



Full wwPDB EM Validation Report ⓘ

May 5, 2025 – 09:40 AM EDT

PDB ID : 9E1M / pdb_00009e1m
EMDB ID : EMD-47413
Title : Snf2h bound nucleosome complex - ClassA2
Authors : Malik, D.; Deshmukh, A.A.; Bilokapic, S.; Halic, M.
Deposited on : 2024-10-21
Resolution : 3.25 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.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

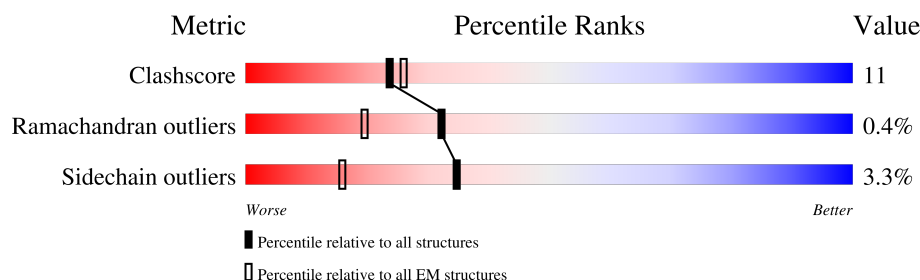
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



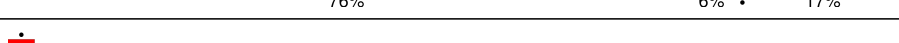





The reported resolution of this entry is 3.25 Å.

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	136	
1	E	136	
2	B	103	
2	F	103	
3	C	130	
3	G	130	
4	D	126	
4	H	126	

Continued on next page...

Mol	Chain	Length	Quality of chain
5	I	149	 <div>50%50%</div>
6	J	152	 <div>57%43%</div>
7	W	1052	 <div>10%23%18%58%</div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15924 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	97	Total	C	N	O	S	0	0
			799	505	153	138	3		
1	E	96	Total	C	N	O	S	0	0
			790	499	151	137	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	85	Total	C	N	O	S	0	0
			679	428	135	115	1		
2	F	80	Total	C	N	O	S	0	0
			641	405	125	110	1		

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	109	Total	C	N	O	0	0
			837	526	165	146		
3	G	109	Total	C	N	O	0	0
			837	526	165	146		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	conflict	UNP P06897
C	123	SER	ALA	conflict	UNP P06897
G	99	ARG	GLY	conflict	UNP P06897
G	123	SER	ALA	conflict	UNP P06897

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	96	Total	C	N	O	S	0	0
			746	469	134	141	2		
4	H	96	Total	C	N	O	S	0	0
			756	475	138	141	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	engineered mutation	UNP P02281
H	29	THR	SER	engineered mutation	UNP P02281

- Molecule 5 is a DNA chain called DNA (149-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	149	Total	C	N	O	P	0	0
			3075	1454	580	892	149		

- Molecule 6 is a DNA chain called DNA (151-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	151	Total	C	N	O	P	0	0
			3077	1461	558	907	151		

- Molecule 7 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily A member 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	W	444	Total	C	N	O	S	0	0
			3656	2340	643	650	23		

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

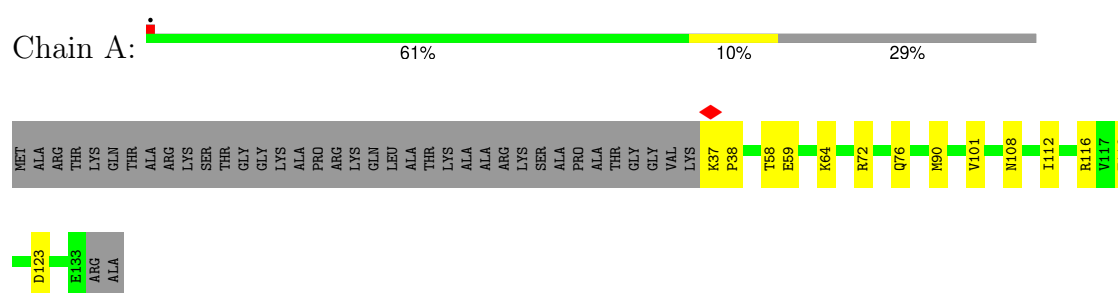


Mol	Chain	Residues	Atoms					AltConf
8	W	1	Total	C	N	O	P	0
			31	10	5	13	3	

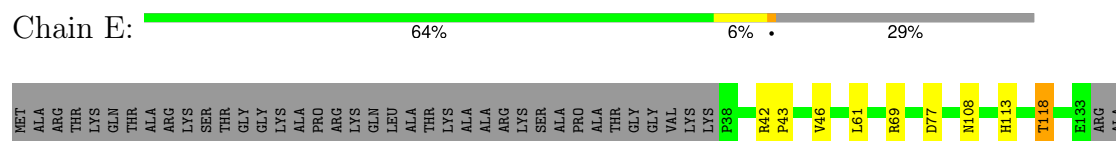
3 Residue-property plots

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.

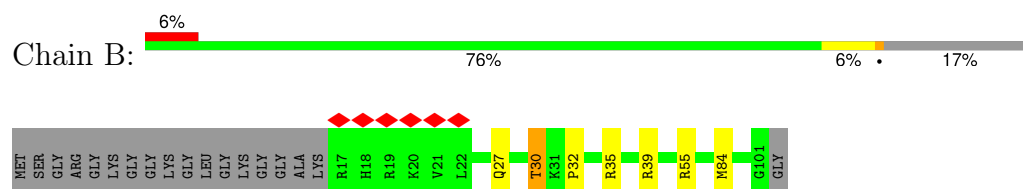
• Molecule 1: Histone H3.2



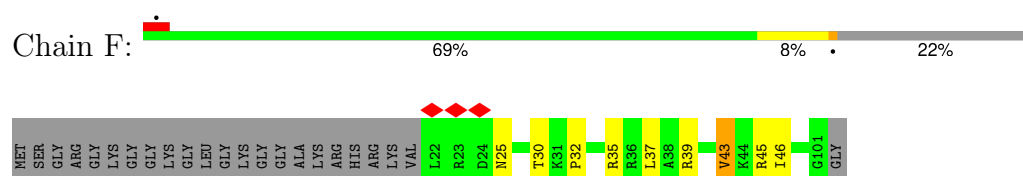
• Molecule 1: Histone H3.2



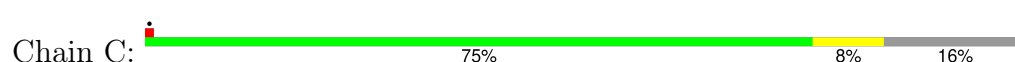
• Molecule 2: Histone H4

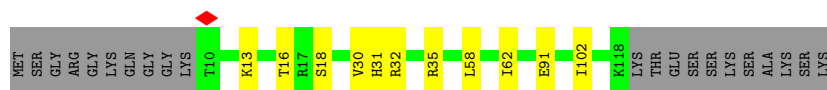


• Molecule 2: Histone H4

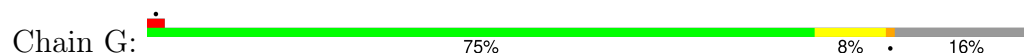


• Molecule 3: Histone H2A type 1

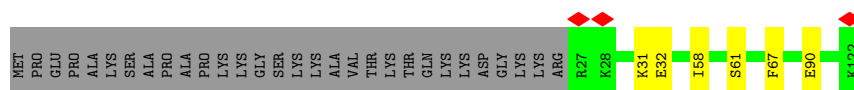




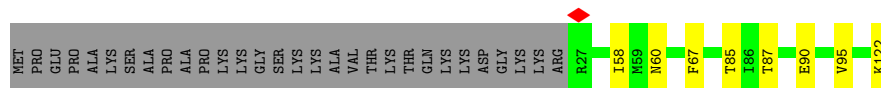
- Molecule 3: Histone H2A type 1



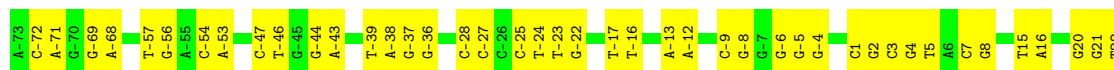
- Molecule 4: Histone H2B 1.1



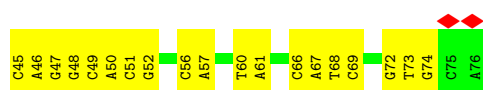
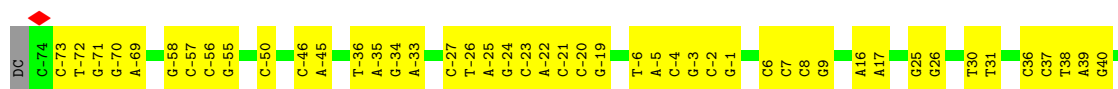
- Molecule 4: Histone H2B 1.1



- Molecule 5: DNA (149-MER)



- Molecule 6: DNA (151-MER)



- Molecule 7: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family A member 5



MET	TLE	LYS	Y183	R267	L354	E422	L492	F555	M623	LYS	ALA	ASN	ASP	THR	PHE	ARG
SER	PHE	PRO	Q194	R271	D357	W423	P493	M556	K624	LYS	VAL	PRO	ASP	ILE	ARG	ARG
ALA	ASP	GLY	W185	D273	N360	Y424	K494	L557	L625	THR	ASP	GLU	ALA	GLY	PHE	PHE
GLU	ALA	ARG	L191	D274	S361	T425	L495	S558	R626	GLU	THR	ASN	PHE	THR	THR	THR
PRO	SER	PRO	I192	L275	A362	R426	K496	T559	E627	MET	ARG	ALA	ARG	LYS	LEU	LEU
PRO	GLY	ILE	S193	L276	D363	I427	Q498	R560	D628	ASN	GLU	ALA	GLU	ALA	LYS	LYS
PRO	LYS	LYS	E196	P277	M429	L428	G499	A561	S829	GLU	ALA	GLN	ARG	GLU	GLU	GLU
PRO	LYS	ASP	G197	D278	PHE	K430	S500	L564	I630	LEU	ALA	GLN	LEU	VAL	VAL	THR
PRO	GLN	GLU	I198	E279	ASP	ASP	R501	G566	V631	SER	ARG	GLN	LEU	ARG	GLY	THR
PRO	ILE	GLN	I199	W280	SER	ASP	V502	L567	I632	MET	VAL	LYS	GLU	GLY	THR	ARG
GLU	GLN	ASN	T202	T285	TRP	ILE	L503	N567	Q633	GLY	PRO	LYS	GLU	GLY	ILE	ILE
GLU	GLN	LEU	A204	S286	PHE	ASP	F504	A569	Q634	ARG	ALA	LYS	GLU	GLY	GLY	GLY
SER	LEU	LEU	D205	L203	TRP	ILE	F505	T570	V634	LEU	VAL	ALA	GLU	GLY	GLY	GLY
PRO	LEU	SER	E206	L200	ASP	ASN	S506	A571	D572	SER	PRO	LYS	GLU	GLY	GLY	GLY
SER	VAL	VAL	G208	L290	ASN	SER	Q567	D573	V574	GLU	PRO	ALA	GLU	GLY	GLY	GLY
ASP	GLY	ASP	M207	E293	CYS	ALA	M508	D574	V575	THR	ALA	ASN	GLU	GLY	GLY	GLY
TYR	THR	TYR	G209	W302	LEU	GLY	T509	V576	Q583	ASN	PRO	LEU	SER	GLY	GLY	GLY
ALA	GLU	ARG	K211	R303	GLY	ASP	V511	D577	Q584	LYS	PRO	ASN	GLU	GLY	GLY	GLY
SER	GLU	ARG	Q214	Y304	L380	MET	L512	D578	Q585	THR	PRO	ASN	GLU	GLY	GLY	GLY
GLY	ASP	THR	L218	L305	V381	ASP	L515	S579	D580	GLU	GLN	ASN	GLU	GLY	GLY	GLY
SER	GLN	THR	M222	L306	K379	K443	E516	D581	N582	GLU	GLN	ASN	GLU	GLY	GLY	GLY
ASN	GLU	GLU	K223	Y307	L386	M444	E517	N583	Q584	THR	GLU	ASN	GLU	GLY	GLY	GLY
SER	GLU	GLU	G224	T307	H385	R445	C619	D584	Q585	GLU	GLU	ASN	GLU	GLY	GLY	GLY
SER	GLU	GLU	Y225	A310	M386	L450	E620	L587	Q586	GLU	GLU	ASN	GLU	GLY	GLY	GLY
LYS	GLU	GLU	R226	H311	R389	L453	W521	D587	Q587	GLU	GLU	ASN	GLU	GLY	GLY	GLY
GLY	LEU	LEU	W227	K314	P390	K455	R522	N588	A590	GLU	GLU	ASN	GLU	GLY	GLY	GLY
GLY	LEU	LEU	T228	E316	F391	C456	E524	M590	Q591	THR	GLU	ASN	GLU	GLY	GLY	GLY
PRO	GLU	GLU	P229	K317	R394	M458	E525	D591	Q592	THR	GLU	ASN	GLU	GLY	GLY	GLY
GLU	SER	SER	G230	E322	R395	R459	Y526	D592	A593	THR	GLU	ASN	GLU	GLY	GLY	GLY
GLY	THR	GLU	P231	V324	R396	Y461	C527	E593	H594	THR	GLU	ASN	GLU	GLY	GLY	GLY
VAL	LYS	LYS	H232	R325	K397	L462	R528	R595	I596	THR	GLU	ASN	GLU	GLY	GLY	GLY
ALA	ALA	ALA	M233	E326	R398	F463	L529	D597	Q598	THR	GLU	ASN	GLU	GLY	GLY	GLY
ALA	THR	THR	V234	F327	D399	D464	D530	G597	Q598	THR	GLU	ASN	GLU	GLY	GLY	GLY
ASN	ASN	VAL	L235	R328	V400	G465	G531	I596	Q598	THR	GLU	ASN	GLU	GLY	GLY	GLY
VAL	VAL	CYS	P237	T330	E401	A466	Q532	G597	Q598	THR	GLU	ASN	GLU	GLY	GLY	GLY
ILE	ILE	ILE	K238	N331	K402	E467	T533	V602	R603	THR	GLU	ASN	GLU	GLY	GLY	GLY
SER	GLN	PRO	S239	L334	L404	P468	H535	V604	F605	THR	GLU	ASN	GLU	GLY	GLY	GLY
ALA	ALA	ALA	H242	L336	K407	G469	D536	R606	F607	THR	GLU	ASN	GLU	GLY	GLY	GLY
SER	ALA	ALA	N243	T336	K408	P470	E537	R607	F608	THR	GLU	ASN	GLU	GLY	GLY	GLY
ALA	GLN	LYS	E247	L340	V410	P471	R538	I608	T609	THR	GLU	ASN	GLU	GLY	GLY	GLY
PRO	PRO	PRO	F248	N343	E409	Y472	Q539	D540	D610	THR	GLU	ASN	GLU	GLY	GLY	GLY
ASP	THR	THR	R249	K411	T473	T474	S541	N611	T612	THR	GLU	ASN	GLU	GLY	GLY	GLY
GLU	SER	SER	W250	E346	I412	D475	I542	N643	V613	THR	GLU	ASN	GLU	GLY	GLY	GLY
PRO	PRO	PRO	W251	L347	V413	L478	A544	E547	R616	THR	GLU	ASN	GLU	GLY	GLY	GLY
LEU	LEU	LEU	L255	W348	G415	M485	E547	S550	E619	THR	GLU	ASN	GLU	GLY	GLY	GLY
MET	LYS	MET	K264	S349	L416	L488	S551	T551	R620	THR	GLU	ASN	GLU	GLY	GLY	GLY
GLU	MET	GLU	L180	L350	S417	D489	K490	K552	A621	THR	GLU	ASN	GLU	GLY	GLY	GLY
GLU	MET	GLU	D182	L350	K418	L491	F553	V554	E622	THR	GLU	ASN	GLU	GLY	GLY	GLY

GLY
ARG
GLY
ARG
LYS
LYS
LYS
LEU
LYS
LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11600	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	28.864	Depositor
Minimum map value	-0.309	Depositor
Average map value	-0.017	Depositor
Map value standard deviation	0.279	Depositor
Recommended contour level	4	Depositor
Map size (Å)	497.0, 497.0, 497.0	wwPDB
Map dimensions	497, 497, 497	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.22	0/811	0.31	0/1088
1	E	0.20	0/802	0.30	0/1076
2	B	0.22	0/687	0.33	0/921
2	F	0.21	0/648	0.31	0/868
3	C	0.20	0/847	0.28	0/1144
3	G	0.21	0/847	0.29	0/1144
4	D	0.20	0/757	0.32	0/1018
4	H	0.20	0/767	0.34	0/1029
5	I	0.31	0/3454	0.43	0/5334
6	J	0.32	0/3447	0.42	0/5313
7	W	0.21	0/3733	0.52	2/5041 (0.0%)
All	All	0.26	0/16800	0.41	2/23976 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	W	596	ILE	N-CA-CB	7.64	122.04	110.58
7	W	596	ILE	CB-CA-C	-7.49	101.88	112.22

There are no chirality outliers.

There are no planarity outliers.

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	799	0	838	10	0
1	E	790	0	826	9	0
2	B	679	0	717	3	0
2	F	641	0	684	9	0
3	C	837	0	891	8	0
3	G	837	0	891	13	0
4	D	746	0	764	4	0
4	H	756	0	786	9	0
5	I	3075	0	1671	55	0
6	J	3077	0	1695	47	0
7	W	3656	0	3730	175	0
8	W	31	0	12	2	0
All	All	15924	0	13505	312	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (312) 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)
7:W:424:TYR:CD2	7:W:453:LEU:HD11	1.47	1.49
7:W:424:TYR:CD2	7:W:453:LEU:CD1	2.36	1.09
7:W:424:TYR:CE2	7:W:453:LEU:HD11	1.88	1.07
7:W:404:LEU:HD11	7:W:596:ILE:HG13	1.36	1.04
7:W:238:LYS:HE2	7:W:535:HIS:CD2	1.98	0.99
7:W:239:SER:HB3	7:W:538:ARG:NH2	1.78	0.98
7:W:596:ILE:HB	8:W:1101:ATP:O3'	1.67	0.94
7:W:528:ARG:HH22	7:W:532:GLN:HB3	1.43	0.83
7:W:202:ILE:HG13	7:W:354:LEU:HD11	1.60	0.81
7:W:238:LYS:CE	7:W:535:HIS:CG	2.63	0.80
7:W:424:TYR:HD2	7:W:453:LEU:HD11	1.44	0.80
7:W:239:SER:HB3	7:W:538:ARG:CZ	2.13	0.78
7:W:534:PRO:HG2	7:W:537:GLU:HG2	1.64	0.77
7:W:510:ARG:HA	7:W:510:ARG:NE	2.00	0.76
7:W:411:LYS:HG3	7:W:608:ILE:HD12	1.69	0.75
5:I:73:DG:N2	6:J:-72:DT:O2	2.20	0.73
7:W:238:LYS:HE2	7:W:535:HIS:CG	2.22	0.72
5:I:74:DG:H2''	5:I:75:DG:H5''	1.72	0.72
5:I:73:DG:H2''	5:I:74:DG:C8	2.25	0.71
7:W:503:LEU:HD22	7:W:568:LEU:HD12	1.73	0.70
7:W:528:ARG:NH1	7:W:532:GLN:OE1	2.23	0.70
7:W:238:LYS:HE3	7:W:535:HIS:CG	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:587:LEU:HA	7:W:590:MET:HE2	1.73	0.69
5:I:-25:DC:H2''	5:I:-24:DT:H71	1.76	0.68
7:W:397:LYS:NZ	7:W:594:HIS:O	2.26	0.67
7:W:264:LYS:HZ3	7:W:267:ARG:HH22	1.43	0.67
5:I:15:DT:H2''	5:I:16:DA:C8	2.30	0.67
7:W:340:LEU:HD23	7:W:628:ASP:HA	1.77	0.67
7:W:424:TYR:HD2	7:W:453:LEU:CD1	2.02	0.66
5:I:73:DG:O6	6:J:-73:DC:N4	2.25	0.66
7:W:457:CYS:HB2	7:W:609:THR:HG21	1.76	0.66
3:G:42:ARG:HB2	4:H:85:THR:HG22	1.77	0.66
7:W:493:PRO:HA	7:W:496:LYS:HG2	1.77	0.66
7:W:496:LYS:HA	7:W:500:SER:HB3	1.77	0.65
7:W:207:MET:HB3	7:W:397:LYS:HE3	1.78	0.65
7:W:500:SER:HB2	7:W:553:PHE:HD1	1.62	0.65
7:W:238:LYS:CE	7:W:535:HIS:CD2	2.78	0.65
7:W:522:ARG:O	7:W:522:ARG:NH1	2.29	0.65
7:W:453:LEU:HG	7:W:453:LEU:O	1.98	0.64
7:W:334:LEU:HD21	7:W:350:LEU:HD22	1.81	0.63
5:I:25:DT:H2''	5:I:26:DA:C8	2.33	0.63
7:W:193:SER:O	7:W:197:ASN:ND2	2.31	0.63
6:J:8:DC:H2''	6:J:9:DG:C8	2.34	0.63
7:W:202:ILE:HG12	7:W:334:LEU:HB3	1.80	0.62
7:W:579:SER:OG	7:W:606:ARG:NH1	2.32	0.62
7:W:235:LEU:HD12	7:W:307:ILE:HG12	1.82	0.62
5:I:23:DG:OP1	7:W:582:ASN:ND2	2.33	0.61
7:W:231:PRO:O	7:W:232:HIS:ND1	2.33	0.61
7:W:424:TYR:CE2	7:W:453:LEU:CD1	2.74	0.61
7:W:316:GLU:OE2	7:W:325:ARG:NH2	2.34	0.60
3:C:13:LYS:NZ	5:I:46:DG:OP1	2.34	0.60
7:W:535:HIS:O	7:W:538:ARG:HG2	2.01	0.60
7:W:267:ARG:NH1	7:W:293:GLU:OE2	2.32	0.59
7:W:210:GLY:O	7:W:214:GLN:NE2	2.36	0.59
7:W:211:LYS:HA	7:W:214:GLN:HE21	1.65	0.59
7:W:603:ARG:HG3	7:W:605:PHE:HE2	1.68	0.59
7:W:404:LEU:HD21	7:W:596:ILE:HA	1.83	0.59
7:W:557:LEU:HD12	7:W:561:ALA:HB3	1.84	0.59
5:I:21:DG:H2'	5:I:22:DT:H71	1.84	0.59
7:W:396:ILE:HD11	7:W:633:GLN:HE22	1.67	0.58
7:W:180:LEU:HD23	7:W:180:LEU:H	1.68	0.58
3:G:20:ARG:HH11	4:H:122:LYS:HB3	1.68	0.58
5:I:-54:DC:H2''	5:I:-53:DA:C8	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:35:DT:H2''	5:I:36:DA:C8	2.39	0.58
3:C:32:ARG:NH2	4:D:32:GLU:OE1	2.36	0.58
7:W:239:SER:CB	7:W:538:ARG:NH2	2.63	0.58
7:W:307:ILE:HD11	7:W:324:VAL:HG21	1.86	0.57
7:W:467:GLU:HG2	7:W:468:PRO:HD2	1.84	0.57
7:W:404:LEU:CD1	7:W:596:ILE:HG13	2.24	0.57
7:W:404:LEU:HD11	7:W:596:ILE:CG1	2.25	0.57
3:G:102:ILE:HG23	4:H:58:ILE:HD13	1.87	0.57
2:F:30:THR:HB	2:F:32:PRO:HD2	1.87	0.57
6:J:-4:DC:H2''	6:J:-3:DG:C8	2.40	0.56
7:W:233:MET:HE3	7:W:305:LEU:HD13	1.87	0.56
3:G:20:ARG:HB3	4:H:122:LYS:HG3	1.88	0.56
5:I:-71:DA:H5'	5:I:-71:DA:C8	2.41	0.56
7:W:505:PHE:CE1	7:W:589:ALA:HB1	2.41	0.56
7:W:191:LEU:HD13	7:W:218:LEU:HD22	1.88	0.55
7:W:233:MET:HB2	7:W:302:TRP:CZ3	2.42	0.55
7:W:495:LEU:O	7:W:498:GLN:C	2.50	0.55
5:I:-47:DC:H2''	5:I:-46:DT:C5	2.43	0.54
3:C:102:ILE:HG23	4:D:58:ILE:HD13	1.90	0.54
7:W:515:LEU:HB3	7:W:556:MET:SD	2.47	0.54
5:I:-9:DC:H2''	5:I:-8:DG:C8	2.42	0.54
5:I:4:DG:H2''	5:I:5:DT:H72	1.90	0.54
2:B:27:GLN:OE1	2:B:55:ARG:NH1	2.41	0.53
5:I:3:DC:H2''	5:I:4:DG:C8	2.43	0.53
6:J:-71:DG:H2''	6:J:-70:DG:H5''	1.89	0.53
5:I:26:DA:H2''	5:I:27:DG:C8	2.44	0.53
1:A:112:ILE:HD12	3:G:114:VAL:HG11	1.91	0.53
5:I:20:DG:H2''	5:I:21:DG:O5'	2.07	0.53
2:B:35:ARG:O	2:B:39:ARG:HG2	2.08	0.53
7:W:396:ILE:HG22	7:W:398:ALA:H	1.73	0.53
7:W:558:SER:H	7:W:561:ALA:HB3	1.74	0.53
7:W:218:LEU:O	7:W:222:MET:HG2	2.09	0.53
7:W:454:ARG:HA	7:W:613:VAL:HG21	1.91	0.53
5:I:-72:DC:H2''	5:I:-71:DA:C8	2.44	0.53
5:I:-6:DG:H2''	5:I:-5:DG:C8	2.44	0.53
7:W:512:LEU:HD13	7:W:556:MET:HE2	1.91	0.52
7:W:348:TRP:NE1	7:W:361:SER:O	2.42	0.52
3:G:10:THR:OG1	3:G:11:ARG:N	2.43	0.52
7:W:238:LYS:HE2	7:W:535:HIS:NE2	2.23	0.52
7:W:380:LEU:HG	7:W:381:VAL:HG23	1.91	0.52
6:J:46:DA:H2''	6:J:47:DG:N7	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:178:GLY:HA2	7:W:251:TRP:HZ3	1.75	0.51
7:W:199:ILE:HD12	7:W:391:PHE:HE1	1.75	0.51
7:W:230:GLY:HA3	7:W:303:ARG:HD2	1.92	0.51
6:J:49:DC:H2''	6:J:50:DA:C8	2.45	0.51
7:W:502:VAL:O	7:W:503:LEU:HB3	2.11	0.51
5:I:-5:DG:H2''	5:I:-4:DG:C8	2.45	0.51
1:A:116:ARG:NH1	1:A:118:THR:O	2.43	0.51
5:I:-57:DT:H2''	5:I:-56:DG:C8	2.46	0.51
5:I:55:DC:H2''	5:I:56:DG:N7	2.26	0.51
6:J:-20:DC:H5'	6:J:-20:DC:C6	2.45	0.51
6:J:-58:DG:C8	6:J:-58:DG:H5'	2.46	0.51
7:W:550:SER:HB3	7:W:552:LYS:HG3	1.93	0.51
5:I:7:DC:H2''	5:I:8:DG:C8	2.46	0.51
6:J:56:DC:H2''	6:J:57:DA:N7	2.26	0.51
7:W:424:TYR:CE2	7:W:453:LEU:HD21	2.46	0.51
6:J:-46:DC:H2''	6:J:-45:DA:C8	2.47	0.50
7:W:529:LEU:HD23	7:W:557:LEU:HD13	1.93	0.50
6:J:-20:DC:H5'	6:J:-20:DC:H6	1.76	0.50
7:W:474:THR:HG1	7:W:521:TRP:CD1	2.30	0.50
7:W:567:ASN:CG	7:W:595:ARG:HB2	2.36	0.50
7:W:248:PHE:HE1	7:W:255:LEU:HD23	1.76	0.50
7:W:610:ASP:OD1	7:W:610:ASP:N	2.40	0.50
3:C:30:VAL:HG13	4:D:67:PHE:HE2	1.77	0.50
5:I:-37:DG:H2''	5:I:-36:DG:C8	2.46	0.50
7:W:280:TRP:H	7:W:280:TRP:CD1	2.30	0.50
5:I:-28:DC:H2''	5:I:-27:DC:C6	2.47	0.50
7:W:181:ARG:HB2	7:W:183:TYR:CE2	2.47	0.50
7:W:596:ILE:CB	8:W:1101:ATP:O3'	2.50	0.50
5:I:45:DT:H2''	5:I:46:DG:N7	2.27	0.50
7:W:574:VAL:HB	7:W:604:VAL:HA	1.93	0.50
5:I:-39:DT:H2''	5:I:-38:DA:H5''	1.94	0.49
6:J:-6:DT:H2''	6:J:-5:DA:C8	2.47	0.49
7:W:416:LEU:H	7:W:416:LEU:HD23	1.76	0.49
5:I:49:DC:H2''	5:I:50:DG:C8	2.47	0.49
5:I:-69:DG:H2''	5:I:-68:DA:C8	2.48	0.49
5:I:35:DT:H2''	5:I:36:DA:N7	2.28	0.49
7:W:528:ARG:NH2	7:W:530:ASP:HB3	2.28	0.49
6:J:60:DT:H2'	6:J:61:DA:C8	2.48	0.48
7:W:503:LEU:HA	7:W:555:PHE:O	2.13	0.48
7:W:596:ILE:O	7:W:598:GLN:N	2.46	0.48
5:I:-57:DT:H2''	5:I:-56:DG:N7	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:-25:DA:H2''	6:J:-24:DG:C8	2.48	0.48
7:W:461:TYR:HB3	7:W:468:PRO:HD3	1.95	0.48
7:W:423:TRP:HA	7:W:426:ARG:HH21	1.77	0.48
5:I:54:DT:H2''	5:I:55:DC:C6	2.49	0.48
6:J:73:DT:N3	6:J:74:DG:O6	2.47	0.48
7:W:334:LEU:HB2	7:W:354:LEU:HD21	1.96	0.48
3:G:30:VAL:HG13	4:H:67:PHE:HE1	1.79	0.48
5:I:47:DA:C8	5:I:47:DA:H5'	2.49	0.48
7:W:360:ASN:N	7:W:360:ASN:OD1	2.47	0.48
6:J:38:DT:H2''	6:J:39:DA:C8	2.47	0.48
1:E:69:ARG:HB3	2:F:25:ASN:ND2	2.29	0.47
5:I:56:DG:H2''	5:I:57:DG:C8	2.49	0.47
3:G:26:PRO:HB2	3:G:29:ARG:HB3	1.96	0.47
7:W:322:GLU:O	7:W:326:GLU:HG2	2.13	0.47
7:W:412:ILE:HD12	7:W:607:PHE:HE1	1.78	0.47
7:W:474:THR:HG1	7:W:521:TRP:CG	2.31	0.47
6:J:16:DA:H2''	6:J:17:DA:C8	2.49	0.47
6:J:6:DC:H2''	6:J:7:DC:C6	2.50	0.47
6:J:46:DA:H2''	6:J:47:DG:C8	2.49	0.47
5:I:24:DC:H2'	5:I:25:DT:C6	2.49	0.47
5:I:34:DC:H2''	5:I:35:DT:H72	1.95	0.47
7:W:271:VAL:HA	7:W:275:LEU:HD23	1.95	0.47
7:W:596:ILE:C	7:W:598:GLN:N	2.70	0.47
6:J:-19:DG:H5'	6:J:-19:DG:C8	2.49	0.47
7:W:203:LEU:HB3	7:W:335:LEU:HD12	1.96	0.47
1:A:101:VAL:HG11	3:G:107:VAL:HG21	1.98	0.46
7:W:616:ARG:O	7:W:619:GLU:HG3	2.15	0.46
7:W:182:ASP:HA	7:W:185:VAL:HG22	1.97	0.46
7:W:250:ARG:CZ	7:W:250:ARG:HB3	2.46	0.46
7:W:500:SER:O	7:W:553:PHE:HA	2.15	0.46
1:E:118:THR:HG22	2:F:45:ARG:HD3	1.97	0.46
6:J:-27:DC:H2''	6:J:-26:DT:H72	1.97	0.46
6:J:45:DC:H2''	6:J:46:DA:C8	2.49	0.46
7:W:310:ALA:HB3	7:W:336:THR:HB	1.96	0.46
6:J:-21:DC:H5''	7:W:508:MET:HE1	1.97	0.46
5:I:20:DG:H2'	5:I:21:DG:H8	1.79	0.46
5:I:64:DG:H2''	5:I:65:DA:C8	2.50	0.46
6:J:-57:DC:H2''	6:J:-56:DC:C5	2.50	0.46
7:W:211:LYS:HB3	7:W:335:LEU:HD11	1.98	0.46
7:W:394:ARG:NH2	7:W:633:GLN:OE1	2.49	0.46
6:J:-70:DG:H2''	6:J:-69:DA:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:-50:DC:H6	6:J:-50:DC:H5'	1.81	0.46
7:W:225:TYR:O	7:W:226:ARG:C	2.59	0.46
7:W:303:ARG:HA	7:W:330:THR:H	1.81	0.46
6:J:-56:DC:H2''	6:J:-55:DG:C8	2.51	0.46
6:J:72:DG:H2''	6:J:73:DT:C6	2.51	0.46
7:W:243:ASN:O	7:W:247:GLU:HG2	2.15	0.46
5:I:20:DG:H4'	5:I:21:DG:OP1	2.15	0.45
6:J:-25:DA:H2''	6:J:-24:DG:H8	1.81	0.45
7:W:564:LEU:HA	7:W:592:ARG:NH2	2.31	0.45
7:W:385:HIS:O	7:W:389:ARG:HG3	2.16	0.45
7:W:572:ASP:CG	7:W:603:ARG:HH12	2.23	0.45
7:W:596:ILE:O	7:W:597:GLY:C	2.58	0.45
3:G:74:LYS:HA	3:G:74:LYS:HD2	1.78	0.45
6:J:-72:DT:H2''	6:J:-71:DG:C8	2.51	0.45
6:J:30:DT:H2'	6:J:31:DT:H71	1.97	0.45
7:W:542:ILE:HB	7:W:566:ILE:HD13	1.98	0.45
1:A:64:LYS:HG2	1:A:90:MET:HE1	1.99	0.45
7:W:459:HIS:NE2	7:W:461:TYR:HB2	2.31	0.45
7:W:578:ASP:OD1	7:W:579:SER:N	2.47	0.45
5:I:67:DT:H2''	5:I:68:DC:C5	2.52	0.45
6:J:25:DG:H2''	6:J:26:DG:C8	2.51	0.45
7:W:264:LYS:HZ3	7:W:267:ARG:NH2	2.13	0.45
4:H:87:THR:OG1	4:H:90:GLU:OE1	2.33	0.45
7:W:490:LYS:O	7:W:493:PRO:HD2	2.17	0.45
7:W:239:SER:CB	7:W:538:ARG:CZ	2.91	0.44
7:W:506:SER:HB3	7:W:512:LEU:HD22	1.99	0.44
6:J:47:DG:H2''	6:J:48:DG:C8	2.53	0.44
7:W:454:ARG:C	7:W:456:CYS:H	2.26	0.44
7:W:592:ARG:NH1	7:W:592:ARG:HA	2.32	0.44
6:J:-23:DC:H2''	6:J:-22:DA:H8	1.82	0.44
6:J:39:DA:H2''	6:J:40:DG:H8	1.82	0.44
7:W:278:GLY:HA2	7:W:280:TRP:NE1	2.33	0.44
7:W:530:ASP:OD1	7:W:531:GLY:N	2.47	0.44
7:W:616:ARG:O	7:W:620:ARG:HG2	2.17	0.44
5:I:37:DC:H2''	5:I:38:DG:C8	2.52	0.44
5:I:69:DT:H2''	5:I:70:DC:C6	2.52	0.44
6:J:-36:DT:H2''	6:J:-35:DA:N7	2.32	0.44
7:W:199:ILE:HD13	7:W:199:ILE:HA	1.88	0.44
1:E:108:ASN:HB2	2:F:43:VAL:HG12	1.99	0.44
7:W:172:PRO:HB2	7:W:174:TYR:HD2	1.82	0.44
7:W:509:THR:HA	7:W:512:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:264:LYS:NZ	7:W:267:ARG:HH22	2.14	0.44
7:W:556:MET:HE2	7:W:556:MET:HB3	1.91	0.44
1:A:72:ARG:HB3	7:W:445:ARG:NH2	2.33	0.43
2:B:30:THR:HG22	2:B:32:PRO:HD2	2.00	0.43
5:I:-44:DG:H2''	5:I:-43:DA:C8	2.53	0.43
5:I:58:DC:H2''	5:I:59:DA:C8	2.53	0.43
1:A:72:ARG:HB3	7:W:445:ARG:HH22	1.83	0.43
2:F:35:ARG:O	2:F:39:ARG:HG2	2.19	0.43
5:I:-13:DA:H2''	5:I:-12:DA:C8	2.52	0.43
7:W:512:LEU:HG	7:W:558:SER:HB2	2.00	0.43
5:I:-38:DA:H2''	5:I:-37:DG:C8	2.54	0.43
7:W:311:HIS:HA	7:W:314:LYS:HB3	2.01	0.43
7:W:485:MET:O	7:W:488:LEU:HG	2.18	0.43
1:E:61:LEU:HD12	2:F:37:LEU:HD12	2.00	0.43
7:W:522:ARG:HG3	7:W:523:ASN:OD1	2.18	0.43
7:W:535:HIS:O	7:W:538:ARG:CG	2.67	0.43
6:J:-2:DC:H2''	6:J:-1:DG:H8	1.84	0.43
3:G:54:VAL:HG21	4:H:95:VAL:HG21	2.00	0.43
7:W:228:ILE:HD11	7:W:303:ARG:HE	1.83	0.43
7:W:278:GLY:HA2	7:W:280:TRP:CD1	2.54	0.43
1:E:118:THR:HG21	2:F:45:ARG:HH11	1.83	0.43
5:I:73:DG:N1	6:J:-72:DT:C2	2.86	0.43
7:W:303:ARG:HA	7:W:330:THR:HG23	2.01	0.43
7:W:343:ASN:OD1	7:W:343:ASN:N	2.51	0.43
7:W:411:LYS:CG	7:W:608:ILE:HD12	2.45	0.43
7:W:495:LEU:O	7:W:498:GLN:O	2.37	0.43
3:C:16:THR:HG22	3:C:18:SER:H	1.83	0.43
1:E:42:ARG:HH21	5:I:70:DC:H3'	1.84	0.43
7:W:290:LEU:HD11	7:W:327:PHE:CE2	2.54	0.43
7:W:302:TRP:O	7:W:329:THR:HA	2.18	0.43
7:W:413:TYR:CE2	7:W:610:ASP:HB3	2.54	0.43
5:I:71:DC:H5''	5:I:71:DC:H6	1.83	0.42
6:J:-2:DC:H2''	6:J:-1:DG:C8	2.53	0.42
5:I:20:DG:H2'	5:I:21:DG:C8	2.53	0.42
7:W:475:ASP:N	7:W:475:ASP:OD1	2.50	0.42
7:W:574:VAL:O	7:W:605:PHE:N	2.39	0.42
5:I:1:DC:H2''	5:I:2:DG:C8	2.54	0.42
6:J:7:DC:H2''	6:J:8:DC:C6	2.54	0.42
7:W:408:LYS:HE2	7:W:408:LYS:HB2	1.92	0.42
7:W:412:ILE:HD12	7:W:607:PHE:CE1	2.54	0.42
7:W:209:LEU:HB2	7:W:395:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:555:PHE:HD1	7:W:556:MET:H	1.66	0.42
7:W:459:HIS:HB3	7:W:462:LEU:HG	2.02	0.42
5:I:-17:DT:H2"	5:I:-16:DT:C6	2.55	0.42
7:W:238:LYS:HE3	7:W:535:HIS:ND1	2.34	0.42
7:W:505:PHE:HA	7:W:557:LEU:O	2.20	0.42
7:W:207:MET:HB3	7:W:208:GLY:H	1.66	0.42
7:W:407:LYS:HB3	7:W:602:VAL:HG23	2.01	0.42
6:J:66:DC:H2"	6:J:67:DA:C8	2.54	0.42
7:W:236:VAL:O	7:W:286:SER:HA	2.20	0.42
1:E:46:VAL:HG21	6:J:9:DG:H3'	2.01	0.41
7:W:609:THR:HG1	7:W:612:THR:HG1	1.65	0.41
6:J:36:DC:H2"	6:J:37:DC:C5	2.55	0.41
7:W:167:ARG:HA	7:W:167:ARG:HD2	1.89	0.41
7:W:276:LEU:HA	7:W:276:LEU:HD13	1.86	0.41
7:W:474:THR:O	7:W:521:TRP:NE1	2.53	0.41
7:W:494:LYS:O	7:W:498:GLN:HG2	2.20	0.41
7:W:580:ASP:OD1	7:W:581:TRP:N	2.52	0.41
2:F:43:VAL:HG21	2:F:46:ILE:HD11	2.01	0.41
4:D:31:LYS:HE3	4:D:31:LYS:HB3	1.93	0.41
2:F:39:ARG:HA	2:F:39:ARG:HD3	1.93	0.41
7:W:572:ASP:O	7:W:603:ARG:NH1	2.53	0.41
1:A:76:GLN:HE21	7:W:445:ARG:CZ	2.33	0.41
3:C:31:HIS:CE1	3:C:35:ARG:HH11	2.38	0.41
1:E:42:ARG:HD3	1:E:43:PRO:HD2	2.03	0.41
1:A:37:LYS:HB3	1:A:38:PRO:HD3	2.02	0.41
6:J:51:DC:H2"	6:J:52:DG:H5"	2.03	0.41
3:G:20:ARG:O	4:H:122:LYS:HE2	2.21	0.41
5:I:-23:DT:H2"	5:I:-22:DG:H8	1.86	0.41
7:W:242:HIS:HB2	7:W:539:GLN:OE1	2.21	0.41
7:W:488:LEU:O	7:W:492:LEU:HG	2.21	0.41
3:G:20:ARG:HD3	4:H:122:LYS:HB3	2.03	0.41
7:W:232:HIS:CE1	7:W:303:ARG:HB2	2.56	0.41
7:W:172:PRO:HB2	7:W:174:TYR:CD2	2.55	0.40
1:A:108:ASN:O	1:A:112:ILE:HG12	2.21	0.40
1:A:123:ASP:OD1	1:E:113:HIS:NE2	2.51	0.40
6:J:-34:DG:H2"	6:J:-33:DA:C8	2.57	0.40
7:W:525:GLU:O	7:W:554:VAL:HB	2.21	0.40
3:C:58:LEU:O	3:C:62:ILE:HG22	2.21	0.40
7:W:305:LEU:HD21	7:W:324:VAL:HG22	2.04	0.40
6:J:68:DT:H2"	6:J:69:DC:C6	2.56	0.40
7:W:389:ARG:N	7:W:390:PRO:HD2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:GLU:H	3:C:91:GLU:HG2	1.60	0.40
7:W:303:ARG:O	7:W:331:ASN:N	2.50	0.40
7:W:450:LEU:HA	7:W:450:LEU:HD12	1.83	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	95/136 (70%)	92 (97%)	3 (3%)	0	100	100
1	E	94/136 (69%)	89 (95%)	5 (5%)	0	100	100
2	B	83/103 (81%)	81 (98%)	2 (2%)	0	100	100
2	F	78/103 (76%)	76 (97%)	2 (3%)	0	100	100
3	C	107/130 (82%)	106 (99%)	1 (1%)	0	100	100
3	G	107/130 (82%)	103 (96%)	4 (4%)	0	100	100
4	D	94/126 (75%)	93 (99%)	1 (1%)	0	100	100
4	H	94/126 (75%)	92 (98%)	2 (2%)	0	100	100
7	W	438/1052 (42%)	398 (91%)	35 (8%)	5 (1%)	12	39
All	All	1190/2042 (58%)	1130 (95%)	55 (5%)	5 (0%)	32	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	W	523	ASN
7	W	455	LYS
7	W	381	VAL
7	W	503	LEU
7	W	566	ILE

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	85/111 (77%)	83 (98%)	2 (2%)	44	66
1	E	84/111 (76%)	82 (98%)	2 (2%)	44	66
2	B	69/79 (87%)	67 (97%)	2 (3%)	37	61
2	F	66/79 (84%)	65 (98%)	1 (2%)	60	75
3	C	85/102 (83%)	85 (100%)	0	100	100
3	G	85/102 (83%)	84 (99%)	1 (1%)	67	79
4	D	80/106 (76%)	78 (98%)	2 (2%)	42	65
4	H	82/106 (77%)	81 (99%)	1 (1%)	67	79
7	W	409/939 (44%)	386 (94%)	23 (6%)	17	44
All	All	1045/1735 (60%)	1011 (97%)	34 (3%)	35	58

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	59	GLU
2	B	30	THR
2	B	84	MET
4	D	61	SER
4	D	90	GLU
1	E	77	ASP
1	E	118	THR
2	F	43	VAL
3	G	74	LYS
4	H	60	ASN
7	W	207	MET
7	W	223	LYS
7	W	276	LEU
7	W	285	THR
7	W	304	TYR
7	W	324	VAL
7	W	346	GLU

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Mol	Chain	Res	Type
7	W	360	ASN
7	W	410	VAL
7	W	428	LEU
7	W	454	ARG
7	W	472	TYR
7	W	474	THR
7	W	478	LEU
7	W	502	VAL
7	W	512	LEU
7	W	515	LEU
7	W	518	TYR
7	W	519	CYS
7	W	537	GLU
7	W	584	GLN
7	W	595	ARG
7	W	612	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	76	GLN
1	A	93	GLN
1	A	108	ASN
1	E	85	GLN
3	G	89	ASN
7	W	214	GLN
7	W	311	HIS
7	W	331	ASN

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

1 ligand 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	$\# Z > 2$
8	ATP	W	1101	-	28,33,33	0.64	0	34,52,52	0.61	1 (2%)

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
8	ATP	W	1101	-	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	W	1101	ATP	C5-C6-N6	2.37	123.91	120.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

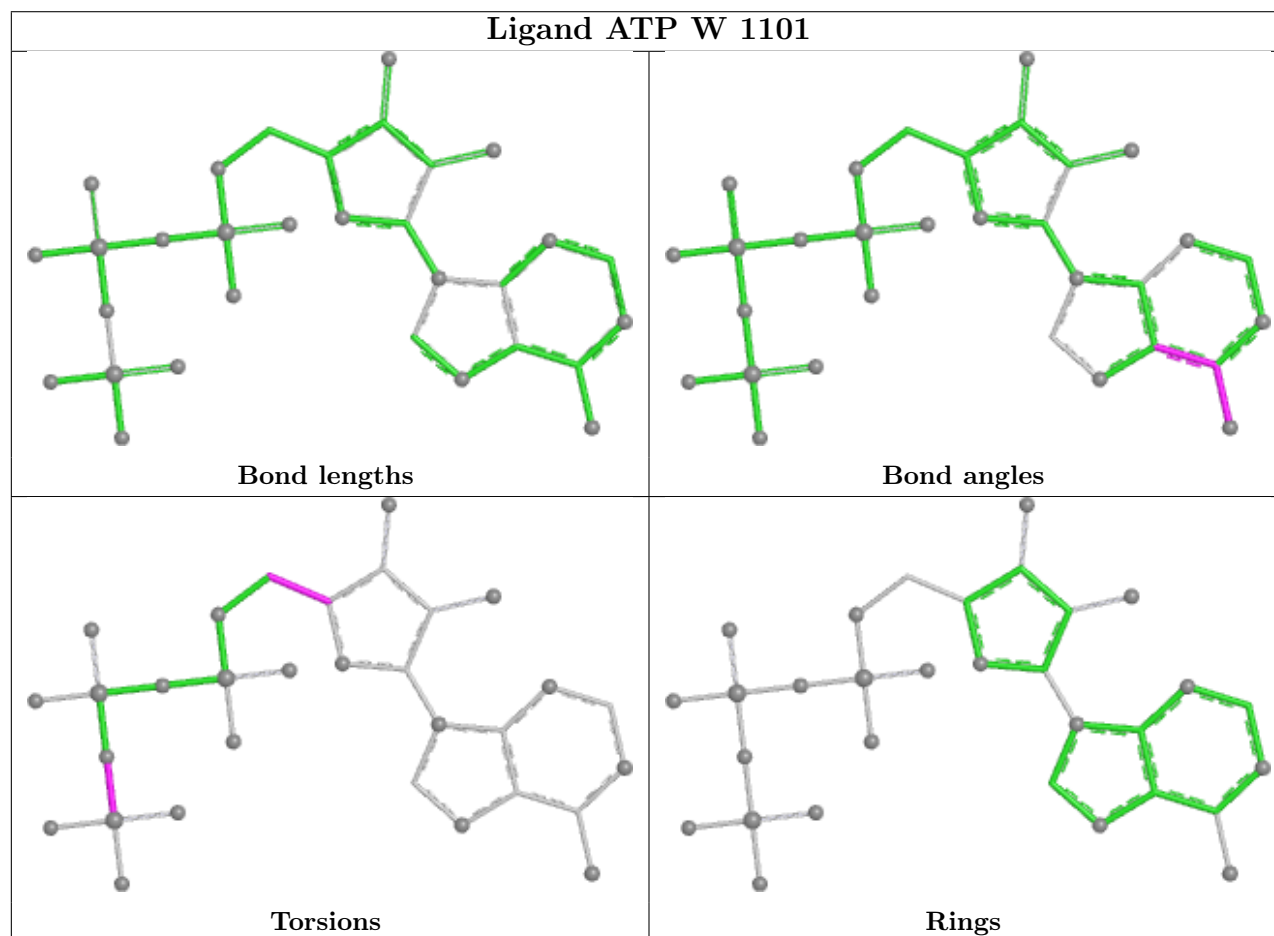
Mol	Chain	Res	Type	Atoms
8	W	1101	ATP	PB-O3B-PG-O2G
8	W	1101	ATP	O4'-C4'-C5'-O5'
8	W	1101	ATP	C3'-C4'-C5'-O5'
8	W	1101	ATP	PB-O3B-PG-O1G

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	W	1101	ATP	2	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

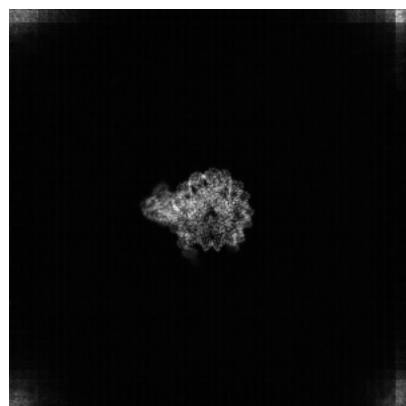
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47413. These allow visual inspection of the internal detail of the map and identification of artifacts.

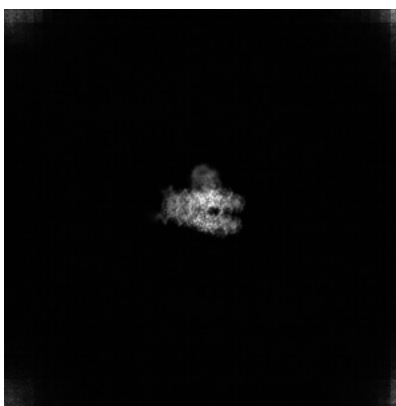
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

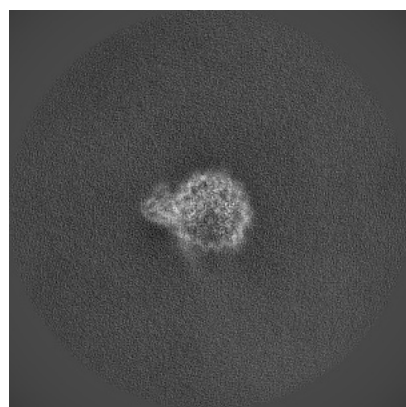


Y

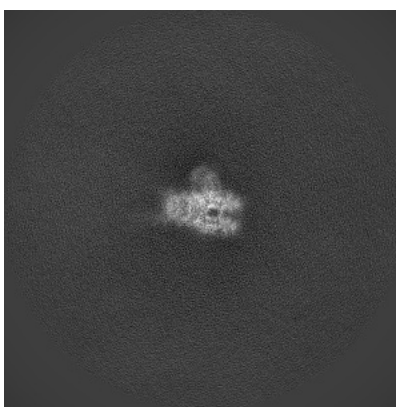


Z

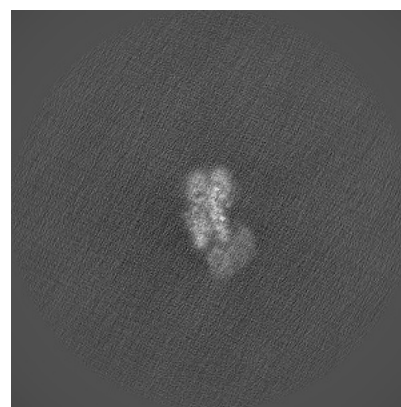
6.1.2 Raw map



X



Y



Z

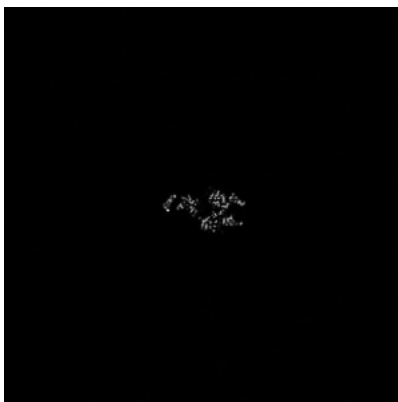
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

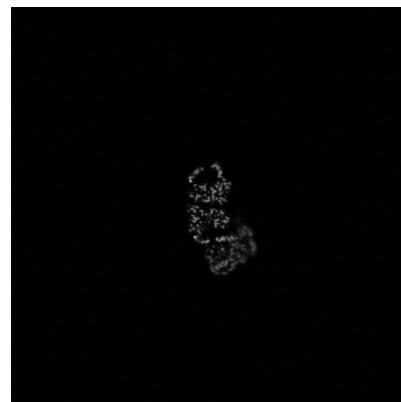
6.2.1 Primary map



X Index: 248

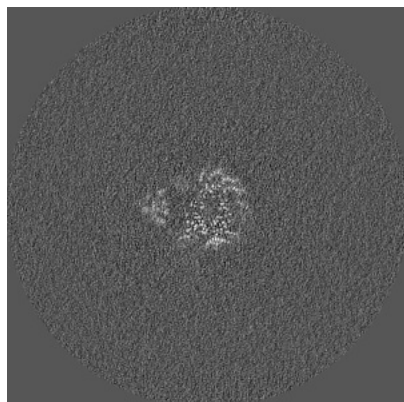


Y Index: 248

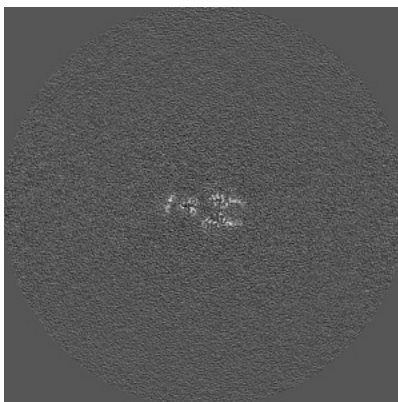


Z Index: 248

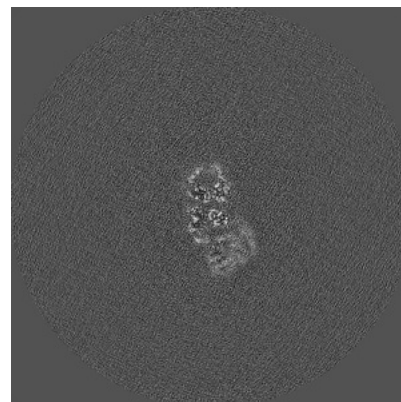
6.2.2 Raw map



X Index: 192



Y Index: 192

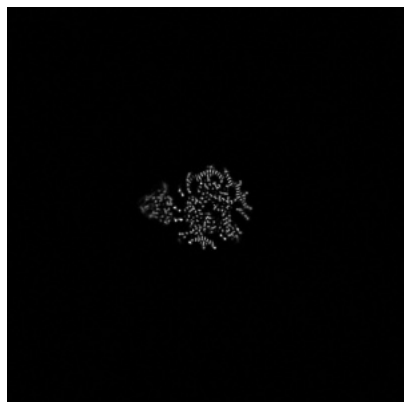


Z Index: 192

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

6.3 Largest variance slices [i](#)

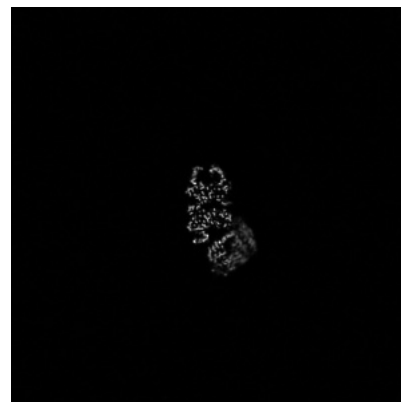
6.3.1 Primary map



X Index: 255

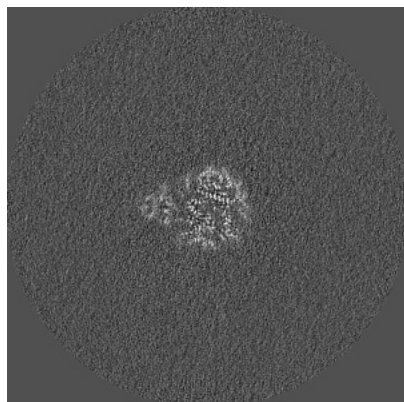


Y Index: 225

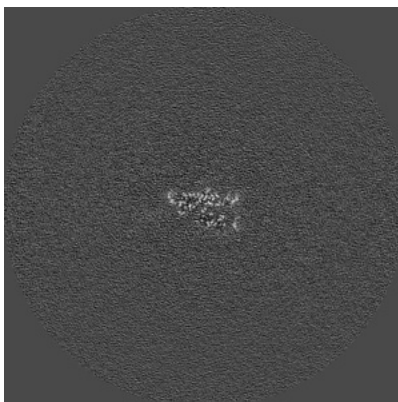


Z Index: 251

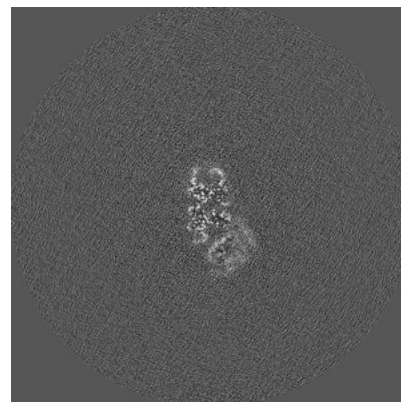
6.3.2 Raw map



X Index: 196



Y Index: 184

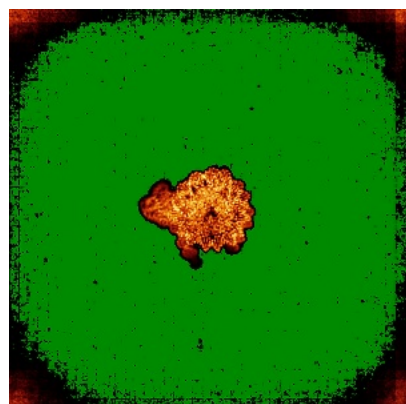


Z Index: 194

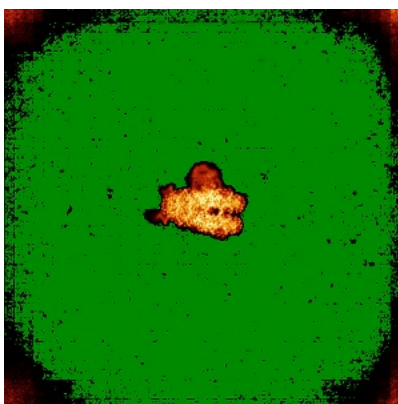
The images above show the largest variance slices of the map in three orthogonal directions.

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

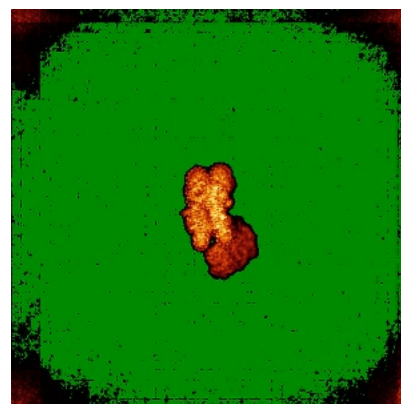
6.4.1 Primary map



X

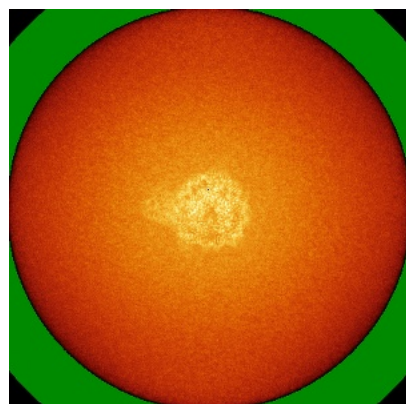


Y

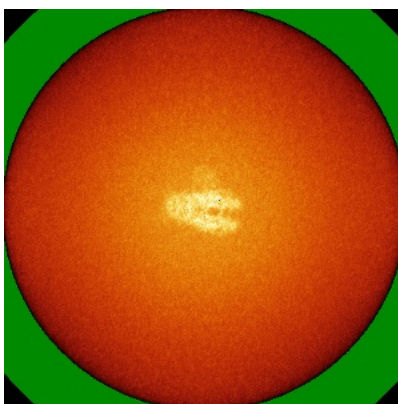


Z

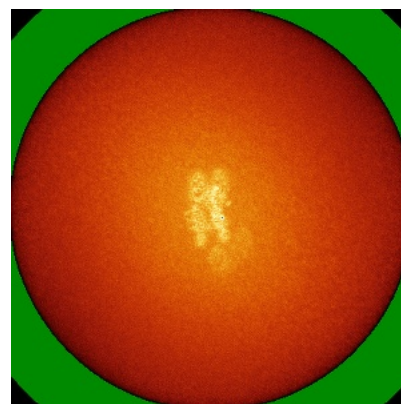
6.4.2 Raw map



X



Y

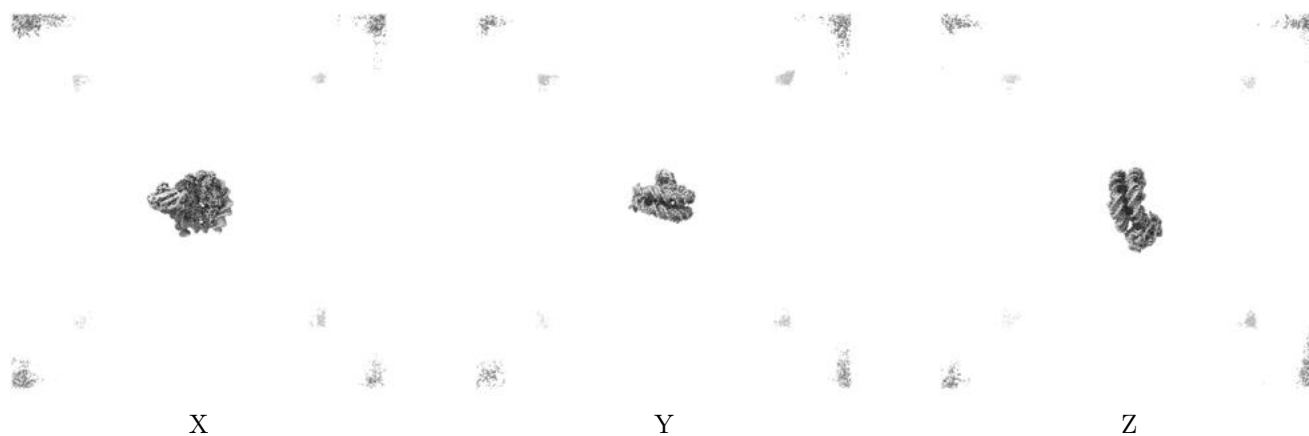


Z

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.

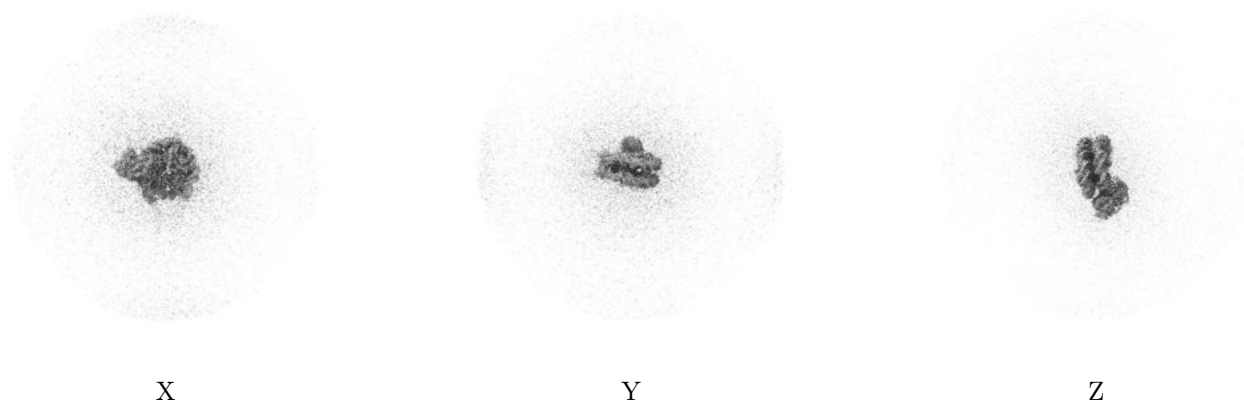
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. 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.

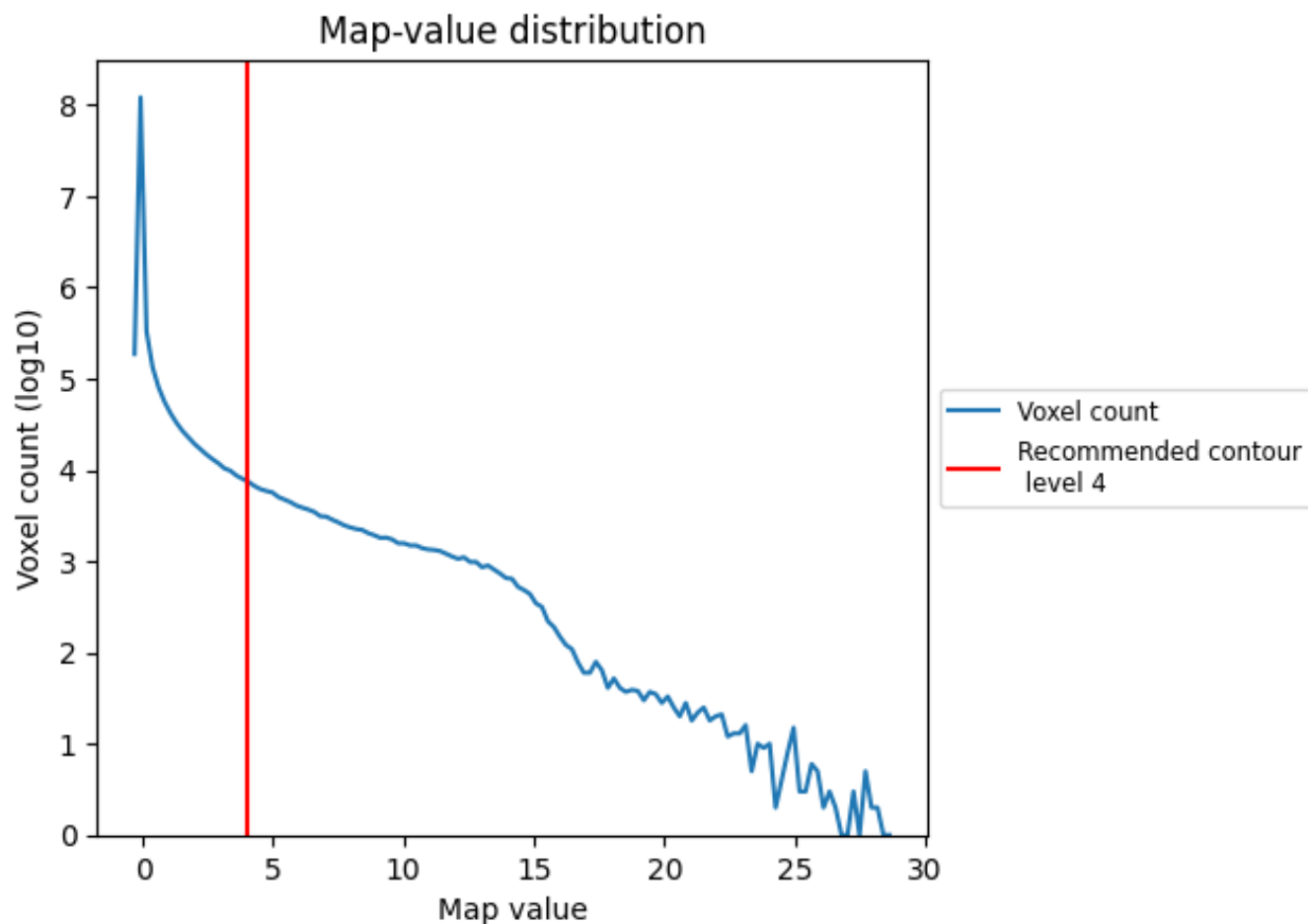
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

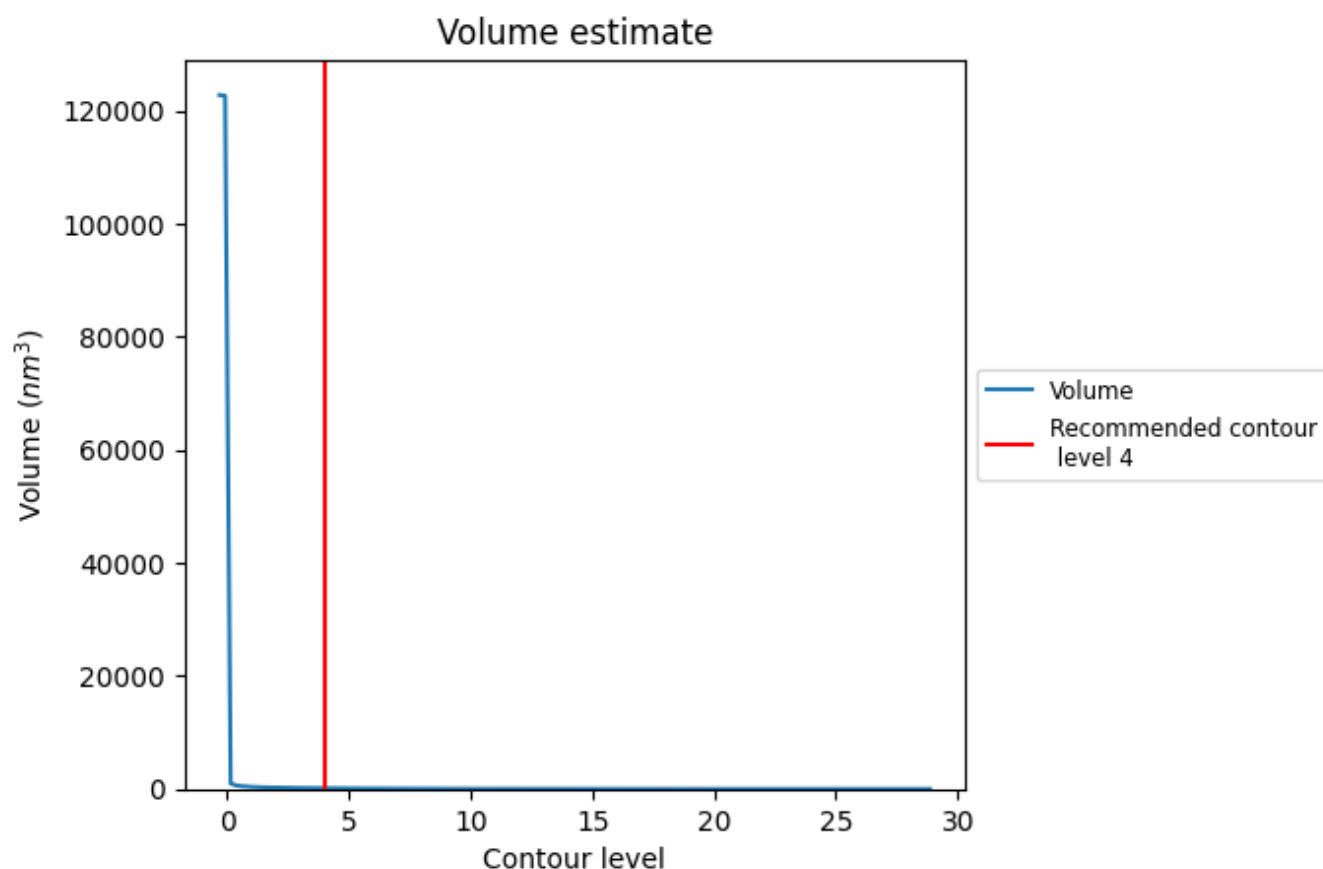
This section contains the results of statistical analysis of the map.

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.

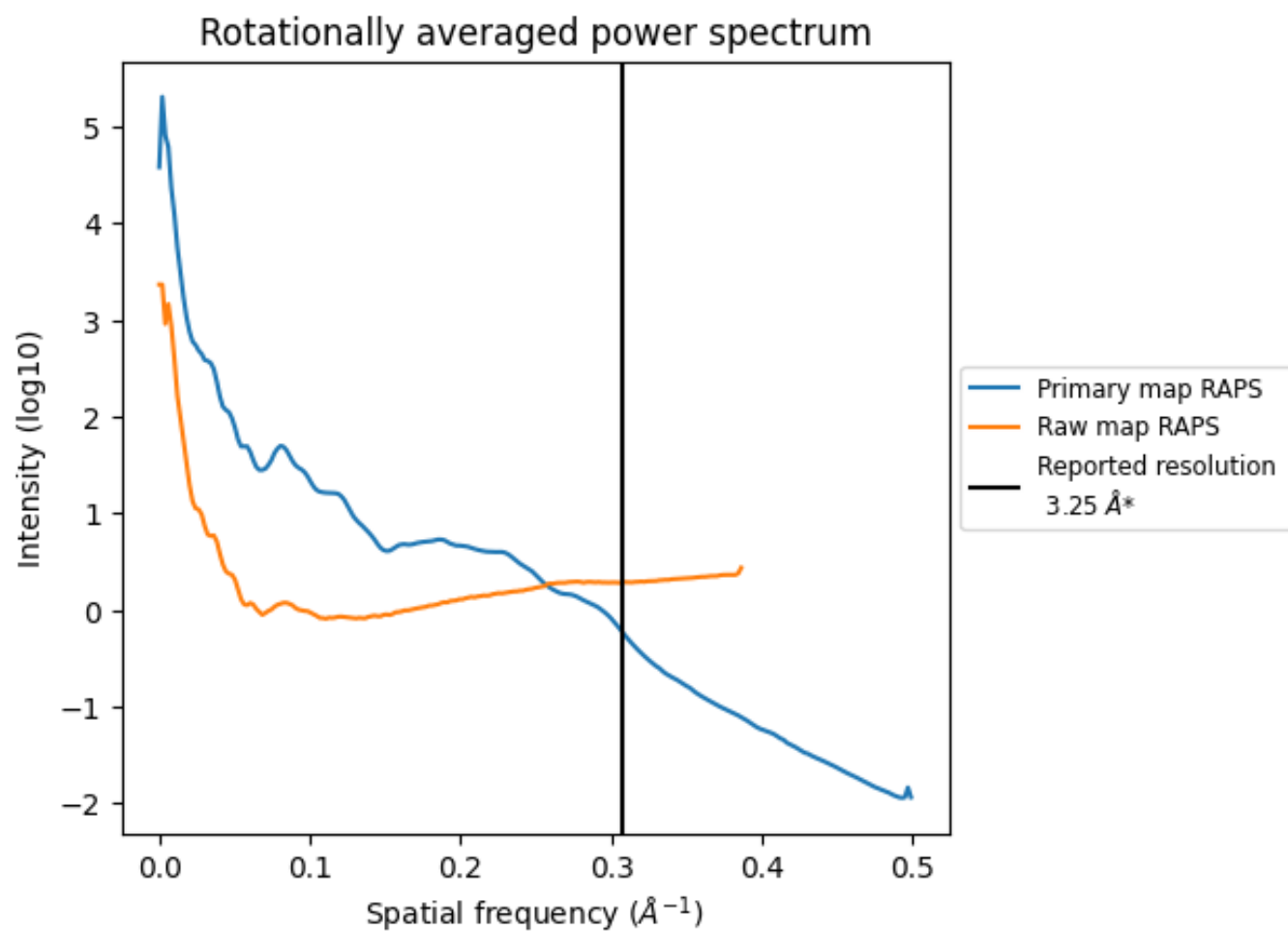
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 120 nm³; this corresponds to an approximate mass of 109 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 ⓘ

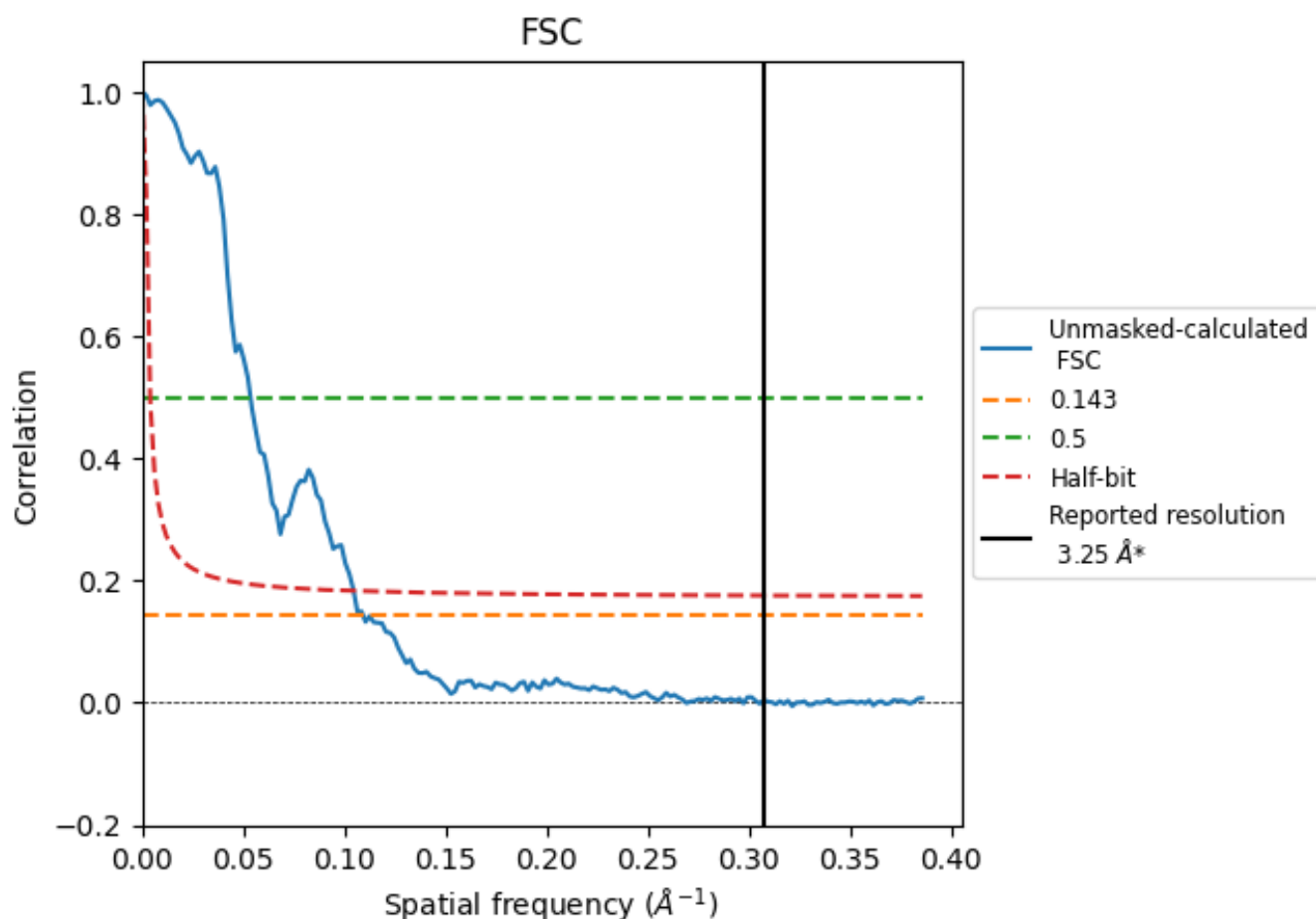


*Reported resolution corresponds to spatial frequency of 0.308 \AA^{-1}

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 0.308 \AA^{-1}

8.2 Resolution estimates [i](#)

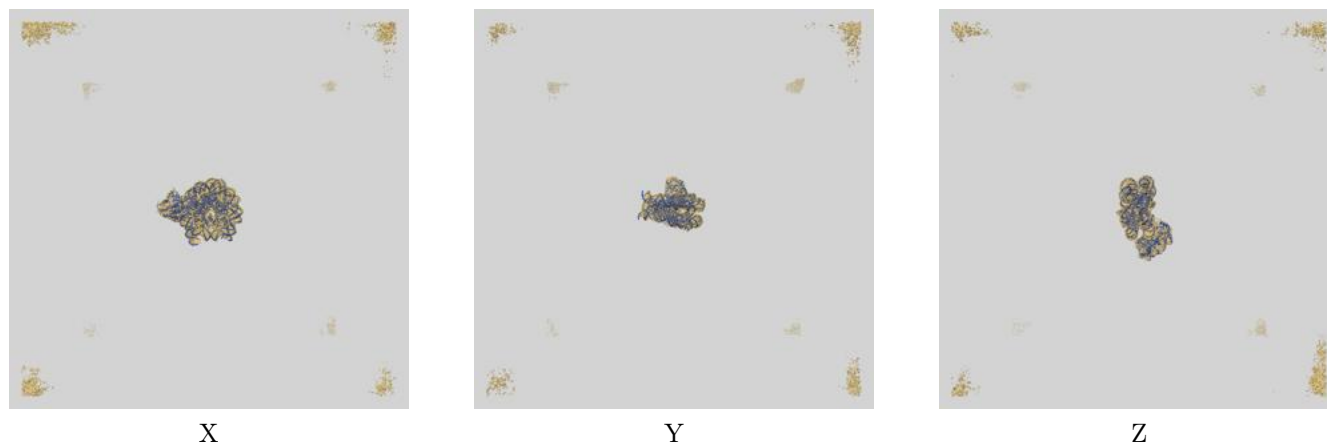
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.16	18.69	9.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.16 differs from the reported value 3.25 by more than 10 %

9 Map-model fit [i](#)

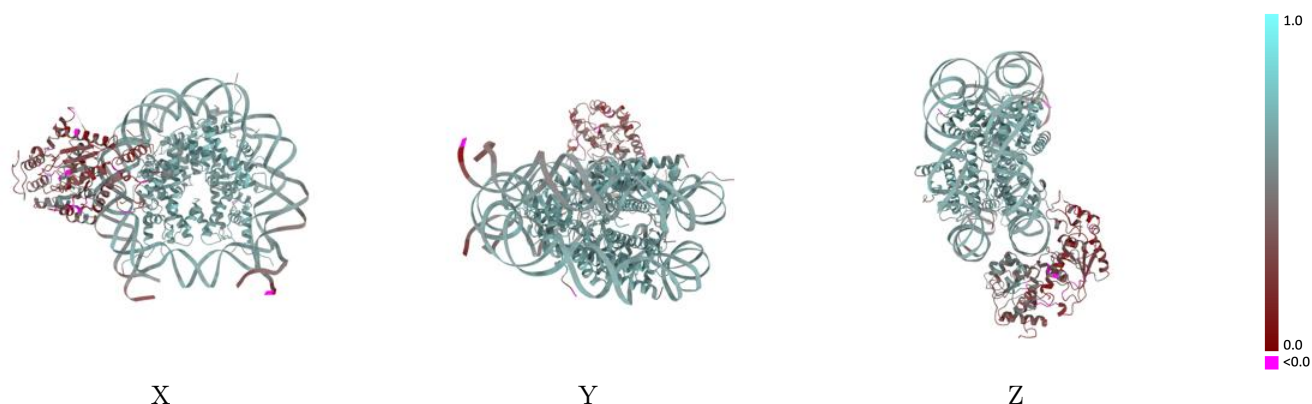
This section contains information regarding the fit between EMDB map EMD-47413 and PDB model 9E1M. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



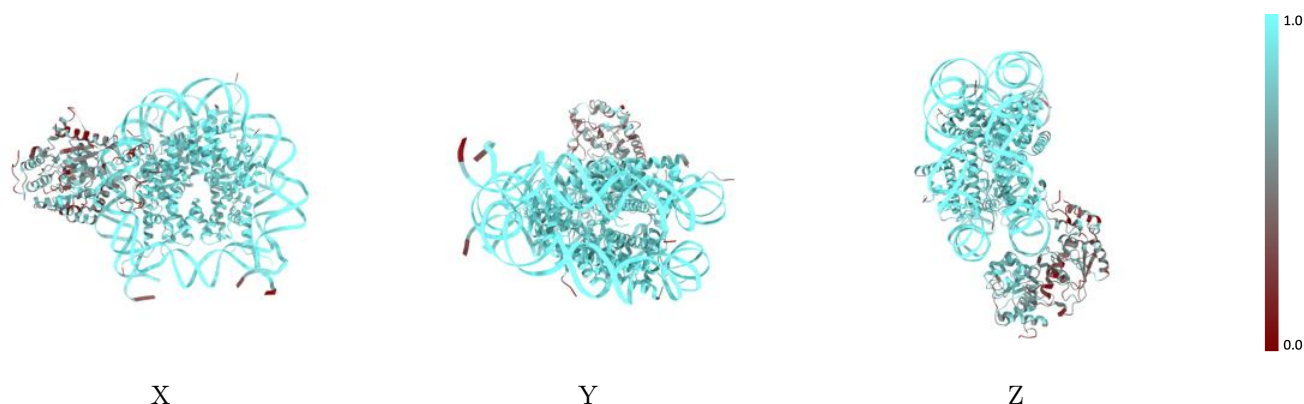
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



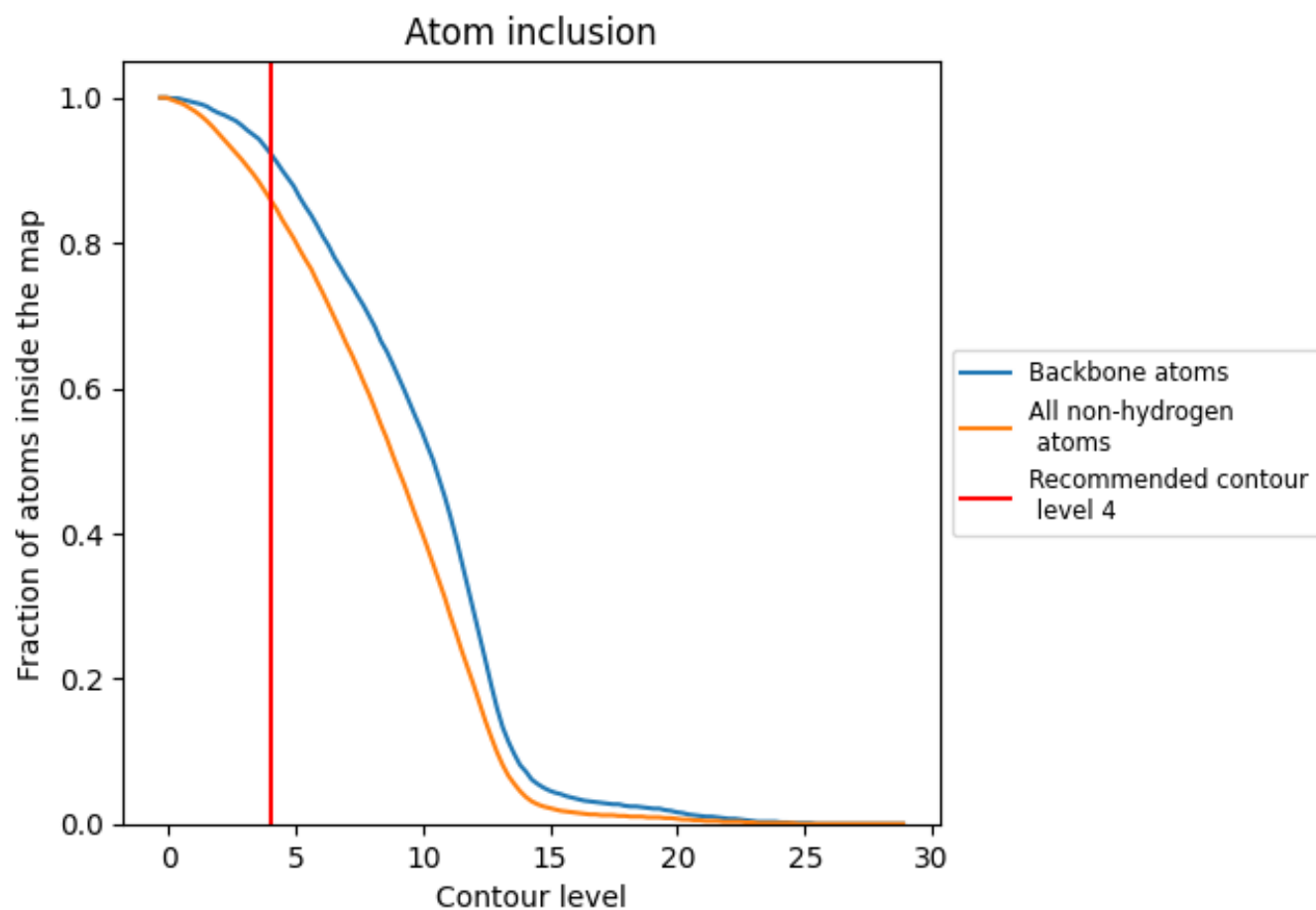
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8600	<div></div> 0.5350
A	<div></div> 0.9480	<div></div> 0.6300
B	<div></div> 0.8950	<div></div> 0.6170
C	<div></div> 0.9490	<div></div> 0.6340
D	<div></div> 0.9380	<div></div> 0.6380
E	<div></div> 0.9650	<div></div> 0.6480
F	<div></div> 0.9430	<div></div> 0.6360
G	<div></div> 0.9380	<div></div> 0.6360
H	<div></div> 0.9160	<div></div> 0.6230
I	<div></div> 0.9560	<div></div> 0.5720
J	<div></div> 0.9450	<div></div> 0.5680
W	<div></div> 0.5780	<div></div> 0.3160

1.0

0.0

<0.0