Full wwPDB EM Validation Report

Nov 19, 2022 – 09:37 pm GMT

PDB ID	:	5JZC
EMDB ID	:	EMD-8183
Title	:	helical filament
Authors	:	Short, J.; Liu, Y.
Deposited on	:	2016-05-16
Resolution	:	4.20 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 (i) 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 (i)) were used in the production of this report:

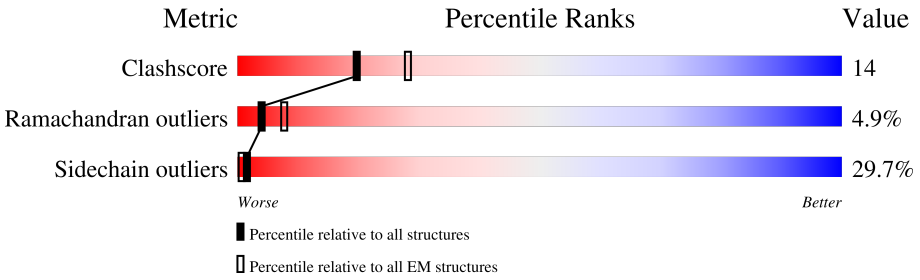
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.20 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	339	17% 69% 19% • • 8%
1	B	339	15% 68% 19% • • 8%
1	C	339	14% 70% 17% • • 8%
1	D	339	15% 68% 19% 5% 8%
1	E	339	14% 69% 18% • • 8%
1	F	339	14% 69% 19% • • 8%
1	G	339	15% 70% 18% • • 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11935 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 DNA repair protein RAD51 homolog 1.

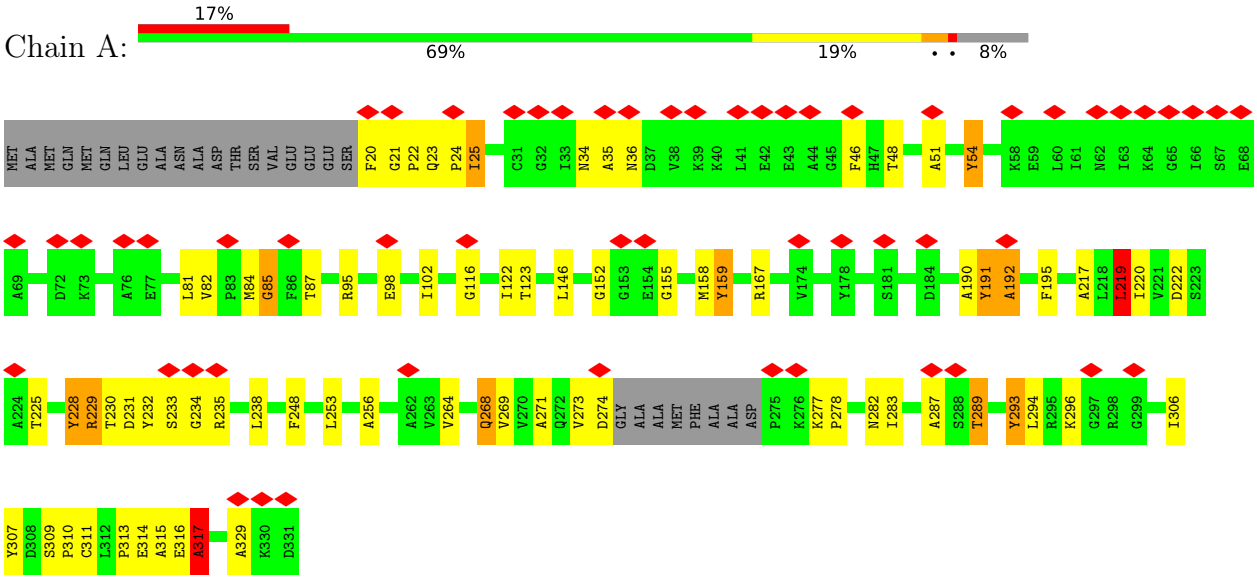
Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	312	Total 1705	C 1043	N 332	O 330	4	0
1	B	312	Total 1705	C 1043	N 332	O 330	4	0
1	C	312	Total 1705	C 1043	N 332	O 330	4	0
1	D	312	Total 1705	C 1043	N 332	O 330	4	0
1	E	312	Total 1705	C 1043	N 332	O 330	4	0
1	F	312	Total 1705	C 1043	N 332	O 330	4	0
1	G	312	Total 1705	C 1043	N 332	O 330	4	0

3 Residue-property plots (i)

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

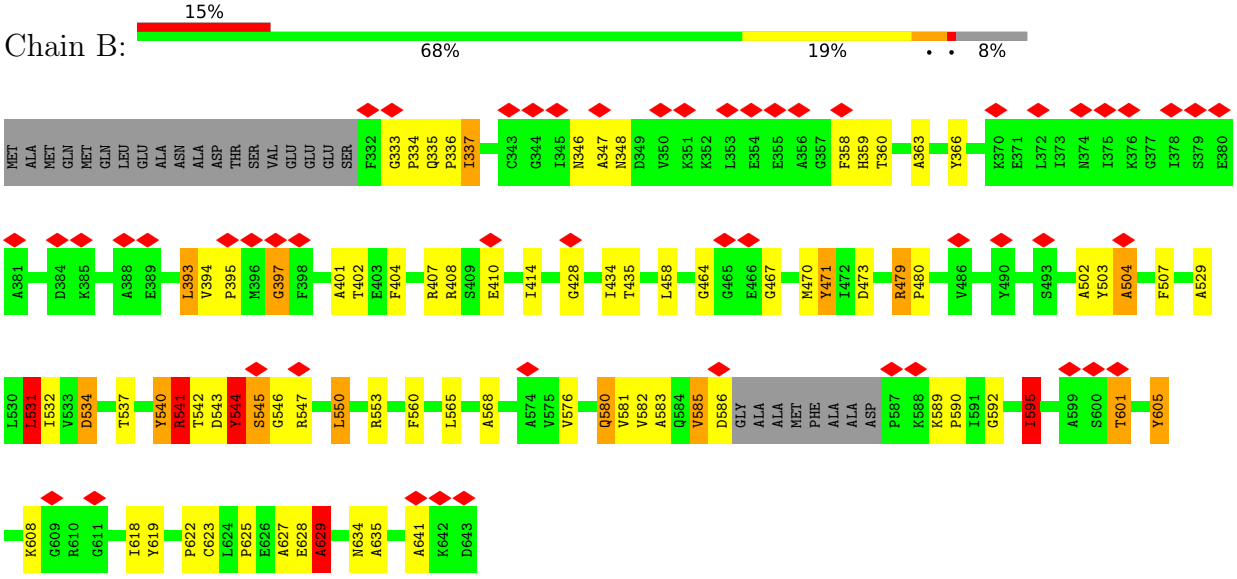
• Molecule 1: DNA repair protein RAD51 homolog 1

Chain A:

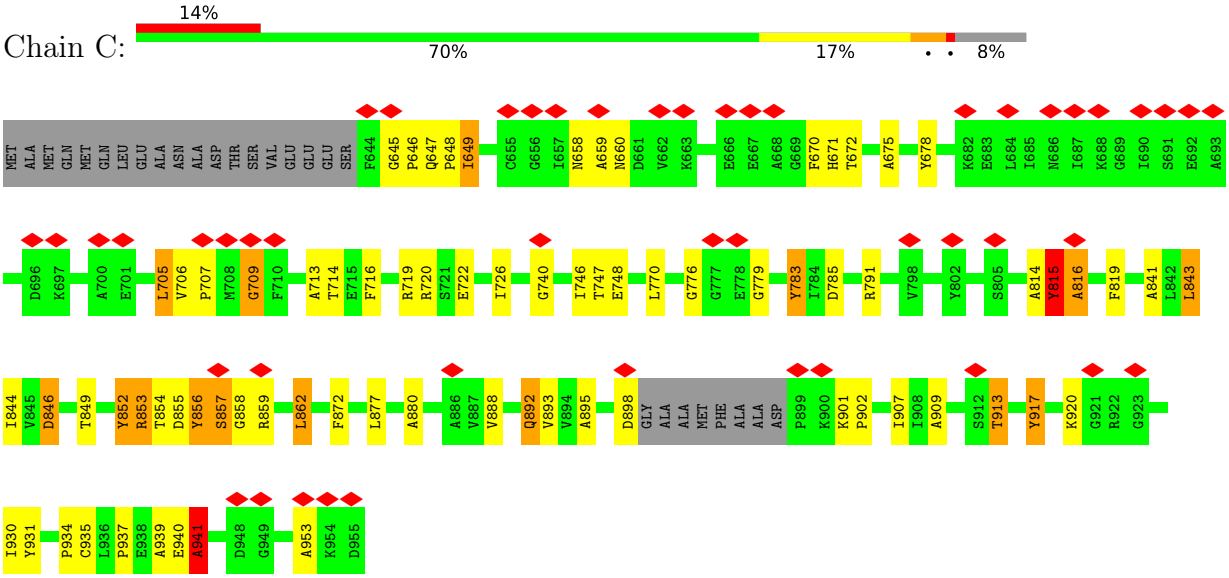


• Molecule 1: DNA repair protein RAD51 homolog 1

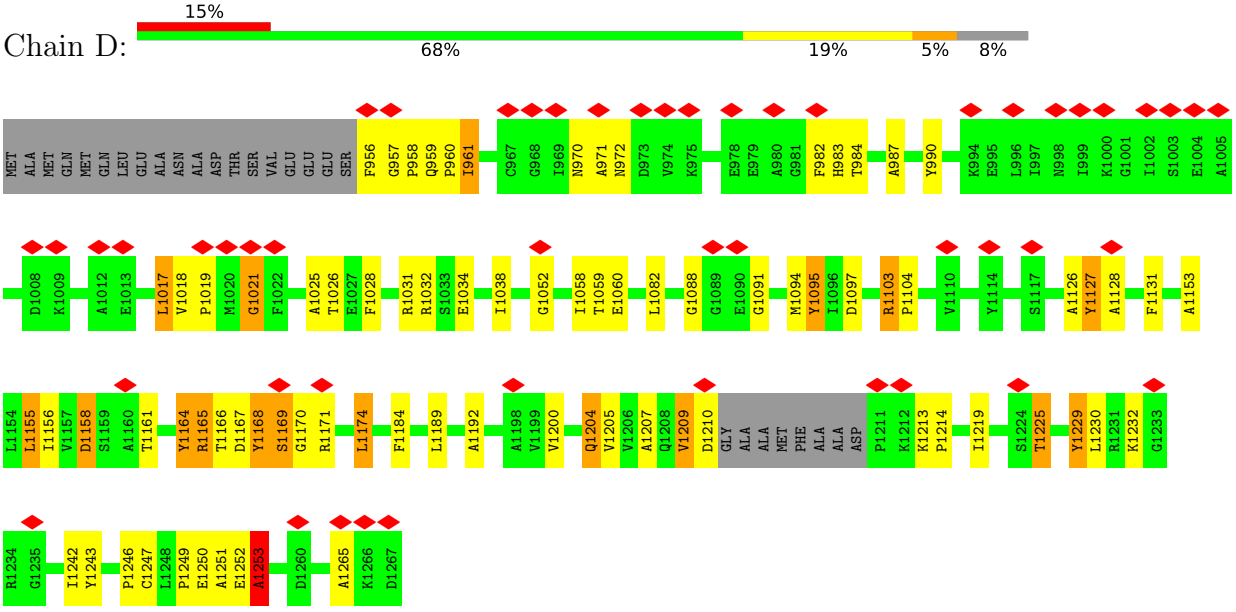
Chain B:



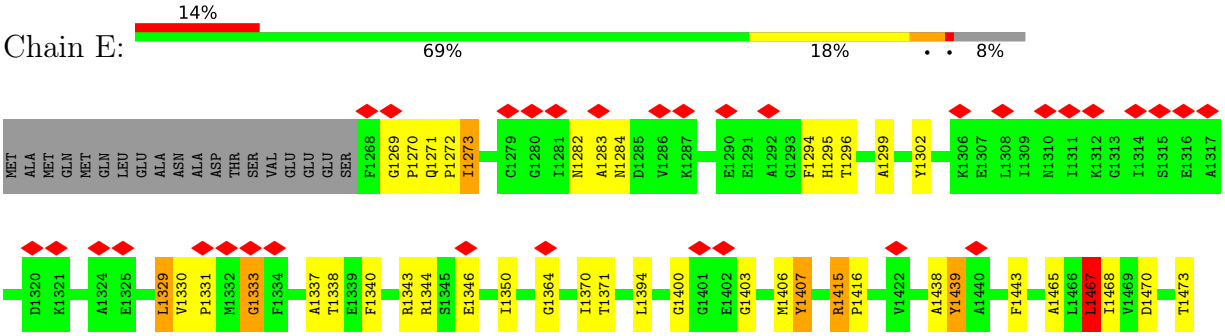
• Molecule 1: DNA repair protein RAD51 homolog 1

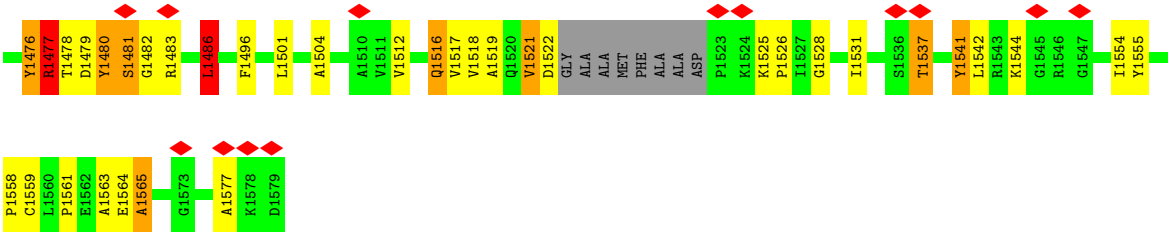


• Molecule 1: DNA repair protein RAD51 homolog 1



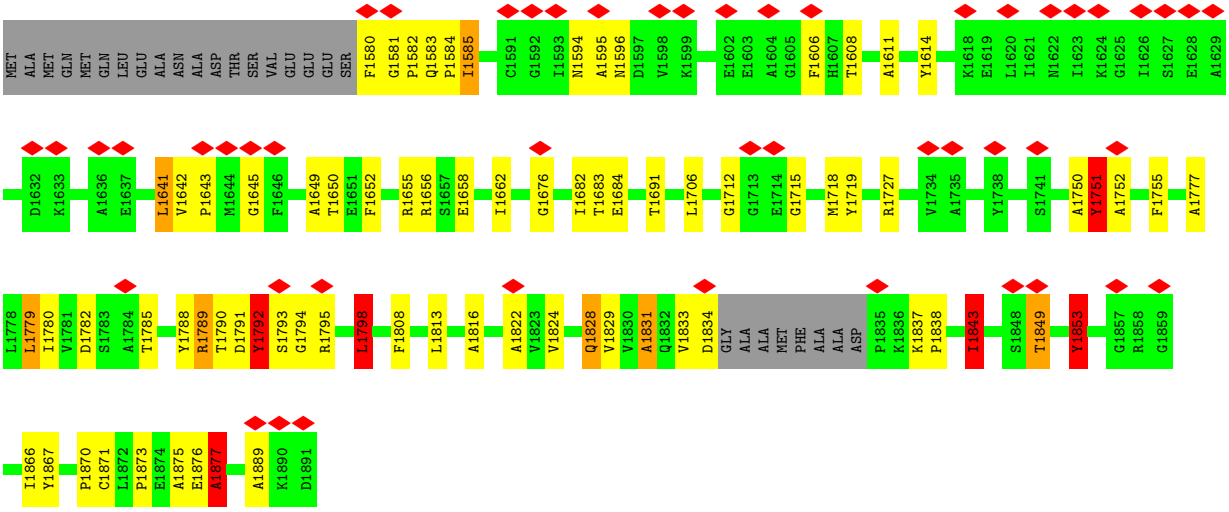
• Molecule 1: DNA repair protein RAD51 homolog 1





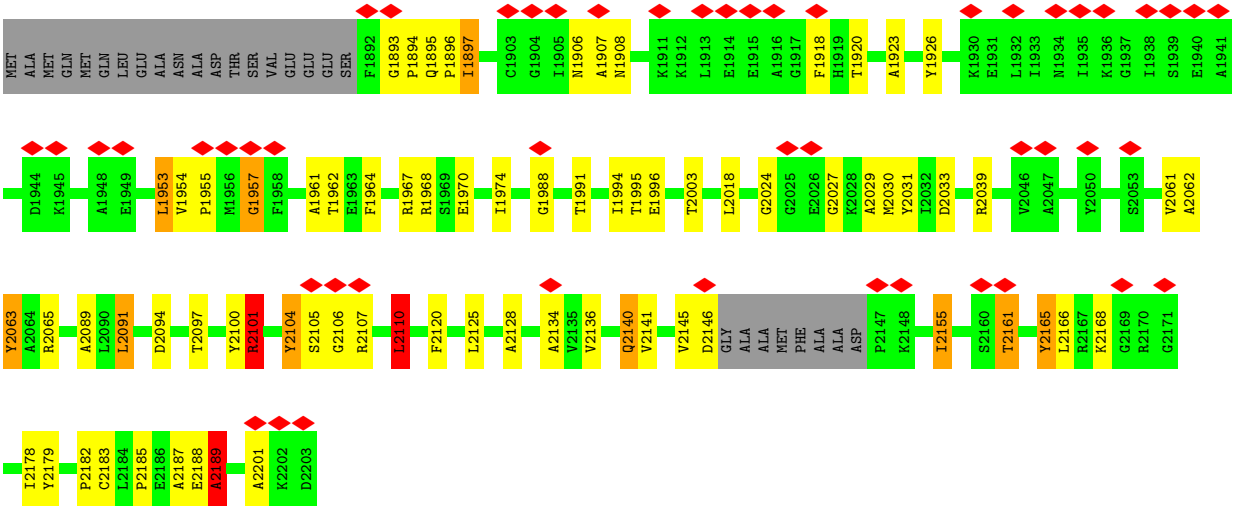
• Molecule 1: DNA repair protein RAD51 homolog 1

Chain F:



• Molecule 1: DNA repair protein RAD51 homolog 1

Chain G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=56.2°, rise=16.05 Å, axial sym=C1	Depositor
Number of segments used	69000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.511	Depositor
Minimum map value	-0.237	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	256.0, 256.0, 256.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.18	11/1725 (0.6%)	1.39	13/2388 (0.5%)
1	B	1.13	3/1725 (0.2%)	1.41	14/2388 (0.6%)
1	C	1.12	1/1725 (0.1%)	1.35	13/2388 (0.5%)
1	D	1.13	2/1725 (0.1%)	1.32	12/2388 (0.5%)
1	E	1.12	2/1725 (0.1%)	1.34	11/2388 (0.5%)
1	F	1.25	11/1725 (0.6%)	1.36	21/2388 (0.9%)
1	G	1.25	13/1725 (0.8%)	1.39	19/2388 (0.8%)
All	All	1.17	43/12075 (0.4%)	1.36	103/16716 (0.6%)

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	A	0	5
1	B	0	5
1	C	0	5
1	D	0	4
1	E	0	4
1	F	0	4
1	G	0	4
All	All	0	31

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	2101	ARG	CD-NE	12.95	1.68	1.46
1	F	1789	ARG	CD-NE	11.68	1.66	1.46
1	A	54	TYR	CE1-CZ	10.50	1.52	1.38
1	F	1789	ARG	CZ-NH2	10.34	1.46	1.33
1	G	2101	ARG	NE-CZ	9.97	1.46	1.33
1	G	2101	ARG	CZ-NH2	9.04	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1789	ARG	NE-CZ	8.96	1.44	1.33
1	F	1789	ARG	CZ-NH1	8.52	1.44	1.33
1	G	2101	ARG	CZ-NH1	8.52	1.44	1.33
1	F	1833	VAL	CA-CB	8.18	1.72	1.54
1	G	2145	VAL	CA-CB	7.81	1.71	1.54
1	A	268	GLN	CG-CD	7.50	1.68	1.51
1	D	1204	GLN	CG-CD	7.48	1.68	1.51
1	B	580	GLN	CG-CD	7.33	1.68	1.51
1	F	1828	GLN	CG-CD	7.29	1.67	1.51
1	C	892	GLN	CG-CD	7.25	1.67	1.51
1	G	2101	ARG	N-CA	7.25	1.60	1.46
1	E	1516	GLN	CG-CD	7.19	1.67	1.51
1	A	54	TYR	CG-CD2	6.86	1.48	1.39
1	F	1789	ARG	N-CA	6.84	1.60	1.46
1	G	2140	GLN	CG-CD	6.54	1.66	1.51
1	A	287	ALA	N-CA	6.42	1.59	1.46
1	F	1789	ARG	CG-CD	6.38	1.68	1.51
1	G	2101	ARG	CG-CD	6.18	1.67	1.51
1	F	1833	VAL	N-CA	6.09	1.58	1.46
1	G	2063	TYR	CE1-CZ	5.85	1.46	1.38
1	G	2145	VAL	N-CA	5.76	1.57	1.46
1	A	229	ARG	CZ-NH2	5.58	1.40	1.33
1	A	229	ARG	NE-CZ	5.41	1.40	1.33
1	A	287	ALA	CA-CB	5.30	1.63	1.52
1	B	541	ARG	CZ-NH2	5.29	1.40	1.33
1	A	314	GLU	N-CA	5.29	1.56	1.46
1	G	2101	ARG	CA-CB	5.28	1.65	1.53
1	G	1996	GLU	N-CA	5.25	1.56	1.46
1	E	1528	GLY	N-CA	5.23	1.53	1.46
1	A	85	GLY	N-CA	5.16	1.53	1.46
1	D	1250	GLU	N-CA	5.09	1.56	1.46
1	B	592	GLY	N-CA	5.08	1.53	1.46
1	F	1789	ARG	CB-CG	5.08	1.66	1.52
1	A	54	TYR	CD1-CE1	5.07	1.47	1.39
1	G	2101	ARG	CB-CG	5.03	1.66	1.52
1	A	228	TYR	CB-CG	-5.03	1.44	1.51
1	F	1789	ARG	CA-CB	5.03	1.65	1.53

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	229	ARG	NE-CZ-NH2	23.16	131.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	541	ARG	NE-CZ-NH2	20.62	130.61	120.30
1	C	853	ARG	NE-CZ-NH2	17.78	129.19	120.30
1	B	541	ARG	NE-CZ-NH1	-16.91	111.84	120.30
1	E	1477	ARG	NE-CZ-NH2	15.01	127.81	120.30
1	G	2101	ARG	NE-CZ-NH1	13.35	126.97	120.30
1	G	2101	ARG	CD-NE-CZ	12.65	141.32	123.60
1	A	229	ARG	NE-CZ-NH1	-12.40	114.10	120.30
1	F	1789	ARG	CD-NE-CZ	11.92	140.28	123.60
1	D	1165	ARG	NE-CZ-NH1	-10.13	115.23	120.30
1	E	1477	ARG	NE-CZ-NH1	-9.74	115.43	120.30
1	D	1155	LEU	CA-CB-CG	9.07	136.16	115.30
1	F	1789	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	E	1467	LEU	CB-CG-CD2	-8.77	96.10	111.00
1	B	531	LEU	CA-CB-CG	8.76	135.45	115.30
1	F	1789	ARG	N-CA-CB	8.65	126.18	110.60
1	G	2101	ARG	N-CA-CB	8.63	126.13	110.60
1	E	1521	VAL	CG1-CB-CG2	-8.33	97.58	110.90
1	F	1789	ARG	CB-CG-CD	8.29	133.17	111.60
1	E	1467	LEU	CA-CB-CG	8.24	134.26	115.30
1	F	1779	LEU	CA-CB-CG	8.10	133.93	115.30
1	D	1155	LEU	CB-CG-CD2	-7.99	97.42	111.00
1	B	531	LEU	CB-CG-CD2	-7.93	97.52	111.00
1	G	2145	VAL	CG1-CB-CG2	-7.80	98.43	110.90
1	G	2101	ARG	CB-CG-CD	7.77	131.79	111.60
1	G	2091	LEU	CA-CB-CG	7.73	133.08	115.30
1	F	1727	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	219	LEU	CA-CB-CG	7.61	132.81	115.30
1	C	843	LEU	CA-CB-CG	7.50	132.56	115.30
1	C	843	LEU	CB-CG-CD2	-7.47	98.29	111.00
1	F	1779	LEU	CB-CG-CD2	-7.37	98.46	111.00
1	D	1165	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	B	479	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	G	2101	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	F	1833	VAL	CG1-CB-CG2	-7.09	99.55	110.90
1	F	1829	VAL	CB-CA-C	-7.04	98.03	111.40
1	C	791	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	E	1415	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	269	VAL	CB-CA-C	-6.96	98.17	111.40
1	B	585	VAL	CG1-CB-CG2	-6.85	99.94	110.90
1	B	581	VAL	CB-CA-C	-6.84	98.41	111.40
1	D	1103	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	G	2141	VAL	CB-CA-C	-6.63	98.81	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	2110	LEU	CB-CG-CD1	-6.54	99.89	111.00
1	G	2039	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	C	853	ARG	NH1-CZ-NH2	-6.51	112.24	119.40
1	D	1209	VAL	CG1-CB-CG2	-6.50	100.50	110.90
1	D	1205	VAL	CB-CA-C	-6.49	99.06	111.40
1	A	287	ALA	N-CA-CB	6.46	119.15	110.10
1	C	893	VAL	CB-CA-C	-6.42	99.20	111.40
1	E	1517	VAL	CB-CA-C	-6.36	99.32	111.40
1	F	1833	VAL	N-CA-CB	6.33	125.43	111.50
1	A	167	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	C	852	TYR	CB-CA-C	-6.20	98.00	110.40
1	B	540	TYR	CB-CA-C	-6.10	98.19	110.40
1	G	2145	VAL	CA-CB-CG2	6.07	120.01	110.90
1	D	1164	TYR	CB-CA-C	-6.03	98.33	110.40
1	G	2101	ARG	CG-CD-NE	6.03	124.45	111.80
1	F	1789	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	B	595	ILE	CB-CA-C	-5.87	99.85	111.60
1	E	1476	TYR	CB-CA-C	-5.85	98.71	110.40
1	E	1486	LEU	CB-CG-CD1	-5.83	101.08	111.00
1	F	1798	LEU	CB-CG-CD1	-5.82	101.10	111.00
1	A	191	TYR	N-CA-C	5.72	126.45	111.00
1	A	219	LEU	CB-CG-CD2	-5.71	101.30	111.00
1	C	815	TYR	N-CA-C	5.64	126.23	111.00
1	B	550	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	G	2155	ILE	CA-CB-CG1	5.53	121.51	111.00
1	B	585	VAL	CA-CB-CG2	-5.52	102.62	110.90
1	D	1127	TYR	N-CA-C	5.51	125.89	111.00
1	F	1789	ARG	CG-CD-NE	5.50	123.36	111.80
1	E	1439	TYR	N-CA-C	5.47	125.78	111.00
1	C	862	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	F	1843	ILE	CA-CB-CG1	5.43	121.31	111.00
1	F	1751	TYR	N-CA-C	5.42	125.63	111.00
1	B	503	TYR	N-CA-C	5.41	125.61	111.00
1	F	1691	THR	C-N-CA	5.35	133.53	122.30
1	C	853	ARG	CB-CG-CD	5.31	125.41	111.60
1	G	2189	ALA	N-CA-C	5.31	125.33	111.00
1	G	2062	ALA	N-CA-CB	5.29	117.51	110.10
1	D	1253	ALA	N-CA-C	5.29	125.28	111.00
1	G	2145	VAL	N-CA-CB	5.28	123.11	111.50
1	C	783	TYR	N-CA-CB	5.27	120.09	110.60
1	A	307	TYR	CB-CA-C	-5.27	99.87	110.40
1	F	1853	TYR	CB-CG-CD2	-5.26	117.84	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	2003	THR	C-N-CA	5.25	133.32	122.30
1	C	941	ALA	N-CA-C	5.23	125.13	111.00
1	G	2091	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	F	1833	VAL	CA-CB-CG2	5.21	118.71	110.90
1	F	1877	ALA	N-CA-C	5.17	124.95	111.00
1	A	159	TYR	N-CA-CB	5.12	119.81	110.60
1	F	1853	TYR	CB-CG-CD1	5.10	124.06	121.00
1	G	2031	TYR	N-CA-CB	5.10	119.77	110.60
1	D	1060	GLU	N-CA-C	5.09	124.76	111.00
1	A	273	VAL	CG1-CB-CG2	-5.09	102.76	110.90
1	B	471	TYR	N-CA-CB	5.09	119.76	110.60
1	A	317	ALA	N-CA-C	5.08	124.70	111.00
1	C	748	GLU	N-CA-C	5.07	124.68	111.00
1	F	1684	GLU	N-CA-C	5.07	124.68	111.00
1	B	629	ALA	N-CA-C	5.03	124.59	111.00
1	D	1095	TYR	N-CA-CB	5.02	119.63	110.60
1	E	1407	TYR	N-CA-CB	5.01	119.62	110.60
1	A	228	TYR	CB-CA-C	-5.00	100.40	110.40

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	ALA	Peptide
1	A	222	ASP	Peptide
1	A	282	ASN	Peptide
1	A	296	LYS	Peptide
1	A	81	LEU	Peptide
1	B	393	LEU	Peptide
1	B	504	ALA	Peptide
1	B	534	ASP	Peptide
1	B	544	TYR	Peptide
1	B	608	LYS	Peptide
1	C	705	LEU	Peptide
1	C	816	ALA	Peptide
1	C	846	ASP	Peptide
1	C	856	TYR	Peptide
1	C	920	LYS	Peptide
1	D	1017	LEU	Peptide
1	D	1158	ASP	Peptide
1	D	1168	TYR	Peptide
1	D	1232	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	E	1329	LEU	Peptide
1	E	1470	ASP	Peptide
1	E	1480	TYR	Peptide
1	E	1544	LYS	Peptide
1	F	1641	LEU	Peptide
1	F	1782	ASP	Peptide
1	F	1792	TYR	Peptide
1	F	1831	ALA	Peptide
1	G	1953	LEU	Peptide
1	G	2094	ASP	Peptide
1	G	2104	TYR	Peptide
1	G	2168	LYS	Peptide

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	1705	0	991	34	0
1	B	1705	0	991	49	0
1	C	1705	0	991	43	0
1	D	1705	0	991	51	0
1	E	1705	0	991	48	0
1	F	1705	0	991	47	0
1	G	1705	0	991	37	0
All	All	11935	0	6937	263	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 14.

All (263) 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:G:2101:ARG:NE	1:G:2101:ARG:CD	1.68	1.54
1:B:541:ARG:HH12	1:B:582:VAL:HG11	1.33	0.94
1:G:1994:ILE:O	1:G:2161:THR:HA	1.70	0.92
1:B:434:ILE:O	1:B:601:THR:HA	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1091:GLY:HA3	1:D:1153:ALA:HB2	1.58	0.86
1:B:583:ALA:HB3	1:C:907:ILE:HD11	1.61	0.83
1:E:1403:GLY:HA3	1:E:1465:ALA:HB2	1.63	0.79
1:E:1438:ALA:HB2	1:F:1649:ALA:HB2	1.65	0.79
1:C:814:ALA:HB2	1:D:1025:ALA:HB2	1.64	0.78
1:F:1682:ILE:O	1:F:1849:THR:HA	1.83	0.78
1:A:155:GLY:HA3	1:A:217:ALA:HB2	1.66	0.78
1:F:1750:ALA:HB2	1:G:1961:ALA:HB2	1.66	0.78
1:B:502:ALA:HB2	1:C:713:ALA:HB2	1.64	0.77
1:A:190:ALA:HB2	1:B:401:ALA:HB2	1.66	0.77
1:C:779:GLY:HA3	1:C:841:ALA:HB2	1.67	0.76
1:B:467:GLY:HA3	1:B:529:ALA:HB2	1.68	0.76
1:D:1126:ALA:HB2	1:E:1337:ALA:HB2	1.68	0.74
1:E:1370:ILE:O	1:E:1537:THR:HA	1.87	0.73
1:F:1715:GLY:HA3	1:F:1777:ALA:HB2	1.70	0.73
1:A:271:ALA:HB3	1:B:595:ILE:HD11	1.71	0.72
1:F:1837:LYS:CB	1:F:1838:PRO:HD2	2.18	0.72
1:D:1161:THR:O	1:D:1164:TYR:HB2	1.89	0.72
1:A:25:ILE:HA	1:A:48:THR:HA	1.71	0.72
1:E:1473:THR:O	1:E:1476:TYR:HB2	1.89	0.70
1:C:649:ILE:HA	1:C:672:THR:HA	1.72	0.70
1:G:2027:GLY:HA3	1:G:2089:ALA:HB2	1.72	0.70
1:B:537:THR:O	1:B:540:TYR:HB2	1.93	0.69
1:D:961:ILE:HA	1:D:984:THR:HA	1.73	0.69
1:A:225:THR:O	1:A:228:TYR:HB2	1.92	0.69
1:B:337:ILE:HA	1:B:360:THR:HA	1.73	0.69
1:E:1443:PHE:H	1:F:1614:TYR:HE2	1.41	0.69
1:F:1585:ILE:HA	1:F:1608:THR:HA	1.74	0.69
1:C:746:ILE:O	1:C:913:THR:HA	1.93	0.69
1:C:849:THR:O	1:C:852:TYR:HB2	1.93	0.68
1:G:1897:ILE:HA	1:G:1920:THR:HA	1.75	0.67
1:D:1058:ILE:O	1:D:1225:THR:HA	1.94	0.67
1:A:102:ILE:O	1:A:116:GLY:HA3	1.95	0.66
1:B:628:GLU:O	1:B:629:ALA:CB	2.43	0.66
1:D:1038:ILE:O	1:D:1052:GLY:HA3	1.96	0.66
1:C:726:ILE:O	1:C:740:GLY:HA3	1.95	0.65
1:E:1273:ILE:HA	1:E:1296:THR:HA	1.78	0.65
1:G:2188:GLU:O	1:G:2189:ALA:CB	2.43	0.65
1:A:277:LYS:CB	1:A:278:PRO:HD2	2.27	0.65
1:B:414:ILE:O	1:B:428:GLY:HA3	1.96	0.65
1:D:1252:GLU:O	1:D:1253:ALA:CB	2.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PHE:CB	1:A:51:ALA:HB1	2.27	0.64
1:D:1131:PHE:H	1:E:1302:TYR:HE2	1.46	0.64
1:F:1876:GLU:O	1:F:1877:ALA:CB	2.45	0.63
1:G:1974:ILE:O	1:G:1988:GLY:HA3	1.97	0.63
1:A:316:GLU:O	1:A:317:ALA:CB	2.46	0.62
1:G:1918:PHE:CB	1:G:1923:ALA:HB1	2.29	0.62
1:F:1853:TYR:HD1	1:F:1853:TYR:C	2.03	0.62
1:E:1564:GLU:O	1:E:1565:ALA:CB	2.48	0.62
1:B:589:LYS:CB	1:B:590:PRO:HD2	2.29	0.62
1:F:1662:ILE:O	1:F:1676:GLY:HA3	2.00	0.61
1:F:1755:PHE:H	1:G:1926:TYR:HE2	1.46	0.61
1:C:819:PHE:CB	1:D:990:TYR:CE2	2.83	0.61
1:E:1350:ILE:O	1:E:1364:GLY:HA3	2.01	0.61
1:G:2165:TYR:C	1:G:2165:TYR:CD1	2.74	0.61
1:B:585:VAL:HG12	1:B:585:VAL:O	2.00	0.60
1:G:2188:GLU:O	1:G:2189:ALA:HB2	2.00	0.60
1:C:819:PHE:CB	1:D:990:TYR:CD2	2.84	0.60
1:F:1853:TYR:C	1:F:1853:TYR:CD1	2.75	0.60
1:B:435:THR:O	1:B:576:VAL:HA	2.01	0.60
1:E:1521:VAL:HG12	1:E:1521:VAL:O	2.03	0.59
1:E:1541:TYR:CD1	1:E:1541:TYR:C	2.76	0.59
1:F:1683:THR:O	1:F:1824:VAL:HA	2.03	0.59
1:C:940:GLU:O	1:C:941:ALA:CB	2.50	0.59
1:E:1371:THR:O	1:E:1512:VAL:HA	2.03	0.58
1:E:1519:ALA:HB3	1:F:1843:ILE:HD11	1.86	0.58
1:C:670:PHE:CB	1:C:675:ALA:HB1	2.34	0.57
1:G:2165:TYR:C	1:G:2165:TYR:HD1	2.07	0.57
1:C:747:THR:O	1:C:888:VAL:HA	2.04	0.57
1:D:1252:GLU:O	1:D:1253:ALA:HB2	2.04	0.57
1:G:2029:ALA:O	1:G:2061:VAL:CB	2.52	0.57
1:D:1229:TYR:CD1	1:D:1229:TYR:C	2.78	0.56
1:F:1785:THR:O	1:F:1788:TYR:HB2	2.04	0.56
1:A:293:TYR:C	1:A:293:TYR:CD1	2.79	0.56
1:A:195:PHE:CB	1:B:366:TYR:CE2	2.89	0.56
1:D:982:PHE:CB	1:D:987:ALA:HB1	2.35	0.56
1:G:2105:SER:O	1:G:2107:ARG:N	2.39	0.56
1:A:195:PHE:CB	1:B:366:TYR:CD2	2.89	0.55
1:F:1606:PHE:CB	1:F:1611:ALA:HB1	2.36	0.55
1:B:507:PHE:H	1:C:678:TYR:HE2	1.54	0.55
1:B:605:TYR:CD1	1:B:605:TYR:C	2.80	0.55
1:D:1131:PHE:CB	1:E:1302:TYR:CD2	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2097:THR:O	1:G:2100:TYR:HB2	2.06	0.55
1:C:917:TYR:CD1	1:C:917:TYR:C	2.80	0.55
1:E:1519:ALA:H	1:F:1843:ILE:HD13	1.71	0.55
1:B:628:GLU:O	1:B:629:ALA:HB2	2.07	0.55
1:E:1481:SER:O	1:E:1483:ARG:N	2.41	0.54
1:A:123:THR:O	1:A:264:VAL:HA	2.07	0.54
1:B:507:PHE:CB	1:C:678:TYR:CE2	2.91	0.54
1:E:1541:TYR:C	1:E:1541:TYR:HD1	2.11	0.54
1:C:716:PHE:O	1:C:720:ARG:N	2.39	0.54
1:E:1443:PHE:CB	1:F:1614:TYR:CD2	2.91	0.54
1:E:1564:GLU:O	1:E:1565:ALA:HB2	2.08	0.54
1:G:2027:GLY:HA3	1:G:2089:ALA:CB	2.37	0.54
1:D:1207:ALA:HB3	1:E:1531:ILE:HD11	1.90	0.53
1:E:1340:PHE:O	1:E:1344:ARG:N	2.40	0.53
1:C:857:SER:O	1:C:859:ARG:N	2.42	0.53
1:G:2030[A]:MET:CB	1:G:2091:LEU:HD13	2.37	0.53
1:F:1876:GLU:O	1:F:1877:ALA:HB2	2.07	0.53
1:D:1131:PHE:CB	1:E:1302:TYR:CE2	2.92	0.53
1:F:1793:SER:O	1:F:1795:ARG:N	2.43	0.52
1:D:1028:PHE:O	1:D:1032:ARG:N	2.41	0.52
1:C:645:GLY:N	1:C:646:PRO:HD2	2.24	0.52
1:C:895:ALA:HB3	1:D:1219:ILE:HD11	1.91	0.52
1:F:1719:TYR:HA	1:F:1780[A]:ILE:O	2.10	0.52
1:A:233:SER:O	1:A:235:ARG:N	2.42	0.52
1:B:404:PHE:O	1:B:408:ARG:N	2.40	0.52
1:D:1169:SER:O	1:D:1171:ARG:N	2.43	0.52
1:D:1059:THR:O	1:D:1200:VAL:HA	2.09	0.51
1:F:1755:PHE:CB	1:G:1926:TYR:CD2	2.93	0.51
1:B:583:ALA:CB	1:C:907:ILE:HD11	2.37	0.51
1:B:507:PHE:CB	1:C:678:TYR:CD2	2.93	0.51
1:E:1294:PHE:CB	1:E:1299:ALA:HB1	2.40	0.51
1:G:1964:PHE:O	1:G:1968:ARG:N	2.40	0.51
1:A:195:PHE:H	1:B:366:TYR:HE2	1.59	0.51
1:G:2033:ASP:O	1:G:2065:ARG:HA	2.11	0.51
1:B:545:SER:O	1:B:547:ARG:N	2.45	0.50
1:B:358:PHE:CB	1:B:363:ALA:HB1	2.41	0.50
1:F:1652:PHE:O	1:F:1656:ARG:N	2.41	0.50
1:F:1719:TYR:HA	1:F:1780[B]:ILE:O	2.11	0.49
1:F:1581:GLY:N	1:F:1582:PRO:HD2	2.28	0.49
1:F:1837:LYS:CB	1:F:1838:PRO:CD	2.90	0.49
1:E:1443:PHE:CB	1:F:1614:TYR:CE2	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:819:PHE:H	1:D:990:TYR:HE2	1.61	0.49
1:D:1017:LEU:HA	1:D:1019:PRO:N	2.28	0.49
1:D:1213:LYS:CB	1:D:1214:PRO:HD2	2.43	0.49
1:G:1893:GLY:N	1:G:1894:PRO:HD2	2.28	0.49
1:D:1095:TYR:HA	1:D:1156[A]:ILE:O	2.14	0.48
1:D:1229:TYR:C	1:D:1229:TYR:HD1	2.15	0.48
1:E:1403:GLY:HA3	1:E:1465:ALA:CB	2.41	0.48
1:E:1519:ALA:HA	1:E:1525:LYS:CB	2.43	0.48
1:B:333:GLY:N	1:B:334:PRO:HD2	2.29	0.48
1:D:1184:PHE:CD1	1:D:1184:PHE:C	2.86	0.48
1:C:895:ALA:H	1:D:1219:ILE:HD13	1.76	0.48
1:F:1715:GLY:HA3	1:F:1777:ALA:CB	2.42	0.48
1:G:1906:ASN:O	1:G:1908:ASN:N	2.47	0.48
1:C:901:LYS:CB	1:C:902:PRO:HD2	2.42	0.48
1:A:158[A]:MET:O	1:A:219:LEU:HA	2.14	0.48
1:F:1594:ASN:O	1:F:1596:ASN:N	2.47	0.48
1:C:719:ARG:O	1:C:722:GLU:N	2.47	0.48
1:E:1407:TYR:HA	1:E:1468[A]:ILE:O	2.14	0.47
1:B:407:ARG:O	1:B:410:GLU:N	2.46	0.47
1:B:541:ARG:NH1	1:B:582:VAL:HG11	2.15	0.47
1:C:770:LEU:O	1:C:776:GLY:HA3	2.14	0.47
1:C:895:ALA:H	1:D:1219:ILE:CD1	2.28	0.47
1:F:1706:LEU:O	1:F:1712:GLY:HA3	2.14	0.47
1:G:1953:LEU:HA	1:G:1955:PRO:N	2.30	0.47
1:A:21:GLY:N	1:A:22:PRO:HD2	2.30	0.47
1:D:1095:TYR:HA	1:D:1156[B]:ILE:O	2.15	0.47
1:D:1082:LEU:O	1:D:1088:GLY:HA3	2.14	0.47
1:E:1343:ARG:O	1:E:1346:GLU:N	2.48	0.47
1:E:1407:TYR:HA	1:E:1468[B]:ILE:O	2.15	0.47
1:G:1995:THR:O	1:G:2136:VAL:HA	2.14	0.47
1:G:2018:LEU:O	1:G:2024:GLY:HA3	2.15	0.47
1:D:1031:ARG:O	1:D:1034:GLU:N	2.48	0.47
1:D:1166:THR:OG1	1:D:1167:ASP:N	2.48	0.47
1:E:1394:LEU:O	1:E:1400:GLY:HA3	2.14	0.47
1:F:1751:TYR:HE2	1:G:1964:PHE:CB	2.27	0.47
1:C:658:ASN:O	1:C:660:ASN:N	2.48	0.47
1:B:560:PHE:CD1	1:B:560:PHE:C	2.88	0.46
1:F:1831:ALA:HA	1:F:1837:LYS:CB	2.45	0.46
1:E:1282:ASN:O	1:E:1284:ASN:N	2.48	0.46
1:E:1496:PHE:CD1	1:E:1496:PHE:C	2.88	0.46
1:E:1501:LEU:O	1:E:1504:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:957:GLY:N	1:D:958:PRO:HD2	2.30	0.46
1:C:705:LEU:HA	1:C:707:PRO:N	2.30	0.46
1:D:970:ASN:O	1:D:972:ASN:N	2.49	0.46
1:E:1329:LEU:HA	1:E:1331:PRO:N	2.30	0.46
1:D:1189:LEU:O	1:D:1192:ALA:HB3	2.16	0.46
1:A:248:PHE:CD1	1:A:248:PHE:C	2.88	0.46
1:F:1655:ARG:O	1:F:1658:GLU:N	2.49	0.46
1:A:316:GLU:O	1:A:317:ALA:HB2	2.15	0.45
1:B:458:LEU:O	1:B:464:GLY:HA3	2.16	0.45
1:C:872:PHE:CD1	1:C:872:PHE:C	2.88	0.45
1:B:393:LEU:HA	1:B:395:PRO:N	2.30	0.45
1:A:146:LEU:O	1:A:152:GLY:HA3	2.17	0.45
1:B:471:TYR:HA	1:B:532[A]:ILE:O	2.17	0.45
1:F:1808:PHE:CD1	1:F:1808:PHE:C	2.88	0.45
1:C:815:TYR:HE2	1:D:1028:PHE:CB	2.29	0.45
1:F:1641:LEU:HA	1:F:1643:PRO:N	2.32	0.45
1:A:253:LEU:O	1:A:256:ALA:HB3	2.17	0.45
1:F:1813:LEU:O	1:F:1816:ALA:HB3	2.17	0.45
1:E:1518:VAL:HA	1:F:1843:ILE:HG21	1.99	0.44
1:F:1798:LEU:O	1:F:1798:LEU:HG	2.17	0.44
1:E:1486:LEU:O	1:E:1486:LEU:HG	2.17	0.44
1:G:2091:LEU:HB3	1:G:2134:ALA:O	2.18	0.44
1:D:956:PHE:CG	1:D:956:PHE:O	2.71	0.44
1:A:34:ASN:O	1:A:36:ASN:N	2.51	0.44
1:G:1918:PHE:CB	1:G:1923:ALA:CB	2.96	0.44
1:G:2063:TYR:CG	1:G:2063:TYR:O	2.69	0.44
1:A:122:ILE:O	1:A:289:THR:HA	2.17	0.44
1:B:471:TYR:HA	1:B:532[B]:ILE:O	2.18	0.44
1:C:854:THR:OG1	1:C:855:ASP:N	2.50	0.44
1:E:1415:ARG:HA	1:E:1416:PRO:HD3	1.91	0.44
1:D:1094[A]:MET:CB	1:D:1155:LEU:HD13	2.48	0.43
1:A:192:ALA:HB2	1:B:397:GLY:C	2.39	0.43
1:G:2165:TYR:HD1	1:G:2166:LEU:N	2.16	0.43
1:A:159:TYR:HA	1:A:220[A]:ILE:O	2.18	0.43
1:E:1269:GLY:N	1:E:1270:PRO:HD2	2.33	0.43
1:G:2125:LEU:O	1:G:2128:ALA:HB3	2.19	0.43
1:G:2120:PHE:CD1	1:G:2120:PHE:C	2.90	0.43
1:B:542:THR:OG1	1:B:543:ASP:N	2.51	0.43
1:B:634:ASN:O	1:B:635:ALA:C	2.56	0.43
1:G:1967:ARG:O	1:G:1970:GLU:N	2.50	0.43
1:A:95:ARG:O	1:A:98:GLU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:783:TYR:HA	1:C:844[A]:ILE:O	2.18	0.43
1:E:1478:THR:OG1	1:E:1479:ASP:N	2.51	0.43
1:F:1718[A]:MET:CB	1:F:1779:LEU:HD13	2.49	0.43
1:F:1779:LEU:HB3	1:F:1822:ALA:O	2.19	0.43
1:G:2110:LEU:O	1:G:2110:LEU:HG	2.18	0.43
1:A:277:LYS:CB	1:A:278:PRO:CD	2.96	0.43
1:B:504:ALA:HB2	1:C:709:GLY:C	2.39	0.43
1:B:565:LEU:O	1:B:568:ALA:HB3	2.19	0.43
1:E:1443:PHE:N	1:F:1614:TYR:HE2	2.13	0.42
1:B:346:ASN:O	1:B:348:ASN:N	2.52	0.42
1:A:293:TYR:C	1:A:293:TYR:HD1	2.22	0.42
1:G:1991:THR:HA	1:G:2134:ALA:HA	2.00	0.42
1:C:819:PHE:CB	1:D:990:TYR:HE2	2.30	0.42
1:B:470[A]:MET:O	1:B:531:LEU:HA	2.20	0.42
1:D:1128:ALA:HB2	1:E:1333:GLY:C	2.39	0.42
1:A:159:TYR:HA	1:A:220[B]:ILE:O	2.20	0.42
1:B:583:ALA:H	1:C:907:ILE:HD13	1.83	0.42
1:E:1541:TYR:HD1	1:E:1542:LEU:N	2.18	0.42
1:F:1791:ASP:O	1:F:1792:TYR:HB2	2.20	0.42
1:C:746:ILE:O	1:C:913:THR:CA	2.66	0.42
1:C:877:LEU:O	1:C:880:ALA:HB3	2.19	0.42
1:E:1406[A]:MET:O	1:E:1467:LEU:HA	2.20	0.42
1:F:1790:THR:OG1	1:F:1791:ASP:N	2.53	0.42
1:C:917:TYR:C	1:C:917:TYR:HD1	2.23	0.41
1:D:1091:GLY:HA3	1:D:1153:ALA:CB	2.38	0.41
1:D:1229:TYR:HD1	1:D:1230:LEU:N	2.18	0.41
1:F:1606:PHE:CB	1:F:1611:ALA:CB	2.98	0.41
1:C:783:TYR:HA	1:C:844[B]:ILE:O	2.19	0.41
1:E:1525:LYS:CB	1:E:1526:PRO:HD2	2.50	0.41
1:A:46:PHE:CB	1:A:51:ALA:CB	2.96	0.41
1:B:605:TYR:C	1:B:605:TYR:HD1	2.24	0.41
1:D:1207:ALA:H	1:E:1531:ILE:HD13	1.85	0.41
1:A:230:THR:OG1	1:A:231:ASP:N	2.53	0.41
1:B:585:VAL:O	1:B:585:VAL:CG1	2.65	0.41
1:B:589:LYS:CB	1:B:590:PRO:CD	2.97	0.41
1:E:1477:ARG:HH11	1:E:1477:ARG:HD2	1.67	0.41
1:F:1580:PHE:O	1:F:1580:PHE:CG	2.74	0.41
1:B:479:ARG:HA	1:B:480:PRO:HD3	1.92	0.41
1:D:1174:LEU:O	1:D:1174:LEU:HG	2.21	0.41
1:C:785:ASP:HA	1:C:846:ASP:O	2.21	0.41
1:D:1097:ASP:HA	1:D:1158:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:PHE:O	1:A:20:PHE:CG	2.73	0.41
1:A:293:TYR:HD1	1:A:294:LEU:N	2.19	0.41
1:D:956:PHE:O	1:D:956:PHE:CD2	2.74	0.41
1:B:473:ASP:HA	1:B:534:ASP:O	2.21	0.40
1:A:84:MET:O	1:A:87:THR:N	2.44	0.40
1:B:544:TYR:CE2	1:B:553:ARG:HA	2.57	0.40
1:C:816:ALA:HB2	1:D:1021:GLY:C	2.41	0.40
1:D:1103:ARG:HA	1:D:1104:PRO:HD3	1.92	0.40
1:D:1131:PHE:N	1:E:1302:TYR:HE2	2.15	0.40
1:B:541:ARG:HH12	1:B:582:VAL:CG1	2.18	0.40
1:D:1209:VAL:HG12	1:D:1209:VAL:O	2.21	0.40
1:F:1752:ALA:HB2	1:G:1957:GLY:C	2.42	0.40
1:F:1755:PHE:CB	1:G:1926:TYR:CE2	3.05	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	312/339 (92%)	264 (85%)	33 (11%)	15 (5%)	2	24
1	B	312/339 (92%)	259 (83%)	38 (12%)	15 (5%)	2	24
1	C	312/339 (92%)	261 (84%)	35 (11%)	16 (5%)	2	22
1	D	312/339 (92%)	265 (85%)	32 (10%)	15 (5%)	2	24
1	E	312/339 (92%)	263 (84%)	34 (11%)	15 (5%)	2	24
1	F	312/339 (92%)	264 (85%)	33 (11%)	15 (5%)	2	24
1	G	312/339 (92%)	260 (83%)	37 (12%)	15 (5%)	2	24
All	All	2184/2373 (92%)	1836 (84%)	242 (11%)	106 (5%)	4	23

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	24	PRO
1	A	35	ALA
1	A	82	VAL
1	A	85	GLY
1	A	311	CYS
1	A	317	ALA
1	B	335	GLN
1	B	336	PRO
1	B	347	ALA
1	B	394	VAL
1	B	618	ILE
1	B	623	CYS
1	B	629	ALA
1	C	647	GLN
1	C	648	PRO
1	C	659	ALA
1	C	706	VAL
1	C	930	ILE
1	C	935	CYS
1	C	941	ALA
1	D	959	GLN
1	D	960	PRO
1	D	971	ALA
1	D	1018	VAL
1	D	1242	ILE
1	D	1247	CYS
1	D	1253	ALA
1	E	1271	GLN
1	E	1272	PRO
1	E	1283	ALA
1	E	1330	VAL
1	E	1333	GLY
1	E	1559	CYS
1	E	1565	ALA
1	F	1583	GLN
1	F	1584	PRO
1	F	1595	ALA
1	F	1642	VAL
1	F	1645	GLY
1	F	1866	ILE
1	F	1871	CYS
1	F	1877	ALA

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Mol	Chain	Res	Type
1	G	1895	GLN
1	G	1896	PRO
1	G	1907	ALA
1	G	1954	VAL
1	G	2178	ILE
1	G	2183	CYS
1	G	2189	ALA
1	A	232	TYR
1	A	234	GLY
1	A	306	ILE
1	B	397	GLY
1	B	402	THR
1	B	544	TYR
1	B	546	GLY
1	B	627	ALA
1	B	641	ALA
1	C	709	GLY
1	C	714	THR
1	C	856	TYR
1	C	858	GLY
1	C	913	THR
1	D	1021	GLY
1	D	1026	THR
1	D	1168	TYR
1	D	1170	GLY
1	D	1251	ALA
1	E	1338	THR
1	E	1482	GLY
1	E	1554	ILE
1	E	1563	ALA
1	F	1650	THR
1	F	1792	TYR
1	F	1794	GLY
1	F	1849	THR
1	G	1957	GLY
1	G	1962	THR
1	G	2104	TYR
1	G	2106	GLY
1	G	2187	ALA
1	G	2201	ALA
1	A	289	THR
1	A	315	ALA

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Mol	Chain	Res	Type
1	A	329	ALA
1	B	601	THR
1	C	939	ALA
1	C	953	ALA
1	D	1225	THR
1	D	1265	ALA
1	E	1480	TYR
1	E	1537	THR
1	E	1577	ALA
1	F	1875	ALA
1	F	1889	ALA
1	G	2161	THR
1	A	25	ILE
1	A	309	SER
1	B	337	ILE
1	C	649	ILE
1	D	961	ILE
1	E	1273	ILE
1	F	1585	ILE
1	G	1897	ILE
1	C	909	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	37/269 (14%)	26 (70%)	11 (30%)	0	2
1	B	37/269 (14%)	25 (68%)	12 (32%)	0	2
1	C	37/269 (14%)	25 (68%)	12 (32%)	0	2
1	D	37/269 (14%)	26 (70%)	11 (30%)	0	2
1	E	37/269 (14%)	25 (68%)	12 (32%)	0	2
1	F	37/269 (14%)	27 (73%)	10 (27%)	0	3
1	G	37/269 (14%)	28 (76%)	9 (24%)	0	4
All	All	259/1883 (14%)	182 (70%)	77 (30%)	1	2

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	TYR
1	A	191	TYR
1	A	219	LEU
1	A	229	ARG
1	A	238	LEU
1	A	268	GLN
1	A	274	ASP
1	A	283	ILE
1	A	293	TYR
1	A	310	PRO
1	A	313	PRO
1	B	359	HIS
1	B	531	LEU
1	B	541	ARG
1	B	545	SER
1	B	550	LEU
1	B	580	GLN
1	B	586	ASP
1	B	595	ILE
1	B	605	TYR
1	B	619	TYR
1	B	622	PRO
1	B	625	PRO
1	C	671	HIS
1	C	815	TYR
1	C	843	LEU
1	C	853	ARG
1	C	857	SER
1	C	862	LEU
1	C	892	GLN
1	C	898	ASP
1	C	917	TYR
1	C	931	TYR
1	C	934	PRO
1	C	937	PRO
1	D	983	HIS
1	D	1127	TYR
1	D	1165	ARG
1	D	1169	SER
1	D	1174	LEU
1	D	1204	GLN
1	D	1210	ASP

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Mol	Chain	Res	Type
1	D	1229	TYR
1	D	1243	TYR
1	D	1246	PRO
1	D	1249	PRO
1	E	1295	HIS
1	E	1439	TYR
1	E	1467	LEU
1	E	1477	ARG
1	E	1481	SER
1	E	1486	LEU
1	E	1516	GLN
1	E	1522	ASP
1	E	1541	TYR
1	E	1555	TYR
1	E	1558	PRO
1	E	1561	PRO
1	F	1751	TYR
1	F	1789	ARG
1	F	1798	LEU
1	F	1828	GLN
1	F	1834	ASP
1	F	1843	ILE
1	F	1853	TYR
1	F	1867	TYR
1	F	1870	PRO
1	F	1873	PRO
1	G	2101	ARG
1	G	2110	LEU
1	G	2140	GLN
1	G	2146	ASP
1	G	2155	ILE
1	G	2165	TYR
1	G	2179	TYR
1	G	2182	PRO
1	G	2185	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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.

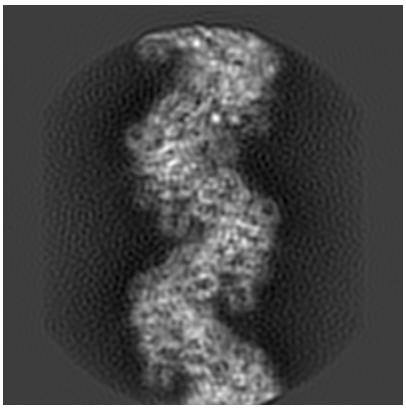
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8183. These allow visual inspection of the internal detail of the map and identification of artifacts.

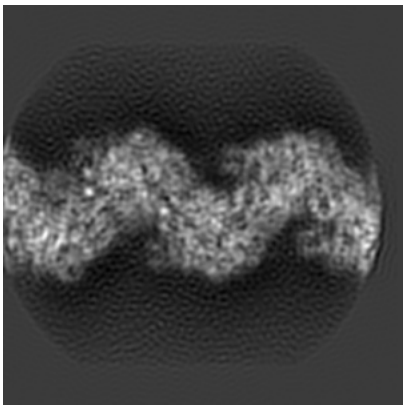
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

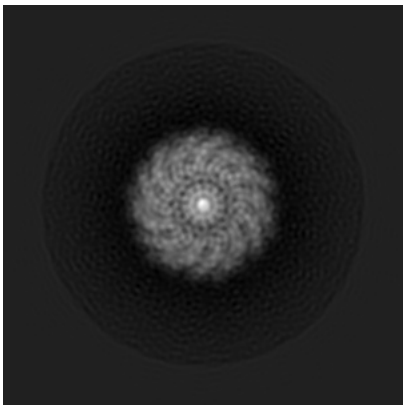
6.1.1 Primary map



X

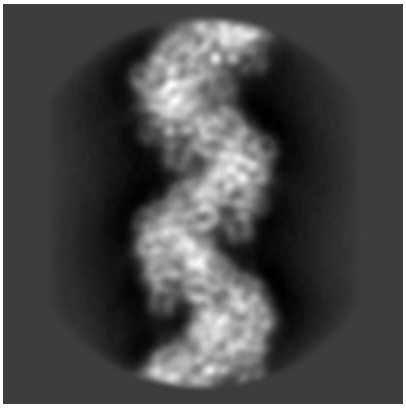


Y

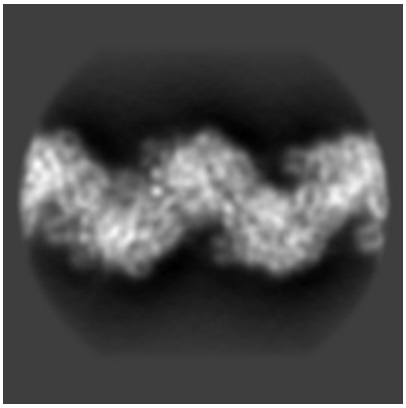


Z

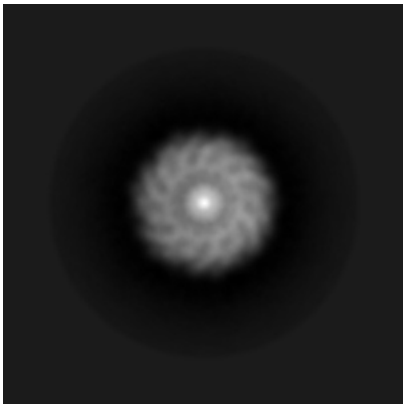
6.1.2 Raw map



X



Y

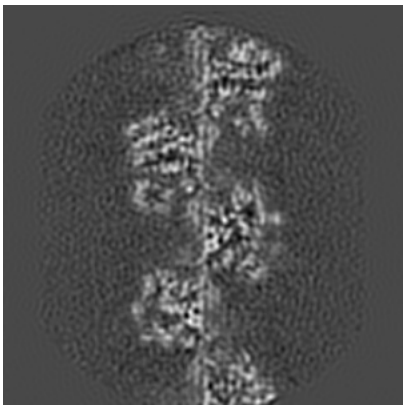


Z

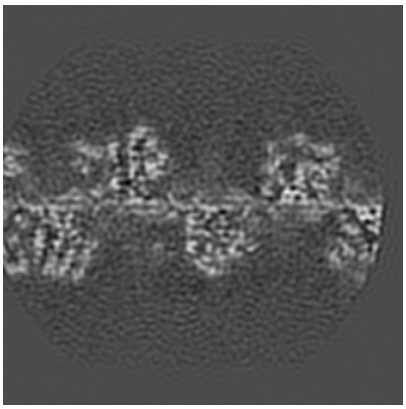
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

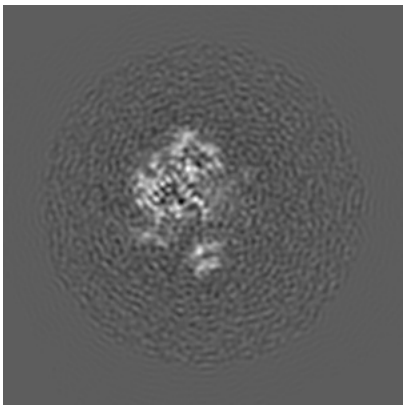
6.2.1 Primary map



X Index: 128

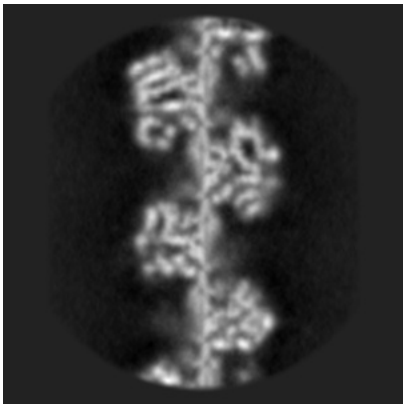


Y Index: 128

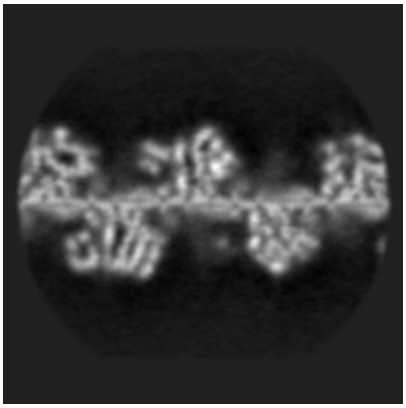


Z Index: 128

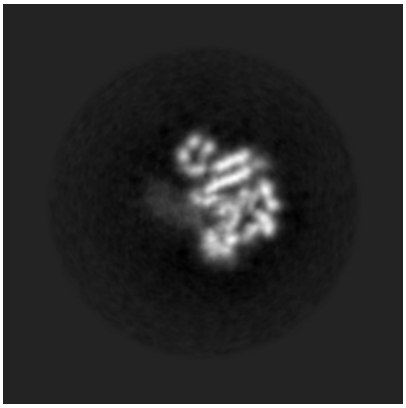
6.2.2 Raw map



X Index: 100



Y Index: 100

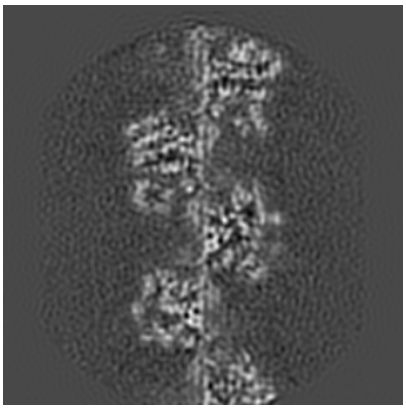


Z Index: 100

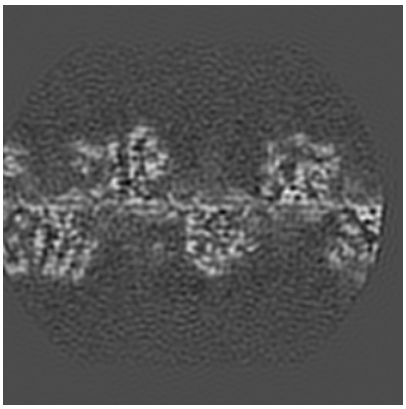
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

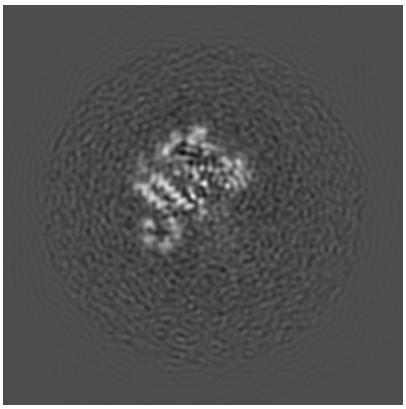
6.3.1 Primary map



X Index: 128

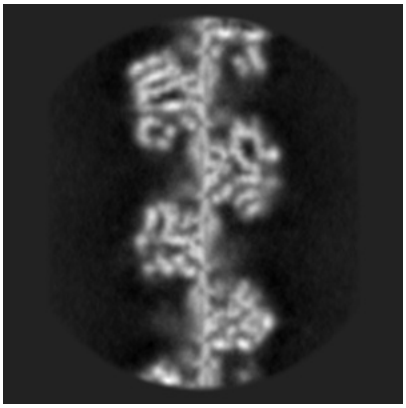


Y Index: 128

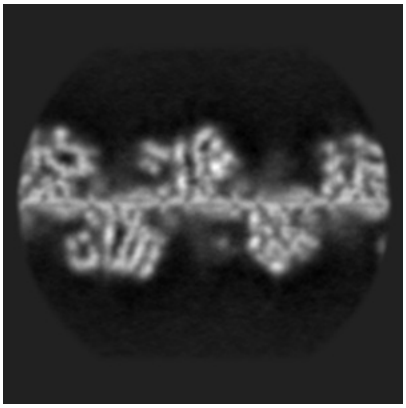


Z Index: 118

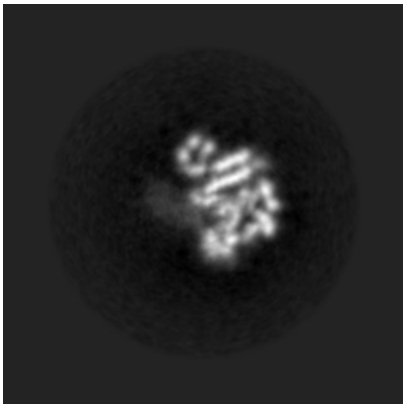
6.3.2 Raw map



X Index: 100



Y Index: 100



Z Index: 100

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 0.16. 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.

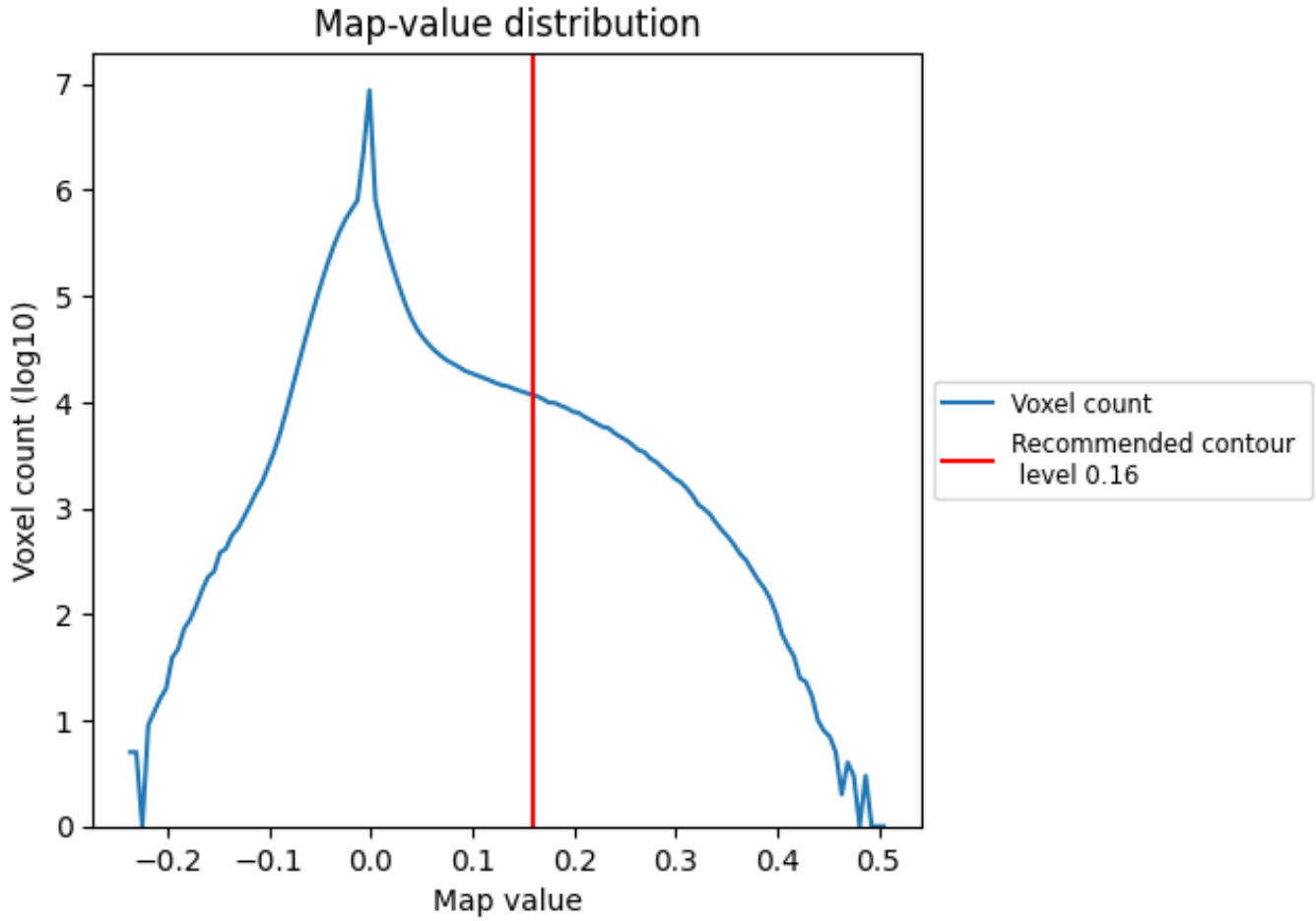
6.5 Mask visualisation (i)

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

7 Map analysis

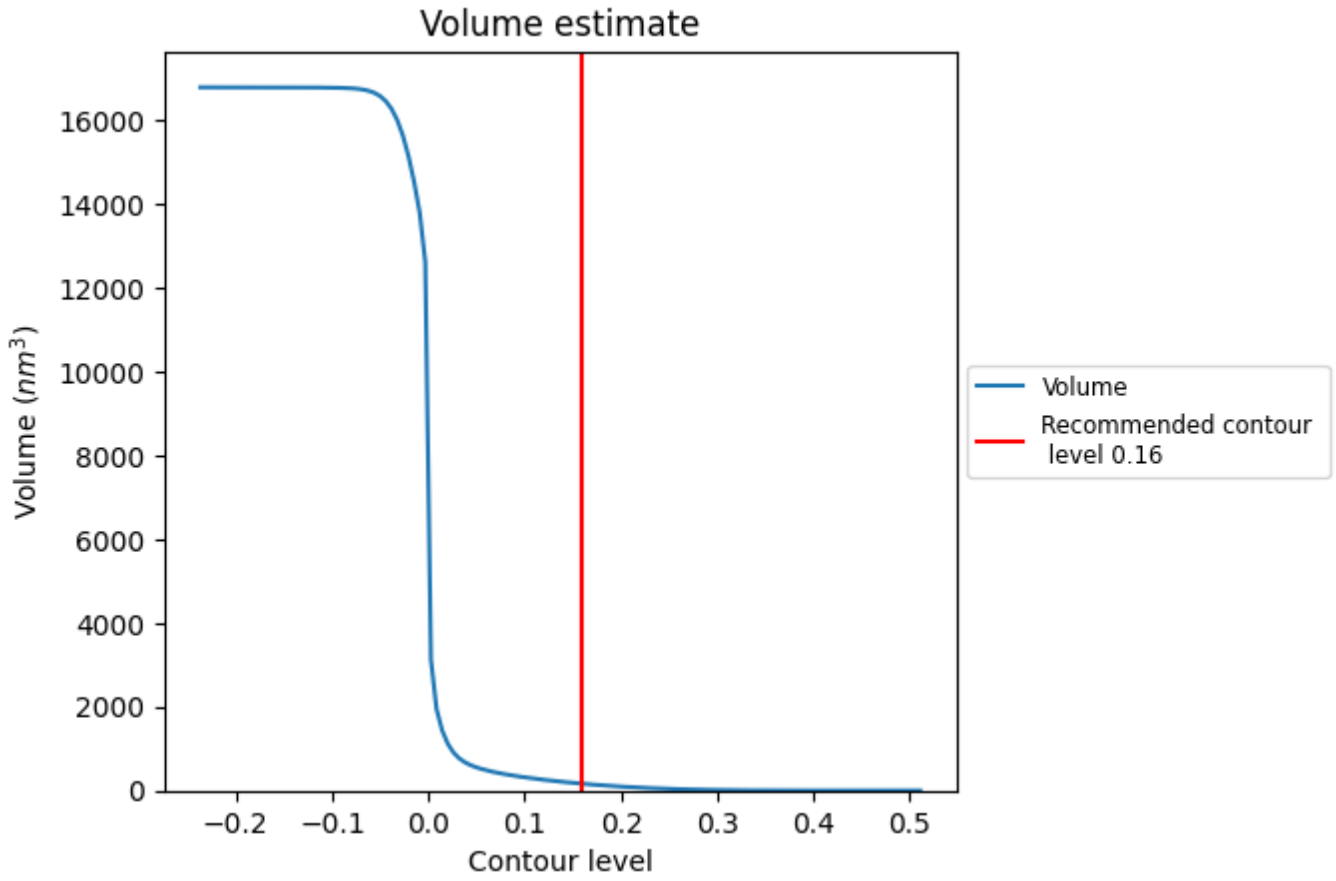
This section contains the results of statistical analysis of the map.

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.

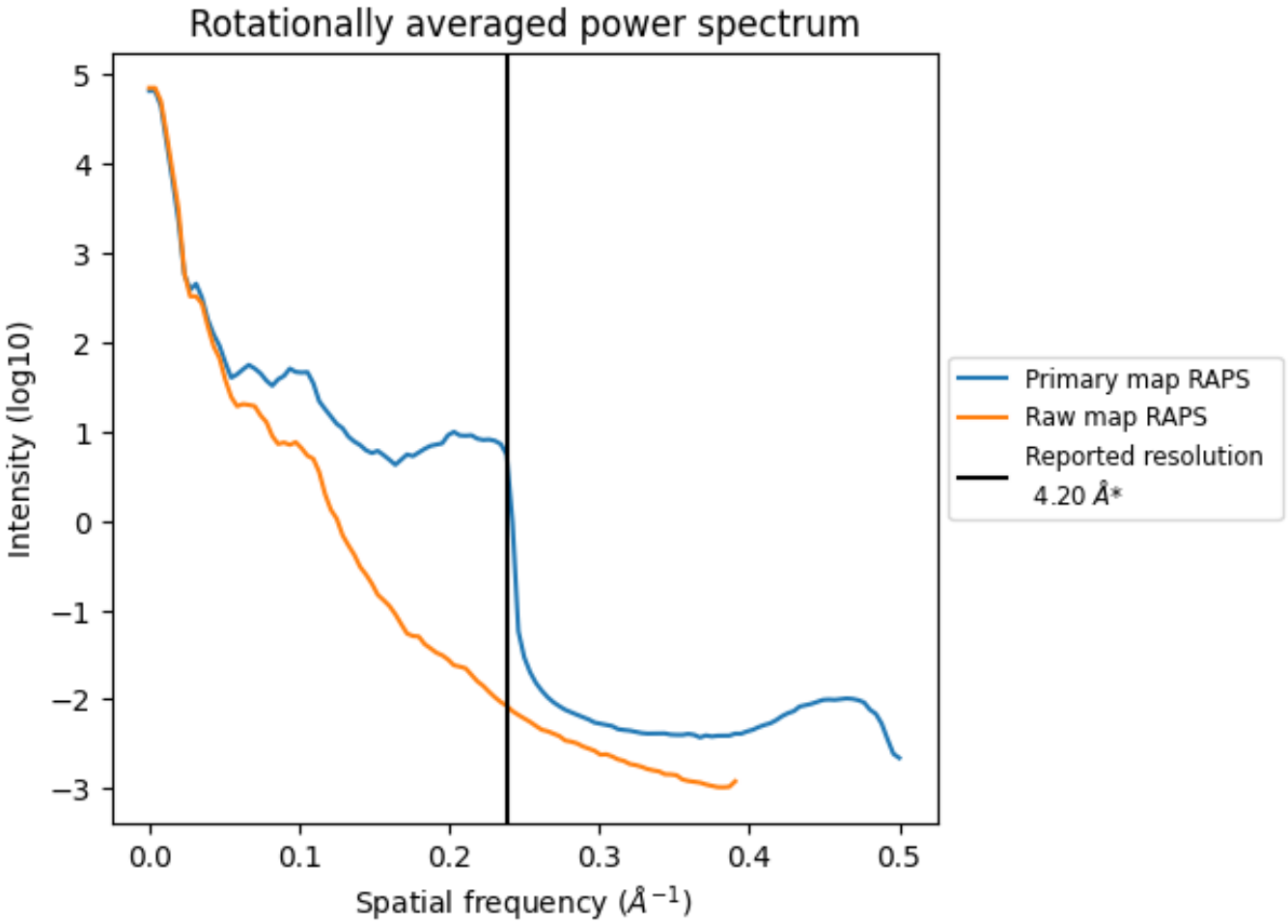
7.2 Volume estimate



The volume at the recommended contour level is 164 nm^3; this corresponds to an approximate mass of 148 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)

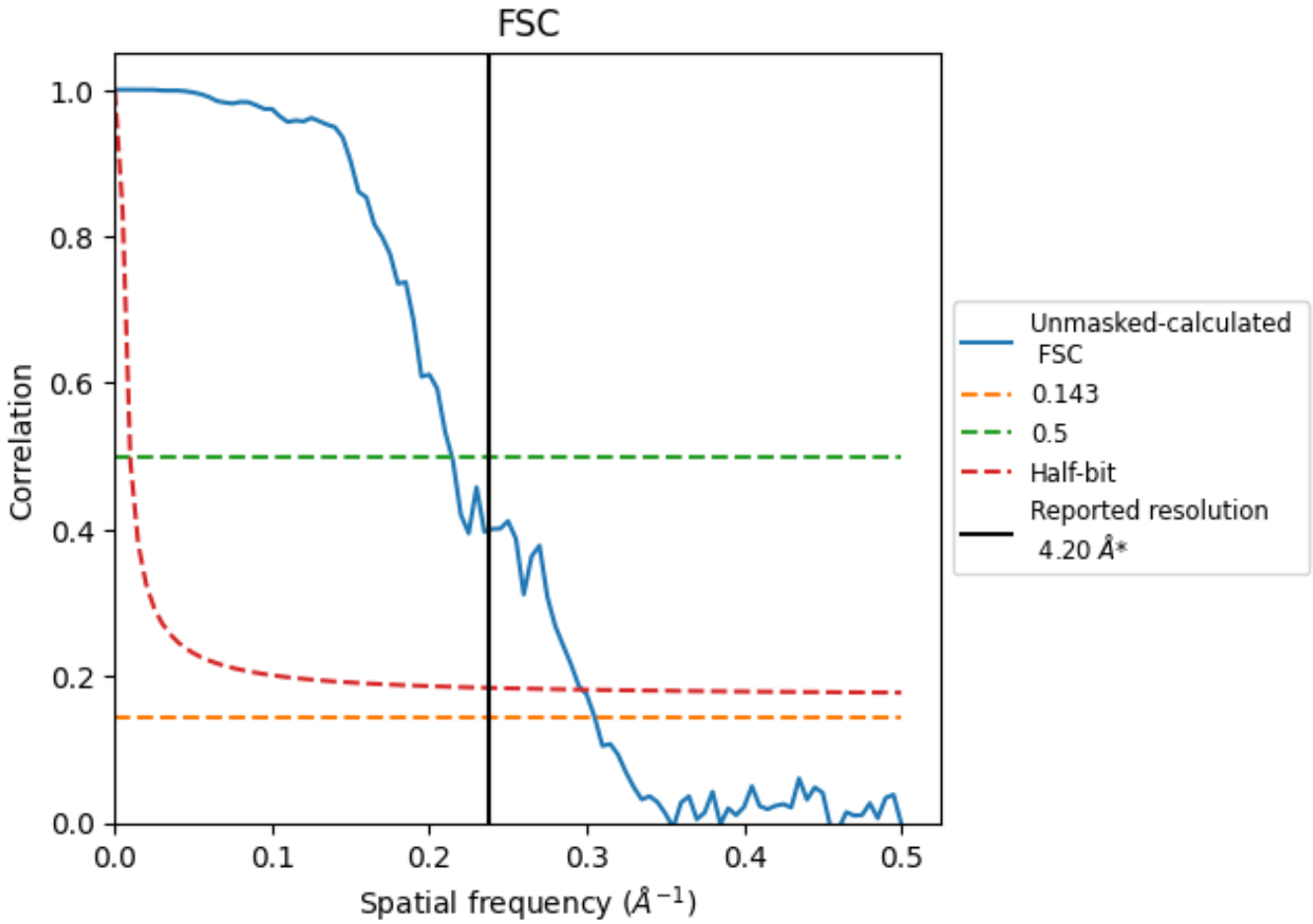


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

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 0.238 Å^{-1}

8.2 Resolution estimates (i)

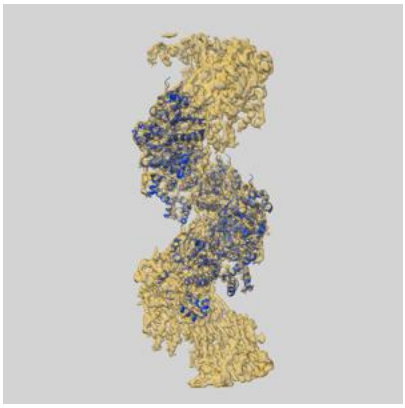
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.28	4.67	3.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.28 differs from the reported value 4.2 by more than 10 %

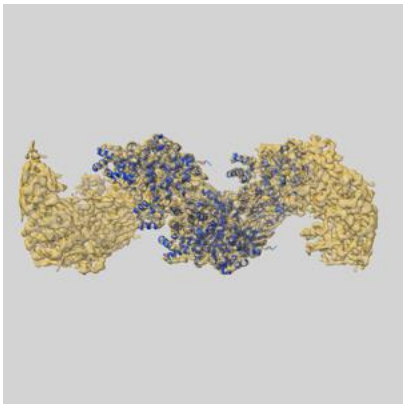
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8183 and PDB model 5JZC. Per-residue inclusion information can be found in section 3 on page 4.

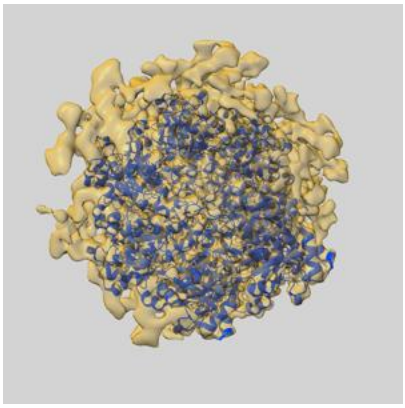
9.1 Map-model overlay



X



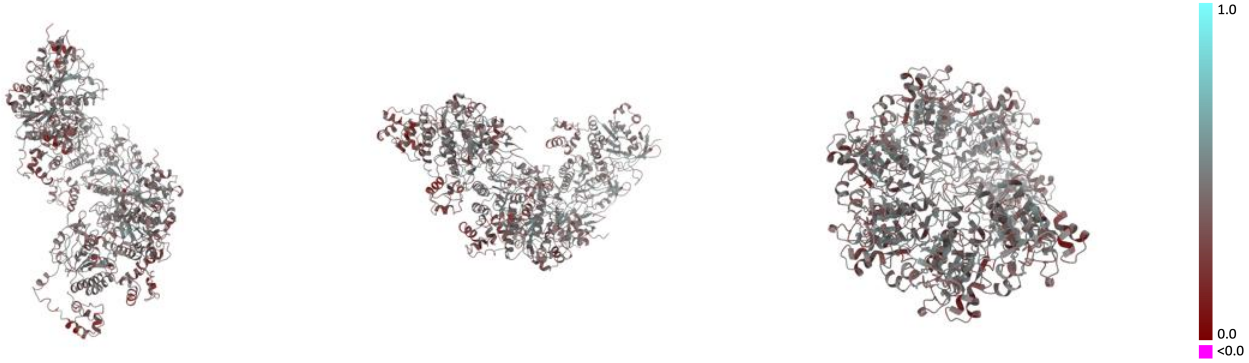
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16 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.

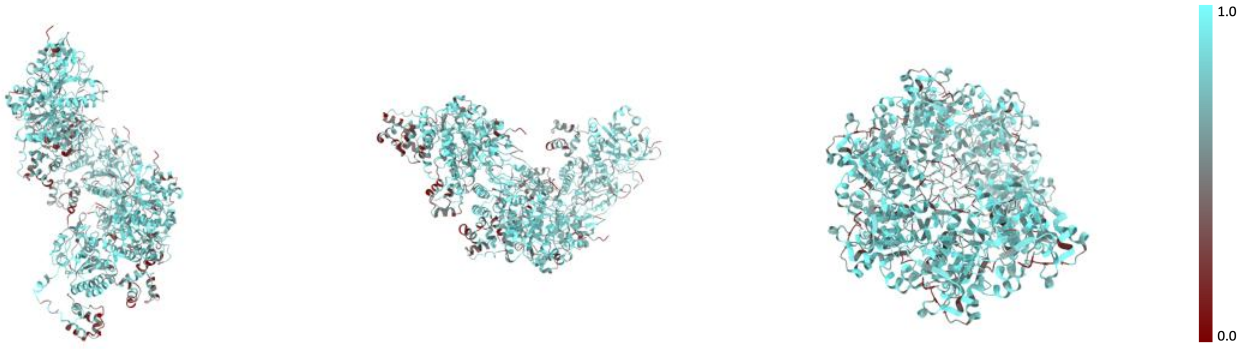
9.2 Q-score mapped to coordinate model (i)



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.

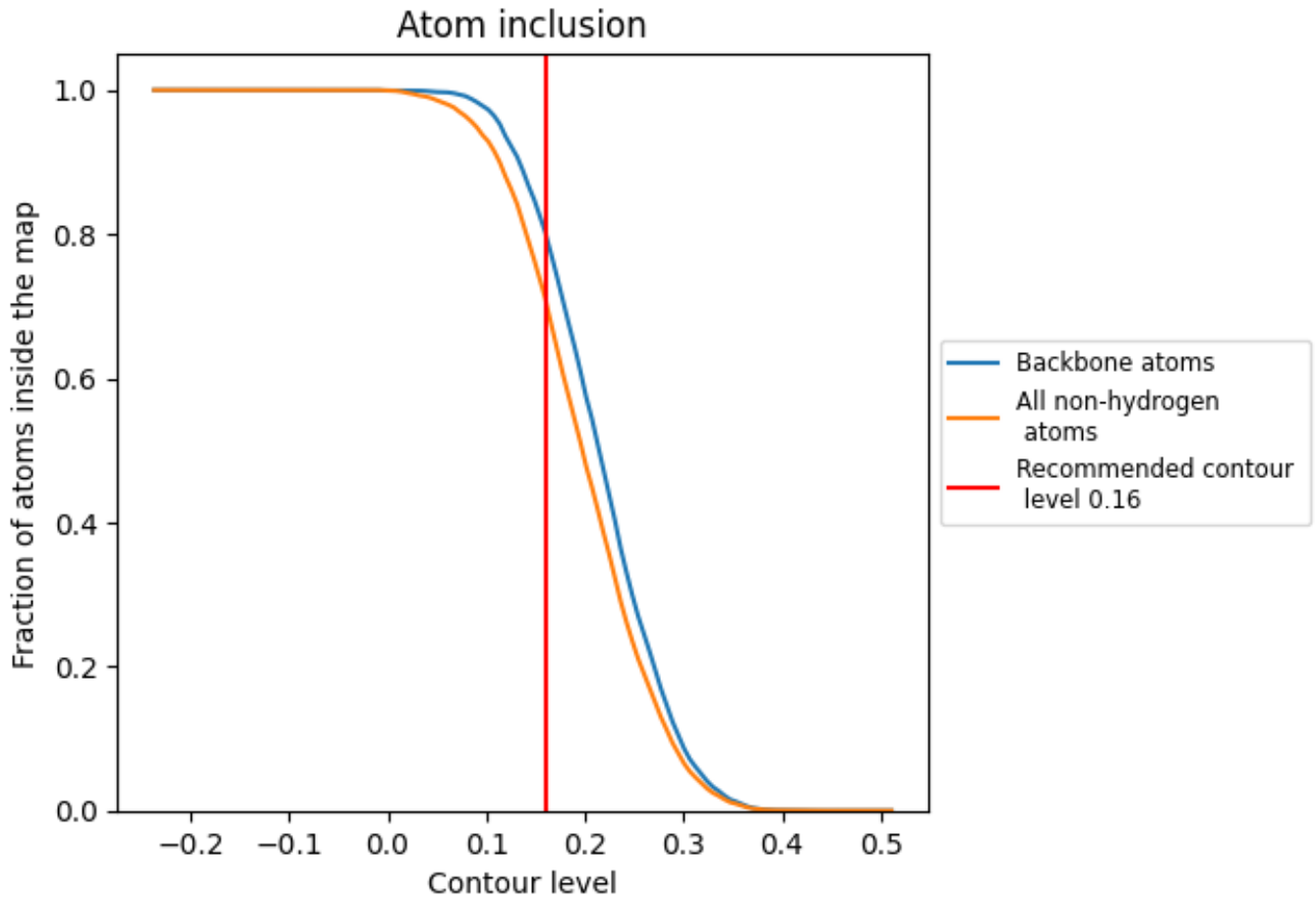
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.16).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 71% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7101	0.4170
A	0.7028	0.4150
B	0.7087	0.4180
C	0.7147	0.4180
D	0.7123	0.4200
E	0.7147	0.4200
F	0.7093	0.4160
G	0.7081	0.4140