



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:45 AM UTC

PDB ID : 8XL0 / pdb_00008xl0
EMDB ID : EMD-38433
Title : Citrate-induced filament of human acetyl-coenzyme A carboxylase 1 (ACC1-citrate)
Authors : Zhou, F.Y.; Zhang, Y.Y.; Zhou, Q.; Hu, Q.
Deposited on : 2023-12-25
Resolution : 4.14 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

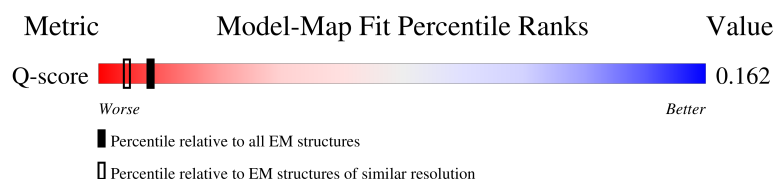
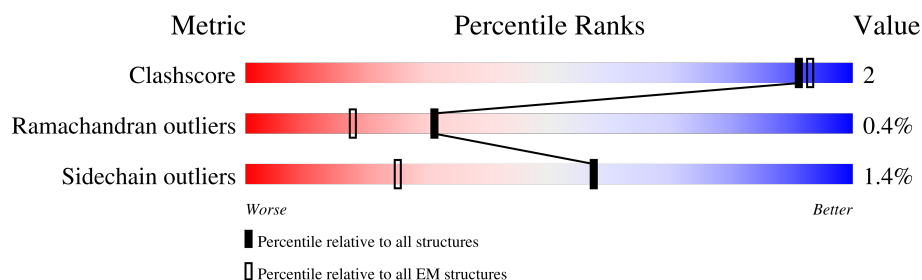
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.14 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5577 (3.64 - 4.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2346	
1	B	2346	
1	C	2346	
1	D	2346	

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Mol	Chain	Length	Quality of chain
1	E	2346	38%74%••22%
1	F	2346	38%53%•45%

2 Entry composition [i](#)

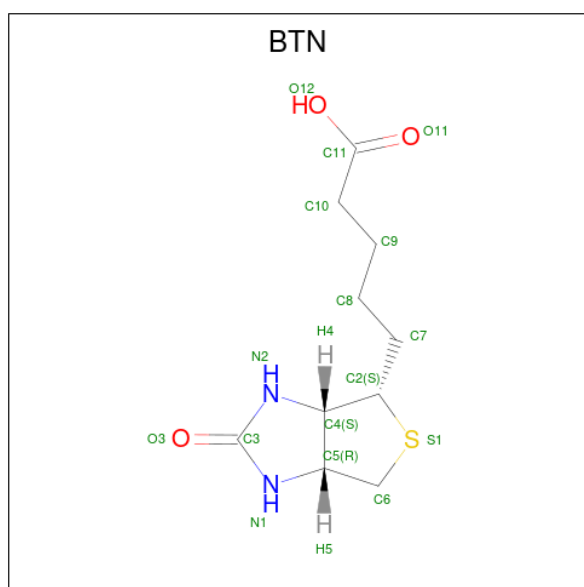
There are 2 unique types of molecules in this entry. The entry contains 93175 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

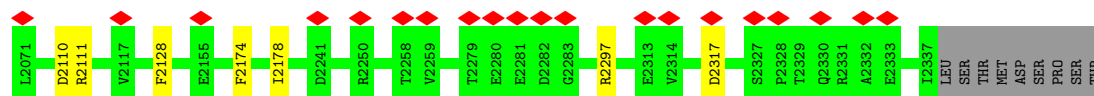
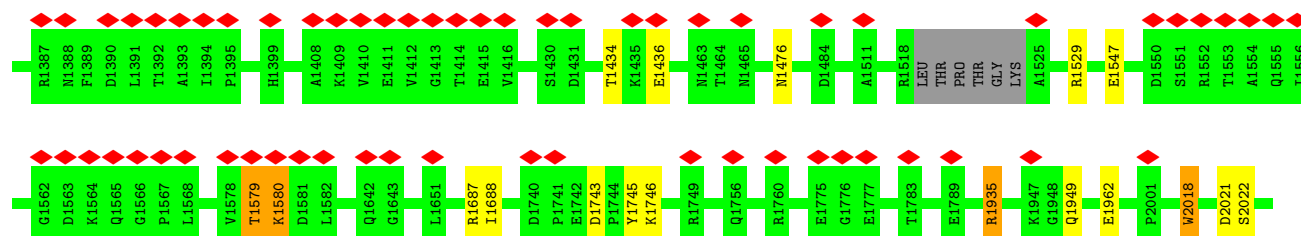
- Molecule 1 is a protein called Acetyl-CoA carboxylase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2146	Total	C	N	O	S	0	0
			17120	10879	2976	3166	99		
1	B	2146	Total	C	N	O	S	0	0
			17120	10879	2976	3166	99		
1	C	2146	Total	C	N	O	S	0	0
			17120	10879	2976	3166	99		
1	D	2146	Total	C	N	O	S	0	0
			17120	10879	2976	3166	99		
1	E	1819	Total	C	N	O	S	0	0
			14435	9170	2503	2676	86		
1	F	1289	Total	C	N	O	S	0	0
			10185	6478	1764	1890	53		

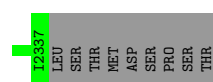
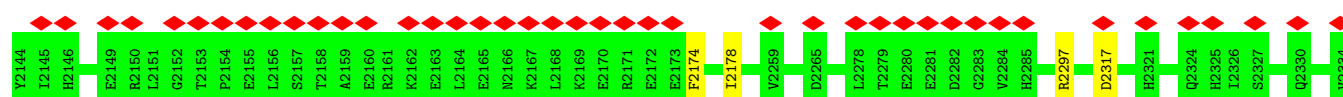
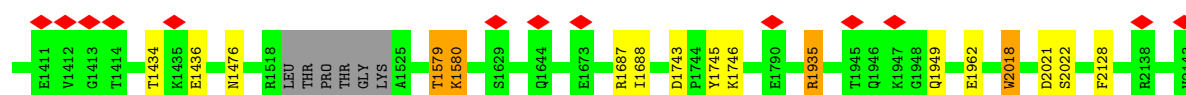
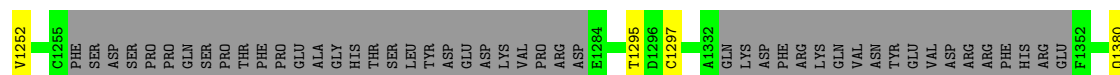
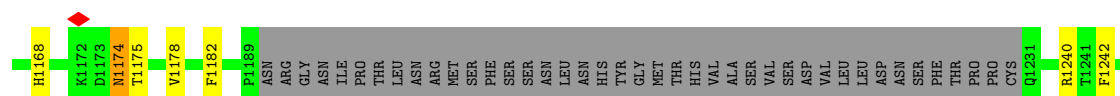
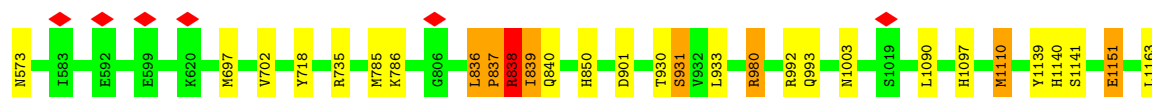
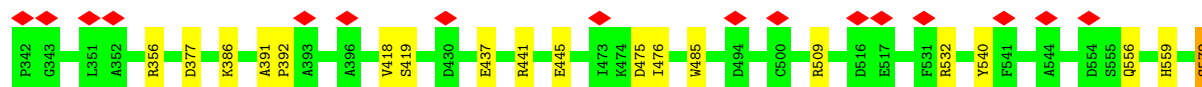
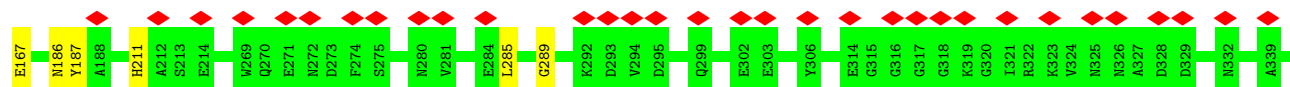
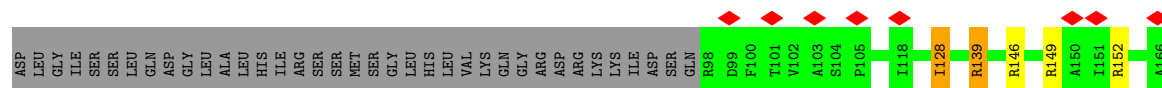
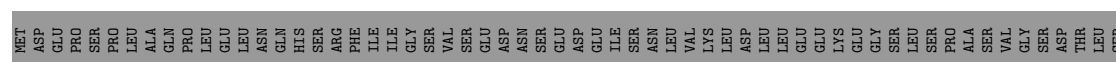
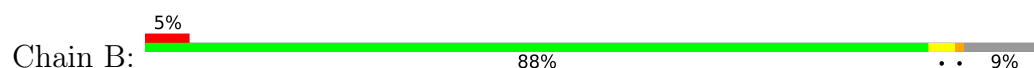
- Molecule 2 is BIOTIN (CCD ID: BTN) (formula: $C_{10}H_{16}N_2O_3S$) (labeled as "Ligand of Interest" by depositor).



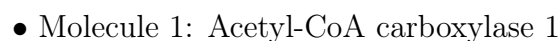
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 15	C 10	N 2	O 2	S 1	0
2	B	1	Total 15	C 10	N 2	O 2	S 1	0
2	C	1	Total 15	C 10	N 2	O 2	S 1	0
2	D	1	Total 15	C 10	N 2	O 2	S 1	0
2	E	1	Total 15	C 10	N 2	O 2	S 1	0



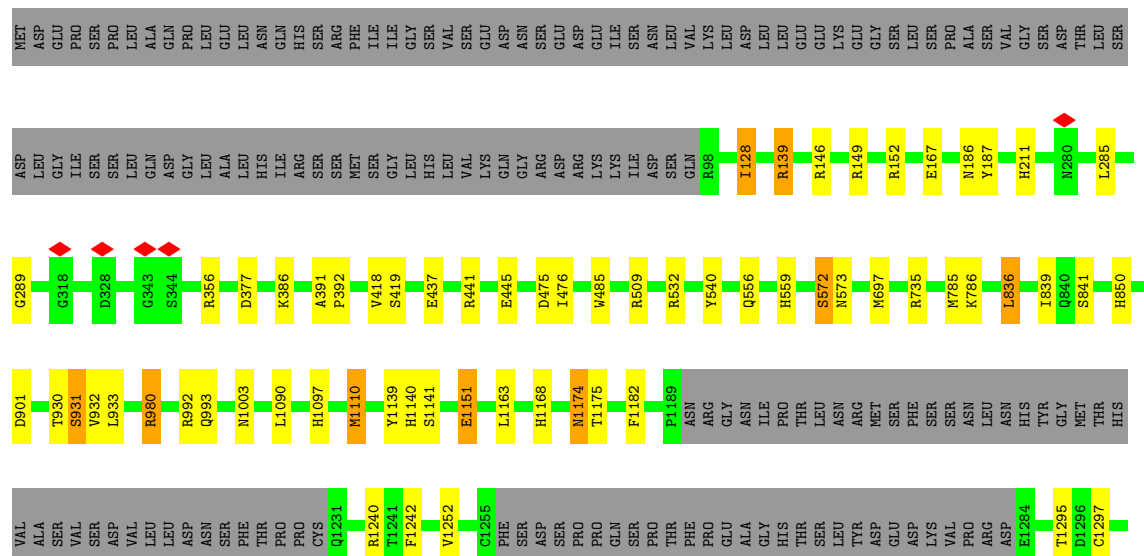
• Molecule 1: Acetyl-CoA carboxylase 1

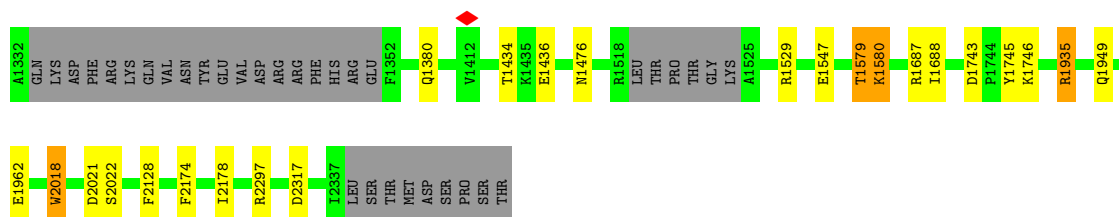


Chain C: 87% . . 9%

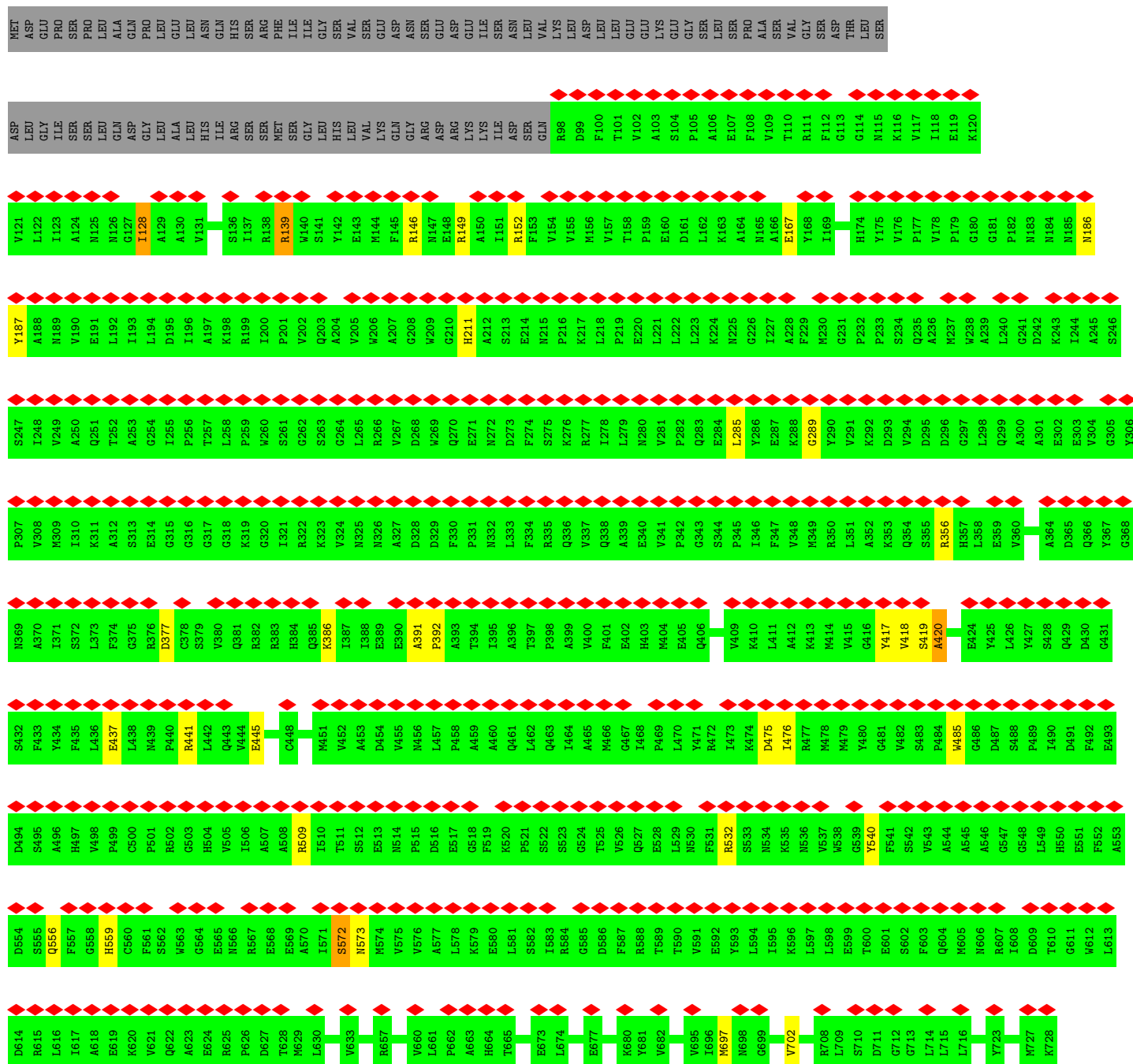
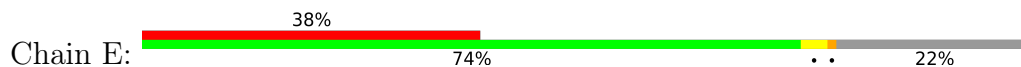


Chain D: 88% .. 9%





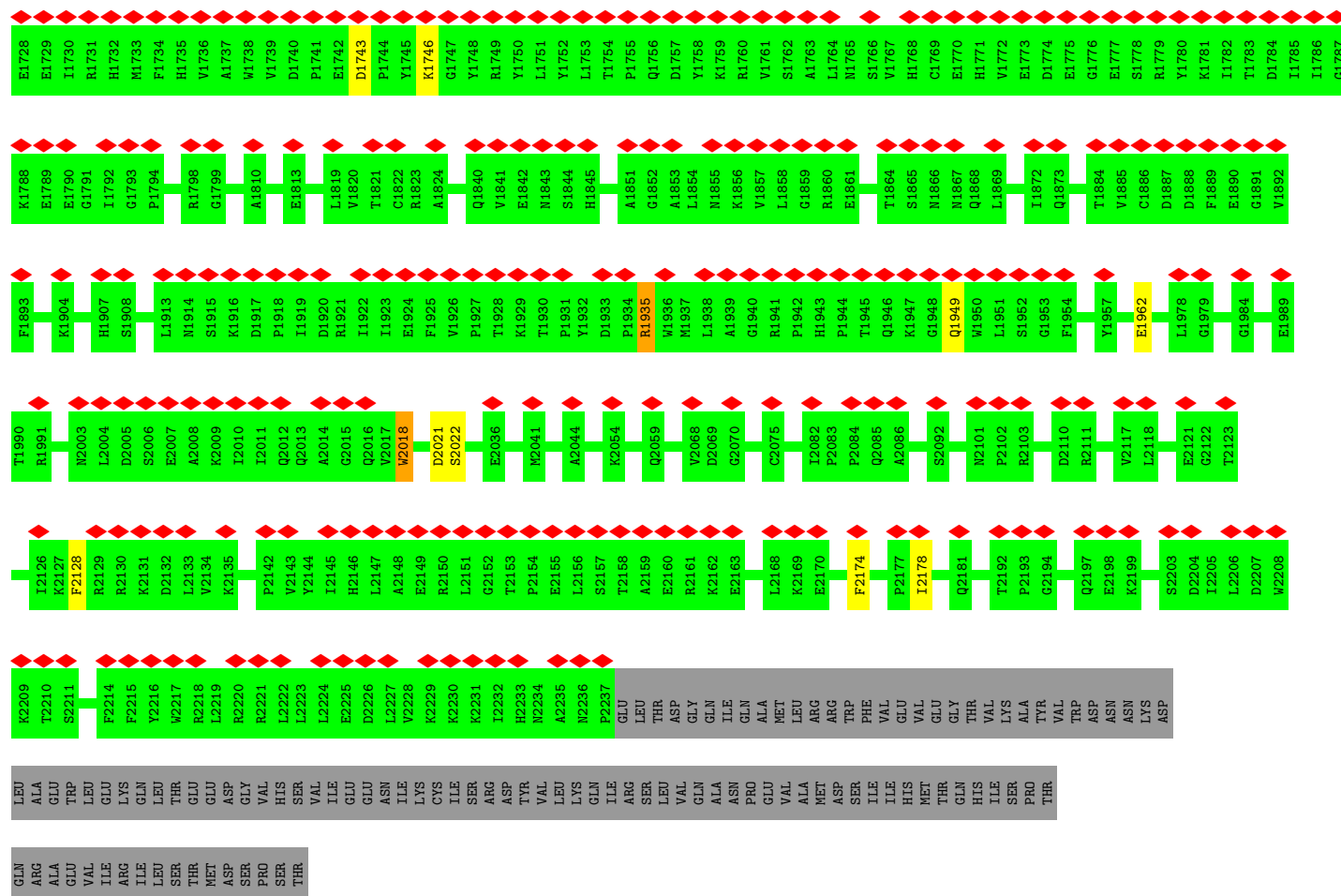
• Molecule 1: Acetyl-CoA carboxylase 1











4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36041	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.719	Depositor
Minimum map value	-0.669	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	525.72235, 525.72235, 525.72235	wwPDB
Map dimensions	488, 488, 488	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0773, 1.0773, 1.0773	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BTN

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	0.45	1/17490 (0.0%)	0.50	6/23691 (0.0%)
1	B	0.44	1/17490 (0.0%)	0.50	6/23691 (0.0%)
1	C	0.45	1/17490 (0.0%)	0.50	6/23691 (0.0%)
1	D	0.44	1/17490 (0.0%)	0.50	6/23691 (0.0%)
1	E	0.44	0/14745	0.50	6/19979 (0.0%)
1	F	0.49	1/10423 (0.0%)	0.48	2/14139 (0.0%)
All	All	0.45	5/95128 (0.0%)	0.50	32/128882 (0.0%)

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	4
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	4
1	F	0	2
All	All	0	22

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	2018	TRP	C-N	-7.42	1.20	1.32
1	F	2018	TRP	C-N	-7.42	1.20	1.32
1	B	2018	TRP	C-N	-7.37	1.20	1.32
1	A	2018	TRP	C-N	-6.79	1.21	1.32
1	C	2018	TRP	C-N	-6.76	1.21	1.32

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	418	VAL	CA-C-N	6.21	133.41	121.54
1	F	418	VAL	C-N-CA	6.21	133.41	121.54
1	B	418	VAL	CA-C-N	6.21	133.40	121.54
1	B	418	VAL	C-N-CA	6.21	133.40	121.54
1	D	418	VAL	CA-C-N	6.21	133.39	121.54
1	D	418	VAL	C-N-CA	6.21	133.39	121.54
1	E	418	VAL	CA-C-N	6.06	133.12	121.54
1	E	418	VAL	C-N-CA	6.06	133.12	121.54
1	C	418	VAL	CA-C-N	6.05	133.10	121.54
1	C	418	VAL	C-N-CA	6.05	133.10	121.54
1	A	418	VAL	CA-C-N	6.03	133.05	121.54
1	A	418	VAL	C-N-CA	6.03	133.05	121.54
1	D	1240	ARG	CA-C-N	5.73	132.48	121.54
1	D	1240	ARG	C-N-CA	5.73	132.48	121.54
1	B	1240	ARG	CA-C-N	5.73	132.48	121.54
1	B	1240	ARG	C-N-CA	5.73	132.48	121.54
1	A	1240	ARG	CA-C-N	5.69	132.41	121.54
1	A	1240	ARG	C-N-CA	5.69	132.41	121.54
1	C	1240	ARG	CA-C-N	5.67	132.38	121.54
1	C	1240	ARG	C-N-CA	5.67	132.38	121.54
1	E	1240	ARG	CA-C-N	5.67	132.38	121.54
1	E	1240	ARG	C-N-CA	5.67	132.38	121.54
1	D	1139	TYR	CA-C-N	5.65	132.34	121.54
1	D	1139	TYR	C-N-CA	5.65	132.34	121.54
1	B	1139	TYR	CA-C-N	5.64	132.31	121.54
1	B	1139	TYR	C-N-CA	5.64	132.31	121.54
1	E	1139	TYR	CA-C-N	5.60	132.23	121.54
1	E	1139	TYR	C-N-CA	5.60	132.23	121.54
1	C	1139	TYR	CA-C-N	5.58	132.21	121.54
1	C	1139	TYR	C-N-CA	5.58	132.21	121.54
1	A	1139	TYR	CA-C-N	5.58	132.20	121.54
1	A	1139	TYR	C-N-CA	5.58	132.20	121.54

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1140	HIS	Peptide
1	A	1579	THR	Mainchain
1	A	1687	ARG	Peptide
1	A	419	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	B	1140	HIS	Peptide
1	B	1579	THR	Mainchain
1	B	1687	ARG	Peptide
1	B	419	SER	Mainchain
1	C	1140	HIS	Peptide
1	C	1579	THR	Mainchain
1	C	1687	ARG	Peptide
1	C	419	SER	Mainchain
1	D	1140	HIS	Peptide
1	D	1579	THR	Mainchain
1	D	1687	ARG	Peptide
1	D	419	SER	Mainchain
1	E	1140	HIS	Peptide
1	E	1579	THR	Mainchain
1	E	1687	ARG	Peptide
1	E	419	SER	Mainchain
1	F	1687	ARG	Peptide
1	F	419	SER	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17120	0	17048	48	0
1	B	17120	0	17047	86	0
1	C	17120	0	17048	71	0
1	D	17120	0	17047	71	0
1	E	14435	0	14365	80	0
1	F	10185	0	10086	20	0
2	A	15	0	15	0	0
2	B	15	0	15	1	0
2	C	15	0	15	0	0
2	D	15	0	15	0	0
2	E	15	0	15	0	0
All	All	93175	0	92716	292	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (292) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:930:THR:HG22	1:E:1168:HIS:HB2	1.23	1.10
1:D:1168:HIS:HB2	1:E:930:THR:HG22	1.44	0.99
1:B:1168:HIS:HB2	1:C:930:THR:HG22	1.51	0.92
1:B:930:THR:HG22	1:C:1168:HIS:HB2	1.49	0.92
1:B:933:LEU:HG	1:C:1151:GLU:OE1	1.72	0.89
1:B:1110:MET:HG2	1:C:980:ARG:HH22	1.40	0.84
1:E:840:GLN:O	1:E:841:SER:HB3	1.78	0.83
1:B:1168:HIS:HD2	1:B:1178:VAL:HG22	1.43	0.83
1:B:931:SER:HA	1:C:1168:HIS:ND1	1.96	0.80
1:B:1110:MET:HB3	1:C:980:ARG:NH2	1.97	0.80
1:D:980:ARG:HD2	1:E:1112:GLY:O	1.83	0.79
1:B:931:SER:HA	1:C:1168:HIS:CE1	2.20	0.77
1:D:933:LEU:HG	1:E:1151:GLU:OE1	1.88	0.74
1:A:702:VAL:HB	1:A:836:LEU:HD12	1.70	0.74
1:B:697:MET:HB3	1:B:836:LEU:CD2	2.18	0.73
1:B:836:LEU:N	1:B:836:LEU:HD23	2.03	0.73
1:D:980:ARG:NH2	1:E:1110:MET:HB3	2.04	0.73
1:E:836:LEU:HD23	1:E:836:LEU:N	2.03	0.73
1:B:930:THR:O	1:C:1168:HIS:ND1	2.20	0.73
1:B:838:ARG:HG2	1:B:838:ARG:O	1.89	0.72
1:B:1168:HIS:HD2	1:B:1178:VAL:CG2	2.02	0.72
1:C:139:ARG:NH1	1:D:573:ASN:OD1	2.23	0.71
1:E:139:ARG:NH1	1:F:573:ASN:OD1	2.23	0.71
1:A:139:ARG:NH1	1:B:573:ASN:OD1	2.23	0.71
1:B:931:SER:HA	1:C:1168:HIS:HD1	1.52	0.71
1:B:697:MET:HE2	1:B:836:LEU:HD22	1.73	0.71
1:E:573:ASN:OD1	1:F:139:ARG:NH1	2.24	0.71
1:B:1110:MET:CG	1:C:980:ARG:HH22	2.04	0.70
1:C:573:ASN:OD1	1:D:139:ARG:NH1	2.24	0.70
1:A:573:ASN:OD1	1:B:139:ARG:NH1	2.24	0.70
1:D:1110:MET:HG2	1:E:980:ARG:NH2	2.06	0.70
1:B:697:MET:HB3	1:B:836:LEU:HD21	1.74	0.70
1:E:838:ARG:O	1:E:838:ARG:HG3	1.90	0.70
1:E:1743:ASP:OD2	1:E:1746:LYS:NZ	2.25	0.69
1:C:1743:ASP:OD2	1:C:1746:LYS:NZ	2.25	0.69
1:D:930:THR:CG2	1:E:1168:HIS:HB2	2.15	0.68
1:B:930:THR:O	1:C:1168:HIS:HB2	1.93	0.68
1:D:1743:ASP:OD2	1:D:1746:LYS:NZ	2.26	0.68
1:F:1743:ASP:OD2	1:F:1746:LYS:NZ	2.26	0.68
1:A:1743:ASP:OD2	1:A:1746:LYS:NZ	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1743:ASP:OD2	1:B:1746:LYS:NZ	2.26	0.67
1:D:931:SER:HA	1:E:1168:HIS:ND1	2.09	0.67
1:D:931:SER:HA	1:E:1168:HIS:HD1	1.58	0.67
1:B:1151:GLU:OE1	1:C:933:LEU:HG	1.93	0.67
1:D:1935:ARG:NH1	1:D:1962:GLU:OE1	2.28	0.67
1:D:697:MET:HB3	1:D:836:LEU:CD2	2.25	0.67
1:B:1935:ARG:NH1	1:B:1962:GLU:OE1	2.28	0.67
1:E:836:LEU:HD23	1:E:836:LEU:H	1.58	0.67
1:F:1935:ARG:NH1	1:F:1962:GLU:OE1	2.28	0.67
1:D:980:ARG:HH22	1:E:1110:MET:HG2	1.62	0.65
1:B:1110:MET:HB3	1:C:980:ARG:HH22	1.59	0.65
1:C:837:PRO:O	1:C:838:ARG:HB3	1.97	0.65
1:D:391:ALA:HB3	1:D:392:PRO:HD3	1.79	0.65
1:E:980:ARG:HH11	1:E:983:MET:CE	2.10	0.64
1:F:391:ALA:HB3	1:F:392:PRO:HD3	1.79	0.64
1:B:391:ALA:HB3	1:B:392:PRO:HD3	1.79	0.64
1:E:697:MET:HB3	1:E:836:LEU:CD2	2.26	0.64
1:A:391:ALA:HB3	1:A:392:PRO:HD3	1.80	0.64
1:B:836:LEU:HD23	1:B:836:LEU:H	1.61	0.64
1:E:391:ALA:HB3	1:E:392:PRO:HD3	1.80	0.64
1:E:697:MET:HE2	1:E:836:LEU:HD22	1.79	0.64
1:A:1935:ARG:NH1	1:A:1962:GLU:OE1	2.31	0.64
1:D:980:ARG:CD	1:E:1112:GLY:O	2.46	0.64
1:D:931:SER:HA	1:E:1168:HIS:CE1	2.32	0.63
1:D:980:ARG:HH22	1:E:1110:MET:HB3	1.61	0.63
1:D:1151:GLU:OE1	1:E:933:LEU:HG	1.99	0.63
1:D:697:MET:HB3	1:D:836:LEU:HD21	1.81	0.63
1:E:1935:ARG:NH1	1:E:1962:GLU:OE1	2.31	0.63
1:C:1935:ARG:NH1	1:C:1962:GLU:OE1	2.31	0.62
1:C:391:ALA:HB3	1:C:392:PRO:HD3	1.80	0.62
1:B:1151:GLU:OE2	1:C:931:SER:HB2	2.01	0.61
1:D:930:THR:HG21	1:E:1168:HIS:O	2.00	0.61
1:A:838:ARG:N	1:A:838:ARG:HD3	2.16	0.60
1:B:836:LEU:O	1:B:837:PRO:O	2.19	0.60
1:D:1168:HIS:HD1	1:E:931:SER:HA	1.66	0.60
1:B:933:LEU:CG	1:C:1151:GLU:OE1	2.49	0.60
1:F:128:ILE:HD11	1:F:556:GLN:O	2.02	0.60
1:B:1110:MET:CB	1:C:980:ARG:HH22	2.15	0.60
1:D:933:LEU:HD12	1:E:1155:ARG:NE	2.17	0.60
1:B:1168:HIS:CD2	1:B:1178:VAL:HG22	2.32	0.59
1:D:128:ILE:HD11	1:D:556:GLN:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1110:MET:HG2	1:E:980:ARG:HH22	1.67	0.59
1:D:186:ASN:OD1	1:D:187:TYR:N	2.36	0.59
1:A:838:ARG:HH21	1:A:838:ARG:HG3	1.67	0.58
1:B:128:ILE:HD11	1:B:556:GLN:O	2.02	0.58
1:F:186:ASN:OD1	1:F:187:TYR:N	2.36	0.58
1:B:186:ASN:OD1	1:B:187:TYR:N	2.36	0.58
1:C:186:ASN:OD1	1:C:187:TYR:N	2.37	0.58
1:A:186:ASN:OD1	1:A:187:TYR:N	2.37	0.57
1:B:838:ARG:C	1:B:839:ILE:HG13	2.29	0.57
1:D:836:LEU:HD23	1:D:836:LEU:H	1.69	0.57
1:E:186:ASN:OD1	1:E:187:TYR:N	2.37	0.57
1:A:128:ILE:HD11	1:A:556:GLN:O	2.05	0.57
1:A:356:ARG:NH1	1:A:377:ASP:OD2	2.38	0.57
1:E:1579:THR:O	1:E:1579:THR:OG1	2.21	0.57
1:D:1168:HIS:ND1	1:E:931:SER:HA	2.20	0.56
1:D:932:VAL:CG2	1:E:1151:GLU:OE1	2.53	0.56
1:E:356:ARG:NH1	1:E:377:ASP:OD2	2.38	0.56
1:E:386:LYS:NZ	1:E:445:GLU:OE2	2.38	0.56
1:C:356:ARG:NH1	1:C:377:ASP:OD2	2.38	0.56
1:C:128:ILE:HD11	1:C:556:GLN:O	2.05	0.56
1:E:285:LEU:O	1:E:289:GLY:N	2.38	0.56
1:A:386:LYS:NZ	1:A:445:GLU:OE2	2.38	0.56
1:A:702:VAL:HB	1:A:836:LEU:CD1	2.36	0.56
1:C:386:LYS:NZ	1:C:445:GLU:OE2	2.38	0.56
1:D:930:THR:O	1:E:1168:HIS:ND1	2.37	0.56
1:E:128:ILE:HD11	1:E:556:GLN:O	2.05	0.55
1:D:932:VAL:HG22	1:E:1151:GLU:OE1	2.06	0.55
1:A:837:PRO:O	1:A:838:ARG:HB3	2.06	0.55
1:A:167:GLU:OE2	1:B:532:ARG:NH1	2.40	0.55
1:C:167:GLU:OE2	1:D:532:ARG:NH1	2.40	0.55
1:E:167:GLU:OE2	1:F:532:ARG:NH1	2.40	0.55
1:A:285:LEU:O	1:A:289:GLY:N	2.38	0.55
1:B:980:ARG:HH21	1:B:980:ARG:CG	2.19	0.55
1:B:285:LEU:O	1:B:289:GLY:N	2.40	0.54
1:E:980:ARG:NH1	1:E:983:MET:HE2	2.23	0.54
1:E:697:MET:HB3	1:E:836:LEU:HD21	1.89	0.54
1:C:285:LEU:O	1:C:289:GLY:N	2.38	0.54
1:C:836:LEU:O	1:C:837:PRO:O	2.26	0.54
1:E:980:ARG:NH1	1:E:983:MET:CE	2.70	0.54
1:B:837:PRO:O	1:B:838:ARG:HB3	2.07	0.53
1:B:980:ARG:NH2	1:C:1110:MET:HB3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:931:SER:CA	1:C:1168:HIS:HD1	2.21	0.53
1:D:785:MET:O	1:D:786:LYS:HB2	2.09	0.53
1:A:1174:ASN:OD1	1:A:1174:ASN:N	2.42	0.53
1:F:285:LEU:O	1:F:289:GLY:N	2.40	0.53
1:C:1174:ASN:N	1:C:1174:ASN:OD1	2.42	0.52
1:D:1110:MET:HG2	1:E:980:ARG:CZ	2.39	0.52
1:E:1174:ASN:N	1:E:1174:ASN:OD1	2.42	0.52
1:D:285:LEU:O	1:D:289:GLY:N	2.40	0.52
1:D:980:ARG:HH22	1:E:1110:MET:CG	2.23	0.51
1:A:702:VAL:HG12	1:A:836:LEU:HD13	1.92	0.51
1:B:785:MET:O	1:B:786:LYS:HB2	2.09	0.51
1:D:1168:HIS:CE1	1:E:931:SER:HA	2.46	0.51
1:F:386:LYS:NZ	1:F:445:GLU:OE2	2.43	0.51
1:A:850:HIS:NE2	1:A:901:ASP:OD2	2.43	0.51
1:E:850:HIS:NE2	1:E:901:ASP:OD2	2.42	0.51
1:B:1174:ASN:OD1	1:B:1174:ASN:N	2.44	0.51
1:B:930:THR:O	1:C:1168:HIS:CB	2.59	0.51
1:D:932:VAL:HG22	1:E:1151:GLU:CD	2.35	0.51
1:D:1174:ASN:OD1	1:D:1174:ASN:N	2.44	0.51
1:B:850:HIS:NE2	1:B:901:ASP:OD2	2.44	0.51
1:B:386:LYS:NZ	1:B:445:GLU:OE2	2.43	0.50
1:B:475:ASP:OD1	1:B:476:ILE:N	2.45	0.50
1:D:386:LYS:NZ	1:D:445:GLU:OE2	2.43	0.50
1:F:2021:ASP:OD1	1:F:2022:SER:N	2.44	0.50
1:A:128:ILE:HD11	1:A:556:GLN:HG3	1.93	0.50
1:A:702:VAL:CG1	1:A:836:LEU:HD13	2.42	0.50
1:D:2021:ASP:OD1	1:D:2022:SER:N	2.44	0.50
1:E:128:ILE:HD11	1:E:556:GLN:HG3	1.94	0.50
1:F:475:ASP:OD1	1:F:476:ILE:N	2.45	0.49
1:B:2021:ASP:OD1	1:B:2022:SER:N	2.44	0.49
1:B:1579:THR:O	1:B:1579:THR:OG1	2.21	0.49
1:C:532:ARG:NH1	1:D:167:GLU:OE2	2.45	0.49
1:F:128:ILE:HD11	1:F:556:GLN:HG3	1.95	0.49
1:D:475:ASP:OD1	1:D:476:ILE:N	2.45	0.49
1:D:980:ARG:HH22	1:E:1110:MET:CB	2.24	0.49
1:C:128:ILE:HD11	1:C:556:GLN:HG3	1.94	0.49
1:B:718:TYR:OH	1:B:837:PRO:HG2	2.13	0.49
1:E:532:ARG:NH1	1:F:167:GLU:OE2	2.45	0.49
1:A:702:VAL:HG12	1:A:836:LEU:CD1	2.43	0.49
1:B:128:ILE:HD11	1:B:556:GLN:HG3	1.95	0.49
1:A:532:ARG:NH1	1:B:167:GLU:OE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:850:HIS:NE2	1:D:901:ASP:OD2	2.44	0.48
1:E:1380:GLN:O	1:E:1476:ASN:ND2	2.46	0.48
1:B:356:ARG:NH1	1:B:377:ASP:OD2	2.46	0.48
1:C:1380:GLN:O	1:C:1476:ASN:ND2	2.46	0.48
1:C:2317:ASP:OD2	1:D:2297:ARG:NH2	2.46	0.48
1:A:1003:ASN:O	1:A:1003:ASN:ND2	2.46	0.48
1:B:702:VAL:HG12	1:B:836:LEU:HD12	1.94	0.48
1:D:128:ILE:HD11	1:D:556:GLN:HG3	1.95	0.48
1:B:930:THR:CG2	1:C:1168:HIS:HB2	2.33	0.48
1:C:1295:THR:O	1:C:1297:CYS:N	2.47	0.48
1:D:836:LEU:HD23	1:D:836:LEU:N	2.27	0.48
1:A:2317:ASP:OD2	1:B:2297:ARG:NH2	2.46	0.48
1:D:356:ARG:NH1	1:D:377:ASP:OD2	2.47	0.48
1:E:1745:TYR:OH	1:F:2174:PHE:O	2.30	0.48
1:A:702:VAL:CG1	1:A:836:LEU:CD1	2.92	0.48
1:A:139:ARG:NH2	1:B:572:SER:OG	2.47	0.48
1:A:2174:PHE:O	1:B:1745:TYR:OH	2.31	0.48
1:C:139:ARG:NH2	1:D:572:SER:OG	2.47	0.48
1:D:1175:THR:HG21	1:D:1252:VAL:HG12	1.96	0.48
1:E:697:MET:HB3	1:E:836:LEU:HD22	1.95	0.48
1:A:1579:THR:O	1:A:1579:THR:OG1	2.21	0.47
1:F:356:ARG:NH1	1:F:377:ASP:OD2	2.47	0.47
1:A:1745:TYR:OH	1:B:2174:PHE:O	2.30	0.47
1:D:509:ARG:HB2	1:D:556:GLN:OE1	2.15	0.47
1:E:139:ARG:NH2	1:F:572:SER:OG	2.47	0.47
1:D:980:ARG:CG	1:D:980:ARG:HH21	2.26	0.47
1:C:1003:ASN:O	1:C:1003:ASN:ND2	2.46	0.47
1:C:1579:THR:O	1:C:1579:THR:OG1	2.21	0.47
1:C:2021:ASP:OD1	1:C:2022:SER:N	2.47	0.47
1:D:930:THR:HG22	1:E:1168:HIS:CB	2.17	0.47
1:B:509:ARG:HB2	1:B:556:GLN:OE1	2.15	0.47
1:B:980:ARG:CG	1:B:980:ARG:NH2	2.76	0.47
1:B:838:ARG:O	1:B:839:ILE:CG1	2.63	0.47
1:A:1295:THR:O	1:A:1297:CYS:N	2.47	0.47
1:C:850:HIS:NE2	1:C:901:ASP:OD2	2.43	0.47
1:F:509:ARG:HB2	1:F:556:GLN:OE1	2.15	0.47
1:B:1175:THR:HG21	1:B:1252:VAL:HG12	1.96	0.46
1:B:836:LEU:O	1:B:837:PRO:C	2.58	0.46
1:A:2021:ASP:OD1	1:A:2022:SER:N	2.47	0.46
1:B:697:MET:HB3	1:B:836:LEU:HD22	1.94	0.46
1:B:1003:ASN:O	1:B:1003:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:841:SER:O	1:E:842:THR:OG1	2.30	0.46
1:C:2297:ARG:NH2	1:D:2317:ASP:OD2	2.47	0.46
1:E:836:LEU:H	1:E:836:LEU:CD2	2.22	0.46
1:A:475:ASP:OD1	1:A:476:ILE:N	2.49	0.46
1:A:2297:ARG:NH2	1:B:2317:ASP:OD2	2.47	0.46
1:C:1745:TYR:OH	1:D:2174:PHE:O	2.30	0.46
1:B:1168:HIS:HB2	1:C:930:THR:CG2	2.34	0.45
1:E:1434:THR:HG22	1:E:1436:GLU:H	1.81	0.45
1:D:1380:GLN:O	1:D:1476:ASN:ND2	2.48	0.45
1:D:1579:THR:O	1:D:1579:THR:OG1	2.21	0.45
1:E:417:TYR:OH	1:E:420:ALA:O	2.23	0.45
1:E:1003:ASN:O	1:E:1003:ASN:ND2	2.46	0.45
1:A:1434:THR:HG22	1:A:1436:GLU:H	1.81	0.45
1:C:475:ASP:OD1	1:C:476:ILE:N	2.49	0.45
1:E:475:ASP:OD1	1:E:476:ILE:N	2.49	0.45
1:D:1003:ASN:ND2	1:D:1003:ASN:O	2.49	0.45
1:B:930:THR:HG22	1:C:1168:HIS:CB	2.34	0.45
1:D:1168:HIS:O	1:E:930:THR:HG21	2.16	0.45
1:A:1380:GLN:O	1:A:1476:ASN:ND2	2.46	0.45
1:C:2174:PHE:O	1:D:1745:TYR:OH	2.31	0.45
1:C:128:ILE:HG22	1:C:540:TYR:CE2	2.52	0.44
1:E:1175:THR:HG21	1:E:1252:VAL:HG12	1.99	0.44
1:A:128:ILE:HG22	1:A:540:TYR:CE2	2.52	0.44
1:C:391:ALA:HB3	1:C:392:PRO:CD	2.47	0.44
1:E:128:ILE:HG22	1:E:540:TYR:CE2	2.52	0.44
1:B:1380:GLN:O	1:B:1476:ASN:ND2	2.48	0.44
1:E:1295:THR:O	1:E:1297:CYS:N	2.47	0.44
1:B:930:THR:O	1:C:1168:HIS:CG	2.71	0.44
1:B:980:ARG:HH22	1:C:1110:MET:HB3	1.83	0.44
1:A:391:ALA:HB3	1:A:392:PRO:CD	2.47	0.44
1:B:1168:HIS:CD2	1:B:1178:VAL:CG2	2.91	0.44
1:C:836:LEU:H	1:C:836:LEU:HG	1.55	0.44
1:A:1175:THR:HG21	1:A:1252:VAL:HG12	1.99	0.44
1:C:1175:THR:HG21	1:C:1252:VAL:HG12	1.99	0.44
1:A:2110:ASP:OD1	1:A:2111:ARG:N	2.46	0.43
1:C:1434:THR:HG22	1:C:1436:GLU:H	1.81	0.43
1:A:1579:THR:O	1:A:1580:LYS:O	2.37	0.43
1:C:1163:LEU:HD23	1:C:1182:PHE:HB3	2.00	0.43
1:C:1579:THR:O	1:C:1580:LYS:O	2.36	0.43
1:E:391:ALA:HB3	1:E:392:PRO:CD	2.47	0.43
1:A:1163:LEU:HD23	1:A:1182:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:838:ARG:O	1:B:839:ILE:HG13	2.18	0.43
1:B:838:ARG:HH21	1:B:838:ARG:HG3	1.82	0.43
1:B:980:ARG:HD2	1:C:1112:GLY:O	2.18	0.43
1:D:1295:THR:O	1:D:1297:CYS:N	2.48	0.43
1:E:1579:THR:O	1:E:1580:LYS:O	2.36	0.43
1:A:509:ARG:HB2	1:A:556:GLN:OE1	2.19	0.42
1:A:1173:ASP:N	1:A:1173:ASP:OD1	2.53	0.42
1:B:1579:THR:O	1:B:1580:LYS:O	2.36	0.42
1:E:509:ARG:HB2	1:E:556:GLN:OE1	2.19	0.42
1:D:1579:THR:O	1:D:1580:LYS:O	2.36	0.42
1:E:572:SER:OG	1:F:139:ARG:NH2	2.53	0.42
1:E:1163:LEU:HD23	1:E:1182:PHE:HB3	2.00	0.42
1:B:1163:LEU:HD23	1:B:1182:PHE:HB3	2.01	0.42
1:B:1434:THR:HG22	1:B:1436:GLU:H	1.84	0.42
1:C:2110:ASP:OD1	1:C:2111:ARG:N	2.46	0.42
1:D:1163:LEU:HD23	1:D:1182:PHE:HB3	2.01	0.42
1:A:572:SER:OG	1:B:139:ARG:NH2	2.53	0.42
1:D:1434:THR:HG22	1:D:1436:GLU:H	1.84	0.42
1:B:836:LEU:C	1:B:837:PRO:O	2.62	0.42
1:C:572:SER:OG	1:D:139:ARG:NH2	2.53	0.41
1:C:702:VAL:CG1	1:C:836:LEU:HD13	2.49	0.41
1:C:509:ARG:HB2	1:C:556:GLN:OE1	2.19	0.41
1:C:1173:ASP:N	1:C:1173:ASP:OD1	2.52	0.41
1:B:1295:THR:O	1:B:1297:CYS:N	2.48	0.41
1:C:980:ARG:HE	1:C:984:LYS:HE3	1.84	0.41
1:E:1164:ASN:ND2	1:E:1181:GLN:O	2.53	0.41
1:E:1173:ASP:N	1:E:1173:ASP:OD1	2.53	0.41
1:A:1164:ASN:ND2	1:A:1181:GLN:O	2.53	0.41
1:C:697:MET:HB3	1:C:836:LEU:HD23	2.02	0.41
1:D:128:ILE:HG22	1:D:540:TYR:CE2	2.56	0.41
1:E:702:VAL:HG12	1:E:836:LEU:HD12	2.01	0.41
1:A:1529:ARG:NH1	1:A:1547:GLU:OE2	2.54	0.41
1:B:980:ARG:HH21	1:B:980:ARG:HG3	1.85	0.41
1:C:1529:ARG:NH1	1:C:1547:GLU:OE2	2.54	0.41
1:F:128:ILE:HG22	1:F:540:TYR:CE2	2.56	0.41
1:B:128:ILE:HG22	1:B:540:TYR:CE2	2.56	0.41
1:A:838:ARG:HH21	1:A:838:ARG:CG	2.33	0.41
1:C:1164:ASN:ND2	1:C:1181:GLN:O	2.53	0.41
1:E:1529:ARG:NH1	1:E:1547:GLU:OE2	2.54	0.41
2:B:2401:BTN:H92	2:B:2401:BTN:H2	1.93	0.41
1:E:980:ARG:HH11	1:E:983:MET:HE1	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:838:ARG:C	1:B:839:ILE:CG1	2.93	0.40
1:B:933:LEU:CD1	1:C:1151:GLU:OE1	2.69	0.40
1:D:1110:MET:HG2	1:E:980:ARG:NH1	2.36	0.40
1:D:1151:GLU:OE1	1:E:932:VAL:CG2	2.69	0.40
1:B:1168:HIS:ND1	1:C:931:SER:HA	2.37	0.40
1:D:1529:ARG:NH1	1:D:1547:GLU:OE2	2.55	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	2136/2346 (91%)	2005 (94%)	122 (6%)	9 (0%)	30	65
1	B	2136/2346 (91%)	1998 (94%)	130 (6%)	8 (0%)	30	65
1	C	2136/2346 (91%)	2004 (94%)	123 (6%)	9 (0%)	30	65
1	D	2136/2346 (91%)	2000 (94%)	129 (6%)	7 (0%)	36	70
1	E	1809/2346 (77%)	1691 (94%)	110 (6%)	8 (0%)	30	65
1	F	1285/2346 (55%)	1226 (95%)	57 (4%)	2 (0%)	43	76
All	All	11638/14076 (83%)	10924 (94%)	671 (6%)	43 (0%)	31	65

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	841	SER
1	A	1580	LYS
1	B	837	PRO
1	B	1580	LYS
1	C	837	PRO
1	C	841	SER

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Mol	Chain	Res	Type
1	C	1580	LYS
1	D	1580	LYS
1	E	840	GLN
1	E	841	SER
1	E	1580	LYS
1	A	1242	PHE
1	A	1688	ILE
1	B	839	ILE
1	B	1242	PHE
1	B	1688	ILE
1	C	838	ARG
1	C	1242	PHE
1	C	1688	ILE
1	D	841	SER
1	D	1242	PHE
1	D	1688	ILE
1	E	1242	PHE
1	E	1688	ILE
1	F	1688	ILE
1	A	838	ARG
1	A	1141	SER
1	B	838	ARG
1	B	1141	SER
1	C	1141	SER
1	D	839	ILE
1	D	1141	SER
1	E	1141	SER
1	A	837	PRO
1	A	1949	GLN
1	B	1949	GLN
1	C	1949	GLN
1	D	1949	GLN
1	E	1949	GLN
1	F	1949	GLN
1	E	420	ALA
1	C	839	ILE
1	A	839	ILE

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	1873/2057 (91%)	1845 (98%)	28 (2%)	57	70
1	B	1873/2057 (91%)	1845 (98%)	28 (2%)	57	70
1	C	1873/2057 (91%)	1847 (99%)	26 (1%)	59	71
1	D	1873/2057 (91%)	1847 (99%)	26 (1%)	59	71
1	E	1581/2057 (77%)	1559 (99%)	22 (1%)	59	71
1	F	1101/2057 (54%)	1085 (98%)	16 (2%)	57	70
All	All	10174/12342 (82%)	10028 (99%)	146 (1%)	57	71

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	ILE
1	A	139	ARG
1	A	146	ARG
1	A	149	ARG
1	A	152	ARG
1	A	211	HIS
1	A	437	GLU
1	A	441	ARG
1	A	485	TRP
1	A	559	HIS
1	A	572	SER
1	A	735	ARG
1	A	836	LEU
1	A	838	ARG
1	A	840	GLN
1	A	841	SER
1	A	980	ARG
1	A	992	ARG
1	A	993	GLN
1	A	1090	LEU
1	A	1097	HIS
1	A	1110	MET
1	A	1151	GLU
1	A	1174	ASN
1	A	1935	ARG
1	A	2018	TRP

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Mol	Chain	Res	Type
1	A	2128	PHE
1	A	2178	ILE
1	B	128	ILE
1	B	139	ARG
1	B	146	ARG
1	B	149	ARG
1	B	152	ARG
1	B	211	HIS
1	B	437	GLU
1	B	441	ARG
1	B	485	TRP
1	B	559	HIS
1	B	572	SER
1	B	735	ARG
1	B	836	LEU
1	B	838	ARG
1	B	840	GLN
1	B	931	SER
1	B	980	ARG
1	B	992	ARG
1	B	993	GLN
1	B	1090	LEU
1	B	1097	HIS
1	B	1110	MET
1	B	1151	GLU
1	B	1174	ASN
1	B	1935	ARG
1	B	2018	TRP
1	B	2128	PHE
1	B	2178	ILE
1	C	128	ILE
1	C	139	ARG
1	C	146	ARG
1	C	149	ARG
1	C	152	ARG
1	C	211	HIS
1	C	437	GLU
1	C	441	ARG
1	C	485	TRP
1	C	559	HIS
1	C	572	SER
1	C	735	ARG

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Mol	Chain	Res	Type
1	C	836	LEU
1	C	840	GLN
1	C	980	ARG
1	C	992	ARG
1	C	993	GLN
1	C	1090	LEU
1	C	1097	HIS
1	C	1110	MET
1	C	1151	GLU
1	C	1174	ASN
1	C	1935	ARG
1	C	2018	TRP
1	C	2128	PHE
1	C	2178	ILE
1	D	128	ILE
1	D	139	ARG
1	D	146	ARG
1	D	149	ARG
1	D	152	ARG
1	D	211	HIS
1	D	437	GLU
1	D	441	ARG
1	D	485	TRP
1	D	559	HIS
1	D	572	SER
1	D	735	ARG
1	D	836	LEU
1	D	931	SER
1	D	980	ARG
1	D	992	ARG
1	D	993	GLN
1	D	1090	LEU
1	D	1097	HIS
1	D	1110	MET
1	D	1151	GLU
1	D	1174	ASN
1	D	1935	ARG
1	D	2018	TRP
1	D	2128	PHE
1	D	2178	ILE
1	E	128	ILE
1	E	139	ARG

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Mol	Chain	Res	Type
1	E	146	ARG
1	E	149	ARG
1	E	152	ARG
1	E	211	HIS
1	E	437	GLU
1	E	441	ARG
1	E	485	TRP
1	E	559	HIS
1	E	572	SER
1	E	735	ARG
1	E	836	LEU
1	E	980	ARG
1	E	992	ARG
1	E	993	GLN
1	E	1090	LEU
1	E	1097	HIS
1	E	1110	MET
1	E	1151	GLU
1	E	1174	ASN
1	E	1935	ARG
1	F	128	ILE
1	F	139	ARG
1	F	146	ARG
1	F	149	ARG
1	F	152	ARG
1	F	211	HIS
1	F	437	GLU
1	F	441	ARG
1	F	485	TRP
1	F	559	HIS
1	F	572	SER
1	F	735	ARG
1	F	1935	ARG
1	F	2018	TRP
1	F	2128	PHE
1	F	2178	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	GLN
1	A	403	HIS

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Mol	Chain	Res	Type
1	A	1000	GLN
1	A	1047	GLN
1	A	1089	HIS
1	A	1164	ASN
1	A	1170	GLN
1	A	1555	GLN
1	A	2285	HIS
1	A	2309	GLN
1	B	354	GLN
1	B	403	HIS
1	B	606	ASN
1	B	939	GLN
1	B	982	HIS
1	B	1164	ASN
1	B	1168	HIS
1	B	1170	GLN
1	B	1555	GLN
1	B	1845	HIS
1	B	1876	HIS
1	B	2016	GLN
1	B	2028	GLN
1	B	2277	GLN
1	B	2285	HIS
1	B	2309	GLN
1	C	354	GLN
1	C	403	HIS
1	C	1047	GLN
1	C	1089	HIS
1	C	1164	ASN
1	C	1170	GLN
1	C	1555	GLN
1	C	2285	HIS
1	C	2309	GLN
1	D	354	GLN
1	D	403	HIS
1	D	606	ASN
1	D	928	ASN
1	D	939	GLN
1	D	982	HIS
1	D	1170	GLN
1	D	1555	GLN
1	D	1845	HIS

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Mol	Chain	Res	Type
1	D	1876	HIS
1	D	2016	GLN
1	D	2028	GLN
1	D	2277	GLN
1	D	2285	HIS
1	D	2309	GLN
1	E	354	GLN
1	E	403	HIS
1	E	840	GLN
1	E	1047	GLN
1	E	1089	HIS
1	E	1164	ASN
1	E	1170	GLN
1	E	1555	GLN
1	F	354	GLN
1	F	403	HIS
1	F	606	ASN
1	F	1845	HIS
1	F	1876	HIS
1	F	2016	GLN
1	F	2028	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BTN	B	2401	1	15,16,17	1.18	1 (6%)	20,21,23	1.49	3 (15%)
2	BTN	A	2401	1	15,16,17	1.19	1 (6%)	20,21,23	1.49	3 (15%)
2	BTN	C	2401	1	15,16,17	1.18	1 (6%)	20,21,23	1.49	3 (15%)
2	BTN	E	2401	1	15,16,17	1.20	1 (6%)	20,21,23	1.49	3 (15%)
2	BTN	D	2401	1	15,16,17	1.18	1 (6%)	20,21,23	1.49	3 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BTN	B	2401	1	-	0/6/27/28	0/2/2/2
2	BTN	A	2401	1	-	0/6/27/28	0/2/2/2
2	BTN	C	2401	1	-	0/6/27/28	0/2/2/2
2	BTN	E	2401	1	-	0/6/27/28	0/2/2/2
2	BTN	D	2401	1	-	0/6/27/28	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2401	BTN	C2-S1	-3.67	1.76	1.82
2	A	2401	BTN	C2-S1	-3.66	1.76	1.82
2	C	2401	BTN	C2-S1	-3.62	1.76	1.82
2	B	2401	BTN	C2-S1	-3.59	1.77	1.82
2	D	2401	BTN	C2-S1	-3.59	1.77	1.82

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2401	BTN	C4-C2-S1	3.21	108.67	105.03
2	A	2401	BTN	C6-S1-C2	3.20	96.65	89.98
2	E	2401	BTN	C6-S1-C2	3.20	96.65	89.98
2	C	2401	BTN	C4-C2-S1	3.20	108.67	105.03
2	C	2401	BTN	C6-S1-C2	3.20	96.63	89.98
2	E	2401	BTN	C4-C2-S1	3.19	108.66	105.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2401	BTN	C6-S1-C2	3.18	96.60	89.98
2	B	2401	BTN	C6-S1-C2	3.18	96.60	89.98
2	B	2401	BTN	C4-C2-S1	3.13	108.58	105.03
2	D	2401	BTN	C4-C2-S1	3.12	108.58	105.03
2	B	2401	BTN	C5-C6-S1	2.18	109.07	106.06
2	D	2401	BTN	C5-C6-S1	2.17	109.05	106.06
2	A	2401	BTN	C5-C6-S1	2.15	109.02	106.06
2	E	2401	BTN	C5-C6-S1	2.14	109.01	106.06
2	C	2401	BTN	C5-C6-S1	2.13	109.00	106.06

There are no chirality outliers.

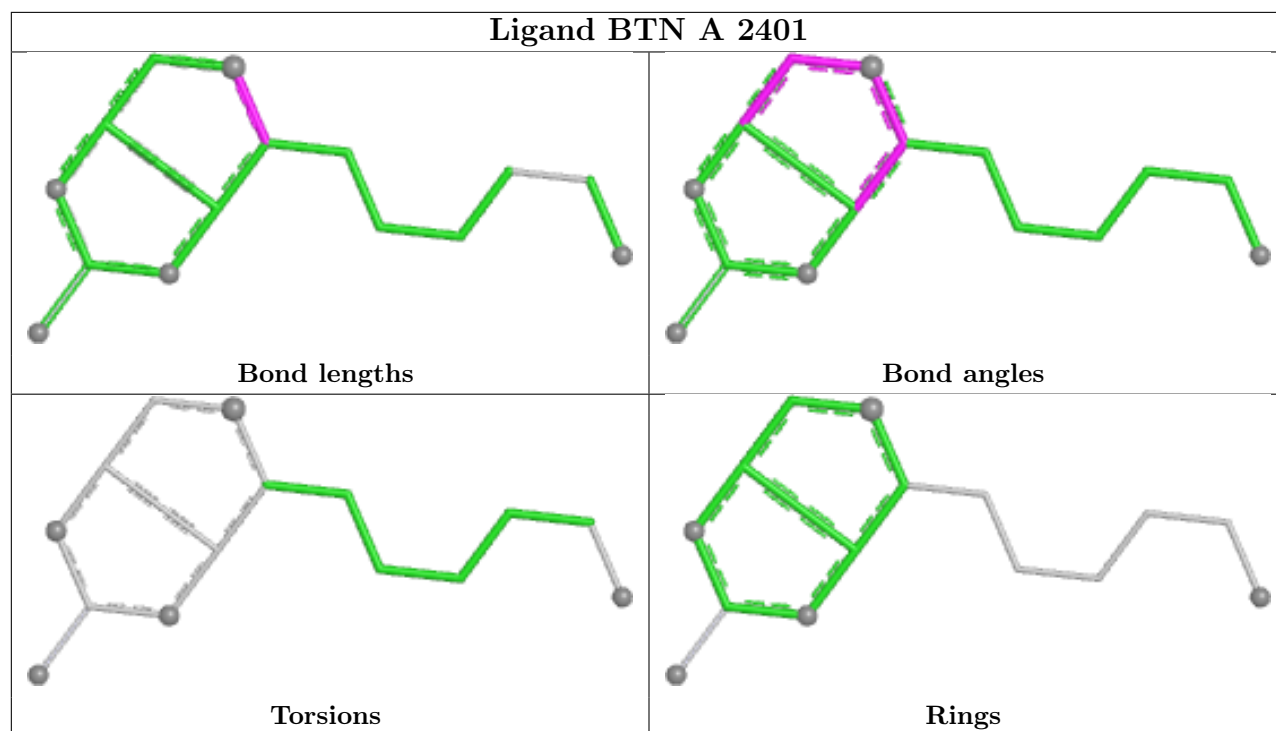
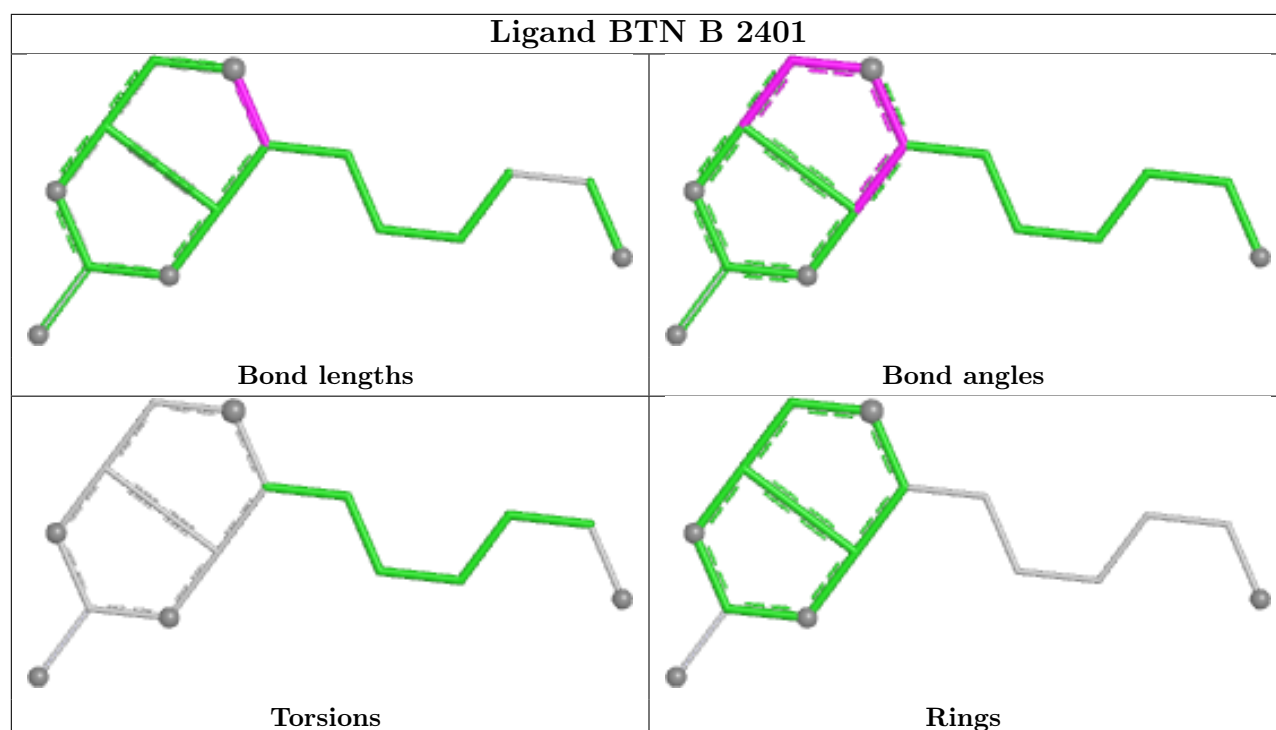
There are no torsion outliers.

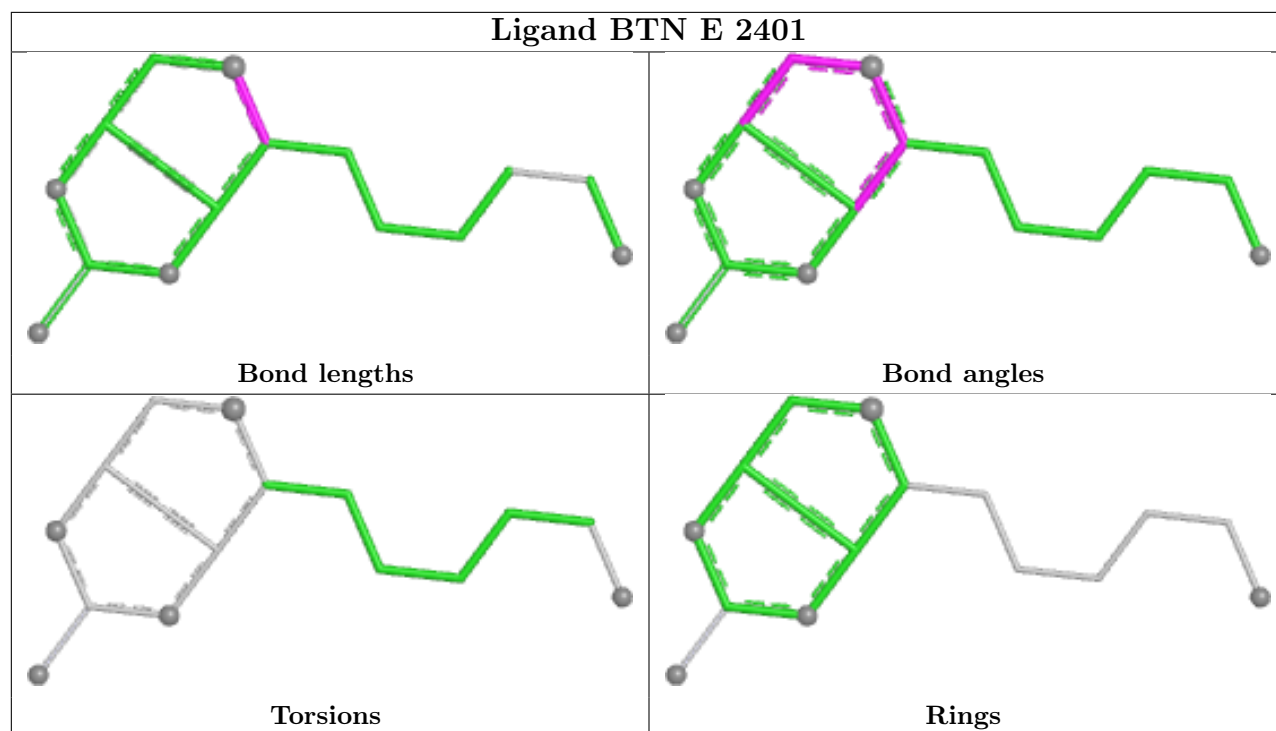
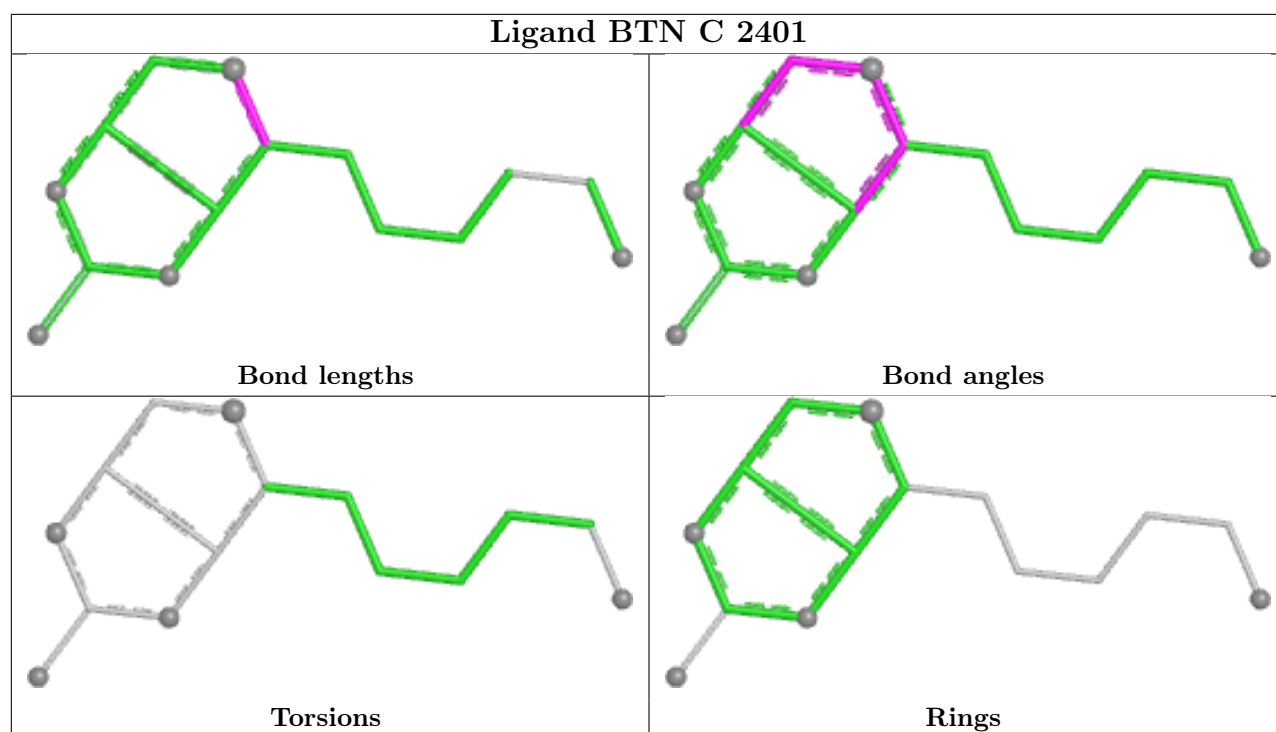
There are no ring outliers.

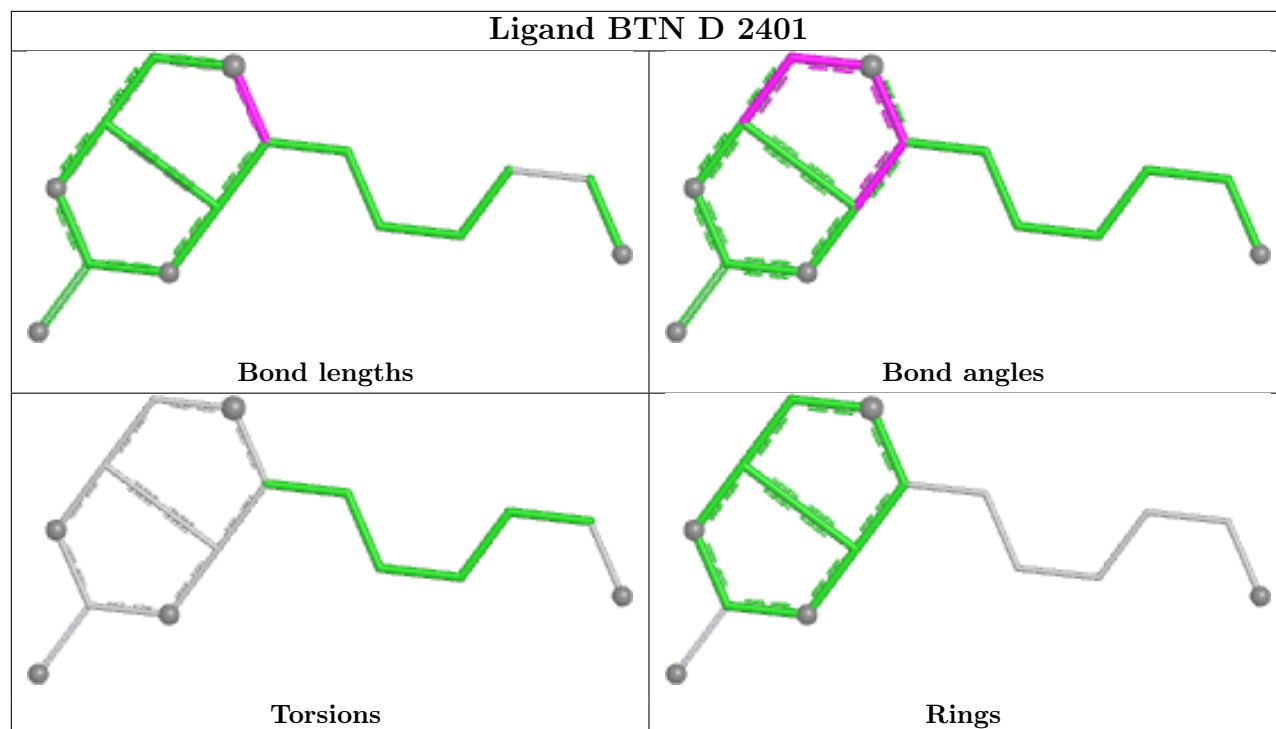
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2401	BTN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

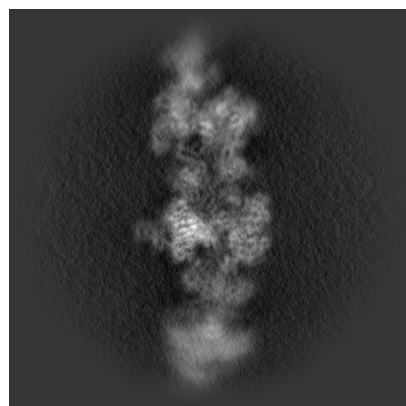
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38433. These allow visual inspection of the internal detail of the map and identification of artifacts.

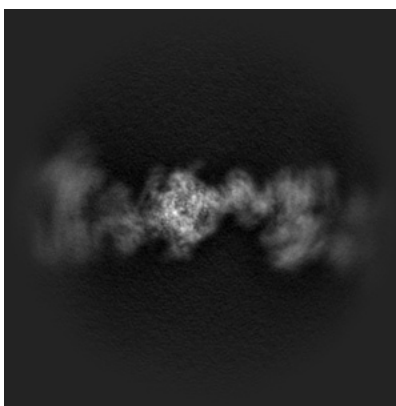
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

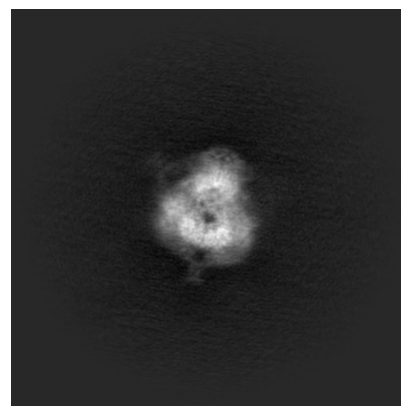
6.1.1 Primary map



X

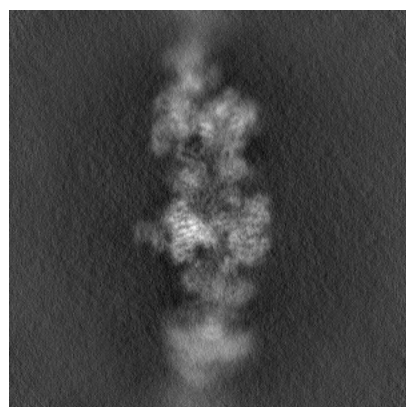


Y

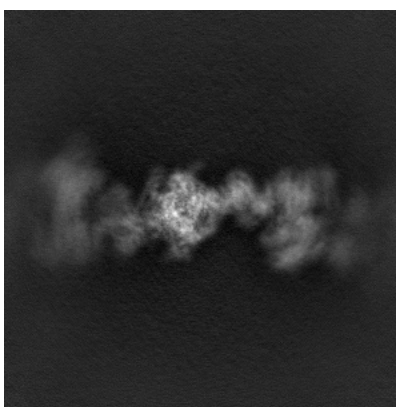


Z

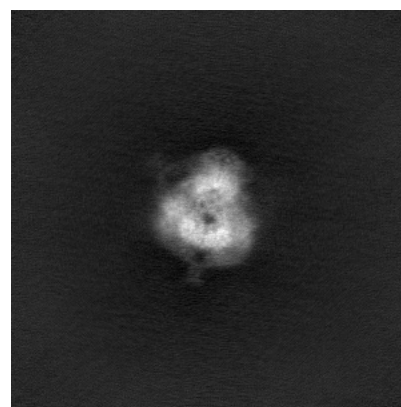
6.1.2 Raw map



X



Y

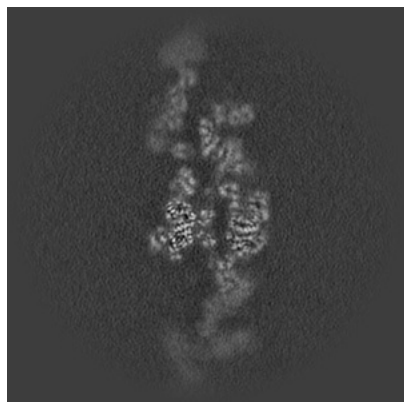


Z

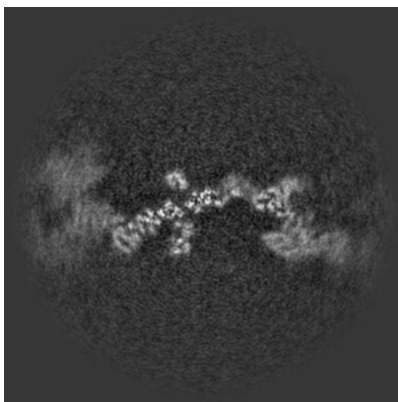
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

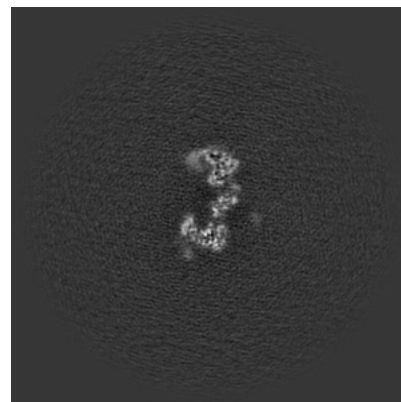
6.2.1 Primary map



X Index: 244

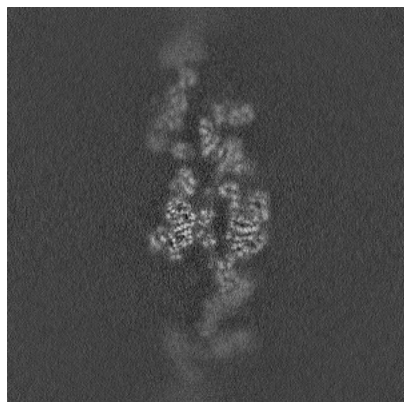


Y Index: 244

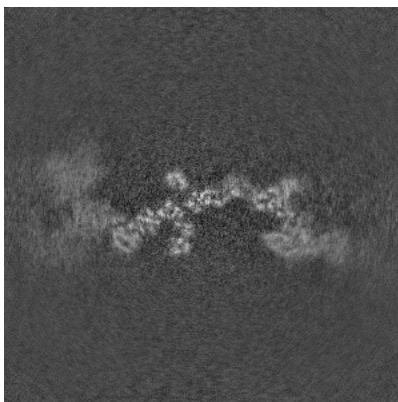


Z Index: 244

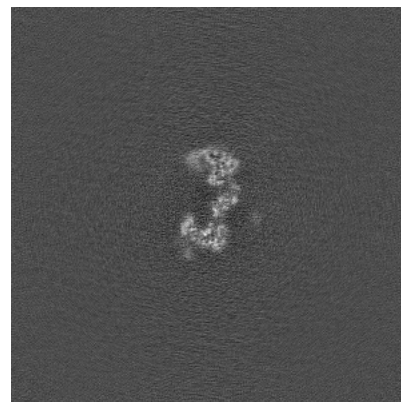
6.2.2 Raw map



X Index: 244



Y Index: 244

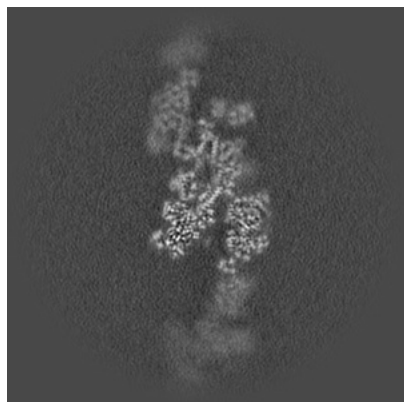


Z Index: 244

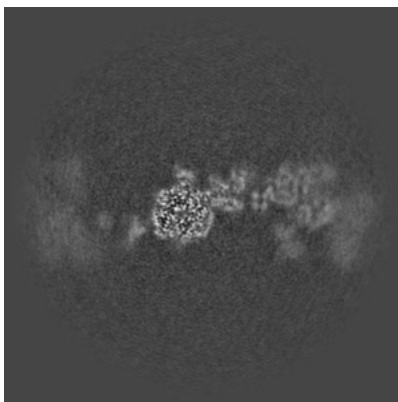
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

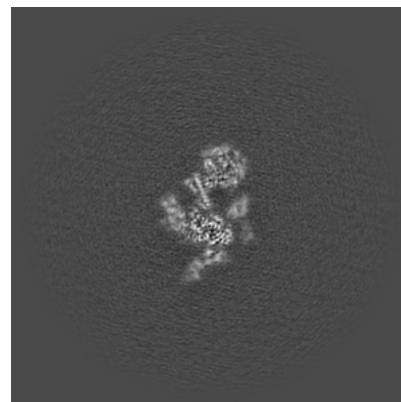
6.3.1 Primary map



X Index: 251

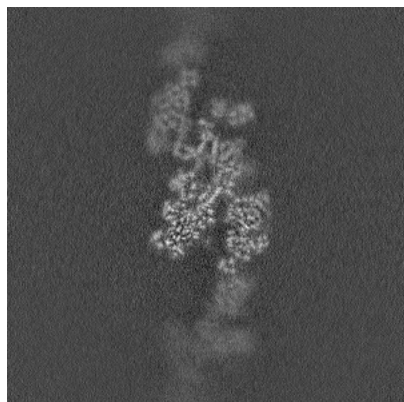


Y Index: 213

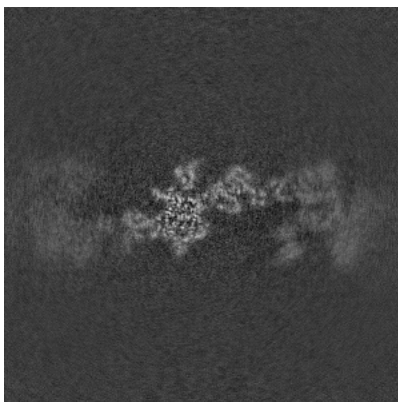


Z Index: 207

6.3.2 Raw map



X Index: 251



Y Index: 220

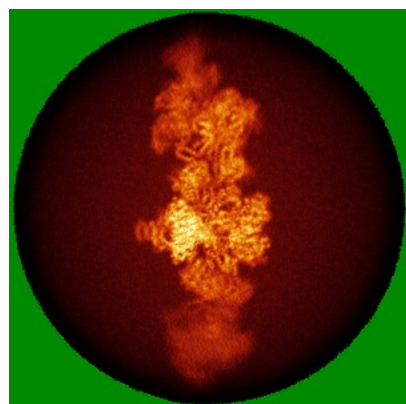


Z Index: 207

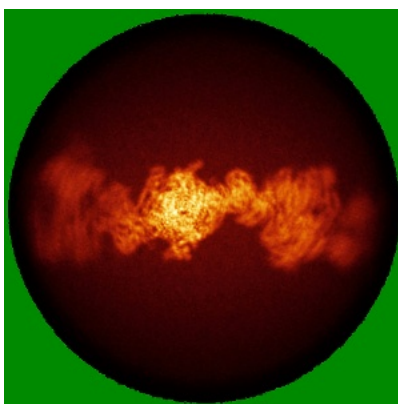
The images above show the largest variance slices of the map in three orthogonal directions.

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

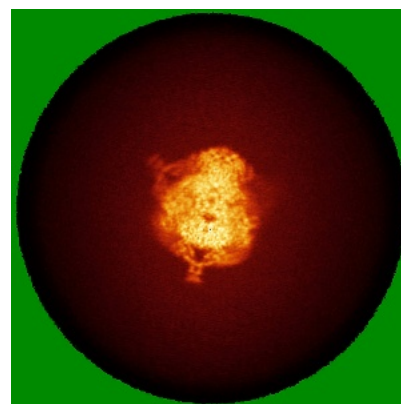
6.4.1 Primary map



X

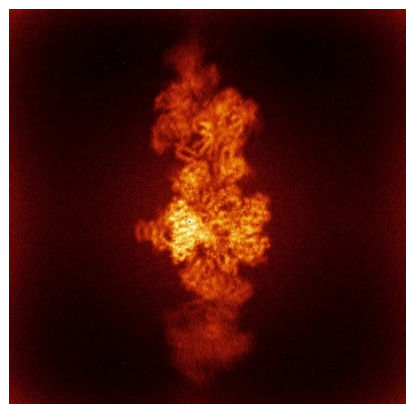


Y

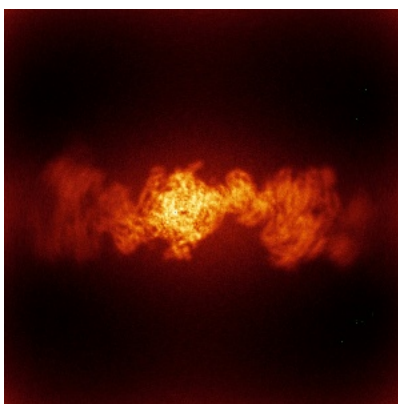


Z

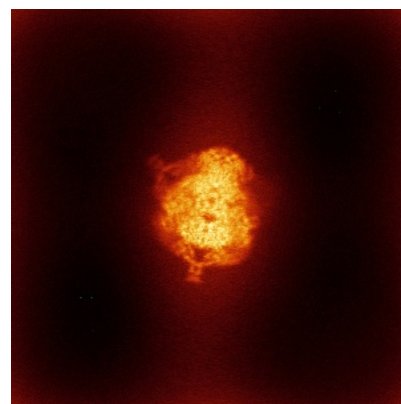
6.4.2 Raw map



X



Y

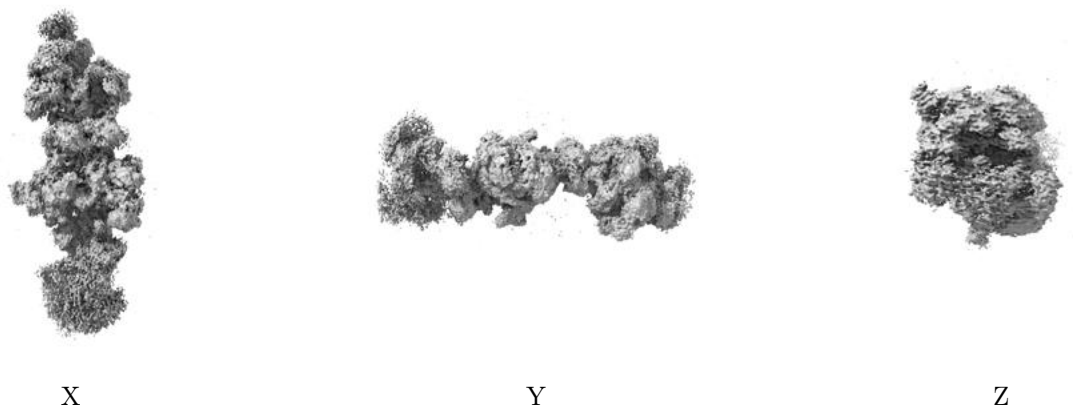


Z

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

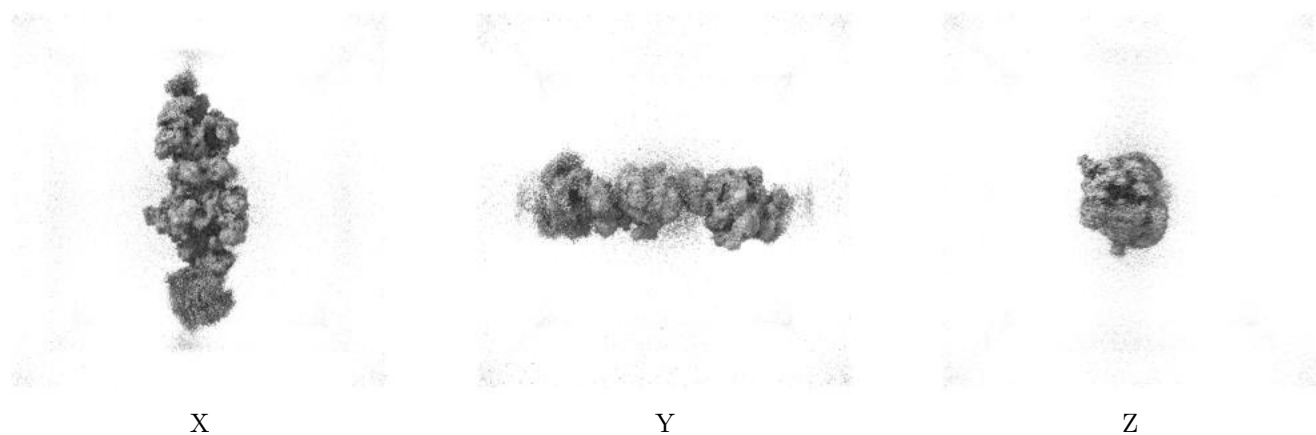
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

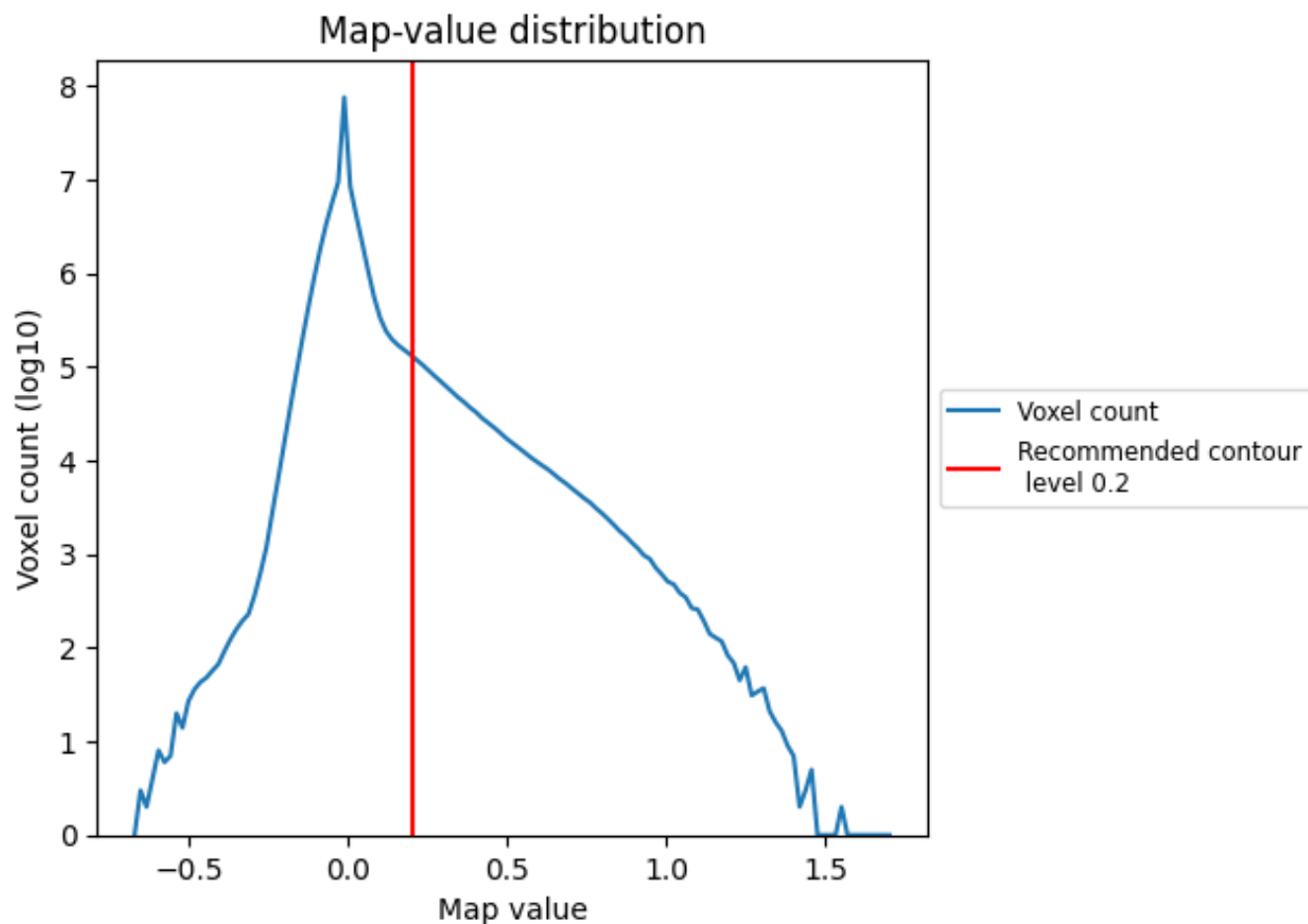
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

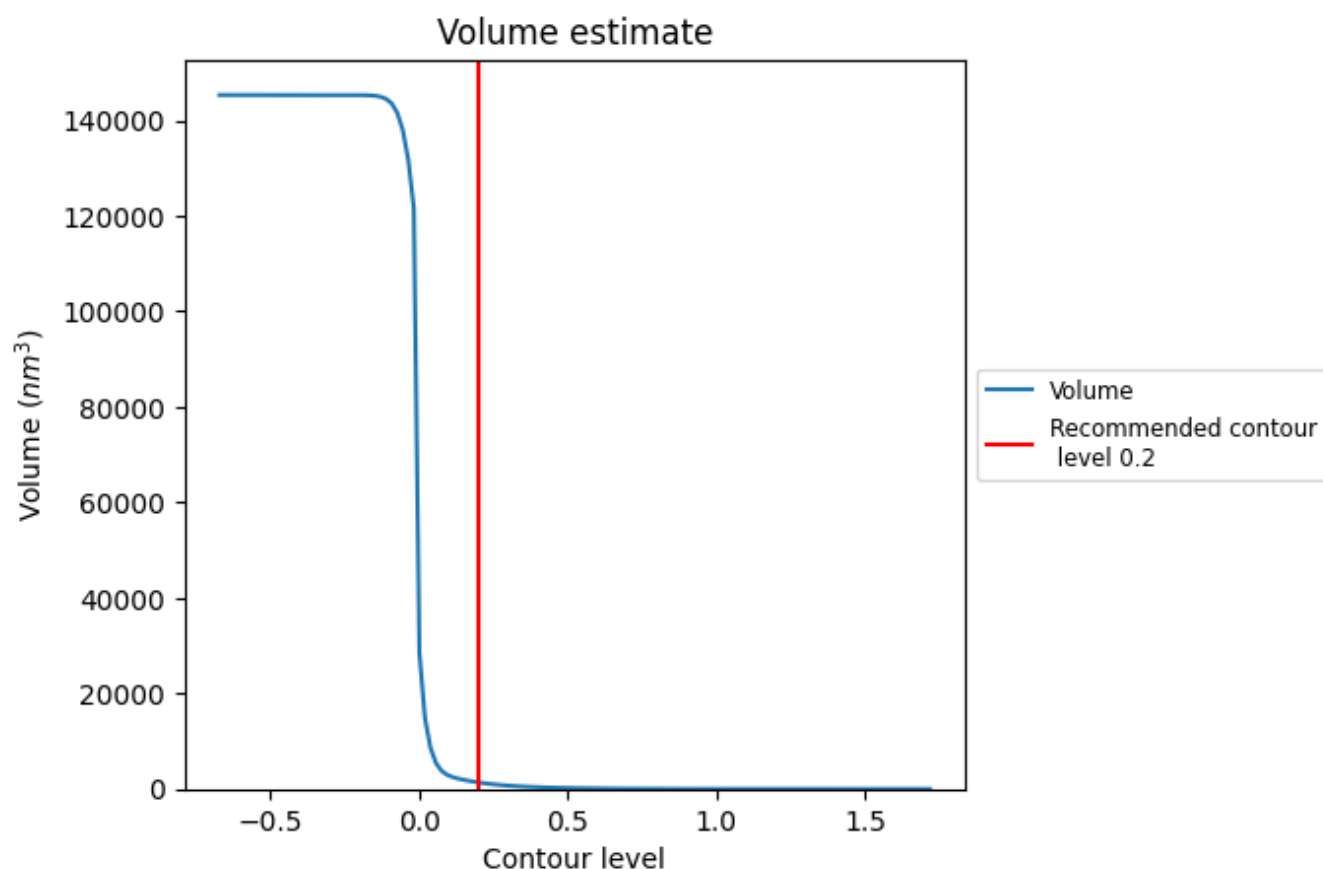
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

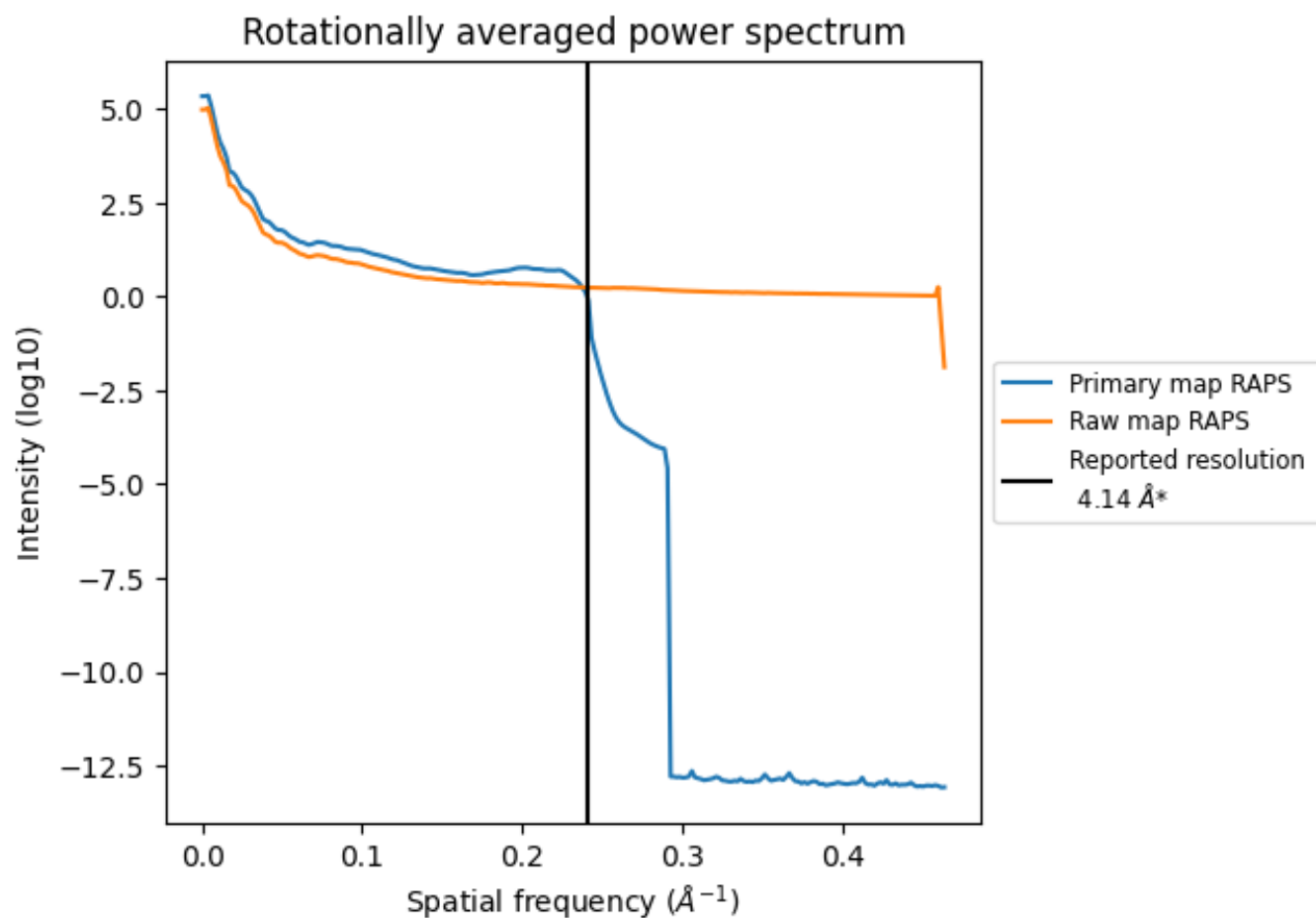
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1379 nm³; this corresponds to an approximate mass of 1246 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

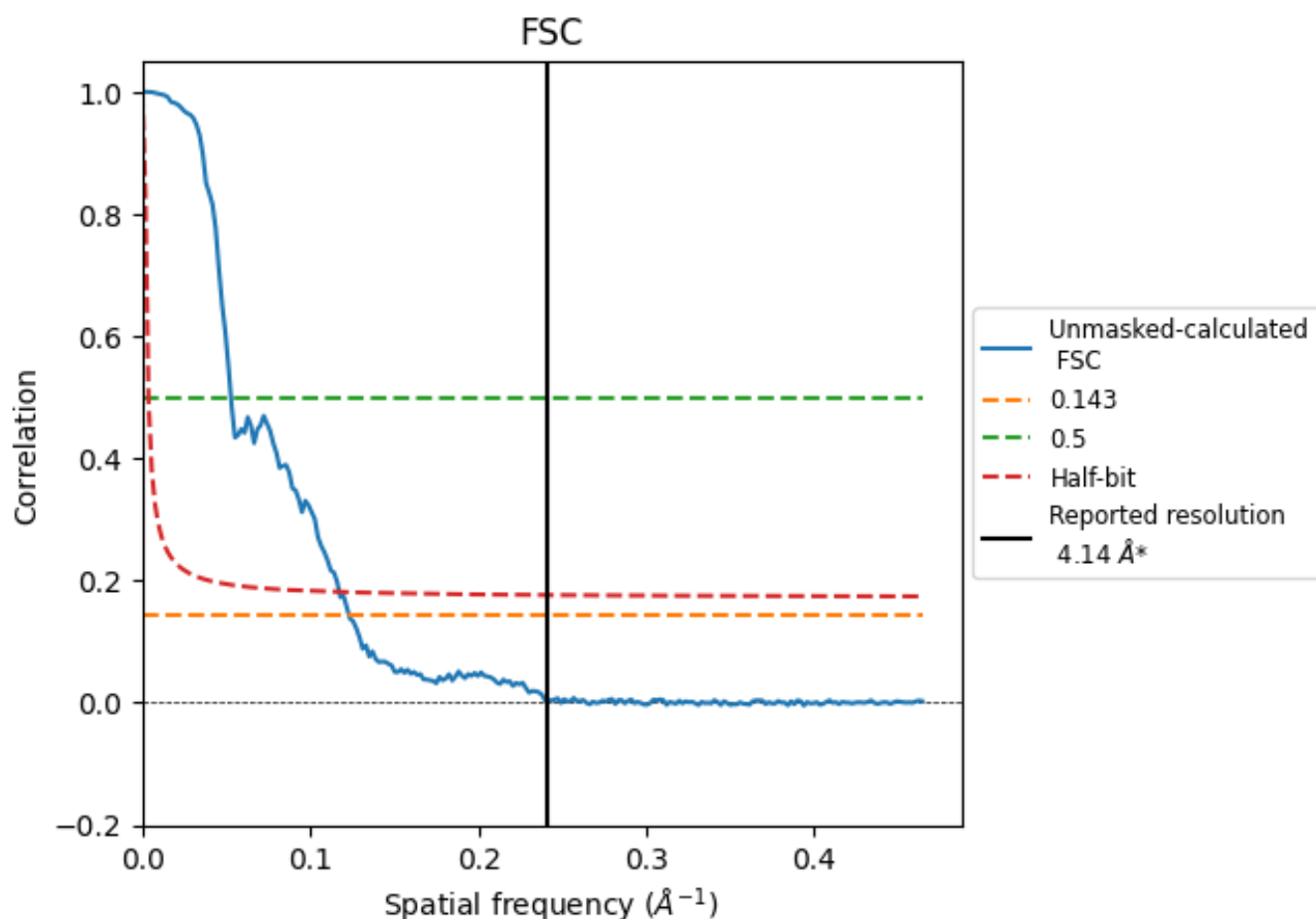


*Reported resolution corresponds to spatial frequency of 0.242 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.242 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

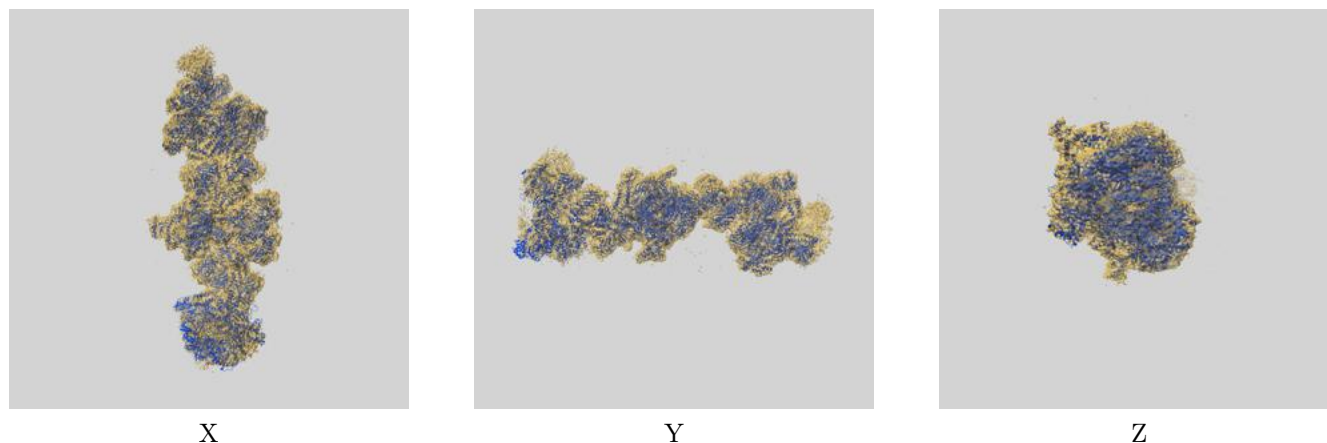
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.14	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.12	18.94	8.53

*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 8.12 differs from the reported value 4.14 by more than 10 %

9 Map-model fit [i](#)

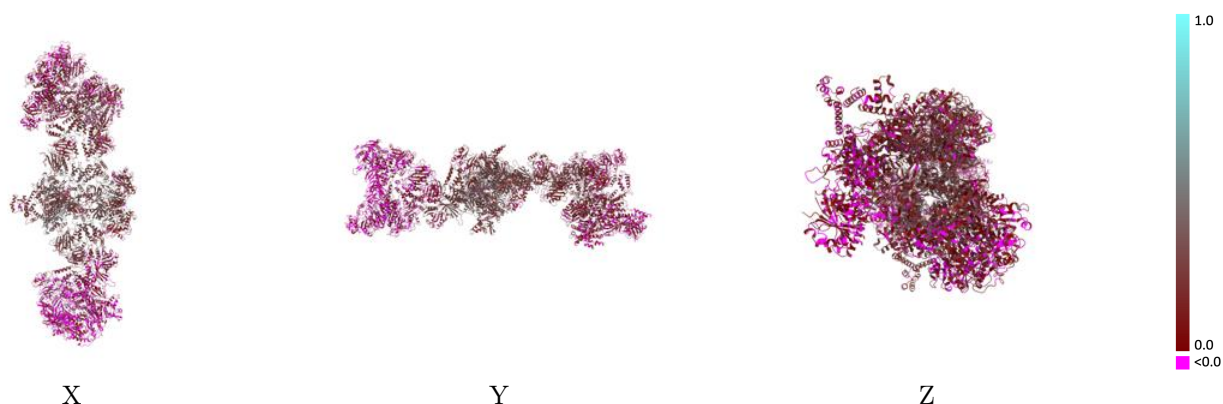
This section contains information regarding the fit between EMDB map EMD-38433 and PDB model 8XL0. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

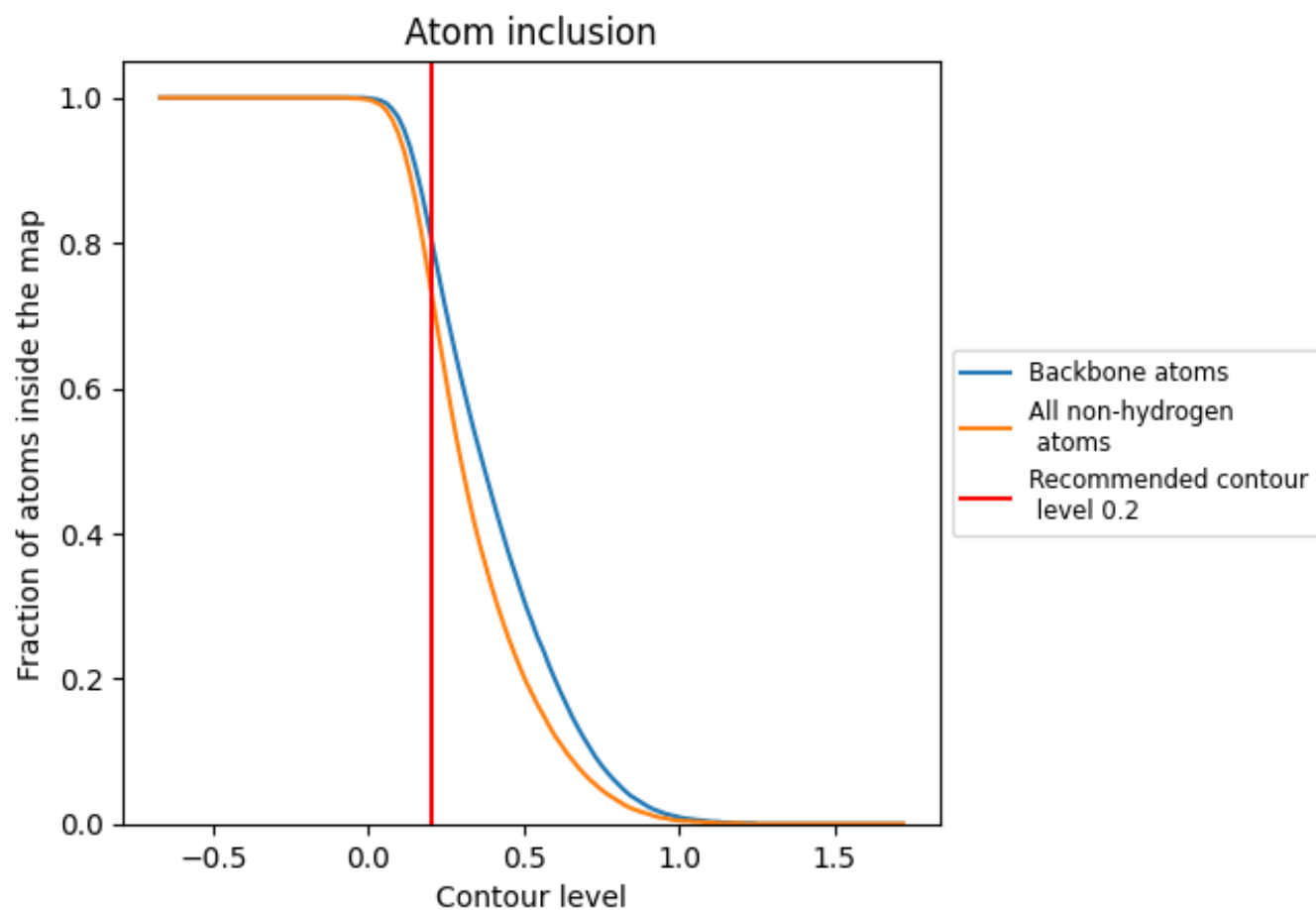


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 74% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7380	0.1620
A	0.7650	0.1060
B	0.8510	0.1530
C	0.9280	0.2830
D	0.9210	0.2770
E	0.4450	0.0520
F	0.2890	0.0270

1.0

0.0

<0.0