



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 05:34 AM UTC

PDB ID : 9HEJ / pdb_00009hej
EMDB ID : EMD-52078
Title : Dimeric CD163 bound to human haptoglobin-haemoglobin complex
Authors : Zhou, R.X.; Higgins, M.K.
Deposited on : 2024-11-14
Resolution : 2.82 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

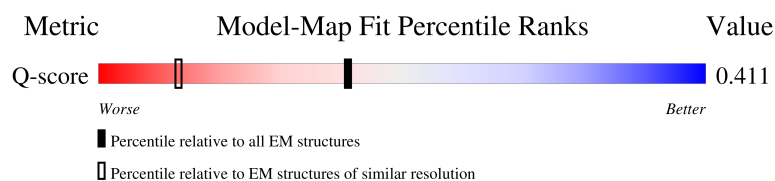
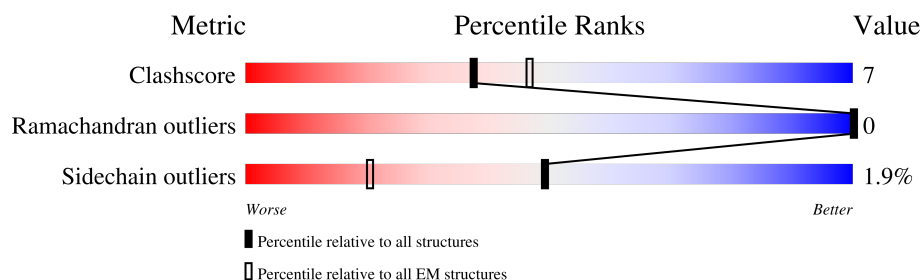
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.82 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11795 (2.32 - 3.32)

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	1156	
1	B	1156	
2	D	142	
3	E	147	

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Mol	Chain	Length	Quality of chain
4	F	347	
4	G	347	
5	C	2	
5	H	2	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 15177 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 Scavenger receptor cysteine-rich type 1 protein M130.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	748	Total	C	N	O	S	0	0
			5661	3476	1022	1101	62		
1	B	631	Total	C	N	O	S	0	0
			4780	2939	868	920	53		

- Molecule 2 is a protein called Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	141	Total	C	N	O	S	0	0
			1069	685	187	194	3		

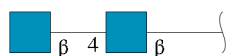
- Molecule 3 is a protein called Hemoglobin subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	142	Total	C	N	O	S	0	0
			1084	698	188	195	3		

- Molecule 4 is a protein called Isoform 2 of Haptoglobin.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	292	Total	C	N	O	S	0	0
			2303	1465	390	436	12		
4	G	9	Total	C	N	O		0	0
			69	46	11	12			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	C	2	Total	C	N	O	0	0
			28	16	2	10		
5	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
7	A	6	Total	Ca	0
			6	6	
7	B	3	Total	Ca	0
			3	3	

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

The diagram illustrates the chemical structure of Heme (HEM). It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with various side chains, including vinyl groups (C3A, C3B, C3C, C3D), methyl groups (C2A, C2B, C2C, C2D), and a long phytol chain (C1A, C1B, C1C, C1D). The central iron atom is also coordinated by a proximal histidine residue (NA) and a distal water molecule (ND). The structure is labeled with various atoms and bonds, including O1A, O2A, O1D, O2D, CAA, CBA, CAD, CBD, CMA, C3A, C3B, C3C, C3D, C2A, C2B, C2C, C2D, C1A, C1B, C1C, C1D, C4A, C4B, C4C, C4D, C4E, C4F, C4G, C4H, C4I, C4J, C4K, C4L, C4M, C4N, C4O, C4P, C4Q, C4R, C4S, C4T, C4U, C4V, C4W, C4X, C4Y, C4Z, C4AA, C4AB, C4AC, C4AD, C4AE, C4AF, C4AG, C4AH, C4AI, C4AJ, C4AK, C4AL, C4AM, C4AN, C4AO, C4AP, C4AQ, C4AR, C4AS, C4AT, C4AU, C4AV, C4AW, C4AX, C4AY, C4AZ, C4BA, C4BB, C4BC, C4BD, C4BE, C4BF, C4BG, C4BH, C4BI, C4BJ, C4BK, C4BL, C4BM, C4BN, C4BO, C4BP, C4BQ, C4BR, C4BS, C4BT, C4BU, C4BV, C4BW, C4BX, C4BY, C4BZ, C4CA, C4CB, C4CC, C4CD, C4CE, C4CF, C4CG, C4CH, C4CI, C4CJ, C4CK, C4CL, C4CM, C4CN, C4CO, C4CP, C4CQ, C4CR, C4CS, C4CT, C4CU, C4CV, C4CW, C4CX, C4CY, C4CZ, C4DA, C4DB, C4DC, C4DD, C4DE, C4DF, C4DG, C4DH, C4DI, C4DJ, C4DK, C4DL, C4DM, C4DN, C4DO, C4DP, C4DQ, C4DR, C4DS, C4DT, C4DU, C4DV, C4DW, C4DX, C4DY, C4DZ, C4EA, C4EB, C4EC, C4ED, C4EE, C4EF, C4EG, C4EH, C4EI, C4EJ, C4EK, C4EL, C4EM, C4EN, C4EO, C4EP, C4EQ, C4ER, C4ES, C4ET, C4EU, C4EV, C4EW, C4EX, C4EY, C4EZ, C4FA, C4FB, C4FC, C4FD, C4FE, C4FF, C4FG, C4FH, C4FI, C4FJ, C4FK, C4FL, C4FM, C4FN, C4FO, C4FP, C4FQ, C4FR, C4FS, C4FT, C4FU, C4FV, C4FW, C4FX, C4FY, C4FZ, C4GA, C4GB, C4GC, C4GD, C4GE, C4GF, C4GG, C4GH, C4GI, C4GJ, C4GK, C4GL, C4GM, C4GN, C4GO, C4GP, C4GQ, C4GR, C4GS, C4GT, C4GU, C4GV, C4GW, C4GX, C4GY, C4GZ, C4HA, C4HB, C4HC, C4HD, C4HE, C4HF, C4HG, C4HH, C4HI, C4HJ, C4HK, C4HL, C4HM, C4HN, C4HO, C4HP, C4HQ, C4HR, C4HS, C4HT, C4HU, C4HV, C4HW, C4HX, C4HY, C4HZ, C4IA, C4IB, C4IC, C4ID, C4IE, C4IF, C4IG, C4IH, C4II, C4IJ, C4IK, C4IL, C4IM, C4IN, C4IO, C4IP, C4IQ, C4IR, C4IS, C4IT, C4IU, C4IV, C4IW, C4IX, C4IY, C4IZ, C4JA, C4JB, C4JC, C4JD, C4JE, C4JF, C4JG, C4JH, C4JI, C4JJ, C4JK, C4JL, C4JM, C4JN, C4JO, C4JP, C4JQ, C4JR, C4JS, C4JT, C4JU, C4JV, C4JW, C4JX, C4JY, C4JZ, C4KA, C4KB, C4KC, C4KD, C4KE, C4KF, C4KG, C4KH, C4KI, C4KJ, C4KK, C4KL, C4KM, C4KN, C4KO, C4KP, C4KQ, C4KR, C4KS, C4KT, C4KU, C4KV, C4KW, C4KX, C4KY, C4KZ, C4LA, C4LB, C4LC, C4LD, C4LE, C4LF, C4LG, C4LH, C4LI, C4LJ, C4LK, C4LL, C4LM, C4LN, C4LO, C4LP, C4LQ, C4LR, C4LS, C4LT, C4LU, C4LV, C4LW, C4LX, C4LY, C4LZ, C4MA, C4MB, C4MC, C4MD, C4ME, C4MF, C4MG, C4MH, C4MI, C4MJ, C4MK, C4ML, C4MN, C4MO, C4MP, C4MQ, C4MR, C4MS, C4MT, C4MU, C4MV, C4MW, C4MX, C4MY, C4MZ, C4NA, C4NB, C4NC, C4ND, C4NE, C4NF, C4NG, C4NH, C4NI, C4NJ, C4NK, C4NL, C4NM, C4NO, C4NP, C4NQ, C4NR, C4NS, C4NT, C4NU, C4NV, C4NW, C4NX, C4NY, C4NZ, C4OA, C4OB, C4OC, C4OD, C4OE, C4OF, C4OG, C4OH, C4OI, C4OJ, C4OK, C4OL, C4OM, C4ON, C4OO, C4OP, C4OQ, C4OR, C4OS, C4OT, C4OU, C4OV, C4OW, C4OX, C4OY, C4OZ, C4PA, C4PB, C4PC, C4PD, C4PE, C4PF, C4PG, C4PH, C4PI, C4PJ, C4PK, C4PL, C4PM, C4PN, C4PO, C4PP, C4PQ, C4PR, C4PS, C4PT, C4PU, C4PV, C4PW, C4PX, C4PY, C4PZ, C4QA, C4QB, C4QC, C4QD, C4QE, C4QF, C4QG, C4QH, C4QI, C4QJ, C4QK, C4QL, C4QM, C4QN, C4QO, C4QP, C4QQ, C4QR, C4QS, C4QT, C4QU, C4QV, C4QW, C4QX, C4QY, C4QZ, C4RA, C4RB, C4RC, C4RD, C4RE, C4RF, C4RG, C4RH, C4RI, C4RJ, C4RK, C4RL, C4RM, C4RN, C4RO, C4RP, C4RQ, C4RR, C4RS, C4RT, C4RU, C4RV, C4RW, C4RX, C4RY, C4RZ, C4SA, C4SB, C4SC, C4SD, C4SE, C4SF, C4SG, C4SH, C4SI, C4SJ, C4SK, C4SL, C4SM, C4SN, C4SO, C4SP, C4SQ, C4SR, C4SS, C4ST, C4SU, C4SV, C4SW, C4SX, C4SY, C4SZ, C4TA, C4TB, C4TC, C4TD, C4TE, C4TF, C4TG, C4TH, C4TI, C4TJ, C4TK, C4TL, C4TM, C4TN, C4TO, C4TP, C4TQ, C4TR, C4TS, C4TT, C4TU, C4TV, C4TW, C4TX, C4TY, C4TZ, C4UA, C4UB, C4UC, C4UD, C4UE, C4UF, C4UG, C4UH, C4UI, C4UJ, C4UK, C4UL, C4UM, C4UN, C4UO, C4UP, C4UQ, C4UR, C4US, C4UT, C4UU, C4UV, C4UW, C4UX, C4UY, C4UZ, C4VA, C4VB, C4VC, C4VD, C4VE, C4VF, C4VG, C4VH, C4VI, C4VJ, C4VK, C4VL, C4VM, C4VN, C4VO, C4VP, C4VQ, C4VR, C4VS, C4VT, C4VU, C4VV, C4VW, C4VX, C4VY, C4VZ, C4WA, C4WB, C4WC, C4WD, C4WE, C4WF, C4WG, C4WH, C4WI, C4WJ, C4WK, C4WL, C4WM, C4WN, C4WO, C4WP, C4WQ, C4WR, C4WS, C4WT, C4WU, C4WV, C4WW, C4WX, C4WY, C4WZ, C4XA, C4XB, C4XC, C4XD, C4XE, C4XF, C4XG, C4XH, C4XI, C4XJ, C4XK, C4XL, C4XM, C4XN, C4XO, C4XP, C4XQ, C4XR, C4XS, C4XT, C4XU, C4XV, C4XW, C4XX, C4XY, C4XZ, C4YA, C4YB, C4YC, C4YD, C4YE, C4YF, C4YG, C4YH, C4YI, C4YJ, C4YK, C4YL, C4YM, C4YN, C4YO, C4YP, C4YQ, C4YR, C4YS, C4YT, C4YU, C4YV, C4YW, C4YX, C4YY, C4YZ, C4ZA, C4ZB, C4ZC, C4ZD, C4ZE, C4ZF, C4ZG, C4ZH, C4ZI, C4ZJ, C4ZK, C4ZL, C4ZM, C4ZN, C4ZO, C4ZP, C4ZQ, C4ZR, C4ZS, C4ZT, C4ZU, C4ZV, C4ZW, C4ZX, C4ZY, C4ZZ.

Mol	Chain	Residues	Atoms					AltConf
8	D	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	E	1	Total 43	C 34	Fe 1	N 4	O 4	0

- OXY
- O1 O=O O2

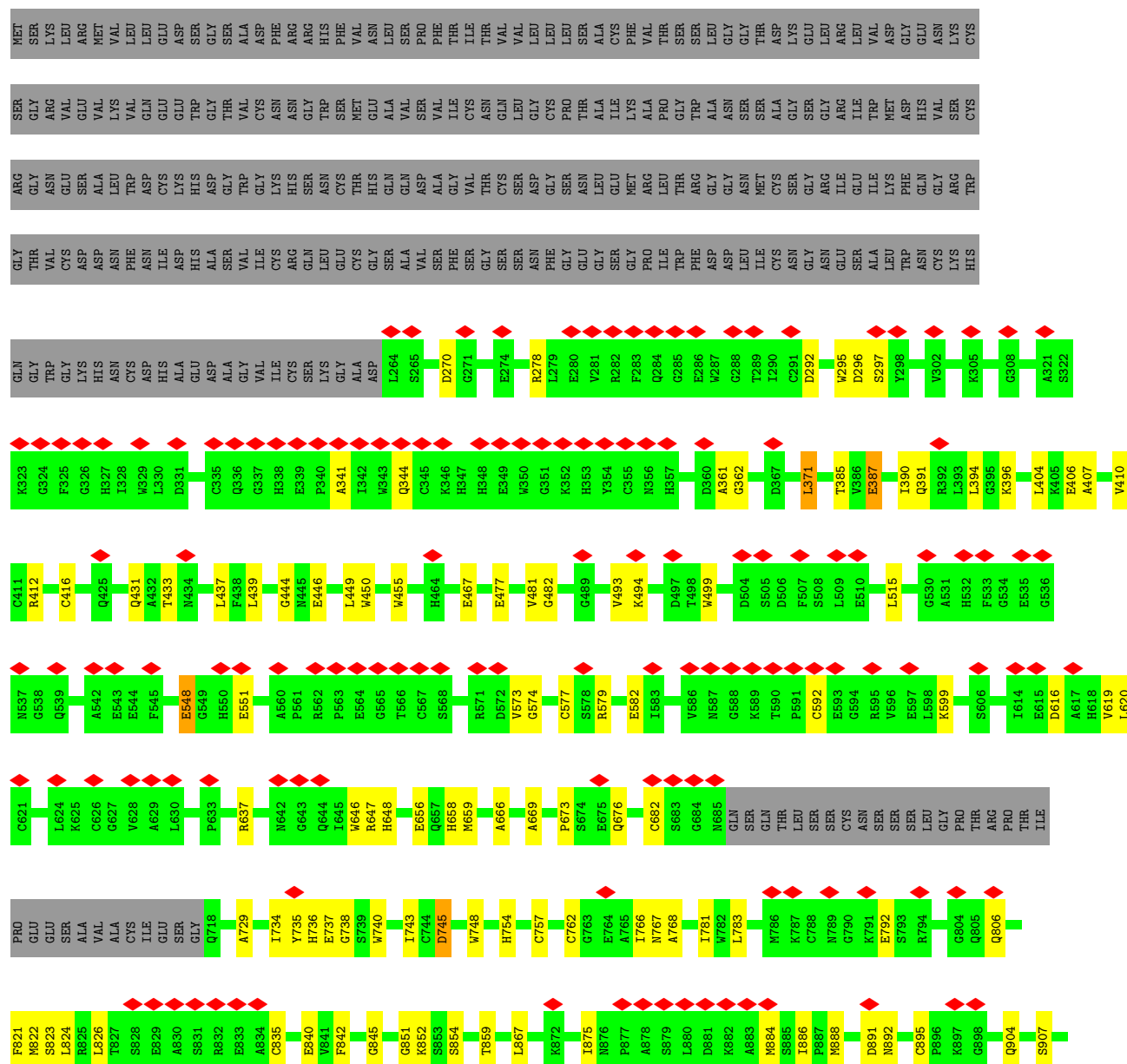
Mol	Chain	Residues	Atoms	AltConf
9	D	1	Total O 2 2	0

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Mol	Chain	Residues	Atoms		AltConf
9	E	1	Total	O	0
			2	2	

- Molecule 1: Scavenger receptor cysteine-rich type 1 protein M130



LEU	THR	GLY	ALA	THR	LEU	ILE	GLN	GLN	TRP	VAL	SER	THR	LEU	VAL	ASN	THR	ALA	LYS	ASN	MET	PRO	ILE	PHE	LEU	ASN	HIS	PRO	SER	GLY	ASN	ALA	THR	ALA	LYS	ASP	ILE	ARG	GLY	VAL	PRO	GLY	THR	LEU	THR	GLY	VAL	ARG	ASN	LYS	GLN	ASN	PHE	LYS	VAL	GLU	THR	ILE	GLU	LYS	VAL	LEU	VAL	TYR	GLY	ASP	HIS	VAL	PRO	ASN	TYR	VAL	SER	ASP	LEU				
VAL	ASP	ILE	GLY	LEU	ILE	LYS	LEU	ASN	GLN	VAL	SER	THR	VAL	ASN	GLU	THR	ARG	VAL	LYS	THR	MET	PRO	ILE	PHE	LEU	ASN	CYS	PRO	SER	GLY	LYS	ASP	ALA	THR	ALA	VAL	GLY	ARG	ILE	VAL	PRO	GLY	THR	LEU	THR	GLY	TRP	TRP	GLY	VAL	ARG	ASN	LYS	GLN	ASN	PHE	LYS	VAL	GLU	THR	ILE	GLU	LYS	VAL	LEU	VAL	TYR	GLY	ASP	HIS	VAL	PRO	ASN	TYR	VAL	SER	ASP	LEU
ASP	GLN	ASP	GLN	CYS	ILE	ARG	HIS	TYR	GLY	ILE	SER	THR	VAL	PRO	GLU	THR	LYS	CYS	ALA	VAL	THR	PRO	LYS	SER	GLY	VAL	GLN	PRO	ILE	ASN	GLU	GLY	HIS	THR	PHE	VAL	CYS	TYR	GLY	ALA	THR	LEU	THR	GLY	MET	SER	TRP	GLY	VAL	ASN	GLN	GLU	ASP	THR	CYS	TYR	GLY	ASP	ALA	GLY	LEU	VAL	ALA	THR	PHE	ALA	VAL	HIS	VAL	ASP	LEU							
GLU	GLU	ASP	THR	TRP	TYR	ALA	THR	GLY	ILE	LEU	SER	PHE	ASP	LYS	SER	CYS	ALA	VAL	ALA	GLU	TYR	GLY	VAL	THR	LYS	VAL	GLN	VAL	THR	SER	ILE	GLN	ASP	TRP	VAL	VAL	GLN	LYS	THR	ILE	ALA	GLU	ASN																																			

● Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

100%

MAG1

MAG2

● Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

50%

50%

50%

MAG1

MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	456124	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 ($e^-/\text{\AA}^2$)	41.68	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.832	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	425.984, 425.984, 425.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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: CA, NAG, OXY, HEM

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	0.17	0/5791	0.43	0/7844
1	B	0.15	0/4890	0.40	0/6625
2	D	0.15	0/1097	0.32	0/1491
3	E	0.15	0/1112	0.30	0/1512
4	F	0.16	0/2357	0.37	0/3199
4	G	0.11	0/72	0.33	0/98
All	All	0.16	0/15319	0.40	0/20769

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	5661	0	5272	101	0
1	B	4780	0	4476	77	0
2	D	1069	0	1070	10	0
3	E	1084	0	1077	8	0
4	F	2303	0	2261	25	0
4	G	69	0	64	2	0
5	C	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	28	0	25	0	0
6	A	28	0	26	0	0
6	B	14	0	13	0	0
6	F	14	0	13	0	0
7	A	6	0	0	0	0
7	B	3	0	0	0	0
8	D	43	0	30	0	0
8	E	43	0	30	2	0
9	D	2	0	0	0	0
9	E	2	0	0	0	0
All	All	15177	0	14382	221	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 7.

The worst 5 of 221 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:GLN:HE22	1:B:433:THR:HG23	1.50	0.77
1:A:857:GLU:N	1:A:857:GLU:OE1	2.21	0.72
1:B:658:HIS:HD2	1:B:659:MET:H	1.35	0.72
1:B:911:GLU:O	1:B:913:ARG:NH1	2.22	0.71
1:B:582:GLU:HB2	1:B:599:LYS:HD3	1.73	0.70

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	744/1156 (64%)	692 (93%)	52 (7%)	0	100	100
1	B	627/1156 (54%)	587 (94%)	40 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
3	E	140/147 (95%)	139 (99%)	1 (1%)	0	100	100
4	F	288/347 (83%)	280 (97%)	8 (3%)	0	100	100
4	G	7/347 (2%)	7 (100%)	0	0	100	100
All	All	1945/3295 (59%)	1841 (95%)	104 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	611/953 (64%)	600 (98%)	11 (2%)	51	80
1	B	514/953 (54%)	505 (98%)	9 (2%)	51	80
2	D	113/114 (99%)	112 (99%)	1 (1%)	70	89
3	E	114/119 (96%)	111 (97%)	3 (3%)	40	73
4	F	252/294 (86%)	245 (97%)	7 (3%)	38	71
4	G	7/294 (2%)	7 (100%)	0	100	100
All	All	1611/2727 (59%)	1580 (98%)	31 (2%)	49	79

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	515	LEU
4	F	95	ASN
1	B	745	ASP
4	F	133	ILE
4	F	59	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	347	HIS
4	F	144	ASN
1	B	391	GLN
4	F	249	GLN
3	E	103	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

4 monosaccharides are 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	$\# Z > 2$
5	NAG	C	1	5,1	14,14,15	0.93	1 (7%)	17,19,21	1.69	2 (11%)
5	NAG	C	2	5	14,14,15	0.75	0	17,19,21	1.04	1 (5%)
5	NAG	H	1	5,1	14,14,15	0.73	0	17,19,21	1.00	2 (11%)
5	NAG	H	2	5	14,14,15	0.72	0	17,19,21	0.86	0

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
5	NAG	C	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	H	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1	NAG	O5-C1	-2.17	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	NAG	C4-C3-C2	4.88	118.17	111.02
5	H	1	NAG	O5-C1-C2	-2.77	107.00	111.29
5	C	1	NAG	C2-N2-C7	2.51	126.26	122.90
5	H	1	NAG	O4-C4-C3	-2.05	105.55	110.38
5	C	2	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

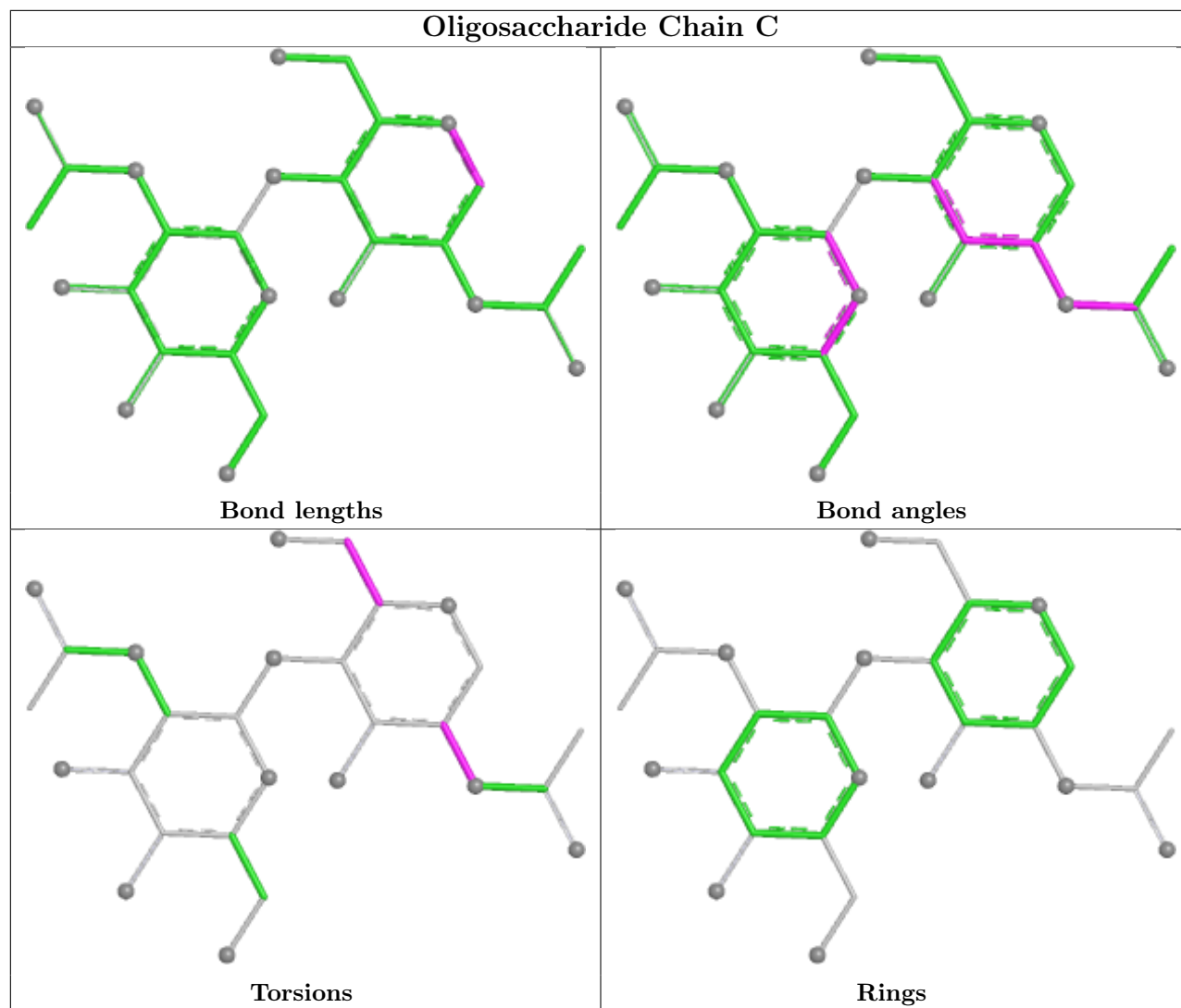
5 of 6 torsion outliers are listed below:

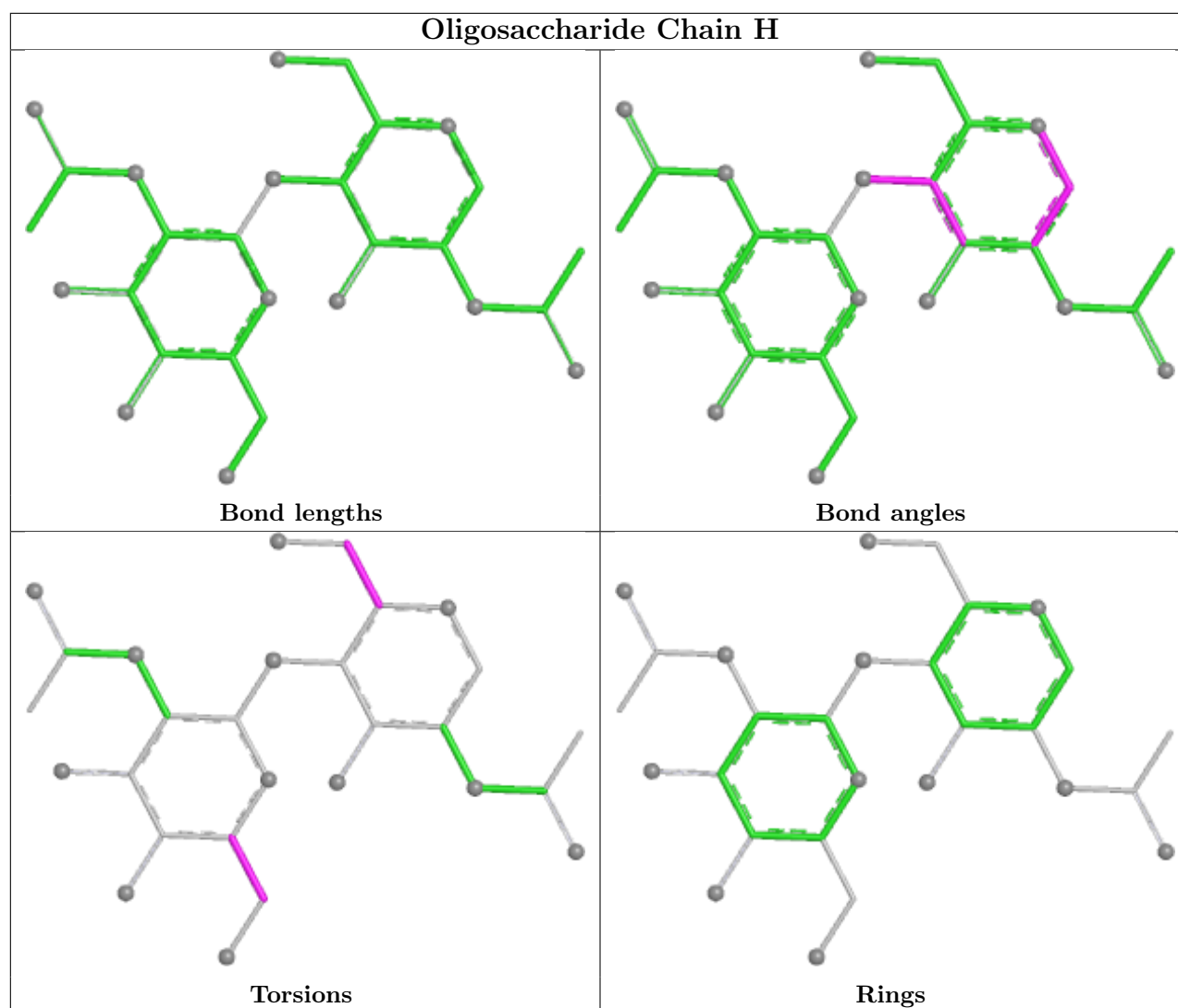
Mol	Chain	Res	Type	Atoms
5	H	1	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
5	C	1	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	B	1201	1	14,14,15	0.72	0	17,19,21	1.16	1 (5%)
9	OXY	D	202	-	1,1,1	0.16	0	-		
6	NAG	A	1202	1	14,14,15	0.69	0	17,19,21	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	HEM	E	201	3	50,50,50	1.39	8 (16%)	67,82,82	0.98	2 (2%)
8	HEM	D	201	2	50,50,50	1.40	8 (16%)	67,82,82	1.07	4 (5%)
6	NAG	A	1201	1	14,14,15	0.76	0	17,19,21	0.80	0
6	NAG	F	401	4	14,14,15	0.73	0	17,19,21	0.80	0
9	OXY	E	202	-	1,1,1	0.16	0	-		

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
6	NAG	B	1201	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1202	1	-	1/6/23/26	0/1/1/1
8	HEM	E	201	3	-	2/14/54/54	-
8	HEM	D	201	2	-	0/14/54/54	-
6	NAG	A	1201	1	-	0/6/23/26	0/1/1/1
6	NAG	F	401	4	-	1/6/23/26	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	201	HEM	FE-NA	3.27	2.05	1.95
8	D	201	HEM	FE-NB	3.16	2.04	1.94
8	D	201	HEM	FE-ND	3.15	2.04	1.94
8	E	201	HEM	FE-NB	3.14	2.04	1.94
8	E	201	HEM	CAB-C3B	3.04	1.55	1.47

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1201	NAG	C2-N2-C7	3.11	127.07	122.90
8	D	201	HEM	C3B-C2B-C1B	2.37	108.19	106.41
8	D	201	HEM	C4D-ND-C1D	2.33	107.97	105.21
8	E	201	HEM	C4D-ND-C1D	2.10	107.69	105.21
8	D	201	HEM	C1B-NB-C4B	2.07	107.66	105.21

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

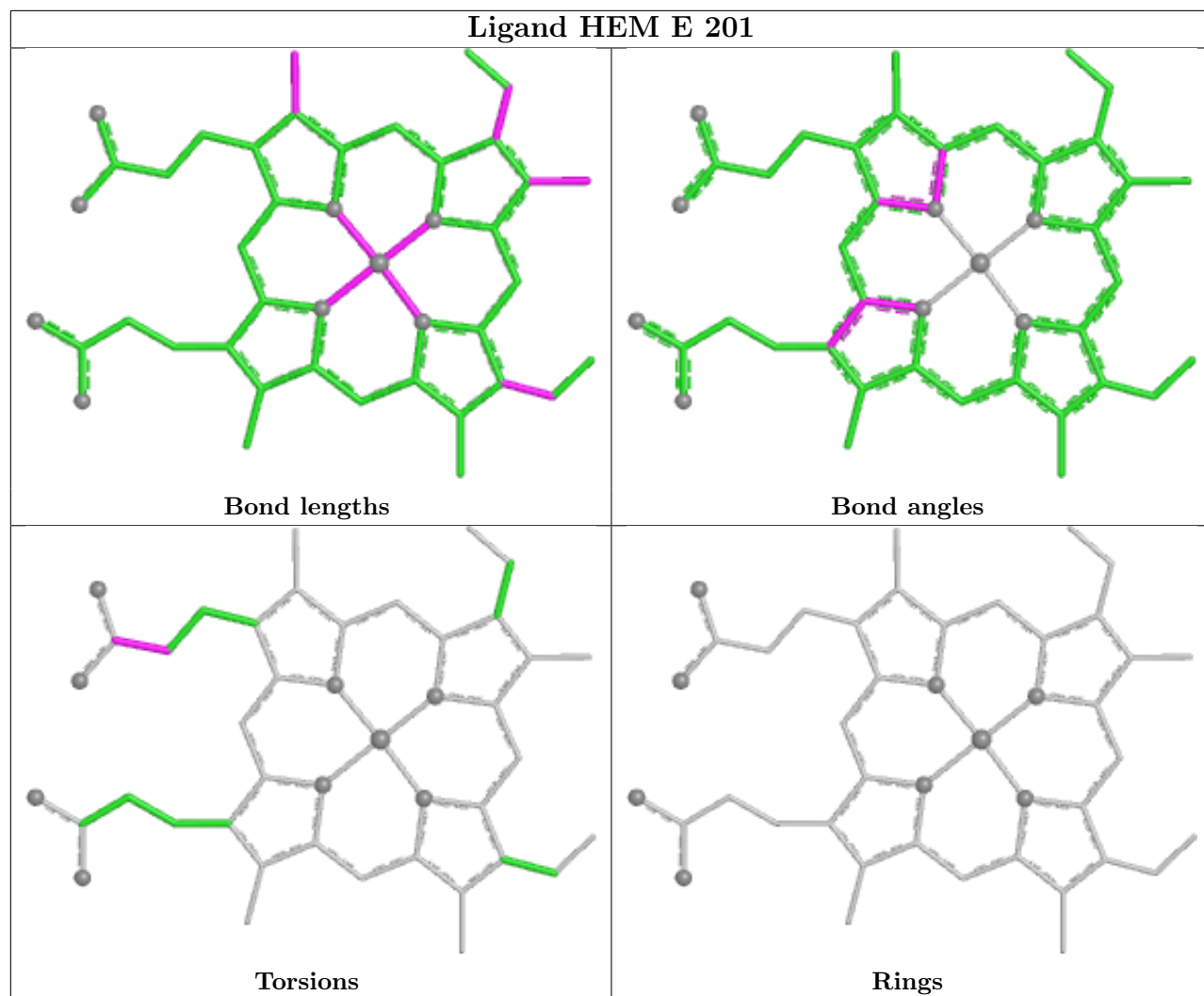
Mol	Chain	Res	Type	Atoms
6	B	1201	NAG	O5-C5-C6-O6
6	B	1201	NAG	C4-C5-C6-O6
6	A	1202	NAG	O5-C5-C6-O6
6	F	401	NAG	O5-C5-C6-O6
6	B	1201	NAG	C3-C2-N2-C7

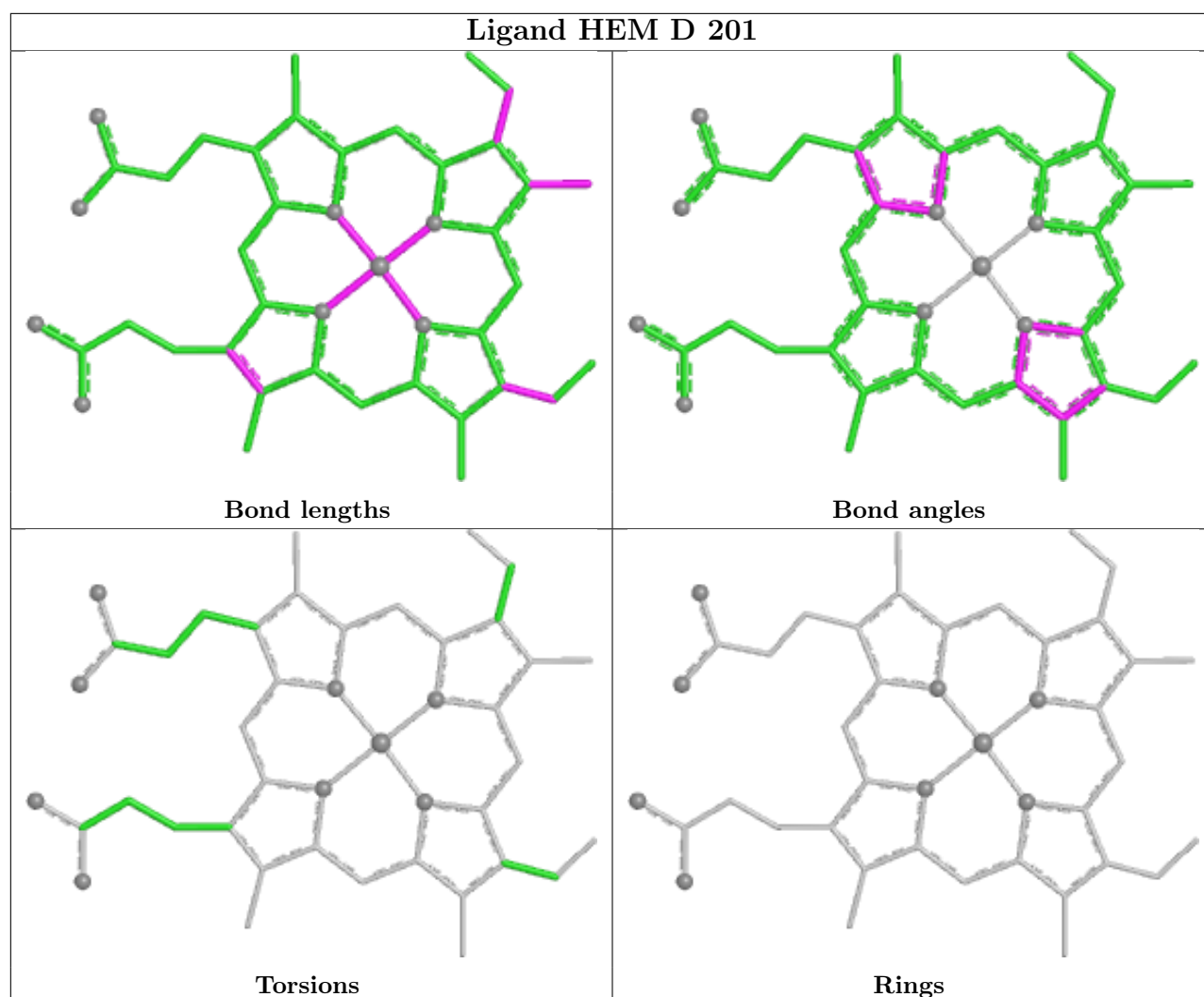
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	201	HEM	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

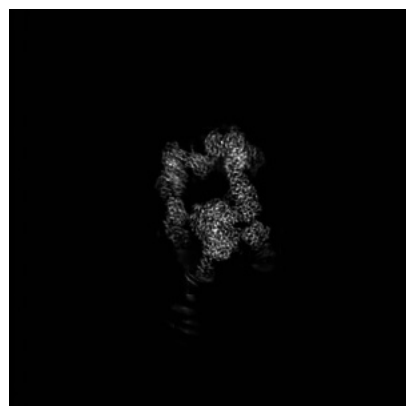
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52078. These allow visual inspection of the internal detail of the map and identification of artifacts.

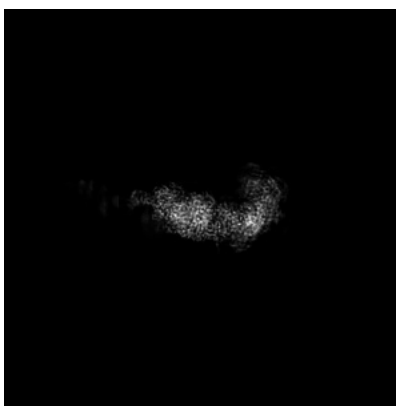
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

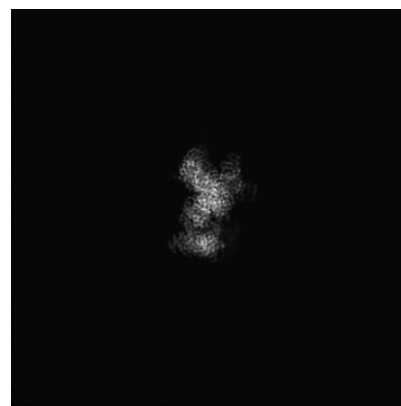
6.1.1 Primary map



X

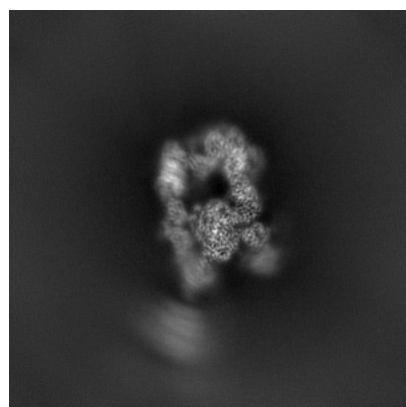


Y

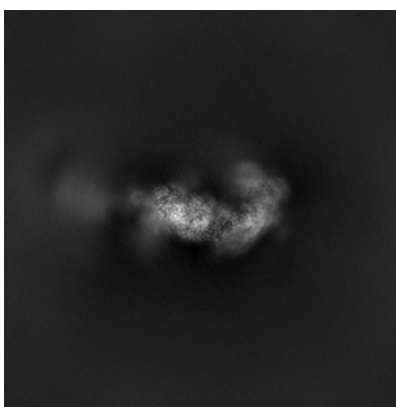


Z

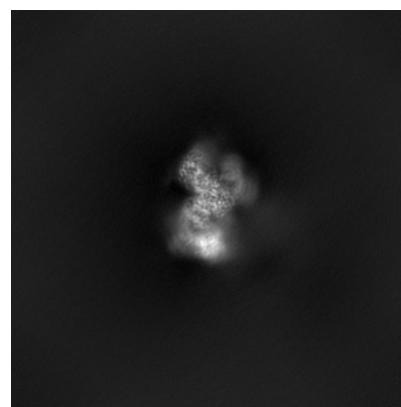
6.1.2 Raw map



X



Y



Z

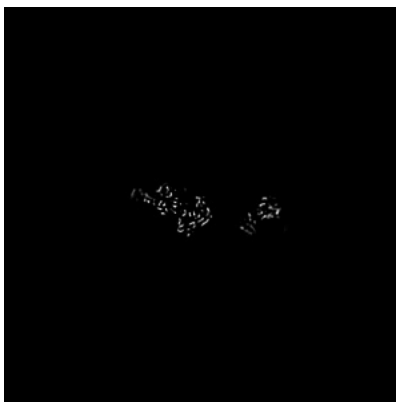
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256

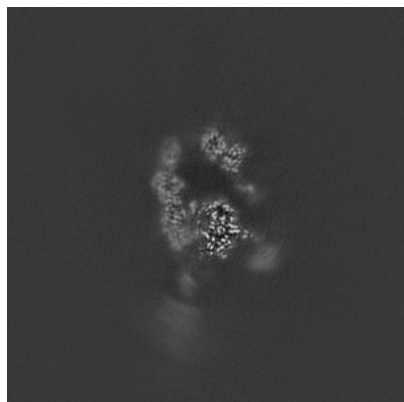


Y Index: 256

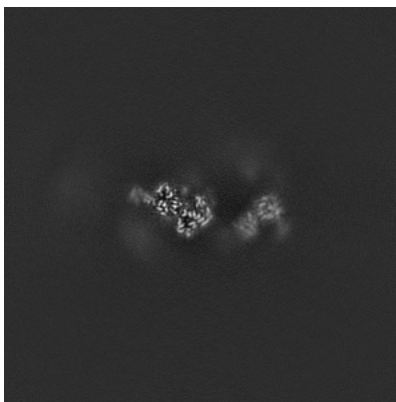


Z Index: 256

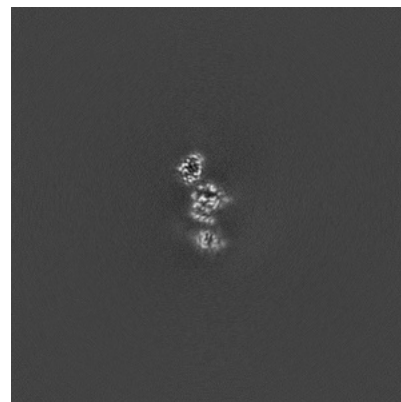
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

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: 239

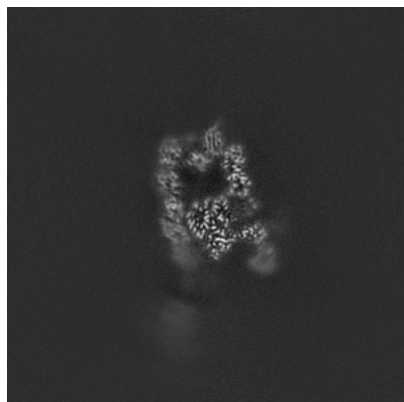


Y Index: 290

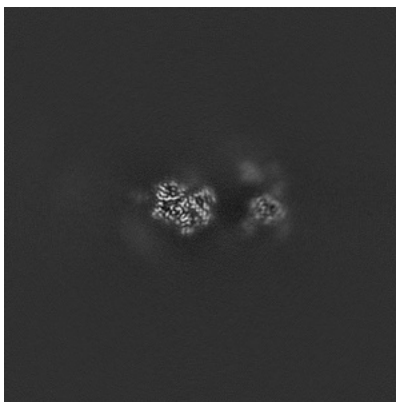


Z Index: 325

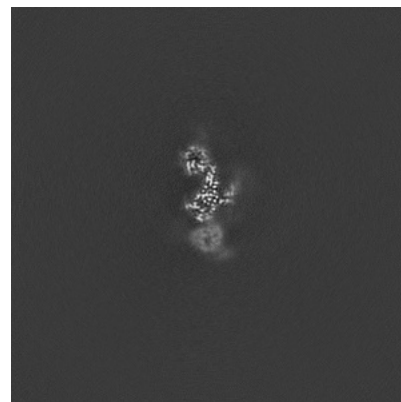
6.3.2 Raw map



X Index: 245



Y Index: 265

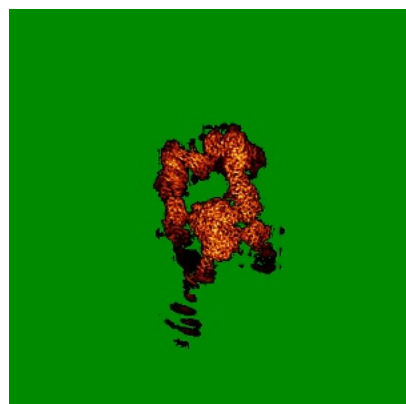


Z Index: 224

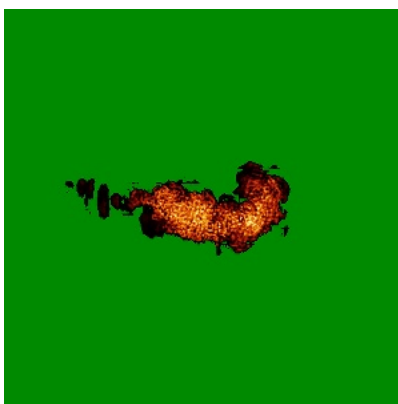
The images above show the largest variance slices of the map in three orthogonal directions.

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

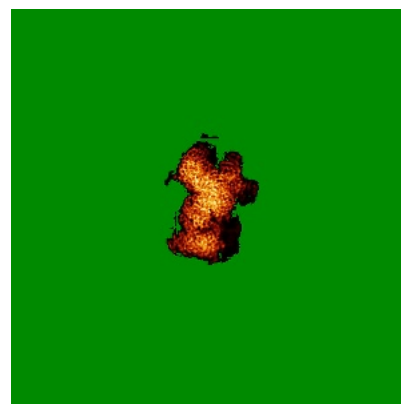
6.4.1 Primary map



X

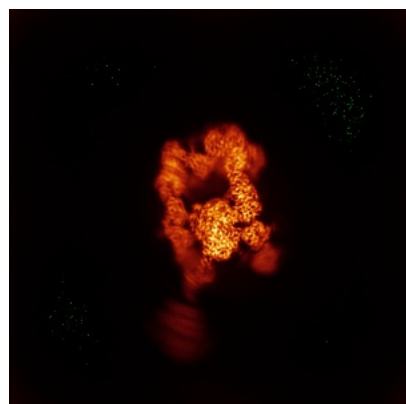


Y

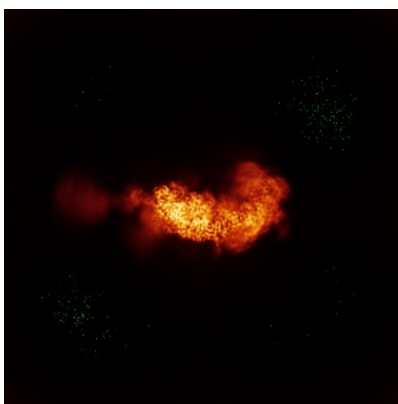


Z

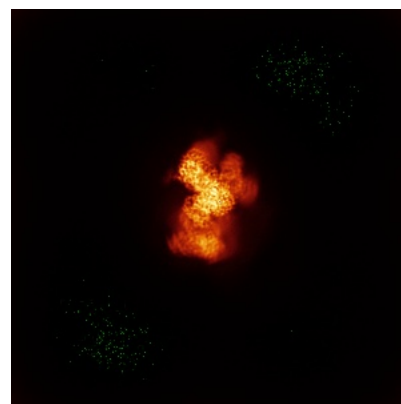
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

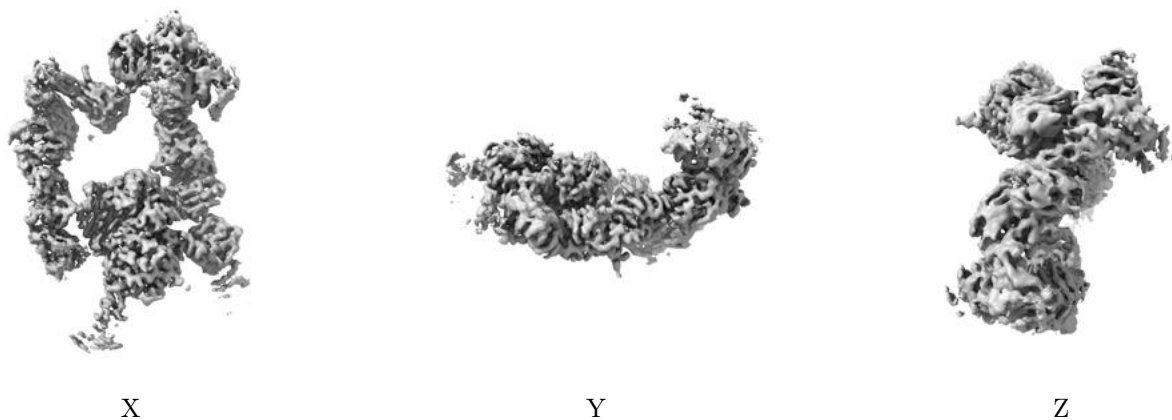
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

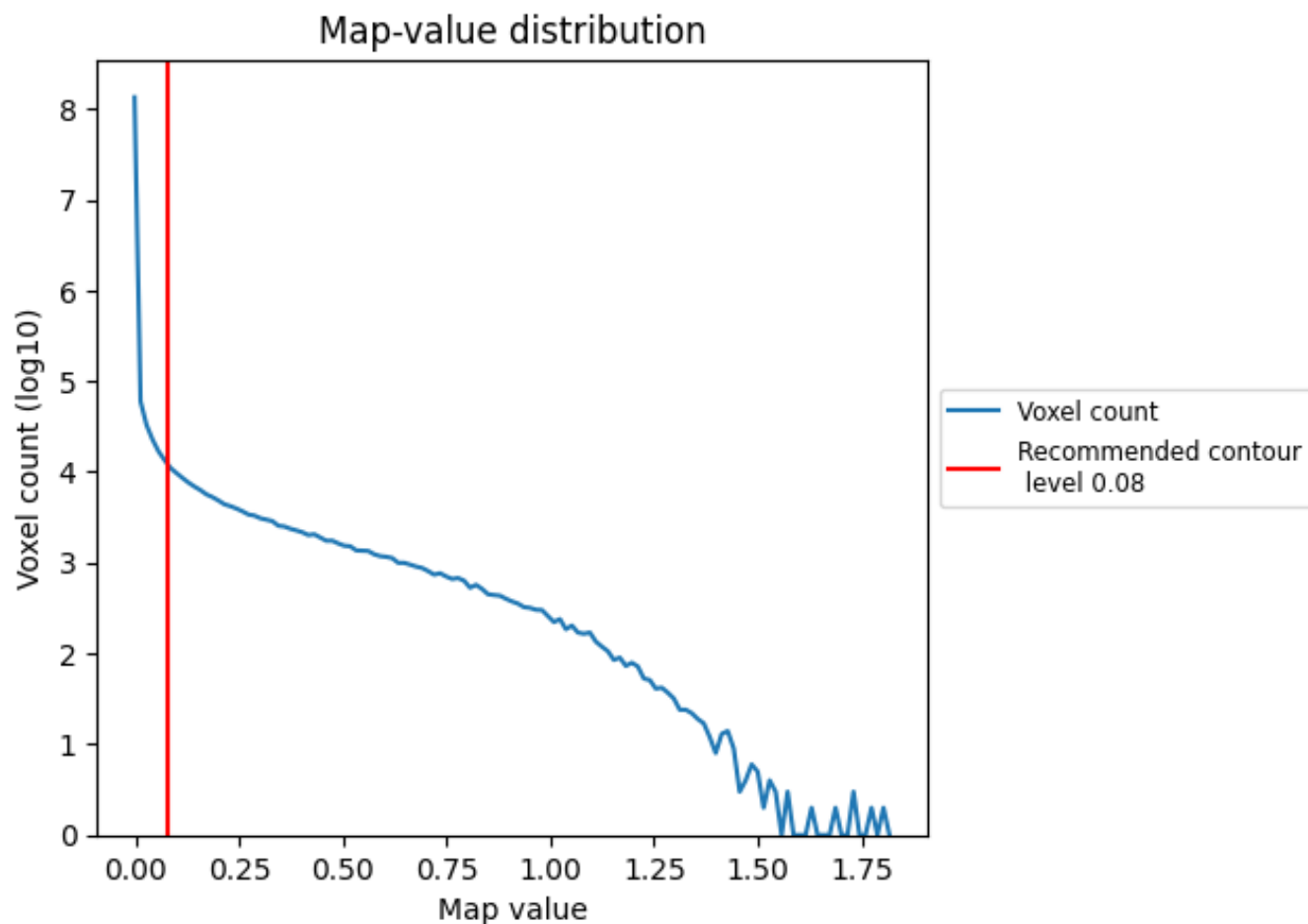
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

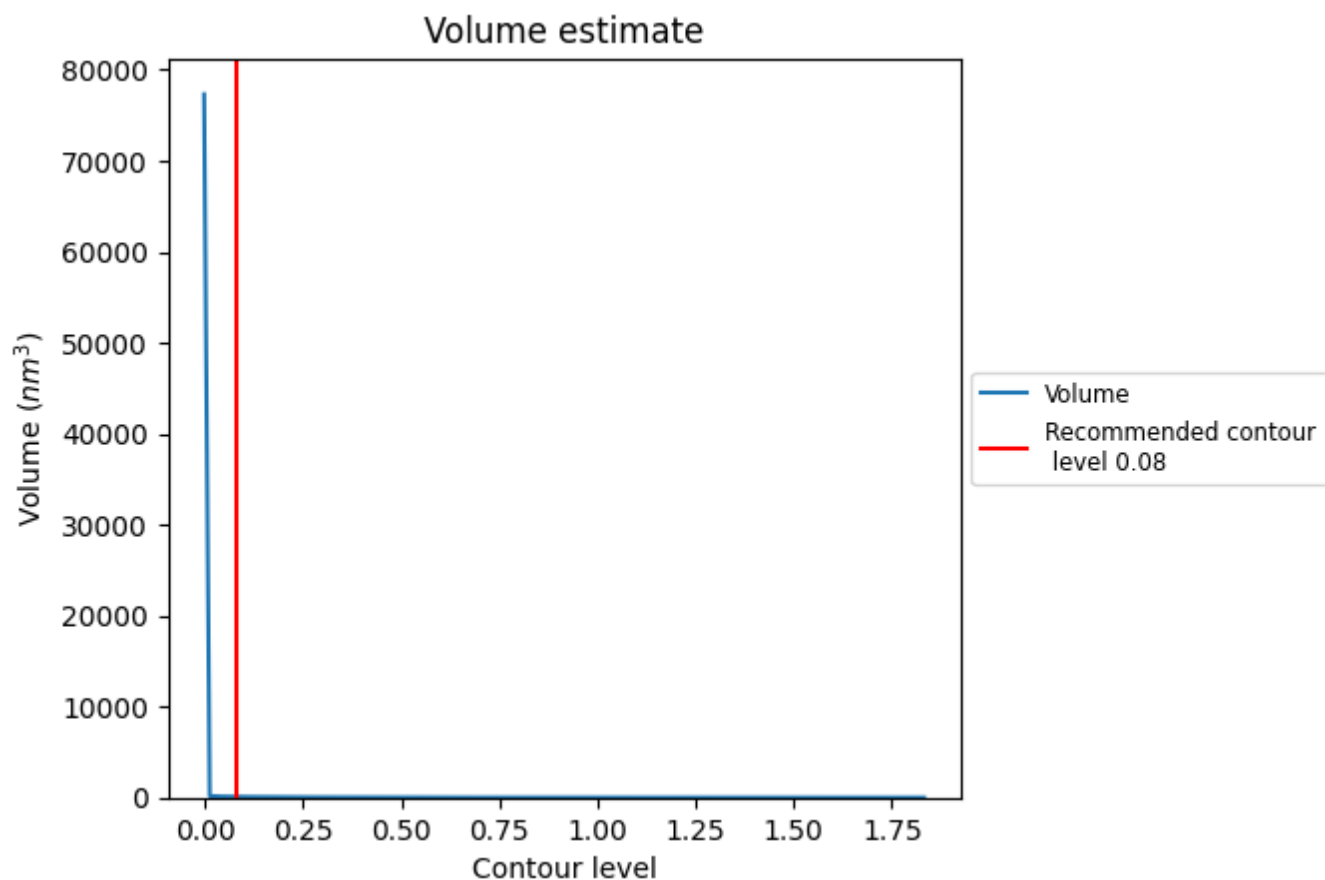
This section contains the results of statistical analysis of the map.

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.

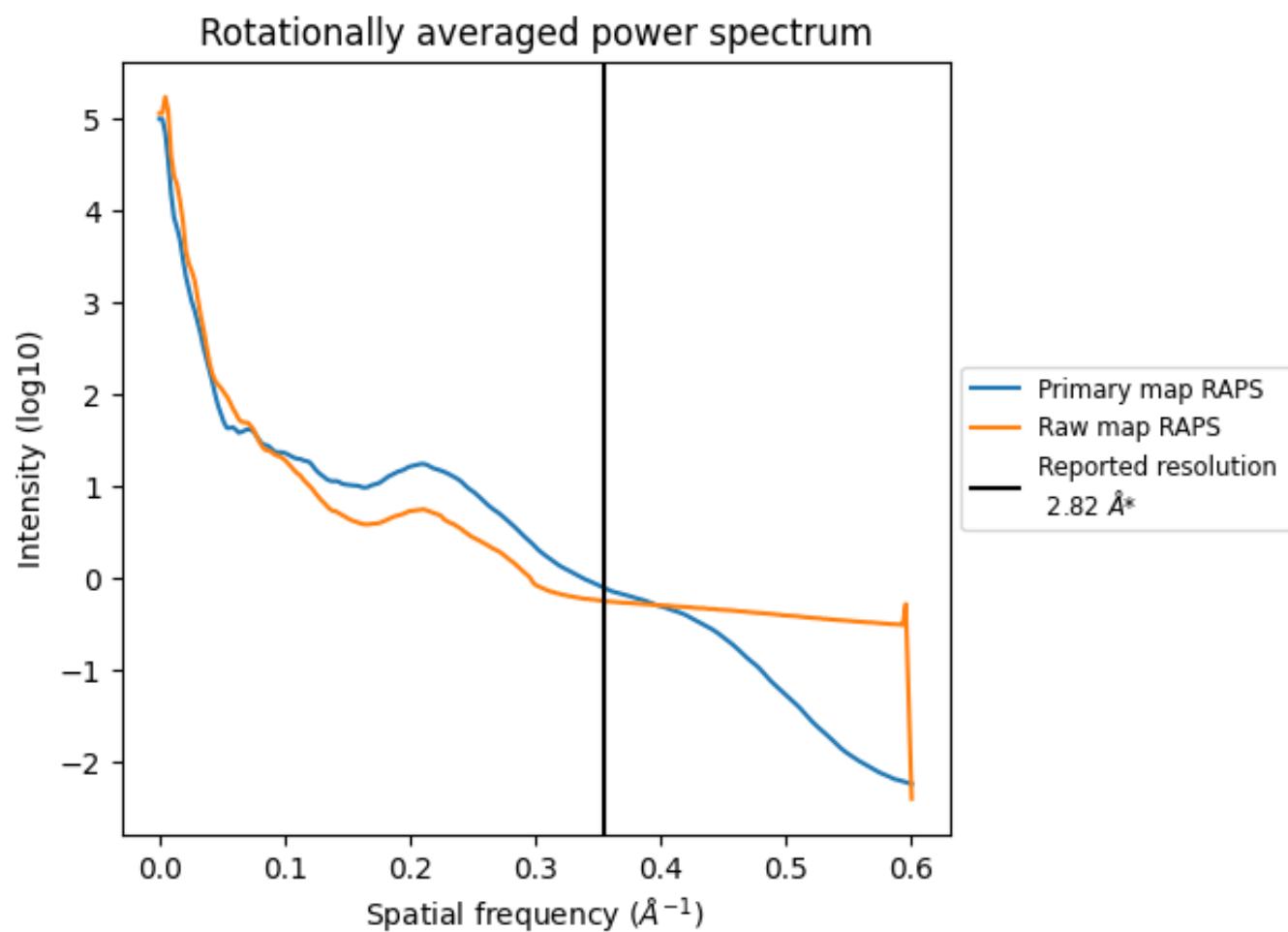
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89 nm^3 ; this corresponds to an approximate mass of 81 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 ⓘ

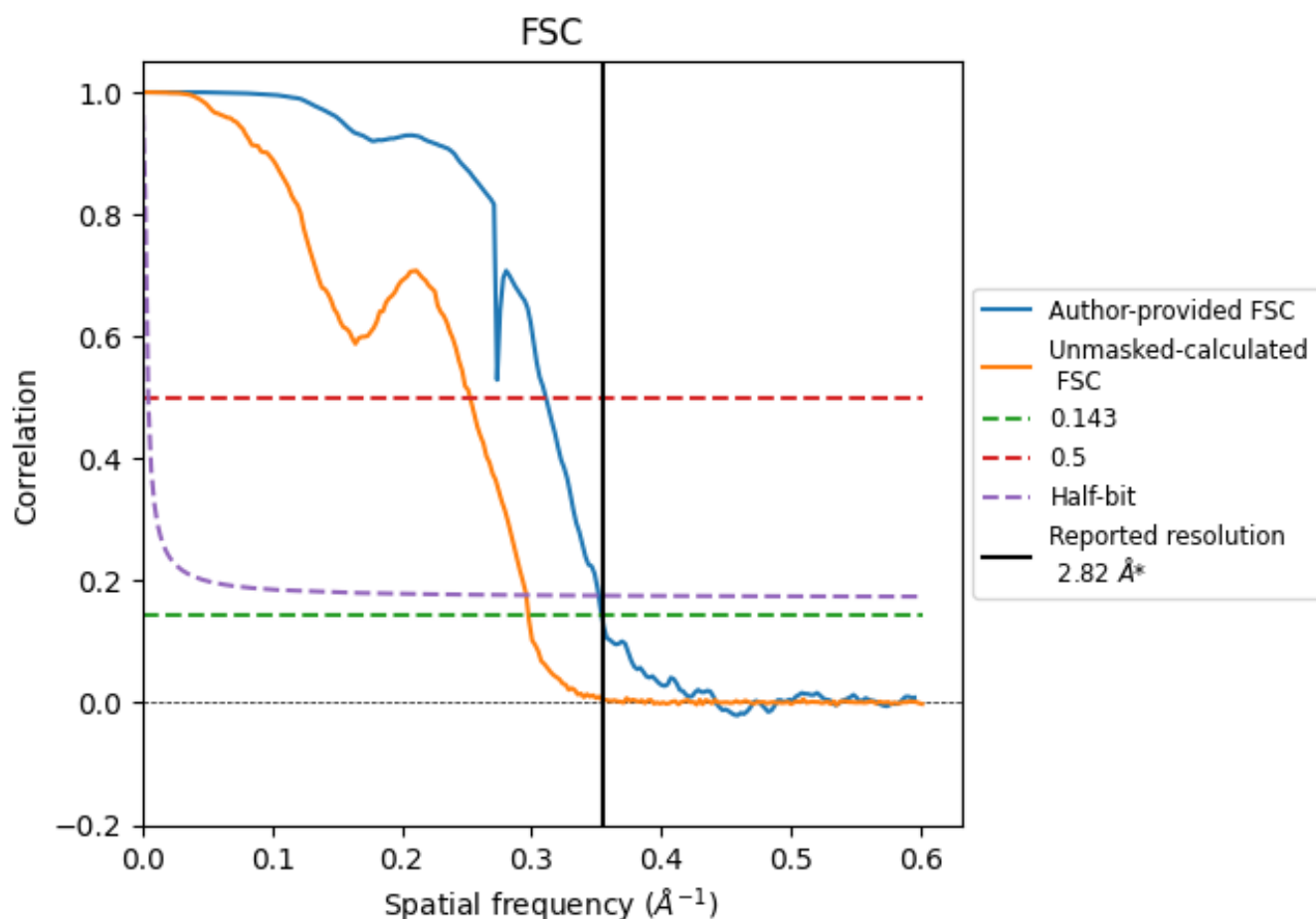


*Reported resolution corresponds to spatial frequency of 0.355 Å⁻¹

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 0.355 \AA^{-1}

8.2 Resolution estimates [i](#)

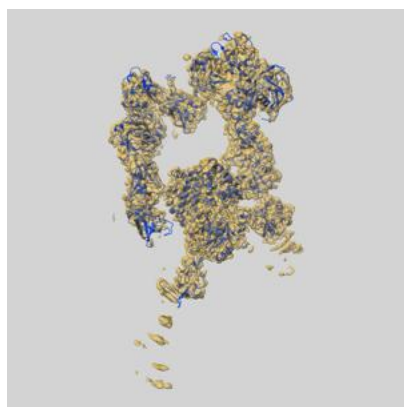
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.82	-	-
Author-provided FSC curve	2.82	3.21	2.84
Unmasked-calculated*	3.36	3.96	3.38

*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 3.36 differs from the reported value 2.82 by more than 10 %

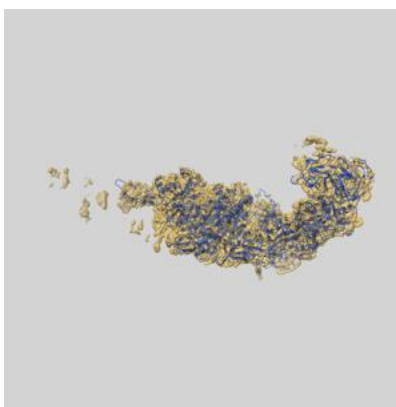
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52078 and PDB model 9HEJ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

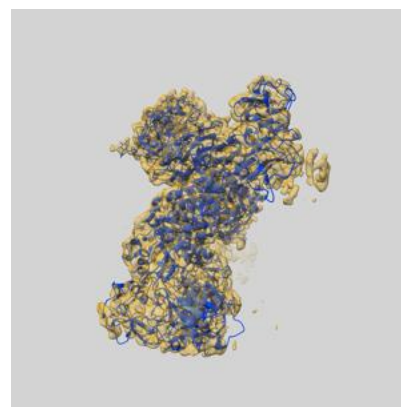
9.1 Map-model overlay [i](#)



X



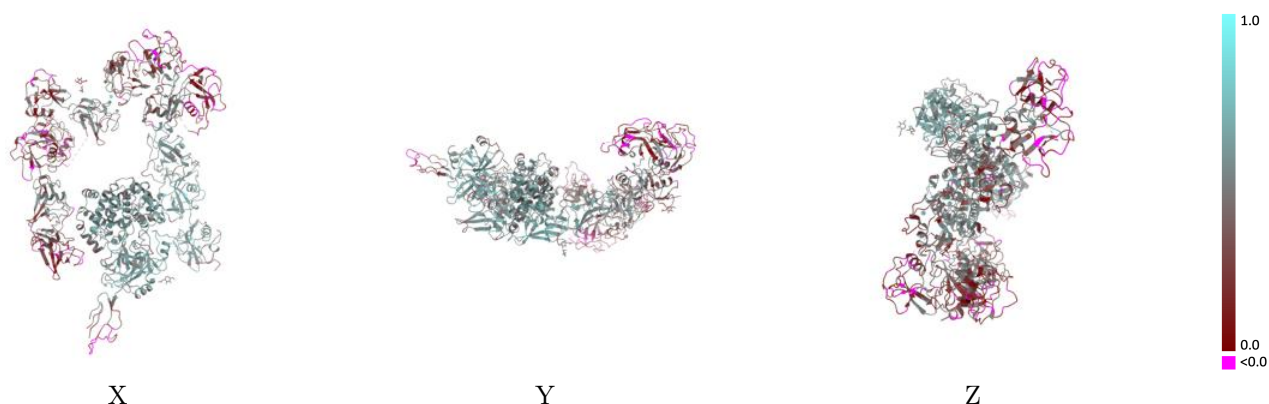
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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](#)



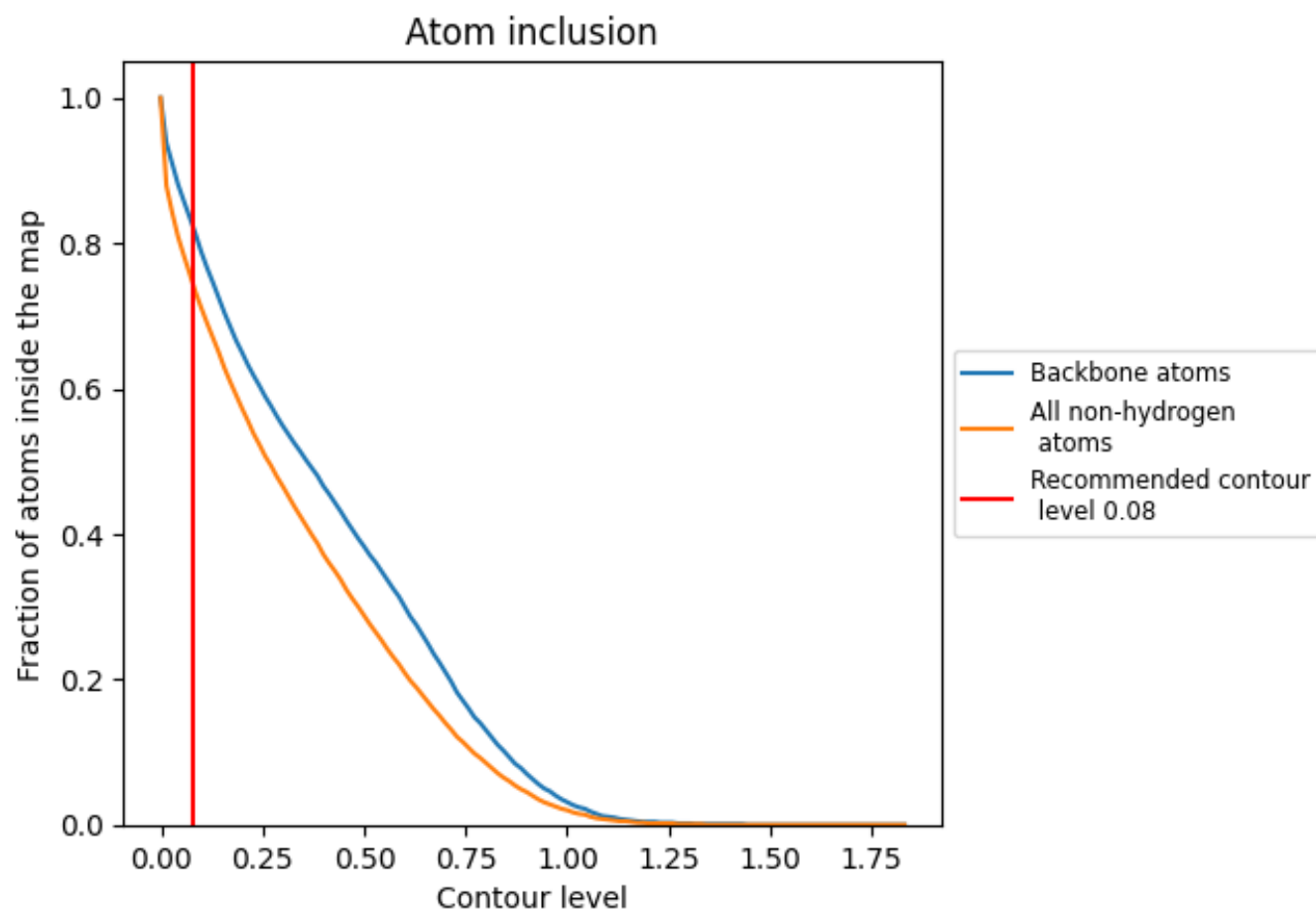
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 74% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7410	<div></div> 0.4110
A	<div></div> 0.7460	<div></div> 0.4080
B	<div></div> 0.6190	<div></div> 0.2990
C	<div></div> 0.8570	<div></div> 0.4640
D	<div></div> 0.8870	<div></div> 0.5530
E	<div></div> 0.8820	<div></div> 0.5440
F	<div></div> 0.8440	<div></div> 0.5200
G	<div></div> 0.7650	<div></div> 0.3690
H	<div></div> 0.5000	<div></div> 0.2270

1.0

0.0

<0.0