Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 05:26 pm GMT

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

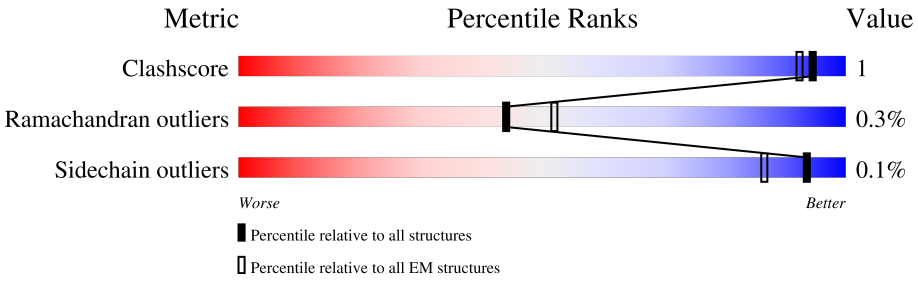
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2516	5% 86% 5% 9%
1	B	2516	6% 85% 6% 9%
1	C	2516	5% 85% 6% 9%
1	D	2516	8% 86% 5% 9%
1	E	2516	5% 86% 5% 9%
2	F	2439	83% 6% 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 108270 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called TcdA1.

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

There are 5 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called TcdB2,TccC3.

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

There are 7 discrepancies between the modelled and reference sequences:

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

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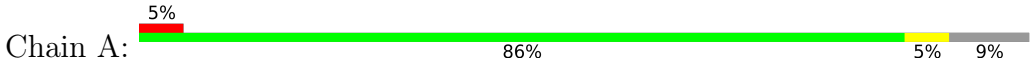
Chain	Residue	Modelled	Actual	Comment	Reference
F	1478	ARG	-	linker	UNP Q8GF99
F	1479	PRO	-	linker	UNP Q8GF99
F	2130	ALA	ASP	engineered mutation	UNP Q8GF97

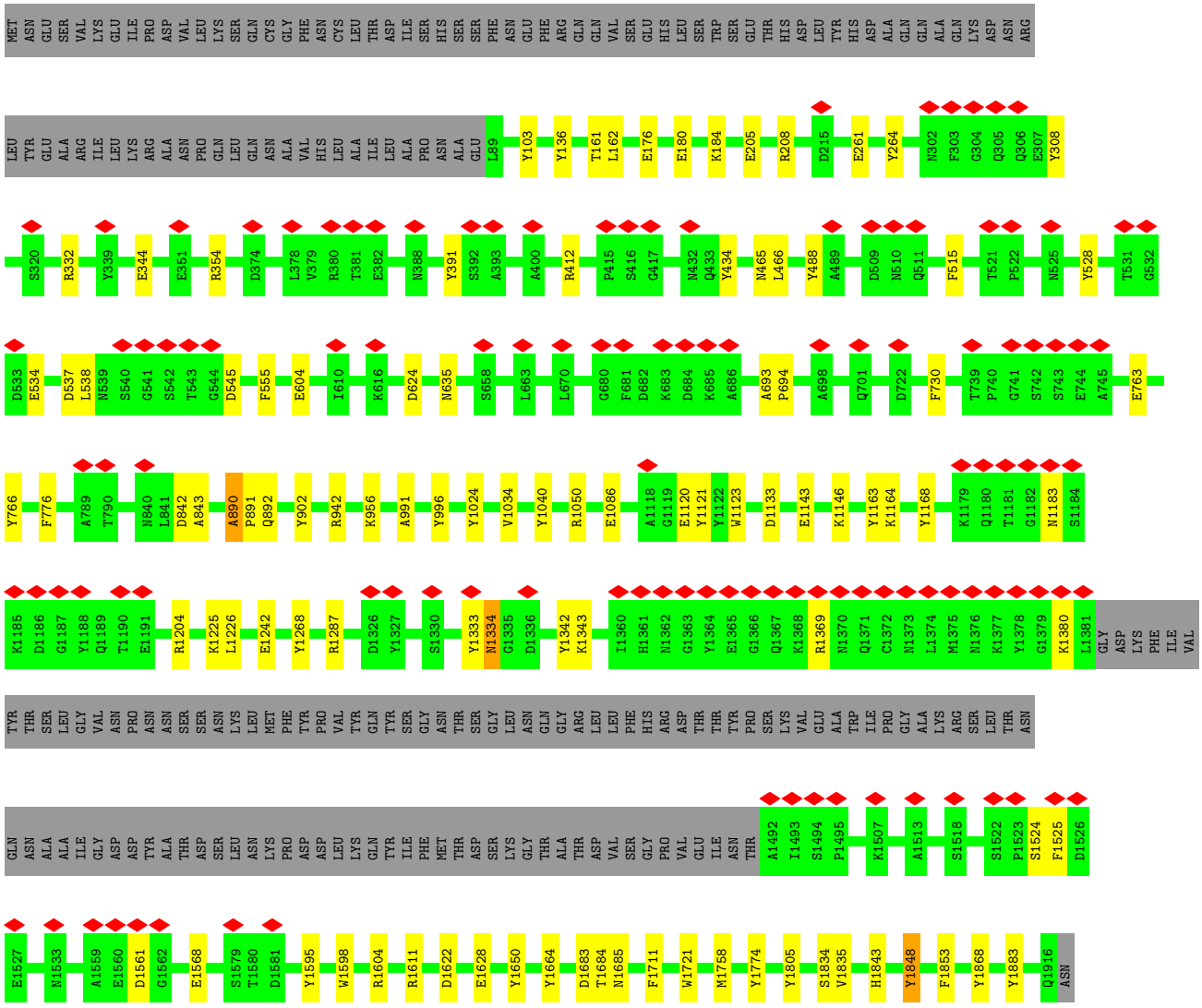
3 Residue-property plots (i)

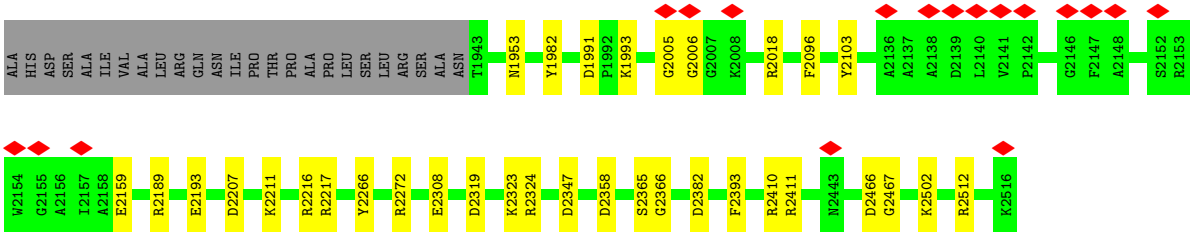
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: TcdA1

Chain A:

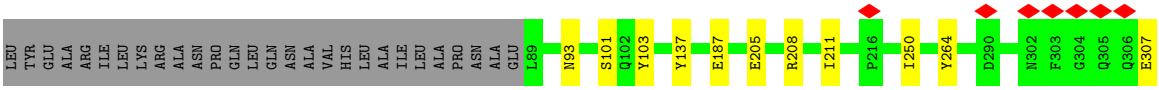


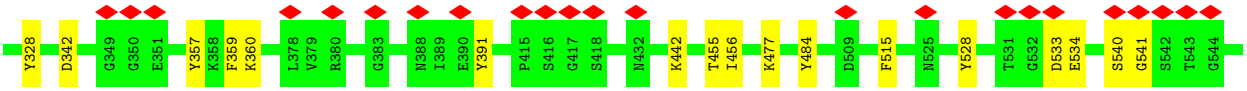


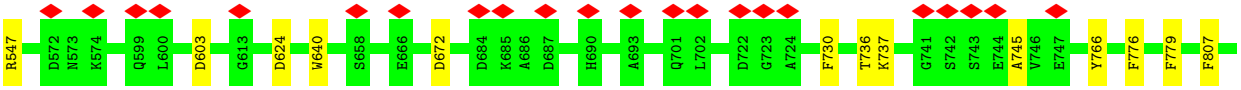


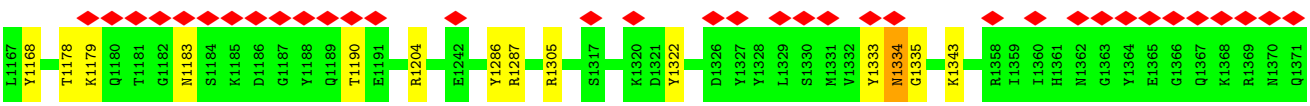
• Molecule 1: TcdA1

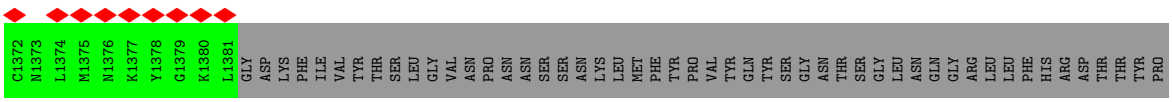
Chain B:

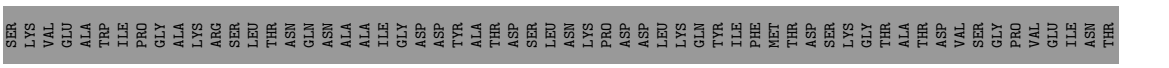


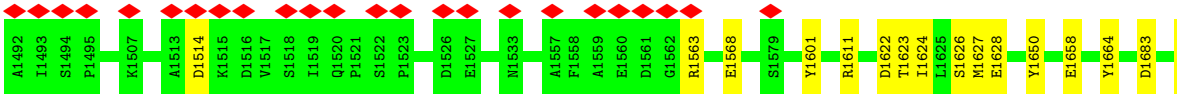


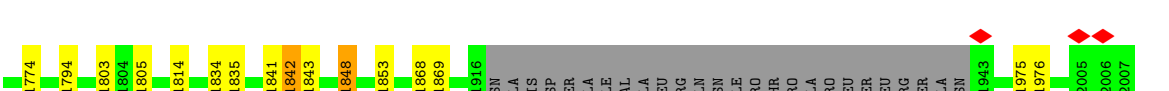


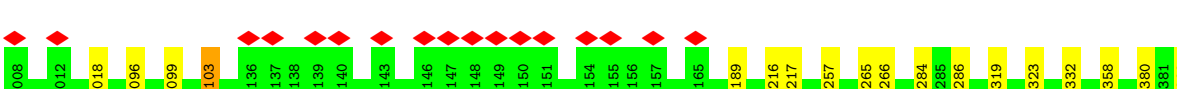






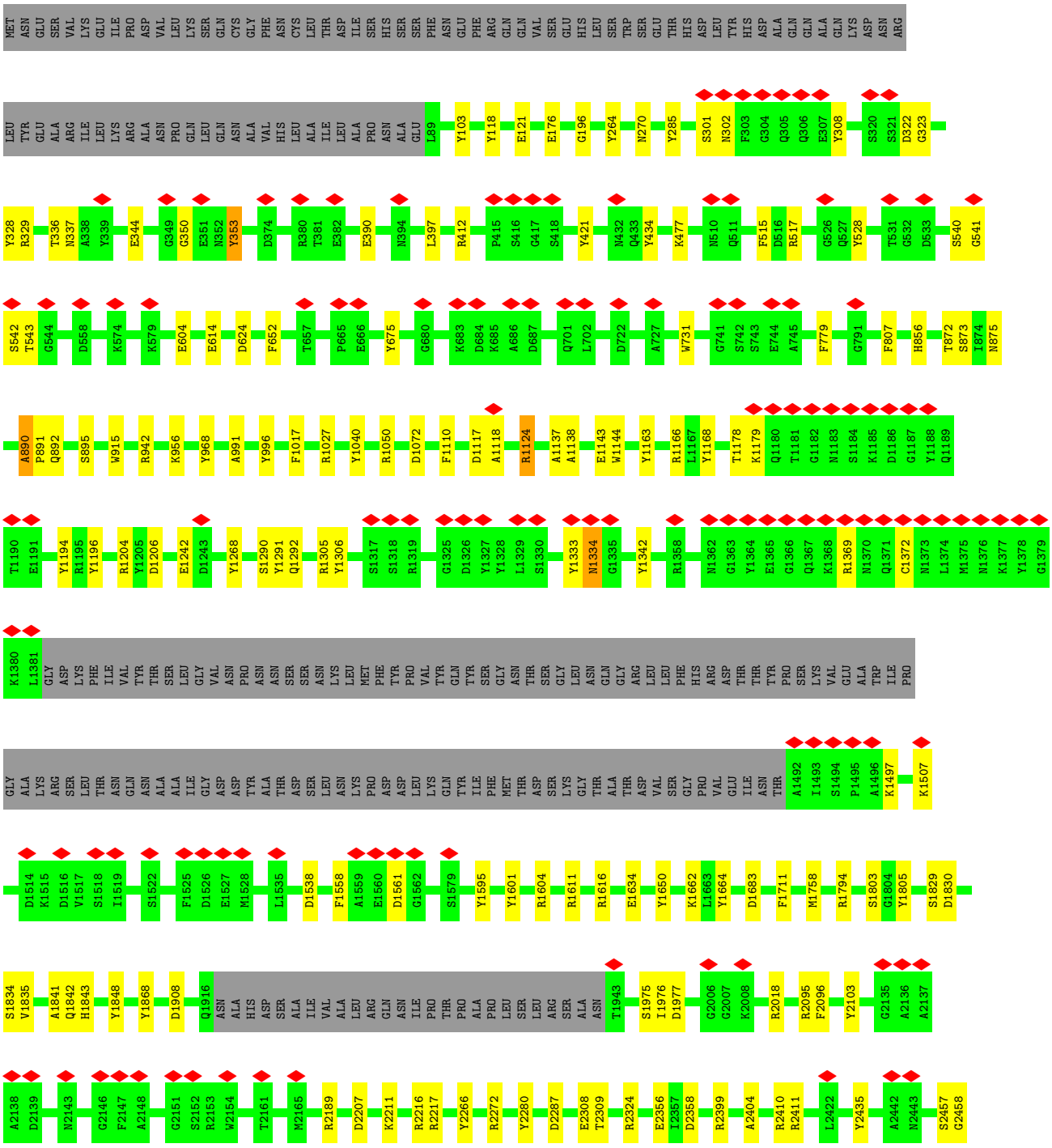






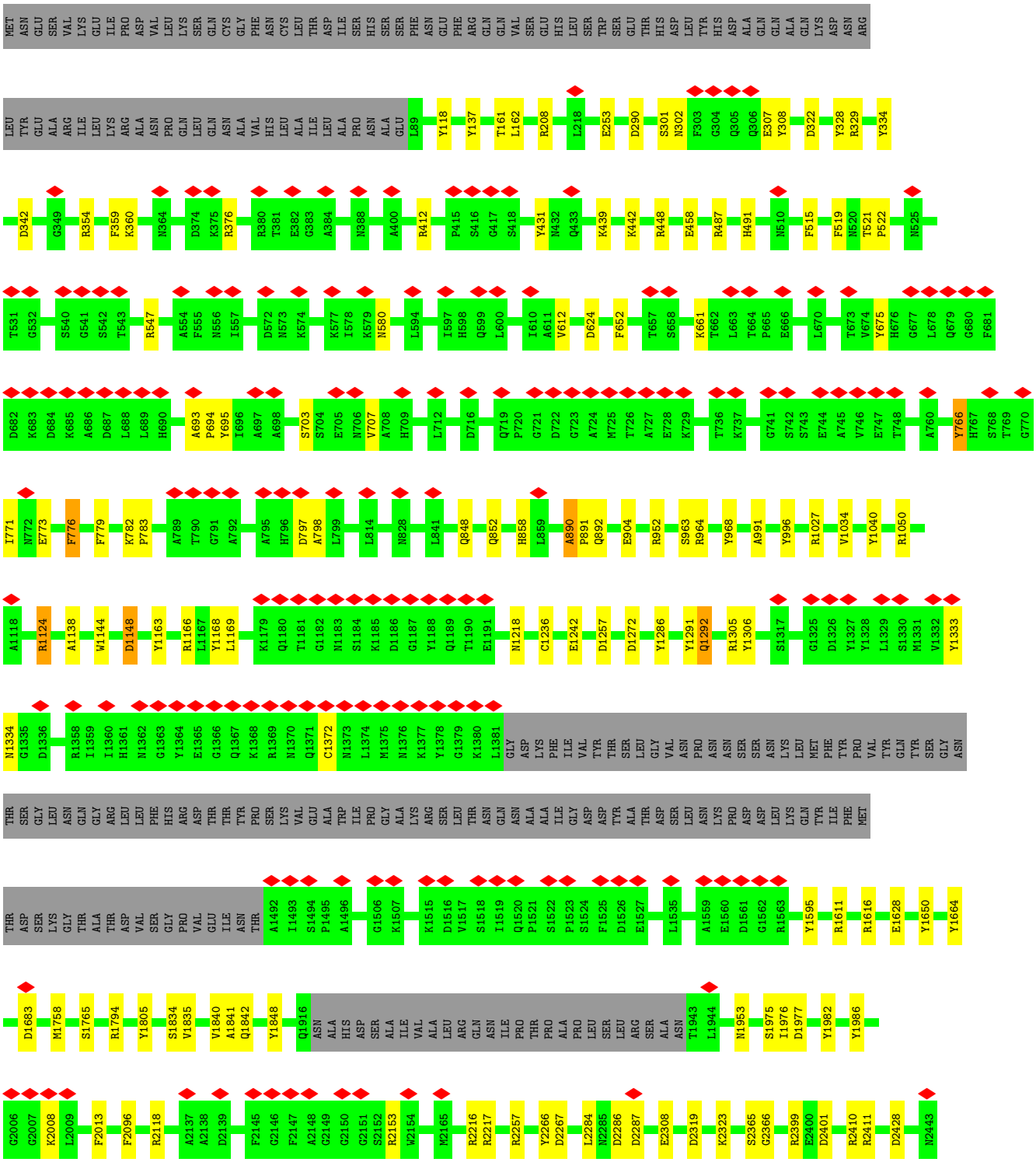
• Molecule 1: TcdA1

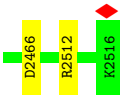
Chain C:



• Molecule 1: TcdA1

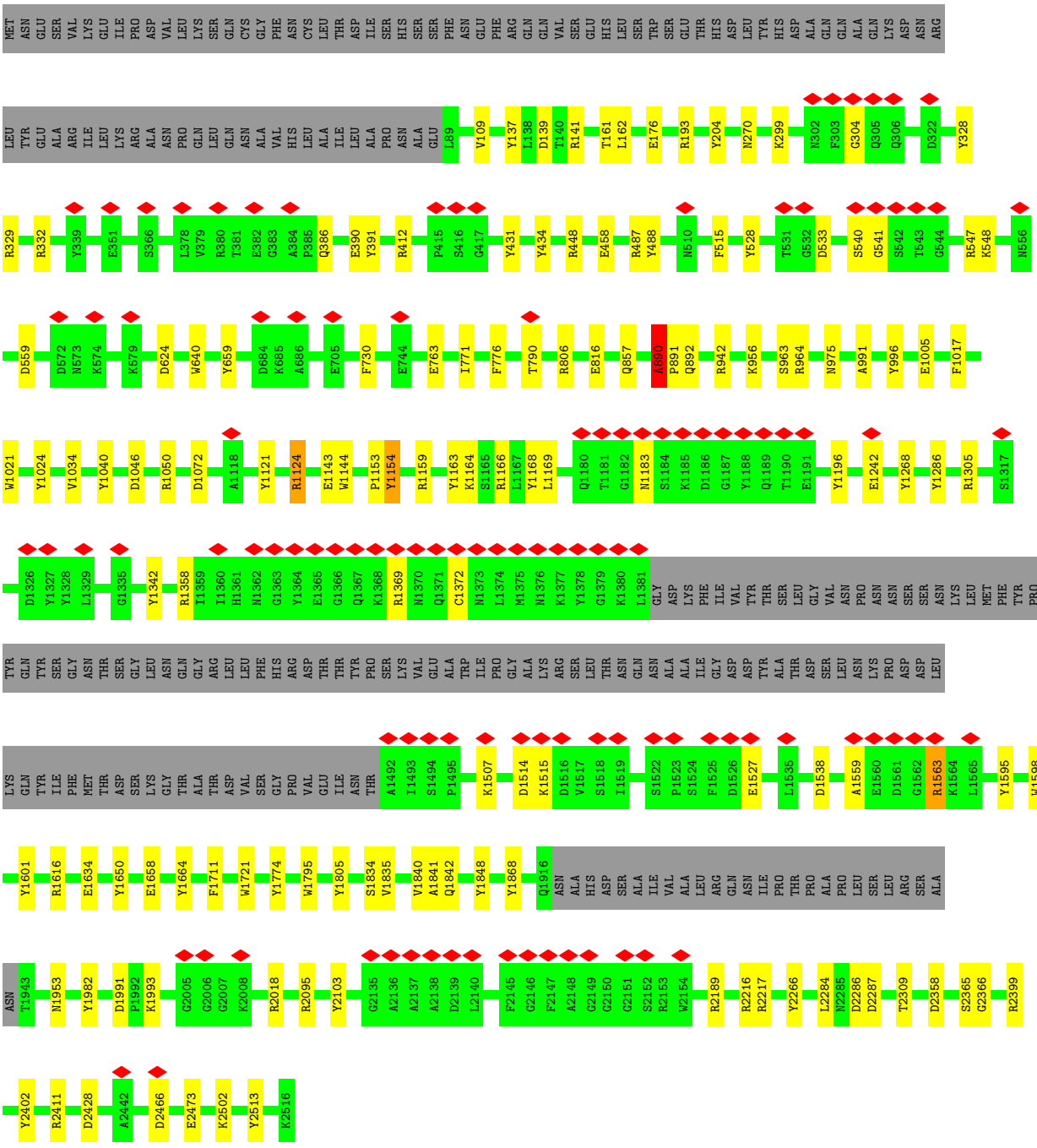
Chain D:





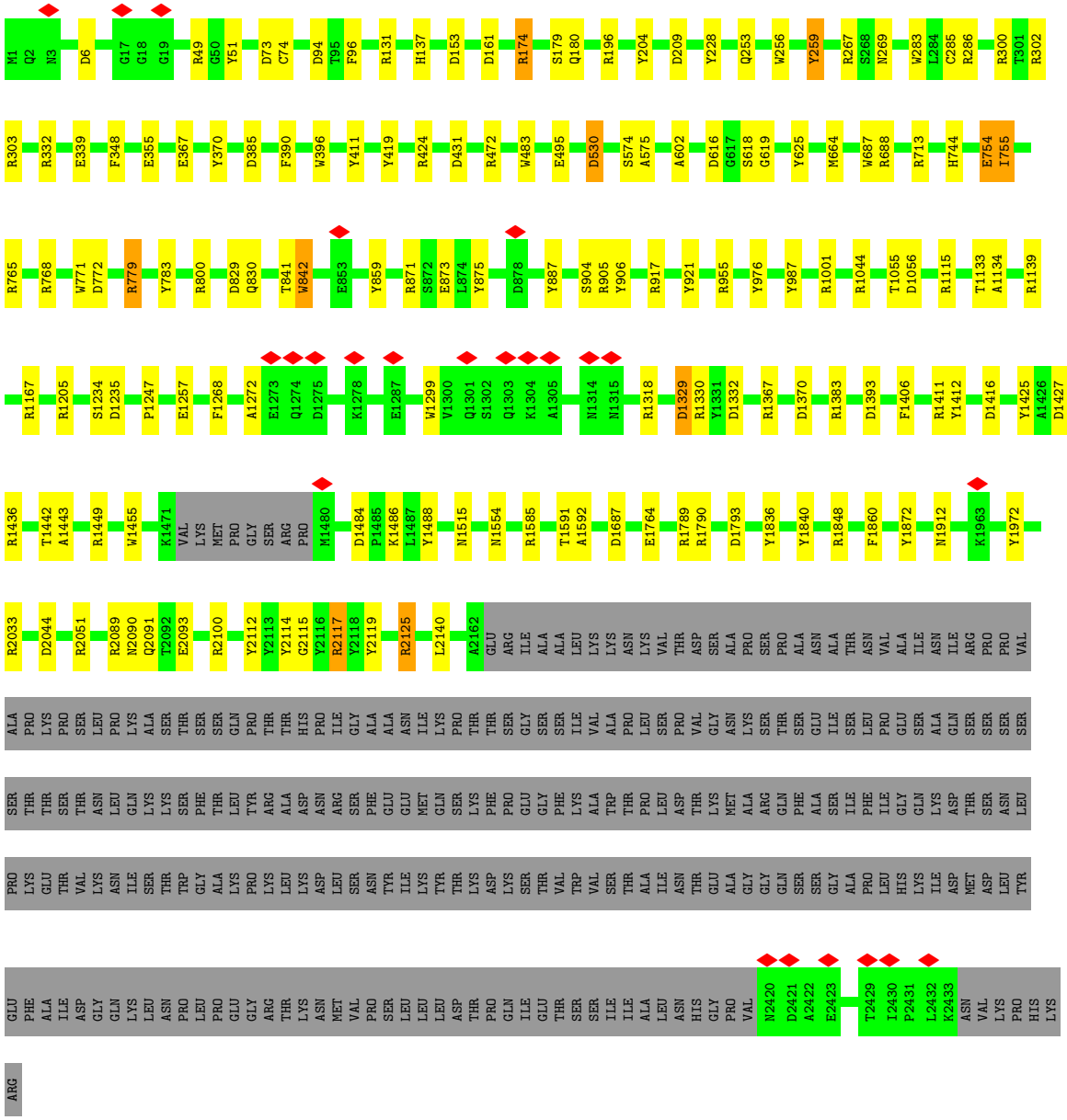
• Molecule 1: TcdA1

Chain E:



• Molecule 2: TcdB2,TccC3

Chain F:


M1 Q2 N3 D6 G17 G18 G19 R49 G50 Y51 D73 C74 D94 T95 F96 R131 H137 D153 D161 R174 S179 Q180 R196 Y204 D209 Y228 Q253 W256 Y259 R267 S268 N269 W283 L284 C285 R286 R300 T301 R302
R303 R332 E339 F348 E355 E367 Y370 D385 F390 W396 Y411 Y419 R424 D431 R472 W483 E495 D530 S574 A575 A602 D616 G617 S618 G619 Y625 M664 W687 R688 R713 H744 E754 I755
R765 R768 W771 D772 R779 Y783 R800 D829 Q830 T841 W842 E853 Y859 R871 S872 E873 L874 Y875 D878 Y887 S904 R905 Y906 R917 Y921 R955 Y976 Y987 R1001 R1044 T1055 D1056 R1115 T1133 A1134 R1139
R1167 R1205 S1234 D1235 P1247 E1257 F1268 A1272 E1273 Q1274 D1275 K1278 E1287 W1299 V1300 Q1301 S1302 Q1303 K1304 A1305 N1314 M1315 R1318 D1329 R1330 Y1331 D1332 R1367 D1370 R1383 D1393 F1406 R1411 Y1412 D1416 Y1425 A1426 D1427
R1436 T1442 A1443 R1449 W1455 K1471 VAL LYS MET PRO GLY SER ARG PRO M1480 D1484 P1485 K1486 L1487 Y1488 N1515 N1554 R1585 T1591 A1592 D1687 E1764 R1789 R1790 D1793 Y1836 Y1840 R1848 F1860 Y1872 N1912 K1963 Y1972
R2033 D2044 R2051 R2089 N2090 Q2091 T2092 E2093 R2100 Y2112 Y2113 Y2114 G2115 Y2116 R2117 Y2118 Y2119 R2125 L2140 A2162 GLU ARG ILE ALA ALA LEU LYS LYS ASN LYS VAL THR ASP SER ALA PRO SER PRO ALA ASN ALA THR ASN VAL ALA ILE ASN ILE ARG PRO PRO VAL
ALA PRO LYS PRO SER LEU PRO LYS ALA SER THR SER GLN PRO THR THR HIS PRO ILE GLY ALA ALA ASN ILE LYS PRO THR THR SER GLY SER SER ILE VAL ALA PRO LEU SER PRO VAL GLY ASN LYS SER THR SER GLU ILE SER LEU PRO GLU SER ALA GLN SER SER SER SER
SER THR THR SER THR ASN LEU GLN LYS LYS SER PHE THR LEU TYR ARG ALA ASP ASN ARG SER PHE GLU GLU MET GLN SER LYS PHE PRO GLU GLY PHE LYS ALA TRP THR PRO LEU ASP THR LYS MET ALA ARG GLN PHE ALA SER ILE PHE ILE GLY GLN LYS ASP THR SER ASN LEU
PRO LYS GLU THR VAL LYS ASN ILE SER THR TRP GLY ALA LYS PRO LYS LEU LYS ASP LEU SER ASN TYR ILE LYS TYR THR LYS ASP LYS SER THR VAL TRP VAL SER THR ALA ILE ASN THR GLU ALA GLY GLY GLN SER SER GLY ALA PRO LEU HIS LYS ILE ASP MET ASP LEU TYR
GLU PHE ALA ILE ASP GLY GLN LYS LEU ASN PRO LEU PRO GLU GLY ARG THR LYS ASN MET VAL PRO SER LEU LEU LEU ASP THR PRO GLN ILE GLU THR SER SER ILE ILE ALA LEU ASN HIS GLY PRO VAL N2420 D2421 A2422 E2423 T2429 I2430 P2431 L2432 K2433 ASN VAL LYS PRO HIS LYS
ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	337823	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.165	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	426.24, 426.24, 426.24	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	46/18587 (0.2%)	0.93	40/25239 (0.2%)
1	B	1.12	47/18587 (0.3%)	0.93	48/25239 (0.2%)
1	C	1.13	54/18587 (0.3%)	0.94	52/25239 (0.2%)
1	D	1.12	38/18587 (0.2%)	0.93	43/25239 (0.2%)
1	E	1.12	43/18587 (0.2%)	0.94	50/25239 (0.2%)
2	F	1.18	46/17708 (0.3%)	0.98	70/24137 (0.3%)
All	All	1.13	274/110643 (0.2%)	0.94	303/150332 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (274) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1242	GLU	CG-CD	-10.17	1.36	1.51
1	A	1242	GLU	CG-CD	-10.04	1.36	1.51
1	A	308	TYR	CB-CG	-9.65	1.37	1.51
1	C	1242	GLU	CG-CD	-9.22	1.38	1.51
2	F	1860	PHE	CB-CG	-9.12	1.35	1.51
1	E	996	TYR	CB-CG	-8.73	1.38	1.51
1	B	1124	ARG	CD-NE	-8.33	1.32	1.46
1	D	1163	TYR	CB-CG	-8.26	1.39	1.51
1	E	1163	TYR	CB-CG	-8.07	1.39	1.51
1	A	902	TYR	CB-CG	-8.06	1.39	1.51
1	E	1664	TYR	CB-CG	-8.02	1.39	1.51
1	B	1163	TYR	CB-CG	-7.99	1.39	1.51
1	A	1242	GLU	CD-OE2	-7.85	1.17	1.25
1	E	1242	GLU	CG-CD	-7.83	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	996	TYR	CB-CG	-7.69	1.40	1.51
1	B	1843	HIS	CB-CG	-7.66	1.36	1.50
1	A	1163	TYR	CB-CG	-7.51	1.40	1.51
1	B	1848	TYR	CG-CD1	-7.46	1.29	1.39
1	E	515	PHE	CB-CG	-7.46	1.38	1.51
1	C	1242	GLU	CD-OE2	-7.45	1.17	1.25
1	C	1163	TYR	CB-CG	-7.44	1.40	1.51
1	E	1372	CYS	CB-SG	-7.44	1.69	1.82
2	F	1872	TYR	CE1-CZ	-7.39	1.28	1.38
1	A	1843	HIS	CB-CG	-7.31	1.36	1.50
2	F	744	HIS	CB-CG	-7.28	1.36	1.50
1	C	1601	TYR	CB-CG	-7.27	1.40	1.51
1	D	1664	TYR	CB-CG	-7.27	1.40	1.51
1	D	1242	GLU	CD-OE2	-7.25	1.17	1.25
1	D	996	TYR	CB-CG	-7.17	1.40	1.51
1	D	1124	ARG	CD-NE	-7.15	1.34	1.46
1	D	776	PHE	CG-CD2	-7.14	1.28	1.38
1	B	640	TRP	CB-CG	-7.12	1.37	1.50
2	F	875	TYR	CB-CG	-7.09	1.41	1.51
1	D	580	ASN	CB-CG	-6.94	1.35	1.51
1	B	1842	GLN	CG-CD	-6.87	1.35	1.51
1	B	776	PHE	CB-CG	-6.86	1.39	1.51
1	C	1843	HIS	CB-CG	-6.85	1.37	1.50
1	B	1664	TYR	CB-CG	-6.84	1.41	1.51
2	F	483	TRP	CB-CG	-6.81	1.38	1.50
1	C	807	PHE	CG-CD1	-6.75	1.28	1.38
1	B	1805	TYR	CB-CG	-6.71	1.41	1.51
1	E	1634	GLU	CD-OE1	-6.68	1.18	1.25
1	D	491	HIS	CB-CG	-6.67	1.38	1.50
1	A	1848	TYR	CE2-CZ	-6.57	1.30	1.38
2	F	348	PHE	CB-CG	-6.55	1.40	1.51
1	A	1268	TYR	CB-CG	-6.54	1.41	1.51
1	B	902	TYR	CB-CG	-6.51	1.41	1.51
1	A	1664	TYR	CB-CG	-6.49	1.42	1.51
2	F	2119	TYR	CB-CG	-6.49	1.42	1.51
1	C	1848	TYR	CE2-CZ	-6.48	1.30	1.38
1	A	776	PHE	CB-CG	-6.45	1.40	1.51
1	E	1595	TYR	CB-CG	-6.43	1.42	1.51
1	A	996	TYR	CB-CG	-6.42	1.42	1.51
2	F	174	ARG	CD-NE	-6.41	1.35	1.46
1	D	515	PHE	CB-CG	-6.35	1.40	1.51
1	A	1721	TRP	CB-CG	-6.33	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1848	TYR	CB-CG	-6.30	1.42	1.51
1	D	1124	ARG	CB-CG	-6.29	1.35	1.52
1	A	1143	GLU	CG-CD	-6.28	1.42	1.51
2	F	285	CYS	CB-SG	-6.25	1.71	1.82
1	D	776	PHE	CG-CD1	-6.21	1.29	1.38
1	D	2013	PHE	CB-CG	-6.20	1.40	1.51
1	A	763	GLU	CG-CD	-6.20	1.42	1.51
1	B	1124	ARG	CB-CG	-6.19	1.35	1.52
1	A	1121	TYR	CB-CG	-6.18	1.42	1.51
1	E	1805	TYR	CB-CG	-6.18	1.42	1.51
1	C	1634	GLU	CD-OE1	-6.17	1.18	1.25
1	A	2272	ARG	CG-CD	-6.16	1.36	1.51
1	E	1005	GLU	CD-OE1	-6.16	1.18	1.25
1	C	779	PHE	CB-CG	-6.16	1.40	1.51
1	D	359	PHE	CB-CG	-6.14	1.41	1.51
2	F	339	GLU	CG-CD	-6.13	1.42	1.51
2	F	259	TYR	CB-CG	-6.12	1.42	1.51
1	C	515	PHE	CB-CG	-6.11	1.41	1.51
2	F	779	ARG	CZ-NH1	-6.11	1.25	1.33
1	B	1848	TYR	CE2-CZ	-6.09	1.30	1.38
1	A	1568	GLU	CG-CD	-6.09	1.42	1.51
1	C	1306	TYR	CB-CG	-6.08	1.42	1.51
1	E	1268	TYR	CB-CG	-6.03	1.42	1.51
1	A	515	PHE	CB-CG	-5.99	1.41	1.51
1	A	344	GLU	CD-OE1	-5.97	1.19	1.25
1	B	515	PHE	CB-CG	-5.97	1.41	1.51
1	C	1664	TYR	CB-CG	-5.97	1.42	1.51
1	A	1595	TYR	CB-CG	-5.95	1.42	1.51
1	E	1658	GLU	CD-OE1	-5.94	1.19	1.25
1	E	1242	GLU	CD-OE1	-5.93	1.19	1.25
1	C	2272	ARG	CG-CD	-5.93	1.37	1.51
1	B	807	PHE	CG-CD1	-5.93	1.29	1.38
1	A	103	TYR	CB-CG	-5.91	1.42	1.51
1	A	1650	TYR	CG-CD1	-5.90	1.31	1.39
1	A	1342	TYR	CB-CG	-5.90	1.42	1.51
2	F	339	GLU	CD-OE2	-5.88	1.19	1.25
1	D	308	TYR	CB-CG	-5.88	1.42	1.51
1	C	968	TYR	CG-CD1	-5.88	1.31	1.39
1	A	1805	TYR	CB-CG	-5.88	1.42	1.51
1	C	1650	TYR	CG-CD1	-5.87	1.31	1.39
1	E	1795	TRP	CB-CG	-5.87	1.39	1.50
2	F	783	TYR	CB-CG	-5.86	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	996	TYR	CG-CD1	-5.82	1.31	1.39
1	E	528	TYR	CB-CG	-5.82	1.43	1.51
2	F	1406	PHE	CB-CG	-5.81	1.41	1.51
1	C	264	TYR	CB-CG	-5.81	1.43	1.51
1	D	307	GLU	CD-OE2	-5.81	1.19	1.25
1	E	1650	TYR	CD1-CE1	-5.80	1.30	1.39
2	F	771	TRP	CB-CG	-5.78	1.39	1.50
1	E	204	TYR	CB-CG	-5.77	1.43	1.51
1	C	604	GLU	CG-CD	-5.77	1.43	1.51
2	F	367	GLU	CD-OE1	-5.75	1.19	1.25
1	C	996	TYR	CG-CD1	-5.75	1.31	1.39
1	B	1322	TYR	CB-CG	-5.74	1.43	1.51
1	D	779	PHE	CB-CG	-5.73	1.41	1.51
1	C	1110	PHE	CB-CG	-5.72	1.41	1.51
1	D	1034	VAL	CB-CG2	-5.72	1.40	1.52
1	A	1650	TYR	CD1-CE1	-5.71	1.30	1.39
1	E	1527	GLU	CD-OE2	-5.71	1.19	1.25
2	F	1554	ASN	CB-CG	-5.67	1.38	1.51
1	B	1628	GLU	CD-OE2	-5.66	1.19	1.25
2	F	411	TYR	CB-CG	-5.66	1.43	1.51
1	B	968	TYR	CG-CD1	-5.64	1.31	1.39
1	C	1595	TYR	CB-CG	-5.64	1.43	1.51
1	E	730	PHE	CB-CG	-5.64	1.41	1.51
1	E	1650	TYR	CG-CD1	-5.63	1.31	1.39
1	B	730	PHE	CB-CG	-5.63	1.41	1.51
1	E	1342	TYR	CB-CG	-5.61	1.43	1.51
2	F	664	MET	CG-SD	-5.59	1.66	1.81
1	B	2099	TYR	CB-CG	-5.59	1.43	1.51
1	D	675	TYR	CB-CG	-5.58	1.43	1.51
2	F	1840	TYR	CB-CG	-5.58	1.43	1.51
1	C	344	GLU	CG-CD	-5.57	1.43	1.51
2	F	1836	TYR	CB-CG	-5.57	1.43	1.51
1	E	141	ARG	CG-CD	-5.56	1.38	1.51
1	E	1124	ARG	CB-CG	-5.56	1.37	1.52
2	F	2093	GLU	CD-OE1	-5.56	1.19	1.25
1	A	902	TYR	CD2-CE2	-5.56	1.31	1.39
1	D	904	GLU	CD-OE1	-5.54	1.19	1.25
2	F	1455	TRP	CB-CG	-5.54	1.40	1.50
1	B	264	TYR	CB-CG	-5.52	1.43	1.51
1	C	1868	TYR	CB-CG	-5.52	1.43	1.51
1	D	612	VAL	CB-CG2	-5.51	1.41	1.52
1	B	2096	PHE	CB-CG	-5.51	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	307	GLU	CD-OE2	-5.49	1.19	1.25
1	C	2356	GLU	CD-OE1	-5.49	1.19	1.25
1	E	328	TYR	CB-CG	-5.48	1.43	1.51
1	C	1848	TYR	CB-CG	-5.47	1.43	1.51
1	A	1598	TRP	CB-CG	-5.46	1.40	1.50
1	A	2393	PHE	CB-CG	-5.45	1.42	1.51
1	C	1268	TYR	CB-CG	-5.45	1.43	1.51
1	A	1034	VAL	CB-CG2	-5.45	1.41	1.52
1	C	1650	TYR	CB-CG	-5.45	1.43	1.51
1	C	1650	TYR	CD1-CE1	-5.44	1.31	1.39
2	F	256	TRP	CD2-CE3	-5.44	1.32	1.40
2	F	174	ARG	CZ-NH2	-5.43	1.25	1.33
1	C	2096	PHE	CB-CG	-5.43	1.42	1.51
2	F	396	TRP	CB-CG	-5.42	1.40	1.50
2	F	204	TYR	CB-CG	-5.41	1.43	1.51
1	C	103	TYR	CB-CG	-5.41	1.43	1.51
1	A	604	GLU	CD-OE1	-5.40	1.19	1.25
2	F	370	TYR	CD1-CE1	-5.40	1.31	1.39
1	C	1342	TYR	CB-CG	-5.38	1.43	1.51
2	F	1383	ARG	CB-CG	-5.38	1.38	1.52
1	E	1124	ARG	CD-NE	-5.37	1.37	1.46
1	B	2103	TYR	CB-CG	-5.37	1.43	1.51
1	C	1805	TYR	CB-CG	-5.37	1.43	1.51
1	A	2159	GLU	CD-OE2	-5.36	1.19	1.25
1	B	766	TYR	CB-CG	-5.35	1.43	1.51
1	B	1005	GLU	CD-OE1	-5.35	1.19	1.25
1	C	353	TYR	CE1-CZ	-5.35	1.31	1.38
1	D	858	HIS	CB-CG	-5.35	1.40	1.50
1	E	640	TRP	CB-CG	-5.34	1.40	1.50
1	E	1121	TYR	CB-CG	-5.34	1.43	1.51
2	F	873	GLU	CD-OE1	-5.34	1.19	1.25
1	A	264	TYR	CB-CG	-5.33	1.43	1.51
2	F	842	TRP	CB-CG	-5.33	1.40	1.50
1	C	353	TYR	CD1-CE1	-5.33	1.31	1.39
1	B	1110	PHE	CB-CG	-5.33	1.42	1.51
2	F	1257	GLU	CD-OE1	-5.33	1.19	1.25
1	A	1123	TRP	CB-CG	-5.32	1.40	1.50
1	D	1218	ASN	CB-CG	-5.32	1.38	1.51
1	B	996	TYR	CB-CG	-5.31	1.43	1.51
1	B	1568	GLU	CG-CD	-5.30	1.44	1.51
1	C	1124	ARG	CB-CG	-5.30	1.38	1.52
1	B	328	TYR	CB-CG	-5.30	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1372	CYS	CB-SG	-5.29	1.73	1.81
1	C	1868	TYR	CD2-CE2	-5.29	1.31	1.39
1	A	766	TYR	CG-CD1	-5.28	1.32	1.39
1	B	2332	GLU	CD-OE1	-5.28	1.19	1.25
1	C	118	TYR	CE2-CZ	-5.27	1.31	1.38
1	E	141	ARG	CD-NE	-5.27	1.37	1.46
2	F	390	PHE	CB-CG	-5.27	1.42	1.51
1	B	1853	PHE	CB-CG	-5.27	1.42	1.51
1	B	137	TYR	CB-CG	-5.26	1.43	1.51
1	D	652	PHE	CB-CG	-5.26	1.42	1.51
1	B	2452	HIS	CB-CG	-5.25	1.40	1.50
1	C	1372	CYS	CB-SG	-5.25	1.73	1.81
1	E	1017	PHE	CB-CG	-5.24	1.42	1.51
1	A	1628	GLU	CD-OE2	-5.24	1.19	1.25
1	B	187	GLU	CD-OE1	-5.24	1.19	1.25
2	F	1764	GLU	CD-OE1	-5.23	1.19	1.25
1	E	1143	GLU	CG-CD	-5.23	1.44	1.51
1	B	1017	PHE	CB-CG	-5.23	1.42	1.51
1	B	1848	TYR	CD1-CE1	-5.22	1.31	1.39
1	D	1848	TYR	CE2-CZ	-5.22	1.31	1.38
1	C	731	TRP	CZ3-CH2	-5.21	1.31	1.40
1	D	1163	TYR	CD1-CE1	-5.21	1.31	1.39
1	C	1124	ARG	CD-NE	-5.21	1.37	1.46
2	F	495	GLU	CD-OE1	-5.20	1.20	1.25
1	A	1868	TYR	CG-CD1	-5.20	1.32	1.39
1	E	2402	TYR	CB-CG	-5.20	1.43	1.51
1	E	1021	TRP	CB-CG	-5.20	1.40	1.50
1	E	1034	VAL	CB-CG2	-5.19	1.42	1.52
2	F	96	PHE	CB-CG	-5.19	1.42	1.51
2	F	687	TRP	CB-CG	-5.19	1.41	1.50
1	A	1853	PHE	CB-CG	-5.18	1.42	1.51
1	C	1017	PHE	CB-CG	-5.17	1.42	1.51
1	B	776	PHE	CG-CD2	-5.16	1.31	1.38
1	C	1143	GLU	CG-CD	-5.15	1.44	1.51
1	D	2096	PHE	CB-CG	-5.15	1.42	1.51
2	F	859	TYR	CE2-CZ	-5.15	1.31	1.38
1	B	2265	PHE	CB-CG	-5.15	1.42	1.51
1	C	2308	GLU	CD-OE2	-5.14	1.20	1.25
1	A	1650	TYR	CB-CG	-5.14	1.44	1.51
1	E	763	GLU	CG-CD	-5.14	1.44	1.51
1	A	1086	GLU	CD-OE1	-5.14	1.20	1.25
2	F	1299	TRP	CZ3-CH2	-5.14	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	390	GLU	CD-OE1	-5.13	1.20	1.25
1	E	390	GLU	CG-CD	-5.13	1.44	1.51
1	D	1805	TYR	CB-CG	-5.13	1.44	1.51
1	C	614	GLU	CD-OE2	-5.12	1.20	1.25
1	B	534	GLU	CD-OE2	-5.12	1.20	1.25
1	B	1143	GLU	CD-OE2	-5.12	1.20	1.25
1	E	2473	GLU	CG-CD	-5.12	1.44	1.51
1	D	1236	CYS	CB-SG	-5.12	1.73	1.81
2	F	228	TYR	CB-CG	-5.11	1.44	1.51
1	D	1595	TYR	CB-CG	-5.11	1.44	1.51
1	E	109	VAL	CB-CG1	-5.11	1.42	1.52
2	F	355	GLU	CD-OE2	-5.11	1.20	1.25
1	B	205	GLU	CD-OE2	-5.11	1.20	1.25
1	E	1721	TRP	CB-CG	-5.11	1.41	1.50
1	B	1658	GLU	CD-OE1	-5.10	1.20	1.25
1	C	652	PHE	CB-CG	-5.10	1.42	1.51
1	D	1628	GLU	CD-OE2	-5.10	1.20	1.25
1	E	816	GLU	CD-OE2	-5.10	1.20	1.25
1	E	1650	TYR	CB-CG	-5.10	1.44	1.51
1	D	703	SER	CB-OG	-5.09	1.35	1.42
2	F	286	ARG	CD-NE	-5.09	1.37	1.46
1	D	2308	GLU	CD-OE2	-5.09	1.20	1.25
1	C	121	GLU	CD-OE2	-5.08	1.20	1.25
1	E	1196	TYR	CB-CG	-5.07	1.44	1.51
1	C	2435	TYR	CB-CG	-5.07	1.44	1.51
1	A	766	TYR	CD1-CE1	-5.06	1.31	1.39
1	C	875	ASN	CB-CG	-5.06	1.39	1.51
1	C	2280	TYR	CB-CG	-5.06	1.44	1.51
1	C	996	TYR	CG-CD2	-5.05	1.32	1.39
1	A	205	GLU	CD-OE2	-5.05	1.20	1.25
1	B	528	TYR	CB-CG	-5.05	1.44	1.51
1	D	695	TYR	CB-CG	-5.05	1.44	1.51
1	A	730	PHE	CB-CG	-5.04	1.42	1.51
1	B	1805	TYR	CD1-CE1	-5.04	1.31	1.39
1	A	1163	TYR	CG-CD1	-5.04	1.32	1.39
1	A	2096	PHE	CB-CG	-5.04	1.42	1.51
1	D	328	TYR	CB-CG	-5.04	1.44	1.51
1	B	1086	GLU	CD-OE1	-5.04	1.20	1.25
1	C	1163	TYR	CD1-CE1	-5.04	1.31	1.39
1	C	915	TRP	CB-CG	-5.03	1.41	1.50
2	F	174	ARG	CB-CG	-5.03	1.39	1.52
1	C	328	TYR	CB-CG	-5.03	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	193	ARG	CG-CD	-5.03	1.39	1.51
1	D	1765	SER	CA-CB	-5.02	1.45	1.52
1	E	1598	TRP	CB-CG	-5.01	1.41	1.50
2	F	887	TYR	CB-CG	-5.01	1.44	1.51
1	B	1042	GLU	CD-OE2	-5.01	1.20	1.25
2	F	495	GLU	CD-OE2	-5.01	1.20	1.25
1	A	2308	GLU	CD-OE2	-5.01	1.20	1.25
1	D	118	TYR	CE2-CZ	-5.01	1.32	1.38

All (303) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	354	ARG	NE-CZ-NH2	-12.65	113.97	120.30
1	E	1616	ARG	NE-CZ-NH2	-11.43	114.59	120.30
2	F	286	ARG	NE-CZ-NH1	-11.17	114.72	120.30
2	F	1585	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	E	2018	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	C	1616	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	B	1869	ARG	NE-CZ-NH2	-10.09	115.25	120.30
1	C	517	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	D	547	ARG	NE-CZ-NH2	-9.77	115.41	120.30
1	C	2018	ARG	NE-CZ-NH2	-9.68	115.46	120.30
2	F	174	ARG	NE-CZ-NH2	-9.59	115.50	120.30
2	F	2117	ARG	NE-CZ-NH1	-9.53	115.53	120.30
2	F	424	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	B	2018	ARG	NE-CZ-NH2	-9.33	115.63	120.30
2	F	1585	ARG	NE-CZ-NH1	9.25	124.93	120.30
1	C	353	TYR	CB-CG-CD1	-9.16	115.50	121.00
1	A	2018	ARG	NE-CZ-NH2	-9.10	115.75	120.30
2	F	871	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	E	1124	ARG	NE-CZ-NH2	-8.99	115.81	120.30
1	C	1124	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	E	2216	ARG	NE-CZ-NH2	-8.93	115.84	120.30
2	F	174	ARG	NE-CZ-NH1	8.89	124.74	120.30
1	B	1124	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	A	1650	TYR	CB-CG-CD1	-8.79	115.73	121.00
1	E	1650	TYR	CB-CG-CD1	-8.78	115.73	121.00
1	C	1204	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	E	1305	ARG	NE-CZ-NH1	8.55	124.57	120.30
1	D	1166	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	B	1322	TYR	CB-CG-CD1	-8.48	115.91	121.00
2	F	1044	ARG	NE-CZ-NH2	-8.47	116.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1650	TYR	CB-CG-CD1	-8.47	115.92	121.00
1	E	547	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	E	1159	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	A	2410	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	B	1159	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	D	487	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	C	1650	TYR	CB-CG-CD1	-8.27	116.04	121.00
2	F	302	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	C	807	PHE	CB-CG-CD2	8.20	126.54	120.80
1	E	1563	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	D	2512	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	E	1601	TYR	CB-CG-CD2	-7.97	116.22	121.00
1	A	1611	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	B	1563	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	A	1868	TYR	CB-CG-CD1	-7.95	116.23	121.00
1	B	137	TYR	CB-CG-CD1	-7.92	116.25	121.00
1	D	1124	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	B	1794	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	E	942	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	2512	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	C	807	PHE	CB-CG-CD1	-7.82	115.32	120.80
2	F	131	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	C	2410	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	D	448	ARG	NE-CZ-NH2	7.71	124.15	120.30
1	B	942	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	C	1611	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	B	1611	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	D	1794	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	B	2512	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	D	208	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	D	1611	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	C	1369	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	A	942	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	A	2216	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	B	2216	ARG	NE-CZ-NH2	-7.50	116.55	120.30
2	F	1383	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	766	TYR	CB-CG-CD1	-7.42	116.55	121.00
2	F	1411	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	E	2216	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	E	1868	TYR	CB-CG-CD1	-7.36	116.58	121.00
2	F	1436	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	E	1050	ARG	NE-CZ-NH1	7.30	123.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	547	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	C	1040	TYR	CB-CG-CD1	-7.24	116.65	121.00
1	B	1305	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	D	1168	TYR	CB-CG-CD2	-7.22	116.67	121.00
1	B	1305	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	B	1166	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	D	2410	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	D	1650	TYR	CB-CG-CD1	-7.05	116.77	121.00
2	F	49	ARG	NE-CZ-NH1	7.04	123.82	120.30
2	F	2051	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	528	TYR	CB-CG-CD1	-7.01	116.79	121.00
1	C	1168	TYR	CB-CG-CD2	-6.99	116.81	121.00
1	E	1305	ARG	NE-CZ-NH2	-6.97	116.82	120.30
2	F	917	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	B	1868	TYR	CB-CG-CD1	-6.94	116.83	121.00
1	B	1050	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	C	2512	ARG	NE-CZ-NH2	-6.87	116.87	120.30
2	F	1139	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	B	1601	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	A	1204	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	E	1286	TYR	CB-CG-CD2	-6.81	116.91	121.00
2	F	800	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	E	1072	ASP	CB-CG-OD1	6.76	124.38	118.30
1	A	1369	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	C	2216	ARG	NE-CZ-NH2	-6.73	116.94	120.30
2	F	625	TYR	CB-CG-CD1	-6.67	117.00	121.00
1	B	1287	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	C	1601	TYR	CB-CG-CD2	-6.62	117.03	121.00
1	E	806	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	434	TYR	CB-CG-CD1	-6.55	117.07	121.00
1	E	1711	PHE	CB-CG-CD2	6.55	125.38	120.80
2	F	2114	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	B	1040	TYR	CB-CG-CD1	-6.47	117.11	121.00
2	F	49	ARG	NE-CZ-NH2	-6.47	117.06	120.30
2	F	1001	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	C	2399	ARG	NE-CZ-NH2	-6.46	117.07	120.30
2	F	1383	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	E	1982	TYR	CB-CG-CD1	-6.41	117.15	121.00
1	E	204	TYR	CB-CG-CD2	-6.41	117.16	121.00
2	F	1205	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	E	1168	TYR	CB-CG-CD2	-6.39	117.17	121.00
1	C	1794	ARG	NE-CZ-NH2	-6.37	117.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	332	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	D	1982	TYR	CB-CG-CD1	-6.35	117.19	121.00
1	D	2512	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	F	768	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	1287	ARG	NE-CZ-NH2	-6.32	117.14	120.30
2	F	196	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	C	517	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	E	448	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	D	1616	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	208	ARG	NE-CZ-NH2	-6.28	117.16	120.30
2	F	859	TYR	CB-CG-CD2	-6.27	117.24	121.00
2	F	1167	ARG	NE-CZ-NH2	-6.26	117.17	120.30
2	F	976	TYR	CB-CG-CD1	-6.26	117.24	121.00
2	F	2051	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	999	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	D	1148	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	2266	TYR	CB-CG-CD2	-6.24	117.26	121.00
1	D	354	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	C	2411	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	208	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	D	2428	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	2512	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	B	484	TYR	CB-CG-CD1	-6.19	117.29	121.00
2	F	131	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	1050	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	E	1358	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	1050	ARG	NE-CZ-NH2	6.15	123.38	120.30
1	C	2512	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	C	1711	PHE	CB-CG-CD2	6.13	125.09	120.80
2	F	1848	ARG	NE-CZ-NH2	6.11	123.36	120.30
2	F	1367	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	D	2411	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	D	1306	TYR	CB-CG-CD2	-6.08	117.35	121.00
2	F	332	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	F	2125	ARG	NE-CZ-NH2	-6.08	117.26	120.30
2	F	1789	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	D	519	PHE	CB-CG-CD2	6.06	125.04	120.80
1	E	488	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	C	1166	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	E	2018	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	B	1159	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	E	1166	ARG	NE-CZ-NH1	5.99	123.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1412	TYR	CB-CG-CD1	-5.99	117.41	121.00
1	A	1711	PHE	CB-CG-CD2	5.98	124.99	120.80
2	F	1790	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	E	1369	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	C	1204	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	B	103	TYR	CB-CG-CD2	-5.96	117.42	121.00
1	A	332	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	E	1711	PHE	CB-CG-CD1	-5.95	116.63	120.80
2	F	1318	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	1883	TYR	CB-CG-CD1	-5.94	117.44	121.00
1	C	1305	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	C	1072	ASP	CB-CG-OD1	5.93	123.64	118.30
1	D	2118	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	C	1305	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	D	1986	TYR	CB-CG-CD1	-5.89	117.47	121.00
1	C	421	TYR	CB-CG-CD1	-5.89	117.47	121.00
2	F	1790	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	2324	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	412	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	E	2411	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	412	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	D	2216	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	E	547	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	F	921	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	A	1024	TYR	CB-CG-CD2	-5.67	117.60	121.00
2	F	259	TYR	CB-CG-CD1	-5.67	117.60	121.00
1	B	890	ALA	C-N-CD	-5.65	108.17	120.60
2	F	754	GLU	N-CA-C	-5.64	95.77	111.00
1	A	555	PHE	CB-CG-CD1	-5.63	116.86	120.80
1	C	942	ARG	NE-CZ-NH2	-5.63	117.49	120.30
2	F	713	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	F	1115	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	C	2266	TYR	CB-CG-CD2	-5.60	117.64	121.00
2	F	1044	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	1168	TYR	CB-CG-CD2	-5.59	117.65	121.00
2	F	906	TYR	CB-CG-CD1	-5.59	117.65	121.00
1	C	1194	TYR	CB-CG-CD2	-5.57	117.66	121.00
1	D	2266	TYR	CB-CG-CD2	-5.56	117.66	121.00
1	C	1072	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	E	1124	ARG	CB-CA-C	-5.55	99.30	110.40
1	A	1982	TYR	CB-CG-CD2	-5.54	117.67	121.00
1	C	1027	ARG	NE-CZ-NH2	-5.54	117.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2217	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	F	2112	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	A	2324	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	F	1972	TYR	CB-CG-CD1	-5.51	117.69	121.00
1	A	136	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	C	353	TYR	CB-CG-CD2	5.50	124.30	121.00
1	C	1124	ARG	CB-CA-C	-5.50	99.39	110.40
1	E	2217	ARG	NE-CZ-NH2	-5.49	117.56	120.30
2	F	94	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	2512	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	E	1024	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	B	2266	TYR	CB-CG-CD2	-5.46	117.73	121.00
1	E	412	ARG	NE-CZ-NH2	-5.45	117.57	120.30
2	F	267	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	D	448	ARG	NE-CZ-NH1	-5.44	117.58	120.30
2	F	2100	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	D	2399	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	2217	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	672	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	825	PHE	CB-CG-CD2	-5.41	117.01	120.80
1	B	2411	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	902	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	C	1050	ARG	NE-CZ-NH1	-5.40	117.60	120.30
2	F	1848	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	C	2399	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	807	PHE	CB-CG-CD2	5.38	124.56	120.80
1	B	779	PHE	CB-CA-C	-5.38	99.65	110.40
1	A	208	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	C	2217	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	D	1272	ASP	N-CA-C	-5.37	96.51	111.00
1	D	2217	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	F	51	TYR	CB-CG-CD1	-5.34	117.79	121.00
2	F	1425	TYR	CB-CG-CD1	-5.34	117.79	121.00
2	F	2033	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	E	2513	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	A	2411	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	E	2266	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	B	1711	PHE	CB-CG-CD2	5.33	124.53	120.80
1	E	2428	ASP	CB-CG-OD1	5.32	123.09	118.30
2	F	1318	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	1168	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	A	2005	GLY	N-CA-C	-5.30	99.85	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1040	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	A	354	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	E	2095	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	B	1286	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	C	890	ALA	C-N-CD	-5.28	108.99	120.60
1	D	1305	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	1040	TYR	CB-CG-CD1	-5.27	117.84	121.00
1	C	2018	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	C	308	TYR	CB-CG-CD1	-5.26	117.85	121.00
2	F	2089	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	2095	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	2006	GLY	N-CA-C	-5.24	100.00	113.10
1	C	1664	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	E	996	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	E	412	ARG	NE-CZ-NH1	5.23	122.92	120.30
2	F	300	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	C	675	TYR	CB-CG-CD2	-5.21	117.88	121.00
1	D	952	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	E	1072	ASP	CB-CG-OD2	-5.20	113.62	118.30
2	F	419	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	D	412	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	E	890	ALA	C-N-CD	-5.19	109.18	120.60
2	F	370	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	A	1604	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	391	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	D	1040	TYR	CB-CG-CD1	-5.16	117.90	121.00
1	B	2018	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	E	1124	ARG	NE-CZ-NH1	5.15	122.87	120.30
2	F	765	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	1814	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	C	1616	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	1711	PHE	CB-CG-CD1	-5.13	117.21	120.80
1	D	1305	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	1204	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	2399	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	D	334	TYR	CB-CG-CD2	-5.10	117.94	121.00
2	F	1488	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	E	2399	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	D	1027	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	E	434	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	D	1794	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	F	1449	ARG	NE-CZ-NH2	-5.07	117.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1650	TYR	CB-CG-CD2	5.06	124.04	121.00
2	F	688	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	E	1616	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	D	2153	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	F	286	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	B	359	PHE	CB-CG-CD1	5.03	124.32	120.80
1	B	2399	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	D	1286	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	E	332	ARG	NE-CZ-NH2	-5.03	117.79	120.30
2	F	987	TYR	CB-CG-CD2	-5.03	117.98	121.00
2	F	1329	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	1664	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	D	376	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	528	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	B	603	ASP	CB-CG-OD2	5.01	122.81	118.30
1	C	1196	TYR	CB-CG-CD2	-5.01	117.99	121.00
1	C	1711	PHE	CB-CG-CD1	-5.01	117.29	120.80
1	D	137	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	E	487	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	B	1805	TYR	CB-CG-CD1	-5.01	118.00	121.00
1	C	1604	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	766	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	18197	0	17794	38	0
1	B	18197	0	17794	47	0
1	C	18197	0	17794	45	0
1	D	18197	0	17794	38	0
1	E	18197	0	17794	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	17285	0	16668	43	0
All	All	108270	0	105638	240	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 (240) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1623:THR:OG1	1:B:1624:ILE:N	2.32	0.61
1:E:1774:TYR:HH	1:E:1848:TYR:HH	1.47	0.60
1:B:2319:ASP:OD2	1:B:2323:LYS:NZ	2.36	0.58
1:B:2358:ASP:OD1	1:B:2502:LYS:NZ	2.38	0.57
2:F:1416:ASP:OD1	2:F:1416:ASP:N	2.37	0.57
1:C:624:ASP:N	1:C:624:ASP:OD1	2.37	0.57
1:E:624:ASP:OD1	1:E:624:ASP:N	2.37	0.57
1:D:1148:ASP:N	1:D:1148:ASP:OD1	2.33	0.56
1:A:2207:ASP:OD2	1:A:2211:LYS:NZ	2.38	0.56
1:D:624:ASP:N	1:D:624:ASP:OD1	2.37	0.56
1:C:329:ARG:NH1	1:C:434:TYR:OH	2.39	0.56
1:C:2207:ASP:OD2	1:C:2211:LYS:NZ	2.38	0.56
1:B:624:ASP:N	1:B:624:ASP:OD1	2.37	0.56
1:B:1072:ASP:OD1	1:B:1072:ASP:N	2.36	0.56
1:D:253:GLU:O	1:D:442:LYS:NZ	2.38	0.56
2:F:73:ASP:OD1	2:F:74:CYS:N	2.39	0.56
1:A:2319:ASP:OD2	1:A:2323:LYS:NZ	2.39	0.56
1:B:1626:SER:OG	1:B:1627:MET:N	2.40	0.55
1:A:2358:ASP:OD1	1:A:2502:LYS:NZ	2.39	0.55
1:A:624:ASP:OD1	1:A:624:ASP:N	2.38	0.55
1:B:1774:TYR:OH	1:B:1848:TYR:OH	2.24	0.54
2:F:385:ASP:OD1	2:F:385:ASP:N	2.39	0.54
2:F:829:ASP:OD1	2:F:829:ASP:N	2.39	0.54
1:B:2257:ARG:NH2	1:C:2309:THR:OG1	2.40	0.54
1:D:890:ALA:O	1:D:892:GLN:N	2.42	0.53
1:A:1225:LYS:NZ	1:A:1226:LEU:O	2.40	0.53
1:D:2257:ARG:NH2	1:E:2309:THR:OG1	2.42	0.53
1:E:2358:ASP:OD1	1:E:2502:LYS:NZ	2.42	0.52
1:C:890:ALA:O	1:C:892:GLN:N	2.41	0.52
1:E:548:LYS:NZ	1:E:559:ASP:OD1	2.42	0.52
1:E:890:ALA:O	1:E:892:GLN:N	2.42	0.52
1:B:1774:TYR:HH	1:B:1848:TYR:HH	1.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:890:ALA:O	1:B:892:GLN:N	2.42	0.52
1:A:1120:GLU:OE2	1:A:1146:LYS:NZ	2.42	0.52
1:D:1683:ASP:OD1	1:D:1683:ASP:N	2.43	0.52
1:D:301:SER:OG	1:D:302:ASN:N	2.42	0.51
2:F:179:SER:OG	2:F:180:GLN:N	2.43	0.51
1:A:1164:LYS:NZ	1:B:1622:ASP:OD2	2.36	0.51
1:C:540:SER:OG	1:C:541:GLY:N	2.44	0.51
1:C:1291:TYR:O	1:C:1292:GLN:HB3	2.11	0.51
1:A:261:GLU:OE1	1:A:1380:LYS:NZ	2.44	0.50
1:D:2319:ASP:OD2	1:D:2323:LYS:NZ	2.45	0.50
1:E:1841:ALA:O	1:E:1842:GLN:HB2	2.11	0.50
1:D:797:ASP:OD1	1:D:798:ALA:N	2.45	0.50
1:D:848:GLN:HE21	1:D:852:GLN:HE21	1.60	0.50
1:A:890:ALA:O	1:A:892:GLN:N	2.45	0.50
1:B:540:SER:OG	1:B:541:GLY:N	2.44	0.50
1:B:1683:ASP:N	1:B:1683:ASP:OD1	2.43	0.50
2:F:754:GLU:O	2:F:755:ILE:HB	2.12	0.50
2:F:1133:THR:OG1	2:F:1134:ALA:N	2.45	0.50
1:B:342:ASP:OD2	1:B:360:LYS:NZ	2.44	0.49
2:F:616:ASP:N	2:F:616:ASP:OD1	2.45	0.49
1:C:1117:ASP:OD1	1:C:1118:ALA:N	2.45	0.49
1:A:180:GLU:OE1	1:A:184:LYS:NZ	2.45	0.49
1:C:301:SER:OG	1:C:302:ASN:N	2.46	0.49
1:E:161:THR:O	1:E:162:LEU:HB3	2.13	0.49
1:D:2466:ASP:N	1:D:2466:ASP:OD1	2.46	0.48
1:E:176:GLU:OE2	1:E:956:LYS:NZ	2.47	0.48
1:E:2287:ASP:N	1:E:2287:ASP:OD1	2.45	0.48
2:F:1687:ASP:N	2:F:1687:ASP:OD1	2.38	0.48
1:E:2466:ASP:N	1:E:2466:ASP:OD1	2.46	0.48
2:F:153:ASP:O	2:F:174:ARG:NH2	2.46	0.48
2:F:1234:SER:OG	2:F:1235:ASP:N	2.46	0.48
1:C:1841:ALA:O	1:C:1842:GLN:HB2	2.14	0.48
1:D:521:THR:H	1:D:522:PRO:HD2	1.79	0.48
1:D:1333:TYR:CG	1:D:1334:ASN:N	2.82	0.48
1:B:2380:GLY:N	1:B:2383:THR:OG1	2.46	0.48
1:A:1774:TYR:OH	1:A:1848:TYR:OH	2.28	0.48
1:B:1841:ALA:O	1:B:1842:GLN:HB2	2.14	0.48
2:F:161:ASP:N	2:F:161:ASP:OD1	2.42	0.48
1:A:1561:ASP:OD1	1:A:1561:ASP:N	2.46	0.47
1:A:1834:SER:OG	1:A:1835:VAL:N	2.47	0.47
1:B:1148:ASP:OD1	1:B:1148:ASP:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1178:THR:OG1	1:B:1179:LYS:N	2.47	0.47
1:C:1178:THR:OG1	1:C:1179:LYS:N	2.46	0.47
1:B:1514:ASP:N	1:B:1514:ASP:OD1	2.46	0.47
1:D:1841:ALA:O	1:D:1842:GLN:HB2	2.13	0.47
1:B:1834:SER:OG	1:B:1835:VAL:N	2.46	0.47
1:E:1991:ASP:OD2	1:E:1993:LYS:NZ	2.45	0.47
1:A:1343:LYS:NZ	1:B:1803:SER:O	2.47	0.47
1:B:1975:SER:OG	1:B:1976:ILE:N	2.48	0.47
2:F:830:GLN:O	2:F:955:ARG:NH2	2.47	0.47
1:B:2103:TYR:O	1:B:2189:ARG:NH1	2.48	0.47
1:B:2284:LEU:O	1:B:2286:ASP:N	2.48	0.47
1:C:1333:TYR:CG	1:C:1334:ASN:N	2.82	0.47
1:E:540:SER:OG	1:E:541:GLY:N	2.47	0.47
1:E:1124:ARG:HD3	1:E:1144:TRP:CD2	2.50	0.47
2:F:431:ASP:OD1	2:F:431:ASP:N	2.44	0.47
1:B:533:ASP:OD1	1:B:533:ASP:N	2.37	0.47
1:C:872:THR:O	1:C:873:SER:HB2	2.15	0.47
1:B:477:LYS:NZ	1:B:624:ASP:OD2	2.40	0.46
1:D:290:ASP:OD1	1:D:290:ASP:N	2.43	0.46
1:E:1840:VAL:C	1:E:1841:ALA:O	2.52	0.46
1:A:2103:TYR:O	1:A:2189:ARG:NH1	2.49	0.46
1:C:1206:ASP:N	1:C:1206:ASP:OD1	2.42	0.46
1:E:270:ASN:OD1	1:E:270:ASN:N	2.46	0.46
2:F:1793:ASP:N	2:F:1793:ASP:OD1	2.47	0.46
1:A:1133:ASP:OD1	1:A:1133:ASP:N	2.40	0.46
1:C:270:ASN:OD1	1:C:270:ASN:N	2.48	0.46
1:D:1834:SER:OG	1:D:1835:VAL:N	2.49	0.46
1:E:1514:ASP:OD2	1:E:1515:LYS:NZ	2.46	0.46
1:B:1183:ASN:OD1	1:B:1183:ASN:N	2.44	0.46
1:C:1975:SER:OG	1:C:1976:ILE:N	2.47	0.46
1:C:1290:SER:C	1:C:1291:TYR:O	2.49	0.46
1:D:161:THR:O	1:D:162:LEU:HB3	2.16	0.46
2:F:1329:ASP:N	2:F:1329:ASP:OD1	2.43	0.46
1:B:1333:TYR:O	1:B:1334:ASN:C	2.54	0.46
1:D:342:ASP:OD2	1:D:360:LYS:NZ	2.46	0.46
1:D:2008:LYS:NZ	1:D:2267:ASP:OD2	2.43	0.46
1:E:2103:TYR:O	1:E:2189:ARG:NH1	2.49	0.45
2:F:1055:THR:OG1	2:F:1056:ASP:N	2.49	0.45
1:C:176:GLU:OE2	1:C:956:LYS:NZ	2.48	0.45
1:A:1683:ASP:N	1:A:1683:ASP:OD1	2.43	0.45
1:E:1046:ASP:OD1	1:E:1046:ASP:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:TYR:CZ	1:B:391:TYR:HB2	2.52	0.45
1:C:1829:SER:OG	1:C:1830:ASP:N	2.50	0.45
1:C:1977:ASP:N	1:C:1977:ASP:OD1	2.45	0.45
1:A:842:ASP:OD1	1:A:843:ALA:N	2.50	0.45
1:C:1834:SER:OG	1:C:1835:VAL:N	2.50	0.45
1:C:1124:ARG:HD3	1:C:1144:TRP:CD2	2.52	0.45
1:C:2103:TYR:O	1:C:2189:ARG:NH1	2.50	0.45
1:D:766:TYR:CD1	1:D:771:ILE:HD11	2.52	0.45
1:E:1834:SER:OG	1:E:1835:VAL:N	2.50	0.45
1:D:329:ARG:HB3	1:D:431:TYR:CE1	2.53	0.44
1:B:250:ILE:O	1:B:442:LYS:NZ	2.50	0.44
1:D:2284:LEU:O	1:D:2286:ASP:N	2.50	0.44
2:F:754:GLU:O	2:F:755:ILE:CB	2.65	0.44
1:A:161:THR:O	1:A:162:LEU:HB3	2.17	0.44
1:E:533:ASP:OD1	1:E:533:ASP:N	2.48	0.44
1:B:1343:LYS:NZ	1:C:1803:SER:O	2.50	0.44
1:C:2457:SER:OG	1:C:2458:GLY:N	2.50	0.44
1:C:2466:ASP:N	1:C:2466:ASP:OD1	2.45	0.44
1:D:1975:SER:OG	1:D:1976:ILE:N	2.50	0.44
1:D:2365:SER:OG	1:D:2366:GLY:N	2.50	0.44
1:E:963:SER:OG	1:E:964:ARG:N	2.48	0.44
1:C:336:THR:OG1	1:C:337:ASN:N	2.49	0.44
2:F:1427:ASP:OD1	2:F:1427:ASP:C	2.55	0.44
1:A:1622:ASP:OD2	1:E:1164:LYS:NZ	2.35	0.44
1:B:963:SER:OG	1:B:964:ARG:N	2.50	0.44
1:D:439:LYS:NZ	1:D:458:GLU:OE2	2.41	0.44
2:F:904:SER:O	2:F:905:ARG:C	2.56	0.44
1:A:537:ASP:OD1	1:A:538:LEU:N	2.51	0.44
1:B:2466:ASP:OD1	1:B:2466:ASP:N	2.47	0.44
1:E:2365:SER:OG	1:E:2366:GLY:N	2.51	0.44
1:C:1683:ASP:OD1	1:C:1683:ASP:N	2.43	0.44
1:D:963:SER:OG	1:D:964:ARG:N	2.49	0.44
2:F:618:SER:OG	2:F:619:GLY:N	2.50	0.44
2:F:1591:THR:OG1	2:F:1592:ALA:N	2.51	0.44
1:A:2466:ASP:N	1:A:2466:ASP:OD1	2.50	0.43
2:F:530:ASP:N	2:F:530:ASP:OD1	2.51	0.43
2:F:209:ASP:OD1	2:F:209:ASP:N	2.46	0.43
2:F:1912:ASN:O	2:F:2125:ARG:NH2	2.51	0.43
1:D:1257:ASP:N	1:D:1257:ASP:OD1	2.46	0.43
1:A:534:GLU:OE1	1:A:534:GLU:N	2.52	0.43
1:C:1662:LYS:NZ	1:C:1830:ASP:OD2	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:693:ALA:HB3	1:D:694:PRO:HD3	2.01	0.43
1:E:1507:LYS:NZ	1:E:1538:ASP:OD2	2.41	0.43
2:F:253:GLN:O	2:F:259:TYR:OH	2.36	0.43
1:A:1183:ASN:OD1	1:A:1183:ASN:N	2.50	0.43
1:C:1507:LYS:NZ	1:C:1538:ASP:OD2	2.39	0.43
1:B:1138:ALA:HB3	1:B:1842:GLN:OE1	2.19	0.43
1:E:975:ASN:N	1:E:975:ASN:OD1	2.42	0.43
1:E:1183:ASN:OD1	1:E:1183:ASN:N	2.48	0.43
1:A:2347:ASP:OD1	1:A:2347:ASP:N	2.47	0.42
1:D:1291:TYR:O	1:D:1292:GLN:HB2	2.19	0.42
2:F:1370:ASP:N	2:F:1370:ASP:OD1	2.48	0.42
2:F:2090:ASN:OD1	2:F:2091:GLN:N	2.52	0.42
1:A:1524:SER:OG	1:A:1525:PHE:N	2.51	0.42
1:C:1561:ASP:N	1:C:1561:ASP:OD1	2.48	0.42
1:E:329:ARG:HB3	1:E:431:TYR:CE1	2.54	0.42
1:C:1137:ALA:O	1:C:1138:ALA:HB3	2.19	0.42
1:E:2284:LEU:O	1:E:2286:ASP:N	2.52	0.42
1:C:196:GLY:N	1:C:285:TYR:OH	2.52	0.42
1:B:1729:ASP:OD2	1:B:1730:LYS:NZ	2.52	0.42
2:F:1442:THR:OG1	2:F:1443:ALA:N	2.52	0.42
1:C:1291:TYR:O	1:C:1292:GLN:CB	2.65	0.42
1:D:1124:ARG:HD2	1:D:1144:TRP:CE2	2.54	0.42
1:E:1774:TYR:OH	1:E:1848:TYR:OH	2.21	0.42
1:A:176:GLU:OE2	1:A:956:LYS:NZ	2.50	0.42
1:E:771:ILE:HD12	1:E:776:PHE:HA	2.00	0.42
1:B:1333:TYR:O	1:B:1335:GLY:N	2.53	0.42
1:C:353:TYR:CE1	1:C:397:LEU:HB2	2.54	0.42
1:E:386:GLN:OE1	1:E:391:TYR:OH	2.38	0.42
1:C:477:LYS:NZ	1:C:624:ASP:OD2	2.39	0.42
1:C:2496:LYS:NZ	1:D:2401:ASP:OD1	2.49	0.42
1:D:773:GLU:HA	1:D:776:PHE:CD1	2.55	0.42
1:D:2287:ASP:OD1	1:D:2287:ASP:N	2.46	0.42
2:F:2117:ARG:NH1	2:F:2140:LEU:O	2.53	0.42
1:A:2382:ASP:OD1	1:A:2382:ASP:N	2.47	0.42
1:B:93:ASN:OD1	1:B:93:ASN:N	2.47	0.42
1:C:1908:ASP:N	1:C:1908:ASP:OD1	2.52	0.42
1:A:488:TYR:OH	1:A:635:ASN:OD1	2.36	0.41
1:B:1124:ARG:HD2	1:B:1144:TRP:CD2	2.55	0.41
1:A:1991:ASP:OD2	1:A:1993:LYS:NZ	2.47	0.41
1:D:1977:ASP:N	1:D:1977:ASP:OD1	2.44	0.41
1:E:857:GLN:CD	1:E:857:GLN:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2358:ASP:OD1	1:C:2502:LYS:NZ	2.49	0.41
1:B:2382:ASP:OD1	1:B:2382:ASP:N	2.51	0.41
1:B:455:THR:OG1	1:B:456:ILE:N	2.53	0.41
1:B:1124:ARG:HG3	1:B:1144:TRP:CE3	2.55	0.41
1:C:856:HIS:NE2	1:C:895:SER:OG	2.54	0.41
1:E:299:LYS:NZ	1:E:458:GLU:OE2	2.53	0.41
1:A:1333:TYR:O	1:A:1334:ASN:C	2.58	0.41
1:A:1684:THR:OG1	1:A:1685:ASN:N	2.54	0.41
1:B:1117:ASP:OD1	1:B:1118:ALA:N	2.53	0.41
1:D:1840:VAL:C	1:D:1841:ALA:O	2.56	0.41
1:A:2365:SER:OG	1:A:2366:GLY:N	2.53	0.41
1:B:736:THR:OG1	1:B:737:LYS:N	2.50	0.41
1:D:782:LYS:N	1:D:783:PRO:HD3	2.36	0.41
2:F:772:ASP:OD1	2:F:779:ARG:NE	2.53	0.41
2:F:574:SER:OG	2:F:575:ALA:N	2.54	0.41
1:A:2103:TYR:CE1	1:A:2193:GLU:HB2	2.55	0.41
1:B:2382:ASP:OD2	1:C:2404:ALA:N	2.54	0.41
1:B:2478:ASP:OD1	1:B:2478:ASP:N	2.40	0.41
1:D:322:ASP:OD1	1:D:322:ASP:N	2.32	0.41
1:D:707:VAL:HG13	1:D:776:PHE:CD2	2.55	0.41
2:F:1484:ASP:OD2	2:F:1486:LYS:NZ	2.37	0.41
1:B:831:THR:OG1	1:B:832:ALA:N	2.54	0.41
2:F:1268:PHE:O	2:F:1272:ALA:N	2.55	0.41
2:F:1515:ASN:N	2:F:1515:ASN:OD1	2.46	0.41
2:F:2044:ASP:OD1	2:F:2044:ASP:N	2.45	0.41
1:A:465:ASN:O	1:A:466:LEU:C	2.58	0.40
1:C:1497:LYS:HB3	1:C:1558:PHE:HB2	2.02	0.40
2:F:1247:PRO:HA	2:F:1332:ASP:OD1	2.21	0.40
1:C:2287:ASP:N	1:C:2287:ASP:OD1	2.45	0.40
1:B:2459:GLN:OE1	1:B:2459:GLN:N	2.53	0.40
1:C:542:SER:OG	1:C:543:THR:N	2.49	0.40
2:F:269:ASN:OD1	2:F:269:ASN:N	2.47	0.40
2:F:283:TRP:CZ3	2:F:303:ARG:HB3	2.56	0.40
2:F:1393:ASP:OD1	2:F:1393:ASP:N	2.49	0.40
1:A:2466:ASP:OD1	1:A:2467:GLY:N	2.55	0.40
1:C:322:ASP:OD1	1:C:323:GLY:N	2.54	0.40
1:E:1153:PRO:O	1:E:1154:TYR:C	2.60	0.40
1:E:1559:ALA:HB3	1:E:1563:ARG:HG2	2.04	0.40
2:F:6:ASP:OD1	2:F:6:ASP:N	2.44	0.40
2:F:1329:ASP:OD1	2:F:1330:ARG:N	2.54	0.40
1:A:545:ASP:C	1:A:545:ASP:OD1	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:ALA:HB3	1:A:694:PRO:HD3	2.03	0.40
1:E:137:TYR:CE2	1:E:139:ASP:HB2	2.57	0.40
2:F:841:THR:OG1	2:F:842:TRP:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2286/2516 (91%)	2240 (98%)	40 (2%)	6 (0%)	41	72
1	B	2286/2516 (91%)	2225 (97%)	54 (2%)	7 (0%)	41	72
1	C	2286/2516 (91%)	2225 (97%)	56 (2%)	5 (0%)	47	78
1	D	2286/2516 (91%)	2233 (98%)	46 (2%)	7 (0%)	41	72
1	E	2286/2516 (91%)	2239 (98%)	39 (2%)	8 (0%)	41	72
2	F	2162/2439 (89%)	2111 (98%)	46 (2%)	5 (0%)	47	78
All	All	13592/15019 (90%)	13273 (98%)	281 (2%)	38 (0%)	44	72

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	891	PRO
1	B	891	PRO
1	C	891	PRO
1	D	891	PRO
1	E	790	THR
1	E	891	PRO
1	A	991	ALA
1	A	1334	ASN
1	B	1138	ALA

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Mol	Chain	Res	Type
1	B	1334	ASN
1	C	991	ALA
1	C	1334	ASN
1	D	991	ALA
1	D	1138	ALA
1	E	991	ALA
1	E	1154	TYR
2	F	755	ILE
1	D	1292	GLN
2	F	137	HIS
2	F	602	ALA
1	B	1190	THR
1	C	1758	MET
1	E	659	TYR
1	A	890	ALA
1	A	1758	MET
1	A	1953	ASN
1	B	101	SER
1	B	2425	PRO
1	D	890	ALA
1	E	1953	ASN
2	F	530	ASP
1	B	745	ALA
1	C	350	GLY
1	D	1758	MET
1	D	1953	ASN
1	E	304	GLY
2	F	2115	GLY
1	E	890	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1960/2157 (91%)	1960 (100%)	0	100 100
1	B	1960/2157 (91%)	1959 (100%)	1 (0%)	93 98

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	1960/2157 (91%)	1960 (100%)	0	100	100
1	D	1960/2157 (91%)	1957 (100%)	3 (0%)	93	98
1	E	1960/2157 (91%)	1959 (100%)	1 (0%)	93	98
2	F	1872/2108 (89%)	1871 (100%)	1 (0%)	93	98
All	All	11672/12893 (90%)	11666 (100%)	6 (0%)	93	98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	211	ILE
1	D	661	LYS
1	D	968	TYR
1	D	1169	LEU
1	E	1169	LEU
2	F	472	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	587	ASN
1	B	679	GLN
1	C	1671	ASN
1	D	848	GLN
1	D	1951	GLN
1	E	854	GLN
1	E	1362	ASN
1	E	1599	GLN
1	E	1951	GLN
2	F	450	ASN
2	F	1546	GLN
2	F	1650	HIS

5.3.3 RNA

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 monosaccharides 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.

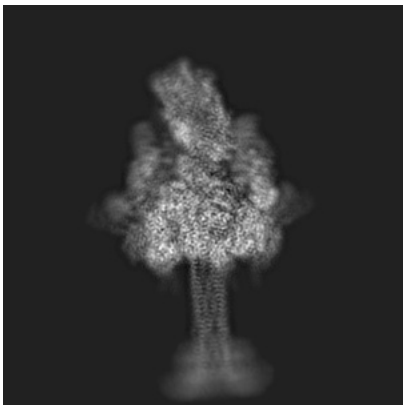
6 Map visualisation

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

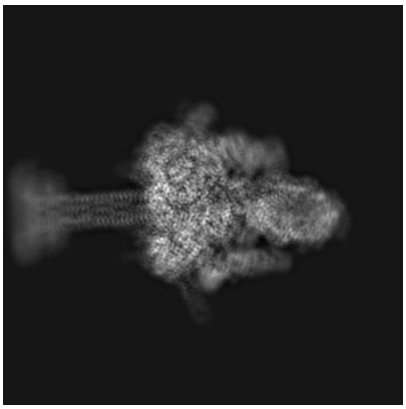
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

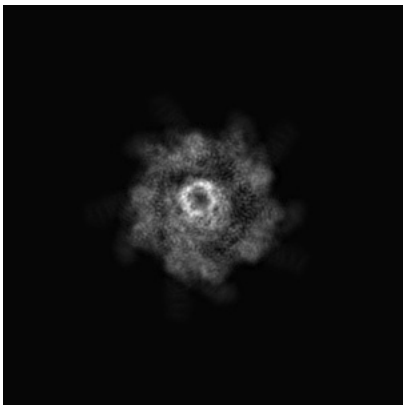
6.1.1 Primary map



X

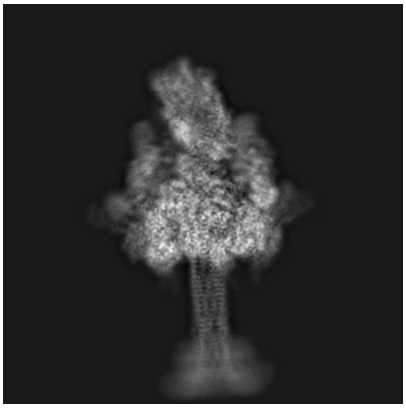


Y

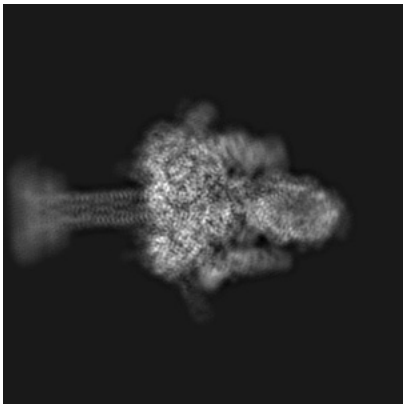


Z

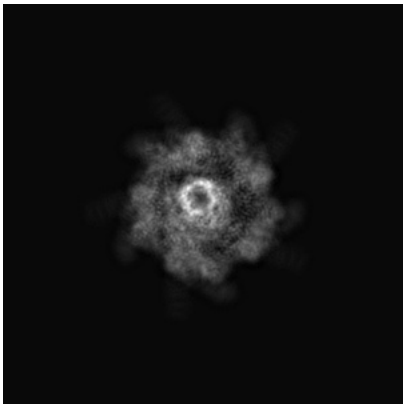
6.1.2 Raw map



X



Y

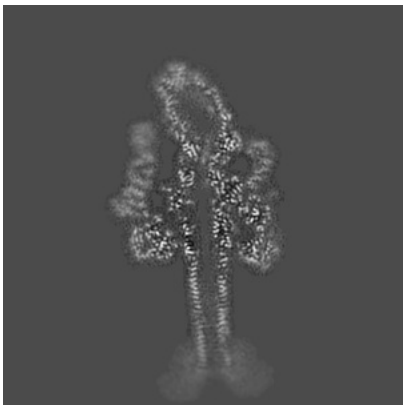


Z

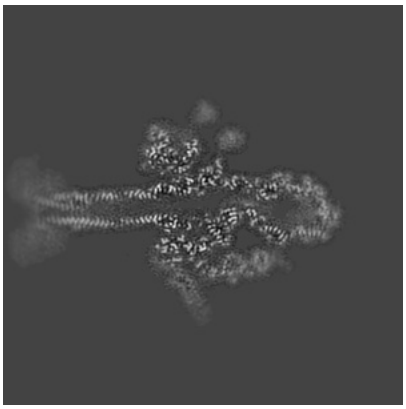
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

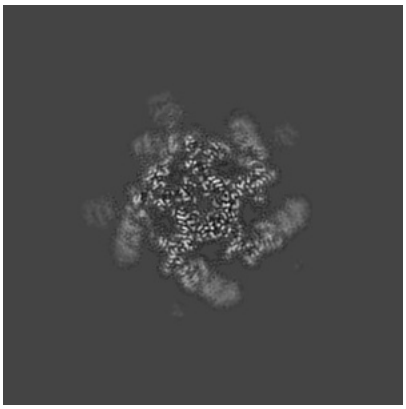
6.2.1 Primary map



X Index: 192

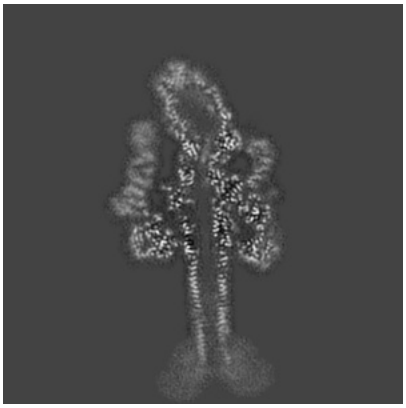


Y Index: 192

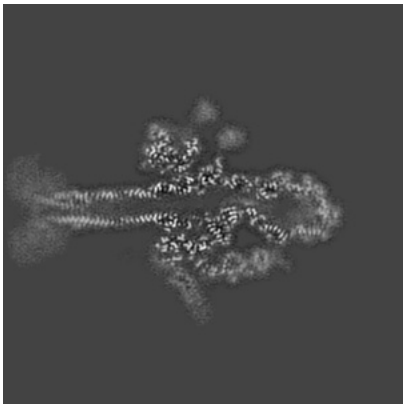


Z Index: 192

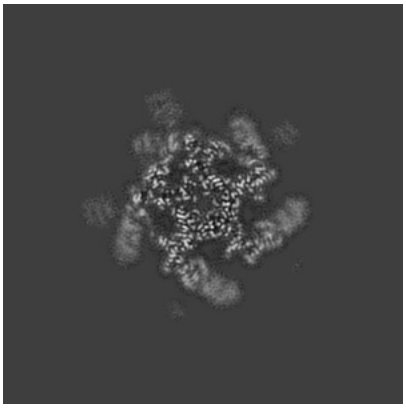
6.2.2 Raw map



X Index: 192



Y Index: 192

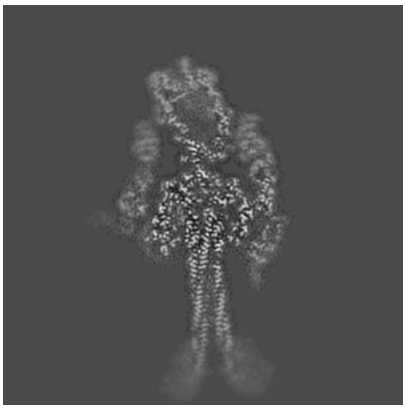


Z Index: 192

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

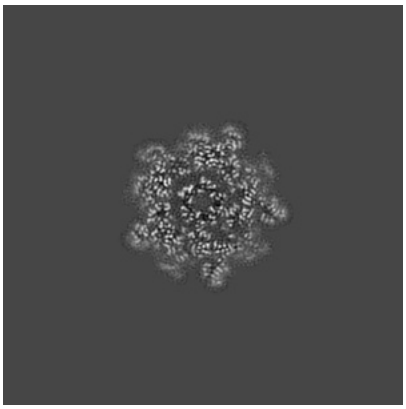
6.3 Largest variance slices (i)

6.3.1 Primary map



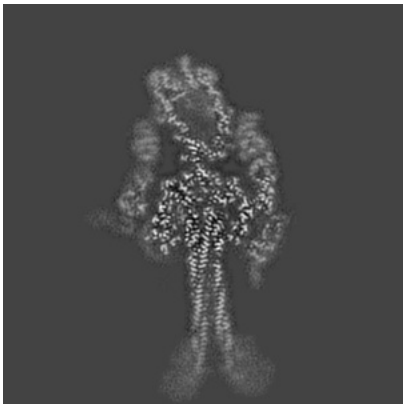
X Index: 179

Y Index: 207

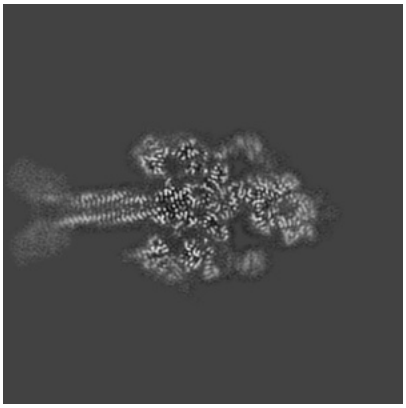


Z Index: 153

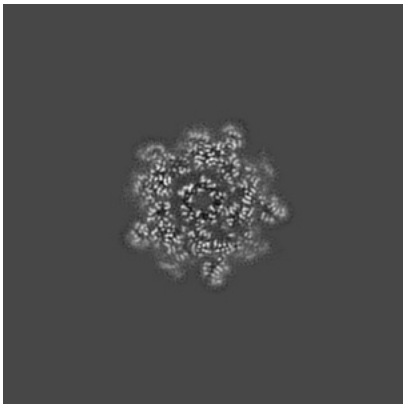
6.3.2 Raw map



X Index: 179



Y Index: 207



Z Index: 153

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

6.4 Orthogonal surface views (i)

6.4.1 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.

6.4.2 Raw map

X Y Z

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

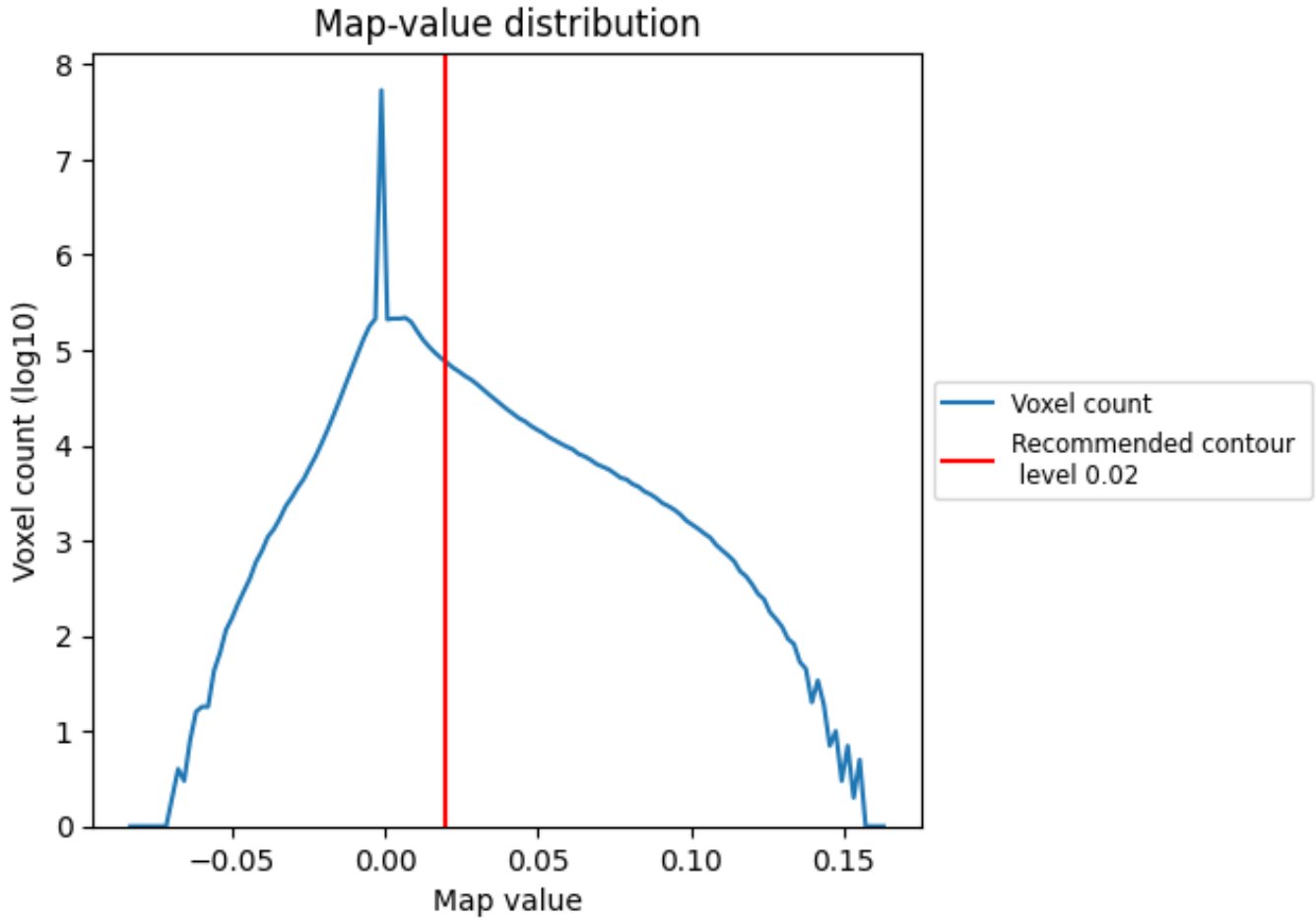
6.5 Mask visualisation (i)

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

7 Map analysis

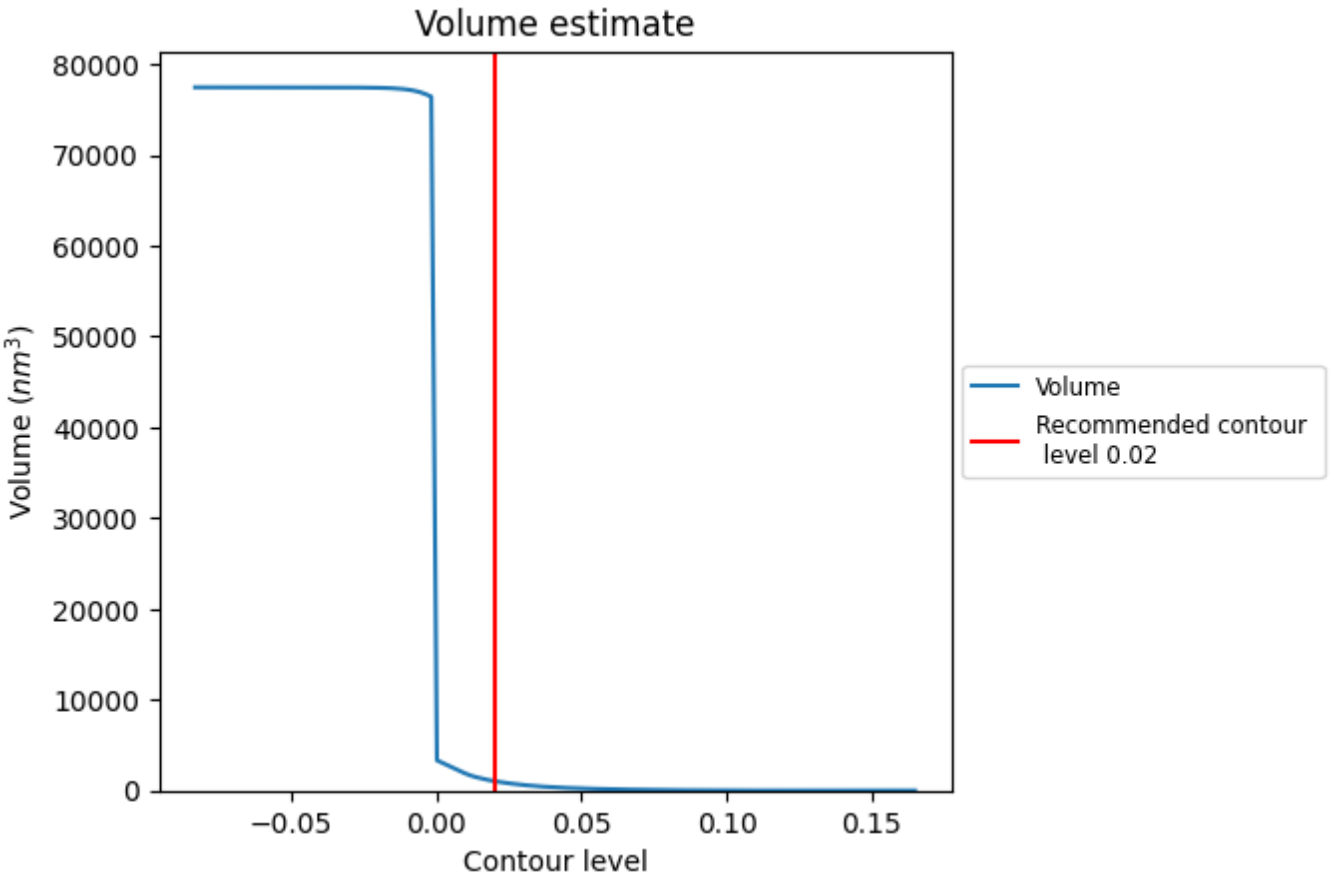
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

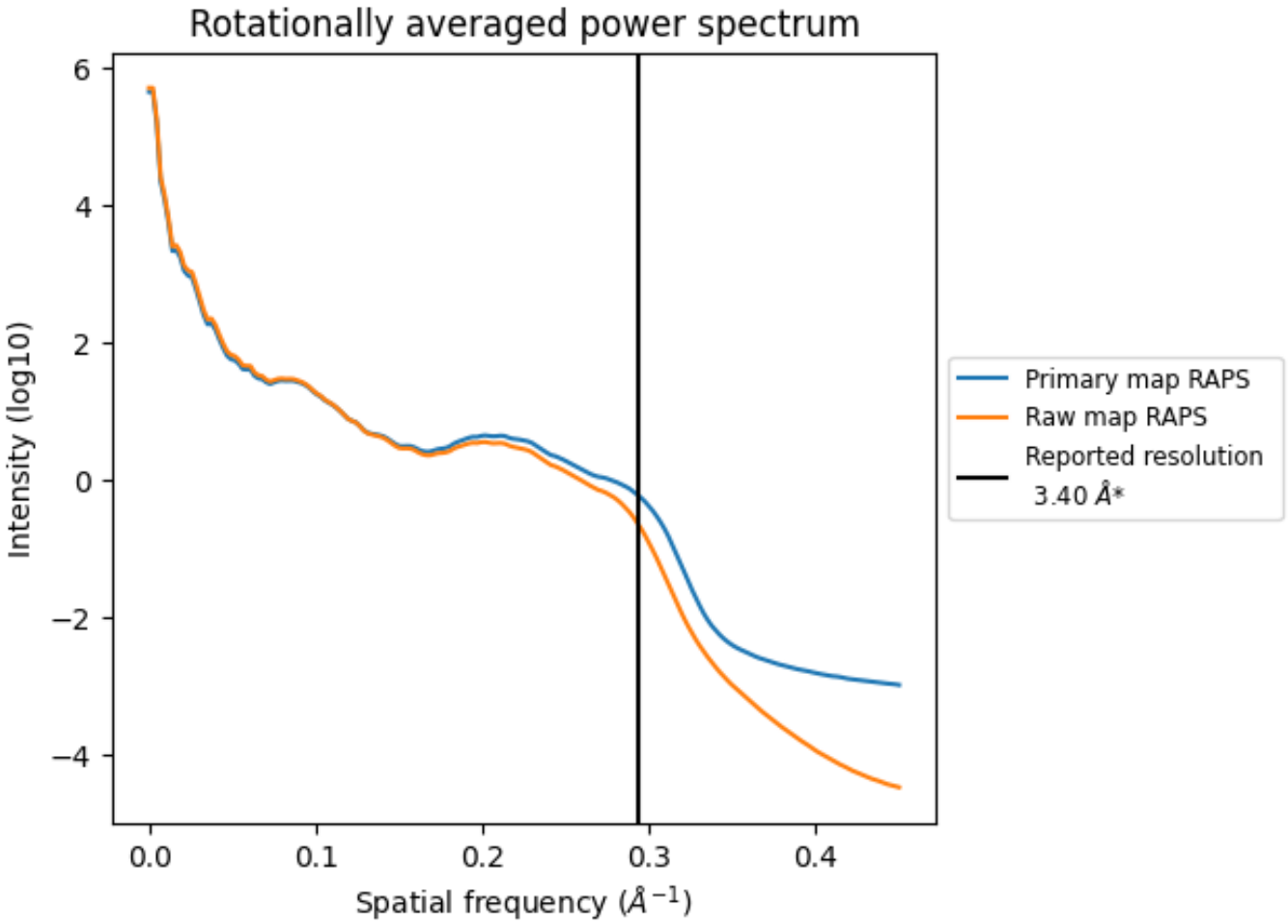
7.2 Volume estimate



The volume at the recommended contour level is 1043 nm^3; this corresponds to an approximate mass of 942 kDa.

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

7.3 Rotationally averaged power spectrum (i)

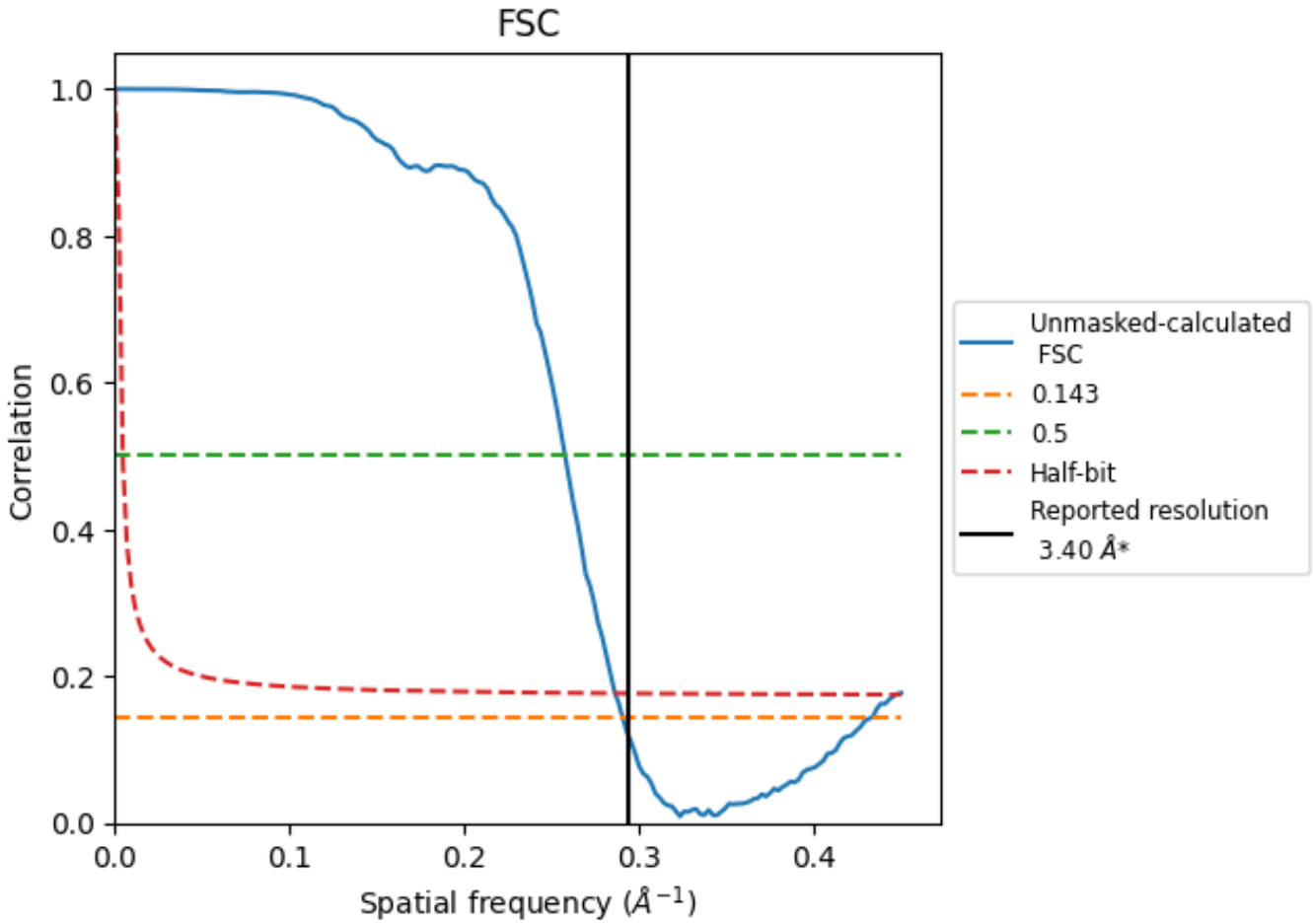


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

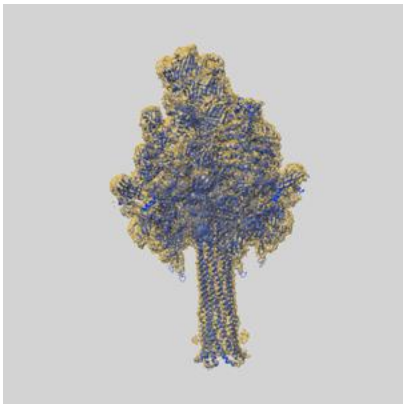
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.44	3.88	3.49

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

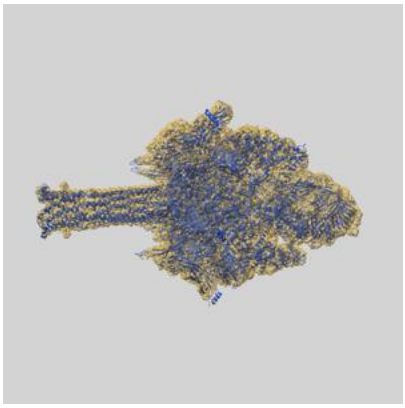
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10312 and PDB model 6SUE. Per-residue inclusion information can be found in section 3 on page 5.

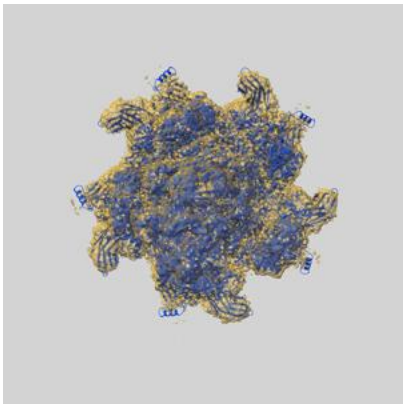
9.1 Map-model overlay



X



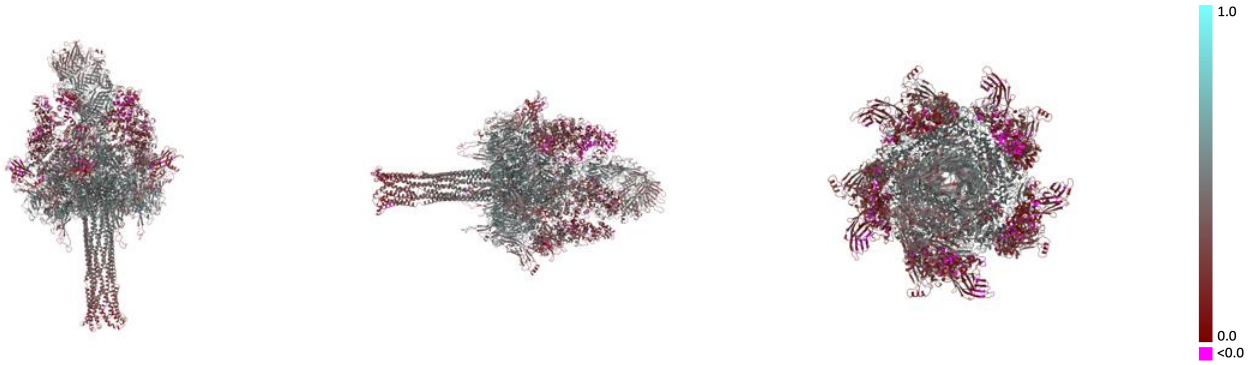
Y



Z

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.

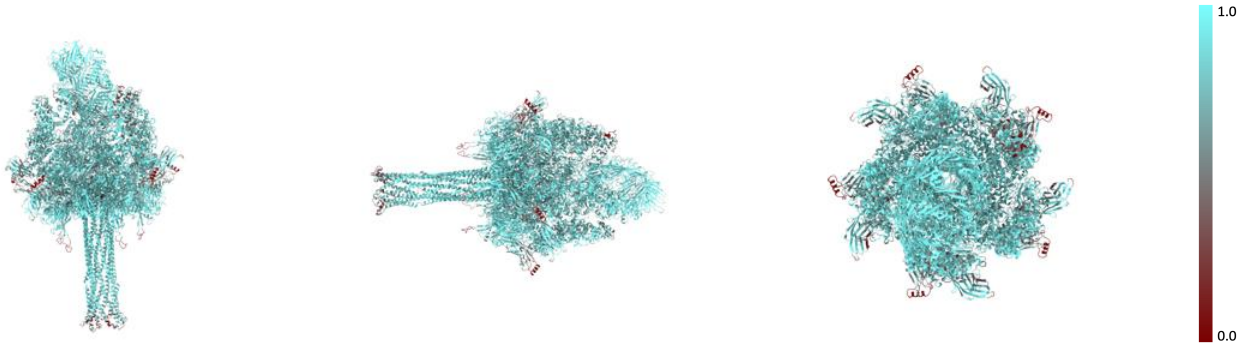
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

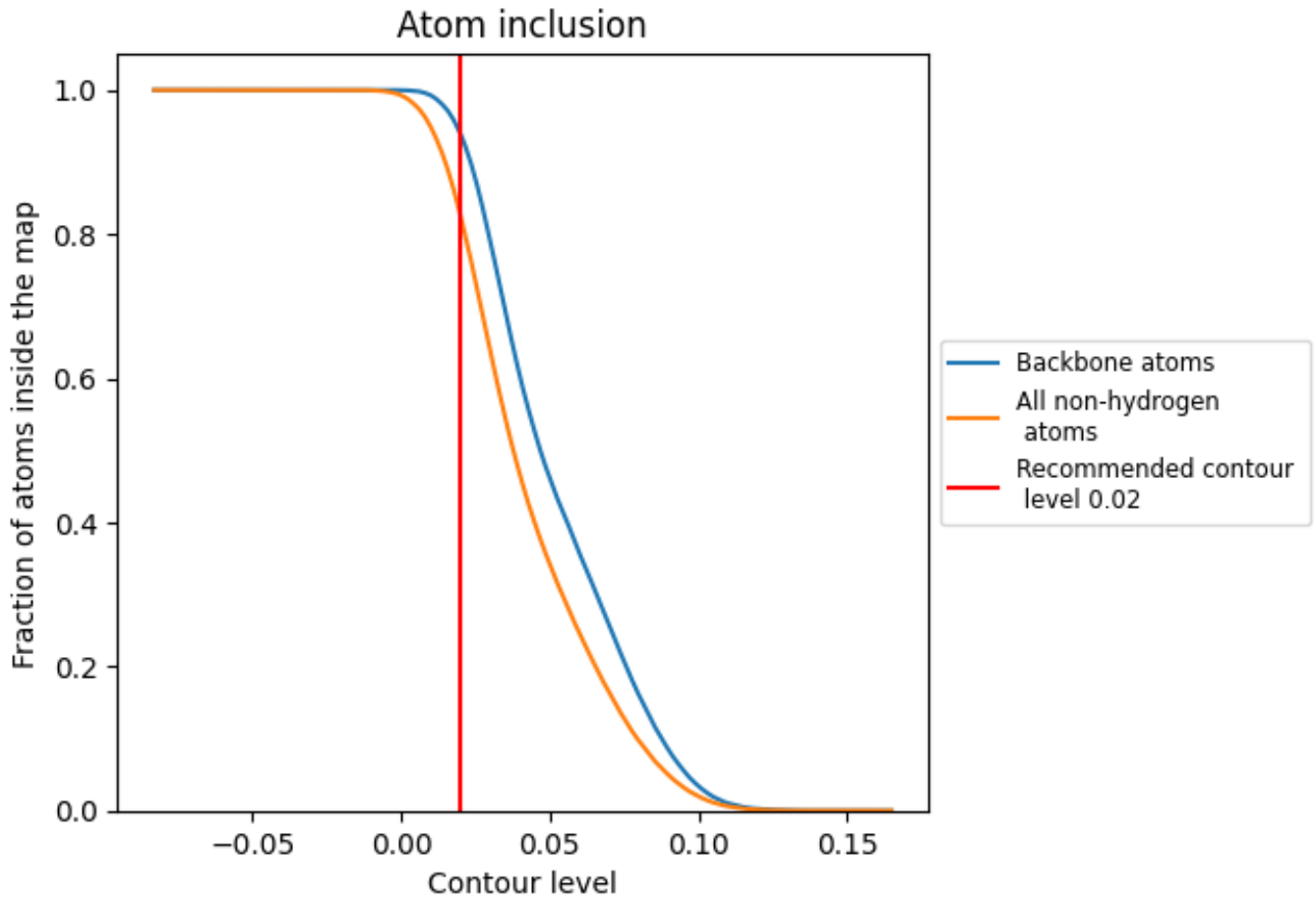
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8250	0.3850
A	0.8097	0.3810
B	0.8146	0.3740
C	0.8145	0.3730
D	0.7948	0.3600
E	0.8212	0.3870
F	0.8992	0.4340