



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:27 AM UTC

PDB ID : 6H6E / pdb_00006h6e
EMDB ID : EMD-0149
Title : PTC3 holotoxin complex from Photorhabdus luminecens in prepore state (TcdA1, TcdB2, TccC3)
Authors : Gatsogiannis, C.; Merino, F.; Roderer, D.; Balchin, D.; Schubert, E.; Kuhlee, A.; Hayer-Hartl, M.; Raunser, S.
Deposited on : 2018-07-27
Resolution : 3.95 Å (reported)
Based on initial models : 1VW1, 4O9X

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:

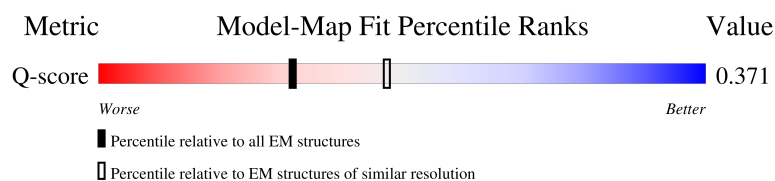
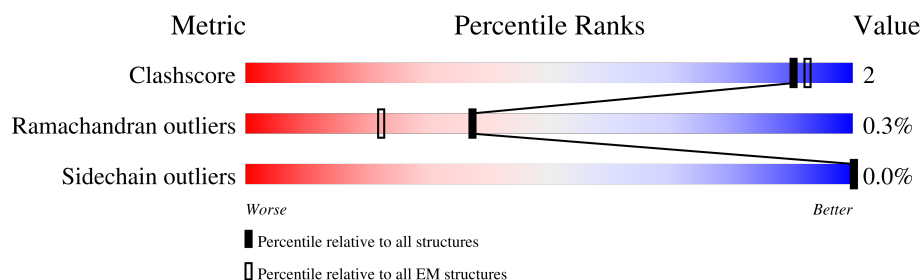
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.95 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	7707 (3.45 - 4.45)

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	
1	B	2516	
1	C	2516	
1	D	2516	

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Mol	Chain	Length	Quality of chain
1	E	2516	88% 8%
2	F	2434	79% 9% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 112922 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	2417	Total	C	N	O	S	0	0
			19161	12136	3248	3716	61		
1	B	2417	Total	C	N	O	S	0	0
			19161	12136	3248	3716	61		
1	C	2417	Total	C	N	O	S	0	0
			19161	12136	3248	3716	61		
1	D	2417	Total	C	N	O	S	0	0
			19161	12136	3248	3716	61		
1	E	2417	Total	C	N	O	S	0	0
			19161	12136	3248	3716	61		

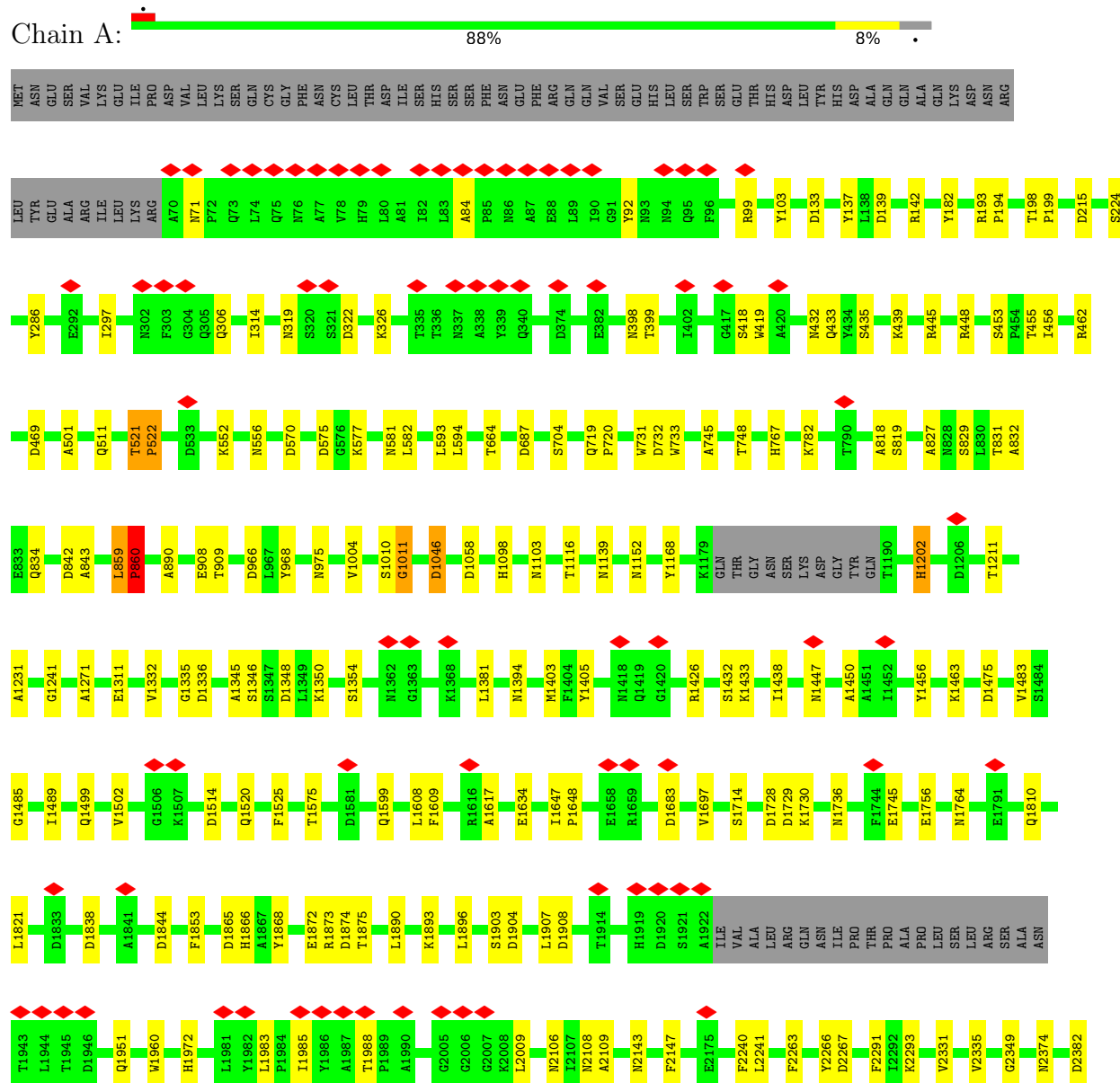
- Molecule 2 is a protein called TcdB2,TccC3.

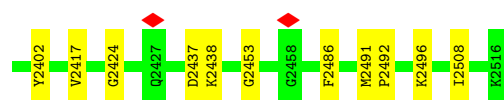
Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	2146	Total	C	N	O	S	0	0
			17117	10722	3038	3322	35		

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.

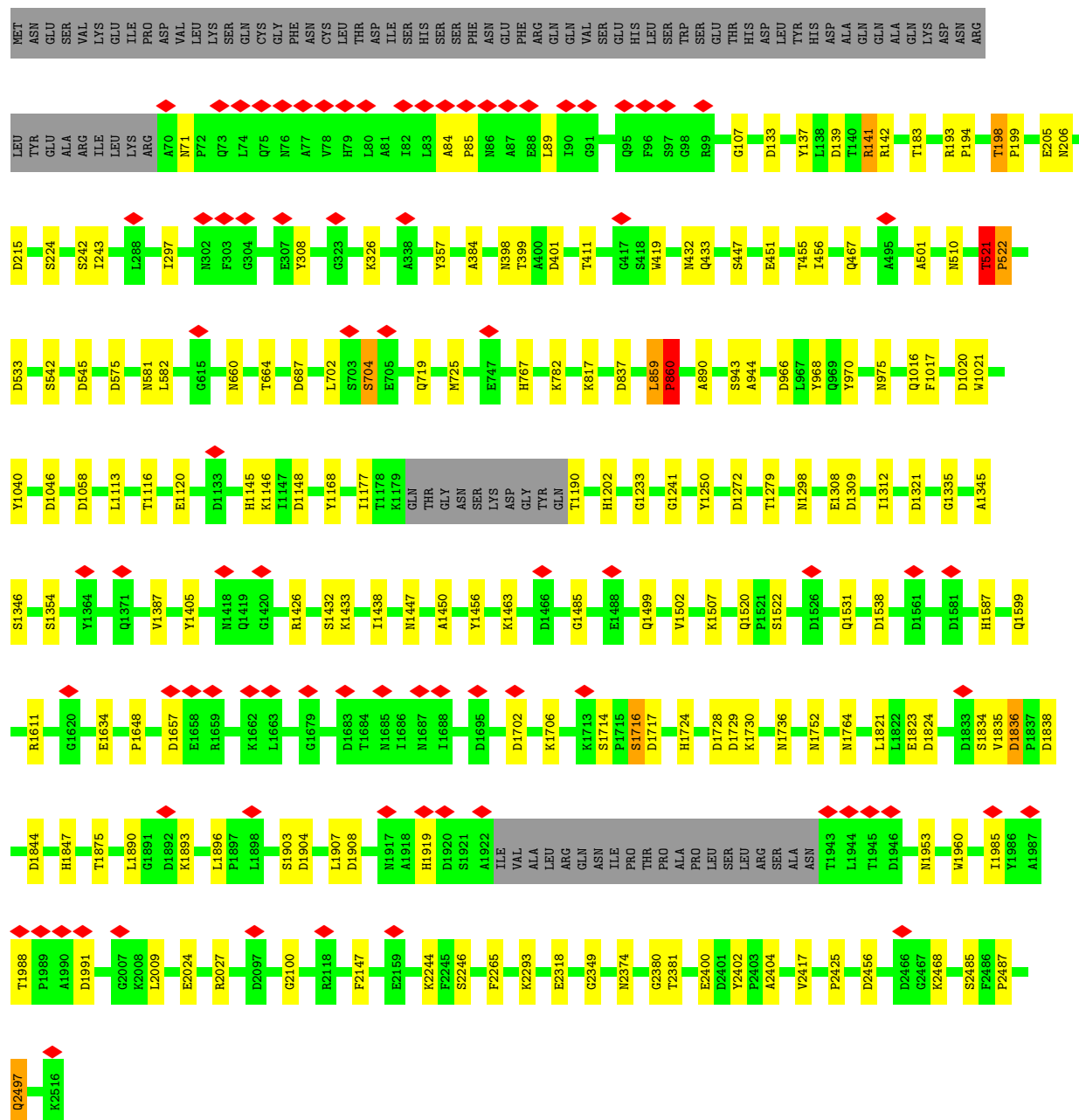
• Molecule 1: TcdA1





• Molecule 1: TcdA1

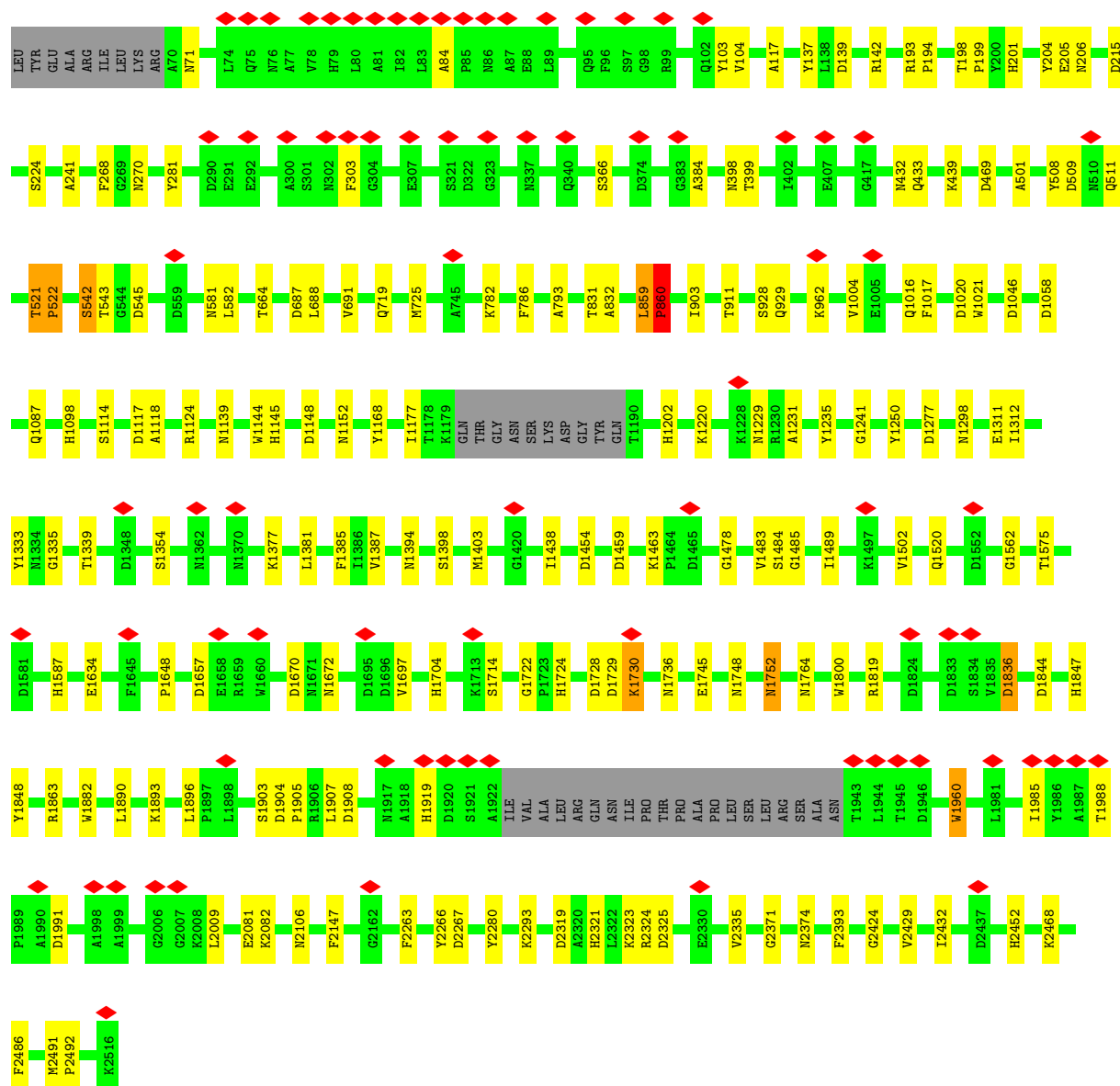
Chain B: 89% 7%



• Molecule 1: TcdA1

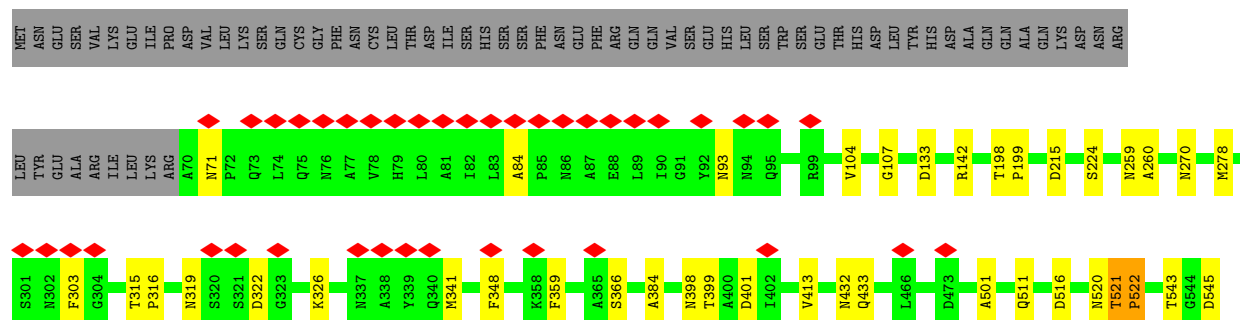
Chain C: 89% 7%

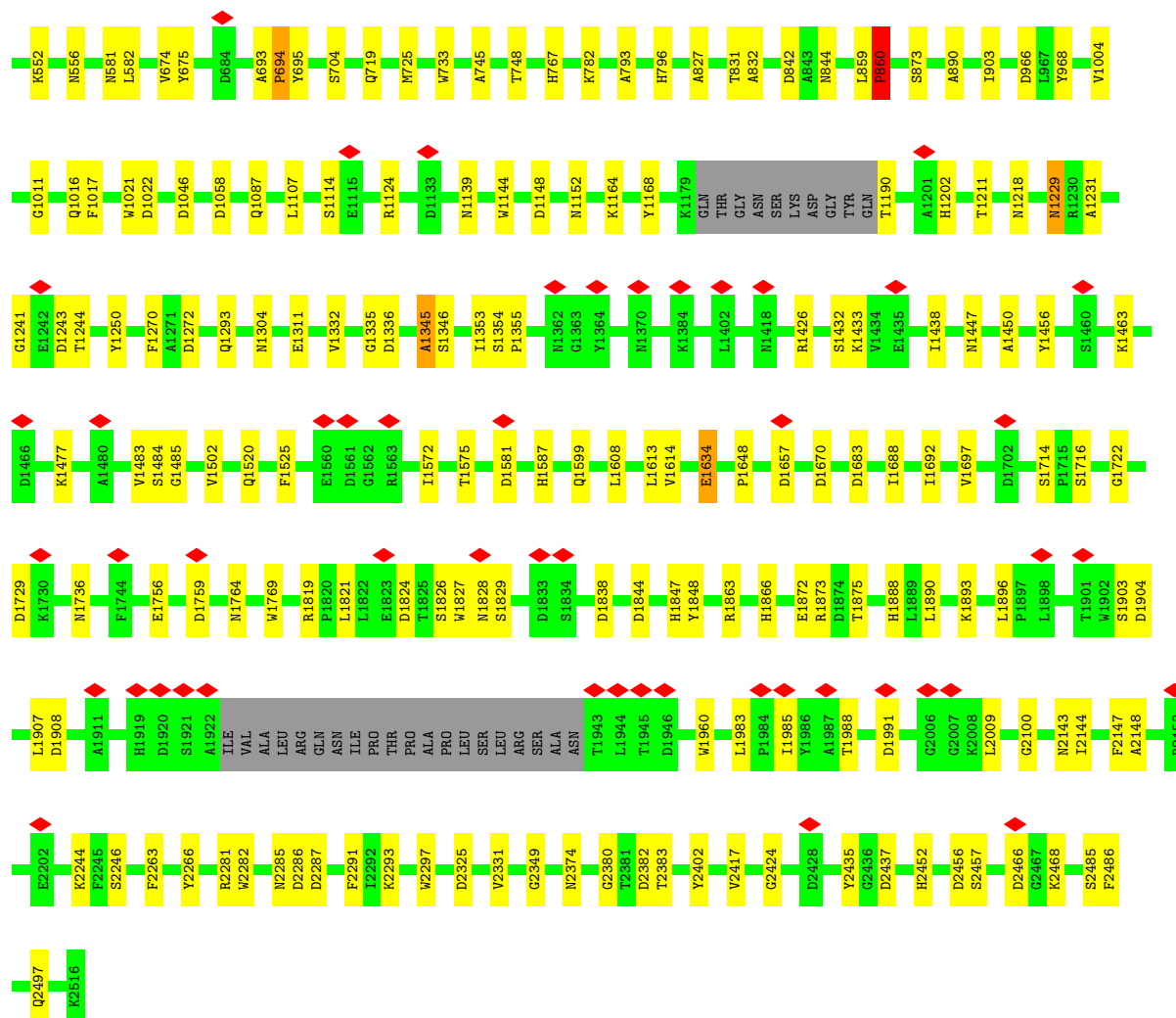




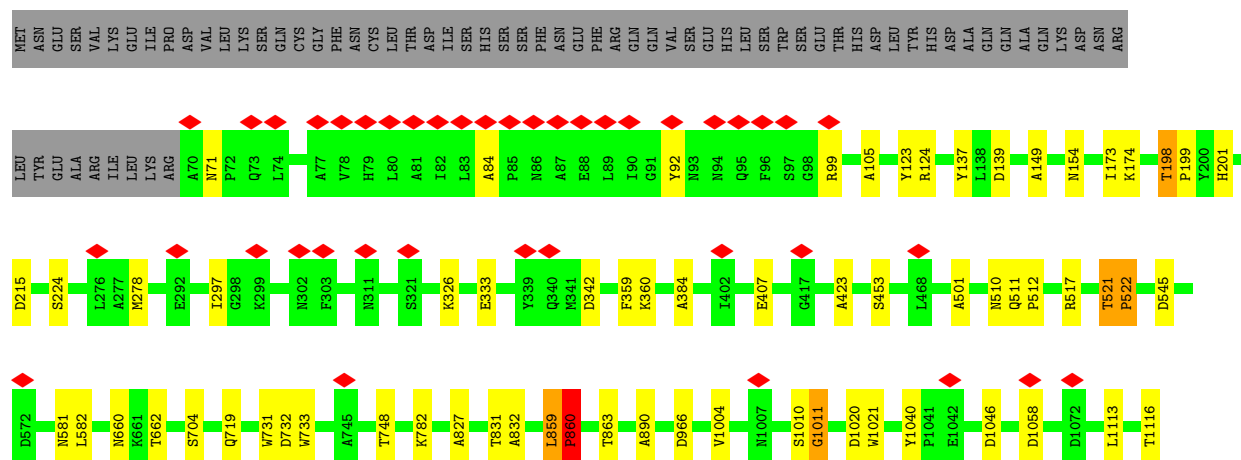
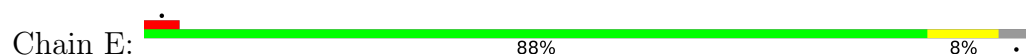
• Molecule 1: TcdA1

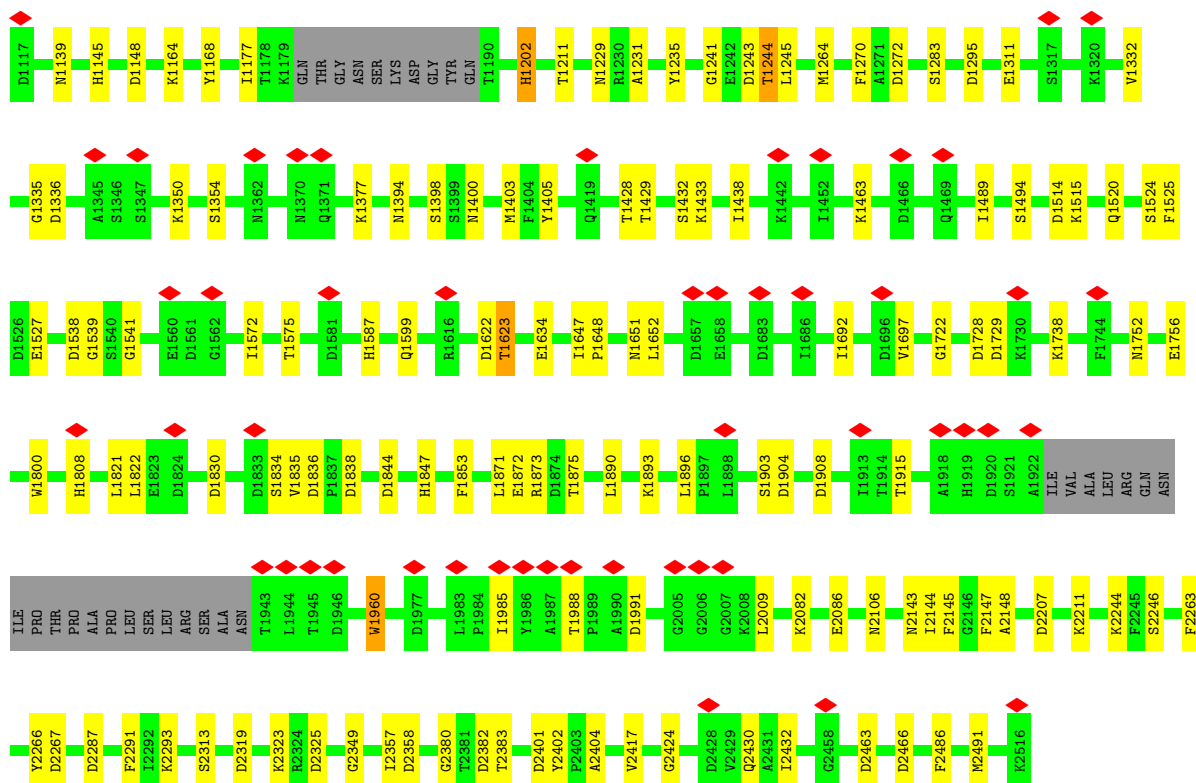
Chain D:  87% 8% .





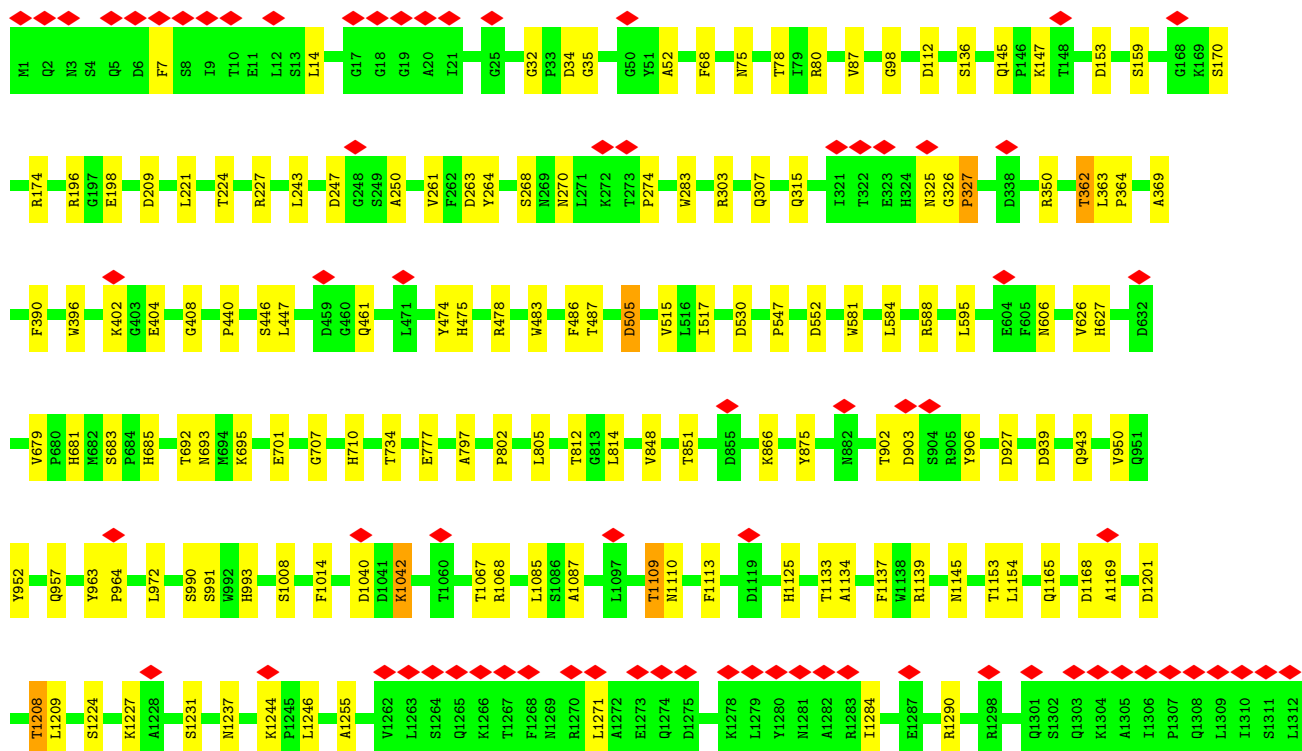
• Molecule 1: TcdA1





• Molecule 2: TcdB2,TccC3

Chain F:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	89148	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 ($e^-/\text{\AA}^2$)	2.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.124	Depositor
Minimum map value	-0.137	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	547.2, 547.2, 547.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.14, 1.14, 1.14	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	1.18	6/19574 (0.0%)	1.25	135/26589 (0.5%)
1	B	1.17	9/19574 (0.0%)	1.23	123/26589 (0.5%)
1	C	1.17	16/19574 (0.1%)	1.23	121/26589 (0.5%)
1	D	1.16	12/19574 (0.1%)	1.25	151/26589 (0.6%)
1	E	1.17	10/19574 (0.1%)	1.25	143/26589 (0.5%)
2	F	1.15	10/17538 (0.1%)	1.35	187/23909 (0.8%)
All	All	1.17	63/115408 (0.1%)	1.26	860/156854 (0.5%)

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1847	HIS	CB-CG	-7.33	1.39	1.50
1	E	1847	HIS	CB-CG	-6.92	1.40	1.50
1	B	1145	HIS	CB-CG	-6.90	1.40	1.50
1	E	1800	TRP	NE1-CE2	-6.81	1.29	1.37
1	C	1724	HIS	CB-CG	-6.79	1.40	1.50
2	F	993	HIS	CB-CG	-6.46	1.41	1.50
1	E	1587	HIS	CB-CG	-6.25	1.41	1.50
2	F	685	HIS	CB-CG	-6.24	1.41	1.50
1	D	1218	ASN	CB-CG	-6.24	1.36	1.52
1	A	1098	HIS	CD2-NE2	-6.18	1.31	1.37
1	C	1587	HIS	CB-CG	-6.18	1.41	1.50
1	C	2321	HIS	CB-CG	-6.17	1.41	1.50
1	E	1960	TRP	NE1-CE2	-6.16	1.30	1.37
2	F	681	HIS	CB-CG	-6.09	1.41	1.50
1	B	968	TYR	CG-CD1	-6.06	1.26	1.39
1	C	1960	TRP	NE1-CE2	-5.95	1.30	1.37
1	D	767	HIS	CB-CG	-5.94	1.41	1.50
1	E	2143	ASN	CB-CG	-5.91	1.37	1.52
1	A	767	HIS	CB-CG	-5.85	1.42	1.50
1	D	1587	HIS	CB-CG	-5.75	1.42	1.50
1	D	968	TYR	CG-CD1	-5.73	1.27	1.39
2	F	627	HIS	CB-CG	-5.71	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1202	HIS	CB-CG	-5.67	1.42	1.50
1	B	141	ARG	CD-NE	-5.67	1.38	1.46
2	F	1824	HIS	CB-CG	-5.63	1.42	1.50
1	C	1863	ARG	CD-NE	-5.58	1.38	1.46
1	D	2452	HIS	CB-CG	-5.57	1.42	1.50
2	F	1125	HIS	CB-CG	-5.53	1.42	1.50
1	B	1919	HIS	CB-CG	-5.52	1.42	1.50
1	B	1724	HIS	CB-CG	-5.52	1.42	1.50
1	A	103	TYR	CB-CG	-5.51	1.39	1.51
1	B	767	HIS	CB-CG	-5.48	1.42	1.50
1	E	1139	ASN	CB-CG	-5.46	1.38	1.52
2	F	1585	ARG	CG-CD	-5.46	1.36	1.52
1	C	1882	TRP	NE1-CE2	-5.44	1.31	1.37
2	F	1684	TRP	NE1-CE2	-5.44	1.31	1.37
1	B	1587	HIS	CB-CG	-5.43	1.42	1.50
1	C	201	HIS	CB-CG	-5.40	1.42	1.50
1	C	2452	HIS	CB-CG	-5.39	1.42	1.50
1	D	2143	ASN	CB-CG	-5.37	1.38	1.52
1	A	1951	GLN	CG-CD	-5.34	1.38	1.52
1	C	1847	HIS	CB-CG	-5.34	1.42	1.50
1	C	1098	HIS	CE1-NE2	-5.33	1.27	1.32
1	E	1145	HIS	CB-CG	-5.33	1.42	1.50
1	C	1800	TRP	NE1-CE2	-5.31	1.31	1.37
1	A	1139	ASN	CB-CG	-5.30	1.38	1.52
1	C	1145	HIS	CB-CG	-5.26	1.42	1.50
1	D	1847	HIS	CB-CG	-5.24	1.42	1.50
1	B	243	ILE	CA-C	-5.24	1.47	1.52
1	E	201	HIS	CB-CG	-5.20	1.42	1.50
1	C	1139	ASN	CB-CG	-5.18	1.39	1.52
1	D	1863	ARG	CD-NE	-5.15	1.39	1.46
1	A	1810	GLN	CG-CD	-5.15	1.39	1.52
1	C	103	TYR	CB-CG	-5.13	1.40	1.51
2	F	710	HIS	CB-CG	-5.12	1.43	1.50
1	E	1853	PHE	CB-CG	-5.12	1.38	1.50
2	F	1290	ARG	CD-NE	-5.12	1.39	1.46
1	D	1866	HIS	CB-CG	-5.11	1.43	1.50
1	C	1919	HIS	CB-CG	-5.11	1.43	1.50
1	D	1888	HIS	CB-CG	-5.07	1.43	1.50
1	C	1819	ARG	CD-NE	-5.07	1.39	1.46
1	D	1819	ARG	CD-NE	-5.03	1.39	1.46
1	D	1139	ASN	CB-CG	-5.00	1.39	1.52

All (860) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1738	LYS	N-CA-C	-10.78	100.40	114.31
1	A	1844	ASP	CA-C-N	9.70	129.46	119.56
1	A	1844	ASP	C-N-CA	9.70	129.46	119.56
1	C	1354	SER	CA-C-N	9.65	129.76	120.31
1	C	1354	SER	C-N-CA	9.65	129.76	120.31
1	A	1011	GLY	N-CA-C	-9.55	97.18	112.66
1	C	1004	VAL	N-CA-C	-9.40	101.22	110.72
1	A	1004	VAL	N-CA-C	-9.26	101.36	110.72
1	B	1354	SER	CA-C-N	9.22	129.16	120.03
1	B	1354	SER	C-N-CA	9.22	129.16	120.03
1	E	1011	GLY	N-CA-C	-9.21	97.74	112.66
1	D	1354	SER	CA-C-N	9.21	129.15	120.03
1	D	1354	SER	C-N-CA	9.21	129.15	120.03
1	D	1477	LYS	N-CA-C	-9.19	102.65	114.04
2	F	1284	ILE	N-CA-C	-9.06	103.03	111.45
2	F	1246	LEU	CA-C-N	8.95	129.18	119.87
2	F	1246	LEU	C-N-CA	8.95	129.18	119.87
1	E	1844	ASP	CA-C-N	8.92	128.66	119.56
1	E	1844	ASP	C-N-CA	8.92	128.66	119.56
1	D	694	PRO	N-CA-C	-8.90	98.76	111.22
2	F	1587	LEU	N-CA-C	-8.90	102.94	113.88
1	A	2291	PHE	N-CA-C	-8.87	103.04	114.04
1	D	1525	PHE	CA-CB-CG	8.72	122.52	113.80
1	C	691	VAL	N-CA-C	-8.64	104.13	111.56
1	D	1241	GLY	N-CA-C	-8.58	101.07	112.14
1	B	2374	ASN	N-CA-C	8.48	119.83	108.38
1	A	1354	SER	CA-C-N	8.44	128.38	120.03
1	A	1354	SER	C-N-CA	8.44	128.38	120.03
1	C	1058	ASP	CA-CB-CG	8.38	120.98	112.60
1	E	1354	SER	CA-C-N	8.14	128.09	120.03
1	E	1354	SER	C-N-CA	8.14	128.09	120.03
1	E	1241	GLY	N-CA-C	-8.14	101.64	112.14
1	C	1046	ASP	CA-C-N	8.13	127.85	119.56
1	C	1046	ASP	C-N-CA	8.13	127.85	119.56
2	F	1894	SER	CA-C-N	8.12	127.85	119.56
2	F	1894	SER	C-N-CA	8.12	127.85	119.56
1	B	1335	GLY	N-CA-C	-8.12	100.17	112.60
1	B	1046	ASP	CA-C-N	8.09	127.81	119.56
1	B	1046	ASP	C-N-CA	8.09	127.81	119.56
1	A	1438	ILE	CA-C-N	7.96	128.39	119.32
1	A	1438	ILE	C-N-CA	7.96	128.39	119.32
2	F	1790	ARG	CA-C-N	7.94	128.68	119.47
2	F	1790	ARG	C-N-CA	7.94	128.68	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1011	GLY	N-CA-C	-7.94	100.07	112.85
1	E	84	ALA	CA-C-N	7.88	127.60	119.56
1	E	84	ALA	C-N-CA	7.88	127.60	119.56
1	D	348	PHE	N-CA-C	-7.84	103.55	113.43
1	D	1438	ILE	CA-C-N	7.79	128.21	119.32
1	D	1438	ILE	C-N-CA	7.79	128.21	119.32
2	F	2078	TYR	N-CA-C	-7.77	98.90	110.24
1	E	1903	SER	N-CA-C	7.72	120.06	107.32
1	A	521	THR	N-CA-C	-7.71	98.81	110.07
1	D	2497	GLN	N-CA-C	-7.69	103.35	112.89
1	A	297	ILE	N-CA-C	7.67	119.48	112.43
1	D	1046	ASP	CA-C-N	7.66	127.38	119.56
1	D	1046	ASP	C-N-CA	7.66	127.38	119.56
1	C	1736	ASN	CA-C-N	7.66	127.37	119.56
1	C	1736	ASN	C-N-CA	7.66	127.37	119.56
1	A	1046	ASP	CA-C-N	7.66	127.32	119.82
1	A	1046	ASP	C-N-CA	7.66	127.32	119.82
1	A	860	PRO	CA-C-N	7.62	127.58	120.03
1	A	860	PRO	C-N-CA	7.62	127.58	120.03
1	B	860	PRO	CA-C-N	7.57	127.52	120.03
1	B	860	PRO	C-N-CA	7.57	127.52	120.03
1	D	2291	PHE	N-CA-C	-7.56	104.67	114.04
1	C	2424	GLY	CA-C-N	7.55	127.26	119.56
1	C	2424	GLY	C-N-CA	7.55	127.26	119.56
1	C	1463	LYS	CA-C-N	7.52	127.23	119.56
1	C	1463	LYS	C-N-CA	7.52	127.23	119.56
1	C	1438	ILE	CA-C-N	7.47	127.18	119.56
1	C	1438	ILE	C-N-CA	7.47	127.18	119.56
2	F	14	LEU	CA-C-N	7.46	127.91	119.92
2	F	14	LEU	C-N-CA	7.46	127.91	119.92
1	B	1736	ASN	CA-C-N	7.45	127.16	119.56
1	B	1736	ASN	C-N-CA	7.45	127.16	119.56
1	A	84	ALA	CA-C-N	7.43	127.14	119.56
1	A	84	ALA	C-N-CA	7.43	127.14	119.56
1	C	860	PRO	CA-C-N	7.42	127.37	120.03
1	C	860	PRO	C-N-CA	7.42	127.37	120.03
1	A	1736	ASN	CA-C-N	7.41	127.12	119.56
1	A	1736	ASN	C-N-CA	7.41	127.12	119.56
2	F	515	VAL	N-CA-C	7.39	118.10	108.35
1	B	1844	ASP	CA-C-N	7.37	129.06	119.84
1	B	1844	ASP	C-N-CA	7.37	129.06	119.84
1	D	1736	ASN	CA-C-N	7.35	127.02	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1736	ASN	C-N-CA	7.35	127.02	119.82
2	F	814	LEU	CA-C-N	7.33	127.97	119.47
2	F	814	LEU	C-N-CA	7.33	127.97	119.47
1	B	1241	GLY	N-CA-C	-7.31	102.70	112.14
1	D	315	THR	CA-C-N	7.31	128.97	119.84
1	D	315	THR	C-N-CA	7.31	128.97	119.84
1	E	2424	GLY	CA-C-N	7.29	127.63	119.32
1	E	2424	GLY	C-N-CA	7.29	127.63	119.32
1	D	84	ALA	CA-C-N	7.27	126.98	119.56
1	D	84	ALA	C-N-CA	7.27	126.98	119.56
2	F	478	ARG	CA-C-N	7.27	126.95	119.82
2	F	478	ARG	C-N-CA	7.27	126.95	119.82
1	C	2009	LEU	CA-C-N	7.25	127.70	120.52
1	C	2009	LEU	C-N-CA	7.25	127.70	120.52
1	B	297	ILE	N-CA-C	7.25	119.10	112.43
1	A	2374	ASN	N-CA-C	7.24	118.15	108.38
1	E	1046	ASP	CA-C-N	7.22	126.89	119.82
1	E	1046	ASP	C-N-CA	7.22	126.89	119.82
2	F	250	ALA	CA-C-N	7.22	127.17	120.03
2	F	250	ALA	C-N-CA	7.22	127.17	120.03
2	F	1432	ASP	CA-C-N	7.20	126.87	119.82
2	F	1432	ASP	C-N-CA	7.20	126.87	119.82
1	C	1844	ASP	CA-C-N	7.19	128.82	119.84
1	C	1844	ASP	C-N-CA	7.19	128.82	119.84
1	D	1004	VAL	N-CA-C	-7.18	103.85	110.82
1	E	1295	ASP	CA-CB-CG	7.16	119.76	112.60
2	F	243	LEU	CA-C-N	7.11	127.26	119.87
2	F	243	LEU	C-N-CA	7.11	127.26	119.87
1	E	860	PRO	CA-C-N	7.11	127.06	120.03
1	E	860	PRO	C-N-CA	7.11	127.06	120.03
1	C	84	ALA	CA-C-N	7.10	126.80	119.56
1	C	84	ALA	C-N-CA	7.10	126.80	119.56
1	D	1983	LEU	CA-C-N	7.06	126.69	119.56
1	D	1983	LEU	C-N-CA	7.06	126.69	119.56
1	E	297	ILE	N-CA-C	7.04	118.91	112.43
1	A	1103	ASN	CA-CB-CG	-7.04	105.56	112.60
1	D	1463	LYS	CA-C-N	7.03	126.73	119.56
1	D	1463	LYS	C-N-CA	7.03	126.73	119.56
1	A	1821	LEU	N-CA-C	-7.01	104.85	113.41
1	D	2009	LEU	CA-C-N	6.98	127.43	120.52
1	D	2009	LEU	C-N-CA	6.98	127.43	120.52
1	D	2486	PHE	CA-C-N	6.96	126.92	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2486	PHE	C-N-CA	6.96	126.92	120.03
1	B	1250	TYR	N-CA-C	6.93	119.60	109.07
1	B	1438	ILE	CA-C-N	6.92	128.49	119.84
1	B	1438	ILE	C-N-CA	6.92	128.49	119.84
1	A	1463	LYS	CA-C-N	6.91	126.61	119.56
1	A	1463	LYS	C-N-CA	6.91	126.61	119.56
1	D	1152	ASN	CA-C-N	6.91	126.82	119.85
1	D	1152	ASN	C-N-CA	6.91	126.82	119.85
1	B	2349	GLY	CA-C-N	6.90	126.86	120.03
1	B	2349	GLY	C-N-CA	6.90	126.86	120.03
1	B	2009	LEU	CA-C-N	6.89	127.06	120.31
1	B	2009	LEU	C-N-CA	6.89	127.06	120.31
1	B	1821	LEU	N-CA-C	-6.87	105.43	113.88
2	F	2082	GLY	N-CA-C	-6.86	102.77	112.37
2	F	734	THR	CA-C-N	6.84	126.80	120.03
2	F	734	THR	C-N-CA	6.84	126.80	120.03
1	E	2402	TYR	CA-C-N	6.84	126.82	119.78
1	E	2402	TYR	C-N-CA	6.84	126.82	119.78
1	E	1463	LYS	CA-C-N	6.83	126.53	119.56
1	E	1463	LYS	C-N-CA	6.83	126.53	119.56
1	E	2009	LEU	CA-C-N	6.81	127.26	120.52
1	E	2009	LEU	C-N-CA	6.81	127.26	120.52
2	F	87	VAL	CA-C-N	6.80	127.20	119.92
2	F	87	VAL	C-N-CA	6.80	127.20	119.92
2	F	2147	ASN	CA-C-N	6.80	126.43	119.56
2	F	2147	ASN	C-N-CA	6.80	126.43	119.56
1	B	1824	ASP	CA-CB-CG	6.79	119.39	112.60
1	B	1502	VAL	N-CA-C	6.78	117.61	108.11
1	A	2009	LEU	CA-C-N	6.77	126.94	120.31
1	A	2009	LEU	C-N-CA	6.77	126.94	120.31
1	B	1463	LYS	CA-C-N	6.77	126.73	119.28
1	B	1463	LYS	C-N-CA	6.77	126.73	119.28
1	C	1896	LEU	CA-C-N	6.77	126.73	120.03
1	C	1896	LEU	C-N-CA	6.77	126.73	120.03
1	A	1489	ILE	N-CA-C	6.76	117.78	107.77
1	B	1988	THR	CA-C-N	6.75	126.92	120.31
1	B	1988	THR	C-N-CA	6.75	126.92	120.31
2	F	1442	THR	N-CA-C	6.75	120.06	110.14
1	D	782	LYS	CA-C-N	6.74	126.37	119.56
1	D	782	LYS	C-N-CA	6.74	126.37	119.56
2	F	1410	TRP	N-CA-C	-6.74	105.62	114.31
1	D	1824	ASP	CA-CB-CG	6.73	119.33	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	782	LYS	CA-C-N	6.70	126.39	119.56
1	C	782	LYS	C-N-CA	6.70	126.39	119.56
1	D	1844	ASP	CA-C-N	6.67	128.17	119.84
1	D	1844	ASP	C-N-CA	6.67	128.17	119.84
1	D	966	ASP	CA-CB-CG	6.66	119.26	112.60
1	A	71	ASN	CA-C-N	6.66	127.19	119.47
1	A	71	ASN	C-N-CA	6.66	127.19	119.47
1	E	1647	ILE	CA-C-N	6.66	127.23	120.38
1	E	1647	ILE	C-N-CA	6.66	127.23	120.38
1	D	2435	TYR	N-CA-C	6.65	120.36	109.06
1	C	1152	ASN	CA-C-N	6.61	126.53	119.85
1	C	1152	ASN	C-N-CA	6.61	126.53	119.85
1	C	1764	ASN	CA-CB-CG	-6.60	106.00	112.60
1	A	1634	GLU	CA-C-N	6.59	126.57	119.78
1	A	1634	GLU	C-N-CA	6.59	126.57	119.78
1	E	966	ASP	CA-CB-CG	6.59	119.19	112.60
1	D	2457	SER	N-CA-C	-6.58	100.47	109.95
1	E	71	ASN	CA-C-N	6.58	127.11	119.47
1	E	71	ASN	C-N-CA	6.58	127.11	119.47
1	C	1502	VAL	N-CA-C	6.56	117.29	108.11
1	E	1335	GLY	N-CA-C	-6.55	102.58	112.41
1	B	215	ASP	CA-C-N	6.55	126.24	119.56
1	B	215	ASP	C-N-CA	6.55	126.24	119.56
1	D	1722	GLY	CA-C-N	6.55	126.53	119.78
1	D	1722	GLY	C-N-CA	6.55	126.53	119.78
2	F	505	ASP	CA-CB-CG	-6.55	106.05	112.60
2	F	595	LEU	CA-C-N	6.54	126.51	120.03
2	F	595	LEU	C-N-CA	6.54	126.51	120.03
2	F	2130	ASP	CA-C-N	6.53	126.22	119.56
2	F	2130	ASP	C-N-CA	6.53	126.22	119.56
1	A	1241	GLY	N-CA-C	-6.53	103.71	112.14
2	F	2120	GLN	CA-C-N	6.52	126.14	119.56
2	F	2120	GLN	C-N-CA	6.52	126.14	119.56
1	E	1896	LEU	CA-C-N	6.51	126.48	120.03
1	E	1896	LEU	C-N-CA	6.51	126.48	120.03
1	C	1991	ASP	CA-C-N	6.50	126.46	120.03
1	C	1991	ASP	C-N-CA	6.50	126.46	120.03
2	F	552	ASP	CA-C-N	6.49	126.18	119.56
2	F	552	ASP	C-N-CA	6.49	126.18	119.56
1	D	71	ASN	CA-C-N	6.49	126.18	119.56
1	D	71	ASN	C-N-CA	6.49	126.18	119.56
2	F	1329	ASP	CA-CB-CG	-6.49	106.11	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	522	PRO	N-CA-C	-6.49	100.90	111.15
2	F	1585	ARG	NE-CZ-NH2	6.48	125.03	119.20
1	D	860	PRO	CA-C-N	6.47	126.45	119.78
1	D	860	PRO	C-N-CA	6.47	126.45	119.78
1	B	1838	ASP	N-CA-C	-6.47	103.51	111.40
2	F	1723	ILE	N-CA-C	6.46	117.15	108.11
1	A	1335	GLY	N-CA-C	-6.43	102.76	112.41
1	A	1903	SER	N-CA-C	6.43	118.13	107.20
1	A	511	GLN	CA-C-N	6.40	126.37	120.03
1	A	511	GLN	C-N-CA	6.40	126.37	120.03
1	E	890	ALA	CA-C-N	6.40	126.90	119.47
1	E	890	ALA	C-N-CA	6.40	126.90	119.47
1	A	2335	VAL	N-CA-C	6.40	117.09	107.75
1	D	1520	GLN	CA-C-N	6.40	126.36	120.03
1	D	1520	GLN	C-N-CA	6.40	126.36	120.03
1	B	2293	LYS	CA-C-N	6.39	126.36	120.03
1	B	2293	LYS	C-N-CA	6.39	126.36	120.03
1	C	1177	ILE	N-CA-C	6.39	117.32	108.12
2	F	1113	PHE	CA-C-N	6.38	126.34	120.03
2	F	1113	PHE	C-N-CA	6.38	126.34	120.03
1	D	501	ALA	CA-C-N	6.37	126.34	120.03
1	D	501	ALA	C-N-CA	6.37	126.34	120.03
2	F	98	GLY	CA-C-N	6.36	126.27	119.28
2	F	98	GLY	C-N-CA	6.36	126.27	119.28
1	A	501	ALA	CA-C-N	6.35	126.32	120.03
1	A	501	ALA	C-N-CA	6.35	126.32	120.03
1	C	71	ASN	CA-C-N	6.35	126.83	119.47
1	C	71	ASN	C-N-CA	6.35	126.83	119.47
1	D	1648	PRO	CA-C-N	6.35	126.30	119.76
1	D	1648	PRO	C-N-CA	6.35	126.30	119.76
1	A	2402	TYR	CA-C-N	6.34	126.31	119.78
1	A	2402	TYR	C-N-CA	6.34	126.31	119.78
1	B	1896	LEU	CA-C-N	6.34	126.31	119.78
1	B	1896	LEU	C-N-CA	6.34	126.31	119.78
1	E	1821	LEU	N-CA-C	-6.33	105.69	113.41
2	F	1322	HIS	N-CA-C	6.33	118.93	108.99
1	C	1335	GLY	N-CA-C	-6.33	102.41	112.66
1	D	1875	THR	N-CA-C	-6.32	105.05	112.89
1	A	445	ARG	NE-CZ-NH2	-6.32	113.52	119.20
2	F	1484	ASP	CA-C-N	6.29	127.70	119.84
2	F	1484	ASP	C-N-CA	6.29	127.70	119.84
1	E	511	GLN	CA-C-N	6.28	126.24	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	511	GLN	C-N-CA	6.28	126.24	120.21
1	C	2263	PHE	CA-CB-CG	-6.27	107.53	113.80
1	E	1822	LEU	N-CA-C	-6.27	104.37	111.14
1	E	1004	VAL	N-CA-C	-6.26	104.40	110.72
1	C	1697	VAL	CA-C-N	6.26	126.61	119.92
1	C	1697	VAL	C-N-CA	6.26	126.61	119.92
1	E	1756	GLU	CA-C-N	6.25	126.22	119.78
1	E	1756	GLU	C-N-CA	6.25	126.22	119.78
2	F	797	ALA	CA-C-N	6.25	126.79	120.04
2	F	797	ALA	C-N-CA	6.25	126.79	120.04
1	E	1394	ASN	CA-C-N	6.24	126.71	119.47
1	E	1394	ASN	C-N-CA	6.24	126.71	119.47
1	E	1893	LYS	CA-C-N	6.24	126.60	119.92
1	E	1893	LYS	C-N-CA	6.24	126.60	119.92
1	A	1745	GLU	N-CA-C	-6.24	104.56	111.36
1	C	2293	LYS	CA-C-N	6.24	126.21	120.03
1	C	2293	LYS	C-N-CA	6.24	126.21	120.03
2	F	1334	ASP	CA-C-N	6.22	126.41	120.31
2	F	1334	ASP	C-N-CA	6.22	126.41	120.31
1	C	1988	THR	CA-C-N	6.21	126.17	119.78
1	C	1988	THR	C-N-CA	6.21	126.17	119.78
2	F	2153	ASP	CA-C-N	6.21	125.89	119.56
2	F	2153	ASP	C-N-CA	6.21	125.89	119.56
1	A	1988	THR	CA-C-N	6.20	126.16	119.78
1	A	1988	THR	C-N-CA	6.20	126.16	119.78
1	E	1904	ASP	CA-C-N	6.20	126.11	119.85
1	E	1904	ASP	C-N-CA	6.20	126.11	119.85
2	F	1255	ALA	CA-C-N	6.20	125.82	119.56
2	F	1255	ALA	C-N-CA	6.20	125.82	119.56
1	A	719	GLN	CA-C-N	6.20	125.82	119.56
1	A	719	GLN	C-N-CA	6.20	125.82	119.56
1	B	704	SER	N-CA-C	6.19	119.64	108.69
1	A	1231	ALA	CA-C-N	6.18	126.15	120.03
1	A	1231	ALA	C-N-CA	6.18	126.15	120.03
1	E	1405	TYR	CA-C-N	6.18	125.94	119.76
1	E	1405	TYR	C-N-CA	6.18	125.94	119.76
1	E	1231	ALA	CA-C-N	6.18	126.09	119.85
1	E	1231	ALA	C-N-CA	6.18	126.09	119.85
2	F	1244	LYS	N-CA-C	6.17	121.27	113.25
1	B	501	ALA	CA-C-N	6.17	126.14	120.03
1	B	501	ALA	C-N-CA	6.17	126.14	120.03
1	B	1634	GLU	CA-C-N	6.17	126.13	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1634	GLU	C-N-CA	6.17	126.13	119.78
1	E	1988	THR	CA-C-N	6.17	126.08	119.85
1	E	1988	THR	C-N-CA	6.17	126.08	119.85
2	F	1165	GLN	N-CA-C	6.17	118.73	111.02
2	F	1829	MET	CA-C-N	6.16	126.08	119.85
2	F	1829	MET	C-N-CA	6.16	126.08	119.85
1	B	859	LEU	N-CA-C	-6.16	101.08	110.07
1	E	1058	ASP	CA-CB-CG	6.15	118.75	112.60
2	F	1139	ARG	CA-C-N	6.15	126.06	119.85
2	F	1139	ARG	C-N-CA	6.15	126.06	119.85
1	B	719	GLN	CA-C-N	6.15	126.12	120.03
1	B	719	GLN	C-N-CA	6.15	126.12	120.03
1	A	462	ARG	NE-CZ-NH2	-6.15	113.67	119.20
1	A	2293	LYS	CA-C-N	6.14	126.11	120.03
1	A	2293	LYS	C-N-CA	6.14	126.11	120.03
1	D	1896	LEU	CA-C-N	6.14	126.10	119.78
1	D	1896	LEU	C-N-CA	6.14	126.10	119.78
1	A	704	SER	N-CA-C	6.13	118.41	108.41
1	D	1697	VAL	CA-C-N	6.13	126.48	119.92
1	D	1697	VAL	C-N-CA	6.13	126.48	119.92
2	F	802	PRO	CA-C-N	6.13	126.48	119.92
2	F	802	PRO	C-N-CA	6.13	126.48	119.92
1	D	1988	THR	CA-C-N	6.13	126.10	120.03
1	D	1988	THR	C-N-CA	6.13	126.10	120.03
1	A	2417	VAL	N-CA-C	6.13	116.95	108.12
1	A	1874	ASP	CA-CB-CG	-6.13	106.47	112.60
1	D	2417	VAL	N-CA-C	6.12	117.29	108.48
1	C	1241	GLY	N-CA-C	-6.11	103.23	111.54
1	D	303	PHE	N-CA-C	-6.11	105.41	112.92
1	E	1403	MET	N-CA-C	6.10	117.16	108.74
1	D	1335	GLY	N-CA-C	-6.10	103.25	112.41
1	B	1321	ASP	CA-CB-CG	6.10	118.70	112.60
2	F	1085	LEU	N-CA-C	-6.09	104.75	111.82
2	F	461	GLN	CA-C-N	-6.08	114.11	122.93
2	F	461	GLN	C-N-CA	-6.08	114.11	122.93
1	B	2417	VAL	N-CA-C	6.08	116.62	108.11
1	B	1875	THR	N-CA-C	-6.08	105.36	112.89
1	E	359	PHE	CA-CB-CG	-6.07	107.73	113.80
2	F	2082	GLY	CA-C-N	-6.07	114.11	122.30
2	F	2082	GLY	C-N-CA	-6.07	114.11	122.30
1	D	1893	LYS	CA-C-N	6.06	126.41	119.92
1	D	1893	LYS	C-N-CA	6.06	126.41	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	606	ASN	CA-C-N	6.06	126.50	119.47
2	F	606	ASN	C-N-CA	6.06	126.50	119.47
2	F	950	VAL	N-CA-C	6.05	116.58	107.80
2	F	1860	PHE	CA-C-N	6.05	126.02	120.03
2	F	1860	PHE	C-N-CA	6.05	126.02	120.03
1	B	521	THR	N-CA-C	-6.05	96.44	109.81
2	F	1109	THR	N-CA-C	6.04	117.37	108.86
2	F	812	THR	N-CA-C	-6.03	106.08	113.50
1	E	1722	GLY	CA-C-N	6.02	125.96	119.76
1	E	1722	GLY	C-N-CA	6.02	125.96	119.76
1	A	1499	GLN	N-CA-C	6.02	119.01	109.50
2	F	1955	GLN	N-CA-C	6.02	118.30	108.55
1	A	1853	PHE	CA-CB-CG	6.01	119.81	113.80
2	F	1137	PHE	CA-C-N	-6.01	112.97	122.23
2	F	1137	PHE	C-N-CA	-6.01	112.97	122.23
1	D	224	SER	CA-C-N	6.01	125.69	119.56
1	D	224	SER	C-N-CA	6.01	125.69	119.56
2	F	75	ASN	N-CA-C	6.01	119.93	111.52
1	A	1525	PHE	CA-CB-CG	6.00	119.80	113.80
1	E	1634	GLU	CA-C-N	6.00	125.96	119.78
1	E	1634	GLU	C-N-CA	6.00	125.96	119.78
1	C	2486	PHE	CA-C-N	6.00	125.91	119.85
1	C	2486	PHE	C-N-CA	6.00	125.91	119.85
2	F	1922	ASP	CA-C-N	5.99	126.42	119.47
2	F	1922	ASP	C-N-CA	5.99	126.42	119.47
1	D	719	GLN	CA-C-N	5.99	125.96	120.03
1	D	719	GLN	C-N-CA	5.99	125.96	120.03
1	A	1405	TYR	CA-C-N	5.98	125.74	119.76
1	A	1405	TYR	C-N-CA	5.98	125.74	119.76
2	F	1804	TYR	N-CA-C	5.98	119.29	109.72
1	E	1908	ASP	CA-CB-CG	5.98	118.58	112.60
2	F	1491	THR	CA-C-N	5.98	126.17	120.31
2	F	1491	THR	C-N-CA	5.98	126.17	120.31
1	B	71	ASN	CA-C-N	5.97	126.40	119.47
1	B	71	ASN	C-N-CA	5.97	126.40	119.47
1	E	704	SER	N-CA-C	5.96	119.25	108.69
1	B	1904	ASP	CA-C-N	5.96	125.87	119.85
1	B	1904	ASP	C-N-CA	5.96	125.87	119.85
1	E	1332	VAL	N-CA-C	-5.96	100.00	108.58
2	F	848	VAL	N-CA-C	5.95	114.44	107.77
1	A	1868	TYR	N-CA-C	-5.94	104.19	112.45
1	C	1520	GLN	CA-C-N	5.94	125.85	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1520	GLN	C-N-CA	5.94	125.85	119.85
1	D	2293	LYS	CA-C-N	5.94	125.91	120.03
1	D	2293	LYS	C-N-CA	5.94	125.91	120.03
1	A	1647	ILE	CA-C-N	5.93	126.49	120.38
1	A	1647	ILE	C-N-CA	5.93	126.49	120.38
2	F	303	ARG	N-CA-C	5.93	117.26	108.60
1	E	2417	VAL	N-CA-C	5.93	116.66	108.12
1	D	1250	TYR	N-CA-C	5.93	118.19	109.24
1	D	2374	ASN	N-CA-C	5.93	116.38	108.38
1	A	1764	ASN	CA-CB-CG	-5.92	106.68	112.60
1	C	521	THR	N-CA-C	-5.92	100.28	109.87
2	F	1777	GLU	CA-C-N	5.92	125.59	119.56
2	F	1777	GLU	C-N-CA	5.92	125.59	119.56
1	C	664	THR	CA-C-N	5.91	126.06	119.32
1	C	664	THR	C-N-CA	5.91	126.06	119.32
1	B	1648	PRO	CA-C-N	5.91	125.82	119.85
1	B	1648	PRO	C-N-CA	5.91	125.82	119.85
1	C	1648	PRO	CA-C-N	5.91	125.82	119.85
1	C	1648	PRO	C-N-CA	5.91	125.82	119.85
1	C	303	PHE	N-CA-C	-5.91	105.66	112.92
1	B	2402	TYR	CA-C-N	5.90	125.92	119.90
1	B	2402	TYR	C-N-CA	5.90	125.92	119.90
1	E	660	ASN	CA-CB-CG	5.90	118.50	112.60
1	C	117	ALA	N-CA-C	-5.89	104.94	111.36
2	F	440	PRO	N-CA-C	-5.89	102.01	111.38
2	F	1494	VAL	N-CA-C	5.89	116.36	107.75
2	F	475	HIS	CA-C-N	-5.89	114.68	122.99
2	F	475	HIS	C-N-CA	-5.89	114.68	122.99
1	D	1764	ASN	CA-CB-CG	-5.88	106.72	112.60
1	E	1599	GLN	CB-CA-C	-5.88	109.78	116.54
1	A	1875	THR	N-CA-C	-5.88	105.60	112.89
1	B	467	GLN	CA-C-N	-5.88	114.60	122.42
1	B	467	GLN	C-N-CA	-5.88	114.60	122.42
1	D	1714	SER	CA-C-N	5.88	125.50	119.56
1	D	1714	SER	C-N-CA	5.88	125.50	119.56
1	B	142	ARG	CA-C-N	5.87	125.55	119.56
1	B	142	ARG	C-N-CA	5.87	125.55	119.56
1	D	316	PRO	CA-C-N	-5.87	115.24	122.93
1	D	316	PRO	C-N-CA	-5.87	115.24	122.93
1	B	1279	THR	CA-C-N	5.86	126.00	119.32
1	B	1279	THR	C-N-CA	5.86	126.00	119.32
1	E	2349	GLY	CA-C-N	5.86	125.77	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2349	GLY	C-N-CA	5.86	125.77	119.85
2	F	1224	SER	CA-C-N	5.86	126.27	119.47
2	F	1224	SER	C-N-CA	5.86	126.27	119.47
1	B	1764	ASN	CA-CB-CG	-5.86	106.74	112.60
1	D	1270	PHE	CA-CB-CG	-5.86	107.94	113.80
1	A	215	ASP	CA-C-N	5.84	125.52	119.56
1	A	215	ASP	C-N-CA	5.84	125.52	119.56
1	B	782	LYS	CA-C-N	5.84	125.95	119.87
1	B	782	LYS	C-N-CA	5.84	125.95	119.87
1	B	660	ASN	CA-CB-CG	5.84	118.44	112.60
1	E	521	THR	N-CA-C	-5.84	101.79	110.20
1	C	1250	TYR	N-CA-C	5.84	117.94	109.07
1	A	453	SER	CA-C-N	5.83	125.51	119.56
1	A	453	SER	C-N-CA	5.83	125.51	119.56
1	B	1991	ASP	CA-C-N	5.83	125.79	119.78
1	B	1991	ASP	C-N-CA	5.83	125.79	119.78
1	A	1983	LEU	CA-C-N	5.83	125.51	119.56
1	A	1983	LEU	C-N-CA	5.83	125.51	119.56
1	C	1562	GLY	N-CA-C	-5.83	106.69	115.32
1	D	1599	GLN	CB-CA-C	-5.83	109.84	116.54
2	F	1780	THR	N-CA-C	-5.83	105.94	114.39
1	B	84	ALA	CA-C-N	5.82	125.92	119.87
1	B	84	ALA	C-N-CA	5.82	125.92	119.87
1	B	1599	GLN	CB-CA-C	-5.81	109.86	116.54
1	D	1525	PHE	CB-CA-C	-5.81	99.52	110.67
1	A	1896	LEU	CA-C-N	5.81	125.71	119.85
1	A	1896	LEU	C-N-CA	5.81	125.71	119.85
1	D	1336	ASP	N-CA-C	5.80	116.05	107.88
1	D	1692	ILE	CA-C-N	5.80	125.70	119.85
1	D	1692	ILE	C-N-CA	5.80	125.70	119.85
2	F	1014	PHE	CA-CB-CG	5.79	119.59	113.80
1	A	1502	VAL	N-CA-C	5.78	116.19	108.11
2	F	957	GLN	CA-C-N	5.77	125.74	120.03
2	F	957	GLN	C-N-CA	5.77	125.74	120.03
2	F	274	PRO	CA-C-N	5.77	125.68	119.85
2	F	274	PRO	C-N-CA	5.77	125.68	119.85
2	F	363	LEU	N-CA-C	-5.77	102.15	110.40
2	F	1145	ASN	N-CA-C	-5.77	105.07	111.36
1	A	1332	VAL	N-CA-C	-5.77	99.44	107.80
1	E	2293	LYS	CA-C-N	5.77	125.74	120.03
1	E	2293	LYS	C-N-CA	5.77	125.74	120.03
1	C	1704	HIS	CA-CB-CG	-5.77	108.03	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	719	GLN	CA-C-N	5.76	125.67	119.85
1	E	719	GLN	C-N-CA	5.76	125.67	119.85
2	F	943	GLN	CA-C-N	5.76	127.04	119.84
2	F	943	GLN	C-N-CA	5.76	127.04	119.84
1	E	1520	GLN	CA-C-N	5.75	125.66	119.85
1	E	1520	GLN	C-N-CA	5.75	125.66	119.85
1	E	1539	GLY	N-CA-C	-5.75	105.23	113.86
1	C	1483	VAL	N-CA-C	5.75	116.14	107.80
2	F	1227	LYS	N-CA-C	-5.75	106.81	113.88
1	D	511	GLN	CA-C-N	5.75	125.72	120.03
1	D	511	GLN	C-N-CA	5.75	125.72	120.03
1	A	1058	ASP	CA-CB-CG	5.75	118.34	112.60
1	E	1244	THR	N-CA-C	5.74	116.96	108.86
1	D	1231	ALA	CA-C-N	5.74	125.65	119.85
1	D	1231	ALA	C-N-CA	5.74	125.65	119.85
2	F	68	PHE	CA-CB-CG	-5.74	108.06	113.80
2	F	1237	ASN	CA-CB-CG	-5.73	106.87	112.60
1	C	1893	LYS	CA-C-N	5.72	126.04	119.92
1	C	1893	LYS	C-N-CA	5.72	126.04	119.92
1	B	1177	ILE	N-CA-C	5.71	116.11	108.11
1	D	890	ALA	CA-C-N	5.71	126.10	119.47
1	D	890	ALA	C-N-CA	5.71	126.10	119.47
1	A	326	LYS	CA-C-N	-5.71	115.00	122.37
1	A	326	LYS	C-N-CA	-5.71	115.00	122.37
1	B	384	ALA	CA-C-N	5.71	125.62	119.85
1	B	384	ALA	C-N-CA	5.71	125.62	119.85
1	C	224	SER	CA-C-N	5.71	125.56	119.28
1	C	224	SER	C-N-CA	5.71	125.56	119.28
1	D	1821	LEU	N-CA-C	-5.71	105.42	112.90
2	F	2038	GLU	N-CA-C	-5.70	106.46	113.41
1	E	1838	ASP	N-CA-C	-5.69	104.46	111.40
1	E	2432	ILE	N-CA-C	5.69	116.07	108.11
2	F	1785	GLY	N-CA-C	5.67	118.78	110.38
1	B	725	MET	N-CA-C	5.65	118.64	110.28
1	E	2486	PHE	CA-C-N	5.63	125.54	119.85
1	E	2486	PHE	C-N-CA	5.63	125.54	119.85
1	D	2402	TYR	CA-C-N	5.63	125.54	119.85
1	D	2402	TYR	C-N-CA	5.63	125.54	119.85
1	C	793	ALA	N-CA-C	-5.62	102.70	109.83
1	E	1697	VAL	CA-C-N	5.62	125.93	119.92
1	E	1697	VAL	C-N-CA	5.62	125.93	119.92
1	D	1759	ASP	N-CA-C	5.61	117.79	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1808	HIS	CA-CB-CG	5.61	119.41	113.80
1	B	1893	LYS	CA-C-N	5.60	125.91	119.92
1	B	1893	LYS	C-N-CA	5.60	125.91	119.92
1	E	1915	THR	N-CA-C	-5.60	105.17	111.28
1	D	693	ALA	CA-C-N	5.60	125.59	120.21
1	D	693	ALA	C-N-CA	5.60	125.59	120.21
2	F	145	GLN	CA-C-N	5.59	126.83	119.84
2	F	145	GLN	C-N-CA	5.59	126.83	119.84
1	D	1332	VAL	N-CA-C	-5.59	100.54	108.58
1	D	2331	VAL	N-CA-C	5.59	115.93	108.11
2	F	364	PRO	CA-C-N	5.59	125.49	119.85
2	F	364	PRO	C-N-CA	5.59	125.49	119.85
1	B	1823	GLU	N-CA-C	-5.58	100.61	109.76
1	A	782	LYS	CA-C-N	5.58	125.67	119.87
1	A	782	LYS	C-N-CA	5.58	125.67	119.87
1	C	2432	ILE	N-CA-C	5.57	116.14	108.12
1	C	1730	LYS	N-CA-C	-5.57	106.15	113.17
1	A	1904	ASP	CA-C-N	5.57	125.47	119.85
1	A	1904	ASP	C-N-CA	5.57	125.47	119.85
1	B	975	ASN	CA-CB-CG	-5.56	107.04	112.60
1	E	326	LYS	CA-C-N	-5.56	114.02	121.80
1	E	326	LYS	C-N-CA	-5.56	114.02	121.80
1	B	1058	ASP	CA-CB-CG	5.55	118.15	112.60
1	B	2497	GLN	N-CA-C	-5.55	106.35	113.23
1	C	719	GLN	CA-C-N	5.54	125.52	120.03
1	C	719	GLN	C-N-CA	5.54	125.52	120.03
1	A	1838	ASP	N-CA-C	-5.54	104.88	111.69
2	F	990	SER	N-CA-C	5.54	116.69	108.60
1	E	501	ALA	CA-C-N	5.53	125.51	120.03
1	E	501	ALA	C-N-CA	5.53	125.51	120.03
1	D	2424	GLY	CA-C-N	5.53	125.88	119.47
1	D	2424	GLY	C-N-CA	5.53	125.88	119.47
1	E	198	THR	N-CA-C	5.53	122.02	109.81
1	D	521	THR	N-CA-C	-5.52	97.60	109.81
2	F	283	TRP	CA-C-N	-5.52	114.92	122.93
2	F	283	TRP	C-N-CA	-5.52	114.92	122.93
2	F	851	THR	N-CA-C	-5.52	101.57	109.24
1	C	725	MET	N-CA-C	5.52	118.45	110.28
2	F	695	LYS	CA-C-N	5.52	125.46	119.78
2	F	695	LYS	C-N-CA	5.52	125.46	119.78
1	B	1903	SER	N-CA-C	5.51	119.31	107.67
1	C	1385	PHE	N-CA-C	5.51	117.45	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	903	ILE	N-CA-C	-5.51	105.74	111.58
1	B	224	SER	CA-C-N	5.51	125.86	119.47
1	B	224	SER	C-N-CA	5.51	125.86	119.47
1	D	2485	SER	N-CA-C	5.50	117.93	109.07
1	E	827	ALA	CA-C-N	-5.49	113.92	122.05
1	E	827	ALA	C-N-CA	-5.49	113.92	122.05
2	F	170	SER	CA-C-N	5.49	125.16	119.56
2	F	170	SER	C-N-CA	5.49	125.16	119.56
1	A	1485	GLY	CA-C-N	5.49	126.70	119.84
1	A	1485	GLY	C-N-CA	5.49	126.70	119.84
1	C	501	ALA	CA-C-N	5.49	125.47	120.03
1	C	501	ALA	C-N-CA	5.49	125.47	120.03
1	D	215	ASP	CA-C-N	5.49	125.83	119.47
1	D	215	ASP	C-N-CA	5.49	125.83	119.47
1	E	224	SER	CA-C-N	5.49	125.31	119.28
1	E	224	SER	C-N-CA	5.49	125.31	119.28
1	A	2263	PHE	CA-CB-CG	-5.48	108.32	113.80
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	863	THR	N-CA-C	-5.48	99.56	109.09
1	E	1991	ASP	CA-C-N	5.48	125.38	119.85
1	E	1991	ASP	C-N-CA	5.48	125.38	119.85
1	B	542	SER	N-CA-C	5.48	119.22	112.54
1	E	1623	THR	N-CA-C	-5.47	106.65	113.55
2	F	581	TRP	CA-C-N	5.47	125.40	119.76
2	F	581	TRP	C-N-CA	5.47	125.40	119.76
1	B	1836	ASP	CA-C-N	5.47	125.08	119.56
1	B	1836	ASP	C-N-CA	5.47	125.08	119.56
2	F	1316	GLY	CA-C-N	5.47	125.41	119.78
2	F	1316	GLY	C-N-CA	5.47	125.41	119.78
1	B	1716	SER	N-CA-C	5.47	118.43	110.17
1	A	1714	SER	CA-C-N	5.47	125.08	119.56
1	A	1714	SER	C-N-CA	5.47	125.08	119.56
1	D	104	VAL	N-CA-C	5.47	117.97	108.95
1	D	704	SER	N-CA-C	5.46	117.30	108.34
2	F	1397	GLN	CA-C-N	5.46	125.22	119.76
2	F	1397	GLN	C-N-CA	5.46	125.22	119.76
1	A	2453	GLY	CA-C-N	-5.46	114.88	123.13
1	A	2453	GLY	C-N-CA	-5.46	114.88	123.13
2	F	952	TYR	CA-C-N	5.46	125.37	119.85
2	F	952	TYR	C-N-CA	5.46	125.37	119.85
1	A	1617	ALA	CA-C-N	5.46	127.60	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1617	ALA	C-N-CA	5.46	127.60	120.28
1	B	664	THR	CA-C-N	5.46	125.80	119.47
1	B	664	THR	C-N-CA	5.46	125.80	119.47
1	B	401	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	1113	LEU	N-CA-C	5.45	118.34	108.69
2	F	875	TYR	N-CA-CB	-5.45	102.21	110.77
1	E	1336	ASP	N-CA-C	5.45	115.74	108.38
1	D	326	LYS	CA-C-N	-5.45	114.17	121.80
1	D	326	LYS	C-N-CA	-5.45	114.17	121.80
1	C	384	ALA	CA-C-N	5.45	125.42	120.03
1	C	384	ALA	C-N-CA	5.45	125.42	120.03
2	F	1349	PHE	N-CA-C	-5.44	106.31	113.17
2	F	972	LEU	N-CA-C	-5.44	104.89	112.45
1	E	2106	ASN	CA-C-N	-5.44	116.05	123.12
1	E	2106	ASN	C-N-CA	-5.44	116.05	123.12
1	C	1312	ILE	CA-C-N	5.43	125.36	119.76
1	C	1312	ILE	C-N-CA	5.43	125.36	119.76
1	E	859	LEU	N-CA-C	-5.43	102.15	110.07
1	A	2486	PHE	CA-C-N	5.42	125.37	119.78
1	A	2486	PHE	C-N-CA	5.42	125.37	119.78
1	D	1483	VAL	N-CA-C	5.42	115.65	107.80
1	E	1541	GLY	N-CA-C	-5.42	108.03	114.48
2	F	707	GLY	CA-C-N	-5.41	115.90	123.10
2	F	707	GLY	C-N-CA	-5.41	115.90	123.10
2	F	408	GLY	N-CA-C	-5.41	105.34	112.81
1	E	453	SER	CA-C-N	5.41	125.08	119.56
1	E	453	SER	C-N-CA	5.41	125.08	119.56
1	A	1394	ASN	CA-C-N	5.41	125.74	119.47
1	A	1394	ASN	C-N-CA	5.41	125.74	119.47
1	B	2485	SER	N-CA-C	5.40	117.32	108.52
1	E	1489	ILE	N-CA-C	5.39	115.66	108.11
1	B	326	LYS	CA-C-N	-5.39	115.63	122.37
1	B	326	LYS	C-N-CA	-5.39	115.63	122.37
1	C	1454	ASP	N-CA-C	5.39	117.31	108.52
1	D	2466	ASP	CA-CB-CG	5.39	117.99	112.60
1	E	1270	PHE	CA-CB-CG	-5.39	108.41	113.80
1	D	1107	LEU	N-CA-C	5.38	118.18	109.40
2	F	1042	LYS	CA-C-N	5.38	125.33	119.78
2	F	1042	LYS	C-N-CA	5.38	125.33	119.78
2	F	307	GLN	N-CA-C	5.38	117.26	108.55
1	E	782	LYS	CA-C-N	5.37	125.46	119.87
1	E	782	LYS	C-N-CA	5.37	125.46	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	384	ALA	CA-C-N	5.37	125.35	120.03
1	E	384	ALA	C-N-CA	5.37	125.35	120.03
2	F	1424	ALA	CA-C-N	-5.37	115.15	122.93
2	F	1424	ALA	C-N-CA	-5.37	115.15	122.93
1	A	966	ASP	CA-CB-CG	5.36	117.96	112.60
2	F	517	ILE	N-CA-C	5.36	115.61	108.11
1	B	1522	SER	N-CA-C	-5.36	103.03	109.83
1	E	1692	ILE	CA-C-N	5.35	125.25	119.85
1	E	1692	ILE	C-N-CA	5.35	125.25	119.85
1	E	2401	ASP	CA-CB-CG	5.34	117.94	112.60
1	C	1403	MET	N-CA-C	5.34	116.39	108.60
1	A	1599	GLN	CB-CA-C	-5.33	110.41	116.54
1	C	1904	ASP	CA-C-N	5.33	125.23	119.85
1	C	1904	ASP	C-N-CA	5.33	125.23	119.85
2	F	159	SER	CA-C-N	5.33	125.65	119.47
2	F	159	SER	C-N-CA	5.33	125.65	119.47
1	E	333	GLU	CA-C-N	-5.32	113.81	121.42
1	E	333	GLU	C-N-CA	-5.32	113.81	121.42
1	B	1485	GLY	CA-C-N	5.32	126.49	119.84
1	B	1485	GLY	C-N-CA	5.32	126.49	119.84
1	B	1714	SER	CA-C-N	5.32	124.93	119.56
1	B	1714	SER	C-N-CA	5.32	124.93	119.56
1	E	1113	LEU	N-CA-C	5.32	118.10	109.06
2	F	327	PRO	CA-C-N	-5.32	114.69	122.19
2	F	327	PRO	C-N-CA	-5.32	114.69	122.19
1	A	2349	GLY	CA-C-N	5.31	125.22	119.85
1	A	2349	GLY	C-N-CA	5.31	125.22	119.85
1	E	1494	SER	CA-C-N	5.31	124.98	119.56
1	E	1494	SER	C-N-CA	5.31	124.98	119.56
1	D	1572	ILE	CB-CA-C	-5.31	105.08	111.18
2	F	7	PHE	N-CA-C	-5.31	106.85	113.38
1	D	1229	ASN	CA-CB-CG	-5.30	107.30	112.60
1	C	1394	ASN	CA-C-N	5.30	125.39	119.87
1	C	1394	ASN	C-N-CA	5.30	125.39	119.87
1	A	224	SER	CA-C-N	5.30	125.11	119.28
1	A	224	SER	C-N-CA	5.30	125.11	119.28
1	D	1829	SER	N-CA-C	-5.30	108.08	114.75
1	C	1745	GLU	N-CA-C	-5.30	105.59	111.36
1	E	215	ASP	CA-C-N	5.30	124.96	119.56
1	E	215	ASP	C-N-CA	5.30	124.96	119.56
1	A	664	THR	CA-C-N	5.29	125.36	119.32
1	A	664	THR	C-N-CA	5.29	125.36	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2331	VAL	N-CA-C	5.28	115.46	107.75
2	F	1231	SER	CA-C-N	5.28	123.46	119.66
2	F	1231	SER	C-N-CA	5.28	123.46	119.66
1	E	278	MET	CA-C-N	5.27	125.33	119.32
1	E	278	MET	C-N-CA	5.27	125.33	119.32
1	A	890	ALA	CA-C-N	5.27	125.58	119.47
1	A	890	ALA	C-N-CA	5.27	125.58	119.47
1	A	142	ARG	CA-C-N	5.27	124.88	119.56
1	A	142	ARG	C-N-CA	5.27	124.88	119.56
1	A	1756	GLU	CA-C-N	5.26	125.20	119.78
1	A	1756	GLU	C-N-CA	5.26	125.20	119.78
1	B	890	ALA	CA-C-N	5.26	125.57	119.47
1	B	890	ALA	C-N-CA	5.26	125.57	119.47
2	F	927	ASP	CA-C-N	5.26	125.46	120.31
2	F	927	ASP	C-N-CA	5.26	125.46	120.31
1	B	1702	ASP	CA-CB-CG	5.25	117.86	112.60
1	B	357	TYR	N-CA-C	5.25	117.05	109.07
1	C	1387	VAL	CA-C-N	-5.25	114.79	122.19
1	C	1387	VAL	C-N-CA	-5.25	114.79	122.19
1	D	384	ALA	CA-C-N	5.25	125.19	119.78
1	D	384	ALA	C-N-CA	5.25	125.19	119.78
1	C	786	PHE	CA-CB-CG	-5.25	108.55	113.80
1	C	1489	ILE	N-CA-C	5.25	115.46	108.11
2	F	32	GLY	N-CA-C	-5.25	101.64	112.34
1	A	1381	LEU	N-CA-C	-5.24	102.10	109.96
1	D	725	MET	N-CA-C	5.24	118.03	110.28
2	F	362	THR	N-CA-C	5.24	117.37	109.41
1	E	2466	ASP	CA-CB-CG	5.23	117.83	112.60
1	D	1903	SER	N-CA-C	5.23	115.95	107.32
1	D	278	MET	CA-C-N	5.23	125.28	119.32
1	D	278	MET	C-N-CA	5.23	125.28	119.32
1	E	1438	ILE	CA-C-N	5.22	126.37	119.84
1	E	1438	ILE	C-N-CA	5.22	126.37	119.84
2	F	1532	HIS	N-CA-C	-5.22	103.14	110.50
2	F	1741	LEU	CA-C-N	-5.22	113.51	121.66
2	F	1741	LEU	C-N-CA	-5.22	113.51	121.66
1	C	281	TYR	N-CA-C	-5.22	105.50	111.14
1	D	1688	ILE	N-CA-C	5.22	115.48	108.17
1	C	1231	ALA	CA-C-N	5.22	125.12	119.85
1	C	1231	ALA	C-N-CA	5.22	125.12	119.85
1	B	242	SER	CA-C-N	-5.22	116.48	122.95
1	B	242	SER	C-N-CA	-5.22	116.48	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1520	GLN	CA-C-N	5.22	125.12	119.85
1	A	1520	GLN	C-N-CA	5.22	125.12	119.85
1	D	142	ARG	CA-C-N	5.22	125.29	119.87
1	D	142	ARG	C-N-CA	5.22	125.29	119.87
2	F	927	ASP	CA-CB-CG	5.21	117.81	112.60
1	C	542	SER	N-CA-C	5.21	119.12	112.87
1	D	359	PHE	CA-CB-CG	-5.21	108.59	113.80
2	F	906	TYR	CA-C-N	5.21	125.14	119.78
2	F	906	TYR	C-N-CA	5.21	125.14	119.78
2	F	261	VAL	N-CA-C	5.20	115.39	108.11
1	A	1202	HIS	N-CA-C	5.20	117.09	109.24
1	C	215	ASP	CA-C-N	5.20	125.50	119.47
1	C	215	ASP	C-N-CA	5.20	125.50	119.47
2	F	483	TRP	N-CA-C	5.20	117.92	109.24
1	B	1387	VAL	CA-C-N	-5.19	115.51	122.42
1	B	1387	VAL	C-N-CA	-5.19	115.51	122.42
2	F	1538	ASP	CA-C-N	5.19	124.81	119.56
2	F	1538	ASP	C-N-CA	5.19	124.81	119.56
1	D	1756	GLU	CA-C-N	5.19	125.12	119.78
1	D	1756	GLU	C-N-CA	5.19	125.12	119.78
1	E	1808	HIS	CB-CA-C	-5.18	103.32	111.51
1	C	1748	ASN	N-CA-C	5.18	116.86	108.26
1	D	93	ASN	CA-CB-CG	-5.18	107.42	112.60
1	D	2263	PHE	CA-CB-CG	-5.18	108.62	113.80
1	A	2424	GLY	CA-C-N	5.18	126.31	119.84
1	A	2424	GLY	C-N-CA	5.18	126.31	119.84
2	F	2109	THR	N-CA-C	-5.18	106.97	113.28
1	A	720	PRO	N-CA-C	5.17	120.33	113.86
2	F	486	PHE	N-CA-C	5.17	117.84	110.24
1	C	142	ARG	CA-C-N	5.17	124.78	119.56
1	C	142	ARG	C-N-CA	5.17	124.78	119.56
1	C	1722	GLY	CA-C-N	5.16	125.08	119.76
1	C	1722	GLY	C-N-CA	5.16	125.08	119.76
1	D	341	MET	N-CA-C	5.16	116.36	108.52
1	C	268	PHE	CA-CB-CG	-5.16	108.64	113.80
1	C	2393	PHE	N-CA-C	-5.16	105.74	111.36
1	D	522	PRO	N-CA-C	-5.16	102.86	111.26
1	D	1991	ASP	CA-C-N	5.15	125.09	119.78
1	D	1991	ASP	C-N-CA	5.15	125.09	119.78
1	A	1648	PRO	CA-C-N	5.15	125.05	119.85
1	A	1648	PRO	C-N-CA	5.15	125.05	119.85
1	A	1697	VAL	CA-C-N	5.15	125.13	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1697	VAL	C-N-CA	5.15	125.13	120.03
1	B	966	ASP	CA-CB-CG	5.14	117.75	112.60
1	A	1483	VAL	N-CA-C	5.14	115.26	107.80
1	C	511	GLN	CA-C-N	5.14	125.12	120.03
1	C	511	GLN	C-N-CA	5.14	125.12	120.03
1	C	366	SER	N-CA-C	-5.14	105.76	112.23
1	B	1233	GLY	N-CA-C	-5.13	105.18	112.37
1	D	903	ILE	N-CA-C	-5.13	106.14	111.58
1	D	1904	ASP	CA-C-N	5.13	125.11	120.03
1	D	1904	ASP	C-N-CA	5.13	125.11	120.03
1	A	1336	ASP	N-CA-C	5.13	115.11	107.88
1	D	2456	ASP	CA-CB-CG	5.13	117.73	112.60
1	D	1716	SER	N-CA-C	5.13	118.03	110.59
2	F	547	PRO	N-CA-C	-5.13	103.23	111.38
1	A	1403	MET	N-CA-C	5.12	116.59	108.96
1	B	1405	TYR	CA-C-N	5.12	125.02	119.85
1	B	1405	TYR	C-N-CA	5.12	125.02	119.85
1	C	1634	GLU	CA-C-N	5.12	125.05	119.78
1	C	1634	GLU	C-N-CA	5.12	125.05	119.78
2	F	474	TYR	N-CA-C	5.12	116.07	108.60
2	F	679	VAL	CA-C-N	5.12	125.19	119.87
2	F	679	VAL	C-N-CA	5.12	125.19	119.87
1	D	873	SER	N-CA-C	-5.11	105.78	111.36
1	B	1499	GLN	N-CA-C	5.11	116.84	109.07
1	C	1672	ASN	CA-C-N	-5.11	115.40	122.30
1	C	1672	ASN	C-N-CA	-5.11	115.40	122.30
2	F	805	LEU	N-CA-C	5.11	117.39	108.76
1	E	1830	ASP	CA-CB-CG	-5.11	107.49	112.60
1	E	1871	LEU	N-CA-C	5.11	118.78	112.24
1	B	2265	PHE	N-CA-C	-5.10	105.80	111.36
2	F	626	VAL	N-CA-C	5.10	115.65	108.36
1	D	401	ASP	CA-CB-CG	5.10	117.70	112.60
1	D	1581	ASP	CA-CB-CG	5.10	117.70	112.60
1	E	2491	MET	CA-C-N	5.09	124.76	119.56
1	E	2491	MET	C-N-CA	5.09	124.76	119.56
1	B	1312	ILE	CA-C-N	5.09	125.03	119.78
1	B	1312	ILE	C-N-CA	5.09	125.03	119.78
1	D	1345	ALA	N-CA-C	-5.09	103.96	110.53
1	E	2263	PHE	CA-CB-CG	-5.09	108.71	113.80
1	D	543	THR	N-CA-C	-5.09	104.66	111.02
1	A	859	LEU	N-CA-C	-5.08	102.64	110.01
2	F	1660	GLU	N-CA-C	-5.08	106.76	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1521	ARG	CA-C-N	-5.08	116.52	123.12
2	F	1521	ARG	C-N-CA	-5.08	116.52	123.12
1	A	909	THR	CA-C-N	5.08	125.01	119.78
1	A	909	THR	C-N-CA	5.08	125.01	119.78
1	C	1848	TYR	N-CA-C	-5.07	105.84	112.23
1	C	1714	SER	CA-C-N	5.07	125.14	119.87
1	C	1714	SER	C-N-CA	5.07	125.14	119.87
1	D	1848	TYR	N-CA-C	-5.07	105.84	112.23
1	C	104	VAL	N-CA-C	5.07	117.31	108.95
1	C	1333	TYR	N-CA-C	5.07	116.76	108.55
1	D	1058	ASP	CA-CB-CG	5.07	117.67	112.60
1	D	1838	ASP	N-CA-C	-5.06	105.67	111.14
2	F	1271	LEU	CA-C-N	5.06	127.57	120.28
2	F	1271	LEU	C-N-CA	5.06	127.57	120.28
2	F	1673	SER	N-CA-C	5.06	116.76	109.07
1	C	1339	THR	N-CA-C	5.06	117.64	108.69
1	C	2429	VAL	CA-C-N	-5.06	115.66	123.14
1	C	2429	VAL	C-N-CA	-5.06	115.66	123.14
1	D	1244	THR	N-CA-C	5.05	115.99	108.86
1	A	1152	ASN	CA-C-N	5.05	124.95	119.85
1	A	1152	ASN	C-N-CA	5.05	124.95	119.85
1	D	793	ALA	N-CA-C	-5.05	103.11	110.08
1	E	1040	TYR	CA-C-N	5.05	124.71	119.56
1	E	1040	TYR	C-N-CA	5.05	124.71	119.56
1	E	105	ALA	CA-C-N	5.05	126.15	119.84
1	E	105	ALA	C-N-CA	5.05	126.15	119.84
1	B	107	GLY	CA-C-N	-5.05	114.62	122.09
1	B	107	GLY	C-N-CA	-5.05	114.62	122.09
1	A	1972	HIS	CA-CB-CG	-5.04	108.75	113.80
1	B	1520	GLN	CA-C-N	5.04	124.95	119.85
1	B	1520	GLN	C-N-CA	5.04	124.95	119.85
1	B	2100	GLY	N-CA-C	-5.04	106.65	112.50
1	C	859	LEU	N-CA-C	-5.04	102.94	110.20
1	E	407	GLU	N-CA-C	5.04	116.74	108.52
1	D	1502	VAL	N-CA-C	5.04	115.23	108.17
1	E	423	ALA	N-CA-C	5.04	116.50	108.79
1	A	570	ASP	N-CA-C	5.03	115.64	107.23
1	E	1177	ILE	N-CA-C	5.03	115.16	108.11
1	E	1648	PRO	CA-C-N	5.03	124.93	119.85
1	E	1648	PRO	C-N-CA	5.03	124.93	119.85
2	F	52	ALA	CA-C-N	5.03	125.30	119.92
2	F	52	ALA	C-N-CA	5.03	125.30	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1836	ASP	CB-CA-C	-5.03	104.08	111.01
1	C	1752	ASN	CA-CB-CG	-5.02	107.58	112.60
2	F	2078	TYR	CA-C-N	5.02	126.12	119.84
2	F	2078	TYR	C-N-CA	5.02	126.12	119.84
1	C	2335	VAL	N-CA-C	5.02	115.08	107.75
1	D	2100	GLY	N-CA-C	-5.02	106.68	112.50
1	A	2508	ILE	N-CA-C	5.01	115.13	108.11
1	B	183	THR	N-CA-C	-5.01	105.92	112.23
1	D	2349	GLY	CA-C-N	5.01	124.91	119.85
1	D	2349	GLY	C-N-CA	5.01	124.91	119.85
2	F	221	LEU	N-CA-C	5.01	117.23	108.52
1	A	1893	LYS	CA-C-N	5.01	124.94	119.78
1	A	1893	LYS	C-N-CA	5.01	124.94	119.78
1	E	1875	THR	N-CA-C	-5.00	106.68	112.89
2	F	487	THR	CA-C-N	5.00	124.98	120.03
2	F	487	THR	C-N-CA	5.00	124.98	120.03
2	F	1562	THR	N-CA-C	-5.00	106.59	113.30
1	B	2456	ASP	CA-CB-CG	5.00	117.60	112.60
1	E	1572	ILE	N-CA-C	5.00	112.95	107.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	19161	0	18735	65	0
1	B	19161	0	18735	67	0
1	C	19161	0	18735	54	0
1	D	19161	0	18735	80	0
1	E	19161	0	18735	77	0
2	F	17117	0	16479	60	0
All	All	112922	0	110154	369	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 (369) 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:D:2147:PHE:CD1	1:E:2147:PHE:CE1	1.83	1.63
1:D:2147:PHE:CD1	1:E:2147:PHE:HE1	0.95	1.59
1:D:2147:PHE:HD1	1:E:2147:PHE:CE1	1.29	1.24
1:D:2144:ILE:HG22	1:D:2148:ALA:O	1.65	0.95
1:D:2147:PHE:HB3	1:E:2147:PHE:HD1	1.33	0.93
1:D:2147:PHE:HB3	1:E:2147:PHE:CD1	2.10	0.86
1:D:2147:PHE:CE1	1:E:2147:PHE:CE1	2.66	0.81
1:D:2147:PHE:CG	1:E:2147:PHE:CE1	2.69	0.80
1:A:2147:PHE:HD1	1:E:2147:PHE:HB3	1.55	0.71
2:F:1442:THR:OG1	2:F:1443:ALA:N	2.26	0.68
1:B:2147:PHE:HB3	1:C:2147:PHE:CD1	2.32	0.65
1:D:2147:PHE:CD1	1:E:2147:PHE:CZ	2.76	0.65
1:B:859:LEU:O	1:B:860:PRO:C	2.40	0.64
1:E:521:THR:O	1:E:522:PRO:C	2.41	0.62
1:A:521:THR:O	1:A:522:PRO:C	2.41	0.62
1:C:521:THR:O	1:C:522:PRO:C	2.41	0.61
1:E:859:LEU:O	1:E:860:PRO:C	2.44	0.61
1:A:859:LEU:O	1:A:860:PRO:C	2.45	0.60
1:D:859:LEU:O	1:D:860:PRO:C	2.45	0.59
1:A:1211:THR:OG1	1:B:1116:THR:OG1	2.19	0.59
1:B:411:THR:HG1	1:B:419:TRP:CD1	2.19	0.59
1:C:859:LEU:O	1:C:860:PRO:C	2.44	0.58
1:E:1148:ASP:OD1	1:E:1148:ASP:N	2.32	0.58
1:A:1116:THR:HG1	1:E:1211:THR:HG1	1.47	0.58
1:A:834:GLN:NE2	1:E:662:THR:OG1	2.37	0.58
1:B:1716:SER:OG	1:B:1717:ASP:N	2.37	0.58
1:B:1706:LYS:NZ	1:B:1717:ASP:OD1	2.36	0.56
1:D:2144:ILE:CG2	1:D:2148:ALA:O	2.48	0.56
1:C:1087:GLN:NE2	1:C:1114:SER:OG	2.38	0.56
1:A:1683:ASP:OD2	1:E:1377:LYS:NZ	2.39	0.56
1:B:2147:PHE:HA	1:D:1190:THR:HG21	1.88	0.55
1:B:817:LYS:NZ	1:B:837:ASP:OD2	2.35	0.55
1:B:1298:ASN:OD1	1:B:1298:ASN:N	2.37	0.55
1:D:733:TRP:CD1	1:D:748:THR:HG1	2.24	0.55
1:E:1514:ASP:OD2	1:E:1515:LYS:NZ	2.40	0.55
1:D:733:TRP:NE1	1:D:748:THR:OG1	2.40	0.54
1:C:1377:LYS:NZ	1:D:1683:ASP:OD2	2.40	0.54
1:D:2285:ASN:O	1:D:2286:ASP:C	2.49	0.54
2:F:1557:TRP:CD1	2:F:1568:THR:HG1	2.25	0.54
1:C:1148:ASP:OD1	1:C:1148:ASP:N	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1350:LYS:NZ	1:E:1538:ASP:OD1	2.38	0.53
2:F:777:GLU:OE2	2:F:866:LYS:NZ	2.41	0.53
1:B:1148:ASP:OD1	1:B:1148:ASP:N	2.33	0.53
1:E:1622:ASP:OD1	1:E:1623:THR:N	2.41	0.53
2:F:1975:SER:OG	2:F:1977:ASP:OD1	2.26	0.53
1:B:1190:THR:HG21	1:E:2147:PHE:HA	1.90	0.53
2:F:78:THR:OG1	2:F:80:ARG:NH2	2.42	0.53
1:E:2144:ILE:HG22	1:E:2148:ALA:O	2.09	0.52
1:D:2147:PHE:CD1	1:E:2147:PHE:CD1	2.80	0.52
1:C:1311:GLU:HB3	1:C:1575:THR:HB	1.90	0.52
1:D:2287:ASP:OD1	1:D:2287:ASP:N	2.40	0.52
1:D:521:THR:O	1:D:522:PRO:C	2.51	0.52
1:A:733:TRP:CD1	1:A:748:THR:HG1	2.27	0.52
1:A:439:LYS:NZ	1:A:469:ASP:OD1	2.43	0.52
1:B:1120:GLU:OE2	1:B:1146:LYS:NZ	2.43	0.52
1:D:1087:GLN:NE2	1:D:1114:SER:OG	2.43	0.52
1:E:2207:ASP:OD2	1:E:2211:LYS:NZ	2.43	0.52
1:A:2147:PHE:O	1:B:2147:PHE:HD2	1.94	0.51
1:E:1398:SER:OG	1:E:1400:ASN:O	2.28	0.51
1:B:1447:ASN:ND2	1:B:1456:TYR:O	2.42	0.51
2:F:1914:ALA:O	2:F:2125:ARG:NH2	2.43	0.51
1:C:2280:TYR:OH	1:C:2324:ARG:NH1	2.44	0.51
1:C:1836:ASP:OD1	1:C:1836:ASP:C	2.53	0.51
1:A:2437:ASP:O	1:A:2438:LYS:C	2.54	0.51
1:D:2281:ARG:O	1:D:2282:TRP:C	2.53	0.51
2:F:991:SER:OG	2:F:1008:SER:OG	2.28	0.51
2:F:268:SER:OG	2:F:270:ASN:OD1	2.29	0.50
2:F:263:ASP:C	2:F:263:ASP:OD1	2.52	0.50
1:A:92:TYR:OH	1:A:99:ARG:NH1	2.45	0.50
1:D:198:THR:N	1:D:199:PRO:CD	2.75	0.50
2:F:505:ASP:OD1	2:F:505:ASP:C	2.51	0.50
1:A:1729:ASP:OD1	1:A:1729:ASP:N	2.43	0.50
1:A:398:ASN:O	1:A:399:THR:C	2.54	0.49
1:C:2468:LYS:NZ	1:D:2325:ASP:OD2	2.39	0.49
1:D:733:TRP:NE1	1:D:748:THR:HG1	2.10	0.49
1:D:1164:LYS:NZ	1:D:1243:ASP:OD2	2.45	0.49
1:E:1428:THR:OG1	1:E:1429:THR:N	2.45	0.49
2:F:446:SER:O	2:F:447:LEU:C	2.53	0.49
1:A:198:THR:N	1:A:199:PRO:CD	2.76	0.49
1:B:141:ARG:HD3	1:B:970:TYR:O	2.11	0.49
1:C:1168:TYR:CD2	1:C:1202:HIS:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1907:LEU:O	1:D:1908:ASP:C	2.54	0.49
1:B:943:SER:O	1:B:944:ALA:C	2.55	0.49
2:F:692:THR:OG1	2:F:693:ASN:N	2.45	0.49
1:E:1311:GLU:HB3	1:E:1575:THR:HB	1.93	0.49
1:E:1524:SER:OG	1:E:1525:PHE:N	2.45	0.49
2:F:1329:ASP:N	2:F:1329:ASP:OD1	2.35	0.49
1:E:1229:ASN:OD1	1:E:1229:ASN:N	2.42	0.49
1:D:2468:LYS:NZ	1:E:2325:ASP:OD2	2.42	0.48
1:B:1657:ASP:OD1	1:B:1657:ASP:N	2.42	0.48
1:D:398:ASN:O	1:D:399:THR:C	2.56	0.48
2:F:224:THR:O	2:F:227:ARG:NH1	2.46	0.48
1:D:1168:TYR:CD2	1:D:1202:HIS:HB3	2.49	0.48
2:F:530:ASP:OD1	2:F:530:ASP:N	2.40	0.48
1:A:182:TYR:C	1:A:182:TYR:CD1	2.90	0.48
1:A:193:ARG:N	1:A:194:PRO:CD	2.77	0.48
1:A:418:SER:OG	1:A:419:TRP:N	2.45	0.48
1:B:533:ASP:OD1	1:B:533:ASP:N	2.40	0.48
1:D:842:ASP:OD1	1:D:844:ASN:N	2.45	0.48
1:E:2382:ASP:OD1	1:E:2382:ASP:N	2.46	0.48
2:F:2018:ASP:OD1	2:F:2018:ASP:C	2.56	0.48
1:B:521:THR:O	1:B:522:PRO:C	2.54	0.48
1:B:1907:LEU:O	1:B:1908:ASP:C	2.54	0.48
1:D:694:PRO:O	1:D:695:TYR:HB2	2.14	0.48
1:D:1148:ASP:N	1:D:1148:ASP:OD1	2.35	0.48
2:F:693:ASN:N	2:F:693:ASN:OD1	2.47	0.48
1:A:1311:GLU:HB3	1:A:1575:THR:HB	1.95	0.48
1:B:1426:ARG:NH2	1:B:1450:ALA:O	2.47	0.48
1:B:1507:LYS:NZ	1:B:1538:ASP:OD2	2.45	0.48
1:E:2319:ASP:OD2	1:E:2323:LYS:NZ	2.46	0.48
1:E:2082:LYS:NZ	1:E:2086:GLU:OE2	2.43	0.48
2:F:1882:ASP:OD1	2:F:1882:ASP:C	2.56	0.48
1:C:198:THR:N	1:C:199:PRO:CD	2.77	0.47
1:D:2380:GLY:N	1:D:2383:THR:OG1	2.47	0.47
1:A:1907:LEU:O	1:A:1908:ASP:C	2.55	0.47
1:E:2287:ASP:N	1:E:2287:ASP:OD1	2.45	0.47
1:B:1168:TYR:CD2	1:B:1202:HIS:HB3	2.49	0.47
1:E:342:ASP:OD2	1:E:360:LYS:NZ	2.38	0.47
2:F:209:ASP:C	2:F:209:ASP:OD1	2.56	0.47
1:B:2147:PHE:HA	1:D:1190:THR:CG2	2.44	0.47
1:C:1016:GLN:O	1:C:1017:PHE:C	2.58	0.47
1:C:1728:ASP:OD1	1:C:1728:ASP:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1670:ASP:OD1	1:D:1670:ASP:C	2.57	0.47
1:B:2147:PHE:HB3	1:C:2147:PHE:CG	2.49	0.47
1:C:581:ASN:O	1:C:582:LEU:C	2.56	0.47
1:D:1872:GLU:O	1:D:1873:ARG:C	2.56	0.47
1:E:1272:ASP:OD1	1:E:1272:ASP:N	2.43	0.47
1:E:545:ASP:C	1:E:545:ASP:OD1	2.58	0.47
1:A:581:ASN:O	1:A:582:LEU:C	2.58	0.47
1:B:398:ASN:O	1:B:399:THR:C	2.56	0.47
1:B:447:SER:O	1:B:451:GLU:N	2.48	0.47
1:B:1890:LEU:HB3	1:B:1960:TRP:CH2	2.50	0.47
1:D:2147:PHE:CE1	1:E:2147:PHE:CZ	3.02	0.47
1:B:1272:ASP:OD1	1:B:1272:ASP:N	2.45	0.46
1:C:439:LYS:NZ	1:C:469:ASP:OD1	2.48	0.46
1:C:1670:ASP:OD1	1:C:1670:ASP:C	2.58	0.46
1:D:1657:ASP:OD1	1:D:1657:ASP:N	2.43	0.46
1:A:1890:LEU:HB3	1:A:1960:TRP:CH2	2.51	0.46
1:D:796:HIS:ND1	1:D:796:HIS:N	2.64	0.46
1:E:512:PRO:O	1:E:517:ARG:NH1	2.48	0.46
2:F:1729:ASP:OD1	2:F:1729:ASP:C	2.59	0.46
1:A:306:GLN:NE2	1:A:314:ILE:O	2.48	0.46
1:E:831:THR:OG1	1:E:832:ALA:N	2.48	0.46
1:C:2319:ASP:OD2	1:C:2323:LYS:NZ	2.47	0.46
1:D:581:ASN:O	1:D:582:LEU:C	2.58	0.46
1:D:1426:ARG:NH2	1:D:1450:ALA:O	2.49	0.46
2:F:1087:ALA:HB1	2:F:1558:GLN:HB3	1.97	0.46
1:A:731:TRP:O	1:A:732:ASP:C	2.58	0.46
1:C:1220:LYS:NZ	1:C:1277:ASP:OD1	2.48	0.46
2:F:263:ASP:OD1	2:F:264:TYR:N	2.49	0.46
1:A:1432:SER:OG	1:A:1433:LYS:N	2.49	0.46
1:A:1514:ASP:N	1:A:1514:ASP:OD1	2.47	0.46
2:F:902:THR:OG1	2:F:903:ASP:N	2.49	0.46
1:D:319:ASN:HB2	1:D:322:ASP:HB3	1.98	0.45
2:F:1109:THR:OG1	2:F:1110:ASN:N	2.49	0.45
2:F:1133:THR:OG1	2:F:1134:ALA:N	2.49	0.45
2:F:1698:ASP:OD1	2:F:1698:ASP:N	2.47	0.45
1:A:2143:ASN:OD1	1:A:2143:ASN:N	2.46	0.45
2:F:1208:THR:OG1	2:F:1209:LEU:N	2.49	0.45
1:B:2244:LYS:NZ	1:B:2246:SER:O	2.50	0.45
1:E:731:TRP:O	1:E:732:ASP:C	2.59	0.45
2:F:390:PHE:CE1	2:F:396:TRP:HB3	2.51	0.45
2:F:584:LEU:O	2:F:588:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ASN:O	1:A:433:GLN:C	2.59	0.45
1:A:1348:ASP:OD1	1:A:1350:LYS:NZ	2.47	0.45
1:C:928:SER:OG	1:C:929:GLN:N	2.48	0.45
1:D:1272:ASP:OD1	1:D:1272:ASP:N	2.44	0.45
1:D:1769:TRP:CE3	1:D:1827:TRP:CZ2	3.04	0.45
1:D:831:THR:OG1	1:D:832:ALA:N	2.50	0.45
1:E:92:TYR:OH	1:E:99:ARG:NE	2.49	0.45
2:F:2120:GLN:HE21	2:F:2122:TRP:HE1	1.65	0.45
1:C:1907:LEU:O	1:C:1908:ASP:C	2.57	0.45
2:F:153:ASP:O	2:F:174:ARG:NH2	2.49	0.45
1:A:1168:TYR:CD2	1:A:1202:HIS:HB3	2.53	0.44
1:E:1235:TYR:CD2	1:E:1235:TYR:C	2.94	0.44
1:B:2380:GLY:O	1:B:2381:THR:C	2.60	0.44
1:C:432:ASN:O	1:C:433:GLN:C	2.57	0.44
1:D:545:ASP:OD1	1:D:545:ASP:C	2.59	0.44
1:A:455:THR:OG1	1:A:456:ILE:N	2.50	0.44
1:B:581:ASN:O	1:B:582:LEU:C	2.60	0.44
1:B:1016:GLN:O	1:B:1017:PHE:C	2.58	0.44
1:E:173:ILE:O	1:E:174:LYS:C	2.60	0.44
1:E:1432:SER:OG	1:E:1433:LYS:N	2.50	0.44
1:C:193:ARG:N	1:C:194:PRO:CD	2.81	0.44
1:D:1447:ASN:ND2	1:D:1456:TYR:O	2.51	0.44
2:F:1444:LYS:HB3	2:F:1446:TRP:CE3	2.52	0.44
1:B:2487:PRO:O	1:B:2497:GLN:HG2	2.18	0.44
1:B:432:ASN:O	1:B:433:GLN:C	2.59	0.44
1:B:1729:ASP:OD1	1:B:1729:ASP:N	2.49	0.44
1:D:270:ASN:OD1	1:D:270:ASN:N	2.48	0.44
1:E:1010:SER:C	1:E:1011:GLY:O	2.57	0.44
2:F:34:ASP:OD1	2:F:35:GLY:N	2.50	0.44
2:F:1687:ASP:OD1	2:F:1687:ASP:N	2.39	0.44
2:F:2066:ASP:OD1	2:F:2066:ASP:C	2.60	0.44
1:E:137:TYR:CE2	1:E:139:ASP:HB2	2.53	0.44
1:A:575:ASP:OD2	1:A:577:LYS:NZ	2.36	0.44
1:A:1729:ASP:OD2	1:A:1730:LYS:NZ	2.50	0.44
1:B:193:ARG:HB2	1:B:194:PRO:HD3	2.00	0.44
1:B:575:ASP:C	1:B:575:ASP:OD1	2.61	0.44
1:B:1752:ASN:OD1	1:B:1752:ASN:N	2.43	0.44
1:D:2147:PHE:CB	1:E:2147:PHE:CD1	2.91	0.44
1:E:1168:TYR:CD2	1:E:1202:HIS:HB3	2.53	0.44
2:F:1805:ASP:OD1	2:F:1805:ASP:C	2.61	0.44
1:B:2024:GLU:OE1	1:B:2027:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1890:LEU:HB3	1:C:1960:TRP:CH2	2.53	0.43
2:F:1040:ASP:OD1	2:F:1042:LYS:HG3	2.18	0.43
2:F:1446:TRP:CZ3	2:F:1806:PRO:HA	2.53	0.43
2:F:1560:ASP:OD1	2:F:1560:ASP:C	2.60	0.43
1:B:137:TYR:CE2	1:B:139:ASP:HB2	2.53	0.43
1:C:398:ASN:O	1:C:399:THR:C	2.58	0.43
2:F:1347:ASP:C	2:F:1347:ASP:OD1	2.60	0.43
1:A:1010:SER:C	1:A:1011:GLY:O	2.56	0.43
1:B:1836:ASP:C	1:B:1836:ASP:OD1	2.61	0.43
1:C:542:SER:O	1:C:543:THR:C	2.62	0.43
1:E:733:TRP:NE1	1:E:748:THR:OG1	2.51	0.43
1:E:1728:ASP:OD1	1:E:1728:ASP:C	2.61	0.43
2:F:326:GLY:N	2:F:327:PRO:HD2	2.32	0.43
1:A:2382:ASP:OD2	1:B:2404:ALA:N	2.51	0.43
2:F:1432:ASP:OD1	2:F:1432:ASP:C	2.62	0.43
1:C:1235:TYR:CD2	1:C:1235:TYR:C	2.96	0.43
1:D:366:SER:N	1:D:413:VAL:O	2.52	0.43
1:D:1729:ASP:OD1	1:D:1729:ASP:N	2.49	0.43
1:E:2380:GLY:N	1:E:2383:THR:OG1	2.52	0.43
1:A:2491:MET:N	1:A:2492:PRO:HD2	2.34	0.43
1:B:1345:ALA:O	1:B:1346:SER:C	2.59	0.43
1:E:1264:MET:HB2	1:E:1283:SER:OG	2.19	0.43
1:E:2244:LYS:NZ	1:E:2246:SER:O	2.51	0.43
2:F:369:ALA:HB3	2:F:701:GLU:HB2	2.01	0.43
1:B:1308:GLU:O	1:B:1309:ASP:C	2.61	0.43
1:C:1903:SER:O	1:C:1905:PRO:HD3	2.19	0.43
1:D:1890:LEU:HB3	1:D:1960:TRP:CZ2	2.54	0.43
1:A:818:ALA:O	1:A:819:SER:C	2.60	0.43
1:A:2108:ASN:O	1:A:2109:ALA:C	2.60	0.43
1:B:455:THR:OG1	1:B:456:ILE:N	2.49	0.43
1:A:286:TYR:O	1:A:448:ARG:NH1	2.52	0.43
1:A:831:THR:OG1	1:A:832:ALA:N	2.49	0.43
1:A:1872:GLU:O	1:A:1873:ARG:C	2.61	0.43
1:D:1211:THR:OG1	1:E:1116:THR:OG1	2.29	0.43
1:D:1432:SER:OG	1:D:1433:LYS:N	2.49	0.43
1:A:1608:LEU:O	1:A:1609:PHE:C	2.61	0.43
1:B:702:LEU:HG	1:B:704:SER:H	1.84	0.43
1:C:1729:ASP:OD1	1:C:1729:ASP:N	2.45	0.43
1:C:1752:ASN:OD1	1:C:1752:ASN:N	2.41	0.43
1:D:2148:ALA:HA	1:E:2145:PHE:O	2.19	0.43
1:C:270:ASN:N	1:C:270:ASN:OD1	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:545:ASP:OD1	1:C:545:ASP:C	2.62	0.42
1:D:1229:ASN:N	1:D:1229:ASN:OD1	2.42	0.42
1:E:1729:ASP:OD1	1:E:1729:ASP:N	2.49	0.42
1:E:1836:ASP:OD1	1:E:1836:ASP:C	2.62	0.42
1:E:1244:THR:OG1	1:E:1245:LEU:N	2.52	0.42
1:E:1872:GLU:O	1:E:1873:ARG:C	2.61	0.42
1:B:2027:ARG:NH2	1:B:2318:GLU:OE1	2.52	0.42
1:D:674:VAL:O	1:D:675:TYR:C	2.61	0.42
1:D:2147:PHE:CG	1:E:2147:PHE:CD1	3.07	0.42
1:D:2244:LYS:NZ	1:D:2246:SER:O	2.50	0.42
1:A:1271:ALA:O	1:B:1611:ARG:NH1	2.53	0.42
1:D:516:ASP:O	1:D:520:ASN:N	2.52	0.42
1:D:1311:GLU:HB3	1:D:1575:THR:HB	2.01	0.42
2:F:1153:THR:OG1	2:F:1154:LEU:N	2.51	0.42
1:A:432:ASN:O	1:A:435:SER:N	2.52	0.42
1:A:827:ALA:O	1:A:829:SER:N	2.52	0.42
1:A:1345:ALA:O	1:A:1346:SER:C	2.62	0.42
1:B:308:TYR:CD1	1:B:308:TYR:C	2.97	0.42
1:B:1531:GLN:OE1	1:C:1752:ASN:ND2	2.53	0.42
1:C:1657:ASP:OD1	1:C:1657:ASP:N	2.44	0.42
1:D:133:ASP:OD1	1:D:133:ASP:N	2.46	0.42
1:E:581:ASN:O	1:E:582:LEU:C	2.59	0.42
2:F:1549:ASN:OD1	2:F:1549:ASN:N	2.51	0.42
2:F:2044:ASP:OD1	2:F:2044:ASP:N	2.46	0.42
1:A:319:ASN:HB3	1:A:322:ASP:HB3	2.01	0.42
1:A:1475:ASP:C	1:A:1475:ASP:OD1	2.60	0.42
1:D:1293:GLN:HE22	1:D:1304:ASN:HB2	1.83	0.42
1:D:1890:LEU:HB3	1:D:1960:TRP:CH2	2.55	0.42
1:E:1752:ASN:OD1	1:E:1752:ASN:N	2.43	0.42
1:E:2291:PHE:O	1:E:2313:SER:OG	2.35	0.42
2:F:315:GLN:HB2	2:F:325:ASN:ND2	2.35	0.42
2:F:1168:ASP:OD1	2:F:1169:ALA:N	2.52	0.42
2:F:1388:GLY:O	2:F:1389:ARG:C	2.62	0.42
1:B:133:ASP:OD1	1:B:133:ASP:N	2.47	0.42
1:B:2468:LYS:NZ	1:C:2325:ASP:OD2	2.53	0.42
1:C:1229:ASN:OD1	1:C:1229:ASN:N	2.45	0.42
1:C:1484:SER:OG	1:C:1485:GLY:N	2.52	0.42
1:C:2371:GLY:O	1:C:2374:ASN:ND2	2.53	0.42
1:D:1016:GLN:O	1:D:1017:PHE:C	2.63	0.42
1:E:2463:ASP:C	1:E:2463:ASP:OD1	2.62	0.42
2:F:1432:ASP:HB2	2:F:1433:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:TYR:CE2	1:C:139:ASP:HB2	2.55	0.42
2:F:1201:ASP:OD1	2:F:1201:ASP:C	2.61	0.42
2:F:2114:TYR:O	2:F:2116:TYR:N	2.51	0.42
1:B:1728:ASP:OD1	1:B:1728:ASP:C	2.62	0.42
1:B:1729:ASP:OD2	1:B:1730:LYS:NZ	2.43	0.42
1:C:2081:GLU:O	1:C:2082:LYS:C	2.61	0.42
1:D:694:PRO:O	1:D:695:TYR:CB	2.65	0.42
1:E:123:TYR:O	1:E:124:ARG:C	2.61	0.42
1:B:85:PRO:HG2	1:B:89:LEU:HB2	2.02	0.42
1:B:687:ASP:OD1	1:B:687:ASP:C	2.63	0.42
1:B:1020:ASP:O	1:B:1021:TRP:C	2.61	0.42
1:C:1729:ASP:OD2	1:C:1730:LYS:NZ	2.53	0.42
1:D:432:ASN:O	1:D:433:GLN:C	2.59	0.42
1:A:842:ASP:C	1:A:842:ASP:OD1	2.62	0.41
1:B:510:ASN:OD1	1:B:510:ASN:N	2.51	0.41
1:D:1826:SER:OG	1:D:1828:ASN:O	2.38	0.41
1:E:1168:TYR:CE2	1:E:1202:HIS:HB3	2.55	0.41
2:F:196:ARG:HB2	2:F:198:GLU:OE1	2.19	0.41
1:B:205:GLU:O	1:B:206:ASN:C	2.62	0.41
1:C:962:LYS:NZ	1:C:1398:SER:O	2.47	0.41
1:D:1124:ARG:HD2	1:D:1144:TRP:CE2	2.55	0.41
1:A:968:TYR:CD1	1:A:968:TYR:C	2.98	0.41
1:B:1890:LEU:HB3	1:B:1960:TRP:CZ2	2.54	0.41
1:C:205:GLU:O	1:C:206:ASN:C	2.62	0.41
1:A:2240:PHE:O	1:A:2241:LEU:C	2.60	0.41
1:C:831:THR:OG1	1:C:832:ALA:N	2.52	0.41
1:C:1117:ASP:O	1:C:1118:ALA:C	2.62	0.41
1:D:1021:TRP:O	1:D:1022:ASP:C	2.63	0.41
1:E:510:ASN:OD1	1:E:510:ASN:N	2.52	0.41
1:A:133:ASP:N	1:A:133:ASP:OD1	2.46	0.41
1:A:593:LEU:O	1:A:594:LEU:C	2.63	0.41
1:E:1890:LEU:HB3	1:E:1960:TRP:CH2	2.55	0.41
1:A:1426:ARG:NH2	1:A:1450:ALA:O	2.53	0.41
1:A:2496:LYS:NZ	1:B:2400:GLU:OE1	2.54	0.41
1:D:2382:ASP:OD2	1:E:2404:ALA:N	2.54	0.41
1:A:687:ASP:OD1	1:A:687:ASP:C	2.61	0.41
1:A:1046:ASP:C	1:A:1046:ASP:OD1	2.61	0.41
1:B:545:ASP:C	1:B:545:ASP:OD1	2.62	0.41
1:C:508:TYR:O	1:C:509:ASP:C	2.63	0.41
1:D:1345:ALA:O	1:D:1346:SER:C	2.62	0.41
1:A:842:ASP:OD1	1:A:843:ALA:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:ASN:O	1:D:260:ALA:C	2.62	0.41
1:D:1613:LEU:O	1:D:1614:VAL:C	2.64	0.41
1:D:1353:ILE:C	1:D:1355:PRO:HD3	2.46	0.41
1:E:1164:LYS:NZ	1:E:1243:ASP:OD1	2.48	0.41
2:F:350:ARG:NH2	2:F:362:THR:OG1	2.54	0.41
2:F:939:ASP:OD1	2:F:939:ASP:C	2.63	0.41
2:F:1067:THR:OG1	2:F:1068:ARG:N	2.53	0.41
1:A:552:LYS:O	1:A:556:ASN:N	2.54	0.41
1:A:975:ASN:OD1	1:A:975:ASN:N	2.46	0.41
1:A:1447:ASN:ND2	1:A:1456:TYR:O	2.54	0.41
1:C:204:TYR:OH	1:C:241:ALA:O	2.39	0.41
1:C:1020:ASP:O	1:C:1021:TRP:C	2.61	0.41
1:D:552:LYS:O	1:D:556:ASN:N	2.54	0.41
1:D:1608:LEU:H	1:D:1634:GLU:CD	2.29	0.41
1:A:137:TYR:CE2	1:A:139:ASP:HB2	2.57	0.40
1:A:1728:ASP:C	1:A:1728:ASP:OD1	2.64	0.40
1:B:1040:TYR:CE2	1:B:1953:ASN:HB2	2.56	0.40
1:D:1484:SER:OG	1:D:1485:GLY:N	2.54	0.40
1:D:2266:TYR:CZ	1:D:2297:TRP:HB2	2.56	0.40
1:D:2437:ASP:OD1	1:D:2437:ASP:C	2.61	0.40
1:B:198:THR:N	1:B:199:PRO:CD	2.85	0.40
1:B:1834:SER:OG	1:B:1835:VAL:N	2.55	0.40
1:C:2491:MET:N	1:C:2492:PRO:CD	2.85	0.40
1:E:1834:SER:OG	1:E:1835:VAL:N	2.52	0.40
2:F:963:TYR:N	2:F:964:PRO:CD	2.84	0.40
1:A:1865:ASP:O	1:A:1866:HIS:C	2.63	0.40
1:E:1020:ASP:O	1:E:1021:TRP:C	2.64	0.40
1:E:2430:GLN:N	1:E:2430:GLN:CD	2.79	0.40
2:F:112:ASP:OD2	2:F:147:LYS:NZ	2.49	0.40
2:F:153:ASP:C	2:F:153:ASP:OD1	2.63	0.40
1:B:1432:SER:OG	1:B:1433:LYS:N	2.54	0.40
1:C:1124:ARG:HD2	1:C:1144:TRP:CE2	2.56	0.40
1:C:1459:ASP:C	1:C:1459:ASP:OD1	2.63	0.40
1:E:1651:ASN:O	1:E:1652:LEU:C	2.65	0.40
1:E:2266:TYR:O	1:E:2267:ASP:C	2.62	0.40
1:E:2357:ILE:O	1:E:2358:ASP:C	2.63	0.40
1:A:2266:TYR:O	1:A:2267:ASP:C	2.64	0.40
1:C:1298:ASN:OD1	1:C:1298:ASN:N	2.52	0.40
1:C:2266:TYR:O	1:C:2267:ASP:C	2.64	0.40
1:E:149:ALA:O	1:E:154:ASN:ND2	2.48	0.40
1:E:198:THR:N	1:E:199:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:247:ASP:N	2:F:247:ASP:OD1	2.44	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	2411/2516 (96%)	2371 (98%)	34 (1%)	6 (0%)	43	75
1	B	2411/2516 (96%)	2365 (98%)	41 (2%)	5 (0%)	43	75
1	C	2411/2516 (96%)	2359 (98%)	44 (2%)	8 (0%)	36	69
1	D	2411/2516 (96%)	2361 (98%)	45 (2%)	5 (0%)	43	75
1	E	2411/2516 (96%)	2360 (98%)	47 (2%)	4 (0%)	43	75
2	F	2142/2434 (88%)	2077 (97%)	56 (3%)	9 (0%)	30	65
All	All	14197/15014 (95%)	13893 (98%)	267 (2%)	37 (0%)	37	69

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	860	PRO
1	B	860	PRO
1	C	688	LEU
1	C	860	PRO
1	C	911	THR
1	D	860	PRO
1	E	522	PRO
1	E	860	PRO
2	F	1208	THR
1	A	522	PRO
1	A	908	GLU

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Mol	Chain	Res	Type
1	C	522	PRO
2	F	1336	GLU
1	A	745	ALA
1	A	2106	ASN
1	C	2106	ASN
2	F	402	LYS
2	F	1920	THR
1	C	687	ASP
1	C	1985	ILE
1	D	107	GLY
1	D	1985	ILE
1	E	1985	ILE
2	F	136	SER
1	B	521	THR
1	B	1985	ILE
1	B	2425	PRO
1	D	745	ALA
1	E	1527	GLU
2	F	404	GLU
1	A	1985	ILE
1	D	827	ALA
2	F	683	SER
1	B	198	THR
1	C	1478	GLY
2	F	1529	ILE
2	F	2115	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2067/2157 (96%)	2067 (100%)	0	100	100
1	B	2067/2157 (96%)	2067 (100%)	0	100	100
1	C	2067/2157 (96%)	2066 (100%)	1 (0%)	100	100
1	D	2067/2157 (96%)	2067 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	2067/2157 (96%)	2067 (100%)	0	100	100
2	F	1853/2105 (88%)	1853 (100%)	0	100	100
All	All	12188/12890 (95%)	12187 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	C	1381	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	511	GLN
1	A	556	ASN
1	A	701	GLN
1	A	706	ASN
1	A	735	ASN
1	A	854	GLN
1	A	935	HIS
1	A	1103	ASN
1	A	1139	ASN
1	A	1252	GLN
1	A	1304	ASN
1	A	1361	HIS
1	A	1499	GLN
1	A	1520	GLN
1	A	1529	ASN
1	A	1671	ASN
1	A	1680	GLN
1	A	1812	GLN
1	A	1885	GLN
1	A	1965	GLN
1	A	1969	ASN
1	A	1979	GLN
1	A	2035	GLN
1	A	2071	GLN
1	B	306	GLN
1	B	679	GLN
1	B	706	ASN
1	B	854	GLN

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Mol	Chain	Res	Type
1	B	935	HIS
1	B	1087	GLN
1	B	1304	ASN
1	B	1462	ASN
1	B	1965	GLN
1	B	1969	ASN
1	B	2004	GLN
1	B	2230	GLN
1	B	2231	GLN
1	B	2388	GLN
1	C	220	GLN
1	C	306	GLN
1	C	679	GLN
1	C	735	ASN
1	C	854	GLN
1	C	886	GLN
1	C	929	GLN
1	C	935	HIS
1	C	1103	ASN
1	C	1304	ASN
1	C	1448	GLN
1	C	1449	ASN
1	C	1529	ASN
1	C	1808	HIS
1	C	2004	GLN
1	C	2058	ASN
1	C	2113	GLN
1	C	2497	GLN
1	D	95	GLN
1	D	305	GLN
1	D	505	GLN
1	D	751	HIS
1	D	935	HIS
1	D	1087	GLN
1	D	1090	ASN
1	D	1252	GLN
1	D	1265	GLN
1	D	1367	GLN
1	D	1529	ASN
1	D	1636	GLN
1	D	1748	ASN
1	D	1808	HIS

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Mol	Chain	Res	Type
1	D	1866	HIS
1	D	1951	GLN
1	D	2035	GLN
1	D	2321	HIS
1	D	2348	ASN
1	D	2459	GLN
1	E	511	GLN
1	E	527	GLN
1	E	935	HIS
1	E	1087	GLN
1	E	1103	ASN
1	E	1304	ASN
1	E	1361	HIS
1	E	1520	GLN
1	E	1965	GLN
1	E	1969	ASN
1	E	2035	GLN
1	E	2071	GLN
1	E	2388	GLN
1	E	2455	ASN
1	E	2497	GLN
2	F	5	GLN
2	F	65	ASN
2	F	203	GLN
2	F	230	HIS
2	F	567	GLN
2	F	748	GLN
2	F	791	GLN
2	F	884	HIS
2	F	920	HIS
2	F	943	GLN
2	F	951	GLN
2	F	982	GLN
2	F	1108	GLN
2	F	1265	GLN
2	F	1459	ASN
2	F	1482	ASN
2	F	1525	HIS
2	F	1534	ASN
2	F	1535	GLN
2	F	1564	ASN
2	F	1616	GLN

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Mol	Chain	Res	Type
2	F	1680	GLN
2	F	1781	GLN
2	F	1825	ASN
2	F	1904	ASN
2	F	1943	GLN
2	F	1994	GLN
2	F	1996	GLN
2	F	2010	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-0149. These allow visual inspection of the internal detail of the map and identification of artifacts.

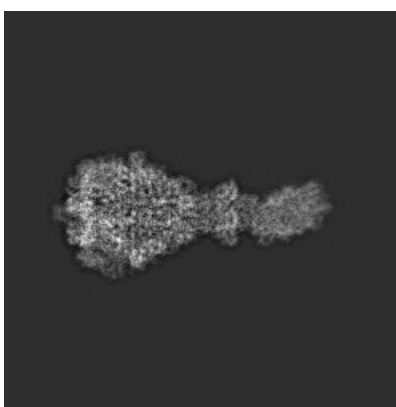
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

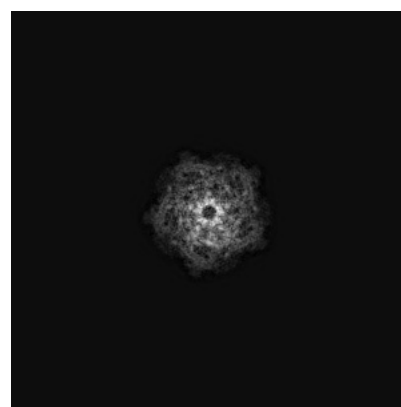
6.1.1 Primary map



X



Y

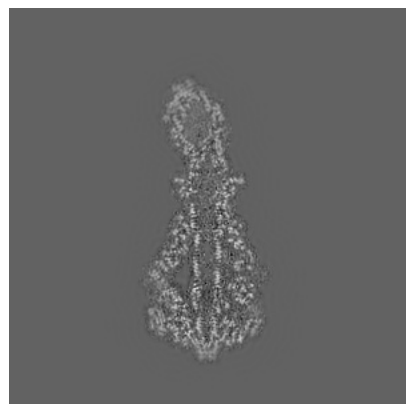


Z

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

6.2 Central slices [i](#)

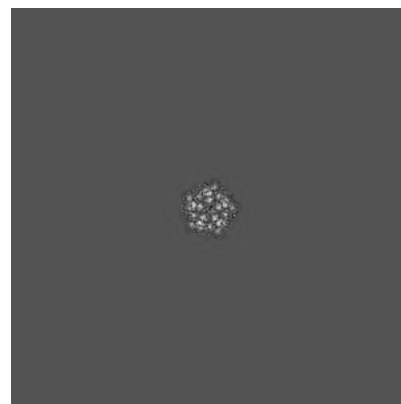
6.2.1 Primary map



X Index: 240



Y Index: 240



Z Index: 240

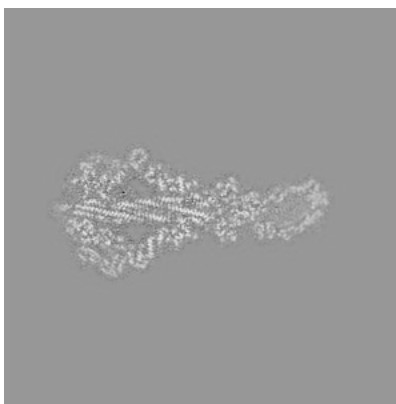
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

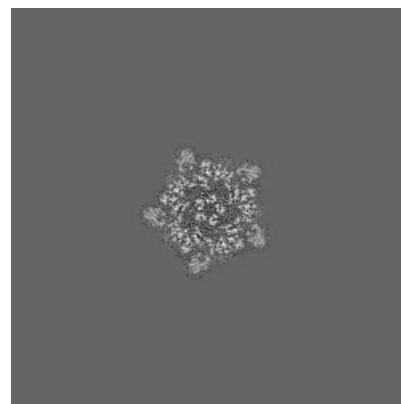
6.3.1 Primary map



X Index: 227



Y Index: 227

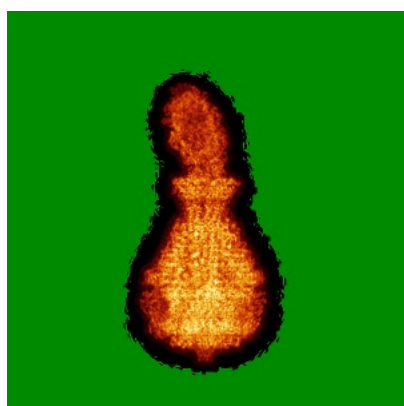


Z Index: 139

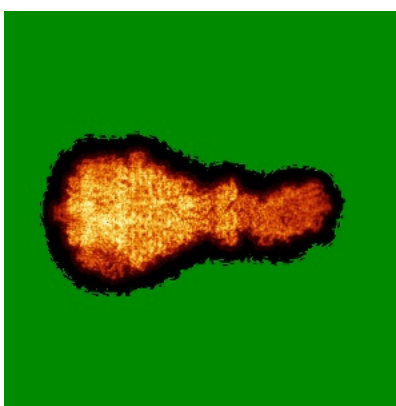
The images above show the largest variance slices of the map in three orthogonal directions.

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

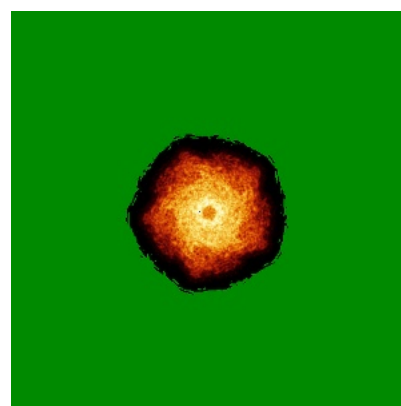
6.4.1 Primary map



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](#)

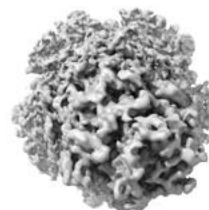
6.5.1 Primary map



X



Y



Z

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.

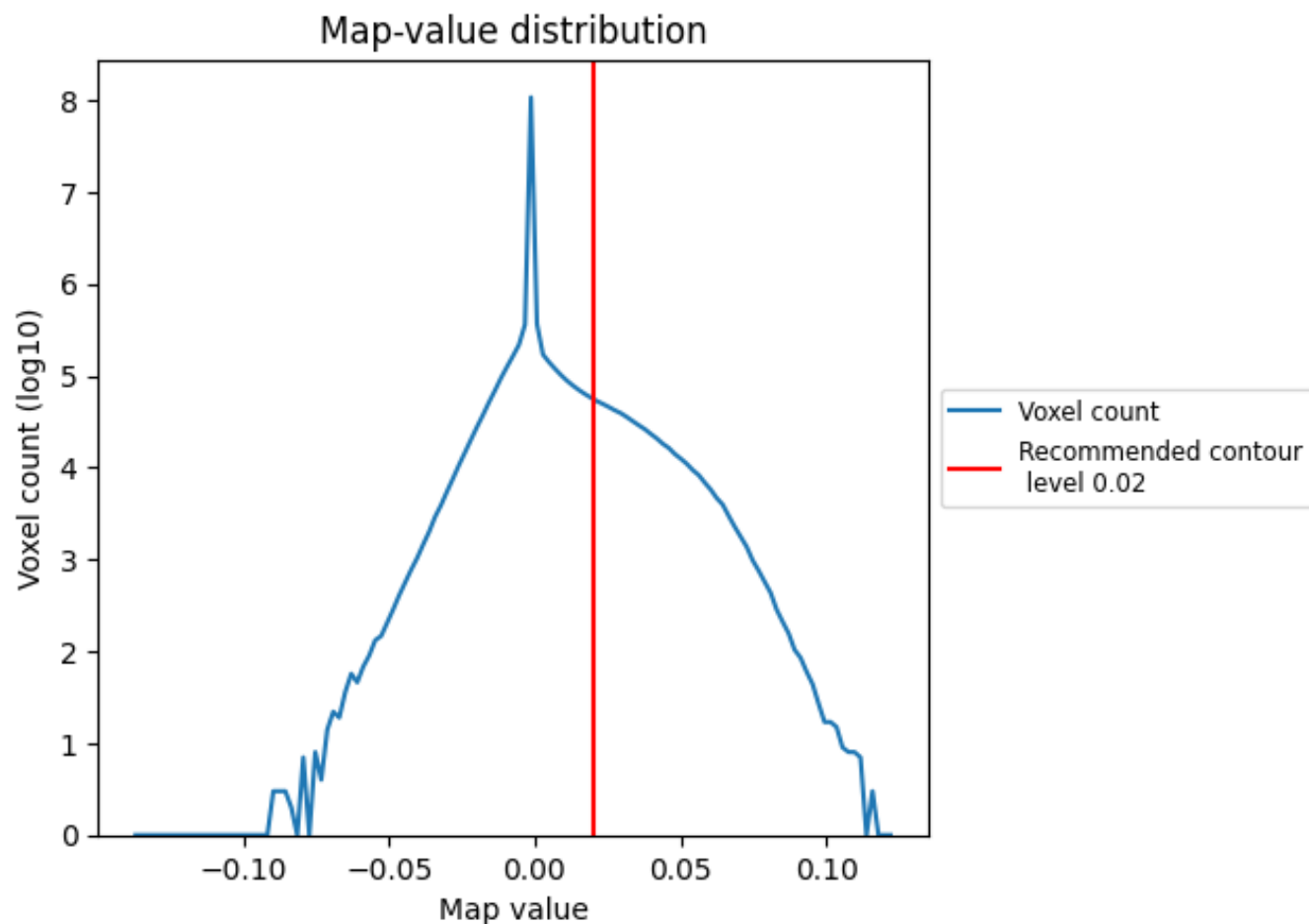
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

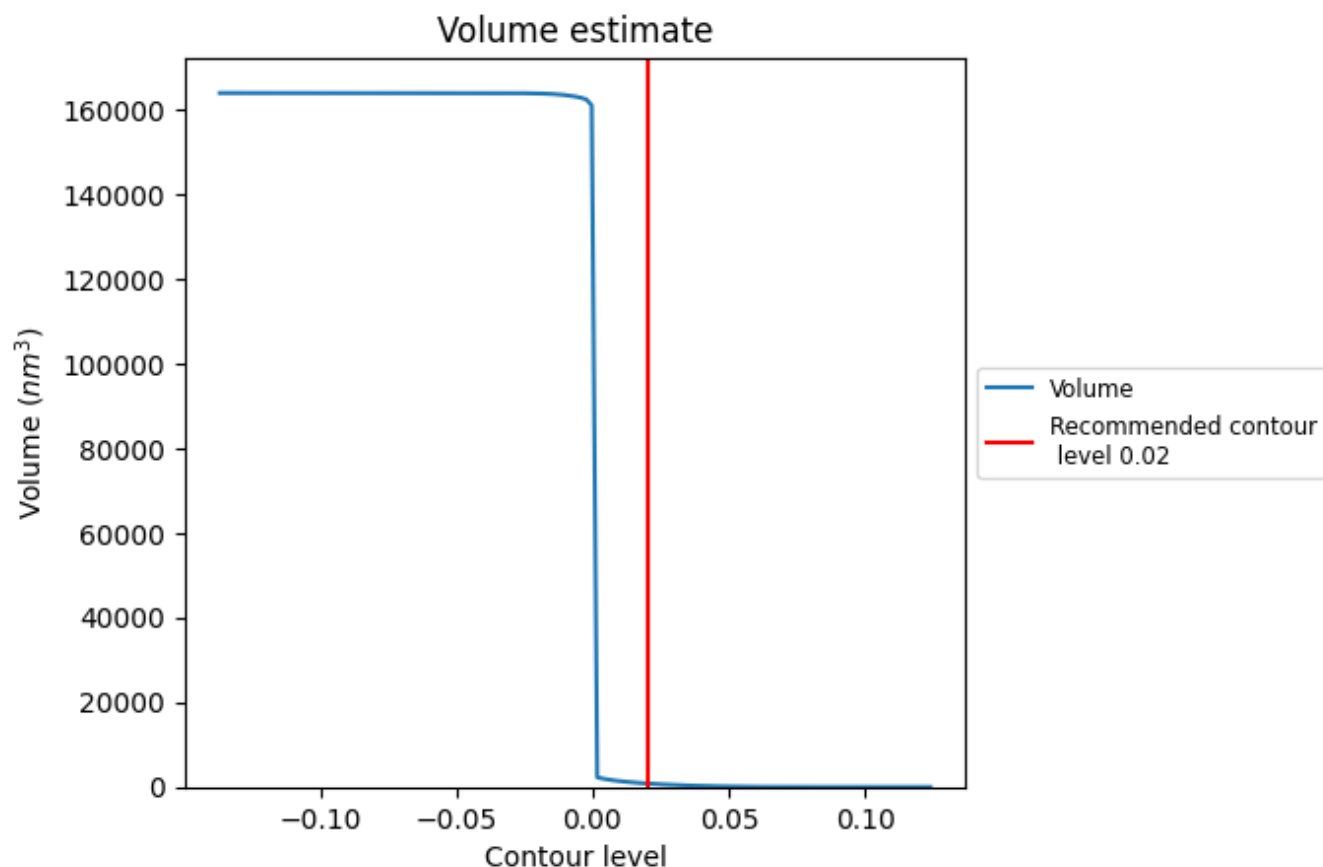
This section contains the results of statistical analysis of the map.

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.

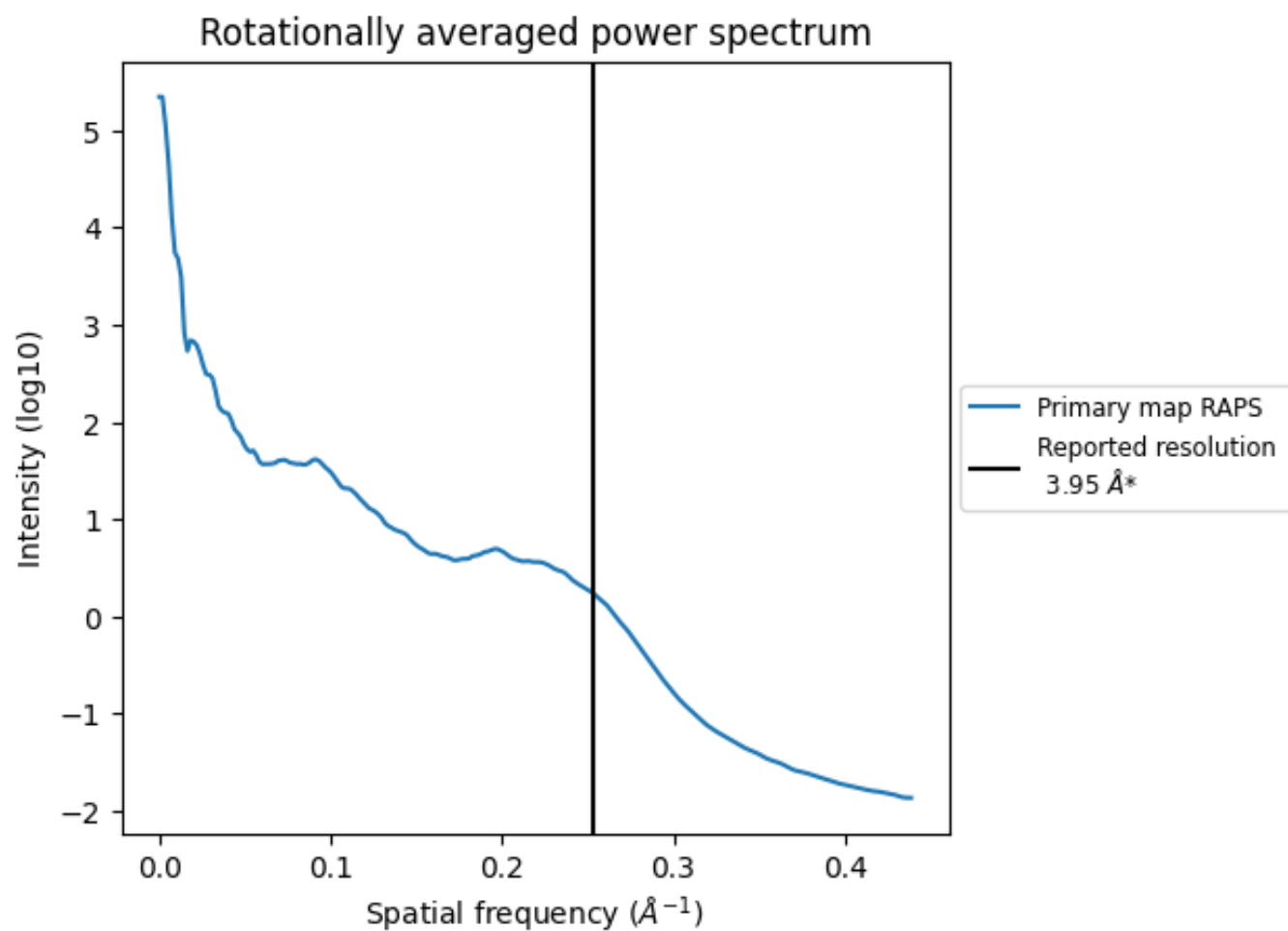
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 825 nm³; this corresponds to an approximate mass of 745 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 0.253 Å⁻¹

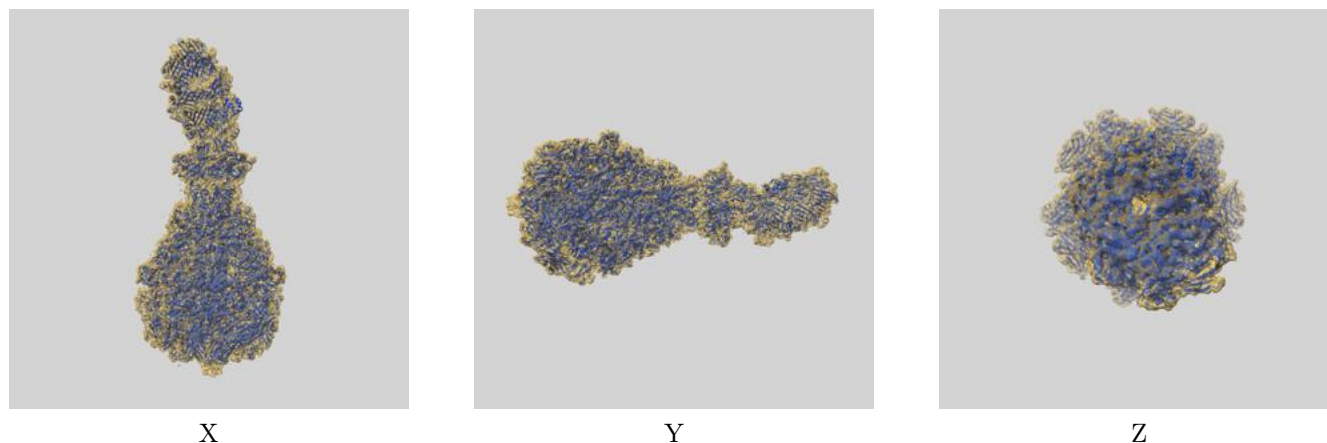
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

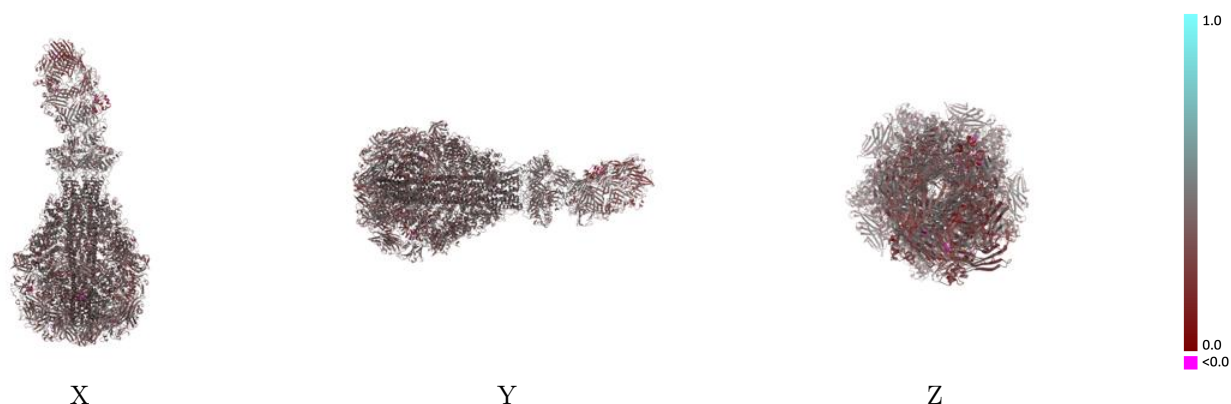
This section contains information regarding the fit between EMDB map EMD-0149 and PDB model 6H6E. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



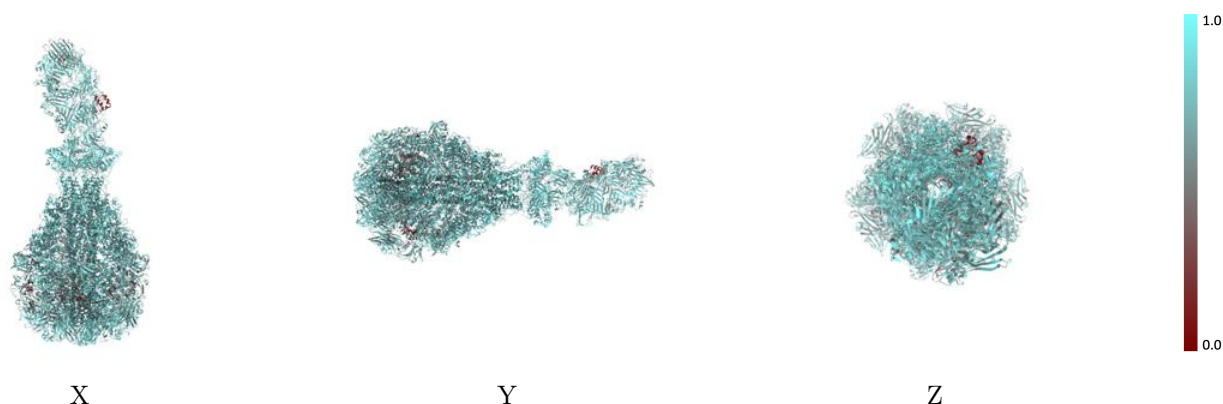
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



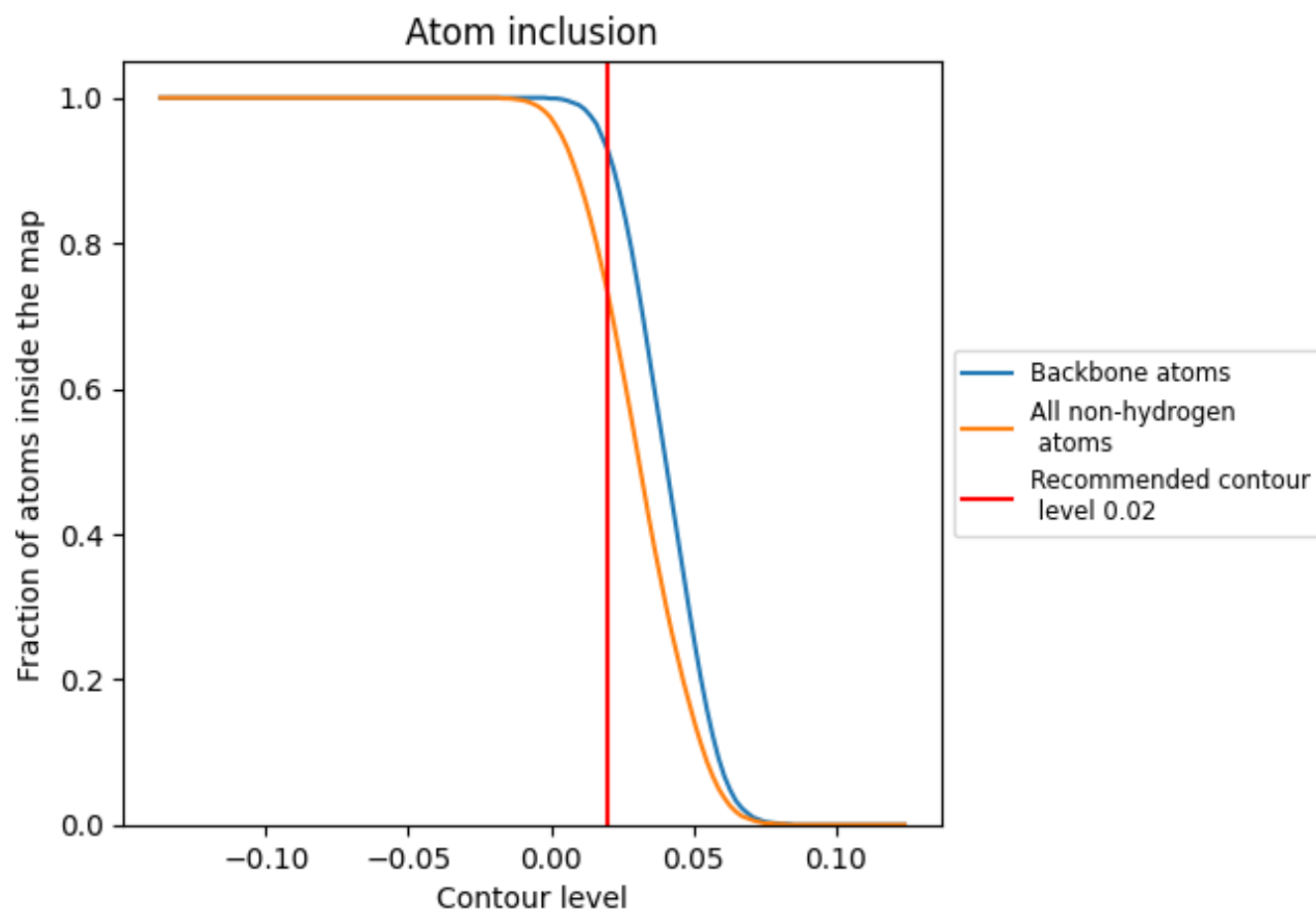
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 93% of all backbone atoms, 73% 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	0.7310	0.3710
A	0.7310	0.3750
B	0.7320	0.3760
C	0.7340	0.3750
D	0.7320	0.3780
E	0.7330	0.3770
F	0.7240	0.3400

1.0

0.0

<0.0