



Full wwPDB EM Validation Report ⓘ

Dec 4, 2022 – 10:26 PM JST

PDB ID : 7X74
EMDB ID : EMD-33031
Title : Cryo-EM structure of Streptomyces coelicolor transcription initial complex with two Zur dimers.
Authors : Yang, X.; Zheng, J.
Deposited on : 2022-03-09
Resolution : 3.70 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

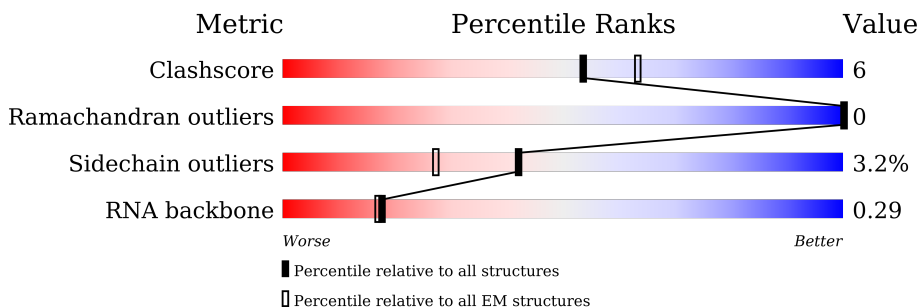
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.



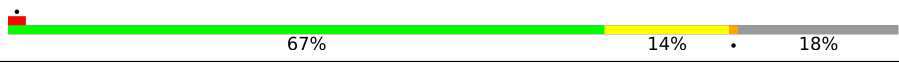


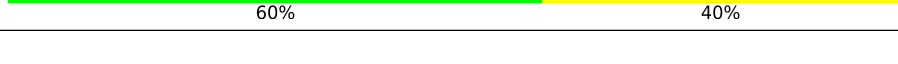
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	340	54% 12% 34%
1	B	340	56% 12% 31%
2	C	1161	80% 16% .
3	D	1307	82% 14% .
4	E	90	. 71% 14% 14%
5	F	531	48% 8% 44%
6	G	159	. 77% 5% . 18%

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Mol	Chain	Length	Quality of chain
6	H	159	 11% 69% 12% 18%
6	M	159	 5% 67% 14% 18%
6	N	159	 5% 69% 14% 18%
7	O	84	 5% 79% 21%
8	P	84	 5% 85% 15%
9	Q	5	 60% 40%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 32550 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	226	Total	C	N	O	S	0	0
			1742	1102	302	334	4		
1	B	233	Total	C	N	O	S	0	0
			1792	1131	309	347	5		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	1116	Total	C	N	O	S	0	0
			8692	5450	1513	1698	31		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	1259	Total	C	N	O	S	0	0
			9846	6161	1787	1857	41		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1300	HIS	-	expression tag	UNP Q8CJT1
D	1301	HIS	-	expression tag	UNP Q8CJT1
D	1302	HIS	-	expression tag	UNP Q8CJT1
D	1303	HIS	-	expression tag	UNP Q8CJT1
D	1304	HIS	-	expression tag	UNP Q8CJT1
D	1305	HIS	-	expression tag	UNP Q8CJT1
D	1306	HIS	-	expression tag	UNP Q8CJT1
D	1307	HIS	-	expression tag	UNP Q8CJT1

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	77	597	382	98	117	0	0

- Molecule 5 is a protein called RNA polymerase principal sigma factor HrdB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	298	2379	1499	423	450	7	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	UNP P18183
F	-18	GLY	-	expression tag	UNP P18183
F	-17	SER	-	expression tag	UNP P18183
F	-16	SER	-	expression tag	UNP P18183
F	-15	HIS	-	expression tag	UNP P18183
F	-14	HIS	-	expression tag	UNP P18183
F	-13	HIS	-	expression tag	UNP P18183
F	-12	HIS	-	expression tag	UNP P18183
F	-11	HIS	-	expression tag	UNP P18183
F	-10	HIS	-	expression tag	UNP P18183
F	-9	SER	-	expression tag	UNP P18183
F	-8	SER	-	expression tag	UNP P18183
F	-7	GLY	-	expression tag	UNP P18183
F	-6	LEU	-	expression tag	UNP P18183
F	-5	VAL	-	expression tag	UNP P18183
F	-4	PRO	-	expression tag	UNP P18183
F	-3	ARG	-	expression tag	UNP P18183
F	-2	GLY	-	expression tag	UNP P18183
F	-1	SER	-	expression tag	UNP P18183
F	0	HIS	-	expression tag	UNP P18183

- Molecule 6 is a protein called Putative metal uptake regulation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	131	984	603	185	190	6	0	0
6	H	131	984	603	185	190	6	0	0
6	M	131	984	603	185	190	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	N	131	984	603	185	190	6	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-19	MET	-	initiating methionine	UNP Q9L2H5
G	-18	GLY	-	expression tag	UNP Q9L2H5
G	-17	SER	-	expression tag	UNP Q9L2H5
G	-16	SER	-	expression tag	UNP Q9L2H5
G	-15	HIS	-	expression tag	UNP Q9L2H5
G	-14	HIS	-	expression tag	UNP Q9L2H5
G	-13	HIS	-	expression tag	UNP Q9L2H5
G	-12	HIS	-	expression tag	UNP Q9L2H5
G	-11	HIS	-	expression tag	UNP Q9L2H5
G	-10	HIS	-	expression tag	UNP Q9L2H5
G	-9	SER	-	expression tag	UNP Q9L2H5
G	-8	SER	-	expression tag	UNP Q9L2H5
G	-7	GLY	-	expression tag	UNP Q9L2H5
G	-6	LEU	-	expression tag	UNP Q9L2H5
G	-5	VAL	-	expression tag	UNP Q9L2H5
G	-4	PRO	-	expression tag	UNP Q9L2H5
G	-3	ARG	-	expression tag	UNP Q9L2H5
G	-2	GLY	-	expression tag	UNP Q9L2H5
G	-1	SER	-	expression tag	UNP Q9L2H5
G	0	HIS	-	expression tag	UNP Q9L2H5
H	-19	MET	-	initiating methionine	UNP Q9L2H5
H	-18	GLY	-	expression tag	UNP Q9L2H5
H	-17	SER	-	expression tag	UNP Q9L2H5
H	-16	SER	-	expression tag	UNP Q9L2H5
H	-15	HIS	-	expression tag	UNP Q9L2H5
H	-14	HIS	-	expression tag	UNP Q9L2H5
H	-13	HIS	-	expression tag	UNP Q9L2H5
H	-12	HIS	-	expression tag	UNP Q9L2H5
H	-11	HIS	-	expression tag	UNP Q9L2H5
H	-10	HIS	-	expression tag	UNP Q9L2H5
H	-9	SER	-	expression tag	UNP Q9L2H5
H	-8	SER	-	expression tag	UNP Q9L2H5
H	-7	GLY	-	expression tag	UNP Q9L2H5
H	-6	LEU	-	expression tag	UNP Q9L2H5
H	-5	VAL	-	expression tag	UNP Q9L2H5
H	-4	PRO	-	expression tag	UNP Q9L2H5

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-3	ARG	-	expression tag	UNP Q9L2H5
H	-2	GLY	-	expression tag	UNP Q9L2H5
H	-1	SER	-	expression tag	UNP Q9L2H5
H	0	HIS	-	expression tag	UNP Q9L2H5
M	-19	MET	-	initiating methionine	UNP Q9L2H5
M	-18	GLY	-	expression tag	UNP Q9L2H5
M	-17	SER	-	expression tag	UNP Q9L2H5
M	-16	SER	-	expression tag	UNP Q9L2H5
M	-15	HIS	-	expression tag	UNP Q9L2H5
M	-14	HIS	-	expression tag	UNP Q9L2H5
M	-13	HIS	-	expression tag	UNP Q9L2H5
M	-12	HIS	-	expression tag	UNP Q9L2H5
M	-11	HIS	-	expression tag	UNP Q9L2H5
M	-10	HIS	-	expression tag	UNP Q9L2H5
M	-9	SER	-	expression tag	UNP Q9L2H5
M	-8	SER	-	expression tag	UNP Q9L2H5
M	-7	GLY	-	expression tag	UNP Q9L2H5
M	-6	LEU	-	expression tag	UNP Q9L2H5
M	-5	VAL	-	expression tag	UNP Q9L2H5
M	-4	PRO	-	expression tag	UNP Q9L2H5
M	-3	ARG	-	expression tag	UNP Q9L2H5
M	-2	GLY	-	expression tag	UNP Q9L2H5
M	-1	SER	-	expression tag	UNP Q9L2H5
M	0	HIS	-	expression tag	UNP Q9L2H5
N	-19	MET	-	initiating methionine	UNP Q9L2H5
N	-18	GLY	-	expression tag	UNP Q9L2H5
N	-17	SER	-	expression tag	UNP Q9L2H5
N	-16	SER	-	expression tag	UNP Q9L2H5
N	-15	HIS	-	expression tag	UNP Q9L2H5
N	-14	HIS	-	expression tag	UNP Q9L2H5
N	-13	HIS	-	expression tag	UNP Q9L2H5
N	-12	HIS	-	expression tag	UNP Q9L2H5
N	-11	HIS	-	expression tag	UNP Q9L2H5
N	-10	HIS	-	expression tag	UNP Q9L2H5
N	-9	SER	-	expression tag	UNP Q9L2H5
N	-8	SER	-	expression tag	UNP Q9L2H5
N	-7	GLY	-	expression tag	UNP Q9L2H5
N	-6	LEU	-	expression tag	UNP Q9L2H5
N	-5	VAL	-	expression tag	UNP Q9L2H5
N	-4	PRO	-	expression tag	UNP Q9L2H5
N	-3	ARG	-	expression tag	UNP Q9L2H5
N	-2	GLY	-	expression tag	UNP Q9L2H5

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-1	SER	-	expression tag	UNP Q9L2H5
N	0	HIS	-	expression tag	UNP Q9L2H5

- Molecule 7 is a DNA chain called DNA (84-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	O	84	1714	810	315	505	84	0	0

- Molecule 8 is a DNA chain called DNA (84-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	P	84	1729	815	325	505	84	0	0

- Molecule 9 is a RNA chain called RNA.

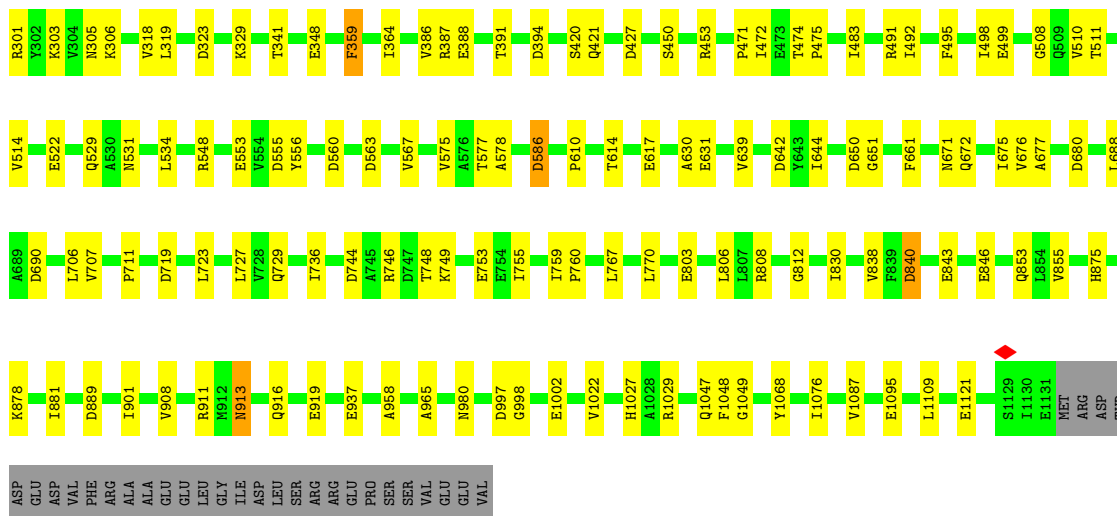
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	Q	5	108	49	22	33	4	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

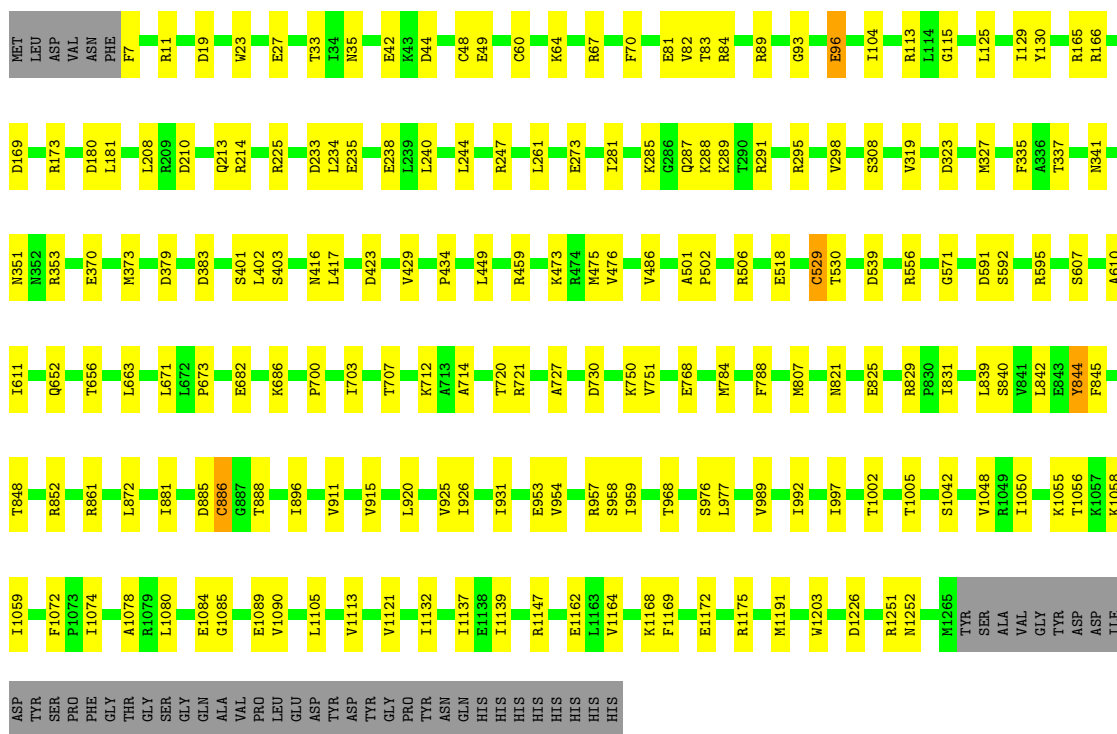
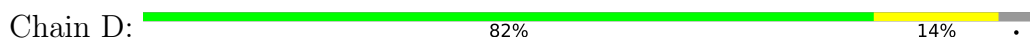
Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	D	2	Total	Zn	0
			2	2	
11	G	3	Total	Zn	0
			3	3	
11	H	3	Total	Zn	0
			3	3	
11	M	3	Total	Zn	0
			3	3	
11	N	3	Total	Zn	0
			3	3	



● Molecule 3: DNA-directed RNA polymerase subunit beta'



● Molecule 4: DNA-directed RNA polymerase subunit omega




● Molecule 5: RNA polymerase principal sigma factor HrdB

Chain N:  69% 14% 18%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER SER GLY LEU VAL PRO ARG GLY SER HIS MET THR ALA GLY P6 Q15 R16 E27 E28 F29 R30 H36 R53 T54 L55 L67 R68 G72 Y76 R77 R78 C79 S80 T81 D82 D83 H84 H85 E98 I126


T129 C130 A131 D132 C133 A134 G135 A136 SER GLY GLY

- Molecule 7: DNA (84-MER)

Chain O:  5% 79% 21%

C1 A2 A3 G4 G11 T19 G20 T21 G25 C29 G30 C31 G32 T33 T34 C37 C47 T48 G53 T54 G71 G72 G79 C84

- Molecule 8: DNA (84-MER)

Chain P:  5% 85% 15%

G1 C7 A19 C20 G21 G22 T27 G49 G53 G54 A59 C60 T61 G62 A63 A64 C81 T82 T83 C84

- Molecule 9: RNA

Chain Q:  60% 40%

G1 U2 A3 G4 G5

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71710	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	3.316	Depositor
Minimum map value	-1.958	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.06	Depositor
Map size (\AA)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	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: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/1768	0.62	0/2400
1	B	0.28	0/1818	0.59	0/2467
2	C	0.28	0/8848	0.57	0/11982
3	D	0.28	0/9998	0.60	0/13490
4	E	0.32	0/607	0.59	0/826
5	F	0.28	0/2414	0.60	0/3253
6	G	0.25	0/1001	0.54	0/1355
6	H	0.26	0/1001	0.55	0/1355
6	M	0.25	0/1001	0.54	0/1355
6	N	0.23	0/1001	0.52	0/1355
7	O	0.68	0/1920	0.92	0/2959
8	P	0.67	0/1940	0.90	0/2994
9	Q	0.20	0/121	0.61	0/188
All	All	0.35	0/33438	0.64	0/45979

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	1742	0	1796	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1792	0	1841	30	0
2	C	8692	0	8632	112	0
3	D	9846	0	10017	109	0
4	E	597	0	604	9	0
5	F	2379	0	2436	29	0
6	G	984	0	947	7	0
6	H	984	0	947	13	0
6	M	984	0	947	15	0
6	N	984	0	947	13	0
7	O	1714	0	940	16	0
8	P	1729	0	940	10	0
9	Q	108	0	55	3	0
10	D	1	0	0	0	0
11	D	2	0	0	0	0
11	G	3	0	0	0	0
11	H	3	0	0	0	0
11	M	3	0	0	0	0
11	N	3	0	0	0	0
All	All	32550	0	31049	351	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 6.

All (351) 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)
2:C:453:ARG:HA	7:O:71:DG:H1'	1.57	0.85
3:D:1058:LYS:NZ	3:D:1059:ILE:O	2.17	0.78
6:G:104:VAL:HG12	6:H:104:VAL:HG12	1.68	0.75
3:D:291:ARG:NH2	7:O:79:DG:OP2	2.21	0.74
2:C:1027:HIS:NE2	2:C:1049:GLY:O	2.21	0.74
1:B:16:GLU:O	1:B:203:ARG:NH1	2.21	0.73
3:D:281:ILE:O	3:D:289:LYS:NZ	2.21	0.73
2:C:421:GLN:N	2:C:421:GLN:OE1	2.22	0.72
3:D:591:ASP:OD1	3:D:592:SER:N	2.22	0.72
6:N:78:ARG:NH1	6:N:79:CYS:O	2.23	0.72
2:C:522:GLU:OE2	2:C:548:ARG:NH2	2.23	0.71
2:C:677:ALA:N	2:C:680:ASP:OD2	2.24	0.71
6:H:16:ARG:HH12	8:P:53:DC:H3'	1.56	0.71
2:C:173:VAL:O	2:C:303:LYS:NZ	2.24	0.70
3:D:1048:VAL:O	3:D:1085:GLY:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:723:LEU:HD13	2:C:727:LEU:HD12	1.74	0.69
2:C:846:GLU:N	2:C:846:GLU:OE2	2.26	0.69
6:M:36:HIS:NE2	6:M:46:VAL:O	2.25	0.69
2:C:107:ILE:HD11	2:C:155:VAL:HG21	1.75	0.68
3:D:19:ASP:OD1	3:D:23:TRP:NE1	2.27	0.68
1:B:224:GLU:N	1:B:224:GLU:OE1	2.26	0.68
3:D:33:THR:HG21	3:D:327:MET:CE	2.24	0.68
3:D:888:THR:O	3:D:957:ARG:NH2	2.27	0.68
2:C:301:ARG:NH1	2:C:323:ASP:OD2	2.27	0.67
3:D:607:SER:O	3:D:611:ILE:HD12	1.95	0.67
3:D:247:ARG:NE	3:D:247:ARG:O	2.26	0.67
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.77	0.66
1:B:81:LYS:NZ	1:B:165:ASP:OD2	2.26	0.66
6:M:50:THR:O	6:M:54:THR:HG23	1.96	0.66
2:C:1068:TYR:OH	3:D:1251:ARG:NE	2.29	0.66
2:C:753:GLU:OE1	2:C:753:GLU:N	2.29	0.66
2:C:491:ARG:NH2	2:C:499:GLU:OE1	2.29	0.65
3:D:165:ARG:NH1	3:D:169:ASP:OD2	2.29	0.65
2:C:744:ASP:OD2	2:C:746:ARG:NH2	2.30	0.64
2:C:41:GLN:NE2	2:C:163:VAL:O	2.30	0.64
2:C:1076:ILE:HG23	2:C:1087:VAL:HG21	1.80	0.64
6:N:28:GLU:OE1	6:N:30:ARG:NH2	2.31	0.64
2:C:86:ASP:OD1	2:C:89:GLY:N	2.31	0.64
6:N:15:GLN:NE2	7:O:11:DG:OP2	2.31	0.64
6:M:77:ARG:HD3	6:M:79:CYS:SG	2.38	0.64
3:D:35:ASN:N	3:D:42:GLU:OE2	2.32	0.63
8:P:19:DA:C2	9:Q:3:A:C2	2.87	0.63
2:C:617:GLU:OE1	2:C:617:GLU:N	2.31	0.63
3:D:953:GLU:OE1	3:D:953:GLU:N	2.31	0.63
6:N:77:ARG:NH1	6:N:79:CYS:SG	2.71	0.63
3:D:959:ILE:HD13	3:D:1139:ILE:HD12	1.81	0.63
2:C:1029:ARG:NH1	2:C:1048:PHE:O	2.31	0.63
2:C:85:GLU:O	2:C:387:ARG:NH1	2.31	0.62
2:C:937:GLU:OE2	2:C:937:GLU:N	2.32	0.62
3:D:287:GLN:N	3:D:287:GLN:OE1	2.32	0.62
2:C:138:GLN:NE2	2:C:139:THR:O	2.32	0.62
2:C:30:GLU:N	2:C:30:GLU:OE1	2.31	0.62
5:F:410:LEU:HD13	5:F:418:PHE:HA	1.81	0.62
2:C:205:ASP:N	2:C:209:MET:O	2.33	0.61
2:C:475:PRO:HG2	2:C:483:ILE:HD13	1.82	0.61
2:C:1095:GLU:OE2	2:C:1095:GLU:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:727:ALA:N	3:D:730:ASP:OD2	2.33	0.61
6:N:27:GLU:OE1	6:N:77:ARG:NH2	2.34	0.61
1:B:46:ILE:HG23	1:B:170:PRO:HD2	1.83	0.61
2:C:280:ALA:O	2:C:284:LEU:HD22	2.01	0.61
3:D:33:THR:HG21	3:D:327:MET:HE3	1.83	0.61
3:D:682:GLU:N	3:D:682:GLU:OE1	2.34	0.61
6:N:55:LEU:HD21	6:N:76:TYR:CD1	2.36	0.60
3:D:337:THR:OG1	3:D:341:ASN:ND2	2.34	0.60
6:G:68:ARG:NH1	6:H:69:THR:O	2.34	0.60
2:C:997:ASP:OD1	2:C:998:GLY:N	2.34	0.60
2:C:202:MET:HG2	2:C:212:VAL:HG22	1.84	0.60
2:C:341:THR:N	2:C:348:GLU:OE2	2.35	0.60
1:B:41:THR:HG21	1:B:215:LEU:HD11	1.85	0.59
2:C:878:LYS:HE3	9:Q:5:G:OP1	2.02	0.59
4:E:32:TYR:CE2	4:E:75:ILE:HD12	2.37	0.59
3:D:115:GLY:CA	3:D:298:VAL:HG21	2.33	0.58
1:A:131:LYS:O	1:A:131:LYS:NZ	2.22	0.58
8:P:60:DC:H2''	8:P:61:DT:H5'	1.84	0.58
1:A:146:TYR:HB2	1:A:167:ILE:HG22	1.85	0.58
2:C:719:ASP:OD2	2:C:911:ARG:NH2	2.37	0.58
3:D:273:GLU:OE1	3:D:295:ARG:NH2	2.37	0.58
2:C:305:ASN:OD1	2:C:306:LYS:N	2.37	0.57
1:A:81:LYS:NZ	2:C:729:GLN:O	2.37	0.57
3:D:959:ILE:HD11	3:D:968:THR:HG21	1.87	0.57
3:D:1162:GLU:N	3:D:1162:GLU:OE1	2.38	0.57
5:F:360:ASN:OD1	5:F:361:LYS:N	2.38	0.56
3:D:844:TYR:O	3:D:848:THR:HG23	2.05	0.56
2:C:803:GLU:OE2	2:C:803:GLU:N	2.38	0.56
3:D:473:LYS:NZ	5:F:431:ALA:HB1	2.19	0.56
2:C:1029:ARG:NE	3:D:423:ASP:OD1	2.39	0.56
3:D:896:ILE:HD12	3:D:954:VAL:HG11	1.86	0.56
5:F:421:LEU:HD23	5:F:421:LEU:O	2.05	0.56
3:D:1089:GLU:N	3:D:1089:GLU:OE1	2.38	0.56
2:C:767:LEU:HA	2:C:770:LEU:HD23	1.86	0.55
5:F:278:LEU:HD12	5:F:315:VAL:HG21	1.88	0.55
1:A:21:PHE:HE2	1:B:225:LEU:HD11	1.70	0.55
5:F:447:LEU:CD2	5:F:455:ALA:HB1	2.36	0.55
7:O:29:DC:H2''	7:O:30:DG:OP2	2.07	0.55
2:C:808:ARG:O	2:C:812:GLY:N	2.39	0.54
1:A:97:LEU:HD13	1:A:110:ILE:HG13	1.88	0.54
1:A:135:GLU:OE2	1:A:136:MET:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:359:PHE:HE1	2:C:498:ILE:HD13	1.71	0.54
3:D:238:GLU:OE1	3:D:238:GLU:N	2.38	0.54
3:D:1074:ILE:HD11	3:D:1078:ALA:HB1	1.90	0.54
1:A:218:LEU:HD23	1:B:34:LEU:HD21	1.89	0.54
3:D:845:PHE:O	3:D:848:THR:OG1	2.21	0.54
3:D:896:ILE:HD12	3:D:954:VAL:CG1	2.37	0.54
1:A:40:ARG:NH1	2:C:889:ASP:OD1	2.37	0.54
3:D:449:LEU:HD11	3:D:476:VAL:HG23	1.89	0.54
2:C:245:SER:O	2:C:249:THR:HG23	2.08	0.54
2:C:1076:ILE:CG2	2:C:1087:VAL:HG21	2.37	0.53
6:M:14:ARG:NH1	7:O:29:DC:OP1	2.41	0.53
1:A:153:LYS:HB3	1:A:163:PRO:HG3	1.90	0.53
2:C:706:LEU:HD23	2:C:707:VAL:N	2.22	0.53
3:D:173:ARG:NE	3:D:208:LEU:HD23	2.23	0.53
1:A:71:GLU:N	1:A:71:GLU:OE1	2.42	0.53
7:O:25:DG:O6	8:P:59:DA:N6	2.41	0.53
5:F:300:PHE:CE2	5:F:304:ILE:HD11	2.44	0.53
2:C:264:ASP:OD1	2:C:267:ARG:NH2	2.41	0.53
2:C:840:ASP:OD1	2:C:843:GLU:N	2.40	0.53
4:E:9:GLU:N	4:E:9:GLU:OE1	2.42	0.53
4:E:32:TYR:CZ	4:E:75:ILE:HD12	2.43	0.52
6:N:81:THR:OG1	6:N:98:GLU:OE1	2.27	0.52
1:A:174:VAL:HG22	1:A:196:VAL:HG23	1.91	0.52
3:D:501:ALA:HB3	3:D:502:PRO:HD3	1.91	0.52
2:C:244:GLU:N	2:C:244:GLU:OE1	2.42	0.52
2:C:875:HIS:NE2	2:C:919:GLU:OE1	2.41	0.52
2:C:878:LYS:CE	9:Q:5:G:OP1	2.56	0.52
5:F:454:GLU:O	5:F:458:VAL:HG23	2.10	0.52
2:C:285:GLU:O	2:C:290:ASN:N	2.42	0.52
1:A:134:LEU:HD12	1:A:135:GLU:N	2.25	0.52
3:D:373:MET:HE2	5:F:301:LEU:HD11	1.91	0.52
3:D:401:SER:OG	3:D:402:LEU:N	2.42	0.52
5:F:362:LEU:HD23	5:F:386:LEU:HG	1.92	0.52
3:D:821:ASN:N	3:D:825:GLU:O	2.43	0.52
2:C:1109:LEU:HD13	3:D:417:LEU:HD11	1.93	0.51
5:F:489:ILE:O	5:F:493:THR:HG23	2.10	0.51
2:C:650:ASP:OD1	2:C:651:GLY:N	2.44	0.51
2:C:508:GLY:N	2:C:560:ASP:OD1	2.44	0.51
3:D:115:GLY:HA2	3:D:298:VAL:HG21	1.90	0.51
3:D:518:GLU:OE1	3:D:518:GLU:N	2.43	0.51
1:A:7:PRO:HG3	1:B:218:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLU:OE2	1:B:6:ARG:NH2	2.44	0.51
2:C:359:PHE:CE1	2:C:498:ILE:HD13	2.45	0.51
3:D:81:GLU:OE2	3:D:82:VAL:N	2.44	0.51
2:C:563:ASP:N	2:C:563:ASP:OD1	2.44	0.51
3:D:881:ILE:HD11	3:D:989:VAL:HG21	1.92	0.51
3:D:115:GLY:HA3	3:D:298:VAL:HG21	1.93	0.51
5:F:460:MET:N	5:F:460:MET:SD	2.84	0.51
3:D:83:THR:HG22	3:D:84:ARG:H	1.75	0.51
3:D:703:ILE:O	3:D:707:THR:HG23	2.11	0.51
6:G:121:ALA:N	6:H:127:PHE:O	2.44	0.51
5:F:490:GLU:O	5:F:493:THR:OG1	2.26	0.50
1:B:117:GLU:OE1	1:B:119:HIS:ND1	2.40	0.50
2:C:149:THR:HG22	2:C:153:THR:O	2.11	0.50
5:F:300:PHE:CZ	5:F:304:ILE:HD11	2.47	0.50
5:F:485:ARG:HB2	7:O:34:DT:H73	1.92	0.50
3:D:353:ARG:NH1	3:D:370:GLU:OE1	2.44	0.50
1:B:120:ASN:OD1	1:B:123:LEU:HD11	2.12	0.50
6:H:58:LEU:HD11	6:H:63:GLU:OE1	2.12	0.50
2:C:675:ILE:HD11	2:C:690:ASP:OD1	2.11	0.50
4:E:60:ASP:OD1	4:E:60:ASP:N	2.44	0.50
6:M:83:ASP:O	6:M:85:HIS:ND1	2.43	0.50
6:M:39:LEU:HD12	6:M:40:LYS:N	2.26	0.49
2:C:173:VAL:HG12	2:C:192:ILE:HD13	1.94	0.49
2:C:553:GLU:N	2:C:553:GLU:OE2	2.46	0.49
7:O:79:DG:N2	8:P:7:DC:O2	2.46	0.49
2:C:578:ALA:O	2:C:614:THR:HG21	2.13	0.49
3:D:353:ARG:NH2	3:D:370:GLU:OE2	2.46	0.49
3:D:49:GLU:OE2	3:D:49:GLU:N	2.38	0.49
6:M:66:VAL:HG12	6:M:76:TYR:HD2	1.78	0.49
3:D:125:LEU:HD12	3:D:261:LEU:HD11	1.95	0.49
2:C:212:VAL:HG23	2:C:222:VAL:HG22	1.95	0.49
6:N:68:ARG:NH2	6:N:72:GLY:O	2.46	0.49
8:P:53:DC:H2"	8:P:54:DG:H8	1.78	0.49
2:C:630:ALA:HB2	2:C:688:LEU:HD11	1.94	0.48
2:C:913:ASN:N	2:C:913:ASN:HD22	2.11	0.48
6:N:83:ASP:O	6:N:85:HIS:ND1	2.45	0.48
2:C:23:ILE:O	2:C:958:ALA:N	2.44	0.48
2:C:192:ILE:HG23	2:C:192:ILE:O	2.13	0.48
2:C:723:LEU:HD21	2:C:881:ILE:HD11	1.95	0.48
2:C:908:VAL:HG22	2:C:916:GLN:NE2	2.28	0.48
1:B:170:PRO:O	1:B:198:THR:OG1	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:652:GLN:NE2	3:D:656:THR:O	2.47	0.48
3:D:671:LEU:HD11	3:D:714:ALA:CB	2.44	0.48
7:O:19:DT:H2''	7:O:20:DG:C8	2.49	0.48
1:A:54:ILE:HD11	1:A:77:ILE:HD11	1.97	0.47
2:C:631:GLU:OE1	2:C:631:GLU:N	2.42	0.47
3:D:1050:ILE:HD13	3:D:1080:LEU:CD2	2.44	0.47
3:D:210:ASP:O	3:D:213:GLN:NE2	2.47	0.47
5:F:314:ALA:HB2	5:F:333:TRP:HB2	1.96	0.47
6:M:122:HIS:HA	6:N:126:ILE:HG22	1.95	0.47
7:O:47:DC:H2'	7:O:48:DT:H71	1.95	0.47
1:A:40:ARG:NH2	1:B:29:GLY:O	2.48	0.47
1:A:150:VAL:O	1:A:153:LYS:HG2	2.14	0.47
5:F:365:VAL:HG21	5:F:386:LEU:HD21	1.95	0.47
1:B:211:ALA:O	1:B:214:THR:OG1	2.28	0.47
2:C:364:ILE:HD11	2:C:492:ILE:CD1	2.45	0.47
3:D:180:ASP:OD1	3:D:181:LEU:N	2.47	0.47
1:A:34:LEU:HD12	1:B:218:LEU:HD21	1.97	0.46
2:C:319:LEU:HD12	2:C:319:LEU:O	2.15	0.46
2:C:388:GLU:O	2:C:391:THR:OG1	2.26	0.46
3:D:997:ILE:HD13	3:D:1132:ILE:CD1	2.46	0.46
7:O:20:DG:H4'	7:O:21:DT:OP1	2.14	0.46
2:C:22:ARG:NH2	2:C:610:PRO:O	2.45	0.46
2:C:838:VAL:HG23	2:C:855:VAL:HG22	1.96	0.46
3:D:976:SER:OG	3:D:977:LEU:N	2.48	0.46
3:D:1074:ILE:HD11	3:D:1078:ALA:CB	2.44	0.46
2:C:913:ASN:HD22	2:C:913:ASN:H	1.64	0.46
3:D:1172:GLU:OE1	3:D:1175:ARG:NH1	2.48	0.46
2:C:661:PHE:HE2	2:C:736:ILE:HD13	1.80	0.46
2:C:130:ASN:OD1	2:C:131:GLU:N	2.48	0.46
2:C:239:GLU:O	2:C:329:LYS:NZ	2.46	0.46
5:F:386:LEU:O	5:F:388:MET:HE3	2.16	0.46
1:B:86:SER:OG	1:B:117:GLU:O	2.23	0.46
2:C:32:LEU:HB3	2:C:567:VAL:HG21	1.97	0.46
2:C:246:MET:SD	2:C:246:MET:N	2.88	0.46
2:C:472:ILE:HD13	2:C:577:THR:HG21	1.97	0.46
2:C:661:PHE:CE2	2:C:736:ILE:HD13	2.50	0.46
3:D:33:THR:HG21	3:D:327:MET:HE1	1.97	0.45
3:D:831:ILE:HG21	3:D:839:LEU:HD22	1.98	0.45
3:D:1252:ASN:OD1	3:D:1252:ASN:N	2.49	0.45
6:M:27:GLU:OE1	6:M:27:GLU:N	2.48	0.45
3:D:911:VAL:HG22	3:D:915:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:VAL:HG12	1:B:198:THR:HB	1.99	0.45
2:C:1022:VAL:HG23	3:D:429:VAL:HG12	1.99	0.45
3:D:234:LEU:HD23	3:D:235:GLU:N	2.32	0.45
3:D:611:ILE:HD12	3:D:611:ILE:H	1.81	0.45
2:C:68:VAL:HG22	2:C:69:PRO:HD2	1.98	0.45
2:C:129:ASN:O	2:C:133:GLY:N	2.49	0.45
5:F:278:LEU:HD12	5:F:315:VAL:CG2	2.46	0.45
6:H:85:HIS:HA	6:H:100:GLU:HB2	1.99	0.45
5:F:383:ALA:O	5:F:387:ASP:N	2.50	0.45
6:G:104:VAL:HG11	6:H:107:TRP:CE3	2.52	0.45
6:H:88:LEU:O	6:H:96:ALA:HA	2.17	0.45
2:C:471:PRO:O	3:D:852:ARG:NH2	2.50	0.44
3:D:751:VAL:HG11	3:D:768:GLU:OE2	2.17	0.44
4:E:63:VAL:HG23	4:E:64:HIS:HD2	1.82	0.44
6:H:39:LEU:HD21	6:H:46:VAL:HG21	1.99	0.44
6:M:55:LEU:HD12	6:M:56:GLN:N	2.32	0.44
2:C:84:ILE:HD12	2:C:93:LEU:HD13	2.00	0.44
6:N:129:THR:OG1	6:N:133:CYS:SG	2.75	0.44
2:C:207:ARG:NH1	2:C:208:ASP:OD2	2.51	0.44
1:B:39:ARG:HA	1:B:174:VAL:HG11	1.99	0.44
1:B:42:LEU:HD12	1:B:42:LEU:HA	1.77	0.44
1:B:171:VAL:HA	1:B:198:THR:HG1	1.83	0.44
1:A:50:ALA:HA	1:A:85:VAL:HG12	1.99	0.44
2:C:246:MET:O	2:C:249:THR:OG1	2.30	0.44
3:D:1203:TRP:CD1	3:D:1226:ASP:HB2	2.53	0.44
3:D:700:PRO:HG2	3:D:703:ILE:HD12	2.00	0.44
3:D:1042:SER:OG	3:D:1090:VAL:O	2.30	0.44
6:G:115:HIS:O	6:G:115:HIS:ND1	2.50	0.44
6:H:65:ASP:OD1	6:H:77:ARG:HG3	2.18	0.44
1:B:107:ALA:N	1:B:123:LEU:O	2.48	0.43
3:D:885:ASP:OD1	3:D:886:CYS:N	2.51	0.43
3:D:1105:LEU:HB2	3:D:1113:VAL:HG11	2.00	0.43
6:M:84:HIS:HE2	6:M:122:HIS:CE1	2.36	0.43
1:A:34:LEU:CD1	1:B:218:LEU:HD21	2.48	0.43
1:A:42:LEU:HD23	1:A:174:VAL:HG21	2.00	0.43
2:C:299:VAL:HG23	2:C:495:PHE:HB3	2.00	0.43
2:C:806:LEU:HD11	5:F:464:LEU:HD11	2.00	0.43
1:A:120:ASN:OD1	1:A:120:ASN:N	2.52	0.43
1:A:80:ILE:HD12	1:A:125:LEU:HD21	2.01	0.43
2:C:228:ALA:HB1	2:C:262:LEU:HD12	1.99	0.43
3:D:240:LEU:O	3:D:244:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:39:LEU:HD13	6:M:46:VAL:HB	2.01	0.43
2:C:806:LEU:HD12	5:F:464:LEU:HD21	2.00	0.43
3:D:129:ILE:HD12	3:D:130:TYR:CD1	2.54	0.43
3:D:434:PRO:O	3:D:712:LYS:NZ	2.31	0.43
3:D:225:ARG:NH1	3:D:235:GLU:OE1	2.52	0.43
1:A:33:THR:HG23	1:B:36:ASN:OD1	2.19	0.42
2:C:21:LEU:HD23	2:C:22:ARG:N	2.34	0.42
2:C:510:VAL:HG21	2:C:534:LEU:HD11	2.00	0.42
2:C:671:ASN:OD1	2:C:672:GLN:N	2.52	0.42
3:D:89:ARG:N	3:D:323:ASP:OD2	2.52	0.42
5:F:301:LEU:HA	5:F:304:ILE:HD12	2.01	0.42
6:M:67:LEU:HD12	6:M:68:ARG:N	2.34	0.42
7:O:53:DG:C8	7:O:54:DT:H72	2.54	0.42
7:O:72:DG:OP2	7:O:72:DG:H3'	2.20	0.42
1:B:129:ASN:OD1	1:B:129:ASN:N	2.53	0.42
3:D:920:LEU:HD23	3:D:920:LEU:HA	1.85	0.42
6:H:38:MET:SD	6:H:39:LEU:N	2.91	0.42
3:D:93:GLY:C	3:D:319:VAL:HG22	2.40	0.42
2:C:289:PHE:HA	2:C:318:VAL:HG21	2.02	0.42
6:G:35:LEU:O	6:G:39:LEU:HD23	2.19	0.42
6:N:67:LEU:HD12	6:N:68:ARG:H	1.84	0.42
1:A:104:LEU:HA	1:A:127:THR:HA	2.02	0.42
3:D:459:ARG:CG	3:D:486:VAL:HG13	2.49	0.42
3:D:473:LYS:HZ3	5:F:431:ALA:HB1	1.84	0.42
2:C:171:PRO:HA	2:C:193:ILE:HG23	2.02	0.42
2:C:1121:GLU:OE1	3:D:11:ARG:NH2	2.52	0.42
3:D:96:GLU:O	3:D:351:ASN:ND2	2.53	0.42
3:D:1164:VAL:HG11	3:D:1169:PHE:HD1	1.85	0.42
6:G:126:ILE:HD12	6:H:122:HIS:HA	2.01	0.42
1:A:62:GLU:HA	1:A:73:VAL:HG11	2.01	0.42
3:D:1084:GLU:OE1	3:D:1084:GLU:N	2.52	0.42
3:D:166:ARG:NH2	3:D:169:ASP:OD2	2.53	0.42
5:F:319:ASP:N	5:F:319:ASP:OD1	2.52	0.42
5:F:361:LYS:O	5:F:365:VAL:HG22	2.20	0.42
2:C:167:LEU:HG	2:C:364:ILE:HG22	2.02	0.41
2:C:294:TYR:O	2:C:318:VAL:HG12	2.20	0.41
2:C:711:PRO:O	3:D:720:THR:HG23	2.20	0.41
3:D:416:ASN:O	3:D:417:LEU:HD23	2.20	0.41
3:D:673:PRO:HD3	3:D:707:THR:HG21	2.02	0.41
2:C:25:PHE:CD2	2:C:965:ALA:HB2	2.55	0.41
3:D:529:CYS:SG	3:D:530:THR:N	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1002:THR:O	3:D:1005:THR:HG23	2.19	0.41
4:E:63:VAL:HG23	4:E:64:HIS:CD2	2.55	0.41
2:C:748:THR:OG1	2:C:749:LYS:N	2.53	0.41
3:D:506:ARG:HD3	3:D:992:ILE:HD13	2.02	0.41
3:D:556:ARG:NH2	4:E:11:ILE:O	2.49	0.41
6:M:52:TYR:OH	7:O:19:DT:OP1	2.38	0.41
6:N:55:LEU:HD21	6:N:76:TYR:CE1	2.55	0.41
2:C:586:ASP:N	2:C:586:ASP:OD1	2.53	0.41
2:C:706:LEU:O	2:C:901:ILE:HG22	2.21	0.41
2:C:806:LEU:CD1	5:F:464:LEU:HD11	2.51	0.41
5:F:292:ARG:O	8:P:27:DT:N3	2.49	0.41
2:C:676:VAL:HG11	2:C:688:LEU:HD22	2.03	0.41
4:E:61:THR:HG23	4:E:70:ILE:HD11	2.02	0.41
4:E:65:GLU:CD	4:E:70:ILE:HD12	2.40	0.41
2:C:84:ILE:HD13	2:C:386:VAL:HG11	2.03	0.41
2:C:213:ARG:NH2	2:C:218:ARG:O	2.47	0.41
2:C:1002:GLU:OE1	3:D:721:ARG:NH2	2.48	0.41
1:B:213:LYS:HA	1:B:213:LYS:HE2	2.02	0.41
3:D:571:GLY:N	3:D:977:LEU:HD23	2.35	0.41
3:D:1055:LYS:O	3:D:1056:THR:OG1	2.37	0.41
5:F:355:MET:O	5:F:359:ILE:HG12	2.21	0.41
8:P:63:DA:H1'	8:P:64:DA:H5'	2.02	0.41
1:A:174:VAL:CG2	1:A:196:VAL:HG23	2.51	0.41
2:C:755:ILE:HD11	2:C:853:GLN:OE1	2.20	0.41
2:C:1047:GLN:OE1	2:C:1047:GLN:N	2.54	0.41
3:D:610:ALA:HB1	3:D:663:LEU:HD13	2.02	0.41
3:D:1080:LEU:HD12	3:D:1080:LEU:C	2.42	0.41
6:M:77:ARG:NH1	6:M:79:CYS:HA	2.36	0.41
7:O:31:DC:H2'	7:O:32:DG:C8	2.55	0.41
1:B:137:GLU:N	1:B:137:GLU:OE1	2.54	0.41
3:D:285:LYS:O	3:D:288:LYS:NZ	2.47	0.41
3:D:383:ASP:HB3	3:D:403:SER:HB3	2.02	0.41
3:D:1042:SER:OG	3:D:1089:GLU:O	2.39	0.41
1:B:10:THR:HG23	1:B:22:VAL:HG22	2.02	0.40
6:H:55:LEU:HD12	6:H:56:GLN:N	2.36	0.40
7:O:37:DC:O2	8:P:49:DG:N2	2.55	0.40
1:A:43:LEU:HA	1:A:171:VAL:HG21	2.04	0.40
1:A:181:THR:OG1	1:A:189:PHE:O	2.31	0.40
1:B:50:ALA:HA	1:B:85:VAL:HG22	2.03	0.40
3:D:67:ARG:HD3	3:D:67:ARG:HA	1.92	0.40
3:D:807:MET:SD	3:D:807:MET:N	2.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1121:VAL:HG11	3:D:1137:ILE:HD13	2.03	0.40
8:P:21:DG:N2	8:P:22:DG:O6	2.54	0.40
1:B:108:ALA:N	1:B:121:PRO:O	2.54	0.40
2:C:759:ILE:HG22	2:C:760:PRO:HD2	2.04	0.40
3:D:591:ASP:N	3:D:682:GLU:OE2	2.54	0.40
3:D:926:ILE:HG22	3:D:931:ILE:HD11	2.02	0.40
1:A:172:LEU:HB2	1:A:197:GLU:O	2.21	0.40
1:B:118:VAL:O	1:B:118:VAL:HG23	2.20	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	224/340 (66%)	213 (95%)	11 (5%)	0	100	100
1	B	231/340 (68%)	225 (97%)	6 (3%)	0	100	100
2	C	1114/1161 (96%)	1071 (96%)	43 (4%)	0	100	100
3	D	1257/1307 (96%)	1208 (96%)	49 (4%)	0	100	100
4	E	75/90 (83%)	72 (96%)	3 (4%)	0	100	100
5	F	296/531 (56%)	290 (98%)	6 (2%)	0	100	100
6	G	129/159 (81%)	125 (97%)	4 (3%)	0	100	100
6	H	129/159 (81%)	127 (98%)	2 (2%)	0	100	100
6	M	129/159 (81%)	128 (99%)	1 (1%)	0	100	100
6	N	129/159 (81%)	128 (99%)	1 (1%)	0	100	100
All	All	3713/4405 (84%)	3587 (97%)	126 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/279 (70%)	188 (97%)	6 (3%)	40	65
1	B	199/279 (71%)	195 (98%)	4 (2%)	55	74
2	C	942/979 (96%)	915 (97%)	27 (3%)	42	66
3	D	1054/1095 (96%)	1020 (97%)	34 (3%)	39	65
4	E	64/74 (86%)	61 (95%)	3 (5%)	26	56
5	F	257/430 (60%)	248 (96%)	9 (4%)	36	63
6	G	99/120 (82%)	96 (97%)	3 (3%)	41	66
6	H	99/120 (82%)	95 (96%)	4 (4%)	31	60
6	M	99/120 (82%)	94 (95%)	5 (5%)	24	55
6	N	99/120 (82%)	96 (97%)	3 (3%)	41	66
All	All	3106/3616 (86%)	3008 (97%)	98 (3%)	42	65

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	TYR
1	A	104	LEU
1	A	122	ASP
1	A	146	TYR
1	A	177	LYS
1	A	182	ARG
1	B	17	PHE
1	B	55	ARG
1	B	122	ASP
1	B	148	SER
2	C	87	PHE
2	C	91	MET
2	C	176	ASP
2	C	207	ARG
2	C	256	GLN
2	C	270	ARG

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Mol	Chain	Res	Type
2	C	359	PHE
2	C	394	ASP
2	C	420	SER
2	C	427	ASP
2	C	450	SER
2	C	474	THR
2	C	511	THR
2	C	514	VAL
2	C	529	GLN
2	C	531	ASN
2	C	555	ASP
2	C	556	TYR
2	C	575	VAL
2	C	586	ASP
2	C	639	VAL
2	C	642	ASP
2	C	644	ILE
2	C	830	ILE
2	C	840	ASP
2	C	913	ASN
2	C	980	ASN
3	D	7	PHE
3	D	27	GLU
3	D	44	ASP
3	D	48	CYS
3	D	60	CYS
3	D	64	LYS
3	D	70	PHE
3	D	96	GLU
3	D	113	ARG
3	D	214	ARG
3	D	233	ASP
3	D	308	SER
3	D	335	PHE
3	D	475	MET
3	D	529	CYS
3	D	539	ASP
3	D	595	ARG
3	D	686	LYS
3	D	750	LYS
3	D	784	MET
3	D	788	PHE

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Mol	Chain	Res	Type
3	D	829	ARG
3	D	840	SER
3	D	842	LEU
3	D	844	TYR
3	D	861	ARG
3	D	872	LEU
3	D	886	CYS
3	D	925	VAL
3	D	958	SER
3	D	1072	PHE
3	D	1147	ARG
3	D	1168	LYS
3	D	1191	MET
4	E	24	ASP
4	E	43	TYR
4	E	62	HIS
5	F	276	ASN
5	F	293	TYR
5	F	309	LEU
5	F	326	PHE
5	F	354	HIS
5	F	441	GLU
5	F	490	GLU
5	F	492	LYS
5	F	502	ARG
6	G	9	LYS
6	G	68	ARG
6	G	91	ARG
6	H	16	ARG
6	H	37	ASP
6	H	83	ASP
6	H	127	PHE
6	M	28	GLU
6	M	52	TYR
6	M	60	ASP
6	M	76	TYR
6	M	90	CYS
6	N	16	ARG
6	N	36	HIS
6	N	53	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	465	HIS
2	C	913	ASN
2	C	916	GLN
4	E	64	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	Q	4/5 (80%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 15 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

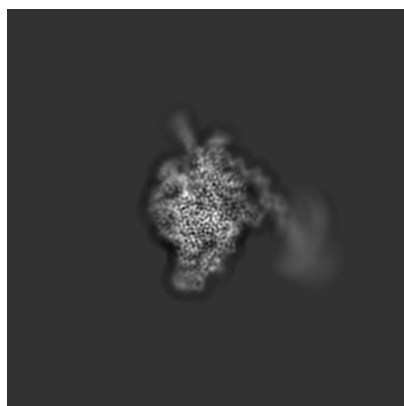
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33031. 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](#)

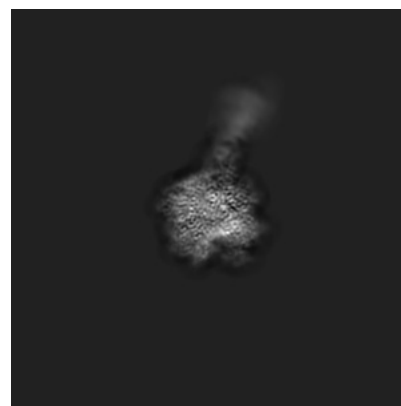
6.1.1 Primary map



X

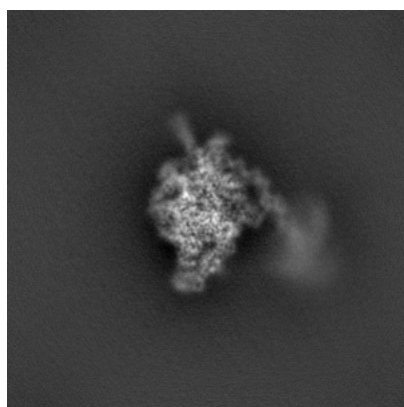


Y

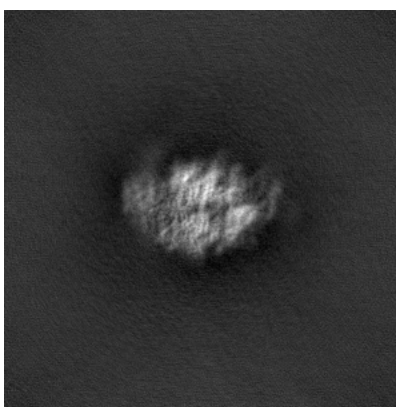


Z

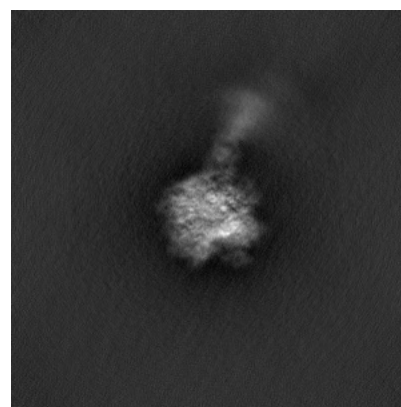
6.1.2 Raw map



X



Y

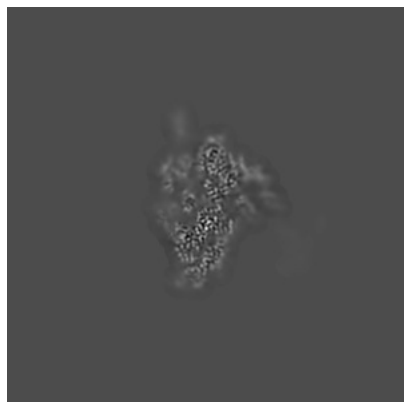


Z

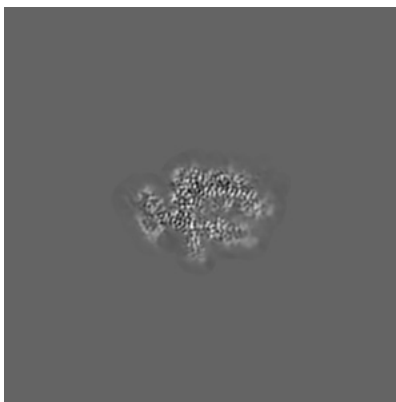
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

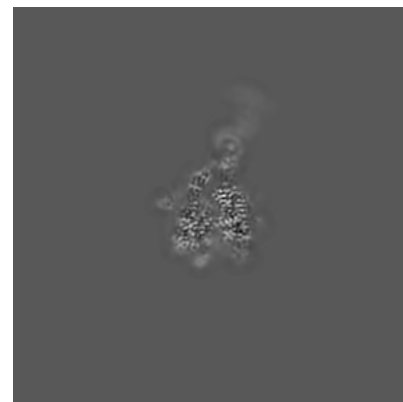
6.2.1 Primary map



X Index: 192

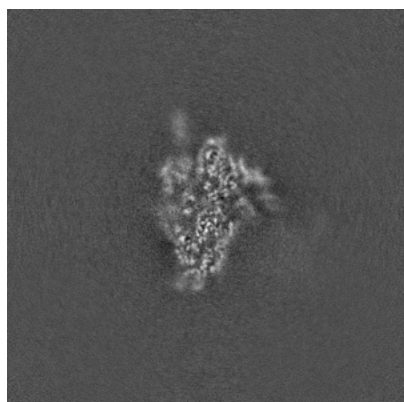


Y Index: 192

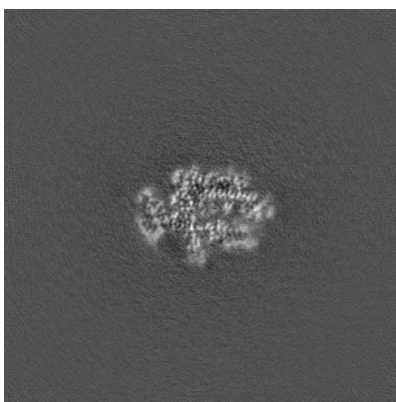


Z Index: 192

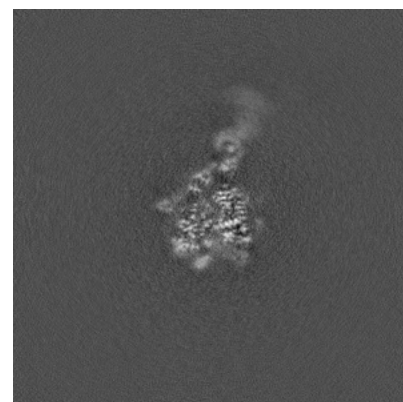
6.2.2 Raw map



X Index: 192



Y Index: 192

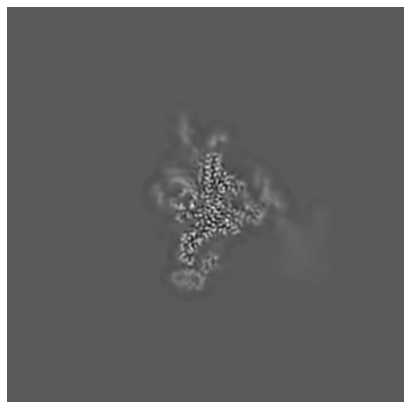


Z Index: 192

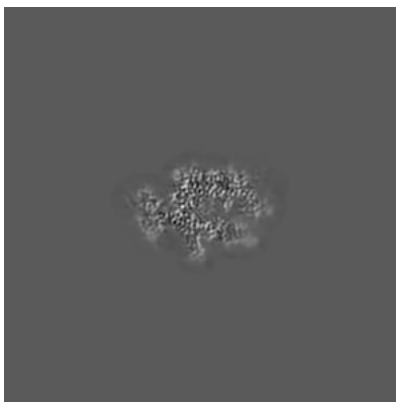
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 204

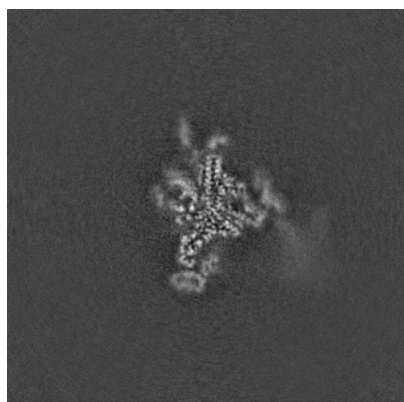


Y Index: 191

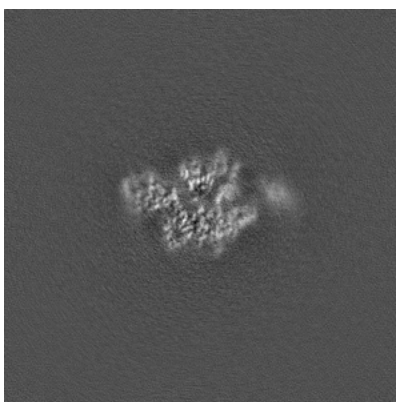


Z Index: 179

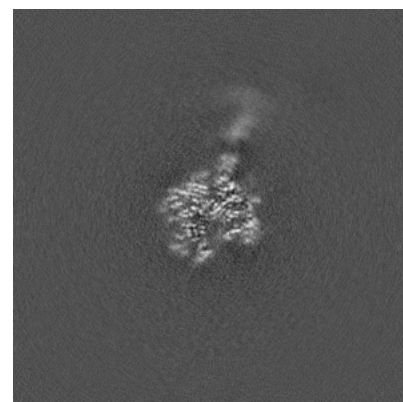
6.3.2 Raw map



X Index: 204



Y Index: 171

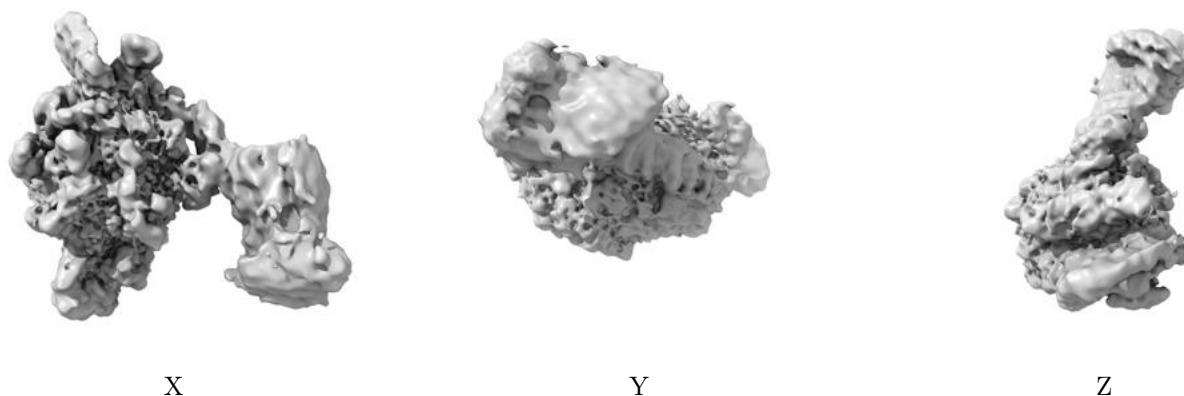


Z Index: 179

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

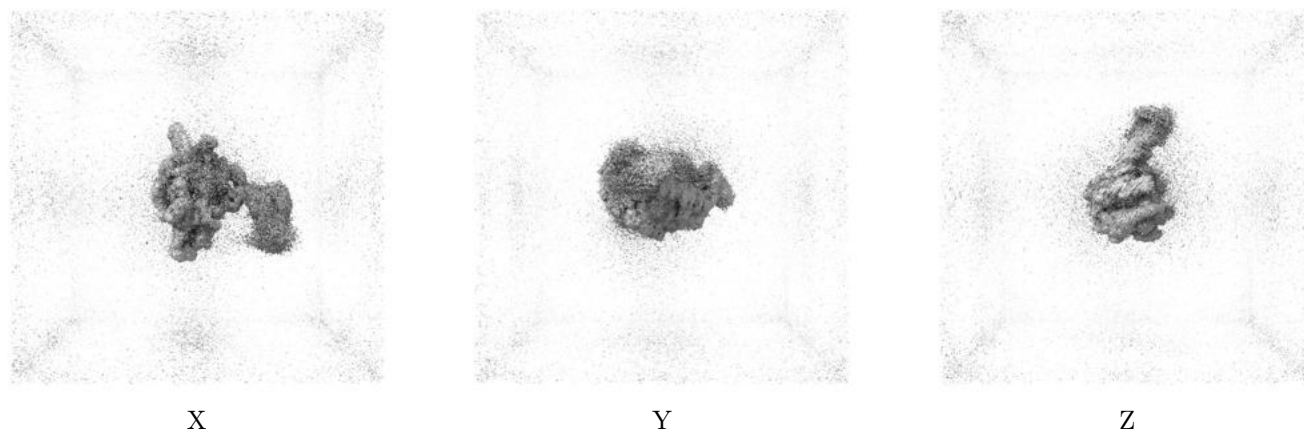
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

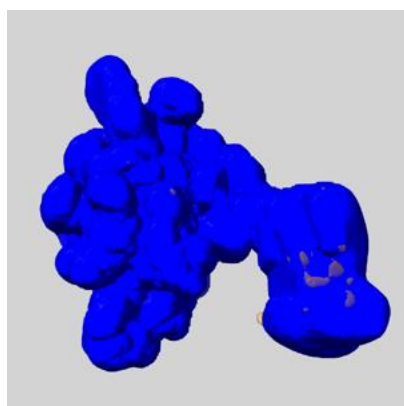
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

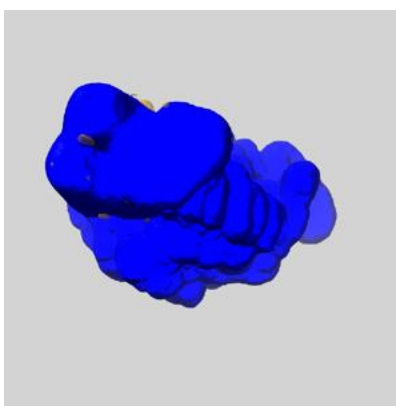
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

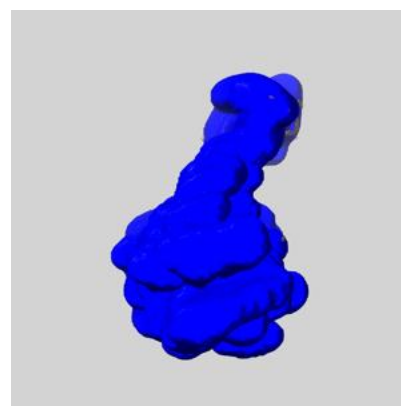
6.5.1 emd_33031_msk_1.map [i](#)



X



Y

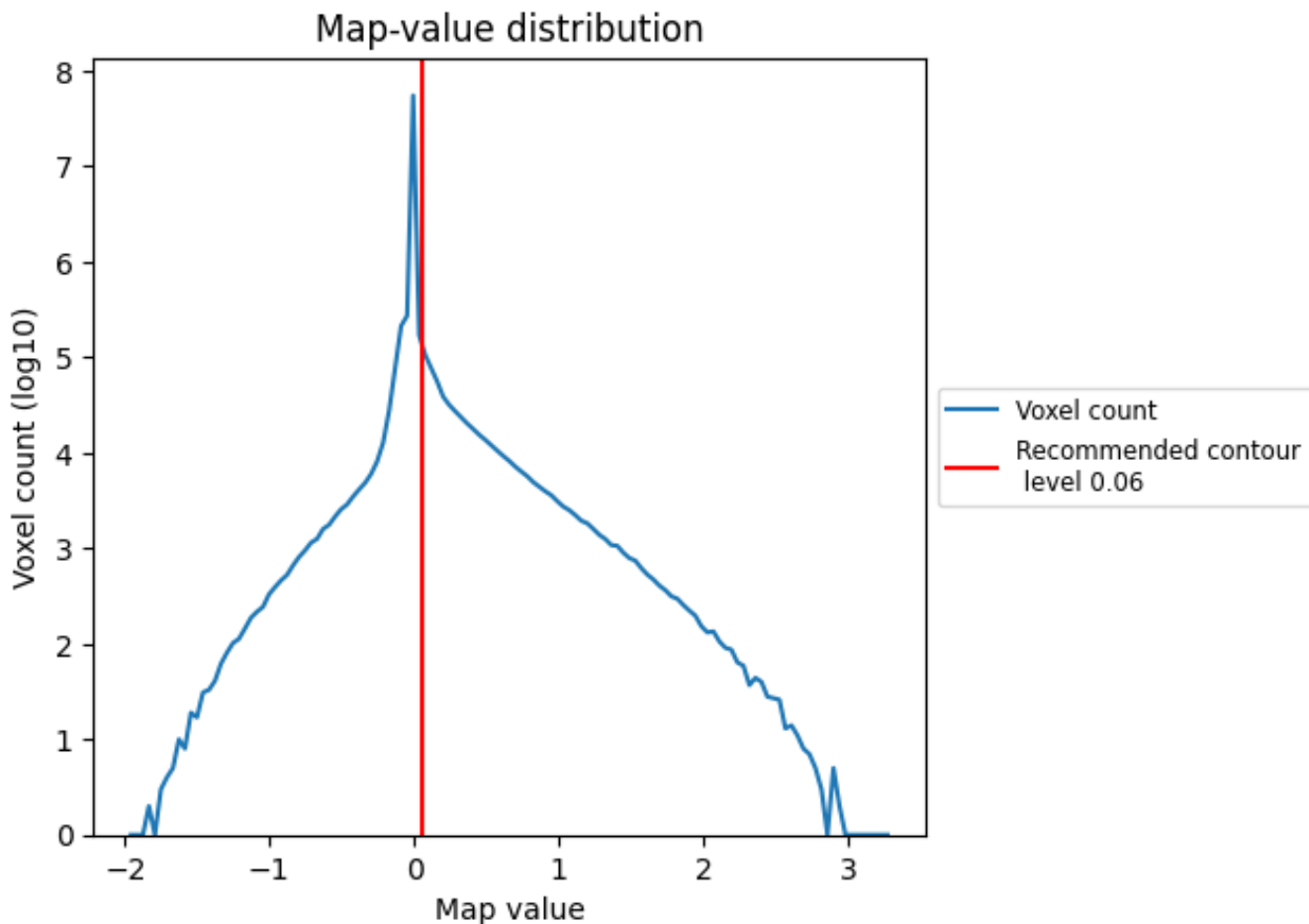


Z

7 Map analysis [i](#)

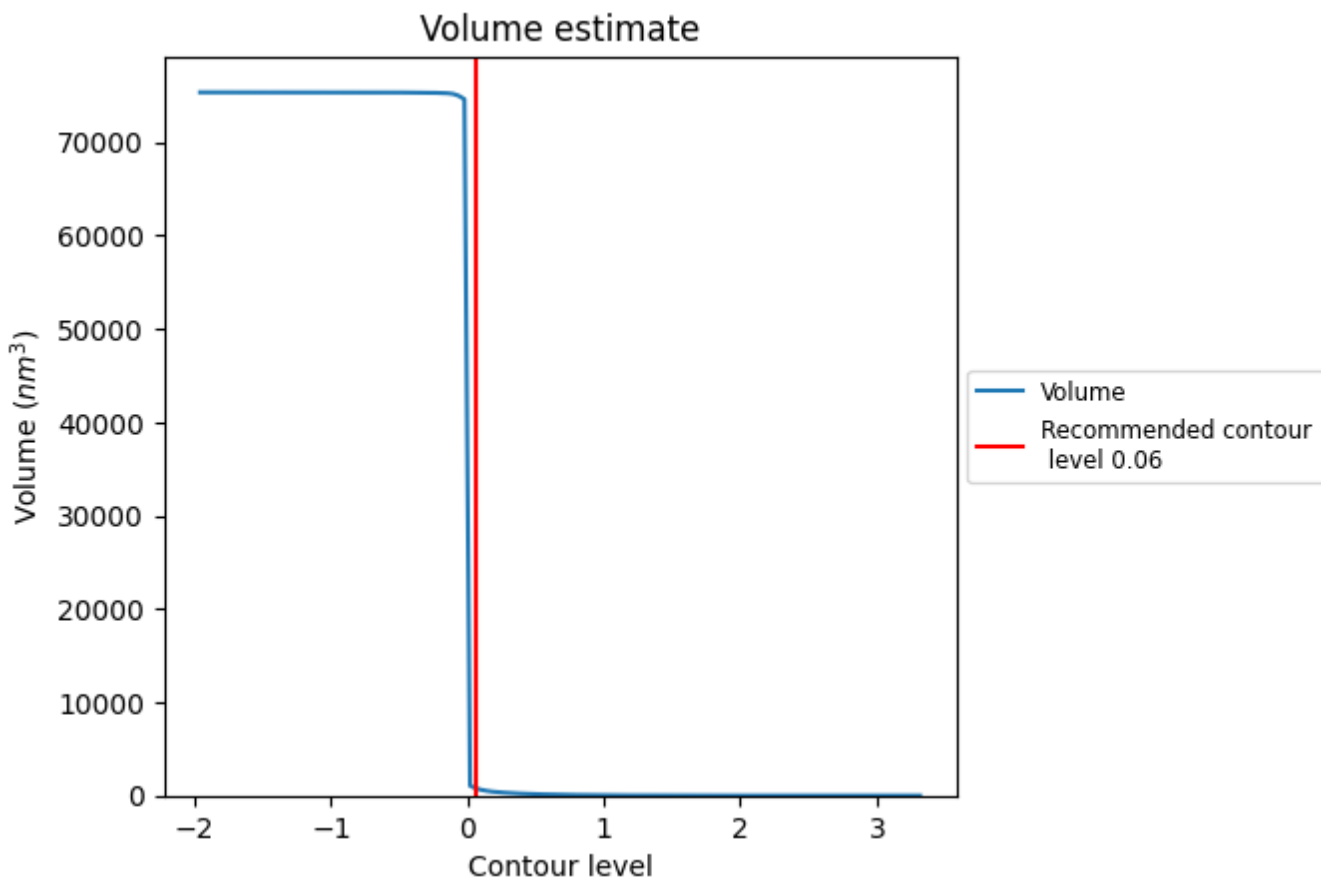
This section contains the results of statistical analysis of the map.

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.

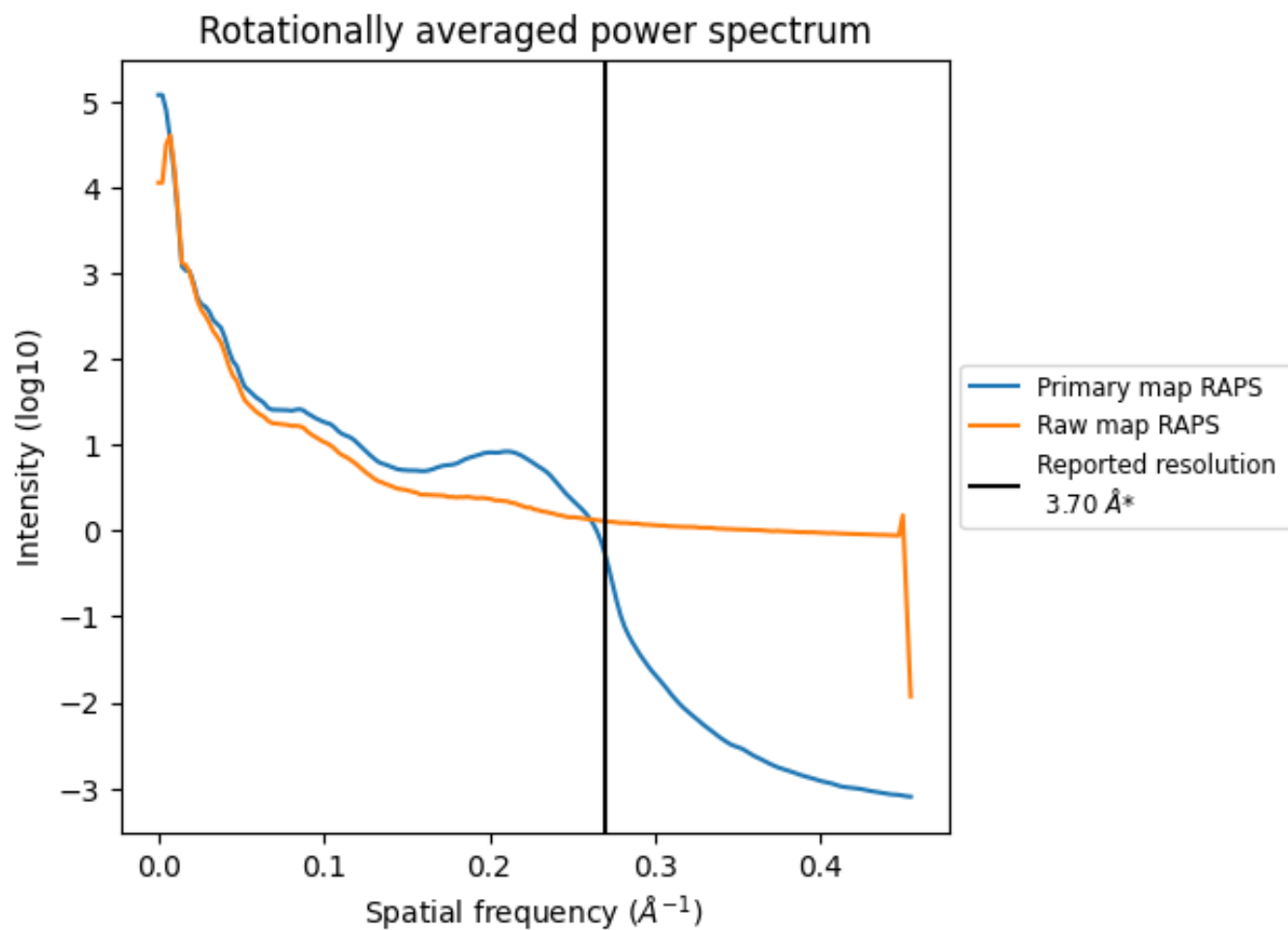
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 789 nm³; this corresponds to an approximate mass of 713 kDa.

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

7.3 Rotationally averaged power spectrum i

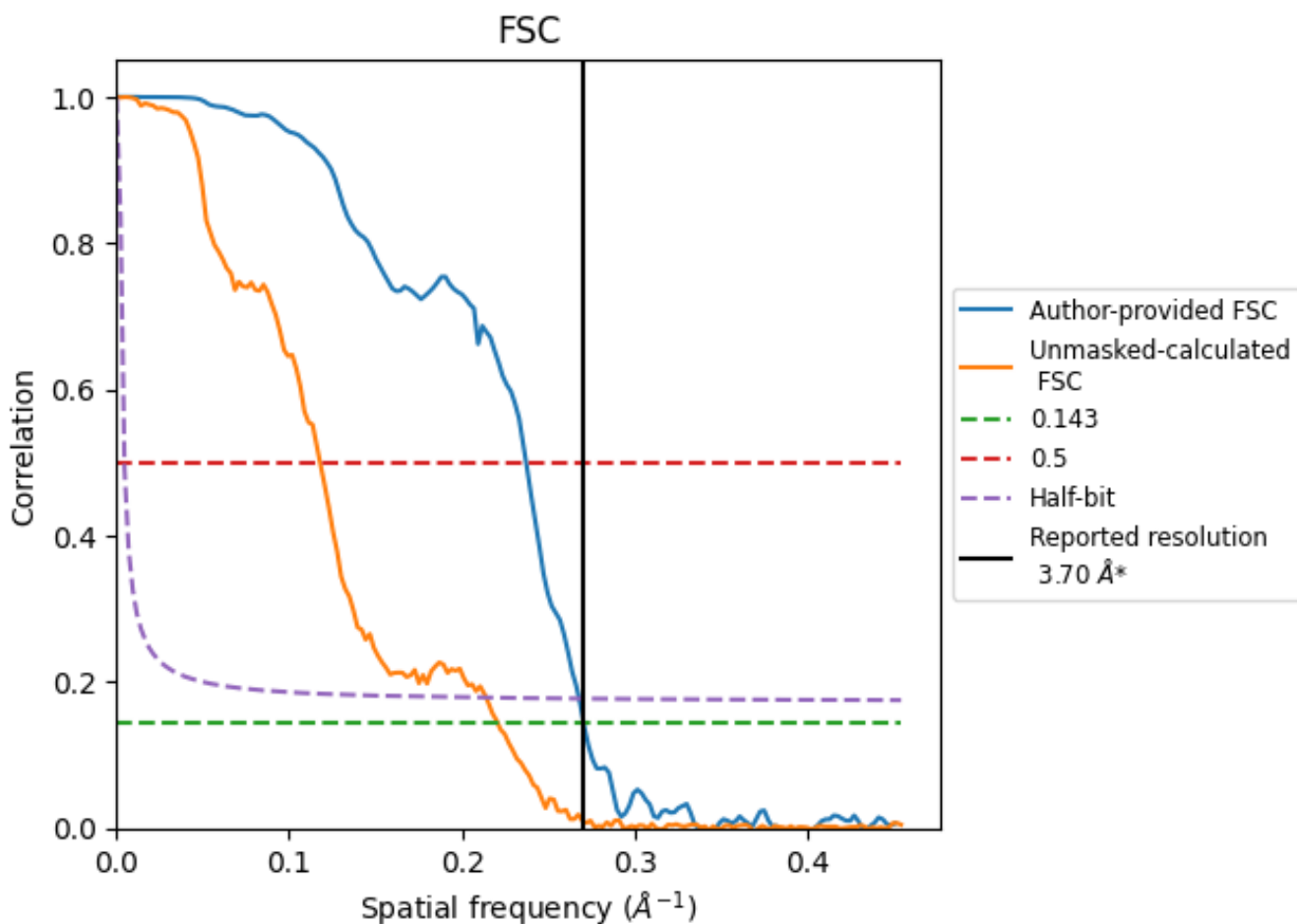


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

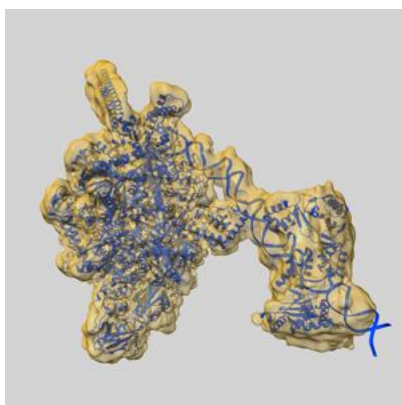
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.70	4.21	3.73
Unmasked-calculated*	4.53	8.48	4.67

*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 4.53 differs from the reported value 3.7 by more than 10 %

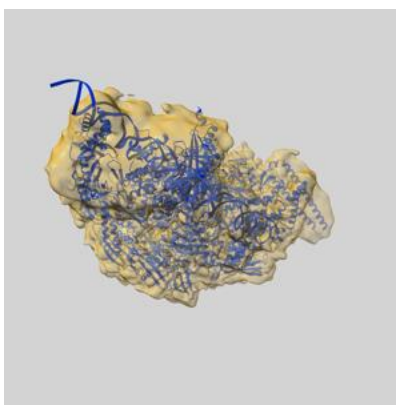
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33031 and PDB model 7X74. Per-residue inclusion information can be found in section 3 on page 9.

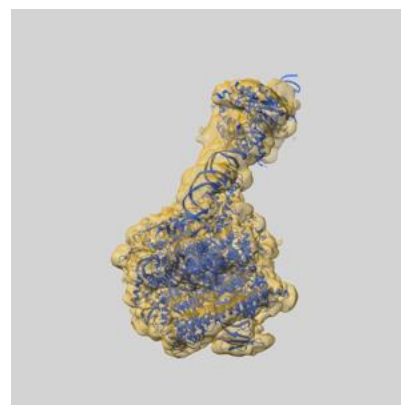
9.1 Map-model overlay [i](#)



X



Y



Z

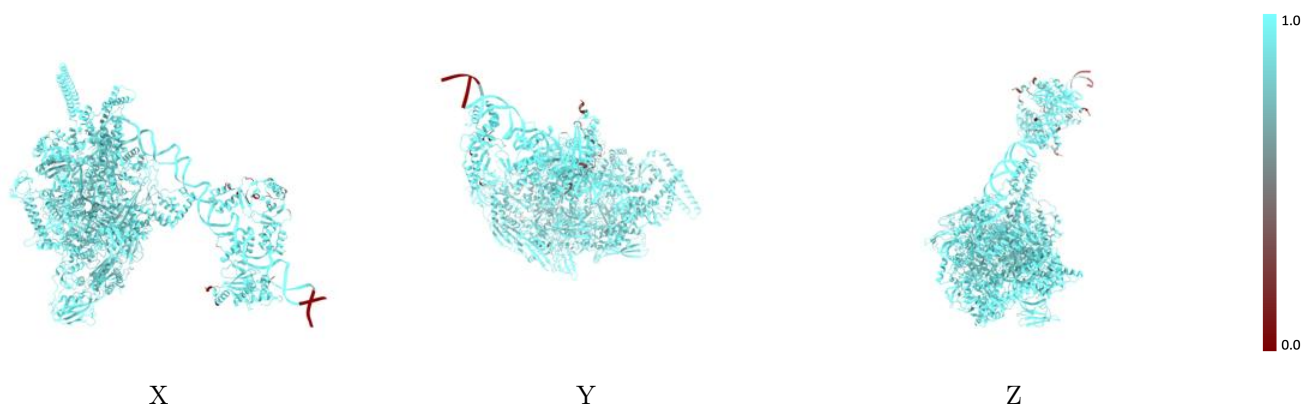
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



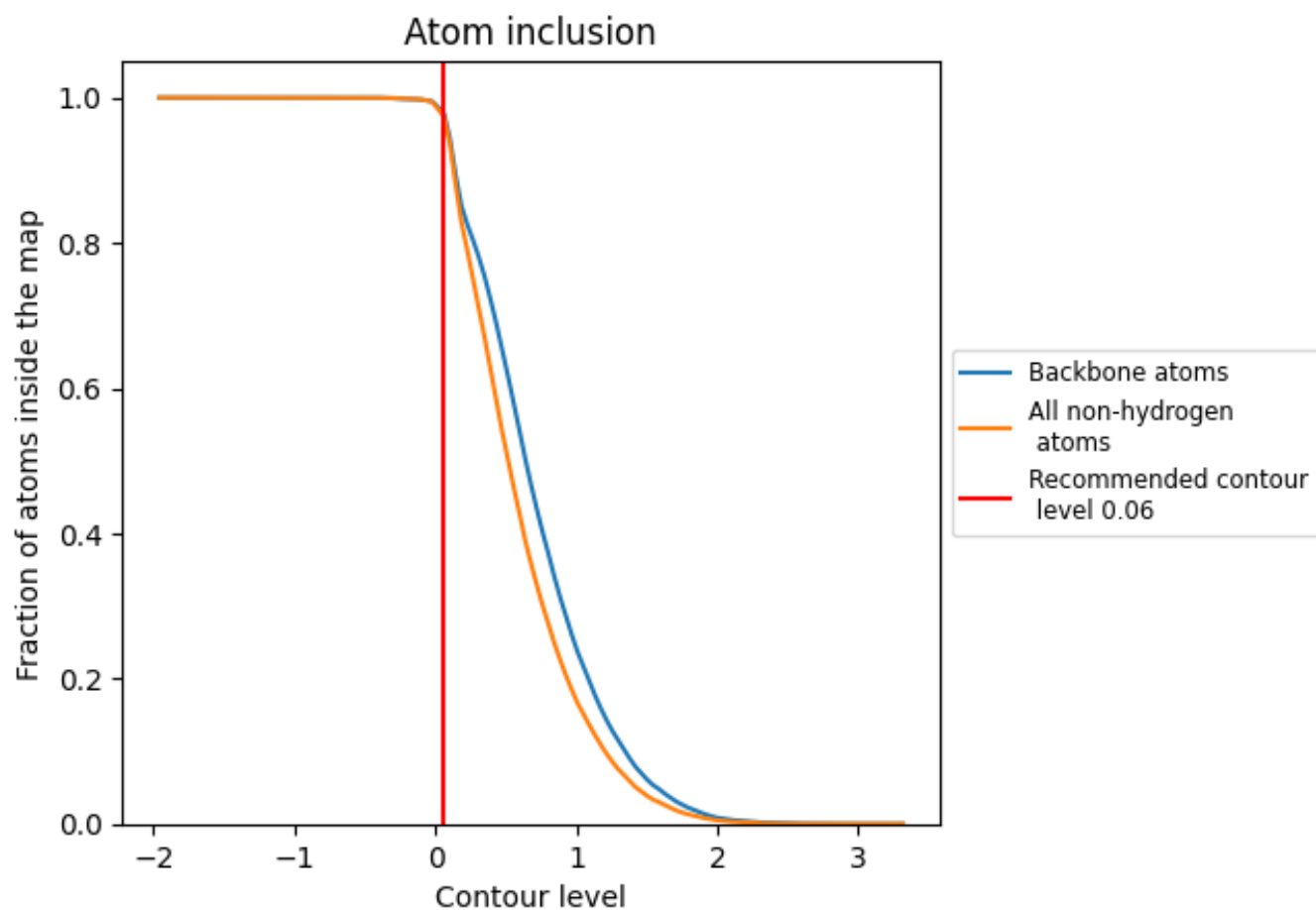
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9742	 0.3170
A	 0.9883	 0.3590
B	 0.9778	 0.3100
C	 0.9873	 0.4090
D	 0.9850	 0.3820
E	 0.9693	 0.3880
F	 0.9789	 0.2840
G	 0.9596	 0.0710
H	 0.8497	 0.0680
M	 0.9658	 0.0640
N	 0.9720	 0.0450
O	 0.9428	 0.1870
P	 0.9427	 0.1810
Q	 0.9537	 0.3920

