



Full wwPDB EM Validation Report ⓘ

May 26, 2025 – 07:26 AM EDT

PDB ID : 8GAE / pdb_00008gae
EMDB ID : EMD-29895
Title : Hsp90 provides platform for CRaf dephosphorylation by PP5
Authors : Jaime-Garza, M.; Nowotny, C.A.; Coutandin, D.; Wang, F.; Tabios, M.;
Agard, D.A.
Deposited on : 2023-02-22
Resolution : 3.30 Å (reported)
Based on initial models : 5FWL, 1WAO, 1S95

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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
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) : 2.43.1

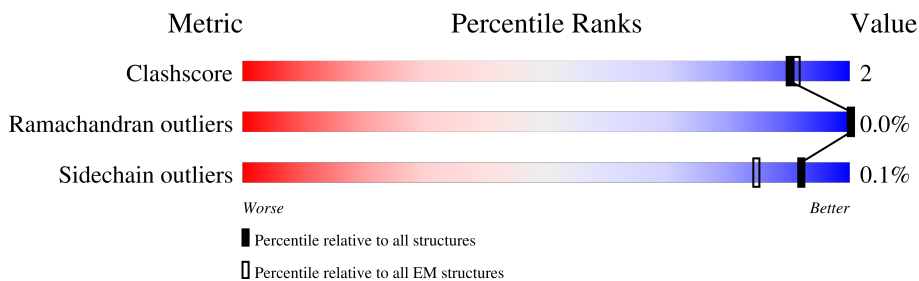
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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
Sidechain outliers	206894	16415

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	727	
1	B	727	
2	C	384	
3	D	207	
4	E	503	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 35406 atoms, of which 17658 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 Heat shock protein HSP 90-beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	635	Total	C	H	N	O	S	0	0
			10338	3263	5189	865	998	23		
1	B	633	Total	C	H	N	O	S	0	0
			10284	3249	5155	859	998	23		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P08238
A	-1	PRO	-	expression tag	UNP P08238
A	0	GLY	-	expression tag	UNP P08238
B	-2	GLY	-	expression tag	UNP P08238
B	-1	PRO	-	expression tag	UNP P08238
B	0	GLY	-	expression tag	UNP P08238

- Molecule 2 is a protein called Hsp90 co-chaperone Cdc37.

Mol	Chain	Residues	Atoms							AltConf	Trace
2	C	259	Total	C	H	N	O	P	S	0	0
			4307	1358	2125	383	425	1	15		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	379	LEU	-	expression tag	UNP Q16543
C	380	GLU	-	expression tag	UNP Q16543
C	381	VAL	-	expression tag	UNP Q16543
C	382	LEU	-	expression tag	UNP Q16543
C	383	PHE	-	expression tag	UNP Q16543
C	384	GLN	-	expression tag	UNP Q16543

- Molecule 3 is a protein called RAF proto-oncogene serine/threonine-protein kinase.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	189	Total	C	H	N	O	S	0	0
			3072	985	1541	258	275	13		

- Molecule 4 is a protein called Serine/threonine-protein phosphatase 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	459	Total	C	H	N	O	S	0	0
			7317	2347	3624	628	699	19		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP P53041
E	-2	PRO	-	expression tag	UNP P53041
E	-1	GLY	-	expression tag	UNP P53041
E	0	SER	-	expression tag	UNP P53041
E	304	ALA	HIS	engineered mutation	UNP P53041

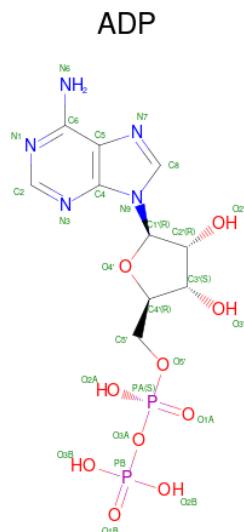
- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	K	0
			1	1	
5	B	1	Total	K	0
			1	1	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

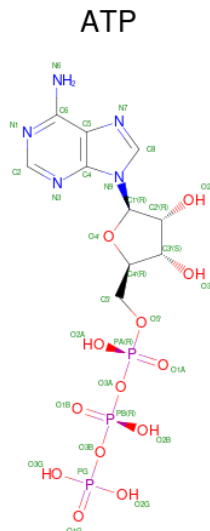
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	
6	B	1	Total	Mg	0
			1	1	

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

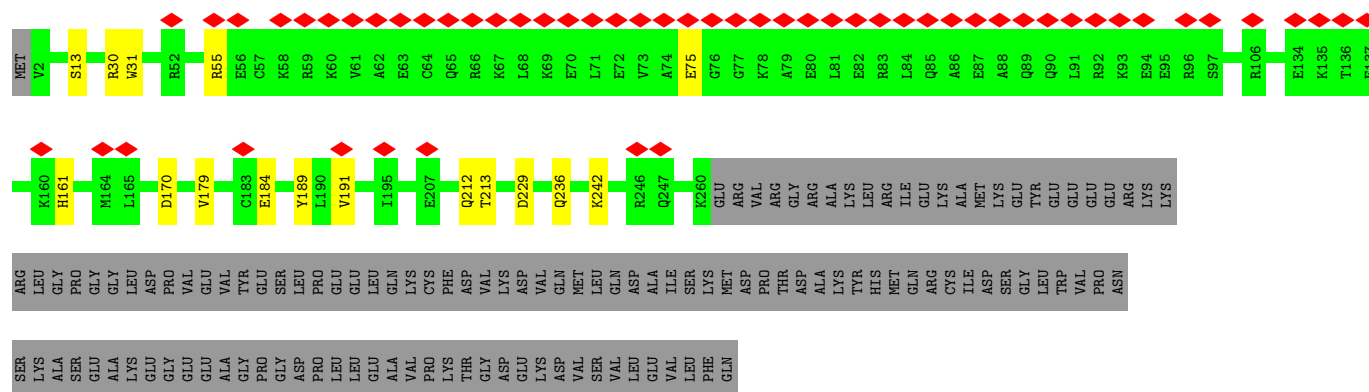
- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
8	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 9 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	E	2	Total	Mn	0
			2	2	



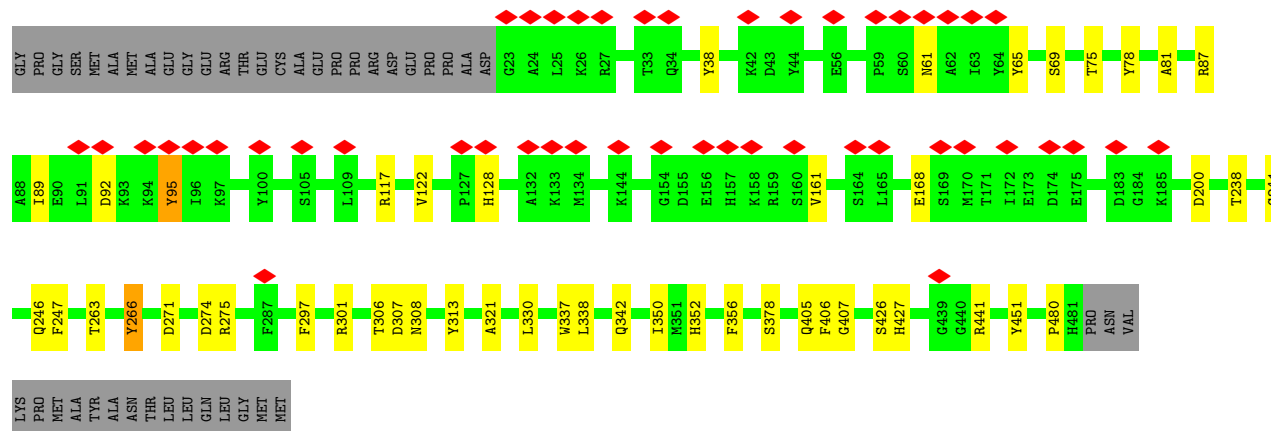
- Molecule 3: RAF proto-oncogene serine/threonine-protein kinase

Chain D: 82% 9% 9%



- Molecule 4: Serine/threonine-protein phosphatase 5

Chain E: 9% 82% 9% 9%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	522000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	69.00	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00615	Depositor
Map size (Å)	267.2, 267.2, 267.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83500004, 0.83500004, 0.83500004	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: SEP, ATP, MN, ADP, MG, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.05	24/5233 (0.5%)	1.59	64/7032 (0.9%)
1	B	0.93	7/5213 (0.1%)	1.46	34/7007 (0.5%)
2	C	0.81	2/2209 (0.1%)	1.44	20/2955 (0.7%)
3	D	0.90	2/1564 (0.1%)	1.54	22/2107 (1.0%)
4	E	0.97	8/3774 (0.2%)	1.59	46/5088 (0.9%)
All	All	0.96	43/17993 (0.2%)	1.53	186/24189 (0.8%)

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	3
1	B	0	3
3	D	0	1
4	E	0	5
All	All	0	12

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	378	SER	CB-OG	-12.87	1.16	1.42
1	B	291	ARG	CZ-NH2	-11.83	1.18	1.33
1	A	177	ARG	CZ-NH2	-10.84	1.19	1.33
1	A	191	GLU	N-CA	-10.47	1.33	1.46
1	A	197	ARG	CZ-NH2	-9.47	1.21	1.33
1	B	615	SER	CB-OG	-9.35	1.23	1.42
1	A	177	ARG	NE-CZ	-7.85	1.24	1.33
1	A	291	ARG	CZ-NH2	-7.82	1.23	1.33
1	A	338	ARG	CZ-NH2	-7.51	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	612	ARG	CZ-NH2	-7.50	1.23	1.33
1	A	604	ARG	CZ-NH2	-7.46	1.23	1.33
1	A	456	ARG	CZ-NH2	-7.45	1.23	1.33
1	A	449	ARG	CZ-NH2	-7.32	1.24	1.33
1	B	67	SER	CB-OG	-7.30	1.27	1.42
4	E	87	ARG	CZ-NH2	-7.26	1.24	1.33
1	A	448	ARG	CZ-NH2	-7.15	1.24	1.33
1	A	450	ARG	CZ-NH2	-7.12	1.24	1.33
1	A	291	ARG	CZ-NH1	-7.06	1.22	1.32
1	B	676	HIS	CE1-NE2	-7.00	1.25	1.32
1	A	338	ARG	CZ-NH1	-6.98	1.23	1.32
4	E	441	ARG	CZ-NH2	-6.95	1.24	1.33
1	A	449	ARG	CZ-NH1	-6.93	1.23	1.32
1	A	604	ARG	CZ-NH1	-6.93	1.23	1.32
4	E	87	ARG	CZ-NH1	-6.86	1.23	1.32
4	E	117	ARG	CZ-NH1	-6.80	1.23	1.32
4	E	441	ARG	CZ-NH1	-6.70	1.23	1.32
1	A	612	ARG	CZ-NH1	-6.70	1.23	1.32
1	A	456	ARG	CZ-NH1	-6.69	1.23	1.32
1	A	632	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	450	ARG	CZ-NH1	-6.59	1.23	1.32
1	A	448	ARG	CZ-NH1	-6.58	1.23	1.32
1	A	562	ASN	N-CA	-6.42	1.38	1.46
1	A	177	ARG	CZ-NH1	-6.01	1.24	1.32
1	B	389	ASN	N-CA	-5.77	1.38	1.46
2	C	212	GLN	CD-NE2	-5.67	1.21	1.33
4	E	271	ASP	CA-CB	-5.62	1.45	1.53
3	D	427	SER	CB-OG	-5.52	1.31	1.42
4	E	117	ARG	CZ-NH2	-5.48	1.26	1.33
1	A	158	GLU	CB-CG	-5.27	1.36	1.52
3	D	523	ASN	N-CA	-5.26	1.41	1.46
2	C	236	GLN	CD-NE2	-5.12	1.22	1.33
1	B	676	HIS	CD2-NE2	-5.09	1.32	1.37
1	B	57	GLU	N-CA	-5.07	1.40	1.46

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	THR	CA-C-N	14.02	139.59	120.38
1	A	190	THR	C-N-CA	14.02	139.59	120.38
1	A	60	THR	CA-C-N	10.83	131.81	122.28
1	A	60	THR	C-N-CA	10.83	131.81	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	388	LEU	CA-C-N	10.31	136.32	120.75
1	B	388	LEU	C-N-CA	10.31	136.32	120.75
4	E	61	ASN	CA-C-N	10.16	133.65	120.44
4	E	61	ASN	C-N-CA	10.16	133.65	120.44
1	A	561	GLU	CA-C-N	9.67	133.01	120.44
1	A	561	GLU	C-N-CA	9.67	133.01	120.44
1	A	300	GLU	CA-C-N	9.52	133.04	120.28
1	A	300	GLU	C-N-CA	9.52	133.04	120.28
1	B	82	ARG	CA-C-N	9.36	135.91	123.00
1	B	82	ARG	C-N-CA	9.36	135.91	123.00
2	C	212	GLN	CB-CG-CD	8.91	127.74	112.60
3	D	522	ASN	CA-C-N	8.85	134.76	123.34
3	D	522	ASN	C-N-CA	8.85	134.76	123.34
4	E	480	PRO	CA-C-N	8.72	137.40	121.70
4	E	480	PRO	C-N-CA	8.72	137.40	121.70
4	E	271	ASP	CA-CB-CG	8.60	121.20	112.60
4	E	65	TYR	CB-CA-C	-8.55	97.45	110.88
4	E	307	ASP	CA-CB-CG	8.39	120.99	112.60
2	C	184	GLU	N-CA-C	8.30	120.41	111.36
1	A	333	LEU	CA-C-N	8.07	134.67	122.65
1	A	333	LEU	C-N-CA	8.07	134.67	122.65
4	E	75	THR	CA-C-N	7.88	134.91	122.61
4	E	75	THR	C-N-CA	7.88	134.91	122.61
1	A	158	GLU	CA-CB-CG	7.84	129.77	114.10
1	B	154	GLN	CA-C-N	7.76	134.72	122.62
1	B	154	GLN	C-N-CA	7.76	134.72	122.62
1	A	186	LYS	CA-C-N	7.67	130.89	120.38
1	A	186	LYS	C-N-CA	7.67	130.89	120.38
1	B	314	ASP	CA-CB-CG	7.59	120.19	112.60
1	A	158	GLU	CB-CG-CD	7.52	125.38	112.60
1	B	545	GLU	CB-CG-CD	7.51	125.37	112.60
4	E	306	THR	CA-C-N	7.39	135.66	121.54
4	E	306	THR	C-N-CA	7.39	135.66	121.54
1	A	191	GLU	N-CA-CB	7.15	120.79	110.06
1	A	311	ASP	CA-C-N	7.06	132.65	120.58
1	A	311	ASP	C-N-CA	7.06	132.65	120.58
1	A	312	TRP	N-CA-CB	7.03	120.68	110.20
4	E	122	VAL	CB-CA-C	-6.93	103.00	111.88
1	B	151	ASP	CA-CB-CG	6.85	119.45	112.60
1	A	519	GLU	CA-C-N	6.69	129.54	120.44
1	A	519	GLU	C-N-CA	6.69	129.54	120.44
1	A	191	GLU	N-CA-C	-6.68	103.25	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	TYR	CA-C-N	6.64	127.36	119.98
1	A	301	TYR	C-N-CA	6.64	127.36	119.98
4	E	263	THR	CA-C-N	6.63	134.22	122.48
4	E	263	THR	C-N-CA	6.63	134.22	122.48
4	E	356	PHE	CA-CB-CG	6.60	120.40	113.80
2	C	75	GLU	CB-CG-CD	-6.49	101.56	112.60
4	E	306	THR	O-C-N	-6.40	115.50	122.79
1	A	351	ASN	CA-CB-CG	6.33	118.93	112.60
1	B	664	LEU	CA-C-N	6.33	129.92	120.31
1	B	664	LEU	C-N-CA	6.33	129.92	120.31
3	D	434	HIS	CA-CB-CG	6.28	120.08	113.80
3	D	539	TYR	CA-CB-CG	6.26	125.17	113.90
3	D	406	LEU	N-CA-C	6.22	118.14	111.36
1	A	334	PHE	CA-CB-CG	6.18	119.98	113.80
4	E	407	GLY	CA-C-N	6.17	126.63	119.47
4	E	407	GLY	C-N-CA	6.17	126.63	119.47
2	C	212	GLN	OE1-CD-NE2	-6.16	116.44	122.60
1	A	158	GLU	CG-CD-OE2	6.11	132.45	118.40
4	E	95	TYR	CA-C-N	6.08	128.79	120.46
4	E	95	TYR	C-N-CA	6.08	128.79	120.46
4	E	122	VAL	N-CA-CB	6.02	117.19	110.51
3	D	432	HIS	CA-CB-CG	6.00	119.80	113.80
1	A	447	ASN	CA-C-N	5.99	128.31	120.28
1	A	447	ASN	C-N-CA	5.99	128.31	120.28
4	E	38	TYR	CA-C-N	5.96	128.19	120.44
4	E	38	TYR	C-N-CA	5.96	128.19	120.44
4	E	321	ALA	CA-C-N	5.96	128.26	120.28
4	E	321	ALA	C-N-CA	5.96	128.26	120.28
3	D	526	SER	CA-C-N	5.95	129.07	120.38
3	D	526	SER	C-N-CA	5.95	129.07	120.38
1	A	346	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	A	388	LEU	CA-C-N	5.91	131.72	120.97
1	A	388	LEU	C-N-CA	5.91	131.72	120.97
4	E	427	HIS	CA-CB-CG	5.80	119.60	113.80
1	A	411	LYS	O-C-N	-5.75	115.59	122.15
2	C	170	ASP	CB-CA-C	5.71	121.83	110.17
2	C	161	HIS	CA-CB-CG	5.70	119.50	113.80
3	D	531	VAL	O-C-N	-5.69	116.34	121.91
4	E	308	ASN	CA-C-N	5.68	127.89	120.28
4	E	308	ASN	C-N-CA	5.68	127.89	120.28
1	B	352	ASN	CA-C-N	5.65	130.20	123.19
1	B	352	ASN	C-N-CA	5.65	130.20	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ILE	CA-C-N	5.62	126.07	119.94
1	A	209	ILE	C-N-CA	5.62	126.07	119.94
1	A	301	TYR	CA-CB-CG	5.60	123.97	113.90
1	B	459	THR	CA-C-N	5.59	127.77	120.28
1	B	459	THR	C-N-CA	5.59	127.77	120.28
4	E	274	ASP	CA-CB-CG	-5.58	107.02	112.60
1	A	346	ASN	CB-CG-ND2	5.57	124.76	116.40
2	C	31	TRP	N-CA-CB	-5.57	101.92	110.16
1	B	571	LEU	CA-C-N	5.57	128.51	120.38
1	B	571	LEU	C-N-CA	5.57	128.51	120.38
3	D	438	THR	CA-C-N	5.52	130.62	123.00
3	D	438	THR	C-N-CA	5.52	130.62	123.00
1	B	623	LYS	CA-C-N	5.52	129.72	121.72
1	B	623	LYS	C-N-CA	5.52	129.72	121.72
2	C	31	TRP	CA-CB-CG	5.51	124.07	113.60
3	D	431	LYS	CA-C-N	5.50	128.10	120.29
3	D	431	LYS	C-N-CA	5.50	128.10	120.29
1	A	39	PHE	N-CA-C	-5.46	105.48	111.82
4	E	168	GLU	CB-CA-C	-5.45	102.29	110.90
4	E	406	PHE	CA-CB-CG	5.44	119.24	113.80
4	E	65	TYR	N-CA-CB	5.41	117.85	110.01
1	A	491	LYS	CA-C-N	5.40	128.06	120.28
1	A	491	LYS	C-N-CA	5.40	128.06	120.28
1	B	392	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	A	278	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	477	LYS	CA-C-N	5.37	128.01	120.28
1	B	477	LYS	C-N-CA	5.37	128.01	120.28
2	C	242	LYS	CA-C-N	5.35	127.99	120.28
2	C	242	LYS	C-N-CA	5.35	127.99	120.28
1	A	462	SER	CA-C-N	5.34	129.28	120.25
1	A	462	SER	C-N-CA	5.34	129.28	120.25
1	A	635	VAL	CA-C-N	5.34	127.38	120.44
1	A	635	VAL	C-N-CA	5.34	127.38	120.44
4	E	297	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	346	ASN	CA-C-N	5.33	128.17	120.38
1	A	346	ASN	C-N-CA	5.33	128.17	120.38
1	B	509	GLU	N-CA-CB	-5.33	102.18	110.55
3	D	527	PHE	CA-C-N	5.33	127.69	120.38
3	D	527	PHE	C-N-CA	5.33	127.69	120.38
2	C	55	ARG	NE-CZ-NH2	5.32	123.99	119.20
2	C	229	ASP	CA-C-N	5.32	126.49	119.84
2	C	229	ASP	C-N-CA	5.32	126.49	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	128	HIS	CE1-NE2-CD2	5.32	114.32	109.00
1	A	278	ASP	N-CA-C	5.30	117.92	110.23
2	C	30	ARG	CA-C-N	5.29	127.80	120.29
2	C	30	ARG	C-N-CA	5.29	127.80	120.29
2	C	189	TYR	CA-C-N	5.28	128.34	120.31
2	C	189	TYR	C-N-CA	5.28	128.34	120.31
1	B	388	LEU	O-C-N	-5.28	117.00	122.96
1	A	67	SER	CA-C-N	5.27	128.78	121.09
1	A	67	SER	C-N-CA	5.27	128.78	121.09
2	C	236	GLN	OE1-CD-NE2	-5.26	117.34	122.60
3	D	531	VAL	CA-C-N	5.24	127.73	120.29
3	D	531	VAL	C-N-CA	5.24	127.73	120.29
1	A	177	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	A	628	ILE	CA-C-N	5.21	128.62	121.74
1	A	628	ILE	C-N-CA	5.21	128.62	121.74
4	E	122	VAL	CA-CB-CG2	5.21	119.26	110.40
1	A	274	GLU	CB-CG-CD	5.21	121.45	112.60
2	C	189	TYR	N-CA-C	5.21	116.76	111.14
4	E	338	LEU	CA-C-N	5.20	125.20	119.90
4	E	338	LEU	C-N-CA	5.20	125.20	119.90
1	B	276	TYR	N-CA-C	5.19	117.14	108.99
4	E	337	TRP	CH2-CZ2-CE2	5.17	124.22	117.50
4	E	247	PHE	CA-CB-CG	5.16	118.96	113.80
4	E	246	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	B	347	LYS	CA-C-N	5.15	129.86	122.40
1	B	347	LYS	C-N-CA	5.15	129.86	122.40
3	D	532	TYR	N-CA-CB	5.14	117.78	110.16
1	B	329	PHE	CA-CB-CG	5.14	118.94	113.80
4	E	200	ASP	CA-C-N	5.13	129.48	122.34
4	E	200	ASP	C-N-CA	5.13	129.48	122.34
4	E	352	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	B	435	LYS	CA-C-N	5.12	127.14	120.28
1	B	435	LYS	C-N-CA	5.12	127.14	120.28
4	E	405	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	A	623	LYS	CA-C-N	5.11	130.81	122.07
1	A	623	LYS	C-N-CA	5.11	130.81	122.07
3	D	564	GLY	CA-C-N	5.11	131.12	122.79
3	D	564	GLY	C-N-CA	5.11	131.12	122.79
1	B	396	GLN	CA-CB-CG	-5.11	103.88	114.10
4	E	78	TYR	CA-C-N	5.11	125.61	119.94
4	E	78	TYR	C-N-CA	5.11	125.61	119.94
3	D	408	PHE	CA-C-N	5.11	127.38	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	408	PHE	C-N-CA	5.11	127.38	120.38
1	A	528	PHE	CA-C-N	5.10	129.60	122.36
1	A	528	PHE	C-N-CA	5.10	129.60	122.36
1	A	300	GLU	O-C-N	5.09	127.59	122.09
1	A	177	ARG	CD-NE-CZ	5.08	131.51	124.40
1	A	197	ARG	CA-C-N	5.08	128.50	120.47
1	A	197	ARG	C-N-CA	5.08	128.50	120.47
1	B	284	LYS	CA-C-N	5.08	128.06	120.95
1	B	284	LYS	C-N-CA	5.08	128.06	120.95
2	C	179	VAL	N-CA-CB	5.07	119.32	110.65
1	B	56	TYR	O-C-N	-5.06	116.76	122.12
1	A	612	ARG	CA-C-N	5.05	129.36	122.34
1	A	612	ARG	C-N-CA	5.05	129.36	122.34
1	A	493	GLN	OE1-CD-NE2	-5.03	117.57	122.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	ARG	Sidechain
1	A	301	TYR	Sidechain
1	A	330	ARG	Sidechain
1	B	126	ILE	Mainchain
1	B	192	TYR	Sidechain
1	B	291	ARG	Sidechain
3	D	539	TYR	Sidechain
4	E	275	ARG	Sidechain
4	E	301	ARG	Sidechain
4	E	313	TYR	Sidechain
4	E	451	TYR	Sidechain
4	E	95	TYR	Sidechain

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	5149	5189	5186	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5129	5155	5153	14	0
2	C	2182	2125	2124	1	0
3	D	1531	1541	1537	6	0
4	E	3693	3624	3622	7	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	27	12	12	0	0
8	B	31	12	12	0	0
9	E	2	0	0	0	0
All	All	17748	17658	17646	56	0

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

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:LEU:HD21	1:B:654:LEU:HD11	1.78	0.65
1:B:149:HIS:ND1	1:B:150:ASN:O	2.30	0.64
1:A:487:THR:HG22	1:A:513:MET:HB2	1.81	0.63
1:A:78:ASN:ND2	1:A:81:GLU:OE1	2.33	0.62
1:A:83:THR:HG21	1:A:182:ILE:HG23	1.82	0.62
1:A:80:GLN:N	1:A:80:GLN:OE1	2.34	0.61
1:A:83:THR:CG2	1:A:182:ILE:HG23	2.33	0.59
1:B:638:LEU:HD13	1:B:654:LEU:HD12	1.86	0.58
1:B:332:LEU:O	1:B:333:LEU:HD23	2.03	0.58
1:A:11:GLU:N	1:A:11:GLU:OE1	2.37	0.57
1:A:53:LYS:HG3	1:A:125:MET:HE1	1.87	0.56
1:B:626:LEU:HD12	1:B:627:GLU:N	2.21	0.56
3:D:531:VAL:HG22	3:D:599:PHE:CE1	2.41	0.56
1:B:439:LEU:O	1:B:439:LEU:HD12	2.06	0.55
1:A:601:ASN:OD1	1:A:604:ARG:NH1	2.40	0.55
3:D:531:VAL:HG22	3:D:599:PHE:CD1	2.44	0.52
1:A:70:GLU:OE1	1:A:70:GLU:N	2.40	0.52
1:B:680:ILE:HD12	1:B:683:MET:HB2	1.90	0.52
1:A:578:VAL:HG22	1:A:626:LEU:HB3	1.93	0.51
1:A:89:THR:O	1:A:89:THR:HG22	2.10	0.51
1:A:145:VAL:HG12	1:A:147:THR:HG23	1.93	0.51
4:E:69:SER:HA	4:E:81:ALA:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:ARG:O	1:A:450:ARG:HG2	2.15	0.46
1:A:147:THR:HG22	1:A:179:THR:HG22	1.96	0.46
3:D:536:ILE:HG12	3:D:539:TYR:CZ	2.51	0.46
1:A:519:GLU:OE2	1:A:519:GLU:HA	2.14	0.46
4:E:238:THR:HG21	4:E:266:TYR:CE2	2.50	0.46
1:B:600:ALA:HB2	1:B:668:PHE:CZ	2.51	0.46
1:B:332:LEU:C	1:B:333:LEU:HD23	2.40	0.45
1:A:409:VAL:HA	1:A:412:CYS:SG	2.56	0.45
3:D:539:TYR:CZ	3:D:568:PRO:HG3	2.52	0.45
1:A:612:ARG:O	1:A:613:ASP:OD1	2.34	0.45
1:A:581:SER:HB3	1:A:627:GLU:HB3	1.99	0.45
1:A:613:ASP:OD1	1:A:613:ASP:C	2.59	0.45
1:B:626:LEU:HD12	1:B:627:GLU:H	1.81	0.44
4:E:241:GLY:HA2	4:E:426:SER:HB3	2.00	0.44
1:A:14:THR:HG23	1:B:164:SER:OG	2.18	0.43
1:A:148:LYS:HE3	1:A:152:ASP:O	2.18	0.43
1:A:374:LEU:HD21	1:A:412:CYS:SG	2.59	0.42
1:A:438:LYS:HE2	1:A:455:LEU:HD22	2.01	0.42
1:B:413:LEU:HD23	1:B:413:LEU:HA	1.82	0.42
1:A:291:ARG:HG3	1:A:291:ARG:HH11	1.85	0.42
3:D:472:ASN:OD1	3:D:472:ASN:C	2.61	0.42
2:C:191:VAL:CG2	2:C:213:THR:HG21	2.50	0.42
1:A:448:ARG:HG3	1:A:449:ARG:N	2.34	0.42
1:A:505:LYS:HB2	1:A:505:LYS:HE2	1.92	0.42
4:E:161:VAL:HG13	4:E:330:LEU:HG	2.02	0.42
1:A:613:ASP:OD1	1:A:613:ASP:O	2.37	0.41
4:E:89:ILE:HA	4:E:92:ASP:O	2.20	0.41
1:A:326:GLN:OE1	1:A:326:GLN:N	2.49	0.41
4:E:342:GLN:HG3	4:E:350:ILE:HD11	2.01	0.41
1:B:93:MET:HE3	1:B:147:THR:HG21	2.03	0.41
1:A:181:VAL:HG12	1:A:183:LEU:CD1	2.51	0.41
3:D:428:SER:HB2	3:D:472:ASN:HA	2.03	0.40
1:B:305:TYR:HB2	1:B:334:PHE:CE2	2.56	0.40
4:E:238:THR:HG21	4:E:266:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	631/727 (87%)	624 (99%)	6 (1%)	1 (0%)	44	71
1	B	629/727 (86%)	620 (99%)	9 (1%)	0	100	100
2	C	256/384 (67%)	250 (98%)	6 (2%)	0	100	100
3	D	185/207 (89%)	181 (98%)	4 (2%)	0	100	100
4	E	457/503 (91%)	439 (96%)	18 (4%)	0	100	100
All	All	2158/2548 (85%)	2114 (98%)	43 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	GLN

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	574/653 (88%)	574 (100%)	0	100	100
1	B	572/653 (88%)	572 (100%)	0	100	100
2	C	238/346 (69%)	238 (100%)	0	100	100
3	D	170/186 (91%)	170 (100%)	0	100	100
4	E	397/431 (92%)	396 (100%)	1 (0%)	91	94
All	All	1951/2269 (86%)	1950 (100%)	1 (0%)	92	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	266	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	351	ASN
1	A	397	GLN
1	A	436	ASN
1	A	442	HIS
1	A	458	HIS
1	A	609	GLN
1	B	30	ASN
1	B	35	ASN
1	B	207	GLN
1	B	396	GLN
1	B	458	HIS
1	B	523	GLN
1	B	632	HIS
2	C	9	HIS
2	C	161	HIS
3	D	434	HIS
4	E	106	ASN
4	E	298	HIS
4	E	326	GLN
4	E	342	GLN
4	E	419	ASN
4	E	438	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SEP	C	13	2	8,9,10	1.12	0	7,12,14	2.22	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	C	13	2	-	2/6/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	13	SEP	OG-CB-CA	4.98	113.00	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	13	SEP	C-CA-CB-OG
2	C	13	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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$
7	ADP	A	803	6	24,29,29	1.29	2 (8%)	29,45,45	1.53	3 (10%)
8	ATP	B	803	6	28,33,33	1.46	3 (10%)	34,52,52	1.25	2 (5%)

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
7	ADP	A	803	6	-	0/12/32/32	0/3/3/3
8	ATP	B	803	6	-	2/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	803	ATP	PA-O3A	-3.97	1.55	1.59
8	B	803	ATP	PB-O3A	-3.81	1.55	1.59
7	A	803	ADP	PA-O3A	-3.47	1.55	1.59
7	A	803	ADP	C1'-N9	-2.66	1.43	1.49
8	B	803	ATP	O4'-C1'	2.31	1.43	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	803	ADP	C4-C5-N7	4.69	114.30	109.34
7	A	803	ADP	C4'-O4'-C1'	-4.62	105.69	109.92
8	B	803	ATP	C4-C5-N7	4.28	113.86	109.34
8	B	803	ATP	O2A-PA-O3A	2.63	114.38	107.27
7	A	803	ADP	O2A-PA-O3A	2.32	113.54	107.27

There are no chirality outliers.

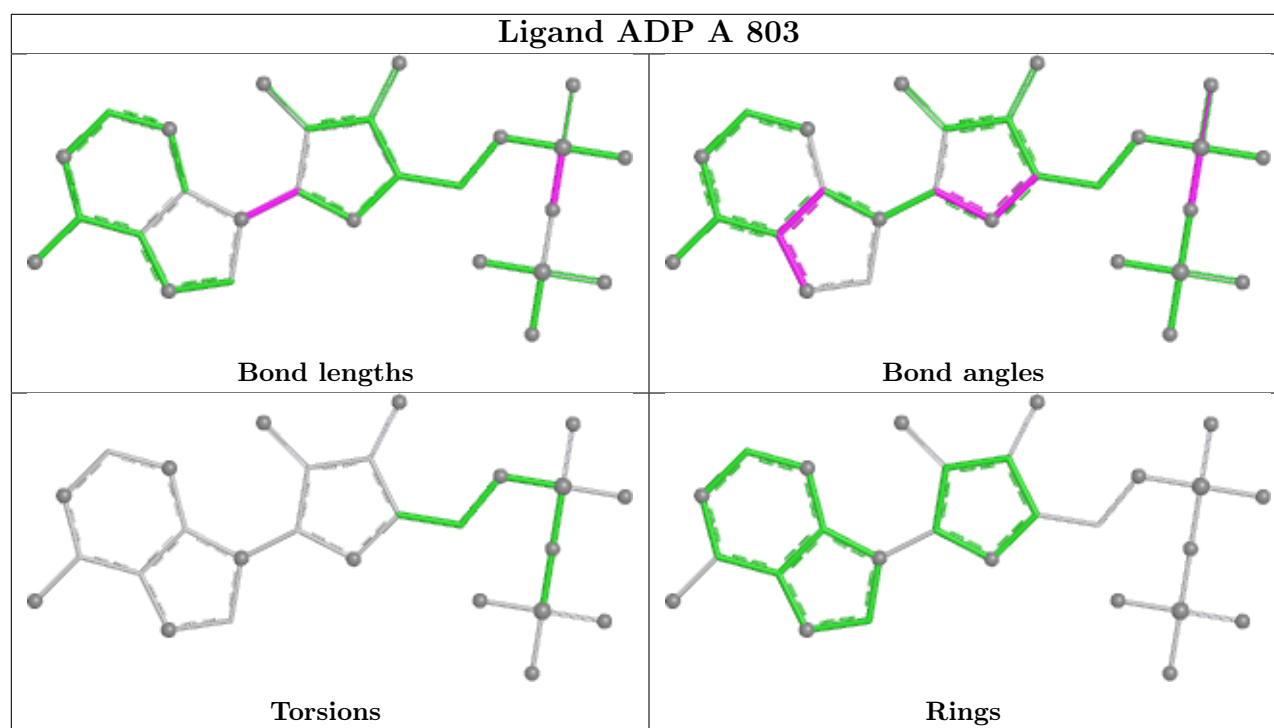
All (2) torsion outliers are listed below:

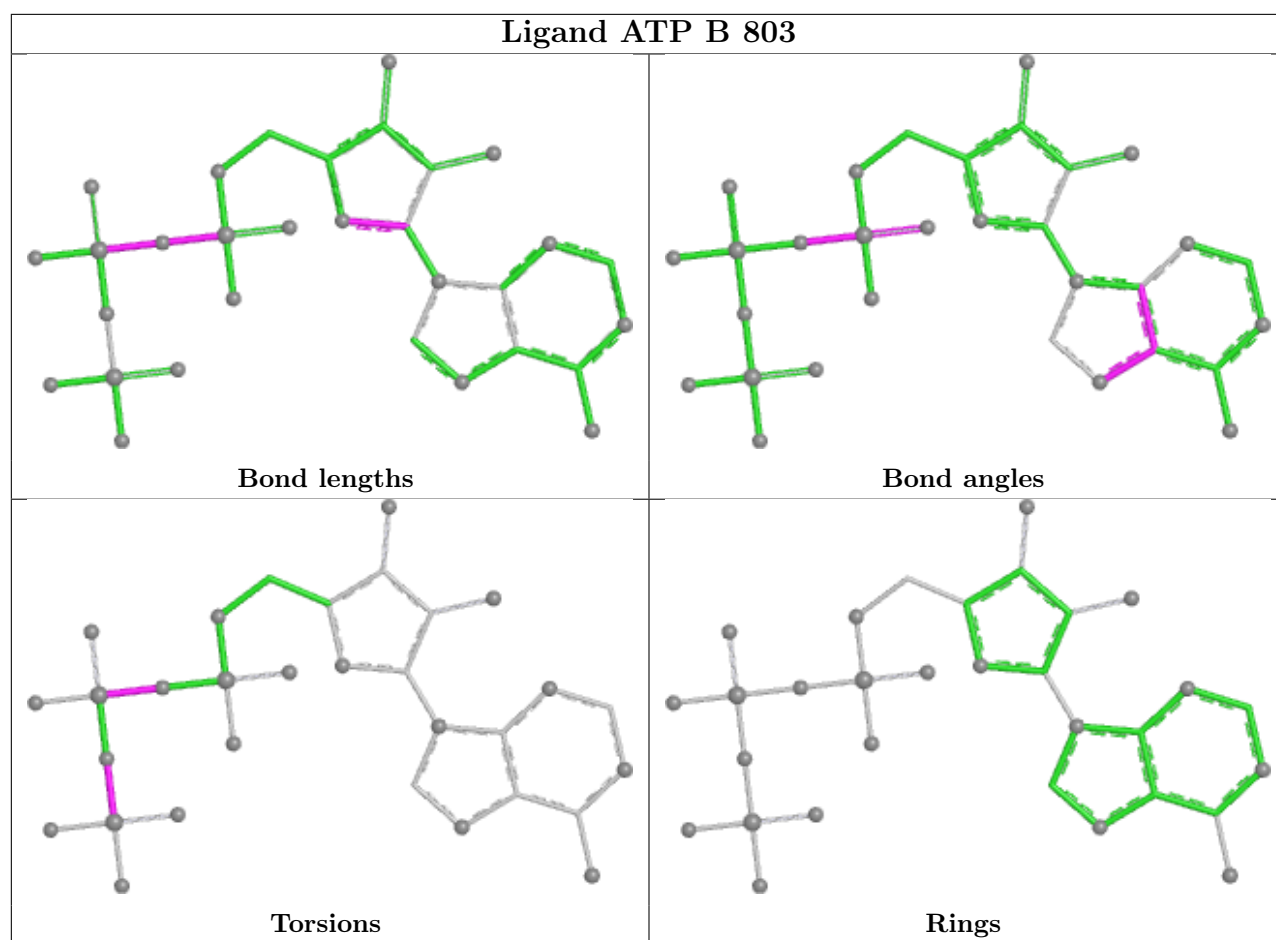
Mol	Chain	Res	Type	Atoms
8	B	803	ATP	PA-O3A-PB-O1B
8	B	803	ATP	PB-O3B-PG-O1G

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

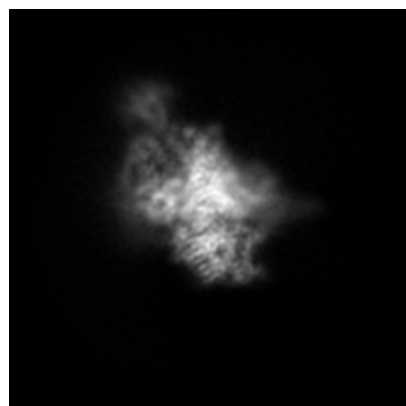
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29895. These allow visual inspection of the internal detail of the map and identification of artifacts.

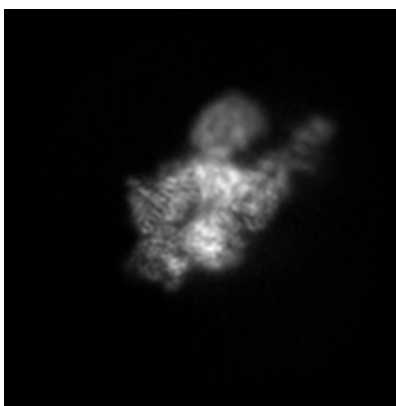
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

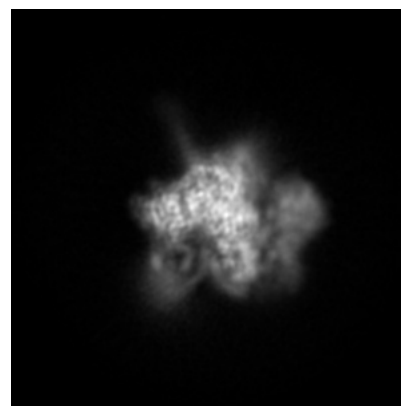
6.1.1 Primary map



X

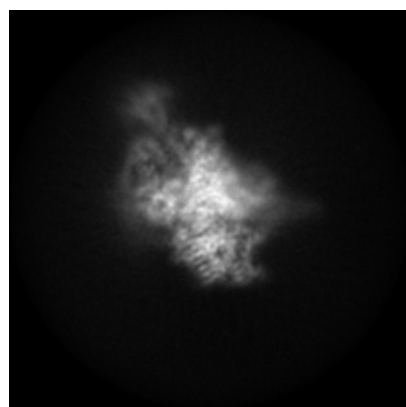


Y

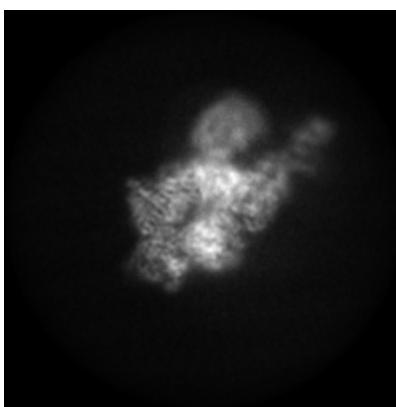


Z

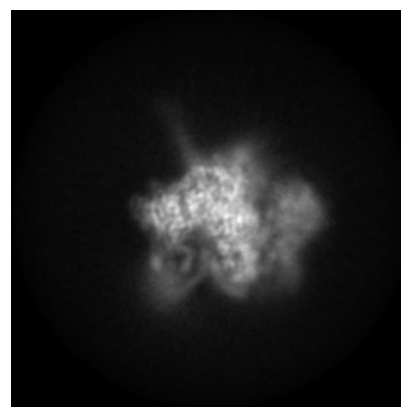
6.1.2 Raw map



X



Y

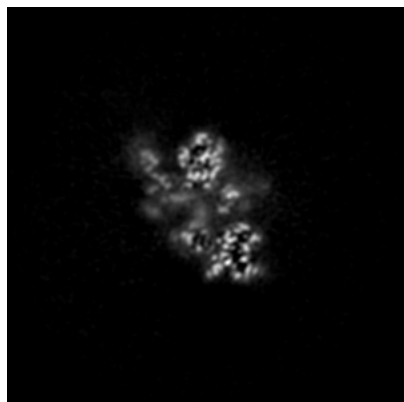


Z

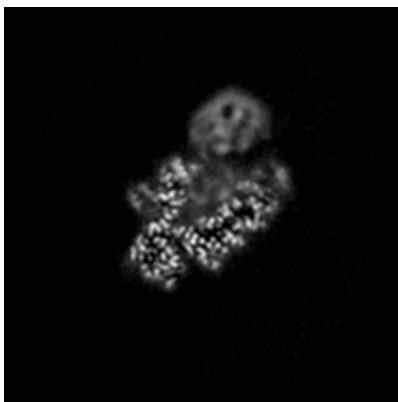
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

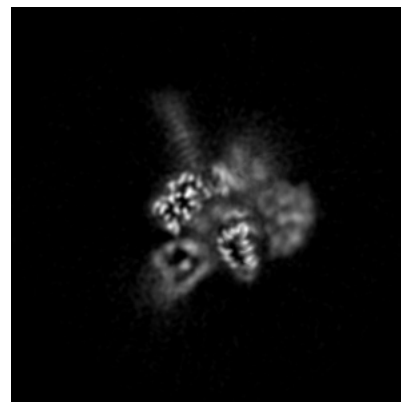
6.2.1 Primary map



X Index: 160

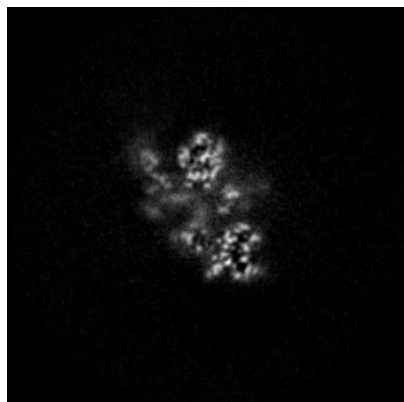


Y Index: 160

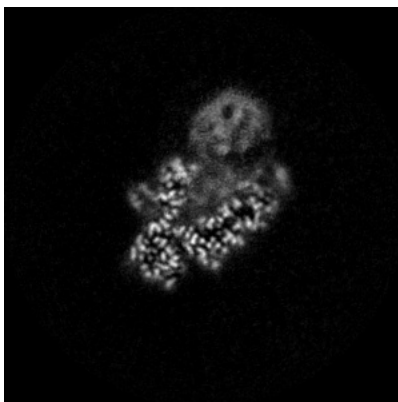


Z Index: 160

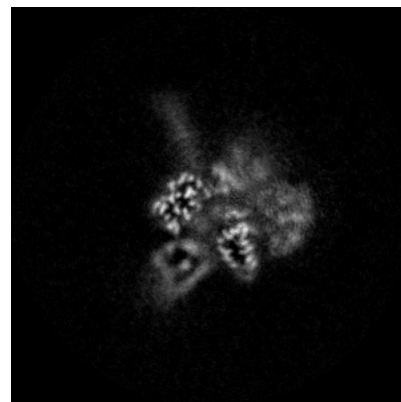
6.2.2 Raw map



X Index: 160



Y Index: 160

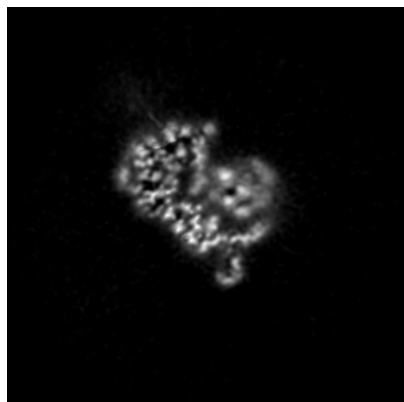


Z Index: 160

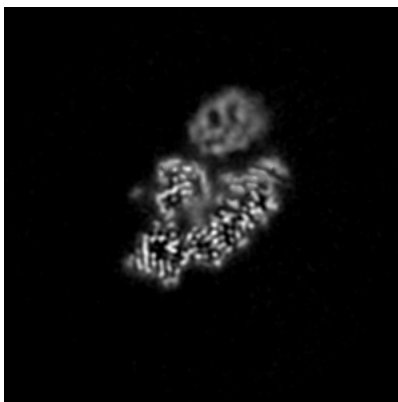
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

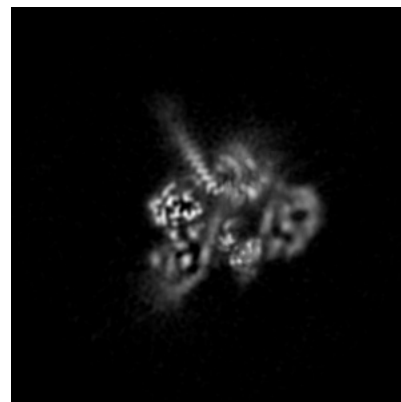
6.3.1 Primary map



X Index: 183

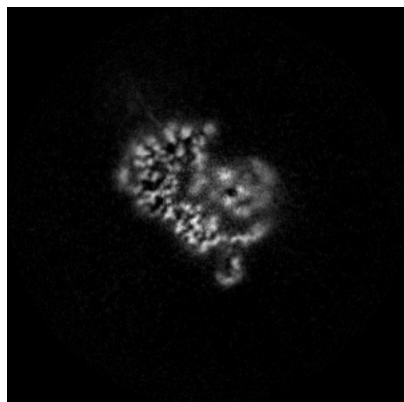


Y Index: 154

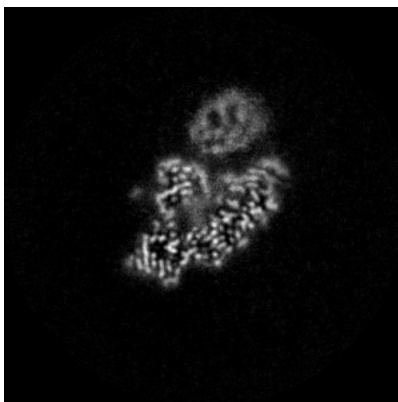


Z Index: 168

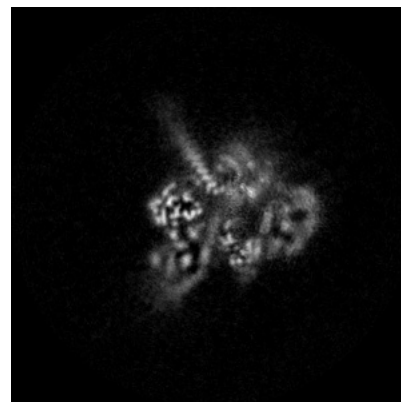
6.3.2 Raw map



X Index: 183



Y Index: 154

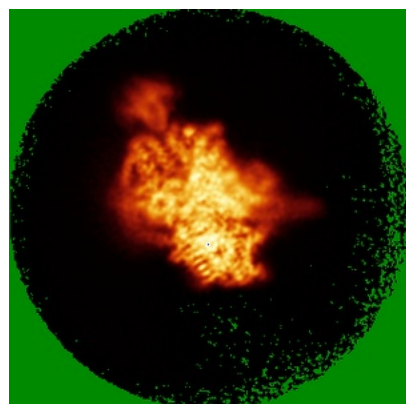


Z Index: 168

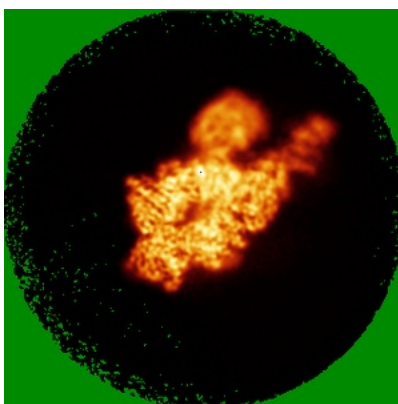
The images above show the largest variance slices of the map in three orthogonal directions.

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

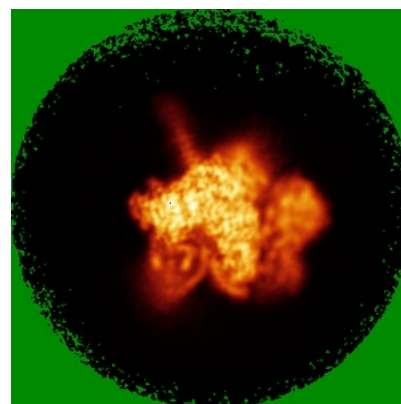
6.4.1 Primary map



X

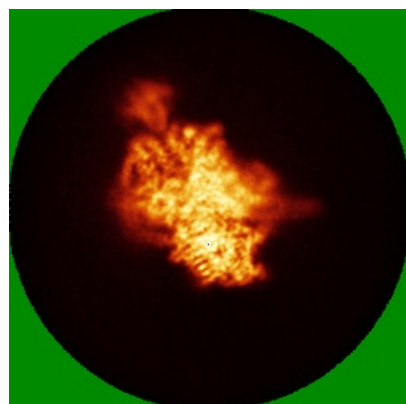


Y



Z

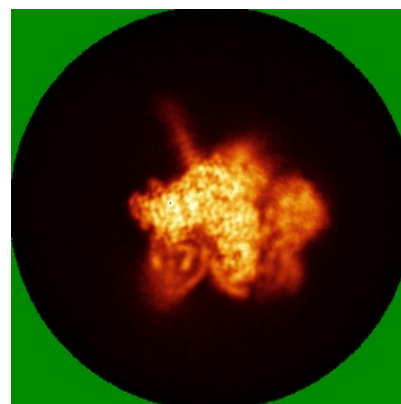
6.4.2 Raw map



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 0.00615. 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.

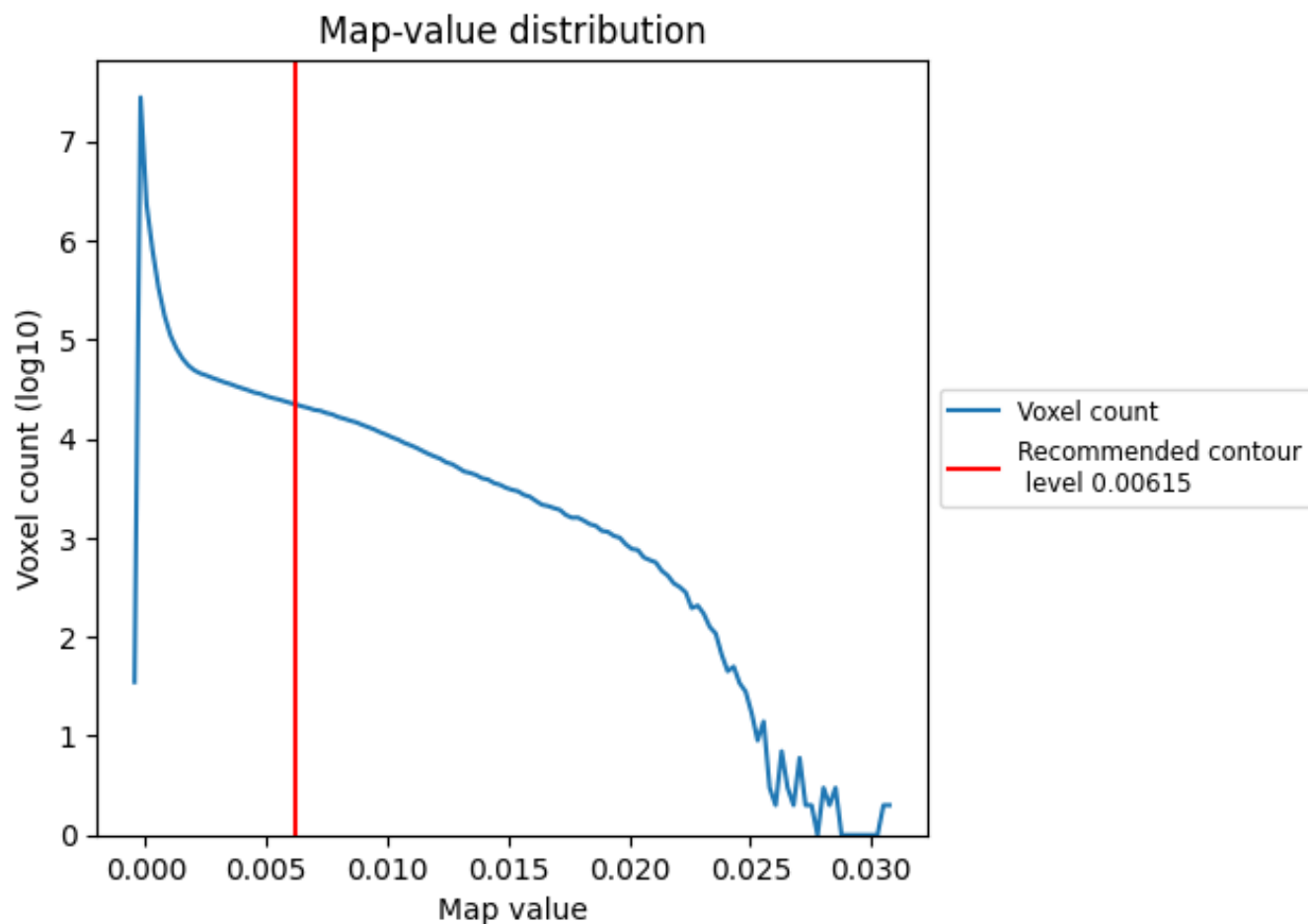
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

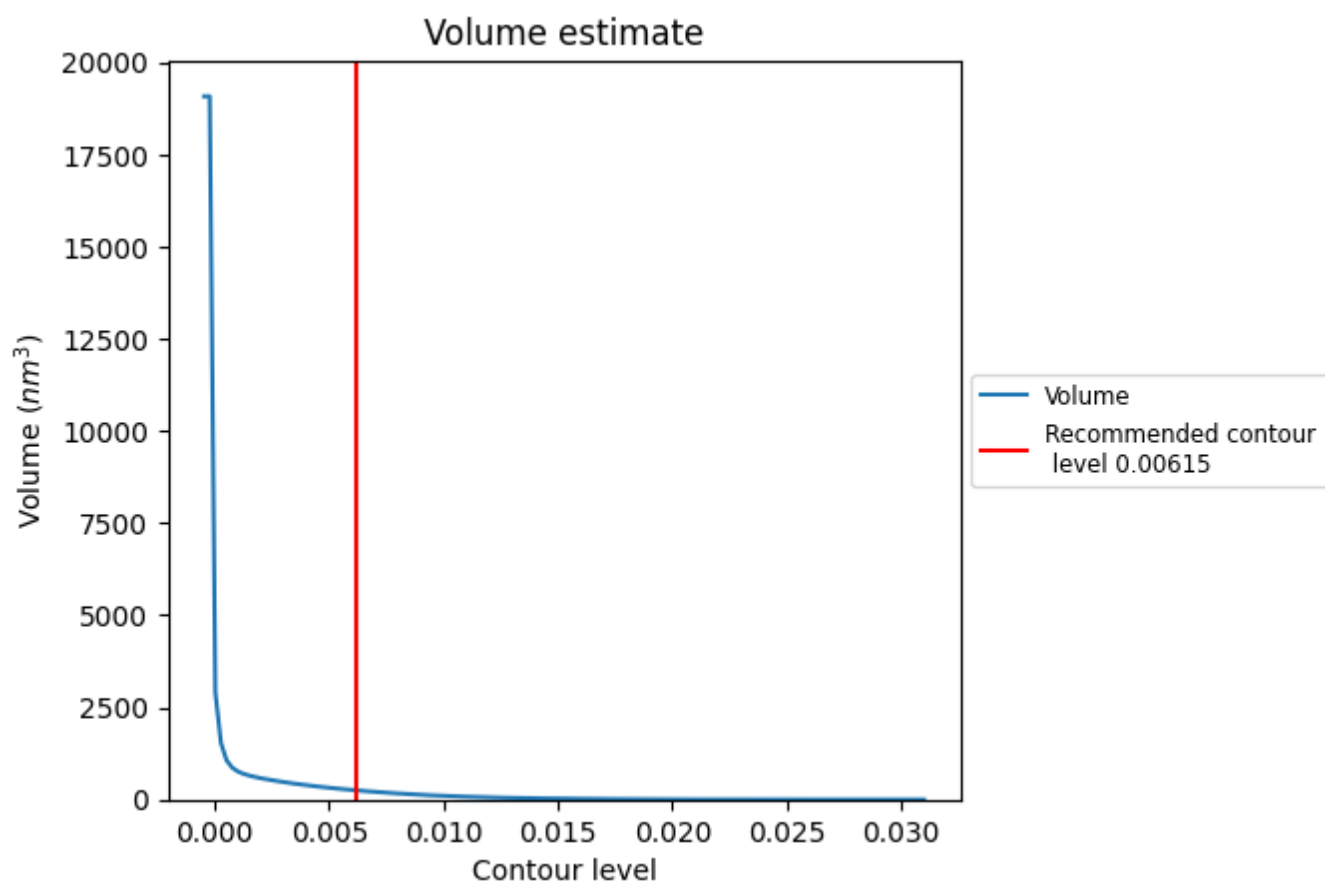
This section contains the results of statistical analysis of the map.

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.

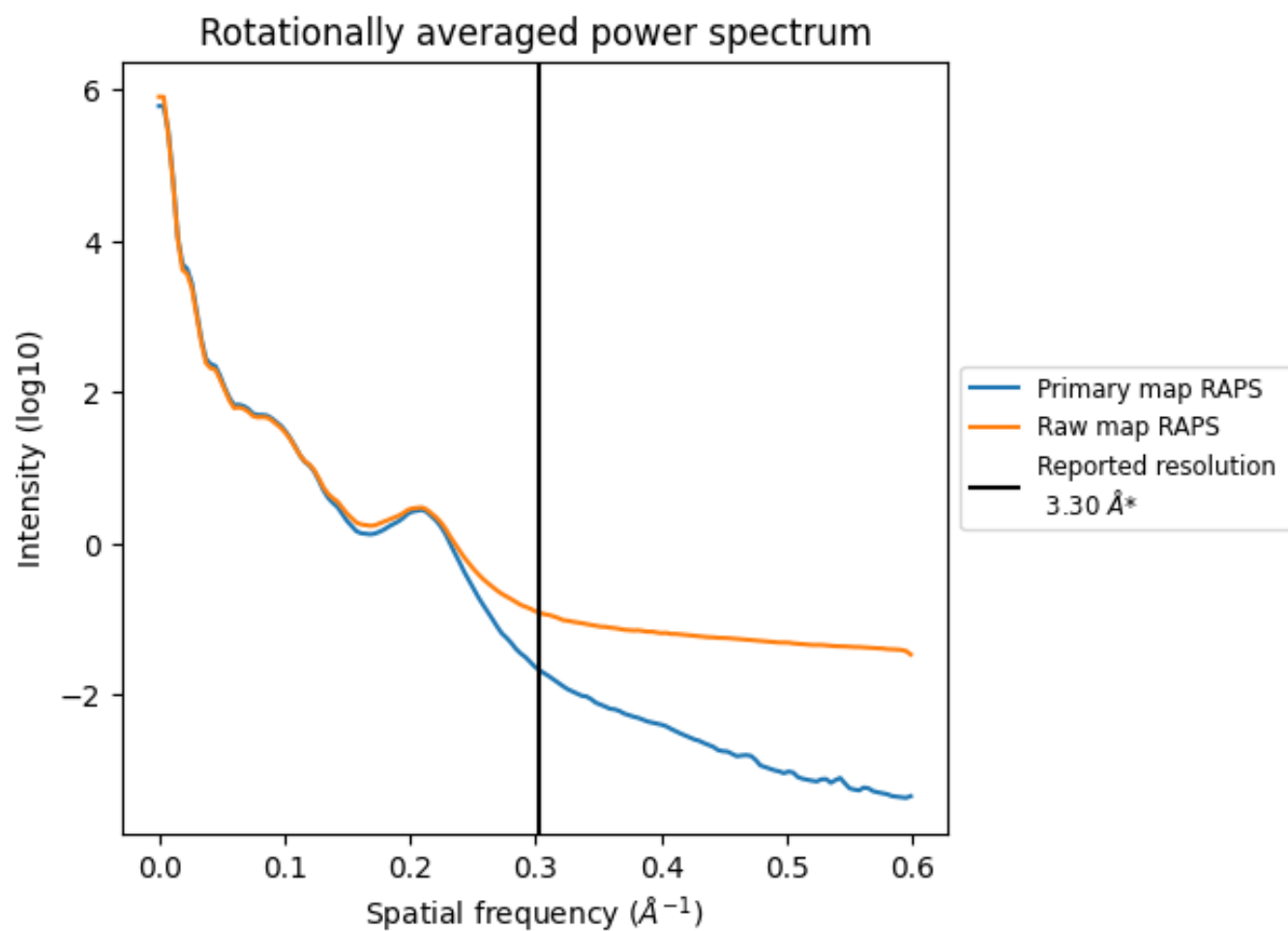
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 252 nm^3 ; this corresponds to an approximate mass of 228 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 ⓘ

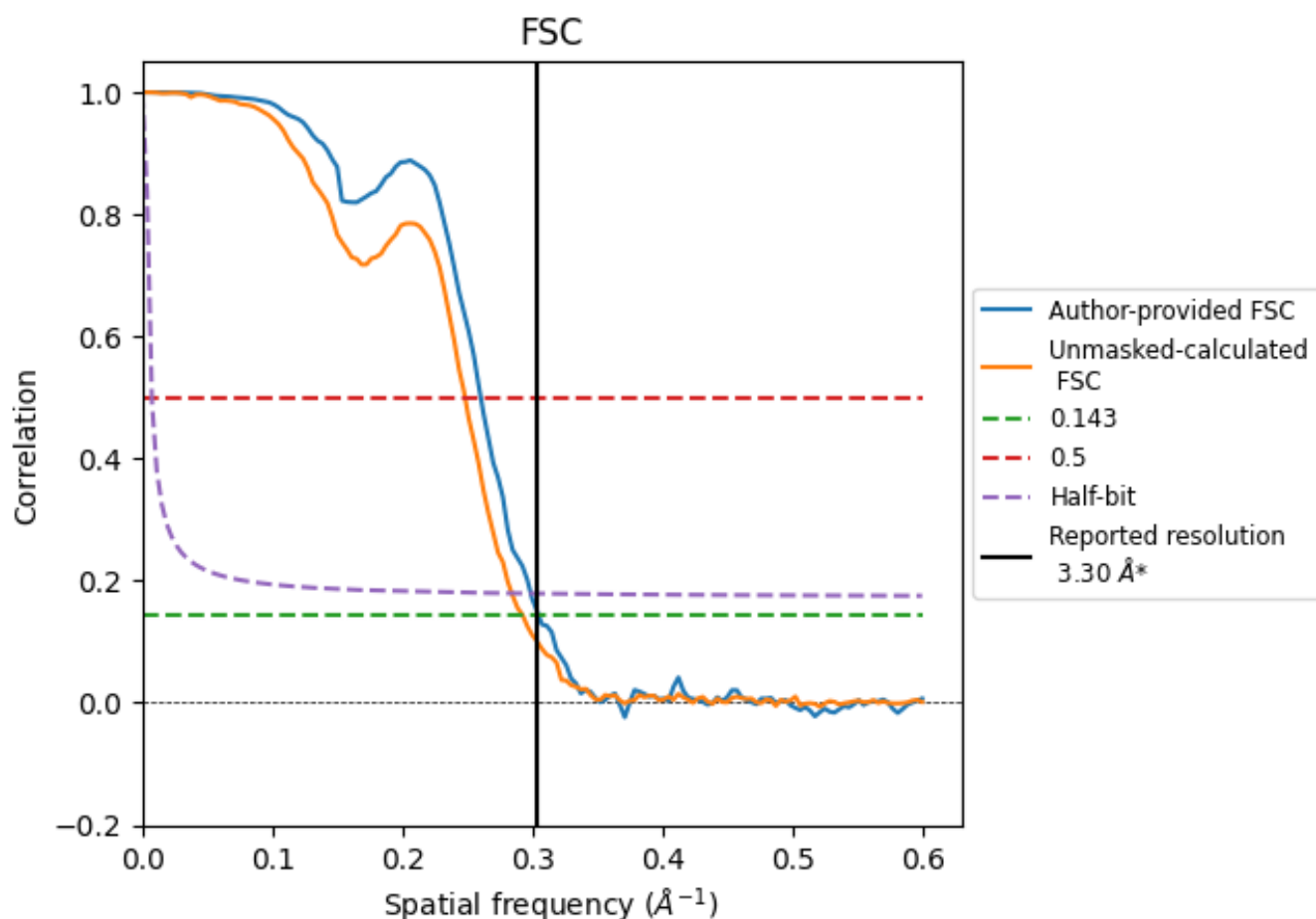


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

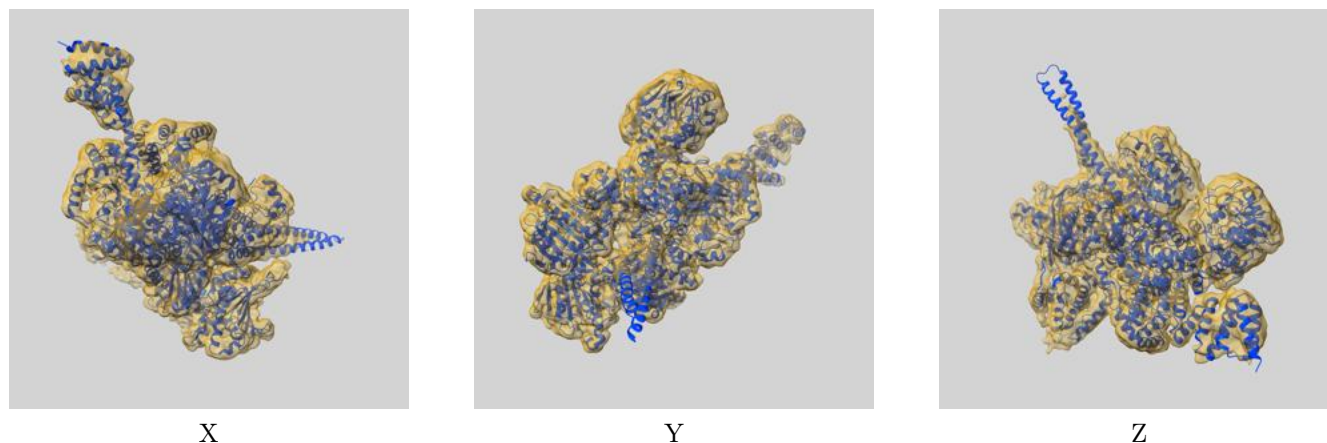
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.85	3.35
Unmasked-calculated*	3.42	4.03	3.52

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

9 Map-model fit [i](#)

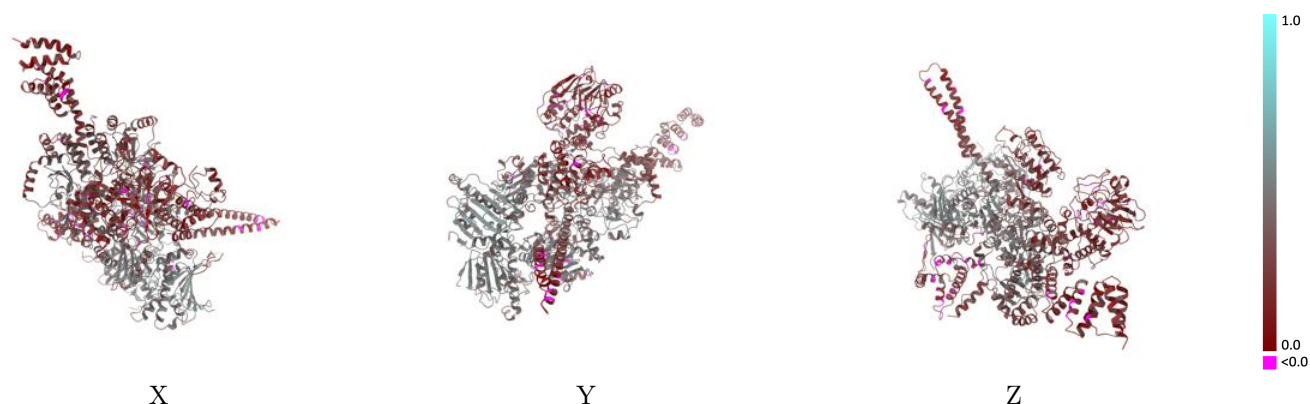
This section contains information regarding the fit between EMDB map EMD-29895 and PDB model 8GAE. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



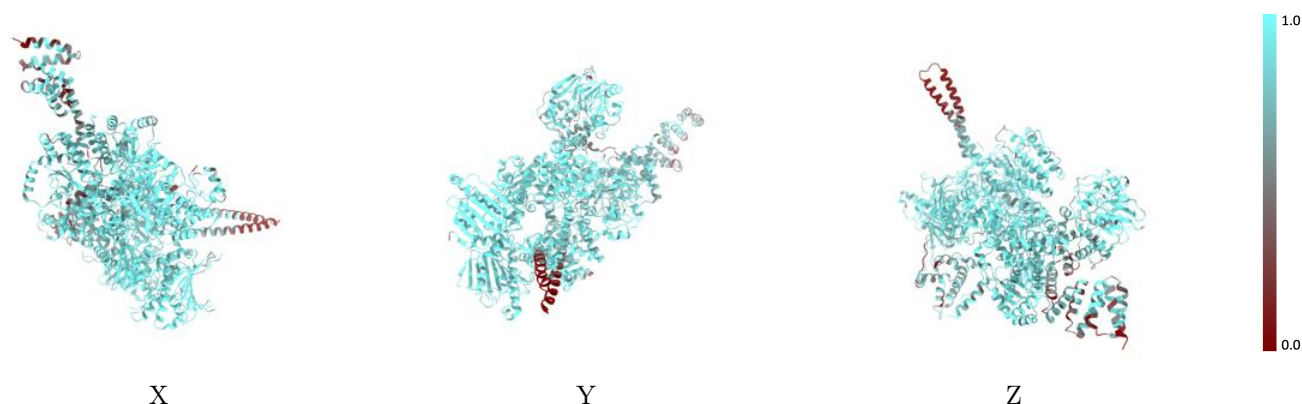
The images above show the 3D surface view of the map at the recommended contour level 0.00615 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



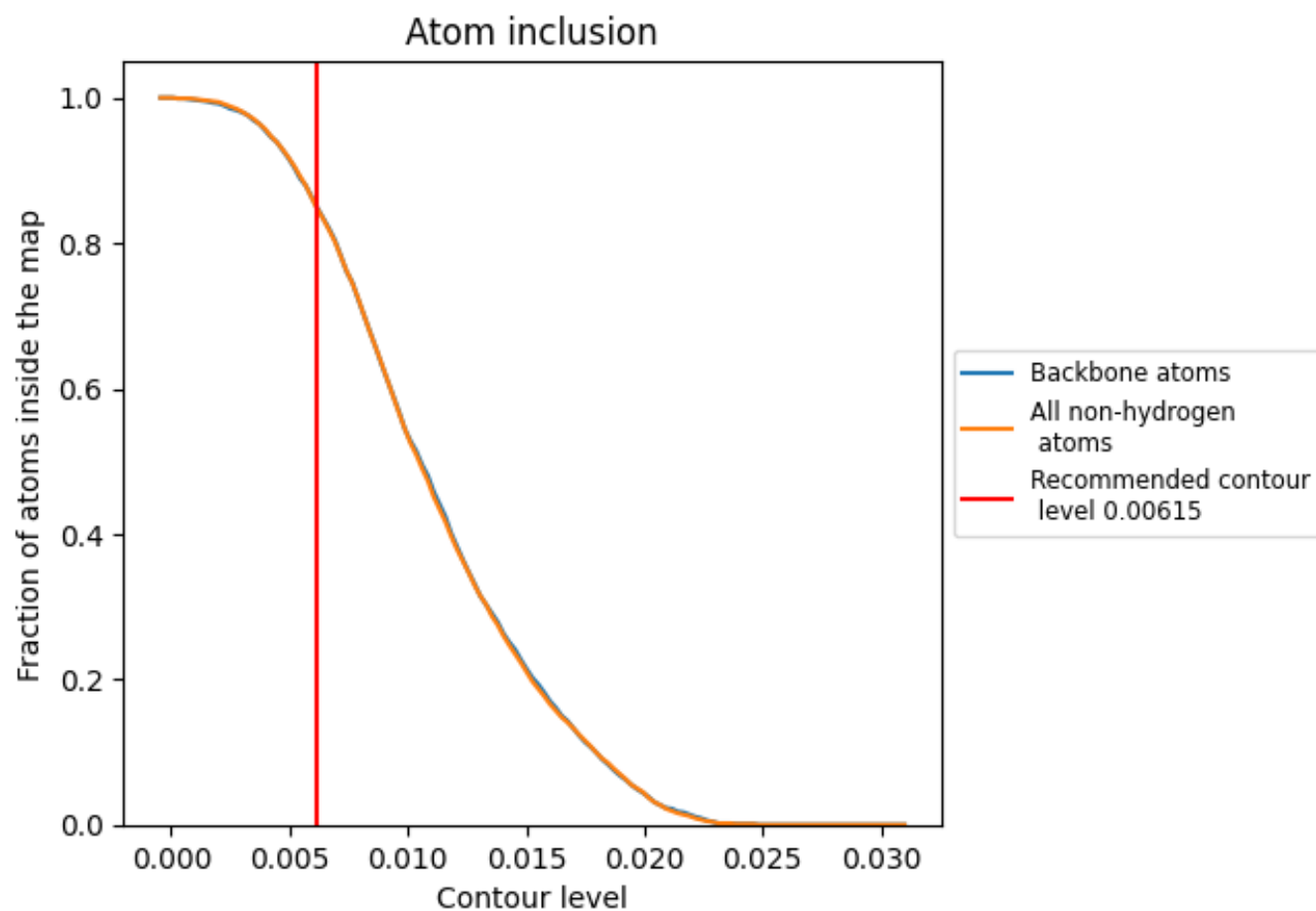
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00615).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.00615) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8480	<div></div> 0.3260
A	<div></div> 0.9130	<div></div> 0.4110
B	<div></div> 0.9140	<div></div> 0.4190
C	<div></div> 0.6470	<div></div> 0.2150
D	<div></div> 0.9170	<div></div> 0.2320
E	<div></div> 0.7710	<div></div> 0.1800

