



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:18 AM UTC

PDB ID : 9QZC / pdb_00009qzc
EMDB ID : EMD-53467
Title : Proximal A-C linker of Tetrahymena centriole, one repeating unit
Authors : Cai, B.; Xu, J.W.; Luo, L.; Aarts, E.; Leitner, A.; Ishikawa, T.; Beltro, P.;
Pilhofer, M.; Wieczorek, M.
Deposited on : 2025-04-22
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

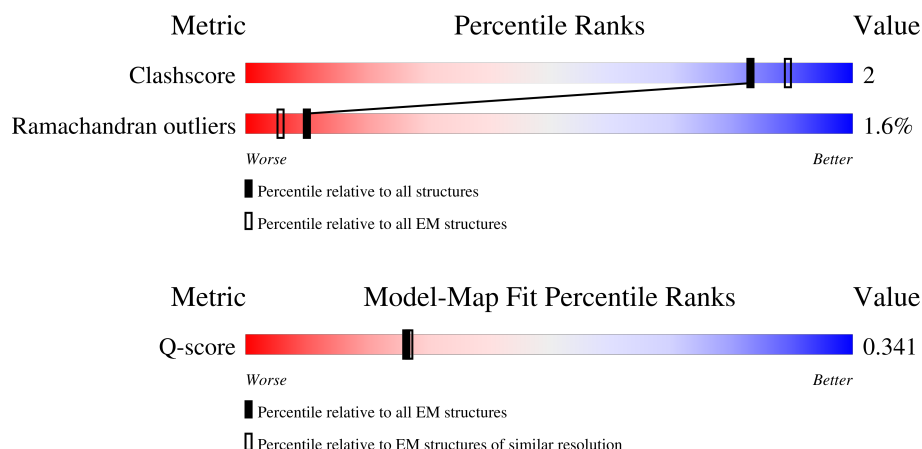
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	10198 (3.30 - 4.30)

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

Mol	Chain	Length	Quality of chain
1	i	452	85% 9% • 5%
2	q	380	68% 5% • 25%
2	y	380	6% 56% 10% • 32%
3	7	937	14% 73% 12% • 13%
4	AE	1202	36% 5% • 57%

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Mol	Chain	Length	Quality of chain
4	AU	1202	
5	AM	634	
6	Ac	32	
7	As	153	
8	A7	230	
8	Az	230	
9	Bw	151	
10	B4	164	
11	CA	167	
12	CH	161	
13	CO	105	
14	CV	127	
15	Cc	102	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 22355 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called WD repeat WRAP73-like protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	i	429	Total	C	N	O	0	0
			2129	1271	429	429		

- Molecule 2 is a protein called Centrosomal protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	q	284	Total	C	N	O	0	0
			1415	847	284	284		
2	y	258	Total	C	N	O	0	0
			1288	772	258	258		

- Molecule 3 is a protein called Rab-GAP TBC domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	7	813	Total	C	N	O	0	0
			4040	2414	813	813		

- Molecule 4 is a protein called TBC1 domain family member 31.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	AE	518	Total	C	N	O	0	0
			2584	1548	518	518		
4	AU	354	Total	C	N	O	0	0
			1752	1044	354	354		

- Molecule 5 is a protein called POC1 centriolar protein homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	AM	365	Total	C	N	O	0	0
			1806	1076	365	365		

- Molecule 6 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	Ac	32	Total	C	N	O	0	0
			160	96	32	32		

- Molecule 7 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	As	153	Total	C	N	O	0	0
			765	459	153	153		

- Molecule 8 is a protein called SWIM-type domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	Az	151	Total	C	N	O	0	0
			748	446	151	151		
8	A7	158	Total	C	N	O	0	0
			783	467	158	158		

- Molecule 9 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Bw	151	Total	C	N	O	0	0
			755	453	151	151		

- Molecule 10 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	B4	164	Total	C	N	O	0	0
			820	492	164	164		

- Molecule 11 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	CA	167	Total	C	N	O	0	0
			835	501	167	167		

- Molecule 12 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	CH	161	Total	C	N	O	0	0
			805	483	161	161		

- Molecule 13 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	CO	105	Total 525	C 315	N 105	O 105	0	0

- Molecule 14 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	CV	127	Total 635	C 381	N 127	O 127	0	0

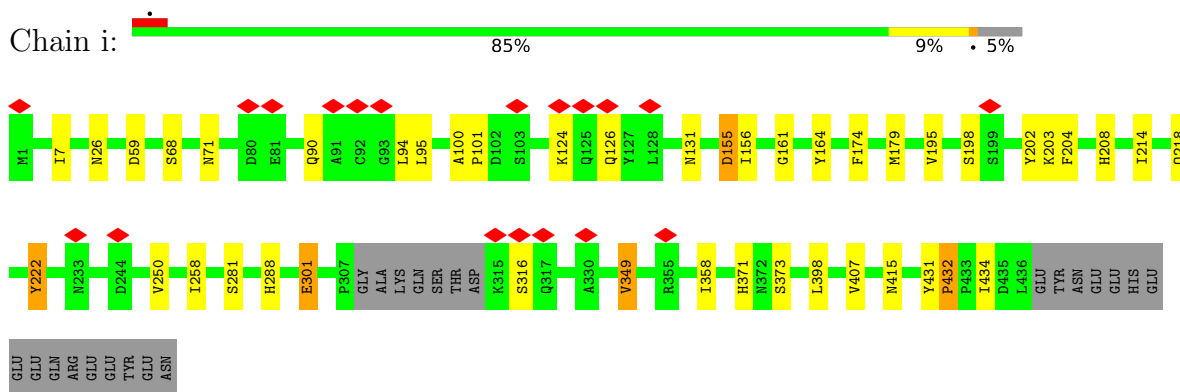
- Molecule 15 is a protein called Unknown Protein Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	Cc	102	Total 510	C 306	N 102	O 102	0	0

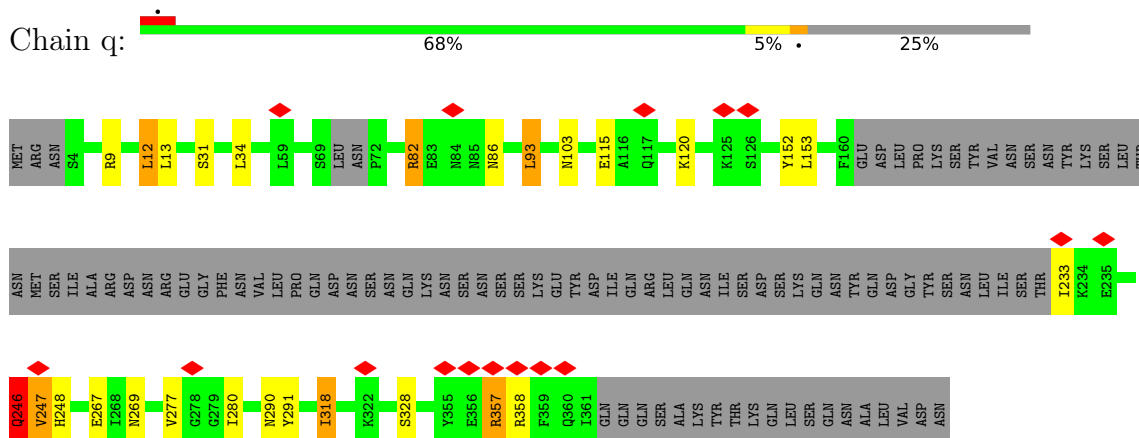
3 Residue-property plots [i](#)

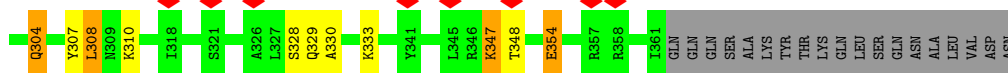
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: WD repeat WRAP73-like protein, putative

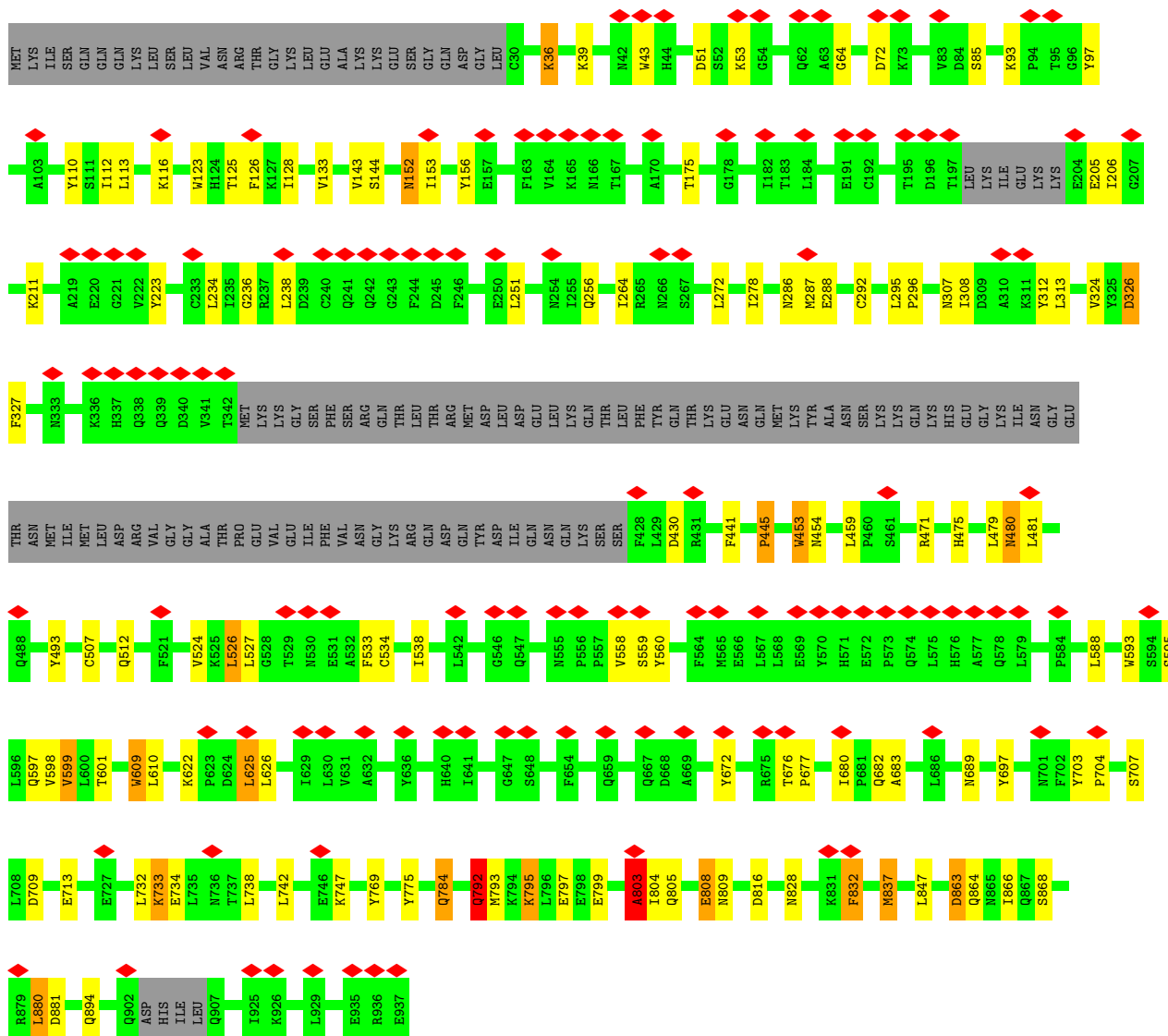


- Molecule 2: Centrosomal protein, putative

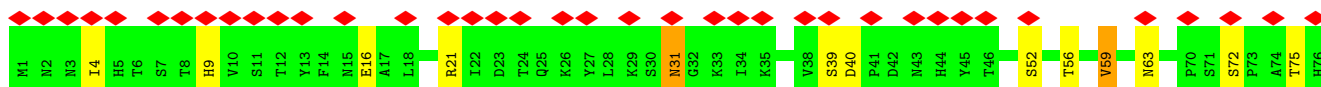




Chain 7: 14% 73% 12% 1%

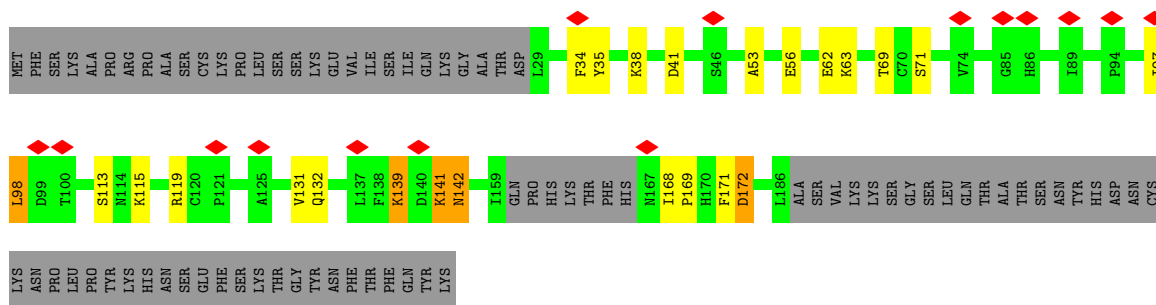


Chain AE:

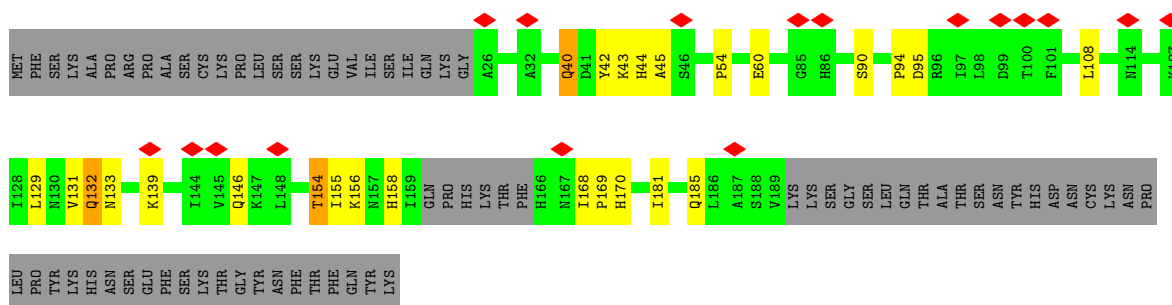


[illegible]

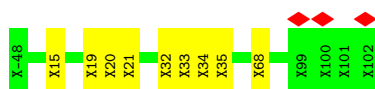
- Molecule 5: POC1 centriolar protein homolog



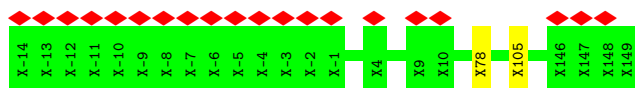
• Molecule 8: SWIM-type domain-containing protein



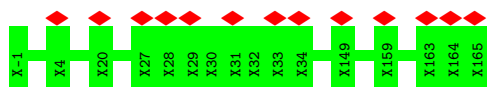
• Molecule 9: Unknown Protein Chain



• Molecule 10: Unknown Protein Chain



• Molecule 11: Unknown Protein Chain

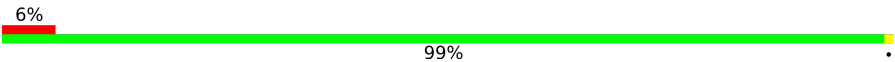


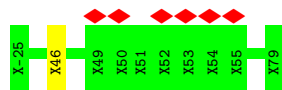
• Molecule 12: Unknown Protein Chain



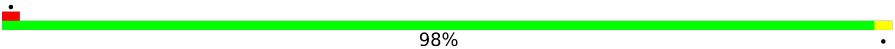
There are no outlier residues recorded for this chain.

• Molecule 13: Unknown Protein Chain

Chain CO:  6% 99% .

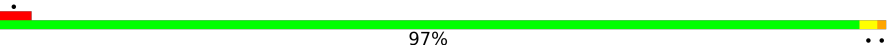


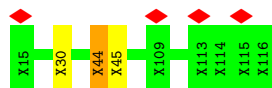
• Molecule 14: Unknown Protein Chain

Chain CV:  98% .



• Molecule 15: Unknown Protein Chain

Chain Cc:  97% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155485	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	13.599	Depositor
Minimum map value	0.000	Depositor
Average map value	0.223	Depositor
Map value standard deviation	1.035	Depositor
Recommended contour level	5	Depositor
Map size (Å)	631.2, 631.2, 631.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.315, 1.315, 1.315	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	i	1.59	4/2127 (0.2%)	1.88	38/2965 (1.3%)
2	q	1.30	0/1412	1.65	21/1969 (1.1%)
2	y	1.42	0/1285	2.07	44/1793 (2.5%)
3	7	1.34	6/4036 (0.1%)	1.84	112/5629 (2.0%)
4	AE	1.33	1/2582 (0.0%)	1.91	82/3608 (2.3%)
4	AU	1.38	9/1751 (0.5%)	1.99	70/2439 (2.9%)
5	AM	1.55	2/1803 (0.1%)	2.05	74/2508 (3.0%)
8	A7	1.49	1/781 (0.1%)	2.03	26/1086 (2.4%)
8	Az	1.35	0/746	2.02	25/1037 (2.4%)
All	All	1.41	23/16523 (0.1%)	1.92	492/23034 (2.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	i	0	6
2	q	0	7
2	y	0	11
3	7	0	18
4	AE	0	18
4	AU	0	9
5	AM	0	13
7	As	0	3
8	A7	0	5
8	Az	0	3
9	Bw	0	1
10	B4	0	3
13	CO	0	1
15	Cc	0	2
All	All	0	100

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	i	198	SER	CA-C	-6.23	1.45	1.52
4	AU	300	ILE	CA-C	-6.17	1.45	1.52
4	AU	181	ASN	CA-CB	-6.10	1.45	1.52
4	AU	301	VAL	CA-C	-5.87	1.45	1.52
4	AU	295	ASN	CA-C	-5.83	1.45	1.52
4	AU	88	ALA	CA-C	-5.75	1.45	1.52
3	7	598	VAL	CA-C	5.75	1.60	1.52
5	AM	192	SER	CA-CB	-5.70	1.44	1.53
3	7	272	LEU	CA-C	-5.61	1.45	1.52
3	7	234	LEU	CA-C	-5.58	1.46	1.52
3	7	113	LEU	CA-C	-5.37	1.46	1.52
4	AU	301	VAL	CA-CB	-5.34	1.47	1.54
1	i	195	VAL	CA-CB	-5.26	1.48	1.54
3	7	610	LEU	CA-C	-5.22	1.45	1.52
5	AM	149	SER	CA-CB	-5.21	1.46	1.52
8	A7	181	ILE	CA-C	-5.18	1.46	1.52
4	AU	181	ASN	N-CA	-5.16	1.40	1.46
1	i	204	PHE	CA-C	-5.15	1.46	1.52
4	AE	500	PHE	CA-C	-5.12	1.46	1.52
3	7	223	TYR	CA-C	-5.10	1.46	1.52
4	AU	155	TYR	CA-C	-5.09	1.46	1.52
4	AU	301	VAL	N-CA	-5.09	1.40	1.46
1	i	7	ILE	CA-C	-5.04	1.47	1.52

All (492) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	i	301	GLU	CA-C-O	-33.51	84.04	121.58
2	y	294	GLN	CA-C-N	19.38	146.80	120.44
2	y	294	GLN	C-N-CA	19.38	146.80	120.44
2	y	29	ILE	CA-C-N	18.04	153.47	122.26
2	y	29	ILE	C-N-CA	18.04	153.47	122.26
8	Az	35	TYR	CA-C-N	16.92	153.86	121.54
8	Az	35	TYR	C-N-CA	16.92	153.86	121.54
4	AE	641	PHE	N-CA-C	13.62	126.20	111.36
8	A7	131	VAL	N-CA-C	-12.82	99.45	113.43
3	7	559	SER	N-CA-C	12.59	128.65	113.28
4	AE	433	VAL	N-CA-C	11.98	121.86	111.56
3	7	238	LEU	N-CA-C	11.97	127.19	112.59
3	7	559	SER	CA-C-N	11.85	143.04	121.70
3	7	559	SER	C-N-CA	11.85	143.04	121.70
3	7	512	GLN	N-CA-C	11.54	127.70	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7	479	LEU	CA-C-N	11.16	141.78	121.70
3	7	479	LEU	C-N-CA	11.16	141.78	121.70
8	A7	90	SER	CA-C-N	11.10	141.69	121.70
8	A7	90	SER	C-N-CA	11.10	141.69	121.70
5	AM	58	LYS	N-CA-C	-11.06	99.82	113.97
8	Az	141	LYS	CA-C-N	10.96	141.43	121.70
8	Az	141	LYS	C-N-CA	10.96	141.43	121.70
1	i	431	TYR	CA-C-N	10.18	130.87	120.38
1	i	431	TYR	C-N-CA	10.18	130.87	120.38
4	AE	545	HIS	CA-C-N	9.98	130.66	120.38
4	AE	545	HIS	C-N-CA	9.98	130.66	120.38
4	AU	39	SER	N-CA-C	9.91	123.95	108.79
8	A7	154	THR	N-CA-C	-9.77	97.93	110.53
4	AU	321	ASN	N-CA-C	-9.61	97.09	110.35
3	7	112	ILE	N-CA-C	-9.56	104.62	113.71
5	AM	328	TYR	N-CA-C	9.47	122.21	108.86
8	A7	156	LYS	N-CA-C	-9.41	96.60	110.52
4	AU	329	ARG	N-CA-C	-9.25	102.50	113.88
2	y	354	GLU	CA-C-O	-9.18	112.37	122.01
2	q	115	GLU	N-CA-C	-9.16	100.23	111.40
4	AE	622	ILE	N-CA-C	-9.12	97.40	108.53
1	i	398	LEU	CA-C-N	9.03	128.88	120.21
1	i	398	LEU	C-N-CA	9.03	128.88	120.21
3	7	206	ILE	N-CA-C	-8.99	103.09	111.45
5	AM	328	TYR	CA-C-N	8.98	137.32	120.97
5	AM	328	TYR	C-N-CA	8.98	137.32	120.97
8	A7	154	THR	CA-C-O	-8.98	111.61	121.94
3	7	527	LEU	N-CA-C	-8.96	101.88	113.17
4	AE	519	GLN	CA-C-N	8.83	137.59	121.70
4	AE	519	GLN	C-N-CA	8.83	137.59	121.70
4	AE	641	PHE	CA-C-N	8.75	137.45	121.70
4	AE	641	PHE	C-N-CA	8.75	137.45	121.70
4	AE	622	ILE	CB-CA-C	8.67	123.57	110.91
4	AU	292	ASN	CA-C-N	8.61	129.46	119.47
4	AU	292	ASN	C-N-CA	8.61	129.46	119.47
3	7	558	VAL	N-CA-C	8.60	119.41	110.72
4	AE	646	ASN	CA-C-N	8.56	128.21	119.56
4	AE	646	ASN	C-N-CA	8.56	128.21	119.56
4	AE	762	LEU	N-CA-C	-8.54	102.05	111.36
4	AE	877	GLN	N-CA-C	-8.54	101.47	112.23
8	Az	113	SER	N-CA-C	-8.53	99.03	110.55
3	7	703	TYR	CA-C-N	8.52	130.49	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7	703	TYR	C-N-CA	8.52	130.49	119.84
2	q	269	ASN	CA-C-N	8.46	136.92	121.70
2	q	269	ASN	C-N-CA	8.46	136.92	121.70
3	7	205	GLU	N-CA-C	8.46	120.41	108.74
4	AU	298	ILE	N-CA-C	8.42	119.90	108.11
4	AU	158	THR	N-CA-C	8.38	119.30	108.24
3	7	175	THR	CA-C-N	8.37	128.10	119.56
3	7	175	THR	C-N-CA	8.37	128.10	119.56
4	AE	484	GLN	N-CA-C	-8.32	101.74	112.23
2	y	43	LEU	N-CA-C	-8.28	103.30	113.41
2	y	290	ASN	CA-C-N	8.22	136.50	121.70
2	y	290	ASN	C-N-CA	8.22	136.50	121.70
3	7	475	HIS	CA-C-N	8.18	127.90	119.56
3	7	475	HIS	C-N-CA	8.18	127.90	119.56
2	y	87	LEU	N-CA-C	-8.12	103.51	113.50
3	7	808	GLU	CA-C-O	-8.12	111.94	120.55
3	7	793	MET	N-CA-C	-8.07	102.06	112.23
2	q	103	ASN	N-CA-C	-8.05	102.58	111.36
1	i	349	VAL	CA-C-O	-8.04	112.15	120.27
2	y	54	ASN	N-CA-C	-8.04	102.37	112.90
2	y	295	ASN	N-CA-C	-8.04	102.46	111.14
4	AE	928	ARG	N-CA-C	-8.04	102.10	112.23
2	q	120	LYS	N-CA-C	-8.01	101.84	111.69
4	AE	728	GLN	CA-C-O	-8.01	111.93	120.42
2	y	266	GLY	N-CA-C	-7.97	101.91	113.86
4	AE	893	LYS	CA-C-O	-7.97	112.11	120.55
2	y	33	GLU	N-CA-C	-7.95	102.21	112.23
3	7	601	THR	N-CA-C	-7.93	104.08	114.31
4	AE	475	TYR	CA-C-N	7.87	129.24	120.66
4	AE	475	TYR	C-N-CA	7.87	129.24	120.66
2	q	269	ASN	N-CA-C	7.86	120.31	109.54
5	AM	522	PHE	CA-C-O	-7.86	112.57	120.82
4	AU	4	ILE	N-CA-C	7.86	119.60	108.36
3	7	454	ASN	N-CA-C	-7.81	102.38	112.23
3	7	264	ILE	N-CA-C	7.80	119.03	108.11
4	AE	767	LYS	N-CA-C	-7.78	102.80	111.28
3	7	512	GLN	CA-C-N	7.76	135.67	121.70
3	7	512	GLN	C-N-CA	7.76	135.67	121.70
4	AU	308	PHE	CA-C-N	7.75	135.66	121.70
4	AU	308	PHE	C-N-CA	7.75	135.66	121.70
4	AE	876	GLN	CA-C-O	-7.75	112.21	120.42
4	AE	432	LYS	CA-C-N	-7.72	115.28	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AE	432	LYS	C-N-CA	-7.72	115.28	123.08
4	AE	562	ASP	CA-C-N	7.72	127.44	119.56
4	AE	562	ASP	C-N-CA	7.72	127.44	119.56
3	7	441	PHE	N-CA-C	-7.72	102.80	111.14
5	AM	553	TYR	N-CA-C	-7.72	103.47	113.12
2	q	318	ILE	CA-C-O	-7.70	111.85	120.32
5	AM	542	GLN	N-CA-C	-7.70	103.89	113.28
2	y	347	LYS	N-CA-C	-7.68	102.84	112.90
8	Az	139	LYS	CA-C-N	-7.67	110.18	122.53
8	Az	139	LYS	C-N-CA	-7.67	110.18	122.53
4	AE	783	ILE	N-CA-C	-7.66	101.55	112.35
3	7	868	SER	N-CA-C	-7.66	99.70	110.50
2	q	12	LEU	CA-C-O	-7.65	112.44	120.55
5	AM	274	GLN	N-CA-C	-7.61	102.99	111.28
4	AU	253	ASN	CA-C-O	-7.59	112.84	122.63
4	AE	857	ARG	CA-C-O	-7.51	111.61	120.10
3	7	453	TRP	CA-C-O	-7.51	111.34	119.97
3	7	622	LYS	CA-C-N	7.50	128.18	119.47
3	7	622	LYS	C-N-CA	7.50	128.18	119.47
5	AM	250	PHE	N-CA-C	-7.49	103.94	113.23
5	AM	329	PHE	N-CA-C	7.48	120.40	110.53
3	7	524	VAL	N-CA-C	-7.47	103.00	110.62
4	AE	462	LYS	CA-C-N	-7.47	109.69	120.97
4	AE	462	LYS	C-N-CA	-7.47	109.69	120.97
3	7	85	SER	N-CA-C	7.45	120.61	110.55
5	AM	70	ILE	N-CA-C	7.45	119.48	108.45
4	AU	236	ALA	CA-C-O	-7.45	112.93	121.72
8	Az	171	PHE	CA-C-N	7.41	135.04	121.70
8	Az	171	PHE	C-N-CA	7.41	135.04	121.70
3	7	36	LYS	CA-C-O	-7.40	112.70	120.55
4	AE	503	SER	CA-C-O	-7.40	112.80	121.16
5	AM	77	LYS	CA-C-N	7.39	129.08	119.84
5	AM	77	LYS	C-N-CA	7.39	129.08	119.84
4	AE	492	CYS	CA-C-O	-7.38	112.73	120.55
4	AU	142	SER	N-CA-C	7.38	121.70	111.74
1	i	288	HIS	N-CA-C	7.32	115.78	108.75
3	7	445	PRO	CA-C-O	-7.32	113.05	122.12
4	AU	72	SER	CA-C-N	7.31	127.47	120.31
4	AU	72	SER	C-N-CA	7.31	127.47	120.31
2	y	348	THR	N-CA-C	-7.30	103.34	112.90
1	i	100	ALA	CA-C-N	7.30	128.96	119.84
1	i	100	ALA	C-N-CA	7.30	128.96	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	y	83	GLU	N-CA-C	-7.29	103.34	111.28
4	AU	283	ASN	CA-C-N	7.26	134.77	121.70
4	AU	283	ASN	C-N-CA	7.26	134.77	121.70
4	AE	919	THR	CA-C-O	-7.25	112.86	120.55
2	q	86	ASN	N-CA-C	-7.21	102.43	112.45
3	7	251	LEU	CA-C-N	7.17	127.12	120.03
3	7	251	LEU	C-N-CA	7.17	127.12	120.03
5	AM	76	PHE	CA-C-O	-7.16	112.94	120.89
2	y	89	SER	N-CA-C	-7.16	103.56	111.36
4	AE	920	GLU	N-CA-C	-7.15	103.57	111.36
2	q	357	ARG	CA-C-O	-7.13	111.76	122.38
4	AE	546	PRO	CA-C-N	7.09	128.70	119.84
4	AE	546	PRO	C-N-CA	7.09	128.70	119.84
3	7	803	ALA	N-CA-C	-7.06	104.27	113.17
5	AM	98	SER	CA-C-N	7.06	126.74	119.82
5	AM	98	SER	C-N-CA	7.06	126.74	119.82
5	AM	333	GLY	CA-C-N	7.04	131.01	120.31
5	AM	333	GLY	C-N-CA	7.04	131.01	120.31
1	i	155	ASP	CA-C-O	-7.03	113.38	121.54
3	7	881	ASP	N-CA-C	-7.00	102.72	112.45
8	A7	54	PRO	N-CA-C	-6.99	100.23	111.14
1	i	349	VAL	O-C-N	-6.99	115.91	123.18
3	7	864	GLN	N-CA-C	-6.97	104.90	113.41
5	AM	204	PHE	N-CA-C	-6.97	105.40	114.04
2	y	53	LYS	CA-C-O	-6.96	113.17	120.55
4	AE	576	PHE	N-CA-C	-6.96	101.36	110.33
3	7	238	LEU	CA-C-N	6.95	134.22	121.70
3	7	238	LEU	C-N-CA	6.95	134.22	121.70
4	AU	40	ASP	CA-C-N	6.94	126.64	119.56
4	AU	40	ASP	C-N-CA	6.94	126.64	119.56
3	7	792	GLN	CA-C-O	-6.87	112.07	119.97
8	Az	71	SER	N-CA-C	-6.80	103.95	111.36
4	AE	463	GLY	N-CA-C	6.79	120.66	110.75
3	7	453	TRP	CA-C-N	-6.76	109.19	120.68
3	7	453	TRP	C-N-CA	-6.76	109.19	120.68
4	AU	175	GLY	N-CA-C	-6.75	106.01	115.32
4	AE	782	LYS	CA-C-O	-6.71	111.65	119.24
4	AU	351	PHE	N-CA-C	6.69	119.37	108.26
4	AU	213	ILE	N-CA-C	6.65	117.47	108.17
3	7	312	TYR	N-CA-C	6.63	119.75	109.07
5	AM	39	LEU	N-CA-C	-6.63	100.22	110.10
5	AM	81	ARG	CA-C-N	6.63	126.54	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AM	81	ARG	C-N-CA	6.63	126.54	119.85
4	AE	585	SER	N-CA-C	-6.59	105.05	113.23
2	q	82	ARG	CA-C-O	-6.58	111.97	120.00
5	AM	533	THR	CA-C-N	-6.56	110.81	122.42
5	AM	533	THR	C-N-CA	-6.56	110.81	122.42
1	i	415	ASN	N-CA-C	-6.55	96.96	108.23
4	AE	483	TYR	CA-C-O	-6.55	114.16	120.90
8	Az	56	GLU	N-CA-C	6.55	120.53	112.54
1	i	214	ILE	N-CA-C	-6.53	105.46	111.67
5	AM	190	SER	N-CA-C	6.53	118.99	109.07
8	Az	172	ASP	CA-C-N	6.51	131.29	120.62
8	Az	172	ASP	C-N-CA	6.51	131.29	120.62
4	AU	261	ASN	N-CA-C	-6.50	104.92	112.92
1	i	126	GLN	N-CA-C	6.48	119.69	109.39
2	y	239	GLN	CA-C-O	-6.48	112.78	120.10
3	7	236	GLY	N-CA-C	-6.47	101.31	112.06
4	AU	293	PRO	N-CA-C	6.47	123.20	113.81
4	AU	121	ASN	CA-C-N	6.46	126.59	119.87
4	AU	121	ASN	C-N-CA	6.46	126.59	119.87
8	A7	108	LEU	CB-CA-C	-6.46	102.09	111.91
5	AM	278	ILE	N-CA-C	6.43	118.41	108.44
5	AM	68	ASP	N-CA-C	6.43	118.13	107.20
8	A7	155	ILE	N-CA-C	6.42	118.64	108.87
4	AE	927	MET	CA-C-O	-6.40	111.51	119.38
2	q	13	LEU	N-CA-C	-6.39	104.18	112.23
4	AE	858	MET	N-CA-C	-6.37	104.20	112.23
5	AM	120	VAL	N-CA-C	6.36	117.98	108.96
2	y	91	ILE	N-CA-C	-6.35	104.31	110.72
5	AM	306	GLN	N-CA-C	-6.35	100.44	109.96
2	q	34	LEU	N-CA-C	-6.34	104.29	111.14
8	Az	53	ALA	CA-C-N	6.34	126.30	120.03
8	Az	53	ALA	C-N-CA	6.34	126.30	120.03
3	7	112	ILE	CB-CA-C	-6.33	104.68	110.63
4	AU	320	MET	N-CA-C	-6.33	97.32	110.80
3	7	507	CYS	CA-C-N	6.32	127.74	119.84
3	7	507	CYS	C-N-CA	6.32	127.74	119.84
4	AU	31	ASN	CA-C-O	-6.32	115.11	122.37
4	AU	162	THR	CA-C-N	6.30	127.71	119.84
4	AU	162	THR	C-N-CA	6.30	127.71	119.84
4	AU	274	ILE	N-CA-C	6.29	117.85	108.23
1	i	218	GLN	CA-C-N	6.28	126.47	120.31
1	i	218	GLN	C-N-CA	6.28	126.47	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AU	212	VAL	N-CA-C	6.28	117.81	108.46
3	7	809	ASN	N-CA-C	-6.27	104.68	112.90
3	7	805	GLN	N-CA-C	-6.26	104.90	112.54
4	AE	519	GLN	N-CA-C	6.26	121.08	113.38
2	y	73	LEU	N-CA-C	-6.25	104.71	112.90
2	y	258	LYS	N-CA-C	-6.25	104.47	111.28
4	AU	75	THR	N-CA-C	-6.25	103.77	112.45
4	AE	609	ASP	N-CA-C	-6.23	103.08	111.87
5	AM	144	GLY	N-CA-C	-6.23	105.08	113.24
4	AU	59	VAL	CA-C-O	-6.22	113.87	120.53
5	AM	182	SER	CA-C-N	6.22	126.13	119.85
5	AM	182	SER	C-N-CA	6.22	126.13	119.85
3	7	697	TYR	CA-C-N	6.17	126.14	120.03
3	7	697	TYR	C-N-CA	6.17	126.14	120.03
2	y	25	GLN	CA-C-N	6.17	126.08	119.85
2	y	25	GLN	C-N-CA	6.17	126.08	119.85
4	AU	134	GLN	N-CA-C	6.17	118.55	109.24
4	AU	303	GLY	N-CA-C	-6.17	107.24	115.32
3	7	152	ASN	CA-C-N	6.16	128.90	120.46
3	7	152	ASN	C-N-CA	6.16	128.90	120.46
3	7	880	LEU	CA-C-O	-6.16	113.89	120.42
2	q	246	GLN	CA-C-N	6.14	132.76	121.70
2	q	246	GLN	C-N-CA	6.14	132.76	121.70
3	7	133	VAL	N-CA-C	6.14	116.96	108.12
3	7	64	GLY	N-CA-C	-6.14	106.85	115.32
5	AM	47	GLU	N-CA-C	6.13	117.96	111.28
3	7	327	PHE	N-CA-C	-6.11	103.95	112.45
4	AU	124	THR	CA-C-O	-6.10	112.19	118.90
5	AM	510	VAL	N-CA-C	-6.08	105.13	111.58
8	Az	168	ILE	CB-CA-C	-6.07	105.31	111.08
3	7	53	LYS	N-CA-C	-6.07	105.37	112.89
4	AE	496	PHE	N-CA-C	-6.05	104.01	111.40
5	AM	55	PHE	N-CA-C	6.05	118.61	109.23
4	AE	894	GLN	N-CA-C	-6.05	104.61	112.23
3	7	51	ASP	N-CA-C	6.04	118.71	110.55
8	Az	119	ARG	N-CA-C	-6.03	105.47	114.64
1	i	371	HIS	N-CA-C	-6.02	101.56	110.48
8	Az	34	PHE	N-CA-C	-6.02	104.83	111.82
4	AU	325	ARG	N-CA-C	-6.02	104.28	111.69
4	AE	456	PHE	N-CA-C	-6.01	104.80	111.36
1	i	208	HIS	N-CA-C	-5.99	102.50	109.93
3	7	680	ILE	N-CA-C	5.99	115.12	108.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	y	240	LEU	N-CA-C	-5.99	104.13	112.45
3	7	598	VAL	N-CA-C	5.98	121.78	109.34
2	y	38	LEU	N-CA-C	-5.98	105.07	112.90
3	7	863	ASP	CA-C-O	-5.96	113.37	120.10
4	AE	782	LYS	CA-C-N	-5.95	111.59	120.82
4	AE	782	LYS	C-N-CA	-5.95	111.59	120.82
3	7	707	SER	N-CA-C	5.95	119.95	109.96
8	A7	94	PRO	CA-C-N	5.95	132.90	121.54
8	A7	94	PRO	C-N-CA	5.95	132.90	121.54
3	7	256	GLN	N-CA-C	-5.92	106.70	114.04
8	Az	115	LYS	N-CA-C	-5.91	107.88	114.62
3	7	480	ASN	N-CA-CB	5.91	120.55	110.50
5	AM	202	LEU	N-CA-C	5.91	119.74	112.54
8	A7	90	SER	N-CA-C	5.91	123.38	110.80
3	7	837	MET	O-C-N	-5.90	118.10	123.41
4	AU	286	ILE	CB-CA-C	-5.90	102.04	110.83
4	AE	597	TRP	N-CA-C	-5.88	105.77	113.17
2	y	304	GLN	N-CA-C	-5.87	104.97	111.36
3	7	689	ASN	N-CA-C	-5.86	104.33	112.30
5	AM	90	GLY	N-CA-C	-5.86	104.12	112.55
4	AU	186	GLU	CA-C-N	-5.84	115.07	122.37
4	AU	186	GLU	C-N-CA	-5.84	115.07	122.37
8	A7	158	HIS	N-CA-C	-5.83	101.65	110.28
8	Az	131	VAL	N-CA-C	-5.83	102.02	109.30
3	7	43	TRP	N-CA-C	5.80	117.34	108.12
3	7	610	LEU	N-CA-C	-5.80	105.70	112.89
4	AE	621	PHE	CA-C-N	5.79	131.39	123.46
4	AE	621	PHE	C-N-CA	5.79	131.39	123.46
1	i	26	ASN	N-CA-C	-5.78	101.17	110.14
3	7	93	LYS	CA-C-N	5.77	125.44	119.56
3	7	93	LYS	C-N-CA	5.77	125.44	119.56
4	AU	252	GLY	CA-C-N	-5.77	113.52	122.05
4	AU	252	GLY	C-N-CA	-5.77	113.52	122.05
2	y	272	LYS	CA-C-N	5.76	129.06	120.31
2	y	272	LYS	C-N-CA	5.76	129.06	120.31
2	y	86	ASN	CA-C-O	-5.75	113.85	120.24
8	A7	168	ILE	CA-C-N	5.75	125.71	119.78
8	A7	168	ILE	C-N-CA	5.75	125.71	119.78
3	7	795	LYS	N-CA-C	-5.75	105.16	111.82
4	AU	52	SER	N-CA-C	-5.74	103.78	112.04
8	A7	132	GLN	CA-C-O	-5.74	112.30	120.51
4	AU	194	GLU	CA-C-N	-5.74	113.98	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AU	194	GLU	C-N-CA	-5.74	113.98	122.41
3	7	481	LEU	N-CA-C	5.71	117.50	111.28
3	7	97	TYR	N-CA-C	-5.71	103.36	111.24
3	7	769	TYR	CB-CA-C	-5.71	100.97	110.68
5	AM	558	GLU	N-CA-C	-5.71	105.96	114.64
5	AM	281	HIS	CA-C-N	5.71	126.09	119.47
5	AM	281	HIS	C-N-CA	5.71	126.09	119.47
2	y	333	LYS	N-CA-C	-5.70	105.14	111.36
4	AE	664	THR	CA-C-N	5.70	125.65	119.78
4	AE	664	THR	C-N-CA	5.70	125.65	119.78
2	y	265	ASP	CA-C-O	-5.70	113.42	119.97
3	7	526	LEU	O-C-N	-5.70	115.50	122.11
2	y	291	TYR	N-CA-C	5.68	126.89	111.00
8	A7	60	GLU	N-CA-C	5.68	118.92	110.52
3	7	125	THR	N-CA-C	-5.66	100.74	109.52
5	AM	48	ASP	CA-C-O	-5.66	112.41	120.51
4	AE	623	ILE	CA-C-N	5.66	128.13	120.38
4	AE	623	ILE	C-N-CA	5.66	128.13	120.38
1	i	179	MET	N-CA-C	-5.64	104.60	112.45
3	7	313	LEU	CA-C-N	-5.64	115.75	123.14
3	7	313	LEU	C-N-CA	-5.64	115.75	123.14
4	AU	40	ASP	N-CA-C	5.64	119.45	109.58
4	AU	209	SER	N-CA-C	-5.64	106.24	113.23
5	AM	534	GLU	N-CA-C	-5.63	107.06	114.04
4	AE	888	ARG	N-CA-C	-5.61	105.16	111.28
4	AE	493	LEU	N-CA-C	-5.61	105.16	112.23
5	AM	126	ILE	N-CA-C	5.60	116.80	108.23
4	AE	765	GLN	CA-C-O	-5.60	111.94	119.11
1	i	250	VAL	N-CA-C	5.58	115.93	108.11
2	q	267	GLU	N-CA-C	-5.57	107.02	113.88
2	y	310	LYS	N-CA-C	-5.57	105.84	113.30
1	i	258	ILE	N-CA-C	-5.54	105.70	111.58
3	7	832	PHE	N-CA-C	-5.54	105.32	111.36
3	7	894	GLN	N-CA-C	-5.54	105.32	111.36
4	AU	163	PRO	N-CA-C	5.54	123.88	112.47
1	i	281	SER	N-CA-C	5.53	115.41	108.45
4	AE	442	ILE	N-CA-C	-5.52	106.81	111.56
5	AM	174	ASN	N-CA-C	5.52	121.89	113.61
4	AE	546	PRO	N-CA-C	5.52	117.43	110.70
2	y	56	ASN	N-CA-C	-5.51	105.42	111.82
1	i	95	LEU	N-CA-C	-5.51	105.28	112.23
2	q	358	ARG	N-CA-C	5.50	120.68	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	q	277	VAL	N-CA-C	5.50	116.56	111.45
1	i	202	TYR	CA-C-N	-5.50	114.04	122.62
1	i	202	TYR	C-N-CA	-5.50	114.04	122.62
4	AU	16	GLU	N-CA-C	5.50	117.98	111.33
1	i	203	LYS	N-CA-C	5.49	118.18	109.50
8	Az	142	ASN	N-CA-CB	5.48	119.82	110.50
3	7	588	LEU	N-CA-C	-5.48	104.95	111.69
3	7	538	ILE	CA-C-N	-5.48	112.94	120.28
3	7	538	ILE	C-N-CA	-5.48	112.94	120.28
3	7	296	PRO	N-CA-C	-5.47	101.92	110.50
5	AM	259	ILE	N-CA-C	5.46	115.97	107.99
3	7	713	GLU	N-CA-C	-5.46	105.33	111.28
3	7	733	LYS	N-CA-C	-5.46	107.19	112.97
4	AE	611	PRO	N-CA-C	5.46	123.71	112.47
5	AM	513	ASN	N-CA-C	5.46	118.77	111.24
4	AE	588	PHE	N-CA-C	5.46	119.68	113.19
4	AE	641	PHE	CA-C-O	-5.46	114.64	120.42
3	7	609	TRP	CA-C-O	-5.45	111.97	119.05
4	AE	787	THR	N-CA-C	-5.44	105.35	111.28
3	7	672	TYR	N-CA-C	-5.44	105.77	112.90
8	Az	38	LYS	N-CA-C	-5.44	105.74	112.38
5	AM	38	ALA	CA-C-N	-5.44	113.15	120.82
5	AM	38	ALA	C-N-CA	-5.44	113.15	120.82
1	i	358	ILE	N-CA-C	5.43	115.67	107.80
5	AM	38	ALA	N-CA-C	5.42	118.72	111.24
2	q	328	SER	N-CA-C	-5.41	107.33	114.31
4	AE	597	TRP	CA-C-O	-5.40	113.03	119.35
5	AM	114	ARG	CA-C-N	-5.39	115.16	123.14
5	AM	114	ARG	C-N-CA	-5.39	115.16	123.14
5	AM	545	SER	N-CA-C	-5.39	105.40	111.28
3	7	493	TYR	N-CA-C	-5.39	105.57	111.82
4	AE	506	PHE	N-CA-C	-5.38	106.84	113.41
5	AM	151	ASP	N-CA-C	5.38	122.25	110.80
3	7	144	SER	N-CA-C	-5.37	102.25	110.14
4	AE	926	GLN	N-CA-C	-5.37	105.99	112.54
4	AE	503	SER	O-C-N	-5.37	116.40	123.16
8	A7	185	GLN	CA-C-N	-5.37	112.15	120.31
8	A7	185	GLN	C-N-CA	-5.37	112.15	120.31
3	7	866	ILE	N-CA-C	-5.36	105.16	111.00
4	AE	465	TYR	CA-C-N	5.34	126.52	119.84
4	AE	465	TYR	C-N-CA	5.34	126.52	119.84
4	AU	319	GLU	CA-C-N	5.34	131.74	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AU	319	GLU	C-N-CA	5.34	131.74	121.54
3	7	459	LEU	CA-C-N	5.34	125.03	119.64
3	7	459	LEU	C-N-CA	5.34	125.03	119.64
8	Az	169	PRO	N-CA-C	-5.33	102.83	111.14
4	AU	102	GLY	N-CA-C	-5.32	105.65	114.48
2	y	14	LEU	CA-C-N	5.31	127.39	120.28
2	y	14	LEU	C-N-CA	5.31	127.39	120.28
2	q	9	ARG	N-CA-C	-5.30	105.50	111.28
1	i	174	PHE	N-CA-C	5.29	118.06	108.69
4	AU	141	GLN	CA-C-N	5.29	129.65	122.19
4	AU	141	GLN	C-N-CA	5.29	129.65	122.19
5	AM	285	TYR	CA-C-N	-5.29	114.60	122.74
5	AM	285	TYR	C-N-CA	-5.29	114.60	122.74
2	y	86	ASN	N-CA-C	-5.29	105.19	111.69
4	AE	622	ILE	CA-C-O	-5.29	115.89	121.44
3	7	816	ASP	N-CA-C	-5.28	105.60	111.36
1	i	131	ASN	CA-C-N	5.28	125.20	119.76
1	i	131	ASN	C-N-CA	5.28	125.20	119.76
4	AU	289	PHE	N-CA-C	5.28	117.09	109.07
2	y	308	LEU	CA-C-N	5.26	131.17	121.70
2	y	308	LEU	C-N-CA	5.26	131.17	121.70
4	AE	756	TYR	CA-C-O	-5.25	113.41	119.56
1	i	90	GLN	N-CA-C	5.25	119.69	113.28
4	AU	59	VAL	O-C-N	-5.25	116.96	123.10
5	AM	126	ILE	CB-CA-C	-5.25	104.61	110.96
4	AE	435	PRO	N-CA-C	-5.24	102.97	111.19
4	AU	290	ASP	CB-CA-C	-5.24	102.71	110.62
4	AE	584	LEU	CA-C-O	-5.23	113.65	119.40
3	7	211	LYS	N-CA-C	-5.22	105.19	112.45
5	AM	187	LEU	N-CA-C	5.22	118.46	110.20
4	AE	729	ILE	N-CA-C	-5.22	105.62	110.53
3	7	677	PRO	N-CA-C	-5.21	105.46	110.47
5	AM	180	VAL	N-CA-C	5.21	115.36	107.75
5	AM	345	PHE	CA-C-O	-5.21	112.99	119.18
5	AM	325	SER	CA-C-N	-5.20	113.79	122.62
5	AM	325	SER	C-N-CA	-5.20	113.79	122.62
3	7	128	ILE	N-CA-C	-5.19	102.04	108.89
5	AM	239	HIS	N-CA-C	-5.19	102.63	109.84
8	A7	129	LEU	N-CA-C	5.18	117.01	111.36
1	i	164	TYR	N-CA-C	-5.18	100.72	108.96
5	AM	521	ASN	CA-C-N	5.16	127.15	120.44
5	AM	521	ASN	C-N-CA	5.16	127.15	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7	797	GLU	N-CA-C	-5.16	105.66	111.28
3	7	676	THR	CA-C-N	5.15	123.42	119.66
3	7	676	THR	C-N-CA	5.15	123.42	119.66
8	A7	146	GLN	CA-C-N	-5.15	112.98	120.29
8	A7	146	GLN	C-N-CA	-5.15	112.98	120.29
3	7	479	LEU	N-CA-C	5.15	119.64	112.90
3	7	324	VAL	N-CA-CB	-5.14	104.98	111.41
4	AE	504	ASP	N-CA-C	-5.14	106.16	112.90
2	y	265	ASP	O-C-N	-5.14	115.95	122.27
2	y	307	TYR	N-CA-C	5.14	119.26	112.89
3	7	625	LEU	CA-C-N	-5.14	112.38	120.60
3	7	625	LEU	C-N-CA	-5.14	112.38	120.60
4	AU	56	THR	CA-C-N	-5.13	115.95	122.37
4	AU	56	THR	C-N-CA	-5.13	115.95	122.37
3	7	153	ILE	CB-CA-C	-5.13	105.21	112.14
5	AM	506	GLN	CA-C-N	5.12	124.78	119.56
5	AM	506	GLN	C-N-CA	5.12	124.78	119.56
5	AM	534	GLU	CA-C-N	-5.12	113.43	120.28
5	AM	534	GLU	C-N-CA	-5.12	113.43	120.28
4	AU	63	ASN	CA-C-N	5.11	131.41	122.82
4	AU	63	ASN	C-N-CA	5.11	131.41	122.82
3	7	775	TYR	N-CA-C	-5.11	105.71	111.28
1	i	71	ASN	CA-C-N	-5.10	114.88	122.74
1	i	71	ASN	C-N-CA	-5.10	114.88	122.74
8	A7	132	GLN	N-CA-C	-5.10	99.93	110.80
3	7	110	TYR	N-CA-CB	-5.10	102.25	110.71
3	7	143	VAL	N-CA-C	5.10	115.19	107.80
4	AU	21	ARG	CA-C-N	-5.10	116.01	122.43
4	AU	21	ARG	C-N-CA	-5.10	116.01	122.43
1	i	161	GLY	N-CA-C	-5.09	103.64	111.64
5	AM	252	HIS	N-CA-CB	-5.09	102.44	110.49
2	y	82	ARG	N-CA-C	-5.08	105.83	112.23
4	AU	181	ASN	N-CA-C	-5.08	99.05	107.99
8	A7	133	ASN	CA-C-N	5.07	127.97	120.82
8	A7	133	ASN	C-N-CA	5.07	127.97	120.82
1	i	288	HIS	CA-C-O	5.07	121.53	118.33
4	AE	611	PRO	CA-C-N	5.07	130.83	121.70
4	AE	611	PRO	C-N-CA	5.07	130.83	121.70
2	q	93	LEU	CA-C-O	-5.07	112.46	119.05
5	AM	125	SER	CA-C-N	5.06	128.70	122.37
5	AM	125	SER	C-N-CA	5.06	128.70	122.37
4	AE	608	ASN	O-C-N	-5.06	115.23	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AM	294	SER	CA-C-O	-5.05	113.31	119.32
4	AU	295	ASN	N-CA-C	-5.05	106.27	114.09
1	i	222	TYR	CA-C-O	-5.03	113.49	121.94
8	A7	139	LYS	N-CA-C	-5.03	106.92	113.16
2	y	249	THR	N-CA-C	-5.02	105.88	111.36
4	AU	337	TYR	CA-C-O	-5.02	113.39	119.27
8	Az	97	ILE	N-CA-C	-5.02	105.53	111.00
4	AE	741	GLU	N-CA-C	-5.01	105.89	111.36
4	AU	153	ALA	CA-C-N	-5.01	113.75	120.82
4	AU	153	ALA	C-N-CA	-5.01	113.75	120.82
3	7	326	ASP	CA-C-O	-5.01	115.05	120.81
4	AU	328	GLU	N-CA-C	-5.01	107.11	113.18
8	Az	98	LEU	CA-C-O	-5.01	112.69	119.11
5	AM	324	GLN	CA-C-N	5.00	131.10	121.54
5	AM	324	GLN	C-N-CA	5.00	131.10	121.54

There are no chirality outliers.

All (100) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	7	326	ASP	Mainchain
3	7	36	LYS	Mainchain
3	7	445	PRO	Mainchain
3	7	453	TRP	Mainchain
3	7	471	ARG	Mainchain
3	7	526	LEU	Mainchain
3	7	609	TRP	Mainchain
3	7	733	LYS	Mainchain
3	7	784	GLN	Peptide,Mainchain
3	7	792	GLN	Mainchain
3	7	803	ALA	Mainchain
3	7	808	GLU	Mainchain
3	7	837	MET	Peptide,Mainchain
3	7	847	LEU	Mainchain
3	7	863	ASP	Mainchain
3	7	880	LEU	Mainchain
8	A7	132	GLN	Peptide,Mainchain
8	A7	154	THR	Peptide,Mainchain
8	A7	40	GLN	Mainchain
4	AE	475	TYR	Mainchain
4	AE	483	TYR	Mainchain
4	AE	492	CYS	Mainchain

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Mol	Chain	Res	Type	Group
4	AE	503	SER	Mainchain
4	AE	584	LEU	Mainchain
4	AE	597	TRP	Mainchain
4	AE	608	ASN	Mainchain
4	AE	649	SER	Peptide,Mainchain
4	AE	728	GLN	Mainchain
4	AE	756	TYR	Mainchain
4	AE	765	GLN	Mainchain
4	AE	782	LYS	Mainchain
4	AE	857	ARG	Mainchain
4	AE	876	GLN	Mainchain
4	AE	893	LYS	Mainchain
4	AE	919	THR	Mainchain
4	AE	927	MET	Mainchain
5	AM	294	SER	Mainchain
5	AM	304	GLY	Mainchain
5	AM	325	SER	Peptide,Mainchain
5	AM	345	PHE	Mainchain
5	AM	48	ASP	Peptide,Mainchain
5	AM	522	PHE	Mainchain
5	AM	533	THR	Mainchain
5	AM	541	GLN	Mainchain
5	AM	557	LEU	Mainchain
5	AM	76	PHE	Peptide,Mainchain
4	AU	124	THR	Mainchain
4	AU	236	ALA	Mainchain
4	AU	253	ASN	Mainchain
4	AU	283	ASN	Peptide,Mainchain
4	AU	31	ASN	Peptide,Mainchain
4	AU	337	TYR	Mainchain
4	AU	59	VAL	Mainchain
7	As	11	UNK	Mainchain
7	As	62	UNK	Mainchain
7	As	84	UNK	Mainchain
8	Az	132	GLN	Mainchain
8	Az	139	LYS	Mainchain
8	Az	98	LEU	Mainchain
10	B4	105	UNK	Mainchain
10	B4	78	UNK	Peptide,Mainchain
9	Bw	68	UNK	Mainchain
13	CO	46	UNK	Mainchain
15	Cc	30	UNK	Mainchain

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Mol	Chain	Res	Type	Group
15	Cc	44	UNK	Mainchain
1	i	155	ASP	Mainchain
1	i	222	TYR	Mainchain
1	i	301	GLU	Mainchain
1	i	349	VAL	Peptide,Mainchain
1	i	94	LEU	Mainchain
2	q	12	LEU	Mainchain
2	q	233	ILE	Peptide,Mainchain
2	q	318	ILE	Mainchain
2	q	357	ARG	Mainchain
2	q	82	ARG	Mainchain
2	q	93	LEU	Mainchain
2	y	239	GLN	Mainchain
2	y	265	ASP	Mainchain
2	y	32	ALA	Mainchain
2	y	329	GLN	Mainchain
2	y	347	LYS	Mainchain
2	y	354	GLU	Mainchain
2	y	37	LYS	Mainchain
2	y	44	LYS	Peptide,Mainchain
2	y	53	LYS	Mainchain
2	y	86	ASN	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	i	2129	0	926	1	0
2	q	1415	0	597	4	0
2	y	1288	0	542	5	0
3	7	4040	0	1741	15	0
4	AE	2584	0	1093	11	0
4	AU	1752	0	772	5	0
5	AM	1806	0	792	17	0
6	Ac	160	0	35	0	0
7	As	765	0	158	3	0
8	A7	783	0	350	3	0
8	Az	748	0	330	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	Bw	755	0	158	5	0
10	B4	820	0	167	0	0
11	CA	835	0	169	0	0
12	CH	805	0	165	0	0
13	CO	525	0	107	0	0
14	CV	635	0	129	1	0
15	Cc	510	0	104	1	0
All	All	22355	0	8335	72	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 2.

All (72) 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:q:152:TYR:O	2:q:153:LEU:C	2.41	0.60
7:As:72:UNK:O	7:As:73:UNK:C	2.49	0.58
7:As:5:UNK:HA	7:As:6:UNK:C	2.36	0.56
4:AU:230:LEU:N	4:AU:351:PHE:O	2.40	0.55
5:AM:553:TYR:O	5:AM:557:LEU:N	2.40	0.55
2:y:84:ASN:O	2:y:88:GLN:N	2.38	0.54
4:AU:153:ALA:O	4:AU:154:SER:C	2.46	0.54
5:AM:544:TYR:O	5:AM:545:SER:C	2.51	0.54
3:7:682:GLN:O	3:7:683:ALA:C	2.51	0.53
3:7:287:MET:O	3:7:288:GLU:C	2.53	0.51
4:AE:466:PRO:O	4:AE:705:GLU:N	2.44	0.51
5:AM:553:TYR:O	5:AM:554:MET:C	2.53	0.50
3:7:792:GLN:O	3:7:795:LYS:N	2.44	0.49
2:y:328:SER:C	2:y:330:ALA:H	2.19	0.49
5:AM:524:PRO:O	5:AM:525:LYS:CB	2.61	0.49
2:y:304:GLN:O	2:y:308:LEU:N	2.41	0.48
3:7:799:GLU:O	3:7:803:ALA:N	2.47	0.48
4:AE:927:MET:O	4:AE:930:ILE:N	2.46	0.48
2:y:328:SER:C	2:y:330:ALA:N	2.71	0.48
4:AE:575:LYS:C	4:AE:576:PHE:O	2.53	0.48
5:AM:517:THR:O	5:AM:518:TYR:C	2.56	0.47
9:Bw:15:UNK:O	9:Bw:19:UNK:N	2.47	0.47
3:7:595:SER:O	3:7:599:VAL:HA	2.15	0.46
5:AM:280:ILE:O	5:AM:281:HIS:C	2.56	0.46
15:Cc:44:UNK:O	15:Cc:45:UNK:C	2.62	0.46
5:AM:342:LYS:O	5:AM:343:THR:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:246:GLN:HA	2:q:248:HIS:N	2.30	0.46
5:AM:231:ASP:O	5:AM:232:THR:C	2.59	0.46
8:A7:42:TYR:O	8:A7:43:LYS:C	2.58	0.45
4:AU:285:GLY:O	4:AU:303:GLY:N	2.48	0.45
3:7:795:LYS:O	3:7:799:GLU:N	2.50	0.45
3:7:828:ASN:O	3:7:832:PHE:N	2.44	0.44
4:AU:320:MET:C	4:AU:321:ASN:O	2.56	0.44
5:AM:45:GLY:O	5:AM:46:HIS:C	2.57	0.44
5:AM:320:VAL:O	5:AM:321:GLN:C	2.59	0.44
9:Bw:20:UNK:O	9:Bw:21:UNK:C	2.65	0.44
9:Bw:34:UNK:O	9:Bw:35:UNK:C	2.61	0.44
9:Bw:33:UNK:CB	9:Bw:34:UNK:HA	2.48	0.43
14:CV:-7:UNK:O	14:CV:-6:UNK:C	2.65	0.43
4:AE:523:LEU:O	4:AE:524:ALA:C	2.58	0.43
4:AE:773:LYS:O	4:AE:774:GLN:C	2.60	0.43
4:AE:728:GLN:O	4:AE:731:SER:N	2.52	0.43
4:AE:610:THR:C	4:AE:612:GLU:HA	2.43	0.43
5:AM:534:GLU:O	5:AM:535:ALA:C	2.60	0.43
4:AE:626:LYS:O	4:AE:627:HIS:C	2.60	0.43
3:7:738:LEU:O	3:7:742:LEU:N	2.52	0.42
5:AM:163:LYS:O	5:AM:164:LYS:C	2.62	0.42
1:i:432:PRO:O	1:i:434:ILE:N	2.52	0.42
4:AE:786:LEU:O	4:AE:787:THR:C	2.60	0.42
9:Bw:32:UNK:O	9:Bw:33:UNK:C	2.68	0.42
3:7:533:PHE:O	3:7:534:CYS:C	2.61	0.42
3:7:593:TRP:O	3:7:597:GLN:N	2.53	0.42
8:A7:169:PRO:O	8:A7:170:HIS:C	2.62	0.42
5:AM:138:SER:O	5:AM:147:LEU:N	2.53	0.42
4:AU:9:HIS:CB	4:AU:279:ARG:H	2.33	0.41
3:7:278:ILE:O	3:7:292:CYS:HA	2.20	0.41
2:q:246:GLN:HA	2:q:247:VAL:C	2.45	0.41
5:AM:69:SER:HA	5:AM:88:HIS:O	2.20	0.41
7:As:11:UNK:O	7:As:14:UNK:N	2.54	0.41
2:y:286:VAL:O	2:y:287:GLN:C	2.63	0.41
4:AE:706:THR:O	4:AE:707:GLU:C	2.63	0.41
3:7:625:LEU:O	3:7:626:LEU:C	2.62	0.41
3:7:732:LEU:C	3:7:734:GLU:H	2.28	0.41
4:AE:876:GLN:O	4:AE:879:ARG:N	2.54	0.41
5:AM:243:THR:O	5:AM:244:CYS:C	2.64	0.41
8:A7:44:HIS:O	8:A7:45:ALA:C	2.63	0.41
2:q:290:ASN:O	2:q:291:TYR:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:152:ASN:O	3:7:156:TYR:N	2.53	0.41
5:AM:536:ILE:O	5:AM:537:ALA:C	2.61	0.40
8:Az:62:GLU:O	8:Az:63:LYS:C	2.62	0.40
3:7:307:ASN:O	3:7:308:ILE:C	2.61	0.40
5:AM:553:TYR:O	5:AM:556:ASN:N	2.52	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	i	425/452 (94%)	371 (87%)	45 (11%)	9 (2%)	5	31
2	q	278/380 (73%)	266 (96%)	8 (3%)	4 (1%)	9	37
2	y	252/380 (66%)	244 (97%)	6 (2%)	2 (1%)	16	48
3	7	805/937 (86%)	761 (94%)	28 (4%)	16 (2%)	6	32
4	AE	514/1202 (43%)	479 (93%)	27 (5%)	8 (2%)	7	35
4	AU	352/1202 (29%)	334 (95%)	15 (4%)	3 (1%)	14	45
5	AM	359/634 (57%)	319 (89%)	36 (10%)	4 (1%)	11	41
8	A7	154/230 (67%)	143 (93%)	9 (6%)	2 (1%)	9	38
8	Az	147/230 (64%)	129 (88%)	13 (9%)	5 (3%)	3	23
All	All	3286/5647 (58%)	3046 (93%)	187 (6%)	53 (2%)	10	35

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	i	68	SER
3	7	72	ASP
3	7	430	ASP

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Mol	Chain	Res	Type
4	AE	583	PHE
4	AE	598	LEU
5	AM	325	SER
4	AU	110	HIS
8	Az	141	LYS
8	A7	40	GLN
8	A7	95	ASP
1	i	101	PRO
1	i	316	SER
2	q	247	VAL
3	7	295	LEU
3	7	480	ASN
3	7	560	TYR
3	7	709	ASP
4	AE	454	ASP
4	AE	650	VAL
4	AE	901	TYR
5	AM	512	ASN
8	Az	142	ASN
8	Az	172	ASP
2	q	280	ILE
2	y	290	ASN
3	7	116	LYS
3	7	286	ASN
3	7	704	PRO
4	AE	465	TYR
4	AE	642	ILE
5	AM	158	TRP
5	AM	232	THR
1	i	124	LYS
1	i	373	SER
2	q	246	GLN
2	y	45	THR
3	7	39	LYS
3	7	123	TRP
3	7	784	GLN
3	7	804	ILE
4	AU	309	LYS
8	Az	41	ASP
8	Az	69	THR
2	q	31	SER
3	7	126	PHE

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Mol	Chain	Res	Type
3	7	747	LYS
4	AE	649	SER
4	AU	153	ALA
1	i	59	ASP
1	i	407	VAL
1	i	432	PRO
3	7	599	VAL
1	i	156	ILE

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

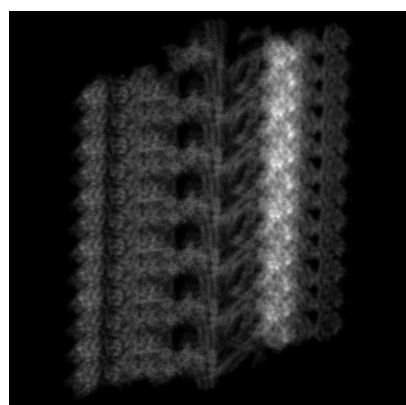
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53467. These allow visual inspection of the internal detail of the map and identification of artifacts.

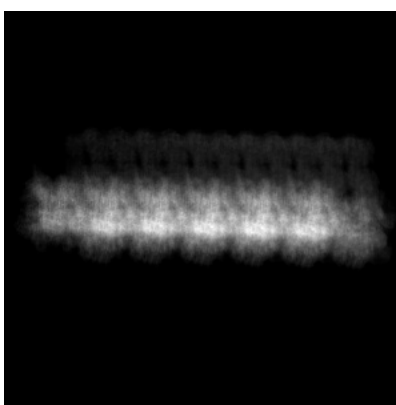
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

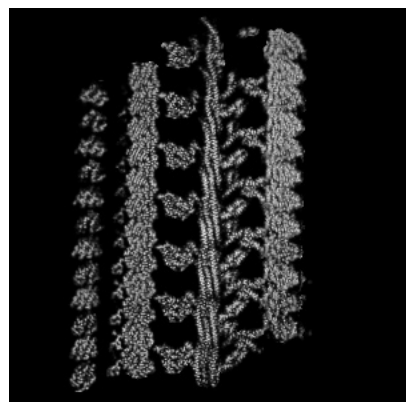


Z

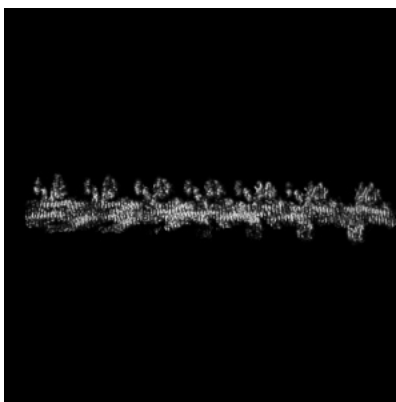
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240



Y Index: 240

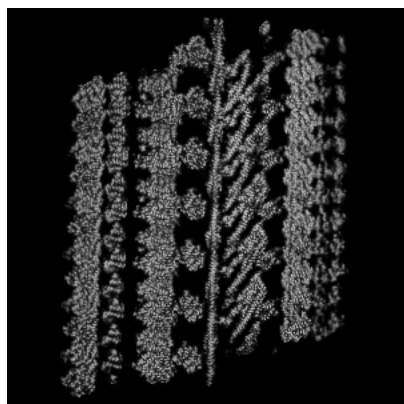


Z Index: 240

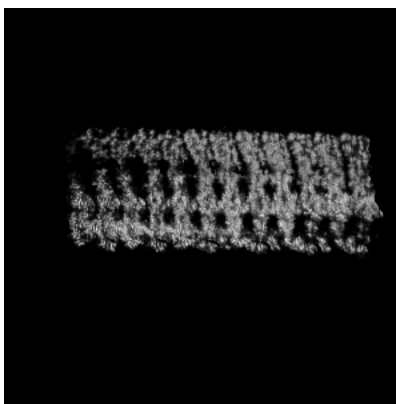
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

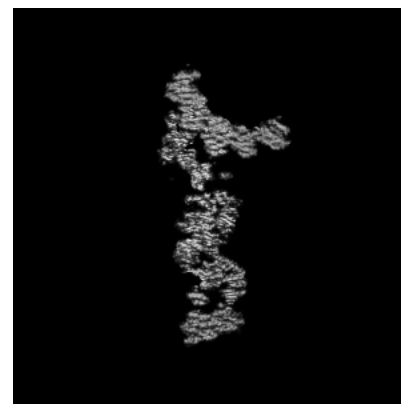
6.3.1 Primary map



X Index: 218



Y Index: 335

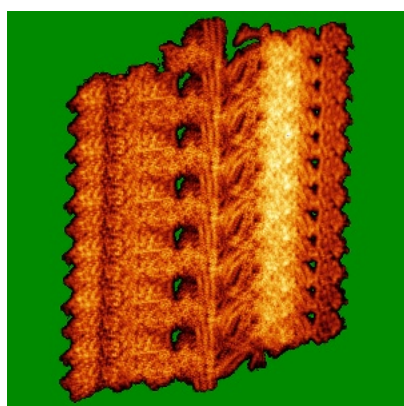


Z Index: 311

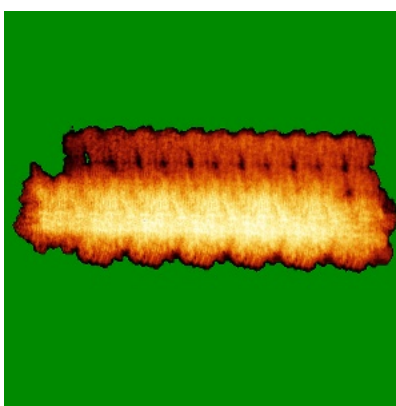
The images above show the largest variance slices of the map in three orthogonal directions.

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

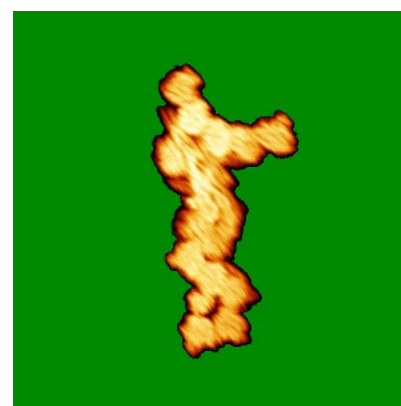
6.4.1 Primary map



X



Y

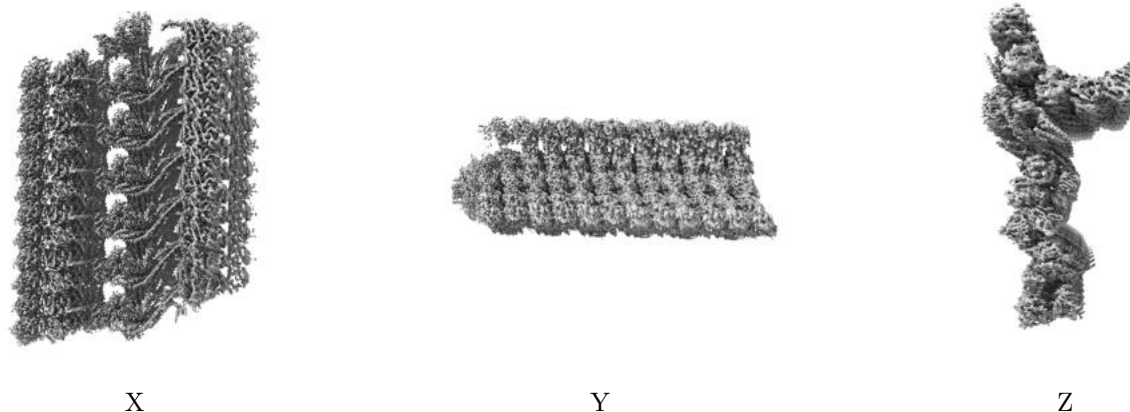


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

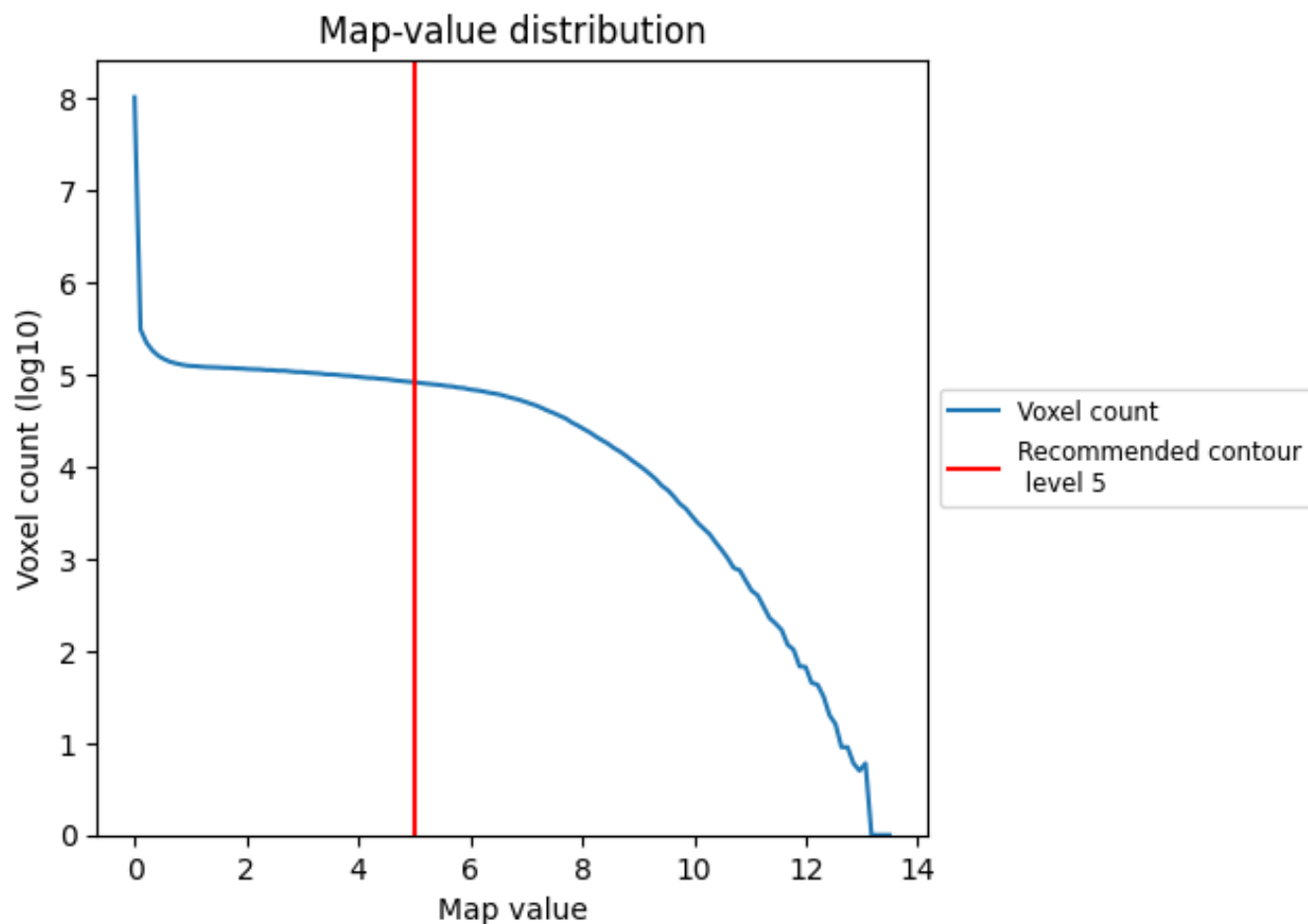
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

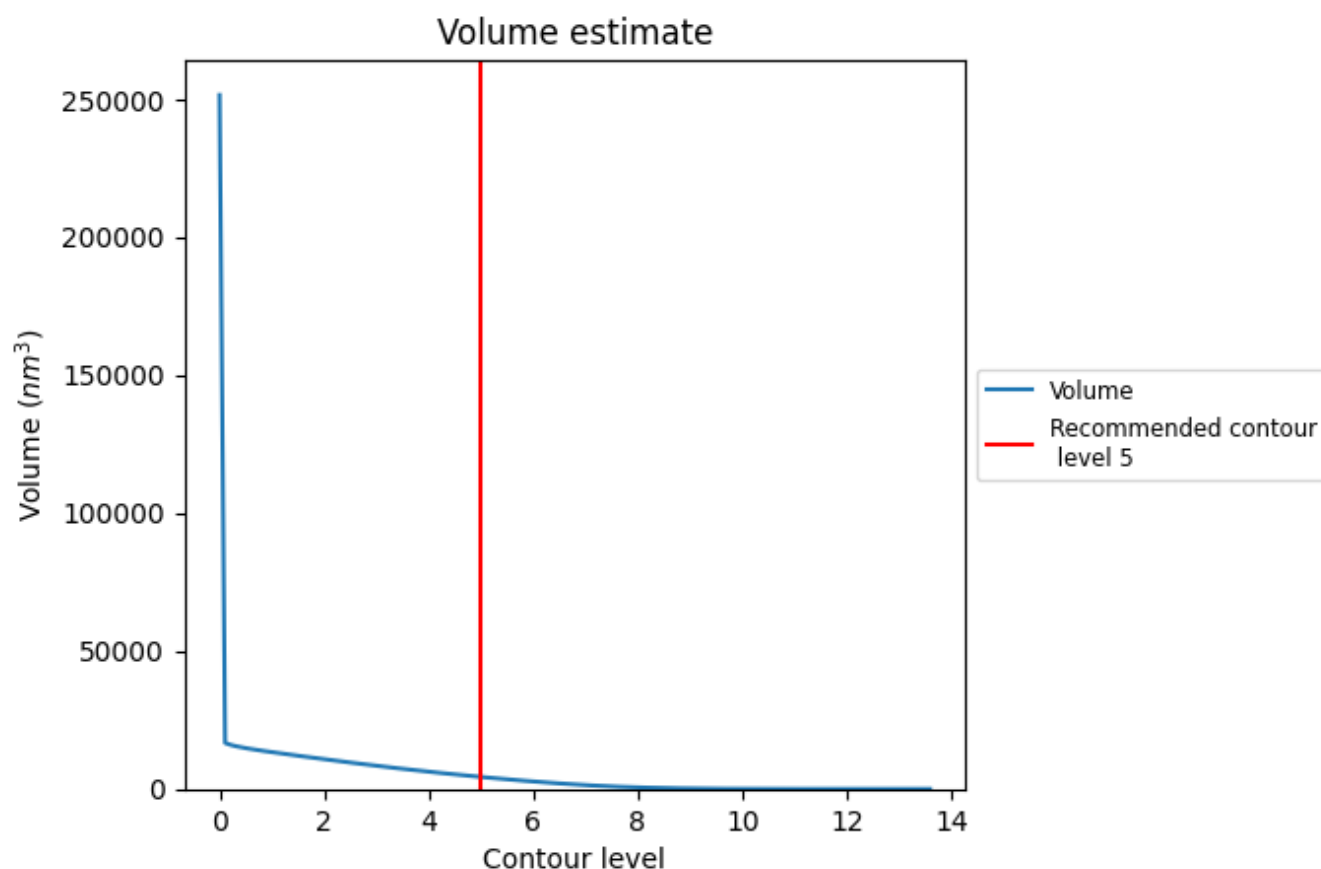
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

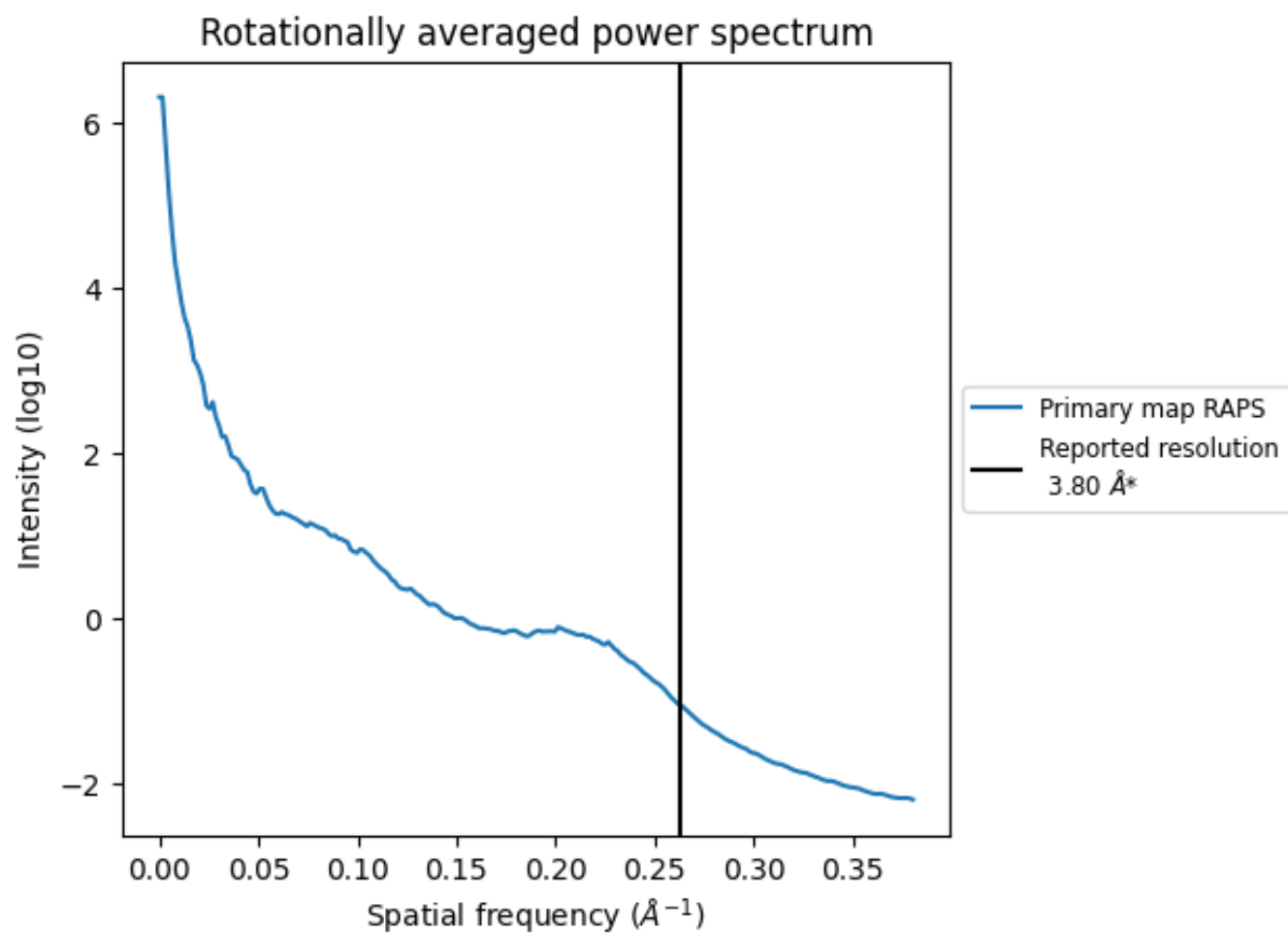
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4355 nm^3 ; this corresponds to an approximate mass of 3934 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

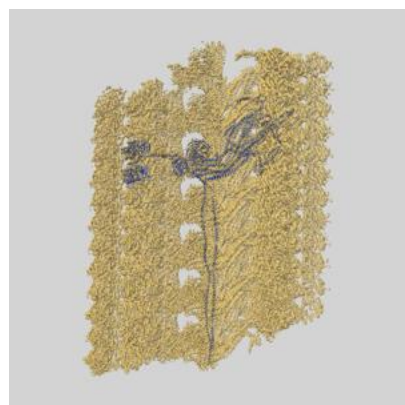
8 Fourier-Shell correlation

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

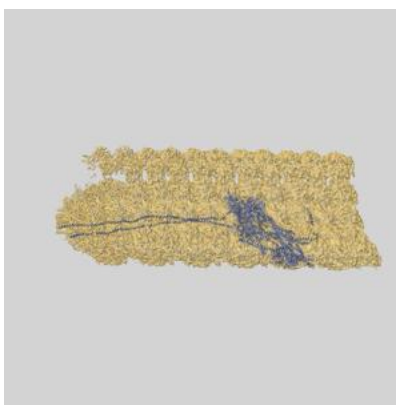
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53467 and PDB model 9QZC. Per-residue inclusion information can be found in section 3 on page 7.

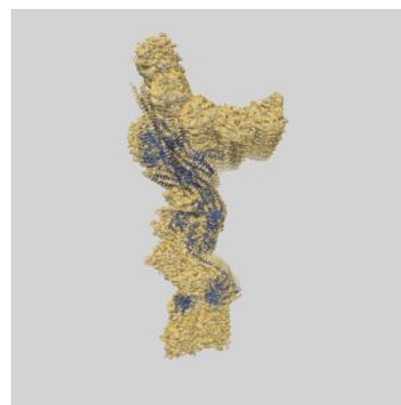
9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

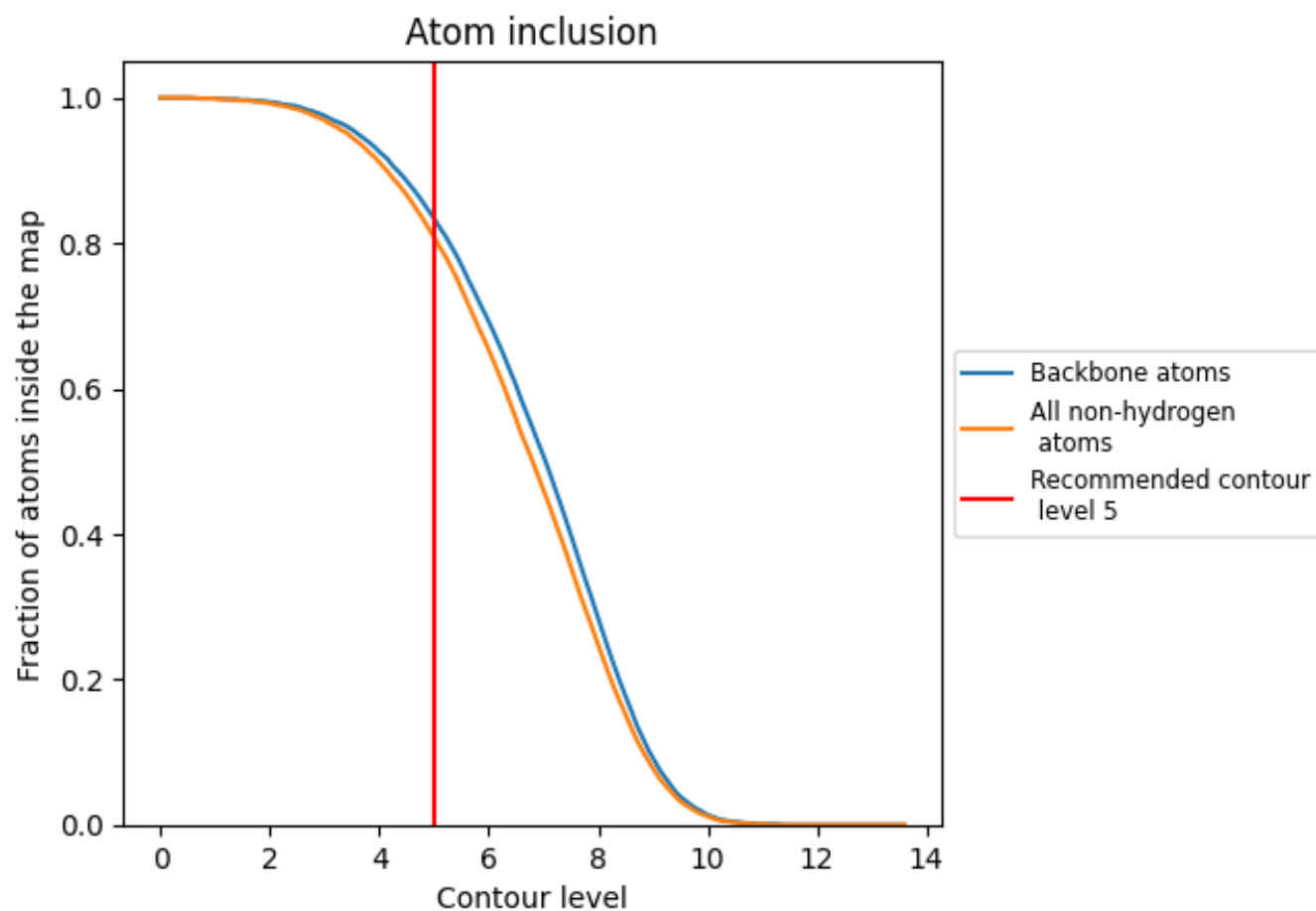


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 81% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8080	 0.3410
7	 0.7440	 0.3410
A7	 0.7940	 0.3400
AE	 0.8500	 0.3580
AM	 0.7320	 0.2870
AU	 0.5010	 0.2140
Ac	 0.8440	 0.4140
As	 0.8990	 0.3380
Az	 0.7940	 0.3240
B4	 0.8520	 0.3670
Bw	 0.9430	 0.3710
CA	 0.8520	 0.3760
CH	 0.9430	 0.3910
CO	 0.9330	 0.3750
CV	 0.9200	 0.3590
Cc	 0.9250	 0.3730
i	 0.8760	 0.3990
q	 0.8820	 0.3490
y	 0.8370	 0.3210

