



Full wwPDB EM Validation Report ⓘ

Aug 17, 2026 – 04:56 PM JST

PDB ID : 9X0R / pdb_00009x0r
EMDB ID : EMD-66440
Title : Cryo-EM Structure of Alcohol Dehydrogenase Variant from *Gluconobacter oxydans* Truncating Membrane-Binding Regions (Form 2)
Authors : Ichikawa, K.; Adachi, T.; Miyata, T.; Makino, F.; Namba, K.; Kitazumi, Y.; Shirai, O.; Sowa, K.
Deposited on : 2025-09-30
Resolution : 2.69 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

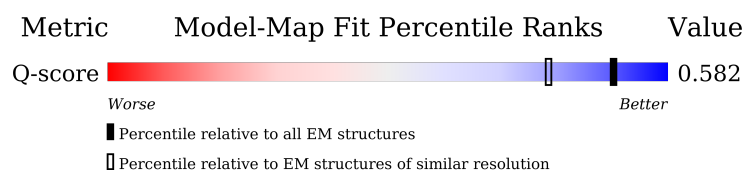
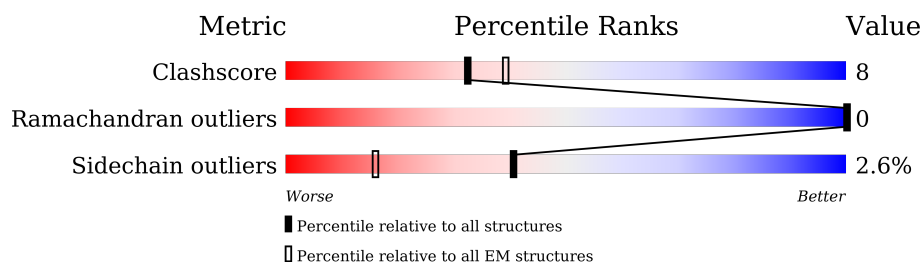
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.69 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	9309 (2.19 - 3.19)

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	757	
2	B	462	
3	C	133	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	HEC	A	801	X	-	-	-
4	HEC	B	501	X	-	-	-
4	HEC	B	502	X	-	-	-
4	HEC	B	503	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8969 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 Alcohol dehydrogenase (quinone), dehydrogenase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	723	Total	C	N	O	S	0	0
			5621	3592	952	1060	17		

- Molecule 2 is a protein called Alcohol dehydrogenase (quinone), cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	313	Total	C	N	O	S	0	0
			2335	1453	411	455	16		

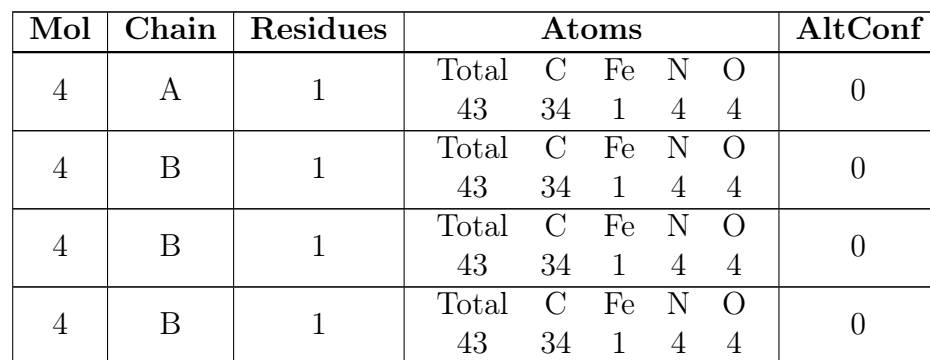
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	77	GLY	PRO	conflict	UNP Q47945
B	78	GLY	ILE	conflict	UNP Q47945
B	159	GLY	-	linker	UNP Q47945
B	160	GLY	-	linker	UNP Q47945
B	161	GLY	-	linker	UNP Q47945
B	162	GLY	-	linker	UNP Q47945
B	?	-	GLY	deletion	UNP Q47945
B	?	-	PHE	deletion	UNP Q47945
B	?	-	GLY	deletion	UNP Q47945
B	?	-	MET	deletion	UNP Q47945

- Molecule 3 is a protein called Small subunit of alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	107	Total	C	N	O	S	0	0
			816	515	135	162	4		

- Molecule 4 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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- The chemical structure of PQQ (Pyrroloquinoline quinone) is shown, featuring a fused ring system with two nitrogen atoms (N1, N6) and four carbonyl groups. The structure is labeled with atom names and numbers:
- Carbonyl groups: C7X=O7A, C9X=O9B, C2X=O2A, C4=O4.
 - Hydroxyl groups: OH (O7B) at C7X, HO (O2B) at C2X.
 - Ring atoms: N1, N6, C2, C3, C4, C5, C6A, C7, C8, C9, C9A, C9B, C9C, C9D, C9E, C9F, C9G, C9H, C9I, C9J, C9K, C9L, C9M, C9N, C9O, C9P, C9Q, C9R, C9S, C9T, C9U, C9V, C9W, C9X, C9Y, C9Z, C9AA, C9AB, C9AC, C9AD, C9AE, C9AF, C9AG, C9AH, C9AI, C9AJ, C9AK, C9AL, C9AM, C9AN, C9AO, C9AP, C9AQ, C9AR, C9AS, C9AT, C9AU, C9AV, C9AW, C9AX, C9AY, C9AZ, C9BA, C9BB, C9BC, C9BD, C9BE, C9BF, C9BG, C9BH, C9BI, C9BJ, C9BK, C9BL, C9BM, C9BN, C9BO, C9BP, C9BQ, C9BR, C9BS, C9BT, C9BU, C9BV, C9BW, C9BX, C9BY, C9BZ, C9CA, C9CB, C9CC, C9CD, C9CE, C9CF, C9CG, C9CH, C9CI, C9CJ, C9CK, C9CL, C9CM, C9CN, C9CO, C9CP, C9CQ, C9CR, C9CS, C9CT, C9CU, C9CV, C9CW, C9CX, C9CY, C9CZ, C9DA, C9DB, C9DC, C9DD, C9DE, C9DF, C9DG, C9DH, C9DI, C9DJ, C9DK, C9DL, C9DM, C9DN, C9DO, C9DP, C9DQ, C9DR, C9DS, C9DT, C9DU, C9DV, C9DW, C9DX, C9DY, C9DZ, C9EA, C9EB, C9EC, C9ED, C9EE, C9EF, C9EG, C9EH, C9EI, C9EJ, C9EK, C9EL, C9EM, C9EN, C9EO, C9EP, C9EQ, C9ER, C9ES, C9ET, C9EU, C9EV, C9EW, C9EX, C9EY, C9EZ, C9FA, C9FB, C9FC, C9FD, C9FE, C9FF, C9FG, C9FH, C9FI, C9FJ, C9FK, C9FL, C9FM, C9FN, C9FO, C9FP, C9FQ, C9FR, C9FS, C9FT, C9FU, C9FV, C9FW, C9FX, C9FY, C9FZ, C9GA, C9GB, C9GC, C9GD, C9GE, C9GF, C9GG, C9GH, C9GI, C9GJ, C9GK, C9GL, C9GM, C9GN, C9GO, C9GP, C9GQ, C9GR, C9GS, C9GT, C9GU, C9GV, C9GW, C9GX, C9GY, C9GZ, C9HA, C9HB, C9HC, C9HD, C9HE, C9HF, C9HG, C9HH, C9HI, C9HJ, C9HK, C9HL, C9HM, C9HN, C9HO, C9HP, C9HQ, C9HR, C9HS, C9HT, C9HU, C9HV, C9HW, C9HX, C9HY, C9HZ, C9IA, C9IB, C9IC, C9ID, C9IE, C9IF, C9IG, C9IH, C9II, C9IJ, C9IK, C9IL, C9IM, C9IN, C9IO, C9IP, C9IQ, C9IR, C9IS, C9IT, C9IU, C9IV, C9IW, C9IX, C9IY, C9IZ, C9JA, C9JB, C9JC, C9JD, C9JE, C9JF, C9JG, C9JH, C9JI, C9JJ, C9JK, C9JL, C9JM, C9JN, C9JO, C9JP, C9JQ, C9JR, C9JS, C9JT, C9JU, C9JV, C9JW, C9JX, C9JY, C9JZ, C9KA, C9KB, C9KC, C9KD, C9KE, C9KF, C9KG, C9KH, C9KI, C9KJ, C9KK, C9KL, C9KM, C9KN, C9KO, C9KP, C9KQ, C9KR, C9KS, C9KT, C9KU, C9KV, C9KW, C9KX, C9KY, C9KZ, C9LA, C9LB, C9LC, C9LD, C9LE, C9LF, C9LG, C9LH, C9LI, C9LJ, C9LK, C9LL, C9LM, C9LN, C9LO, C9LP, C9LQ, C9LR, C9LS, C9LT, C9LU, C9LV, C9LW, C9LX, C9LY, C9LZ, C9MA, C9MB, C9MC, C9MD, C9ME, C9MF, C9MG, C9MH, C9MI, C9MJ, C9MK, C9ML, C9MM, C9MN, C9MO, C9MP, C9MQ, C9MR, C9MS, C9MT, C9MU, C9MV, C9MW, C9MX, C9MY, C9MZ, C9NA, C9NB, C9NC, C9ND, C9NE, C9NF, C9NG, C9NH, C9NI, C9NJ, C9NK, C9NL, C9NM, C9NO, C9NP, C9NQ, C9NR, C9NS, C9NT, C9NU, C9NV, C9NW, C9NX, C9NY, C9NZ, C9OA, C9OB, C9OC, C9OD, C9OE, C9OF, C9OG, C9OH, C9OI, C9OJ, C9OK, C9OL, C9OM, C9ON, C9OO, C9OP, C9OQ, C9OR, C9OS, C9OT, C9OU, C9OV, C9OW, C9OX, C9OY, C9OZ, C9PA, C9PB, C9PC, C9PD, C9PE, C9PF, C9PG, C9PH, C9PI, C9PJ, C9PK, C9PL, C9PM, C9PN, C9PO, C9PP, C9PQ, C9PR, C9PS, C9PT, C9PU, C9PV, C9PW, C9PX, C9PY, C9PZ, C9QA, C9QB, C9QC, C9QD, C9QE, C9QF, C9QG, C9QH, C9QI, C9QJ, C9QK, C9QL, C9QM, C9QN, C9QO, C9QP, C9QQ, C9QR, C9QS, C9QT, C9QU, C9QV, C9QW, C9QX, C9QY, C9QZ, C9RA, C9RB, C9RC, C9RD, C9RE, C9RF, C9RG, C9RH, C9RI, C9RJ, C9RK, C9RL, C9RM, C9RN, C9RO, C9RP, C9RQ, C9RR, C9RS, C9RT, C9RU, C9RV, C9RW, C9RX, C9RY, C9RZ, C9SA, C9SB, C9SC, C9SD, C9SE, C9SF, C9SG, C9SH, C9SI, C9SJ, C9SK, C9SL, C9SM, C9SN, C9SO, C9SP, C9SQ, C9SR, C9SS, C9ST, C9SU, C9SV, C9SW, C9SX, C9SY, C9SZ, C9TA, C9TB, C9TC, C9TD, C9TE, C9TF, C9TG, C9TH, C9TI, C9TJ, C9TK, C9TL, C9TM, C9TN, C9TO, C9TP, C9TQ, C9TR, C9TS, C9TT, C9TU, C9TV, C9TW, C9TX, C9TY, C9TZ, C9UA, C9UB, C9UC, C9UD, C9UE, C9UF, C9UG, C9UH, C9UI, C9UJ, C9UK, C9UL, C9UM, C9UN, C9UO, C9UP, C9UQ, C9UR, C9US, C9UT, C9UU, C9UV, C9UW, C9UX, C9UY, C9UZ, C9VA, C9VB, C9VC, C9VD, C9VE, C9VF, C9VG, C9VH, C9VI, C9VJ, C9VK, C9VL, C9VM, C9VN, C9VO, C9VP, C9VQ, C9VR, C9VS, C9VT, C9VU, C9VV, C9VW, C9VX, C9VY, C9VZ, C9WA, C9WB, C9WC, C9WD, C9WE, C9WF, C9WG, C9WH, C9WI, C9WJ, C9WK, C9WL, C9WM, C9WN, C9WO, C9WP, C9WQ, C9WR, C9WS, C9WT, C9WU, C9WV, C9WW, C9WX, C9WY, C9WZ, C9XA, C9XB, C9XC, C9XD, C9XE, C9XF, C9XG, C9XH, C9XI, C9XJ, C9XK, C9XL, C9XM, C9XN, C9XO, C9XP, C9XQ, C9XR, C9XS, C9XT, C9XU, C9XV, C9XW, C9XX, C9XY, C9XZ, C9YA, C9YB, C9YC, C9YD, C9YE, C9YF, C9YG, C9YH, C9YI, C9YJ, C9YK, C9YL, C9YM, C9YN, C9YO, C9YP, C9YQ, C9YR, C9YS, C9YT, C9YU, C9YV, C9YW, C9YX, C9YY, C9YZ, C9ZA, C9ZB, C9ZC, C9ZD, C9ZE, C9ZF, C9ZG, C9ZH, C9ZI, C9ZJ, C9ZK, C9ZL, C9ZM, C9ZN, C9ZO, C9ZP, C9ZQ, C9ZR, C9ZS, C9ZT, C9ZU, C9ZV, C9ZW, C9ZX, C9ZY, C9ZZ.

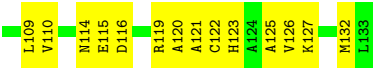
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			24	14	2	8	

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	



• Molecule 3: Small subunit of alcohol dehydrogenase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	119667	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	56754	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.240	Depositor
Minimum map value	-0.091	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	274.88, 274.88, 274.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.859, 0.859, 0.859	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, PQQ, HEC

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	0.11	0/5792	0.27	0/7892
2	B	0.13	0/2396	0.35	1/3267 (0.0%)
3	C	0.12	0/838	0.41	0/1141
All	All	0.12	0/9026	0.31	1/12300 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	58	ALA	CB-CA-C	-5.17	110.63	116.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	125	GLU	Peptide

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	5621	0	5364	85	0
2	B	2335	0	2202	44	0
3	C	816	0	765	24	0
4	A	43	0	30	2	0
4	B	129	0	90	6	0
5	A	24	0	3	1	0
6	A	1	0	0	0	0
All	All	8969	0	8454	148	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 8.

All (148) 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:B:128:ARG:HG3	2:B:129:LEU:HG	1.73	0.70
1:A:215:GLU:OE2	5:A:802:PQQ:C7X	2.39	0.70
2:B:117:VAL:HG23	2:B:119:PRO:HD3	1.74	0.69
1:A:65:ARG:HH22	1:A:97:THR:HG21	1.58	0.68
2:B:126:PHE:HB3	2:B:132:ASP:HA	1.76	0.67
1:A:73:ASN:H	1:A:76:ASN:HB2	1.62	0.64
3:C:87:VAL:HG12	3:C:88:GLY:H	1.62	0.64
1:A:401:VAL:HG23	1:A:402:THR:HG23	1.82	0.62
3:C:64:VAL:HG23	3:C:65:SER:H	1.65	0.61
1:A:365:VAL:HG12	1:A:375:ILE:HG12	1.82	0.61
1:A:64:GLN:HA	1:A:350:MET:HE2	1.82	0.60
1:A:222:VAL:HG21	1:A:293:LEU:HD22	1.84	0.60
1:A:297:ASN:CG	1:A:342:ASP:OD1	2.45	0.59
1:A:304:LYS:H	1:A:414:THR:HG21	1.67	0.59
1:A:229:THR:HG23	1:A:231:LYS:H	1.66	0.59
2:B:125:GLU:HB2	2:B:189:PRO:HG3	1.84	0.59
2:B:295:ASN:HB3	2:B:349:ILE:HG23	1.84	0.59
1:A:142:CYS:HB3	1:A:588:ILE:HD13	1.83	0.59
1:A:241:ASN:HD21	1:A:245:LYS:H	1.49	0.59
2:B:363:GLY:HA3	2:B:378:MET:O	2.04	0.58
4:B:502:HEC:HBD2	4:B:502:HEC:HHA	1.84	0.58
1:A:304:LYS:HE2	3:C:83:THR:HB	1.86	0.57
2:B:348:VAL:HG13	2:B:356:LEU:HD21	1.87	0.57
1:A:685:LEU:HD22	1:A:690:ALA:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:LEU:HB3	1:A:568:PRO:HG2	1.88	0.55
2:B:191:HIS:HB3	2:B:194:GLU:HG3	1.88	0.55
1:A:253:ASP:O	1:A:257:SER:HB3	2.07	0.55
1:A:469:TRP:HE3	1:A:471:LEU:HD11	1.71	0.55
2:B:123:TYR:HB3	2:B:124:PRO:HD3	1.89	0.55
1:A:143:ASP:HB3	1:A:145:VAL:HG13	1.89	0.54
1:A:152:TRP:HB2	1:A:202:ILE:HD12	1.90	0.54
3:C:120:ALA:HA	3:C:123:HIS:HB2	1.89	0.54
1:A:526:GLY:HA3	1:A:567:PRO:HB3	1.88	0.54
1:A:546:ALA:HB3	1:A:556:TYR:HB3	1.90	0.53
1:A:387:LYS:HD2	1:A:511:MET:HB3	1.90	0.53
1:A:302:ASN:HB3	1:A:305:PHE:HB2	1.91	0.53
2:B:56:CYS:HB3	4:B:501:HEC:HHC	1.91	0.52
2:B:240:GLU:OE1	2:B:282:LYS:HG2	2.09	0.52
1:A:649:TYR:HE2	1:A:670:LEU:HD12	1.73	0.52
2:B:247:LEU:HD22	2:B:269:THR:HG21	1.92	0.52
1:A:91:ASN:HB3	2:B:439:TYR:CZ	2.45	0.52
1:A:624:ASN:HD21	1:A:626:LEU:HG	1.74	0.52
1:A:582:GLU:HG2	1:A:609:VAL:HG22	1.91	0.51
2:B:346:PRO:HA	2:B:349:ILE:HB	1.92	0.51
1:A:240:PRO:HA	1:A:255:LEU:HD13	1.93	0.51
1:A:629:THR:HG23	2:B:370:ASN:HB3	1.93	0.51
1:A:682:PHE:CD2	1:A:712:ARG:HB2	2.46	0.50
1:A:511:MET:HB2	3:C:30:PRO:HG2	1.93	0.50
1:A:696:MET:HG2	4:A:801:HEC:ND	2.27	0.50
2:B:305:ALA:O	2:B:309:LYS:HG3	2.12	0.50
1:A:583:VAL:O	1:A:607:SER:HA	2.12	0.49
3:C:35:VAL:HG21	3:C:110:VAL:HG12	1.93	0.49
3:C:28:SER:OG	3:C:29:PRO:HD3	2.13	0.49
1:A:329:TYR:HE2	1:A:332:HIS:HB3	1.78	0.49
3:C:43:PHE:HD2	3:C:46:VAL:HG21	1.77	0.49
1:A:426:GLU:HB3	1:A:453:LEU:HD22	1.94	0.49
2:B:398:ARG:HB3	2:B:405:ALA:HB3	1.95	0.49
2:B:244:VAL:HG21	2:B:278:ARG:HD2	1.95	0.48
1:A:95:GLU:HA	1:A:566:ALA:HB2	1.94	0.48
1:A:338:MET:HB3	1:A:338:MET:HE2	1.73	0.48
3:C:43:PHE:CD2	3:C:46:VAL:HG21	2.49	0.48
2:B:354:THR:HG23	2:B:417:LEU:HD21	1.96	0.48
3:C:51:LEU:HD11	3:C:125:ALA:HB1	1.96	0.48
1:A:279:TRP:CE2	1:A:346:VAL:HG21	2.49	0.47
1:A:471:LEU:HD12	1:A:473:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:HD11	1:A:322:ILE:HD13	1.96	0.47
1:A:408:VAL:HG22	1:A:411:ALA:HB2	1.97	0.47
1:A:443:LEU:HD13	1:A:505:ALA:HB1	1.97	0.47
2:B:131:ASP:HB2	2:B:134:ILE:HG22	1.97	0.47
2:B:360:VAL:HA	2:B:378:MET:HE1	1.97	0.47
1:A:421:LEU:HD23	1:A:454:LEU:HD23	1.97	0.47
3:C:123:HIS:O	3:C:127:LYS:HD3	2.14	0.47
1:A:141:CYS:HB2	1:A:215:GLU:HG3	1.96	0.46
1:A:426:GLU:HG2	1:A:427:LEU:HD23	1.97	0.46
2:B:207:ALA:HB3	2:B:212:TYR:HB2	1.96	0.46
1:A:375:ILE:HB	1:A:385:THR:HG22	1.96	0.46
3:C:114:ASN:HD22	3:C:114:ASN:C	2.22	0.46
1:A:298:GLY:HA2	1:A:316:LEU:HD11	1.97	0.46
1:A:370:ASN:HB2	1:A:394:TRP:CZ2	2.50	0.46
1:A:459:LYS:HA	1:A:459:LYS:HD3	1.81	0.46
3:C:87:VAL:HG12	3:C:88:GLY:N	2.29	0.46
2:B:378:MET:HG3	4:B:503:HEC:NC	2.31	0.46
2:B:413:ASP:HA	2:B:416:LYS:HD2	1.98	0.46
2:B:51:ALA:HB1	2:B:52:ARG:HE	1.81	0.45
1:A:542:GLY:HA2	1:A:563:ALA:HA	1.99	0.45
3:C:76:LEU:HD12	3:C:76:LEU:HA	1.86	0.45
1:A:217:GLY:HA2	1:A:299:SER:OG	2.17	0.45
2:B:320:TYR:HA	2:B:324:CYS:SG	2.57	0.45
1:A:516:THR:HG21	1:A:751:VAL:HG11	1.99	0.45
1:A:696:MET:HG2	4:A:801:HEC:C4D	2.46	0.45
2:B:134:ILE:HD12	2:B:134:ILE:HA	1.89	0.45
2:B:309:LYS:HB2	2:B:309:LYS:HZ3	1.81	0.45
3:C:52:ALA:HB2	3:C:76:LEU:HB3	1.99	0.45
1:A:348:GLN:HE21	1:A:348:GLN:HB2	1.64	0.45
2:B:335:VAL:HG11	2:B:338:MET:HE3	1.98	0.44
1:A:739:ASP:HB3	1:A:744:VAL:HB	1.99	0.44
3:C:72:VAL:O	3:C:76:LEU:HB2	2.17	0.44
1:A:314:LEU:HD12	1:A:314:LEU:HA	1.83	0.44
1:A:413:TRP:CE2	1:A:455:TYR:HB3	2.53	0.44
1:A:124:LEU:HD11	1:A:127:SER:HB3	1.98	0.44
1:A:668:PRO:HG2	2:B:374:SER:HB3	1.98	0.44
1:A:292:TYR:CZ	1:A:364:ILE:HD11	2.53	0.44
2:B:434:LYS:HB3	2:B:434:LYS:HE3	1.81	0.44
1:A:280:ASP:HB3	1:A:346:VAL:O	2.18	0.43
1:A:368:PRO:HD2	1:A:372:PHE:O	2.18	0.43
1:A:527:LEU:HD13	1:A:537:GLN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:TRP:CZ2	1:A:346:VAL:HG21	2.52	0.43
1:A:630:PRO:HA	1:A:672:TRP:CG	2.54	0.43
3:C:119:ARG:C	3:C:121:ALA:H	2.26	0.43
1:A:119:ALA:HB1	1:A:571:TYR:CE2	2.53	0.43
1:A:243:GLU:HB2	1:A:245:LYS:HG3	1.99	0.43
2:B:347:VAL:HG21	4:B:503:HEC:HBA2	2.00	0.43
1:A:97:THR:HG22	1:A:567:PRO:HG2	2.01	0.43
1:A:262:THR:HG22	3:C:66:TYR:OH	2.19	0.42
2:B:228:ARG:HA	2:B:228:ARG:HD2	1.76	0.42
2:B:219:ILE:HD12	2:B:219:ILE:N	2.34	0.42
2:B:356:LEU:HD23	2:B:394:VAL:HG13	2.02	0.42
2:B:426:THR:HG21	2:B:440:MET:HE1	2.00	0.42
3:C:48:PRO:C	3:C:50:ASN:H	2.27	0.42
1:A:350:MET:SD	1:A:437:TYR:HB2	2.59	0.42
1:A:438:SER:HB2	1:A:445:TYR:HE2	1.85	0.42
2:B:274:ASP:O	2:B:278:ARG:HG2	2.19	0.42
1:A:92:ARG:HB2	1:A:110:ASN:CG	2.45	0.42
2:B:196:HIS:CE1	2:B:224:ALA:HB1	2.55	0.42
2:B:348:VAL:HG22	2:B:356:LEU:HD11	2.02	0.42
1:A:475:MET:HG3	1:A:651:THR:HA	2.01	0.42
2:B:339:PHE:HD1	4:B:503:HEC:HMD2	1.85	0.42
2:B:340:PRO:HG3	4:B:503:HEC:HAD2	2.03	0.41
2:B:356:LEU:HD12	2:B:356:LEU:HA	1.92	0.41
3:C:60:GLU:H	3:C:60:GLU:HG2	1.57	0.41
3:C:122:CYS:O	3:C:126:VAL:HG23	2.21	0.41
1:A:66:TYR:HB2	1:A:437:TYR:O	2.20	0.41
1:A:354:MET:HG3	1:A:356:VAL:HG23	2.02	0.41
1:A:486:PRO:HA	1:A:489:VAL:HG22	2.03	0.41
3:C:48:PRO:HG3	3:C:132:MET:HG2	2.02	0.41
1:A:419:PRO:HB3	1:A:454:LEU:HD11	2.02	0.41
1:A:423:ILE:HG12	1:A:452:PRO:HB3	2.02	0.41
1:A:617:LYS:HE3	1:A:617:LYS:HB3	1.86	0.41
2:B:321:LEU:HD12	2:B:321:LEU:HA	1.95	0.41
1:A:528:LEU:HD11	1:A:570:THR:HG22	2.03	0.41
1:A:585:TRP:CZ2	1:A:590:PRO:HB3	2.56	0.41
2:B:368:PRO:HD3	2:B:375:ALA:HB2	2.03	0.41
1:A:162:ASP:OD2	1:A:164:ARG:HD3	2.21	0.41
3:C:109:LEU:HD23	3:C:109:LEU:HA	1.88	0.40
1:A:105:MET:O	1:A:116:ALA:HA	2.21	0.40
1:A:254:ILE:HD12	1:A:254:ILE:HA	1.87	0.40
1:A:368:PRO:HG2	1:A:370:ASN:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:ASN:C	3:C:116:ASP:H	2.30	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	721/757 (95%)	695 (96%)	26 (4%)	0	100	100
2	B	307/462 (66%)	283 (92%)	24 (8%)	0	100	100
3	C	105/133 (79%)	89 (85%)	16 (15%)	0	100	100
All	All	1133/1352 (84%)	1067 (94%)	66 (6%)	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	580/605 (96%)	562 (97%)	18 (3%)	35	65
2	B	245/355 (69%)	241 (98%)	4 (2%)	55	80
3	C	84/102 (82%)	82 (98%)	2 (2%)	43	72
All	All	909/1062 (86%)	885 (97%)	24 (3%)	41	70

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	VAL
1	A	108	THR
1	A	117	LEU
1	A	141	CYS
1	A	142	CYS
1	A	178	SER
1	A	262	THR
1	A	340	GLU
1	A	348	GLN
1	A	408	VAL
1	A	421	LEU
1	A	454	LEU
1	A	471	LEU
1	A	530	THR
1	A	636	THR
1	A	653	CYS
1	A	685	LEU
1	A	750	ASP
2	B	134	ILE
2	B	240	GLU
2	B	300	ASP
2	B	324	CYS
3	C	68	GLU
3	C	115	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	GLN
1	A	347	GLN
1	A	450	GLN
1	A	476	ASN
1	A	650	GLN
1	A	746	GLN
1	A	756	HIS
3	C	130	GLN

5.3.3 RNA ⓘ

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](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
4	HEC	A	801	1	50,50,50	1.32	6 (12%)	68,82,82	1.15	5 (7%)
5	PQQ	A	802	6	26,26,26	1.09	2 (7%)	33,40,40	1.53	10 (30%)
4	HEC	B	501	2	50,50,50	1.34	8 (16%)	68,82,82	1.13	6 (8%)
4	HEC	B	503	2	50,50,50	1.31	4 (8%)	68,82,82	1.24	8 (11%)
4	HEC	B	502	2	50,50,50	1.35	8 (16%)	68,82,82	1.27	8 (11%)

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
4	HEC	A	801	1	1/1/3/7	1/14/54/54	-
5	PQQ	A	802	6	-	6/12/28/28	0/3/3/3
4	HEC	B	501	2	1/1/3/7	3/14/54/54	-
4	HEC	B	503	2	1/1/3/7	4/14/54/54	-
4	HEC	B	502	2	1/1/3/7	2/14/54/54	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	HEC	CBC-CAC	-3.31	1.36	1.51
4	B	503	HEC	CBC-CAC	-3.31	1.36	1.51
4	B	502	HEC	CBC-CAC	-3.27	1.36	1.51
4	B	501	HEC	CBC-CAC	-3.27	1.36	1.51
4	B	501	HEC	CAC-C3C	2.92	1.58	1.51
4	B	502	HEC	CAC-C3C	2.88	1.58	1.51
4	B	503	HEC	CAC-C3C	2.87	1.58	1.51
4	A	801	HEC	CAC-C3C	2.83	1.58	1.51
4	B	501	HEC	CAB-C3B	2.83	1.58	1.51
4	A	801	HEC	CBB-CAB	-2.36	1.41	1.51
4	B	503	HEC	CBB-CAB	-2.35	1.41	1.51
4	B	502	HEC	CBB-CAB	-2.35	1.41	1.51
4	B	501	HEC	CBB-CAB	-2.30	1.41	1.51
4	B	502	HEC	CAB-C3B	2.30	1.57	1.51
4	B	503	HEC	CAB-C3B	2.24	1.56	1.51
4	A	801	HEC	CAB-C3B	2.23	1.56	1.51
4	B	502	HEC	FE-ND	2.18	2.01	1.94
5	A	802	PQQ	C1A-N1	-2.18	1.33	1.37
4	B	501	HEC	CMD-C2D	2.15	1.55	1.50
4	B	502	HEC	CMD-C2D	2.13	1.55	1.50
4	A	801	HEC	CMD-C2D	2.12	1.55	1.50
4	B	501	HEC	CMB-C2B	2.11	1.55	1.50
4	B	501	HEC	FE-ND	2.09	2.01	1.94
4	B	502	HEC	CMB-C2B	2.06	1.55	1.50
4	A	801	HEC	FE-ND	2.05	2.01	1.94
4	B	501	HEC	CMA-C3A	2.03	1.55	1.50
5	A	802	PQQ	O2B-C2X	-2.02	1.24	1.30
4	B	502	HEC	CMA-C3A	2.01	1.55	1.50

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	HEC	CBD-CAD-C3D	4.20	124.29	112.63
5	A	802	PQQ	C9A-C9-C9X	3.12	128.39	121.46
4	B	503	HEC	O1D-CGD-CBD	-3.00	113.45	123.08
4	B	502	HEC	O1D-CGD-CBD	-2.98	113.50	123.08
5	A	802	PQQ	O9A-C9X-C9	-2.88	114.95	121.94
4	B	503	HEC	C1D-ND-C4D	2.83	108.00	105.07
4	B	501	HEC	O1D-CGD-CBD	-2.82	114.03	123.08
4	A	801	HEC	O1D-CGD-CBD	-2.75	114.23	123.08
4	B	503	HEC	CBD-CAD-C3D	2.73	120.22	112.63
5	A	802	PQQ	C8-C9-C9A	-2.59	116.90	120.34
4	B	502	HEC	O1A-CGA-CBA	-2.59	114.77	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	802	PQQ	O2A-C2X-C2	-2.52	115.89	121.09
5	A	802	PQQ	O7A-C7X-C7	-2.51	116.15	121.24
4	B	501	HEC	CBD-CAD-C3D	2.37	119.22	112.63
5	A	802	PQQ	C9-C8-C7	2.34	121.85	119.93
4	A	801	HEC	O1A-CGA-CBA	-2.34	115.56	123.08
4	B	501	HEC	O1A-CGA-CBA	-2.32	115.62	123.08
4	B	503	HEC	O1A-CGA-CBA	-2.31	115.65	123.08
4	B	501	HEC	C1D-ND-C4D	2.30	107.45	105.07
4	A	801	HEC	C1D-ND-C4D	2.28	107.43	105.07
5	A	802	PQQ	O7B-C7X-O7A	2.28	128.40	123.35
4	B	502	HEC	CMD-C2D-C1D	-2.26	121.59	125.04
4	A	801	HEC	CHC-C4B-NB	2.23	127.13	124.37
4	B	502	HEC	C1D-ND-C4D	2.21	107.36	105.07
4	B	503	HEC	C4B-NB-C1B	2.17	107.32	105.07
4	B	501	HEC	CAB-C3B-C4B	2.11	127.54	124.81
5	A	802	PQQ	C3A-C4-C5	-2.09	114.66	117.04
5	A	802	PQQ	O4-C4-C3A	2.07	126.50	122.03
4	B	502	HEC	O2A-CGA-O1A	2.07	128.46	123.30
4	B	503	HEC	CHC-C4B-NB	2.07	126.93	124.37
4	B	503	HEC	CMC-C2C-C3C	2.06	130.06	125.61
5	A	802	PQQ	O2B-C2X-O2A	2.05	128.31	123.61
4	B	502	HEC	C1D-C2D-C3D	2.04	109.10	106.96
4	B	503	HEC	C3D-C4D-ND	-2.02	108.39	110.36
4	B	501	HEC	O2A-CGA-O1A	2.02	128.33	123.30
4	A	801	HEC	C3D-C4D-ND	-2.02	108.40	110.36
4	B	502	HEC	CHC-C4B-NB	2.01	126.85	124.37

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	801	HEC	NA
4	B	501	HEC	NA
4	B	502	HEC	NA
4	B	503	HEC	NA

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	502	HEC	C2D-C3D-CAD-CBD
4	B	502	HEC	C4D-C3D-CAD-CBD
4	B	503	HEC	C2A-CAA-CBA-CGA
5	A	802	PQQ	N1-C2-C2X-O2A

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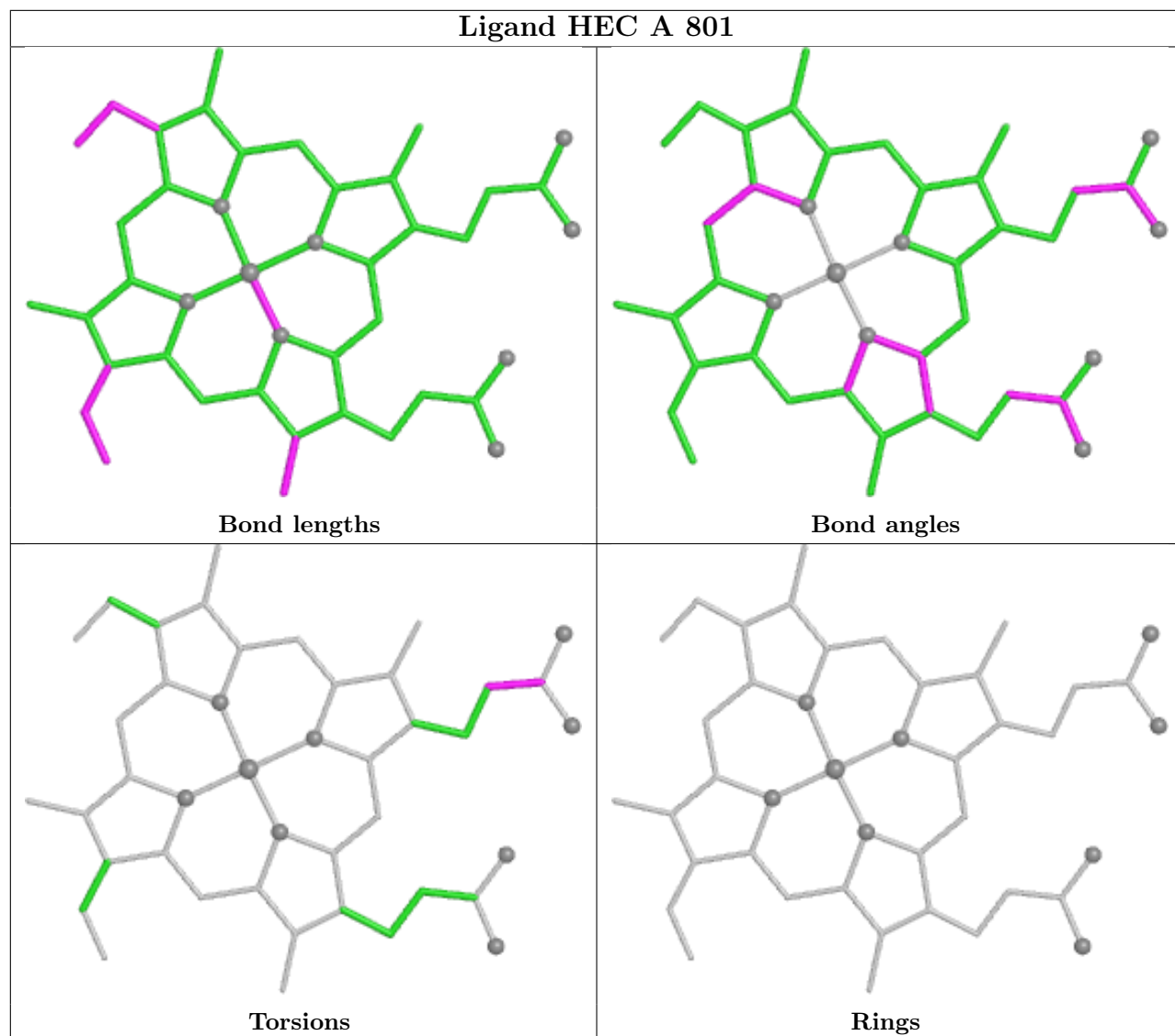
Mol	Chain	Res	Type	Atoms
4	B	501	HEC	C3D-CAD-CBD-CGD
4	B	503	HEC	C3D-CAD-CBD-CGD
4	B	503	HEC	C4D-C3D-CAD-CBD
5	A	802	PQQ	N1-C2-C2X-O2B
5	A	802	PQQ	C3-C2-C2X-O2B
4	B	503	HEC	C2D-C3D-CAD-CBD
5	A	802	PQQ	C3-C2-C2X-O2A
4	B	501	HEC	CAD-CBD-CGD-O1D
4	B	501	HEC	CAD-CBD-CGD-O2D
5	A	802	PQQ	C8-C9-C9X-O9B
5	A	802	PQQ	C8-C9-C9X-O9A
4	A	801	HEC	CAA-CBA-CGA-O2A

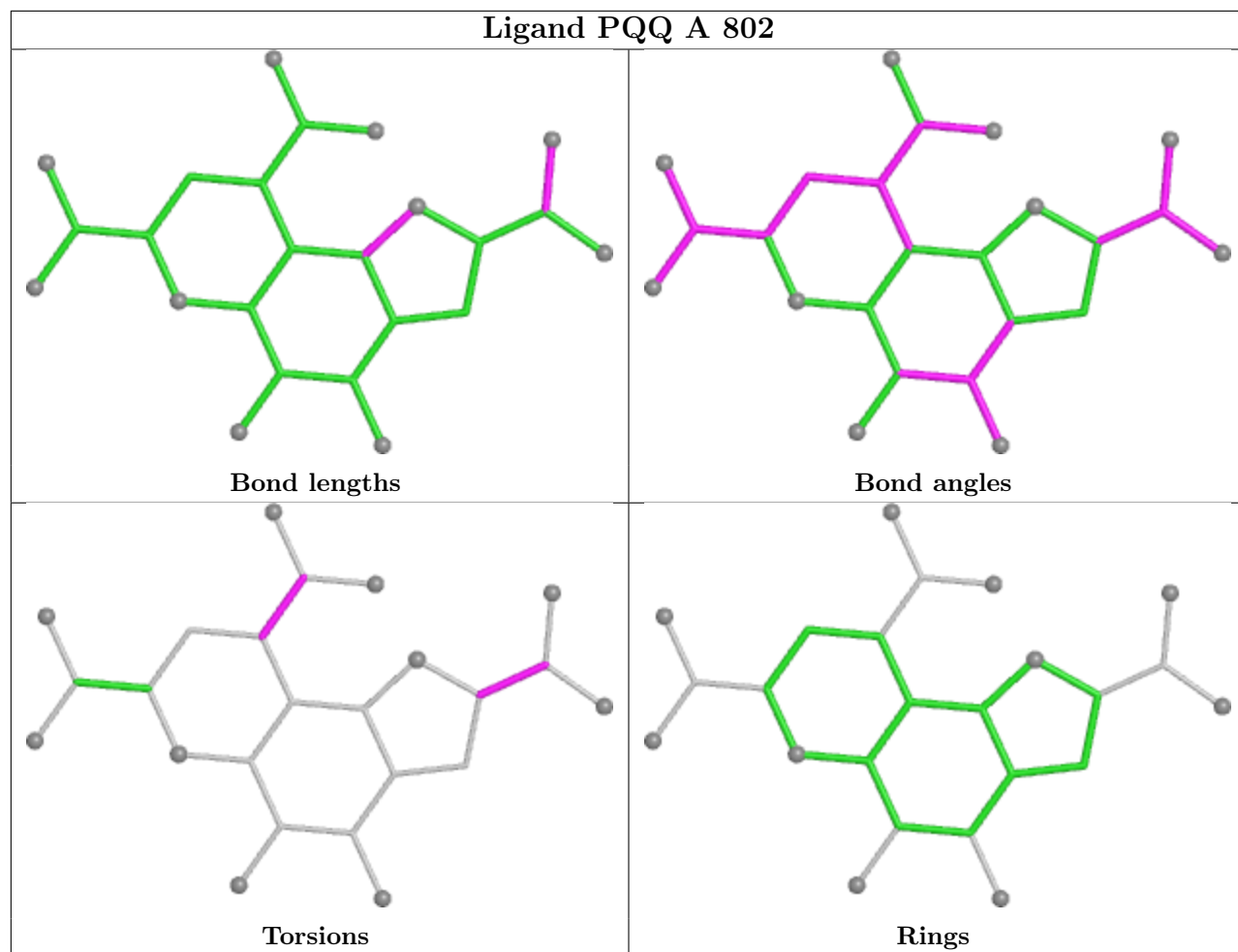
There are no ring outliers.

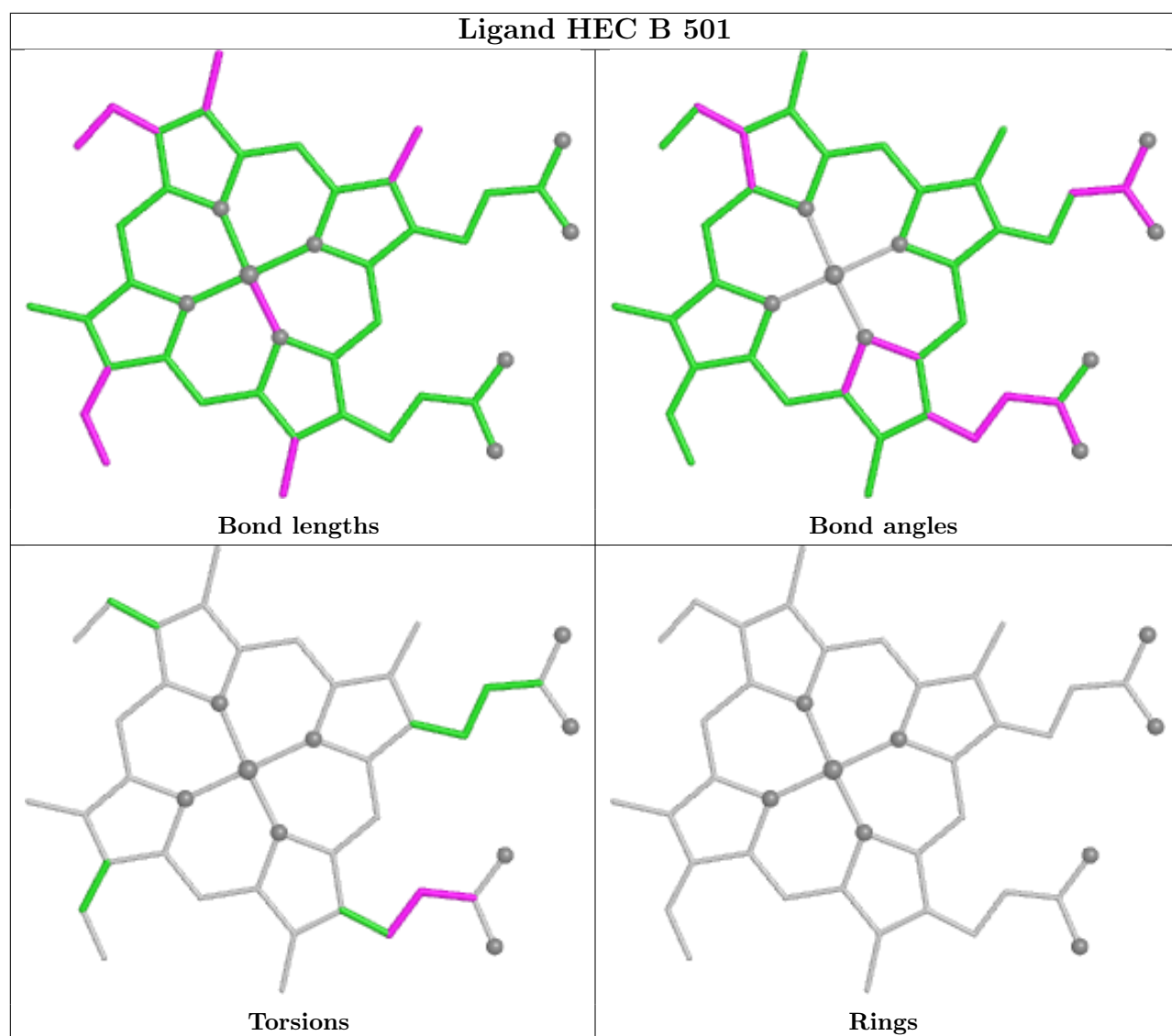
5 monomers are involved in 9 short contacts:

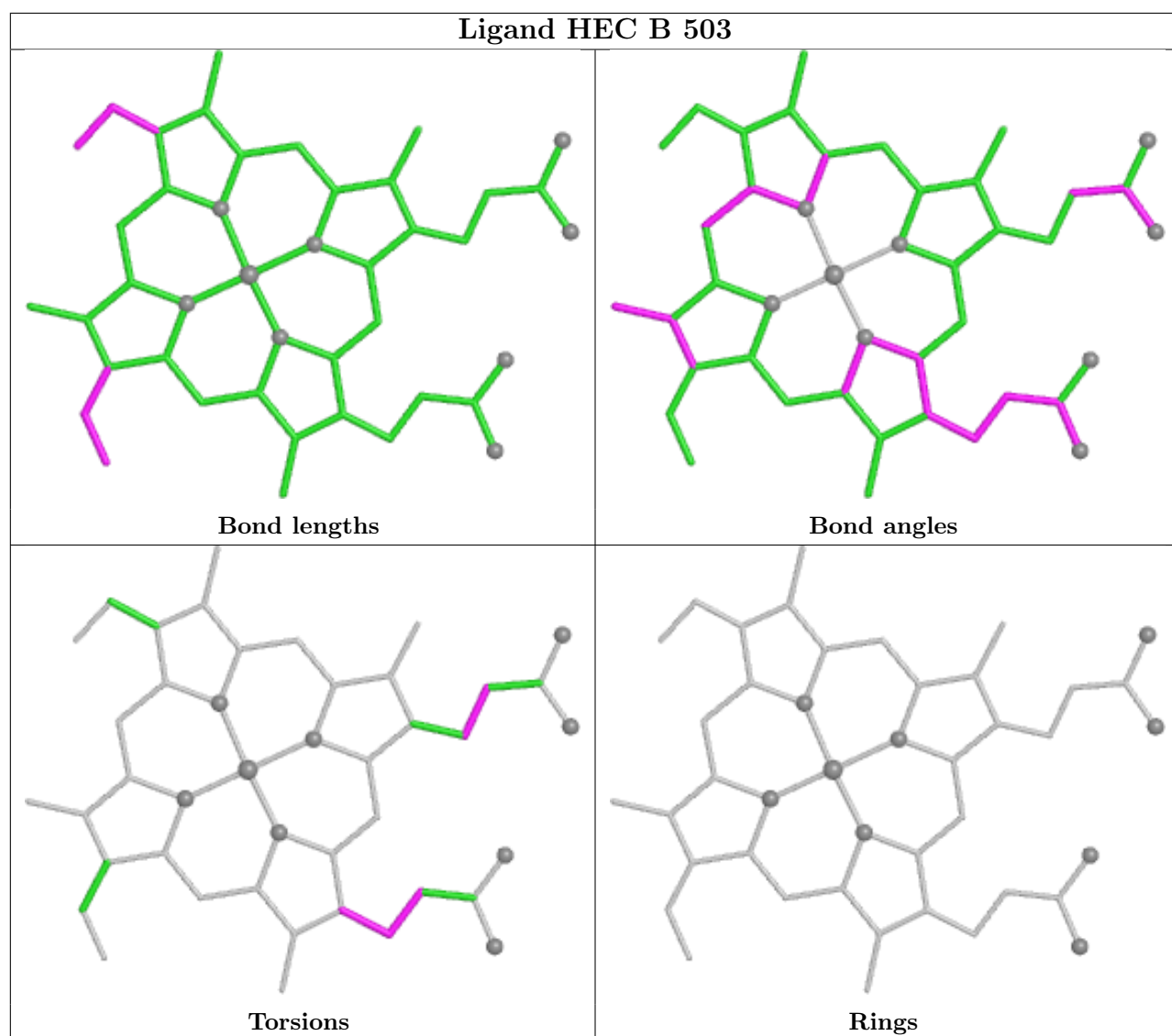
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	HEC	2	0
5	A	802	PQQ	1	0
4	B	501	HEC	1	0
4	B	503	HEC	4	0
4	B	502	HEC	1	0

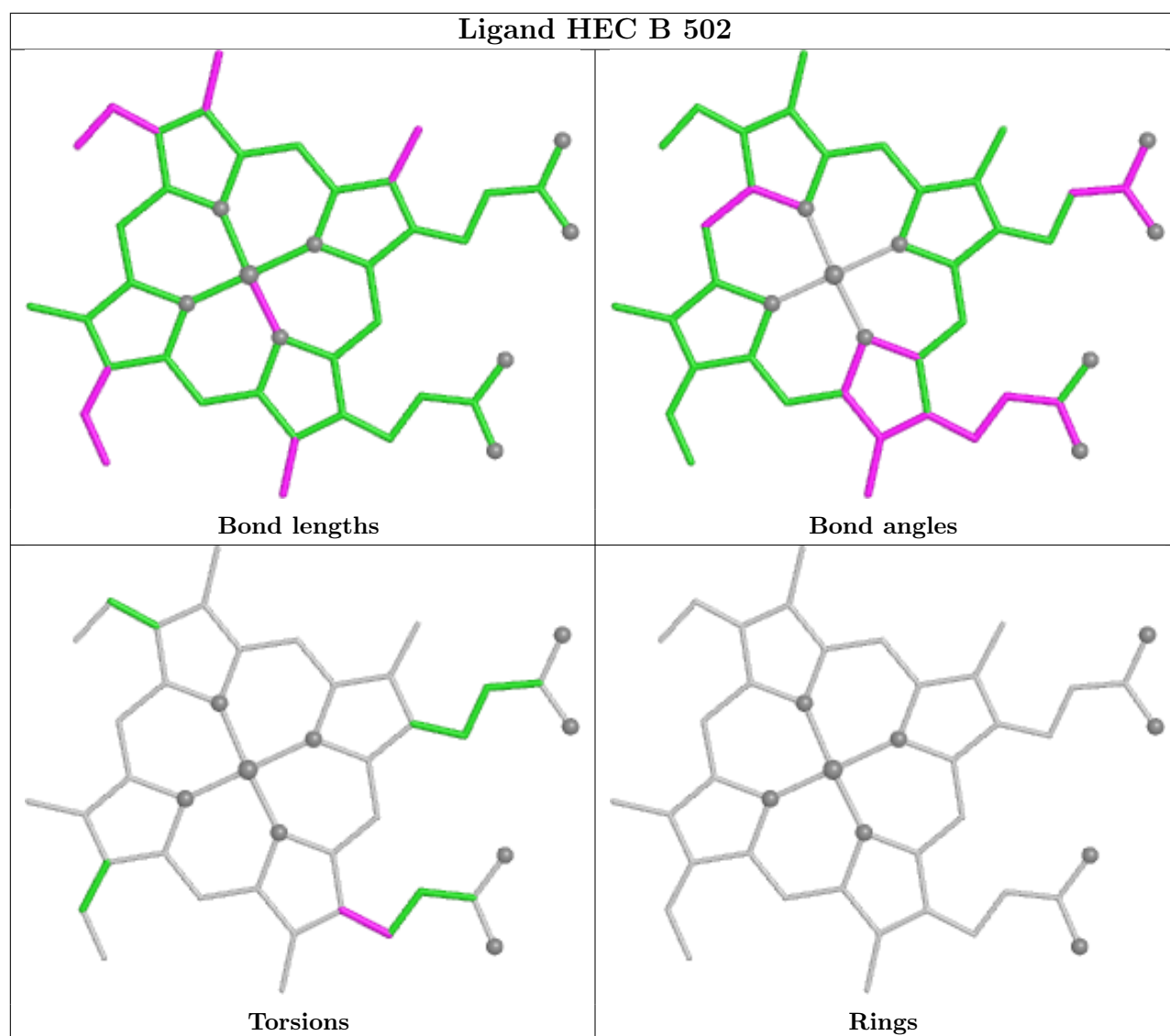
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

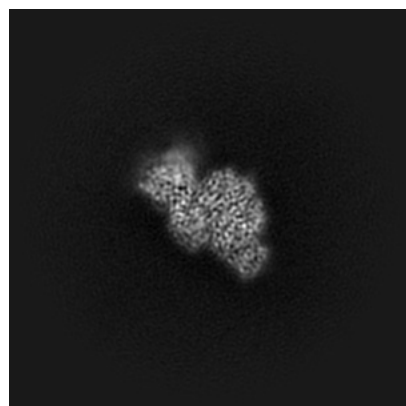
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66440. These allow visual inspection of the internal detail of the map and identification of artifacts.

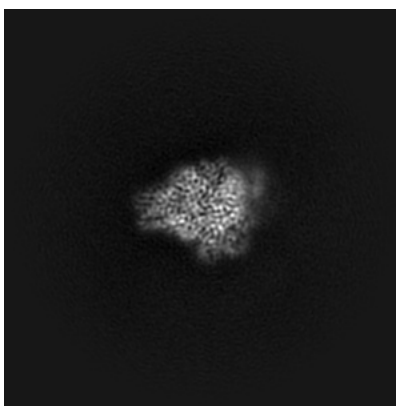
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

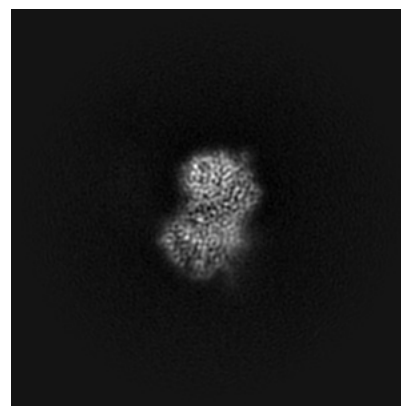
6.1.1 Primary map



X

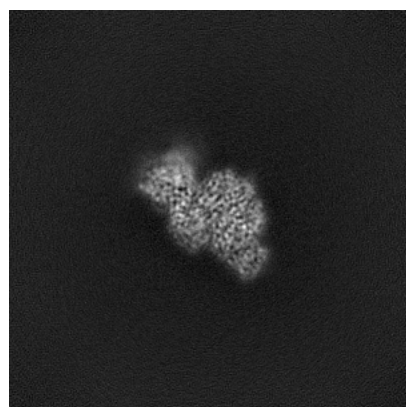


Y

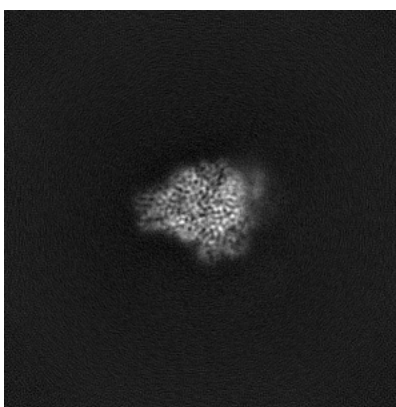


Z

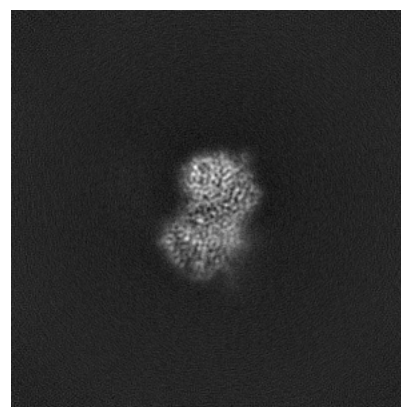
6.1.2 Raw map



X



Y

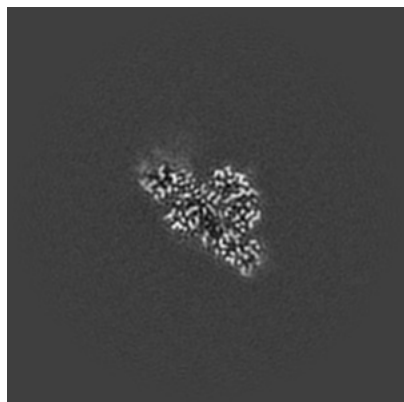


Z

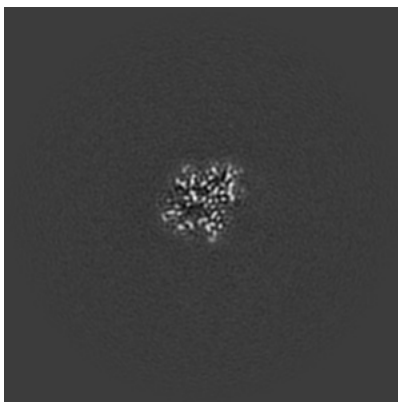
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

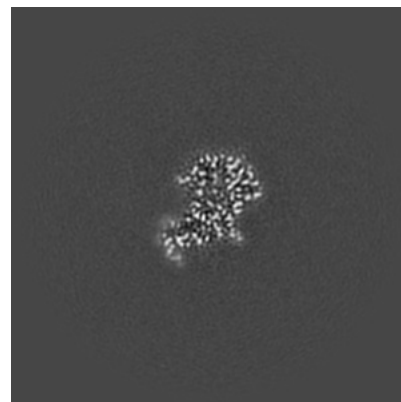
6.2.1 Primary map



X Index: 160

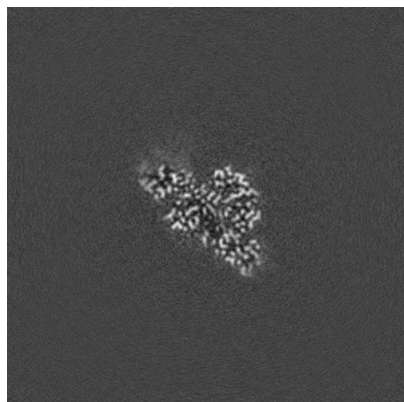


Y Index: 160

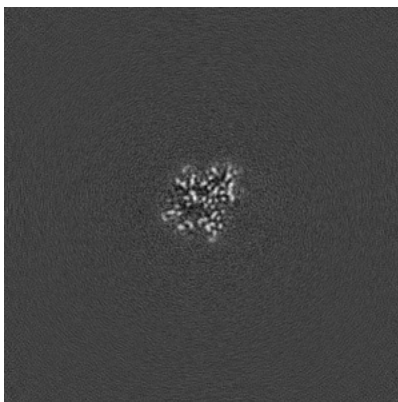


Z Index: 160

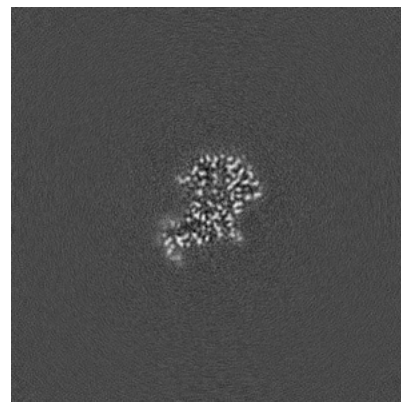
6.2.2 Raw map



X Index: 160



Y Index: 160

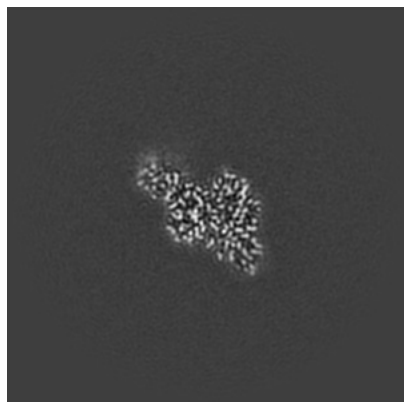


Z Index: 160

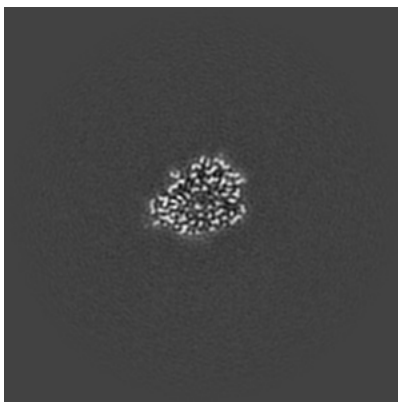
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

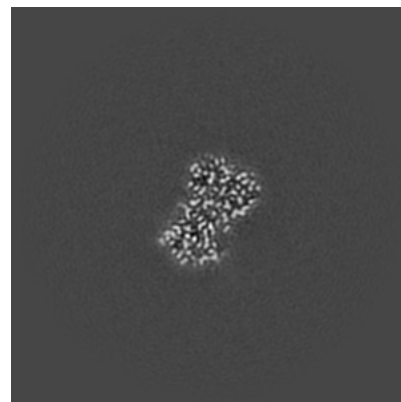
6.3.1 Primary map



X Index: 150

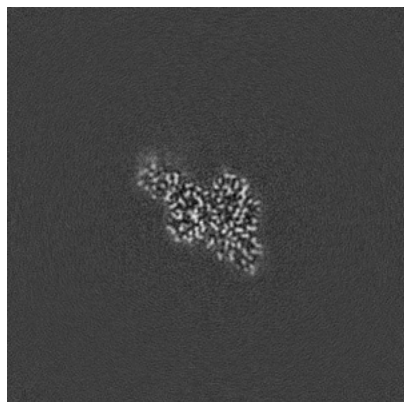


Y Index: 175

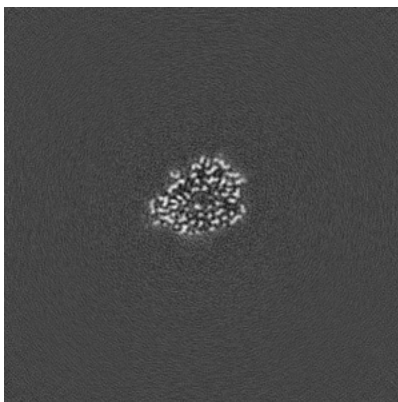


Z Index: 169

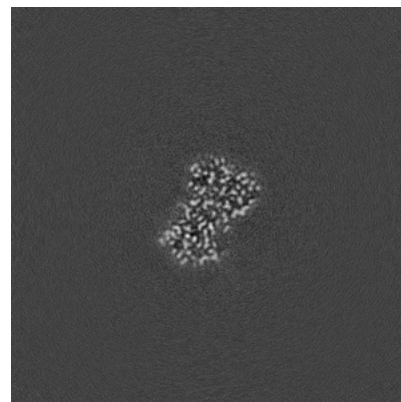
6.3.2 Raw map



X Index: 150



Y Index: 175

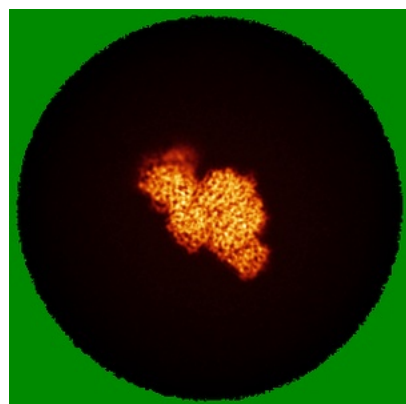


Z Index: 169

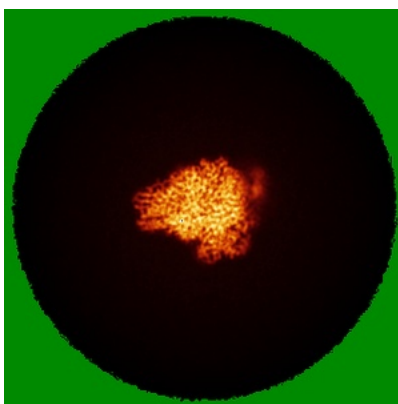
The images above show the largest variance slices of the map in three orthogonal directions.

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

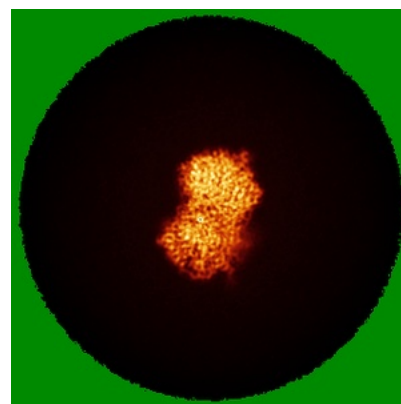
6.4.1 Primary map



X

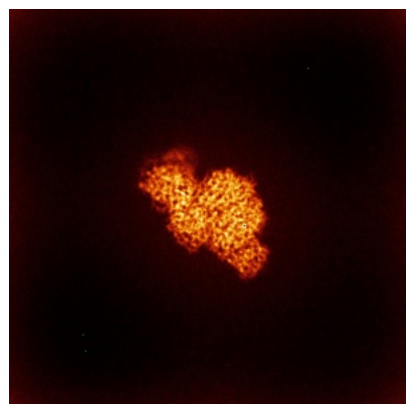


Y

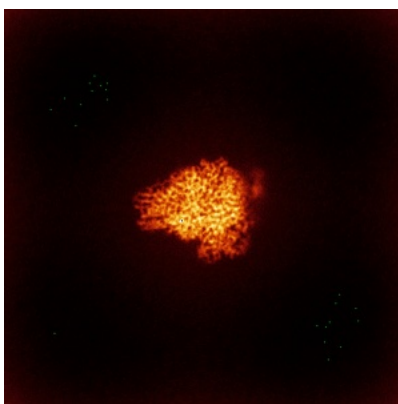


Z

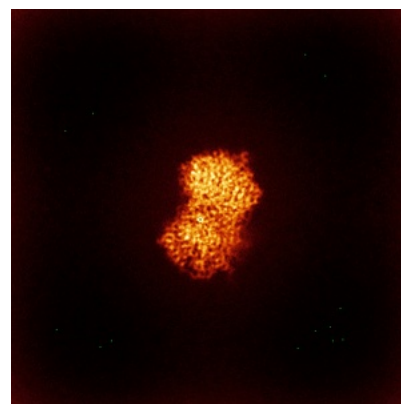
6.4.2 Raw map



X



Y

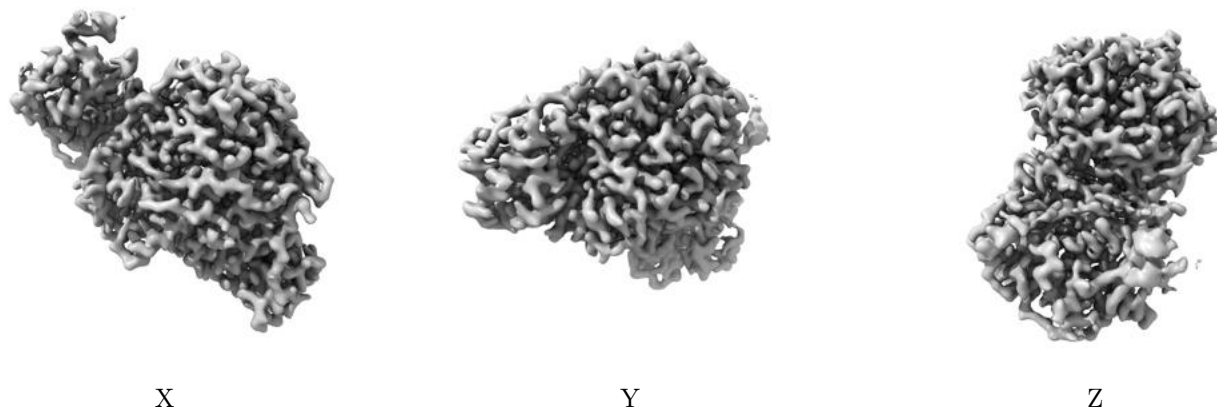


Z

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.

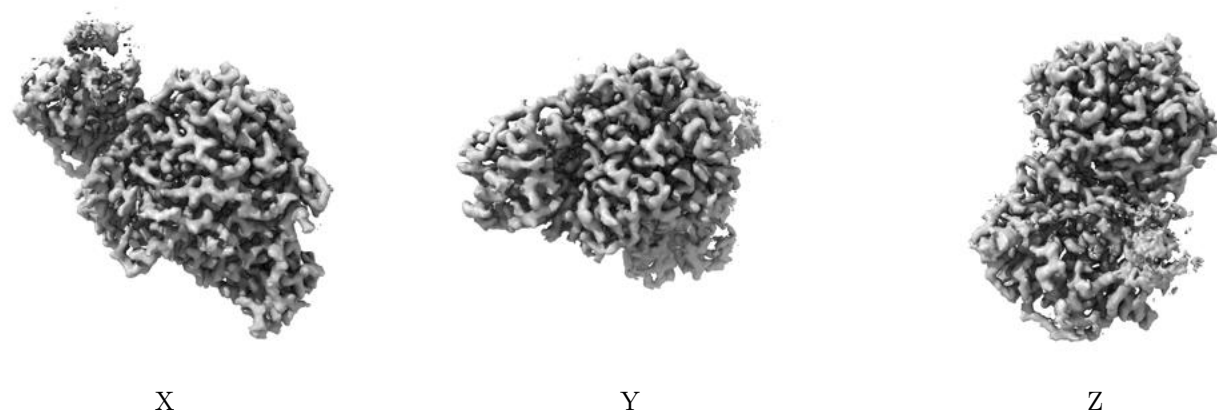
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

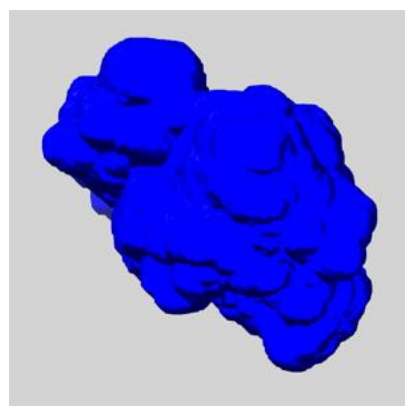
6.6 Mask visualisation [i](#)

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

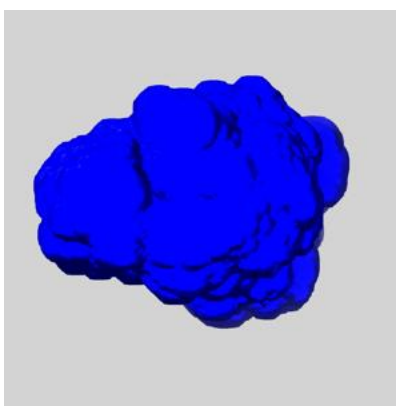
A mask typically either:

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

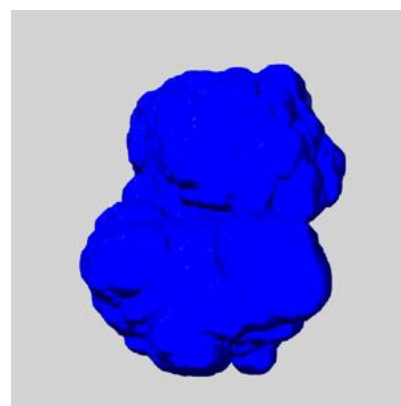
6.6.1 emd_66440_msk_1.map [i](#)



X



Y

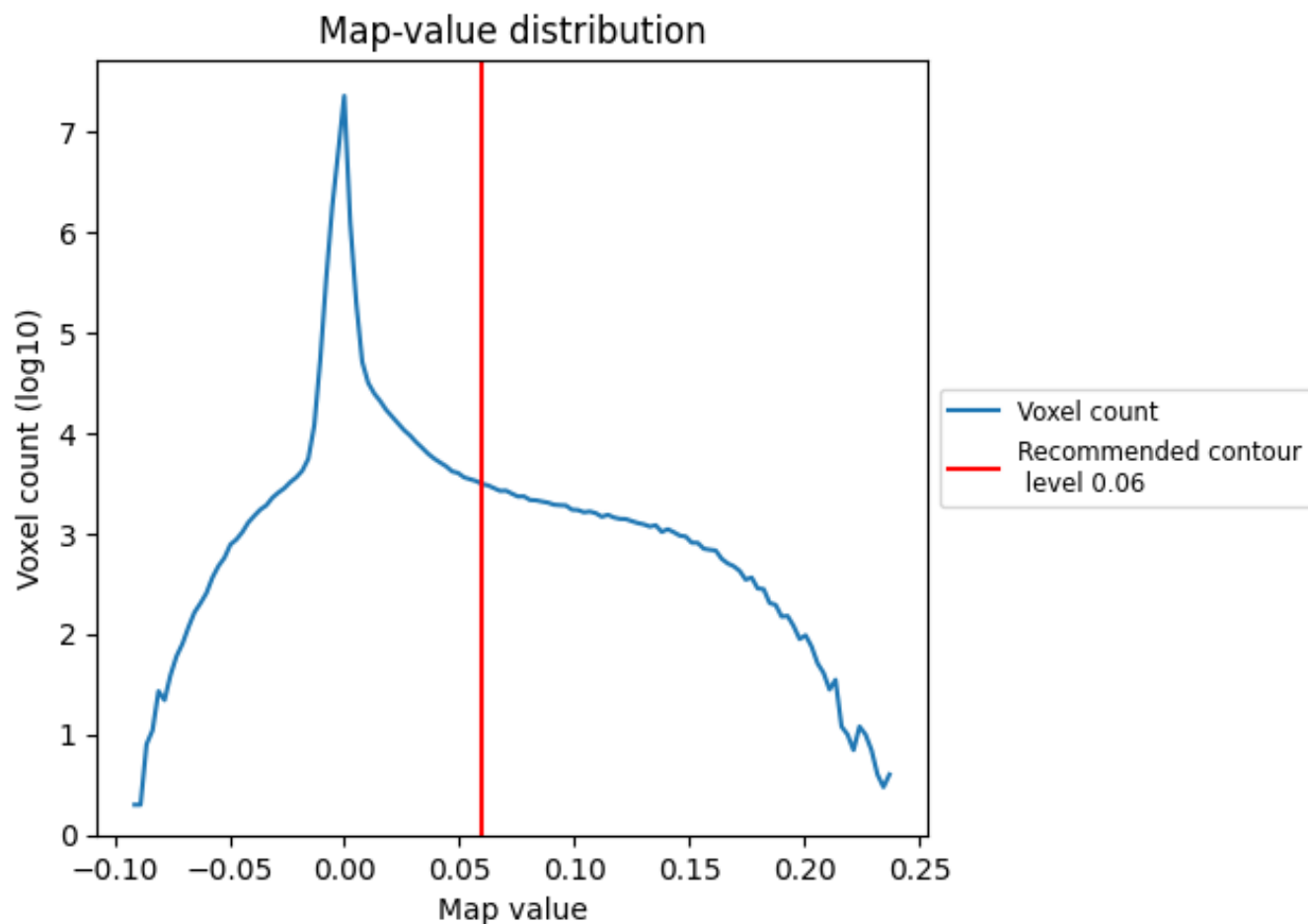


Z

7 Map analysis [i](#)

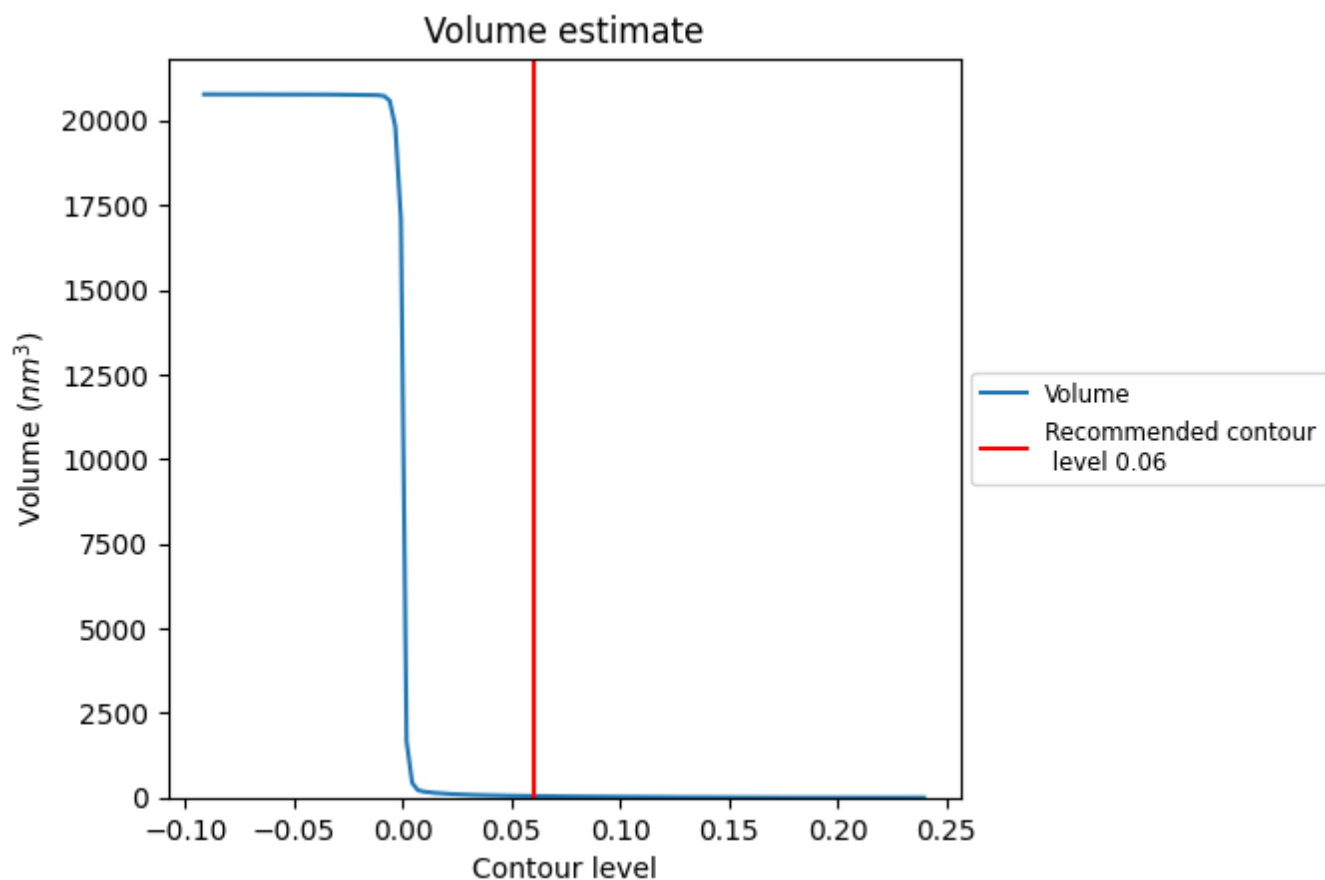
This section contains the results of statistical analysis of the map.

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.

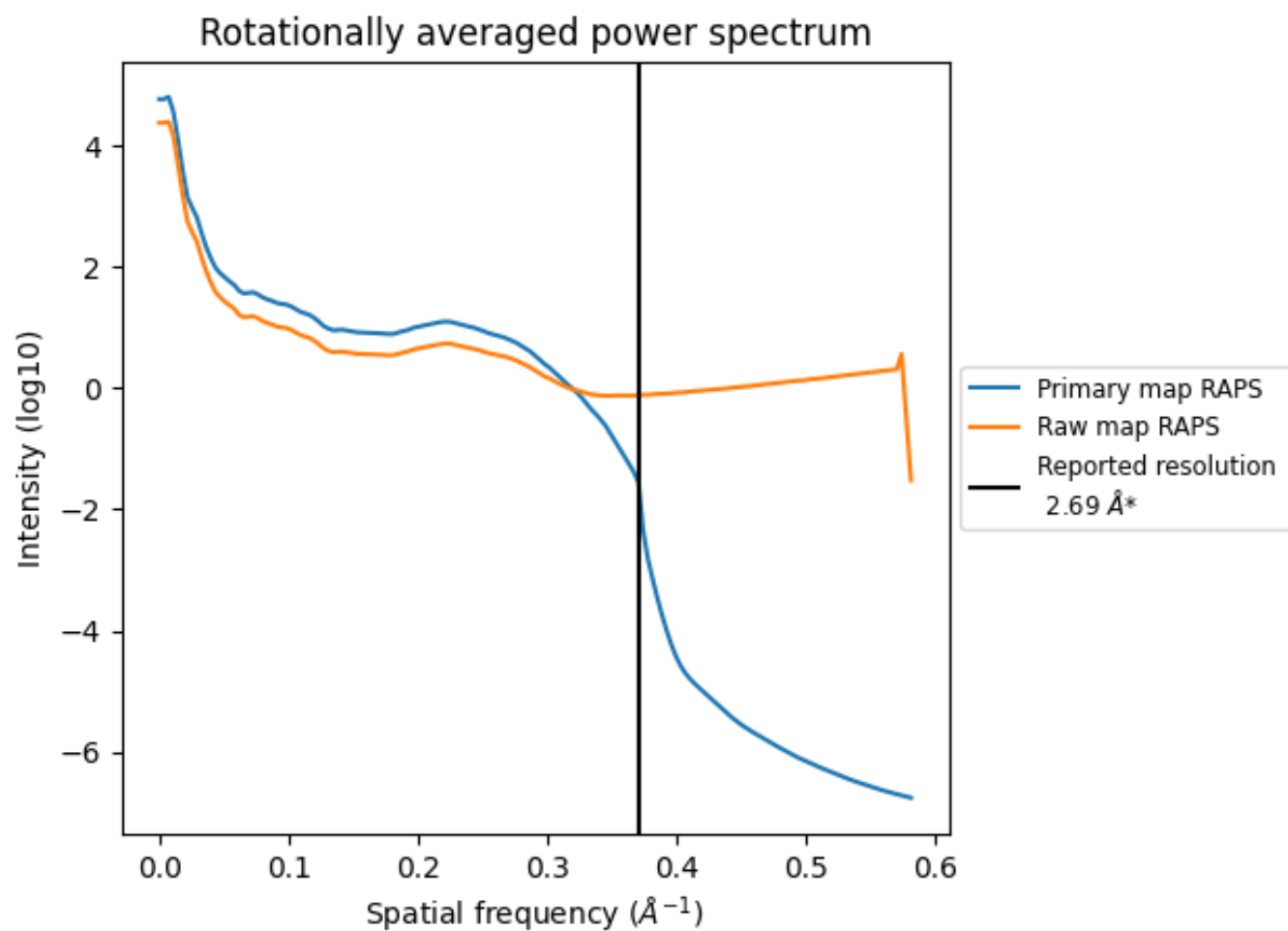
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 45 nm^3 ; this corresponds to an approximate mass of 40 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 ⓘ

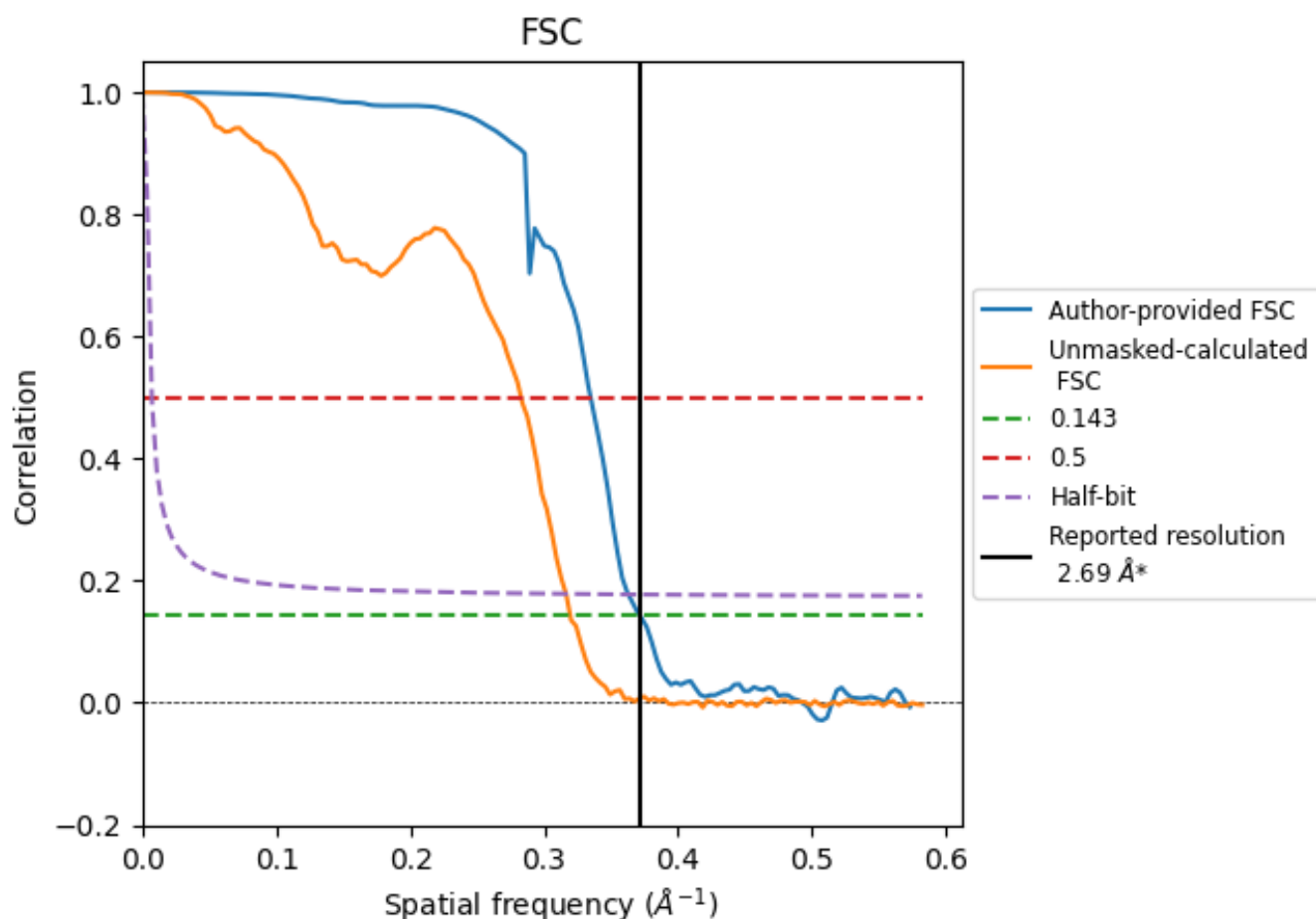


*Reported resolution corresponds to spatial frequency of $0.372 \text{ \AA}^{-1}$

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 0.372 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

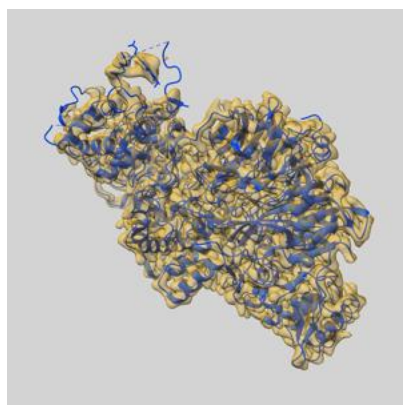
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	2.69	2.99	2.76
Unmasked-calculated*	3.13	3.54	3.16

*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 3.13 differs from the reported value 2.69 by more than 10 %

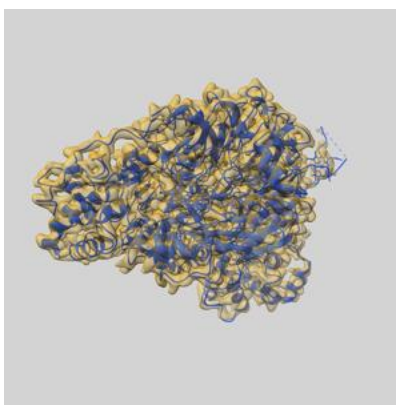
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66440 and PDB model 9X0R. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

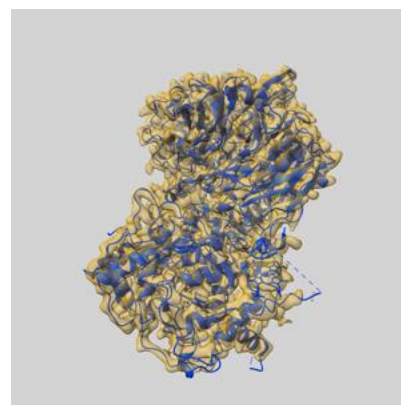
9.1 Map-model overlay [i](#)



X



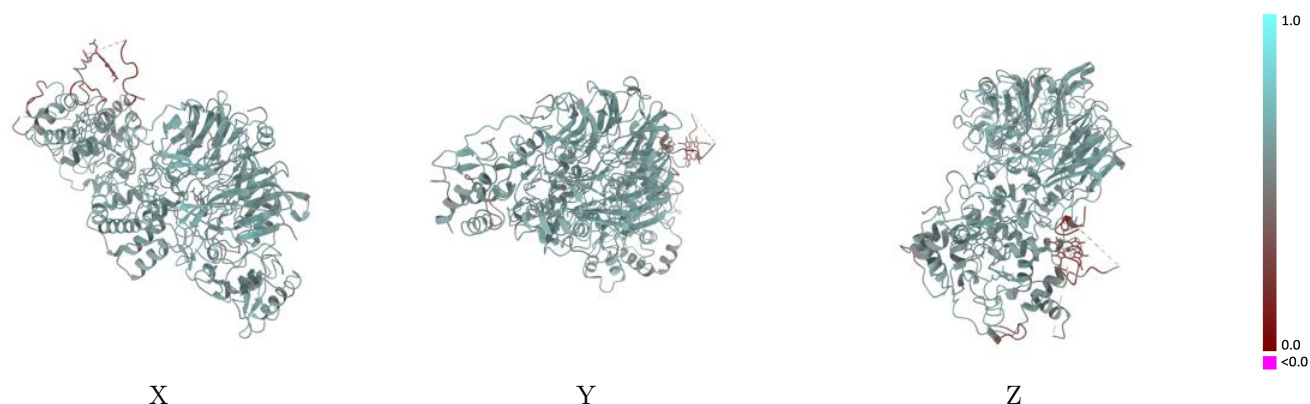
Y



Z

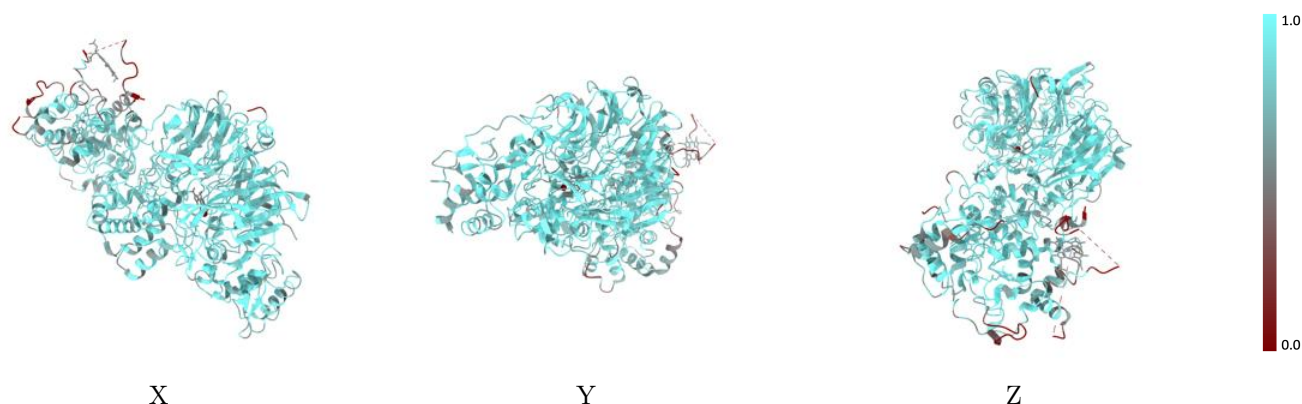
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



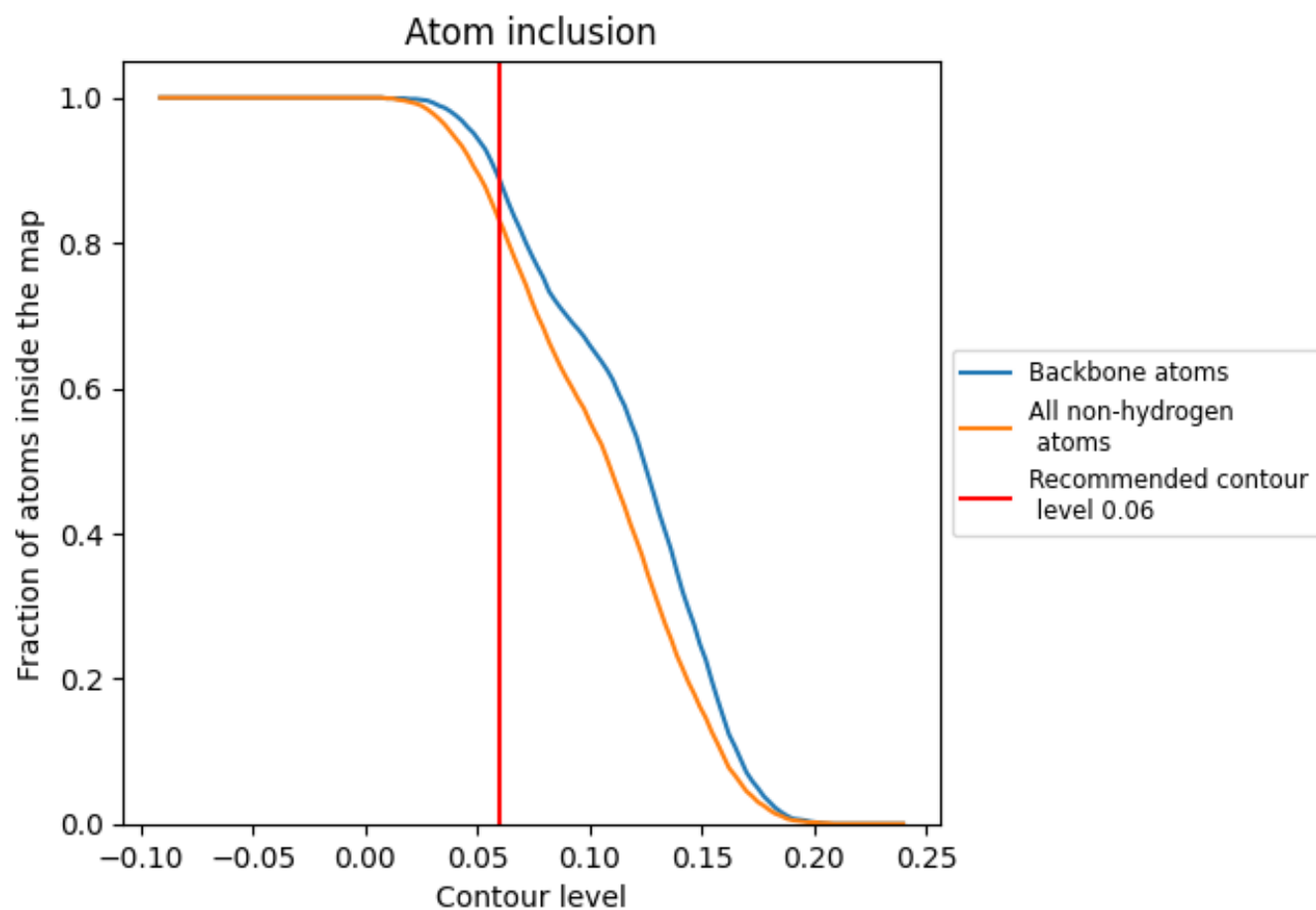
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 83% 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	0.8290	0.5820
A	0.8790	0.6080
B	0.7300	0.5350
C	0.7800	0.5500

