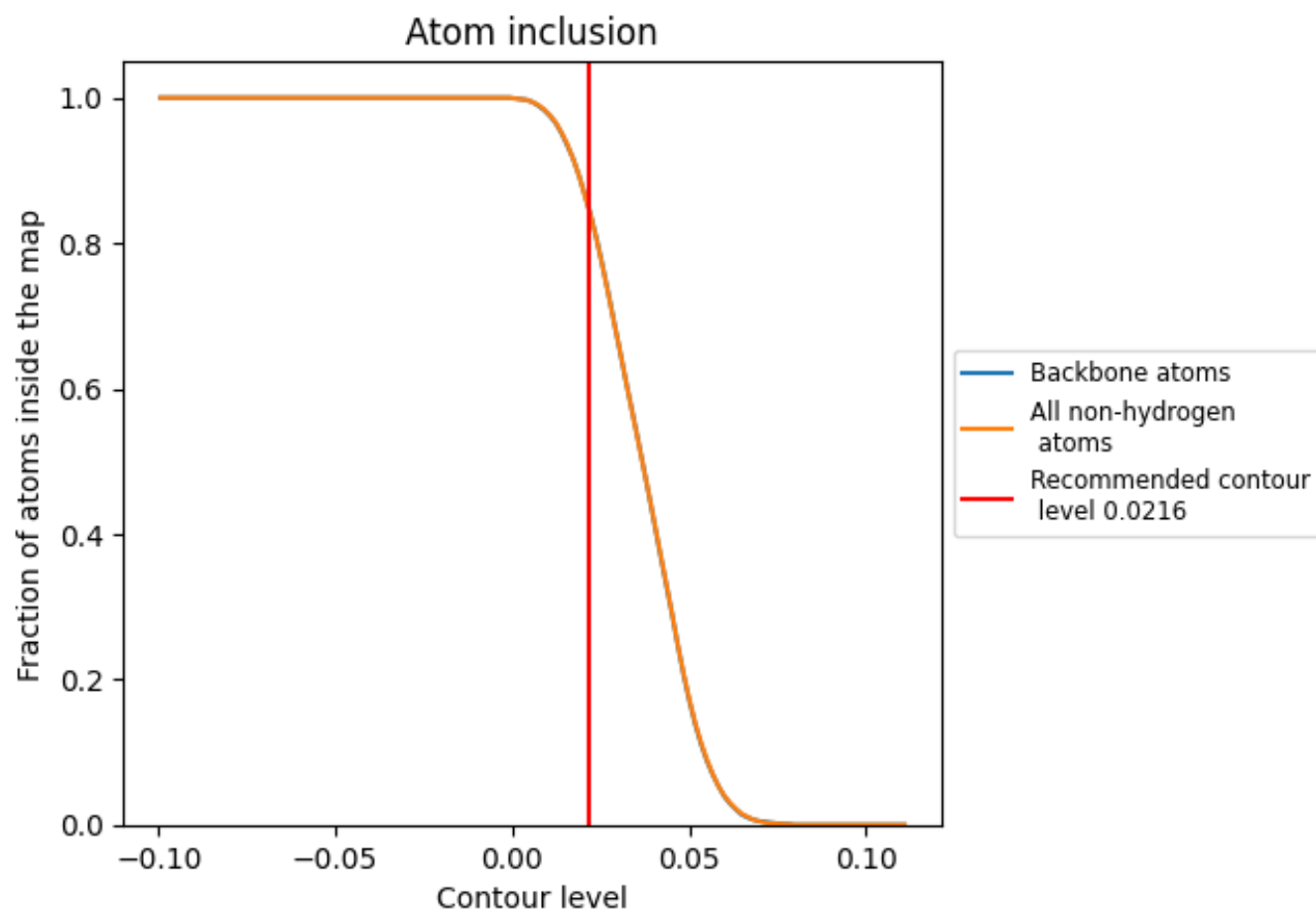
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0216).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.0216) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8480	 0.5020
1	 0.8200	 0.4290
2	 0.5540	 0.4150
3	 0.7120	 0.3890
4	 0.6820	 0.3790
5	 0.5890	 0.3710
6	 0.5770	 0.3260
7	 0.5970	 0.3490
8	 0.6220	 0.3830
A	 0.8600	 0.5100
B	 0.8450	 0.4910
C	 0.8450	 0.4920
D	 0.8810	 0.5240
E	 0.8630	 0.5010
F	 0.8680	 0.5070
G	 0.8690	 0.5070
H	 0.8820	 0.5290
I	 0.8610	 0.5050
J	 0.8700	 0.5180
K	 0.8610	 0.4990
L	 0.8600	 0.4990
M	 0.8080	 0.4860
N	 0.7300	 0.4460
O	 0.8910	 0.5260
P	 0.8900	 0.5220
Q	 0.5870	 0.3250
R	 0.7080	 0.4060
S	 0.7770	 0.4120
T	 0.4940	 0.2850

