



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 02:55 AM UTC

PDB ID : 6SUE / pdb_00006sue
EMDB ID : EMD-10312
Title : Structure of Photorhabdus luminescens Tc holotoxin pore, Mutation TccC3-D651A
Authors : Roderer, D.; Raunser, S.
Deposited on : 2019-09-13
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

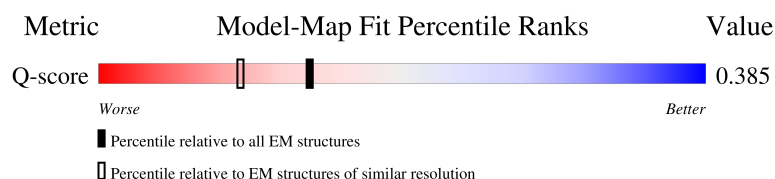
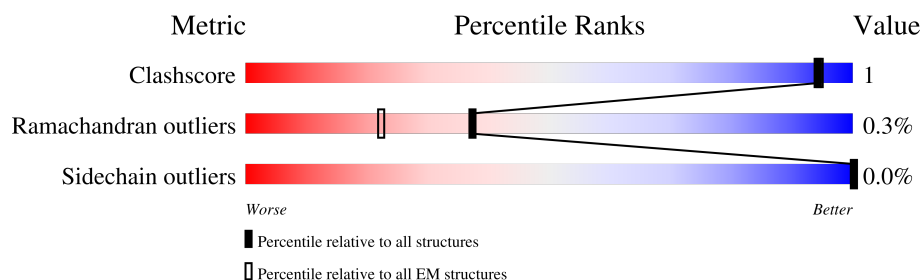
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	A	2516	 5% 85% 5% 9%
1	B	2516	 6% 85% 6% 9%
1	C	2516	 5% 84% 7% 9%
1	D	2516	 8% 85% 6% 9%

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Mol	Chain	Length	Quality of chain
1	E	2516	5% 85% 6% 9%
2	F	2439	81% 7% 11%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 108270 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 TcdA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2292	Total	C	N	O	S	0	0
			18197	11530	3083	3525	59		
1	B	2292	Total	C	N	O	S	0	0
			18197	11530	3083	3525	59		
1	C	2292	Total	C	N	O	S	0	0
			18197	11530	3083	3525	59		
1	D	2292	Total	C	N	O	S	0	0
			18197	11530	3083	3525	59		
1	E	2292	Total	C	N	O	S	0	0
			18197	11530	3083	3525	59		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	904	GLU	GLN	conflict	UNP Q9RN43
B	904	GLU	GLN	conflict	UNP Q9RN43
C	904	GLU	GLN	conflict	UNP Q9RN43
D	904	GLU	GLN	conflict	UNP Q9RN43
E	904	GLU	GLN	conflict	UNP Q9RN43

- Molecule 2 is a protein called TcdB2,TccC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	2168	Total	C	N	O	S	0	0
			17285	10833	3064	3351	37		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	543	GLU	ASP	conflict	UNP Q8GF99
F	1475	PRO	-	linker	UNP Q8GF99
F	1476	GLY	-	linker	UNP Q8GF99
F	1477	SER	-	linker	UNP Q8GF99

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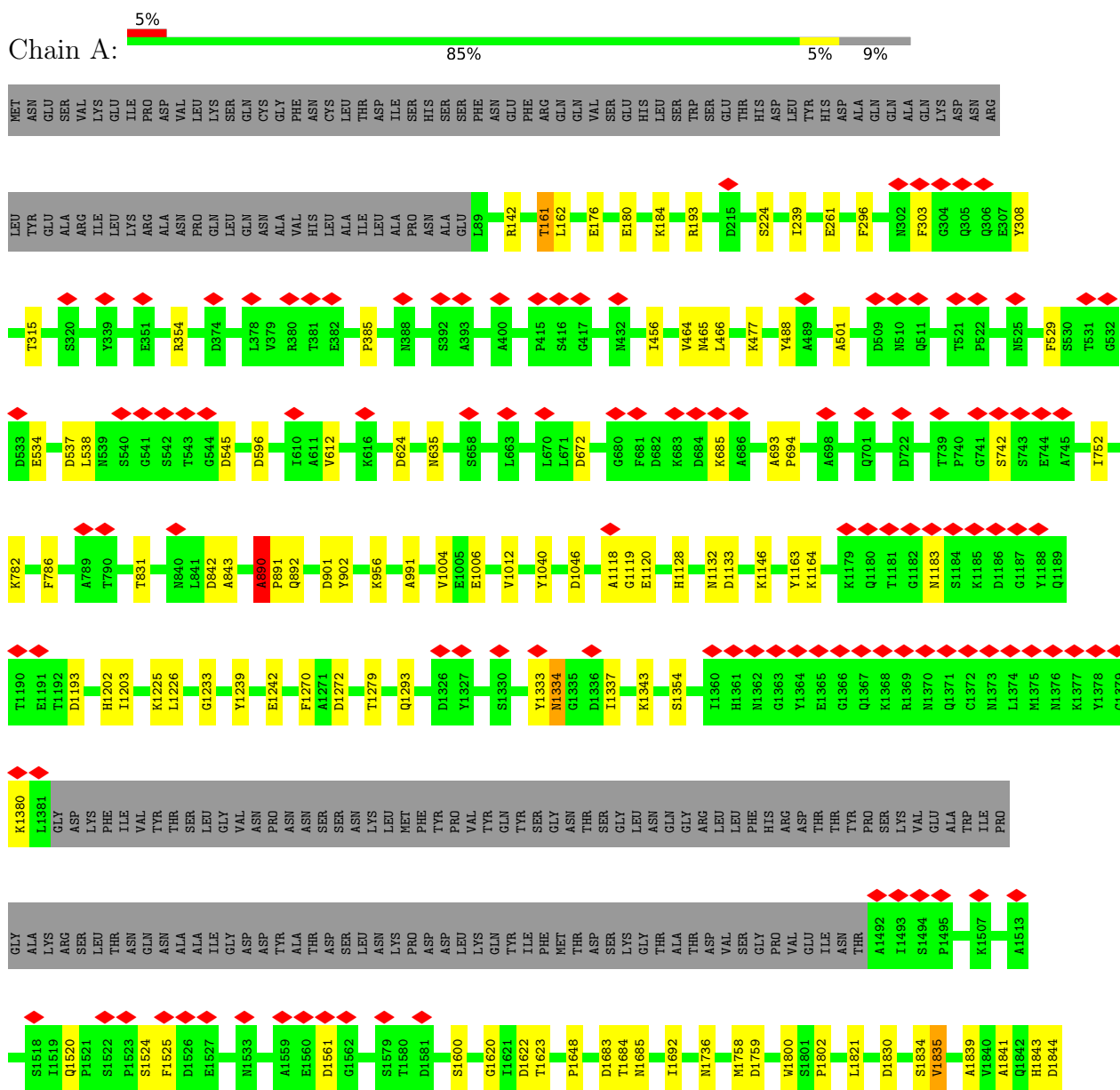
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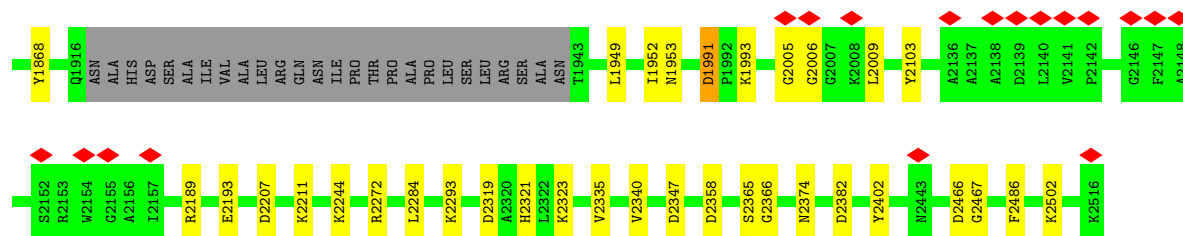
Chain	Residue	Modelled	Actual	Comment	Reference
F	1478	ARG	-	linker	UNP Q8GF99
F	1479	PRO	-	linker	UNP Q8GF99
F	2130	ALA	ASP	engineered mutation	UNP Q8GF97

3 Residue-property plots

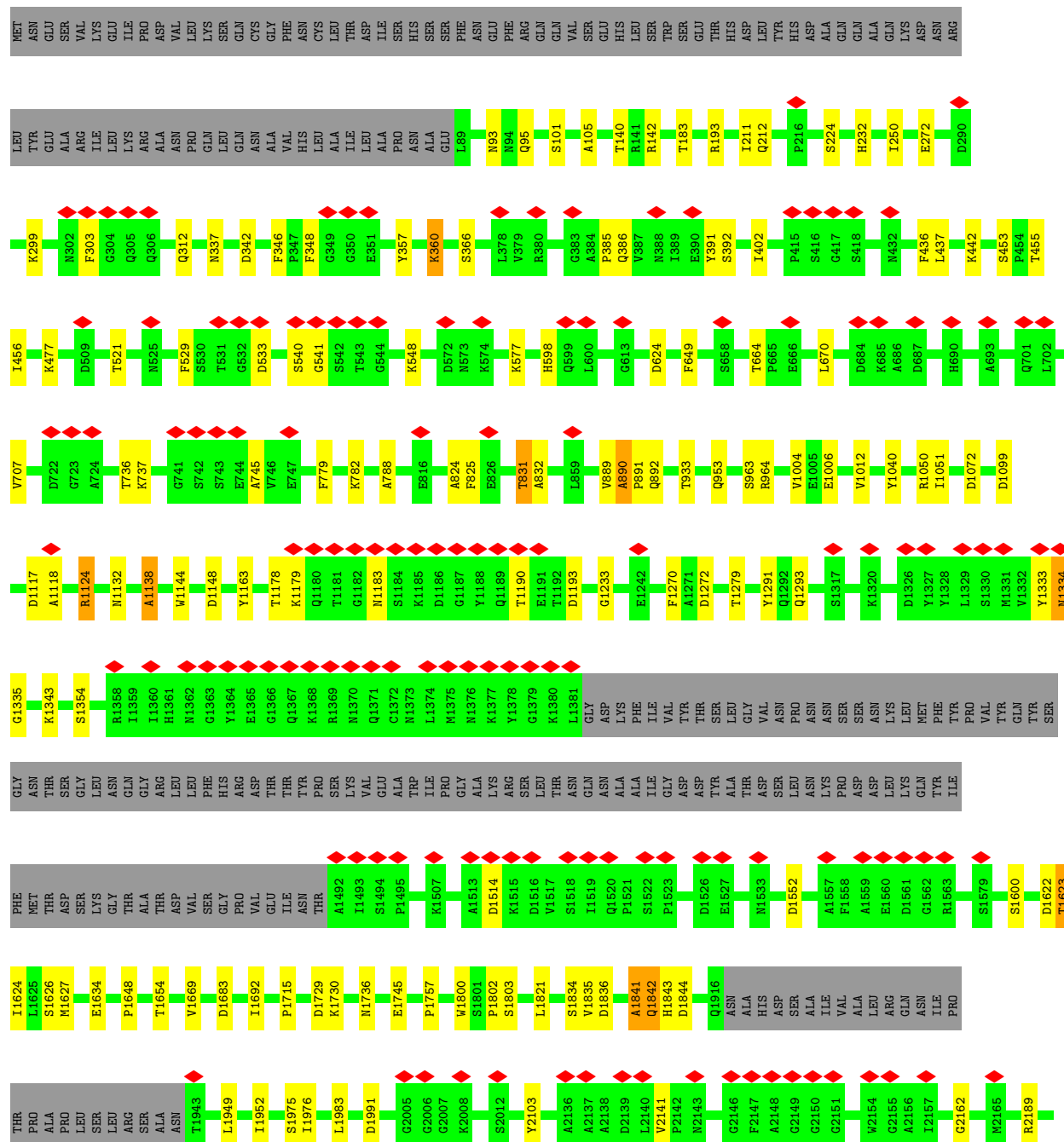
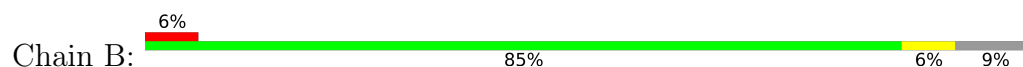
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: TcdA1



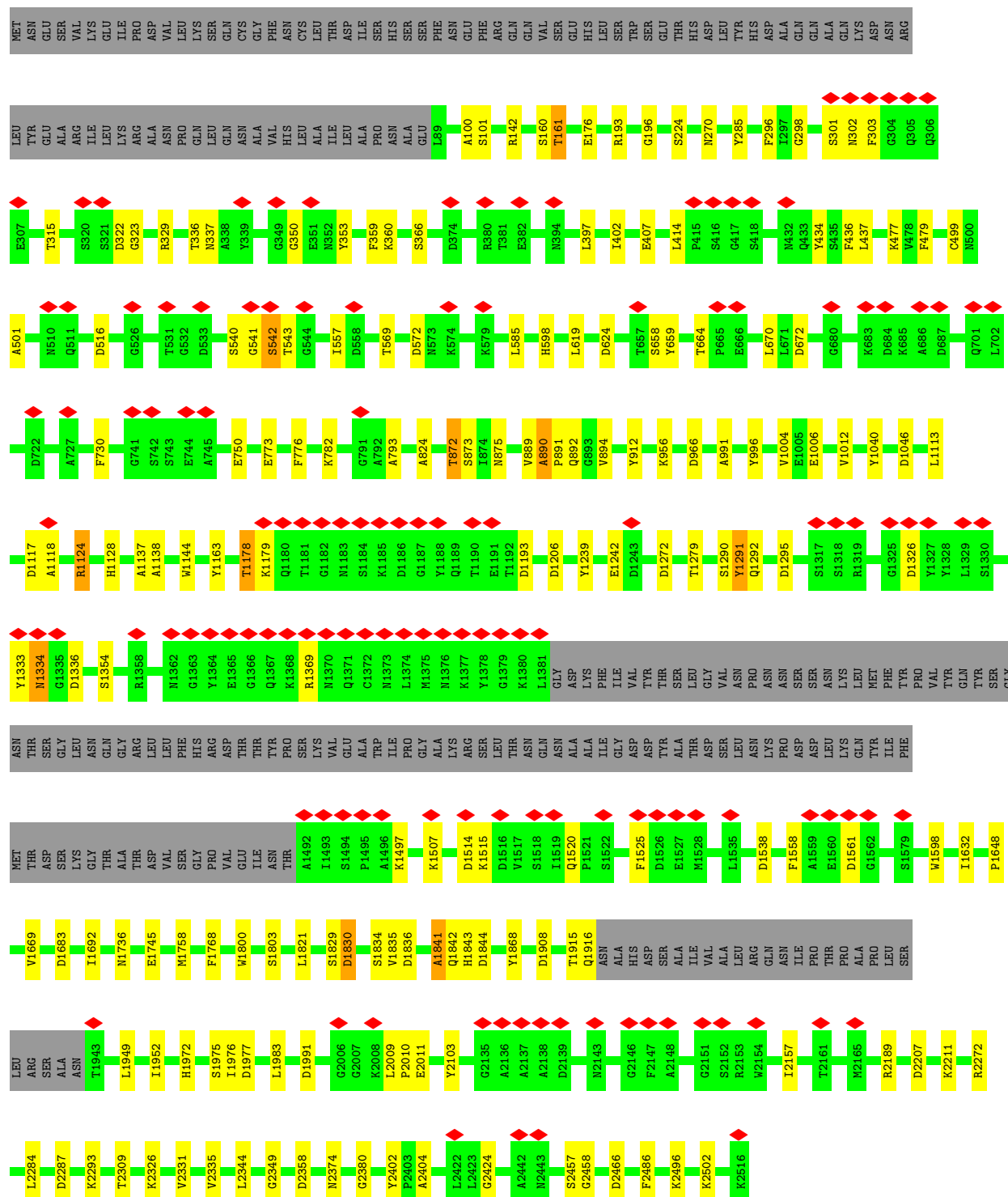
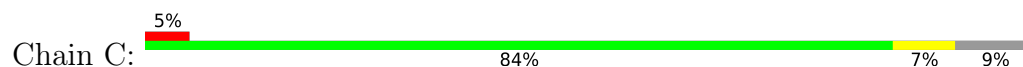


• Molecule 1: TcdA1





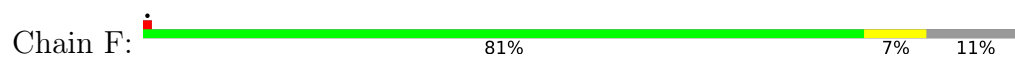
• Molecule 1: TcdA1

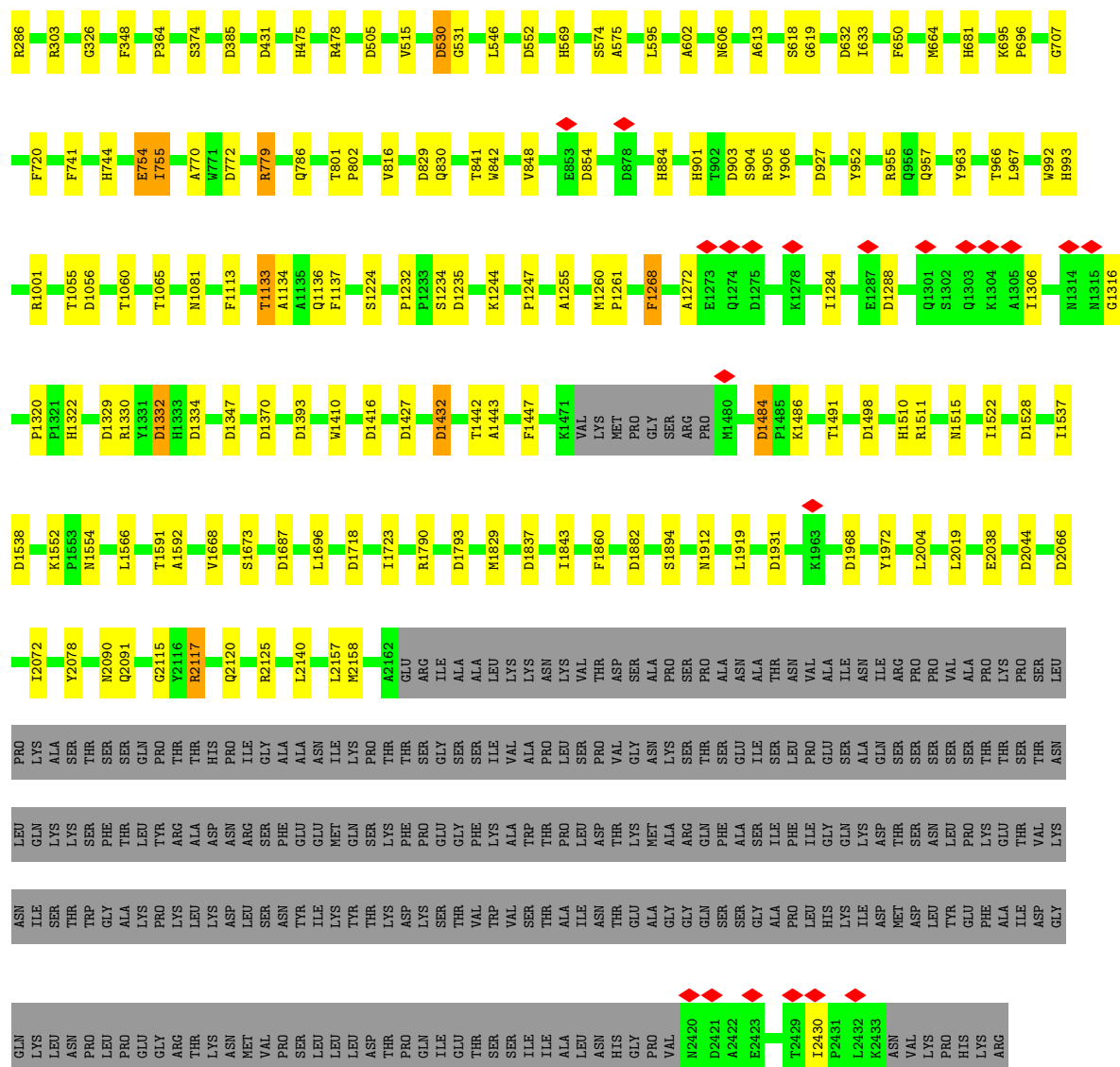


Chain D: 8% 85% 6% 9%



Chain E: 5% 85% 6% 9%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	337823	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.165	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	426.24, 426.24, 426.24	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	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	A	1.11	13/18587 (0.1%)	1.22	99/25239 (0.4%)
1	B	1.11	8/18587 (0.0%)	1.22	113/25239 (0.4%)
1	C	1.13	11/18587 (0.1%)	1.23	131/25239 (0.5%)
1	D	1.11	14/18587 (0.1%)	1.23	113/25239 (0.4%)
1	E	1.11	12/18587 (0.1%)	1.23	109/25239 (0.4%)
2	F	1.18	19/17708 (0.1%)	1.30	164/24137 (0.7%)
All	All	1.13	77/110643 (0.1%)	1.24	729/150332 (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	D	0	1

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1124	ARG	CD-NE	-9.97	1.32	1.46
1	B	1843	HIS	CB-CG	-9.91	1.36	1.50
1	A	1843	HIS	CB-CG	-9.47	1.36	1.50
2	F	744	HIS	CB-CG	-9.43	1.36	1.50
1	C	1843	HIS	CB-CG	-8.88	1.37	1.50
1	D	491	HIS	CB-CG	-8.64	1.38	1.50
1	D	1124	ARG	CD-NE	-8.54	1.34	1.46
2	F	174	ARG	CD-NE	-7.64	1.35	1.46
1	D	858	HIS	CB-CG	-6.95	1.40	1.50
1	B	2452	HIS	CB-CG	-6.82	1.40	1.50
1	D	580	ASN	CB-CG	-6.78	1.35	1.52
1	B	1842	GLN	CG-CD	-6.72	1.35	1.52
1	A	308	TYR	CB-CG	-6.58	1.37	1.51
2	F	1860	PHE	CB-CG	-6.43	1.35	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1124	ARG	CD-NE	-6.38	1.37	1.46
1	E	141	ARG	CD-NE	-6.26	1.37	1.46
2	F	884	HIS	CB-CG	-6.21	1.41	1.50
1	C	1124	ARG	CD-NE	-6.18	1.37	1.46
1	D	1242	GLU	CG-CD	-6.14	1.36	1.52
1	A	1242	GLU	CG-CD	-6.06	1.36	1.52
2	F	286	ARG	CD-NE	-6.04	1.37	1.46
2	F	681	HIS	CB-CG	-6.01	1.41	1.50
1	E	996	TYR	CB-CG	-5.95	1.38	1.51
1	D	1128	HIS	CB-CG	-5.86	1.42	1.50
1	B	1800	TRP	NE1-CE2	-5.82	1.31	1.37
1	C	1800	TRP	NE1-CE2	-5.77	1.31	1.37
2	F	174	ARG	CZ-NH2	-5.74	1.25	1.33
1	A	161	THR	CA-C	-5.72	1.45	1.53
1	A	1128	HIS	CB-CG	-5.72	1.42	1.50
1	A	1800	TRP	NE1-CE2	-5.70	1.31	1.37
2	F	664	MET	CG-SD	-5.65	1.66	1.80
1	D	1163	TYR	CB-CG	-5.63	1.39	1.51
1	D	1124	ARG	CB-CG	-5.63	1.35	1.52
1	C	585	LEU	CB-CG	-5.62	1.42	1.53
2	F	1554	ASN	CB-CG	-5.62	1.38	1.52
2	F	992	TRP	NE1-CE2	-5.59	1.31	1.37
1	C	1242	GLU	CG-CD	-5.57	1.38	1.52
2	F	475	HIS	CB-CG	-5.54	1.42	1.50
1	B	1124	ARG	CB-CG	-5.53	1.35	1.52
1	E	2321	HIS	CB-CG	-5.52	1.42	1.50
1	E	1163	TYR	CB-CG	-5.50	1.39	1.51
1	A	902	TYR	CB-CG	-5.50	1.39	1.51
2	F	901	HIS	CB-CG	-5.49	1.42	1.50
1	E	1664	TYR	CB-CG	-5.47	1.39	1.51
2	F	1322	HIS	CB-CG	-5.46	1.42	1.50
2	F	779	ARG	CZ-NH1	-5.46	1.25	1.32
1	B	1163	TYR	CB-CG	-5.45	1.39	1.51
1	C	1692	ILE	N-CA	-5.42	1.42	1.46
1	C	1128	HIS	CB-CG	-5.38	1.42	1.50
2	F	1510	HIS	CB-CG	-5.38	1.42	1.50
1	A	1203	ILE	CB-CG1	-5.33	1.42	1.53
1	D	608	LEU	CB-CG	5.33	1.64	1.53
1	D	1800	TRP	NE1-CE2	-5.33	1.31	1.37
1	A	2272	ARG	CG-CD	-5.30	1.36	1.52
1	D	1218	ASN	CB-CG	-5.29	1.38	1.52
1	A	1692	ILE	N-CA	-5.25	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	996	TYR	CB-CG	-5.24	1.40	1.51
1	E	1843	HIS	CB-CG	-5.24	1.42	1.50
1	E	1128	HIS	CB-CG	-5.21	1.42	1.50
1	A	2321	HIS	CB-CG	-5.21	1.42	1.50
1	E	515	PHE	CB-CG	-5.21	1.38	1.50
1	A	2272	ARG	CD-NE	-5.19	1.39	1.46
2	F	993	HIS	CB-CG	-5.18	1.43	1.50
1	D	776	PHE	CG-CD2	-5.15	1.28	1.38
1	B	1692	ILE	N-CA	-5.14	1.42	1.46
1	A	1163	TYR	CB-CG	-5.12	1.40	1.51
1	C	2272	ARG	CG-CD	-5.11	1.37	1.52
1	C	1163	TYR	CB-CG	-5.07	1.40	1.51
1	E	2018	ARG	CD-NE	-5.06	1.39	1.46
1	C	875	ASN	CB-CG	-5.05	1.39	1.52
1	E	1800	TRP	NE1-CE2	-5.05	1.31	1.37
1	D	99	ARG	NE-CZ	5.04	1.38	1.33
1	D	880	TRP	NE1-CE2	-5.04	1.31	1.37
2	F	256	TRP	CD2-CE3	-5.04	1.32	1.40
1	E	313	LEU	CB-CG	-5.03	1.43	1.53
2	F	569	HIS	CB-CG	-5.03	1.43	1.50
2	F	1511	ARG	CD-NE	-5.01	1.39	1.46

All (729) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	816	VAL	N-CA-C	-13.10	101.27	113.71
2	F	754	GLU	N-CA-C	-10.44	95.77	110.50
1	D	664	THR	CA-C-N	10.13	129.89	119.56
1	D	664	THR	C-N-CA	10.13	129.89	119.56
1	E	161	THR	N-CA-C	-9.82	98.33	110.41
1	C	1354	SER	CA-C-N	9.69	129.63	120.03
1	C	1354	SER	C-N-CA	9.69	129.63	120.03
1	E	619	LEU	N-CA-C	-9.54	102.15	113.88
1	C	872	THR	N-CA-C	-9.42	98.83	110.41
1	E	436	PHE	N-CA-C	-9.41	102.30	113.88
1	E	1952	ILE	N-CA-C	9.38	120.19	110.62
1	E	1841	ALA	N-CA-C	-9.36	98.90	110.41
1	E	1006	GLU	N-CA-C	9.29	121.41	111.28
1	A	1354	SER	CA-C-N	9.20	129.14	120.03
1	A	1354	SER	C-N-CA	9.20	129.14	120.03
1	B	1354	SER	CA-C-N	9.16	129.10	120.03
1	B	1354	SER	C-N-CA	9.16	129.10	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1006	GLU	N-CA-C	9.07	121.25	111.36
1	E	1354	SER	CA-C-N	9.07	129.01	120.03
1	E	1354	SER	C-N-CA	9.07	129.01	120.03
1	A	1952	ILE	N-CA-C	9.02	119.82	110.62
1	D	1841	ALA	N-CA-C	-9.01	99.33	110.41
1	A	612	VAL	N-CA-C	-8.95	104.75	113.53
1	D	1952	ILE	N-CA-C	8.94	119.73	110.62
1	D	1354	SER	CA-C-N	8.71	128.65	120.03
1	D	1354	SER	C-N-CA	8.71	128.65	120.03
1	B	303	PHE	N-CA-C	-8.59	103.23	114.31
1	E	664	THR	CA-C-N	8.58	129.42	119.47
1	E	664	THR	C-N-CA	8.58	129.42	119.47
1	C	776	PHE	CA-CB-CG	8.37	122.17	113.80
2	F	632	ASP	CA-CB-CG	8.34	120.94	112.60
1	C	360	LYS	N-CA-C	-8.31	103.66	113.88
1	B	664	THR	CA-C-N	8.28	129.08	119.47
1	B	664	THR	C-N-CA	8.28	129.08	119.47
1	A	2340	VAL	N-CA-C	-8.22	103.86	111.67
1	B	312	GLN	N-CA-C	8.18	119.42	108.38
1	D	1844	ASP	CA-C-N	8.14	127.86	119.56
1	D	1844	ASP	C-N-CA	8.14	127.86	119.56
1	C	1841	ALA	N-CA-C	-8.12	99.81	110.53
2	F	2120	GLN	CA-C-N	8.12	127.76	119.56
2	F	2120	GLN	C-N-CA	8.12	127.76	119.56
1	C	730	PHE	CA-CB-CG	8.05	121.85	113.80
1	D	1004	VAL	N-CA-C	-7.94	102.35	111.00
2	F	1510	HIS	N-CA-C	7.93	121.44	108.99
1	D	1272	ASP	N-CA-C	-7.84	96.51	108.67
2	F	1136	GLN	N-CA-C	-7.83	98.05	109.18
1	A	1841	ALA	N-CA-C	-7.83	100.20	110.53
1	C	619	LEU	N-CA-C	-7.80	103.98	113.97
1	C	1952	ILE	N-CA-C	7.78	118.55	110.62
1	E	1844	ASP	CA-C-N	7.77	127.48	119.56
1	E	1844	ASP	C-N-CA	7.77	127.48	119.56
1	B	224	SER	CA-C-N	7.76	127.48	119.56
1	B	224	SER	C-N-CA	7.76	127.48	119.56
1	A	303	PHE	N-CA-C	-7.76	103.34	114.12
1	A	456	ILE	N-CA-C	-7.73	103.32	110.82
1	B	890	ALA	CA-C-N	7.73	129.50	119.84
1	B	890	ALA	C-N-CA	7.73	129.50	119.84
1	C	782	LYS	CA-C-N	7.73	127.44	119.56
1	C	782	LYS	C-N-CA	7.73	127.44	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	782	LYS	CA-C-N	7.72	127.90	119.87
1	B	782	LYS	C-N-CA	7.72	127.90	119.87
2	F	1484	ASP	CA-C-N	7.66	127.37	119.56
2	F	1484	ASP	C-N-CA	7.66	127.37	119.56
1	A	1006	GLU	N-CA-C	7.65	120.50	111.71
1	B	402	ILE	N-CA-C	7.53	121.08	113.47
1	D	224	SER	CA-C-N	7.53	127.17	119.56
1	D	224	SER	C-N-CA	7.53	127.17	119.56
2	F	966	THR	N-CA-C	-7.51	103.23	113.30
1	A	890	ALA	CA-C-N	7.46	129.17	119.84
1	A	890	ALA	C-N-CA	7.46	129.17	119.84
1	C	1291	TYR	N-CA-C	-7.42	100.75	110.33
1	A	1004	VAL	N-CA-C	-7.42	102.91	111.00
1	C	1004	VAL	N-CA-C	-7.38	102.95	111.00
1	C	1669	VAL	N-CA-C	-7.37	106.02	113.47
1	C	224	SER	CA-C-N	7.37	127.07	119.56
1	C	224	SER	C-N-CA	7.37	127.07	119.56
1	A	1844	ASP	CA-C-N	7.36	127.04	119.82
1	A	1844	ASP	C-N-CA	7.36	127.04	119.82
2	F	1723	ILE	N-CA-C	7.35	118.49	107.75
1	B	1293	GLN	N-CA-C	-7.35	105.22	114.56
1	A	1843	HIS	N-CA-C	-7.35	103.31	112.72
1	A	224	SER	CA-C-N	7.34	127.05	119.56
1	A	224	SER	C-N-CA	7.34	127.05	119.56
2	F	1843	ILE	N-CA-C	-7.34	105.50	111.81
1	B	386	GLN	N-CA-C	7.34	121.38	110.52
1	E	1293	GLN	N-CA-C	-7.34	103.75	114.39
1	D	1006	GLU	N-CA-C	7.31	120.12	111.71
1	C	1844	ASP	CA-C-N	7.31	127.01	119.56
1	C	1844	ASP	C-N-CA	7.31	127.01	119.56
1	D	890	ALA	CA-C-N	7.27	128.93	119.84
1	D	890	ALA	C-N-CA	7.27	128.93	119.84
1	A	1293	GLN	N-CA-C	-7.26	104.94	114.31
2	F	801	THR	CA-C-N	7.20	124.92	119.66
2	F	801	THR	C-N-CA	7.20	124.92	119.66
2	F	1060	THR	N-CA-C	-7.16	105.08	114.31
2	F	552	ASP	CA-C-N	7.14	126.84	119.56
2	F	552	ASP	C-N-CA	7.14	126.84	119.56
1	A	1239	TYR	N-CA-C	-7.14	99.72	110.28
1	B	779	PHE	CA-CB-CG	7.12	120.92	113.80
1	A	142	ARG	CA-C-N	7.11	126.81	119.56
1	A	142	ARG	C-N-CA	7.11	126.81	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1802	PRO	N-CA-C	-7.11	99.91	111.21
1	C	2009	LEU	CA-C-N	7.10	127.03	120.21
1	C	2009	LEU	C-N-CA	7.10	127.03	120.21
1	E	2043	ILE	N-CA-C	-7.09	105.71	111.81
1	E	224	SER	CA-C-N	7.08	126.78	119.56
1	E	224	SER	C-N-CA	7.08	126.78	119.56
1	C	402	ILE	N-CA-C	7.07	119.68	112.90
1	B	825	PHE	CA-CB-CG	7.06	120.86	113.80
1	C	142	ARG	CA-C-N	7.06	126.76	119.56
1	C	142	ARG	C-N-CA	7.06	126.76	119.56
2	F	32	GLY	CA-C-N	7.04	126.74	119.56
2	F	32	GLY	C-N-CA	7.04	126.74	119.56
1	A	239	ILE	N-CA-C	-7.03	105.76	111.81
1	E	1520	GLN	CA-C-N	7.01	126.97	120.03
1	E	1520	GLN	C-N-CA	7.01	126.97	120.03
1	E	213	LEU	N-CA-C	-7.01	103.40	112.23
1	D	1233	GLY	N-CA-C	-7.00	102.01	111.54
1	A	1193	ASP	N-CA-C	-7.00	98.89	110.17
1	B	1736	ASN	CA-C-N	7.00	126.68	119.82
1	B	1736	ASN	C-N-CA	7.00	126.68	119.82
1	E	315	THR	N-CA-C	7.00	117.14	108.11
1	A	1736	ASN	CA-C-N	6.98	126.66	119.82
1	A	1736	ASN	C-N-CA	6.98	126.66	119.82
2	F	1894	SER	CA-C-N	6.96	127.55	119.47
2	F	1894	SER	C-N-CA	6.96	127.55	119.47
2	F	1288	ASP	CA-CB-CG	6.96	119.56	112.60
1	E	890	ALA	CA-C-N	6.95	128.53	119.84
1	E	890	ALA	C-N-CA	6.95	128.53	119.84
1	E	1736	ASN	CA-C-N	6.95	126.63	119.82
1	E	1736	ASN	C-N-CA	6.95	126.63	119.82
1	C	2424	GLY	CA-C-N	6.94	126.57	119.56
1	C	2424	GLY	C-N-CA	6.94	126.57	119.56
1	E	2456	ASP	CA-CB-CG	6.94	119.54	112.60
1	D	340	GLN	N-CA-C	-6.92	103.72	112.93
1	E	456	ILE	N-CA-C	-6.92	104.11	110.82
1	E	1233	GLY	N-CA-C	-6.91	102.14	111.54
1	B	1949	LEU	CA-C-N	6.89	126.85	120.03
1	B	1949	LEU	C-N-CA	6.89	126.85	120.03
1	C	890	ALA	CA-C-N	6.88	128.44	119.84
1	C	890	ALA	C-N-CA	6.88	128.44	119.84
1	C	1736	ASN	CA-C-N	6.86	126.54	119.82
1	C	1736	ASN	C-N-CA	6.86	126.54	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1949	LEU	CA-C-N	6.86	126.82	120.03
1	A	1949	LEU	C-N-CA	6.86	126.82	120.03
1	B	1648	PRO	CA-C-N	6.84	126.76	119.85
1	B	1648	PRO	C-N-CA	6.84	126.76	119.85
1	E	548	LYS	N-CA-C	-6.83	103.92	111.36
1	C	1239	TYR	N-CA-C	-6.82	100.19	110.28
1	E	1949	LEU	CA-C-N	6.81	126.77	120.03
1	E	1949	LEU	C-N-CA	6.81	126.77	120.03
1	B	1844	ASP	CA-C-N	6.81	126.95	119.87
1	B	1844	ASP	C-N-CA	6.81	126.95	119.87
2	F	100	GLU	N-CA-C	-6.81	98.31	109.40
1	C	750	GLU	N-CA-C	-6.79	103.68	112.23
2	F	286	ARG	NE-CZ-NH1	-6.79	114.72	121.50
2	F	1860	PHE	CA-C-N	6.78	126.70	119.85
2	F	1860	PHE	C-N-CA	6.78	126.70	119.85
1	E	1632	ILE	N-CA-C	-6.78	100.82	109.30
2	F	364	PRO	CA-C-N	6.77	126.73	120.03
2	F	364	PRO	C-N-CA	6.77	126.73	120.03
1	D	672	ASP	CA-CB-CG	6.76	119.36	112.60
2	F	1860	PHE	CA-CB-CG	6.75	120.55	113.80
1	D	1736	ASN	CA-C-N	6.74	126.43	119.82
1	D	1736	ASN	C-N-CA	6.74	126.43	119.82
1	C	359	PHE	CA-CB-CG	6.73	120.53	113.80
1	B	779	PHE	CB-CA-C	-6.71	99.65	110.79
2	F	98	GLY	CA-C-N	6.71	126.33	119.56
2	F	98	GLY	C-N-CA	6.71	126.33	119.56
1	E	1118	ALA	N-CA-C	-6.70	104.80	114.12
1	C	664	THR	CA-C-N	6.70	126.39	119.56
1	C	664	THR	C-N-CA	6.70	126.39	119.56
1	D	501	ALA	CA-C-N	6.69	126.66	120.03
1	D	501	ALA	C-N-CA	6.69	126.66	120.03
1	D	1949	LEU	CA-C-N	6.69	126.66	120.03
1	D	1949	LEU	C-N-CA	6.69	126.66	120.03
1	B	577	LYS	N-CA-C	6.69	118.69	108.52
1	A	1648	PRO	CA-C-N	6.68	126.60	119.85
1	A	1648	PRO	C-N-CA	6.68	126.60	119.85
1	B	1004	VAL	N-CA-C	-6.68	103.72	111.00
1	A	1118	ALA	N-CA-C	-6.68	105.04	113.72
1	D	1326	ASP	CA-CB-CG	6.68	119.28	112.60
1	E	2293	LYS	CA-C-N	6.67	126.81	119.87
1	E	2293	LYS	C-N-CA	6.67	126.81	119.87
1	B	1841	ALA	N-CA-C	-6.67	102.20	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	14	LEU	CA-C-N	6.67	126.64	120.03
2	F	14	LEU	C-N-CA	6.67	126.64	120.03
1	D	1291	TYR	N-CA-C	-6.67	101.28	110.35
1	D	1745	GLU	N-CA-C	-6.67	104.09	111.36
1	E	2424	GLY	CA-C-N	6.66	126.35	119.56
1	E	2424	GLY	C-N-CA	6.66	126.35	119.56
1	E	1821	LEU	N-CA-C	-6.65	105.30	113.41
1	C	1991	ASP	CA-C-N	6.63	126.33	119.56
1	C	1991	ASP	C-N-CA	6.63	126.33	119.56
1	D	2009	LEU	CA-C-N	6.63	126.60	120.03
1	D	2009	LEU	C-N-CA	6.63	126.60	120.03
1	B	1600	SER	N-CA-C	-6.63	105.19	113.28
1	D	789	ALA	N-CA-C	6.62	119.32	111.71
2	F	720	PHE	N-CA-C	-6.62	103.55	111.69
1	B	360	LYS	N-CA-C	-6.61	105.75	113.88
1	C	542	SER	N-CA-C	6.61	116.77	108.45
1	E	239	ILE	N-CA-C	-6.60	104.58	111.58
1	A	1830	ASP	CA-C-N	6.60	126.52	119.85
1	A	1830	ASP	C-N-CA	6.60	126.52	119.85
1	C	1525	PHE	CA-CB-CG	6.60	120.40	113.80
1	E	340	GLN	N-CA-C	-6.59	105.78	113.88
1	E	521	THR	N-CA-C	-6.58	103.80	112.75
1	E	1040	TYR	CA-C-N	6.58	126.20	119.56
1	E	1040	TYR	C-N-CA	6.58	126.20	119.56
1	B	1272	ASP	N-CA-C	-6.57	99.20	109.25
1	A	1839	ALA	N-CA-C	-6.56	104.31	112.90
1	E	776	PHE	CA-CB-CG	6.56	120.36	113.80
2	F	374	SER	CA-C-N	6.55	126.24	119.56
2	F	374	SER	C-N-CA	6.55	126.24	119.56
1	E	1239	TYR	N-CA-C	-6.54	100.60	110.28
1	A	161	THR	N-CA-C	-6.54	101.33	110.35
2	F	906	TYR	CA-C-N	6.54	126.50	120.03
2	F	906	TYR	C-N-CA	6.54	126.50	120.03
1	D	2456	ASP	CA-CB-CG	6.53	119.13	112.60
1	C	2293	LYS	CA-C-N	6.52	126.65	119.87
1	C	2293	LYS	C-N-CA	6.52	126.65	119.87
2	F	159	SER	CA-C-N	6.51	126.20	119.56
2	F	159	SER	C-N-CA	6.51	126.20	119.56
2	F	595	LEU	CA-C-N	6.51	126.47	120.03
2	F	595	LEU	C-N-CA	6.51	126.47	120.03
1	D	2300	THR	N-CA-C	-6.51	100.65	110.28
2	F	212	CYS	N-CA-C	6.50	118.64	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1306	ILE	CA-C-N	6.50	127.00	119.47
2	F	1306	ILE	C-N-CA	6.50	127.00	119.47
1	B	1991	ASP	CA-C-N	6.49	126.18	119.56
1	B	1991	ASP	C-N-CA	6.49	126.18	119.56
1	C	1113	LEU	N-CA-C	6.49	119.75	109.50
1	D	1100	ASN	CA-CB-CG	6.49	119.09	112.60
1	C	1648	PRO	CA-C-N	6.47	126.39	119.85
1	C	1648	PRO	C-N-CA	6.47	126.39	119.85
1	A	1119	GLY	N-CA-C	-6.47	103.24	112.55
2	F	695	LYS	CA-C-N	6.46	126.09	119.56
2	F	695	LYS	C-N-CA	6.46	126.09	119.56
2	F	1284	ILE	N-CA-C	-6.44	105.46	111.45
1	C	2284	LEU	N-CA-C	-6.44	99.20	109.76
1	D	1648	PRO	CA-C-N	6.43	126.40	120.03
1	D	1648	PRO	C-N-CA	6.43	126.40	120.03
1	D	1239	TYR	N-CA-C	-6.42	100.77	110.28
1	B	212	GLN	N-CA-C	-6.42	105.27	113.23
1	C	557	ILE	N-CA-C	6.42	118.17	108.80
1	C	1949	LEU	CA-C-N	6.38	126.34	120.03
1	C	1949	LEU	C-N-CA	6.38	126.34	120.03
1	D	414	LEU	CA-C-N	6.38	126.50	119.87
1	D	414	LEU	C-N-CA	6.38	126.50	119.87
1	A	901	ASP	N-CA-C	6.36	119.13	110.55
2	F	1137	PHE	CA-CB-CG	-6.36	107.44	113.80
2	F	927	ASP	CB-CA-C	-6.35	104.74	110.71
1	E	1756	GLU	CA-C-N	6.35	126.71	119.92
1	E	1756	GLU	C-N-CA	6.35	126.71	119.92
2	F	1432	ASP	CA-C-N	6.34	126.04	119.82
2	F	1432	ASP	C-N-CA	6.34	126.04	119.82
2	F	66	SER	CA-C-N	6.34	126.03	119.56
2	F	66	SER	C-N-CA	6.34	126.03	119.56
1	A	1802	PRO	N-CA-C	-6.33	101.14	111.21
1	E	572	ASP	N-CA-C	-6.33	104.61	112.90
2	F	2078	TYR	N-CA-C	-6.32	101.10	110.20
1	D	2374	ASN	N-CA-C	6.30	116.89	108.38
1	E	1272	ASP	N-CA-C	-6.30	99.61	109.25
2	F	1137	PHE	N-CA-C	-6.30	100.30	110.32
1	C	303	PHE	N-CA-C	-6.29	105.26	114.39
1	D	142	ARG	CA-C-N	6.27	125.95	119.56
1	D	142	ARG	C-N-CA	6.27	125.95	119.56
1	A	1040	TYR	CA-C-N	6.26	125.95	119.56
1	A	1040	TYR	C-N-CA	6.26	125.95	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	569	THR	N-CA-C	-6.26	105.29	113.12
1	E	1911	ALA	CA-C-N	6.25	130.97	122.84
1	E	1911	ALA	C-N-CA	6.25	130.97	122.84
1	C	875	ASN	CA-CB-CG	-6.25	106.35	112.60
1	D	1040	TYR	CA-C-N	6.22	125.91	119.56
1	D	1040	TYR	C-N-CA	6.22	125.91	119.56
1	C	1830	ASP	CA-C-N	6.22	126.40	120.31
1	C	1830	ASP	C-N-CA	6.22	126.40	120.31
1	E	1648	PRO	CA-C-N	6.20	126.11	119.85
1	E	1648	PRO	C-N-CA	6.20	126.11	119.85
1	C	100	ALA	N-CA-C	6.20	120.42	112.86
1	A	1272	ASP	N-CA-C	-6.20	99.77	109.25
1	E	193	ARG	CA-C-N	6.19	125.81	119.56
1	E	193	ARG	C-N-CA	6.19	125.81	119.56
2	F	770	ALA	N-CA-C	6.19	118.71	108.99
1	E	782	LYS	CA-C-N	6.19	126.09	119.28
1	E	782	LYS	C-N-CA	6.19	126.09	119.28
1	E	2374	ASN	N-CA-C	6.18	116.72	108.38
1	B	1132	ASN	CA-CB-CG	6.17	118.77	112.60
1	D	386	GLN	N-CA-C	6.17	119.59	109.85
1	D	1494	SER	CA-C-N	6.17	126.62	119.47
1	D	1494	SER	C-N-CA	6.17	126.62	119.47
1	B	2293	LYS	CA-C-N	6.15	126.27	119.87
1	B	2293	LYS	C-N-CA	6.15	126.27	119.87
1	A	193	ARG	CA-C-N	6.15	125.77	119.56
1	A	193	ARG	C-N-CA	6.15	125.77	119.56
1	C	889	VAL	N-CA-C	6.15	119.06	113.10
2	F	952	TYR	CA-C-N	6.14	126.11	120.03
2	F	952	TYR	C-N-CA	6.14	126.11	120.03
1	C	366	SER	N-CA-C	-6.13	104.68	111.36
2	F	1224	SER	CA-C-N	6.12	125.81	119.56
2	F	1224	SER	C-N-CA	6.12	125.81	119.56
1	D	385	PRO	CB-CA-C	6.12	118.97	110.95
2	F	963	TYR	CA-C-N	6.12	126.23	119.87
2	F	963	TYR	C-N-CA	6.12	126.23	119.87
1	E	1004	VAL	N-CA-C	-6.09	104.36	111.00
1	A	1991	ASP	CA-C-N	6.09	125.77	119.56
1	A	1991	ASP	C-N-CA	6.09	125.77	119.56
1	C	773	GLU	N-CA-C	6.07	117.56	111.07
1	C	315	THR	CA-C-N	6.07	125.98	119.85
1	C	315	THR	C-N-CA	6.07	125.98	119.85
1	B	272	GLU	CA-C-N	6.06	125.74	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	272	GLU	C-N-CA	6.06	125.74	119.56
1	E	2009	LEU	CA-C-N	6.06	126.52	120.52
1	E	2009	LEU	C-N-CA	6.06	126.52	120.52
1	A	786	PHE	CA-CB-CG	-6.06	107.74	113.80
1	B	1821	LEU	N-CA-C	-6.05	106.03	113.41
1	A	1233	GLY	N-CA-C	-6.05	103.31	111.54
1	E	1991	ASP	CA-C-N	6.04	125.72	119.56
1	E	1991	ASP	C-N-CA	6.04	125.72	119.56
2	F	212	CYS	CA-C-N	6.04	129.87	120.75
2	F	212	CYS	C-N-CA	6.04	129.87	120.75
1	A	385	PRO	N-CA-C	-6.03	101.80	111.38
1	A	782	LYS	CA-C-N	6.03	125.91	119.28
1	A	782	LYS	C-N-CA	6.03	125.91	119.28
1	B	2424	GLY	CA-C-N	6.03	127.37	119.84
1	B	2424	GLY	C-N-CA	6.03	127.37	119.84
1	C	1006	GLU	N-CA-C	6.02	117.85	111.28
1	C	501	ALA	CA-C-N	6.02	125.99	120.03
1	C	501	ALA	C-N-CA	6.02	125.99	120.03
1	E	1600	SER	N-CA-C	-6.01	105.94	113.28
1	A	672	ASP	CA-CB-CG	6.01	118.61	112.60
1	D	1821	LEU	N-CA-C	-6.01	106.08	113.41
1	D	825	PHE	CA-CB-CG	6.00	119.80	113.80
2	F	478	ARG	CA-C-N	6.00	125.68	119.56
2	F	478	ARG	C-N-CA	6.00	125.68	119.56
1	E	1702	ASP	N-CA-C	-5.99	105.06	112.90
2	F	741	PHE	CA-C-N	5.99	126.01	119.90
2	F	741	PHE	C-N-CA	5.99	126.01	119.90
1	C	793	ALA	CA-C-N	5.99	125.90	119.85
1	C	793	ALA	C-N-CA	5.99	125.90	119.85
1	C	572	ASP	N-CA-C	-5.98	105.65	113.12
1	C	1745	GLU	N-CA-C	-5.98	104.84	111.36
1	C	598	HIS	N-CA-C	-5.98	101.68	110.52
1	E	1279	THR	CA-C-N	5.97	126.40	119.47
1	E	1279	THR	C-N-CA	5.97	126.40	119.47
1	B	1669	VAL	N-CA-C	-5.97	107.44	113.47
2	F	2117	ARG	NE-CZ-NH1	-5.97	115.53	121.50
1	A	1012	VAL	N-CA-C	-5.96	107.08	111.90
1	E	1333	TYR	N-CA-C	5.96	118.94	108.75
2	F	613	ALA	N-CA-C	5.95	118.16	108.76
1	A	1623	THR	N-CA-C	-5.95	105.69	113.12
1	C	1040	TYR	CA-C-N	5.95	125.56	119.56
1	C	1040	TYR	C-N-CA	5.95	125.56	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	966	ASP	N-CA-C	-5.93	104.75	112.23
1	E	1119	GLY	N-CA-C	-5.93	104.01	112.55
1	E	366	SER	N-CA-C	-5.93	104.90	111.36
2	F	1232	PRO	CA-C-N	5.92	125.90	120.03
2	F	1232	PRO	C-N-CA	5.92	125.90	120.03
1	A	2293	LYS	CA-C-N	5.91	126.02	119.87
1	A	2293	LYS	C-N-CA	5.91	126.02	119.87
1	B	1233	GLY	N-CA-C	-5.91	103.51	111.54
2	F	957	GLN	CA-C-N	5.91	126.10	120.31
2	F	957	GLN	C-N-CA	5.91	126.10	120.31
1	D	612	VAL	N-CA-C	-5.89	106.74	111.81
1	A	1600	SER	N-CA-C	-5.89	106.09	113.28
1	D	1525	PHE	CA-CB-CG	5.89	119.69	113.80
1	B	142	ARG	CA-C-N	5.89	126.00	119.87
1	B	142	ARG	C-N-CA	5.89	126.00	119.87
2	F	1113	PHE	CA-C-N	5.89	125.86	120.03
2	F	1113	PHE	C-N-CA	5.89	125.86	120.03
1	E	649	PHE	CA-CB-CG	-5.89	107.91	113.80
1	C	161	THR	N-CA-C	-5.88	102.89	110.19
1	E	142	ARG	CA-C-N	5.88	125.99	119.87
1	E	142	ARG	C-N-CA	5.88	125.99	119.87
1	E	739	THR	N-CA-C	-5.88	99.99	109.58
1	E	1802	PRO	N-CA-C	-5.88	101.97	111.14
1	D	1991	ASP	CA-C-N	5.88	125.56	119.56
1	D	1991	ASP	C-N-CA	5.88	125.56	119.56
2	F	1316	GLY	CA-C-N	5.88	125.89	119.90
2	F	1316	GLY	C-N-CA	5.88	125.89	119.90
1	C	1972	HIS	CA-CB-CG	-5.87	107.93	113.80
1	D	730	PHE	CA-CB-CG	5.87	119.67	113.80
1	B	140	THR	N-CA-C	-5.87	105.21	112.90
2	F	1244	LYS	N-CA-C	5.87	120.88	113.25
2	F	1332	ASP	CB-CA-C	-5.86	100.72	110.68
1	A	1692	ILE	CA-C-N	5.86	125.77	119.85
1	A	1692	ILE	C-N-CA	5.86	125.77	119.85
1	B	392	SER	N-CA-C	5.86	117.16	108.60
1	B	831	THR	N-CA-C	5.86	115.83	108.45
1	D	2335	VAL	N-CA-C	5.85	116.30	107.75
1	B	2162	GLY	N-CA-C	-5.85	105.41	112.49
1	C	1272	ASP	N-CA-C	-5.84	100.31	109.25
2	F	2430	ILE	CA-C-N	5.84	125.75	119.85
2	F	2430	ILE	C-N-CA	5.84	125.75	119.85
1	C	1836	ASP	CA-C-N	5.82	125.44	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1836	ASP	C-N-CA	5.82	125.44	119.56
1	D	1972	HIS	CA-CB-CG	-5.82	107.98	113.80
2	F	1552	LYS	CA-C-N	5.81	125.79	120.21
2	F	1552	LYS	C-N-CA	5.81	125.79	120.21
1	D	667	ILE	N-CA-C	-5.81	107.20	111.90
1	A	354	ARG	NE-CZ-NH2	-5.81	113.97	119.20
1	B	1040	TYR	CA-C-N	5.80	125.48	119.56
1	B	1040	TYR	C-N-CA	5.80	125.48	119.56
1	A	1337	ILE	CA-C-N	5.80	125.93	119.32
1	A	1337	ILE	C-N-CA	5.80	125.93	119.32
2	F	515	VAL	N-CA-C	5.78	117.01	108.45
2	F	1931	ASP	CA-CB-CG	5.78	118.38	112.60
1	D	272	GLU	CA-C-N	5.78	125.39	119.56
1	D	272	GLU	C-N-CA	5.78	125.39	119.56
2	F	1255	ALA	CA-C-N	5.77	125.39	119.56
2	F	1255	ALA	C-N-CA	5.77	125.39	119.56
2	F	1065	THR	CA-C-N	5.76	125.73	120.03
2	F	1065	THR	C-N-CA	5.76	125.73	120.03
2	F	650	PHE	CA-C-N	5.76	125.67	119.85
2	F	650	PHE	C-N-CA	5.76	125.67	119.85
1	B	193	ARG	CA-C-N	5.76	125.37	119.56
1	B	193	ARG	C-N-CA	5.76	125.37	119.56
1	C	407	GLU	CA-C-N	-5.76	115.18	122.43
1	C	407	GLU	C-N-CA	-5.76	115.18	122.43
1	C	2402	TYR	CA-C-N	5.75	125.70	119.78
1	C	2402	TYR	C-N-CA	5.75	125.70	119.78
2	F	848	VAL	N-CA-C	5.75	114.58	108.95
2	F	1133	THR	N-CA-C	5.74	117.96	109.69
1	B	366	SER	N-CA-C	-5.73	105.01	112.23
1	C	414	LEU	CA-C-N	5.73	125.40	119.56
1	C	414	LEU	C-N-CA	5.73	125.40	119.56
2	F	802	PRO	CA-C-N	5.73	125.68	119.78
2	F	802	PRO	C-N-CA	5.73	125.68	119.78
1	A	1193	ASP	CA-C-N	-5.73	114.98	123.11
1	A	1193	ASP	C-N-CA	-5.73	114.98	123.11
1	C	1983	LEU	CA-C-N	5.72	125.70	120.03
1	C	1983	LEU	C-N-CA	5.72	125.70	120.03
1	D	824	ALA	CA-C-N	5.72	128.41	120.29
1	D	824	ALA	C-N-CA	5.72	128.41	120.29
1	C	1295	ASP	CA-CB-CG	5.71	118.31	112.60
2	F	1919	LEU	N-CA-C	-5.71	105.08	112.68
1	B	788	ALA	CA-C-O	5.71	121.25	117.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	479	PHE	CA-CB-CG	5.69	119.49	113.80
2	F	1829	MET	CA-C-N	5.69	125.64	119.78
2	F	1829	MET	C-N-CA	5.69	125.64	119.78
1	E	468	LEU	CB-CA-C	-5.69	103.65	111.73
1	B	1193	ASP	N-CA-C	-5.69	99.85	108.67
1	B	1654	THR	N-CA-C	-5.68	100.77	109.41
1	E	315	THR	CA-C-N	5.68	125.59	119.85
1	E	315	THR	C-N-CA	5.68	125.59	119.85
1	D	161	THR	N-CA-C	-5.68	102.51	110.35
1	B	529	PHE	N-CA-C	5.67	121.22	113.97
2	F	1491	THR	CA-C-N	5.66	125.86	120.31
2	F	1491	THR	C-N-CA	5.66	125.86	120.31
1	C	2326	LYS	CA-C-N	-5.66	113.51	121.72
1	C	2326	LYS	C-N-CA	-5.66	113.51	121.72
2	F	967	LEU	CA-C-N	5.66	125.63	120.03
2	F	967	LEU	C-N-CA	5.66	125.63	120.03
2	F	1537	ILE	N-CA-C	5.65	116.26	108.12
1	C	2349	GLY	CA-C-N	5.64	125.59	119.78
1	C	2349	GLY	C-N-CA	5.64	125.59	119.78
1	A	2486	PHE	CA-C-N	5.64	125.61	120.03
1	A	2486	PHE	C-N-CA	5.64	125.61	120.03
1	D	732	ASP	CA-CB-CG	5.64	118.24	112.60
1	B	1952	ILE	N-CA-C	5.63	120.32	113.00
1	E	824	ALA	CA-C-N	5.63	128.10	120.44
1	E	824	ALA	C-N-CA	5.63	128.10	120.44
1	A	2005	GLY	N-CA-C	-5.62	99.85	113.18
1	C	1632	ILE	N-CA-C	-5.62	102.27	109.30
1	E	242	SER	N-CA-C	5.62	118.57	108.17
1	B	889	VAL	N-CA-C	5.62	118.55	113.10
1	A	1520	GLN	CA-C-N	5.62	125.52	119.85
1	A	1520	GLN	C-N-CA	5.62	125.52	119.85
1	B	933	THR	N-CA-C	-5.61	106.27	113.23
1	D	1520	GLN	CA-C-N	5.61	125.51	119.85
1	D	1520	GLN	C-N-CA	5.61	125.51	119.85
1	D	384	ALA	CA-C-N	5.60	125.58	120.03
1	D	384	ALA	C-N-CA	5.60	125.58	120.03
1	A	2009	LEU	CA-C-N	5.59	125.56	120.03
1	A	2009	LEU	C-N-CA	5.59	125.56	120.03
1	C	1193	ASP	N-CA-C	-5.59	99.41	108.41
1	A	2402	TYR	CA-C-N	5.59	125.60	119.90
1	A	2402	TYR	C-N-CA	5.59	125.60	119.90
1	C	2486	PHE	CA-C-N	5.58	125.55	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2486	PHE	C-N-CA	5.58	125.55	120.03
1	D	2391	VAL	N-CA-C	5.57	116.14	108.12
1	E	501	ALA	CA-C-N	5.57	125.54	120.03
1	E	501	ALA	C-N-CA	5.57	125.54	120.03
1	A	2006	GLY	N-CA-C	-5.56	100.00	113.18
1	D	431	TYR	N-CA-C	5.56	117.47	108.41
1	E	1124	ARG	CB-CA-C	-5.56	99.30	110.30
2	F	1322	HIS	N-CA-C	5.56	116.41	108.74
2	F	848	VAL	CA-C-N	5.55	125.48	119.76
2	F	848	VAL	C-N-CA	5.55	125.48	119.76
1	D	739	THR	N-CA-C	-5.55	99.44	109.09
1	B	346	PHE	CA-C-N	5.54	125.74	120.31
1	B	346	PHE	C-N-CA	5.54	125.74	120.31
1	A	501	ALA	CA-C-N	5.53	125.73	120.31
1	A	501	ALA	C-N-CA	5.53	125.73	120.31
1	C	1279	THR	CA-C-N	5.53	125.88	119.47
1	C	1279	THR	C-N-CA	5.53	125.88	119.47
1	E	2335	VAL	N-CA-C	5.52	115.81	107.75
1	E	1623	THR	N-CA-C	-5.51	106.72	113.50
1	A	529	PHE	N-CA-C	5.51	120.88	113.72
1	B	521	THR	N-CA-C	-5.51	106.09	113.25
1	D	1836	ASP	CA-C-N	5.51	125.18	119.56
1	D	1836	ASP	C-N-CA	5.51	125.18	119.56
1	D	448	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	D	1632	ILE	N-CA-C	-5.50	102.43	109.30
1	A	296	PHE	CA-CB-CG	5.50	119.30	113.80
1	D	1193	ASP	N-CA-C	-5.50	101.38	109.62
1	C	1692	ILE	CA-C-N	5.49	125.40	119.85
1	C	1692	ILE	C-N-CA	5.49	125.40	119.85
2	F	243	LEU	CA-C-N	5.49	125.11	119.56
2	F	243	LEU	C-N-CA	5.49	125.11	119.56
2	F	1081	ASN	N-CA-C	-5.49	101.85	110.36
1	E	299	LYS	CA-C-N	5.49	130.88	121.87
1	E	299	LYS	C-N-CA	5.49	130.88	121.87
1	A	1132	ASN	CA-CB-CG	5.49	118.09	112.60
2	F	29	THR	N-CA-C	5.49	116.58	109.72
1	C	1336	ASP	N-CA-C	5.49	115.79	108.38
1	A	1279	THR	N-CA-C	-5.48	103.13	109.93
1	D	1634	GLU	CA-C-N	5.48	125.42	119.78
1	D	1634	GLU	C-N-CA	5.48	125.42	119.78
1	E	1759	ASP	N-CA-C	5.48	117.23	108.41
1	E	1972	HIS	CA-CB-CG	-5.47	108.33	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	824	ALA	CA-C-N	5.47	127.87	120.44
1	B	824	ALA	C-N-CA	5.47	127.87	120.44
2	F	633	ILE	N-CA-C	5.46	115.71	107.80
1	A	1868	TYR	CB-CA-C	-5.45	102.32	110.88
1	C	672	ASP	CA-CB-CG	5.45	118.05	112.60
2	F	1968	ASP	N-CA-C	-5.45	102.22	110.28
1	C	2331	VAL	N-CA-C	5.45	115.73	108.11
2	F	2117	ARG	N-CA-C	5.44	117.46	109.24
1	A	685	LYS	N-CA-C	-5.44	107.19	113.88
1	E	2380	GLY	N-CA-C	-5.44	104.25	112.41
1	B	649	PHE	CA-CB-CG	-5.44	108.36	113.80
1	A	1202	HIS	N-CA-C	5.44	117.45	109.24
1	D	520	ASN	CA-CB-CG	-5.44	107.16	112.60
1	D	596	ASP	N-CA-C	5.43	118.37	111.69
1	C	1520	GLN	CA-C-N	5.42	125.33	119.85
1	C	1520	GLN	C-N-CA	5.42	125.33	119.85
1	D	1148	ASP	CA-CB-CG	-5.42	107.18	112.60
1	B	105	ALA	CA-C-N	5.41	125.02	119.56
1	B	105	ALA	C-N-CA	5.41	125.02	119.56
1	D	1692	ILE	CA-C-N	5.41	125.31	119.85
1	D	1692	ILE	C-N-CA	5.41	125.31	119.85
1	D	2402	TYR	CA-C-N	5.41	125.35	119.78
1	D	2402	TYR	C-N-CA	5.41	125.35	119.78
1	D	572	ASP	N-CA-C	-5.39	105.83	112.90
1	E	512	PRO	N-CA-C	-5.39	102.81	111.38
1	A	831	THR	N-CA-C	5.37	115.38	108.34
2	F	531	GLY	N-CA-C	-5.37	102.95	110.63
1	B	1745	GLU	N-CA-C	-5.37	105.51	111.36
1	B	1836	ASP	CA-C-N	5.36	125.02	119.56
1	B	1836	ASP	C-N-CA	5.36	125.02	119.56
2	F	1522	ILE	N-CA-C	5.35	115.56	107.80
2	F	2066	ASP	CA-CB-CG	5.35	117.95	112.60
1	B	548	LYS	N-CA-C	-5.35	105.53	111.36
1	A	1046	ASP	CA-C-N	5.34	125.01	119.56
1	A	1046	ASP	C-N-CA	5.34	125.01	119.56
1	D	1835	VAL	N-CA-C	-5.34	108.08	113.47
1	E	235	SER	N-CA-C	-5.34	105.35	111.07
1	E	1291	TYR	N-CA-C	-5.34	102.98	110.35
2	F	2038	GLU	N-CA-C	-5.34	106.90	113.41
1	C	824	ALA	CA-C-N	5.33	127.69	120.44
1	C	824	ALA	C-N-CA	5.33	127.69	120.44
1	D	1520	GLN	N-CA-C	-5.33	103.31	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1012	VAL	N-CA-C	-5.33	107.58	111.90
1	D	901	ASP	N-CA-C	5.33	117.29	109.24
1	A	1821	LEU	N-CA-C	-5.32	105.93	112.90
2	F	1668	VAL	N-CA-C	5.32	116.37	108.23
1	D	740	PRO	N-CA-C	-5.32	102.85	111.14
1	B	1270	PHE	CA-CB-CG	-5.31	108.49	113.80
1	C	1178	THR	N-CA-C	5.31	115.25	108.24
1	B	1623	THR	N-CA-C	-5.30	104.40	112.04
2	F	348	PHE	CA-CB-CG	5.30	119.10	113.80
1	D	193	ARG	CA-C-N	5.30	125.76	120.04
1	D	193	ARG	C-N-CA	5.30	125.76	120.04
2	F	2019	LEU	N-CA-C	5.30	117.53	108.90
1	B	1692	ILE	CA-C-N	5.29	125.19	119.85
1	B	1692	ILE	C-N-CA	5.29	125.19	119.85
1	C	193	ARG	CA-C-N	5.27	124.89	119.56
1	C	193	ARG	C-N-CA	5.27	124.89	119.56
1	C	1768	PHE	N-CA-C	-5.27	106.69	113.23
2	F	546	LEU	CA-C-N	5.27	125.17	119.85
2	F	546	LEU	C-N-CA	5.27	125.17	119.85
1	A	742	SER	N-CA-C	5.26	117.26	108.99
2	F	1268	PHE	CA-CB-CG	-5.26	108.54	113.80
1	B	453	SER	CA-C-N	5.26	124.87	119.56
1	B	453	SER	C-N-CA	5.26	124.87	119.56
1	D	1702	ASP	N-CA-C	-5.26	106.01	112.90
2	F	1538	ASP	CA-C-N	5.26	124.92	119.56
2	F	1538	ASP	C-N-CA	5.26	124.92	119.56
1	B	2331	VAL	N-CA-C	5.25	115.47	108.11
1	A	2335	VAL	N-CA-C	5.25	115.41	107.75
2	F	2072	ILE	N-CA-C	-5.24	106.69	111.67
1	B	348	PHE	CA-CB-CG	5.24	119.04	113.80
1	D	802	ILE	CB-CA-C	-5.24	105.27	111.97
2	F	1261	PRO	CB-CA-C	5.23	117.84	110.98
2	F	1320	PRO	CA-C-N	5.23	125.15	119.76
2	F	1320	PRO	C-N-CA	5.23	125.15	119.76
1	B	1279	THR	N-CA-C	-5.23	102.55	110.39
1	D	185	VAL	N-CA-C	-5.23	106.70	111.67
1	B	1983	LEU	CA-C-N	5.21	125.18	120.03
1	B	1983	LEU	C-N-CA	5.21	125.18	120.03
1	D	105	ALA	CA-C-N	5.21	124.82	119.56
1	D	105	ALA	C-N-CA	5.21	124.82	119.56
1	B	299	LYS	CA-C-N	5.20	130.38	122.11
1	B	299	LYS	C-N-CA	5.20	130.38	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	322	ASP	CA-CB-CG	-5.20	107.40	112.60
1	C	298	GLY	N-CA-C	-5.20	105.92	114.76
1	C	1821	LEU	N-CA-C	-5.20	106.09	112.90
2	F	41	LEU	CA-C-N	5.20	125.41	120.31
2	F	41	LEU	C-N-CA	5.20	125.41	120.31
1	C	296	PHE	CA-CB-CG	5.20	119.00	113.80
1	C	598	HIS	CA-C-N	-5.19	114.23	122.23
1	C	598	HIS	C-N-CA	-5.19	114.23	122.23
1	A	1620	GLY	N-CA-C	5.19	117.34	112.04
1	E	670	LEU	N-CA-C	-5.19	106.10	112.90
1	C	2374	ASN	N-CA-C	5.18	116.17	108.60
1	C	2344	LEU	CA-C-N	5.18	125.12	119.78
1	C	2344	LEU	C-N-CA	5.18	125.12	119.78
1	B	1099	ASP	N-CA-C	5.18	117.83	111.82
2	F	1790	ARG	CA-C-N	5.18	124.79	119.56
2	F	1790	ARG	C-N-CA	5.18	124.79	119.56
1	C	894	VAL	N-CA-C	-5.18	105.36	111.00
1	C	101	SER	N-CA-C	5.18	121.83	110.80
1	C	499	CYS	N-CA-C	-5.17	106.56	112.92
1	E	696	ILE	N-CA-C	-5.17	104.62	111.09
2	F	1447	PHE	N-CA-C	5.17	116.93	109.07
1	D	782	LYS	CA-C-N	5.17	124.83	119.56
1	D	782	LYS	C-N-CA	5.17	124.83	119.56
1	E	1868	TYR	CB-CA-C	-5.17	102.20	110.79
2	F	1837	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	1051	ILE	N-CA-C	5.17	115.75	108.36
1	E	383	GLY	N-CA-C	-5.17	106.08	112.33
1	B	232	HIS	N-CA-C	-5.16	103.23	110.50
1	B	1291	TYR	N-CA-C	-5.16	103.23	110.35
1	A	752	ILE	N-CA-C	-5.15	105.36	110.62
1	B	1715	PRO	N-CA-C	-5.15	105.53	112.48
1	E	272	GLU	CA-C-N	5.15	124.81	119.56
1	E	272	GLU	C-N-CA	5.15	124.81	119.56
1	B	385	PRO	CB-CA-C	5.15	117.72	110.98
1	C	402	ILE	CB-CA-C	-5.14	104.82	111.20
1	D	696	ILE	N-CA-C	-5.14	104.84	112.04
2	F	1410	TRP	N-CA-C	-5.14	107.67	114.31
1	B	953	GLN	N-CA-C	5.14	120.55	113.97
1	A	2244	LYS	N-CA-C	-5.14	103.62	110.55
1	E	1692	ILE	CA-C-N	5.14	125.04	119.85
1	E	1692	ILE	C-N-CA	5.14	125.04	119.85
1	A	315	THR	CA-C-N	5.13	125.58	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	THR	C-N-CA	5.13	125.58	120.14
1	A	1835	VAL	N-CA-C	-5.13	108.28	113.47
1	B	183	THR	N-CA-C	-5.13	106.18	112.90
2	F	1001	ARG	CA-C-N	-5.13	116.13	123.11
2	F	1001	ARG	C-N-CA	-5.13	116.13	123.11
2	F	1334	ASP	CA-C-N	5.13	124.74	119.56
2	F	1334	ASP	C-N-CA	5.13	124.74	119.56
1	C	1598	TRP	CB-CA-C	5.13	115.78	109.16
1	A	2374	ASN	N-CA-C	5.13	116.09	108.60
1	C	1046	ASP	CA-C-N	5.13	124.74	119.56
1	C	1046	ASP	C-N-CA	5.13	124.74	119.56
2	F	1696	LEU	N-CA-C	5.13	118.10	109.95
1	B	2335	VAL	N-CA-C	5.12	115.23	107.75
1	E	1616	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	B	1634	GLU	CA-C-N	5.12	125.02	119.85
1	B	1634	GLU	C-N-CA	5.12	125.02	119.85
1	D	1012	VAL	N-CA-C	-5.12	107.76	111.90
1	B	1012	VAL	N-CA-C	-5.11	107.76	111.90
2	F	274	PRO	CA-C-N	5.11	125.02	119.85
2	F	274	PRO	C-N-CA	5.11	125.02	119.85
2	F	1673	SER	N-CA-C	5.11	116.84	109.07
1	B	598	HIS	N-CA-C	-5.11	102.95	110.52
1	C	1326	ASP	N-CA-C	5.11	116.85	111.28
1	D	1655	HIS	CA-CB-CG	5.11	118.91	113.80
1	B	337	ASN	N-CA-C	5.11	117.28	109.62
1	B	1843	HIS	N-CA-C	-5.10	105.61	111.07
1	D	779	PHE	CA-CB-CG	5.10	118.90	113.80
1	A	596	ASP	N-CA-C	5.10	116.92	111.36
1	B	2141	VAL	CA-C-N	5.10	124.77	119.56
1	B	2141	VAL	C-N-CA	5.10	124.77	119.56
1	E	584	ASN	CA-CB-CG	-5.10	107.50	112.60
2	F	606	ASN	CA-C-N	5.10	126.21	119.84
2	F	606	ASN	C-N-CA	5.10	126.21	119.84
2	F	1566	LEU	N-CA-C	-5.09	107.19	113.41
1	A	1759	ASP	N-CA-C	5.09	116.56	108.67
2	F	786	GLN	N-CA-C	5.09	116.82	108.52
1	B	707	VAL	N-CA-C	-5.09	105.75	110.53
1	D	1801	SER	CA-C-N	5.08	124.75	119.56
1	D	1801	SER	C-N-CA	5.08	124.75	119.56
1	E	1634	GLU	CA-C-N	5.08	124.98	119.85
1	E	1634	GLU	C-N-CA	5.08	124.98	119.85
2	F	34	ASP	CA-CB-CG	-5.08	107.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	670	LEU	N-CA-C	-5.08	105.44	111.69
1	E	453	SER	N-CA-C	-5.08	103.19	109.64
1	C	1124	ARG	CB-CA-C	-5.07	99.39	109.79
1	D	2240	PHE	N-CA-C	-5.07	105.22	111.40
2	F	696	PRO	CA-C-N	-5.07	114.69	122.60
2	F	696	PRO	C-N-CA	-5.07	114.69	122.60
1	E	1841	ALA	CA-C-O	-5.07	116.22	121.99
2	F	1972	TYR	N-CA-C	5.07	117.37	109.52
1	E	590	ILE	CB-CA-C	-5.06	105.49	111.97
2	F	505	ASP	CA-CB-CG	5.05	117.66	112.60
1	C	2380	GLY	N-CA-C	-5.05	104.83	112.41
1	D	1623	THR	N-CA-C	-5.05	104.77	112.04
1	A	2284	LEU	N-CA-C	-5.04	101.49	109.76
1	D	1316	VAL	N-CA-C	5.04	115.38	108.12
1	D	1697	VAL	CA-C-N	5.04	125.02	120.03
1	D	1697	VAL	C-N-CA	5.04	125.02	120.03
1	B	1050	ARG	NE-CZ-NH2	5.04	123.73	119.20
2	F	326	GLY	CA-C-N	5.04	124.95	119.76
2	F	326	GLY	C-N-CA	5.04	124.95	119.76
1	C	2335	VAL	N-CA-C	5.03	115.10	107.80
2	F	707	GLY	CA-C-N	-5.03	116.58	123.12
2	F	707	GLY	C-N-CA	-5.03	116.58	123.12
2	F	1260	MET	CA-C-N	5.03	124.94	119.85
2	F	1260	MET	C-N-CA	5.03	124.94	119.85
2	F	2004	LEU	N-CA-C	5.03	117.53	108.48
1	D	909	THR	CA-C-N	5.03	124.92	119.85
1	D	909	THR	C-N-CA	5.03	124.92	119.85
1	B	95	GLN	N-CA-C	-5.02	102.33	110.32
2	F	87	VAL	CA-C-N	5.02	124.93	119.76
2	F	87	VAL	C-N-CA	5.02	124.93	119.76
1	C	670	LEU	N-CA-C	-5.02	105.91	112.23
1	C	1369	ARG	N-CA-C	-5.02	105.89	111.36
1	E	1099	ASP	N-CA-C	5.02	117.64	111.82
1	C	516	ASP	CA-CB-CG	5.02	117.62	112.60
1	D	1295	ASP	CA-CB-CG	5.01	117.61	112.60
1	B	1757	PRO	N-CA-C	5.01	121.70	112.33
1	B	1552	ASP	CA-CB-CG	5.01	117.61	112.60
1	C	2157	ILE	N-CA-C	-5.01	105.96	110.82
1	A	1270	PHE	CA-CB-CG	-5.00	108.80	113.80
1	A	464	VAL	N-CA-C	5.00	115.95	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	766	TYR	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	A	18197	0	17794	38	0
1	B	18197	0	17794	46	0
1	C	18197	0	17794	52	0
1	D	18197	0	17794	41	0
1	E	18197	0	17794	39	0
2	F	17285	0	16668	51	0
All	All	108270	0	105638	259	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 (259) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1623:THR:OG1	1:B:1624:ILE:N	2.32	0.61
1:B:2319:ASP:OD2	1:B:2323:LYS:NZ	2.36	0.58
1:B:2358:ASP:OD1	1:B:2502:LYS:NZ	2.38	0.57
2:F:1416:ASP:N	2:F:1416:ASP:OD1	2.37	0.57
1:C:624:ASP:N	1:C:624:ASP:OD1	2.37	0.57
1:E:624:ASP:OD1	1:E:624:ASP:N	2.37	0.57
1:D:1148:ASP:OD1	1:D:1148:ASP:N	2.33	0.56
1:A:2207:ASP:OD2	1:A:2211:LYS:NZ	2.38	0.56
1:D:624:ASP:OD1	1:D:624:ASP:N	2.37	0.56
1:C:329:ARG:NH1	1:C:434:TYR:OH	2.39	0.56
1:C:2207:ASP:OD2	1:C:2211:LYS:NZ	2.38	0.56
1:B:624:ASP:OD1	1:B:624:ASP:N	2.37	0.56
1:B:1072:ASP:OD1	1:B:1072:ASP:N	2.36	0.56
1:D:253:GLU:O	1:D:442:LYS:NZ	2.38	0.56
2:F:73:ASP:OD1	2:F:74:CYS:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2319:ASP:OD2	1:A:2323:LYS:NZ	2.39	0.56
1:B:1626:SER:OG	1:B:1627:MET:N	2.40	0.55
1:A:2358:ASP:OD1	1:A:2502:LYS:NZ	2.39	0.55
1:A:624:ASP:N	1:A:624:ASP:OD1	2.38	0.55
2:F:385:ASP:N	2:F:385:ASP:OD1	2.39	0.54
1:B:2257:ARG:NH2	1:C:2309:THR:OG1	2.40	0.54
1:D:890:ALA:O	1:D:892:GLN:N	2.42	0.53
1:A:1225:LYS:NZ	1:A:1226:LEU:O	2.40	0.53
1:D:1774:TYR:HH	1:D:1848:TYR:HH	1.54	0.53
1:D:2257:ARG:NH2	1:E:2309:THR:OG1	2.42	0.53
1:E:2358:ASP:OD1	1:E:2502:LYS:NZ	2.42	0.52
1:C:890:ALA:O	1:C:892:GLN:N	2.41	0.52
1:E:548:LYS:NZ	1:E:559:ASP:OD1	2.42	0.52
1:E:890:ALA:O	1:E:892:GLN:N	2.42	0.52
1:B:890:ALA:O	1:B:892:GLN:N	2.42	0.52
1:A:1120:GLU:OE2	1:A:1146:LYS:NZ	2.42	0.52
1:D:1683:ASP:OD1	1:D:1683:ASP:N	2.43	0.52
1:D:301:SER:OG	1:D:302:ASN:N	2.42	0.51
2:F:179:SER:OG	2:F:180:GLN:N	2.43	0.51
1:C:1507:LYS:NZ	1:C:1538:ASP:OD2	2.39	0.51
1:A:1164:LYS:NZ	1:B:1622:ASP:OD2	2.36	0.51
1:C:540:SER:OG	1:C:541:GLY:N	2.44	0.51
1:C:1290:SER:C	1:C:1291:TYR:O	2.49	0.51
1:C:1291:TYR:O	1:C:1292:GLN:HB3	2.11	0.51
1:A:261:GLU:OE1	1:A:1380:LYS:NZ	2.44	0.50
1:B:342:ASP:OD2	1:B:360:LYS:NZ	2.44	0.50
1:D:2319:ASP:OD2	1:D:2323:LYS:NZ	2.45	0.50
1:E:1841:ALA:O	1:E:1842:GLN:HB2	2.11	0.50
1:B:1333:TYR:O	1:B:1334:ASN:C	2.54	0.50
1:D:797:ASP:OD1	1:D:798:ALA:N	2.45	0.50
1:D:848:GLN:HE21	1:D:852:GLN:HE21	1.60	0.50
1:A:890:ALA:O	1:A:892:GLN:N	2.45	0.50
1:B:540:SER:OG	1:B:541:GLY:N	2.44	0.50
2:F:754:GLU:O	2:F:755:ILE:HB	2.12	0.50
1:C:1117:ASP:OD1	1:C:1118:ALA:N	2.45	0.49
1:A:180:GLU:OE1	1:A:184:LYS:NZ	2.45	0.49
1:C:301:SER:OG	1:C:302:ASN:N	2.46	0.49
1:E:161:THR:O	1:E:162:LEU:HB3	2.13	0.49
2:F:1427:ASP:OD1	2:F:1427:ASP:C	2.55	0.49
1:E:176:GLU:OE2	1:E:956:LYS:NZ	2.47	0.48
1:E:2287:ASP:OD1	1:E:2287:ASP:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1687:ASP:OD1	2:F:1687:ASP:N	2.38	0.48
2:F:153:ASP:O	2:F:174:ARG:NH2	2.46	0.48
2:F:1234:SER:OG	2:F:1235:ASP:N	2.46	0.48
1:C:1841:ALA:O	1:C:1842:GLN:HB2	2.14	0.48
1:D:521:THR:H	1:D:522:PRO:HD2	1.79	0.48
1:D:1333:TYR:CG	1:D:1334:ASN:N	2.82	0.48
1:E:2466:ASP:OD1	1:E:2466:ASP:N	2.46	0.48
1:B:2380:GLY:N	1:B:2383:THR:OG1	2.46	0.48
1:B:1841:ALA:O	1:B:1842:GLN:HB2	2.14	0.48
1:A:1561:ASP:OD1	1:A:1561:ASP:N	2.46	0.47
1:A:1834:SER:OG	1:A:1835:VAL:N	2.47	0.47
1:B:1148:ASP:OD1	1:B:1148:ASP:N	2.45	0.47
1:B:1178:THR:OG1	1:B:1179:LYS:N	2.47	0.47
2:F:1133:THR:OG1	2:F:1134:ALA:N	2.45	0.47
1:B:1514:ASP:OD1	1:B:1514:ASP:N	2.46	0.47
1:C:1178:THR:OG1	1:C:1179:LYS:N	2.46	0.47
1:D:1841:ALA:O	1:D:1842:GLN:HB2	2.13	0.47
1:B:1834:SER:OG	1:B:1835:VAL:N	2.46	0.47
1:E:1991:ASP:OD2	1:E:1993:LYS:NZ	2.45	0.47
1:A:1343:LYS:NZ	1:B:1803:SER:O	2.47	0.47
1:B:1975:SER:OG	1:B:1976:ILE:N	2.48	0.47
2:F:830:GLN:O	2:F:955:ARG:NH2	2.47	0.47
1:B:2103:TYR:O	1:B:2189:ARG:NH1	2.48	0.47
1:B:2284:LEU:O	1:B:2286:ASP:N	2.48	0.47
1:C:1333:TYR:CG	1:C:1334:ASN:N	2.82	0.47
1:E:540:SER:OG	1:E:541:GLY:N	2.47	0.47
1:E:1124:ARG:HD3	1:E:1144:TRP:CD2	2.50	0.47
1:E:1046:ASP:C	1:E:1046:ASP:OD1	2.55	0.47
2:F:431:ASP:OD1	2:F:431:ASP:N	2.44	0.47
1:B:533:ASP:OD1	1:B:533:ASP:N	2.37	0.47
1:C:872:THR:O	1:C:873:SER:HB2	2.15	0.47
2:F:829:ASP:N	2:F:829:ASP:OD1	2.39	0.47
1:B:477:LYS:NZ	1:B:624:ASP:OD2	2.40	0.46
1:D:290:ASP:OD1	1:D:290:ASP:N	2.43	0.46
1:A:2103:TYR:O	1:A:2189:ARG:NH1	2.49	0.46
1:C:1206:ASP:OD1	1:C:1206:ASP:N	2.42	0.46
1:E:270:ASN:OD1	1:E:270:ASN:N	2.46	0.46
1:A:1133:ASP:OD1	1:A:1133:ASP:N	2.40	0.46
1:C:270:ASN:OD1	1:C:270:ASN:N	2.48	0.46
1:D:1834:SER:OG	1:D:1835:VAL:N	2.49	0.46
1:E:857:GLN:N	1:E:857:GLN:CD	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1514:ASP:OD2	1:E:1515:LYS:NZ	2.46	0.46
1:B:1183:ASN:OD1	1:B:1183:ASN:N	2.44	0.46
1:D:161:THR:O	1:D:162:LEU:HB3	2.16	0.46
2:F:1329:ASP:N	2:F:1329:ASP:OD1	2.43	0.46
1:A:1333:TYR:O	1:A:1334:ASN:C	2.58	0.46
1:C:1975:SER:OG	1:C:1976:ILE:N	2.47	0.46
1:D:2466:ASP:OD1	1:D:2466:ASP:N	2.46	0.45
1:E:2103:TYR:O	1:E:2189:ARG:NH1	2.49	0.45
2:F:1055:THR:OG1	2:F:1056:ASP:N	2.49	0.45
1:C:176:GLU:OE2	1:C:956:LYS:NZ	2.48	0.45
1:A:1683:ASP:OD1	1:A:1683:ASP:N	2.43	0.45
2:F:283:TRP:CD1	2:F:283:TRP:H	2.33	0.45
1:A:465:ASN:O	1:A:466:LEU:C	2.58	0.45
1:B:357:TYR:CZ	1:B:391:TYR:HB2	2.52	0.45
1:C:1829:SER:OG	1:C:1830:ASP:N	2.50	0.45
1:C:1977:ASP:N	1:C:1977:ASP:OD1	2.45	0.45
1:A:842:ASP:OD1	1:A:843:ALA:N	2.50	0.45
1:C:1834:SER:OG	1:C:1835:VAL:N	2.50	0.45
1:C:1124:ARG:HD3	1:C:1144:TRP:CD2	2.52	0.45
1:C:2103:TYR:O	1:C:2189:ARG:NH1	2.50	0.45
1:D:766:TYR:CD1	1:D:771:ILE:HD11	2.52	0.45
1:E:1834:SER:OG	1:E:1835:VAL:N	2.50	0.45
1:A:176:GLU:OE2	1:A:956:LYS:NZ	2.50	0.44
1:D:329:ARG:HB3	1:D:431:TYR:CE1	2.53	0.44
1:B:250:ILE:O	1:B:442:LYS:NZ	2.50	0.44
1:D:2284:LEU:O	1:D:2286:ASP:N	2.50	0.44
2:F:754:GLU:O	2:F:755:ILE:CB	2.65	0.44
1:A:161:THR:O	1:A:162:LEU:HB3	2.17	0.44
1:E:533:ASP:OD1	1:E:533:ASP:N	2.48	0.44
2:F:904:SER:O	2:F:905:ARG:C	2.56	0.44
2:F:1793:ASP:N	2:F:1793:ASP:OD1	2.47	0.44
1:B:1343:LYS:NZ	1:C:1803:SER:O	2.50	0.44
1:C:2457:SER:OG	1:C:2458:GLY:N	2.50	0.44
1:C:2466:ASP:N	1:C:2466:ASP:OD1	2.45	0.44
1:D:1290:SER:O	1:D:1291:TYR:C	2.57	0.44
1:D:1975:SER:OG	1:D:1976:ILE:N	2.50	0.44
1:D:2365:SER:OG	1:D:2366:GLY:N	2.50	0.44
1:E:963:SER:OG	1:E:964:ARG:N	2.48	0.44
1:C:336:THR:OG1	1:C:337:ASN:N	2.49	0.44
1:A:1622:ASP:OD2	1:E:1164:LYS:NZ	2.35	0.44
1:A:537:ASP:OD1	1:A:538:LEU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2466:ASP:N	1:B:2466:ASP:OD1	2.47	0.44
1:D:658:SER:O	1:D:659:TYR:C	2.60	0.44
1:E:1153:PRO:O	1:E:1154:TYR:C	2.60	0.44
1:E:2365:SER:OG	1:E:2366:GLY:N	2.51	0.44
1:C:1683:ASP:OD1	1:C:1683:ASP:N	2.43	0.44
1:D:963:SER:OG	1:D:964:ARG:N	2.49	0.44
2:F:618:SER:OG	2:F:619:GLY:N	2.50	0.44
2:F:1591:THR:OG1	2:F:1592:ALA:N	2.51	0.44
1:A:545:ASP:OD1	1:A:545:ASP:C	2.60	0.43
1:A:2466:ASP:OD1	1:A:2466:ASP:N	2.50	0.43
2:F:1347:ASP:C	2:F:1347:ASP:OD1	2.61	0.43
2:F:530:ASP:OD1	2:F:530:ASP:N	2.51	0.43
2:F:903:ASP:C	2:F:904:SER:O	2.60	0.43
1:C:2358:ASP:OD1	1:C:2502:LYS:NZ	2.49	0.43
2:F:209:ASP:OD1	2:F:209:ASP:N	2.46	0.43
2:F:1912:ASN:O	2:F:2125:ARG:NH2	2.51	0.43
1:D:1257:ASP:N	1:D:1257:ASP:OD1	2.46	0.43
1:A:534:GLU:N	1:A:534:GLU:OE1	2.52	0.43
1:C:1290:SER:O	1:C:1291:TYR:C	2.60	0.43
1:D:693:ALA:HB3	1:D:694:PRO:HD3	2.01	0.43
2:F:1882:ASP:OD1	2:F:1882:ASP:C	2.60	0.43
1:C:912:TYR:CD1	1:C:912:TYR:C	2.97	0.43
1:E:912:TYR:CD1	1:E:912:TYR:C	2.95	0.43
1:E:1507:LYS:NZ	1:E:1538:ASP:OD2	2.41	0.43
2:F:1528:ASP:OD1	2:F:1528:ASP:C	2.60	0.43
1:B:963:SER:OG	1:B:964:ARG:N	2.50	0.43
1:C:2010:PRO:O	1:C:2011:GLU:C	2.62	0.43
1:D:342:ASP:OD2	1:D:360:LYS:NZ	2.46	0.43
2:F:253:GLN:O	2:F:259:TYR:OH	2.36	0.43
1:A:1183:ASN:OD1	1:A:1183:ASN:N	2.50	0.43
2:F:2157:LEU:O	2:F:2158:MET:C	2.62	0.43
1:B:1138:ALA:HB3	1:B:1842:GLN:OE1	2.19	0.43
1:E:975:ASN:N	1:E:975:ASN:OD1	2.42	0.43
1:E:1183:ASN:OD1	1:E:1183:ASN:N	2.48	0.43
1:A:2347:ASP:OD1	1:A:2347:ASP:N	2.47	0.42
1:D:1291:TYR:O	1:D:1292:GLN:HB2	2.19	0.42
2:F:1370:ASP:OD1	2:F:1370:ASP:N	2.48	0.42
2:F:2090:ASN:OD1	2:F:2091:GLN:N	2.52	0.42
1:A:1524:SER:OG	1:A:1525:PHE:N	2.51	0.42
1:C:1561:ASP:OD1	1:C:1561:ASP:N	2.48	0.42
1:E:329:ARG:HB3	1:E:431:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:436:PHE:O	1:E:437:LEU:C	2.62	0.42
1:C:1137:ALA:O	1:C:1138:ALA:HB3	2.19	0.42
1:E:2284:LEU:O	1:E:2286:ASP:N	2.52	0.42
1:C:196:GLY:N	1:C:285:TYR:OH	2.52	0.42
2:F:1432:ASP:OD1	2:F:1432:ASP:C	2.62	0.42
1:B:1729:ASP:OD2	1:B:1730:LYS:NZ	2.52	0.42
2:F:1442:THR:OG1	2:F:1443:ALA:N	2.52	0.42
1:C:1291:TYR:O	1:C:1292:GLN:CB	2.65	0.42
1:D:968:TYR:CD1	1:D:968:TYR:C	2.96	0.42
1:D:1124:ARG:HD2	1:D:1144:TRP:CE2	2.54	0.42
1:E:160:SER:C	1:E:161:THR:O	2.54	0.42
1:E:771:ILE:HD12	1:E:776:PHE:HA	2.00	0.42
1:B:1333:TYR:O	1:B:1335:GLY:N	2.53	0.42
1:C:353:TYR:CE1	1:C:397:LEU:HB2	2.54	0.42
1:C:1514:ASP:OD2	1:C:1515:LYS:NZ	2.48	0.42
1:E:386:GLN:OE1	1:E:391:TYR:OH	2.38	0.42
2:F:854:ASP:C	2:F:854:ASP:OD1	2.61	0.42
1:C:477:LYS:NZ	1:C:624:ASP:OD2	2.39	0.42
1:C:2496:LYS:NZ	1:D:2401:ASP:OD1	2.49	0.42
1:D:773:GLU:HA	1:D:776:PHE:CD1	2.55	0.42
1:D:2287:ASP:OD1	1:D:2287:ASP:N	2.46	0.42
2:F:2117:ARG:NH1	2:F:2140:LEU:O	2.53	0.42
1:A:2382:ASP:OD1	1:A:2382:ASP:N	2.47	0.42
1:B:93:ASN:OD1	1:B:93:ASN:N	2.47	0.42
1:C:1908:ASP:OD1	1:C:1908:ASP:N	2.52	0.42
1:E:1840:VAL:C	1:E:1841:ALA:O	2.52	0.42
1:A:488:TYR:OH	1:A:635:ASN:OD1	2.36	0.41
1:B:1124:ARG:HD2	1:B:1144:TRP:CD2	2.55	0.41
1:A:1991:ASP:OD2	1:A:1993:LYS:NZ	2.47	0.41
1:C:1868:TYR:CD2	1:C:1868:TYR:C	2.98	0.41
1:D:2140:LEU:O	1:D:2141:VAL:C	2.63	0.41
2:F:1718:ASP:C	2:F:1718:ASP:OD1	2.62	0.41
1:B:2382:ASP:OD1	1:B:2382:ASP:N	2.51	0.41
1:D:1872:GLU:O	1:D:1873:ARG:C	2.63	0.41
1:E:608:LEU:O	1:E:609:LEU:C	2.62	0.41
1:A:477:LYS:NZ	1:A:624:ASP:OD2	2.46	0.41
1:B:455:THR:OG1	1:B:456:ILE:N	2.53	0.41
1:B:1124:ARG:HG3	1:B:1144:TRP:CE3	2.55	0.41
1:E:299:LYS:NZ	1:E:458:GLU:OE2	2.53	0.41
1:A:1684:THR:OG1	1:A:1685:ASN:N	2.54	0.41
1:B:1117:ASP:OD1	1:B:1118:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2365:SER:OG	1:A:2366:GLY:N	2.53	0.41
1:B:736:THR:OG1	1:B:737:LYS:N	2.50	0.41
1:D:782:LYS:N	1:D:783:PRO:HD3	2.36	0.41
2:F:772:ASP:OD1	2:F:779:ARG:NE	2.53	0.41
1:C:436:PHE:O	1:C:437:LEU:C	2.63	0.41
2:F:574:SER:OG	2:F:575:ALA:N	2.54	0.41
1:A:2103:TYR:CE1	1:A:2193:GLU:HB2	2.55	0.41
1:B:436:PHE:O	1:B:437:LEU:C	2.64	0.41
1:B:2382:ASP:OD2	1:C:2404:ALA:N	2.54	0.41
1:B:2478:ASP:OD1	1:B:2478:ASP:N	2.40	0.41
1:D:322:ASP:OD1	1:D:322:ASP:N	2.32	0.41
1:D:707:VAL:HG13	1:D:776:PHE:CD2	2.55	0.41
2:F:1484:ASP:OD2	2:F:1486:LYS:NZ	2.37	0.41
1:B:831:THR:OG1	1:B:832:ALA:N	2.54	0.41
2:F:1268:PHE:O	2:F:1272:ALA:N	2.55	0.41
2:F:1515:ASN:N	2:F:1515:ASN:OD1	2.46	0.41
2:F:2044:ASP:OD1	2:F:2044:ASP:N	2.45	0.41
1:C:658:SER:O	1:C:659:TYR:C	2.64	0.40
1:C:1497:LYS:HB3	1:C:1558:PHE:HB2	2.02	0.40
1:C:1915:THR:O	1:C:1916:GLN:C	2.61	0.40
1:D:436:PHE:O	1:D:437:LEU:C	2.63	0.40
2:F:1247:PRO:HA	2:F:1332:ASP:OD1	2.21	0.40
1:C:2287:ASP:N	1:C:2287:ASP:OD1	2.45	0.40
1:B:2459:GLN:OE1	1:B:2459:GLN:N	2.53	0.40
1:C:542:SER:OG	1:C:543:THR:N	2.49	0.40
2:F:269:ASN:OD1	2:F:269:ASN:N	2.47	0.40
2:F:283:TRP:CZ3	2:F:303:ARG:HB3	2.56	0.40
2:F:1393:ASP:OD1	2:F:1393:ASP:N	2.49	0.40
1:A:2466:ASP:OD1	1:A:2467:GLY:N	2.55	0.40
1:C:322:ASP:OD1	1:C:323:GLY:N	2.54	0.40
1:E:1559:ALA:HB3	1:E:1563:ARG:HG2	2.04	0.40
2:F:6:ASP:OD1	2:F:6:ASP:N	2.44	0.40
2:F:1329:ASP:OD1	2:F:1330:ARG:N	2.54	0.40
1:A:693:ALA:HB3	1:A:694:PRO:HD3	2.03	0.40
1:B:1683:ASP:OD1	1:B:1683:ASP:N	2.43	0.40
1:C:160:SER:C	1:C:161:THR:O	2.60	0.40
1:E:137:TYR:CE2	1:E:139:ASP:HB2	2.57	0.40
2:F:841:THR:OG1	2:F:842:TRP:N	2.53	0.40
2:F:1498:ASP:OD1	2:F:1498:ASP:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	A	2286/2516 (91%)	2240 (98%)	40 (2%)	6 (0%)	36	65
1	B	2286/2516 (91%)	2225 (97%)	54 (2%)	7 (0%)	36	65
1	C	2286/2516 (91%)	2225 (97%)	56 (2%)	5 (0%)	43	71
1	D	2286/2516 (91%)	2233 (98%)	46 (2%)	7 (0%)	36	65
1	E	2286/2516 (91%)	2239 (98%)	39 (2%)	8 (0%)	36	65
2	F	2162/2439 (89%)	2111 (98%)	46 (2%)	5 (0%)	43	71
All	All	13592/15019 (90%)	13273 (98%)	281 (2%)	38 (0%)	37	65

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	891	PRO
1	B	891	PRO
1	C	891	PRO
1	D	891	PRO
1	E	790	THR
1	E	891	PRO
1	A	991	ALA
1	A	1334	ASN
1	B	1138	ALA
1	B	1334	ASN
1	C	991	ALA
1	C	1334	ASN
1	D	991	ALA
1	D	1138	ALA
1	E	991	ALA
1	E	1154	TYR
2	F	755	ILE
1	D	1292	GLN
2	F	137	HIS
2	F	602	ALA

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Mol	Chain	Res	Type
1	B	1190	THR
1	C	1758	MET
1	E	659	TYR
1	A	890	ALA
1	A	1758	MET
1	A	1953	ASN
1	B	101	SER
1	B	2425	PRO
1	D	890	ALA
1	E	1953	ASN
2	F	530	ASP
1	B	745	ALA
1	C	350	GLY
1	D	1758	MET
1	D	1953	ASN
1	E	304	GLY
2	F	2115	GLY
1	E	890	ALA

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	A	1960/2157 (91%)	1960 (100%)	0	100	100
1	B	1960/2157 (91%)	1959 (100%)	1 (0%)	88	89
1	C	1960/2157 (91%)	1960 (100%)	0	100	100
1	D	1960/2157 (91%)	1960 (100%)	0	100	100
1	E	1960/2157 (91%)	1960 (100%)	0	100	100
2	F	1872/2108 (89%)	1872 (100%)	0	100	100
All	All	11672/12893 (90%)	11671 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	211	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	642	HIS
1	A	709	HIS
1	A	854	GLN
1	A	1132	ASN
1	A	1240	GLN
1	A	1252	GLN
1	A	1293	GLN
1	A	1520	GLN
1	A	1743	HIS
1	A	1817	ASN
1	A	1888	HIS
1	A	1965	GLN
1	A	1969	ASN
1	A	2248	GLN
1	A	2348	ASN
1	A	2363	GLN
1	B	102	GLN
1	B	233	GLN
1	B	352	ASN
1	B	885	GLN
1	B	886	GLN
1	B	1087	GLN
1	B	1102	ASN
1	B	1132	ASN
1	B	1252	GLN
1	B	1253	GLN
1	B	1293	GLN
1	B	1499	GLN
1	B	1520	GLN
1	B	1587	HIS
1	B	1599	GLN
1	B	1743	HIS
1	B	1781	GLN
1	B	1787	GLN
1	B	1885	GLN
1	B	1888	HIS
1	B	1979	GLN
1	B	2032	GLN

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Mol	Chain	Res	Type
1	B	2093	GLN
1	B	2230	GLN
1	B	2248	GLN
1	B	2348	ASN
1	B	2461	GLN
1	C	128	ASN
1	C	212	GLN
1	C	312	GLN
1	C	404	GLN
1	C	709	HIS
1	C	875	ASN
1	C	886	GLN
1	C	1043	ASN
1	C	1252	GLN
1	C	1297	ASN
1	C	1303	ASN
1	C	1885	GLN
1	C	1951	GLN
1	C	1965	GLN
1	C	1969	ASN
1	C	2032	GLN
1	C	2071	GLN
1	C	2248	GLN
1	C	2348	ASN
1	C	2363	GLN
1	D	206	ASN
1	D	212	GLN
1	D	214	GLN
1	D	267	ASN
1	D	312	GLN
1	D	441	ASN
1	D	635	ASN
1	D	679	GLN
1	D	701	GLN
1	D	848	GLN
1	D	885	GLN
1	D	886	GLN
1	D	953	GLN
1	D	1293	GLN
1	D	1531	GLN
1	D	1764	ASN
1	D	1793	ASN

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Mol	Chain	Res	Type
1	D	1842	GLN
1	D	1888	HIS
1	D	1951	GLN
1	D	2093	GLN
1	D	2248	GLN
1	D	2348	ASN
1	E	102	GLN
1	E	854	GLN
1	E	886	GLN
1	E	1132	ASN
1	E	1252	GLN
1	E	1743	HIS
1	E	1787	GLN
1	E	1808	HIS
1	E	1888	HIS
1	E	1951	GLN
1	E	1965	GLN
1	E	1969	ASN
1	E	2248	GLN
1	E	2348	ASN
1	E	2497	GLN
2	F	5	GLN
2	F	89	HIS
2	F	391	ASN
2	F	412	GLN
2	F	600	GLN
2	F	661	GLN
2	F	663	GLN
2	F	943	GLN
2	F	1050	GLN
2	F	1082	GLN
2	F	1108	GLN
2	F	1354	GLN
2	F	1546	GLN
2	F	1634	ASN
2	F	1650	HIS
2	F	1832	ASN
2	F	1856	GLN
2	F	1891	GLN
2	F	1936	GLN
2	F	1937	ASN
2	F	1992	ASN

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Mol	Chain	Res	Type
2	F	2010	GLN
2	F	2120	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

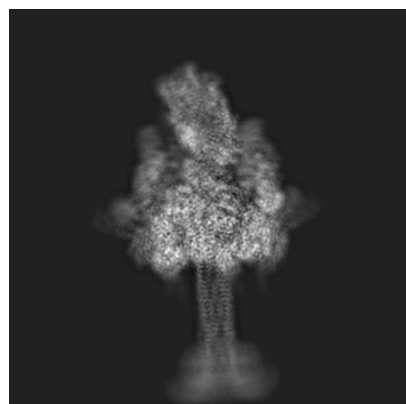
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10312. These allow visual inspection of the internal detail of the map and identification of artifacts.

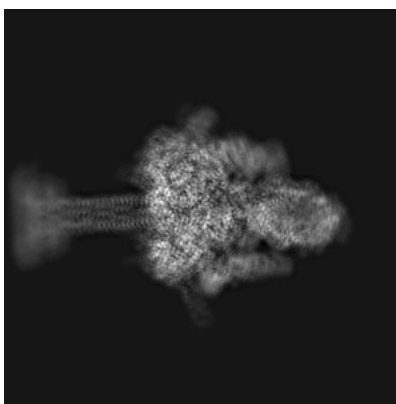
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

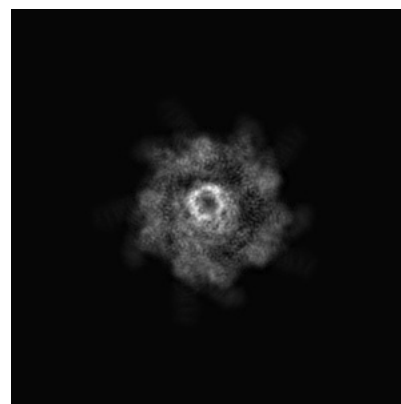
6.1.1 Primary map



X

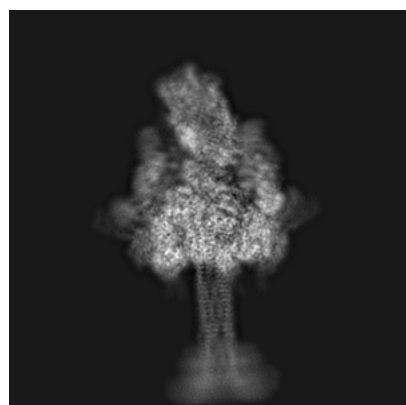


Y

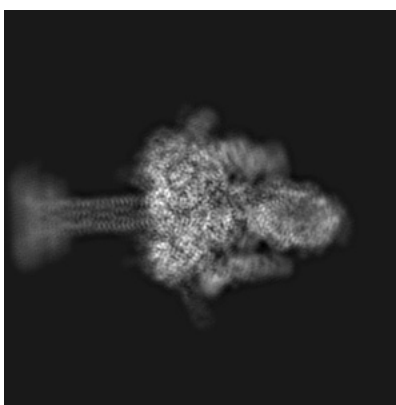


Z

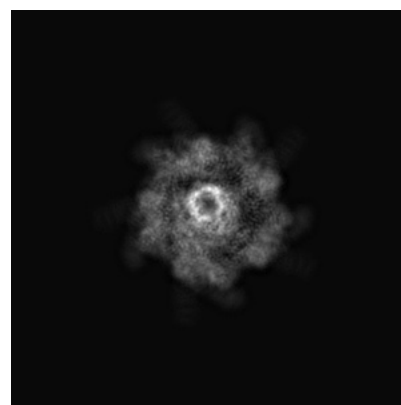
6.1.2 Raw map



X



Y

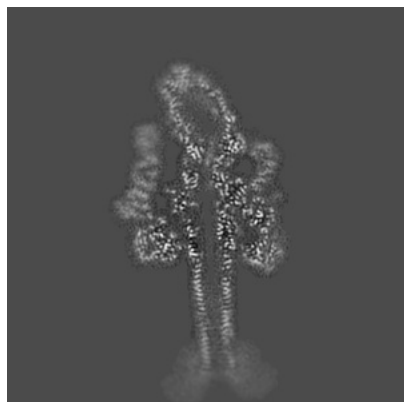


Z

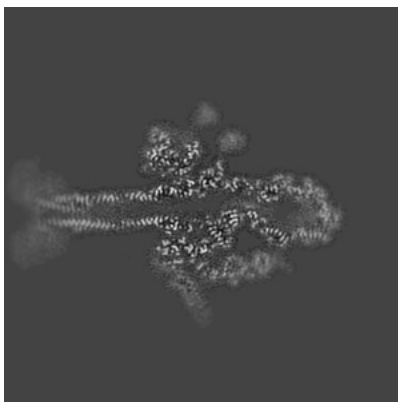
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

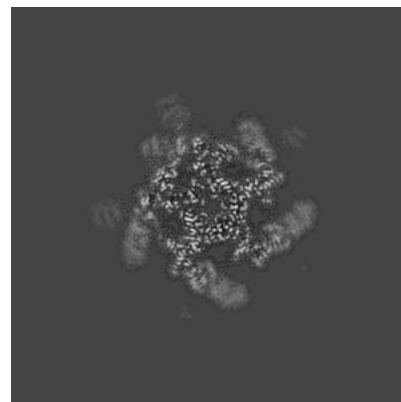
6.2.1 Primary map



X Index: 192

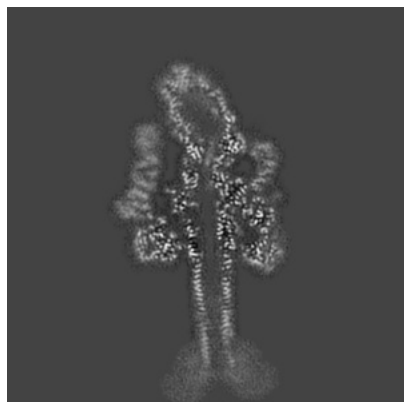


Y Index: 192

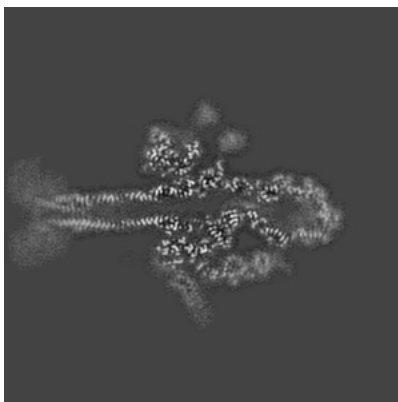


Z Index: 192

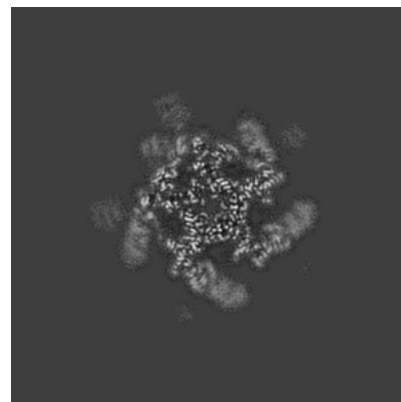
6.2.2 Raw map



X Index: 192



Y Index: 192

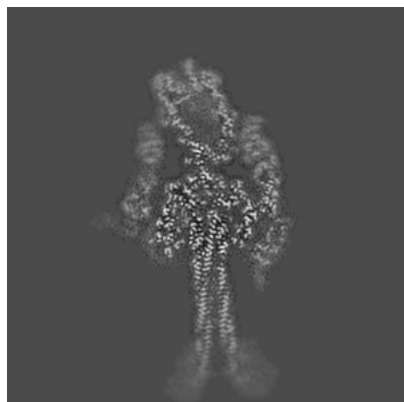


Z Index: 192

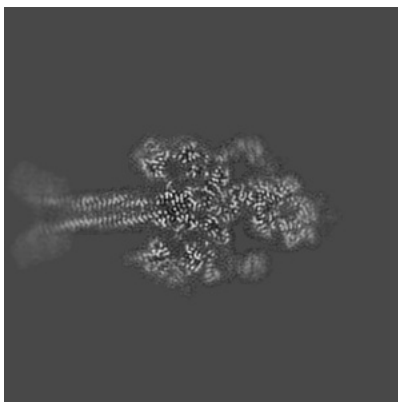
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

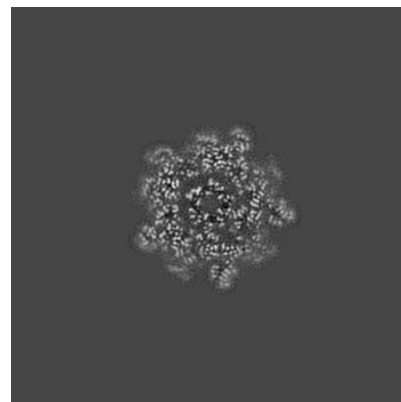
6.3.1 Primary map



X Index: 179

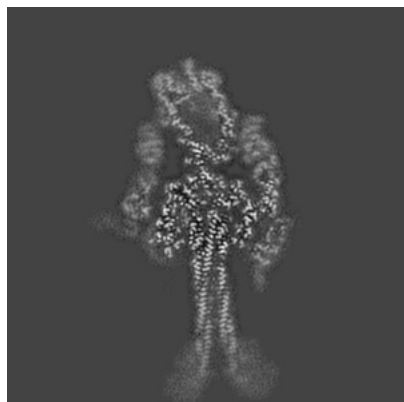


Y Index: 207

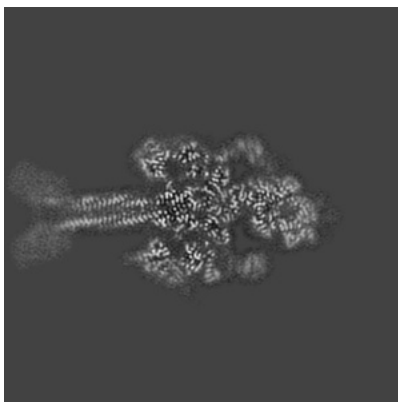


Z Index: 153

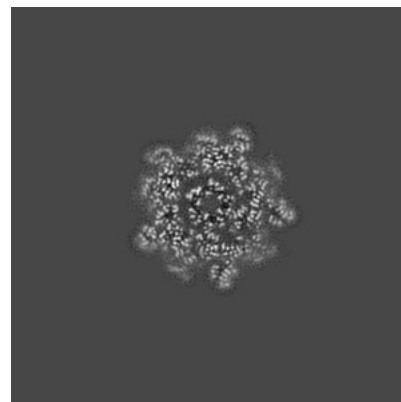
6.3.2 Raw map



X Index: 179



Y Index: 207

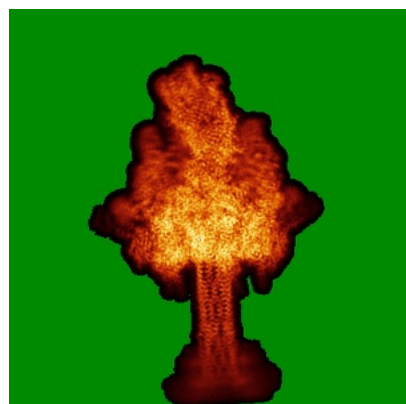


Z Index: 153

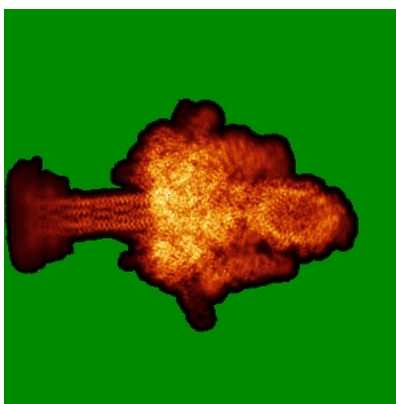
The images above show the largest variance slices of the map in three orthogonal directions.

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

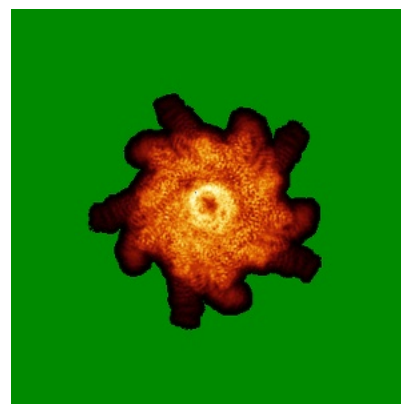
6.4.1 Primary map



X

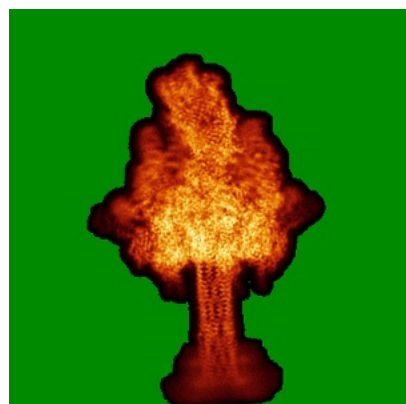


Y

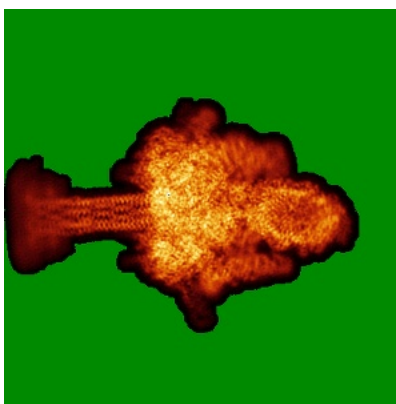


Z

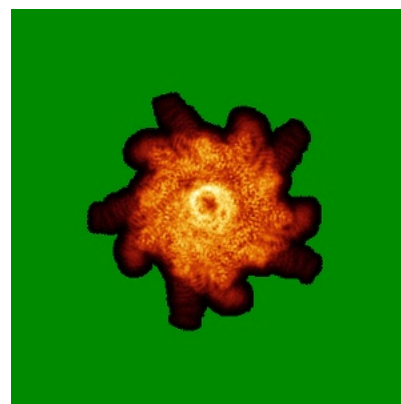
6.4.2 Raw map



X



Y

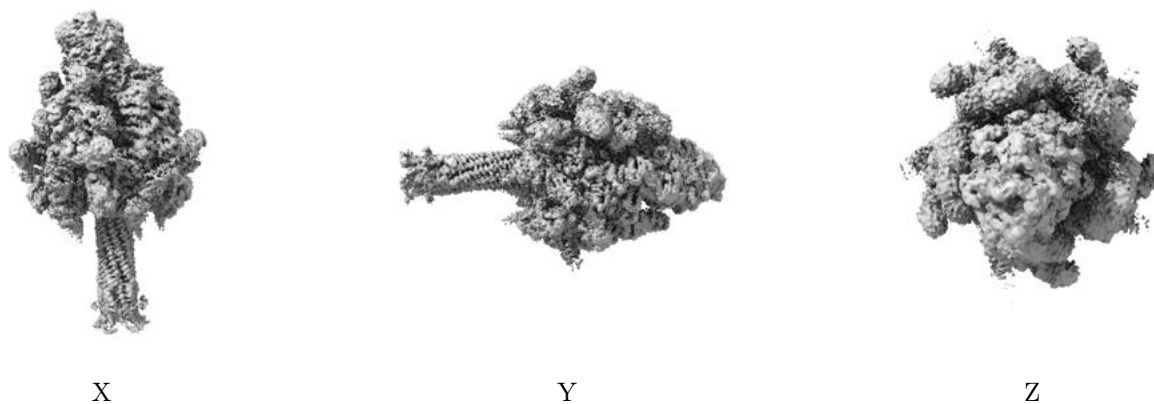


Z

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

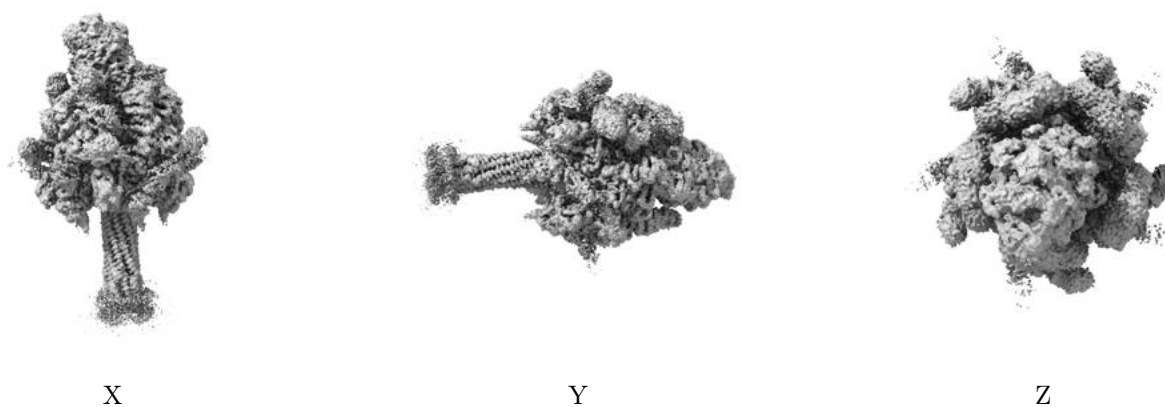
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

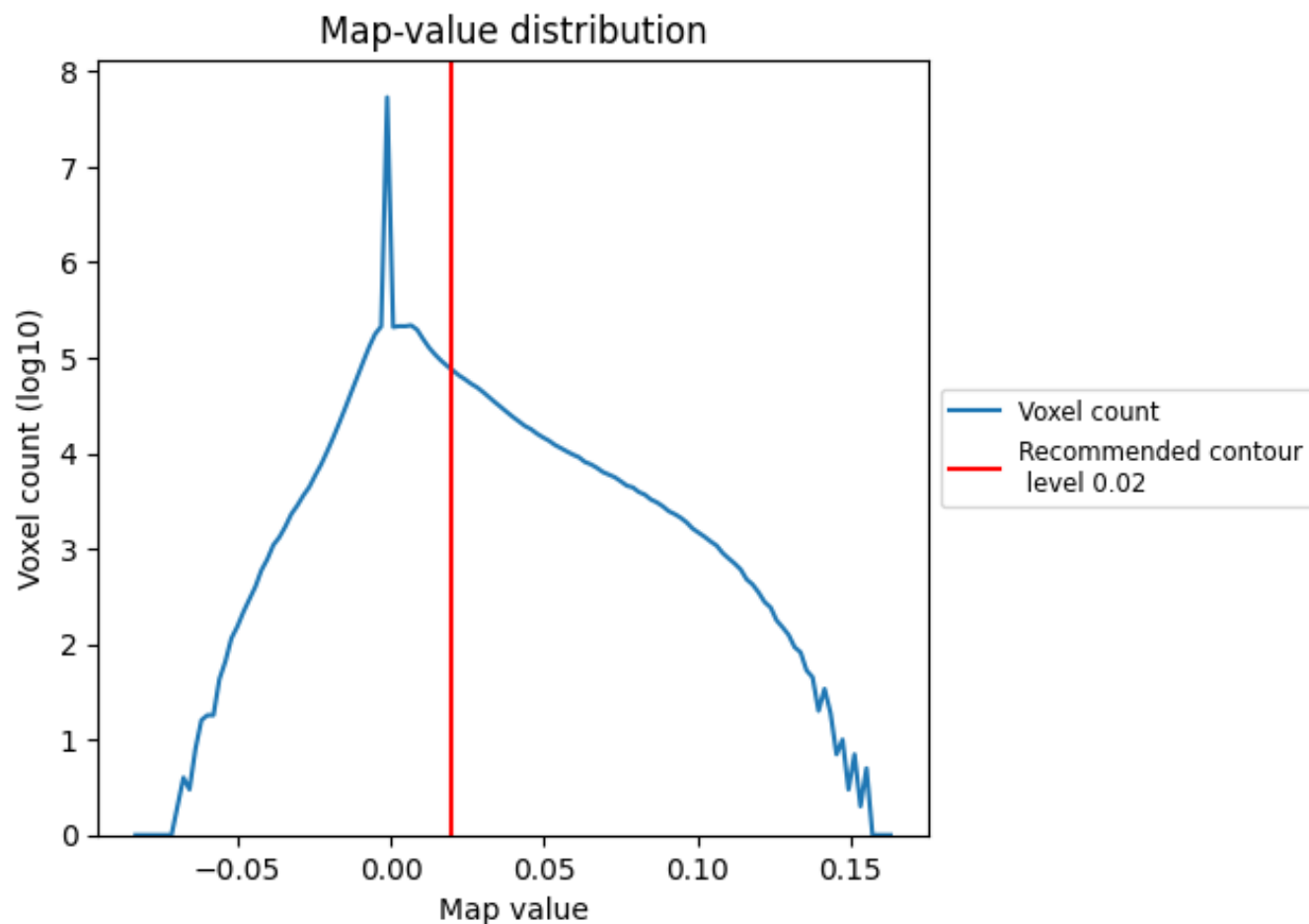
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

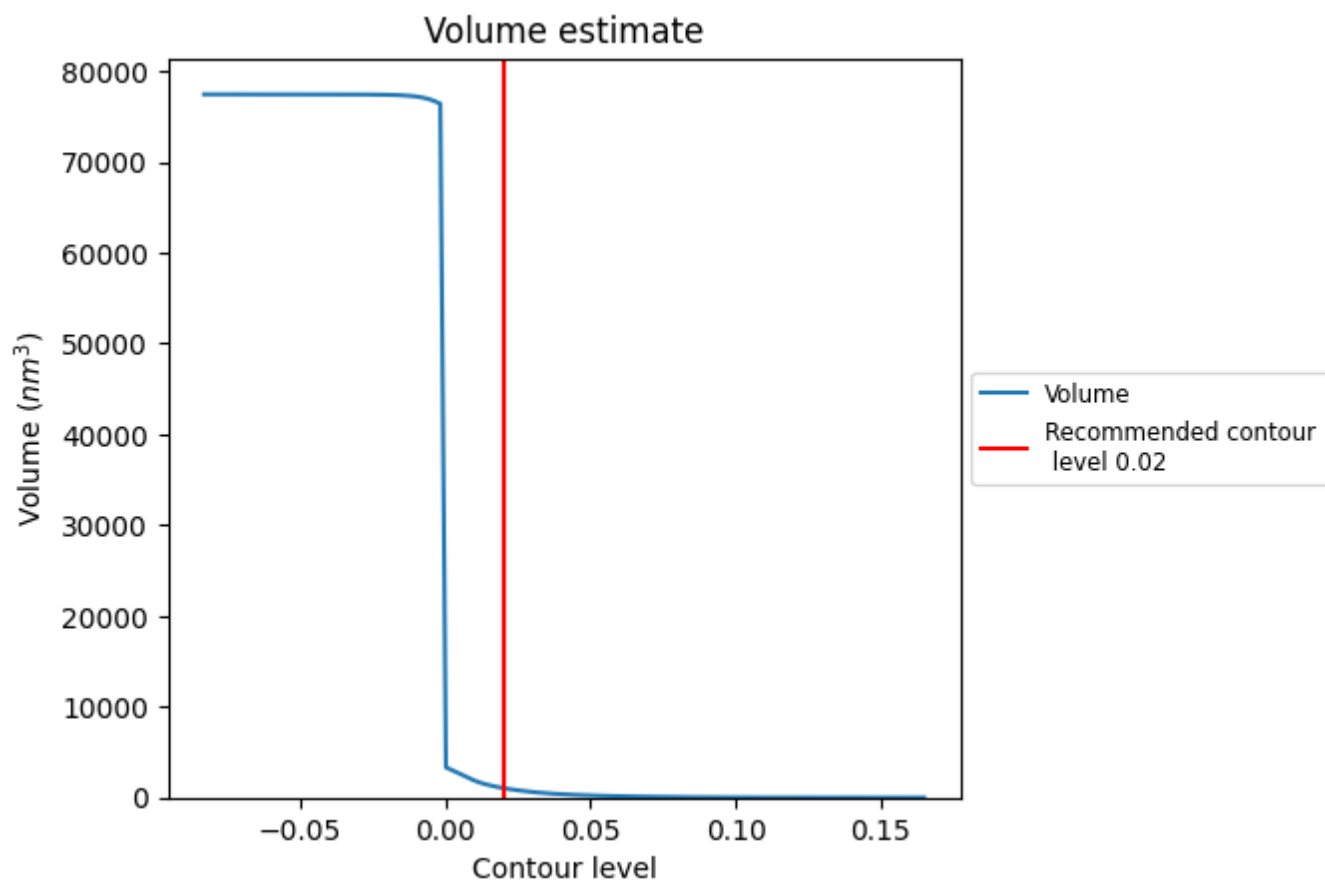
This section contains the results of statistical analysis of the map.

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.

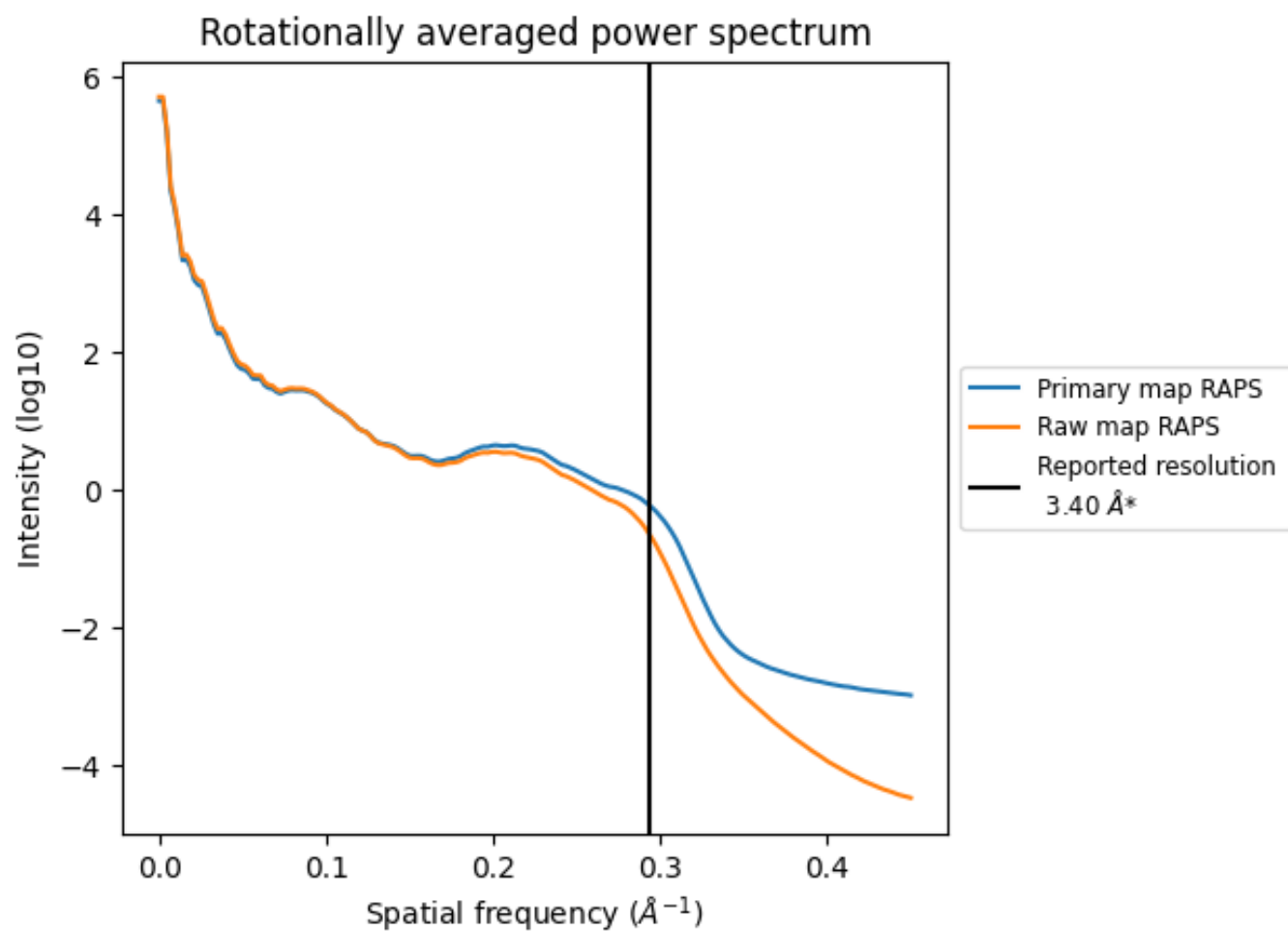
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1043 nm³; this corresponds to an approximate mass of 942 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 ⓘ

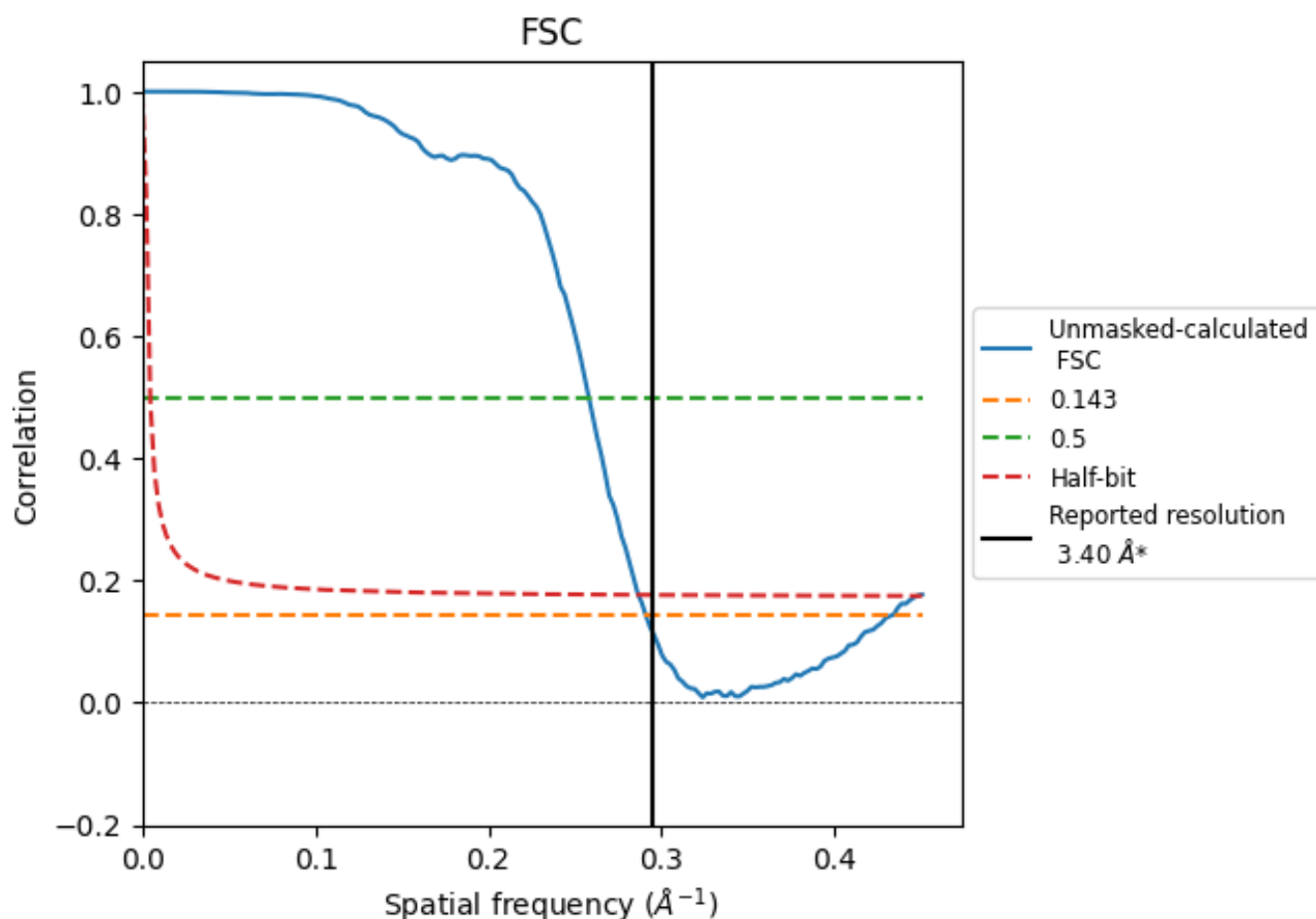


*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

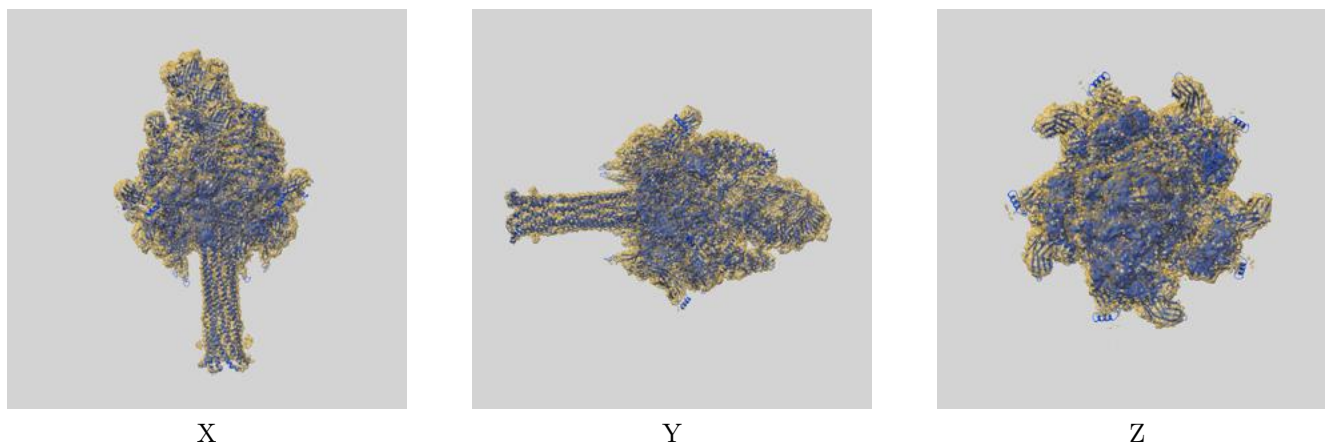
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.44	3.88	3.49

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

9 Map-model fit [i](#)

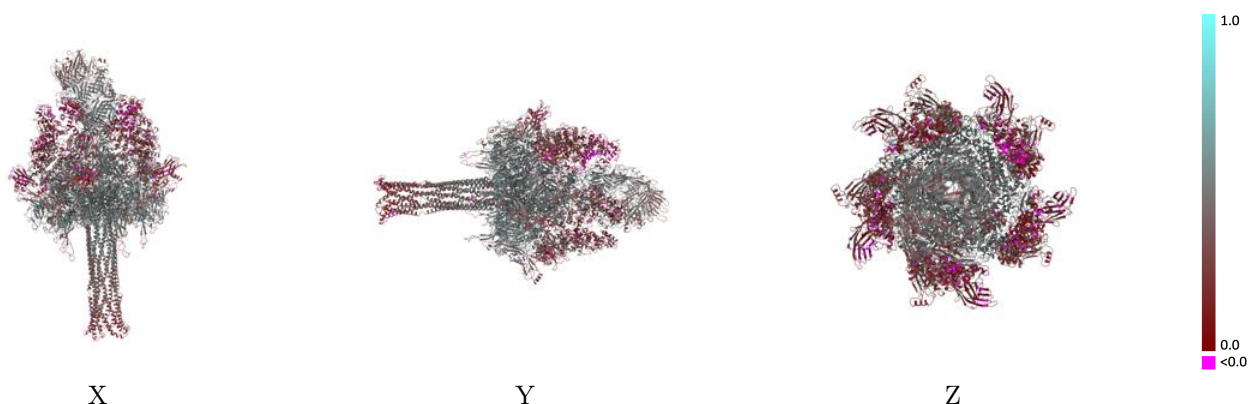
This section contains information regarding the fit between EMDB map EMD-10312 and PDB model 6SUE. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



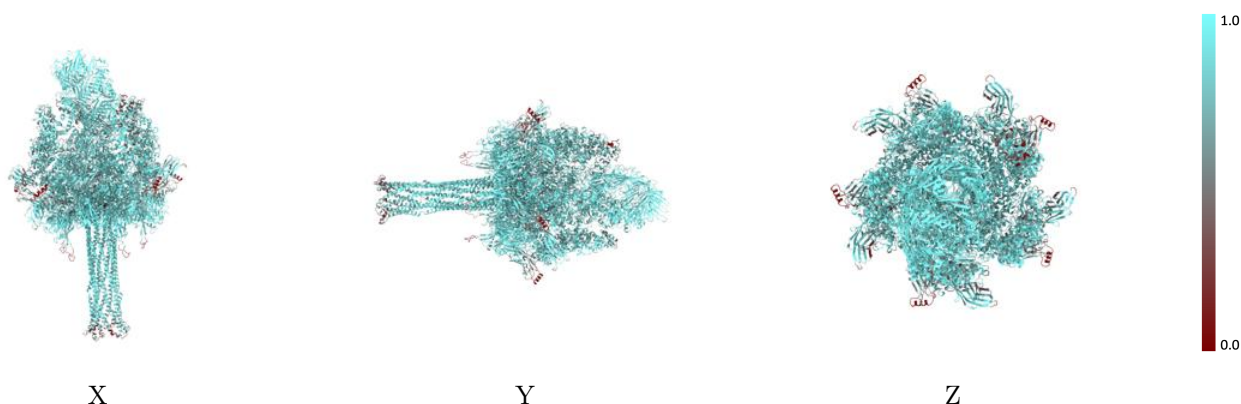
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



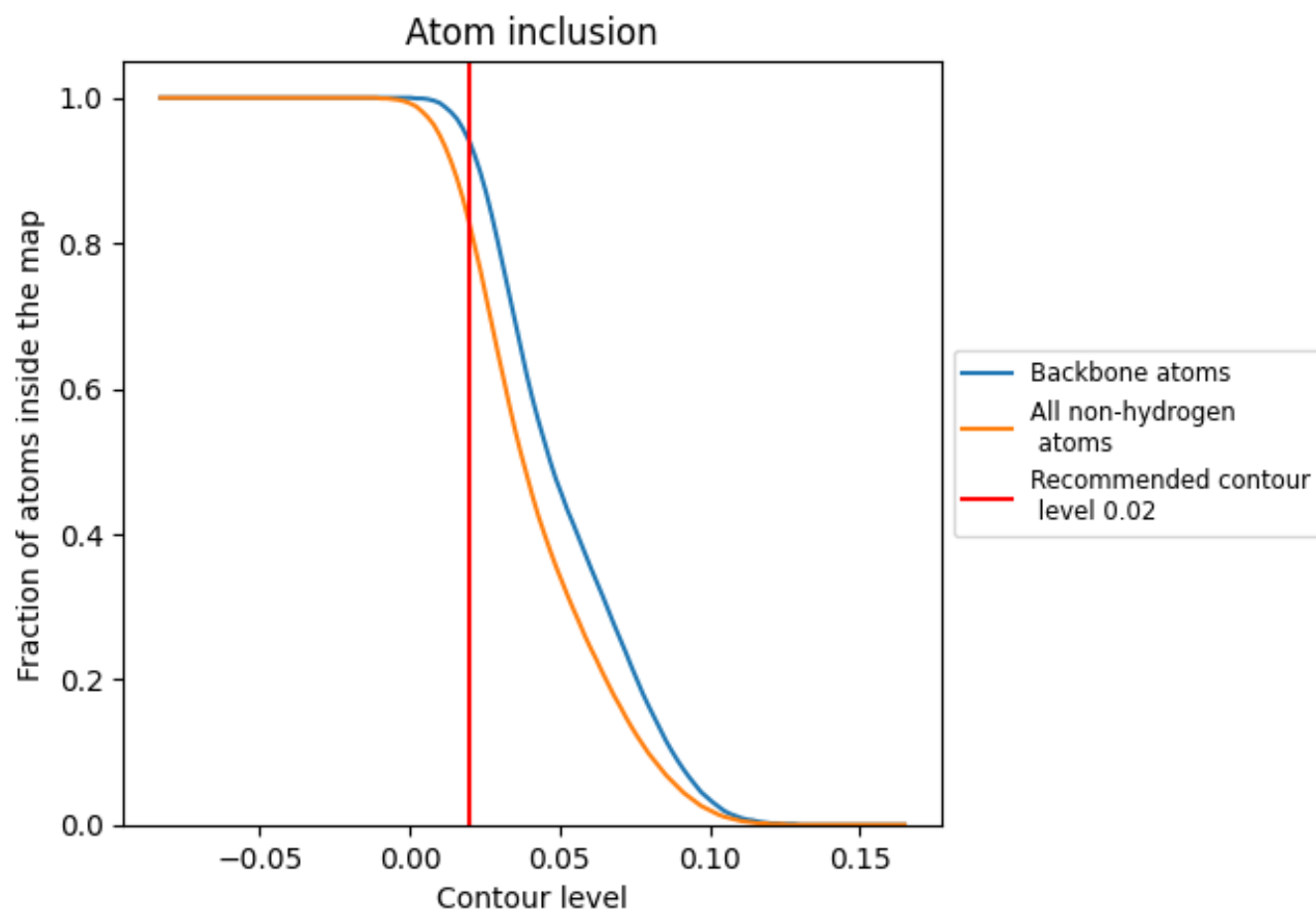
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 82% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8250	0.3850
A	0.8100	0.3810
B	0.8150	0.3740
C	0.8150	0.3730
D	0.7950	0.3600
E	0.8210	0.3870
F	0.8990	0.4340

1.0

0.0

<0.0