



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:41 PM UTC

PDB ID : 8U1M / pdb_00008u1m
EMDB ID : EMD-41817
Title : Cryo-EM structure of the HSP90 dimer (NTD-MD) in the semi-open state
Authors : Finci, L.I.; Simanshu, D.K.
Deposited on : 2023-09-01
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

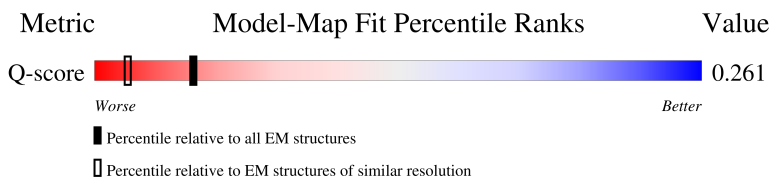
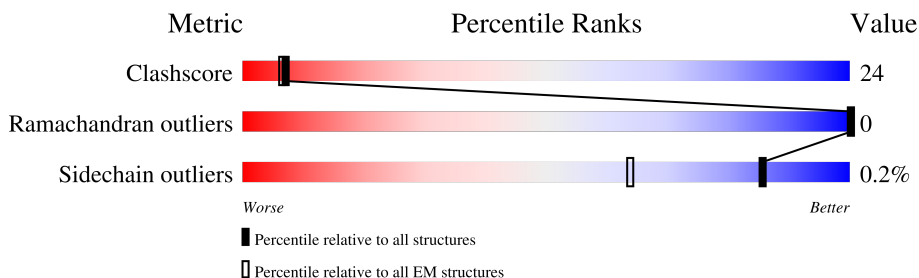
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

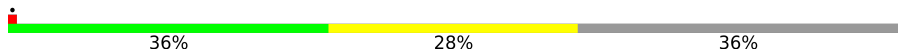
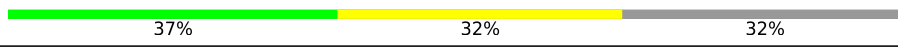
The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	722	
1	B	722	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	A	801	-	-	X	-

2 Entry composition [i](#)

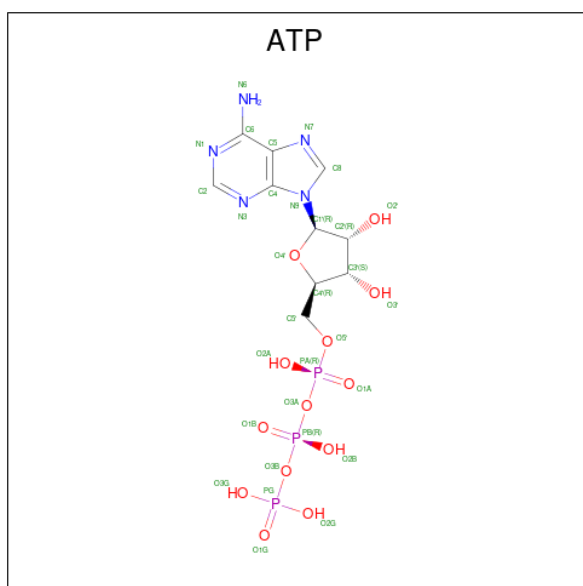
There are 3 unique types of molecules in this entry. The entry contains 7882 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Heat shock protein 83.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	463	Total	C	N	O	S	0	0
			3789	2410	633	732	14		
1	B	494	Total	C	N	O	S	0	0
			4029	2558	675	782	14		

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
3	B	1	1	1	0

ASP	GLU	PRO	ILE	SER	ASN	Q492	G396	V322	GLU	F165	K74	MET
GLU	VAL	GLU	VAL	ILE	LYS	V499	N397	V327	ASP	F175	I75	PRO
ILE	GLU	GLU	GLU	GLU	VAL	E500	K398	E327	LYS	L175	I76	GLU
GLN	THR	THR	THR	THR	LYS	R501	I399	R328	GLU	L176	T83	GLN
VAL	THR	THR	THR	THR	LYS	V502	L400	R329	ASP	R177	F84	THR
GLU	VAL	VAL	VAL	VAL	VAL	K503	K401	A330	GLU	G178	T85	ASP
SER	VAL	VAL	VAL	VAL	VAL	R404	R404	L331	LYS	T179	I86	SER
SER	LYS	SER	SER	SER	ASN	E508	L407	L332	GLU	K180	I87	SER
SER	ALA	ALA	ALA	ALA	ASN	M612	V408	F333	ASP	I181	D88	GLU
VAL	GLU	GLU	GLU	GLU	LEU	T513	L407	V334	GLU	V182	E11	V12
GLY	ASP	ASP	ASP	ASP	VAL	E514	L412	P335	LYS	L183	G90	E13
VAL	LYS	LYS	LYS	LYS	GLU	P515	E413	R336	LYS	H184	G92	T14
PRO	ASN	ASN	ASN	ASN	GLU	I516	L414	P339	ILE	I185	M93	F15
PRO	ASP	ASP	ASP	ASP	PRO	D617	F415	D341	ASP	E187	T94	A16
LEU	LYS	LYS	LYS	LYS	CYS	E518	E416	D341	ASP	D188	K95	F17
GLU	ALA	ALA	ALA	ALA	CYS	Y519	E417	K346	VAL	L189	A96	E20
GLY	VAL	VAL	VAL	VAL	ILE	V520	L418	K347	GLY	A190	E20	I21
ASP	LYS	LYS	LYS	LYS	VAL	V521	L418	K348	GLU	E191	I21	A22
ALA	ASP	ASP	ASP	ASP	THR	Y425	Y425	K349	ASP	E191	I105	Q23
ASP	LEU	LEU	LEU	LEU	ALA	M524	Y428	K350	ASP	A106	Q23	L24
ASP	VAL	VAL	VAL	VAL	GLN	R525	Y428	N351	GLU	I198	L24	M25
ALA	ILE	ILE	ILE	ILE	TYR	E526	F432	I352	GLU	T110	S26	L27
SER	GLY	GLY	GLY	GLY	TRP	K530	S433	K353	ASP	M114	L27	I28
ARG	LEU	LEU	LEU	LEU	TRP	T531	K437	L354	LYS	K203	I29	N30
LEU	TYR	TYR	TYR	TYR	ALA	F531	L438	R357	LYS	R204	N30	F32
GLU	THR	THR	THR	THR	ASN	V533	L438	K358	LYS	K206	T31	Y33
VAL	ALA	ALA	ALA	ALA	MET	S534	G439	I361	ASP	Q207	M125	S34
ASP	ALA	ALA	ALA	ALA	GLU	K537	I440	M362	GLY	Q207	I126	S34
LEU	LEU	LEU	LEU	LEU	ARG	Y441	H441	D363	GLU	T209	G127	N35
SER	ILE	ILE	ILE	ILE	ILE	D545	L450	N364	ASP	G210	G130	K36
SER	GLY	GLY	GLY	GLY	LYS	GLU	L450	C365	LYS	I211	V131	E37
PHE	ALA	ALA	ALA	ALA	ALA	GLU	L454	E366	LYS	I213	Y134	I38
THR	GLN	GLN	GLN	GLN	ALA	GLU	R455	D367	LYS	K214	S135	F39
LEU	ALA	ALA	ALA	ALA	ALA	LYS	Y456	Y372	LYS	L215	C136	L40
ASP	LEU	LEU	LEU	LEU	LEU	LYS	S459	N374	LYS	T216	Y137	R41
GLU	GLU	GLU	GLU	GLU	ARG	ARG	A460	L373	LYS	V217	L138	S45
PRO	ASP	ASP	ASP	ASP	THR	GLU	S461	N374	LYS	K219	V139	N46
GLN	GLN	GLN	GLN	GLN	THR	GLU	G462	A292	LYS	E220	S47	S47
VAL	VAL	VAL	VAL	VAL	SER	ASP	K377	I295	LYS	E221	S48	D49
HIS	ALA	ALA	ALA	ALA	THR	LYS	C466	T296	LYS	E222	A50	L51
ALA	ALA	ALA	ALA	ALA	MET	LYS	V379	T296	LYS	K223	D52	K53
SER	GLY	GLY	GLY	GLY	GLY	VAL	Y471	D381	ASP	E224	I54	I54
ARG	ARG	ARG	ARG	ARG	MET	PHE	V472	S382	ASP	ALA	K148	L65
TYR	TYR	TYR	TYR	TYR	ALA	GLU	M475	E383	ASP	TYR	H149	D66
ARG	ARG	ARG	ARG	ARG	ALA	GLY	GLY	L387	ASP	ASP	K148	G68
MET	MET	MET	MET	MET	LYS	LEU	LEU	N388	ASP	ASP	H149	I54
ILE	ILE	ILE	ILE	ILE	LYS	CYS	I482	Y483	GLU	GLU	N150	L65
LYS	LYS	LYS	LYS	LYS	HIS	LYS	Y483	N389	GLU	GLU	D151	D66
HIS	HIS	HIS	HIS	HIS	LEU	VAL	Y484	I389	GLU	GLU	D152	G68
LEU	LEU	LEU	LEU	LEU	LEU	VAL	GLY	S390	GLU	GLU	E153	S45
GLY	GLY	GLY	GLY	GLY	GLY	MET	G487	R391	LYS	LYS	Q154	N46
ILE	ILE	ILE	ILE	ILE	ILE	LYS	E488	E392	LYS	LYS	Q154	S47
ASN	ASN	ASN	ASN	ASN	ASN	ASN	N489	N393	GLU	GLU	H157	L71
PRO	PRO	PRO	PRO	PRO	PRO	ASN	R490	L394	GLU	GLU	E158	Y72
ASP	ASP	ASP	ASP	ASP	ASP	LEU	D491	Q395	GLU	GLU	Y72	I73
GLU	HIS	HIS	HIS	HIS	HIS	ASP			GLU	GLU	S159	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	325732	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.318	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	219.648, 219.648, 219.648	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.858, 0.858, 0.858	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: ATP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/3856	0.35	0/5181
1	B	0.12	0/4099	0.34	0/5510
All	All	0.12	0/7955	0.34	0/10691

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3789	0	3772	190	0
1	B	4029	0	4018	201	0
2	A	31	0	12	10	0
2	B	31	0	12	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	7882	0	7814	375	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 24.

All (375) 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:B:159:SER:CB	1:B:165:PHE:CD1	1.78	1.60
1:B:159:SER:CB	1:B:165:PHE:HD1	1.05	1.55
1:B:159:SER:HB2	1:B:165:PHE:CD1	1.43	1.36
1:B:159:SER:HB3	1:B:165:PHE:CD1	1.49	1.26
1:B:159:SER:HB2	1:B:165:PHE:CE1	1.74	1.21
1:B:159:SER:CB	1:B:165:PHE:CE1	2.31	1.11
1:A:213:ILE:H	1:A:282:ASN:HD21	1.16	0.93
1:B:202:VAL:CG1	1:B:282:ASN:OD1	2.19	0.91
1:B:202:VAL:HG11	1:B:282:ASN:OD1	1.72	0.89
1:B:50:ALA:HB1	1:B:91:ILE:H	1.43	0.84
1:A:50:ALA:HB1	1:A:91:ILE:H	1.42	0.82
1:B:397:ASN:HA	1:B:400:LEU:HB2	1.60	0.82
1:B:137:TYR:OH	1:B:165:PHE:CE1	2.33	0.81
1:B:159:SER:HB3	1:B:165:PHE:HD1	0.62	0.79
1:A:334:VAL:HG11	1:A:428:TYR:HE2	1.44	0.79
1:A:267:LYS:HG3	1:A:268:LYS:H	1.52	0.75
1:B:51:LEU:HD22	1:B:71:LEU:HB3	1.71	0.73
1:A:97:ASP:OD1	1:A:101:ASN:ND2	2.22	0.72
1:B:137:TYR:OH	1:B:165:PHE:CZ	2.43	0.72
1:B:21:ILE:O	1:B:24:LEU:N	2.23	0.71
1:A:455:ARG:HB3	1:A:465:ALA:HB1	1.73	0.70
1:B:354:LEU:HB3	1:B:362:MET:HB2	1.72	0.70
1:B:483:TYR:HA	1:B:533:VAL:HB	1.73	0.70
1:A:168:ARG:HE	1:B:12:VAL:HA	1.56	0.70
1:A:28:ILE:HD11	1:A:105:ILE:HD12	1.75	0.68
1:B:41:ARG:HD3	1:B:205:HIS:HD2	1.58	0.68
1:A:433:SER:HG	1:A:513:THR:HG1	1.39	0.68
1:A:40:LEU:HD23	1:A:201:ILE:HD11	1.74	0.68
1:B:361:ILE:HD12	1:B:391:ARG:HB3	1.76	0.68
1:A:316:ALA:HB1	1:A:414:LEU:HD11	1.75	0.67
1:B:401:LYS:HA	1:B:404:ARG:HD2	1.77	0.67
1:B:215:LEU:HD13	1:B:282:ASN:HD22	1.61	0.66
1:A:93:MET:HE1	2:A:801:ATP:C4	2.30	0.66
1:A:334:VAL:HG11	1:A:428:TYR:CE2	2.30	0.66
1:A:421:ASP:OD2	1:A:424:ASN:ND2	2.29	0.65
1:A:25:MET:HG2	1:A:28:ILE:HD12	1.78	0.65
1:B:159:SER:OG	1:B:165:PHE:CE1	2.49	0.64
1:A:332:LEU:HB3	1:A:376:ILE:HD11	1.79	0.64
1:B:283:LYS:O	1:B:283:LYS:HG2	1.97	0.63
1:B:501:ARG:HH21	1:B:502:VAL:HG22	1.62	0.63
1:A:222:GLU:HB3	1:A:267:LYS:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:SER:HB3	1:B:126:ILE:HG21	1.81	0.63
1:A:25:MET:HA	1:A:28:ILE:HB	1.79	0.63
1:A:24:LEU:HD21	1:A:105:ILE:HG21	1.81	0.62
1:A:348:ARG:NH1	1:A:363:ASP:OD1	2.31	0.62
1:A:351:ASN:ND2	1:A:376:ILE:O	2.31	0.62
1:A:267:LYS:HG3	1:A:268:LYS:N	2.13	0.62
1:B:210:GLY:HA2	1:B:286:PRO:HB3	1.80	0.62
1:B:388:ASN:ND2	1:B:390:SER:OG	2.32	0.62
1:A:370:PRO:HD3	1:A:404:ARG:HG3	1.81	0.62
1:A:219:LYS:O	1:A:221:ARG:NH1	2.33	0.61
1:A:447:ARG:HD3	1:A:523:GLN:HB3	1.82	0.61
1:A:126:ILE:HD11	1:A:361:ILE:HD11	1.83	0.61
1:A:213:ILE:N	1:A:282:ASN:HD21	1.94	0.61
1:B:20:GLU:OE2	1:B:23:GLN:NE2	2.32	0.61
1:A:146:HIS:ND1	1:A:170:ASP:OD2	2.34	0.61
1:B:110:THR:OG1	1:B:125:MET:SD	2.54	0.61
1:B:124:SER:O	1:B:358:ARG:NH2	2.31	0.61
1:B:348:ARG:NH2	1:B:363:ASP:O	2.34	0.61
1:B:512:MET:SD	1:B:517:ASP:HB3	2.41	0.60
1:A:46:ASN:ND2	2:A:801:ATP:O2A	2.29	0.60
1:A:202:VAL:HG11	1:A:281:LEU:HD13	1.83	0.60
1:B:454:LEU:O	1:B:455:ARG:NH1	2.34	0.60
1:A:95:LYS:HA	1:A:98:LEU:HD12	1.84	0.60
1:B:41:ARG:HD3	1:B:205:HIS:CD2	2.37	0.60
1:B:83:THR:HG23	1:B:182:VAL:HG13	1.82	0.60
1:B:489:ASN:O	1:B:492:GLN:NE2	2.34	0.60
1:B:202:VAL:HG11	1:B:282:ASN:CG	2.27	0.60
1:A:371:GLU:HG3	1:A:438:LEU:HD21	1.84	0.59
1:B:341:ASP:HB3	1:B:347:LYS:HD3	1.84	0.59
1:A:46:ASN:HB3	2:A:801:ATP:C6	2.36	0.59
1:B:137:TYR:OH	1:B:165:PHE:HE1	1.84	0.59
1:A:125:MET:HA	1:A:125:MET:HE3	1.83	0.59
1:B:351:ASN:HA	1:B:377:LYS:HE2	1.85	0.59
1:A:362:MET:SD	1:A:363:ASP:N	2.76	0.59
1:B:86:ILE:N	1:B:181:ILE:O	2.35	0.58
1:A:362:MET:SD	1:A:364:ASN:N	2.76	0.58
1:B:499:VAL:O	1:B:503:LYS:N	2.36	0.58
1:A:145:VAL:HG22	1:A:181:ILE:HG23	1.85	0.58
1:A:355:TYR:CZ	1:A:360:PHE:HB2	2.38	0.58
1:A:458:THR:HG22	1:A:510:VAL:HG22	1.86	0.58
1:B:54:ILE:HD11	1:B:90:GLY:C	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:THR:HG23	1:A:517:ASP:HB2	1.85	0.57
1:B:212:PRO:HB3	1:B:283:LYS:HG3	1.85	0.57
1:A:90:GLY:O	1:A:177:ARG:NE	2.28	0.57
1:A:122:ASP:O	1:A:329:ARG:NH2	2.37	0.57
1:A:46:ASN:HB3	2:A:801:ATP:C5	2.40	0.57
1:A:91:ILE:O	1:A:149:HIS:ND1	2.32	0.57
1:B:459:SER:O	1:B:490:ARG:NH2	2.38	0.57
1:A:54:ILE:HG21	1:A:177:ARG:HH22	1.70	0.57
1:A:73:ILE:HG13	1:A:213:ILE:HG23	1.87	0.57
1:B:38:ILE:HG23	1:B:135:SER:HB2	1.87	0.57
1:B:146:HIS:HB2	1:B:180:LYS:HB3	1.87	0.57
1:B:393:MET:SD	1:B:395:GLN:NE2	2.78	0.57
1:A:335:PRO:HG3	1:A:377:LYS:HE2	1.86	0.56
1:B:137:TYR:HH	1:B:165:PHE:HZ	1.47	0.56
1:B:75:ILE:HB	1:B:215:LEU:HD12	1.87	0.56
1:A:166:THR:HB	1:A:168:ARG:HH22	1.70	0.56
1:B:35:ASN:OD1	1:B:36:LYS:N	2.39	0.56
1:B:143:VAL:HG12	1:B:183:LEU:HG	1.87	0.56
1:A:92:GLY:HA3	1:A:149:HIS:HA	1.88	0.56
1:A:290:ARG:NH2	1:A:299:GLU:OE2	2.38	0.56
1:A:51:LEU:HD22	1:A:71:LEU:HB3	1.88	0.56
1:A:146:HIS:O	1:A:180:LYS:N	2.36	0.56
1:A:358:ARG:NH2	1:A:383:GLU:OE2	2.40	0.55
1:B:144:THR:HG23	1:B:158:GLU:HB2	1.87	0.55
1:A:50:ALA:HB1	1:A:91:ILE:N	2.19	0.55
1:B:215:LEU:HD13	1:B:282:ASN:ND2	2.22	0.55
1:B:441:HIS:HB2	1:B:520:VAL:HG12	1.88	0.55
1:A:267:LYS:NZ	1:A:268:LYS:HB3	2.21	0.55
1:B:139:VAL:HG13	1:B:189:LEU:HD23	1.89	0.55
1:A:57:GLU:O	1:A:61:ASP:N	2.39	0.55
1:B:302:ASP:OD1	1:B:305:LYS:NZ	2.32	0.55
1:A:281:LEU:C	1:A:282:ASN:HD22	2.14	0.55
1:B:318:LYS:HB2	1:B:414:LEU:HD22	1.89	0.55
1:B:361:ILE:HG21	1:B:387:LEU:HD22	1.89	0.54
1:A:73:ILE:HG22	1:A:88:ASP:HB2	1.89	0.54
1:A:388:ASN:OD1	1:A:392:GLU:N	2.36	0.54
1:B:460:ALA:N	1:B:508:GLU:OE2	2.41	0.54
1:B:73:ILE:HB	1:B:213:ILE:HG12	1.90	0.54
1:A:524:MET:SD	1:A:524:MET:N	2.80	0.54
1:B:354:LEU:HB3	1:B:362:MET:CB	2.38	0.54
1:A:344:GLU:OE2	1:B:441:HIS:NE2	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ASN:ND2	1:A:373:LEU:O	2.38	0.54
1:B:292:ALA:HA	1:B:295:ILE:HD12	1.89	0.54
1:A:213:ILE:H	1:A:282:ASN:ND2	1.97	0.54
1:B:471:TYR:OH	1:B:508:GLU:O	2.17	0.54
1:A:101:ASN:HB3	2:A:801:ATP:H4'	1.89	0.53
1:A:157:TRP:HA	1:A:167:VAL:HG12	1.89	0.53
1:A:387:LEU:HD13	1:A:391:ARG:HD3	1.90	0.53
1:A:168:ARG:NH2	1:B:13:GLU:O	2.41	0.53
1:A:39:PHE:HB2	1:A:136:CYS:HA	1.90	0.53
1:B:145:VAL:HG22	1:B:181:ILE:HG23	1.91	0.53
1:A:140:ALA:HA	1:A:185:ILE:HA	1.90	0.52
1:A:166:THR:HG22	1:B:14:THR:HG23	1.90	0.52
1:B:49:ASP:OD2	1:B:127:GLY:N	2.40	0.52
1:B:373:LEU:HD12	1:B:408:VAL:HG12	1.90	0.52
1:B:351:ASN:ND2	1:B:374:ASN:O	2.32	0.52
1:B:487:GLY:HA3	1:B:492:GLN:HE22	1.74	0.52
1:A:429:TYR:O	1:A:433:SER:HB3	2.09	0.52
1:A:440:ILE:HG21	1:A:520:VAL:HG13	1.91	0.52
1:A:90:GLY:C	1:A:177:ARG:HH21	2.17	0.52
1:A:300:TYR:CZ	1:A:317:VAL:HB	2.44	0.52
1:A:300:TYR:CE1	1:A:317:VAL:HB	2.44	0.52
1:B:331:LEU:N	1:B:379:VAL:O	2.43	0.52
1:B:388:ASN:HB3	1:B:393:MET:SD	2.50	0.52
1:A:318:LYS:HB2	1:A:414:LEU:HD13	1.91	0.52
1:A:357:ARG:HG3	1:A:383:GLU:HA	1.92	0.52
1:A:385:LEU:HD13	1:A:386:PRO:HD2	1.90	0.52
1:A:372:TYR:HB3	1:A:438:LEU:HG	1.92	0.52
1:B:288:TRP:HA	1:B:300:TYR:HE1	1.74	0.51
1:A:50:ALA:HB2	2:A:801:ATP:C2	2.45	0.51
1:A:145:VAL:O	1:A:157:TRP:N	2.43	0.51
1:A:468:LEU:HA	1:A:471:TYR:HB3	1.92	0.51
1:A:350:ASN:HB2	1:A:363:ASP:HB2	1.93	0.51
1:A:425:TYR:OH	1:A:453:LEU:O	2.20	0.51
1:B:516:ILE:HD12	1:B:519:TYR:HD2	1.75	0.51
1:B:105:ILE:HD12	1:B:105:ILE:H	1.76	0.51
1:B:212:PRO:HB3	1:B:283:LYS:CG	2.40	0.51
1:B:223:LYS:HE2	1:B:224:GLU:HG3	1.93	0.51
1:A:43:LEU:HD13	1:A:86:ILE:HD13	1.92	0.51
1:A:437:LYS:NZ	1:A:513:THR:H	2.09	0.51
1:B:514:GLU:HB2	1:B:517:ASP:CG	2.36	0.51
1:A:208:PHE:CZ	1:A:307:LEU:HG	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:TYR:OH	1:A:524:MET:O	2.28	0.51
1:B:159:SER:OG	1:B:165:PHE:HE1	1.92	0.51
1:B:21:ILE:HG22	1:B:25:MET:SD	2.51	0.50
1:B:85:THR:HG23	1:B:180:LYS:HG3	1.92	0.50
1:B:307:LEU:O	1:B:353:LYS:NZ	2.43	0.50
1:B:105:ILE:HG13	1:B:134:TYR:CE2	2.47	0.50
1:B:114:MET:HE2	1:B:125:MET:HE1	1.94	0.50
1:B:145:VAL:N	1:B:157:TRP:O	2.44	0.50
1:A:218:GLU:OE1	1:A:221:ARG:NH2	2.44	0.50
1:A:36:LYS:HA	1:A:138:LEU:HD13	1.92	0.50
1:B:76:ILE:HG23	1:B:217:VAL:HG13	1.94	0.50
1:A:187:GLU:OE2	1:A:187:GLU:N	2.44	0.50
1:A:395:GLN:NE2	1:B:30:ASN:O	2.45	0.50
1:A:91:ILE:HG12	1:A:149:HIS:CE1	2.47	0.50
1:B:86:ILE:HB	1:B:181:ILE:HB	1.93	0.50
1:B:28:ILE:O	1:B:32:PHE:HB2	2.12	0.49
1:B:440:ILE:HG13	1:B:454:LEU:HD11	1.93	0.49
1:A:41:ARG:NH2	1:A:42:GLU:OE2	2.33	0.49
1:A:28:ILE:HG12	1:A:32:PHE:CE2	2.48	0.49
1:A:74:LYS:HB3	1:A:87:ILE:HG23	1.94	0.49
1:A:484:TYR:HE2	1:A:520:VAL:HG12	1.77	0.49
1:B:68:GLY:O	1:B:177:ARG:NE	2.45	0.49
1:A:50:ALA:HB2	2:A:801:ATP:H2	1.78	0.49
1:A:405:LYS:O	1:A:409:LYS:HG2	2.11	0.49
1:A:175:LEU:HD11	1:A:180:LYS:HB3	1.94	0.49
1:A:32:PHE:N	1:B:395:GLN:OE1	2.46	0.49
2:A:801:ATP:O1B	2:A:801:ATP:O3'	2.23	0.49
1:B:84:PHE:HB3	1:B:183:LEU:HB2	1.94	0.49
1:B:388:ASN:OD1	1:B:392:GLU:N	2.36	0.49
1:B:388:ASN:CG	1:B:392:GLU:H	2.19	0.49
1:B:521:VAL:HA	1:B:524:MET:SD	2.53	0.49
1:A:18:GLN:HB3	1:B:104:THR:HG23	1.95	0.49
1:B:95:LYS:HD2	1:B:96:ALA:N	2.27	0.49
1:B:136:CYS:SG	1:B:143:VAL:HG11	2.53	0.49
1:B:534:SER:HB3	1:B:537:LYS:HB2	1.95	0.49
1:A:88:ASP:OD1	1:A:179:THR:OG1	2.24	0.48
1:B:22:ALA:HA	1:B:25:MET:HE1	1.95	0.48
1:B:456:TYR:O	1:B:466:CYS:N	2.43	0.48
1:B:188:ASP:OD1	1:B:188:ASP:N	2.45	0.48
1:B:352:ILE:N	1:B:365:CYS:SG	2.86	0.48
1:A:28:ILE:O	1:A:32:PHE:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:HIS:N	1:A:180:LYS:O	2.35	0.48
1:A:389:ILE:HD13	1:B:27:LEU:HD11	1.96	0.48
2:A:801:ATP:H5'1	2:A:801:ATP:C8	2.49	0.48
1:B:41:ARG:HB2	1:B:205:HIS:HB3	1.94	0.48
1:A:93:MET:HB3	1:A:98:LEU:HG	1.96	0.48
1:A:485:ILE:O	1:A:512:MET:HB2	2.13	0.48
1:A:215:LEU:HB2	1:A:281:LEU:HD11	1.96	0.48
1:A:110:THR:OG1	1:A:127:GLY:O	2.23	0.48
1:A:280:GLU:HA	1:A:283:LYS:HE3	1.97	0.47
1:A:157:TRP:CH2	1:A:159:SER:HB3	2.50	0.47
1:B:47:SER:HA	2:B:801:ATP:N6	2.29	0.47
1:B:202:VAL:HG12	1:B:282:ASN:OD1	2.11	0.47
1:A:105:ILE:HG13	1:A:131:VAL:HG12	1.97	0.47
1:B:372:TYR:HB3	1:B:438:LEU:HD22	1.96	0.47
1:B:391:ARG:NH1	2:B:801:ATP:O1G	2.48	0.47
1:A:71:LEU:O	1:A:212:PRO:HD2	2.15	0.47
1:B:433:SER:O	1:B:437:LYS:HG2	2.14	0.47
1:A:146:HIS:HB2	1:A:180:LYS:HB3	1.96	0.47
1:A:197:LYS:O	1:A:201:ILE:HG23	2.14	0.47
1:B:191:GLU:HB2	1:B:197:LYS:HE3	1.97	0.47
1:B:203:LYS:O	1:B:207:GLN:HB2	2.14	0.47
1:B:362:MET:SD	1:B:393:MET:HA	2.55	0.47
1:A:73:ILE:HD11	1:A:213:ILE:HG12	1.96	0.47
1:B:302:ASP:HA	1:B:305:LYS:HD2	1.97	0.46
1:A:98:LEU:HD23	1:A:102:LEU:HD12	1.97	0.46
1:B:66:ASP:OD1	1:B:150:ASN:ND2	2.34	0.46
1:B:313:ASP:HB2	1:B:336:ARG:HH21	1.80	0.46
1:A:408:VAL:O	1:A:412:LEU:HG	2.15	0.46
1:B:350:ASN:OD1	1:B:350:ASN:N	2.43	0.46
1:B:388:ASN:HB3	1:B:395:GLN:HE21	1.80	0.46
1:A:281:LEU:C	1:A:282:ASN:ND2	2.73	0.46
1:A:213:ILE:HG13	1:A:282:ASN:ND2	2.29	0.46
1:B:212:PRO:CB	1:B:283:LYS:HG3	2.45	0.46
1:A:123:ILE:HD12	1:A:123:ILE:HA	1.85	0.46
1:B:459:SER:OG	1:B:460:ALA:N	2.48	0.46
1:B:472:VAL:O	1:B:475:MET:HE2	2.16	0.46
1:A:425:TYR:CE1	1:A:428:TYR:HD1	2.34	0.46
1:A:315:LEU:N	1:A:334:VAL:O	2.44	0.46
1:A:126:ILE:HG21	1:A:359:VAL:HG21	1.97	0.45
1:B:126:ILE:HD12	1:B:357:ARG:HD2	1.98	0.45
1:A:72:TYR:HB2	1:A:212:PRO:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:MET:HE1	1:B:17:PHE:HB3	1.99	0.45
1:A:273:GLU:OE1	1:A:274:LYS:N	2.50	0.45
1:A:146:HIS:CD2	1:A:180:LYS:HE2	2.52	0.45
1:B:75:ILE:HG21	1:B:198:ILE:HG21	1.98	0.45
1:A:312:GLU:HG2	1:A:313:ASP:H	1.82	0.45
1:B:367:ASP:O	1:B:404:ARG:NH2	2.38	0.45
1:B:106:ALA:H	1:B:131:VAL:HG12	1.82	0.45
1:A:52:ASP:OD1	1:A:211:TYR:OH	2.32	0.45
1:A:318:LYS:HE2	1:A:413:GLU:HB2	1.99	0.45
1:B:122:ASP:OD1	1:B:122:ASP:N	2.49	0.45
1:B:339:PRO:HD2	1:B:432:PHE:HE1	1.82	0.45
1:B:221:ARG:HH22	1:B:223:LYS:HA	1.81	0.44
1:A:25:MET:HE1	1:B:17:PHE:CG	2.53	0.44
1:A:64:LYS:HA	1:A:64:LYS:HD2	1.73	0.44
1:A:331:LEU:HB3	1:A:333:PHE:HE1	1.82	0.44
1:A:388:ASN:CG	1:A:393:MET:H	2.26	0.44
1:B:105:ILE:HD12	1:B:105:ILE:N	2.32	0.44
1:A:175:LEU:HD21	1:A:180:LYS:HB2	1.99	0.44
1:B:65:LEU:HA	1:B:177:ARG:HH22	1.81	0.44
1:B:418:LEU:O	1:B:425:TYR:HB2	2.17	0.44
1:A:124:SER:HB2	1:A:357:ARG:HB3	1.99	0.44
1:A:208:PHE:HE1	1:A:307:LEU:HA	1.83	0.44
1:B:329:ARG:HG2	1:B:381:ASP:HB3	2.00	0.44
1:A:517:ASP:HA	1:A:520:VAL:HB	2.00	0.44
1:B:350:ASN:HA	1:B:363:ASP:O	2.18	0.44
1:A:41:ARG:HB2	1:A:205:HIS:CD2	2.52	0.44
1:A:71:LEU:O	1:A:211:TYR:HB3	2.17	0.44
1:A:316:ALA:HB2	1:A:418:LEU:HD11	2.00	0.44
1:B:48:SER:HB2	1:B:209:ILE:HG23	2.00	0.44
1:A:291:ASN:OD1	1:A:292:ALA:N	2.51	0.43
1:A:355:TYR:O	1:A:381:ASP:HA	2.17	0.43
1:A:415:PHE:HB3	1:A:425:TYR:OH	2.17	0.43
1:A:440:ILE:HG23	1:A:524:MET:SD	2.58	0.43
1:B:52:ASP:OD2	1:B:211:TYR:OH	2.28	0.43
1:B:73:ILE:O	1:B:214:LYS:N	2.51	0.43
1:B:37:GLU:HB3	1:B:205:HIS:CE1	2.52	0.43
1:B:517:ASP:HA	1:B:520:VAL:HG22	2.00	0.43
1:A:32:PHE:C	1:B:395:GLN:HE22	2.26	0.43
1:A:421:ASP:HB3	1:A:424:ASN:HB2	2.00	0.43
1:A:447:ARG:HG2	1:A:524:MET:HE1	2.01	0.43
1:A:484:TYR:OH	1:A:524:MET:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LEU:HD23	1:A:31:THR:HG21	2.01	0.43
1:A:73:ILE:HG22	1:A:88:ASP:CB	2.49	0.43
1:B:149:HIS:HB2	1:B:152:ASP:HB3	1.99	0.43
1:B:335:PRO:HG3	1:B:377:LYS:HG3	2.01	0.43
1:A:320:PHE:CZ	1:A:330:ALA:HB3	2.53	0.43
1:B:36:LYS:HD2	1:B:189:LEU:HD21	1.99	0.43
1:B:213:ILE:N	1:B:283:LYS:HA	2.33	0.43
1:B:408:VAL:O	1:B:412:LEU:HG	2.18	0.43
1:B:471:TYR:CE1	1:B:482:ILE:HG23	2.53	0.43
1:A:66:ASP:HA	1:A:69:LYS:HE3	2.01	0.43
1:A:352:ILE:HG13	1:A:369:ILE:HD13	2.00	0.43
1:B:300:TYR:HA	1:B:303:PHE:HB3	2.01	0.43
1:A:102:LEU:HD21	2:A:801:ATP:C8	2.54	0.43
1:B:484:TYR:CE1	1:B:532:LEU:HB3	2.53	0.43
1:A:267:LYS:HZ2	1:A:268:LYS:HD3	1.84	0.43
1:B:93:MET:HE1	2:B:801:ATP:C4	2.54	0.43
1:B:148:LYS:HG2	1:B:176:GLY:H	1.84	0.43
1:B:175:LEU:HD11	1:B:180:LYS:HB3	2.01	0.43
1:A:53:LYS:HB3	1:A:91:ILE:HD12	2.01	0.43
1:A:149:HIS:CD2	1:A:151:ASP:H	2.37	0.43
1:A:483:TYR:HB3	1:A:509:VAL:HA	2.01	0.43
1:A:125:MET:C	1:A:357:ARG:HD2	2.44	0.42
1:A:185:ILE:HD11	1:A:190:ALA:HA	2.02	0.42
1:A:188:ASP:OD2	1:B:398:LYS:NZ	2.42	0.42
1:A:338:ALA:N	1:A:431:GLN:OE1	2.41	0.42
1:A:418:LEU:HD22	1:A:424:ASN:HB3	2.01	0.42
1:A:470:GLU:O	1:A:474:ARG:NE	2.52	0.42
1:B:526:GLU:HG3	1:B:530:LYS:C	2.44	0.42
1:B:415:PHE:HA	1:B:418:LEU:HD12	2.02	0.42
1:B:418:LEU:HD13	1:B:428:TYR:CE2	2.54	0.42
1:A:211:TYR:O	1:A:282:ASN:OD1	2.37	0.42
1:A:124:SER:HB3	1:A:358:ARG:HH21	1.84	0.42
1:B:145:VAL:HB	1:B:157:TRP:HB3	2.01	0.42
1:B:219:LYS:NZ	1:B:274:LYS:O	2.47	0.42
1:B:290:ARG:NH1	1:B:296:THR:H	2.18	0.42
1:B:373:LEU:HD23	1:B:373:LEU:HA	1.88	0.42
1:A:273:GLU:CD	1:A:274:LYS:H	2.27	0.42
1:A:425:TYR:HE1	1:A:428:TYR:HD1	1.67	0.42
1:B:72:TYR:H	1:B:89:THR:HG1	1.61	0.42
1:B:74:LYS:N	1:B:87:ILE:O	2.35	0.42
1:A:27:LEU:HB3	1:B:389:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LEU:HD13	1:A:454:LEU:HD22	2.01	0.42
1:B:330:ALA:HB1	1:B:332:LEU:HG	2.02	0.42
1:B:75:ILE:HD12	1:B:86:ILE:HD12	2.02	0.42
1:B:317:VAL:HG23	1:B:333:PHE:CD1	2.55	0.42
1:B:516:ILE:HD12	1:B:516:ILE:HA	1.86	0.42
1:B:154:GLN:OE1	1:B:175:LEU:N	2.42	0.42
1:B:450:LEU:O	1:B:454:LEU:HG	2.19	0.42
1:B:93:MET:HB2	1:B:147:SER:HB3	2.02	0.41
1:A:213:ILE:HB	1:A:281:LEU:HB2	2.00	0.41
1:A:426:LYS:HG3	1:A:457:HIS:NE2	2.35	0.41
1:B:146:HIS:O	1:B:180:LYS:N	2.25	0.41
1:B:414:LEU:O	1:B:418:LEU:HG	2.20	0.41
1:A:418:LEU:HD23	1:A:418:LEU:HA	1.92	0.41
1:B:332:LEU:HD11	1:B:407:LEU:HD22	2.02	0.41
1:A:365:CYS:HB2	1:B:346:LYS:HD3	2.03	0.41
1:B:322:VAL:O	1:B:327:GLU:HA	2.19	0.41
1:B:462:GLY:O	1:B:490:ARG:NH1	2.53	0.41
1:B:382:SER:OG	1:B:383:GLU:N	2.53	0.41
1:A:354:LEU:HG	1:A:356:VAL:HG23	2.01	0.41
1:B:413:GLU:HG3	1:B:417:GLU:OE2	2.20	0.41
1:B:489:ASN:H	1:B:492:GLN:HE21	1.67	0.41
1:A:15:PHE:CD2	1:B:165:PHE:HB2	2.56	0.41
1:A:54:ILE:HD12	1:A:54:ILE:HA	1.87	0.41
1:A:165:PHE:CZ	1:B:15:PHE:HB2	2.56	0.41
1:B:105:ILE:HG13	1:B:134:TYR:CZ	2.56	0.41
1:A:43:LEU:HD22	1:A:181:ILE:HG12	2.02	0.41
1:A:387:LEU:HA	1:A:394:LEU:HD23	2.03	0.41
1:A:437:LYS:HZ3	1:A:513:THR:H	1.69	0.41
1:B:130:GLY:H	2:B:801:ATP:PB	2.44	0.41
1:A:32:PHE:HE1	1:B:389:ILE:HD13	1.86	0.41
1:A:349:LYS:HD3	1:A:374:ASN:ND2	2.35	0.41
1:A:426:LYS:HG3	1:A:457:HIS:CE1	2.55	0.41
1:B:46:ASN:HD21	2:B:801:ATP:C5'	2.34	0.41
1:B:144:THR:N	1:B:182:VAL:O	2.49	0.41
1:B:187:GLU:CD	1:B:187:GLU:H	2.29	0.41
1:A:75:ILE:HG22	1:A:77:PRO:HD3	2.03	0.41
1:A:395:GLN:CD	1:B:34:SER:HA	2.45	0.41
1:B:21:ILE:H	1:B:21:ILE:HD12	1.86	0.40
1:B:76:ILE:HB	1:B:85:THR:HB	2.02	0.40
1:B:39:PHE:HB2	1:B:136:CYS:HA	2.03	0.40
1:B:144:THR:O	1:B:182:VAL:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:VAL:HG12	1:B:185:ILE:HG12	2.04	0.40
1:A:147:SER:HA	1:A:179:THR:HA	2.03	0.40
1:B:37:GLU:HB3	1:B:205:HIS:HE1	1.87	0.40
1:B:89:THR:HA	1:B:178:GLY:HA3	2.03	0.40
1:B:459:SER:H	1:B:508:GLU:HG3	1.87	0.40
1:B:492:GLN:H	1:B:492:GLN:HG3	1.76	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	457/722 (63%)	436 (95%)	21 (5%)	0	100	100
1	B	490/722 (68%)	464 (95%)	26 (5%)	0	100	100
All	All	947/1444 (66%)	900 (95%)	47 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	417/649 (64%)	416 (100%)	1 (0%)	87	85
1	B	445/649 (69%)	444 (100%)	1 (0%)	87	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	862/1298 (66%)	860 (100%)	2 (0%)	85	85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
1	B	149	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	HIS
1	A	282	ASN
1	A	395	GLN
1	A	435	ASN
1	A	457	HIS
1	B	46	ASN
1	B	118	GLN
1	B	149	HIS
1	B	196	ASN
1	B	205	HIS
1	B	345	ASN
1	B	431	GLN
1	B	479	GLN
1	B	492	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 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
2	ATP	B	801	3	32,33,33	2.17	8 (25%)	48,52,52	2.83	13 (27%)
2	ATP	A	801	3	32,33,33	2.13	5 (15%)	48,52,52	2.89	13 (27%)

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	ATP	B	801	3	-	8/22/38/38	0/3/3/3
2	ATP	A	801	3	-	8/22/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	ATP	O5'-C5'	-5.93	1.22	1.44
2	A	801	ATP	O5'-C5'	-5.82	1.22	1.44
2	A	801	ATP	PB-O3B	-5.77	1.53	1.59
2	A	801	ATP	PA-O3A	-5.74	1.53	1.59
2	B	801	ATP	PA-O3A	-5.72	1.53	1.59
2	B	801	ATP	PB-O3B	-5.21	1.53	1.59
2	B	801	ATP	PB-O3A	3.37	1.63	1.59
2	A	801	ATP	PB-O3A	3.18	1.62	1.59
2	B	801	ATP	O4'-C1'	-2.36	1.36	1.42
2	B	801	ATP	C8-N9	2.25	1.41	1.37
2	B	801	ATP	O3'-C3'	-2.24	1.37	1.43
2	B	801	ATP	O4'-C4'	-2.17	1.40	1.45
2	A	801	ATP	C8-N9	2.14	1.41	1.37

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ATP	O5'-C5'-C4'	9.16	140.19	108.99
2	B	801	ATP	C5'-C4'-C3'	-8.81	83.50	115.21
2	A	801	ATP	C5'-C4'-C3'	-8.58	84.32	115.21
2	B	801	ATP	O5'-C5'-C4'	8.49	137.88	108.99
2	A	801	ATP	O5'-PA-O1A	-7.21	80.37	108.94
2	B	801	ATP	O5'-PA-O1A	-6.95	81.40	108.94
2	B	801	ATP	PA-O5'-C5'	5.97	155.59	121.35
2	A	801	ATP	PA-O5'-C5'	5.92	155.25	121.35
2	B	801	ATP	O2B-PB-O3B	5.59	122.38	107.27
2	A	801	ATP	O2B-PB-O3B	5.47	122.05	107.27
2	A	801	ATP	O2A-PA-O3A	4.94	120.62	107.27
2	A	801	ATP	O3A-PB-O1B	-4.72	96.49	110.70
2	B	801	ATP	O2A-PA-O3A	4.63	119.80	107.27
2	B	801	ATP	O3A-PB-O1B	-4.48	97.21	110.70
2	B	801	ATP	O3A-PA-O1A	3.25	120.49	110.70
2	A	801	ATP	C6-C5-C4	-3.05	113.02	117.18
2	B	801	ATP	C6-C5-C4	-3.02	113.06	117.18
2	A	801	ATP	O3A-PA-O1A	2.95	119.58	110.70
2	B	801	ATP	O2A-PA-O5'	-2.79	94.94	107.57
2	A	801	ATP	O2A-PA-O5'	-2.74	95.15	107.57
2	B	801	ATP	C5-C6-N1	2.28	123.31	117.51
2	A	801	ATP	O4'-C4'-C3'	2.25	109.62	105.15
2	B	801	ATP	O4'-C1'-N9	2.18	112.28	108.09
2	A	801	ATP	C5-C6-N1	2.17	123.02	117.51
2	B	801	ATP	O3'-C3'-C2'	2.08	118.49	111.82
2	A	801	ATP	O3'-C3'-C2'	2.07	118.45	111.82

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ATP	C5'-O5'-PA-O1A
2	A	801	ATP	C5'-O5'-PA-O2A
2	A	801	ATP	C5'-O5'-PA-O3A
2	B	801	ATP	C5'-O5'-PA-O1A
2	B	801	ATP	C5'-O5'-PA-O2A
2	A	801	ATP	O4'-C4'-C5'-O5'
2	A	801	ATP	C3'-C4'-C5'-O5'
2	A	801	ATP	PB-O3A-PA-O1A
2	B	801	ATP	O4'-C1'-N9-C8
2	B	801	ATP	C2'-C1'-N9-C8
2	B	801	ATP	PG-O3B-PB-O3A
2	B	801	ATP	C5'-O5'-PA-O3A

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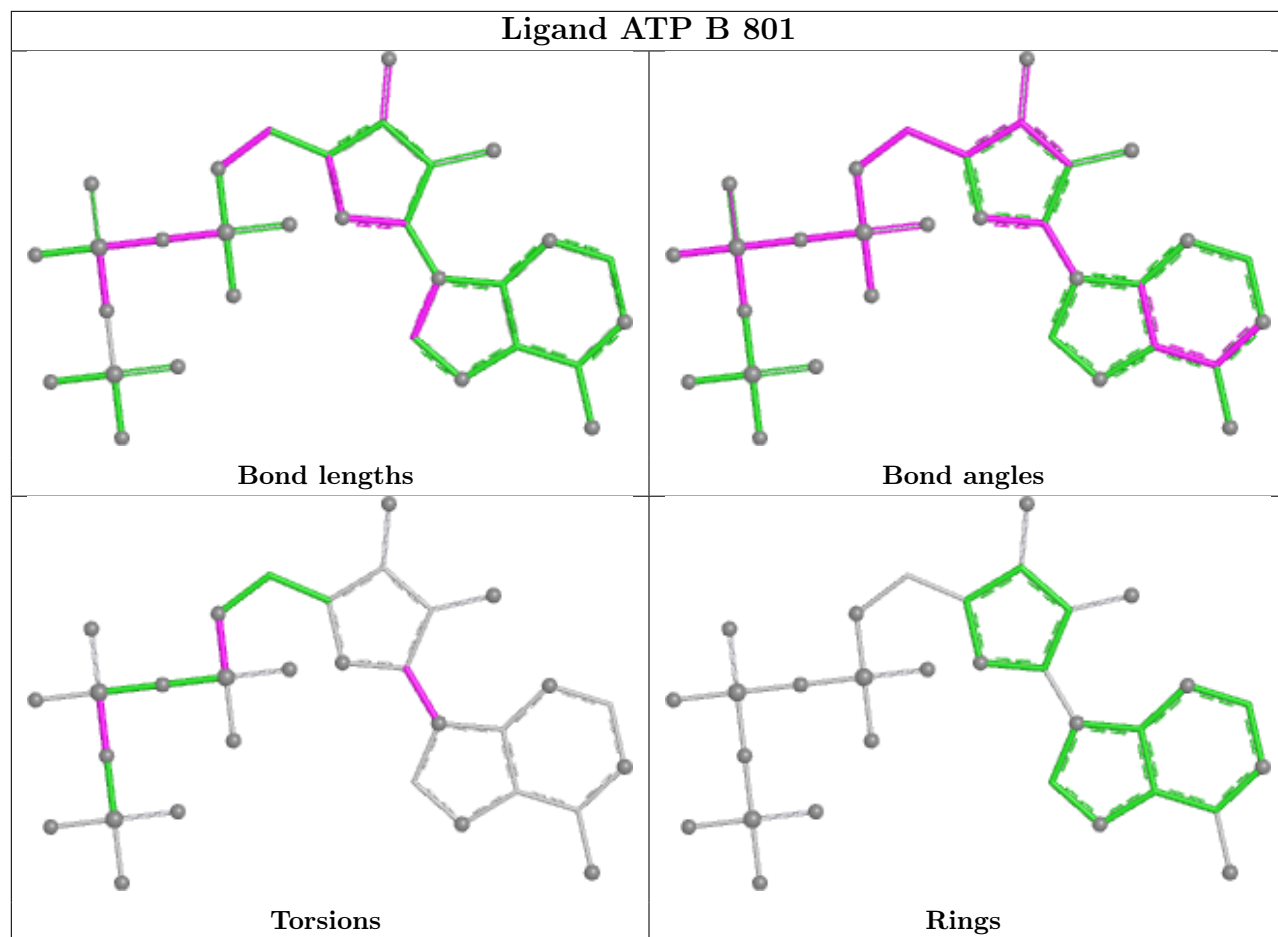
Mol	Chain	Res	Type	Atoms
2	B	801	ATP	O4'-C1'-N9-C4
2	A	801	ATP	PG-O3B-PB-O1B
2	A	801	ATP	PA-O3A-PB-O2B
2	B	801	ATP	PG-O3B-PB-O2B

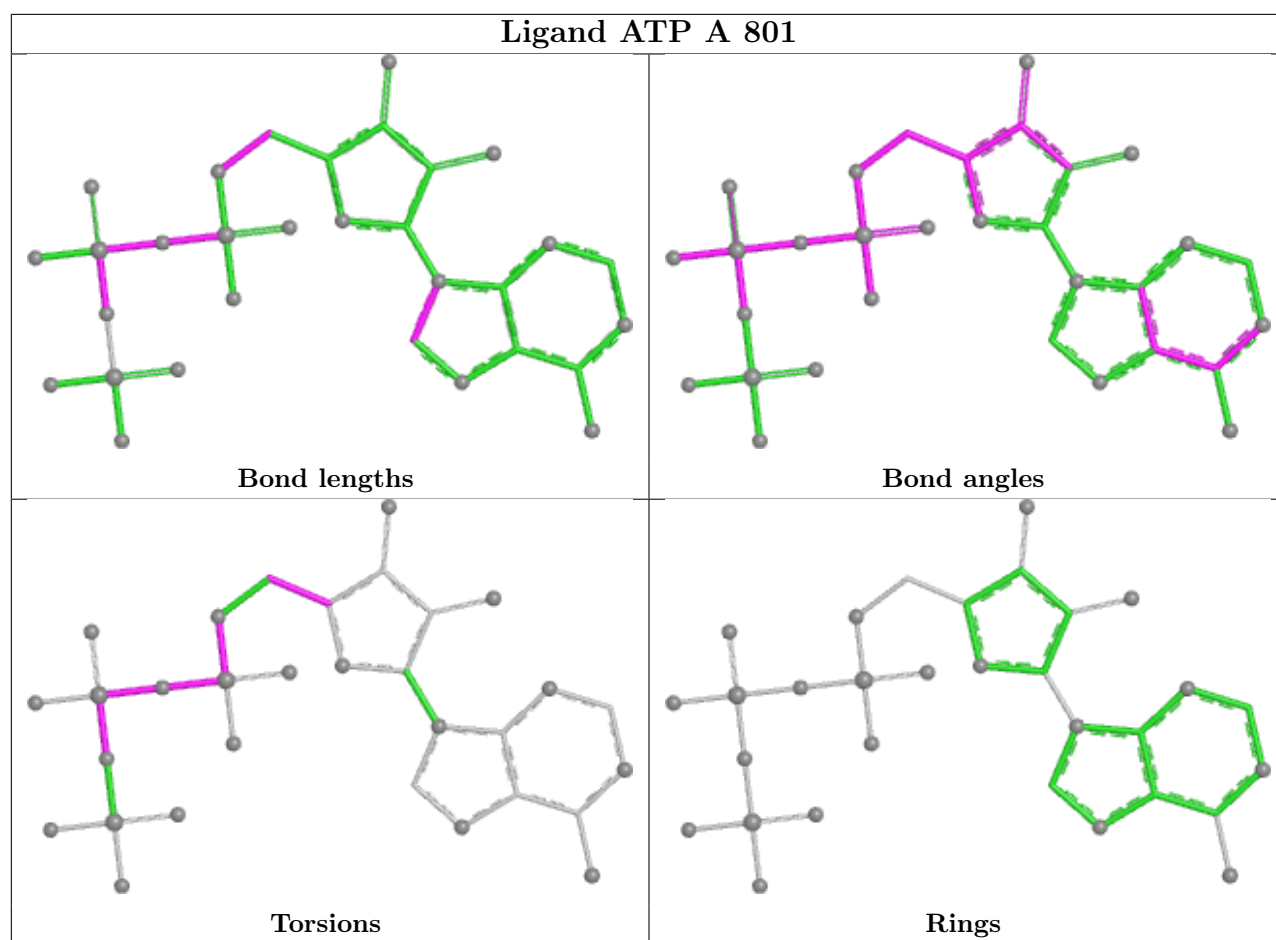
There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	ATP	5	0
2	A	801	ATP	10	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

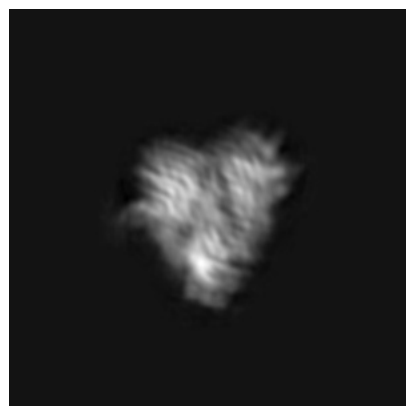
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41817. These allow visual inspection of the internal detail of the map and identification of artifacts.

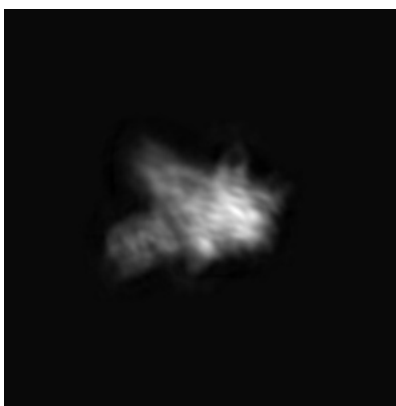
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

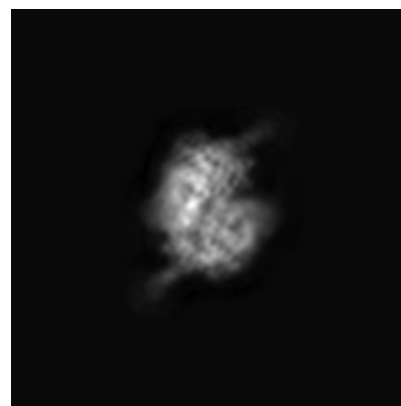
6.1.1 Primary map



X

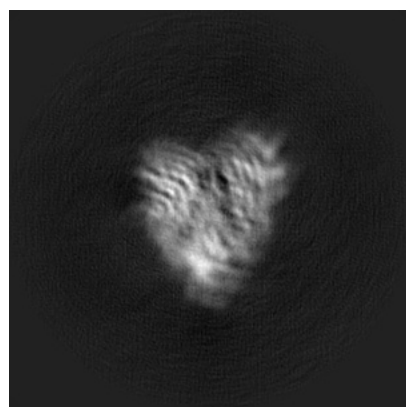


Y

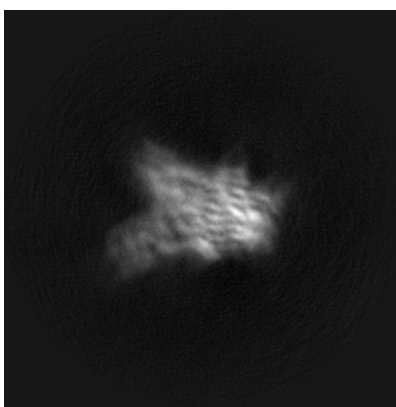


Z

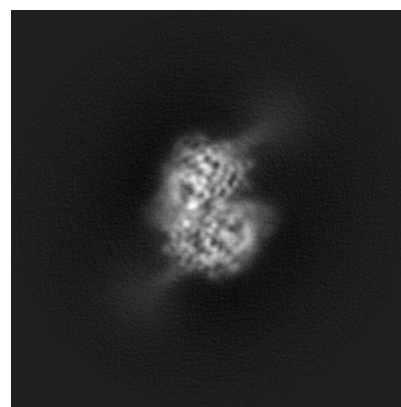
6.1.2 Raw map



X



Y

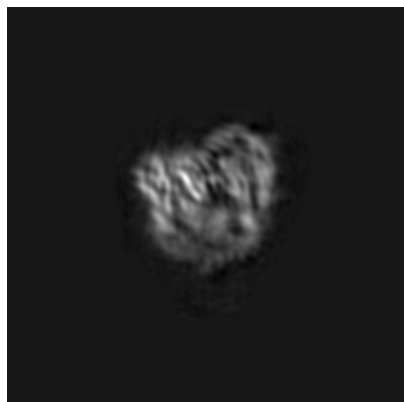


Z

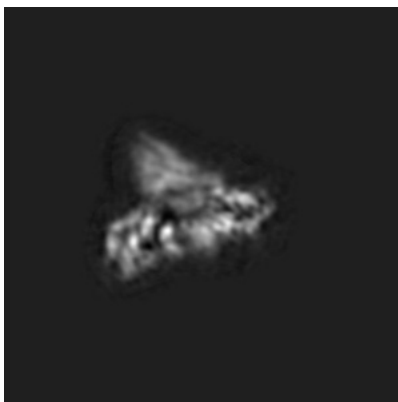
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 128

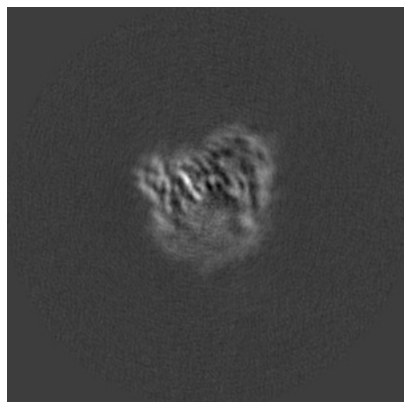


Y Index: 128

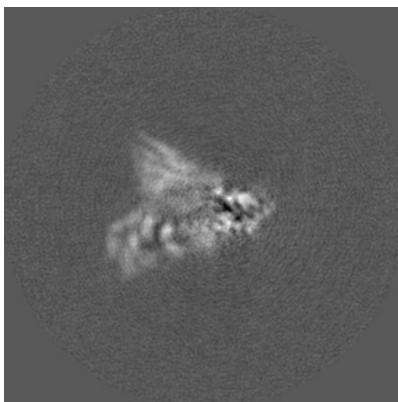


Z Index: 128

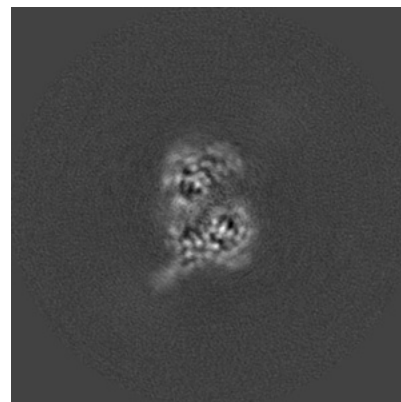
6.2.2 Raw map



X Index: 128



Y Index: 128

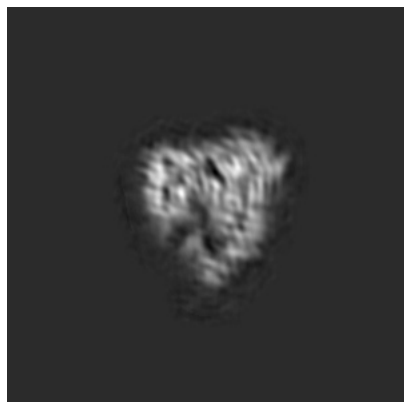


Z Index: 128

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

6.3 Largest variance slices [i](#)

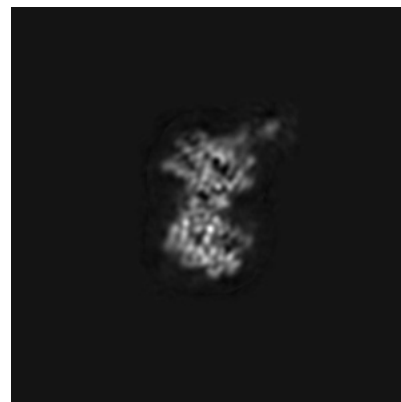
6.3.1 Primary map



X Index: 122

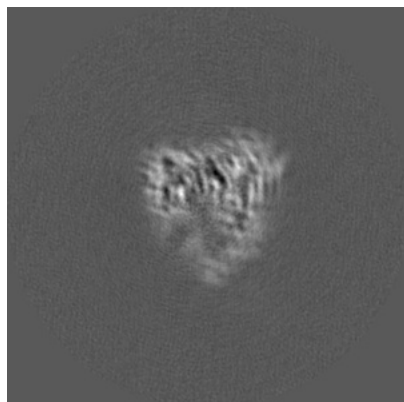


Y Index: 130

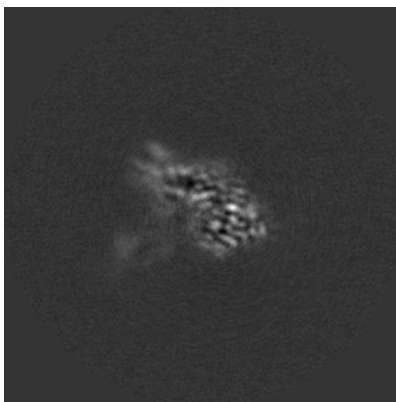


Z Index: 147

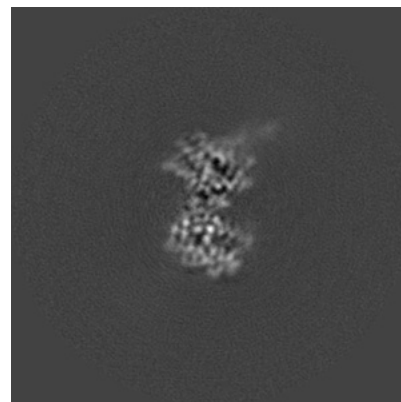
6.3.2 Raw map



X Index: 122



Y Index: 114



Z Index: 147

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

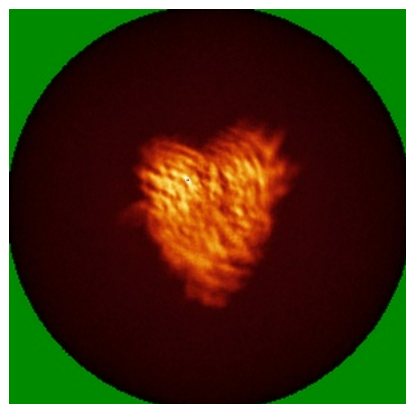


Y

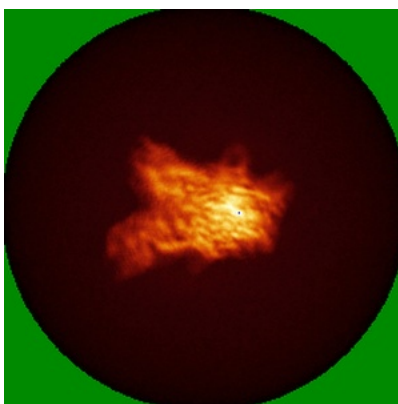


Z

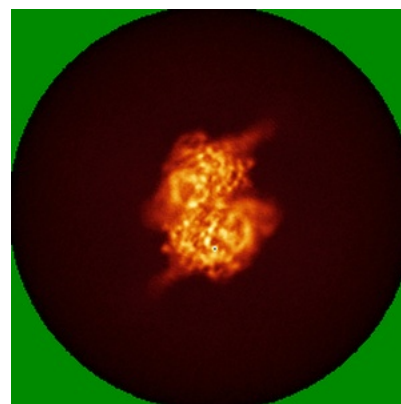
6.4.2 Raw map



X



Y

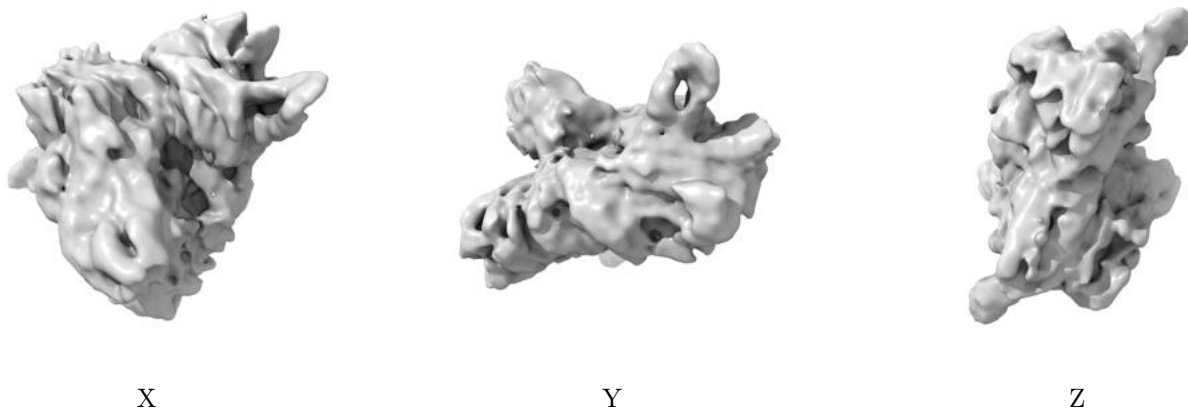


Z

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.

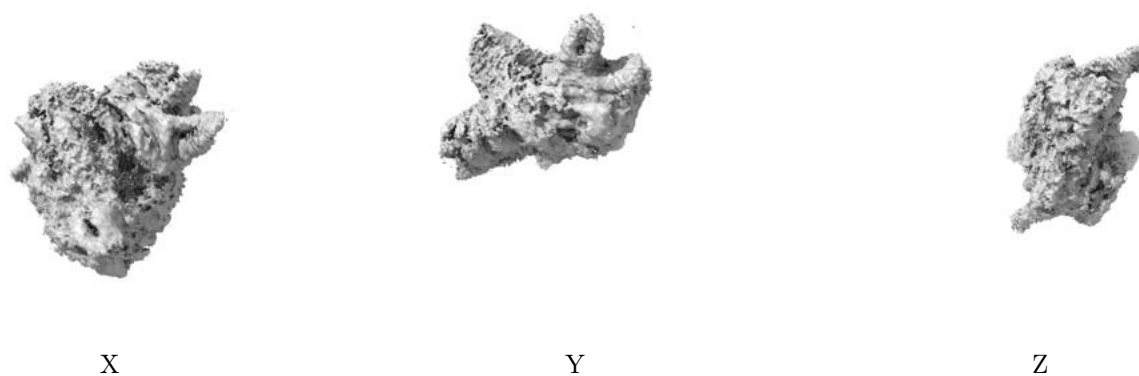
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

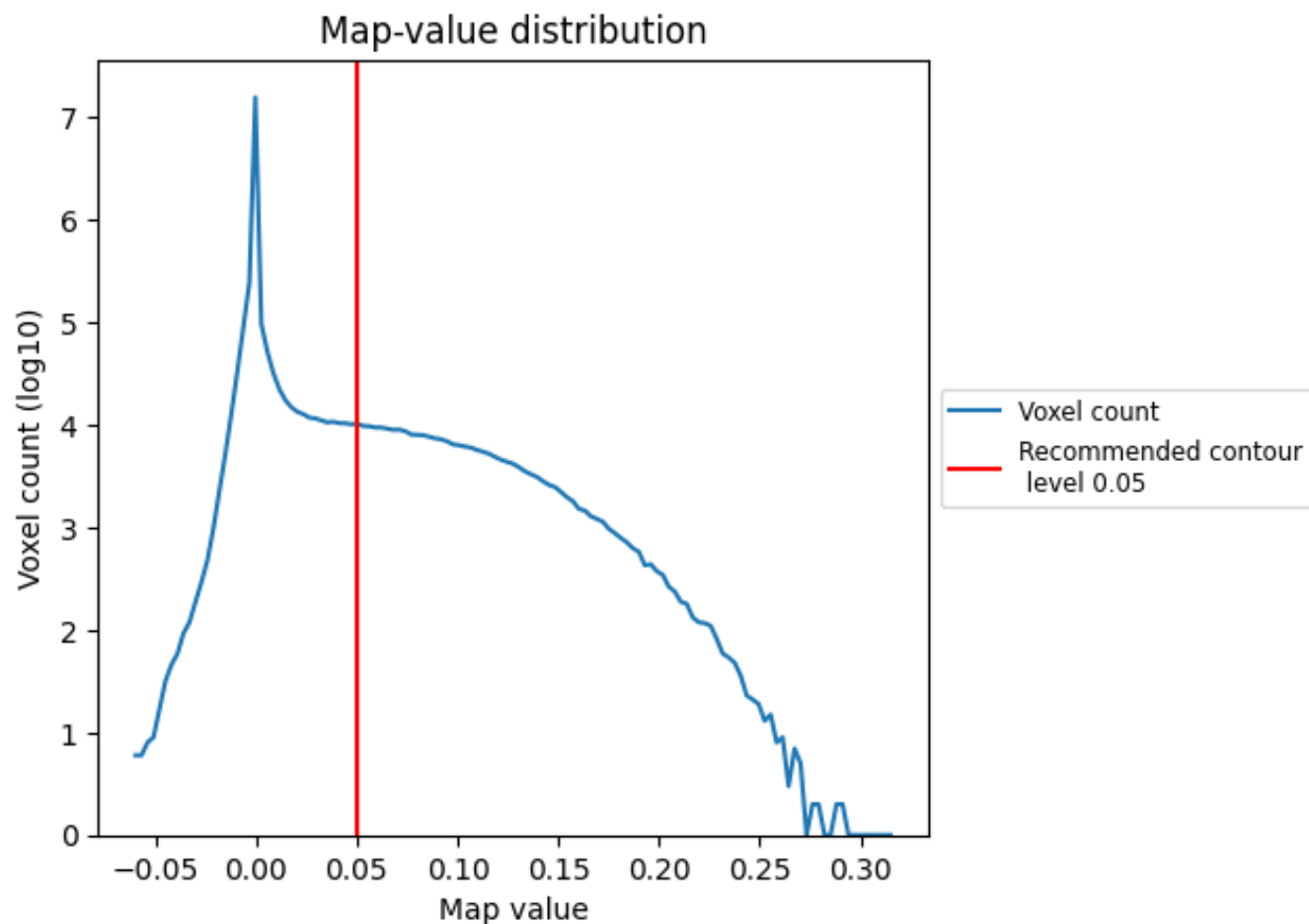
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

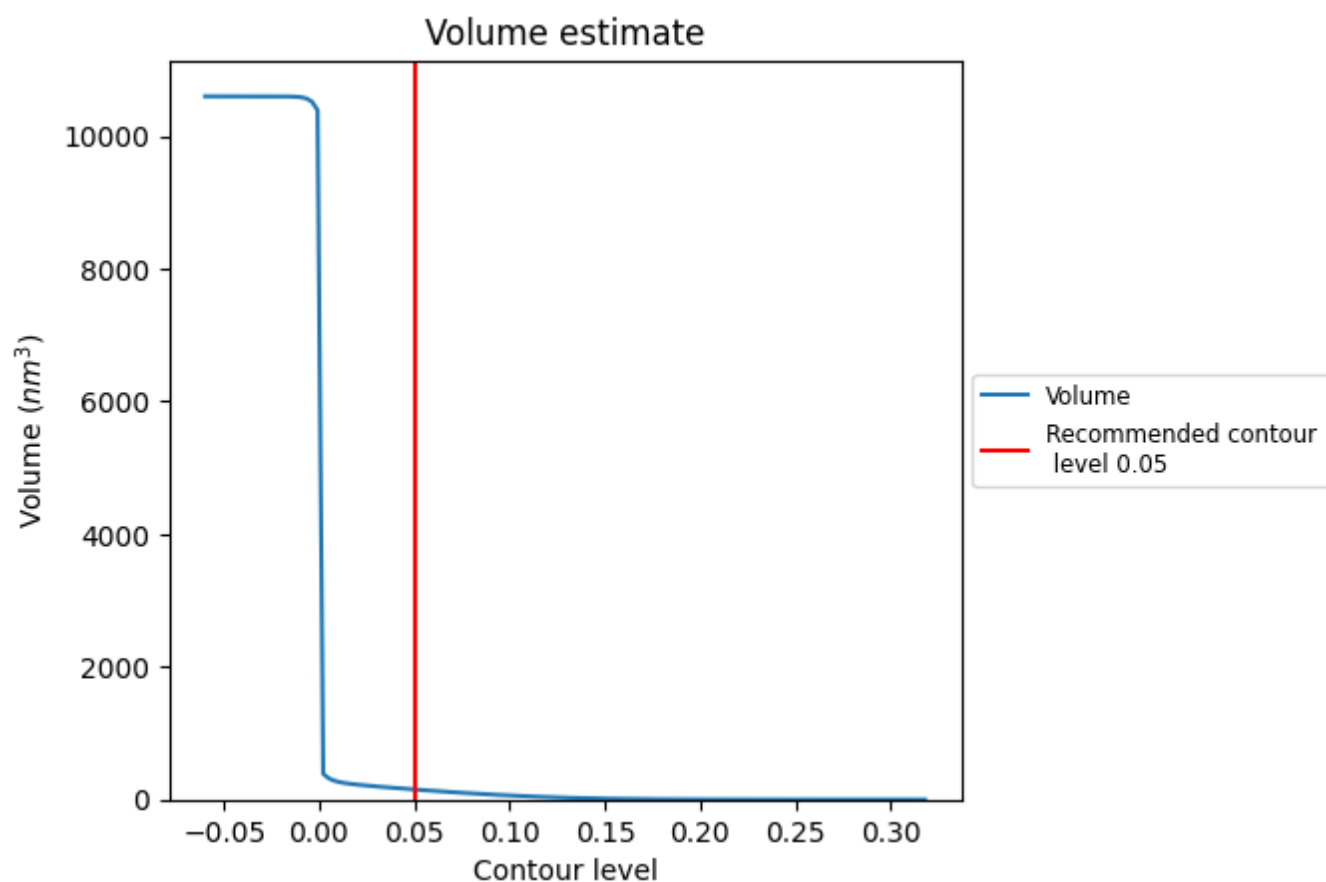
This section contains the results of statistical analysis of the map.

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.

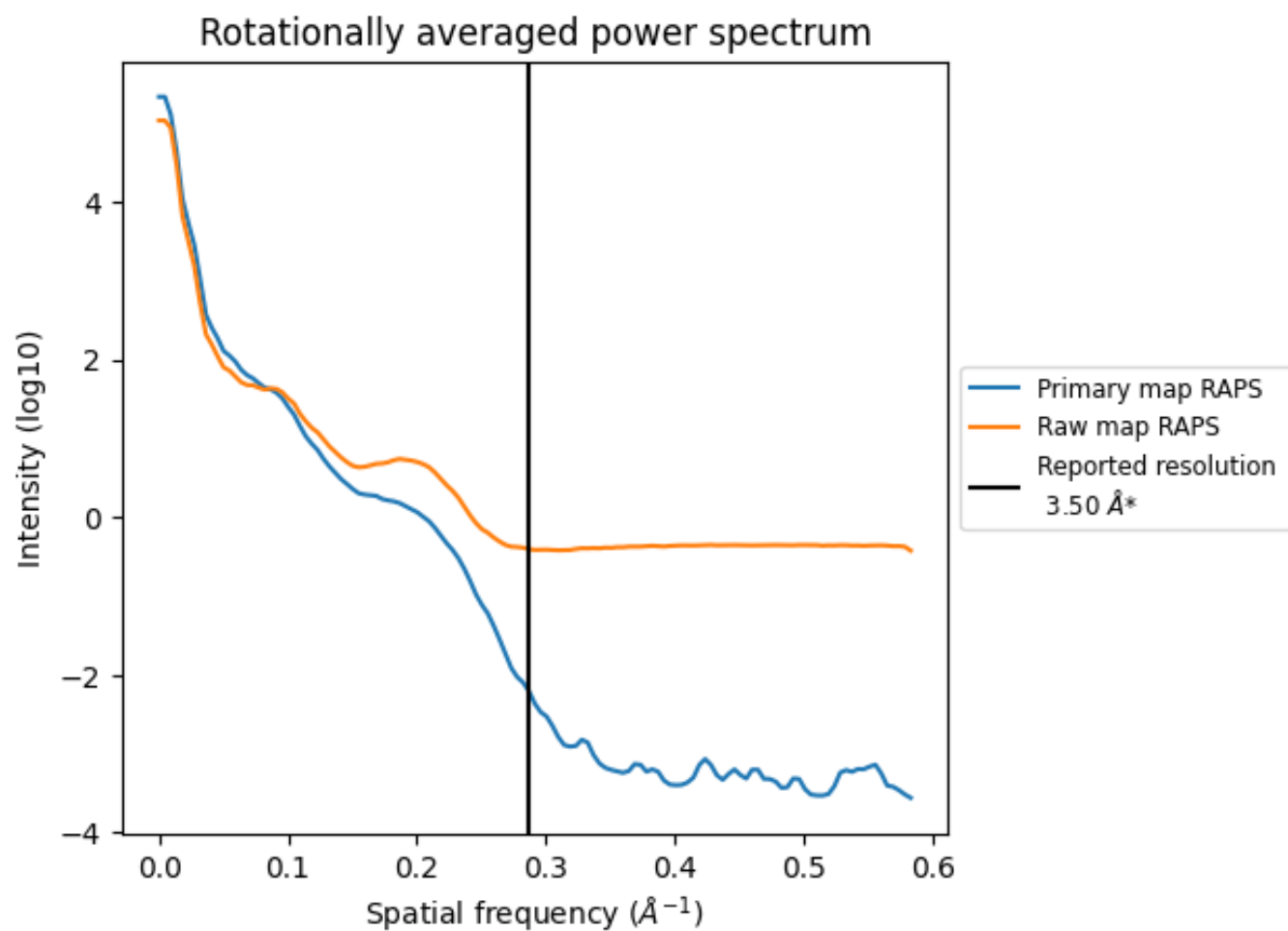
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 152 nm^3 ; this corresponds to an approximate mass of 137 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 ⓘ

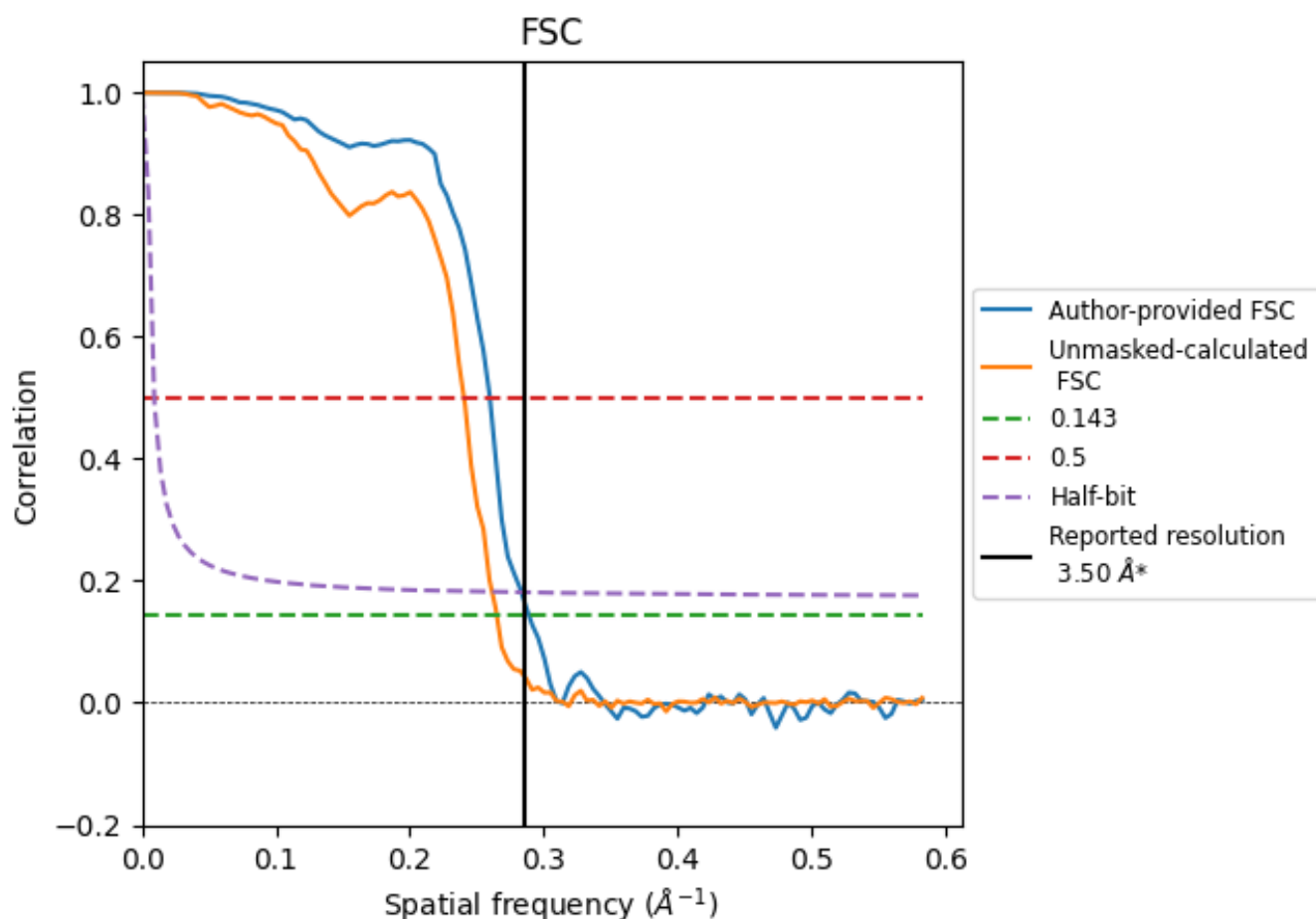


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

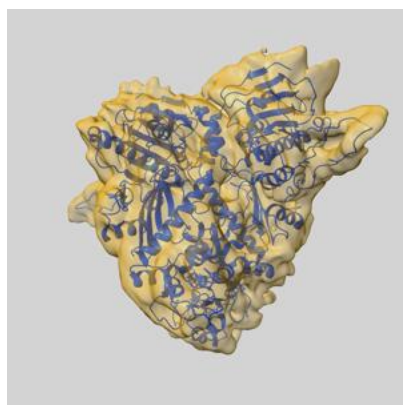
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.46	3.85	3.53
Unmasked-calculated*	3.78	4.16	3.83

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

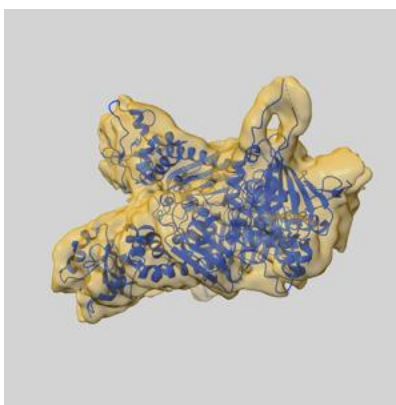
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41817 and PDB model 8U1M. Per-residue inclusion information can be found in section [3](#) on page [6](#).

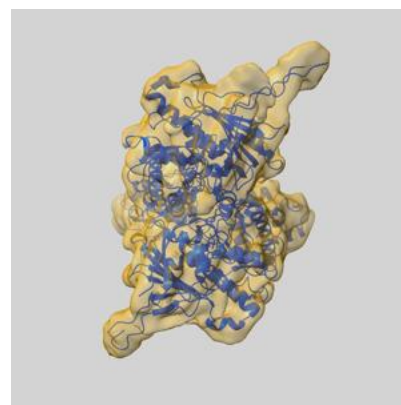
9.1 Map-model overlay [i](#)



X



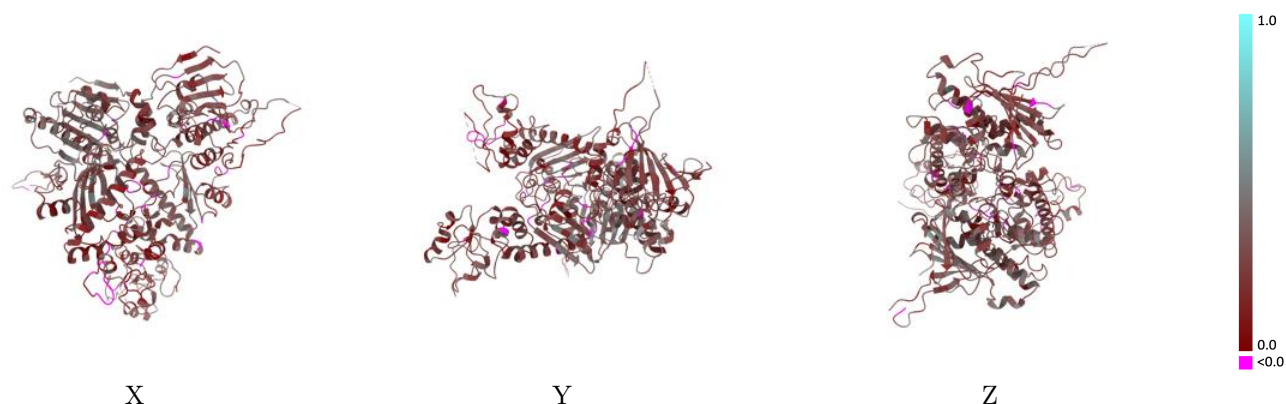
Y



Z

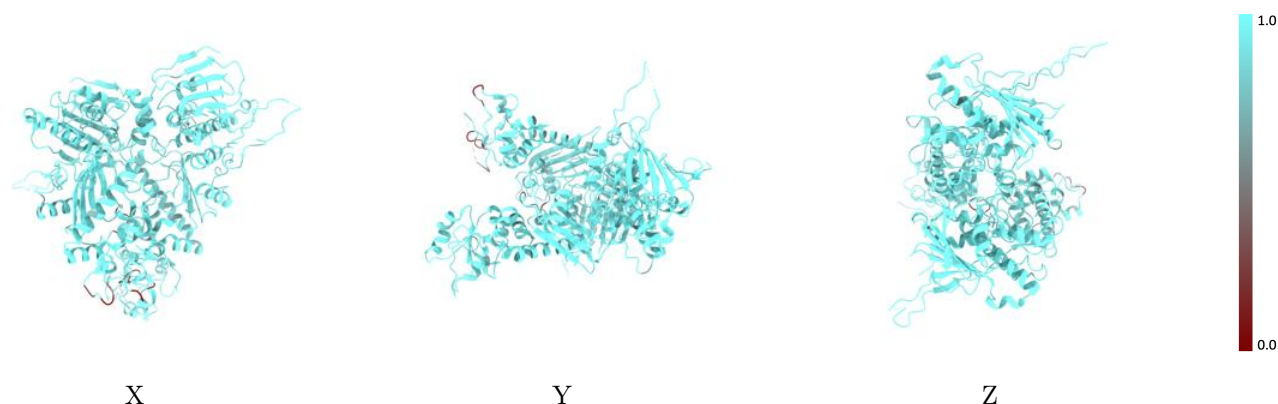
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



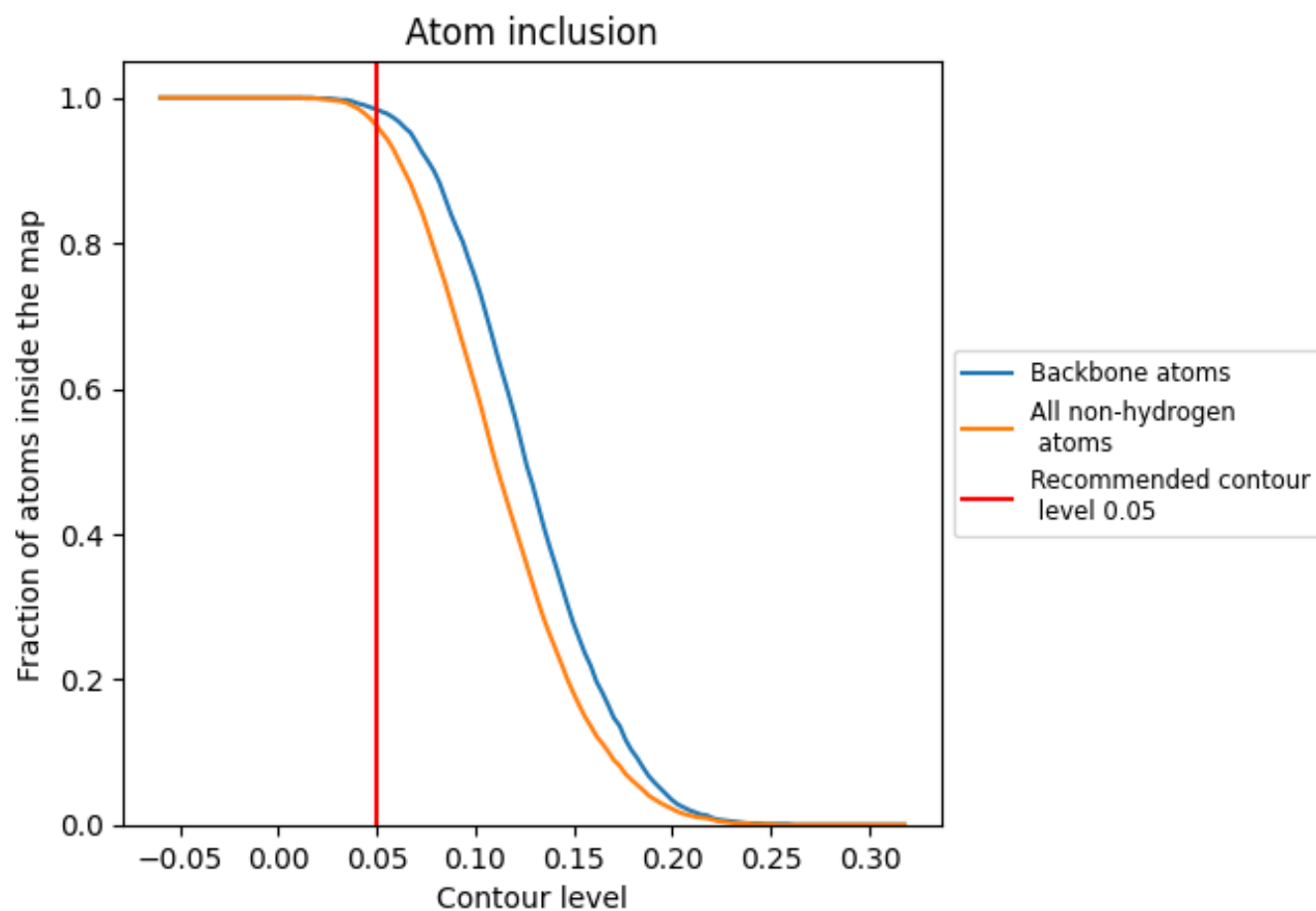
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9610	0.2610
A	0.9520	0.2640
B	0.9690	0.2580

