



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:02 PM UTC

PDB ID : 6H6F / pdb_00006h6f
EMDB ID : EMD-0150
Title : PTC3 holotoxin complex from Photorhabdus luminiscens - Mutant TcC-D651A
Authors : Gatsogiannis, C.; Merino, F.; Roderer, D.; Balchin, D.; Schubert, E.; Kuhlee, A.; Hayer-Hartl, M.; Raunser, S.
Deposited on : 2018-07-27
Resolution : 3.72 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:

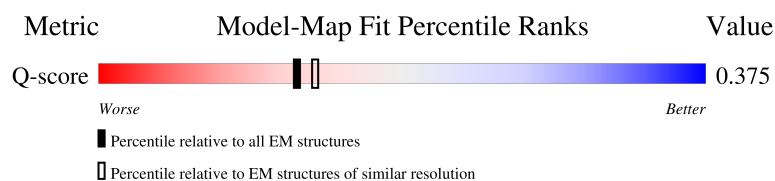
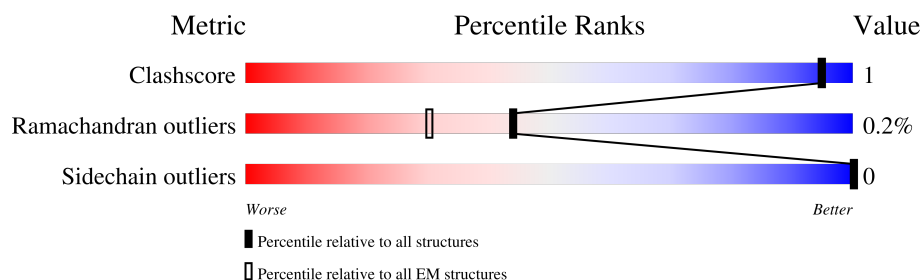
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.72 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	10474 (3.22 - 4.22)

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	22% 92% 5%
1	B	2516	21% 91% 6%
1	C	2516	21% 92% 5%
1	D	2516	19% 92% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	2516	20% 91% 6%
2	F	2434	42% 78% 8% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 114303 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	2454	Total	C	N	O	S	0	0
			19477	12332	3310	3774	61		
1	B	2454	Total	C	N	O	S	0	0
			19477	12332	3310	3774	61		
1	C	2454	Total	C	N	O	S	0	0
			19477	12332	3310	3774	61		
1	D	2454	Total	C	N	O	S	0	0
			19477	12332	3310	3774	61		
1	E	2454	Total	C	N	O	S	0	0
			19477	12332	3310	3774	61		

- Molecule 2 is a protein called TcdB2,TccC3,TccC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	2118	Total	C	N	O	S	0	0
			16918	10601	3006	3277	34		

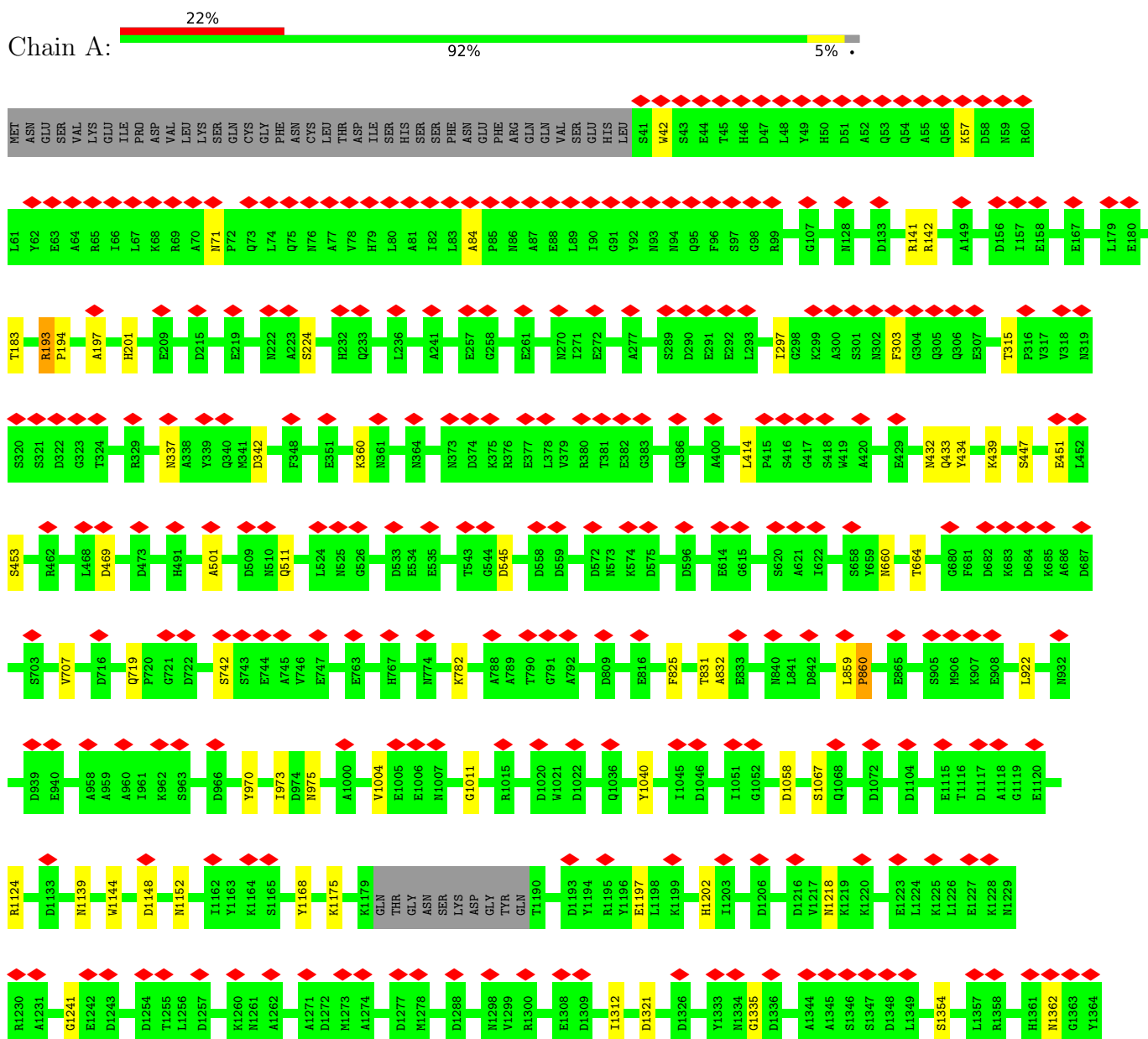
There is a discrepancy between the modelled and reference sequences:

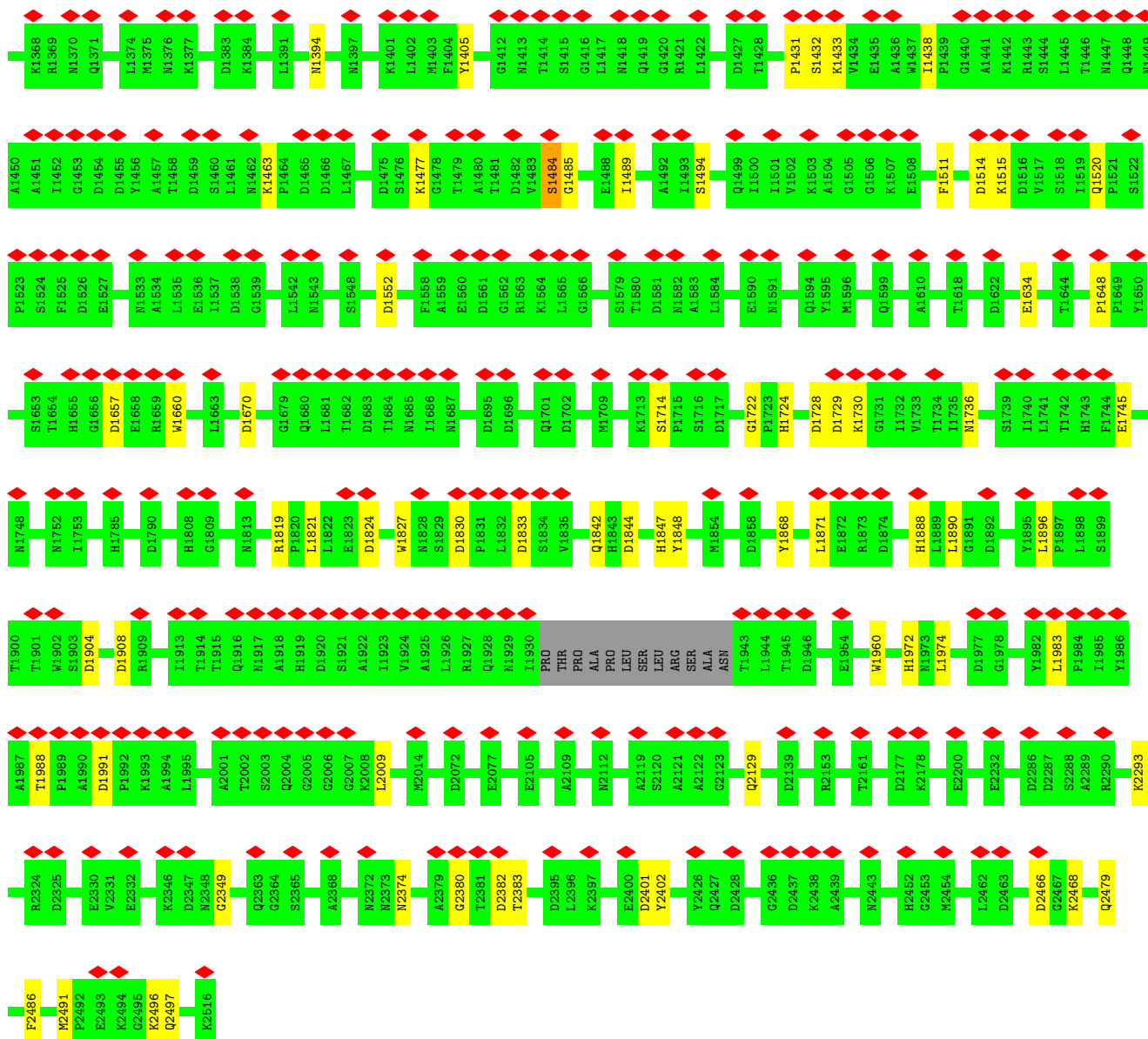
Chain	Residue	Modelled	Actual	Comment	Reference
F	2130	ALA	ASP	engineered mutation	UNP Q8GF97

3 Residue-property plots

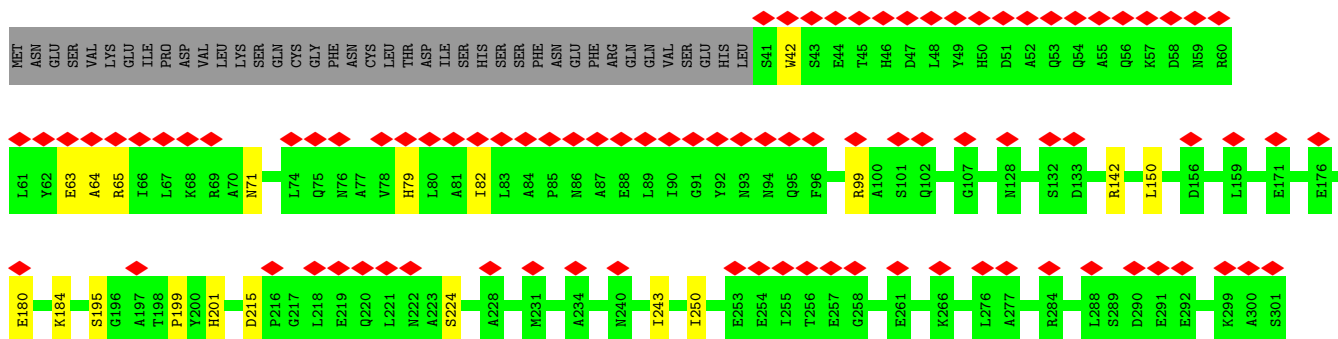
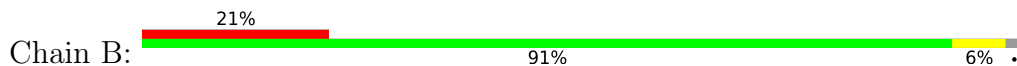
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

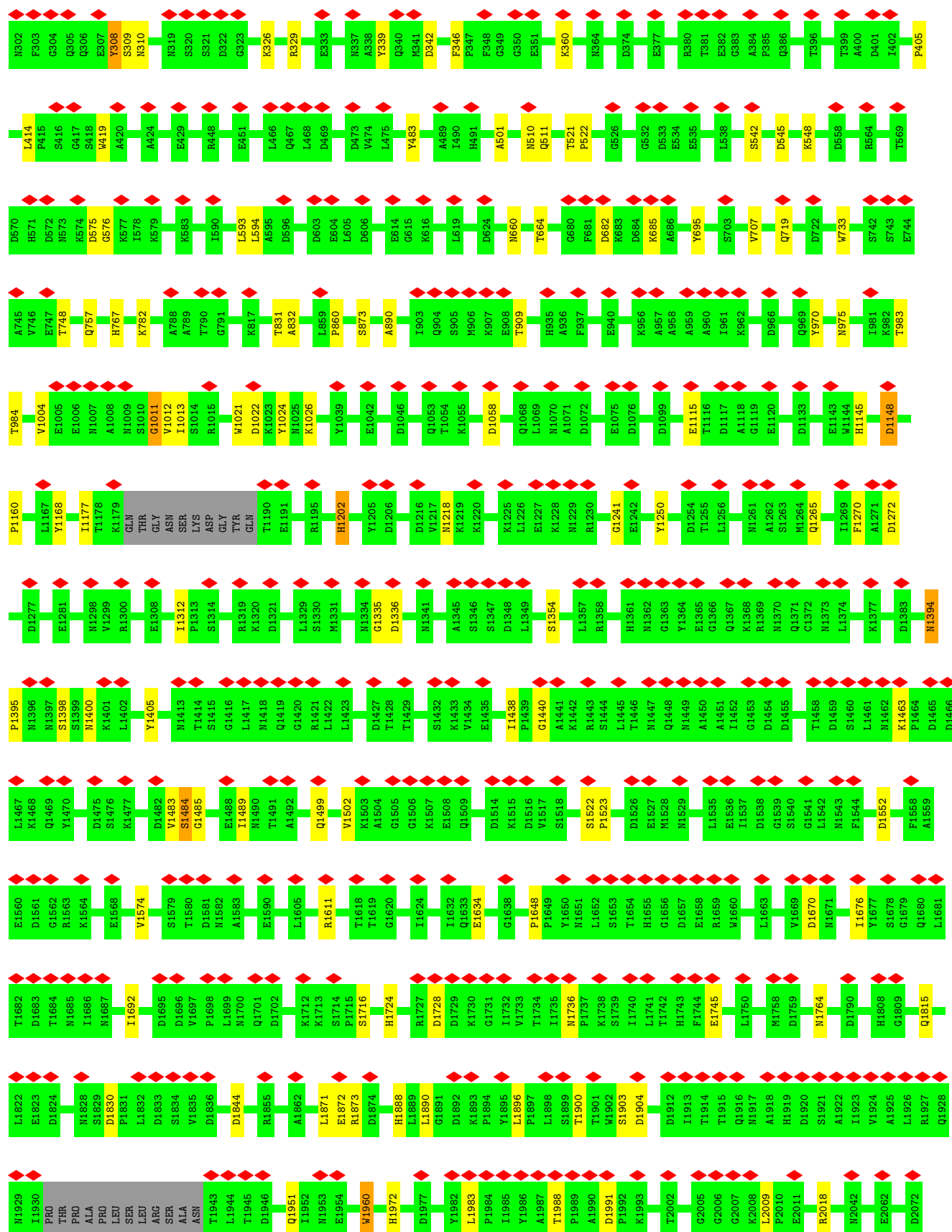
• Molecule 1: TcdA1

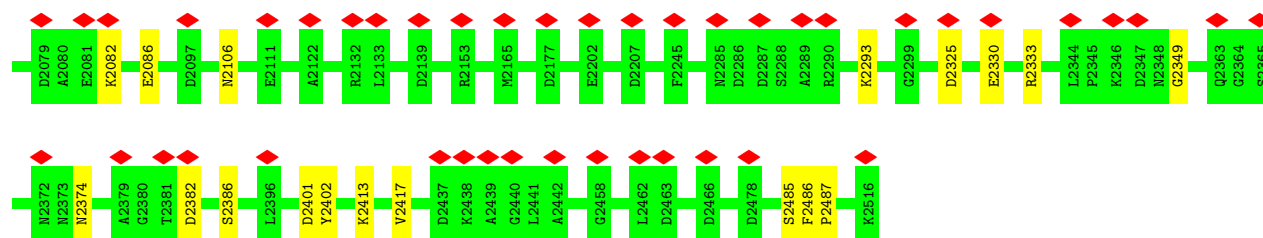




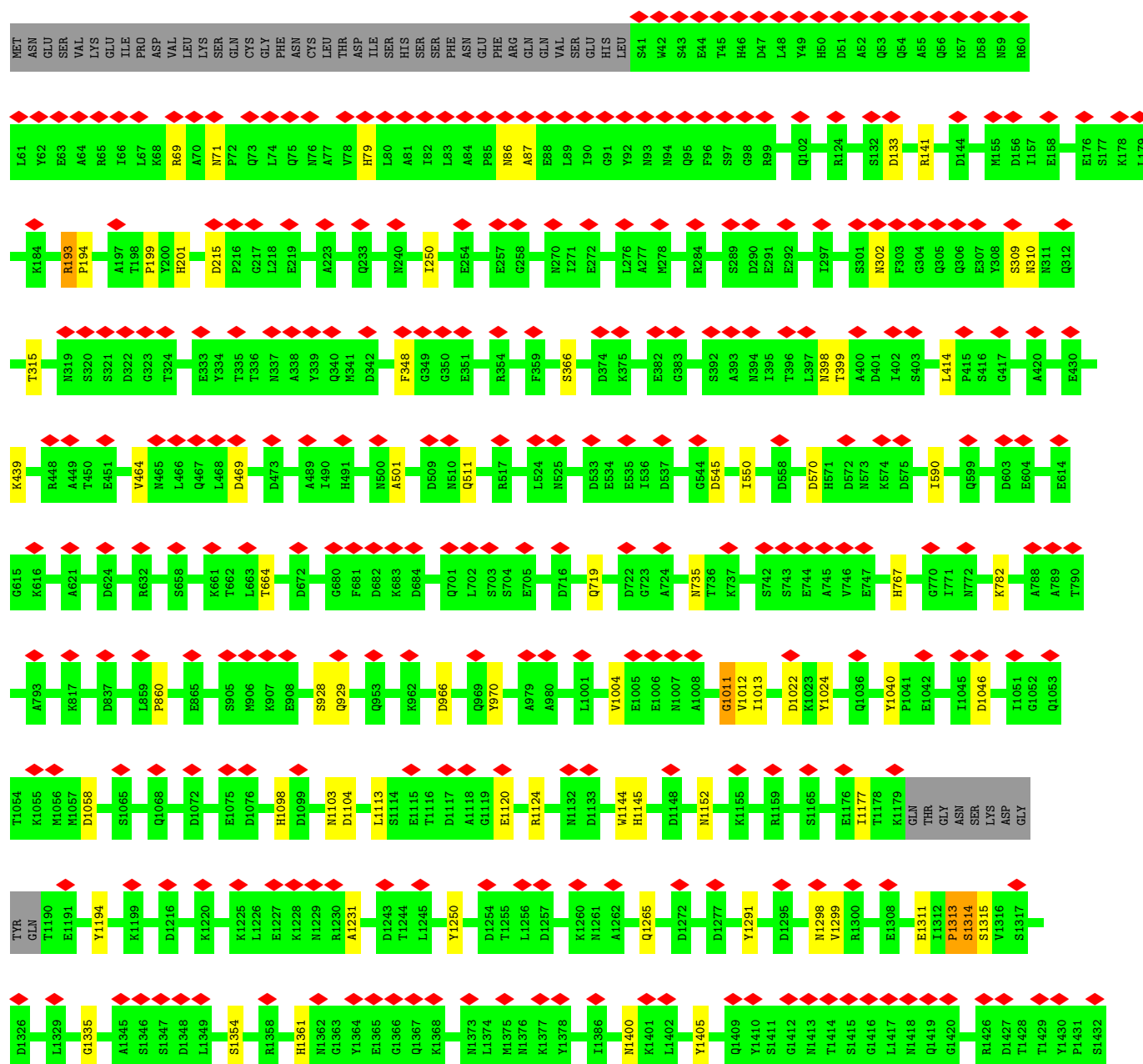
• Molecule 1: TcdA1

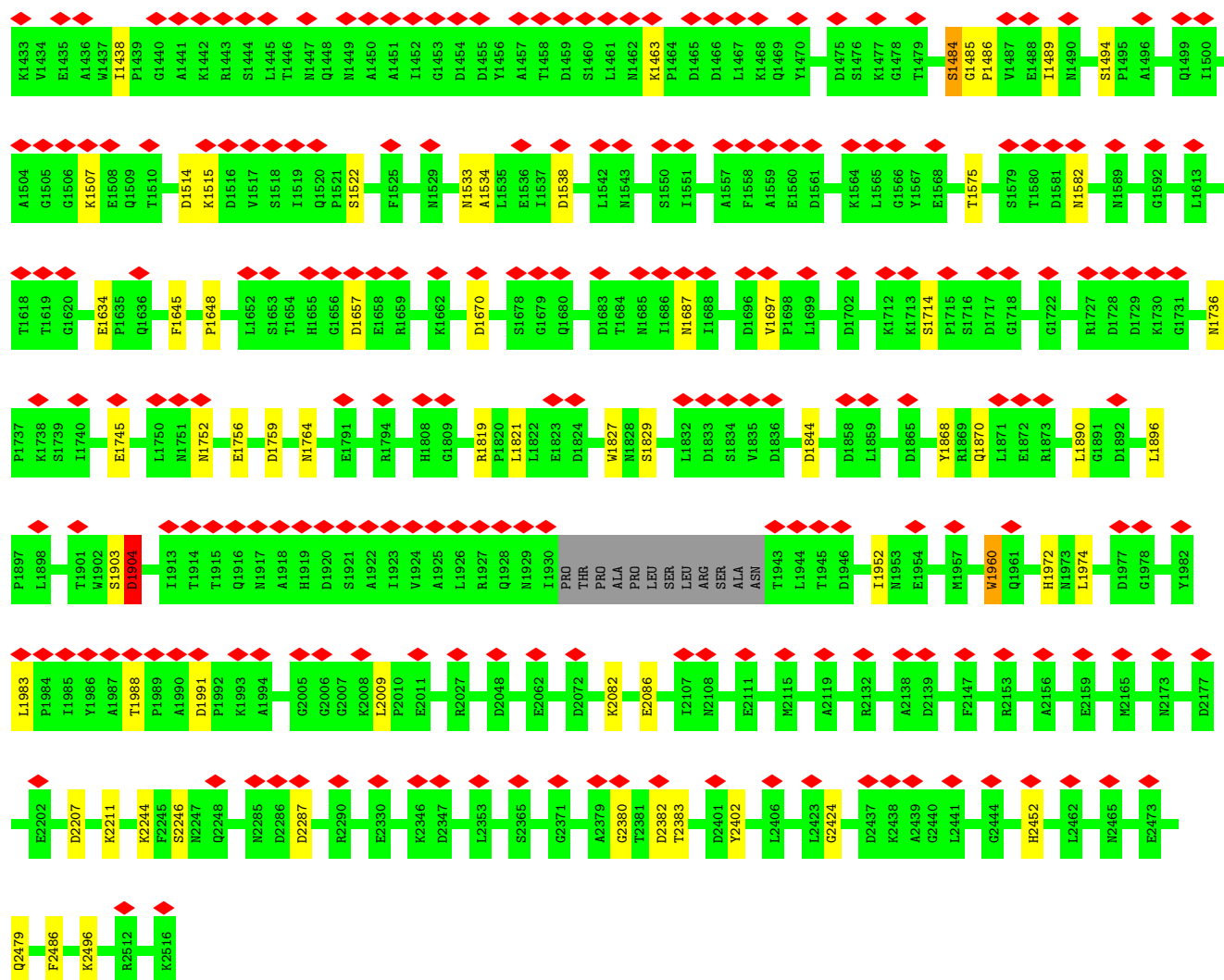




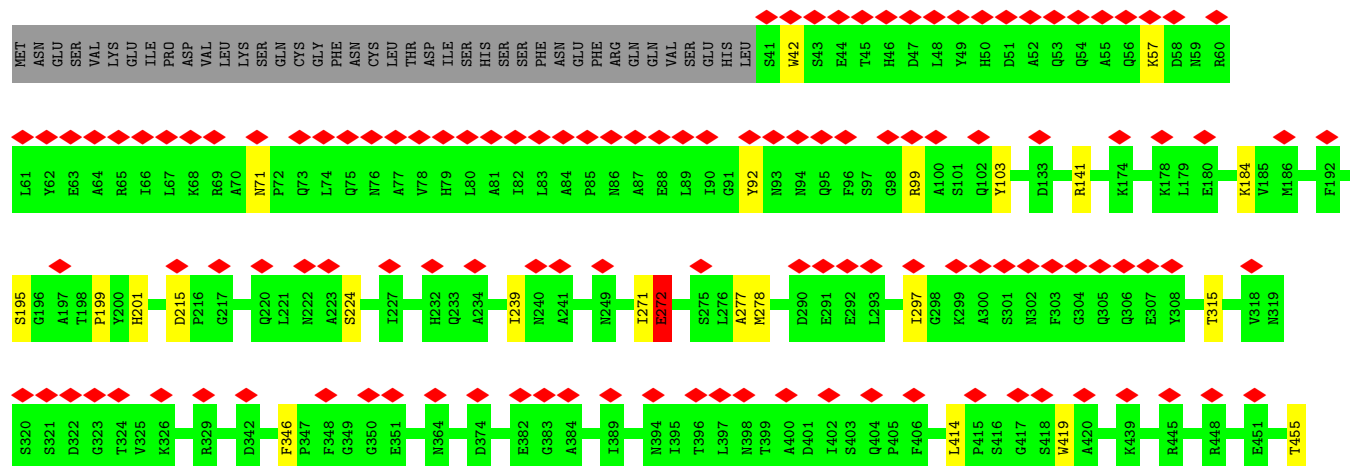


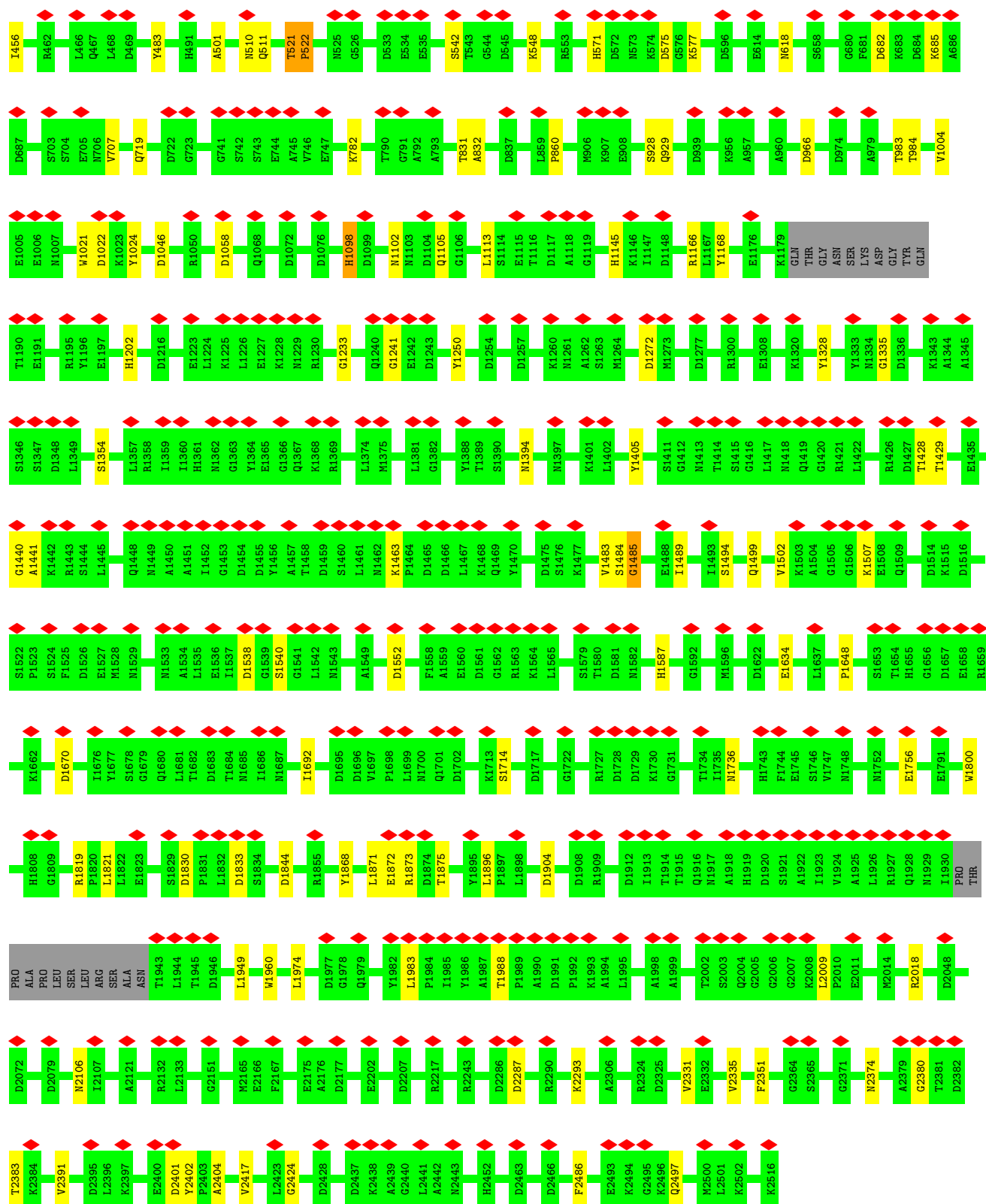
• Molecule 1: TcdA1



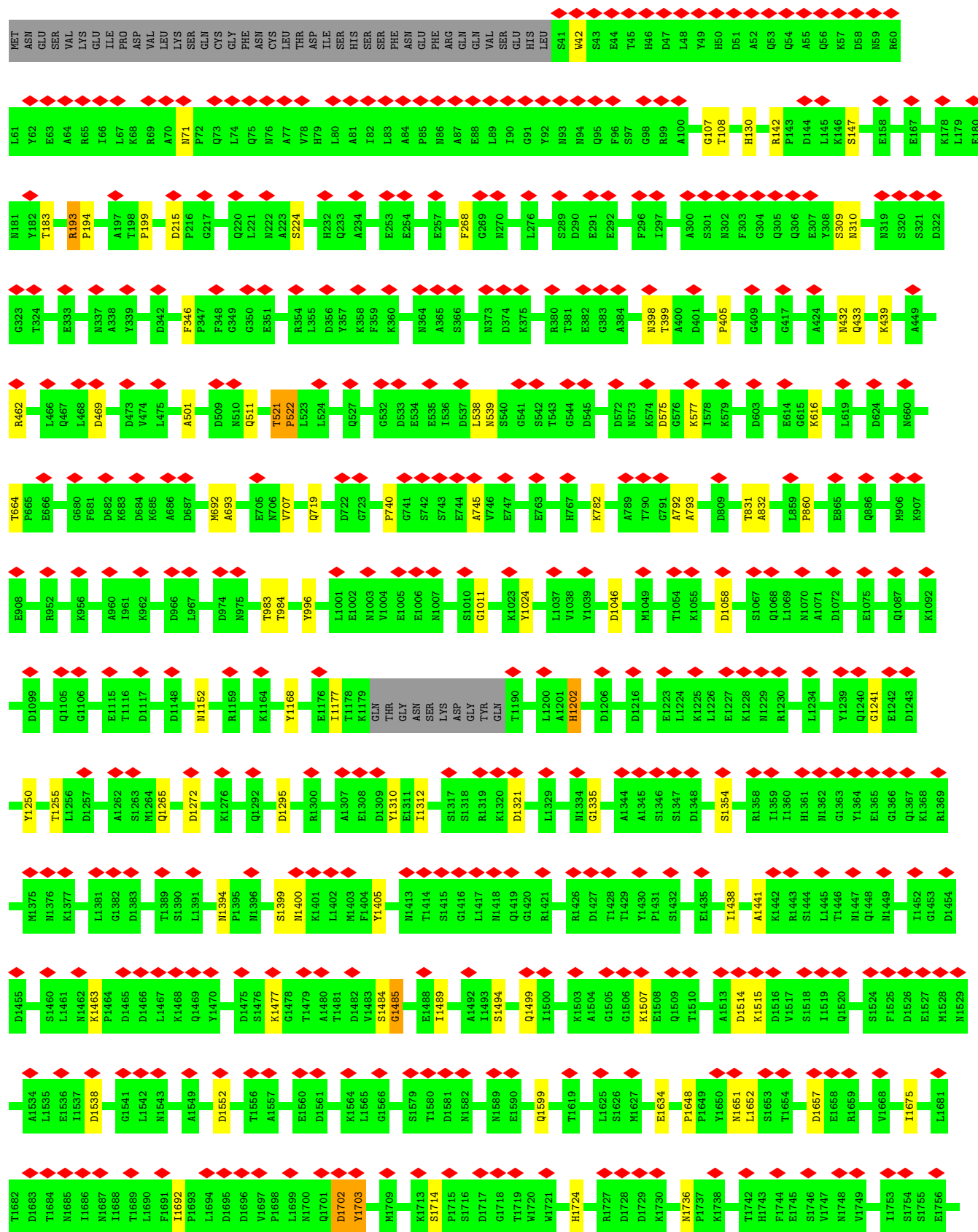


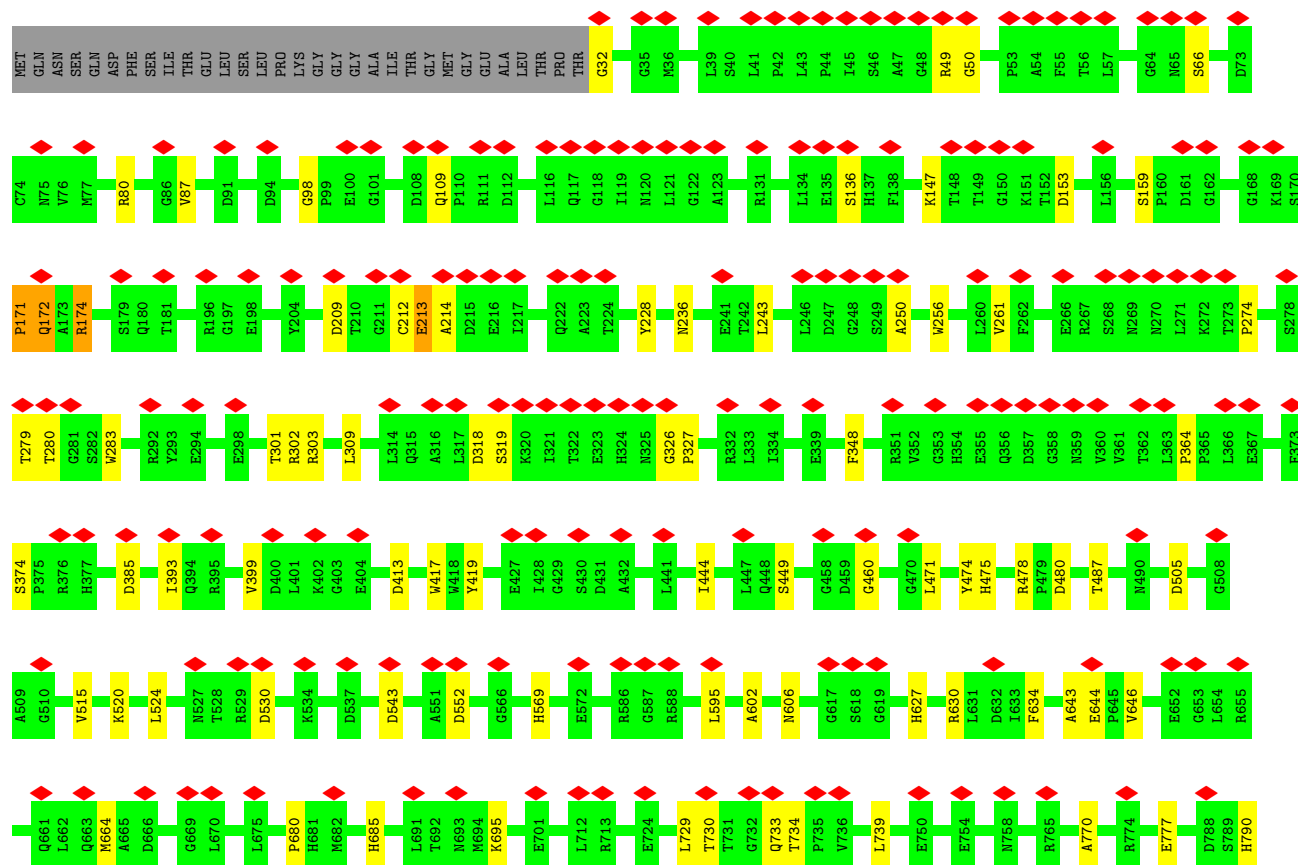
• Molecule 1: TcdA1

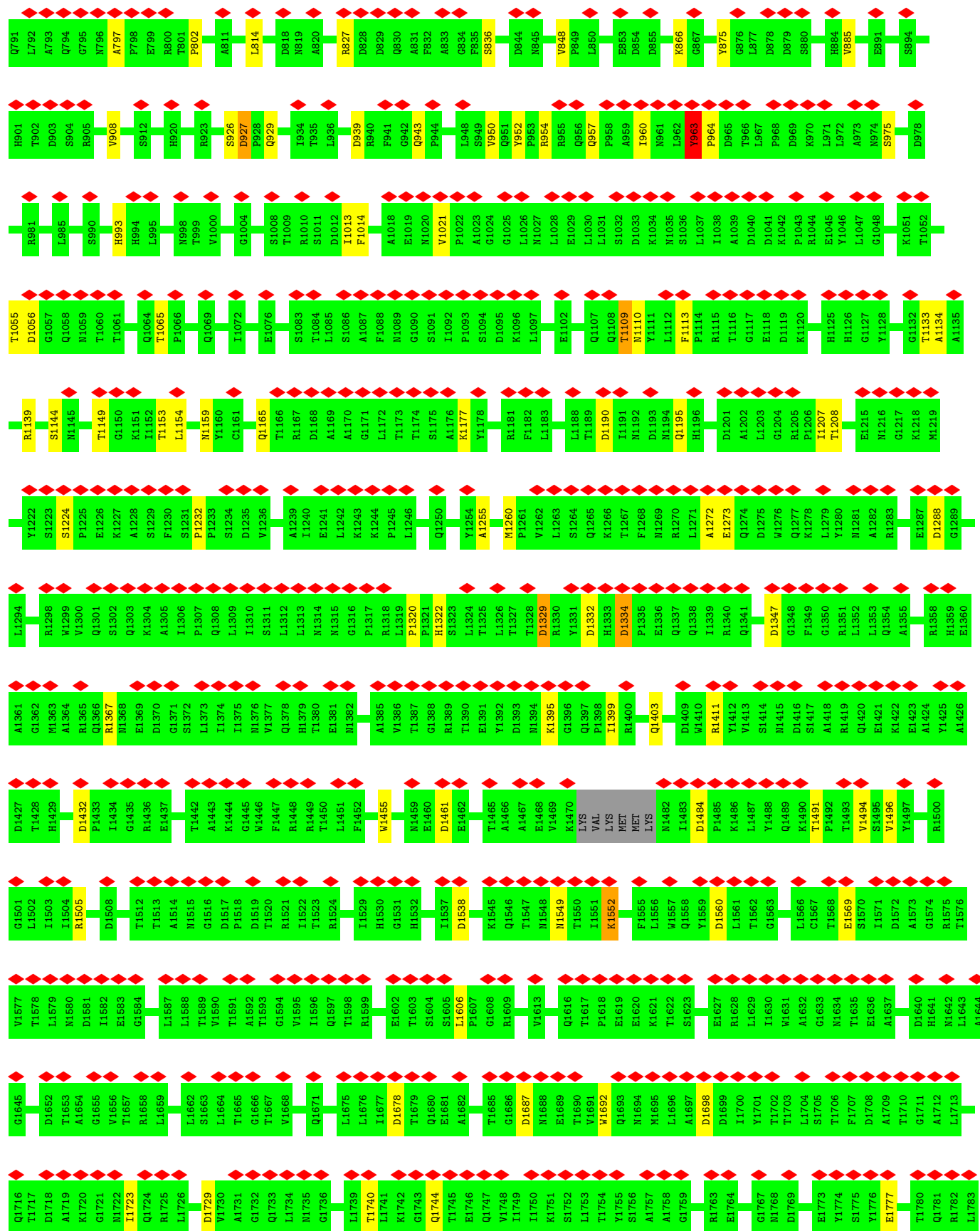




• Molecule 1: TcdA1









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	132000	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	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.141	Depositor
Minimum map value	-0.113	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	528.0, 528.0, 528.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	1.12	8/19896 (0.0%)	1.20	118/27024 (0.4%)
1	B	1.11	13/19896 (0.1%)	1.20	122/27024 (0.5%)
1	C	1.12	13/19896 (0.1%)	1.20	112/27024 (0.4%)
1	D	1.13	15/19896 (0.1%)	1.18	101/27024 (0.4%)
1	E	1.11	5/19896 (0.0%)	1.19	120/27024 (0.4%)
2	F	1.10	15/17337 (0.1%)	1.33	170/23638 (0.7%)
All	All	1.11	69/116817 (0.1%)	1.21	743/158758 (0.5%)

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1724	HIS	CB-CG	-7.47	1.39	1.50
1	C	141	ARG	CD-NE	-7.12	1.36	1.46
1	C	1145	HIS	CB-CG	-6.87	1.40	1.50
1	E	1847	HIS	CB-CG	-6.74	1.40	1.50
1	C	1819	ARG	CD-NE	-6.66	1.36	1.46
2	F	174	ARG	CD-NE	-6.56	1.37	1.46
2	F	627	HIS	CB-CG	-6.44	1.41	1.50
1	A	1819	ARG	CD-NE	-6.40	1.37	1.46
1	D	201	HIS	CB-CG	-6.35	1.41	1.50
2	F	236	ASN	CB-CG	-6.31	1.36	1.52
1	B	201	HIS	CB-CG	-6.27	1.41	1.50
1	B	767	HIS	CB-CG	-6.24	1.41	1.50
1	D	1819	ARG	CD-NE	-6.24	1.37	1.46
1	B	2018	ARG	CD-NE	-6.22	1.37	1.46
1	D	2018	ARG	CD-NE	-6.13	1.37	1.46
1	D	1145	HIS	CB-CG	-6.11	1.41	1.50
1	B	308	TYR	CB-CG	-6.00	1.38	1.51
1	D	1098	HIS	CB-CG	-5.95	1.41	1.50
1	A	1847	HIS	CB-CG	-5.88	1.42	1.50
1	B	1145	HIS	CB-CG	-5.83	1.42	1.50
1	B	1888	HIS	CB-CG	-5.81	1.42	1.50
1	C	767	HIS	CB-CG	-5.81	1.42	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1960	TRP	NE1-CE2	-5.80	1.31	1.37
2	F	685	HIS	CB-CG	-5.78	1.42	1.50
1	C	79	HIS	CB-CG	-5.70	1.42	1.50
2	F	2126	TRP	CD2-CE3	-5.69	1.31	1.40
1	A	141	ARG	CD-NE	-5.68	1.38	1.46
2	F	664	MET	CG-SD	-5.62	1.66	1.80
1	A	1139	ASN	CB-CG	-5.61	1.38	1.52
1	D	1587	HIS	CB-CG	-5.61	1.42	1.50
1	C	1098	HIS	CB-CG	-5.58	1.42	1.50
2	F	2126	TRP	NE1-CE2	-5.56	1.31	1.37
2	F	875	TYR	CB-CG	-5.55	1.39	1.51
1	E	1819	ARG	CD-NE	-5.53	1.38	1.46
1	D	1960	TRP	NE1-CE2	-5.52	1.31	1.37
1	C	1098	HIS	CD2-NE2	-5.49	1.31	1.37
1	C	1960	TRP	NE1-CE2	-5.48	1.31	1.37
1	E	2452	HIS	CB-CG	-5.47	1.42	1.50
1	E	1202	HIS	CB-CG	-5.46	1.42	1.50
2	F	174	ARG	CZ-NH2	-5.46	1.26	1.33
1	D	483	TYR	CB-CG	-5.44	1.39	1.51
1	C	141	ARG	CG-CD	-5.41	1.36	1.52
2	F	256	TRP	CD2-CE3	-5.40	1.31	1.40
1	D	1800	TRP	NE1-CE2	-5.39	1.31	1.37
2	F	1823	TRP	NE1-CE2	-5.38	1.31	1.37
1	D	1166	ARG	CD-NE	-5.38	1.38	1.46
2	F	993	HIS	CB-CG	-5.36	1.42	1.50
1	A	141	ARG	CZ-NH2	-5.30	1.26	1.33
2	F	475	HIS	CB-CG	-5.26	1.42	1.50
1	D	1692	ILE	N-CA	-5.25	1.42	1.46
1	C	69	ARG	CD-NE	5.23	1.53	1.46
1	E	1310	TYR	CB-CG	-5.22	1.40	1.51
1	D	103	TYR	CB-CG	-5.20	1.40	1.51
1	C	1098	HIS	CE1-NE2	-5.14	1.27	1.32
1	B	1218	ASN	CB-CG	-5.13	1.39	1.52
1	A	1218	ASN	CB-CG	-5.13	1.39	1.52
1	B	79	HIS	CB-CG	-5.11	1.43	1.50
2	F	348	PHE	CB-CG	-5.11	1.39	1.50
1	D	1328	TYR	CB-CG	-5.10	1.40	1.51
1	B	483	TYR	CB-CG	-5.10	1.40	1.51
1	B	1202	HIS	CB-CG	-5.09	1.43	1.50
1	A	1888	HIS	CB-CG	-5.09	1.43	1.50
1	B	1724	HIS	CB-CG	-5.05	1.43	1.50
1	C	201	HIS	CB-CG	-5.05	1.43	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1951	GLN	CG-CD	-5.04	1.39	1.52
1	D	141	ARG	CD-NE	-5.04	1.39	1.46
1	C	1952	ILE	CB-CG1	-5.03	1.43	1.53
1	D	1021	TRP	NE1-CE2	-5.03	1.31	1.37
2	F	1322	HIS	CB-CG	-5.00	1.43	1.50

All (743) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1395	LYS	N-CA-C	-9.69	101.57	113.97
1	D	1844	ASP	CA-C-N	9.05	128.79	119.56
1	D	1844	ASP	C-N-CA	9.05	128.79	119.56
1	E	1477	LYS	N-CA-C	-9.05	102.81	114.04
1	D	1004	VAL	N-CA-C	-8.89	101.74	110.72
1	E	1354	SER	CA-C-N	8.85	128.79	120.03
1	E	1354	SER	C-N-CA	8.85	128.79	120.03
1	C	1011	GLY	N-CA-C	-8.80	99.88	112.55
1	E	1844	ASP	CA-C-N	8.79	128.52	119.56
1	E	1844	ASP	C-N-CA	8.79	128.52	119.56
1	A	1844	ASP	CA-C-N	8.74	128.39	119.82
1	A	1844	ASP	C-N-CA	8.74	128.39	119.82
1	E	1011	GLY	N-CA-C	-8.71	100.63	112.57
2	F	952	TYR	CA-C-N	8.67	128.61	120.03
2	F	952	TYR	C-N-CA	8.67	128.61	120.03
1	A	2497	GLN	N-CA-C	-8.66	102.15	112.89
1	D	2497	GLN	N-CA-C	-8.65	102.16	112.89
1	A	1354	SER	CA-C-N	8.61	128.55	120.03
1	A	1354	SER	C-N-CA	8.61	128.55	120.03
1	C	348	PHE	N-CA-C	-8.60	103.38	114.04
1	B	2486	PHE	CA-C-N	8.54	129.38	119.47
1	B	2486	PHE	C-N-CA	8.54	129.38	119.47
2	F	2120	GLN	CA-C-N	8.53	128.26	119.56
2	F	2120	GLN	C-N-CA	8.53	128.26	119.56
1	D	1354	SER	CA-C-N	8.47	128.42	120.03
1	D	1354	SER	C-N-CA	8.47	128.42	120.03
1	B	1844	ASP	CA-C-N	8.39	128.12	119.56
1	B	1844	ASP	C-N-CA	8.39	128.12	119.56
1	C	1844	ASP	CA-C-N	8.30	128.03	119.56
1	C	1844	ASP	C-N-CA	8.30	128.03	119.56
2	F	32	GLY	CA-C-N	8.30	129.10	119.47
2	F	32	GLY	C-N-CA	8.30	129.10	119.47
2	F	1484	ASP	CA-C-N	8.09	127.75	119.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1484	ASP	C-N-CA	8.09	127.75	119.82
1	E	616	LYS	N-CA-C	-8.05	104.33	114.56
1	A	1004	VAL	N-CA-C	-7.93	102.35	111.00
1	B	1354	SER	CA-C-N	7.92	127.88	120.03
1	B	1354	SER	C-N-CA	7.92	127.88	120.03
1	B	1676	ILE	CB-CA-C	-7.90	102.48	111.80
2	F	1723	ILE	N-CA-C	7.81	119.04	108.11
1	B	414	LEU	CA-C-N	7.80	127.47	119.82
1	B	414	LEU	C-N-CA	7.80	127.47	119.82
1	A	1438	ILE	CA-C-N	7.74	127.38	119.56
1	A	1438	ILE	C-N-CA	7.74	127.38	119.56
1	B	1004	VAL	N-CA-C	-7.73	102.57	111.00
1	A	742	SER	N-CA-C	7.72	119.33	111.07
1	A	1011	GLY	N-CA-C	-7.70	102.02	112.57
1	A	782	LYS	CA-C-N	7.66	127.37	119.56
1	A	782	LYS	C-N-CA	7.66	127.37	119.56
1	D	1736	ASN	CA-C-N	7.65	127.36	119.56
1	D	1736	ASN	C-N-CA	7.65	127.36	119.56
1	C	511	GLN	CA-C-N	7.62	127.57	120.03
1	C	511	GLN	C-N-CA	7.62	127.57	120.03
1	B	1011	GLY	N-CA-C	-7.59	101.62	112.55
2	F	2147	ASN	CA-C-N	7.59	127.77	119.87
2	F	2147	ASN	C-N-CA	7.59	127.77	119.87
1	A	1463	LYS	CA-C-N	7.56	127.19	119.56
1	A	1463	LYS	C-N-CA	7.56	127.19	119.56
1	C	2424	GLY	CA-C-N	7.53	127.24	119.56
1	C	2424	GLY	C-N-CA	7.53	127.24	119.56
1	C	1354	SER	CA-C-N	7.51	127.47	120.03
1	C	1354	SER	C-N-CA	7.51	127.47	120.03
1	D	1441	ALA	N-CA-C	-7.50	104.64	114.31
1	D	315	THR	CA-C-N	7.47	129.18	119.84
1	D	315	THR	C-N-CA	7.47	129.18	119.84
2	F	963	TYR	CA-C-N	7.45	127.16	119.56
2	F	963	TYR	C-N-CA	7.45	127.16	119.56
2	F	1860	PHE	CA-C-N	7.43	127.39	120.03
2	F	1860	PHE	C-N-CA	7.43	127.39	120.03
1	C	315	THR	CA-C-N	7.38	129.07	119.84
1	C	315	THR	C-N-CA	7.38	129.07	119.84
2	F	1113	PHE	CA-C-N	7.37	127.33	120.03
2	F	1113	PHE	C-N-CA	7.37	127.33	120.03
2	F	399	VAL	N-CA-C	7.33	120.69	108.81
2	F	1922	ASP	CA-C-N	7.33	127.04	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1922	ASP	C-N-CA	7.33	127.04	119.56
2	F	1552	LYS	CA-C-N	7.33	127.76	119.92
2	F	1552	LYS	C-N-CA	7.33	127.76	119.92
1	A	1904	ASP	CA-C-N	7.31	127.26	120.03
1	A	1904	ASP	C-N-CA	7.31	127.26	120.03
1	B	1463	LYS	CA-C-N	7.28	126.99	119.56
1	B	1463	LYS	C-N-CA	7.28	126.99	119.56
1	E	1463	LYS	CA-C-N	7.26	127.89	119.47
1	E	1463	LYS	C-N-CA	7.26	127.89	119.47
1	C	1736	ASN	CA-C-N	7.25	126.93	119.82
1	C	1736	ASN	C-N-CA	7.25	126.93	119.82
1	D	521	THR	N-CA-C	-7.24	99.50	110.07
2	F	243	LEU	CA-C-N	7.23	126.86	119.56
2	F	243	LEU	C-N-CA	7.23	126.86	119.56
2	F	2130	ALA	CA-C-N	7.23	127.39	119.87
2	F	2130	ALA	C-N-CA	7.23	127.39	119.87
1	D	2009	LEU	CA-C-N	7.22	127.67	120.52
1	D	2009	LEU	C-N-CA	7.22	127.67	120.52
1	A	511	GLN	CA-C-N	7.20	127.15	120.03
1	A	511	GLN	C-N-CA	7.20	127.15	120.03
1	D	297	ILE	N-CA-C	7.19	119.04	112.43
2	F	595	LEU	CA-C-N	7.18	127.14	120.03
2	F	595	LEU	C-N-CA	7.18	127.14	120.03
1	C	1463	LYS	CA-C-N	7.17	127.78	119.47
1	C	1463	LYS	C-N-CA	7.17	127.78	119.47
1	B	1438	ILE	CA-C-N	7.15	126.78	119.56
1	B	1438	ILE	C-N-CA	7.15	126.78	119.56
1	D	199	PRO	N-CA-C	-7.15	100.01	111.38
1	A	71	ASN	CA-C-N	7.12	127.73	119.47
1	A	71	ASN	C-N-CA	7.12	127.73	119.47
1	C	1004	VAL	N-CA-C	-7.10	103.26	111.00
1	E	1441	ALA	N-CA-C	-7.10	105.15	114.31
1	D	1463	LYS	CA-C-N	7.10	126.73	119.56
1	D	1463	LYS	C-N-CA	7.10	126.73	119.56
1	D	2331	VAL	N-CA-C	7.09	118.04	108.11
1	B	1483	VAL	N-CA-C	7.08	118.02	108.11
1	E	1152	ASN	CA-C-N	7.07	126.99	119.85
1	E	1152	ASN	C-N-CA	7.07	126.99	119.85
1	B	2009	LEU	CA-C-N	7.06	127.02	120.03
1	B	2009	LEU	C-N-CA	7.06	127.02	120.03
1	B	511	GLN	CA-C-N	7.05	127.01	120.03
1	B	511	GLN	C-N-CA	7.05	127.01	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1736	ASN	CA-C-N	7.04	126.72	119.82
1	B	1736	ASN	C-N-CA	7.04	126.72	119.82
2	F	1399	ILE	N-CA-C	-7.04	106.63	113.53
1	B	1896	LEU	CA-C-N	7.00	126.95	120.03
1	B	1896	LEU	C-N-CA	7.00	126.95	120.03
1	D	860	PRO	N-CA-C	-6.97	102.20	110.70
1	B	2382	ASP	CA-CB-CG	6.93	119.53	112.60
2	F	515	VAL	N-CA-C	6.92	118.69	108.45
1	A	1896	LEU	CA-C-N	6.92	126.88	120.03
1	A	1896	LEU	C-N-CA	6.92	126.88	120.03
1	E	1904	ASP	CA-C-N	6.92	126.88	120.03
1	E	1904	ASP	C-N-CA	6.92	126.88	120.03
1	C	1058	ASP	CA-CB-CG	6.92	119.52	112.60
1	A	414	LEU	CA-C-N	6.92	126.60	119.82
1	A	414	LEU	C-N-CA	6.92	126.60	119.82
1	A	1736	ASN	CA-C-N	6.91	126.59	119.82
1	A	1736	ASN	C-N-CA	6.91	126.59	119.82
1	B	1522	SER	CA-C-N	6.91	127.79	120.12
1	B	1522	SER	C-N-CA	6.91	127.79	120.12
1	E	521	THR	N-CA-C	-6.88	100.02	110.07
1	D	1875	THR	N-CA-C	-6.87	104.71	113.23
1	C	1983	LEU	CA-C-N	6.87	127.04	120.31
1	C	1983	LEU	C-N-CA	6.87	127.04	120.31
1	B	199	PRO	N-CA-C	-6.87	101.11	111.41
1	C	1438	ILE	CA-C-N	6.85	126.48	119.56
1	C	1438	ILE	C-N-CA	6.85	126.48	119.56
1	A	860	PRO	N-CA-C	-6.85	102.35	110.70
1	E	1893	LYS	CA-C-N	6.84	126.54	119.56
1	E	1893	LYS	C-N-CA	6.84	126.54	119.56
2	F	1065	THR	CA-C-N	6.84	126.80	120.03
2	F	1065	THR	C-N-CA	6.84	126.80	120.03
2	F	460	GLY	N-CA-C	-6.82	106.58	114.69
1	E	1875	THR	N-CA-C	-6.81	104.78	113.23
2	F	957	GLN	CA-C-N	6.81	126.98	120.31
2	F	957	GLN	C-N-CA	6.81	126.98	120.31
1	E	2466	ASP	CA-CB-CG	6.80	119.40	112.60
1	E	1489	ILE	N-CA-C	6.79	117.62	108.11
2	F	236	ASN	CA-CB-CG	-6.76	105.83	112.60
1	C	1405	TYR	CA-C-N	6.76	126.67	119.85
1	C	1405	TYR	C-N-CA	6.76	126.67	119.85
1	E	71	ASN	CA-C-N	6.75	127.29	119.47
1	E	71	ASN	C-N-CA	6.75	127.29	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	159	SER	CA-C-N	6.75	128.27	119.84
2	F	159	SER	C-N-CA	6.75	128.27	119.84
1	B	2374	ASN	N-CA-C	6.72	117.45	108.38
1	C	1904	ASP	CA-C-N	6.71	126.63	119.85
1	C	1904	ASP	C-N-CA	6.71	126.63	119.85
1	E	199	PRO	N-CA-C	-6.70	100.72	111.38
2	F	1894	SER	CA-C-N	6.70	127.24	119.47
2	F	1894	SER	C-N-CA	6.70	127.24	119.47
1	C	2402	TYR	CA-C-N	6.69	126.67	119.78
1	C	2402	TYR	C-N-CA	6.69	126.67	119.78
1	B	71	ASN	CA-C-N	6.68	127.22	119.47
1	B	71	ASN	C-N-CA	6.68	127.22	119.47
2	F	960	ILE	N-CA-C	6.67	117.47	107.80
1	E	2009	LEU	CA-C-N	6.64	127.03	119.92
1	E	2009	LEU	C-N-CA	6.64	127.03	119.92
2	F	1777	GLU	CA-C-N	6.63	127.17	119.47
2	F	1777	GLU	C-N-CA	6.63	127.17	119.47
1	C	193	ARG	CA-C-N	6.63	126.57	120.21
1	C	193	ARG	C-N-CA	6.63	126.57	120.21
1	C	71	ASN	CA-C-N	6.62	127.15	119.47
1	C	71	ASN	C-N-CA	6.62	127.15	119.47
1	A	1335	GLY	N-CA-C	-6.62	102.48	112.41
1	A	315	THR	CA-C-N	6.61	128.11	119.84
1	A	315	THR	C-N-CA	6.61	128.11	119.84
1	C	199	PRO	N-CA-C	-6.60	100.88	111.38
1	B	860	PRO	N-CA-C	-6.59	102.65	110.70
2	F	1139	ARG	CA-C-N	6.58	126.50	119.85
2	F	1139	ARG	C-N-CA	6.58	126.50	119.85
1	E	1736	ASN	CA-C-N	6.57	126.26	119.82
1	E	1736	ASN	C-N-CA	6.57	126.26	119.82
1	B	1335	GLY	N-CA-C	-6.57	102.55	112.41
1	D	414	LEU	CA-C-N	6.57	126.70	119.87
1	D	414	LEU	C-N-CA	6.57	126.70	119.87
1	B	707	VAL	N-CA-C	-6.57	103.84	111.00
1	A	297	ILE	N-CA-C	6.56	118.46	112.43
2	F	1491	THR	CA-C-N	6.55	126.73	120.31
2	F	1491	THR	C-N-CA	6.55	126.73	120.31
1	B	1394	ASN	CA-C-N	6.54	126.23	119.56
1	B	1394	ASN	C-N-CA	6.54	126.23	119.56
1	B	1904	ASP	CA-C-N	6.52	126.44	119.85
1	B	1904	ASP	C-N-CA	6.52	126.44	119.85
1	E	1241	GLY	N-CA-C	-6.52	103.73	112.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2479	GLN	N-CA-C	6.51	118.97	109.07
2	F	1432	ASP	CA-C-N	6.51	126.20	119.56
2	F	1432	ASP	C-N-CA	6.51	126.20	119.56
1	A	2293	LYS	CA-C-N	6.50	126.45	120.21
1	A	2293	LYS	C-N-CA	6.50	126.45	120.21
1	A	1830	ASP	CA-C-N	6.48	126.17	119.56
1	A	1830	ASP	C-N-CA	6.48	126.17	119.56
1	D	1335	GLY	N-CA-C	-6.47	102.71	112.41
2	F	478	ARG	CA-C-N	6.47	126.16	119.56
2	F	478	ARG	C-N-CA	6.47	126.16	119.56
1	D	707	VAL	N-CA-C	-6.46	103.96	111.00
2	F	274	PRO	CA-C-N	6.46	126.38	119.85
2	F	274	PRO	C-N-CA	6.46	126.38	119.85
2	F	1255	ALA	CA-C-N	6.46	126.08	119.56
2	F	1255	ALA	C-N-CA	6.46	126.08	119.56
1	E	1949	LEU	CA-C-N	6.45	126.40	119.76
1	E	1949	LEU	C-N-CA	6.45	126.40	119.76
2	F	739	LEU	CA-C-N	6.44	126.57	119.87
2	F	739	LEU	C-N-CA	6.44	126.57	119.87
1	D	1714	SER	CA-C-N	6.43	126.99	120.04
1	D	1714	SER	C-N-CA	6.43	126.99	120.04
1	A	1058	ASP	CA-CB-CG	6.43	119.03	112.60
2	F	552	ASP	CA-C-N	6.42	126.10	119.56
2	F	552	ASP	C-N-CA	6.42	126.10	119.56
1	B	2417	VAL	N-CA-C	6.42	117.36	108.12
1	D	1250	TYR	N-CA-C	6.42	118.82	109.07
1	A	664	THR	CA-C-N	6.41	126.63	119.32
1	A	664	THR	C-N-CA	6.41	126.63	119.32
1	A	1714	SER	CA-C-N	6.41	126.96	120.04
1	A	1714	SER	C-N-CA	6.41	126.96	120.04
1	B	2402	TYR	CA-C-N	6.40	126.32	119.85
1	B	2402	TYR	C-N-CA	6.40	126.32	119.85
1	E	1046	ASP	CA-C-N	6.40	126.08	119.56
1	E	1046	ASP	C-N-CA	6.40	126.08	119.56
1	A	1152	ASN	CA-C-N	6.39	126.31	119.85
1	A	1152	ASN	C-N-CA	6.39	126.31	119.85
1	B	1634	GLU	CA-C-N	6.39	126.36	119.78
1	B	1634	GLU	C-N-CA	6.39	126.36	119.78
1	E	1949	LEU	N-CA-C	6.38	119.56	110.24
1	D	346	PHE	CA-C-N	6.38	127.81	119.84
1	D	346	PHE	C-N-CA	6.38	127.81	119.84
1	E	193	ARG	CA-C-N	6.37	126.33	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	193	ARG	C-N-CA	6.37	126.33	120.03
1	C	1714	SER	CA-C-N	6.37	125.99	119.56
1	C	1714	SER	C-N-CA	6.37	125.99	119.56
2	F	474	TYR	N-CA-C	6.37	117.89	108.60
1	B	1489	ILE	N-CA-C	6.36	117.03	107.75
1	D	782	LYS	CA-C-N	6.35	126.47	119.87
1	D	782	LYS	C-N-CA	6.35	126.47	119.87
2	F	374	SER	CA-C-N	6.35	126.03	119.56
2	F	374	SER	C-N-CA	6.35	126.03	119.56
1	A	1489	ILE	N-CA-C	6.34	116.99	108.11
2	F	2011	ASN	N-CA-C	-6.34	101.99	110.55
1	E	782	LYS	CA-C-N	6.33	126.25	119.28
1	E	782	LYS	C-N-CA	6.33	126.25	119.28
2	F	487	THR	CA-C-N	6.33	126.02	119.56
2	F	487	THR	C-N-CA	6.33	126.02	119.56
2	F	1334	ASP	CA-C-N	6.33	127.75	119.84
2	F	1334	ASP	C-N-CA	6.33	127.75	119.84
1	E	2417	VAL	N-CA-C	6.33	116.97	108.11
1	B	719	GLN	CA-C-N	6.30	126.27	120.03
1	B	719	GLN	C-N-CA	6.30	126.27	120.03
1	A	1745	GLU	N-CA-C	-6.27	104.53	111.36
1	D	1489	ILE	N-CA-C	6.25	116.86	108.11
1	C	2479	GLN	N-CA-C	6.23	119.34	109.50
2	F	802	PRO	CA-C-N	6.23	126.20	120.03
2	F	802	PRO	C-N-CA	6.23	126.20	120.03
1	E	1321	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	2009	LEU	CA-C-N	6.21	126.67	120.52
1	A	2009	LEU	C-N-CA	6.21	126.67	120.52
1	C	1250	TYR	N-CA-C	6.21	118.52	109.07
1	B	1058	ASP	CA-CB-CG	6.20	118.80	112.60
1	E	1438	ILE	CA-C-N	6.19	125.87	119.56
1	E	1438	ILE	C-N-CA	6.19	125.87	119.56
1	C	1152	ASN	CA-C-N	6.18	126.09	119.85
1	C	1152	ASN	C-N-CA	6.18	126.09	119.85
1	B	909	THR	CA-C-N	6.18	126.15	120.03
1	B	909	THR	C-N-CA	6.18	126.15	120.03
1	D	1983	LEU	CA-C-N	6.18	126.14	120.03
1	D	1983	LEU	C-N-CA	6.18	126.14	120.03
1	C	1046	ASP	CA-C-N	6.17	125.87	119.82
1	C	1046	ASP	C-N-CA	6.17	125.87	119.82
1	D	1046	ASP	CA-C-N	6.17	125.85	119.56
1	D	1046	ASP	C-N-CA	6.17	125.85	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	664	THR	CA-C-N	6.16	126.35	119.32
1	B	664	THR	C-N-CA	6.16	126.35	119.32
1	C	719	GLN	CA-C-N	6.16	126.13	120.03
1	C	719	GLN	C-N-CA	6.16	126.13	120.03
1	C	1484	SER	N-CA-C	6.15	116.20	108.45
1	B	215	ASP	CA-C-N	6.13	125.81	119.56
1	B	215	ASP	C-N-CA	6.13	125.81	119.56
1	B	1648	PRO	CA-C-N	6.12	126.03	119.85
1	B	1648	PRO	C-N-CA	6.12	126.03	119.85
1	E	1405	TYR	CA-C-N	6.12	126.62	120.14
1	E	1405	TYR	C-N-CA	6.12	126.62	120.14
1	C	1335	GLY	N-CA-C	-6.11	103.24	112.41
1	D	2402	TYR	CA-C-N	6.11	126.02	119.85
1	D	2402	TYR	C-N-CA	6.11	126.02	119.85
2	F	797	ALA	CA-C-N	6.11	125.73	119.56
2	F	797	ALA	C-N-CA	6.11	125.73	119.56
1	E	1335	GLY	N-CA-C	-6.11	103.25	112.41
1	A	1241	GLY	N-CA-C	-6.11	104.26	112.14
1	C	966	ASP	CA-CB-CG	6.10	118.70	112.60
1	D	1494	SER	CA-C-N	6.09	125.78	119.56
1	D	1494	SER	C-N-CA	6.09	125.78	119.56
1	A	1484	SER	N-CA-C	6.09	116.12	108.45
1	B	873	SER	N-CA-C	-6.09	104.72	111.36
1	E	664	THR	CA-C-N	6.09	126.26	119.32
1	E	664	THR	C-N-CA	6.09	126.26	119.32
1	A	1648	PRO	CA-C-N	6.07	125.98	119.85
1	A	1648	PRO	C-N-CA	6.07	125.98	119.85
1	D	2417	VAL	N-CA-C	6.07	116.61	108.11
2	F	848	VAL	N-CA-C	6.07	113.85	108.63
1	C	1764	ASN	CA-CB-CG	-6.05	106.55	112.60
2	F	364	PRO	CA-C-N	6.05	125.96	119.85
2	F	364	PRO	C-N-CA	6.05	125.96	119.85
1	D	1241	GLY	N-CA-C	-6.04	104.34	112.14
1	C	1896	LEU	CA-C-N	6.04	126.01	120.03
1	C	1896	LEU	C-N-CA	6.04	126.01	120.03
1	E	501	ALA	CA-C-N	6.04	126.01	120.03
1	E	501	ALA	C-N-CA	6.04	126.01	120.03
1	E	1988	THR	CA-C-N	6.04	126.00	119.78
1	E	1988	THR	C-N-CA	6.04	126.00	119.78
1	E	1295	ASP	CA-CB-CG	6.04	118.64	112.60
2	F	1207	ILE	CB-CA-C	-6.03	104.39	111.09
1	A	1321	ASP	CA-CB-CG	6.03	118.63	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	511	GLN	CA-C-N	6.03	126.00	120.03
1	E	511	GLN	C-N-CA	6.03	126.00	120.03
2	F	1829	MET	CA-C-N	6.01	125.98	120.03
2	F	1829	MET	C-N-CA	6.01	125.98	120.03
1	D	1058	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	1871	LEU	N-CA-C	6.00	119.92	112.24
1	A	1972	HIS	CA-CB-CG	-6.00	107.80	113.80
1	E	860	PRO	N-CA-C	-6.00	103.39	110.70
1	C	2486	PHE	CA-C-N	5.99	125.96	120.03
1	C	2486	PHE	C-N-CA	5.99	125.96	120.03
1	E	2293	LYS	CA-C-N	5.99	125.95	119.78
1	E	2293	LYS	C-N-CA	5.99	125.95	119.78
1	C	664	THR	CA-C-N	5.99	126.15	119.32
1	C	664	THR	C-N-CA	5.99	126.15	119.32
2	F	1538	ASP	CA-C-N	5.98	126.40	119.47
2	F	1538	ASP	C-N-CA	5.98	126.40	119.47
1	D	1483	VAL	N-CA-C	5.98	116.47	107.80
1	A	719	GLN	CA-C-N	5.96	125.93	120.03
1	A	719	GLN	C-N-CA	5.96	125.93	120.03
1	C	782	LYS	CA-C-N	5.96	126.07	119.87
1	C	782	LYS	C-N-CA	5.96	126.07	119.87
1	C	1648	PRO	CA-C-N	5.95	125.86	119.85
1	C	1648	PRO	C-N-CA	5.95	125.86	119.85
1	E	1648	PRO	CA-C-N	5.95	125.86	119.85
1	E	1648	PRO	C-N-CA	5.95	125.86	119.85
2	F	66	SER	CA-C-N	5.95	125.65	119.82
2	F	66	SER	C-N-CA	5.95	125.65	119.82
1	E	346	PHE	CA-C-N	5.95	127.27	119.84
1	E	346	PHE	C-N-CA	5.95	127.27	119.84
2	F	606	ASN	CA-C-N	5.93	127.25	119.84
2	F	606	ASN	C-N-CA	5.93	127.25	119.84
1	A	1494	SER	CA-C-N	5.92	126.03	119.87
1	A	1494	SER	C-N-CA	5.92	126.03	119.87
1	A	453	SER	CA-C-N	5.92	125.60	119.56
1	A	453	SER	C-N-CA	5.92	125.60	119.56
1	E	215	ASP	CA-C-N	5.92	125.60	119.56
1	E	215	ASP	C-N-CA	5.92	125.60	119.56
1	B	1903	SER	N-CA-C	5.91	117.54	110.44
1	C	570	ASP	N-CA-C	5.90	117.08	107.23
1	D	419	TRP	N-CA-C	5.90	117.21	108.60
1	C	1231	ALA	CA-C-N	5.89	125.86	120.03
1	C	1231	ALA	C-N-CA	5.89	125.86	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	782	LYS	CA-C-N	5.89	125.99	119.87
1	B	782	LYS	C-N-CA	5.89	125.99	119.87
1	E	1714	SER	CA-C-N	5.89	125.99	119.87
1	E	1714	SER	C-N-CA	5.89	125.99	119.87
1	C	2009	LEU	CA-C-N	5.88	125.85	120.03
1	C	2009	LEU	C-N-CA	5.88	125.85	120.03
1	A	1824	ASP	CA-CB-CG	5.87	118.47	112.60
1	D	1904	ASP	CA-C-N	5.87	125.78	119.85
1	D	1904	ASP	C-N-CA	5.87	125.78	119.85
1	C	1634	GLU	CA-C-N	5.86	125.81	119.78
1	C	1634	GLU	C-N-CA	5.86	125.81	119.78
2	F	1109	THR	N-CA-C	5.86	116.82	108.74
2	F	250	ALA	CA-C-N	5.84	126.33	120.14
2	F	250	ALA	C-N-CA	5.84	126.33	120.14
1	C	1829	SER	N-CA-C	-5.84	107.39	114.75
1	E	2402	TYR	CA-C-N	5.84	125.86	119.90
1	E	2402	TYR	C-N-CA	5.84	125.86	119.90
1	B	2349	GLY	CA-C-N	5.83	125.79	119.78
1	B	2349	GLY	C-N-CA	5.83	125.79	119.78
1	C	1299	VAL	N-CA-C	5.83	115.52	108.06
2	F	1165	GLN	N-CA-C	5.81	119.26	111.24
1	A	1405	TYR	CA-C-N	5.81	125.72	119.85
1	A	1405	TYR	C-N-CA	5.81	125.72	119.85
1	D	1499	GLN	N-CA-C	5.81	118.01	109.24
1	D	1634	GLU	CA-C-N	5.80	125.76	119.78
1	D	1634	GLU	C-N-CA	5.80	125.76	119.78
1	C	1988	THR	CA-C-N	5.79	125.76	120.03
1	C	1988	THR	C-N-CA	5.79	125.76	120.03
1	D	511	GLN	CA-C-N	5.78	125.76	120.03
1	D	511	GLN	C-N-CA	5.78	125.76	120.03
1	E	1675	ILE	N-CA-C	5.78	116.52	108.89
1	D	1896	LEU	CA-C-N	5.78	125.69	119.85
1	D	1896	LEU	C-N-CA	5.78	125.69	119.85
1	E	2486	PHE	CA-C-N	5.78	125.73	119.78
1	E	2486	PHE	C-N-CA	5.78	125.73	119.78
1	D	1405	TYR	CA-C-N	5.77	125.68	119.85
1	D	1405	TYR	C-N-CA	5.77	125.68	119.85
1	B	2293	LYS	CA-C-N	5.76	125.74	120.03
1	B	2293	LYS	C-N-CA	5.76	125.74	120.03
1	D	2335	VAL	N-CA-C	5.76	116.17	107.75
1	A	1722	GLY	CA-C-N	5.75	125.70	119.78
1	A	1722	GLY	C-N-CA	5.75	125.70	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2487	PRO	N-CA-C	5.73	122.12	113.81
1	C	1489	ILE	N-CA-C	5.72	116.09	107.80
1	B	1241	GLY	N-CA-C	-5.71	104.77	112.14
1	A	2374	ASN	N-CA-C	5.71	116.09	108.38
2	F	927	ASP	CA-C-N	5.71	125.90	120.31
2	F	927	ASP	C-N-CA	5.71	125.90	120.31
1	A	2491	MET	CA-C-N	5.70	125.80	119.87
1	A	2491	MET	C-N-CA	5.70	125.80	119.87
1	E	1485	GLY	CA-C-N	5.69	126.95	119.84
1	E	1485	GLY	C-N-CA	5.69	126.95	119.84
1	C	1759	ASP	N-CA-C	5.68	117.91	108.20
1	A	1067	SER	N-CA-C	5.67	117.55	111.36
1	B	1991	ASP	CA-C-N	5.67	125.65	120.03
1	B	1991	ASP	C-N-CA	5.67	125.65	120.03
1	D	501	ALA	CA-C-N	5.67	125.65	120.03
1	D	501	ALA	C-N-CA	5.67	125.65	120.03
2	F	1260	MET	CA-C-N	5.67	125.62	119.78
2	F	1260	MET	C-N-CA	5.67	125.62	119.78
1	D	719	GLN	CA-C-N	5.67	125.64	120.03
1	D	719	GLN	C-N-CA	5.67	125.64	120.03
1	D	1648	PRO	CA-C-N	5.66	125.57	119.85
1	D	1648	PRO	C-N-CA	5.66	125.57	119.85
1	A	193	ARG	CA-C-N	5.65	126.91	119.84
1	A	193	ARG	C-N-CA	5.65	126.91	119.84
1	B	1972	HIS	CA-CB-CG	-5.65	108.15	113.80
1	B	1764	ASN	CA-CB-CG	-5.65	106.95	112.60
1	D	71	ASN	CA-C-N	5.65	126.90	119.84
1	D	71	ASN	C-N-CA	5.65	126.90	119.84
2	F	98	GLY	CA-C-N	5.65	125.49	119.28
2	F	98	GLY	C-N-CA	5.65	125.49	119.28
1	C	2452	HIS	N-CA-C	-5.64	104.61	112.45
1	B	501	ALA	CA-C-N	5.64	125.61	120.03
1	B	501	ALA	C-N-CA	5.64	125.61	120.03
1	D	1113	LEU	N-CA-C	5.63	118.28	108.76
1	A	1983	LEU	CA-C-N	5.63	125.61	120.03
1	A	1983	LEU	C-N-CA	5.63	125.61	120.03
1	E	147	SER	N-CA-C	5.63	119.88	112.89
2	F	1332	ASP	CB-CA-C	-5.63	110.06	116.54
1	B	1900	THR	N-CA-C	5.63	117.62	109.07
1	D	1871	LEU	N-CA-C	5.62	119.19	111.54
2	F	147	LYS	N-CA-C	-5.61	105.16	112.23
2	F	1224	SER	CA-C-N	5.61	125.72	119.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1224	SER	C-N-CA	5.61	125.72	119.32
1	B	1716	SER	N-CA-C	5.61	117.62	108.76
1	E	1702	ASP	N-CA-C	-5.61	101.67	110.36
2	F	1013	ILE	N-CA-C	5.60	116.19	108.12
1	C	215	ASP	CA-C-N	5.59	125.96	119.47
1	C	215	ASP	C-N-CA	5.59	125.96	119.47
1	D	1756	GLU	CA-C-N	5.59	125.52	119.76
1	D	1756	GLU	C-N-CA	5.59	125.52	119.76
1	B	1405	TYR	CA-C-N	5.58	125.49	119.85
1	B	1405	TYR	C-N-CA	5.58	125.49	119.85
1	C	1361	HIS	CA-CB-CG	5.58	119.38	113.80
2	F	471	LEU	CB-CA-C	-5.57	103.81	111.73
2	F	569	HIS	CA-CB-CG	-5.55	108.25	113.80
1	C	366	SER	N-CA-C	-5.55	105.23	112.23
1	B	1871	LEU	N-CA-C	5.55	119.63	112.86
1	E	1250	TYR	N-CA-C	5.55	117.50	109.07
2	F	2145	ARG	CA-C-N	5.55	130.01	122.19
2	F	2145	ARG	C-N-CA	5.55	130.01	122.19
1	B	142	ARG	CA-C-N	5.54	125.15	119.56
1	B	142	ARG	C-N-CA	5.54	125.15	119.56
2	F	50	GLY	N-CA-C	-5.54	106.89	114.64
1	E	1499	GLN	N-CA-C	5.53	118.24	109.50
1	E	2374	ASN	N-CA-C	5.53	116.67	108.60
1	D	1988	THR	CA-C-N	5.53	125.47	119.78
1	D	1988	THR	C-N-CA	5.53	125.47	119.78
1	E	1058	ASP	CA-CB-CG	5.53	118.13	112.60
1	B	250	ILE	CB-CA-C	-5.53	104.78	112.02
1	E	1991	ASP	CA-C-N	5.53	125.47	119.78
1	E	1991	ASP	C-N-CA	5.53	125.47	119.78
1	B	1745	GLU	N-CA-C	-5.52	104.90	111.69
1	D	1485	GLY	CA-C-N	5.50	126.71	119.84
1	D	1485	GLY	C-N-CA	5.50	126.71	119.84
1	C	464	VAL	N-CA-C	5.49	116.27	110.72
1	D	239	ILE	N-CA-C	-5.49	105.01	111.00
1	C	1494	SER	CA-C-N	5.49	125.58	119.87
1	C	1494	SER	C-N-CA	5.49	125.58	119.87
1	E	142	ARG	CA-C-N	5.49	125.16	119.56
1	E	142	ARG	C-N-CA	5.49	125.16	119.56
1	C	860	PRO	N-CA-C	-5.49	104.00	110.70
2	F	1494	VAL	N-CA-C	5.48	115.79	108.11
2	F	885	VAL	CA-C-N	5.48	125.46	120.03
2	F	885	VAL	C-N-CA	5.48	125.46	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1320	PRO	CA-C-N	5.48	125.40	119.76
2	F	1320	PRO	C-N-CA	5.48	125.40	119.76
1	A	501	ALA	CA-C-N	5.47	125.44	120.03
1	A	501	ALA	C-N-CA	5.47	125.44	120.03
2	F	875	TYR	N-CA-CB	-5.47	102.12	110.65
1	C	1265	GLN	CA-C-N	-5.47	117.30	122.17
1	C	1265	GLN	C-N-CA	-5.47	117.30	122.17
1	C	1756	GLU	CA-C-N	5.47	125.41	119.78
1	C	1756	GLU	C-N-CA	5.47	125.41	119.78
1	E	1759	ASP	N-CA-C	5.47	117.21	108.41
1	A	1040	TYR	CA-C-N	5.46	125.81	119.47
1	A	1040	TYR	C-N-CA	5.46	125.81	119.47
1	E	2331	VAL	N-CA-C	5.46	115.76	108.11
1	D	184	LYS	N-CA-C	-5.46	105.35	112.23
1	A	201	HIS	CA-CB-CG	5.46	119.26	113.80
2	F	449	SER	N-CA-C	5.46	119.20	112.54
1	B	1270	PHE	CA-CB-CG	-5.45	108.35	113.80
1	E	1255	THR	N-CA-C	5.45	117.47	109.24
2	F	2078	TYR	CA-C-N	5.45	125.79	119.47
2	F	2078	TYR	C-N-CA	5.45	125.79	119.47
1	B	890	ALA	CA-C-N	5.45	125.79	119.47
1	B	890	ALA	C-N-CA	5.45	125.79	119.47
1	A	1312	ILE	CA-C-N	5.44	125.39	119.78
1	A	1312	ILE	C-N-CA	5.44	125.39	119.78
1	C	1313	PRO	N-CA-C	5.44	119.83	112.48
1	D	1540	SER	N-CA-C	-5.44	103.35	110.53
1	B	1265	GLN	CA-C-N	-5.44	117.33	122.17
1	B	1265	GLN	C-N-CA	-5.44	117.33	122.17
1	E	719	GLN	CA-C-N	5.44	125.34	119.85
1	E	719	GLN	C-N-CA	5.44	125.34	119.85
1	E	1634	GLU	CA-C-N	5.44	125.38	119.78
1	E	1634	GLU	C-N-CA	5.44	125.38	119.78
1	E	745	ALA	CB-CA-C	-5.43	110.30	116.54
1	E	1903	SER	N-CA-C	5.42	116.27	107.32
1	B	1484	SER	N-CA-C	5.42	115.28	108.45
1	A	1991	ASP	CA-C-N	5.42	125.39	120.03
1	A	1991	ASP	C-N-CA	5.42	125.39	120.03
1	D	1821	LEU	N-CA-C	-5.41	104.93	112.45
2	F	419	TYR	N-CA-C	5.41	118.00	108.75
2	F	2066	ASP	CA-CB-CG	5.41	118.01	112.60
2	F	602	ALA	N-CA-C	5.40	117.17	111.28
1	E	740	PRO	N-CA-C	-5.40	102.64	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1394	ASN	CA-C-N	5.39	125.01	119.56
1	D	1394	ASN	C-N-CA	5.39	125.01	119.56
1	B	2333	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	B	150	LEU	N-CA-C	-5.39	101.69	110.20
1	E	1692	ILE	CA-C-N	5.39	125.29	119.85
1	E	1692	ILE	C-N-CA	5.39	125.29	119.85
2	F	309	LEU	N-CA-C	5.38	117.58	109.23
1	A	825	PHE	N-CA-C	-5.38	104.29	112.04
1	E	1265	GLN	CA-C-N	-5.36	117.40	122.17
1	E	1265	GLN	C-N-CA	-5.36	117.40	122.17
1	A	224	SER	CA-C-N	5.36	125.03	119.56
1	A	224	SER	C-N-CA	5.36	125.03	119.56
2	F	827	ARG	N-CA-C	5.36	118.55	109.76
1	E	2288	SER	N-CA-C	5.35	119.87	113.23
1	E	405	PRO	N-CA-C	-5.35	102.80	111.14
1	C	1972	HIS	CA-CB-CG	-5.35	108.45	113.80
1	D	2486	PHE	CA-C-N	5.34	125.32	120.03
1	D	2486	PHE	C-N-CA	5.34	125.32	120.03
1	E	1838	ASP	N-CA-C	-5.34	105.13	111.69
2	F	1790	ARG	CA-C-N	5.32	124.99	119.56
2	F	1790	ARG	C-N-CA	5.32	124.99	119.56
1	A	1634	GLU	CA-C-N	5.32	125.22	119.85
1	A	1634	GLU	C-N-CA	5.32	125.22	119.85
1	B	82	ILE	N-CA-C	-5.32	102.65	109.30
1	E	1985	ILE	N-CA-C	5.32	115.51	107.80
2	F	943	GLN	CA-C-N	5.32	126.49	119.84
2	F	943	GLN	C-N-CA	5.32	126.49	119.84
2	F	1329	ASP	CA-CB-CG	-5.32	107.28	112.60
1	D	272	GLU	CA-C-N	5.31	125.63	119.47
1	D	272	GLU	C-N-CA	5.31	125.63	119.47
1	A	197	ALA	CA-C-N	-5.31	116.94	122.89
1	A	197	ALA	C-N-CA	-5.31	116.94	122.89
1	A	707	VAL	N-CA-C	-5.31	105.22	111.00
1	B	1983	LEU	CA-C-N	5.30	125.28	120.03
1	B	1983	LEU	C-N-CA	5.30	125.28	120.03
1	A	337	ASN	N-CA-C	5.30	118.70	111.39
1	A	2349	GLY	CA-C-N	5.29	125.20	119.85
1	A	2349	GLY	C-N-CA	5.29	125.20	119.85
2	F	1014	PHE	CA-CB-CG	5.29	119.09	113.80
1	A	1848	TYR	N-CA-C	-5.29	105.56	112.23
2	F	814	LEU	CA-C-N	5.29	124.96	119.56
2	F	814	LEU	C-N-CA	5.29	124.96	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	SER	CA-C-N	5.28	124.95	119.56
1	B	224	SER	C-N-CA	5.28	124.95	119.56
1	B	1440	GLY	CA-C-N	5.28	127.88	120.28
1	B	1440	GLY	C-N-CA	5.28	127.88	120.28
1	C	1821	LEU	N-CA-C	-5.28	105.20	111.69
1	E	107	GLY	CA-C-N	-5.28	114.79	122.65
1	E	107	GLY	C-N-CA	-5.28	114.79	122.65
1	C	1645	PHE	CA-C-N	-5.28	116.26	123.12
1	C	1645	PHE	C-N-CA	-5.28	116.26	123.12
1	B	1692	ILE	CA-C-N	5.27	125.17	119.85
1	B	1692	ILE	C-N-CA	5.27	125.17	119.85
2	F	646	VAL	CA-C-N	-5.27	115.77	122.77
2	F	646	VAL	C-N-CA	-5.27	115.77	122.77
1	C	1113	LEU	N-CA-C	5.26	117.95	108.48
1	D	224	SER	CA-C-N	5.25	124.92	119.56
1	D	224	SER	C-N-CA	5.25	124.92	119.56
1	A	1362	ASN	CA-CB-CG	-5.25	107.35	112.60
1	A	922	LEU	N-CA-C	5.25	117.08	111.36
1	A	1520	GLN	CA-C-N	5.25	125.19	119.78
1	A	1520	GLN	C-N-CA	5.25	125.19	119.78
1	A	1511	PHE	CA-CB-CG	-5.25	108.55	113.80
2	F	1403	GLN	CA-C-N	5.24	125.14	119.85
2	F	1403	GLN	C-N-CA	5.24	125.14	119.85
1	C	501	ALA	CA-C-N	5.24	125.22	120.03
1	C	501	ALA	C-N-CA	5.24	125.22	120.03
2	F	630	ARG	N-CA-C	5.24	116.80	108.79
1	A	660	ASN	CA-CB-CG	5.24	117.83	112.60
1	C	414	LEU	CA-C-N	5.23	124.90	119.56
1	C	414	LEU	C-N-CA	5.23	124.90	119.56
1	A	2466	ASP	CA-CB-CG	5.23	117.83	112.60
1	E	1907	LEU	N-CA-C	5.23	116.98	111.28
1	B	1148	ASP	CA-CB-CG	-5.22	107.38	112.60
1	C	1040	TYR	CA-C-N	5.22	124.88	119.56
1	C	1040	TYR	C-N-CA	5.22	124.88	119.56
1	D	966	ASP	CA-CB-CG	5.22	117.82	112.60
1	D	2374	ASN	N-CA-C	5.22	116.73	108.96
1	E	183	THR	N-CA-C	-5.22	106.42	112.89
2	F	1917	SER	CA-C-N	5.22	127.27	120.28
2	F	1917	SER	C-N-CA	5.22	127.27	120.28
1	C	1745	GLU	N-CA-C	-5.21	105.28	111.69
1	D	215	ASP	CA-C-N	5.21	124.88	119.56
1	D	215	ASP	C-N-CA	5.21	124.88	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2293	LYS	CA-C-N	5.21	125.19	120.03
1	D	2293	LYS	C-N-CA	5.21	125.19	120.03
2	F	171	PRO	N-CA-C	-5.19	102.86	111.11
1	E	268	PHE	CA-CB-CG	-5.18	108.62	113.80
1	E	1394	ASN	CA-C-N	5.18	125.25	119.87
1	E	1394	ASN	C-N-CA	5.18	125.25	119.87
1	B	329	ARG	NE-CZ-NH2	-5.18	114.54	119.20
1	E	707	VAL	N-CA-C	-5.18	105.36	111.00
2	F	695	LYS	CA-C-N	5.17	125.15	120.03
2	F	695	LYS	C-N-CA	5.17	125.15	120.03
2	F	1232	PRO	CA-C-N	5.17	125.38	120.31
2	F	1232	PRO	C-N-CA	5.17	125.38	120.31
2	F	2072	ILE	N-CA-C	-5.17	106.64	111.45
1	A	303	PHE	N-CA-C	-5.16	106.76	113.16
2	F	2092	THR	N-CA-C	-5.16	105.56	111.14
1	B	1574	VAL	CA-C-N	-5.16	115.88	123.00
1	B	1574	VAL	C-N-CA	-5.16	115.88	123.00
1	B	1499	GLN	N-CA-C	5.16	117.65	109.50
1	C	550	ILE	CB-CA-C	-5.16	105.18	112.14
1	A	1394	ASN	CA-C-N	5.16	124.77	119.56
1	A	1394	ASN	C-N-CA	5.16	124.77	119.56
1	E	1494	SER	CA-C-N	5.16	124.77	119.56
1	E	1494	SER	C-N-CA	5.16	124.77	119.56
1	D	1502	VAL	N-CA-C	5.15	115.27	107.75
2	F	524	LEU	N-CA-C	5.15	117.29	108.90
1	A	142	ARG	CA-C-N	5.14	124.80	119.56
1	A	142	ARG	C-N-CA	5.14	124.80	119.56
2	F	1195	GLN	N-CA-C	5.14	117.62	109.50
1	C	1991	ASP	CA-C-N	5.14	125.07	119.78
1	C	1991	ASP	C-N-CA	5.14	125.07	119.78
1	C	1687	ASN	CA-CB-CG	5.13	117.73	112.60
1	E	1177	ILE	N-CA-C	5.12	115.28	108.11
2	F	80	ARG	N-CA-C	5.12	116.86	109.07
1	C	1870	GLN	N-CA-C	-5.12	106.54	112.89
2	F	2038	GLU	N-CA-C	-5.12	107.16	113.41
2	F	1021	VAL	CA-C-N	5.12	125.05	119.78
2	F	1021	VAL	C-N-CA	5.12	125.05	119.78
1	B	1523	PRO	N-CA-C	5.12	120.34	114.20
1	A	2402	TYR	CA-C-N	5.11	125.04	119.78
1	A	2402	TYR	C-N-CA	5.11	125.04	119.78
1	C	590	ILE	CB-CA-C	-5.11	105.43	111.97
1	A	2486	PHE	CA-C-N	5.11	125.08	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2486	PHE	C-N-CA	5.11	125.08	120.03
2	F	1165	GLN	CB-CA-C	-5.11	104.23	112.09
2	F	1729	ASP	CA-CB-CG	5.11	117.70	112.60
1	B	180	GLU	N-CA-C	5.10	116.84	111.28
1	A	1660	TRP	N-CA-C	5.10	117.83	110.28
1	B	1160	PRO	N-CA-C	-5.09	103.17	111.68
2	F	790	HIS	N-CA-C	5.09	117.55	107.98
1	A	183	THR	N-CA-C	-5.09	106.92	113.23
2	F	393	ILE	N-CA-C	-5.09	106.83	111.67
2	F	1606	LEU	CA-C-N	5.09	124.75	119.56
2	F	1606	LEU	C-N-CA	5.09	124.75	119.56
2	F	770	ALA	N-CA-C	5.09	116.57	108.79
1	E	462	ARG	NE-CZ-NH2	-5.09	114.62	119.20
2	F	87	VAL	CA-C-N	5.09	125.07	120.03
2	F	87	VAL	C-N-CA	5.09	125.07	120.03
1	A	84	ALA	CA-C-N	5.08	124.69	119.56
1	A	84	ALA	C-N-CA	5.08	124.69	119.56
1	B	1177	ILE	N-CA-C	5.08	115.23	108.11
2	F	950	VAL	CB-CA-C	-5.08	104.02	110.98
1	A	973	ILE	N-CA-C	-5.08	100.81	108.12
1	B	243	ILE	N-CA-C	5.07	114.79	106.72
1	E	224	SER	CA-C-N	5.07	124.73	119.56
1	E	224	SER	C-N-CA	5.07	124.73	119.56
1	D	1102	ASN	CA-CB-CG	-5.07	107.53	112.60
2	F	1805	ASP	CA-C-N	5.06	124.72	119.56
2	F	1805	ASP	C-N-CA	5.06	124.72	119.56
1	B	346	PHE	CA-C-N	5.06	126.16	119.84
1	B	346	PHE	C-N-CA	5.06	126.16	119.84
1	B	695	TYR	N-CA-C	-5.06	107.24	113.41
2	F	109	GLN	CA-C-N	5.05	124.95	119.85
2	F	109	GLN	C-N-CA	5.05	124.95	119.85
2	F	1322	HIS	N-CA-C	5.05	115.71	108.74
1	C	1697	VAL	CA-C-N	5.05	125.03	120.03
1	C	1697	VAL	C-N-CA	5.05	125.03	120.03
1	B	1502	VAL	N-CA-C	5.05	115.12	107.75
1	C	1400	ASN	N-CA-C	5.05	115.20	108.38
1	C	1486	PRO	CB-CA-C	-5.05	105.28	111.64
1	E	2491	MET	CA-C-N	5.05	124.71	119.56
1	E	2491	MET	C-N-CA	5.05	124.71	119.56
1	E	108	THR	N-CA-CB	5.04	118.84	110.52
1	B	1250	TYR	N-CA-C	5.04	116.73	109.07
1	B	1336	ASP	CA-CB-CG	5.04	117.64	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	836	SER	CA-C-N	5.04	124.94	119.85
2	F	836	SER	C-N-CA	5.04	124.94	119.85
1	B	184	LYS	N-CA-C	-5.04	105.88	112.23
1	E	1599	GLN	CB-CA-C	-5.04	110.79	116.63
1	D	2424	GLY	CA-C-N	5.04	124.82	119.28
1	D	2424	GLY	C-N-CA	5.04	124.82	119.28
1	D	2391	VAL	N-CA-C	5.03	114.99	108.35
1	E	1312	ILE	CA-C-N	5.03	124.96	119.78
1	E	1312	ILE	C-N-CA	5.03	124.96	119.78
1	C	735	ASN	CA-CB-CG	-5.03	107.57	112.60
1	B	405	PRO	N-CA-C	-5.03	103.29	111.14
2	F	939	ASP	CA-CB-CG	5.03	117.63	112.60
1	C	1194	TYR	N-CA-C	5.03	117.59	109.40
2	F	413	ASP	CA-C-N	-5.03	114.43	121.72
2	F	413	ASP	C-N-CA	-5.03	114.43	121.72
1	C	250	ILE	CB-CA-C	-5.02	105.44	112.02
1	C	1177	ILE	N-CA-C	5.02	115.14	108.11
1	D	2351	PHE	N-CA-C	5.02	116.47	108.79
2	F	634	PHE	CA-C-N	-5.02	114.66	122.09
2	F	634	PHE	C-N-CA	-5.02	114.66	122.09
1	B	419	TRP	N-CA-C	5.02	115.93	108.60
1	A	1988	THR	CA-C-N	5.02	125.00	120.03
1	A	1988	THR	C-N-CA	5.02	125.00	120.03
2	F	261	VAL	N-CA-C	5.01	115.12	108.11
1	B	1988	THR	CA-C-N	5.01	124.94	119.78
1	B	1988	THR	C-N-CA	5.01	124.94	119.78
1	D	1949	LEU	CA-C-N	5.01	124.91	119.85
1	D	1949	LEU	C-N-CA	5.01	124.91	119.85
1	A	1821	LEU	N-CA-C	-5.00	106.34	112.90
1	B	1312	ILE	CA-C-N	5.00	124.94	119.78
1	B	1312	ILE	C-N-CA	5.00	124.94	119.78
1	E	1764	ASN	CA-CB-CG	-5.00	107.59	112.60
1	B	326	LYS	CA-C-N	-5.00	116.50	122.90
1	B	326	LYS	C-N-CA	-5.00	116.50	122.90
1	D	1233	GLY	N-CA-C	-5.00	104.73	111.54
2	F	214	ALA	N-CA-C	5.00	116.73	111.28
1	C	1522	SER	CA-C-N	5.00	125.93	120.83
1	C	1522	SER	C-N-CA	5.00	125.93	120.83

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	19477	0	19046	35	0
1	B	19477	0	19046	39	0
1	C	19477	0	19046	39	0
1	D	19477	0	19046	31	0
1	E	19477	0	19046	42	0
2	F	16918	0	16285	60	0
All	All	114303	0	111515	239	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 (239) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:228:TYR:HH	2:F:301:THR:HG1	1.36	0.70
1:D:92:TYR:OH	1:D:99:ARG:NH1	2.26	0.69
1:D:521:THR:O	1:D:522:PRO:C	2.44	0.61
1:E:521:THR:O	1:E:522:PRO:C	2.44	0.60
1:A:57:LYS:NZ	1:A:1833:ASP:OD1	2.33	0.60
1:E:1868:TYR:OH	1:E:1974:LEU:O	2.19	0.59
1:C:1868:TYR:OH	1:C:1974:LEU:O	2.22	0.58
1:E:1702:ASP:O	1:E:1703:TYR:C	2.46	0.58
1:B:342:ASP:OD1	1:B:360:LYS:NZ	2.38	0.56
2:F:1329:ASP:OD1	2:F:1329:ASP:N	2.30	0.55
1:D:57:LYS:NZ	1:D:1833:ASP:OD1	2.40	0.55
1:A:1868:TYR:OH	1:A:1974:LEU:O	2.24	0.55
2:F:530:ASP:N	2:F:530:ASP:OD1	2.39	0.54
1:C:1011:GLY:O	1:C:1013:ILE:N	2.41	0.54
1:B:1148:ASP:OD1	1:B:1148:ASP:N	2.34	0.54
1:C:2207:ASP:OD2	1:C:2211:LYS:NZ	2.40	0.54
2:F:49:ARG:NH2	2:F:1159:ASN:O	2.41	0.54
1:B:542:SER:O	1:B:548:LYS:NZ	2.41	0.53
1:B:1011:GLY:O	1:B:1013:ILE:N	2.42	0.53
1:C:2244:LYS:NZ	1:C:2246:SER:O	2.42	0.53
1:D:1868:TYR:OH	1:D:1974:LEU:O	2.27	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:TRP:CD1	1:B:748:THR:HG1	2.27	0.52
1:E:309:SER:O	1:E:310:ASN:C	2.53	0.52
2:F:209:ASP:OD1	2:F:302:ARG:NH1	2.43	0.52
2:F:318:ASP:OD1	2:F:1177:LYS:NZ	2.43	0.52
2:F:520:LYS:NZ	2:F:543:ASP:OD1	2.42	0.52
2:F:963:TYR:N	2:F:964:PRO:CD	2.74	0.51
2:F:505:ASP:OD1	2:F:505:ASP:C	2.52	0.51
1:D:2287:ASP:OD1	1:D:2287:ASP:N	2.38	0.51
1:B:682:ASP:OD2	1:B:685:LYS:NZ	2.39	0.51
1:D:1868:TYR:C	1:D:1868:TYR:CD2	2.88	0.51
2:F:1795:LYS:NZ	2:F:1818:GLU:OE1	2.43	0.51
2:F:153:ASP:O	2:F:174:ARG:NH2	2.44	0.50
2:F:1837:ASP:OD1	2:F:1837:ASP:C	2.54	0.50
1:E:42:TRP:N	1:E:1552:ASP:OD2	2.45	0.50
1:A:1514:ASP:OD2	1:A:1515:LYS:NZ	2.42	0.50
1:A:2401:ASP:OD1	1:E:2496:LYS:NZ	2.40	0.50
2:F:1687:ASP:OD1	2:F:1687:ASP:N	2.39	0.50
1:C:1514:ASP:OD2	1:C:1515:LYS:NZ	2.42	0.49
1:E:1514:ASP:OD2	1:E:1515:LYS:NZ	2.42	0.49
2:F:385:ASP:OD1	2:F:385:ASP:N	2.38	0.49
1:A:42:TRP:N	1:A:1552:ASP:OD2	2.46	0.49
1:D:1507:LYS:NZ	1:D:1538:ASP:OD2	2.41	0.48
1:A:432:ASN:O	1:A:434:TYR:N	2.46	0.48
1:B:42:TRP:N	1:B:1552:ASP:OD2	2.47	0.48
2:F:1931:ASP:OD1	2:F:1931:ASP:C	2.55	0.48
1:A:1432:SER:OG	1:A:1433:LYS:N	2.45	0.48
1:E:1774:TYR:HH	1:E:1848:TYR:HH	1.53	0.48
1:A:1431:PRO:O	1:A:1477:LYS:NZ	2.44	0.48
1:D:271:ILE:O	1:D:272:GLU:HB3	2.14	0.48
1:E:1912:ASP:OD1	1:E:1913:ILE:N	2.46	0.48
2:F:2129:SER:OG	2:F:2130:ALA:N	2.46	0.48
1:D:42:TRP:N	1:D:1552:ASP:OD2	2.47	0.48
1:B:575:ASP:OD1	1:B:576:GLY:N	2.47	0.47
2:F:777:GLU:OE2	2:F:866:LYS:NZ	2.47	0.47
1:D:510:ASN:OD1	1:D:510:ASN:N	2.46	0.47
1:E:2029:MET:HG3	1:E:2272:ARG:HG3	1.97	0.47
2:F:926:SER:OG	2:F:927:ASP:N	2.47	0.47
2:F:171:PRO:O	2:F:172:GLN:HB2	2.15	0.47
1:A:1484:SER:OG	1:A:1485:GLY:N	2.48	0.47
1:A:1827:TRP:CE3	1:A:1842:GLN:HG3	2.50	0.47
1:C:1868:TYR:C	1:C:1868:TYR:CD2	2.92	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:326:GLY:N	2:F:327:PRO:HD2	2.29	0.47
2:F:1272:ALA:O	2:F:1273:GLU:C	2.56	0.47
1:C:133:ASP:OD1	1:C:133:ASP:N	2.45	0.47
1:E:1657:ASP:OD1	1:E:1657:ASP:N	2.48	0.47
1:A:2468:LYS:NZ	1:B:2325:ASP:OD2	2.45	0.47
1:C:1311:GLU:HB3	1:C:1575:THR:HB	1.96	0.47
2:F:283:TRP:CE3	2:F:303:ARG:HB3	2.50	0.47
1:A:1868:TYR:CD2	1:A:1868:TYR:C	2.92	0.47
1:B:1272:ASP:OD1	1:B:1272:ASP:N	2.45	0.46
1:B:2386:SER:HG	1:B:2485:SER:HG	1.55	0.46
1:D:2380:GLY:N	1:D:2383:THR:OG1	2.47	0.46
1:C:928:SER:OG	1:C:929:GLN:N	2.48	0.46
1:D:1428:THR:OG1	1:D:1429:THR:N	2.47	0.46
1:E:1399:SER:OG	1:E:1400:ASN:N	2.44	0.46
2:F:1288:ASP:OD1	2:F:1288:ASP:N	2.46	0.46
1:C:1890:LEU:HB3	1:C:1960:TRP:CH2	2.51	0.46
1:D:928:SER:OG	1:D:929:GLN:N	2.48	0.46
2:F:1805:ASP:HB2	2:F:1806:PRO:HD2	1.96	0.46
1:A:2380:GLY:N	1:A:2383:THR:OG1	2.47	0.46
2:F:1461:ASP:C	2:F:1461:ASP:OD1	2.59	0.46
1:C:439:LYS:NZ	1:C:469:ASP:OD1	2.49	0.46
1:A:1148:ASP:N	1:A:1148:ASP:OD1	2.35	0.46
2:F:212:CYS:O	2:F:213:GLU:CB	2.63	0.46
2:F:1055:THR:OG1	2:F:1056:ASP:N	2.49	0.46
2:F:1819:ALA:O	2:F:1820:THR:CB	2.63	0.46
2:F:1909:ASN:N	2:F:1909:ASN:OD1	2.48	0.46
1:B:1115:GLU:OE2	1:B:1611:ARG:NH2	2.48	0.46
1:E:1168:TYR:CD2	1:E:1202:HIS:HB3	2.51	0.46
2:F:279:THR:OG1	2:F:280:THR:N	2.48	0.45
2:F:480:ASP:OD1	2:F:480:ASP:N	2.44	0.45
1:B:1670:ASP:OD1	1:B:1670:ASP:C	2.59	0.45
1:E:792:ALA:O	1:E:793:ALA:C	2.59	0.45
1:C:1670:ASP:OD1	1:C:1670:ASP:C	2.59	0.45
1:E:130:HIS:HD1	1:E:996:TYR:HH	1.64	0.45
1:E:1872:GLU:O	1:E:1873:ARG:C	2.59	0.45
1:E:1908:ASP:N	1:E:1908:ASP:OD1	2.47	0.45
1:C:302:ASN:N	1:C:302:ASN:OD1	2.46	0.45
1:C:545:ASP:OD1	1:C:545:ASP:C	2.59	0.45
2:F:1975:SER:OG	2:F:1976:GLY:N	2.50	0.45
1:B:1484:SER:OG	1:B:1485:GLY:N	2.50	0.45
1:B:1021:TRP:O	1:B:1026:LYS:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:THR:OG1	1:D:456:ILE:N	2.50	0.45
1:E:2228:LYS:NZ	1:E:2232:GLU:OE2	2.48	0.45
2:F:1552:LYS:NZ	2:F:1569:GLU:OE2	2.40	0.45
1:A:1908:ASP:N	1:A:1908:ASP:OD1	2.49	0.45
1:C:1104:ASP:OD1	1:C:1104:ASP:N	2.42	0.45
1:A:1729:ASP:OD1	1:A:1729:ASP:N	2.50	0.44
1:E:2082:LYS:NZ	1:E:2086:GLU:OE2	2.48	0.44
2:F:1367:ARG:NH1	2:F:1411:ARG:O	2.50	0.44
2:F:1882:ASP:OD1	2:F:1882:ASP:C	2.60	0.44
1:A:1728:ASP:OD1	1:A:1728:ASP:C	2.59	0.44
1:E:1868:TYR:C	1:E:1868:TYR:CD2	2.94	0.44
2:F:1740:THR:OG1	2:F:1744:GLN:O	2.36	0.44
1:E:2365:SER:OG	1:E:2366:GLY:N	2.50	0.44
2:F:1133:THR:OG1	2:F:1134:ALA:N	2.49	0.44
2:F:1190:ASP:OD1	2:F:1190:ASP:C	2.61	0.44
1:C:1484:SER:OG	1:C:1485:GLY:N	2.49	0.44
1:B:1890:LEU:HB3	1:B:1960:TRP:CH2	2.53	0.44
1:C:1314:SER:OG	1:C:1315:SER:N	2.51	0.44
1:A:1168:TYR:CD2	1:A:1202:HIS:HB3	2.53	0.44
1:B:1815:GLN:N	1:B:1815:GLN:OE1	2.51	0.44
1:E:193:ARG:N	1:E:194:PRO:CD	2.81	0.44
2:F:733:GLN:O	2:F:734:THR:C	2.61	0.44
1:A:1729:ASP:OD2	1:A:1730:LYS:NZ	2.42	0.44
1:D:831:THR:OG1	1:D:832:ALA:N	2.51	0.44
1:D:1484:SER:OG	1:D:1485:GLY:N	2.50	0.44
1:A:193:ARG:N	1:A:194:PRO:CD	2.81	0.43
1:A:342:ASP:OD2	1:A:360:LYS:NZ	2.52	0.43
1:A:1124:ARG:HD2	1:A:1144:TRP:CE2	2.53	0.43
1:B:831:THR:OG1	1:B:832:ALA:N	2.51	0.43
1:B:1728:ASP:OD1	1:B:1728:ASP:C	2.61	0.43
1:C:309:SER:O	1:C:310:ASN:HB2	2.18	0.43
1:C:1313:PRO:O	1:C:1315:SER:N	2.51	0.43
2:F:1549:ASN:N	2:F:1549:ASN:OD1	2.49	0.43
1:E:983:THR:OG1	1:E:984:THR:N	2.51	0.43
1:A:2496:LYS:NZ	1:B:2401:ASP:OD1	2.47	0.43
1:B:521:THR:N	1:B:522:PRO:CD	2.81	0.43
2:F:963:TYR:N	2:F:964:PRO:HD3	2.33	0.43
1:B:975:ASN:OD1	1:B:975:ASN:N	2.40	0.43
1:C:1903:SER:O	1:C:1904:ASP:C	2.61	0.43
1:C:2382:ASP:OD2	1:D:2404:ALA:N	2.51	0.43
1:E:2380:GLY:N	1:E:2383:THR:OG1	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:963:TYR:N	2:F:963:TYR:CD2	2.85	0.43
1:B:309:SER:O	1:B:310:ASN:C	2.60	0.43
1:B:1168:TYR:CD2	1:B:1202:HIS:HB3	2.53	0.43
1:E:1895:TYR:CG	1:E:1896:LEU:N	2.86	0.43
2:F:954:ARG:NH1	2:F:975:SER:O	2.50	0.43
2:F:2114:TYR:O	2:F:2115:GLY:C	2.56	0.43
2:F:1109:THR:OG1	2:F:1110:ASN:N	2.50	0.43
1:C:2496:LYS:NZ	1:D:2401:ASP:OD1	2.41	0.43
1:B:2330:GLU:OE2	1:B:2413:LYS:NZ	2.49	0.43
1:D:575:ASP:OD2	1:D:577:LYS:NZ	2.42	0.43
1:B:545:ASP:OD1	1:B:545:ASP:C	2.61	0.42
1:D:542:SER:O	1:D:548:LYS:NZ	2.52	0.42
2:F:2118:TYR:CD1	2:F:2118:TYR:N	2.86	0.42
1:D:1872:GLU:O	1:D:1873:ARG:C	2.62	0.42
1:E:1890:LEU:HB3	1:E:1960:TRP:CH2	2.55	0.42
1:A:1890:LEU:HB3	1:A:1960:TRP:CH2	2.54	0.42
1:C:2380:GLY:N	1:C:2383:THR:OG1	2.52	0.42
1:D:277:ALA:O	1:D:278:MET:C	2.62	0.42
1:A:439:LYS:NZ	1:A:469:ASP:OD1	2.52	0.42
1:E:439:LYS:NZ	1:E:469:ASP:OD1	2.51	0.42
2:F:1496:VAL:HB	2:F:1505:ARG:HB2	2.02	0.42
1:A:1175:LYS:NZ	1:A:1197:GLU:OE2	2.45	0.42
1:B:510:ASN:OD1	1:B:510:ASN:N	2.51	0.42
1:E:1507:LYS:NZ	1:E:1538:ASP:OD2	2.50	0.42
2:F:1698:ASP:OD1	2:F:1698:ASP:N	2.43	0.42
1:B:983:THR:OG1	1:B:984:THR:N	2.51	0.42
1:B:2082:LYS:NZ	1:B:2086:GLU:OE2	2.48	0.42
2:F:1692:TRP:CD1	2:F:1692:TRP:N	2.86	0.42
2:F:417:TRP:H	2:F:444:ILE:CD1	2.32	0.42
1:C:1507:LYS:NZ	1:C:1538:ASP:OD2	2.52	0.42
1:E:1272:ASP:OD1	1:E:1272:ASP:N	2.45	0.42
2:F:1560:ASP:C	2:F:1560:ASP:OD1	2.62	0.42
1:C:1752:ASN:OD1	1:C:1752:ASN:N	2.50	0.41
1:D:1098:HIS:NE2	1:D:1105:GLN:O	2.53	0.41
1:A:1670:ASP:OD1	1:A:1670:ASP:C	2.63	0.41
1:D:1022:ASP:OD2	1:E:1797:LYS:NZ	2.47	0.41
1:D:1168:TYR:CD2	1:D:1202:HIS:HB3	2.55	0.41
1:E:2143:ASN:OD1	1:E:2143:ASN:N	2.49	0.41
1:A:545:ASP:OD1	1:A:545:ASP:C	2.61	0.41
1:C:1124:ARG:HD2	1:C:1144:TRP:CE2	2.55	0.41
1:B:1394:ASN:HA	1:B:1395:PRO:HD3	1.91	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1298:ASN:OD1	1:C:1298:ASN:N	2.49	0.41
1:D:1272:ASP:OD1	1:D:1272:ASP:N	2.47	0.41
1:E:692:MET:O	1:E:693:ALA:C	2.63	0.41
1:E:1484:SER:OG	1:E:1485:GLY:N	2.54	0.41
1:E:2308:GLU:OE1	1:E:2308:GLU:N	2.50	0.41
2:F:2117:ARG:HG2	2:F:2126:TRP:CE3	2.55	0.41
1:B:1872:GLU:O	1:B:1873:ARG:C	2.59	0.41
1:A:1657:ASP:OD1	1:A:1657:ASP:N	2.44	0.41
1:A:2129:GLN:NE2	1:C:1120:GLU:OE2	2.54	0.41
1:C:86:ASN:O	1:C:87:ALA:C	2.62	0.41
1:C:398:ASN:O	1:C:399:THR:C	2.64	0.41
1:E:432:ASN:O	1:E:433:GLN:C	2.63	0.41
1:E:1703:TYR:HB3	1:E:1724:HIS:HB3	2.02	0.41
1:B:64:ALA:O	1:B:65:ARG:C	2.64	0.41
1:D:983:THR:OG1	1:D:984:THR:N	2.53	0.41
2:F:1144:SER:OG	2:F:1149:THR:OG1	2.32	0.41
1:A:831:THR:OG1	1:A:832:ALA:N	2.54	0.41
1:B:593:LEU:O	1:B:594:LEU:C	2.63	0.41
1:C:1022:ASP:OD1	1:C:1022:ASP:N	2.46	0.41
1:C:1103:ASN:ND2	1:C:1582:ASN:O	2.54	0.41
1:C:1291:TYR:CD1	1:C:1291:TYR:C	2.99	0.41
1:C:1657:ASP:OD1	1:C:1657:ASP:N	2.47	0.41
1:C:1827:TRP:O	1:C:1827:TRP:CG	2.74	0.41
1:C:2082:LYS:NZ	1:C:2086:GLU:OE2	2.49	0.41
1:D:1670:ASP:OD1	1:D:1670:ASP:C	2.64	0.41
1:E:575:ASP:OD2	1:E:577:LYS:NZ	2.41	0.41
2:F:1334:ASP:OD1	2:F:1334:ASP:C	2.63	0.41
2:F:1347:ASP:OD1	2:F:1347:ASP:C	2.63	0.41
1:B:660:ASN:O	1:B:757:GLN:NE2	2.52	0.41
2:F:643:ALA:O	2:F:644:GLU:C	2.64	0.41
1:A:859:LEU:HB3	1:A:860:PRO:CD	2.51	0.40
1:B:308:TYR:CD1	1:B:308:TYR:C	2.99	0.40
1:E:538:LEU:O	1:E:539:ASN:C	2.64	0.40
1:A:975:ASN:OD1	1:A:975:ASN:N	2.41	0.40
1:C:193:ARG:N	1:C:194:PRO:CD	2.84	0.40
1:C:1533:ASN:O	1:C:1534:ALA:C	2.64	0.40
1:C:2287:ASP:N	1:C:2287:ASP:OD1	2.39	0.40
1:D:682:ASP:OD2	1:D:685:LYS:NZ	2.43	0.40
1:E:398:ASN:O	1:E:399:THR:C	2.63	0.40
2:F:929:GLN:HG2	2:F:1455:TRP:CZ2	2.56	0.40
1:B:1398:SER:OG	1:B:1400:ASN:O	2.38	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:571:HIS:ND1	1:D:618:ASN:OD1	2.55	0.40
1:E:831:THR:OG1	1:E:832:ALA:N	2.54	0.40
1:B:63:GLU:OE2	1:B:99:ARG:NH1	2.55	0.40
1:B:1830:ASP:OD1	1:B:1830:ASP:C	2.62	0.40
1:D:1830:ASP:OD1	1:D:1830:ASP:C	2.63	0.40
1:E:1827:TRP:O	1:E:1827:TRP:CG	2.74	0.40
2:F:729:LEU:O	2:F:730:THR:HB	2.21	0.40
1:A:447:SER:O	1:A:451:GLU:N	2.55	0.40
1:A:2382:ASP:OD1	1:A:2382:ASP:N	2.48	0.40
1:B:1022:ASP:N	1:B:1022:ASP:OD1	2.50	0.40
1:E:1651:ASN:O	1:E:1652:LEU:C	2.64	0.40
2:F:1153:THR:OG1	2:F:1154:LEU:N	2.53	0.40
2:F:2158:MET:N	2:F:2159:PRO:CD	2.84	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	2448/2516 (97%)	2401 (98%)	45 (2%)	2 (0%)	48	78
1	B	2448/2516 (97%)	2410 (98%)	32 (1%)	6 (0%)	43	71
1	C	2448/2516 (97%)	2413 (99%)	30 (1%)	5 (0%)	43	71
1	D	2448/2516 (97%)	2408 (98%)	34 (1%)	6 (0%)	43	71
1	E	2448/2516 (97%)	2407 (98%)	38 (2%)	3 (0%)	48	78
2	F	2114/2434 (87%)	2046 (97%)	58 (3%)	10 (0%)	24	56
All	All	14354/15014 (96%)	14085 (98%)	237 (2%)	32 (0%)	44	71

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	GLN
1	C	1314	SER
1	D	522	PRO
1	E	522	PRO
2	F	680	PRO
2	F	908	VAL
2	F	1820	THR
1	B	970	TYR
1	E	1703	TYR
2	F	172	GLN
2	F	319	SER
1	B	1024	TYR
1	C	1012	VAL
1	C	1024	TYR
1	D	1024	TYR
2	F	213	GLU
1	A	970	TYR
1	B	195	SER
1	B	1012	VAL
1	B	2106	ASN
1	D	272	GLU
1	D	1440	GLY
1	D	2106	ASN
1	E	1024	TYR
2	F	136	SER
2	F	1208	THR
2	F	1678	ASP
1	B	339	TYR
1	C	970	TYR
1	C	1904	ASP
1	D	195	SER
2	F	963	TYR

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	2100/2157 (97%)	2100 (100%)	0	100	100
1	B	2100/2157 (97%)	2100 (100%)	0	100	100
1	C	2100/2157 (97%)	2100 (100%)	0	100	100
1	D	2100/2157 (97%)	2100 (100%)	0	100	100
1	E	2100/2157 (97%)	2100 (100%)	0	100	100
2	F	1831/2104 (87%)	1831 (100%)	0	100	100
All	All	12331/12889 (96%)	12331 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	433	GLN
1	A	505	GLN
1	A	679	GLN
1	A	735	ASN
1	A	751	HIS
1	A	892	GLN
1	A	1068	GLN
1	A	1105	GLN
1	A	1132	ASN
1	A	1252	GLN
1	A	1499	GLN
1	A	1547	ASN
1	A	1587	HIS
1	A	1636	GLN
1	A	1671	ASN
1	A	1965	GLN
1	A	1969	ASN
1	A	2230	GLN
1	A	2237	GLN
1	A	2321	HIS
1	A	2388	GLN
1	A	2452	HIS
1	B	46	HIS
1	B	306	GLN
1	B	505	GLN
1	B	527	GLN
1	B	676	HIS
1	B	679	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	735	ASN
1	B	1053	GLN
1	B	1252	GLN
1	B	1631	ASN
1	B	1671	ASN
1	B	1866	HIS
1	B	1885	GLN
1	B	1965	GLN
1	B	1969	ASN
1	B	2004	GLN
1	B	2230	GLN
1	B	2459	GLN
1	C	319	ASN
1	C	394	ASN
1	C	676	HIS
1	C	751	HIS
1	C	828	ASN
1	C	904	GLN
1	C	953	GLN
1	C	1499	GLN
1	C	1531	GLN
1	C	1636	GLN
1	C	1965	GLN
1	C	1969	ASN
1	C	2035	GLN
1	C	2071	GLN
1	C	2459	GLN
1	D	220	GLN
1	D	676	HIS
1	D	679	GLN
1	D	735	ASN
1	D	886	GLN
1	D	1520	GLN
1	D	1529	ASN
1	D	1671	ASN
1	D	1752	ASN
1	D	1951	GLN
1	D	2321	HIS
1	D	2459	GLN
1	E	46	HIS
1	E	220	GLN
1	E	679	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	886	GLN
1	E	1303	ASN
1	E	1547	ASN
1	E	1815	GLN
1	E	1866	HIS
1	E	1929	ASN
1	E	2021	HIS
1	E	2071	GLN
1	E	2112	ASN
1	E	2230	GLN
1	E	2348	ASN
1	E	2388	GLN
2	F	199	GLN
2	F	236	ASN
2	F	287	GLN
2	F	461	GLN
2	F	700	ASN
2	F	748	GLN
2	F	843	GLN
2	F	974	ASN
2	F	1125	HIS
2	F	1187	GLN
2	F	1397	GLN
2	F	1482	ASN
2	F	1534	ASN
2	F	1535	GLN
2	F	1558	GLN
2	F	1564	ASN
2	F	1680	GLN
2	F	1716	GLN
2	F	1994	GLN
2	F	1996	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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.

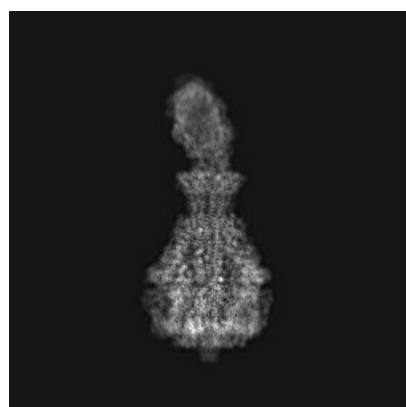
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0150. These allow visual inspection of the internal detail of the map and identification of artifacts.

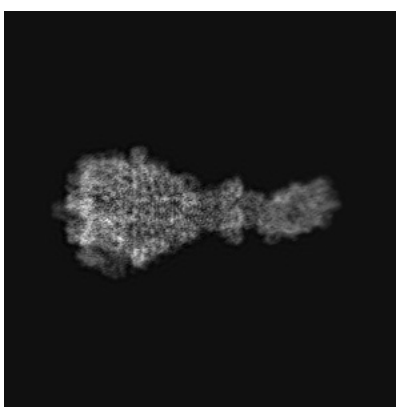
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

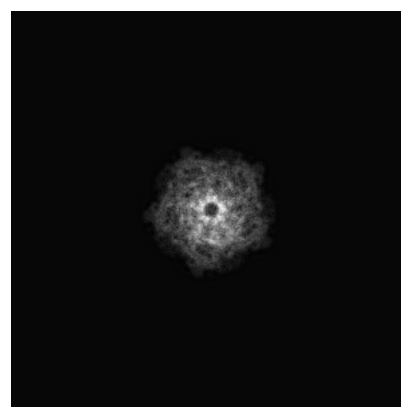
6.1.1 Primary map



X



Y



Z

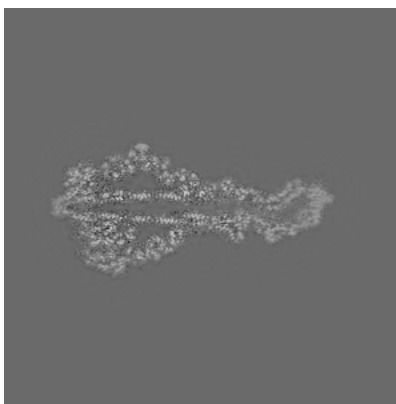
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240



Y Index: 240

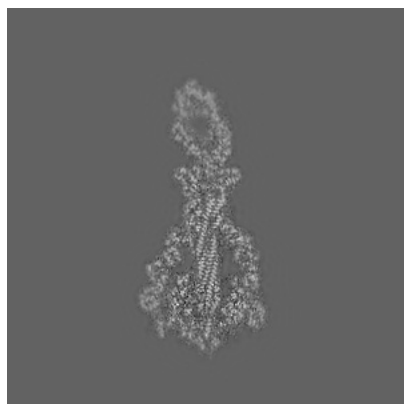


Z Index: 240

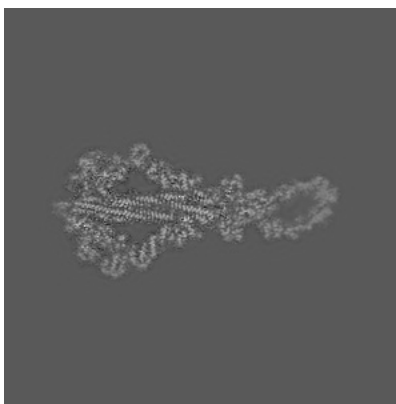
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

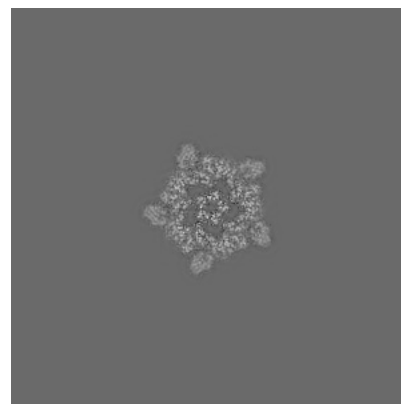
6.3.1 Primary map



X Index: 228



Y Index: 230

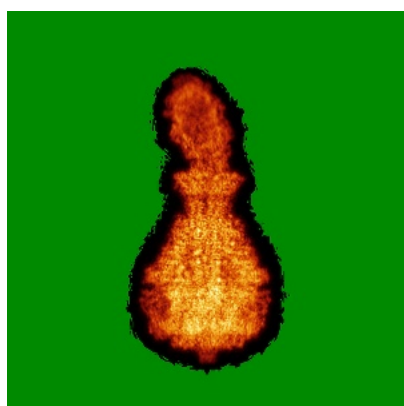


Z Index: 140

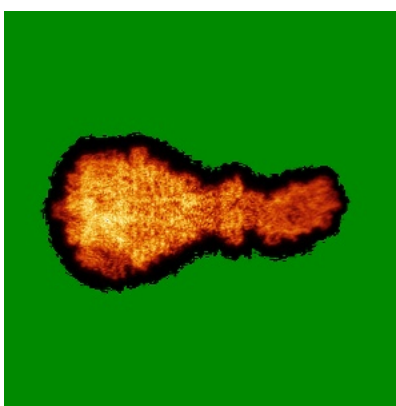
The images above show the largest variance slices of the map in three orthogonal directions.

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

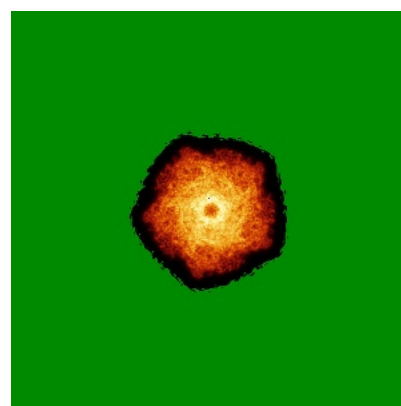
6.4.1 Primary map



X



Y

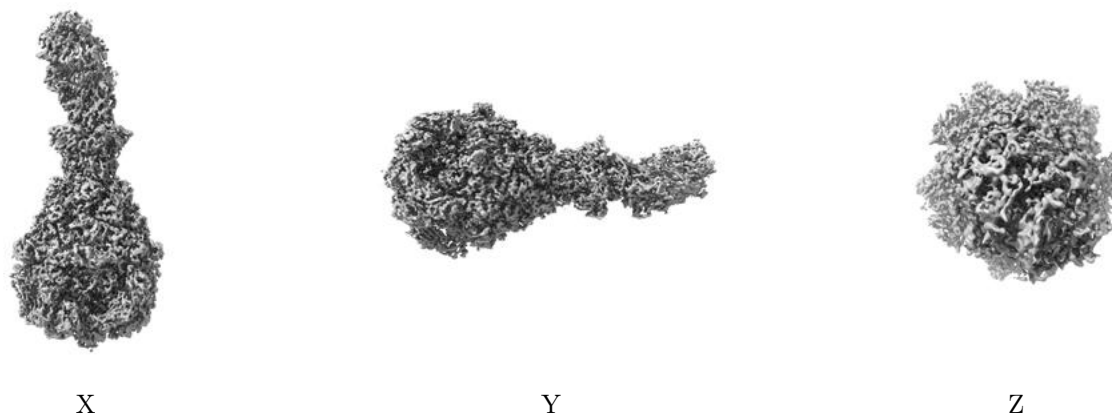


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

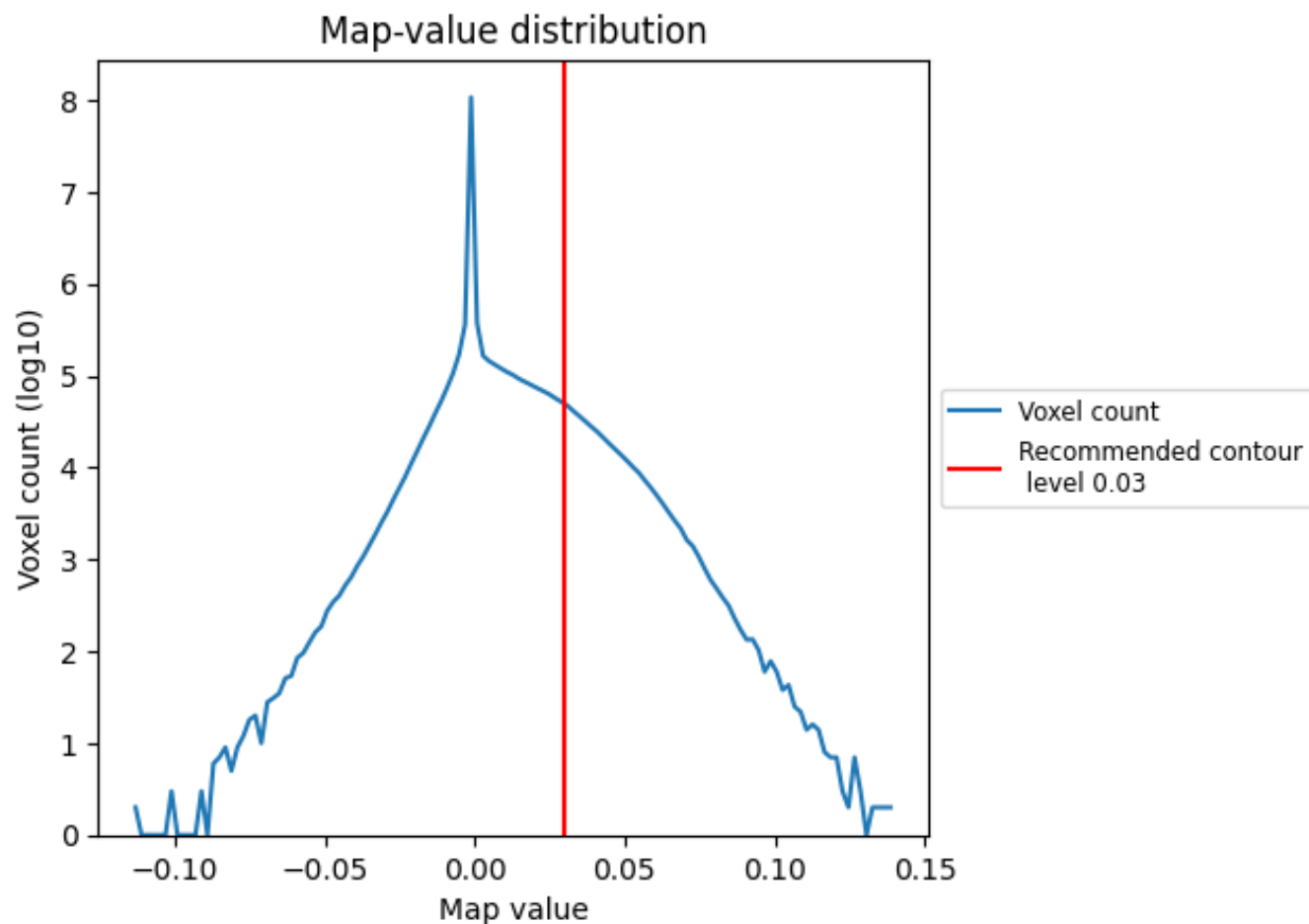
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

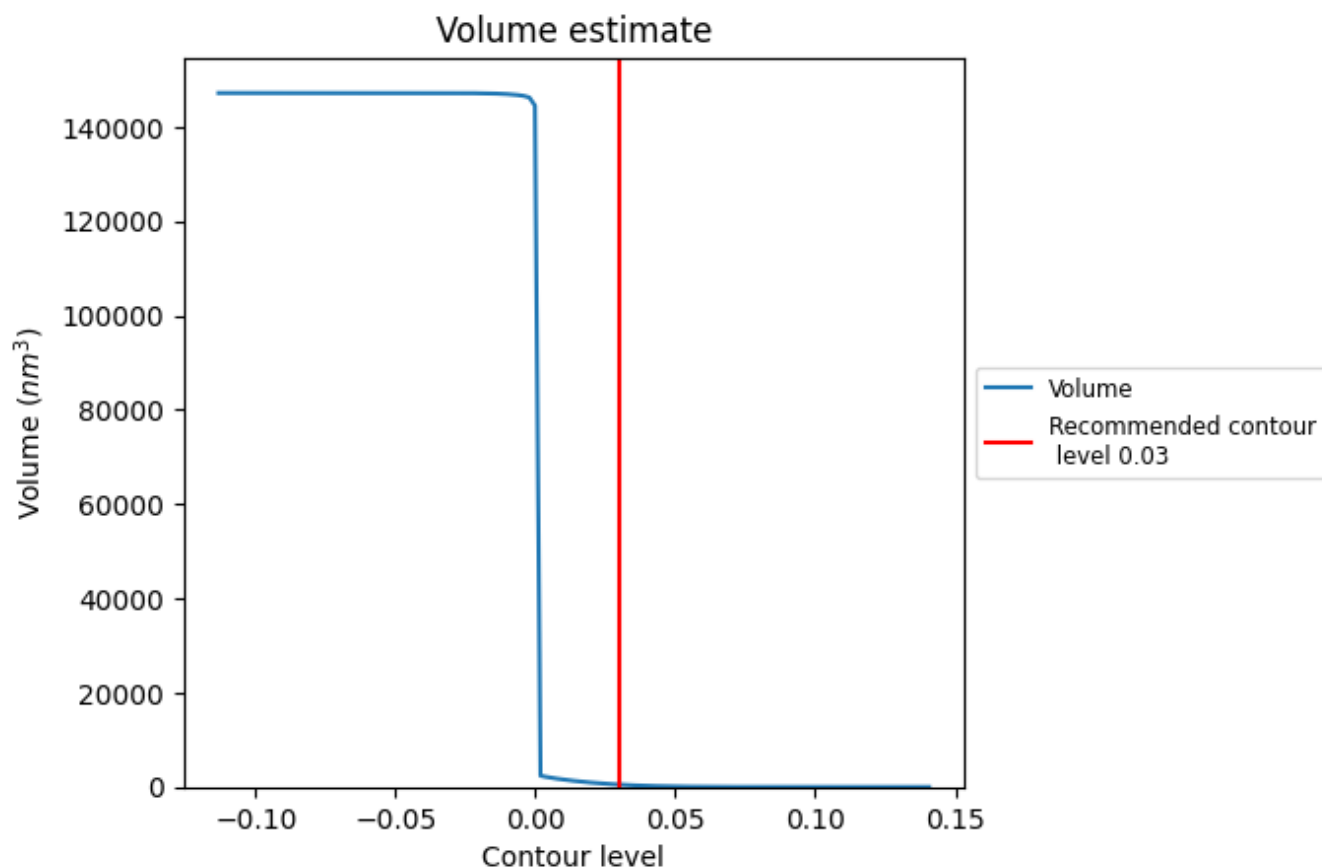
This section contains the results of statistical analysis of the map.

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.

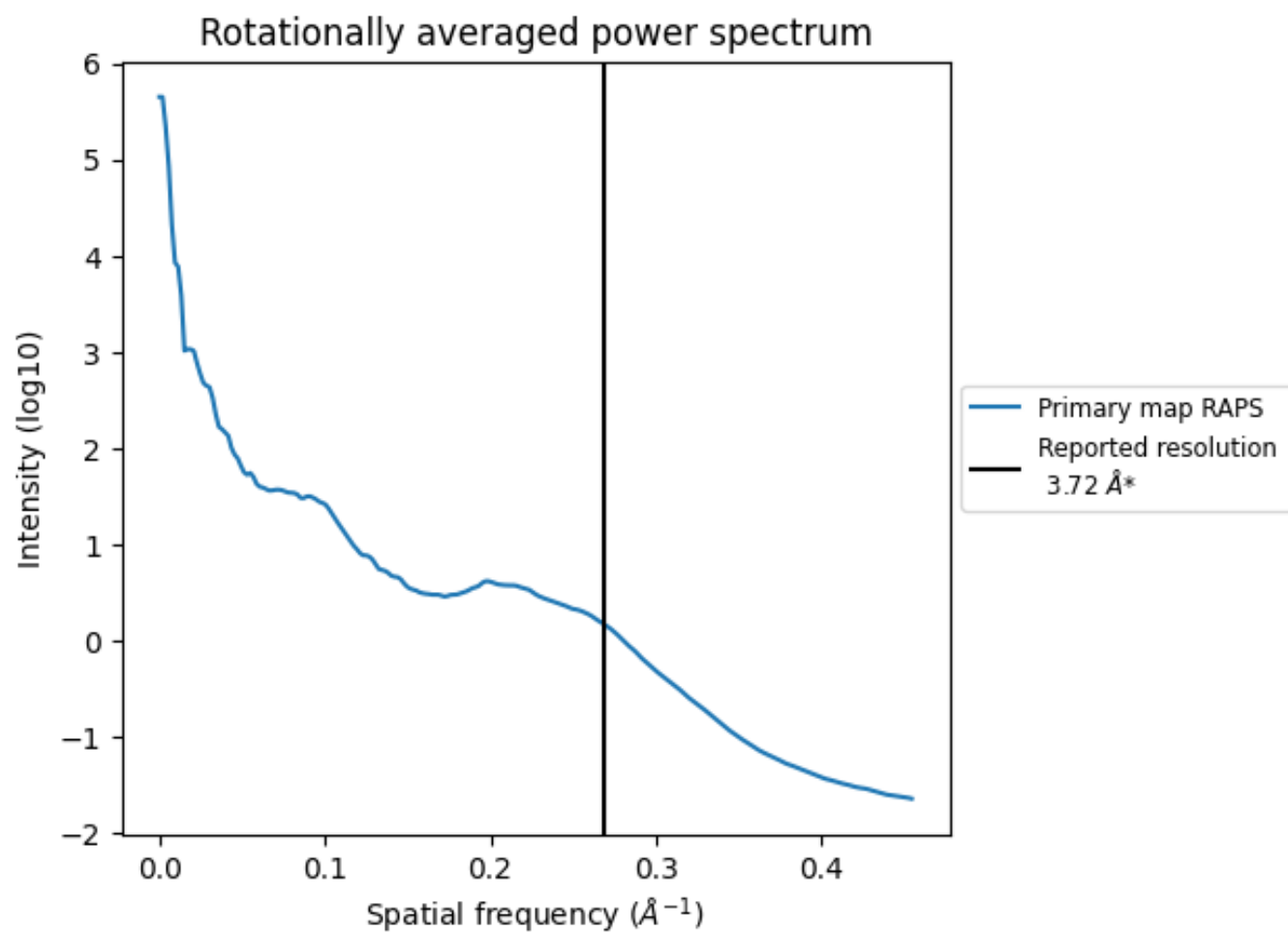
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 491 nm³; this corresponds to an approximate mass of 444 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 0.269 Å⁻¹

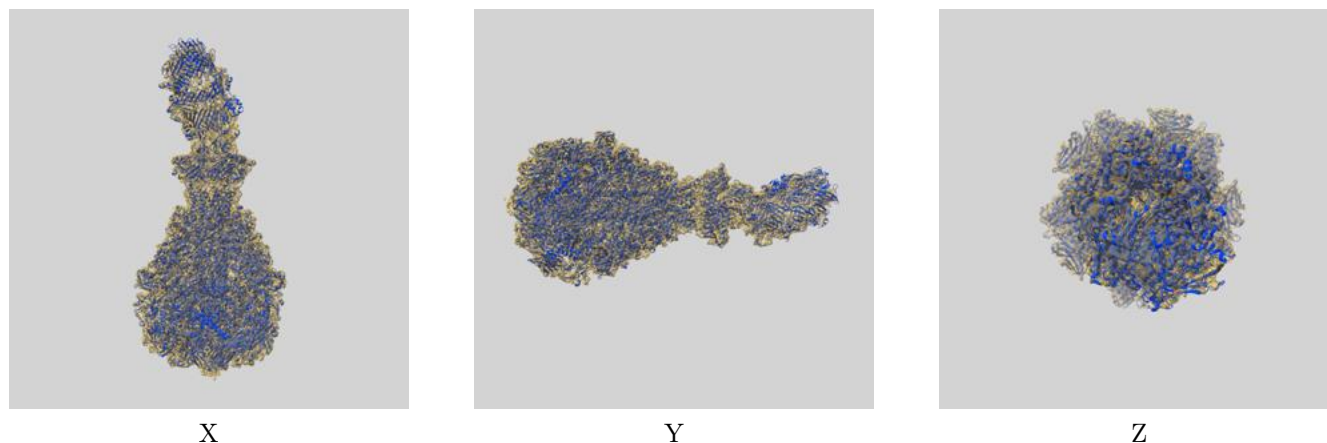
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

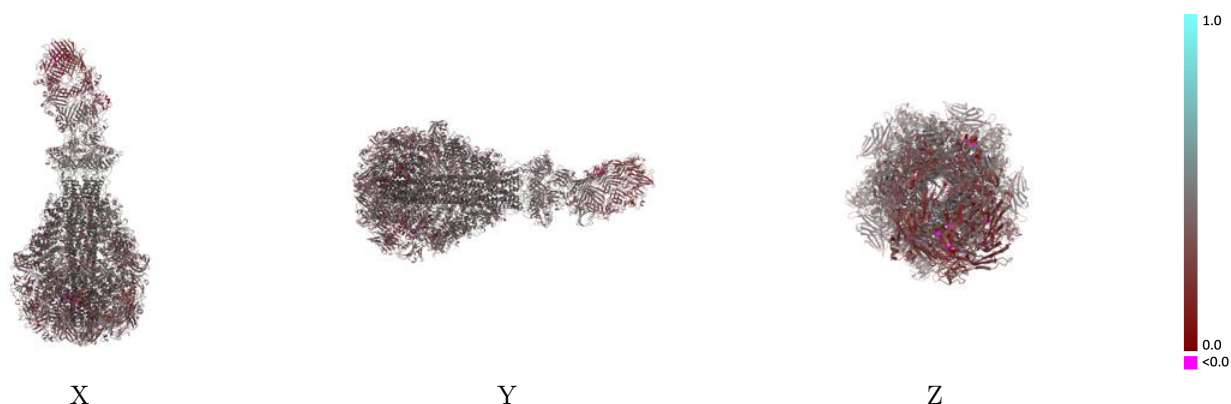
This section contains information regarding the fit between EMDB map EMD-0150 and PDB model 6H6F. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



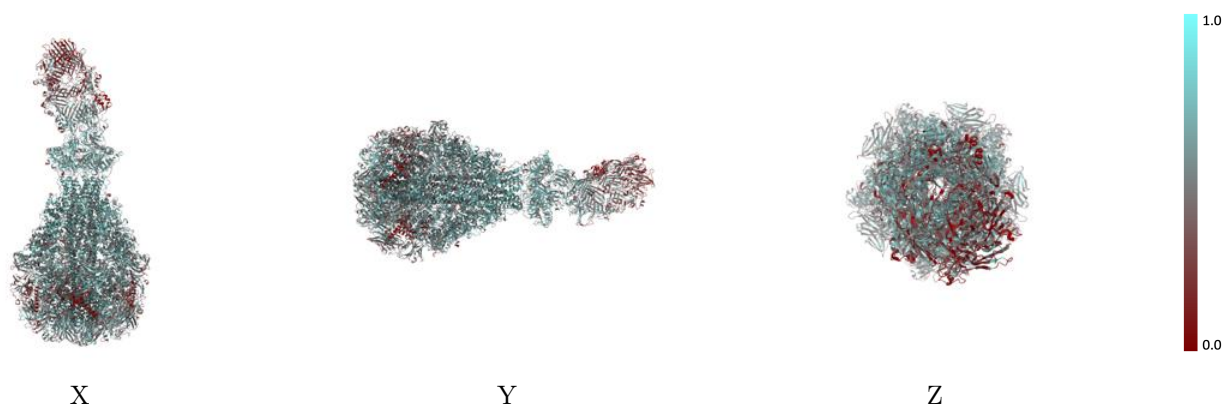
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



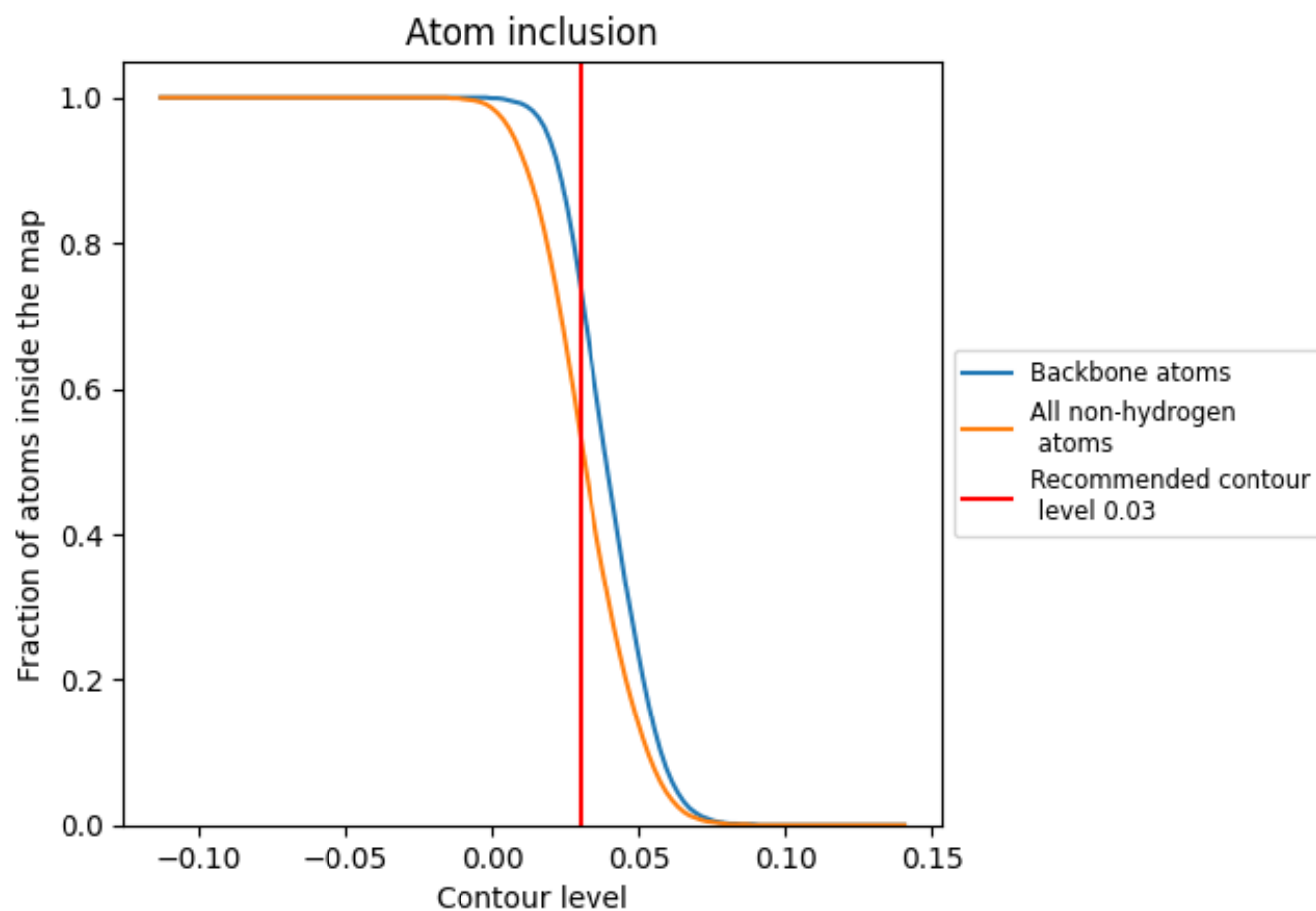
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 54% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5350	0.3750
A	0.5510	0.3850
B	0.5570	0.3840
C	0.5570	0.3850
D	0.5620	0.3910
E	0.5580	0.3890
F	0.4080	0.3090

1.0

0.0

<0.0