Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 12:52 pm GMT

PDB ID	:	6QB8
EMDB ID	:	EMD-4489
Title	:	Human CCT:mLST8 complex
Authors	:	Cuellar, J.; Santiago, C.; Ludlam, W.G.; Bueno-Carrasco, M.T.; Valpuesta, J.M.; Willardson, B.M.
Deposited on	:	2018-12-20
Resolution	:	3.97 Å(reported)
Based on initial model	:	5GW5

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

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

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

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

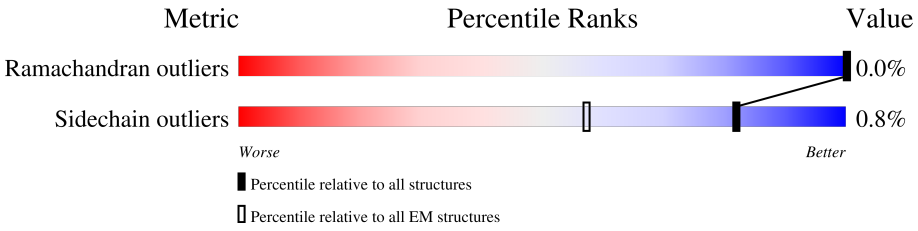
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.97 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	556	88% · 11%
1	a	556	87% · 12%
2	B	535	91% · 8%
2	b	535	89% · 11%
3	D	539	90% · 10%
3	d	539	90% · 9%
4	E	541	92% · 7%
4	e	541	93% · 7%
5	G	544	89% 11%

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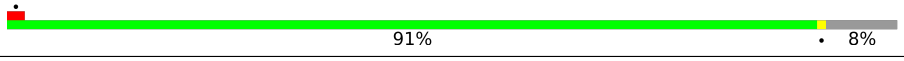
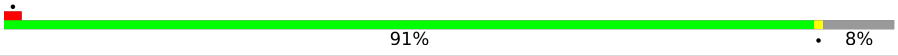
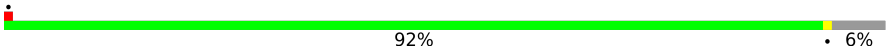
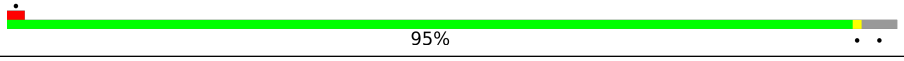
Mol	Chain	Length	Quality of chain
5	g	544	
6	H	543	
6	h	543	
7	Q	548	
7	q	548	
8	Z	531	
8	z	531	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 60035 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	490	Total	C	N	O	S	0	0
			3709	2323	651	713	22		
1	A	494	Total	C	N	O	S	0	0
			3742	2345	656	719	22		

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	478	Total	C	N	O	S	0	0
			3590	2248	630	694	18		
2	B	492	Total	C	N	O	S	0	0
			3698	2311	648	720	19		

- Molecule 3 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	489	Total	C	N	O	S	0	0
			3673	2302	636	714	21		
3	D	487	Total	C	N	O	S	0	0
			3655	2292	634	708	21		

- Molecule 4 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	505	Total	C	N	O	S	0	0
			3882	2422	678	752	30		
4	E	503	Total	C	N	O	S	0	0
			3863	2412	672	749	30		

- Molecule 5 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	477	Total	C	N	O	S	0	0
			3678	2295	654	700	29		
5	G	485	Total	C	N	O	S	0	0
			3741	2335	664	713	29		

- Molecule 6 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	500	Total	C	N	O	S	0	0
			3834	2422	662	727	23		
6	H	499	Total	C	N	O	S	0	0
			3825	2417	661	724	23		

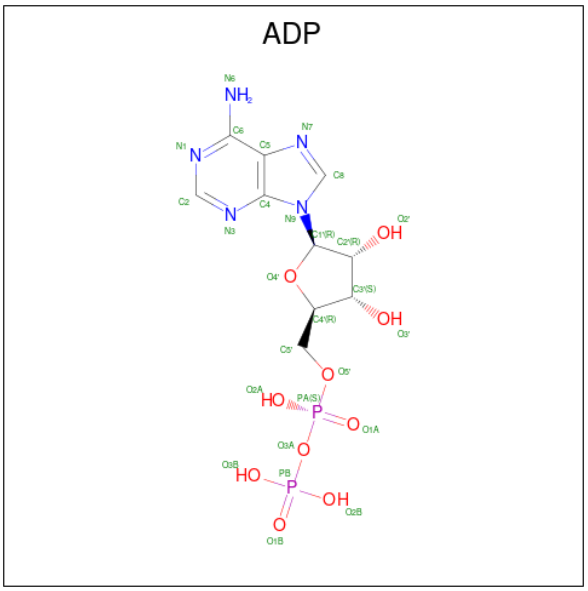
- Molecule 7 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	q	483	Total	C	N	O	S	0	0
			3692	2327	628	712	25		
7	Q	483	Total	C	N	O	S	0	0
			3692	2327	628	712	25		

- Molecule 8 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	z	508	Total	C	N	O	S	0	0
			3894	2447	680	747	20		
8	Z	497	Total	C	N	O	S	0	0
			3813	2395	670	728	20		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



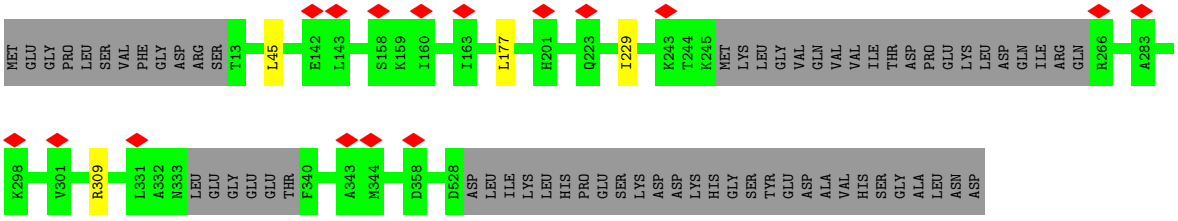
Mol	Chain	Residues	Atoms					AltConf
9	q	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	Q	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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

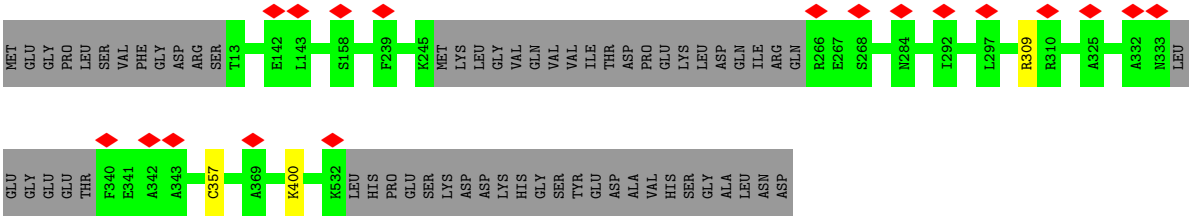
• Molecule 1: T-complex protein 1 subunit alpha

Chain a:



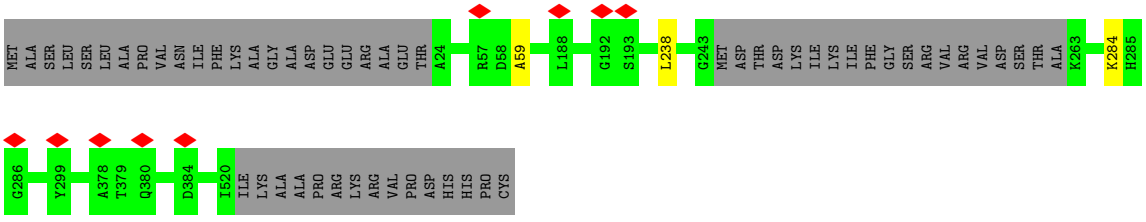
• Molecule 1: T-complex protein 1 subunit alpha

Chain A:



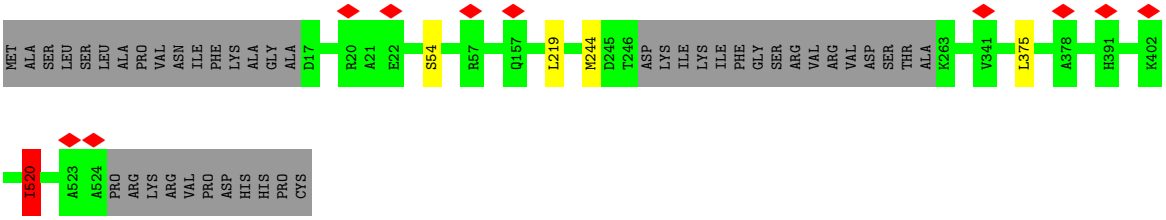
• Molecule 2: T-complex protein 1 subunit beta

Chain b:

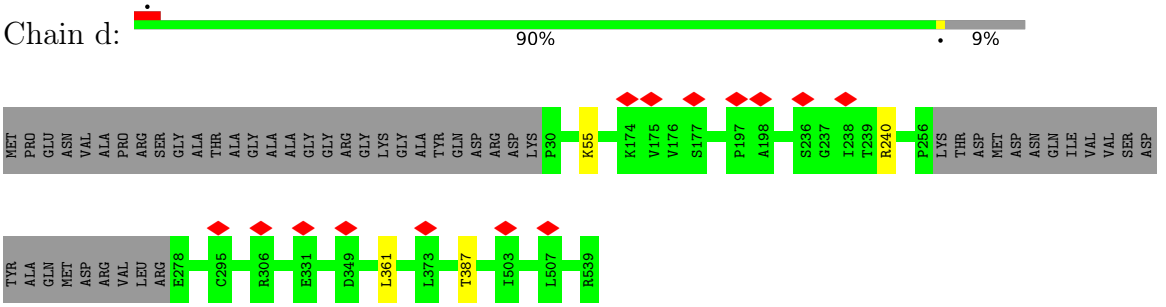


• Molecule 2: T-complex protein 1 subunit beta

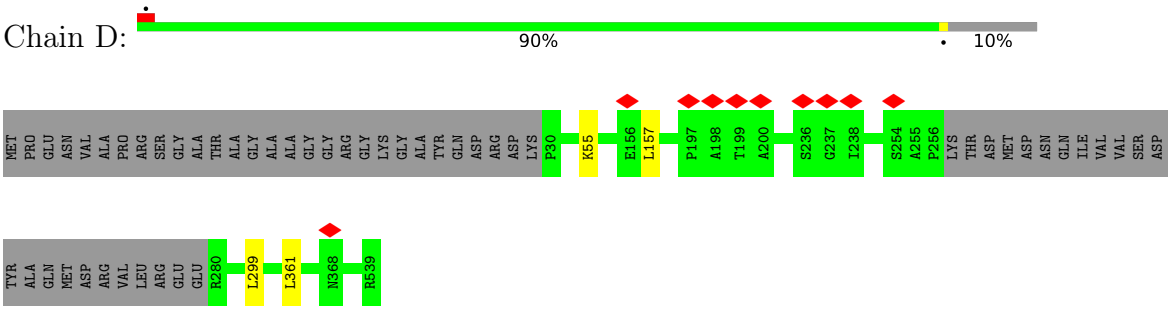
Chain B:



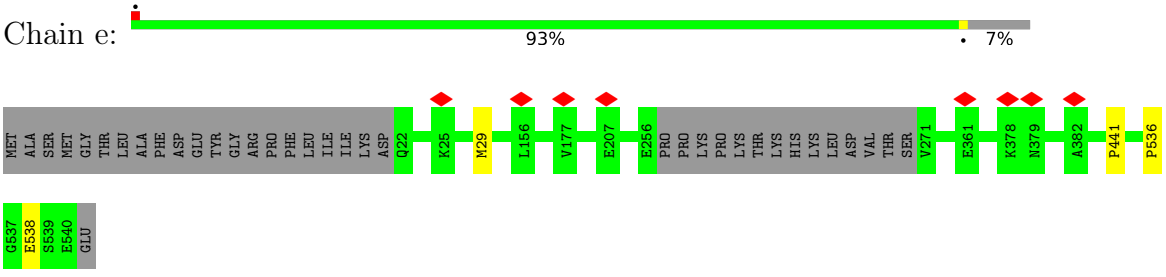
• Molecule 3: T-complex protein 1 subunit delta



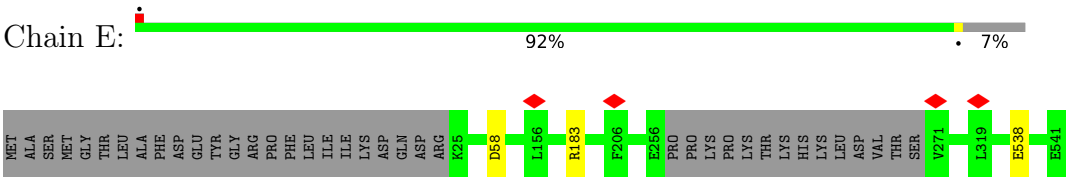
• Molecule 3: T-complex protein 1 subunit delta



• Molecule 4: T-complex protein 1 subunit epsilon

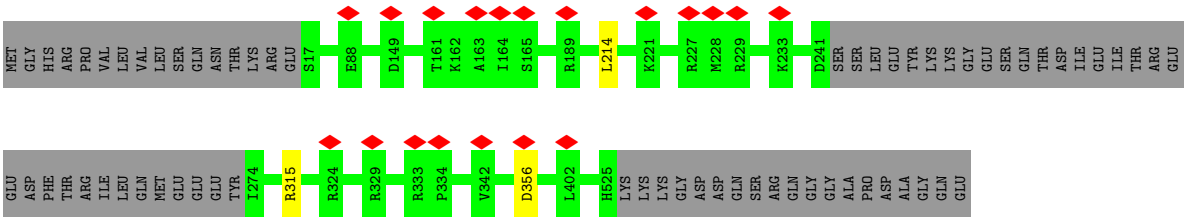


• Molecule 4: T-complex protein 1 subunit epsilon



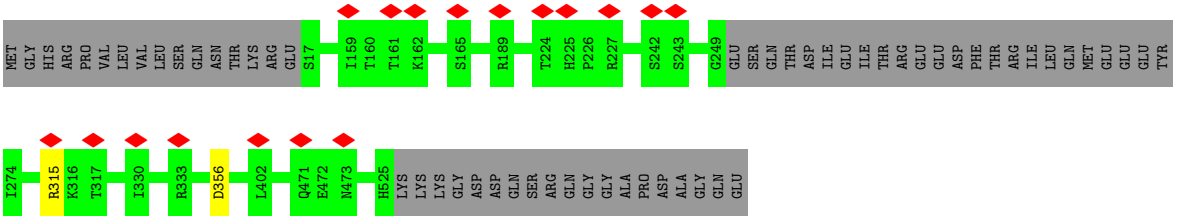
• Molecule 5: T-complex protein 1 subunit gamma

Chain g:



• Molecule 5: T-complex protein 1 subunit gamma

Chain G:

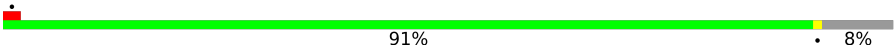


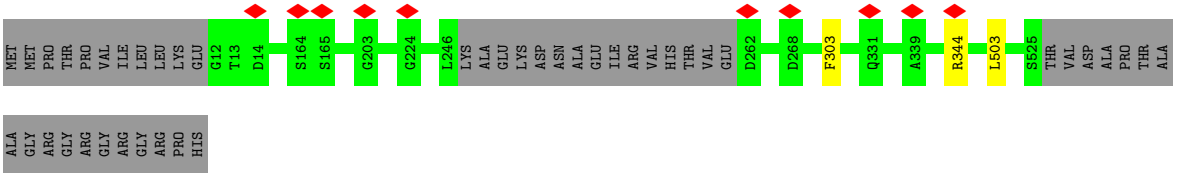
• Molecule 6: T-complex protein 1 subunit eta

Chain h:

• Molecule 6: T-complex protein 1 subunit eta

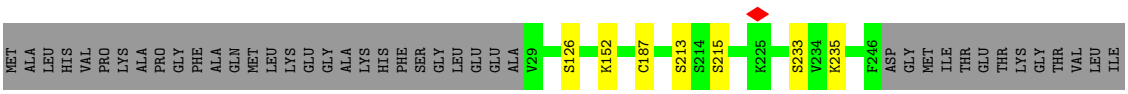
Chain H:

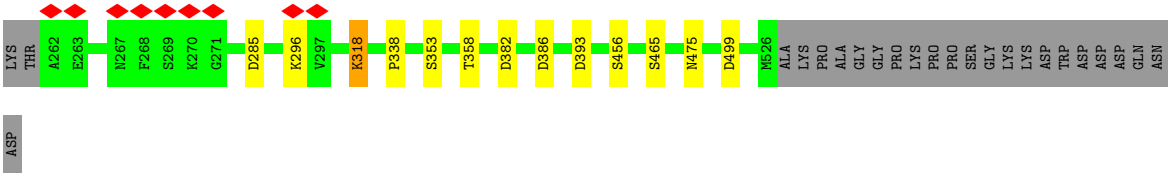




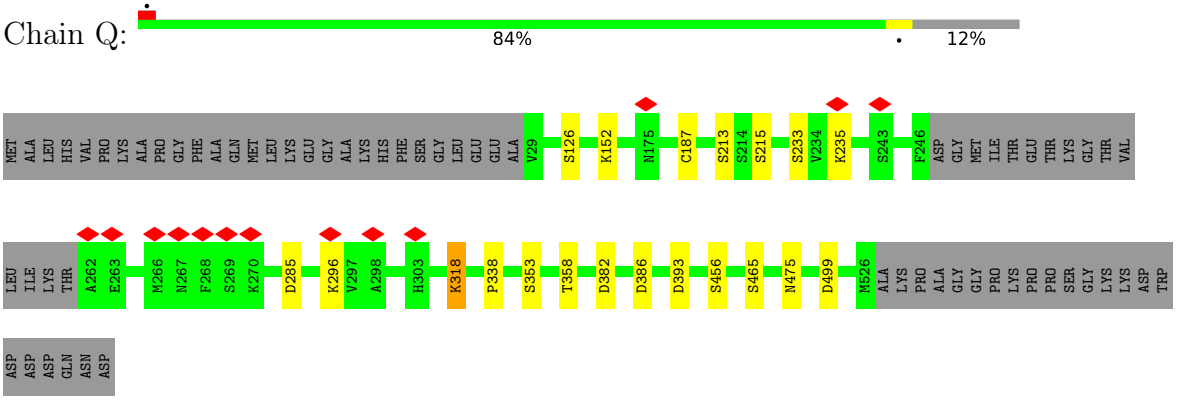
• Molecule 7: T-complex protein 1 subunit theta

Chain q:

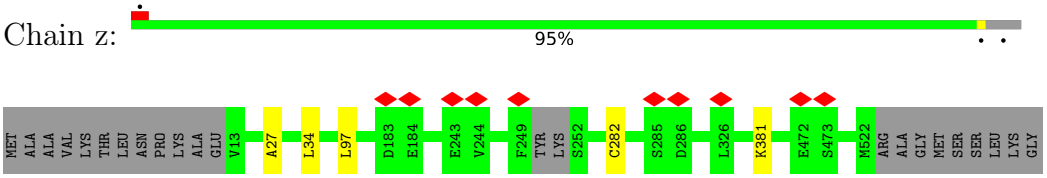




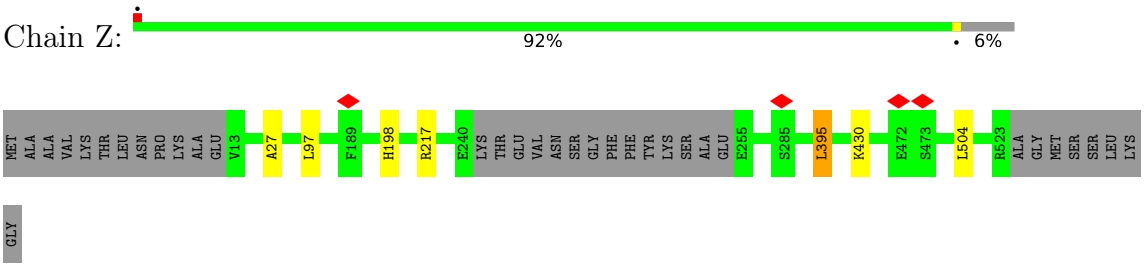
• Molecule 7: T-complex protein 1 subunit theta



• Molecule 8: T-complex protein 1 subunit zeta



• Molecule 8: T-complex protein 1 subunit zeta



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	452000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	36	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.533	Depositor
Minimum map value	-0.670	Depositor
Average map value	0.042	Depositor
Map value standard deviation	0.162	Depositor
Recommended contour level	0.36	Depositor
Map size (Å)	274.0, 274.0, 274.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.28	0/3775	0.53	1/5093 (0.0%)
1	a	0.28	0/3742	0.55	2/5049 (0.0%)
2	B	0.29	0/3736	0.58	3/5036 (0.1%)
2	b	0.28	0/3628	0.57	1/4891 (0.0%)
3	D	0.28	0/3684	0.57	3/4972 (0.1%)
3	d	0.29	0/3702	0.55	1/4996 (0.0%)
4	E	0.29	0/3904	0.56	0/5256
4	e	0.28	0/3923	0.55	0/5281
5	G	0.29	0/3783	0.54	1/5104 (0.0%)
5	g	0.29	0/3719	0.56	2/5020 (0.0%)
6	H	0.29	0/3878	0.53	0/5232
6	h	0.29	0/3887	0.54	1/5244 (0.0%)
7	Q	0.29	0/3742	0.54	1/5059 (0.0%)
7	q	0.29	0/3742	0.55	1/5059 (0.0%)
8	Z	0.29	0/3855	0.54	3/5197 (0.1%)
8	z	0.30	0/3938	0.57	3/5309 (0.1%)
All	All	0.29	0/60638	0.55	23/81798 (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
2	B	0	3
2	b	0	1
3	d	0	1
4	E	0	2
4	e	0	5
6	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	h	0	3
7	Q	0	2
7	q	0	2
8	Z	0	2
8	z	0	1
All	All	0	24

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	g	356	ASP	CB-CG-OD2	8.33	125.79	118.30
8	z	34	LEU	CA-CB-CG	-7.70	97.59	115.30
3	D	157	LEU	CA-CB-CG	7.05	131.52	115.30
2	B	219	LEU	CA-CB-CG	7.00	131.40	115.30
7	Q	318	LYS	CD-CE-NZ	6.18	125.92	111.70
7	q	318	LYS	CD-CE-NZ	6.17	125.90	111.70
8	Z	504	LEU	CA-CB-CG	6.04	129.18	115.30
8	Z	395	LEU	CA-CB-CG	5.99	129.09	115.30
2	B	520	ILE	CG1-CB-CG2	-5.92	98.38	111.40
5	g	214	LEU	CA-CB-CG	5.91	128.89	115.30
3	d	361	LEU	CA-CB-CG	5.88	128.83	115.30
6	h	378	LEU	CA-CB-CG	5.72	128.45	115.30
8	z	97	LEU	CA-CB-CG	5.69	128.39	115.30
1	A	357	CYS	CA-CB-SG	5.67	124.20	114.00
2	B	375	LEU	CA-CB-CG	5.63	128.25	115.30
5	G	356	ASP	CB-CG-OD2	5.62	123.36	118.30
3	D	361	LEU	CA-CB-CG	5.55	128.06	115.30
1	a	45	LEU	CA-CB-CG	5.43	127.80	115.30
2	b	238	LEU	CA-CB-CG	5.43	127.78	115.30
8	Z	97	LEU	CA-CB-CG	5.26	127.39	115.30
8	z	282	CYS	CA-CB-SG	5.13	123.24	114.00
3	D	299	LEU	CA-CB-CG	5.02	126.84	115.30
1	a	177	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	244	MET	Peptide
2	B	520	ILE	Peptide

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Mol	Chain	Res	Type	Group
2	B	54	SER	Peptide
4	E	538	GLU	Peptide
4	E	58	ASP	Peptide
6	H	303	PHE	Peptide
7	Q	338	PRO	Peptide
7	Q	475	ASN	Peptide
8	Z	198	HIS	Peptide
8	Z	27	ALA	Mainchain
1	a	229	ILE	Peptide
2	b	59	ALA	Peptide
3	d	387	THR	Peptide
4	e	29	MET	Peptide
4	e	441	PRO	Peptide
4	e	536	PRO	Peptide
4	e	538	GLU	Peptide,Mainchain
6	h	318	VAL	Peptide
6	h	527	PRO	Peptide,Mainchain
7	q	338	PRO	Peptide
7	q	475	ASN	Peptide
8	z	27	ALA	Mainchain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	488/556 (88%)	453 (93%)	35 (7%)	0	100	100
1	a	484/556 (87%)	450 (93%)	34 (7%)	0	100	100
2	B	488/535 (91%)	447 (92%)	41 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	474/535 (89%)	432 (91%)	42 (9%)	0	100	100
3	D	483/539 (90%)	440 (91%)	43 (9%)	0	100	100
3	d	485/539 (90%)	452 (93%)	33 (7%)	0	100	100
4	E	499/541 (92%)	448 (90%)	51 (10%)	0	100	100
4	e	501/541 (93%)	448 (89%)	53 (11%)	0	100	100
5	G	481/544 (88%)	443 (92%)	38 (8%)	0	100	100
5	g	473/544 (87%)	438 (93%)	35 (7%)	0	100	100
6	H	495/543 (91%)	453 (92%)	42 (8%)	0	100	100
6	h	496/543 (91%)	452 (91%)	44 (9%)	0	100	100
7	Q	479/548 (87%)	441 (92%)	38 (8%)	0	100	100
7	q	479/548 (87%)	441 (92%)	38 (8%)	0	100	100
8	Z	493/531 (93%)	453 (92%)	39 (8%)	1 (0%)	47	79
8	z	504/531 (95%)	471 (94%)	33 (6%)	0	100	100
All	All	7802/8674 (90%)	7162 (92%)	639 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	Z	430	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	409/463 (88%)	407 (100%)	2 (0%)	88	93
1	a	405/463 (88%)	404 (100%)	1 (0%)	93	96
2	B	391/427 (92%)	390 (100%)	1 (0%)	92	95
2	b	380/427 (89%)	379 (100%)	1 (0%)	92	95
3	D	413/452 (91%)	412 (100%)	1 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	d	415/452 (92%)	413 (100%)	2 (0%)	88 93
4	E	422/456 (92%)	421 (100%)	1 (0%)	93 96
4	e	424/456 (93%)	424 (100%)	0	100 100
5	G	416/468 (89%)	415 (100%)	1 (0%)	93 96
5	g	409/468 (87%)	408 (100%)	1 (0%)	93 96
6	H	408/443 (92%)	406 (100%)	2 (0%)	88 93
6	h	409/443 (92%)	407 (100%)	2 (0%)	88 93
7	Q	402/452 (89%)	384 (96%)	18 (4%)	27 54
7	q	402/452 (89%)	384 (96%)	18 (4%)	27 54
8	Z	416/442 (94%)	414 (100%)	2 (0%)	88 93
8	z	425/442 (96%)	424 (100%)	1 (0%)	93 96
All	All	6546/7206 (91%)	6492 (99%)	54 (1%)	82 88

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	309	ARG
2	b	284	LYS
3	d	55	LYS
3	d	240	ARG
5	g	315	ARG
6	h	53	ARG
6	h	507	LEU
7	q	126	SER
7	q	152	LYS
7	q	187	CYS
7	q	213	SER
7	q	215	SER
7	q	233	SER
7	q	235	LYS
7	q	285	ASP
7	q	296	LYS
7	q	318	LYS
7	q	353	SER
7	q	358	THR
7	q	382	ASP
7	q	386	ASP
7	q	393	ASP

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Mol	Chain	Res	Type
7	q	456	SER
7	q	465	SER
7	q	499	ASP
8	z	381	LYS
1	A	309	ARG
1	A	400	LYS
2	B	520	ILE
3	D	55	LYS
4	E	183	ARG
5	G	315	ARG
6	H	344	ARG
6	H	503	LEU
7	Q	126	SER
7	Q	152	LYS
7	Q	187	CYS
7	Q	213	SER
7	Q	215	SER
7	Q	233	SER
7	Q	235	LYS
7	Q	285	ASP
7	Q	296	LYS
7	Q	318	LYS
7	Q	353	SER
7	Q	358	THR
7	Q	382	ASP
7	Q	386	ASP
7	Q	393	ASP
7	Q	456	SER
7	Q	465	SER
7	Q	499	ASP
8	Z	217	ARG
8	Z	395	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	135	ASN
1	a	164	ASN
1	a	353	GLN
1	a	472	ASN
2	b	174	HIS
2	b	175	HIS

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Mol	Chain	Res	Type
2	b	285	HIS
2	b	292	ASN
2	b	298	ASN
2	b	426	ASN
2	b	453	ASN
2	b	473	ASN
3	d	172	ASN
3	d	231	GLN
3	d	318	ASN
3	d	472	ASN
4	e	290	GLN
4	e	495	HIS
5	g	25	ASN
5	g	275	GLN
5	g	300	GLN
5	g	405	GLN
5	g	433	GLN
5	g	480	ASN
5	g	503	GLN
6	h	30	GLN
6	h	245	ASN
6	h	335	GLN
6	h	384	GLN
6	h	505	ASN
7	q	41	GLN
7	q	145	ASN
7	q	219	HIS
7	q	274	ASN
7	q	306	ASN
7	q	383	ASN
7	q	461	ASN
8	z	68	GLN
8	z	84	GLN
8	z	105	GLN
8	z	346	HIS
8	z	460	GLN
1	A	30	ASN
1	A	135	ASN
1	A	139	ASN
1	A	150	ASN
1	A	193	ASN
1	A	196	ASN

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Mol	Chain	Res	Type
1	A	242	GLN
1	A	276	GLN
1	A	472	ASN
2	B	78	ASN
3	D	37	ASN
3	D	85	HIS
3	D	172	ASN
3	D	231	GLN
3	D	318	ASN
3	D	472	ASN
4	E	37	HIS
4	E	86	GLN
4	E	98	GLN
4	E	191	ASN
4	E	311	ASN
4	E	312	HIS
4	E	316	GLN
4	E	411	ASN
4	E	481	GLN
5	G	25	ASN
5	G	156	ASN
5	G	405	GLN
5	G	480	ASN
6	H	25	ASN
6	H	119	GLN
6	H	134	ASN
6	H	241	ASN
7	Q	41	GLN
7	Q	145	ASN
7	Q	219	HIS
7	Q	274	ASN
7	Q	306	ASN
7	Q	383	ASN
8	Z	37	ASN
8	Z	65	HIS
8	Z	84	GLN
8	Z	497	ASN
8	Z	514	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	ADP	q	5000	-	24,29,29	0.91	1 (4%)	29,45,45	1.50	4 (13%)
9	ADP	Q	5000	-	24,29,29	0.90	1 (4%)	29,45,45	1.51	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	q	5000	-	-	2/12/32/32	0/3/3/3
9	ADP	Q	5000	-	-	2/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Q	5000	ADP	C5-C4	2.24	1.46	1.40
9	q	5000	ADP	C5-C4	2.23	1.46	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Q	5000	ADP	PA-O3A-PB	-4.07	118.87	132.83
9	q	5000	ADP	PA-O3A-PB	-4.06	118.90	132.83
9	Q	5000	ADP	N3-C2-N1	-3.45	123.29	128.68
9	q	5000	ADP	N3-C2-N1	-3.40	123.36	128.68
9	q	5000	ADP	C4-C5-N7	-2.63	106.65	109.40
9	Q	5000	ADP	C4-C5-N7	-2.61	106.67	109.40
9	q	5000	ADP	C3'-C2'-C1'	2.47	104.70	100.98
9	Q	5000	ADP	C3'-C2'-C1'	2.46	104.69	100.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

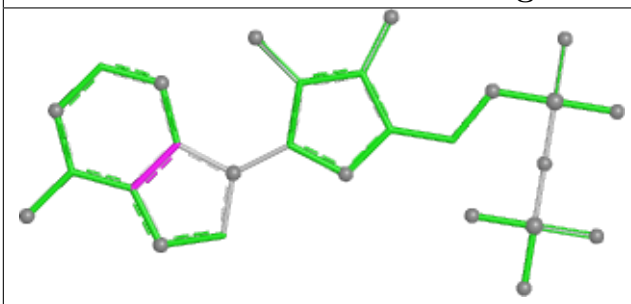
Mol	Chain	Res	Type	Atoms
9	q	5000	ADP	C5'-O5'-PA-O2A
9	q	5000	ADP	C5'-O5'-PA-O3A
9	Q	5000	ADP	C5'-O5'-PA-O3A
9	Q	5000	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

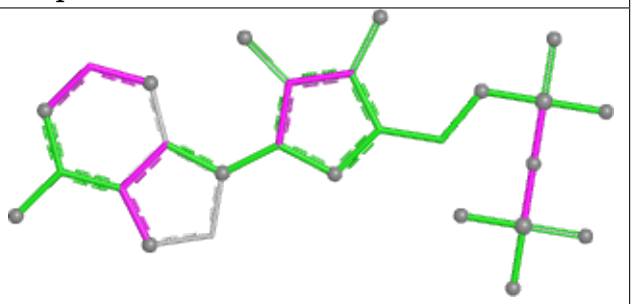
No monomer is involved in short contacts.

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

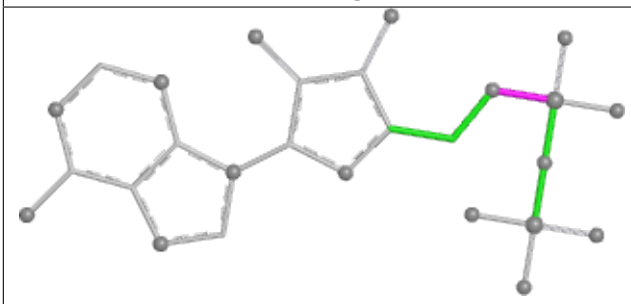
Ligand ADP q 5000



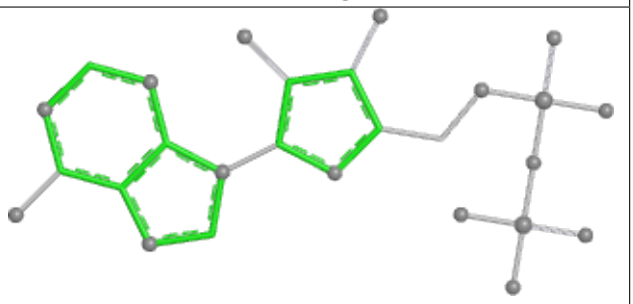
Bond lengths



Bond angles

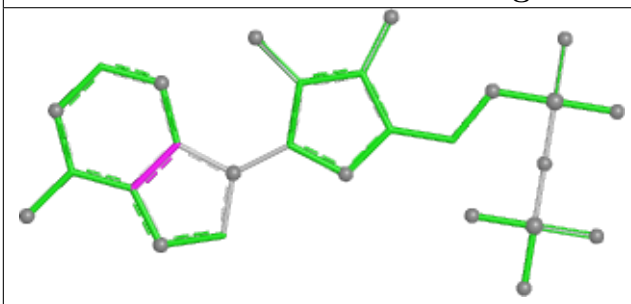


Torsions

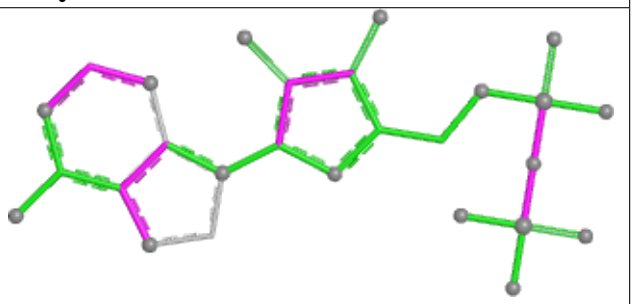


Rings

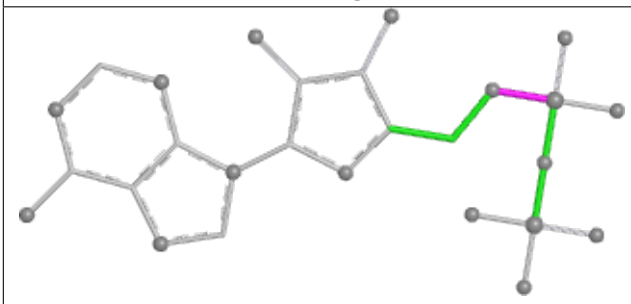
Ligand ADP Q 5000



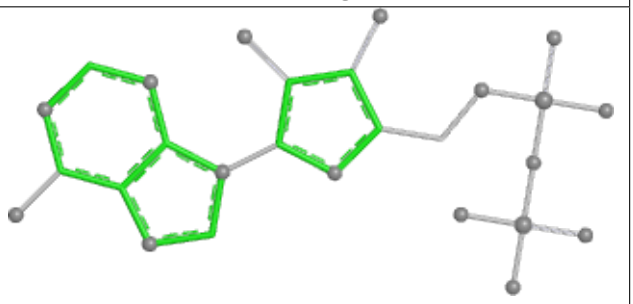
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

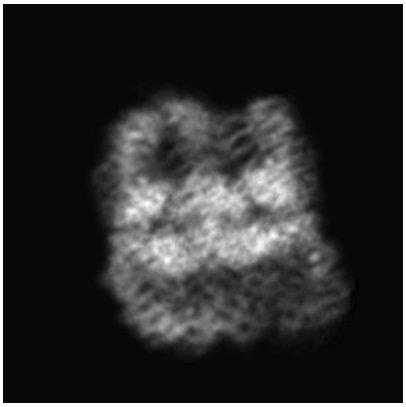
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4489. These allow visual inspection of the internal detail of the map and identification of artifacts.

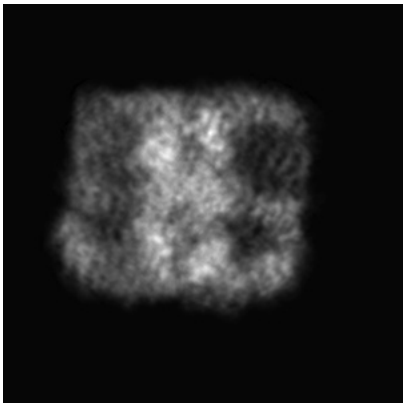
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

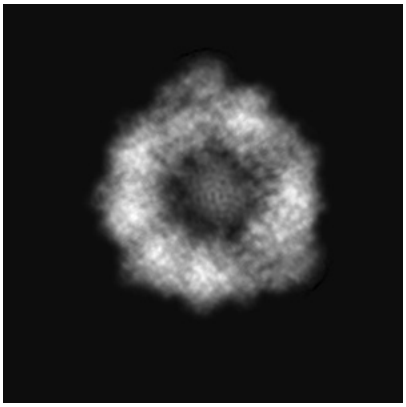
6.1.1 Primary map



X



Y

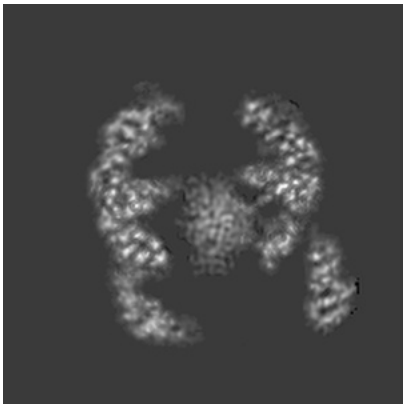


Z

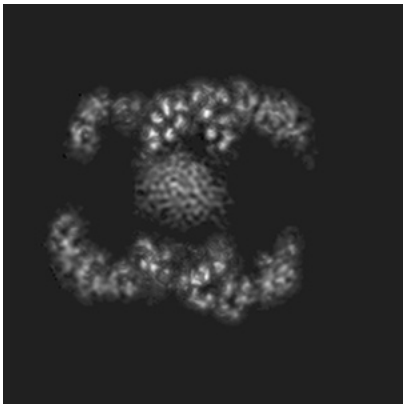
The images above show the map projected in three orthogonal directions.

6.2 Central slices

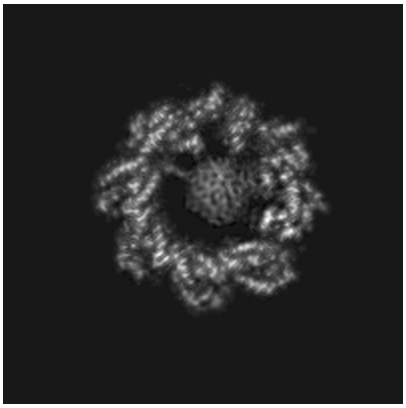
6.2.1 Primary map



X Index: 100



Y Index: 100

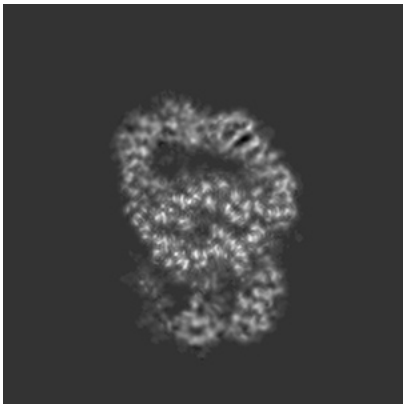


Z Index: 100

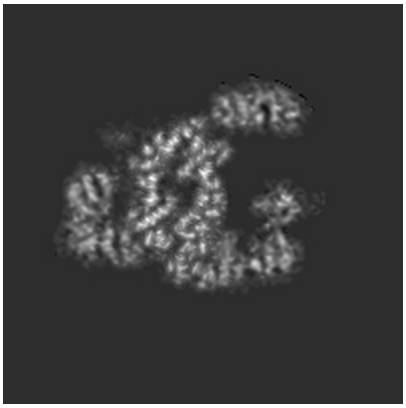
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

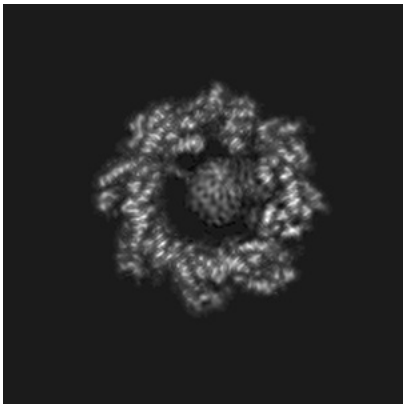
6.3.1 Primary map



X Index: 69



Y Index: 70



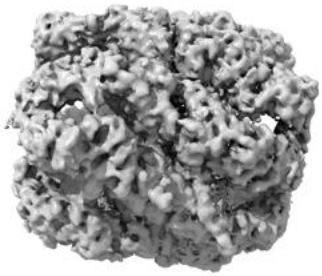
Z Index: 101

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

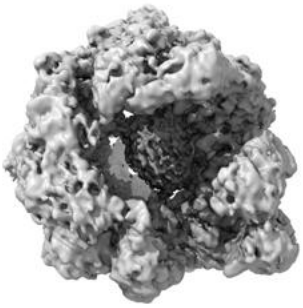
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.36. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

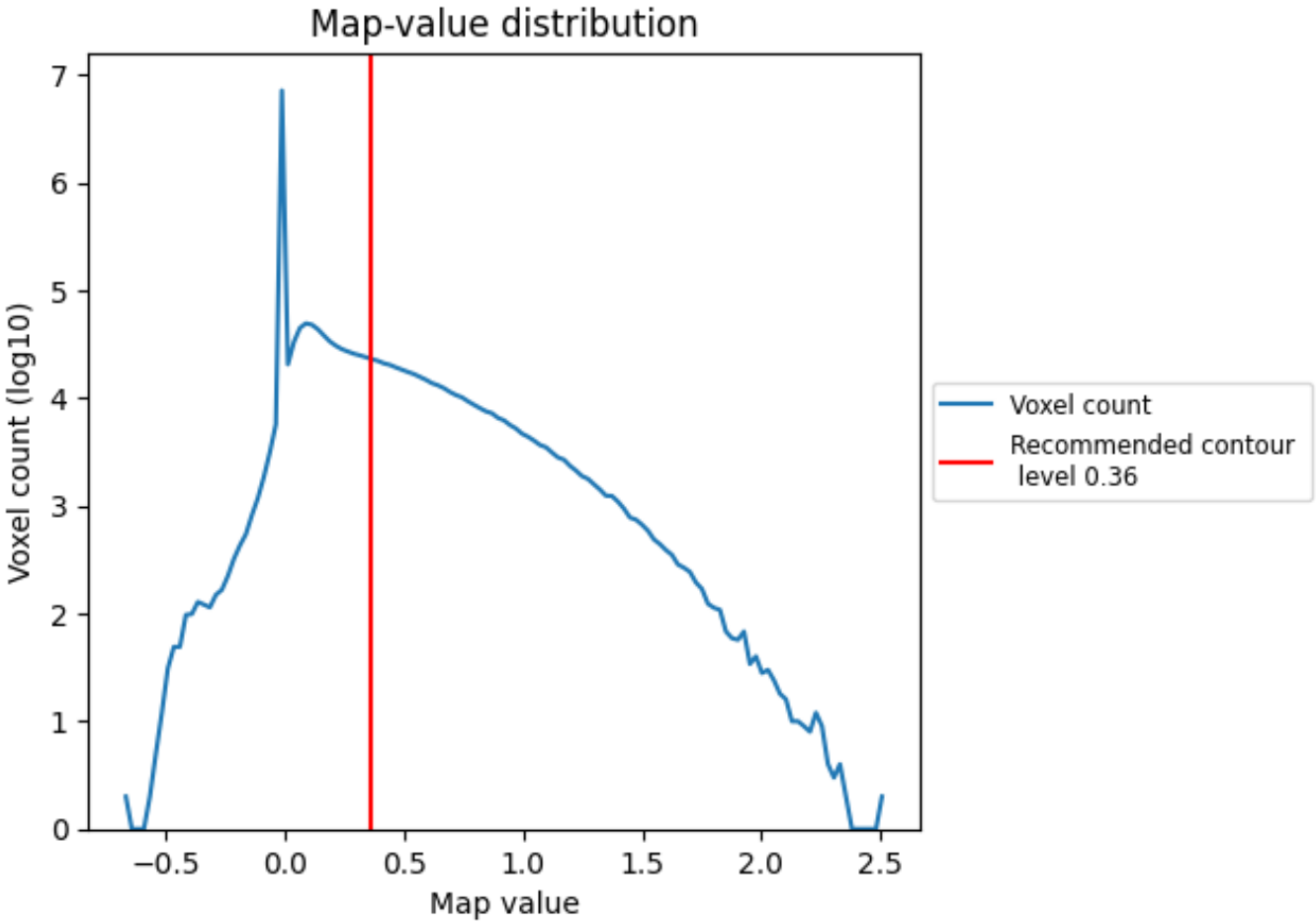
6.5 Mask visualisation (i)

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

7 Map analysis

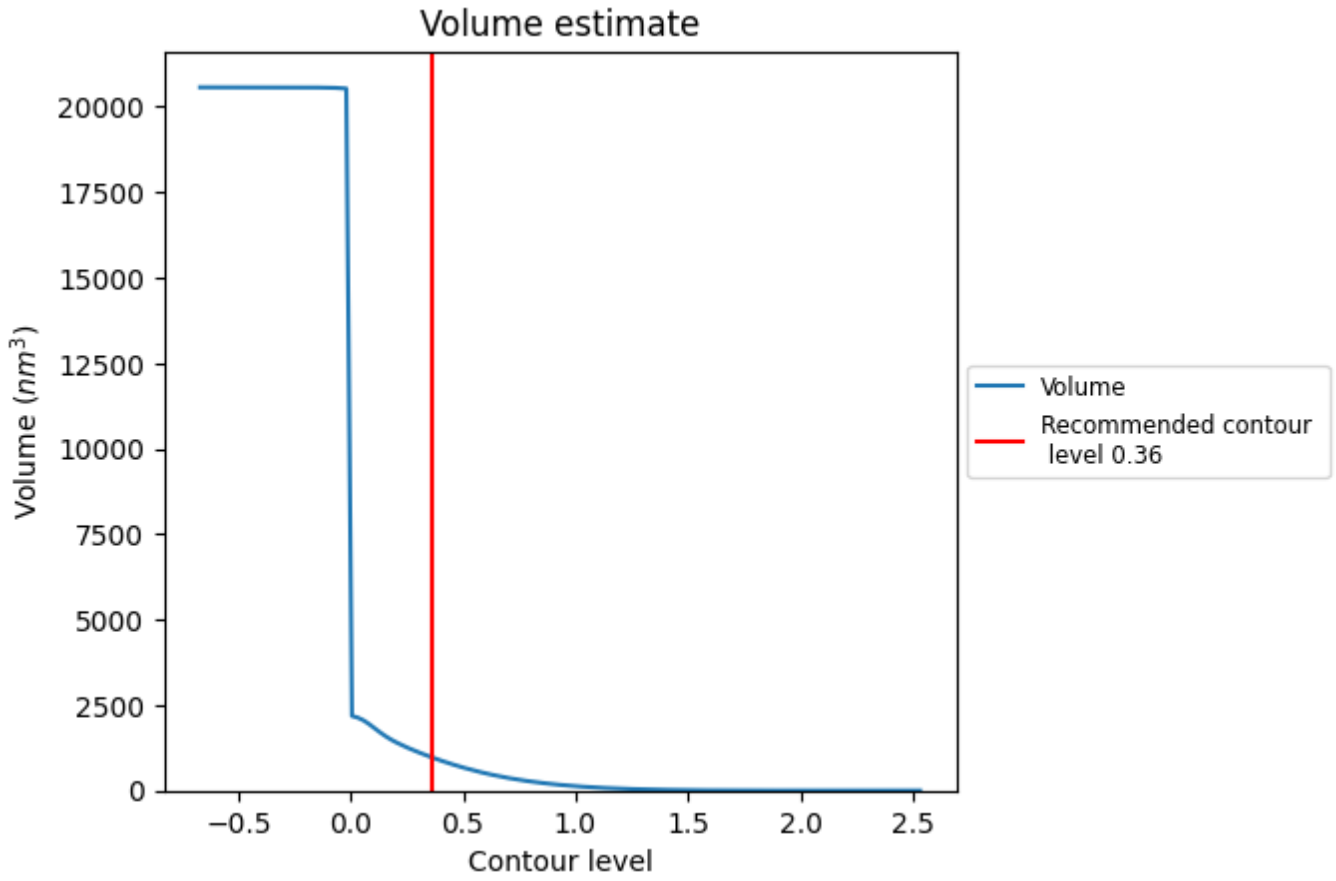
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

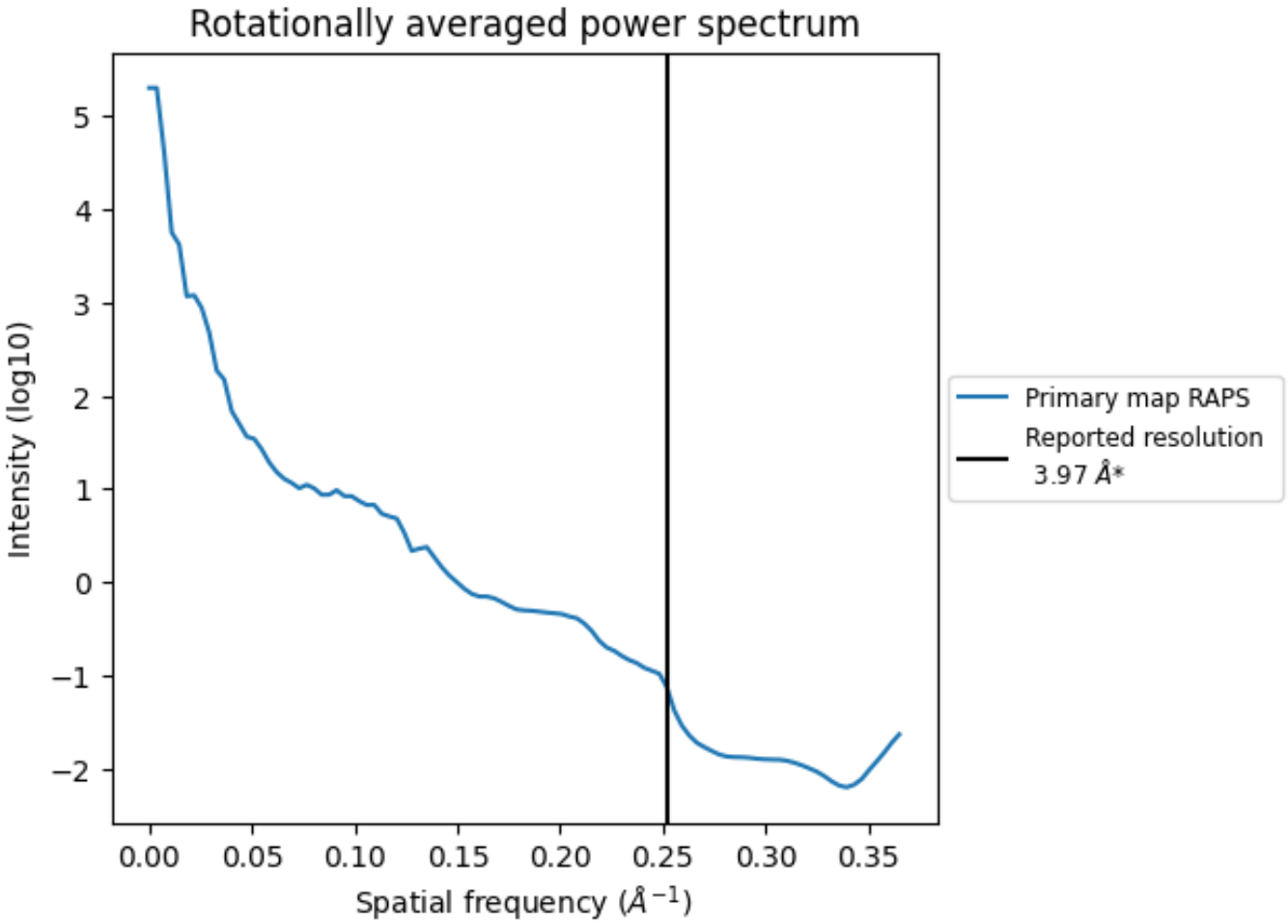
7.2 Volume estimate



The volume at the recommended contour level is 974 nm^3; this corresponds to an approximate mass of 880 kDa.

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

7.3 Rotationally averaged power spectrum (i)

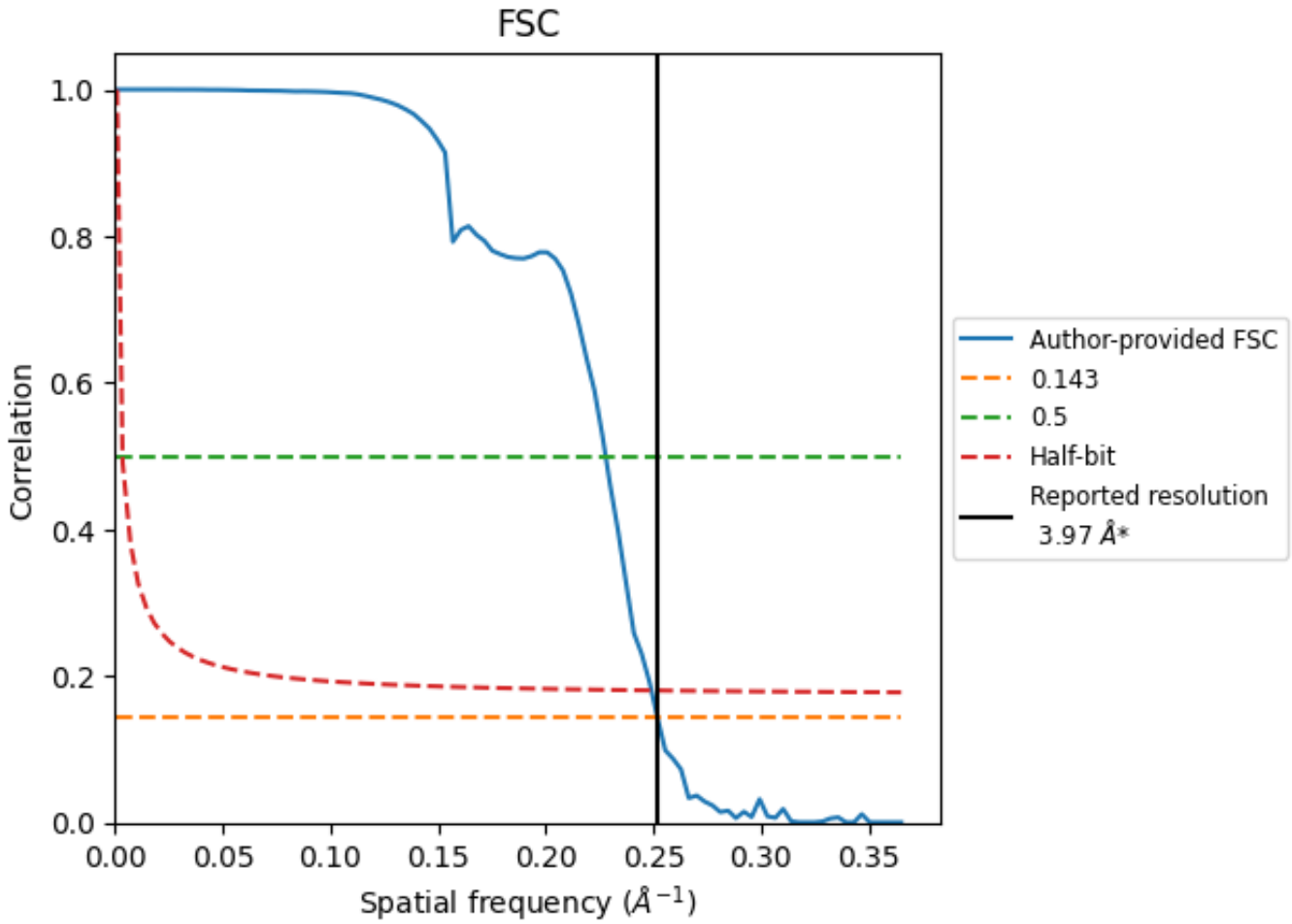


*Reported resolution corresponds to spatial frequency of 0.252 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.252 Å^{-1}

8.2 Resolution estimates (i)

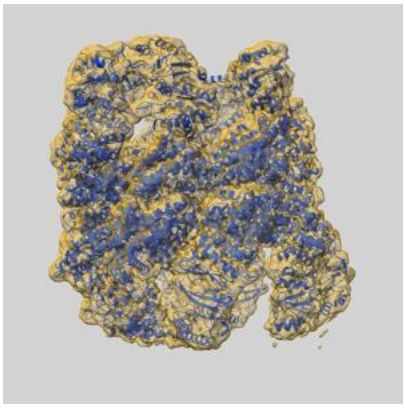
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.97	-	-
Author-provided FSC curve	3.97	4.39	4.02
Unmasked-calculated*	-	-	-

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

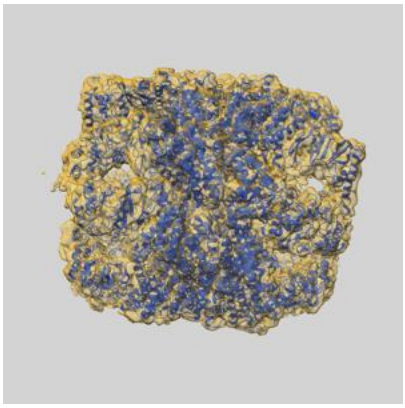
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4489 and PDB model 6QB8. Per-residue inclusion information can be found in section 3 on page 7.

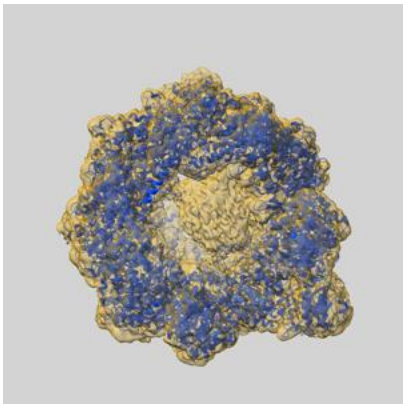
9.1 Map-model overlay



X



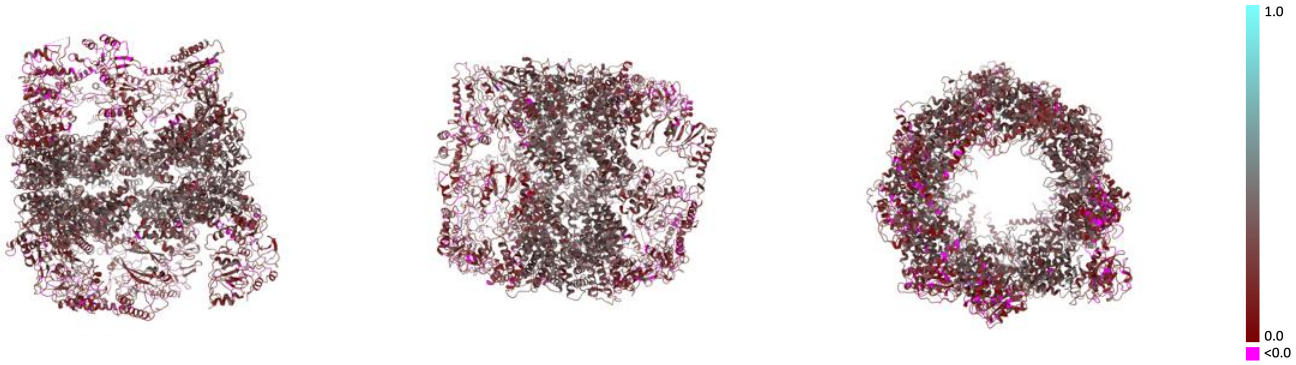
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.36 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

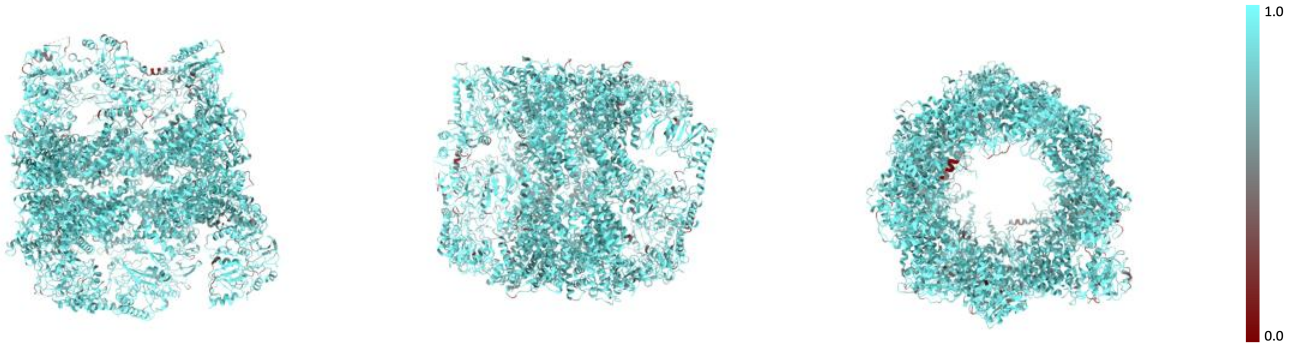
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

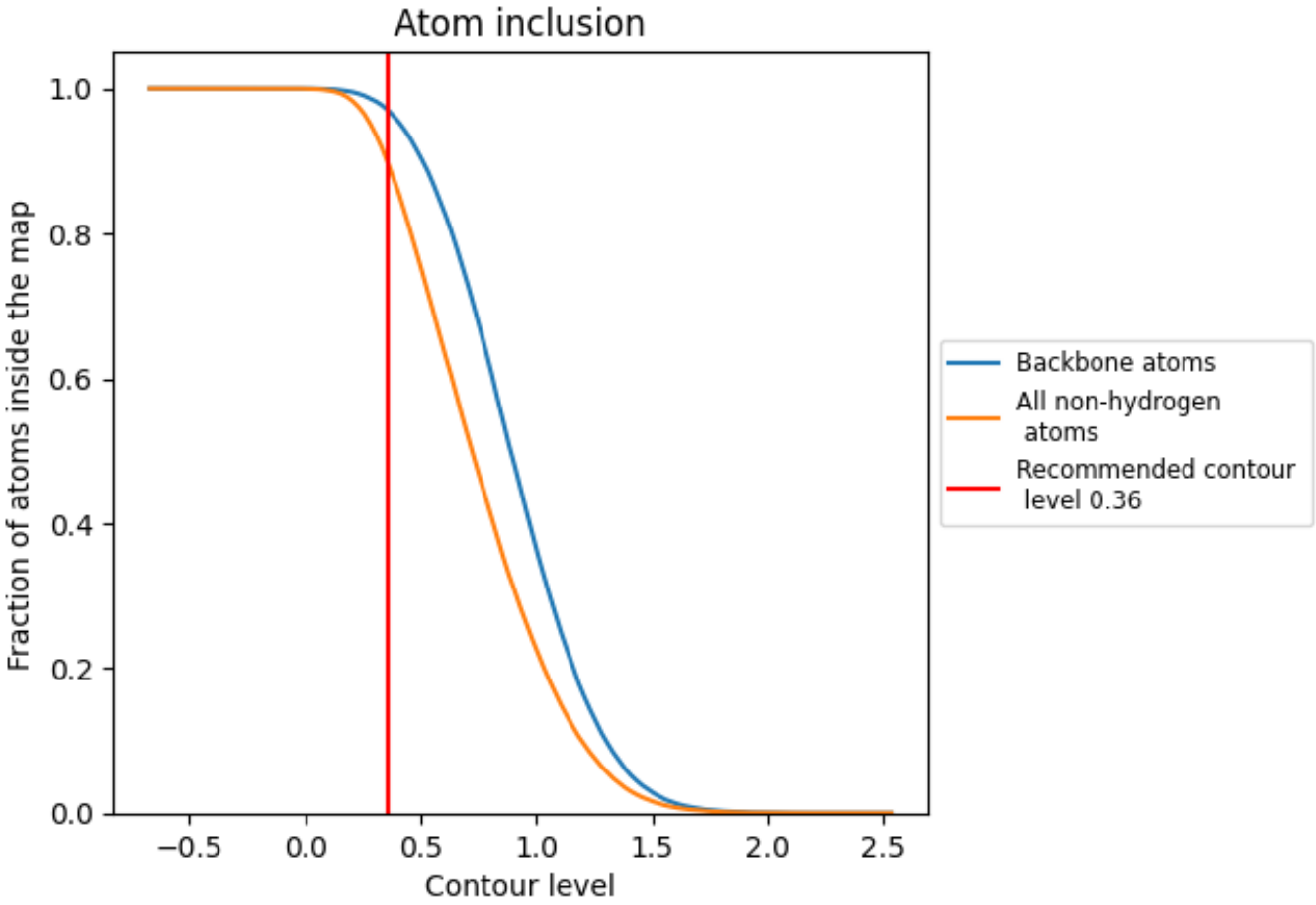
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.36).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 90% 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 (0.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8951	0.2580
A	0.8762	0.2650
B	0.8892	0.2580
D	0.9091	0.2650
E	0.9102	0.2490
G	0.8932	0.2720
H	0.9103	0.2520
Q	0.8991	0.2820
Z	0.9276	0.2870
a	0.8814	0.2480
b	0.8904	0.2500
d	0.8902	0.2290
e	0.9065	0.2470
g	0.8600	0.2180
h	0.8912	0.2560
q	0.8904	0.2790
z	0.8937	0.2720