



Full wwPDB EM Validation Report ⓘ

Apr 10, 2025 – 04:37 PM EDT

PDB ID : 9N9R / pdb_00009n9r
EMDB ID : EMD-48928
Title : Model of APC/C-CDC20-UBE2C from H2A/H2B-bound complex
Authors : Skrajna, A.; Bodrug, T.; Brown, N.G.; McGinty, R.K.
Deposited on : 2025-02-11
Resolution : 3.90 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.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

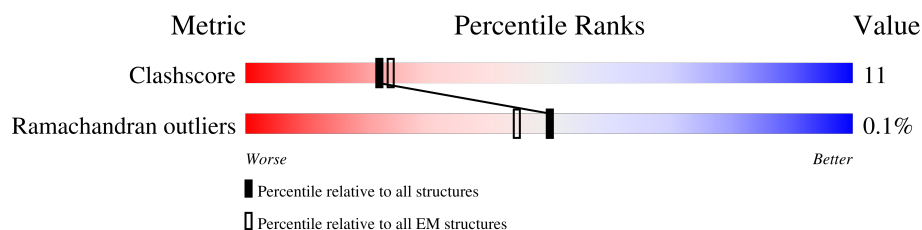
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


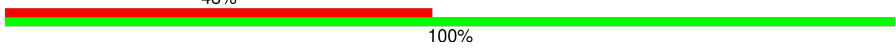
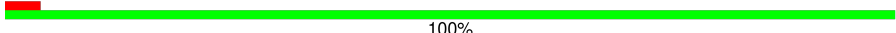

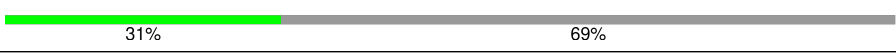




The reported resolution of this entry is 3.90 Å.

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




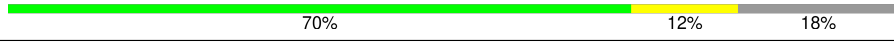
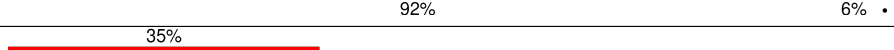
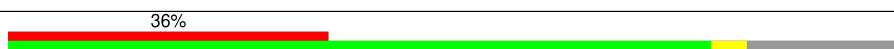

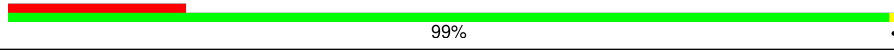

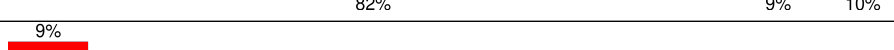




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835

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	1944	
2	C	84	
3	D	56	
4	G	85	
4	W	85	
5	H	58	
6	I	808	
7	J	824	
7	P	824	

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Mol	Chain	Length	Quality of chain
8	K	620	
8	S	620	
9	L	185	
10	M	74	
11	N	822	
12	O	755	
13	Q	145	
14	R	499	
15	U	597	
15	V	597	
16	Y	565	
16	Z	565	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 53107 atoms, of which 17125 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 Anaphase-promoting complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
1	A	1648	9883	3296	3291	1648	1648	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	GLU	SER	engineered mutation	UNP Q9H1A4
A	286	GLU	SER	engineered mutation	UNP Q9H1A4
A	291	GLU	THR	engineered mutation	UNP Q9H1A4
A	313	GLU	SER	engineered mutation	UNP Q9H1A4
A	316	GLU	THR	engineered mutation	UNP Q9H1A4
A	317	GLU	SER	engineered mutation	UNP Q9H1A4
A	334	GLU	SER	engineered mutation	UNP Q9H1A4
A	341	GLU	SER	engineered mutation	UNP Q9H1A4
A	343	GLU	SER	engineered mutation	UNP Q9H1A4
A	355	GLU	SER	engineered mutation	UNP Q9H1A4
A	362	GLU	SER	engineered mutation	UNP Q9H1A4
A	372	GLU	SER	engineered mutation	UNP Q9H1A4
A	377	GLU	SER	engineered mutation	UNP Q9H1A4
A	537	GLU	THR	engineered mutation	UNP Q9H1A4
A	547	GLU	SER	engineered mutation	UNP Q9H1A4
A	555	GLU	SER	engineered mutation	UNP Q9H1A4
A	569	GLU	SER	engineered mutation	UNP Q9H1A4
A	688	GLU	SER	engineered mutation	UNP Q9H1A4
A	699	GLU	SER	engineered mutation	UNP Q9H1A4
A	916	GLU	SER	engineered mutation	UNP Q9H1A4
A	1347	GLU	SER	engineered mutation	UNP Q9H1A4

- Molecule 2 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
2	C	84	508	168	171	84	85	0	0

- Molecule 3 is a protein called Anaphase-promoting complex subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	56	Total	C	H	N	O	0	0
			335	112	110	56	57		

- Molecule 4 is a protein called Anaphase-promoting complex subunit CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	27	Total	C	H	N	O	0	0
			163	54	55	27	27		
4	W	26	Total	C	H	N	O	0	0
			157	52	53	26	26		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	51	GLU	SER	engineered mutation	UNP Q8NHZ8
G	52	GLU	SER	engineered mutation	UNP Q8NHZ8
G	82	GLU	SER	engineered mutation	UNP Q8NHZ8
W	51	GLU	SER	engineered mutation	UNP Q8NHZ8
W	52	GLU	SER	engineered mutation	UNP Q8NHZ8
W	82	GLU	SER	engineered mutation	UNP Q8NHZ8

- Molecule 5 is a protein called Anaphase-promoting complex subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	58	Total	C	H	N	O	0	0
			348	116	116	58	58		

- Molecule 6 is a protein called Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	742	Total	C	H	N	O	0	0
			4458	1484	1490	742	742		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	777	GLU	SER	engineered mutation	UNP Q9UJX5
I	779	GLU	SER	engineered mutation	UNP Q9UJX5

- Molecule 7 is a protein called Cell division cycle protein 27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	510	Total	C	H	N	O	0	0
			3067	1020	1027	510	510		
7	P	496	Total	C	H	N	O	0	0
			2982	992	998	496	496		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	200	GLU	THR	engineered mutation	UNP P30260
J	205	GLU	THR	engineered mutation	UNP P30260
J	220	GLU	SER	engineered mutation	UNP P30260
J	241	GLU	SER	engineered mutation	UNP P30260
J	276	GLU	SER	engineered mutation	UNP P30260
J	320	GLU	SER	engineered mutation	UNP P30260
J	336	GLU	SER	engineered mutation	UNP P30260
J	339	GLU	SER	engineered mutation	UNP P30260
J	386	GLU	SER	engineered mutation	UNP P30260
J	387	GLU	SER	engineered mutation	UNP P30260
J	393	GLU	SER	engineered mutation	UNP P30260
J	426	GLU	SER	engineered mutation	UNP P30260
J	435	GLU	SER	engineered mutation	UNP P30260
J	446	GLU	THR	engineered mutation	UNP P30260
P	200	GLU	THR	engineered mutation	UNP P30260
P	205	GLU	THR	engineered mutation	UNP P30260
P	220	GLU	SER	engineered mutation	UNP P30260
P	241	GLU	SER	engineered mutation	UNP P30260
P	276	GLU	SER	engineered mutation	UNP P30260
P	320	GLU	SER	engineered mutation	UNP P30260
P	336	GLU	SER	engineered mutation	UNP P30260
P	339	GLU	SER	engineered mutation	UNP P30260
P	386	GLU	SER	engineered mutation	UNP P30260
P	387	GLU	SER	engineered mutation	UNP P30260
P	393	GLU	SER	engineered mutation	UNP P30260
P	426	GLU	SER	engineered mutation	UNP P30260
P	435	GLU	SER	engineered mutation	UNP P30260
P	446	GLU	THR	engineered mutation	UNP P30260

- Molecule 8 is a protein called Cell division cycle protein 16 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	531	Total	C	H	N	O	0	0
			3190	1062	1066	531	531		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	506	Total	C	H	N	O	0	0
			3043	1012	1019	506	506		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	112	GLU	SER	engineered mutation	UNP Q13042
K	560	GLU	SER	engineered mutation	UNP Q13042
K	581	GLU	THR	engineered mutation	UNP Q13042
K	585	GLU	THR	engineered mutation	UNP Q13042
K	586	GLU	SER	engineered mutation	UNP Q13042
S	112	GLU	SER	engineered mutation	UNP Q13042
S	560	GLU	SER	engineered mutation	UNP Q13042
S	581	GLU	THR	engineered mutation	UNP Q13042
S	585	GLU	THR	engineered mutation	UNP Q13042
S	586	GLU	SER	engineered mutation	UNP Q13042

- Molecule 9 is a protein called Anaphase-promoting complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	183	Total	C	H	N	O	0	0
			1097	366	364	183	184		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	3	GLU	THR	engineered mutation	UNP Q9UM13

- Molecule 10 is a protein called Anaphase-promoting complex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	68	Total	C	H	N	O	0	0
			409	136	137	68	68		

- Molecule 11 is a protein called Anaphase-promoting complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	682	Total	C	H	N	O	0	0
			4091	1364	1363	682	682		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	218	GLU	SER	engineered mutation	UNP Q9UJX6
N	314	GLU	SER	engineered mutation	UNP Q9UJX6
N	470	GLU	SER	engineered mutation	UNP Q9UJX6
N	534	GLU	SER	engineered mutation	UNP Q9UJX6
N	811	GLU	SER	engineered mutation	UNP Q9UJX6

- Molecule 12 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	707	Total	C	H	N	O	0	0
			4254	1414	1425	707	708		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	178	GLU	THR	engineered mutation	UNP Q9UJX4
O	179	GLU	SER	engineered mutation	UNP Q9UJX4
O	195	GLU	SER	engineered mutation	UNP Q9UJX4
O	202	GLU	SER	engineered mutation	UNP Q9UJX4
O	221	GLU	SER	engineered mutation	UNP Q9UJX4
O	232	GLU	THR	engineered mutation	UNP Q9UJX4
O	364	GLU	SER	engineered mutation	UNP Q9UJX4

- Molecule 13 is a protein called Ubiquitin-conjugating enzyme E2 C.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	145	Total	C	H	N	O	0	0
			870	290	290	145	145		

- Molecule 14 is a protein called Cell division cycle protein 20 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	R	375	Total	C	N	O	0	0
			1846	1095	375	376		

- Molecule 15 is a protein called Cell division cycle protein 23 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	540	Total	C	H	N	O	0	0
			3244	1080	1084	540	540		
15	V	534	Total	C	H	N	O	0	0
			3211	1068	1075	534	534		

There are 10 discrepancies between the modelled and reference sequences:

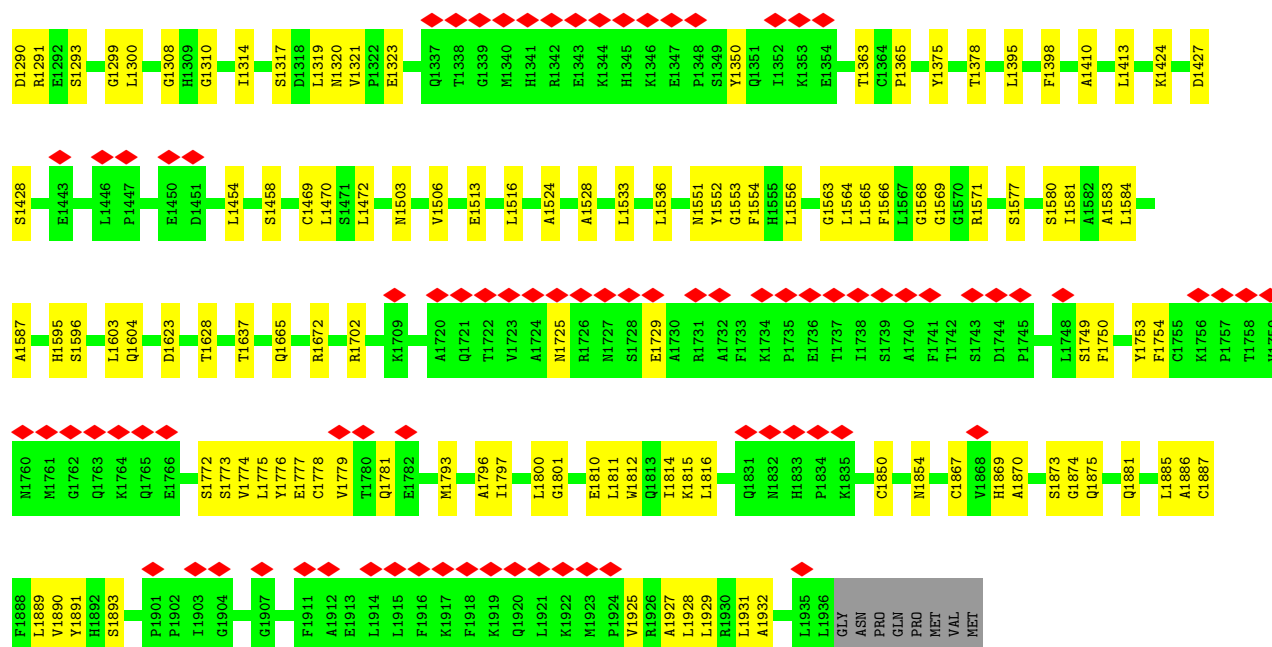
Chain	Residue	Modelled	Actual	Comment	Reference
U	542	GLU	THR	engineered mutation	UNP Q9UJX2
U	562	GLU	THR	engineered mutation	UNP Q9UJX2
U	582	GLU	THR	engineered mutation	UNP Q9UJX2
U	588	GLU	SER	engineered mutation	UNP Q9UJX2
U	596	GLU	THR	engineered mutation	UNP Q9UJX2
V	542	GLU	THR	engineered mutation	UNP Q9UJX2
V	562	GLU	THR	engineered mutation	UNP Q9UJX2
V	582	GLU	THR	engineered mutation	UNP Q9UJX2
V	588	GLU	SER	engineered mutation	UNP Q9UJX2
V	596	GLU	THR	engineered mutation	UNP Q9UJX2

- Molecule 16 is a protein called Anaphase-promoting complex subunit 7.

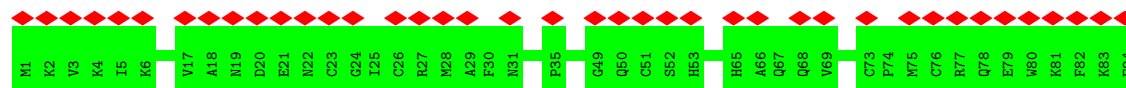
Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	501	Total	C	H	N	O	0	0
			3012	1002	1008	501	501		
16	Z	488	Total	C	H	N	O	0	0
			2935	976	983	488	488		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

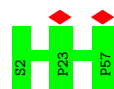
Mol	Chain	Residues	Atoms		AltConf
17	C	3	Total	Zn	0
			3	3	
17	N	1	Total	Zn	0
			1	1	



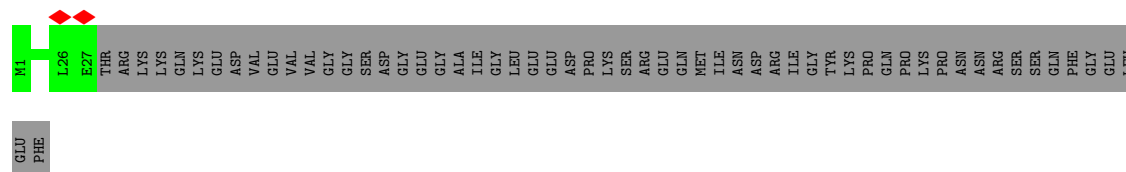
• Molecule 2: Anaphase-promoting complex subunit 11



• Molecule 3: Anaphase-promoting complex subunit 15

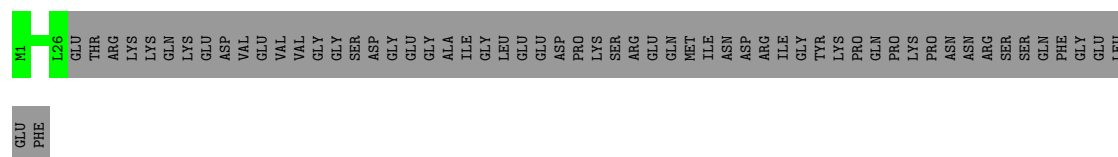


• Molecule 4: Anaphase-promoting complex subunit CDC26



• Molecule 4: Anaphase-promoting complex subunit CDC26





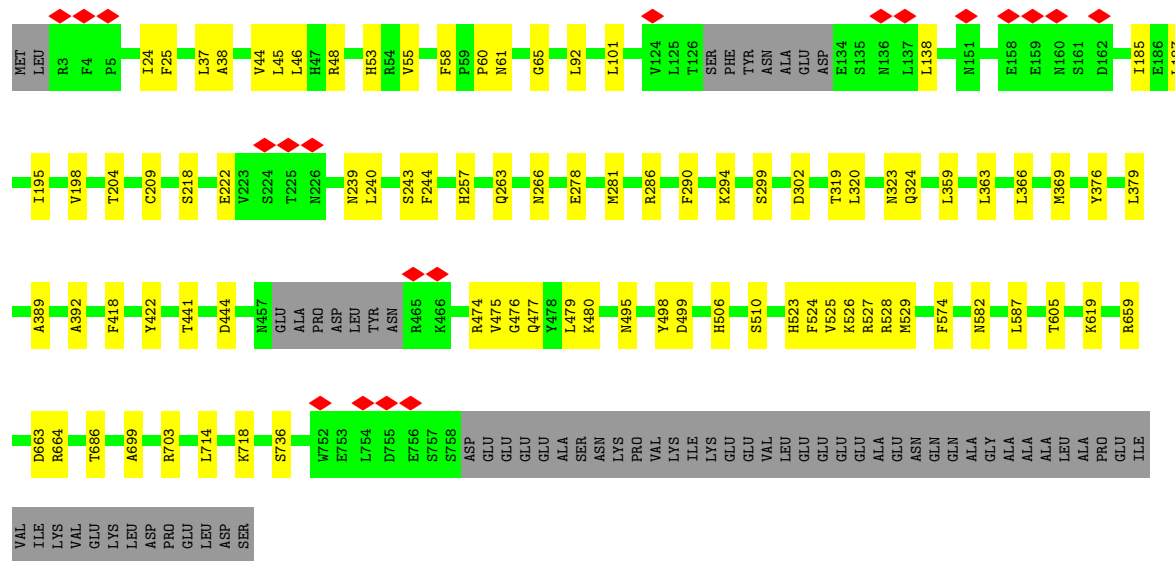
• Molecule 5: Anaphase-promoting complex subunit 16

Chain H: 100%

There are no outlier residues recorded for this chain.

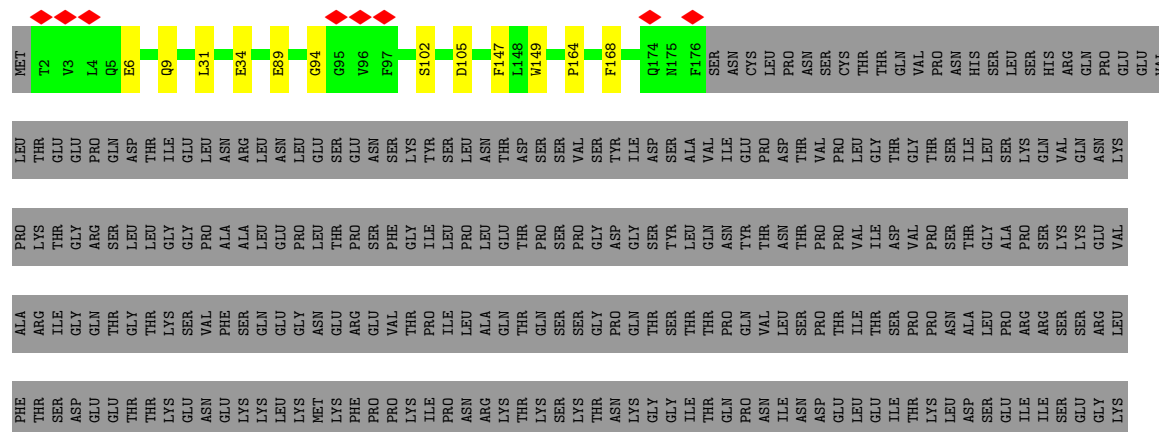
• Molecule 6: Anaphase-promoting complex subunit 4

Chain I: 81% 11% 8%

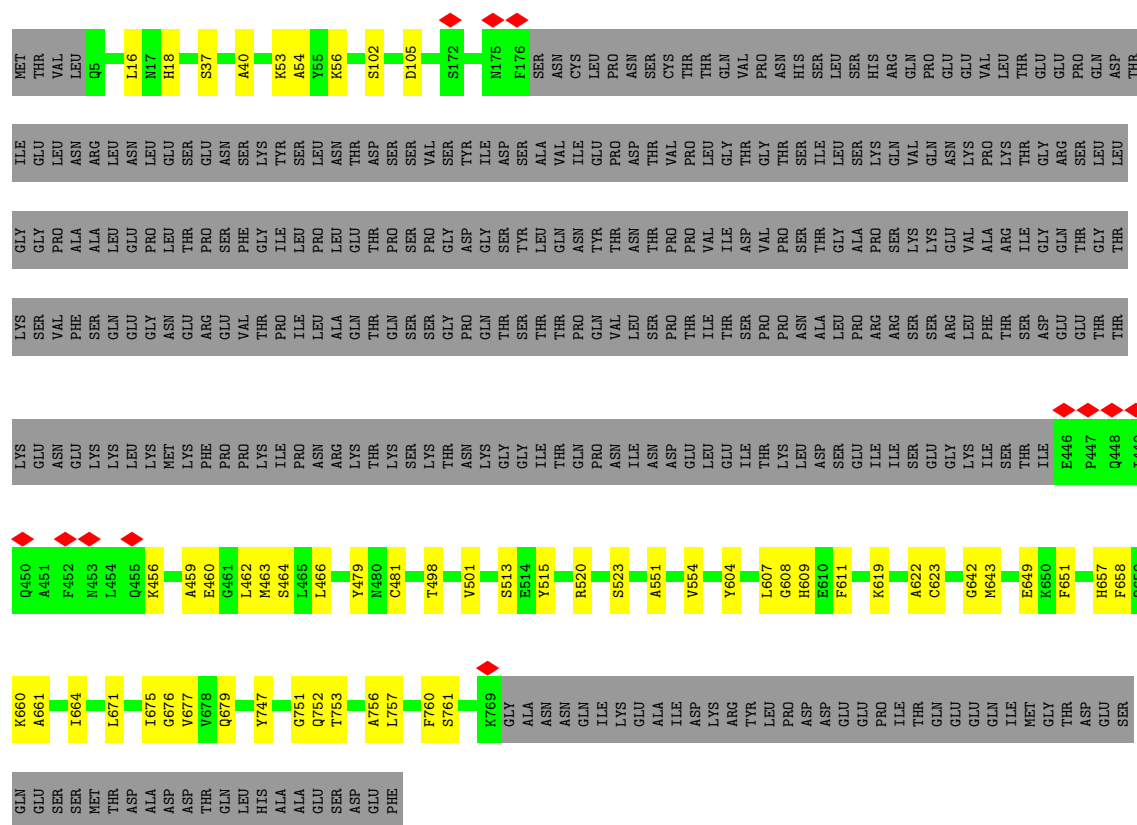


• Molecule 7: Cell division cycle protein 27 homolog

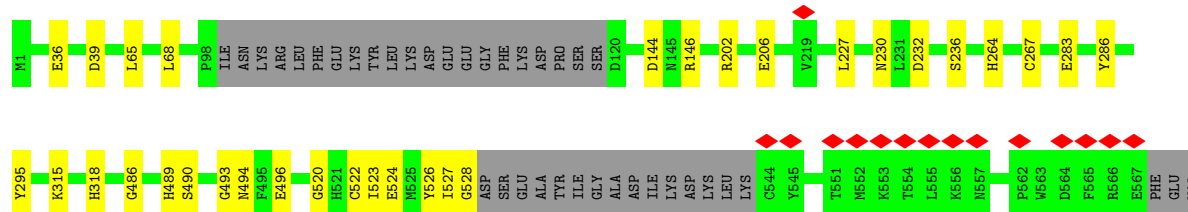
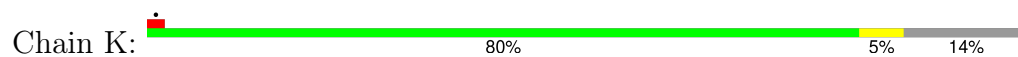
Chain J: 56% 5% 38%



- Molecule 7: Cell division cycle protein 27 homolog



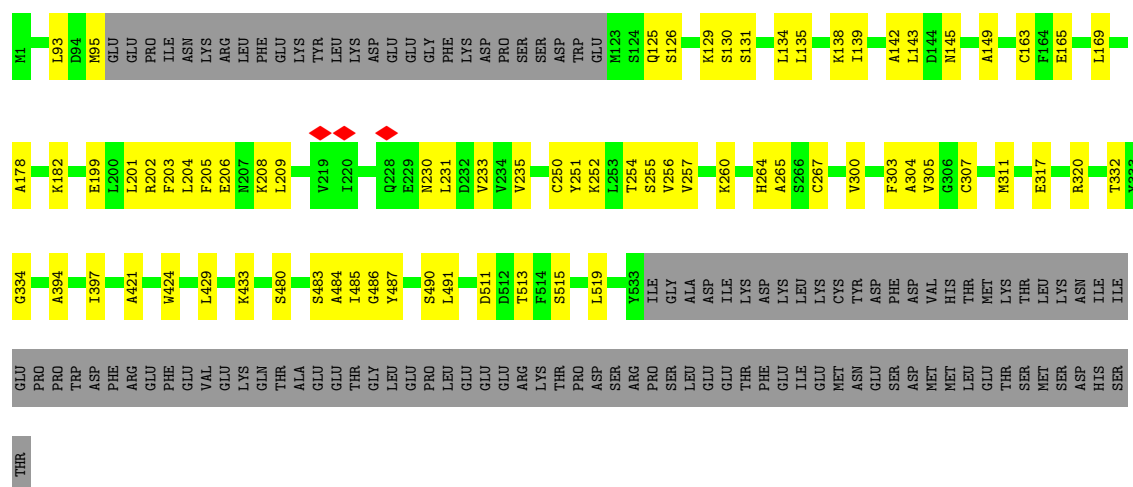
- Molecule 8: Cell division cycle protein 16 homolog



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

• Molecule 8: Cell division cycle protein 16 homolog

Chain S:  70% 12% 18%




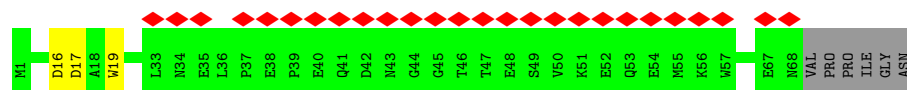
• Molecule 9: Anaphase-promoting complex subunit 10

Chain L:  92% 6%




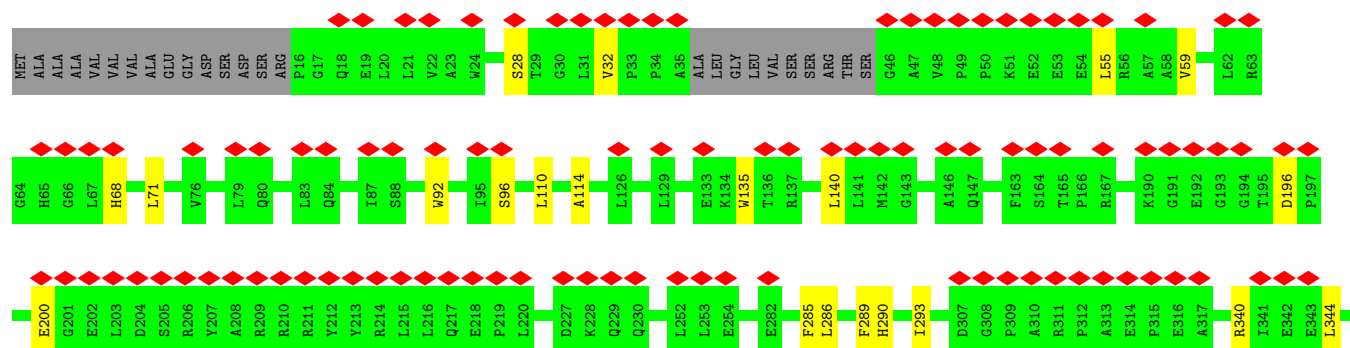
• Molecule 10: Anaphase-promoting complex subunit 13

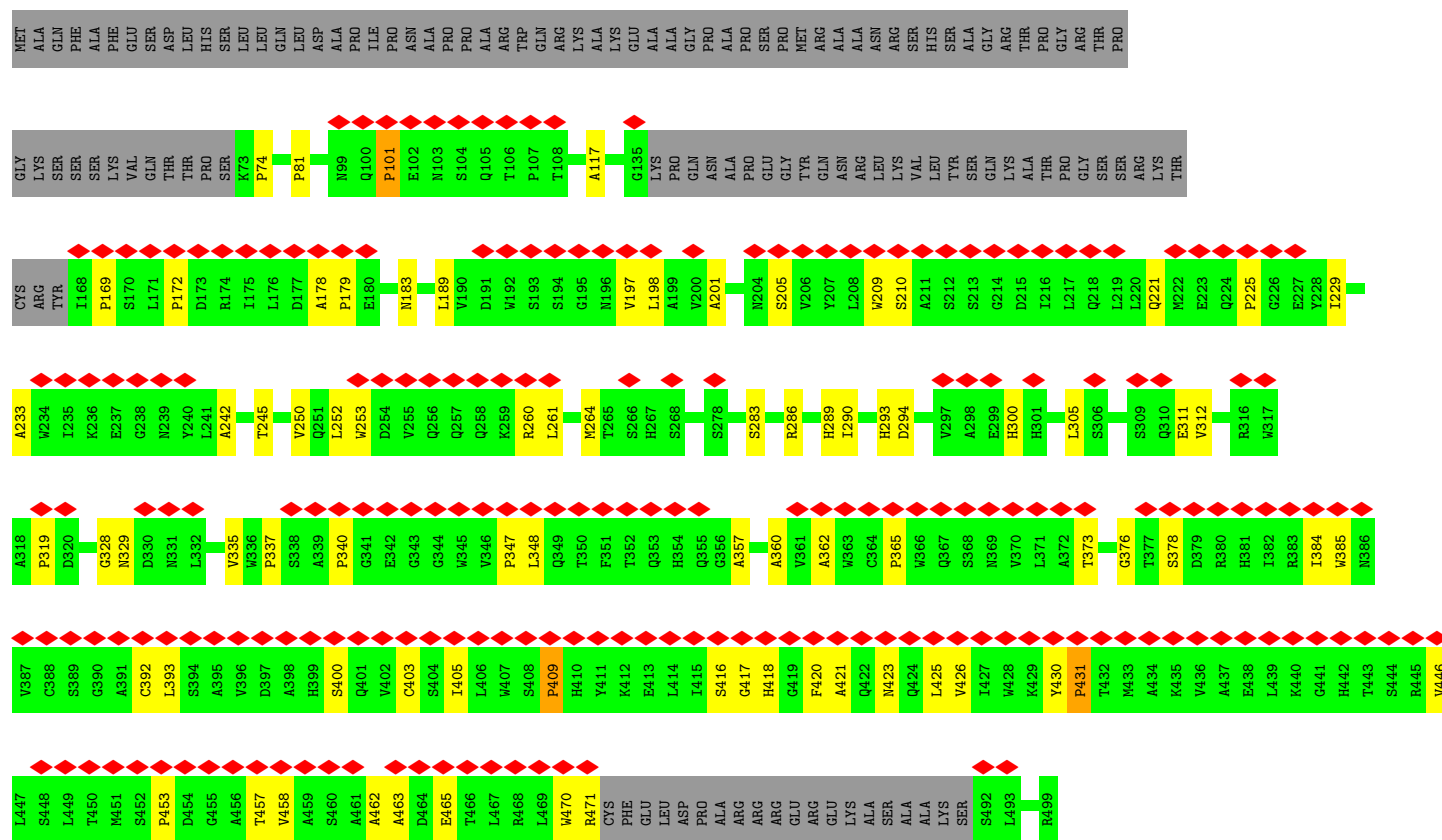
Chain M:  35% 88% 8%



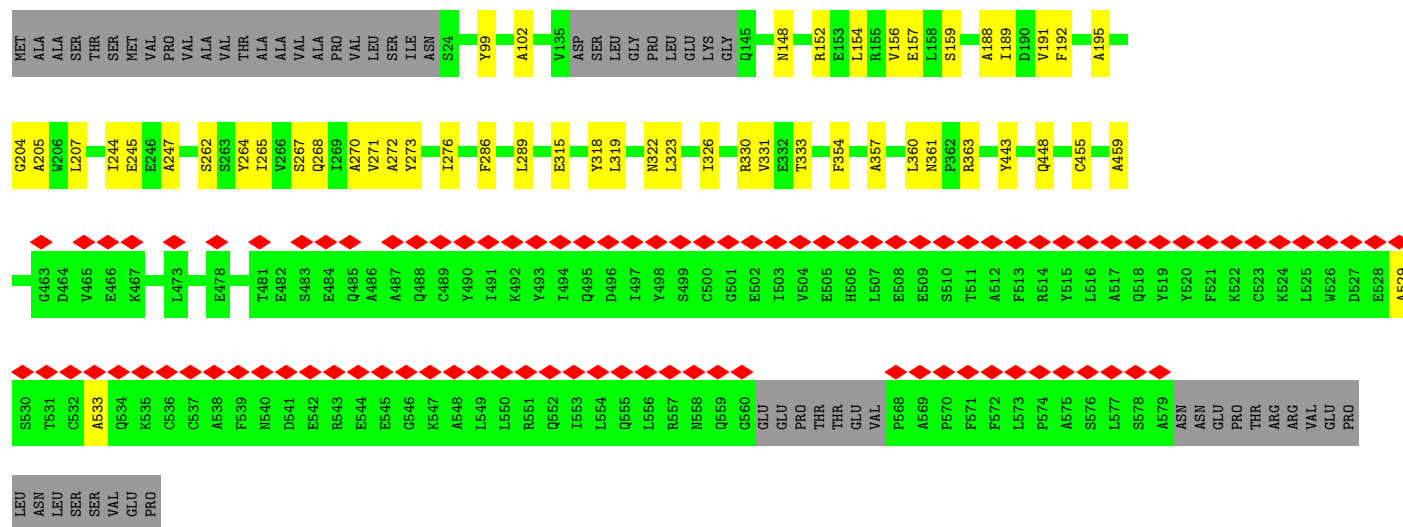
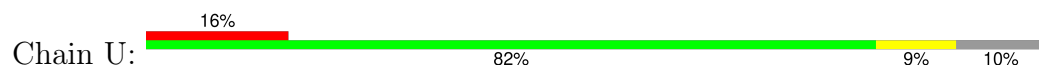
• Molecule 11: Anaphase-promoting complex subunit 2

Chain N:  36% 79% 17%

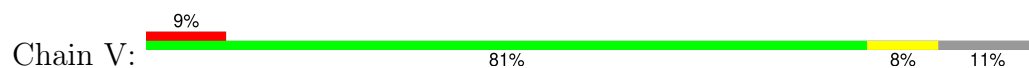


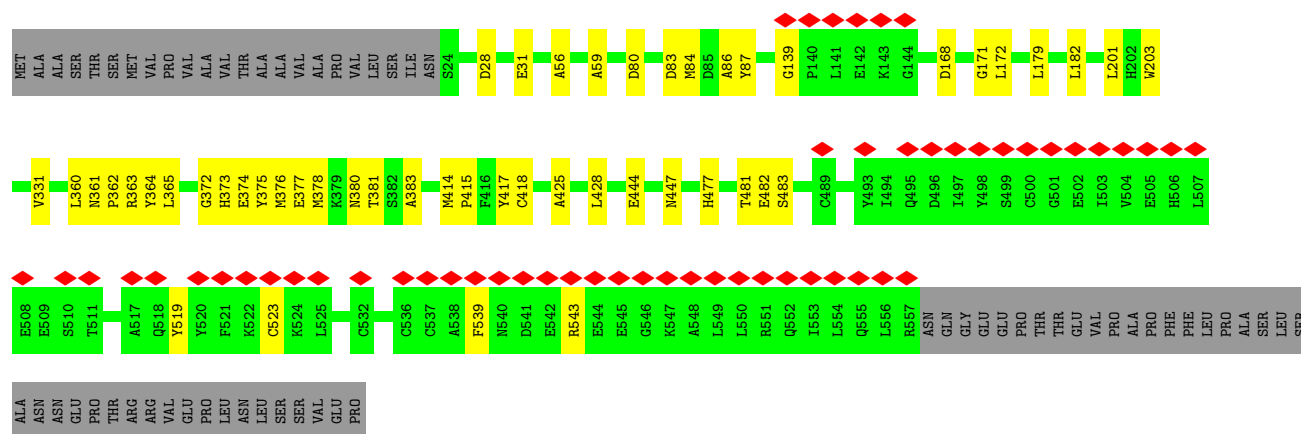


• Molecule 15: Cell division cycle protein 23 homolog

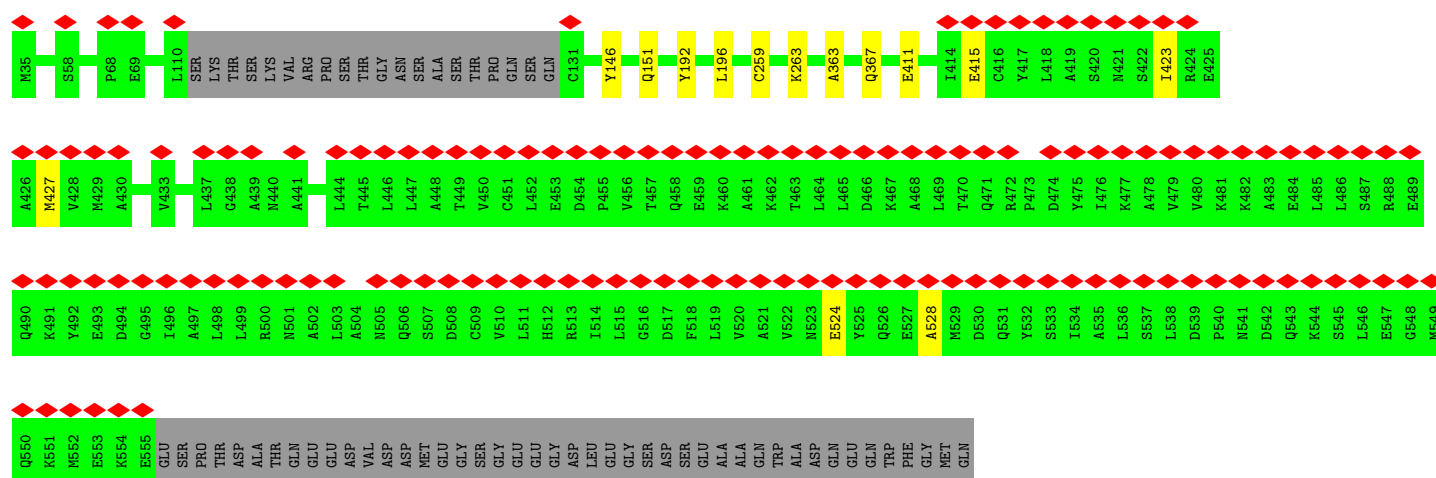
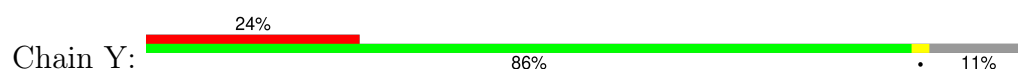


• Molecule 15: Cell division cycle protein 23 homolog

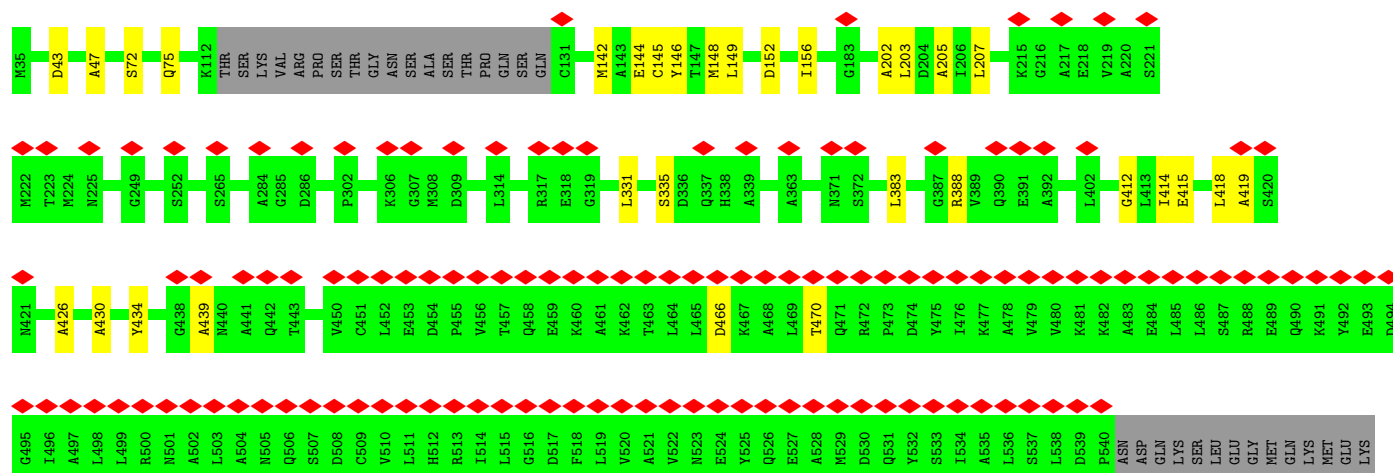
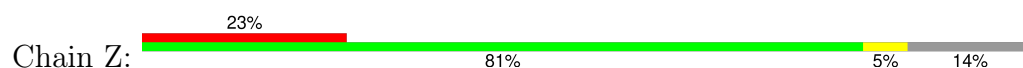




• Molecule 16: Anaphase-promoting complex subunit 7



• Molecule 16: Anaphase-promoting complex subunit 7



GLU
GLU
SER
PRO
THR
ASP
ALA
THR
GLN
GLU
GLU
ASP
VAL
ASP
ASP
MET
GLU
GLY
SER
GLY
GLU
GLY
GLY
ASP
LEU
GLU
GLY
SER
SER
SER
GLU
ALA
ALA
GLN
TRP
ALA
ASP
GLN
GLU
GLN
TRP
PHE
GLY
MET
GLN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	183499	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.020	Depositor
Minimum map value	-0.009	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0026	Depositor
Map size (Å)	436.80002, 436.80002, 436.80002	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.91, 0.91, 0.91	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.27	0/6582	0.49	0/8210
2	C	0.26	0/336	0.50	0/417
3	D	0.26	0/224	0.45	0/277
4	G	0.28	0/107	0.39	0/132
4	W	0.27	0/103	0.44	0/127
5	H	0.23	0/231	0.42	0/287
6	I	0.25	0/2965	0.50	0/3701
7	J	0.26	0/2038	0.44	0/2544
7	P	0.26	0/1982	0.45	0/2474
8	K	0.26	0/2121	0.44	0/2646
8	S	0.27	0/2022	0.45	0/2524
9	L	0.24	0/732	0.51	0/912
10	M	0.26	0/271	0.51	0/337
11	N	0.24	0/2724	0.44	0/3398
12	O	0.27	0/2825	0.45	0/3523
13	Q	0.23	0/579	0.47	0/722
14	R	0.31	0/1842	0.76	16/2553 (0.6%)
15	U	0.25	0/2157	0.45	0/2691
15	V	0.29	0/2135	0.47	0/2667
16	Y	0.23	0/2002	0.42	0/2499
16	Z	0.23	0/1950	0.41	0/2434
All	All	0.26	0/35928	0.48	16/45075 (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
15	V	0	1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	R	74	PRO	N-CA-CB	6.32	110.88	103.30
14	R	431	PRO	N-CA-CB	6.16	110.69	103.30
14	R	337	PRO	N-CA-CB	6.15	110.68	103.30
14	R	81	PRO	N-CA-CB	6.15	110.68	103.30
14	R	169	PRO	N-CA-CB	6.11	110.63	103.30
14	R	179	PRO	N-CA-CB	6.06	110.57	103.30
14	R	319	PRO	N-CA-CB	6.03	110.54	103.30
14	R	340	PRO	N-CA-CB	6.00	110.50	103.30
14	R	225	PRO	N-CA-CB	5.97	110.46	103.30
14	R	172	PRO	N-CA-CB	5.94	110.42	103.30
14	R	101	PRO	N-CA-CB	5.86	110.34	103.30
14	R	365	PRO	N-CA-CB	5.80	110.26	103.30
14	R	409	PRO	N-CA-CB	5.72	110.17	103.30
14	R	347	PRO	N-CA-CB	5.66	110.09	103.30
14	R	453	PRO	N-CA-CB	5.64	110.07	103.30
14	R	117	ALA	N-CA-CB	-5.09	102.98	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	V	377	GLU	Peptide

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	6592	3291	1722	172	0
2	C	337	171	92	0	0
3	D	225	110	52	0	0
4	G	108	55	28	0	0
4	W	104	53	27	0	0
5	H	232	116	59	0	0
6	I	2968	1490	776	47	0
7	J	2040	1027	538	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P	1984	998	522	34	0
8	K	2124	1066	552	17	0
8	S	2024	1019	531	41	0
9	L	733	364	190	6	0
10	M	272	137	72	2	0
11	N	2728	1363	713	18	0
12	O	2829	1425	744	55	0
13	Q	580	290	154	1	0
14	R	1846	0	862	44	0
15	U	2160	1084	561	30	0
15	V	2136	1075	560	38	0
16	Y	2004	1008	526	7	0
16	Z	1952	983	511	16	0
17	C	3	0	0	0	0
17	N	1	0	0	0	0
All	All	35982	17125	9792	516	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 11.

All (516) 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)
14:R:229:ILE:HA	14:R:245:THR:HA	1.17	1.14
14:R:253:TRP:HA	14:R:260:ARG:HA	1.53	0.90
1:A:1070:LEU:O	1:A:1074:CYS:N	2.05	0.89
1:A:27:HIS:O	12:O:263:ARG:N	2.07	0.88
6:I:582:ASN:O	6:I:605:THR:N	2.10	0.85
14:R:233:ALA:HB3	14:R:242:ALA:HB3	1.59	0.85
8:S:145:ASN:O	8:S:149:ALA:N	2.10	0.84
1:A:460:SER:N	1:A:465:GLN:O	2.10	0.84
1:A:793:LEU:O	1:A:797:LEU:N	2.13	0.82
7:P:608:GLY:O	7:P:611:PHE:N	2.13	0.82
1:A:1887:CYS:O	1:A:1891:TYR:N	2.14	0.81
7:J:499:GLY:O	7:J:503:CYS:N	2.14	0.81
12:O:254:HIS:O	12:O:258:TYR:N	2.12	0.81
14:R:458:VAL:O	14:R:470:TRP:N	2.13	0.80
7:P:551:ALA:O	7:P:554:VAL:N	2.14	0.80
15:V:372:GLY:O	15:V:375:TYR:N	2.15	0.80
6:I:44:VAL:O	6:I:58:PHE:N	2.14	0.80
13:Q:105:PRO:O	13:Q:148:LEU:N	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:747:TYR:O	7:P:751:GLY:N	2.16	0.78
1:A:1073:LEU:O	1:A:1077:THR:N	2.16	0.78
14:R:294:ASP:H	14:R:300:HIS:HA	1.49	0.78
1:A:1284:GLU:O	1:A:1350:TYR:N	2.18	0.77
16:Z:145:CYS:O	16:Z:149:LEU:N	2.17	0.77
1:A:790:LEU:O	1:A:794:ALA:N	2.17	0.77
7:P:676:GLY:O	7:P:679:GLN:N	2.16	0.77
8:S:204:LEU:O	8:S:208:LYS:N	2.16	0.77
15:V:477:HIS:O	15:V:482:GLU:N	2.17	0.77
1:A:1870:ALA:O	1:A:1875:GLN:N	2.19	0.76
1:A:1881:GLN:O	1:A:1885:LEU:N	2.18	0.76
14:R:183:ASN:HA	14:R:463:ALA:HB1	1.67	0.76
6:I:46:LEU:O	6:I:55:VAL:N	2.19	0.76
9:L:10:GLY:N	9:L:119:TRP:O	2.19	0.75
1:A:791:VAL:O	1:A:795:ARG:N	2.20	0.75
6:I:61:ASN:O	6:I:65:GLY:N	2.20	0.75
8:K:524:GLU:O	8:K:528:GLY:N	2.20	0.75
12:O:12:PRO:CA	15:V:139:GLY:O	2.35	0.75
8:S:139:ILE:O	8:S:143:LEU:N	2.20	0.74
12:O:147:SER:O	12:O:150:GLN:N	2.21	0.74
1:A:1886:ALA:O	1:A:1890:VAL:N	2.20	0.74
12:O:357:SER:O	12:O:360:LEU:N	2.22	0.73
14:R:198:LEU:N	14:R:209:TRP:O	2.18	0.73
16:Z:383:LEU:O	16:Z:388:ARG:N	2.22	0.73
1:A:1810:GLU:O	1:A:1814:ILE:N	2.18	0.73
1:A:1067:GLU:O	1:A:1071:LEU:N	2.21	0.72
6:I:299:SER:O	6:I:302:ASP:N	2.21	0.72
7:P:459:ALA:O	7:P:463:MET:N	2.23	0.72
14:R:283:SER:O	14:R:290:ILE:HA	1.90	0.71
1:A:792:GLN:O	1:A:796:ASP:N	2.23	0.71
12:O:12:PRO:O	15:V:139:GLY:N	2.23	0.71
1:A:15:ARG:O	12:O:534:GLY:N	2.23	0.71
1:A:1073:LEU:O	1:A:1076:ARG:N	2.24	0.70
12:O:208:SER:O	12:O:211:GLN:N	2.24	0.70
15:U:323:LEU:O	15:U:326:ILE:N	2.23	0.70
1:A:15:ARG:O	12:O:533:THR:N	2.24	0.70
14:R:289:HIS:HA	14:R:305:LEU:O	1.92	0.70
1:A:1130:ASN:O	1:A:1133:SER:N	2.24	0.70
1:A:704:ASP:O	1:A:708:GLU:N	2.22	0.70
6:I:525:VAL:O	6:I:529:MET:N	2.22	0.69
8:S:202:ARG:O	8:S:206:GLU:N	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1290:ASP:O	1:A:1293:SER:N	2.26	0.69
14:R:417:GLY:HA2	14:R:425:LEU:HA	1.74	0.68
15:U:192:PHE:O	15:U:195:ALA:N	2.25	0.68
12:O:255:TYR:O	12:O:259:LEU:N	2.25	0.68
1:A:1672:ARG:O	1:A:1702:ARG:N	2.27	0.67
6:I:718:LYS:O	6:I:736:SER:N	2.28	0.67
12:O:679:ASP:O	12:O:683:LYS:N	2.27	0.67
1:A:31:HIS:CA	12:O:260:ASN:C	2.63	0.67
1:A:133:ILE:N	1:A:146:GLU:O	2.24	0.67
1:A:1797:ILE:O	1:A:1801:GLY:N	2.28	0.67
7:P:460:GLU:O	7:P:464:SER:N	2.23	0.67
14:R:293:HIS:HA	14:R:300:HIS:O	1.95	0.66
7:J:31:LEU:O	7:J:34:GLU:N	2.28	0.66
8:S:304:ALA:O	8:S:307:CYS:N	2.28	0.66
1:A:1246:PRO:O	1:A:1249:VAL:N	2.29	0.66
6:I:506:HIS:O	6:I:510:SER:N	2.28	0.66
7:P:53:LYS:O	7:P:56:LYS:N	2.28	0.66
1:A:24:GLY:O	12:O:264:VAL:O	2.14	0.66
1:A:1308:GLY:O	1:A:1310:GLY:N	2.28	0.66
6:I:187:LEU:O	6:I:195:ILE:N	2.29	0.66
14:R:233:ALA:O	14:R:242:ALA:N	2.29	0.66
6:I:290:PHE:O	6:I:294:LYS:N	2.29	0.65
8:S:486:GLY:O	8:S:490:SER:N	2.28	0.65
11:N:682:SER:O	11:N:686:LYS:N	2.29	0.65
16:Y:146:TYR:O	16:Y:151:GLN:N	2.30	0.65
7:P:657:HIS:O	7:P:660:LYS:N	2.29	0.65
8:S:165:GLU:O	8:S:169:LEU:N	2.28	0.65
10:M:16:ASP:O	10:M:19:TRP:N	2.29	0.65
1:A:44:PRO:O	15:V:362:PRO:N	2.30	0.65
1:A:1140:GLY:O	1:A:1143:ALA:N	2.30	0.64
11:N:110:LEU:O	11:N:114:ALA:N	2.28	0.64
1:A:709:TYR:O	1:A:713:SER:N	2.31	0.64
15:U:188:ALA:O	15:U:191:VAL:N	2.31	0.64
15:U:156:VAL:O	15:U:159:SER:N	2.30	0.63
1:A:802:TYR:O	1:A:805:HIS:N	2.32	0.63
6:I:474:ARG:O	6:I:477:GLN:N	2.31	0.63
1:A:1775:LEU:O	1:A:1779:VAL:N	2.31	0.63
6:I:48:ARG:N	6:I:53:HIS:O	2.32	0.63
12:O:530:SER:O	12:O:532:VAL:N	2.32	0.63
14:R:205:SER:HA	14:R:221:GLN:HA	1.80	0.63
8:S:484:ALA:O	8:S:487:TYR:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:458:VAL:N	14:R:470:TRP:O	2.23	0.63
1:A:1066:LYS:O	1:A:1070:LEU:N	2.22	0.63
12:O:348:TYR:O	12:O:352:GLN:N	2.32	0.62
8:S:300:VAL:O	8:S:303:PHE:N	2.32	0.62
1:A:1424:LYS:O	1:A:1427:ASP:N	2.31	0.62
8:S:250:CYS:O	8:S:254:THR:N	2.30	0.62
16:Y:411:GLU:O	16:Y:415:GLU:N	2.29	0.62
14:R:362:ALA:HB2	14:R:405:ILE:O	2.00	0.61
14:R:416:SER:O	14:R:426:VAL:N	2.31	0.61
6:I:523:HIS:O	6:I:527:ARG:N	2.29	0.61
7:J:744:GLY:O	7:J:748:LYS:N	2.33	0.61
1:A:972:GLU:O	1:A:976:LEU:N	2.28	0.61
8:S:487:TYR:O	8:S:491:LEU:N	2.27	0.61
1:A:860:TYR:N	1:A:895:TYR:O	2.33	0.60
6:I:320:LEU:O	6:I:324:GLN:N	2.33	0.60
14:R:189:LEU:CB	14:R:201:ALA:HB3	2.31	0.60
1:A:769:VAL:O	1:A:772:GLU:N	2.34	0.60
6:I:24:ILE:N	6:I:38:ALA:O	2.31	0.60
16:Y:259:CYS:O	16:Y:263:LYS:N	2.34	0.60
12:O:258:TYR:O	12:O:261:ASN:N	2.31	0.60
1:A:1584:LEU:O	1:A:1587:ALA:N	2.34	0.59
1:A:707:TRP:O	1:A:711:LEU:N	2.29	0.59
1:A:1869:HIS:O	1:A:1873:SER:N	2.32	0.59
16:Z:144:GLU:O	16:Z:148:MET:N	2.31	0.59
1:A:708:GLU:O	1:A:712:ASN:N	2.28	0.59
7:P:513:SER:O	7:P:515:TYR:N	2.34	0.59
1:A:1553:GLY:O	1:A:1556:LEU:N	2.36	0.59
1:A:1469:CYS:O	1:A:1472:LEU:N	2.36	0.59
14:R:294:ASP:H	14:R:300:HIS:CA	2.15	0.59
7:J:702:ASN:O	7:J:706:LYS:N	2.33	0.59
14:R:335:VAL:O	14:R:348:LEU:N	2.28	0.58
1:A:1749:SER:O	1:A:1753:TYR:N	2.30	0.58
6:I:524:PHE:O	6:I:528:ARG:N	2.29	0.58
1:A:1812:TRP:O	1:A:1816:LEU:N	2.36	0.58
16:Y:524:GLU:O	16:Y:528:ALA:N	2.32	0.58
1:A:878:ALA:O	1:A:882:LEU:N	2.36	0.58
8:S:251:TYR:O	8:S:255:SER:N	2.35	0.58
15:U:357:ALA:O	15:U:360:LEU:N	2.36	0.58
14:R:329:ASN:HA	14:R:357:ALA:HB1	1.84	0.58
16:Z:152:ASP:O	16:Z:156:ILE:N	2.28	0.58
1:A:30:HIS:O	12:O:260:ASN:CA	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1395:LEU:O	1:A:1398:PHE:N	2.37	0.57
1:A:1623:ASP:N	1:A:1628:THR:O	2.37	0.57
15:U:204:GLY:O	15:U:207:LEU:N	2.36	0.57
1:A:27:HIS:N	12:O:265:GLN:H	2.00	0.57
1:A:1047:VAL:O	1:A:1110:ARG:N	2.32	0.57
1:A:1069:ARG:O	1:A:1073:LEU:N	2.35	0.57
1:A:1109:GLY:N	1:A:1118:VAL:O	2.34	0.57
1:A:1725:ASN:O	1:A:1729:GLU:N	2.36	0.57
7:J:89:GLU:O	7:J:94:GLY:N	2.37	0.57
11:N:382:LEU:O	11:N:387:LEU:N	2.33	0.57
7:P:747:TYR:O	7:P:752:GLN:N	2.36	0.57
7:P:459:ALA:O	7:P:462:LEU:N	2.37	0.57
16:Y:423:ILE:O	16:Y:427:MET:N	2.33	0.57
6:I:441:THR:O	6:I:444:ASP:N	2.37	0.57
8:K:144:ASP:O	8:K:146:ARG:N	2.37	0.57
14:R:197:VAL:HA	14:R:210:SER:HA	1.86	0.57
1:A:1774:VAL:O	1:A:1778:CYS:N	2.33	0.57
6:I:659:ARG:O	6:I:663:ASP:N	2.38	0.57
12:O:750:PRO:O	12:O:754:HIS:N	2.36	0.57
1:A:478:ASP:O	1:A:491:LEU:N	2.35	0.57
12:O:110:GLN:O	12:O:114:ASP:N	2.32	0.57
1:A:1870:ALA:O	1:A:1874:GLY:N	2.37	0.56
7:P:479:TYR:O	7:P:481:CYS:N	2.39	0.56
6:I:475:VAL:O	6:I:479:LEU:N	2.31	0.56
7:J:605:THR:O	7:J:608:GLY:N	2.38	0.56
14:R:457:THR:HA	14:R:471:ARG:HA	1.86	0.56
8:S:130:SER:O	8:S:134:LEU:N	2.34	0.56
9:L:81:ALA:O	9:L:118:GLY:N	2.35	0.56
14:R:418:HIS:O	14:R:423:ASN:HA	2.05	0.56
15:U:455:CYS:O	15:U:459:ALA:N	2.37	0.56
1:A:1320:ASN:O	1:A:1323:GLU:N	2.39	0.55
1:A:675:LEU:O	1:A:679:ARG:N	2.35	0.55
6:I:92:LEU:O	6:I:101:LEU:N	2.38	0.55
15:U:354:PHE:O	15:U:357:ALA:N	2.37	0.55
1:A:1796:ALA:O	1:A:1800:LEU:N	2.34	0.55
15:V:201:LEU:O	15:V:203:TRP:N	2.39	0.55
14:R:360:ALA:HB2	14:R:403:CYS:O	2.06	0.55
14:R:329:ASN:HA	14:R:357:ALA:CB	2.36	0.55
15:V:539:PHE:O	15:V:543:ARG:N	2.40	0.55
1:A:1533:LEU:O	1:A:1536:LEU:N	2.40	0.55
1:A:1577:SER:O	1:A:1580:SER:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:360:ALA:O	14:R:373:THR:HA	2.07	0.54
1:A:940:THR:O	1:A:943:ASP:N	2.39	0.54
8:K:520:GLY:O	8:K:524:GLU:N	2.34	0.54
15:U:244:ILE:O	15:U:247:ALA:N	2.40	0.54
1:A:1319:LEU:O	1:A:1321:VAL:N	2.39	0.54
1:A:1033:ARG:O	1:A:1036:ASP:N	2.40	0.54
8:S:252:LYS:O	8:S:256:VAL:N	2.34	0.54
6:I:686:THR:N	6:I:699:ALA:O	2.39	0.54
1:A:1811:LEU:O	1:A:1815:LYS:N	2.32	0.54
8:K:283:GLU:O	8:K:286:TYR:N	2.39	0.54
11:N:289:PHE:O	11:N:293:ILE:N	2.38	0.54
8:S:257:VAL:O	8:S:260:LYS:N	2.39	0.54
8:S:515:SER:O	8:S:519:LEU:N	2.36	0.54
12:O:12:PRO:CA	15:V:139:GLY:C	2.76	0.54
1:A:1551:ASN:O	1:A:1554:PHE:N	2.41	0.53
8:S:264:HIS:O	8:S:267:CYS:N	2.42	0.53
16:Z:43:ASP:O	16:Z:47:ALA:N	2.38	0.53
14:R:312:VAL:HA	14:R:328:GLY:HA2	1.91	0.53
16:Z:203:LEU:O	16:Z:207:LEU:N	2.33	0.53
1:A:1513:GLU:O	1:A:1516:LEU:N	2.42	0.53
6:I:37:LEU:N	6:I:45:LEU:O	2.37	0.53
11:N:196:ASP:O	11:N:200:GLU:N	2.36	0.53
12:O:630:ALA:O	12:O:634:LEU:N	2.38	0.53
8:S:480:SER:O	8:S:483:SER:N	2.42	0.53
1:A:26:ASP:H	12:O:265:GLN:CA	2.21	0.53
1:A:782:GLY:O	1:A:784:CYS:N	2.41	0.53
15:V:28:ASP:O	15:V:31:GLU:N	2.41	0.53
12:O:388:ARG:O	12:O:391:ALA:N	2.41	0.53
15:U:262:SER:O	15:U:265:ILE:N	2.42	0.53
7:J:508:ALA:O	7:J:512:LEU:N	2.35	0.52
14:R:183:ASN:HA	14:R:463:ALA:CB	2.36	0.52
14:R:286:ARG:HA	14:R:311:GLU:CB	2.39	0.52
8:S:131:SER:O	8:S:135:LEU:N	2.34	0.52
1:A:45:ALA:CA	15:V:363:ARG:N	2.73	0.52
6:I:495:ASN:O	6:I:499:ASP:N	2.43	0.52
16:Y:363:ALA:O	16:Y:367:GLN:N	2.35	0.52
1:A:706:ASP:O	1:A:710:LEU:N	2.30	0.52
6:I:319:THR:O	6:I:323:ASN:N	2.42	0.52
7:P:37:SER:O	7:P:40:ALA:N	2.40	0.52
12:O:255:TYR:O	12:O:258:TYR:N	2.42	0.52
6:I:619:LYS:N	6:I:703:ARG:O	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Z:426:ALA:O	16:Z:430:ALA:N	2.37	0.52
16:Z:142:MET:O	16:Z:146:TYR:N	2.31	0.52
1:A:45:ALA:CA	15:V:362:PRO:N	2.73	0.52
1:A:48:LEU:CA	15:V:331:VAL:CA	2.88	0.51
11:N:285:PHE:O	11:N:289:PHE:N	2.37	0.51
12:O:544:VAL:O	12:O:547:LYS:N	2.43	0.51
1:A:45:ALA:CA	15:V:362:PRO:CA	2.88	0.51
16:Y:192:TYR:O	16:Y:196:LEU:N	2.40	0.51
1:A:27:HIS:O	12:O:260:ASN:O	2.29	0.51
6:I:476:GLY:HA2	6:I:480:LYS:H	1.74	0.51
9:L:82:ASP:O	9:L:86:ASP:N	2.44	0.51
11:N:340:ARG:O	11:N:344:LEU:N	2.43	0.51
1:A:46:SER:CA	15:V:360:LEU:O	2.58	0.51
6:I:523:HIS:O	6:I:526:LYS:N	2.44	0.51
6:I:574:PHE:O	6:I:587:LEU:N	2.32	0.51
15:U:319:LEU:O	15:U:322:ASN:N	2.44	0.51
6:I:240:LEU:O	6:I:244:PHE:N	2.34	0.51
1:A:22:PRO:CA	1:A:113:VAL:CA	2.89	0.51
1:A:460:SER:O	1:A:463:LYS:N	2.38	0.51
1:A:1927:ALA:O	1:A:1931:LEU:N	2.36	0.50
6:I:263:GLN:O	6:I:266:ASN:N	2.45	0.50
14:R:384:ILE:O	14:R:392:CYS:HA	2.11	0.50
1:A:846:GLN:O	1:A:849:SER:N	2.45	0.50
8:K:65:LEU:O	8:K:68:LEU:N	2.44	0.50
7:P:649:GLU:O	7:P:651:PHE:N	2.42	0.50
1:A:27:HIS:N	12:O:265:GLN:N	2.59	0.50
1:A:793:LEU:O	1:A:797:LEU:CA	2.59	0.50
1:A:640:LYS:O	1:A:644:VAL:N	2.30	0.50
11:N:135:TRP:O	11:N:140:LEU:N	2.42	0.50
7:P:608:GLY:O	7:P:609:HIS:C	2.49	0.50
15:V:179:LEU:O	15:V:182:LEU:N	2.45	0.50
12:O:481:GLY:O	12:O:483:PHE:N	2.43	0.50
14:R:178:ALA:O	14:R:465:GLU:HA	2.11	0.50
1:A:1061:GLU:O	1:A:1065:GLU:N	2.36	0.50
1:A:1637:THR:N	1:A:1665:GLN:O	2.40	0.50
6:I:209:CYS:N	6:I:218:SER:O	2.45	0.50
7:J:661:ALA:O	7:J:665:ASN:N	2.40	0.50
11:N:55:LEU:O	11:N:59:VAL:N	2.44	0.50
7:P:757:LEU:O	7:P:761:SER:N	2.33	0.49
15:V:56:ALA:O	15:V:59:ALA:N	2.44	0.49
1:A:789:LEU:O	1:A:793:LEU:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1886:ALA:O	1:A:1889:LEU:N	2.46	0.49
7:P:456:LYS:O	7:P:460:GLU:N	2.44	0.49
7:P:756:ALA:O	7:P:760:PHE:N	2.41	0.49
1:A:1867:CYS:O	1:A:1870:ALA:N	2.46	0.49
6:I:185:ILE:O	6:I:198:VAL:N	2.45	0.49
6:I:239:ASN:O	6:I:243:SER:N	2.39	0.49
8:S:138:LYS:O	8:S:142:ALA:N	2.40	0.49
1:A:26:ASP:O	12:O:263:ARG:C	2.50	0.49
15:U:272:ALA:O	15:U:276:ILE:N	2.42	0.49
15:V:380:ASN:O	15:V:383:ALA:N	2.45	0.49
11:N:92:TRP:O	11:N:96:SER:N	2.44	0.49
15:V:372:GLY:O	15:V:373:HIS:C	2.51	0.49
16:Z:331:LEU:O	16:Z:335:SER:N	2.34	0.49
1:A:28:CYS:O	1:A:31:HIS:O	2.31	0.49
1:A:704:ASP:O	1:A:707:TRP:N	2.46	0.49
1:A:1140:GLY:O	1:A:1142:ALA:N	2.46	0.49
1:A:1216:LYS:O	1:A:1219:THR:N	2.37	0.49
8:K:490:SER:O	8:K:493:GLY:N	2.44	0.49
11:N:542:VAL:O	11:N:546:LYS:N	2.44	0.48
1:A:1410:ALA:O	1:A:1413:LEU:N	2.45	0.48
11:N:286:LEU:O	11:N:290:HIS:N	2.43	0.48
12:O:41:LEU:O	12:O:45:SER:N	2.33	0.48
16:Z:466:ASP:O	16:Z:470:THR:N	2.42	0.48
1:A:31:HIS:CA	12:O:261:ASN:N	2.76	0.48
8:S:125:GLN:O	8:S:129:LYS:N	2.26	0.48
15:V:83:ASP:O	15:V:86:ALA:N	2.39	0.48
1:A:14:ALA:O	12:O:530:SER:C	2.52	0.48
1:A:1246:PRO:O	1:A:1247:HIS:C	2.51	0.48
7:J:705:CYS:O	7:J:709:ARG:N	2.39	0.48
1:A:1041:LEU:O	1:A:1043:SER:N	2.47	0.48
14:R:446:VAL:HA	14:R:462:ALA:HA	1.96	0.48
14:R:420:PHE:HA	14:R:421:ALA:HA	1.55	0.48
7:J:164:PRO:O	7:J:168:PHE:N	2.46	0.48
1:A:798:LYS:O	1:A:800:GLY:N	2.46	0.48
1:A:1772:SER:O	1:A:1776:TYR:N	2.34	0.48
8:K:227:LEU:O	8:K:230:ASN:N	2.47	0.48
14:R:233:ALA:CB	14:R:242:ALA:HB3	2.37	0.48
1:A:824:ASP:O	1:A:828:THR:N	2.45	0.48
6:I:376:TYR:O	6:I:379:LEU:N	2.45	0.48
8:S:231:LEU:O	8:S:235:VAL:N	2.34	0.48
15:V:168:ASP:O	15:V:172:LEU:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:SER:CA	15:V:361:ASN:CA	2.91	0.47
6:I:138:LEU:O	6:I:257:HIS:CA	2.61	0.47
8:S:202:ARG:O	8:S:205:PHE:N	2.45	0.47
1:A:31:HIS:C	12:O:257:SER:O	2.53	0.47
1:A:23:PHE:O	1:A:26:ASP:N	2.48	0.47
6:I:286:ARG:O	6:I:290:PHE:N	2.39	0.47
1:A:27:HIS:C	12:O:261:ASN:C	2.73	0.47
1:A:28:CYS:O	1:A:31:HIS:N	2.47	0.47
12:O:253:ALA:O	12:O:257:SER:N	2.41	0.47
12:O:617:GLN:O	12:O:620:ALA:N	2.47	0.47
8:K:523:ILE:O	8:K:527:ILE:N	2.37	0.47
1:A:1551:ASN:O	1:A:1552:TYR:C	2.52	0.47
1:A:1314:ILE:O	1:A:1317:SER:N	2.42	0.47
12:O:290:SER:O	12:O:337:HIS:N	2.48	0.47
12:O:543:GLY:O	12:O:547:LYS:N	2.46	0.47
7:P:753:THR:O	7:P:757:LEU:N	2.34	0.46
15:U:264:TYR:O	15:U:268:GLN:N	2.38	0.46
15:V:519:TYR:O	15:V:523:CYS:N	2.47	0.46
7:J:601:ALA:O	7:J:604:TYR:N	2.48	0.46
7:P:604:TYR:O	7:P:607:LEU:N	2.48	0.46
7:J:507:ARG:O	7:J:511:GLU:N	2.38	0.46
1:A:32:PRO:N	12:O:257:SER:O	2.47	0.46
1:A:460:SER:CA	1:A:465:GLN:O	2.64	0.46
1:A:591:VAL:O	1:A:592:HIS:C	2.53	0.46
1:A:1890:VAL:O	1:A:1893:SER:N	2.43	0.46
15:U:361:ASN:O	15:U:363:ARG:N	2.49	0.46
8:K:202:ARG:O	8:K:206:GLU:N	2.32	0.46
14:R:250:VAL:O	14:R:264:MET:N	2.49	0.46
1:A:804:ASP:O	1:A:808:ARG:N	2.43	0.46
1:A:973:ALA:O	1:A:977:LEU:N	2.28	0.46
6:I:37:LEU:O	6:I:45:LEU:N	2.32	0.46
8:K:36:GLU:O	8:K:39:ASP:N	2.49	0.46
7:P:671:LEU:O	7:P:675:ILE:N	2.44	0.46
8:S:332:THR:O	8:S:334:GLY:N	2.48	0.46
1:A:23:PHE:H	1:A:113:VAL:N	2.14	0.46
1:A:1140:GLY:O	1:A:1141:VAL:C	2.54	0.46
1:A:1777:GLU:O	1:A:1781:GLN:N	2.47	0.46
10:M:16:ASP:O	10:M:17:ASP:C	2.55	0.46
7:P:498:THR:O	7:P:501:VAL:N	2.49	0.46
14:R:233:ALA:HB3	14:R:242:ALA:O	2.16	0.46
1:A:46:SER:N	15:V:361:ASN:CA	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:LEU:O	1:A:506:VAL:N	2.49	0.46
1:A:711:LEU:CA	1:A:734:GLU:O	2.64	0.46
1:A:1111:ALA:O	1:A:1115:ASN:N	2.48	0.46
1:A:1925:VAL:O	1:A:1929:LEU:N	2.42	0.46
1:A:46:SER:H	15:V:362:PRO:N	2.14	0.45
11:N:28:SER:O	11:N:32:VAL:N	2.49	0.45
15:U:204:GLY:O	15:U:205:ALA:C	2.54	0.45
1:A:27:HIS:CA	12:O:262:LEU:CA	2.95	0.45
6:I:495:ASN:O	6:I:498:TYR:N	2.49	0.45
7:J:568:GLU:O	7:J:571:CYS:N	2.49	0.45
8:K:486:GLY:O	8:K:489:HIS:N	2.50	0.45
8:S:511:ASP:O	8:S:513:THR:N	2.49	0.45
8:K:522:CYS:O	8:K:526:TYR:N	2.36	0.45
8:S:421:ALA:O	8:S:424:TRP:N	2.49	0.45
15:V:444:GLU:O	15:V:447:ASN:N	2.47	0.45
1:A:1083:GLY:O	1:A:1084:ARG:C	2.54	0.45
1:A:1201:HIS:O	1:A:1204:THR:N	2.50	0.45
6:I:278:GLU:O	6:I:281:MET:N	2.50	0.45
12:O:57:ARG:O	12:O:61:ASN:N	2.38	0.45
11:N:382:LEU:O	11:N:386:LEU:N	2.47	0.45
16:Z:414:ILE:O	16:Z:418:LEU:N	2.41	0.45
1:A:41:GLN:O	12:O:10:PHE:CA	2.65	0.45
8:K:264:HIS:O	8:K:267:CYS:N	2.50	0.45
14:R:233:ALA:HB3	14:R:242:ALA:CB	2.40	0.45
12:O:425:LYS:O	12:O:428:ILE:N	2.50	0.45
15:U:188:ALA:O	15:U:189:ILE:C	2.54	0.45
15:V:425:ALA:O	15:V:428:LEU:N	2.49	0.45
1:A:1928:LEU:O	1:A:1932:ALA:N	2.41	0.45
1:A:1299:GLY:O	1:A:1300:LEU:C	2.54	0.45
7:J:611:PHE:O	7:J:616:GLU:N	2.50	0.45
6:I:60:PRO:CA	6:I:65:GLY:O	2.65	0.44
1:A:23:PHE:H	1:A:113:VAL:H	1.64	0.44
1:A:44:PRO:O	1:A:46:SER:N	2.49	0.44
12:O:251:ALA:O	12:O:252:GLU:C	2.55	0.44
15:U:315:GLU:O	15:U:318:TYR:N	2.50	0.44
15:V:363:ARG:O	15:V:365:LEU:N	2.50	0.44
1:A:1793:MET:O	1:A:1797:ILE:N	2.39	0.44
8:K:315:LYS:O	8:K:318:HIS:N	2.51	0.44
8:S:199:GLU:O	8:S:203:PHE:N	2.34	0.44
8:S:205:PHE:O	8:S:209:LEU:N	2.51	0.44
8:S:201:LEU:O	8:S:205:PHE:N	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1256:GLY:O	1:A:1259:LEU:N	2.50	0.44
7:P:462:LEU:O	7:P:466:LEU:N	2.36	0.44
1:A:714:ASP:O	1:A:718:ASN:N	2.39	0.44
7:J:147:PHE:O	7:J:149:TRP:N	2.51	0.44
7:J:538:ILE:O	7:J:541:THR:N	2.51	0.44
8:K:232:ASP:O	8:K:236:SER:N	2.47	0.44
8:S:178:ALA:O	8:S:182:LYS:N	2.36	0.44
8:S:230:ASN:O	8:S:233:VAL:N	2.51	0.44
12:O:719:ARG:O	12:O:723:THR:N	2.49	0.43
8:S:126:SER:O	8:S:130:SER:N	2.34	0.43
7:J:722:ALA:O	7:J:726:LEU:N	2.38	0.43
14:R:376:GLY:O	14:R:378:SER:N	2.52	0.43
14:R:384:ILE:O	14:R:393:LEU:N	2.43	0.43
1:A:1146:LYS:O	1:A:1147:ILE:C	2.57	0.43
1:A:1363:THR:O	1:A:1365:PRO:O	2.35	0.43
1:A:1850:CYS:O	1:A:1854:ASN:N	2.49	0.43
7:P:16:LEU:O	7:P:18:HIS:N	2.51	0.43
7:P:53:LYS:O	7:P:54:ALA:C	2.56	0.43
15:V:361:ASN:O	15:V:363:ARG:N	2.51	0.43
1:A:24:GLY:O	12:O:265:GLN:CA	2.65	0.43
7:J:6:GLU:O	7:J:9:GLN:N	2.52	0.43
8:K:520:GLY:O	8:K:523:ILE:N	2.52	0.43
8:S:93:LEU:O	8:S:95:MET:N	2.51	0.43
14:R:430:TYR:HA	14:R:431:PRO:HA	1.65	0.43
8:S:484:ALA:O	8:S:485:ILE:C	2.57	0.43
15:U:529:ALA:O	15:U:533:ALA:N	2.43	0.43
1:A:1132:THR:O	1:A:1133:SER:C	2.57	0.43
1:A:1773:SER:O	1:A:1777:GLU:N	2.35	0.43
12:O:273:SER:O	12:O:276:HIS:N	2.51	0.43
16:Z:415:GLU:O	16:Z:419:ALA:N	2.50	0.43
1:A:1174:GLY:O	1:A:1175:PHE:C	2.57	0.43
6:I:359:LEU:O	6:I:363:LEU:N	2.37	0.43
14:R:416:SER:O	14:R:425:LEU:HA	2.19	0.43
15:V:374:GLU:O	15:V:376:MET:O	2.37	0.43
15:U:286:PHE:O	15:U:289:LEU:N	2.52	0.43
15:U:443:TYR:O	15:U:448:GLN:N	2.45	0.43
1:A:1595:HIS:O	1:A:1596:SER:C	2.57	0.42
7:J:728:GLU:O	7:J:731:GLN:N	2.52	0.42
7:P:657:HIS:O	7:P:658:PHE:C	2.57	0.42
15:U:330:ARG:O	15:U:331:VAL:C	2.57	0.42
14:R:385:TRP:HA	14:R:392:CYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:60:GLN:O	9:L:62:HIS:N	2.50	0.42
7:P:642:GLY:O	7:P:643:MET:C	2.58	0.42
8:S:163:CYS:O	8:S:165:GLU:N	2.53	0.42
16:Z:72:SER:O	16:Z:75:GLN:N	2.53	0.42
14:R:252:LEU:O	14:R:261:LEU:N	2.46	0.42
1:A:279:GLU:O	1:A:283:LEU:N	2.46	0.42
1:A:591:VAL:O	1:A:593:ASN:N	2.53	0.42
1:A:1021:HIS:CA	11:N:486:ASP:CA	2.97	0.42
1:A:1244:ASP:O	1:A:1246:PRO:N	2.52	0.42
7:P:520:ARG:O	7:P:523:SER:N	2.52	0.42
8:S:264:HIS:O	8:S:265:ALA:C	2.57	0.42
1:A:15:ARG:O	12:O:531:LEU:C	2.58	0.42
12:O:563:LEU:O	12:O:566:LYS:N	2.53	0.42
8:S:394:ALA:O	8:S:397:ILE:N	2.53	0.42
15:U:264:TYR:O	15:U:267:SER:N	2.53	0.42
15:V:481:THR:O	15:V:483:SER:N	2.51	0.42
1:A:27:HIS:H	12:O:265:GLN:CA	2.32	0.42
6:I:366:LEU:O	6:I:369:MET:N	2.53	0.42
9:L:90:THR:O	9:L:145:HIS:N	2.35	0.42
7:P:459:ALA:O	7:P:462:LEU:CA	2.68	0.42
1:A:1290:ASP:O	1:A:1291:ARG:C	2.58	0.42
1:A:1320:ASN:O	1:A:1321:VAL:C	2.58	0.42
1:A:1503:ASN:O	1:A:1506:VAL:N	2.51	0.42
1:A:1524:ALA:O	1:A:1528:ALA:N	2.53	0.42
7:J:626:ASN:O	7:J:630:VAL:N	2.45	0.42
14:R:400:SER:CB	14:R:420:PHE:O	2.68	0.41
1:A:1469:CYS:O	1:A:1470:LEU:C	2.59	0.41
1:A:1563:GLY:O	1:A:1566:PHE:N	2.53	0.41
1:A:1568:GLY:O	1:A:1571:ARG:N	2.54	0.41
7:J:102:SER:O	7:J:105:ASP:N	2.53	0.41
12:O:316:HIS:O	12:O:317:TYR:C	2.57	0.41
7:P:661:ALA:O	7:P:664:ILE:N	2.52	0.41
7:P:676:GLY:O	7:P:677:VAL:C	2.58	0.41
8:S:429:LEU:O	8:S:433:LYS:N	2.42	0.41
6:I:25:PHE:O	6:I:38:ALA:N	2.41	0.41
7:J:740:TYR:O	7:J:744:GLY:N	2.41	0.41
12:O:357:SER:O	12:O:358:TYR:C	2.59	0.41
15:V:86:ALA:O	15:V:87:TYR:C	2.58	0.41
1:A:1424:LYS:O	1:A:1428:SER:N	2.53	0.41
1:A:1563:GLY:O	1:A:1565:LEU:N	2.54	0.41
9:L:78:CYS:O	9:L:157:LYS:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:503:SER:O	11:N:507:SER:N	2.52	0.41
7:P:619:LYS:O	7:P:622:ALA:N	2.49	0.41
15:U:154:LEU:O	15:U:156:VAL:N	2.54	0.41
15:V:80:ASP:O	15:V:84:MET:N	2.50	0.41
15:V:414:MET:O	15:V:415:PRO:C	2.59	0.41
1:A:1750:PHE:O	1:A:1754:PHE:N	2.51	0.41
8:K:494:ASN:O	8:K:496:GLU:N	2.53	0.41
15:V:168:ASP:O	15:V:171:GLY:N	2.53	0.41
15:V:380:ASN:O	15:V:381:THR:C	2.59	0.41
1:A:49:TRP:CA	15:V:364:TYR:CA	2.99	0.41
1:A:1563:GLY:O	1:A:1564:LEU:C	2.58	0.41
1:A:1580:SER:O	1:A:1583:ALA:N	2.53	0.41
1:A:1603:LEU:O	1:A:1604:GLN:C	2.59	0.41
12:O:161:TYR:O	12:O:165:GLY:N	2.44	0.41
15:U:99:TYR:O	15:U:102:ALA:N	2.53	0.41
1:A:1256:GLY:O	1:A:1257:ILE:C	2.57	0.41
1:A:1454:LEU:O	1:A:1458:SER:N	2.43	0.41
7:P:102:SER:O	7:P:105:ASP:N	2.54	0.41
8:S:304:ALA:O	8:S:305:VAL:C	2.58	0.41
8:S:307:CYS:O	8:S:311:MET:N	2.40	0.41
1:A:1580:SER:O	1:A:1581:ILE:C	2.59	0.41
6:I:664:ARG:O	6:I:714:LEU:N	2.40	0.41
11:N:68:HIS:O	11:N:71:LEU:N	2.52	0.41
12:O:600:ALA:O	12:O:601:LEU:C	2.57	0.41
15:U:244:ILE:O	15:U:245:GLU:C	2.59	0.41
11:N:570:ILE:O	11:N:574:ILE:N	2.54	0.40
15:U:156:VAL:O	15:U:157:GLU:C	2.59	0.40
15:U:270:ALA:O	15:U:273:TYR:N	2.54	0.40
1:A:1566:PHE:O	1:A:1569:GLY:N	2.53	0.40
6:I:389:ALA:O	6:I:392:ALA:N	2.54	0.40
7:P:622:ALA:O	7:P:623:CYS:C	2.59	0.40
15:U:330:ARG:O	15:U:333:THR:N	2.55	0.40
1:A:802:TYR:O	1:A:804:ASP:N	2.55	0.40
6:I:204:THR:N	6:I:222:GLU:O	2.45	0.40
6:I:418:PHE:O	6:I:422:TYR:N	2.36	0.40
7:J:475:ALA:O	7:J:479:TYR:N	2.55	0.40
8:S:317:GLU:O	8:S:320:ARG:N	2.55	0.40
15:V:417:TYR:O	15:V:418:CYS:C	2.59	0.40
16:Z:434:TYR:O	16:Z:439:ALA:N	2.50	0.40
1:A:633:ILE:O	1:A:636:GLN:N	2.54	0.40
1:A:1375:TYR:O	1:A:1378:THR:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:148:ASN:O	15:U:152:ARG:N	2.45	0.40
15:U:270:ALA:O	15:U:271:VAL:C	2.60	0.40
15:V:378:MET:O	15:V:380:ASN:N	2.54	0.40
16:Z:202:ALA:O	16:Z:205:ALA:N	2.55	0.40
16:Z:412:GLY:O	16:Z:415:GLU:N	2.54	0.40
1:A:19:GLU:N	1:A:110:ALA:H	2.19	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	1628/1944 (84%)	1464 (90%)	162 (10%)	2 (0%)	48	80
2	C	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
3	D	54/56 (96%)	48 (89%)	6 (11%)	0	100	100
4	G	25/85 (29%)	23 (92%)	2 (8%)	0	100	100
4	W	24/85 (28%)	23 (96%)	1 (4%)	0	100	100
5	H	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
6	I	736/808 (91%)	691 (94%)	45 (6%)	0	100	100
7	J	506/824 (61%)	481 (95%)	25 (5%)	0	100	100
7	P	492/824 (60%)	437 (89%)	55 (11%)	0	100	100
8	K	525/620 (85%)	496 (94%)	28 (5%)	1 (0%)	44	75
8	S	502/620 (81%)	462 (92%)	40 (8%)	0	100	100
9	L	181/185 (98%)	169 (93%)	12 (7%)	0	100	100
10	M	66/74 (89%)	57 (86%)	9 (14%)	0	100	100
11	N	674/822 (82%)	651 (97%)	22 (3%)	1 (0%)	48	80
12	O	699/755 (93%)	645 (92%)	53 (8%)	1 (0%)	48	80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Q	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
14	R	367/499 (74%)	346 (94%)	19 (5%)	2 (0%)	25	60
15	U	534/597 (89%)	484 (91%)	50 (9%)	0	100	100
15	V	532/597 (89%)	485 (91%)	47 (9%)	0	100	100
16	Y	497/565 (88%)	487 (98%)	10 (2%)	0	100	100
16	Z	484/565 (86%)	472 (98%)	12 (2%)	0	100	100
All	All	8807/10812 (82%)	8193 (93%)	607 (7%)	7 (0%)	50	80

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	N	473	ASP
14	R	101	PRO
1	A	109	GLN
12	O	531	LEU
1	A	121	SER
8	K	295	TYR
14	R	409	PRO

5.3.2 Protein sidechains [i](#)

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

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](#)

Of 4 ligands modelled in this entry, 4 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	388:CYS	C	389:SER	N	3.54

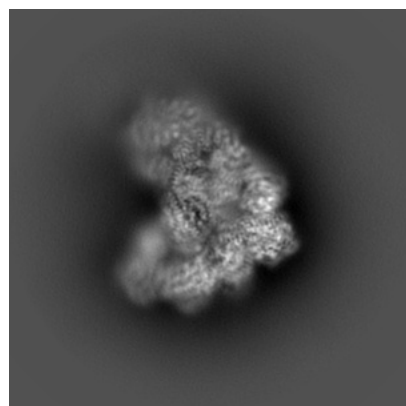
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48928. These allow visual inspection of the internal detail of the map and identification of artifacts.

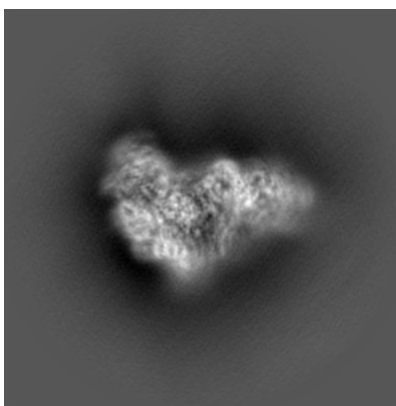
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

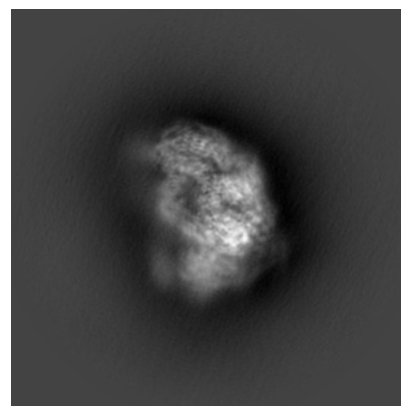
6.1.1 Primary map



X

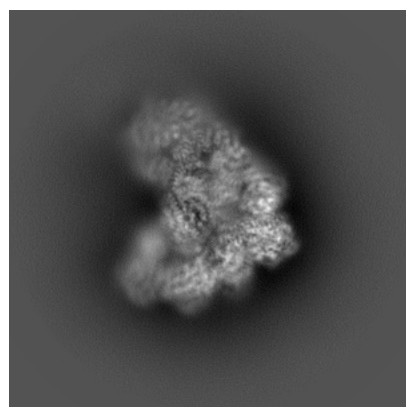


Y

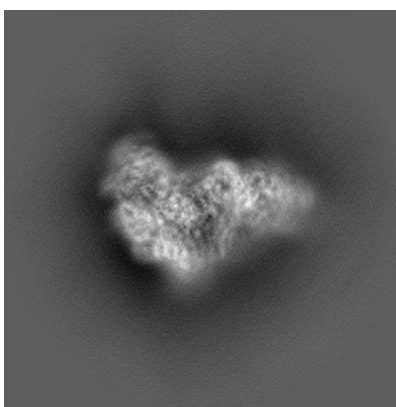


Z

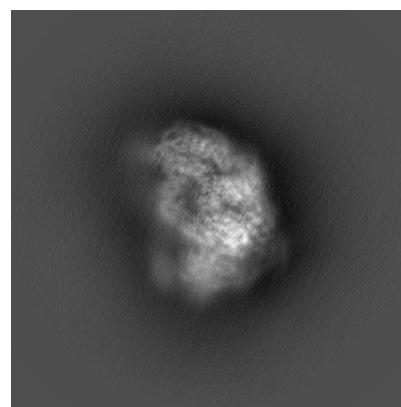
6.1.2 Raw map



X



Y

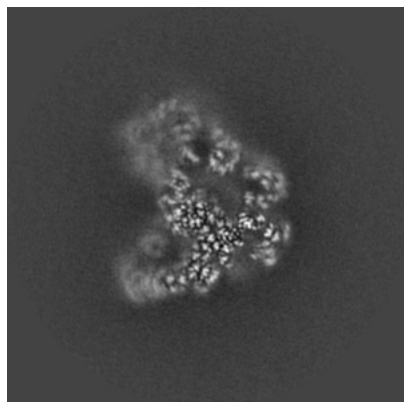


Z

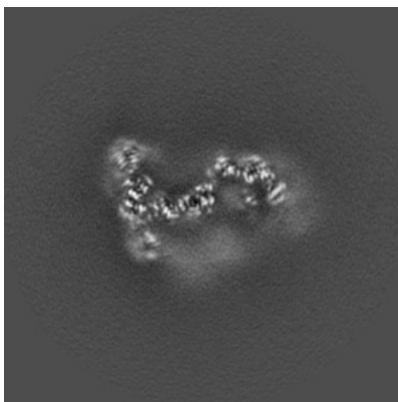
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

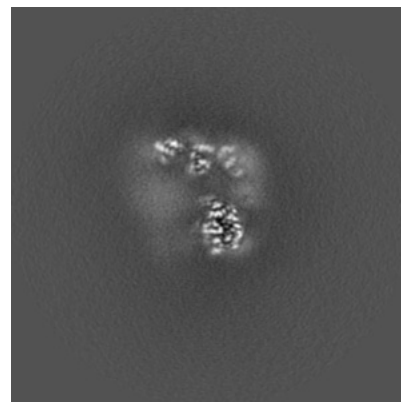
6.2.1 Primary map



X Index: 240

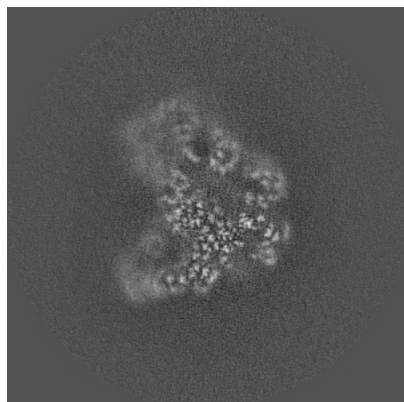


Y Index: 240

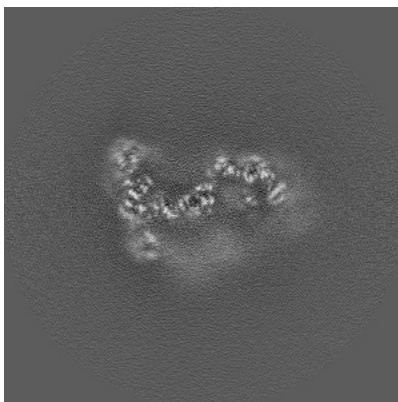


Z Index: 240

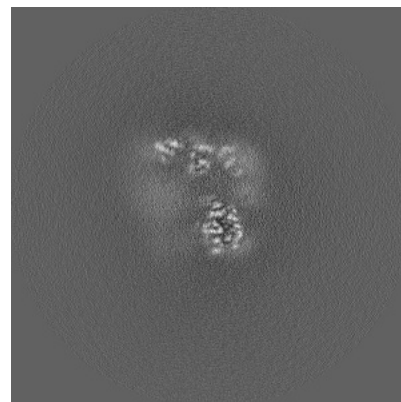
6.2.2 Raw map



X Index: 240



Y Index: 240

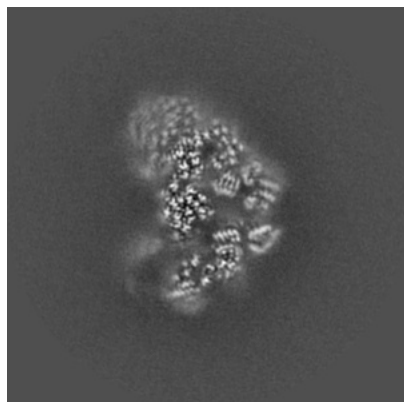


Z Index: 240

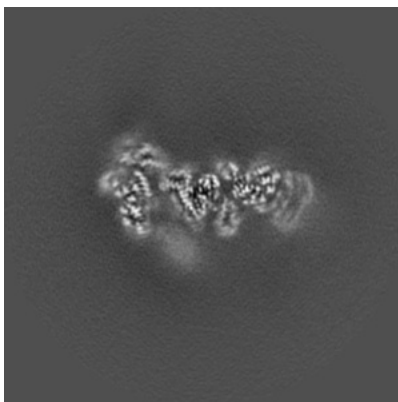
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

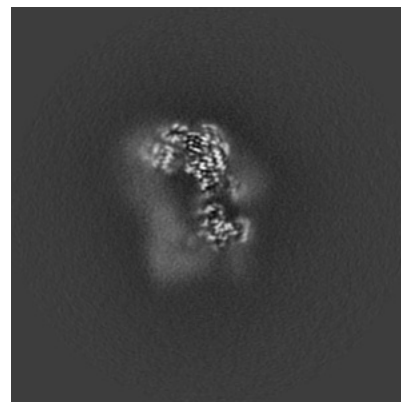
6.3.1 Primary map



X Index: 258

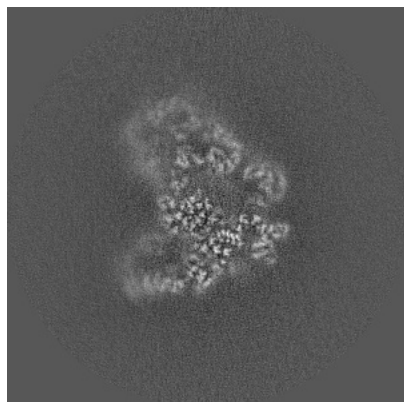


Y Index: 212

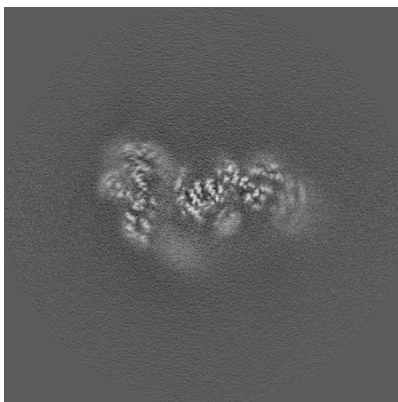


Z Index: 215

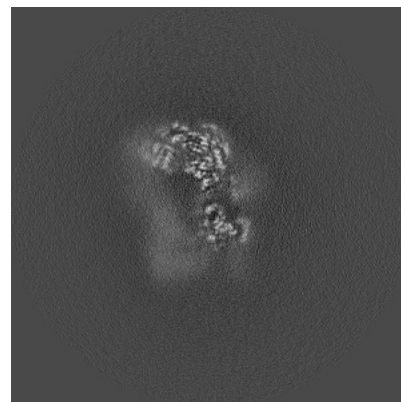
6.3.2 Raw map



X Index: 244



Y Index: 220

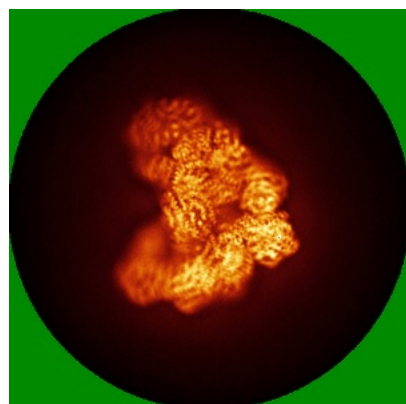


Z Index: 214

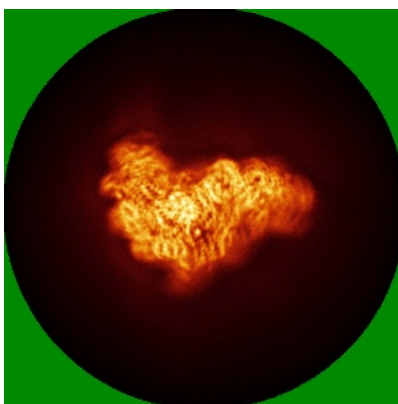
The images above show the largest variance slices of the map in three orthogonal directions.

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

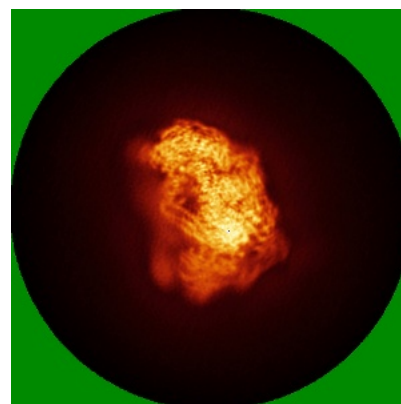
6.4.1 Primary map



X

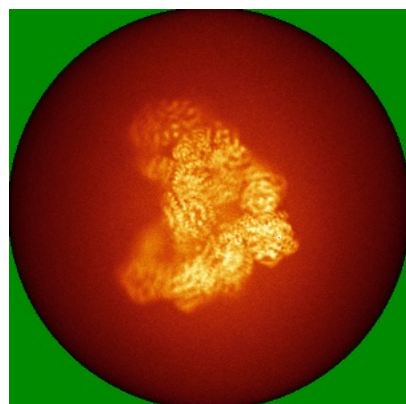


Y

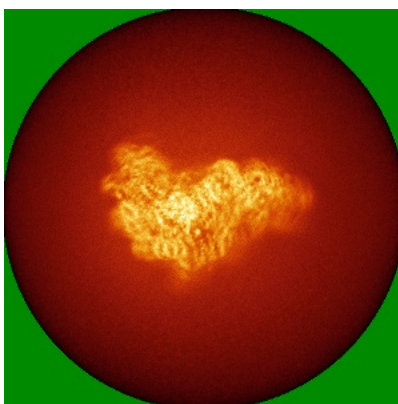


Z

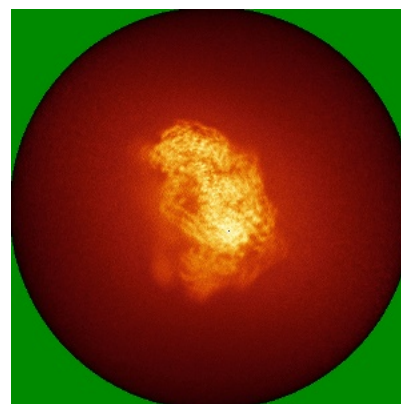
6.4.2 Raw map



X



Y

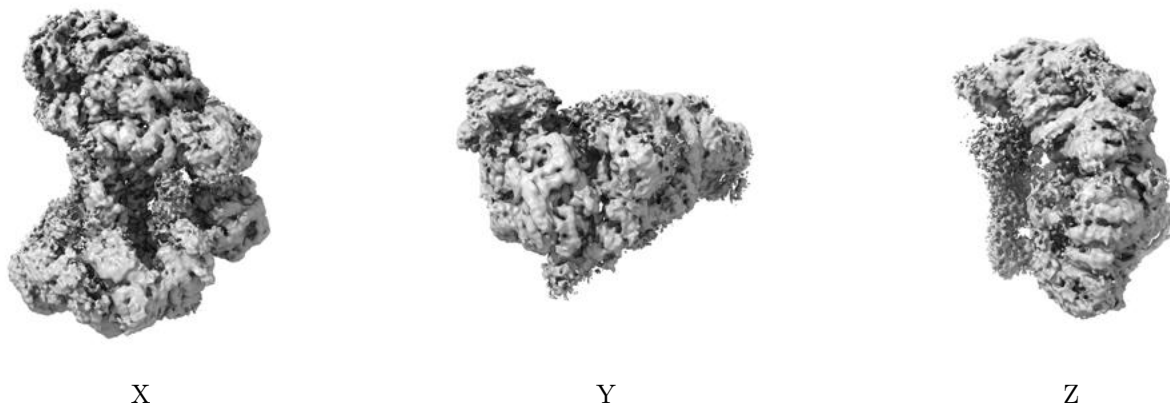


Z

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.

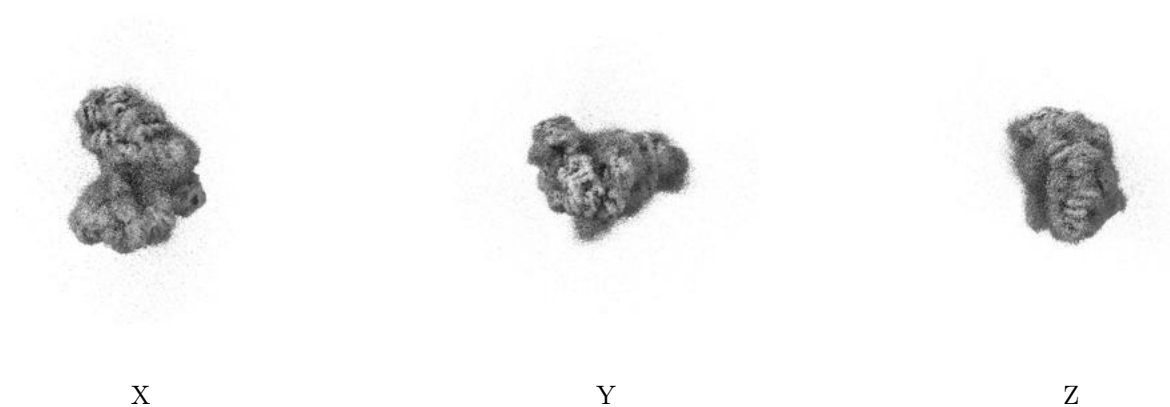
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0026. 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.

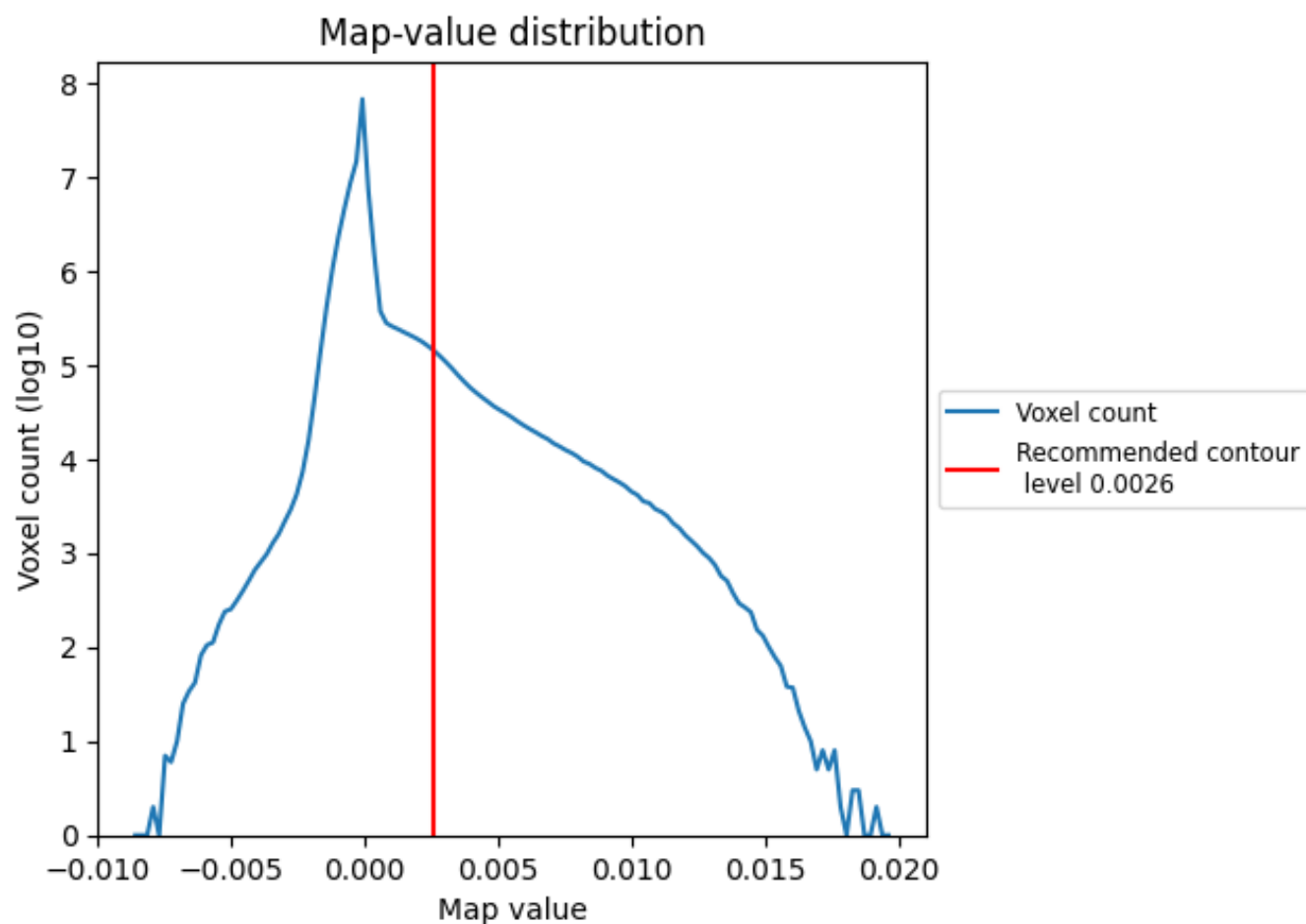
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

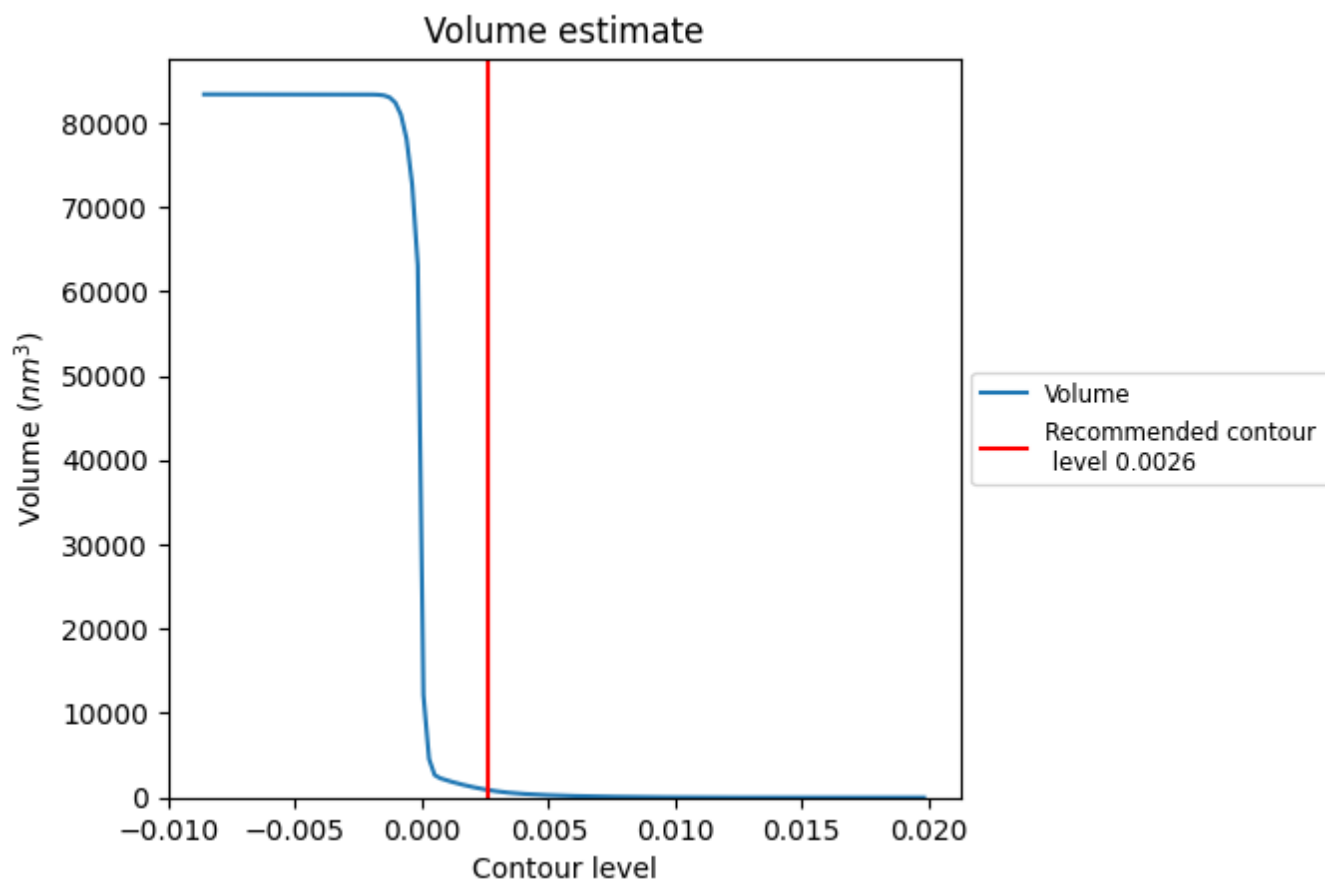
This section contains the results of statistical analysis of the map.

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.

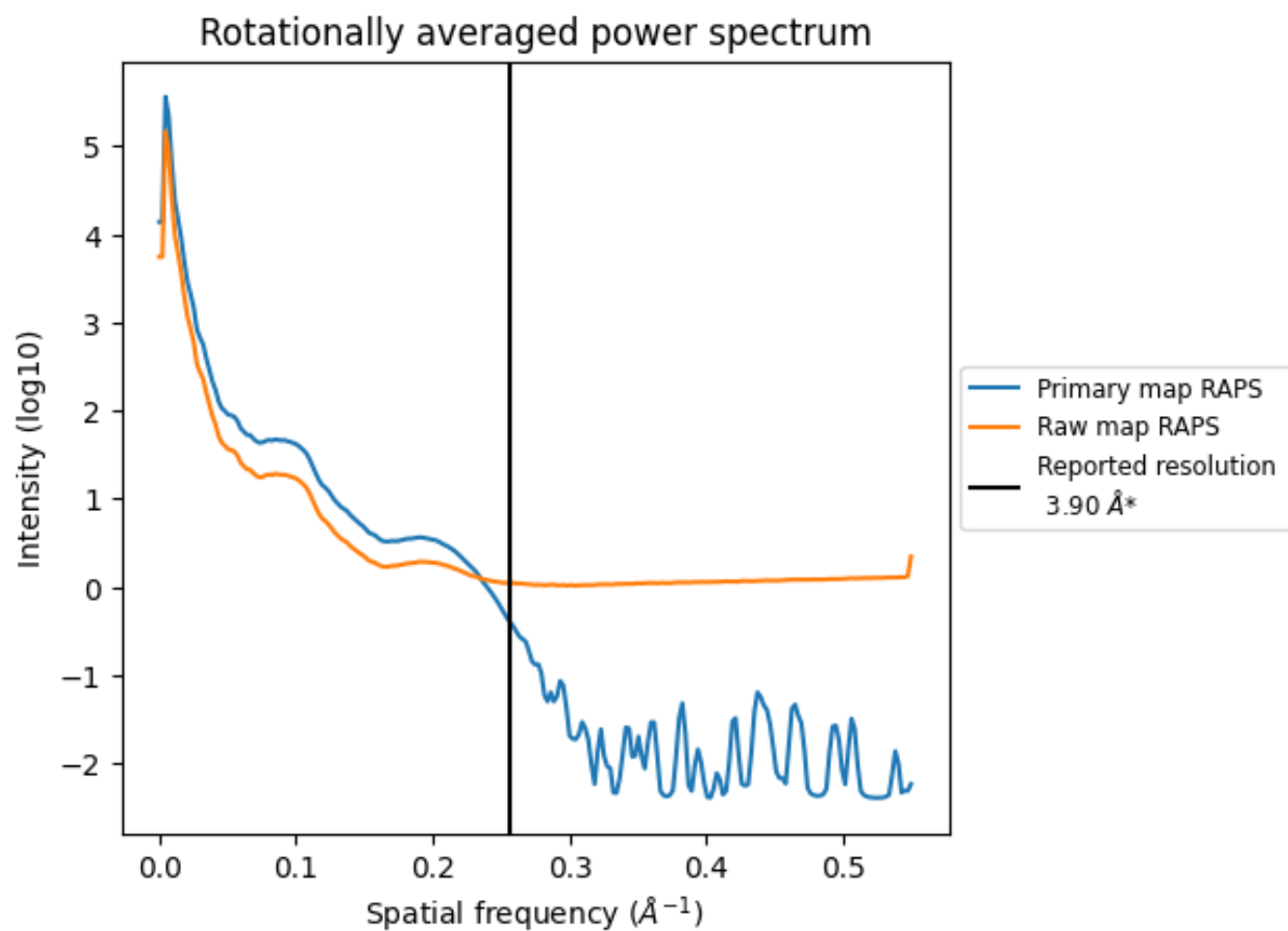
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 906 nm³; this corresponds to an approximate mass of 818 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 ⓘ

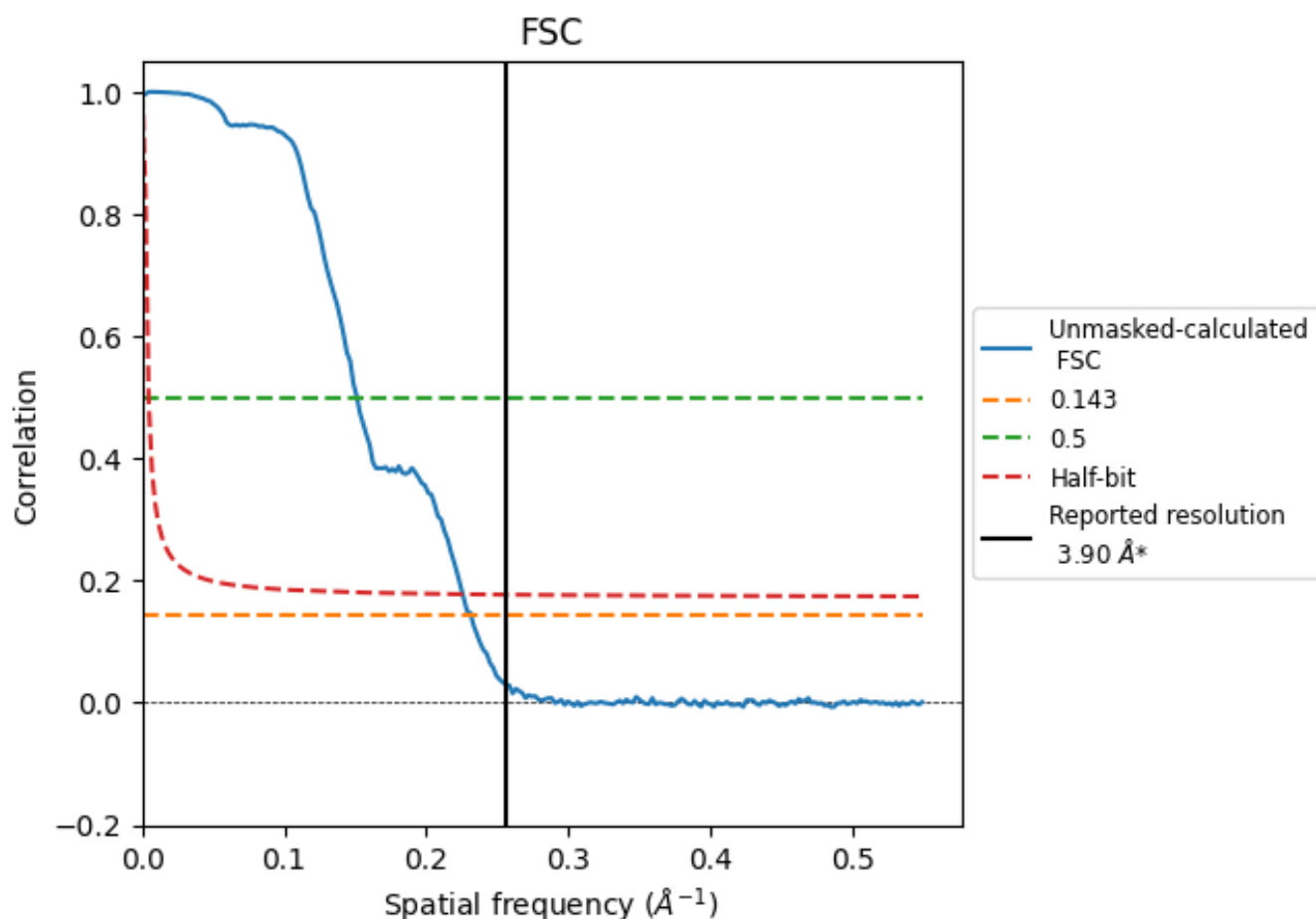


*Reported resolution corresponds to spatial frequency of 0.256 \AA^{-1}

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 0.256 \AA^{-1}

8.2 Resolution estimates [i](#)

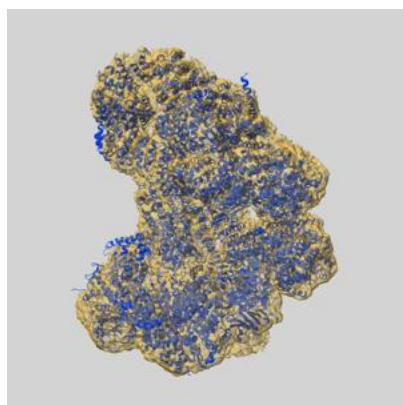
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.32	6.61	4.43

*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 4.32 differs from the reported value 3.9 by more than 10 %

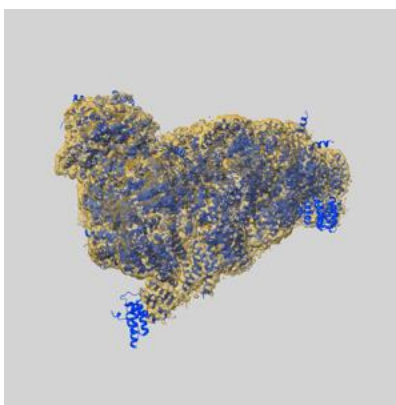
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48928 and PDB model 9N9R. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

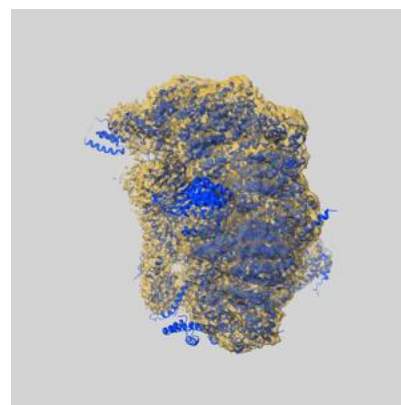
9.1 Map-model overlay [i](#)



X



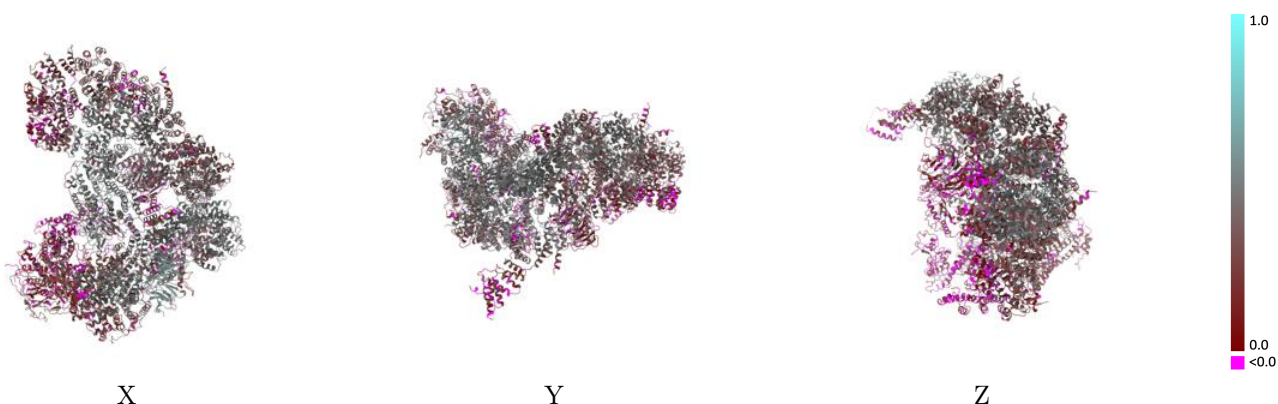
Y



Z

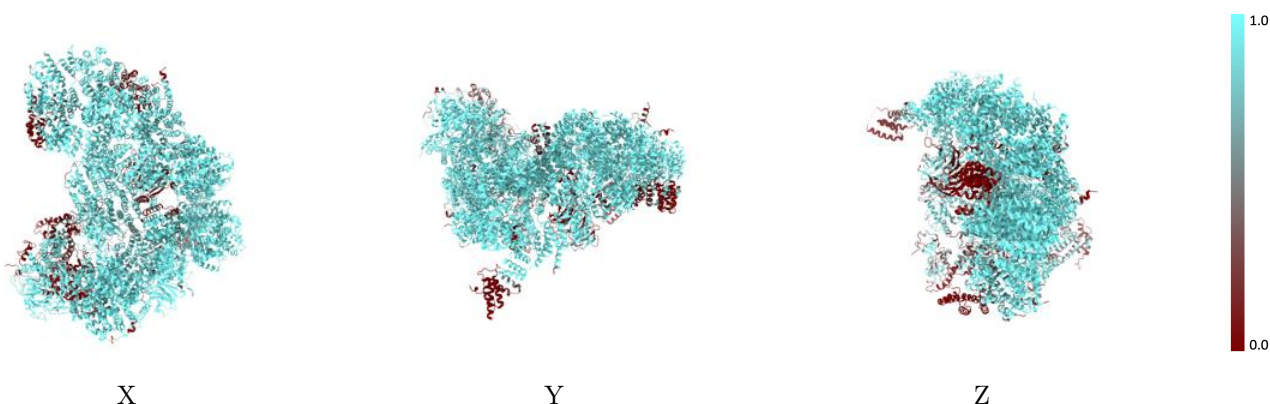
The images above show the 3D surface view of the map at the recommended contour level 0.0026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



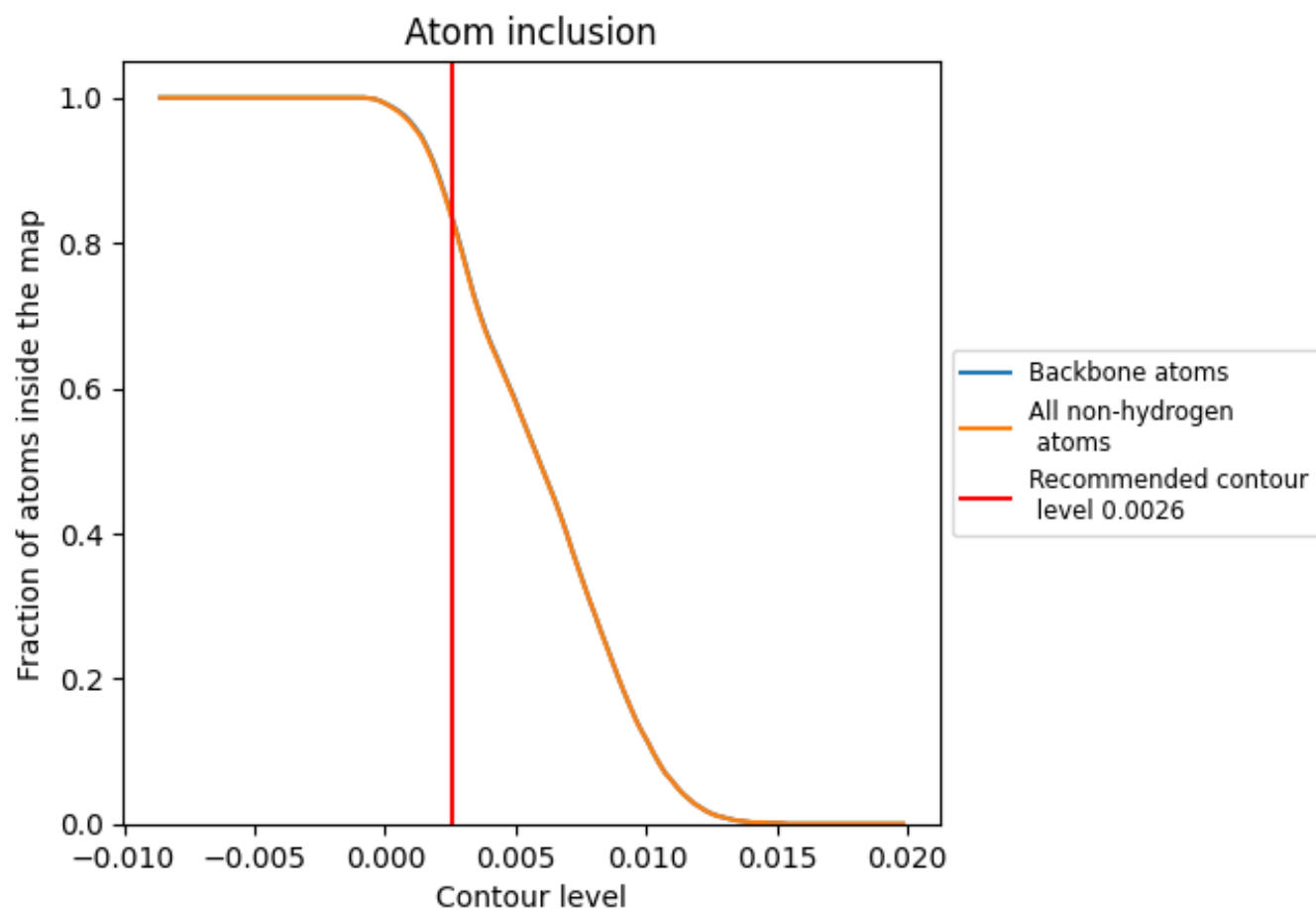
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0026).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% 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 (0.0026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8290	 0.3360
A	 0.8890	 0.3890
C	 0.4730	 0.0800
D	 0.9560	 0.4380
G	 0.9170	 0.4050
H	 0.9400	 0.3130
I	 0.9550	 0.3170
J	 0.9330	 0.3640
K	 0.9650	 0.4070
L	 0.9580	 0.4040
M	 0.5920	 0.3360
N	 0.5150	 0.1510
O	 0.9550	 0.4390
P	 0.9730	 0.4390
Q	 0.7120	 0.0830
R	 0.4080	 0.1620
S	 0.9900	 0.3870
U	 0.8170	 0.3850
V	 0.8980	 0.4160
W	 1.0000	 0.4800
Y	 0.7140	 0.2650
Z	 0.7000	 0.1980

