



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 03:20 PM UTC

PDB ID : 7OO3 / pdb_00007oo3
EMDB ID : EMD-13004
Title : Pol II-CSB-CSA-DDB1-UVSSA (Structure1)
Authors : Kokic, G.; Cramer, P.
Deposited on : 2021-05-26
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

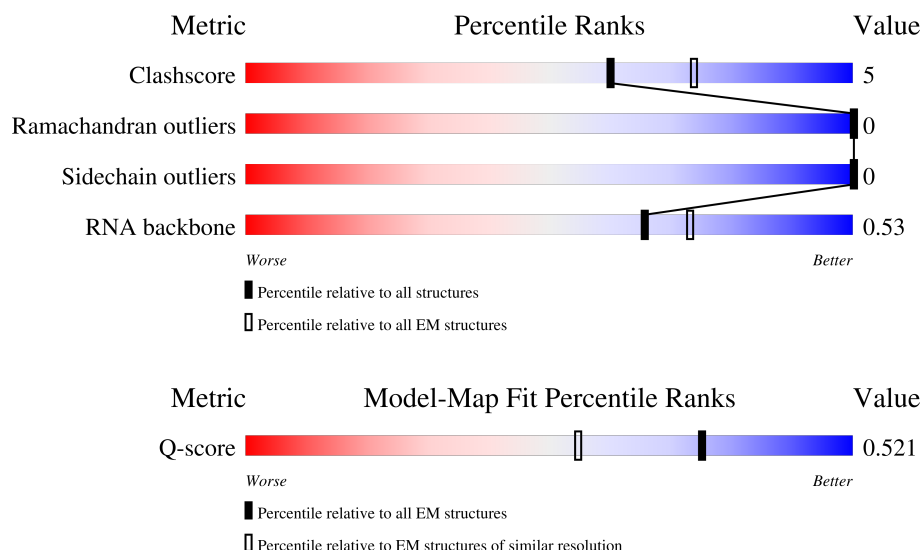
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	1970	
2	B	1174	
3	C	275	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	N	47	
14	T	47	
15	P	10	
16	a	396	
17	b	1493	
18	x	35	
19	c	709	
20	d	1143	

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 95988 atoms, of which 46598 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-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1412	Total	C	H	N	O	S	0	0
			22493	7033	11314	2002	2074	70		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1131	Total	C	H	N	O	S	0	0
			18140	5727	9088	1592	1669	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	260	Total	C	H	N	O	S	0	0
			4119	1309	2030	359	415	6		

- Molecule 4 is a protein called RPOL4c domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	126	Total	C	H	N	O	S	0	0
			2046	642	1016	175	209	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	209	Total	C	H	N	O	S	0	0
			3457	1089	1737	300	323	8		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	82	Total	C	H	N	O	S	0	0
			1341	418	684	113	121	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	171	Total	C	H	N	O	S	0	0
			2709	875	1358	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	148	Total	C	H	N	O	S	0	0
			2333	750	1147	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	117	Total	C	H	N	O	S	0	0
			1828	587	879	169	182	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	67	Total	C	H	N	O	S	0	0
			1086	345	553	90	92	6		

- Molecule 11 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	115	Total	C	H	N	O	S	0	0
			1862	593	942	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	46	Total	C	H	N	O	S	0	0
			781	241	393	75	66	6		

- Molecule 13 is a DNA chain called NTS.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	35	Total	C	N	O	P	0	0
			727	344	142	206	35		

- Molecule 14 is a DNA chain called TS.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	47	Total	C	N	O	P	0	0
			947	453	159	288	47		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	10	Total	C	H	N	O	P	0
			329	98	109	45	67	10	0

- Molecule 16 is a protein called DNA excision repair protein ERCC-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	365	Total	C	H	N	O	S	0
			5541	1775	2692	507	548	19	0

- Molecule 17 is a protein called DNA excision repair protein ERCC-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	534	Total	C	H	N	O	S	0
			8744	2803	4390	761	769	21	0

- Molecule 18 is a protein called CSB element.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	x	35	Total	C	H	N	O		0
			317	105	142	35	35		0

- Molecule 19 is a protein called UV-stimulated scaffold protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	c	141	Total	C	H	N	O	0	0
			707	282	143	141	141		

- Molecule 20 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	d	1096	Total	C	H	N	O	S	0
			16472	5397	7981	1423	1625	46	0

There are 3 discrepancies between the modelled and reference sequences:

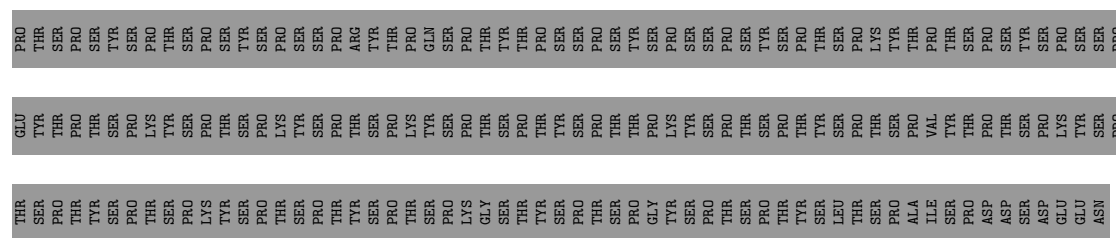
Chain	Residue	Modelled	Actual	Comment	Reference
d	-2	SER	-	expression tag	UNP Q16531
d	-1	ASN	-	expression tag	UNP Q16531
d	0	ALA	-	expression tag	UNP Q16531

- Molecule 21 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
21	A	2	Total 2	Zn 2	0
21	B	1	Total 1	Zn 1	0
21	C	1	Total 1	Zn 1	0
21	I	2	Total 2	Zn 2	0
21	J	1	Total 1	Zn 1	0
21	L	1	Total 1	Zn 1	0

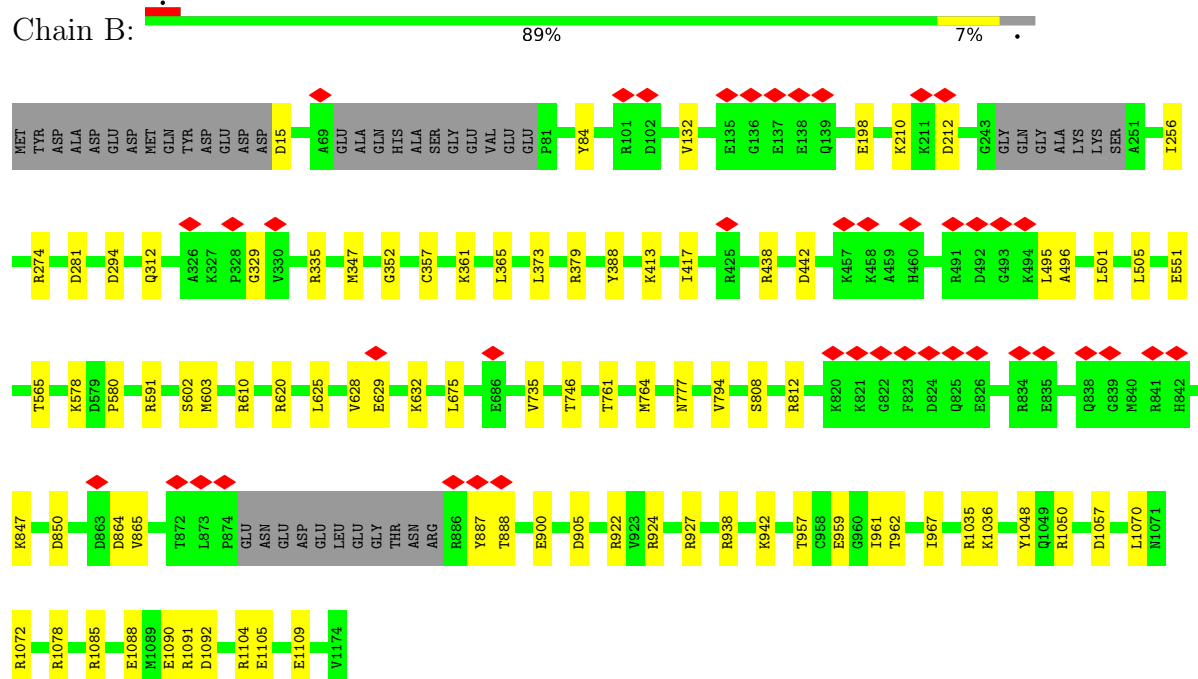
- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total 1	Mg 1	0



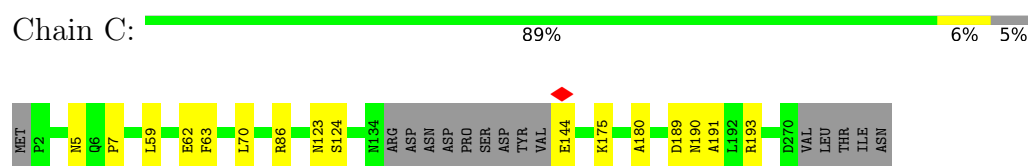
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:



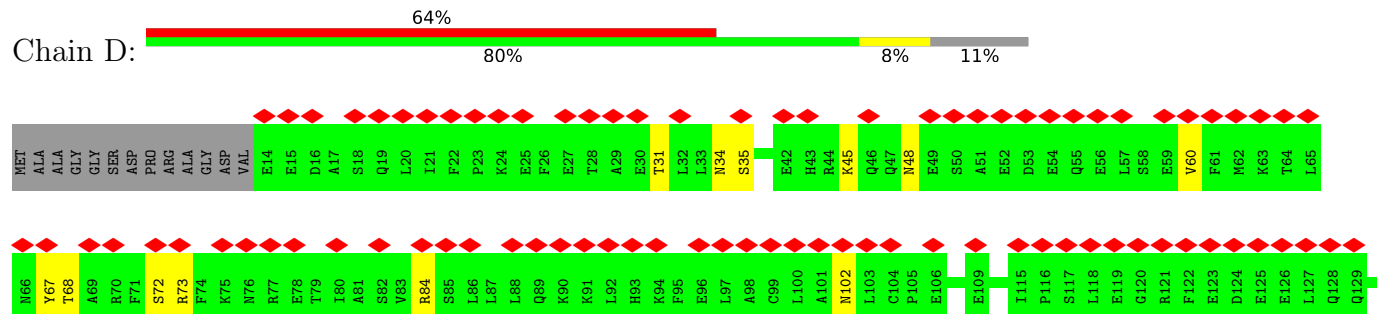
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

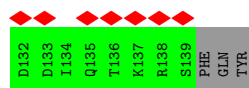
Chain C:



• Molecule 4: RPOL4c domain-containing protein

Chain D:





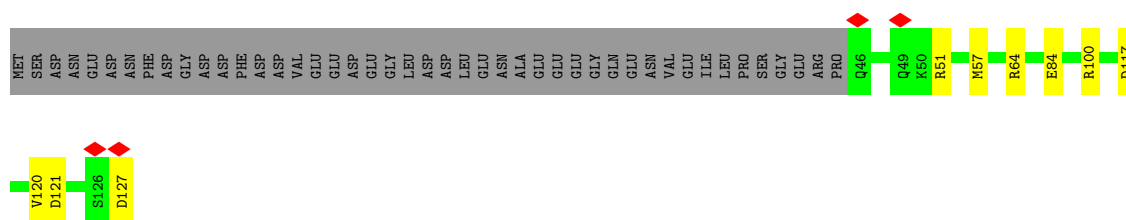
- Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E: 93% 7%



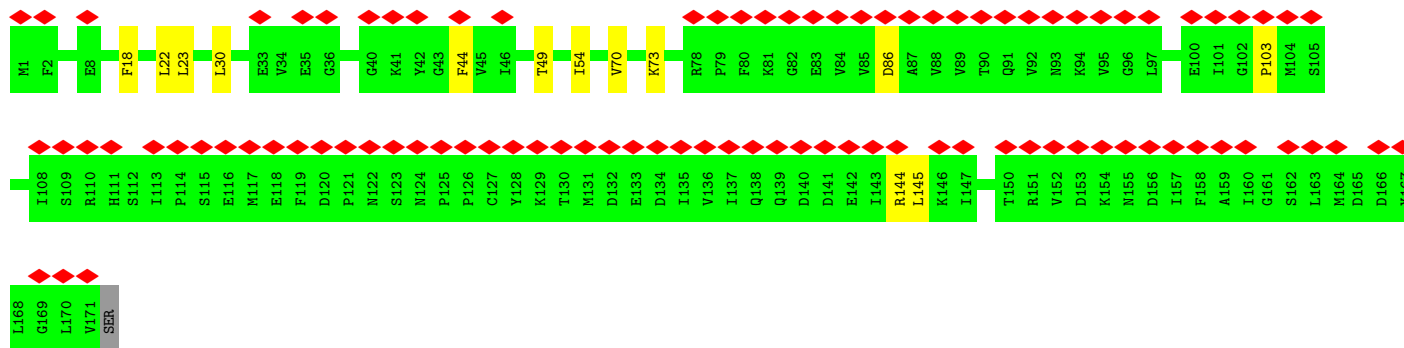
- Molecule 6: DNA-directed RNA polymerase II subunit F

Chain F: 57% 7% 35%



- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G: 55% 92% 8%



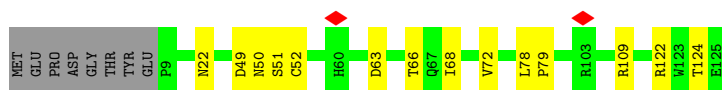
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 87% 11%

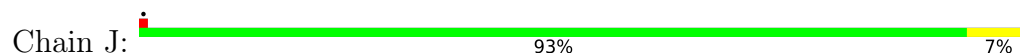


- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 82% 11% 6%



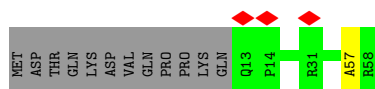
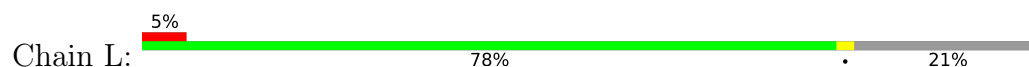
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



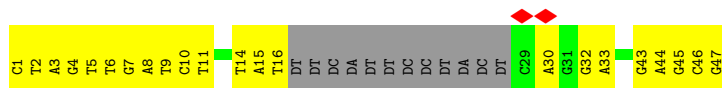
- Molecule 11: RNA_pol_L_2 domain-containing protein



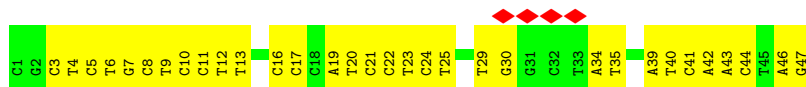
- Molecule 12: RNA polymerase II subunit K



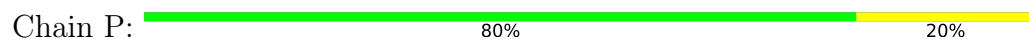
- Molecule 13: NTS



- Molecule 14: TS

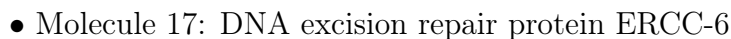


- Molecule 15: RNA



- Molecule 16: DNA excision repair protein ERCC-8

Frequency	Percentage
Daily	85%
Weekly	7%
Monthly	8%



Frequency	Percentage
Daily	31%
Weekly	5%
Monthly	64%



ASN	ALA	ILE	SER	GLU	MET	LEU	ARG	SER	ARG	HIS	ILE	THR	PHE	ALA	GLY	LYS	PHE	GLU	PRO	VAL	GLN	ASP	GLN	HIS	TRP	CYS	ARG	ALA	PRO	ARG	PRO	PRO	GLY	LEU	CYS	GLU	ARG	GLN	ASP	ASP	LEU	LYS	CYS	GLY	LYS	ILE	VAL	HIS	GLY	GLY	ASP	ASP	GLU	GLY	ARG	PRO	ASN	PRO	THR	LEU	LEU
ASP	PRO	GLU	ASP	ALA	ARG	GLU	GLN	ARG	ARG	GLN	ARG	LEU	GLN	LYS	GLN	ARG	PRO	GLU	GLU	TRP	GLN	ASP	PRO	GLU	LEU	MET	ARG	ALA	ASP	VAL	GLU	ALA	ALA	GLY	GLN	ASP	LEU	LEU	GLY	SER	SER	ARG	ARG	TYR	SER	GLY	LYS	VAL	ARG	ARG	TYR	PRO	SER	LEU	THR	ASN	LEU				
LYS	ALA	GLN	ALA	ASP	THR	ALA	ARG	ALA	ARG	ILE	GLY	ARG	VAL	PHE	LYS	LYS	ALA	ALA	VAL	ARG	ARG	VAL	ARG	VAL	VAL	ALA	ALA	ALA	MET	ASN	ARG	MET	GLN	LYS	LYS	HIS	GLU	LYS	PHE	SER	ASN	ASN	GLN	PHE	ASN	TYR	ALA	ALA	LEU	ASN											

• Molecule 20: DNA damage-binding protein 1

Chain d:  81% 14%

SER	ASN	ALA	M1	C18	N36	E40	V43	T45	A46	E47	R50	E54	L80	D99	I100	I101	T102	E117	T118	G119	I120	M130	R134	D146	K150	D166	V167	P176	Q186	L197	E213	I231	Q234	H240	D243	K244	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100000	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 ($e^-/\text{\AA}^2$)	40.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.181	Depositor
Minimum map value	-0.105	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.22	0/11382	0.40	0/15368
2	B	0.23	0/9233	0.39	0/12463
3	C	0.25	0/2132	0.41	0/2896
4	D	0.16	0/1043	0.31	0/1400
5	E	0.18	0/1751	0.34	0/2366
6	F	0.21	0/667	0.35	0/901
7	G	0.17	0/1382	0.39	0/1874
8	H	0.21	0/1207	0.36	0/1628
9	I	0.18	0/972	0.40	0/1316
10	J	0.22	0/542	0.37	0/730
11	K	0.20	0/939	0.34	0/1271
12	L	0.22	0/394	0.41	0/524
13	N	0.19	0/817	0.35	0/1258
14	T	0.25	0/1056	0.41	0/1624
15	P	0.23	0/247	0.25	0/384
16	a	0.24	0/2908	0.43	0/3939
17	b	0.21	0/4458	0.46	0/6021
19	c	0.08	0/563	0.26	0/702
20	d	0.88	2/8646 (0.0%)	0.82	8/11725 (0.1%)
All	All	0.41	2/50339 (0.0%)	0.50	8/68390 (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	1
16	a	0	1
17	b	0	2
20	d	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	d	659	ILE	CG1-CD1	-6.56	1.26	1.51
20	d	623	LEU	CG-CD2	-5.73	1.33	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	d	705	ASP	N-CA-C	6.05	117.67	111.14
20	d	707	ILE	N-CA-C	5.70	121.19	109.34
20	d	930	VAL	N-CA-CB	5.66	120.57	111.23
20	d	394	ILE	CB-CG1-CD1	-5.56	102.13	113.80
20	d	929	SER	N-CA-C	5.48	122.47	110.80
20	d	708	GLN	CB-CA-C	-5.27	101.70	110.81
20	d	563	ASP	N-CA-C	-5.16	104.25	110.44
20	d	1054	MET	N-CA-CB	5.03	117.52	110.12

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	VAL	Peptide
16	a	174	LYS	Peptide
17	b	912	LEU	Peptide
17	b	995	PHE	Peptide
20	d	884	ILE	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	11179	11314	11313	85	0
2	B	9052	9088	9087	61	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2089	2030	2031	12	0
4	D	1030	1016	1016	9	0
5	E	1720	1737	1737	10	0
6	F	657	684	684	6	0
7	G	1351	1358	1358	10	0
8	H	1186	1147	1147	9	0
9	I	949	879	879	10	0
10	J	533	553	553	5	0
11	K	920	942	942	6	0
12	L	388	393	393	1	0
13	N	727	0	394	22	0
14	T	947	0	532	48	0
15	P	220	109	109	1	0
16	a	2849	2692	2778	26	0
17	b	4354	4390	4390	49	0
18	x	175	142	40	0	0
19	c	564	143	143	1	0
20	d	8491	7981	8402	124	0
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	C	1	0	0	0	0
21	I	2	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
22	A	1	0	0	0	0
All	All	49390	46598	47928	441	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 5.

All (441) 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:A:114:CYS:SG	1:A:184:CYS:HB3	1.83	1.19
16:a:174:LYS:HE2	17:b:1384:LEU:CD2	2.03	0.88
14:T:8:DC:H2'	14:T:9:DT:H71	1.54	0.88
1:A:338:SER:OG	1:A:341:GLN:OE1	1.92	0.87
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.57	0.86
2:B:565:THR:OG1	2:B:610:ARG:O	1.95	0.85
1:A:114:CYS:SG	1:A:184:CYS:CB	2.68	0.81
1:A:1190:GLN:O	1:A:1194:ASN:ND2	2.16	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:d:275:ASP:OD2	20:d:279:ARG:NH1	2.16	0.78
9:I:68:ILE:O	9:I:122:ARG:NH1	2.17	0.78
14:T:3:DC:H2'	14:T:4:DT:H71	1.65	0.77
16:a:174:LYS:HE2	17:b:1384:LEU:CD1	2.14	0.76
2:B:357:CYS:SG	2:B:361:LYS:NZ	2.58	0.76
20:d:660:TYR:CD1	20:d:707:ILE:HD12	2.20	0.76
20:d:186:GLN:N	20:d:186:GLN:OE1	2.18	0.76
14:T:11:DC:H2'	14:T:12:DT:H71	1.69	0.74
20:d:18:CYS:SG	20:d:315:THR:OG1	2.42	0.74
20:d:394:ILE:HG12	20:d:670:ASN:O	1.87	0.74
20:d:706:GLU:HB3	20:d:708:GLN:NE2	2.03	0.74
2:B:924:ARG:NH1	3:C:62:GLU:OE1	2.21	0.74
20:d:706:GLU:OE2	20:d:708:GLN:NE2	2.20	0.73
1:A:538:VAL:HG12	1:A:539:GLN:H	1.53	0.73
16:a:174:LYS:HE2	17:b:1384:LEU:HD22	1.69	0.73
20:d:36:ASN:ND2	20:d:1002:GLU:OE2	2.21	0.73
1:A:70:ARG:NH2	1:A:75:ALA:O	2.21	0.72
1:A:576:GLN:O	1:A:590:GLN:NE2	2.23	0.72
1:A:374:SER:OG	1:A:376:ASP:OD1	2.06	0.72
2:B:942:LYS:NZ	15:P:10:A:OP1	2.19	0.72
3:C:180:ALA:O	10:J:42:ARG:NH2	2.23	0.71
20:d:102:THR:OG1	20:d:1065:VAL:O	2.09	0.71
1:A:549:THR:O	1:A:589:LYS:NZ	2.24	0.70
17:b:920:GLY:O	17:b:950:ARG:NH2	2.24	0.70
1:A:233:CYS:SG	1:A:244:ARG:NH1	2.64	0.70
1:A:461:GLN:NE2	2:B:1090:GLU:OE2	2.24	0.70
8:H:92:MET:HE2	8:H:143:LEU:HD22	1.74	0.69
16:a:174:LYS:CE	17:b:1384:LEU:HD13	2.22	0.69
1:A:321:GLU:OE1	1:A:341:GLN:NE2	2.26	0.69
14:T:6:DT:H2'	14:T:7:DG:C8	2.27	0.69
16:a:17:ARG:NH1	20:d:117:GLU:O	2.24	0.69
1:A:413:TYR:OH	1:A:450:MET:O	2.08	0.69
20:d:415:SER:O	20:d:481:GLN:NE2	2.26	0.69
2:B:957:THR:OG1	2:B:959:GLU:O	2.11	0.68
2:B:198:GLU:OE2	2:B:388:TYR:OH	2.09	0.68
17:b:686:TRP:CE3	17:b:700:LEU:HD12	2.29	0.68
2:B:352:GLY:O	2:B:361:LYS:NZ	2.20	0.67
2:B:591:ARG:HE	2:B:603:MET:HE2	1.59	0.67
20:d:394:ILE:CD1	20:d:707:ILE:HA	2.23	0.67
2:B:551:GLU:OE2	2:B:578:LYS:NZ	2.28	0.67
4:D:67:TYR:OH	7:G:86:ASP:O	2.13	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:12:DT:H2''	14:T:13:DT:H5''	1.77	0.66
20:d:47:GLU:OE1	20:d:47:GLU:N	2.28	0.66
20:d:477:ARG:HB3	20:d:486:LEU:HD11	1.77	0.66
20:d:659:ILE:HD13	20:d:668:PHE:CE1	2.30	0.66
1:A:457:ILE:HD11	1:A:515:ILE:HD12	1.76	0.66
2:B:329:GLY:O	2:B:335:ARG:NE	2.29	0.65
16:a:174:LYS:CE	17:b:1384:LEU:HD22	2.27	0.65
20:d:381:ALA:O	20:d:385:GLY:N	2.30	0.65
2:B:746:THR:HG21	14:T:25:DT:H5''	1.79	0.65
17:b:913:THR:OG1	17:b:916:VAL:HG13	1.97	0.65
1:A:413:TYR:O	1:A:415:GLY:N	2.30	0.64
1:A:373:LEU:O	1:A:485:ASN:ND2	2.30	0.64
1:A:1182:GLN:O	1:A:1190:GLN:NE2	2.29	0.64
1:A:1198:GLU:OE1	1:A:1198:GLU:N	2.29	0.64
20:d:546:LEU:HB3	20:d:600:HIS:CE1	2.33	0.64
20:d:1002:GLU:OE1	20:d:1034:ASN:ND2	2.29	0.64
2:B:1104:ARG:NH1	2:B:1109:GLU:OE2	2.31	0.63
9:I:50:ASN:O	9:I:51:SER:OG	2.16	0.63
20:d:567:ARG:HE	20:d:579:LYS:CB	2.10	0.63
14:T:7:DG:H2''	14:T:8:DC:H5''	1.81	0.63
14:T:42:DA:H4'	14:T:43:DA:OP1	1.97	0.63
1:A:41:ILE:HD12	1:A:255:VAL:HG11	1.81	0.63
16:a:174:LYS:HE2	17:b:1384:LEU:HD13	1.80	0.63
14:T:8:DC:H5''	14:T:8:DC:H6	1.64	0.62
20:d:456:GLN:O	20:d:472:THR:OG1	2.03	0.62
1:A:1311:LEU:HD12	1:A:1332:GLN:HG3	1.82	0.62
13:N:44:DA:H2''	13:N:45:DG:H5''	1.81	0.62
14:T:7:DG:H4'	14:T:8:DC:OP1	2.00	0.62
2:B:927:ARG:NH1	2:B:1057:ASP:OD1	2.33	0.61
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.82	0.61
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.14	0.61
8:H:71:ASP:OD2	8:H:142:TYR:OH	2.18	0.61
1:A:507:GLN:N	2:B:1105:GLU:OE2	2.33	0.61
2:B:210:LYS:NZ	2:B:212:ASP:O	2.34	0.61
1:A:668:PHE:CE1	1:A:672:ILE:HD11	2.35	0.61
1:A:332:SER:HB3	14:T:29:DT:H5''	1.83	0.61
1:A:659:GLU:OE2	1:A:985:ARG:NH1	2.34	0.61
3:C:190:ASN:O	3:C:193:ARG:NH1	2.33	0.61
17:b:665:PHE:O	17:b:670:ARG:NH2	2.34	0.61
20:d:130:MET:HE3	20:d:176:PRO:HG2	1.83	0.61
1:A:808:PRO:HG2	2:B:675:LEU:HD12	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:10:DC:C6	13:N:11:DT:H72	2.36	0.61
2:B:347:MET:HE1	2:B:365:LEU:HD22	1.82	0.61
20:d:706:GLU:HB3	20:d:708:GLN:HE22	1.65	0.61
14:T:16:DC:H2'	14:T:17:DC:C6	2.36	0.61
14:T:20:DT:H2'	14:T:21:DC:C6	2.36	0.60
16:a:37:ASP:OD2	16:a:81:TYR:OH	2.16	0.60
20:d:708:GLN:O	20:d:709:LYS:HB2	2.01	0.60
20:d:396:ILE:HG21	20:d:673:LEU:HD23	1.84	0.60
16:a:211:VAL:HB	16:a:226:LEU:HD22	1.83	0.60
20:d:1135:GLU:HA	20:d:1138:ARG:HH11	1.67	0.60
20:d:394:ILE:HD11	20:d:669:SER:OG	2.02	0.60
14:T:34:DA:H1'	17:b:800:ILE:HD13	1.83	0.59
17:b:902:ASN:ND2	17:b:922:ASN:O	2.35	0.59
2:B:501:LEU:HD12	2:B:505:LEU:CD1	2.33	0.59
14:T:34:DA:H2'	14:T:35:DT:C6	2.38	0.59
1:A:862:ARG:NH2	1:A:1432:PHE:O	2.34	0.58
17:b:1394:ARG:O	17:b:1398:HIS:ND1	2.33	0.58
20:d:1053:ASP:OD2	20:d:1057:ARG:NH2	2.36	0.58
5:E:134:GLU:OE2	5:E:181:ARG:NH2	2.36	0.58
2:B:794:VAL:HG12	2:B:967:ILE:HG22	1.83	0.58
13:N:4:DG:C8	13:N:5:DT:H72	2.37	0.58
5:E:56:THR:OG1	5:E:78:GLU:OE2	2.18	0.58
20:d:659:ILE:HD13	20:d:668:PHE:CD1	2.38	0.58
1:A:521:VAL:HG13	1:A:535:MET:HE1	1.84	0.58
8:H:102:ASP:OD2	8:H:110:THR:OG1	2.21	0.58
14:T:34:DA:H2'	14:T:35:DT:H6	1.69	0.58
20:d:603:LEU:HD12	20:d:611:LEU:HD21	1.85	0.58
2:B:413:LYS:O	2:B:417:ILE:HD12	2.04	0.58
14:T:9:DT:H2''	14:T:10:DC:C6	2.38	0.57
20:d:407:ILE:HD11	20:d:699:LEU:HD11	1.86	0.57
16:a:114:MET:HE3	16:a:126:VAL:HG13	1.86	0.57
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.86	0.57
1:A:904:GLN:NE2	1:A:981:CYS:O	2.37	0.57
20:d:40:GLU:HG2	20:d:54:GLU:HG3	1.87	0.57
20:d:432:GLN:OE1	20:d:432:GLN:N	2.37	0.57
14:T:39:DA:C2'	14:T:40:DT:H71	2.35	0.57
19:c:137:PHE:O	19:c:141:ASN:N	2.37	0.57
2:B:1078:ARG:HG3	14:T:23:DT:H5''	1.85	0.57
5:E:120:ASP:OD1	5:E:121:MET:N	2.38	0.57
14:T:24:DC:H2'	14:T:25:DT:C6	2.39	0.56
2:B:565:THR:HG21	2:B:580:PRO:HB3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:b:859:LEU:HB2	17:b:929:VAL:HG12	1.86	0.56
20:d:99:ASP:OD1	20:d:100:ILE:N	2.38	0.56
20:d:213:GLU:OE1	20:d:234:GLN:N	2.38	0.56
13:N:14:DT:H72	14:T:34:DA:N1	2.20	0.56
2:B:1090:GLU:OE1	2:B:1090:GLU:N	2.39	0.56
1:A:421:ARG:NH1	1:A:444:TYR:OH	2.39	0.55
2:B:959:GLU:O	2:B:961:ILE:N	2.40	0.55
1:A:1180:ASN:ND2	1:A:1183:SER:OG	2.38	0.55
1:A:54:LEU:O	1:A:61:ARG:NH2	2.40	0.55
17:b:531:GLY:O	17:b:744:ARG:NH1	2.38	0.55
5:E:78:GLU:OE1	5:E:78:GLU:N	2.41	0.54
6:F:84:GLU:OE2	6:F:84:GLU:N	2.40	0.54
3:C:59:LEU:HD13	3:C:63:PHE:CD1	2.42	0.54
17:b:872:GLU:OE1	17:b:884:LYS:NZ	2.39	0.54
4:D:31:THR:O	4:D:84:ARG:NH2	2.40	0.54
1:A:358:ARG:NH1	14:T:22:DC:OP1	2.40	0.54
20:d:704:ILE:HD12	20:d:707:ILE:CG2	2.38	0.54
13:N:5:DT:H2'	13:N:6:DT:H71	1.90	0.54
17:b:921:VAL:HG23	17:b:923:LEU:HD13	1.89	0.54
20:d:288:GLU:HB2	20:d:298:LYS:HB2	1.89	0.54
2:B:602:SER:OG	2:B:620:ARG:NH1	2.41	0.54
17:b:539:THR:O	17:b:543:ILE:HD12	2.08	0.54
1:A:413:TYR:O	1:A:449:HIS:ND1	2.41	0.53
4:D:60:VAL:HG13	7:G:103:PRO:HB3	1.91	0.53
20:d:538:VAL:O	20:d:561:TRP:NE1	2.42	0.53
14:T:19:DA:H2'	14:T:20:DT:C6	2.44	0.53
2:B:274:ARG:NH2	2:B:281:ASP:OD1	2.41	0.53
20:d:516:LEU:O	20:d:531:HIS:ND1	2.41	0.53
2:B:625:LEU:HD13	2:B:675:LEU:HD21	1.90	0.53
2:B:847:LYS:NZ	2:B:864:ASP:OD2	2.22	0.53
20:d:542:ASP:OD2	20:d:592:LEU:HD12	2.09	0.53
1:A:108:ARG:NH2	1:A:191:ILE:O	2.41	0.53
9:I:109:ARG:HE	9:I:124:THR:HG21	1.74	0.53
20:d:243:ASP:OD1	20:d:244:LYS:N	2.41	0.53
1:A:114:CYS:HG	1:A:184:CYS:CB	2.20	0.53
14:T:41:DC:H2''	14:T:42:DA:C8	2.44	0.52
1:A:862:ARG:NH1	2:B:1088:GLU:OE2	2.42	0.52
1:A:865:ILE:HD13	1:A:1092:ALA:HB3	1.91	0.52
20:d:706:GLU:CD	20:d:708:GLN:HE22	2.18	0.52
1:A:1433:GLU:OE1	14:T:17:DC:H4'	2.10	0.52
16:a:70:LEU:O	16:a:87:VAL:N	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:7:DG:H2''	13:N:8:DA:H5''	1.90	0.52
3:C:86:ARG:HD3	11:K:11:LEU:HD11	1.91	0.52
1:A:461:GLN:OE1	1:A:502:ASN:ND2	2.42	0.52
20:d:503:CYS:SG	20:d:504:ASN:N	2.83	0.52
3:C:7:PRO:O	11:K:104:ARG:NH1	2.43	0.51
20:d:542:ASP:OD1	20:d:543:ILE:N	2.43	0.51
1:A:601:ASN:ND2	1:A:989:ASN:OD1	2.43	0.51
14:T:46:DA:H2'	14:T:47:DG:O4'	2.10	0.51
1:A:889:LEU:O	1:A:890:ARG:NH1	2.42	0.51
13:N:46:DC:H2''	13:N:47:DG:N7	2.26	0.51
14:T:12:DT:H2''	14:T:13:DT:C6	2.46	0.51
17:b:867:MET:HE2	17:b:932:TYR:CE2	2.45	0.51
14:T:7:DG:H2''	14:T:8:DC:C5'	2.41	0.50
16:a:42:HIS:HE2	16:a:61:SER:HG	1.54	0.50
1:A:951:GLU:OE2	1:A:954:ARG:NH2	2.44	0.50
2:B:746:THR:CG2	14:T:25:DT:H5''	2.42	0.50
5:E:141:GLU:N	5:E:141:GLU:OE1	2.45	0.50
17:b:971:LYS:NZ	17:b:1003:GLU:O	2.44	0.50
5:E:209:VAL:O	5:E:210:GLN:NE2	2.44	0.50
20:d:546:LEU:HD21	20:d:594:THR:HA	1.94	0.50
13:N:8:DA:H2''	13:N:9:DT:H5'	1.94	0.50
2:B:777:ASN:O	10:J:47:ARG:NH1	2.40	0.49
7:G:23:LEU:CD1	7:G:54:ILE:HG21	2.42	0.49
17:b:921:VAL:HG23	17:b:923:LEU:CD1	2.41	0.49
17:b:761:GLU:OE2	17:b:961:ARG:NH1	2.45	0.49
4:D:34:ASN:OD1	4:D:35:SER:N	2.46	0.49
16:a:78:ARG:NE	20:d:944:GLU:O	2.41	0.49
20:d:659:ILE:HD12	20:d:667:VAL:O	2.13	0.49
14:T:11:DC:C2'	14:T:12:DT:H71	2.42	0.49
2:B:312:GLN:NE2	9:I:22:ASN:OD1	2.46	0.49
13:N:16:DT:OP1	17:b:975:ARG:NH1	2.40	0.49
20:d:929:SER:O	20:d:930:VAL:HG13	2.12	0.49
20:d:690:SER:HA	20:d:703:THR:HG22	1.95	0.49
8:H:136:GLU:O	8:H:139:SER:OG	2.27	0.49
14:T:43:DA:H2''	14:T:44:DC:C6	2.48	0.49
17:b:751:LYS:O	17:b:754:LEU:O	2.31	0.49
20:d:467:GLN:NE2	20:d:479:VAL:O	2.46	0.49
9:I:50:ASN:ND2	9:I:52:CYS:O	2.46	0.48
16:a:174:LYS:CE	17:b:1384:LEU:CD1	2.83	0.48
16:a:174:LYS:NZ	17:b:1384:LEU:HD13	2.27	0.48
17:b:945:ARG:HB2	17:b:959:VAL:HG21	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:LYS:NZ	12:L:57:ALA:O	2.44	0.48
20:d:546:LEU:HD21	20:d:594:THR:CA	2.43	0.48
1:A:481:THR:O	1:A:483:ARG:NE	2.46	0.48
17:b:614:VAL:HG11	17:b:621:LEU:HB2	1.93	0.48
17:b:647:GLU:N	17:b:673:LEU:O	2.46	0.48
1:A:1005:HIS:ND1	1:A:1007:ILE:HG22	2.29	0.48
2:B:812:ARG:NH2	2:B:900:GLU:OE2	2.45	0.48
13:N:1:DC:C2	13:N:2:DT:H72	2.48	0.48
2:B:764:MET:HE1	2:B:938:ARG:NH1	2.29	0.48
9:I:72:VAL:HG22	9:I:78:LEU:HD11	1.95	0.48
14:T:5:DC:H2''	14:T:6:DT:O4'	2.14	0.48
20:d:629:VAL:HG11	20:d:668:PHE:CZ	2.49	0.48
9:I:109:ARG:NE	9:I:124:THR:HG21	2.29	0.47
17:b:921:VAL:HG22	17:b:947:ARG:HE	1.79	0.47
20:d:558:ILE:HG13	20:d:569:LEU:HD11	1.97	0.47
2:B:629:GLU:N	2:B:632:LYS:O	2.41	0.47
1:A:728:THR:H	1:A:736:THR:HG21	1.78	0.47
13:N:8:DA:H2'	13:N:9:DT:H71	1.95	0.47
1:A:523:ARG:NH1	6:F:127:ASP:OD2	2.47	0.47
14:T:20:DT:H2'	14:T:21:DC:H6	1.79	0.47
16:a:93:ASP:OD1	16:a:93:ASP:N	2.47	0.47
17:b:604:THR:O	17:b:605:HIS:ND1	2.48	0.47
2:B:808:SER:OG	2:B:1050:ARG:NH1	2.48	0.47
1:A:98:GLY:HA3	1:A:1440:MET:HE3	1.97	0.47
3:C:189:ASP:O	3:C:191:ALA:N	2.48	0.47
1:A:455:ILE:HG23	1:A:520:MET:HE1	1.96	0.47
4:D:68:THR:O	4:D:72:SER:OG	2.21	0.47
14:T:39:DA:H2''	14:T:40:DT:H71	1.96	0.47
16:a:126:VAL:HG11	17:b:1393:MET:HE1	1.97	0.47
17:b:935:ASP:OD1	17:b:936:TRP:N	2.46	0.47
20:d:599:SER:OG	20:d:600:HIS:N	2.48	0.47
7:G:18:PHE:HA	7:G:22:LEU:HD13	1.97	0.46
2:B:15:ASP:OD1	2:B:15:ASP:N	2.47	0.46
17:b:777:GLN:HA	17:b:780:VAL:HG12	1.96	0.46
2:B:294:ASP:OD1	2:B:379:ARG:NH2	2.47	0.46
2:B:1035:ARG:NH1	2:B:1036:LYS:O	2.47	0.46
4:D:60:VAL:HG11	7:G:44:PHE:CE2	2.51	0.46
20:d:413:LEU:HD13	20:d:426:VAL:HG23	1.98	0.46
20:d:616:LEU:HD21	20:d:623:LEU:CD2	2.45	0.46
20:d:706:GLU:HB3	20:d:708:GLN:CD	2.39	0.46
1:A:1166:LEU:O	1:A:1170:THR:OG1	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:114:ALA:O	5:E:117:SER:OG	2.26	0.46
16:a:273:ASN:O	16:a:277:GLY:N	2.49	0.46
17:b:600:THR:HG23	17:b:601:GLY:H	1.80	0.46
3:C:144:GLU:OE1	3:C:144:GLU:N	2.48	0.46
13:N:43:DG:H2''	13:N:44:DA:C8	2.51	0.46
17:b:494:ASP:OD1	17:b:495:GLU:N	2.47	0.46
20:d:45:THR:OG1	20:d:47:GLU:O	2.32	0.46
20:d:119:GLY:O	20:d:134:ARG:NH2	2.44	0.46
1:A:78:MET:O	2:B:1072:ARG:NH2	2.49	0.46
20:d:832:GLY:HA3	20:d:873:MET:HE3	1.98	0.46
1:A:1297:THR:HG23	1:A:1297:THR:O	2.15	0.46
20:d:612:PHE:HE2	20:d:628:LYS:HD2	1.80	0.46
20:d:660:TYR:CG	20:d:707:ILE:HD12	2.51	0.46
14:T:34:DA:H2''	14:T:35:DT:O5'	2.16	0.45
20:d:679:MET:SD	20:d:680:CYS:N	2.89	0.45
1:A:760:LEU:HD22	1:A:764:ASN:HD22	1.80	0.45
20:d:394:ILE:HD12	20:d:707:ILE:HA	1.98	0.45
2:B:438:ARG:NH2	2:B:442:ASP:OD1	2.48	0.45
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.52	0.45
1:A:823:VAL:CG1	1:A:831:LEU:HD22	2.46	0.45
20:d:150:LYS:O	20:d:150:LYS:HG3	2.15	0.45
16:a:111:ASP:OD1	16:a:112:THR:N	2.49	0.45
17:b:533:GLU:OE2	17:b:747:LYS:N	2.49	0.45
20:d:231:ILE:HD13	20:d:240:HIS:CE1	2.51	0.45
1:A:823:VAL:HG11	1:A:831:LEU:HD22	1.99	0.45
1:A:883:ILE:HD11	1:A:1424:THR:HA	1.99	0.45
8:H:88:PHE:CD1	8:H:144:LEU:HD12	2.51	0.45
16:a:174:LYS:HE2	17:b:1384:LEU:HD21	1.91	0.45
17:b:857:ARG:NH2	17:b:901:TYR:O	2.44	0.45
20:d:673:LEU:HD11	20:d:676:VAL:CG2	2.46	0.45
1:A:1189:ASP:OD2	1:A:1258:ARG:NE	2.50	0.45
8:H:49:PRO:O	8:H:147:LYS:NZ	2.50	0.45
20:d:407:ILE:CD1	20:d:699:LEU:HD11	2.47	0.45
1:A:321:GLU:OE1	1:A:321:GLU:N	2.50	0.45
1:A:844:ARG:NH2	2:B:501:LEU:HD13	2.31	0.45
20:d:661:SER:HB2	20:d:666:LEU:HD23	1.98	0.45
20:d:875:GLU:OE2	20:d:878:GLY:N	2.38	0.45
20:d:1055:GLN:HG3	20:d:1093:LEU:HD23	1.99	0.45
17:b:928:ARG:NH1	17:b:958:THR:OG1	2.42	0.45
20:d:341:ASN:O	20:d:343:GLN:NE2	2.49	0.45
1:A:1471:PHE:O	6:F:64:ARG:NH1	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:LEU:O	10:J:6:ARG:NE	2.40	0.45
13:N:44:DA:H2''	13:N:45:DG:C8	2.51	0.45
20:d:396:ILE:HG13	20:d:397:HIS:N	2.32	0.45
20:d:421:THR:OG1	20:d:683:ASN:O	2.28	0.45
20:d:538:VAL:HG11	20:d:541:LEU:HD11	1.99	0.45
20:d:720:SER:O	20:d:720:SER:OG	2.32	0.45
17:b:635:ILE:O	17:b:640:TRP:NE1	2.45	0.44
17:b:760:ASN:OD1	17:b:761:GLU:N	2.51	0.44
20:d:426:VAL:C	20:d:427:LEU:HD12	2.42	0.44
20:d:427:LEU:HD13	20:d:436:LEU:HD23	1.99	0.44
20:d:438:LEU:HA	20:d:443:VAL:HA	1.98	0.44
1:A:896:LEU:O	1:A:1396:ARG:NH1	2.50	0.44
13:N:32:DG:H2''	13:N:33:DA:C8	2.52	0.44
14:T:24:DC:H2'	14:T:25:DT:H6	1.83	0.44
20:d:396:ILE:CG2	20:d:673:LEU:HD23	2.47	0.44
20:d:408:LYS:N	20:d:428:SER:O	2.40	0.44
20:d:478:LEU:HD11	20:d:521:ILE:HG23	1.99	0.44
20:d:480:SER:O	20:d:484:LYS:O	2.35	0.44
1:A:1478:GLU:N	1:A:1478:GLU:OE1	2.49	0.44
3:C:5:ASN:OD1	11:K:52:LYS:NZ	2.51	0.44
7:G:144:ARG:C	7:G:145:LEU:HD12	2.42	0.44
17:b:579:HIS:O	17:b:582:VAL:HG12	2.17	0.44
20:d:367:LEU:O	20:d:368:GLU:HB2	2.17	0.44
20:d:884:ILE:HG22	20:d:885:ASN:H	1.83	0.44
3:C:123:ASN:OD1	3:C:124:SER:N	2.51	0.44
13:N:14:DT:H72	14:T:34:DA:C2	2.53	0.44
14:T:42:DA:H2''	14:T:43:DA:H5''	2.00	0.44
1:A:1229:GLU:OE1	1:A:1229:GLU:N	2.45	0.44
7:G:54:ILE:HG23	7:G:54:ILE:O	2.16	0.44
20:d:515:ALA:HA	20:d:533:GLU:HA	1.99	0.44
20:d:986:ASP:OD1	20:d:986:ASP:N	2.50	0.44
1:A:77:ASN:OD1	1:A:80:GLU:N	2.45	0.44
2:B:887:TYR:O	2:B:888:THR:HG22	2.17	0.44
20:d:719:GLU:OE2	20:d:737:SER:OG	2.25	0.44
1:A:1357:THR:O	5:E:142:HIS:NE2	2.45	0.44
8:H:51:ASP:N	8:H:54:ASP:OD2	2.45	0.44
9:I:49:ASP:OD1	9:I:49:ASP:N	2.49	0.44
13:N:32:DG:H2''	13:N:33:DA:H8	1.83	0.43
14:T:34:DA:H2''	14:T:35:DT:C5'	2.48	0.43
20:d:649:VAL:HB	20:d:659:ILE:HG23	2.00	0.43
2:B:256:ILE:HD11	2:B:373:LEU:HD21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:29:DT:H2''	14:T:30:DG:H4'	1.99	0.43
16:a:65:ASP:OD1	16:a:65:ASP:N	2.52	0.43
1:A:467:MET:SD	1:A:524:MET:HB3	2.58	0.43
1:A:937:ASP:OD1	1:A:938:LEU:N	2.50	0.43
2:B:628:VAL:HG12	2:B:629:GLU:O	2.18	0.43
2:B:967:ILE:HG21	2:B:1048:TYR:OH	2.19	0.43
20:d:468:LEU:HD22	20:d:479:VAL:HB	2.00	0.43
2:B:84:TYR:HE1	2:B:132:VAL:HG22	1.83	0.43
20:d:43:VAL:HB	20:d:50:ARG:HG3	2.01	0.43
20:d:256:SER:OG	20:d:275:ASP:OD2	2.37	0.43
4:D:73:ARG:NE	4:D:102:ASN:O	2.47	0.43
20:d:394:ILE:HD12	20:d:394:ILE:HG23	1.34	0.42
13:N:44:DA:H2''	13:N:45:DG:H8	1.82	0.42
20:d:556:CYS:SG	20:d:571:LEU:HD13	2.60	0.42
20:d:570:LYS:O	20:d:574:PHE:N	2.47	0.42
1:A:695:ASP:OD1	1:A:695:ASP:N	2.52	0.42
13:N:6:DT:H2''	13:N:7:DG:C8	2.54	0.42
20:d:518:TYR:HB2	20:d:574:PHE:CZ	2.54	0.42
2:B:905:ASP:N	2:B:922:ARG:O	2.46	0.42
4:D:68:THR:O	4:D:72:SER:N	2.52	0.42
2:B:864:ASP:OD1	2:B:865:VAL:N	2.51	0.42
11:K:7:PHE:CD1	11:K:11:LEU:HD12	2.54	0.42
20:d:252:ILE:HD12	20:d:252:ILE:H	1.85	0.42
20:d:706:GLU:O	20:d:707:ILE:CG1	2.68	0.42
1:A:94:VAL:HG21	1:A:311:GLN:HA	2.01	0.42
2:B:1091:ARG:NH2	2:B:1092:ASP:OD1	2.53	0.42
17:b:667:THR:O	17:b:670:ARG:NE	2.52	0.42
20:d:393:GLY:HA3	20:d:672:ASN:OD1	2.20	0.42
1:A:255:VAL:HG23	1:A:280:LEU:HD22	2.01	0.42
2:B:495:LEU:HD23	13:N:30:DA:H1'	2.01	0.42
8:H:71:ASP:OD1	8:H:72:ASP:N	2.51	0.42
17:b:651:ILE:HG22	17:b:651:ILE:O	2.20	0.42
6:F:100:ARG:NH2	6:F:121:ASP:O	2.52	0.42
9:I:63:ASP:O	9:I:66:THR:OG1	2.37	0.42
20:d:637:VAL:HG12	20:d:652:CYS:HB2	2.01	0.42
6:F:57:MET:HE1	6:F:120:VAL:HG13	2.02	0.41
16:a:244:HIS:NE2	16:a:262:THR:OG1	2.35	0.41
17:b:869:ASP:OD1	17:b:884:LYS:NZ	2.52	0.41
20:d:989:ARG:O	20:d:989:ARG:HG2	2.19	0.41
20:d:539:ALA:N	20:d:559:GLY:O	2.51	0.41
20:d:698:THR:OG1	20:d:699:LEU:N	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:VAL:O	1:A:342:ARG:NH1	2.44	0.41
1:A:349:ARG:NH2	2:B:1070:LEU:HD21	2.35	0.41
20:d:130:MET:HE2	20:d:197:LEU:HD21	2.01	0.41
20:d:455:GLN:HB3	20:d:472:THR:OG1	2.21	0.41
20:d:564:ILE:HD12	20:d:564:ILE:H	1.84	0.41
1:A:413:TYR:HB3	1:A:414:PRO:HD3	2.02	0.41
1:A:883:ILE:O	1:A:883:ILE:HG22	2.20	0.41
2:B:761:THR:H	2:B:764:MET:HE3	1.85	0.41
4:D:45:LYS:O	4:D:48:ASN:N	2.51	0.41
5:E:112:PRO:HB3	14:T:7:DG:H5'	2.02	0.41
17:b:756:LEU:HD23	17:b:756:LEU:HA	1.89	0.41
1:A:381:PRO:HG2	1:A:384:ILE:HD12	2.01	0.41
1:A:883:ILE:HD11	1:A:1424:THR:HG22	2.02	0.41
11:K:81:TYR:OH	11:K:89:ASN:OD1	2.33	0.41
20:d:130:MET:HE3	20:d:176:PRO:CG	2.48	0.41
20:d:469:ILE:HD11	20:d:476:VAL:HG22	2.03	0.41
20:d:658:VAL:HG11	20:d:707:ILE:HG21	2.01	0.41
20:d:1053:ASP:O	20:d:1057:ARG:HG3	2.21	0.41
1:A:848:ILE:HG21	2:B:496:ALA:HB1	2.03	0.41
20:d:616:LEU:CD2	20:d:623:LEU:HD23	2.51	0.41
20:d:654:ASP:OD1	20:d:655:ARG:N	2.54	0.41
1:A:457:ILE:HD11	1:A:515:ILE:HG23	2.03	0.41
1:A:863:ARG:HB3	1:A:1414:ILE:HG22	2.02	0.41
1:A:1212:LEU:HD11	1:A:1289:GLU:HB2	2.03	0.41
2:B:1078:ARG:CD	14:T:23:DT:H5''	2.50	0.41
2:B:1085:ARG:NE	14:T:21:DC:OP1	2.41	0.41
7:G:30:LEU:HD22	7:G:70:VAL:HG21	2.03	0.41
14:T:12:DT:C2'	14:T:13:DT:H71	2.51	0.41
16:a:36:ARG:NH1	16:a:348:GLU:OE1	2.45	0.41
16:a:48:THR:HG23	16:a:105:VAL:HG12	2.02	0.41
1:A:86:GLY:C	1:A:255:VAL:HG12	2.46	0.41
1:A:962:ASP:HB3	1:A:1043:ILE:HG23	2.02	0.41
2:B:850:ASP:OD1	2:B:850:ASP:N	2.53	0.41
2:B:962:THR:O	10:J:9:THR:HG23	2.21	0.41
17:b:754:LEU:HD12	17:b:754:LEU:HA	1.84	0.41
20:d:80:LEU:HD23	20:d:120:ILE:HG21	2.03	0.41
20:d:130:MET:CE	20:d:176:PRO:HG2	2.50	0.41
20:d:402:ILE:HG13	20:d:699:LEU:HD13	2.03	0.41
20:d:616:LEU:CD1	20:d:623:LEU:HD23	2.50	0.41
20:d:631:LEU:HD12	20:d:631:LEU:O	2.21	0.41
20:d:813:ALA:HA	20:d:833:THR:HG22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:d:881:LEU:HD21	20:d:921:ILE:HG21	2.03	0.41
20:d:1136:LEU:O	20:d:1139:ILE:HG12	2.21	0.41
13:N:8:DA:C2'	13:N:9:DT:H5'	2.51	0.41
14:T:12:DT:H2''	14:T:13:DT:H6	1.86	0.41
20:d:407:ILE:HD11	20:d:699:LEU:CD1	2.51	0.41
7:G:49:THR:N	7:G:73:LYS:O	2.46	0.40
14:T:8:DC:H2'	14:T:9:DT:C7	2.38	0.40
14:T:30:DG:N3	14:T:30:DG:H2'	2.36	0.40
20:d:673:LEU:HD12	20:d:673:LEU:C	2.45	0.40
1:A:811:ILE:HD12	9:I:79:PRO:HB3	2.03	0.40
2:B:735:VAL:HG21	10:J:55:LEU:HD13	2.03	0.40
14:T:19:DA:H2'	14:T:20:DT:H6	1.84	0.40
20:d:478:LEU:CD1	20:d:521:ILE:HG23	2.50	0.40
7:G:23:LEU:HD12	7:G:54:ILE:HG21	2.04	0.40
8:H:7:GLU:OE2	8:H:57:ARG:NH1	2.54	0.40
16:a:121:ASP:OD1	16:a:123:THR:OG1	2.27	0.40
16:a:318:VAL:O	16:a:327:ILE:N	2.54	0.40
20:d:296:THR:OG1	20:d:297:LEU:N	2.55	0.40
5:E:110:MET:HG2	5:E:114:ALA:HB3	2.03	0.40
6:F:51:ARG:NH1	6:F:117:ASP:O	2.52	0.40
20:d:166:ASP:OD1	20:d:167:VAL:N	2.54	0.40
13:N:3:DA:H2''	13:N:4:DG:H8	1.86	0.40
13:N:15:DA:H2''	17:b:799:LEU:HG	2.03	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	1402/1970 (71%)	1367 (98%)	35 (2%)	0	100	100
2	B	1123/1174 (96%)	1076 (96%)	47 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	256/275 (93%)	249 (97%)	7 (3%)	0	100	100
4	D	124/142 (87%)	119 (96%)	5 (4%)	0	100	100
5	E	207/210 (99%)	204 (99%)	3 (1%)	0	100	100
6	F	80/127 (63%)	75 (94%)	5 (6%)	0	100	100
7	G	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
8	H	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
9	I	115/125 (92%)	111 (96%)	4 (4%)	0	100	100
10	J	65/67 (97%)	65 (100%)	0	0	100	100
11	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
12	L	44/58 (76%)	40 (91%)	4 (9%)	0	100	100
16	a	363/396 (92%)	348 (96%)	15 (4%)	0	100	100
17	b	526/1493 (35%)	507 (96%)	19 (4%)	0	100	100
19	c	139/709 (20%)	136 (98%)	3 (2%)	0	100	100
20	d	1082/1143 (95%)	1010 (93%)	72 (7%)	0	100	100
All	All	5954/8328 (72%)	5725 (96%)	229 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1242/1749 (71%)	1242 (100%)	0	100	100
2	B	992/1027 (97%)	992 (100%)	0	100	100
3	C	237/252 (94%)	237 (100%)	0	100	100
4	D	116/126 (92%)	116 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	152/153 (99%)	152 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	105/112 (94%)	105 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	43/55 (78%)	43 (100%)	0	100	100
16	a	320/348 (92%)	320 (100%)	0	100	100
17	b	476/1297 (37%)	476 (100%)	0	100	100
20	d	938/1001 (94%)	938 (100%)	0	100	100
All	All	5172/6716 (77%)	5172 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	HIS
1	A	735	GLN
1	A	792	ASN
1	A	1077	ASN
2	B	227	ASN
2	B	319	ASN
4	D	38	HIS
4	D	43	HIS
11	K	36	ASN
16	a	169	GLN
16	a	187	GLN
16	a	235	GLN
17	b	762	GLN
20	d	4	ASN
20	d	261	HIS
20	d	337	ASN
20	d	399	HIS
20	d	467	GLN
20	d	617	ASN
20	d	670	ASN
20	d	711	HIS
20	d	731	GLN
20	d	904	ASN
20	d	991	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	9	G

There are no RNA pucker outliers to report.

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](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

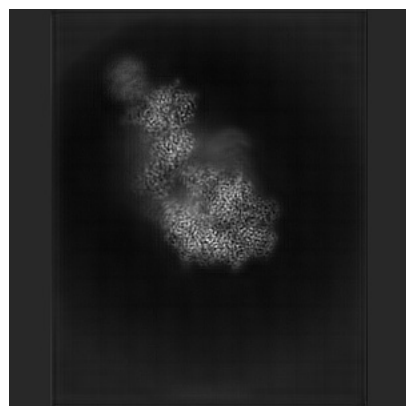
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13004. These allow visual inspection of the internal detail of the map and identification of artifacts.

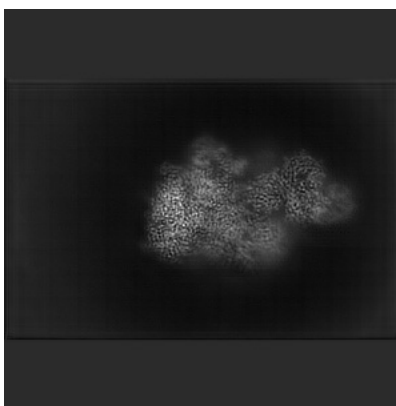
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

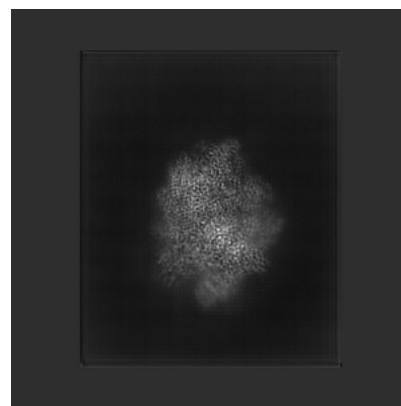
6.1.1 Primary map



X

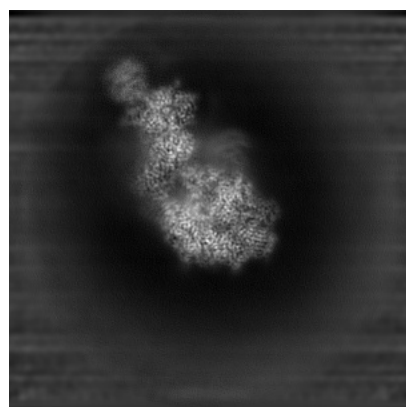


Y

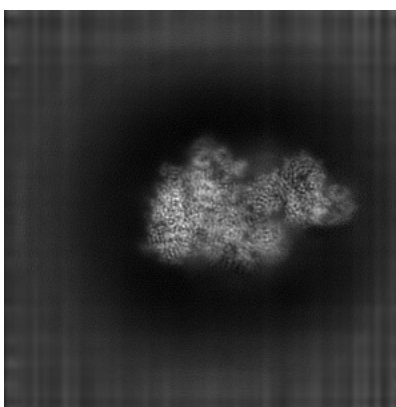


Z

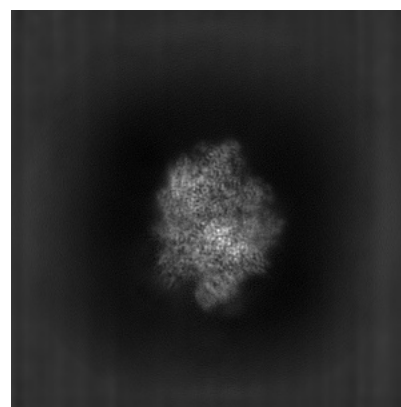
6.1.2 Raw map



X



Y

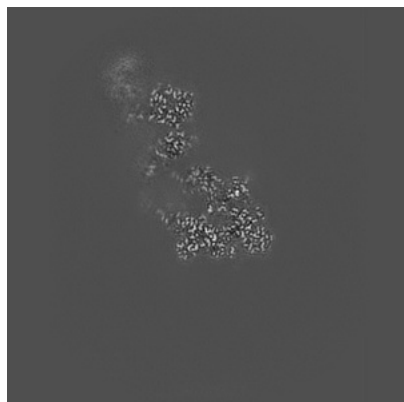


Z

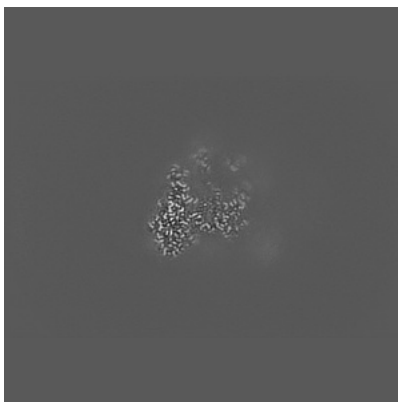
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

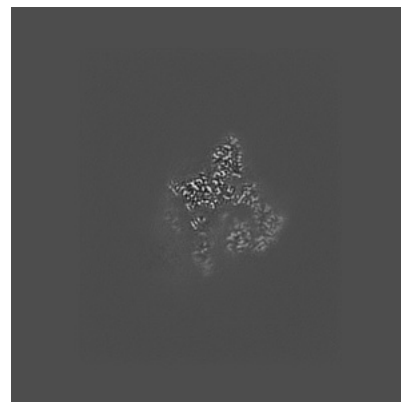
6.2.1 Primary map



X Index: 200

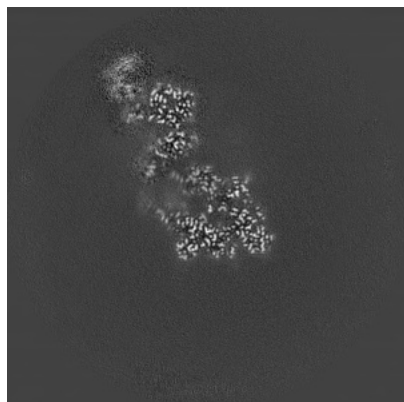


Y Index: 200

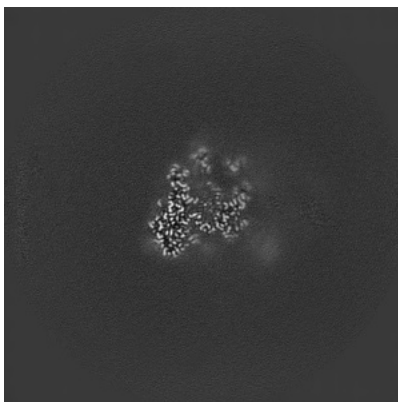


Z Index: 200

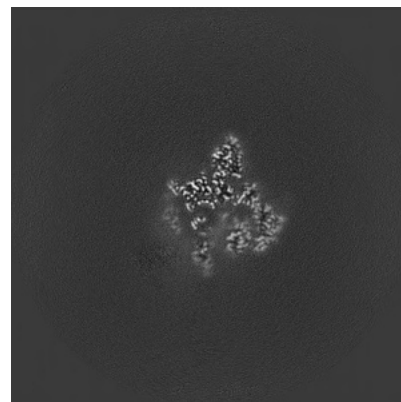
6.2.2 Raw map



X Index: 200



Y Index: 200

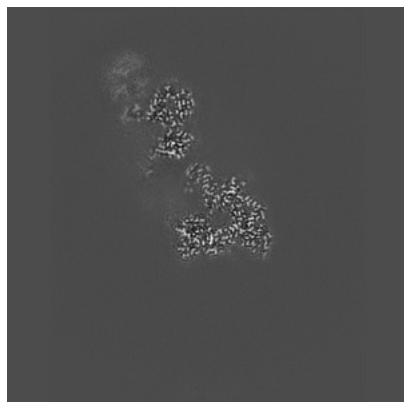


Z Index: 200

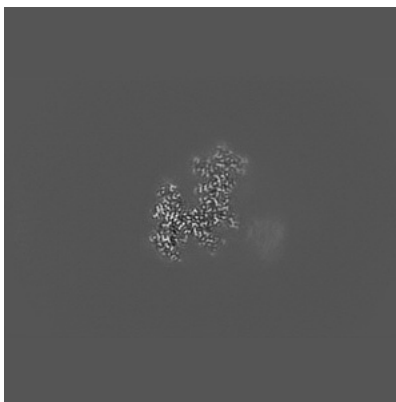
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

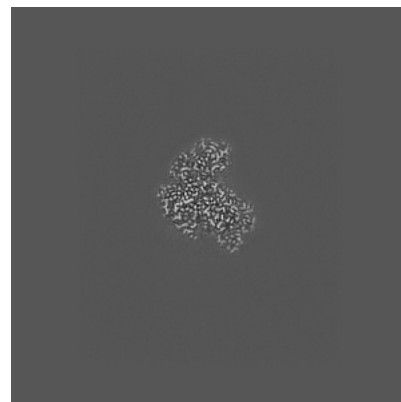
6.3.1 Primary map



X Index: 203

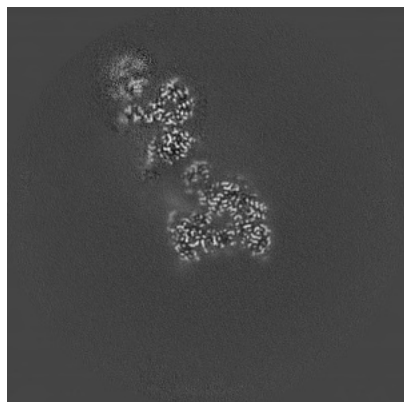


Y Index: 215

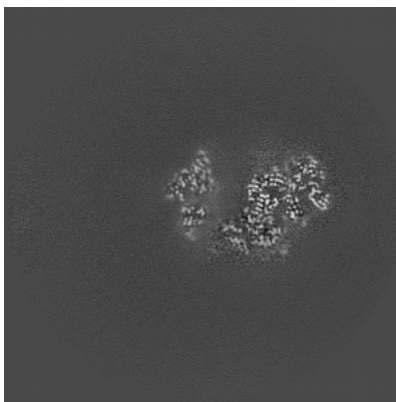


Z Index: 169

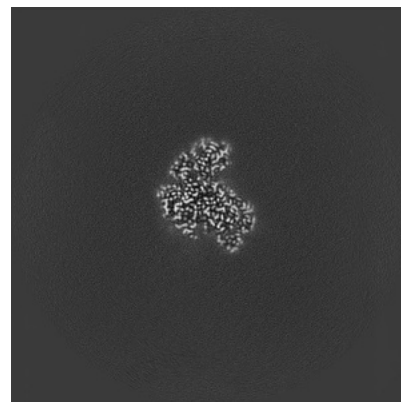
6.3.2 Raw map



X Index: 206



Y Index: 161

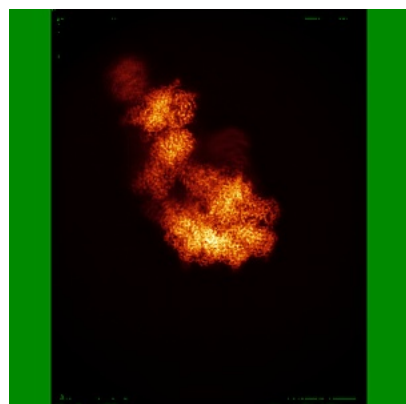


Z Index: 169

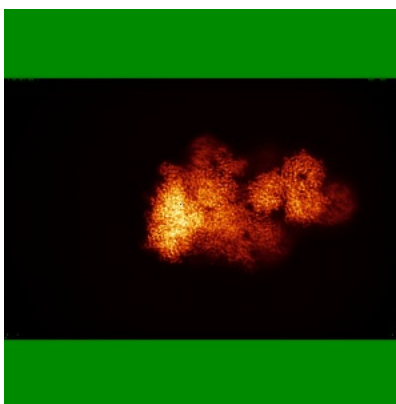
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

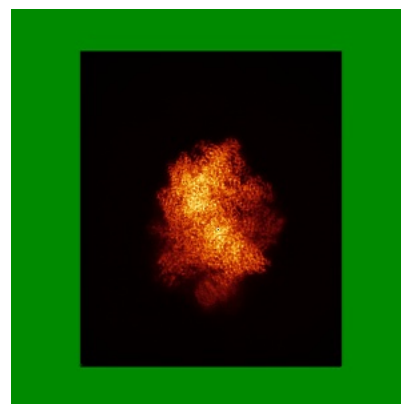
6.4.1 Primary map



X

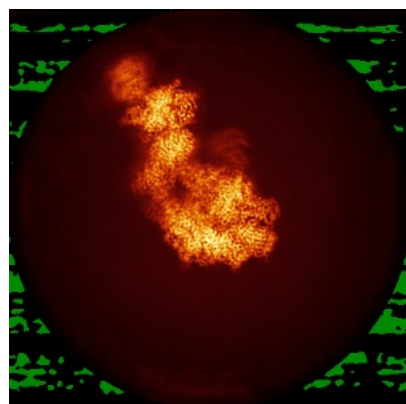


Y

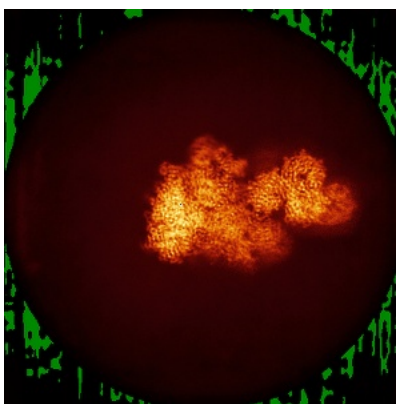


Z

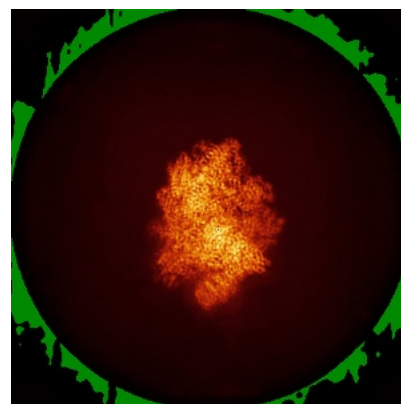
6.4.2 Raw map



X



Y

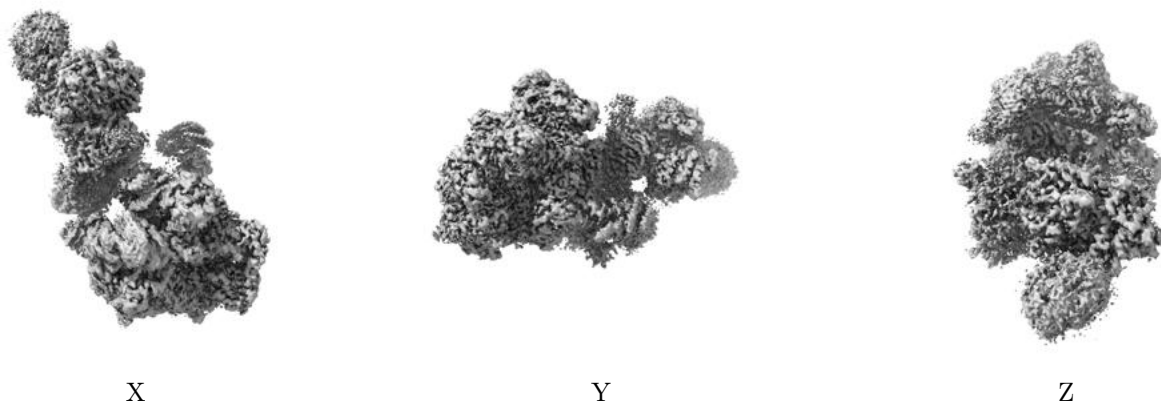


Z

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.

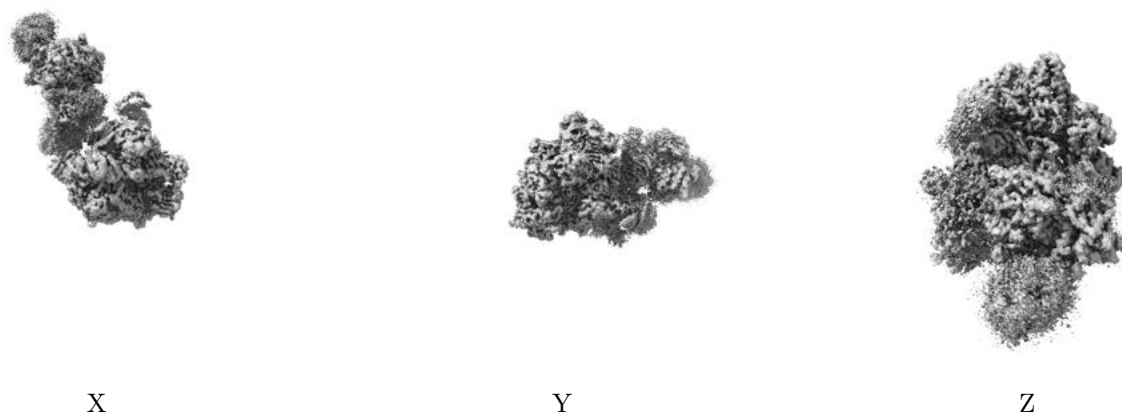
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

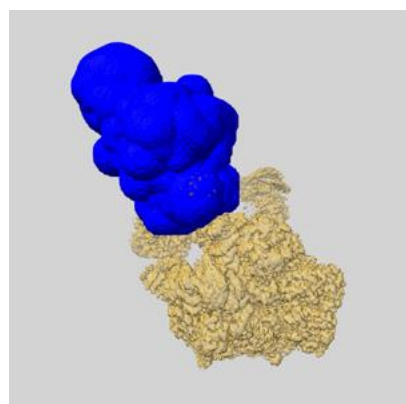
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

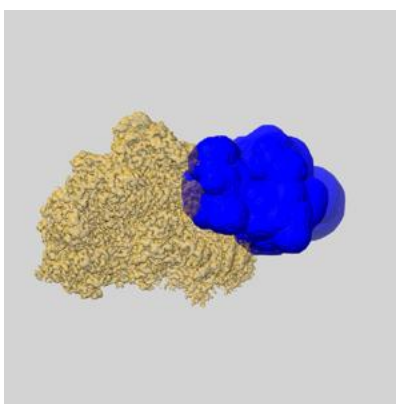
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

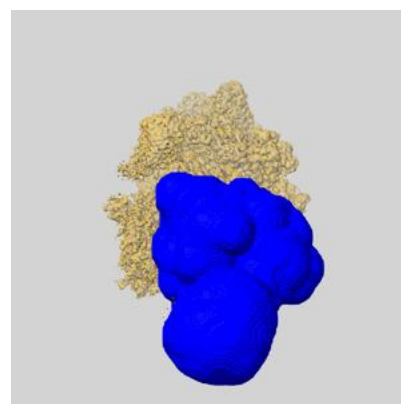
6.6.1 emd_13004_msk_1.map [i](#)



X

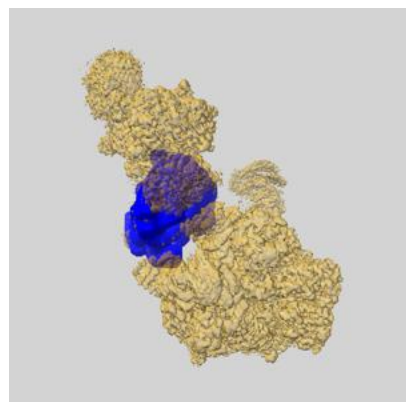


Y

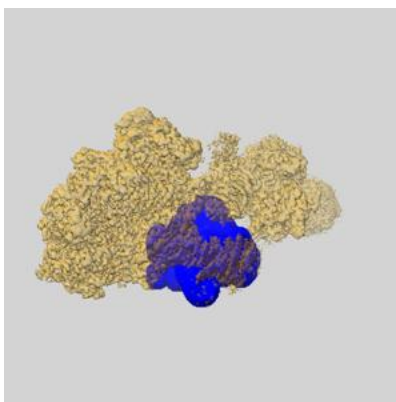


Z

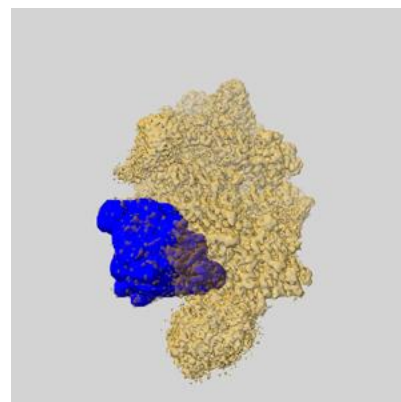
6.6.2 emd_13004_msk_5.map [i](#)



X

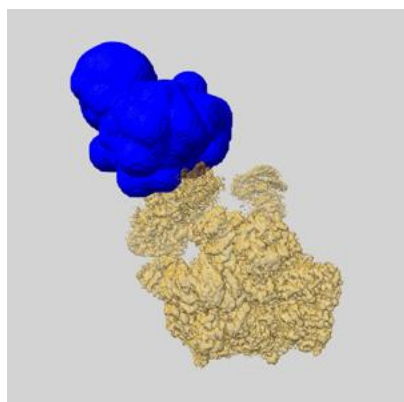


Y

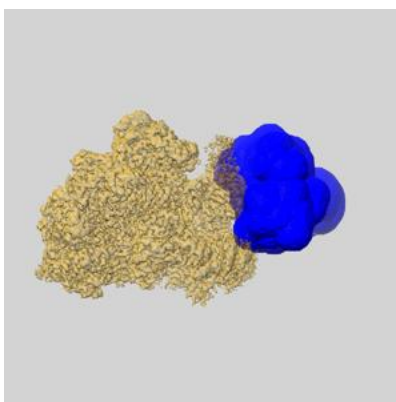


Z

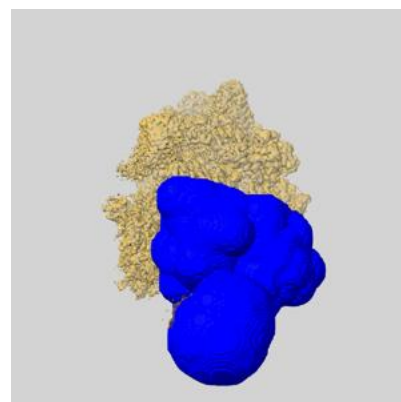
6.6.3 emd_13004_msk_3.map [i](#)



X

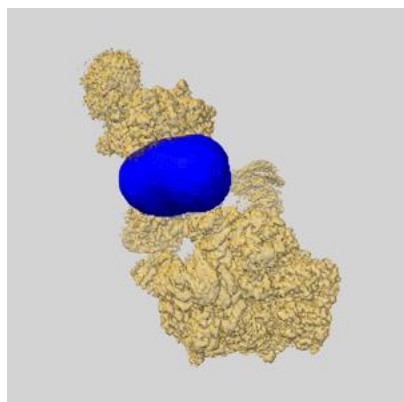


Y

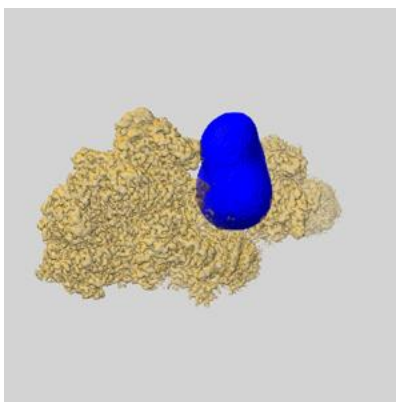


Z

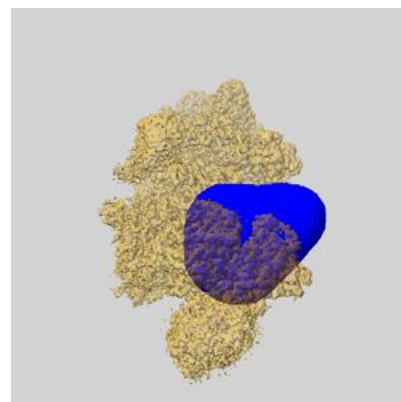
6.6.4 emd_13004_msk_2.map [i](#)



X

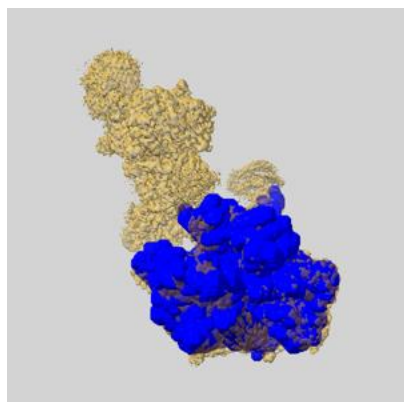


Y

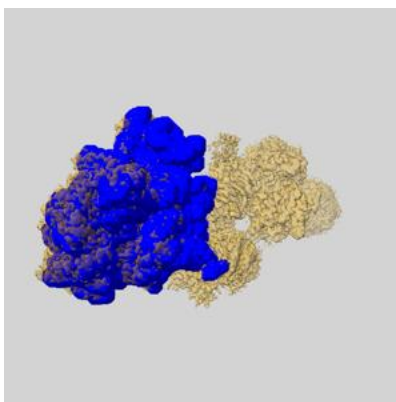


Z

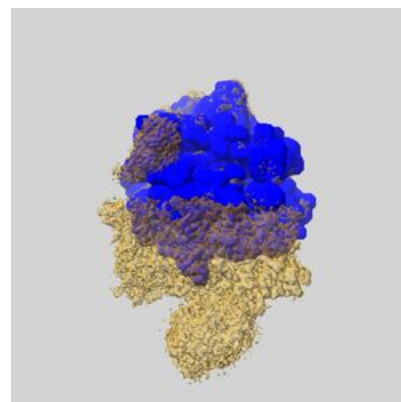
6.6.5 emd_13004_msk_4.map [i](#)



X



Y

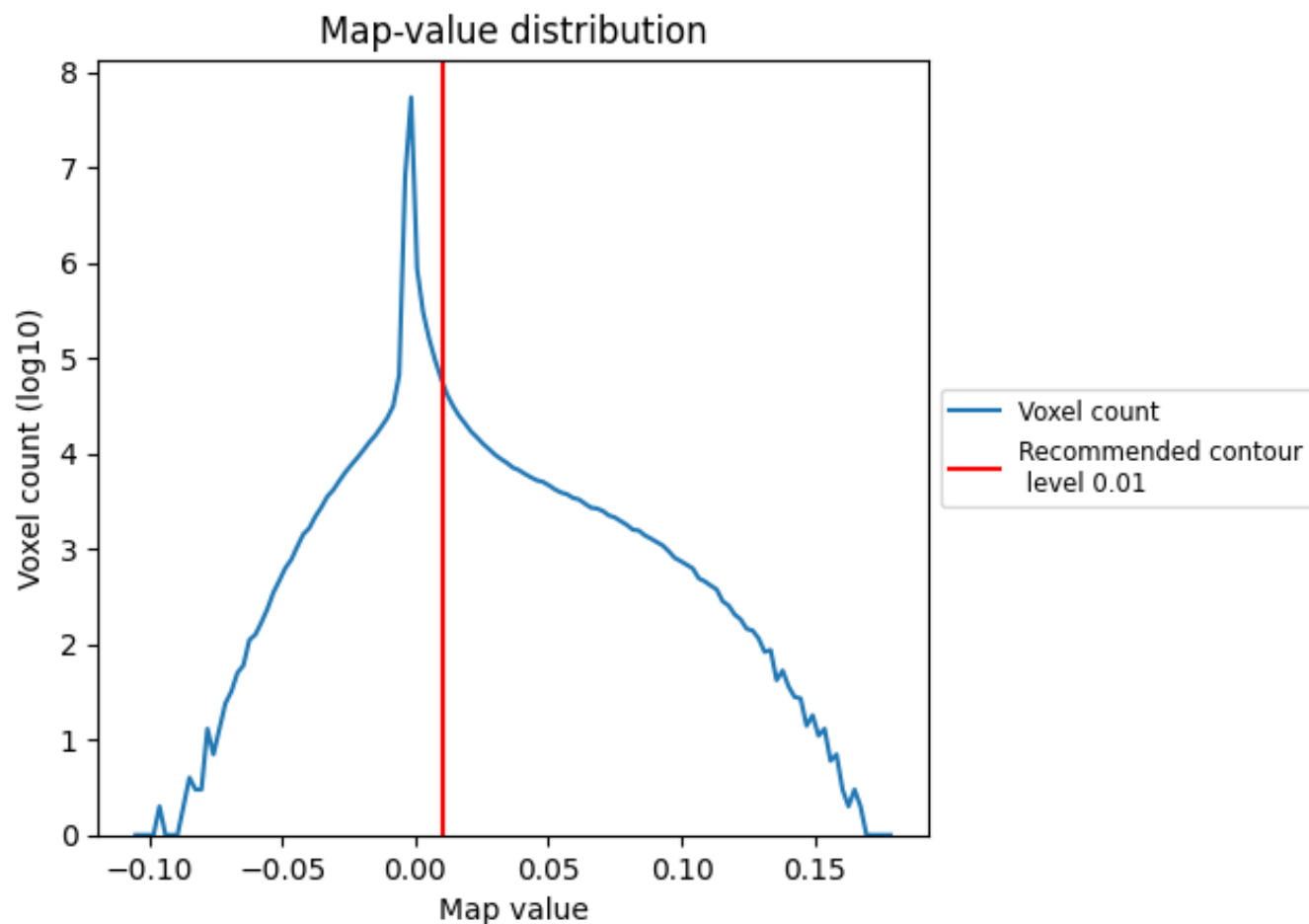


Z

7 Map analysis [i](#)

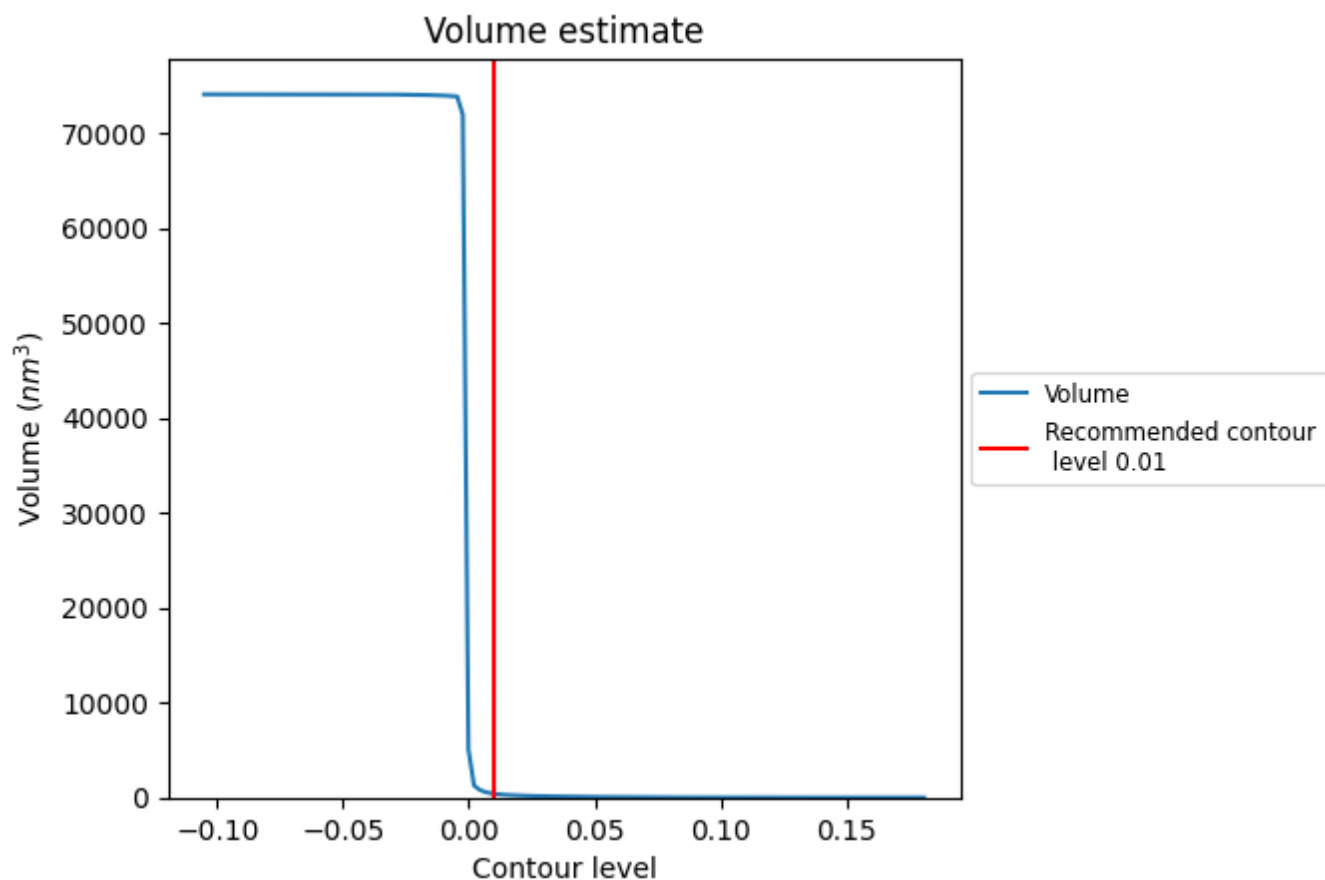
This section contains the results of statistical analysis of the map.

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.

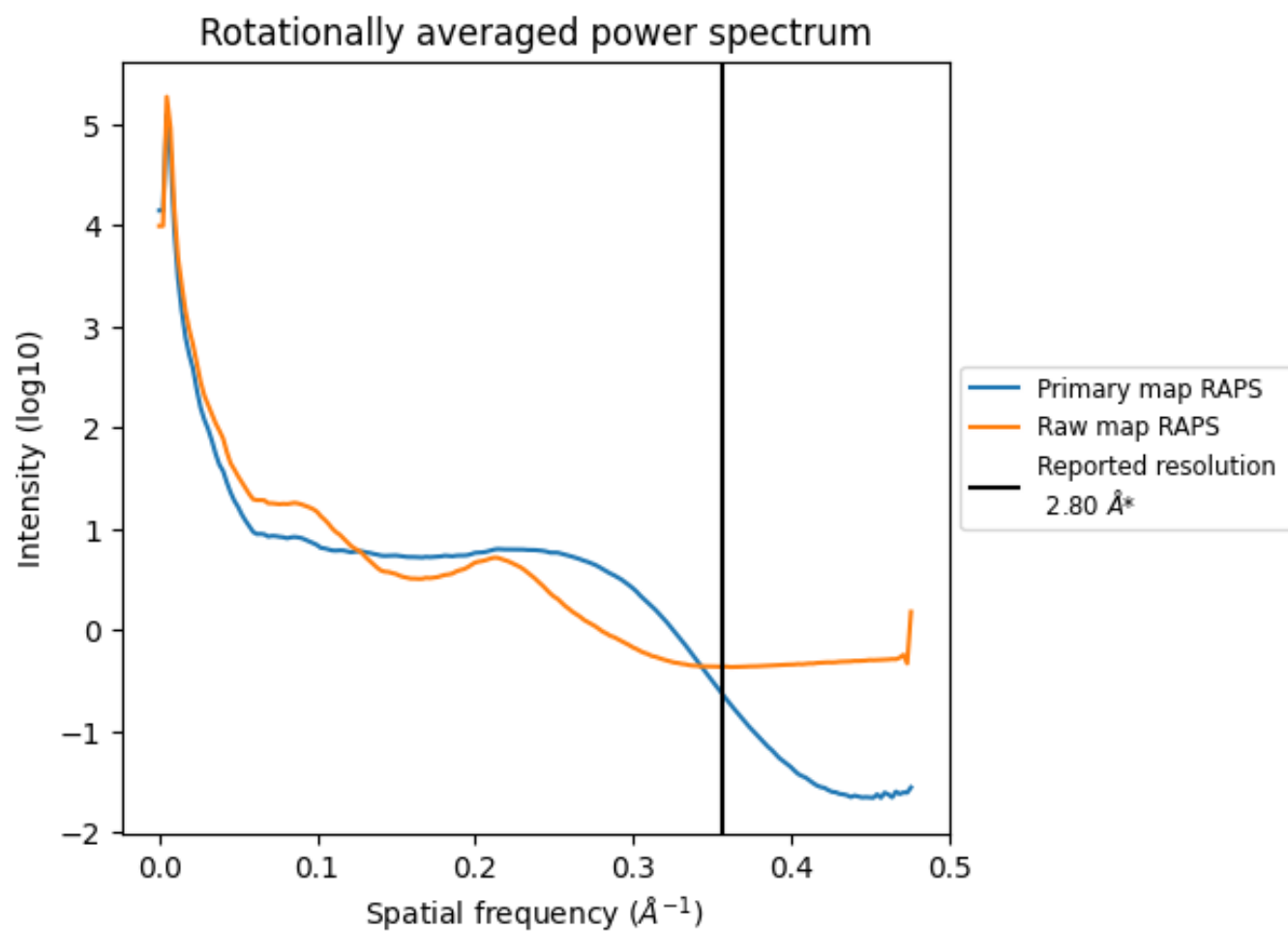
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 401 nm³; this corresponds to an approximate mass of 362 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 ⓘ

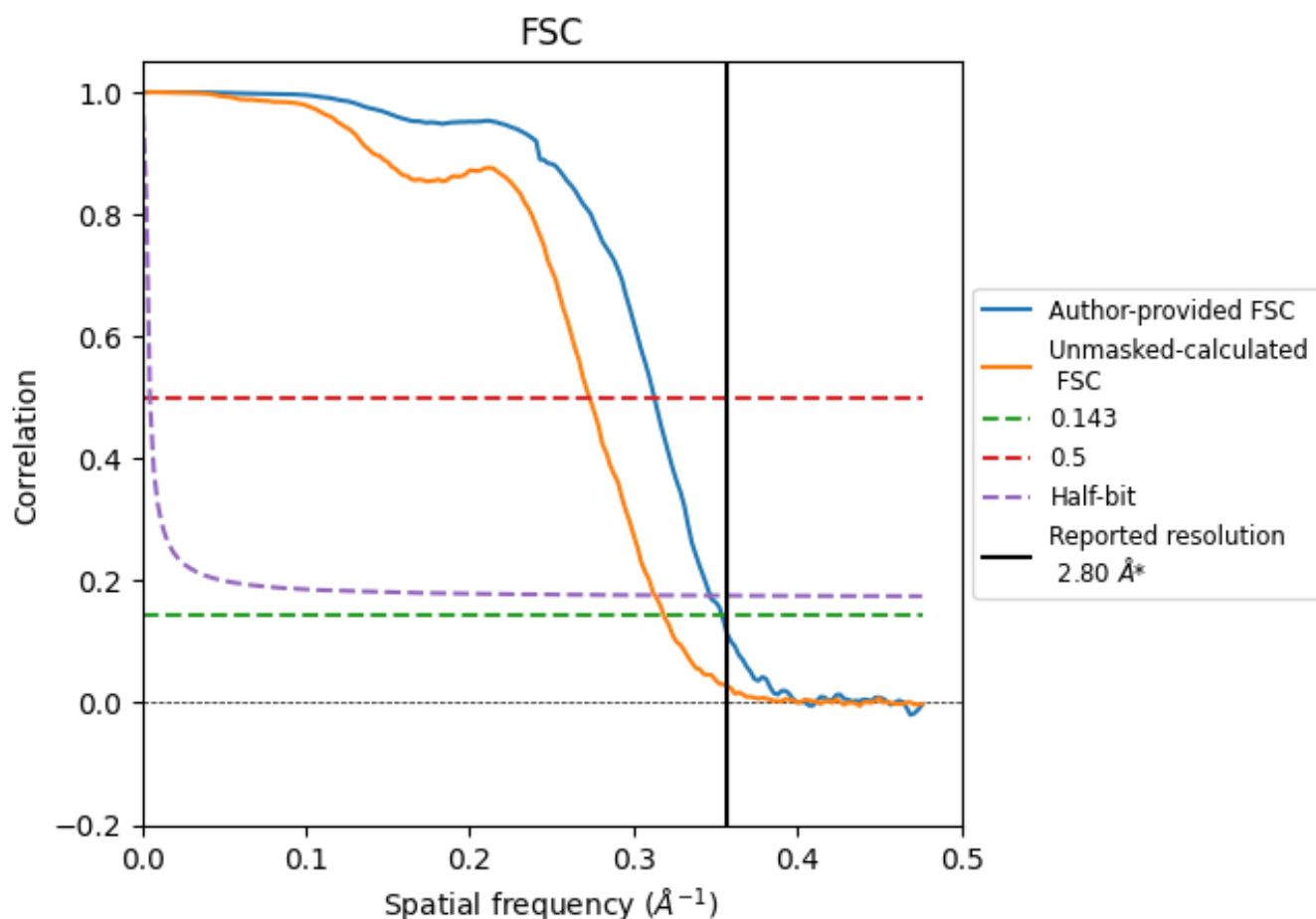


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 $0.357 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

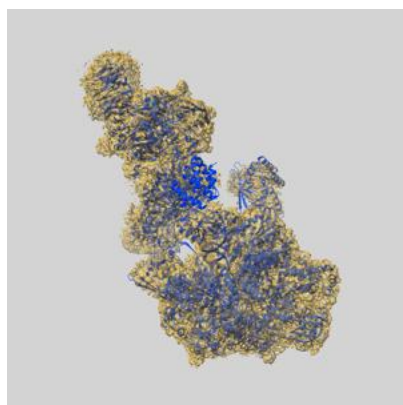
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.83	3.20	2.88
Unmasked-calculated*	3.14	3.66	3.19

*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 3.14 differs from the reported value 2.8 by more than 10 %

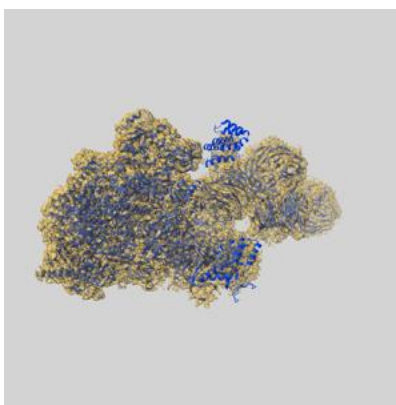
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13004 and PDB model 7OO3. Per-residue inclusion information can be found in section [3](#) on page [8](#).

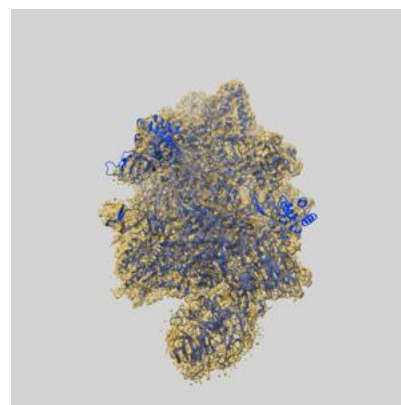
9.1 Map-model overlay [i](#)



X



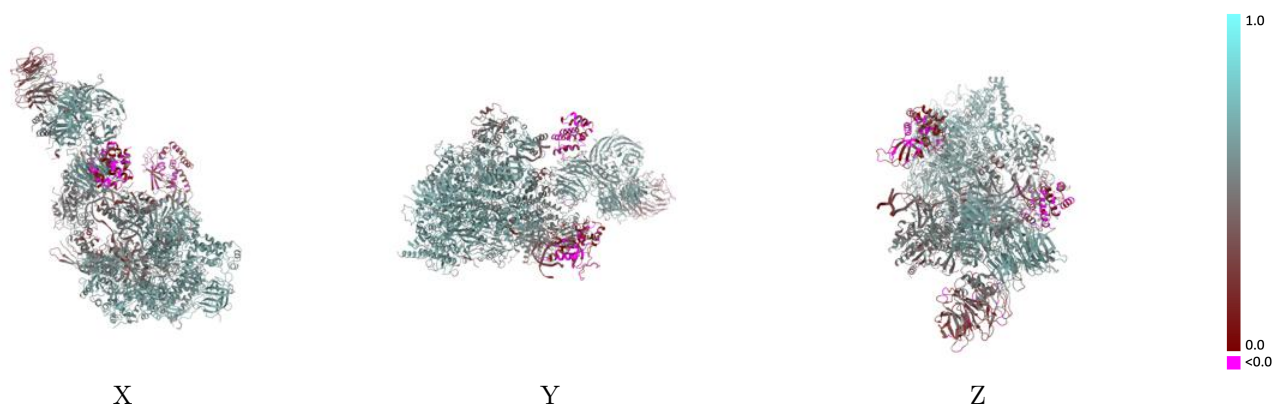
Y



Z

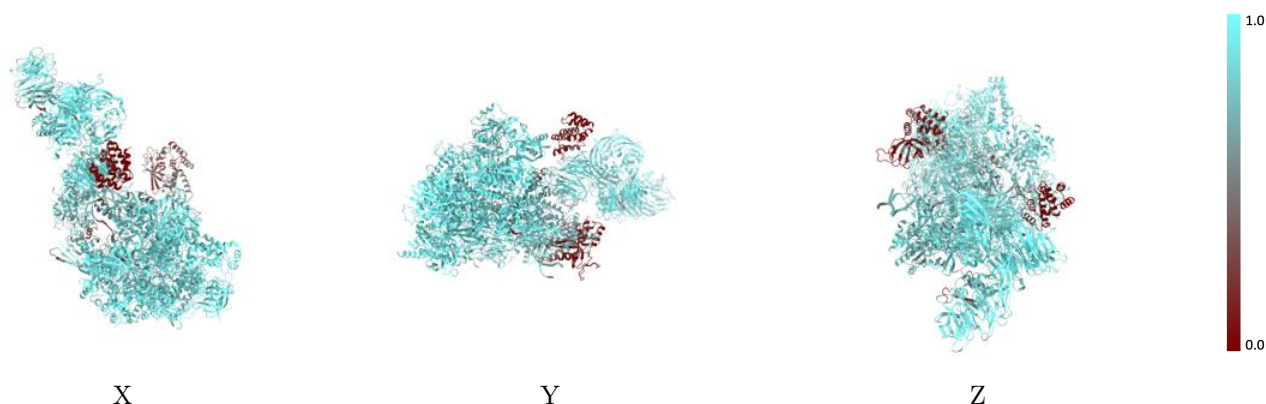
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



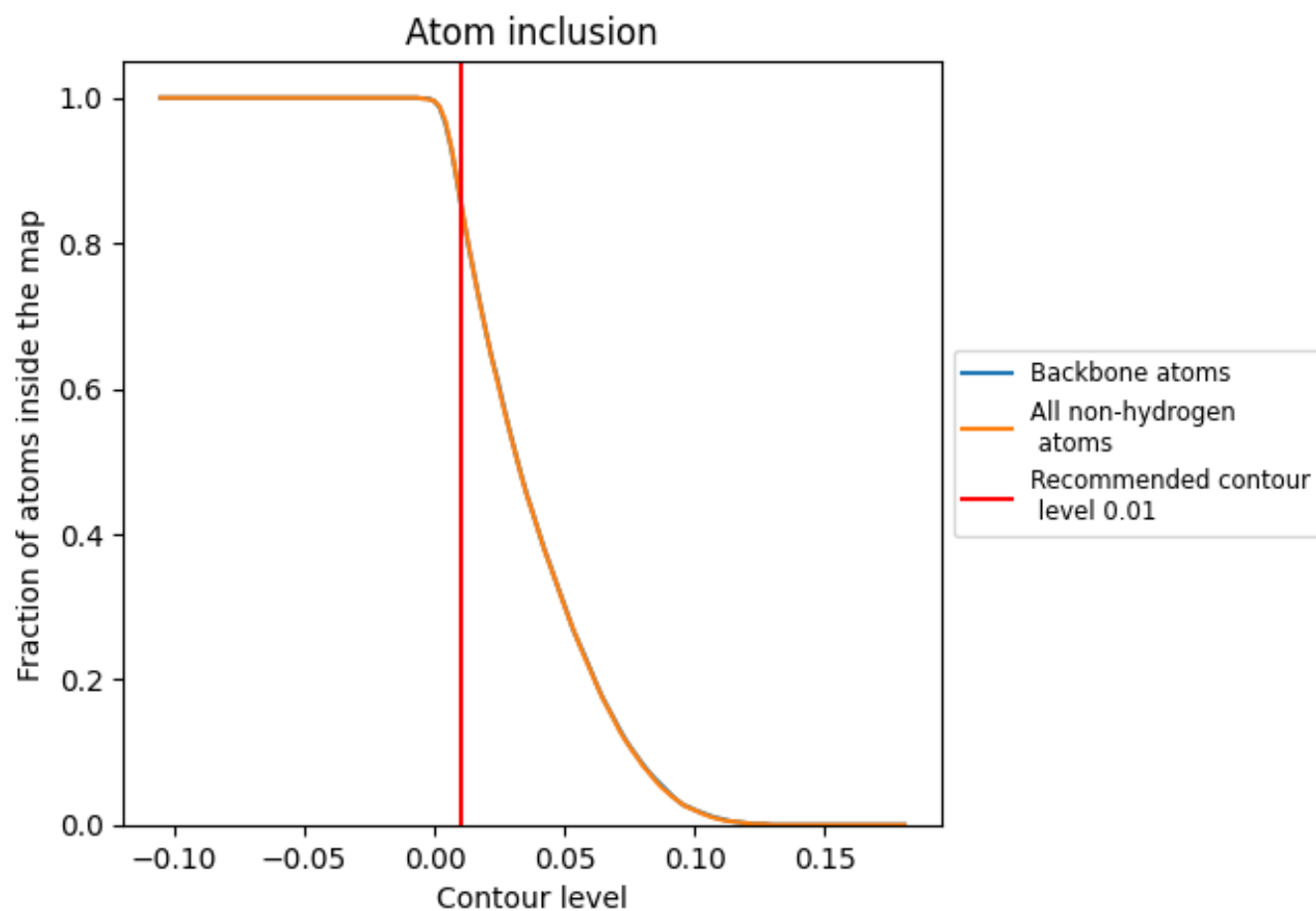
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8610	 0.5210
A	 0.9170	 0.5720
B	 0.9070	 0.5770
C	 0.9440	 0.6080
D	 0.2600	 0.1120
E	 0.9390	 0.5630
F	 0.9010	 0.5830
G	 0.3980	 0.2270
H	 0.9640	 0.6040
I	 0.8900	 0.5200
J	 0.9660	 0.6350
K	 0.9330	 0.6110
L	 0.8200	 0.5160
N	 0.8120	 0.4180
P	 0.9680	 0.6170
T	 0.8130	 0.4330
a	 0.9250	 0.5690
b	 0.8140	 0.4690
c	 0.0480	 0.0140
d	 0.8950	 0.4930
x	 0.8110	 0.4250

