



Full wwPDB EM Validation Report ⓘ

Jan 13, 2025 – 12:23 PM EST

PDB ID : 9E1O
EMDB ID : EMD-47415
Title : Snf2h bound nucleosome complex - ClassB1
Authors : Malik, D.; Deshmukh, A.A.; Bilokapic, S.; Halic, M.
Deposited on : 2024-10-21
Resolution : 3.30 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
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) : 2.40

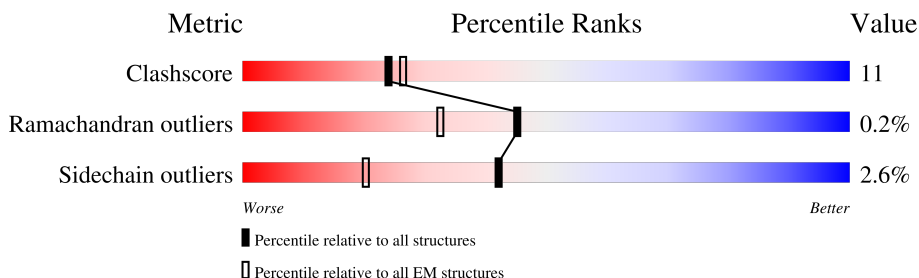
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



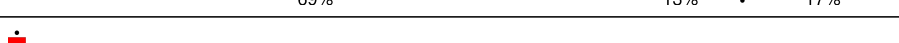



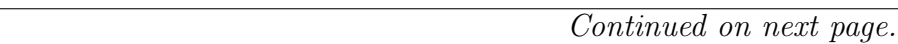

The reported resolution of this entry is 3.30 Å.

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






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	136	
1	E	136	
2	B	103	
2	F	103	
3	C	130	
3	G	130	
4	D	126	
4	H	126	

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Mol	Chain	Length	Quality of chain
5	I	149	 44% 56%
6	J	152	 50% 49%
7	W	1052	 6% 24% 16% 58%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15877 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 (148-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	148	Total	C	N	O	P	0	0
			3053	1444	575	886	148		

- Molecule 6 is a DNA chain called DNA (150-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	150	Total	C	N	O	P	0	0
			3056	1451	553	902	150		

- 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'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

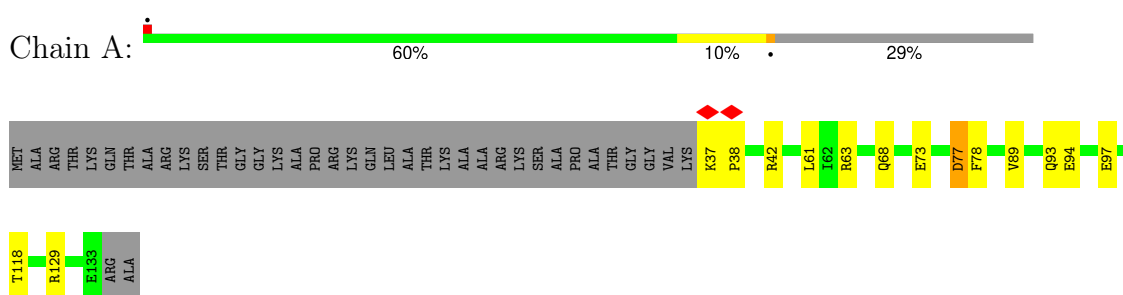


Mol	Chain	Residues	Atoms					AltConf
8	W	1	Total	C	N	O	P	0
			27	10	5	10	2	

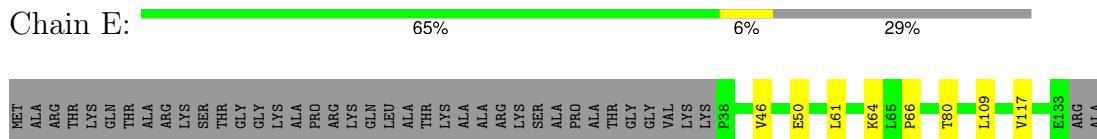
3 Residue-property plots [i](#)

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

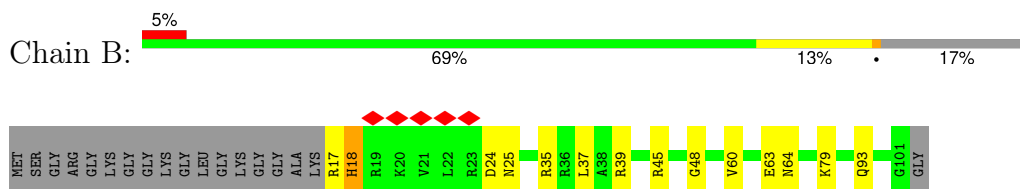
• Molecule 1: Histone H3.2



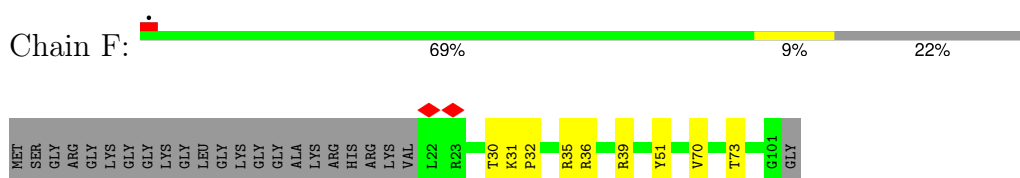
• Molecule 1: Histone H3.2



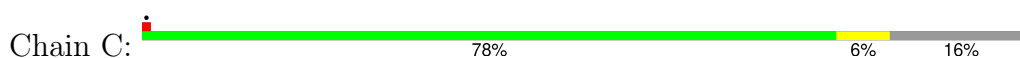
• Molecule 2: Histone H4

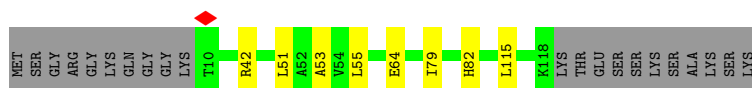


• Molecule 2: Histone H4



• Molecule 3: Histone H2A type 1

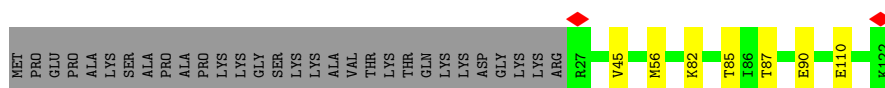




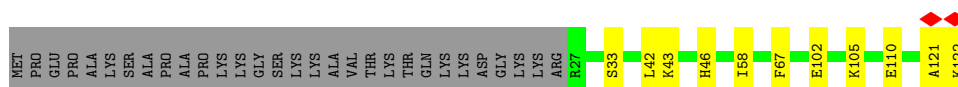
• Molecule 3: Histone H2A type 1



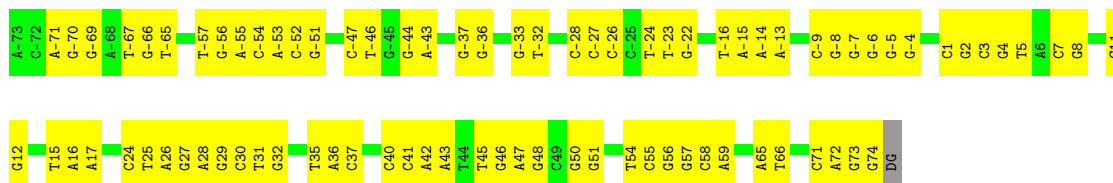
• Molecule 4: Histone H2B 1.1



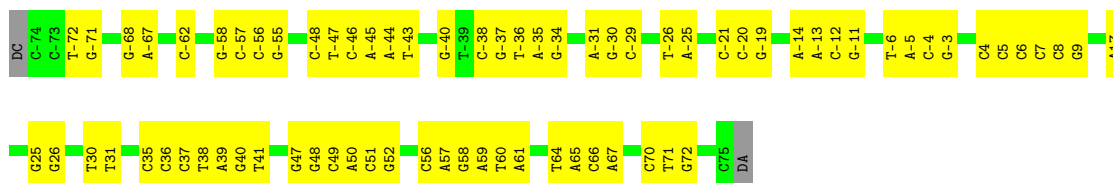
• Molecule 4: Histone H2B 1.1



• Molecule 5: DNA (148-MER)



• Molecule 6: DNA (150-MER)



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



MET	ILE	LYS	R181	E279	GLY	ASP	E516	G597	LYS	ILE	LEU	TRP	GLU	LYS
SER	PHE	PRO	D182	W280	D377	K443	D517	Q598	GLU	ALA	GLU	ASN	ARG	GLY
ALA	ASP	GLY	Y183	D281	Q378	M444	Y518		SER	THR	LYS	LYS	GLY	SER
ALA	ALA	ARG	Q184		K379	R445	C519	V602	ILE	THR	ILE	ILE	GLU	THR
GLU	SER	PRO	V185	S286	L380	R445	M520	V604	THR	ASP	PHE	ASP	LEU	ASP
PRO	PRO	ILE	N189	E288	V381	R454	R521		ASP	GLU	THR	ASN	THR	THR
PRO	GLY	LYS		E289	E382	K455	R522	F605	GLU	PRO	TYR	GLN	GLU	GLU
PRO	LYS	ASP	S193	L290	R383	C456	N523	F607	ASP	PRO	ARG	ARG	LEU	ASP
PRO	GLN	GLU	E196	K294	L384	H458	Y524	I608	ILE	PRO	LYS	LYS	THR	ILE
PRO	GLU	LYS			H385	H459	Y526	T609	GLY	ARG	ALA	ALA	ILE	ARG
PRO	ILE	ASN	I202	V302	N386	P460	C527	D610	ILE	GLU	GLY	ASN	GLY	GLY
GLU	GLN	ASN	L203	R303	R389	Y461	R528	N611	LEU	ARG	TYR	GLU	LEU	LEU
SER	GLU	LEU	A204	P390	F391	L462	D536	T612	GLU	LYS	VAL	LYS	GLU	GLU
ALA	PRO	LEU	D205	L305	L392	F463	E537		ARG	ALA	PRO	GLY	ALA	ALA
PRO	ASP	SER	E206	A310	L393	D464	R538	E615	GLY	TYR	ARG	ASP	ASN	ASN
SER	PRO	VAL	M207	E316	R394	G465	Q539	R616	LYS	ALA	ASN	ASP	ALA	LYS
LYS	THR	GLY	G208		R395	A466	D540	E619	THR	VAL	PRO	ASP	ALA	LYS
PRO	TYR	ASP	L209	R325	D399	E467	I542		THR	ASP	GLU	ASP	GLU	THR
ALA	GLU	TYR		E326	V400	P468	N543	M623	GLU	ALA	GLU	ILE	ALA	ALA
ALA	LYS	HIS	L213	F327	F401	G469	A544	K624	ALA	TYR	GLU	GLU	ALA	GLU
ALA	GLN	ARG	K223	K328	E402	P470	Y546	L625	GLU	PHE	ASN	ALA	ARG	ALA
SER	THR	THR	R226	T329	K403	P471	E547	R626	GLU	GLU	ALA	ALA	GLU	GLU
GLY	ASP	GLN		N331	S403	Y472	E547	L627	LYS	ALA	GLN	VAL	ALA	ALA
ASN	GLU	ALA	P231	L334	L404	T473	P548	S629	SER	ARG	LYS	GLY	GLY	GLY
SER	ASP	GLU	H232	L335		T480	N549	Q633	LYS	SER	LYS	LYS	LEU	LEU
SER	GLU	GLU	V236	T336	K407	D475	F553	Q634	GLY	GLU	GLN	THR	GLU	GLU
ASN	GLU	LEU		G337	K408	M476	F554		THR	PRO	PRO	ALA	PRO	GLU
LYS	TYR	LEU	N243	L340	E409	H477	M556		SER	LYS	ALA	ARG	ASN	GLU
GLY	LEU	THR			V410	L478	L557		THR	ALA	PRO	PRO	ASN	GLU
PRO	GLU	GLN	E247	H345	K411	W479	S558		ARG	LYS	PRO	PRO	ASN	GLU
GLU	THR	SER	F248		L412	N481	S559		ASN	ALA	ASN	ASN	ASN	GLU
GLY	GLN	LYS	K249	W348	L415		T559	I566	GLN	PRO	GLU	GLU	GLU	GLU
VAL	THR	LYS	R250	L354	L416	M485	R560	N567	LYS	ASN	GLU	GLU	GLU	GLU
ALA	PHE	ALA	W251		S417	V486	A561	L568	ASP	ARG	CYS	ASP	GLU	GLU
ALA	ALA	THR			K418	K490	G562		GLU	GLN	GLU	ASN	GLU	GLU
ASN	VAL	ASN	T254	D357	Q420	L491		V573	LEU	PHE	LYS	LEU	LEU	LEU
VAL	CYS	LYS	R256	L255	R421	L492			GLY	GLN	LYS	GLU	GLU	GLU
ILE	T166	ILE	S257	S361	E422	L495	I566		LYS	ASN	LYS	ARG	GLU	GLU
ALA	R167	GLN	C258	A363	W423	K496	N567		ASP	VAL	VAL	VAL	VAL	VAL
ALA	F168	PRO	G259	D363		E497	L568		THR	ASP	GLN	ASP	ASP	ASP
SER	E169	ALA	L260		R426	Q498	V573		ASN	PHE	GLN	PHE	PHE	PHE
ALA		GLN	D263		I427	G499	D578		GLU	GLN	GLU	GLU	GLU	GLU
SER	D170	LYS	R267		M429	S500	S579		GLY	ILE	LYS	LYS	LYS	LYS
PRO	S171	THR			ASP	R501	N582		THR	THR	THR	THR	THR	THR
ALA	P172	PRO			ILE	L503	V585		ARG	GLY	ARG	ARG	ARG	ARG
ASP	S173	THR	V271		ASP	S506	A589		GLU	ALA	GLY	GLY	GLY	GLY
ALA	V174	SER	R272		ILE	R510	R592		GLU	THR	THR	THR	THR	THR
GLU	V175	PRO	D273		ILE	V511	A593		LYS	ALA	ALA	ALA	ALA	ALA
MET	K176	LEU	W274		LEU	L512	H594		GLN	PHE	PHE	PHE	PHE	PHE
GLU	W177	LYS	L275		ASN	D613	R595		VAL	VAL	VAL	VAL	VAL	VAL
MET	G178	MET	L276		SER	I514	I596		PHE	ALA	ALA	ALA	ALA	ALA
GLU	K179	GLY	P277		ALA	I515			SER	SER	SER	SER	SER	SER
GLU	L180	LYS	G278		LYS									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8300	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	26.241	Depositor
Minimum map value	-0.316	Depositor
Average map value	-0.012	Depositor
Map value standard deviation	0.285	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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/811	0.53	0/1088
1	E	0.29	0/802	0.53	0/1076
2	B	0.28	0/687	0.56	0/921
2	F	0.29	0/648	0.57	0/868
3	C	0.27	0/847	0.53	0/1144
3	G	0.27	0/847	0.53	0/1144
4	D	0.28	0/757	0.46	0/1018
4	H	0.29	0/767	0.49	0/1029
5	I	0.63	0/3429	0.92	0/5295
6	J	0.64	0/3423	0.92	0/5276
7	W	0.26	0/3733	0.50	0/5041
All	All	0.46	0/16751	0.72	0/23900

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	799	0	838	12	0
1	E	790	0	826	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	679	0	717	11	0
2	F	641	0	684	8	0
3	C	837	0	891	6	0
3	G	837	0	891	10	0
4	D	746	0	764	5	0
4	H	756	0	786	7	0
5	I	3053	0	1660	72	0
6	J	3056	0	1684	60	0
7	W	3656	0	3730	139	0
8	W	27	0	12	5	0
All	All	15877	0	13483	308	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 (308) 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:455:LYS:HE3	7:W:463:PHE:HE1	1.32	0.92
7:W:455:LYS:HE3	7:W:463:PHE:CE1	2.06	0.91
5:I:73:DG:H2''	5:I:74:DG:C8	2.14	0.83
6:J:35:DC:H2''	6:J:36:DC:C5	2.13	0.83
1:A:68:GLN:HG2	1:A:89:VAL:HG11	1.62	0.81
1:A:73:GLU:OE1	2:B:25:ASN:HB2	1.82	0.80
7:W:560:ARG:HH21	7:W:582:ASN:HB2	1.52	0.75
2:B:17:ARG:HH11	7:W:467:GLU:HG3	1.54	0.73
7:W:357:ASP:OD1	7:W:360:ASN:ND2	2.22	0.72
6:J:-72:DT:H2'	6:J:-71:DG:C8	2.25	0.70
7:W:184:GLN:HG2	7:W:213:LEU:HD23	1.73	0.70
7:W:389:ARG:O	7:W:389:ARG:NH1	2.23	0.70
2:F:36:ARG:NH2	5:I:-13:DA:OP1	2.25	0.69
5:I:40:DC:H42	6:J:-40:DG:H1	1.39	0.69
6:J:-57:DC:H2''	6:J:-56:DC:C5	2.28	0.69
1:A:77:ASP:OD1	1:A:78:PHE:N	2.26	0.68
7:W:183:TYR:HE1	8:W:1101:ADP:H2	1.40	0.67
7:W:411:LYS:HG3	7:W:608:ILE:HD13	1.76	0.67
7:W:546:ASN:ND2	7:W:567:ASN:O	2.28	0.67
6:J:-57:DC:H2''	6:J:-56:DC:C6	2.30	0.67
7:W:305:LEU:HD22	7:W:329:THR:HG21	1.77	0.66
7:W:462:LEU:HD22	7:W:510:ARG:HB3	1.78	0.66
3:C:42:ARG:HB2	4:D:85:THR:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:181:ARG:HD2	7:W:184:GLN:HE22	1.62	0.64
7:W:213:LEU:HD22	7:W:251:TRP:HZ3	1.63	0.64
7:W:208:GLY:HA2	8:W:1101:ADP:H4'	1.79	0.64
5:I:30:DC:H2'	5:I:31:DT:C6	2.33	0.64
2:B:17:ARG:NH2	2:B:18:HIS:O	2.24	0.63
1:E:61:LEU:O	2:F:36:ARG:NH1	2.32	0.63
7:W:478:LEU:HD21	7:W:518:TYR:HA	1.81	0.62
6:J:35:DC:H2''	6:J:36:DC:C6	2.35	0.61
7:W:206:GLU:OE1	7:W:394:ARG:NH2	2.33	0.61
7:W:303:ARG:NH1	7:W:331:ASN:OD1	2.29	0.61
6:J:30:DT:H2'	6:J:31:DT:H71	1.81	0.61
2:B:48:GLY:N	5:I:7:DC:OP1	2.34	0.60
6:J:-4:DC:H2''	6:J:-3:DG:C8	2.36	0.60
7:W:340:LEU:HD23	7:W:628:ASP:HA	1.83	0.60
5:I:-70:DG:H2''	5:I:-69:DG:C8	2.37	0.60
7:W:407:LYS:HG2	7:W:602:VAL:HG23	1.84	0.60
7:W:538:ARG:O	7:W:542:ILE:HG12	2.02	0.59
5:I:-24:DT:H2'	5:I:-23:DT:H71	1.85	0.59
6:J:5:DC:H2''	6:J:6:DC:C5	2.36	0.59
5:I:-71:DA:H2''	5:I:-70:DG:C8	2.37	0.59
7:W:302:TRP:HB2	7:W:329:THR:HG22	1.84	0.59
6:J:49:DC:H2''	6:J:50:DA:C8	2.38	0.59
7:W:258:VAL:HG11	7:W:274:VAL:HG11	1.85	0.59
7:W:623:MET:HG2	7:W:626:ARG:HH22	1.68	0.59
7:W:547:GLU:HG3	7:W:549:ASN:H	1.67	0.59
1:A:94:GLU:OE1	3:G:104:GLN:NE2	2.36	0.58
6:J:71:DT:H2''	6:J:72:DG:C8	2.38	0.58
6:J:4:DC:H2''	6:J:5:DC:C5	2.38	0.58
7:W:316:GLU:OE2	7:W:325:ARG:NH2	2.37	0.58
5:I:-57:DT:OP1	7:W:294:LYS:NZ	2.36	0.58
7:W:467:GLU:HG2	7:W:468:PRO:HD2	1.85	0.58
6:J:-58:DG:H2''	6:J:-57:DC:C6	2.38	0.58
7:W:181:ARG:CZ	8:W:1101:ADP:HN62	2.16	0.58
7:W:609:THR:O	7:W:612:THR:OG1	2.20	0.57
7:W:492:LEU:HD23	7:W:495:LEU:HD12	1.87	0.57
5:I:-5:DG:H2''	5:I:-4:DG:C8	2.40	0.56
5:I:26:DA:H2''	5:I:27:DG:C8	2.40	0.56
5:I:-37:DG:H2''	5:I:-36:DG:C8	2.40	0.56
5:I:29:DG:H1'	5:I:30:DC:O4'	2.05	0.56
7:W:181:ARG:HD2	7:W:181:ARG:H	1.70	0.56
1:E:50:GLU:OE2	2:F:39:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:102:ILE:HG23	4:H:58:ILE:HD13	1.87	0.56
3:G:29:ARG:NH1	4:H:33:SER:O	2.39	0.56
6:J:-38:DC:H2''	6:J:-37:DG:C8	2.41	0.56
7:W:596:ILE:HG23	7:W:597:GLY:N	2.21	0.56
6:J:-37:DG:H2''	6:J:-36:DT:C5	2.41	0.56
6:J:-68:DG:H2'	6:J:-67:DA:C8	2.41	0.56
6:J:-48:DC:H2''	6:J:-47:DT:C5	2.41	0.56
7:W:256:ARG:NH1	7:W:256:ARG:O	2.39	0.56
7:W:615:GLU:O	7:W:619:GLU:HG3	2.06	0.56
5:I:36:DA:H2''	5:I:37:DC:C5	2.40	0.56
5:I:15:DT:H2''	5:I:16:DA:C8	2.40	0.56
6:J:-37:DG:H2''	6:J:-36:DT:C7	2.36	0.55
7:W:560:ARG:NH2	7:W:582:ASN:HB2	2.18	0.55
1:A:93:GLN:O	1:A:97:GLU:HG2	2.07	0.55
7:W:167:ARG:HE	7:W:189:ASN:HB3	1.71	0.55
7:W:380:LEU:O	7:W:382:GLU:N	2.40	0.55
5:I:-54:DC:H2''	5:I:-53:DA:C8	2.40	0.55
5:I:-47:DC:H2''	5:I:-46:DT:C5	2.42	0.55
7:W:422:GLU:O	7:W:426:ARG:HG2	2.07	0.55
6:J:56:DC:H2''	6:J:57:DA:C8	2.42	0.54
2:B:64:ASN:HB3	2:B:93:GLN:HE22	1.72	0.54
7:W:213:LEU:HD13	7:W:251:TRP:CE3	2.43	0.54
7:W:540:ASP:OD1	7:W:540:ASP:N	2.39	0.54
5:I:40:DC:N3	6:J:-40:DG:N2	2.53	0.54
6:J:6:DC:H2''	6:J:7:DC:C6	2.43	0.54
7:W:573:VAL:HG13	7:W:603:ARG:HH22	1.73	0.54
1:A:77:ASP:OD1	1:A:77:ASP:C	2.45	0.54
2:F:70:VAL:HA	2:F:73:THR:HG22	1.89	0.54
7:W:399:ASP:OD1	7:W:400:VAL:N	2.41	0.54
7:W:589:ALA:HA	7:W:592:ARG:HE	1.73	0.54
6:J:8:DC:H2''	6:J:9:DG:C8	2.43	0.54
6:J:59:DA:H2'	6:J:60:DT:H71	1.90	0.53
5:I:55:DC:H2''	5:I:56:DG:C8	2.44	0.53
5:I:-27:DC:H1'	5:I:-26:DC:C6	2.43	0.53
5:I:-9:DC:H2''	5:I:-8:DG:C8	2.44	0.53
7:W:383:ARG:HG3	7:W:384:LEU:HD12	1.91	0.53
5:I:28:DA:H1'	5:I:29:DG:C8	2.44	0.52
6:J:4:DC:H2''	6:J:5:DC:C6	2.43	0.52
2:B:60:VAL:O	2:B:63:GLU:HG2	2.09	0.52
1:E:46:VAL:HG21	6:J:9:DG:H3'	1.92	0.52
7:W:263:ASP:N	7:W:263:ASP:OD1	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:-67:DT:H2''	5:I:-66:DG:C8	2.45	0.52
3:C:53:ALA:HB1	4:D:110:GLU:HG3	1.92	0.52
7:W:202:ILE:HG13	7:W:354:LEU:HD11	1.91	0.52
7:W:213:LEU:HD13	7:W:251:TRP:HE3	1.75	0.52
7:W:310:ALA:HB3	7:W:336:THR:HB	1.91	0.52
7:W:566:ILE:HG22	7:W:568:LEU:HG	1.91	0.52
5:I:35:DT:H2''	5:I:36:DA:C8	2.45	0.52
6:J:-56:DC:H2''	6:J:-55:DG:C8	2.45	0.52
7:W:501:ARG:NH2	7:W:545:TYR:O	2.43	0.52
7:W:303:ARG:NH1	7:W:330:THR:OG1	2.42	0.51
7:W:290:LEU:HD11	7:W:327:PHE:CE2	2.45	0.51
7:W:412:ILE:HD11	7:W:605:PHE:CD1	2.46	0.51
3:C:64:GLU:HB3	4:D:45:VAL:HG21	1.92	0.51
7:W:223:LYS:HD2	7:W:255:LEU:HD13	1.92	0.51
7:W:454:ARG:HH21	7:W:458:ASN:HD21	1.59	0.51
6:J:-36:DT:H2''	6:J:-35:DA:C8	2.46	0.51
6:J:-46:DC:H2''	6:J:-45:DA:C8	2.46	0.51
5:I:45:DT:H2''	5:I:46:DG:C8	2.46	0.51
2:B:24:ASP:OD1	2:B:25:ASN:N	2.44	0.50
7:W:429:MET:SD	7:W:430:LYS:HG3	2.51	0.50
5:I:57:DG:H2''	5:I:58:DC:C5	2.47	0.50
7:W:417:SER:N	7:W:420:GLN:OE1	2.35	0.50
7:W:459:HIS:HD2	7:W:514:ILE:HG21	1.76	0.50
7:W:416:LEU:H	7:W:421:ARG:NH2	2.10	0.50
7:W:474:THR:O	7:W:521:TRP:NE1	2.44	0.50
7:W:479:VAL:HG23	7:W:486:VAL:HA	1.93	0.50
7:W:578:ASP:OD1	7:W:579:SER:N	2.44	0.50
1:A:63:ARG:HD3	5:I:17:DA:H4'	1.93	0.50
3:G:88:ARG:NH1	3:G:94:ASN:OD1	2.42	0.50
5:I:31:DT:C2	5:I:32:DG:C8	3.00	0.50
7:W:179:LYS:HB2	7:W:181:ARG:NE	2.27	0.50
7:W:460:PRO:O	7:W:463:PHE:HB2	2.11	0.50
7:W:516:GLU:HG2	7:W:526:TYR:CE2	2.47	0.50
7:W:558:SER:HB3	7:W:561:ALA:HB3	1.93	0.50
7:W:513:ASP:OD1	7:W:528:ARG:NH1	2.45	0.49
6:J:38:DT:H2''	6:J:39:DA:C8	2.47	0.49
5:I:-55:DA:H2''	5:I:-54:DC:C5	2.47	0.49
5:I:25:DT:H2''	5:I:26:DA:C8	2.47	0.49
5:I:46:DG:H2''	5:I:47:DA:C8	2.48	0.49
7:W:476:MET:O	7:W:481:ASN:ND2	2.46	0.49
5:I:71:DC:H2''	5:I:72:DA:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:623:MET:HG2	7:W:626:ARG:NH2	2.26	0.49
1:E:66:PRO:HD3	6:J:17:DA:H5''	1.95	0.49
7:W:183:TYR:CE1	8:W:1101:ADP:H2	2.26	0.49
7:W:208:GLY:N	8:W:1101:ADP:O2A	2.45	0.49
7:W:256:ARG:HH12	7:W:281:ASP:N	2.10	0.49
5:I:7:DC:H2''	5:I:8:DG:C8	2.48	0.49
3:G:26:PRO:HB2	3:G:29:ARG:HB3	1.95	0.48
5:I:4:DG:H2''	5:I:5:DT:H72	1.94	0.48
7:W:423:TRP:O	7:W:427:ILE:HG12	2.13	0.48
7:W:512:LEU:HD22	7:W:556:MET:HB3	1.93	0.48
1:A:42:ARG:HG2	6:J:70:DC:P	2.53	0.48
7:W:177:TRP:HZ3	7:W:250:ARG:HB3	1.78	0.48
5:I:3:DC:H2''	5:I:4:DG:C8	2.48	0.48
7:W:500:SER:HB2	7:W:553:PHE:HE1	1.77	0.48
6:J:-37:DG:H2''	6:J:-36:DT:H71	1.95	0.48
6:J:-31:DA:H2''	6:J:-30:DG:C8	2.49	0.48
3:G:30:VAL:HG13	4:H:67:PHE:HE1	1.78	0.48
3:C:115:LEU:HD22	1:E:117:VAL:HG13	1.96	0.48
7:W:503:LEU:HD11	7:W:557:LEU:HD13	1.96	0.48
5:I:65:DA:C8	5:I:66:DT:H72	2.49	0.47
5:I:73:DG:C2	5:I:74:DG:C2	3.03	0.47
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.50	0.47
1:A:37:LYS:HB3	1:A:38:PRO:HD3	1.97	0.47
1:A:118:THR:HG22	2:B:45:ARG:HB3	1.95	0.47
6:J:-45:DA:H2''	6:J:-44:DA:H8	1.80	0.47
7:W:454:ARG:C	7:W:456:CYS:H	2.17	0.47
7:W:177:TRP:CZ3	7:W:250:ARG:HB3	2.50	0.47
2:F:31:LYS:NZ	2:F:35:ARG:HH22	2.13	0.47
5:I:-70:DG:H2''	5:I:-69:DG:H8	1.80	0.47
5:I:26:DA:H2''	5:I:27:DG:N7	2.29	0.47
7:W:256:ARG:HH12	7:W:281:ASP:H	1.63	0.47
7:W:271:VAL:HA	7:W:275:LEU:HB3	1.96	0.47
7:W:409:GLU:OE2	7:W:606:ARG:NE	2.34	0.47
7:W:475:ASP:N	7:W:475:ASP:OD1	2.47	0.47
7:W:202:ILE:HG12	7:W:334:LEU:HB2	1.96	0.47
7:W:256:ARG:NH2	7:W:279:GLU:O	2.48	0.47
7:W:500:SER:HB2	7:W:553:PHE:CE1	2.49	0.47
7:W:404:LEU:HG	7:W:594:HIS:CE1	2.51	0.46
5:I:30:DC:H2'	5:I:31:DT:C5	2.50	0.46
7:W:418:LYS:O	7:W:422:GLU:HG2	2.15	0.46
7:W:519:CYS:O	7:W:523:ASN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:24:DC:OP1	7:W:624:LYS:NZ	2.35	0.46
6:J:40:DG:H1'	6:J:41:DT:H5'	1.97	0.46
7:W:256:ARG:NH2	7:W:281:ASP:HB2	2.30	0.46
7:W:231:PRO:HB2	7:W:302:TRP:HA	1.97	0.46
7:W:454:ARG:NH2	7:W:458:ASN:HD21	2.14	0.46
4:D:87:THR:OG1	4:D:90:GLU:OE1	2.27	0.46
5:I:-57:DT:H2''	5:I:-56:DG:C8	2.51	0.46
6:J:51:DC:H2''	6:J:52:DG:H5''	1.97	0.46
5:I:-15:DA:H2''	5:I:-14:DA:C8	2.50	0.46
6:J:-6:DT:H2''	6:J:-5:DA:C8	2.51	0.46
6:J:60:DT:H2''	6:J:61:DA:H8	1.80	0.46
7:W:196:GLU:OE2	7:W:226:ARG:NH2	2.42	0.46
7:W:206:GLU:HA	7:W:337:GLY:HA2	1.97	0.46
6:J:25:DG:H2''	6:J:26:DG:C8	2.50	0.46
4:H:102:GLU:HA	4:H:105:LYS:HG2	1.99	0.45
7:W:416:LEU:HB3	7:W:420:GLN:HB2	1.98	0.45
6:J:36:DC:H2''	6:J:37:DC:C5	2.51	0.45
2:F:30:THR:HB	2:F:32:PRO:HD2	1.99	0.45
3:G:14:ALA:HB1	5:I:-43:DA:H4'	1.97	0.45
5:I:-27:DC:H1'	5:I:-26:DC:C5	2.52	0.45
7:W:522:ARG:HB3	7:W:524:TYR:CZ	2.51	0.45
7:W:204:ALA:HA	7:W:336:THR:O	2.17	0.45
2:B:79:LYS:N	5:I:28:DA:OP1	2.47	0.45
6:J:47:DG:H2''	6:J:48:DG:C8	2.52	0.45
6:J:-35:DA:H2''	6:J:-34:DG:C8	2.52	0.45
7:W:236:VAL:O	7:W:286:SER:HA	2.17	0.45
7:W:560:ARG:HE	7:W:585:VAL:HG11	1.82	0.45
7:W:204:ALA:O	7:W:394:ARG:HD2	2.17	0.44
7:W:243:ASN:O	7:W:247:GLU:HG2	2.16	0.44
7:W:393:LEU:HD21	7:W:395:ARG:HG3	1.98	0.44
7:W:167:ARG:CZ	7:W:193:SER:HB3	2.47	0.44
5:I:1:DC:H2''	5:I:2:DG:C8	2.52	0.44
7:W:478:LEU:HD12	7:W:478:LEU:HA	1.81	0.44
5:I:-16:DT:H1'	5:I:-15:DA:C8	2.52	0.44
5:I:-15:DA:H2''	5:I:-14:DA:H8	1.83	0.44
5:I:15:DT:H2''	5:I:16:DA:N7	2.32	0.44
7:W:427:ILE:HD12	7:W:446:LEU:HD21	1.99	0.44
7:W:475:ASP:HA	7:W:521:TRP:CZ2	2.53	0.44
7:W:180:LEU:HB3	7:W:185:VAL:HG13	2.00	0.44
3:G:63:LEU:HD13	4:H:42:LEU:HB2	1.99	0.44
6:J:8:DC:H2''	6:J:9:DG:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:417:SER:O	7:W:421:ARG:HG2	2.16	0.44
7:W:479:VAL:O	7:W:486:VAL:HG23	2.18	0.44
5:I:-52:DC:H2''	5:I:-51:DG:C8	2.53	0.44
6:J:-45:DA:H2''	6:J:-44:DA:C8	2.53	0.44
7:W:181:ARG:HH11	7:W:184:GLN:NE2	2.16	0.44
7:W:495:LEU:HA	7:W:498:GLN:HG2	1.99	0.44
7:W:538:ARG:NH2	7:W:562:GLY:HA2	2.32	0.44
7:W:629:SER:HA	7:W:633:GLN:HG2	1.99	0.43
1:A:129:ARG:HD3	1:E:109:LEU:HD11	2.00	0.43
5:I:-70:DG:H4'	5:I:-69:DG:OP1	2.17	0.43
6:J:-48:DC:H2''	6:J:-47:DT:C6	2.53	0.43
7:W:232:HIS:CE1	7:W:303:ARG:HB3	2.53	0.43
7:W:348:TRP:NE1	7:W:361:SER:O	2.51	0.43
4:H:121:ALA:C	4:H:122:LYS:HD3	2.39	0.43
7:W:260:LEU:HD11	7:W:267:ARG:HG2	2.00	0.43
7:W:416:LEU:HB2	7:W:421:ARG:CZ	2.49	0.43
7:W:506:SER:O	7:W:559:THR:N	2.51	0.43
5:I:54:DT:H2''	5:I:55:DC:C6	2.53	0.43
5:I:55:DC:H2''	5:I:56:DG:N7	2.34	0.43
6:J:-26:DT:H2''	6:J:-25:DA:C8	2.53	0.43
2:F:31:LYS:HG3	2:F:51:TYR:CE1	2.53	0.43
5:I:-52:DC:H2''	5:I:-51:DG:H8	1.84	0.43
6:J:49:DC:H2''	6:J:50:DA:H8	1.83	0.43
7:W:172:PRO:HG2	7:W:175:VAL:HG22	2.00	0.43
6:J:7:DC:H2''	6:J:8:DC:C6	2.54	0.43
5:I:-23:DT:H2''	5:I:-22:DG:H8	1.83	0.43
4:D:82:LYS:HD2	4:D:82:LYS:HA	1.72	0.43
5:I:-66:DG:C8	5:I:-65:DT:H72	2.53	0.43
6:J:-62:DC:H6	6:J:-62:DC:H5'	1.84	0.42
6:J:-21:DC:H2'	6:J:-20:DC:C6	2.54	0.42
5:I:72:DA:H2''	5:I:73:DG:H8	1.84	0.42
5:I:4:DG:H4'	5:I:5:DT:OP1	2.19	0.42
5:I:40:DC:H1'	5:I:41:DC:H5'	2.01	0.42
6:J:-12:DC:H2''	6:J:-11:DG:C8	2.55	0.42
7:W:209:LEU:HD12	7:W:209:LEU:HA	1.77	0.42
3:G:15:LYS:HE3	3:G:15:LYS:HB3	1.85	0.42
7:W:479:VAL:HA	7:W:485:MET:CB	2.50	0.42
7:W:517:ASP:HA	7:W:520:MET:HG2	2.00	0.42
5:I:72:DA:H2''	5:I:73:DG:C8	2.55	0.42
7:W:408:LYS:HB2	7:W:408:LYS:HE2	1.78	0.42
7:W:275:LEU:HA	7:W:280:TRP:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:490:LYS:HB3	7:W:490:LYS:HE3	1.83	0.42
6:J:-44:DA:H2'	6:J:-43:DT:H71	2.01	0.42
6:J:66:DC:H2''	6:J:67:DA:C8	2.54	0.42
7:W:475:ASP:C	7:W:477:HIS:H	2.23	0.42
5:I:50:DG:H2''	5:I:51:DG:C8	2.55	0.42
6:J:-58:DG:H2''	6:J:-57:DC:C5	2.55	0.42
6:J:-14:DA:H2''	6:J:-13:DA:C8	2.55	0.42
7:W:277:PRO:HB2	7:W:279:GLU:OE1	2.19	0.42
5:I:-44:DG:H2''	5:I:-43:DA:C8	2.55	0.41
6:J:5:DC:H2''	6:J:6:DC:C6	2.55	0.41
6:J:58:DG:H2''	6:J:59:DA:C8	2.54	0.41
5:I:47:DA:H2''	5:I:48:DG:N7	2.36	0.41
5:I:-27:DC:OP2	5:I:-27:DC:H2'	2.20	0.41
5:I:-7:DG:H2''	5:I:-6:DG:N7	2.35	0.41
7:W:304:TYR:HD1	7:W:304:TYR:HA	1.71	0.41
2:B:35:ARG:O	2:B:39:ARG:HG2	2.21	0.41
7:W:390:PRO:HG2	7:W:391:PHE:CZ	2.55	0.41
7:W:573:VAL:HG13	7:W:603:ARG:NH2	2.34	0.41
7:W:596:ILE:CG2	7:W:597:GLY:N	2.83	0.41
1:A:61:LEU:HD12	2:B:37:LEU:HD23	2.02	0.41
3:C:51:LEU:O	3:C:55:LEU:HG	2.21	0.41
6:J:64:DT:H2'	6:J:65:DA:C8	2.56	0.41
4:H:43:LYS:HD3	4:H:43:LYS:HA	1.67	0.41
5:I:-28:DC:H2''	5:I:-27:DC:C6	2.56	0.41
5:I:11:DC:H2''	5:I:12:DG:C8	2.56	0.41
5:I:42:DA:H2''	5:I:43:DA:C5'	2.51	0.41
6:J:-20:DC:H2''	6:J:-19:DG:H8	1.85	0.41
7:W:288:GLU:CD	7:W:288:GLU:H	2.24	0.41
7:W:334:LEU:HG	7:W:354:LEU:HD21	2.02	0.41
7:W:502:VAL:HA	7:W:573:VAL:HB	2.03	0.41
3:G:16:THR:HG22	3:G:18:SER:H	1.87	0.40
6:J:-30:DG:H1'	6:J:-29:DC:H5'	2.02	0.40
5:I:50:DG:H2''	5:I:51:DG:H8	1.87	0.40
5:I:58:DC:H2''	5:I:59:DA:C8	2.56	0.40
7:W:389:ARG:N	7:W:390:PRO:HD2	2.37	0.40
2:F:31:LYS:HE2	2:F:51:TYR:CZ	2.56	0.40
5:I:-33:DG:H2'	5:I:-32:DT:H71	2.03	0.40
7:W:177:TRP:O	7:W:177:TRP:CG	2.75	0.40
7:W:470:PRO:N	7:W:471:PRO:HD2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	95/136 (70%)	90 (95%)	5 (5%)	0	100	100
1	E	94/136 (69%)	90 (96%)	4 (4%)	0	100	100
2	B	83/103 (81%)	80 (96%)	3 (4%)	0	100	100
2	F	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
3	C	107/130 (82%)	104 (97%)	3 (3%)	0	100	100
3	G	107/130 (82%)	104 (97%)	3 (3%)	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%)	401 (92%)	35 (8%)	2 (0%)	25	56
All	All	1190/2042 (58%)	1131 (95%)	57 (5%)	2 (0%)	45	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	W	455	LYS
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%)	84 (99%)	1 (1%)	67	80
1	E	84/111 (76%)	82 (98%)	2 (2%)	44	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	69/79 (87%)	68 (99%)	1 (1%)	62	78
2	F	66/79 (84%)	66 (100%)	0	100	100
3	C	85/102 (83%)	85 (100%)	0	100	100
3	G	85/102 (83%)	84 (99%)	1 (1%)	67	80
4	D	80/106 (76%)	79 (99%)	1 (1%)	65	79
4	H	82/106 (77%)	80 (98%)	2 (2%)	44	68
7	W	409/939 (44%)	390 (95%)	19 (5%)	23	52
All	All	1045/1735 (60%)	1018 (97%)	27 (3%)	42	66

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
2	B	18	HIS
4	D	56	MET
1	E	64	LYS
1	E	80	THR
3	G	72	ASP
4	H	46	HIS
4	H	110	GLU
7	W	177	TRP
7	W	181	ARG
7	W	182	ASP
7	W	183	TYR
7	W	209	LEU
7	W	254	THR
7	W	256	ARG
7	W	304	TYR
7	W	345	HIS
7	W	391	PHE
7	W	408	LYS
7	W	454	ARG
7	W	463	PHE
7	W	474	THR
7	W	479	VAL
7	W	490	LYS
7	W	538	ARG
7	W	555	PHE
7	W	616	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
7	W	232	HIS
7	W	458	ASN
7	W	477	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	ADP	W	1101	-	24,29,29	0.88	0	29,45,45	1.21	2 (6%)

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	ADP	W	1101	-	-	4/12/32/32	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	W	1101	ADP	N3-C2-N1	-3.71	123.64	128.67
8	W	1101	ADP	C4-C5-N7	-2.28	106.92	109.34

There are no chirality outliers.

All (4) torsion outliers are listed below:

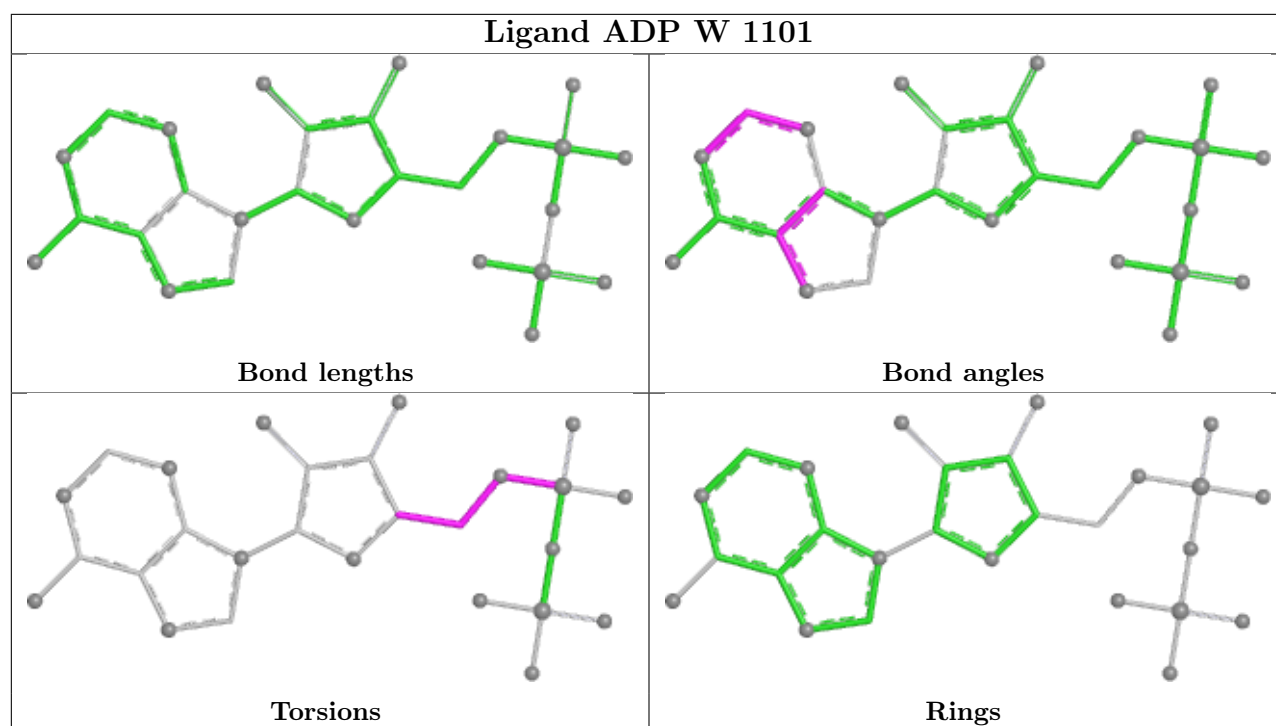
Mol	Chain	Res	Type	Atoms
8	W	1101	ADP	C5'-O5'-PA-O1A
8	W	1101	ADP	O4'-C4'-C5'-O5'
8	W	1101	ADP	C3'-C4'-C5'-O5'
8	W	1101	ADP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	W	1101	ADP	5	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.

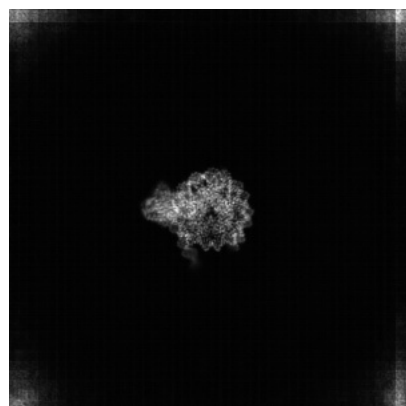
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47415. These allow visual inspection of the internal detail of the map and identification of artifacts.

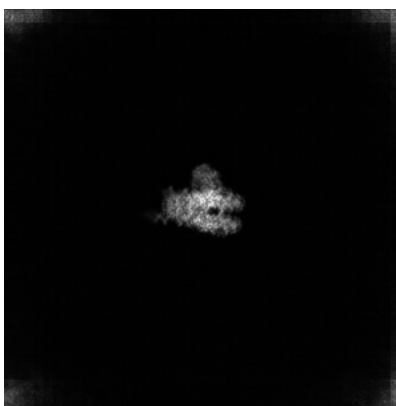
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

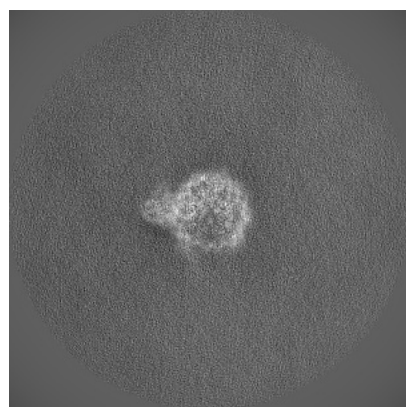


Y

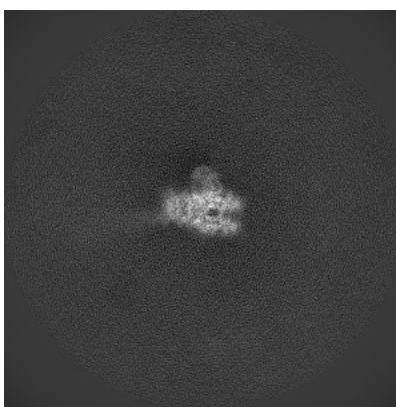


Z

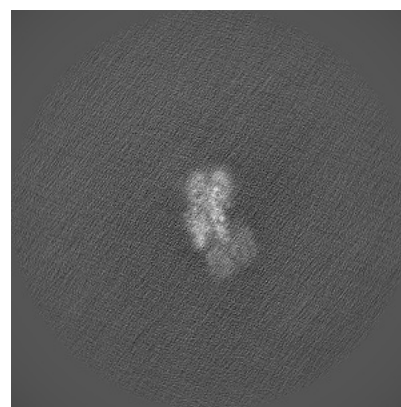
6.1.2 Raw map



X



Y

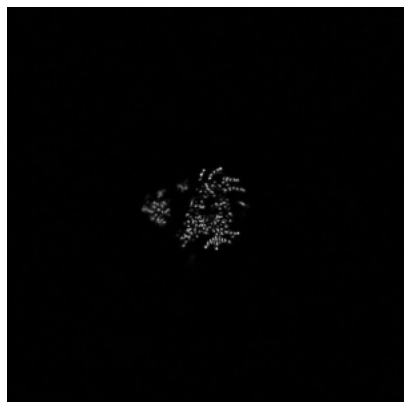


Z

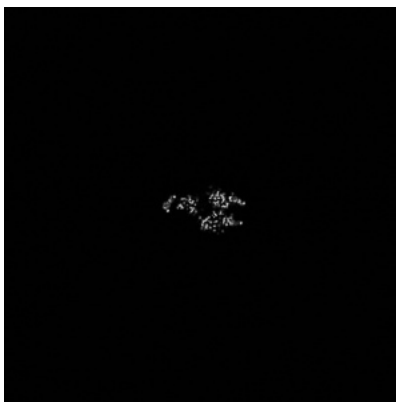
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

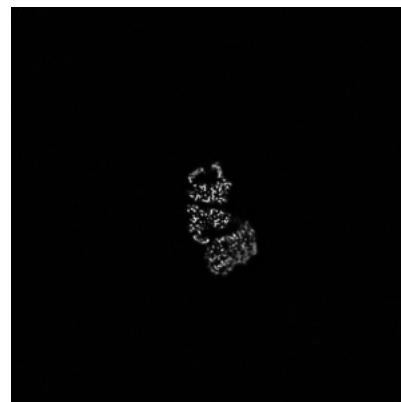
6.2.1 Primary map



X Index: 248

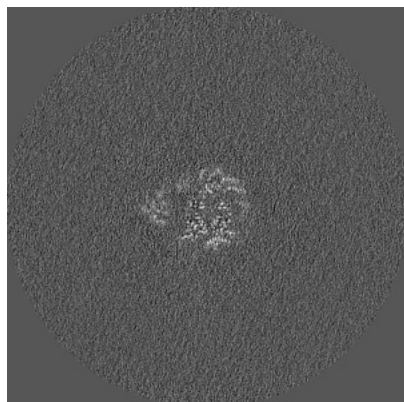


Y Index: 248

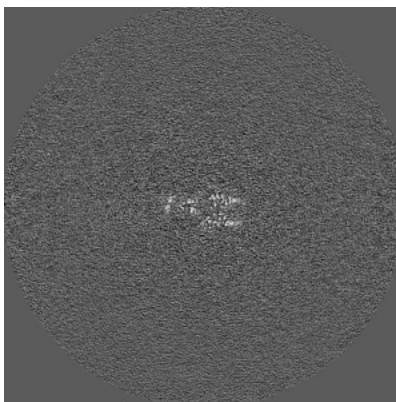


Z Index: 248

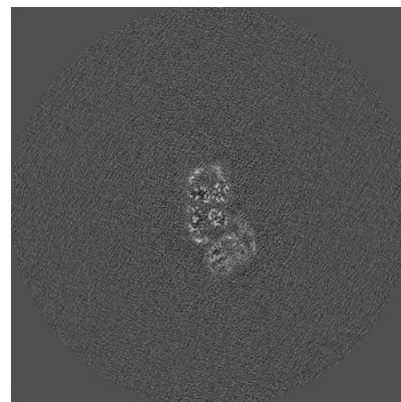
6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

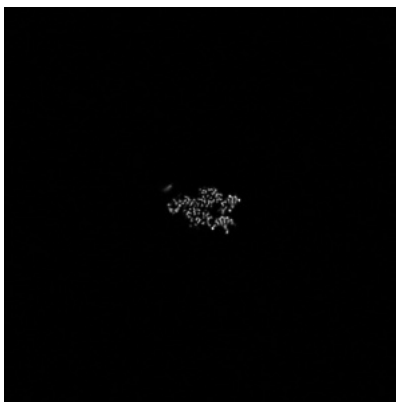
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

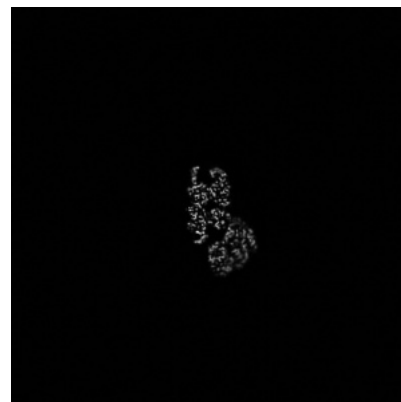
6.3.1 Primary map



X Index: 254

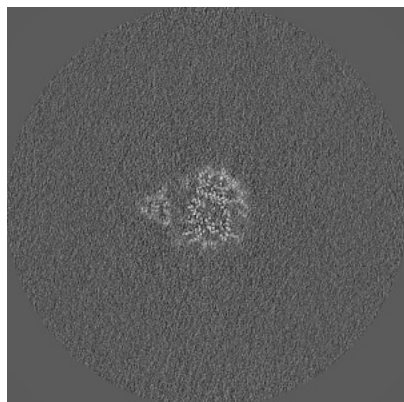


Y Index: 274

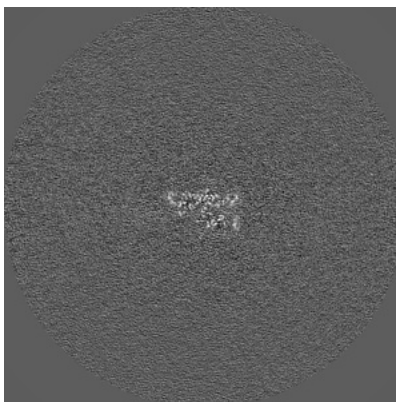


Z Index: 253

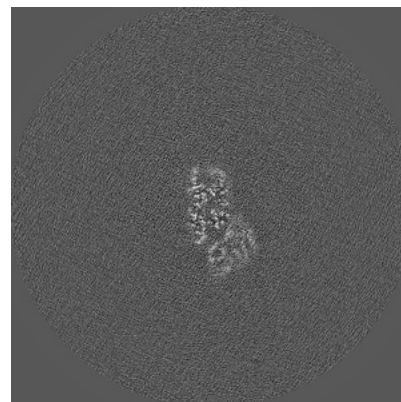
6.3.2 Raw map



X Index: 195



Y Index: 184

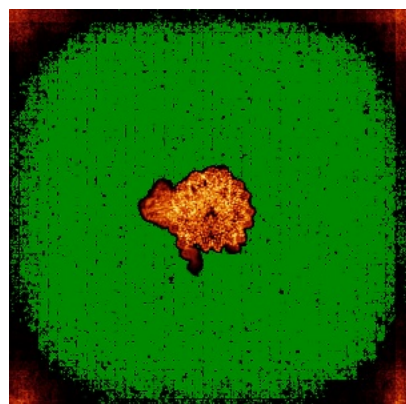


Z Index: 195

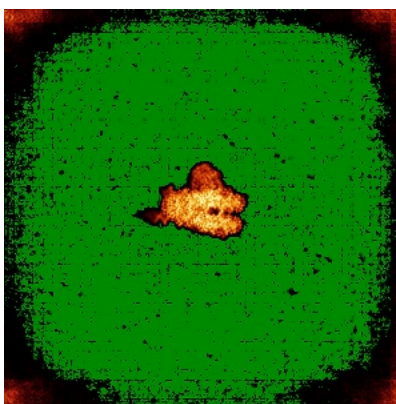
The images above show the largest variance slices of the map in three orthogonal directions.

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

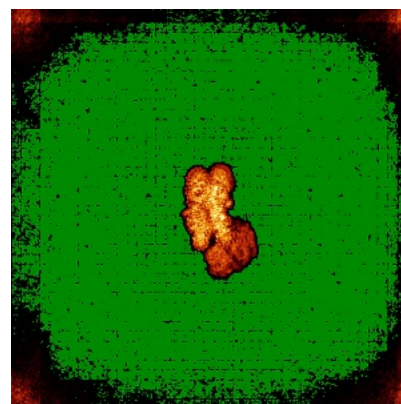
6.4.1 Primary map



X

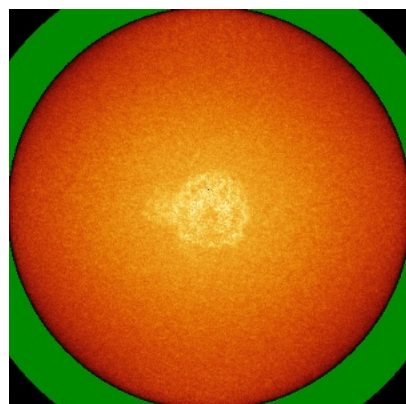


Y

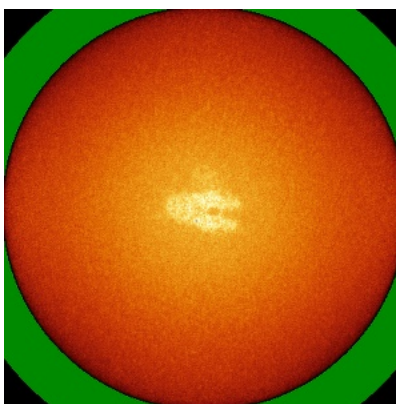


Z

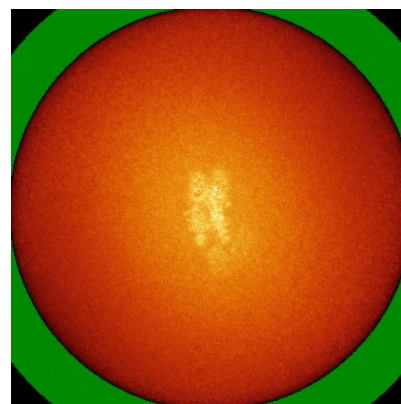
6.4.2 Raw map



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.

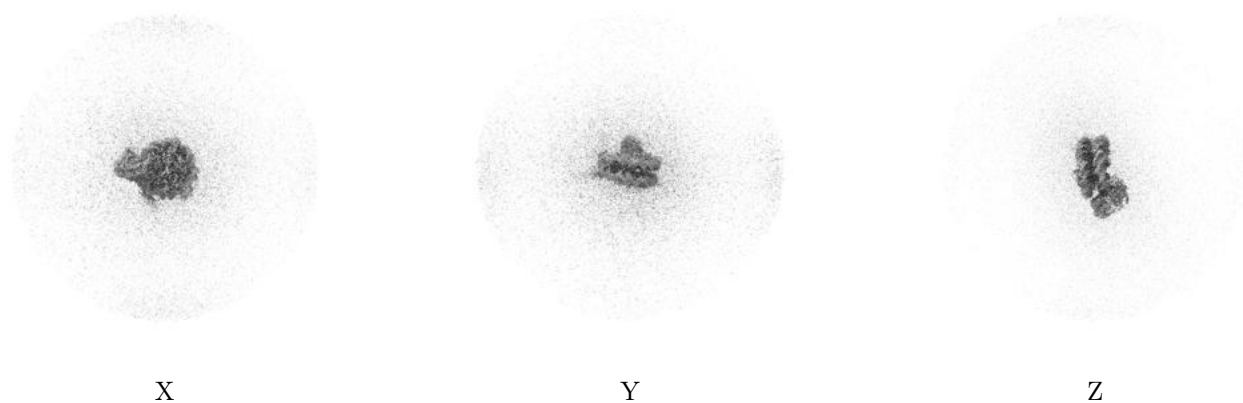
6.5 Orthogonal surface views [i](#)

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.

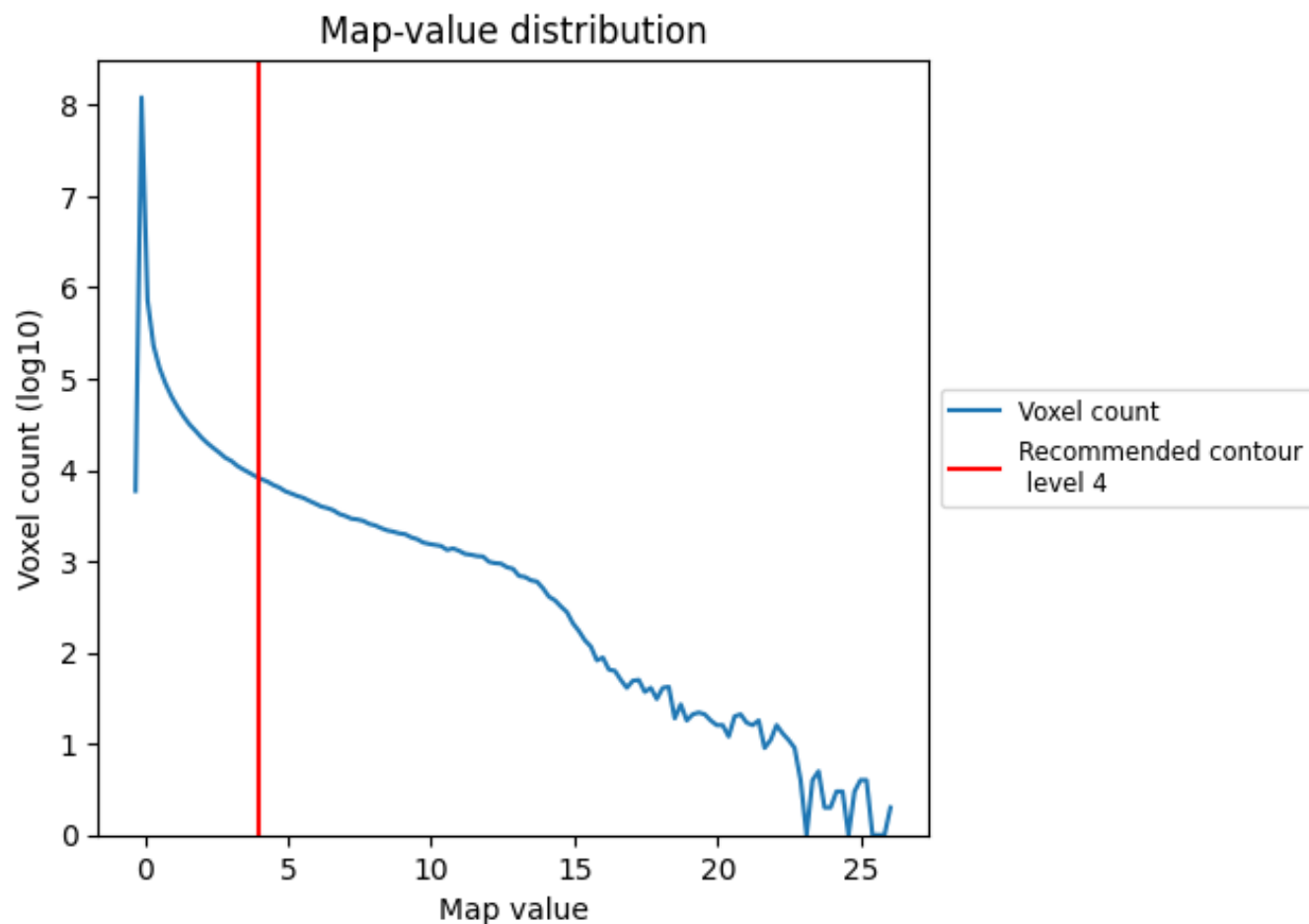
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

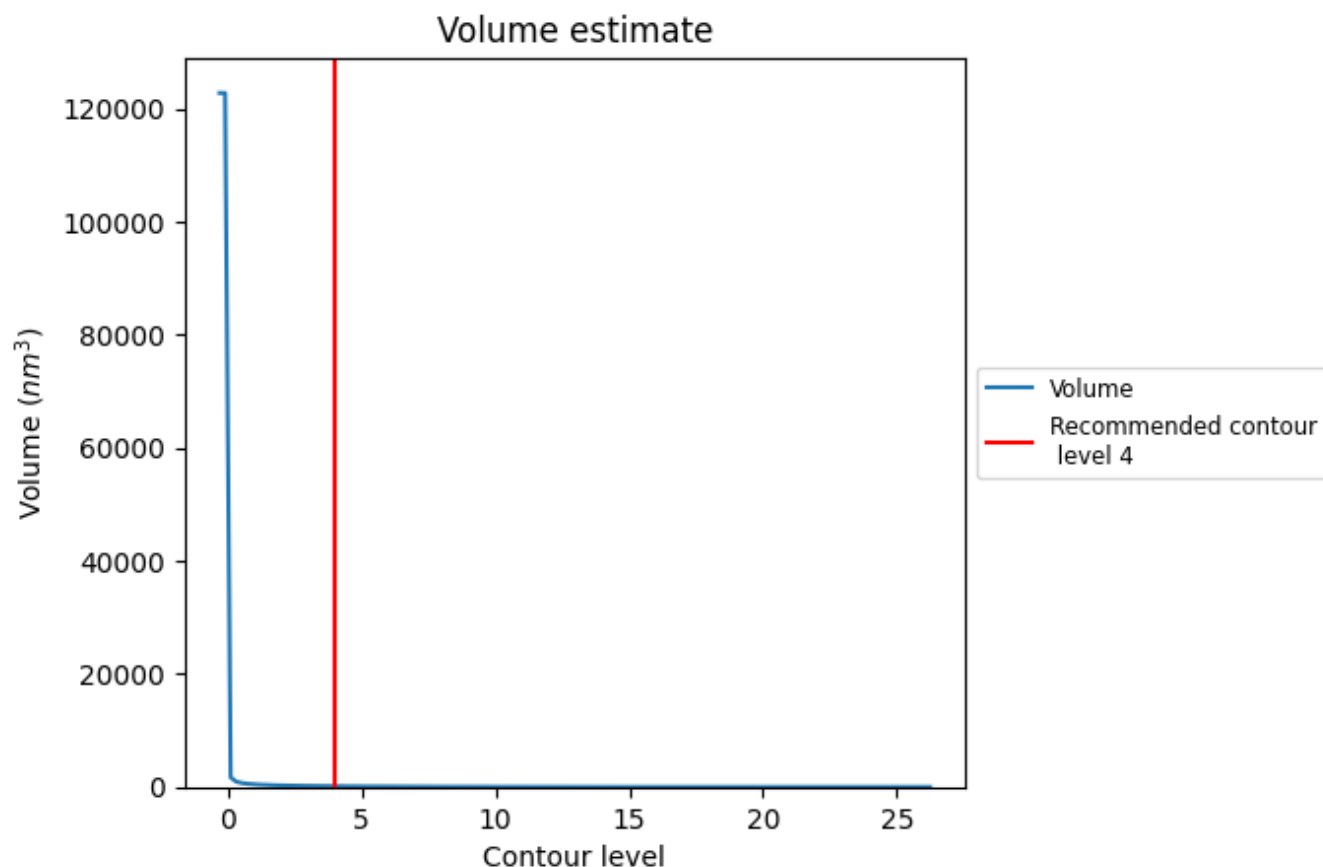
This section contains the results of statistical analysis of the map.

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.

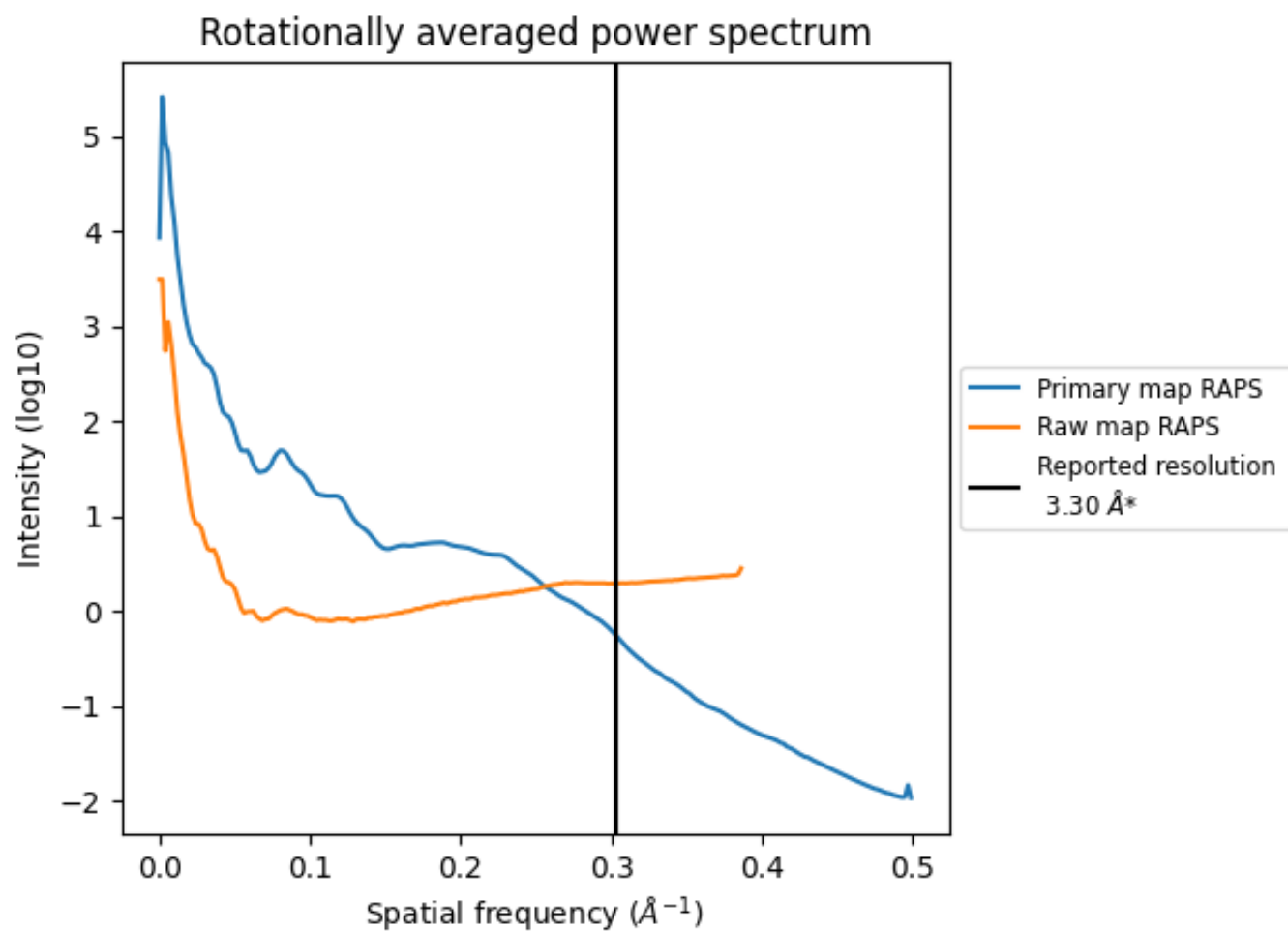
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 133 nm^3 ; this corresponds to an approximate mass of 120 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

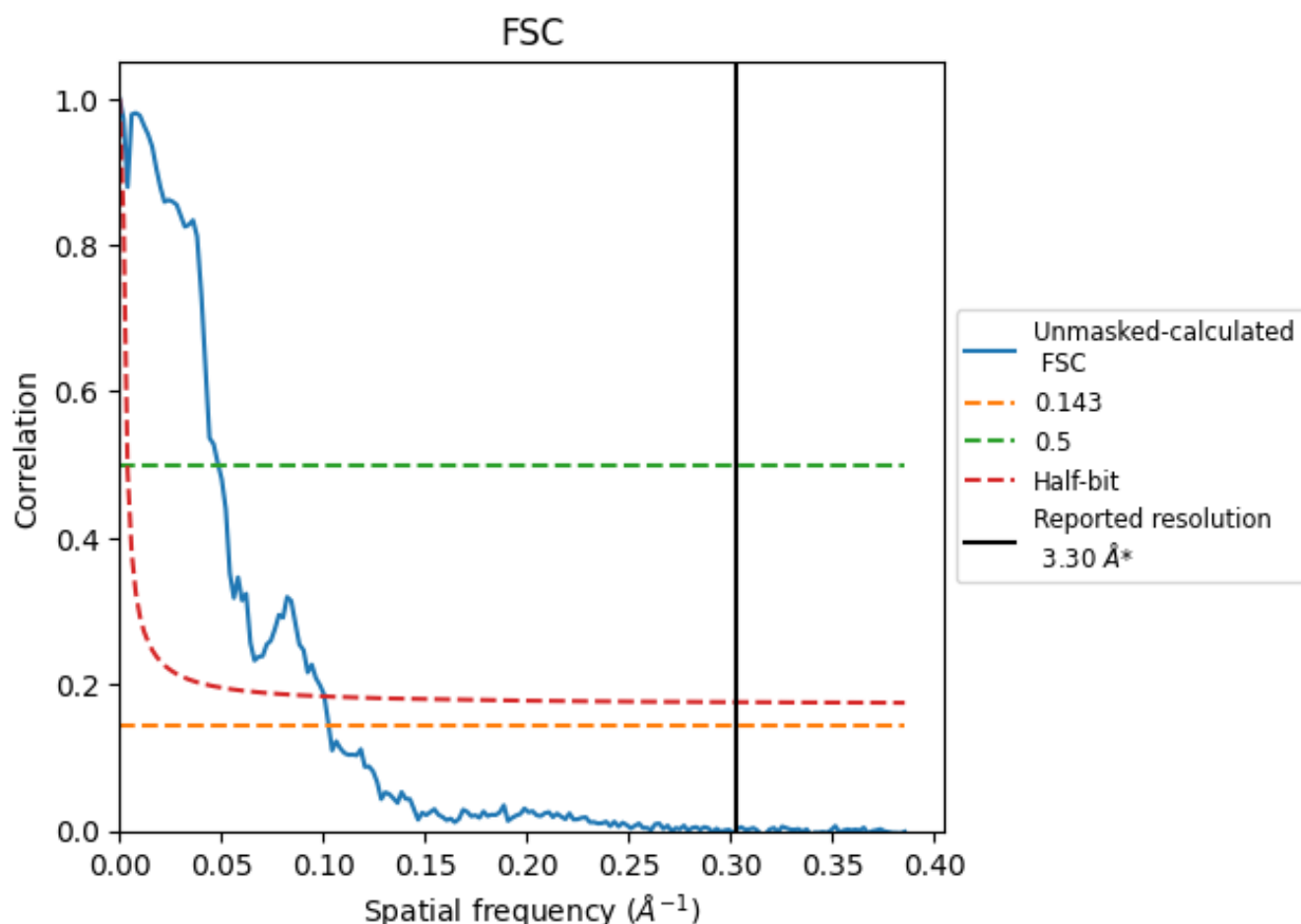


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

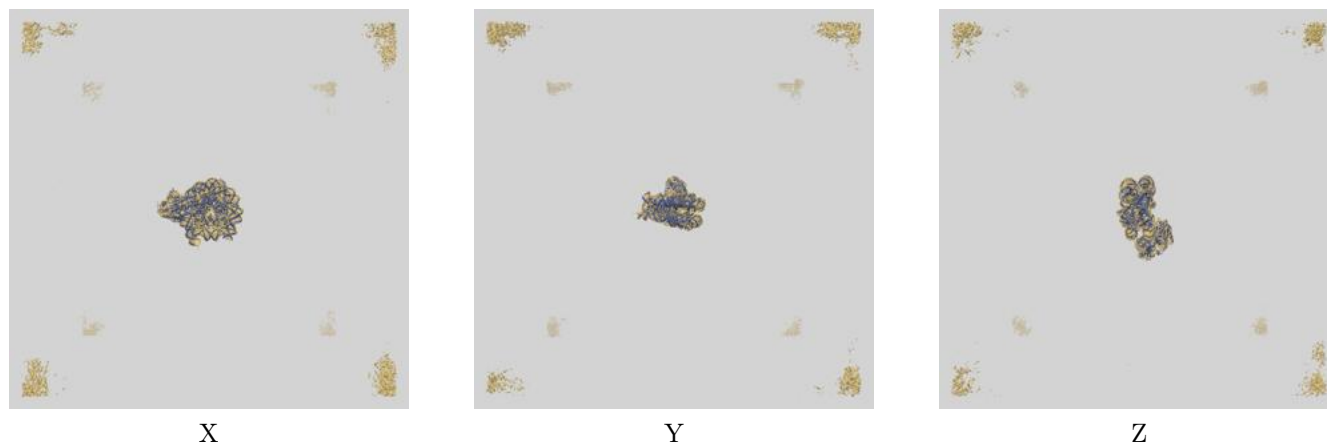
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.74	20.66	9.94

*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 9.74 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

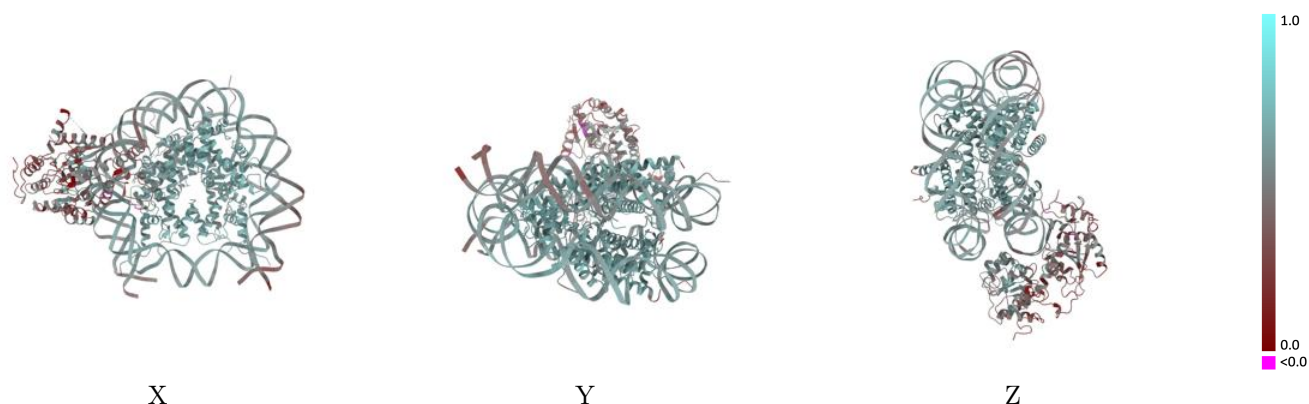
This section contains information regarding the fit between EMDB map EMD-47415 and PDB model 9E1O. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



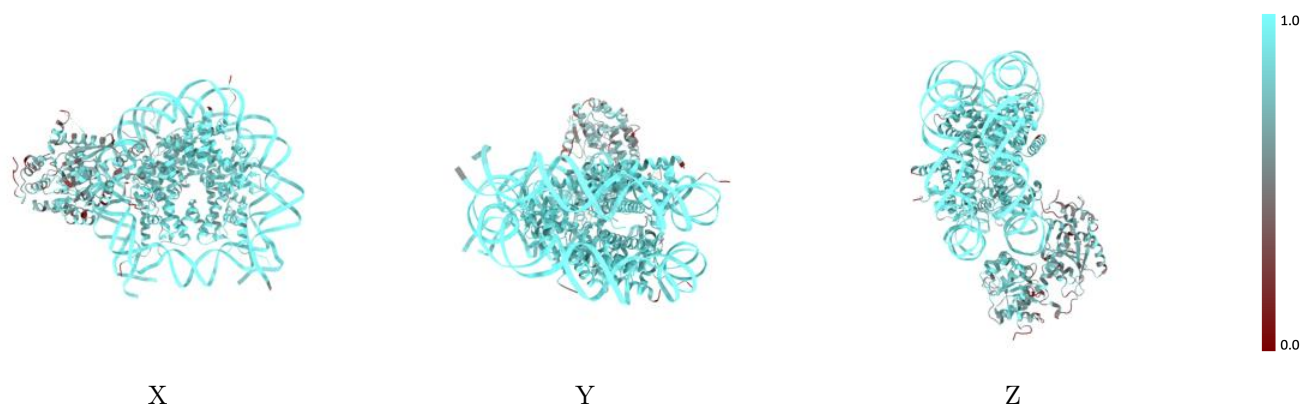
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



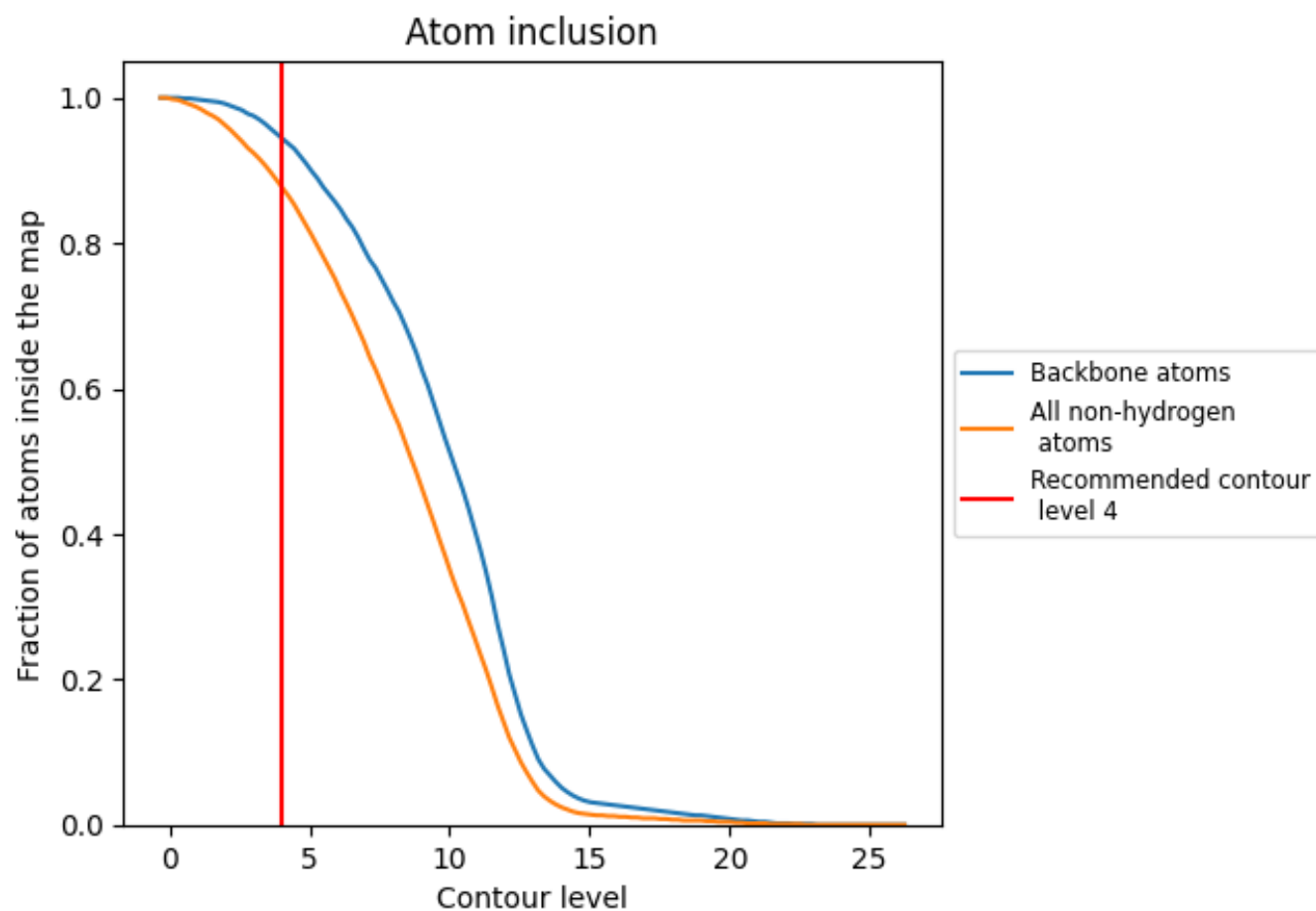
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 94% of all backbone atoms, 88% 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> 0.8780	<div></div> 0.5380
A	<div></div> 0.9260	<div></div> 0.6210
B	<div></div> 0.8920	<div></div> 0.6000
C	<div></div> 0.9350	<div></div> 0.6230
D	<div></div> 0.9340	<div></div> 0.6200
E	<div></div> 0.9490	<div></div> 0.6320
F	<div></div> 0.9460	<div></div> 0.6340
G	<div></div> 0.9180	<div></div> 0.6080
H	<div></div> 0.9120	<div></div> 0.6120
I	<div></div> 0.9560	<div></div> 0.5430
J	<div></div> 0.9530	<div></div> 0.5450
W	<div></div> 0.6670	<div></div> 0.3940

1.0

0.0

<0.0