W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB EM Validation Report (i)

May 15, 2024 – 02:27 PM JST

PDB ID	:	8XCN
EMDB ID	:	EMD-38248
Title	:	Cryo-EM Structure of Membrane-bound Fructose Dehydrogenase from Gluconobacter japonicus variant-N1190A
Authors	:	Fukawa, E.; Miyata, T.; Makino, F.; Adachi, T.; Suzuki, Y.; Tanaka, H.; Namba, K.; Sowa, K.; Kitazumi, Y.; Shirai, O.
Deposited on	:	2023-12-09
Resolution	:	3.02 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2
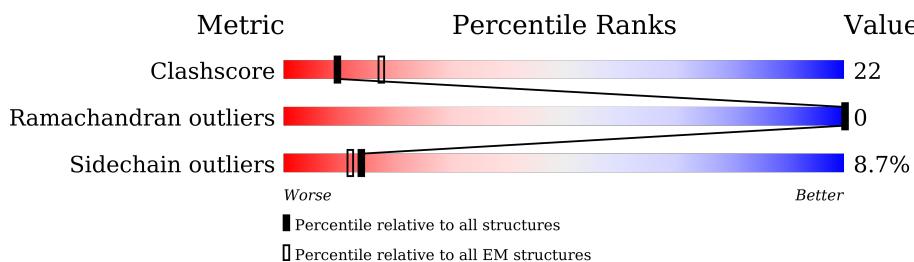
1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY
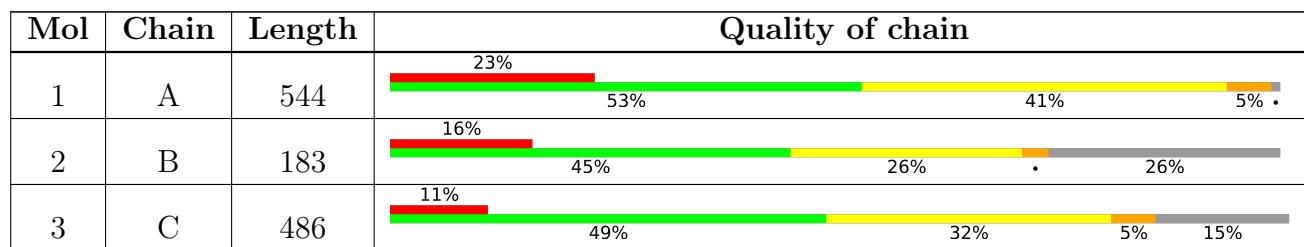
The reported resolution of this entry is 3.02 Å.

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	Percentile Ranks	Value
Clashscore		22
Ramachandran outliers		0
Sidechain outliers		8.7%

Worse   *Better*

■ Percentile relative to all structures
❑ Percentile relative to all EM structures

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

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 <=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	544	23% / 53% 41% 5% •
2	B	183	16% / 45% 26% • 26%
3	C	486	11% / 49% 32% 5% 15%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	F3S	A	602	-	-	X	-

WORLDWIDE wwPDB PROTEIN DATA BANK

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 8601 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 Fructose dehydrogenase large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	540	Total	C	N	O	S	0	0
			4164	2610	736	791	27		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	521	ALA	ASN	variant	UNP M1VMF7
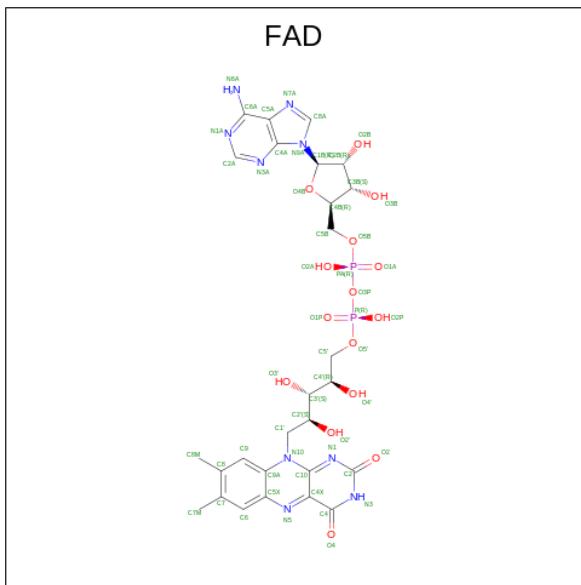
- Molecule 2 is a protein called Fructose dehydrogenase small subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	136	Total	C	N	O	S	0	0
			1080	690	180	206	4		

- Molecule 3 is a protein called Fructose dehydrogenase cytochrome subunit.
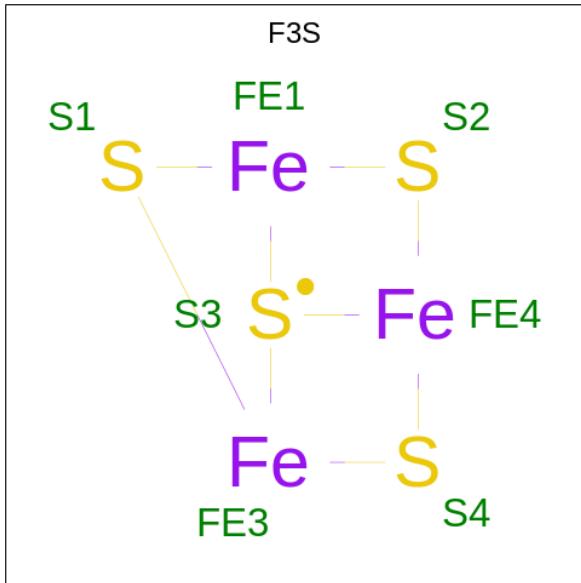
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	413	Total	C	N	O	S	0	0
			3130	1957	552	610	11		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).

FAD
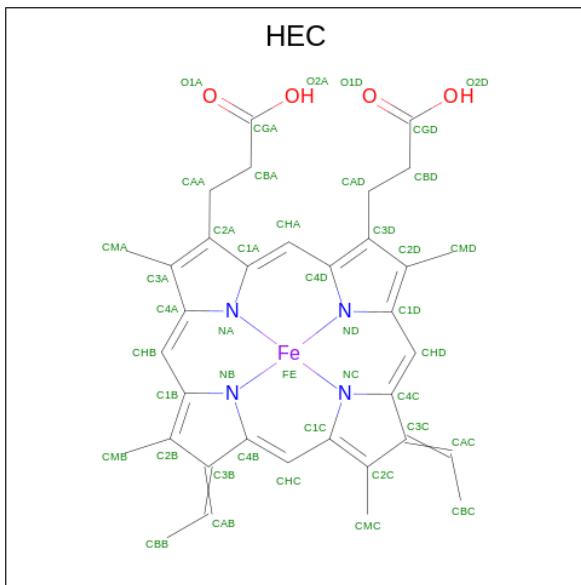
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	53	27	9	15	2	0

- Molecule 5 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).

F3S
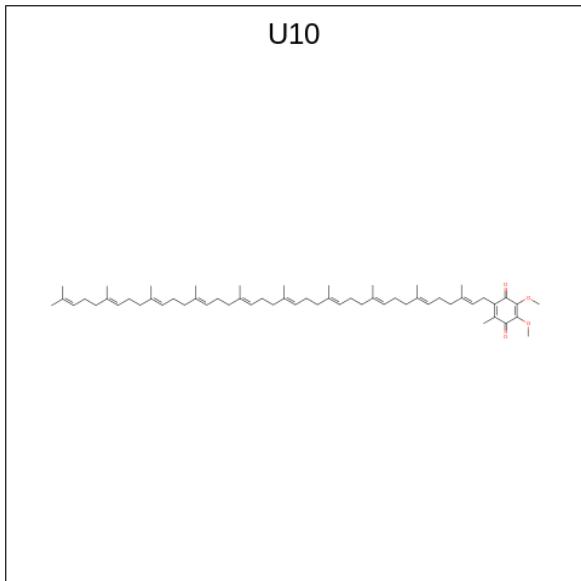
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
5	A	1	7	3	4	0

- Molecule 6 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

HEC

| Mol	Chain	Residues	Atoms					AltConf
6	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
6	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
6	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

U10
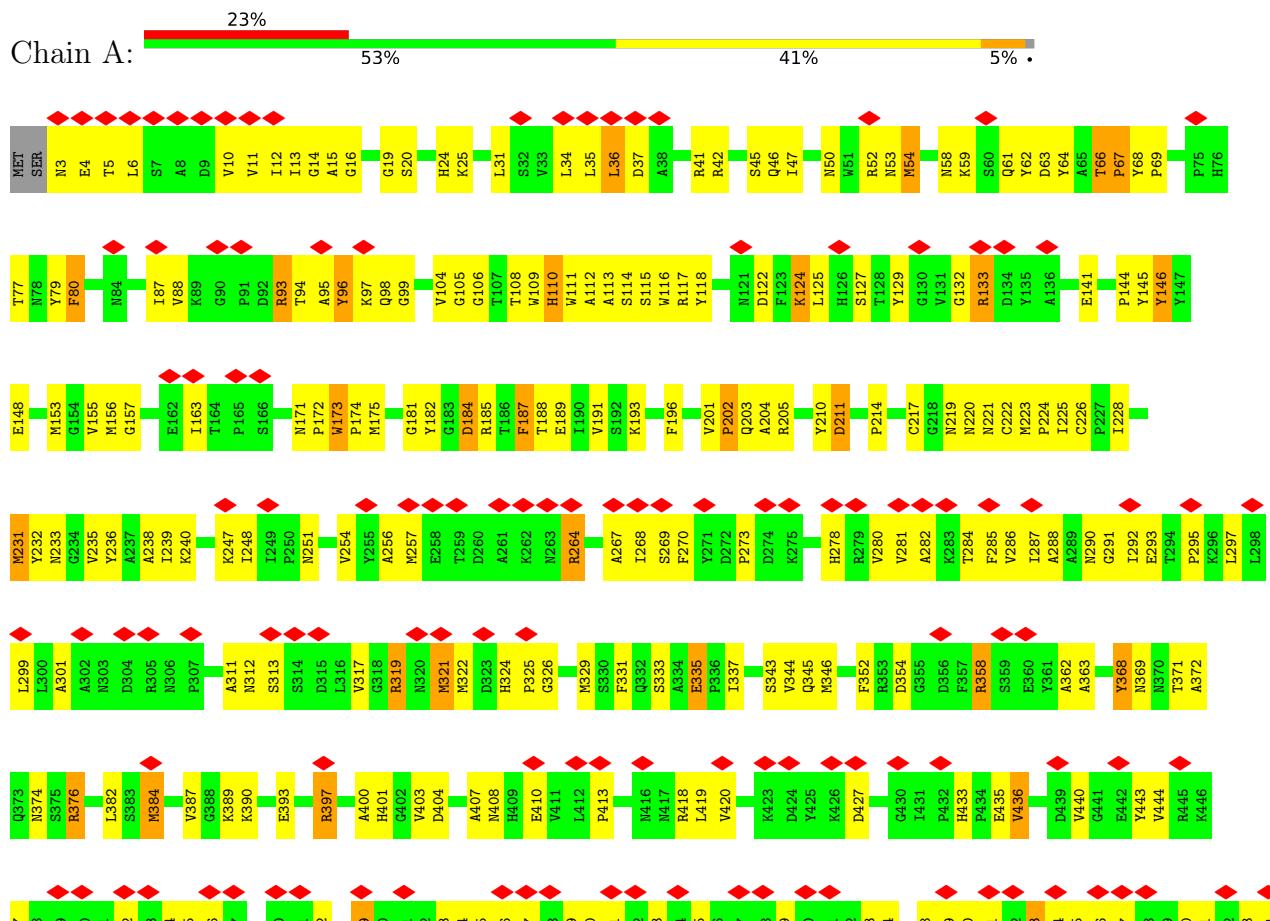
Mol	Chain	Residues	Atoms			AltConf
7	C	1	Total 38	C 34	O 4	0

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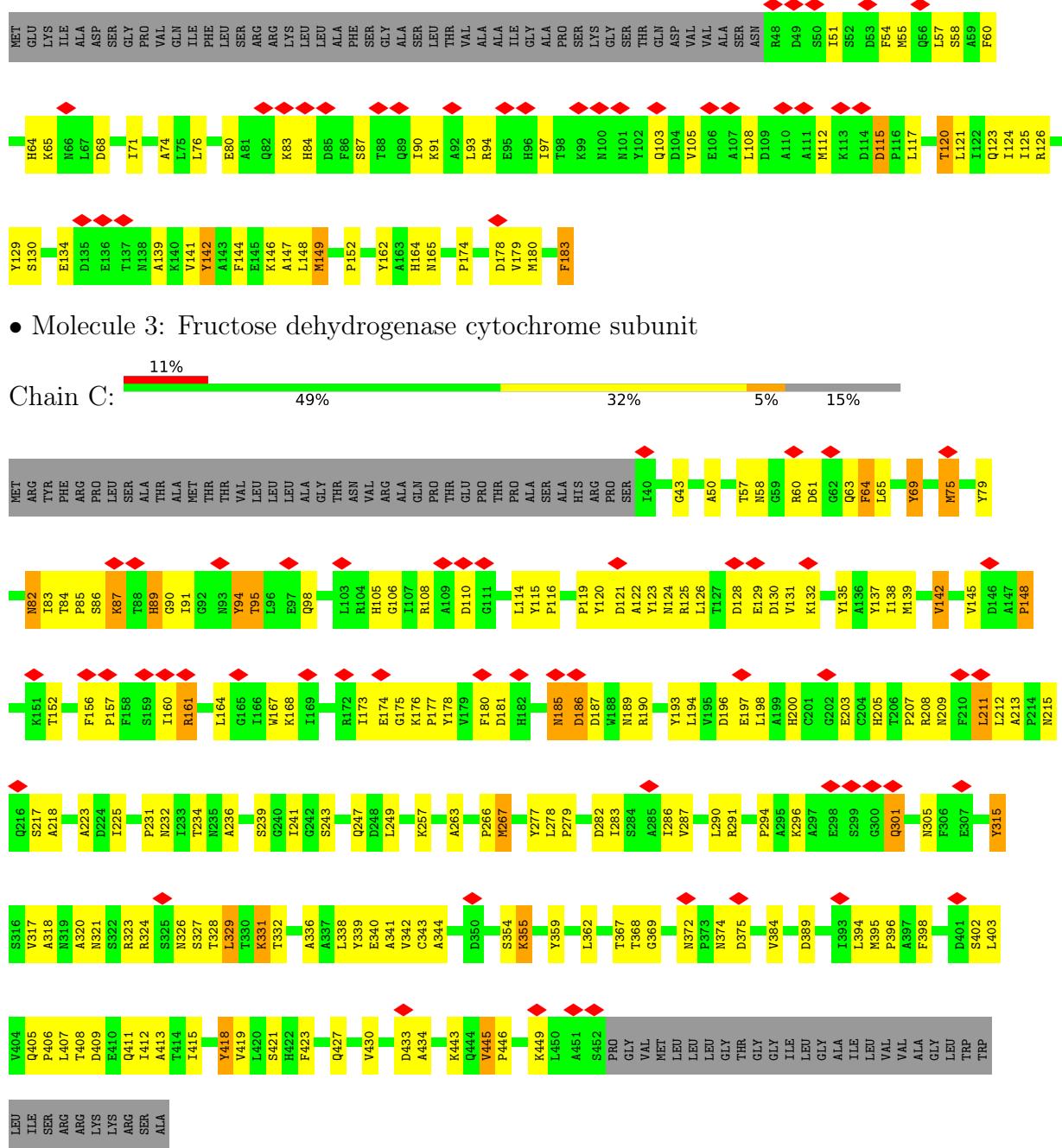
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Fructose dehydrogenase large subunit

- Molecule 2: Fructose dehydrogenase small subunit

MET GLU LYS ILE ALA ASP GLY SER GLY PRO VAL GLN ILE PHE LEU SER ARG ARG LYS LEU LEU ALA PHE SER GLY ALA SER LEU THR VAL ALA ALA ILE GLY ALA PRO SER LYS GLY SER THR GLN ASP VAL VAL ALA SER ASN R48 D49 S50 I51 S52 D53 F54 M55 Q56 L57 S58 A59 F60

H64 K65 N66 L67 D68 I71 A74 L75 L76 E80 A81 Q82 K83 H84 D85 F86 S87 T88 Q89 I90 K91 A92 L93 R94 E95 H96 I97 T98 K99 N100 N101 Y102 Q103 D104 V105 E106 A107 L108 D109 A110 A111 M112 K113 D114 D115 P116 L117 T120 L121 I122 Q123 I124 I125 R126

Y129 S130 E134 D135 E136 T137 N138 A139 K140 V141 Y142 A143 F144 E145 K146 A147 L148 M149 P152 Y162 A163 H164 N165 P174 D178 V179 M180 F183

• Molecule 3: Fructose dehydrogenase cytochrome subunit

Chain C:

11%

49%   32%   5%   15%

MET ARG TYR PHE ARG PRO LEU SER ALA THR ALA MET THR THR VAL LEU LEU ALA GLY THR ASN VAL ARG ALA GLN PRO THR GLU PRO THR PRO ALA SER ALA HIS ARG PRO SER I40 G43 A50 T57 N58 G59 R60 D61 G62 Q63 F64 L65 Y69 M75 Y79

N82 I83 T84 P85 S86 K87 T88 H89 G90 I91 G92 N93 Y94 T95 L96 E97 Q98 L103 R104 H105 G106 I107 R108 A109 D110 G111 L114 Y115 P116 P119 Y120 D121 A122 Y123 N124 R125 L126 T127 D128 E129 D130 V131 K132 Y135 A136 Y137 I138 M139 V142 V145 D146 A147 P148

K151 T152 F156 P157 F158 S159 I160 R161 L164 G165 I166 W167 K168 I169 R172 I173 E174 G175 K176 P177 Y178 V179 F180 D181 H182 N185 D186 D187 W188 N189 R190 Y193 L194 V195 D196 E197 L198 A199 H200 C201 G202 E203 C204 H205 T206 P207 R208 N209 F210 L211 L212 A213 P214 N215

Q216 S217 A218 A223 D224 I225 P231 N232 I233 T234 N235 A236 S239 G240 I241 G242 S243 Q247 D248 L249 K257 A263 P266 M267 Y277 L278 P279 D282 I283 S284 A285 I286 V287 L290 R291 P294 A295 K296 A297 E298 S299 G300 Q301 N305 F306 E307 Y315

S316 V317 A318 N319 A320 N321 S322 R323 R324 S325 N326 S327 T328 L329 T330 K331 T332 A336 A337 L338 Y339 E340 A341 V342 C343 A344 D350 S354 K355 Y359 L362 T367 T368 G369 N372 P373 N374 D375 V384 D389 I393 L394 M395 P396 A397 F398 D401 S402 L403

V404 Q405 P406 L407 T408 D409 E410 Q411 I412 A413 T414 I415 Y418 V419 L420 S421 H422 F423 Q427 V430 D433 A434 K443 Q444 V445 P446 K449 L450 A451 S452 PRO GLY VAL MET LEU LEU LEU GLY THR GLY GLY ILE LEU GLY ALA ILE LEU LEU VAL VAL ALA GLY LEU LEU TRP TRP

LEU ILE SER ARG ARG LYS ARG SER ALA

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	64345	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 $(e^-/\text{Å}^2)$	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	0.846	Depositor
Minimum map value	-0.252	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.127	Depositor
Map size (Å)	240.8, 240.8, 240.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, F3S, HEC, U10

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	0.40	3/4267 (0.1%)	0.81	11/5803 (0.2%)
2	B	0.29	0/1107	0.52	0/1507
3	C	0.29	0/3206	0.61	1/4369 (0.0%)
All	All	0.35	3/8580 (0.0%)	0.70	12/11679 (0.1%)

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
1	A	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	PRO	CB-CG	-10.15	0.99	1.50
1	A	144	PRO	CG-CD	-8.54	1.22	1.50
1	A	172	PRO	CG-CD	-8.46	1.22	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	PRO	CB-CG-CD	18.81	179.85	106.50
1	A	144	PRO	N-CD-CG	-17.73	76.60	103.20
1	A	144	PRO	CA-CB-CG	-17.03	71.64	104.00
1	A	172	PRO	CA-N-CD	-13.08	93.19	111.50
1	A	67	PRO	CA-N-CD	-11.87	94.89	111.50
3	C	148	PRO	CA-N-CD	-10.46	96.85	111.50
1	A	172	PRO	N-CD-CG	-7.68	91.68	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	144	PRO	CA-N-CD	-7.68	100.75	111.50
1	A	202	PRO	CA-N-CD	-6.92	101.81	111.50
1	A	172	PRO	CA-CB-CG	-6.19	92.24	104.00
1	A	211	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	36	LEU	CA-CB-CG	5.35	127.60	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	79	TYR	Peptide
1	A	80	PHE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4164	0	4050	218	0
2	B	1080	0	1046	38	0
3	C	3130	0	3012	140	0
4	A	53	0	31	4	0
5	A	7	0	0	2	0
6	C	129	0	87	13	0
7	C	38	0	47	2	0
All	All	8601	0	8273	376	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 22.

All (376) 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:A:12:ILE:HG22	1:A:286:VAL:HB	1.40	1.03
1:A:46:GLN:NE2	1:A:50:ASN:OD1	1.99	0.95
1:A:31:LEU:HD21	1:A:541:LEU:HD23	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:THR:HG1	4:A:601:FAD:HO4'	1.24	0.81
1:A:418:ARG:HD3	1:A:419:LEU:H	1.44	0.79
1:A:6:LEU:HB2	1:A:280:VAL:HG12	1.64	0.79
1:A:110:HIS:O	1:A:110:HIS:ND1	2.14	0.78
1:A:13:ILE:HD11	1:A:287:ILE:HG12	1.65	0.78
1:A:66:THR:HG23	1:A:67:PRO:HD2	1.66	0.77
1:A:53:ASN:ND2	3:C:317:VAL:O	2.16	0.76
2:B:57:LEU:HD22	2:B:90:ILE:HG13	1.66	0.75
2:B:51:ILE:HG12	2:B:76:LEU:HD23	1.68	0.74
1:A:257:MET:HB2	1:A:268:ILE:HG22	1.70	0.73
2:B:134:GLU:OE1	2:B:134:GLU:N	2.22	0.73
1:A:326:GLY:HA3	1:A:476:ASN:HD21	1.53	0.73
3:C:278:LEU:HD21	3:C:282:ASP:HB2	1.71	0.72
2:B:93:LEU:HD22	2:B:121:LEU:HD22	1.71	0.72
3:C:75:MET:SD	3:C:75:MET:N	2.64	0.71
1:A:156:MET:HA	1:A:175:MET:HB2	1.72	0.71
3:C:98:GLN:N	3:C:98:GLN:OE1	2.24	0.71
1:A:322:MET:HG2	1:A:481:GLY:HA3	1.73	0.70
1:A:418:ARG:HD2	1:A:420:VAL:HG13	1.73	0.70
3:C:234:THR:HG21	3:C:296:LYS:H	1.57	0.70
1:A:286:VAL:HG21	1:A:537:ILE:HD11	1.74	0.70
2:B:74:ALA:HB1	2:B:142:TYR:CE2	2.26	0.70
2:B:144:PHE:H	3:C:317:VAL:HG21	1.57	0.70
1:A:217:CYS:SG	3:C:359:TYR:OH	2.36	0.69
3:C:427:GLN:OE1	3:C:427:GLN:N	2.27	0.68
1:A:133:ARG:HG2	1:A:413:PRO:HG3	1.76	0.68
1:A:319:ARG:HD2	1:A:418:ARG:HG2	1.75	0.68
3:C:234:THR:OG1	3:C:294:PRO:O	2.11	0.68
3:C:50:ALA:O	3:C:123:TYR:OH	2.11	0.68
3:C:249:LEU:HD23	3:C:287:VAL:HG23	1.75	0.67
1:A:223:MET:H	1:A:344:VAL:HG11	1.58	0.67
1:A:268:ILE:HG13	1:A:280:VAL:HG23	1.77	0.66
2:B:108:LEU:HD21	2:B:121:LEU:HD21	1.78	0.66
3:C:340:GLU:HA	3:C:344:ALA:HB2	1.78	0.66
1:A:98:GLN:HG2	1:A:477:ASN:HA	1.78	0.65
1:A:46:GLN:HB2	3:C:329:LEU:HB2	1.77	0.65
1:A:13:ILE:HG12	1:A:287:ILE:HA	1.80	0.64
1:A:418:ARG:HD3	1:A:419:LEU:N	2.12	0.64
3:C:232:ASN:OD1	3:C:234:THR:HG22	1.95	0.64
1:A:47:ILE:HG22	1:A:225:ILE:HG21	1.80	0.63
1:A:358:ARG:O	1:A:443:TYR:OH	2.09	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:VAL:O	1:A:109:TRP:NE1	2.30	0.63
3:C:362:LEU:HG	3:C:368:THR:HG21	1.80	0.63
1:A:326:GLY:O	1:A:474:THR:N	2.26	0.62
3:C:384:VAL:O	3:C:394:LEU:HA	2.00	0.62
1:A:333:SER:OG	1:A:335:GLU:O	2.18	0.62
3:C:119:PRO:HB3	3:C:203:GLU:HG3	1.82	0.62
3:C:57:THR:HG22	3:C:64:PHE:HA	1.81	0.62
3:C:120:TYR:HA	3:C:123:TYR:HB2	1.80	0.62
3:C:126:LEU:HD13	3:C:197:GLU:HB3	1.81	0.62
1:A:96:TYR:HE2	1:A:321:MET:HG3	1.65	0.61
1:A:155:VAL:HA	1:A:204:ALA:HA	1.80	0.61
1:A:4:GLU:HG2	1:A:5:THR:H	1.66	0.61
1:A:133:ARG:HA	1:A:133:ARG:NH1	2.15	0.61
1:A:267:ALA:HB2	1:A:281:VAL:HG22	1.81	0.61
1:A:235:VAL:O	1:A:239:ILE:HG22	2.01	0.61
3:C:82:ASN:OD1	3:C:90:GLY:HA2	2.01	0.61
1:A:493:VAL:HG22	1:A:494:VAL:HG13	1.83	0.61
3:C:241:ILE:HG21	6:C:502:HEC:HMA3	1.83	0.60
2:B:97:ILE:HG22	2:B:108:LEU:HD13	1.84	0.60
1:A:12:ILE:HD13	1:A:35:LEU:HD23	1.84	0.59
1:A:15:ALA:HB3	1:A:37:ASP:HB2	1.84	0.59
1:A:299:LEU:HD13	1:A:418:ARG:HH12	1.65	0.59
1:A:329:MET:HE2	1:A:455:LEU:HD13	1.84	0.59
3:C:128:ASP:HA	3:C:131:VAL:HG22	1.84	0.59
1:A:317:VAL:O	1:A:319:ARG:NH1	2.34	0.59
1:A:25:LYS:HD3	1:A:531:LEU:HD22	1.84	0.59
1:A:111:TRP:CZ2	1:A:113:ALA:HA	2.38	0.58
3:C:65:LEU:HD12	3:C:83:ILE:HB	1.84	0.58
3:C:209:ASN:HD21	3:C:213:ALA:HB3	1.68	0.58
1:A:291:GLY:H	1:A:479:ILE:HD13	1.67	0.58
3:C:125:ARG:HB3	3:C:197:GLU:HG3	1.86	0.58
3:C:433:ASP:OD1	3:C:434:ALA:N	2.37	0.58
1:A:34:LEU:HD12	1:A:247:LYS:HD3	1.86	0.58
3:C:286:ILE:O	3:C:290:LEU:HD23	2.03	0.58
1:A:256:ALA:HA	1:A:301:ALA:HB2	1.85	0.58
3:C:367:THR:HG23	3:C:375:ASP:HB3	1.85	0.58
3:C:234:THR:HG23	3:C:236:ALA:H	1.69	0.57
3:C:105:HIS:O	3:C:168:LYS:NZ	2.36	0.57
3:C:207:PRO:HA	3:C:223:ALA:HB2	1.86	0.57
1:A:47:ILE:HG21	1:A:68:TYR:CZ	2.40	0.57
6:C:502:HEC:HBC1	7:C:504:U10:H303	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:HG22	1:A:284:THR:HB	1.86	0.57
1:A:88:VAL:HG23	1:A:93:ARG:HE	1.68	0.57
2:B:87:SER:O	2:B:91:LYS:HG2	2.04	0.57
3:C:215:ASN:OD1	3:C:217:SER:OG	2.22	0.57
1:A:11:VAL:HG22	1:A:282:ALA:HB3	1.85	0.57
2:B:64:HIS:ND1	2:B:183:PHE:O	2.38	0.57
1:A:97:LYS:HB2	1:A:475:PRO:HG3	1.85	0.57
3:C:323:ARG:CZ	3:C:332:THR:HG23	2.35	0.57
3:C:116:PRO:HD2	3:C:164:LEU:HD21	1.87	0.56
1:A:220:ASN:OD1	1:A:372:ALA:N	2.38	0.56
3:C:205:HIS:CD2	6:C:502:HEC:NB	2.68	0.56
1:A:452:ARG:O	1:A:456:MET:HG3	2.05	0.56
3:C:408:THR:N	3:C:411:GLN:OE1	2.38	0.56
1:A:118:TYR:OH	1:A:517:SER:O	2.22	0.56
3:C:266:PRO:HB2	6:C:502:HEC:HHD	1.88	0.56
1:A:13:ILE:HG22	1:A:36:LEU:HG	1.88	0.56
1:A:257:MET:CB	1:A:268:ILE:HG22	2.36	0.56
1:A:257:MET:HE3	1:A:301:ALA:HB3	1.88	0.56
1:A:205:ARG:HA	1:A:231:MET:HA	1.88	0.56
1:A:498:LEU:HD11	1:A:529:LEU:HD22	1.88	0.56
3:C:193:TYR:O	3:C:197:GLU:HB2	2.06	0.56
3:C:354:SER:HB2	3:C:359:TYR:HB2	1.86	0.56
3:C:187:ASP:OD2	3:C:187:ASP:N	2.39	0.55
3:C:323:ARG:NH1	3:C:332:THR:HG23	2.21	0.55
1:A:214:PRO:HG3	3:C:396:PRO:HD3	1.88	0.55
3:C:323:ARG:NH2	3:C:332:THR:HA	2.21	0.55
1:A:41:ARG:HH22	1:A:248:ILE:HD11	1.72	0.55
1:A:325:PRO:HG2	1:A:444:VAL:HG11	1.87	0.55
3:C:135:TYR:O	3:C:139:MET:HG2	2.06	0.55
1:A:88:VAL:CG2	1:A:93:ARG:HE	2.18	0.55
1:A:522:SER:O	1:A:526:MET:HG2	2.07	0.55
2:B:120:THR:O	2:B:124:ILE:HG22	2.06	0.55
1:A:96:TYR:CE2	1:A:321:MET:HG3	2.41	0.55
1:A:333:SER:O	1:A:401:HIS:ND1	2.30	0.55
3:C:338:LEU:O	3:C:342:VAL:HG12	2.07	0.55
1:A:270:PHE:CE1	1:A:278:HIS:HB2	2.41	0.55
2:B:152:PRO:HB3	2:B:180:MET:HE1	1.89	0.55
1:A:41:ARG:HG2	1:A:104:VAL:HG21	1.89	0.54
1:A:64:TYR:HB3	1:A:224:PRO:HB3	1.89	0.54
2:B:141:VAL:O	3:C:321:ASN:ND2	2.40	0.54
1:A:3:ASN:HB2	1:A:6:LEU:HD11	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:THR:HA	1:A:97:LYS:HD2	1.90	0.54
1:A:201:VAL:HG12	1:A:346:MET:HA	1.88	0.54
3:C:263:ALA:HB1	3:C:267:MET:HB3	1.90	0.54
3:C:167:TRP:NE1	3:C:211:LEU:O	2.30	0.54
3:C:190:ARG:O	3:C:194:LEU:HG	2.07	0.54
1:A:37:ASP:OD1	4:A:601:FAD:O2B	2.24	0.53
1:A:286:VAL:HG22	1:A:507:PHE:HB2	1.89	0.53
3:C:359:TYR:CD2	6:C:501:HEC:HMD3	2.43	0.53
3:C:234:THR:HG21	3:C:296:LYS:N	2.20	0.53
3:C:63:GLN:HG3	3:C:145:VAL:HG11	1.90	0.53
1:A:268:ILE:HG23	1:A:285:PHE:CE2	2.43	0.53
3:C:64:PHE:CD2	3:C:65:LEU:HD23	2.44	0.53
1:A:498:LEU:HD22	1:A:533:ALA:HB2	1.91	0.52
1:A:11:VAL:HG12	1:A:34:LEU:HD22	1.92	0.52
1:A:187:PHE:HE1	1:A:368:TYR:HB2	1.74	0.52
1:A:329:MET:HG2	1:A:331:PHE:HD1	1.75	0.52
1:A:46:GLN:OE1	3:C:329:LEU:HD12	2.08	0.52
1:A:153:MET:HG2	1:A:232:TYR:CE2	2.45	0.52
2:B:105:VAL:HG23	2:B:108:LEU:HD23	1.91	0.52
3:C:84:THR:HG21	3:C:145:VAL:HG22	1.92	0.52
1:A:220:ASN:ND2	1:A:343:SER:O	2.42	0.52
1:A:284:THR:HA	1:A:505:ASN:OD1	2.10	0.52
3:C:125:ARG:HG2	3:C:178:TYR:HB2	1.90	0.52
3:C:418:TYR:HE1	3:C:423:PHE:CZ	2.28	0.51
1:A:115:SER:HB3	1:A:524:LEU:HD22	1.92	0.51
1:A:324:HIS:HB3	1:A:408:ASN:HB3	1.92	0.51
3:C:181:ASP:O	3:C:189:ASN:ND2	2.33	0.51
3:C:359:TYR:HD2	6:C:501:HEC:HMD3	1.75	0.51
3:C:190:ARG:HG3	3:C:190:ARG:HH11	1.76	0.51
1:A:24:HIS:CE1	1:A:240:LYS:HB3	2.46	0.51
1:A:58:ASN:HB3	1:A:63:ASP:HB3	1.92	0.51
3:C:85:PRO:HG3	3:C:139:MET:HA	1.92	0.51
1:A:117:ARG:HA	1:A:146:TYR:CZ	2.46	0.51
1:A:427:ASP:HB3	1:A:433:HIS:NE2	2.26	0.51
3:C:95:THR:HG23	3:C:98:GLN:OE1	2.10	0.51
1:A:45:SER:HB3	3:C:341:ALA:HB1	1.93	0.51
1:A:173:TRP:HD1	1:A:174:PRO:CD	2.24	0.51
1:A:124:LYS:HB2	1:A:127:SER:HB2	1.94	0.50
2:B:129:TYR:HA	2:B:148:LEU:HB2	1.93	0.50
1:A:187:PHE:CE2	1:A:191:VAL:HG11	2.46	0.50
1:A:290:ASN:HB2	1:A:293:GLU:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:372:ASN:HB3	3:C:374:ASN:OD1	2.11	0.50
1:A:205:ARG:NH1	1:A:222:CYS:SG	2.85	0.50
1:A:211:ASP:OD1	3:C:403:LEU:HD12	2.12	0.50
1:A:264:ARG:HG2	1:A:505:ASN:HD22	1.76	0.50
3:C:86:SER:HB2	3:C:90:GLY:HA3	1.94	0.50
1:A:221:ASN:OD1	1:A:221:ASN:O	2.29	0.50
1:A:233:ASN:HB2	1:A:235:VAL:HG12	1.93	0.50
1:A:499:ARG:NH1	1:A:504:SER:O	2.36	0.50
1:A:337:ILE:HG22	1:A:401:HIS:HA	1.94	0.50
1:A:116:TRP:HE1	1:A:201:VAL:HG23	1.76	0.49
1:A:329:MET:HG2	1:A:331:PHE:CD1	2.47	0.49
2:B:94:ARG:O	2:B:97:ILE:HG13	2.13	0.49
1:A:41:ARG:NH2	1:A:248:ILE:HD11	2.28	0.49
3:C:194:LEU:HD23	3:C:198:LEU:HD12	1.95	0.49
1:A:311:ALA:HB1	1:A:493:VAL:HG23	1.94	0.49
1:A:157:GLY:HA3	1:A:173:TRP:CD2	2.48	0.49
1:A:236:TYR:HD1	3:C:403:LEU:HD22	1.78	0.49
1:A:299:LEU:CD1	1:A:418:ARG:HH12	2.26	0.49
1:A:326:GLY:HA2	1:A:407:ALA:O	2.13	0.49
3:C:91:ILE:O	3:C:94:TYR:HB2	2.13	0.49
3:C:115:TYR:HA	3:C:164:LEU:HD21	1.94	0.49
1:A:132:GLY:HA2	1:A:413:PRO:HD2	1.95	0.48
1:A:193:LYS:HB2	1:A:193:LYS:HE2	1.69	0.48
1:A:397:ARG:HB3	1:A:397:ARG:NH1	2.28	0.48
3:C:225:ILE:HD11	3:C:266:PRO:HG2	1.95	0.48
1:A:106:GLY:O	1:A:109:TRP:HB2	2.13	0.48
1:A:312:ASN:HD21	1:A:319:ARG:HH12	1.60	0.48
1:A:184:ASP:O	1:A:188:THR:OG1	2.29	0.48
1:A:187:PHE:CE1	1:A:368:TYR:HB2	2.48	0.48
1:A:191:VAL:HB	1:A:196:PHE:HB2	1.95	0.48
1:A:343:SER:HB2	1:A:346:MET:SD	2.54	0.48
2:B:60:PHE:HE2	2:B:108:LEU:HD22	1.77	0.48
1:A:64:TYR:CE1	1:A:223:MET:HB3	2.49	0.48
1:A:419:LEU:HD12	1:A:436:VAL:HG12	1.96	0.48
1:A:290:ASN:O	1:A:510:THR:OG1	2.32	0.48
1:A:256:ALA:HA	1:A:301:ALA:CB	2.44	0.48
1:A:337:ILE:N	1:A:400:ALA:O	2.37	0.47
2:B:139:ALA:O	3:C:324:ARG:NH1	2.47	0.47
1:A:114:SER:OG	1:A:345:GLN:OE1	2.18	0.47
1:A:291:GLY:N	1:A:479:ILE:HD13	2.29	0.47
1:A:45:SER:N	3:C:405:GLN:OE1	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:CYS:SG	1:A:228:ILE:HB	2.54	0.47
3:C:338:LEU:CB	3:C:415:ILE:HD11	2.45	0.47
1:A:50:ASN:HB3	1:A:67:PRO:HA	1.97	0.47
3:C:320:ALA:HA	3:C:323:ARG:HB2	1.97	0.47
3:C:402:SER:O	3:C:406:PRO:HG3	2.15	0.47
3:C:194:LEU:HD11	3:C:282:ASP:HB3	1.97	0.47
1:A:202:PRO:HD2	1:A:202:PRO:O	2.15	0.47
1:A:113:ALA:O	1:A:203:GLN:HA	2.15	0.46
1:A:129:TYR:OH	1:A:354:ASP:OD1	2.22	0.46
3:C:174:GLU:HA	3:C:175:GLY:HA3	1.45	0.46
3:C:231:PRO:HD3	6:C:502:HEC:C3D	2.45	0.46
1:A:19:GLY:HA3	1:A:35:LEU:HD21	1.98	0.46
1:A:440:VAL:HG22	1:A:444:VAL:HB	1.97	0.46
1:A:196:PHE:CZ	1:A:454:ARG:HG2	2.50	0.46
1:A:389:LYS:O	1:A:393:GLU:HG2	2.16	0.46
1:A:521:ALA:HB1	4:A:601:FAD:O2	2.14	0.46
1:A:69:PRO:HG2	3:C:327:SER:H	1.79	0.46
2:B:162:TYR:CE2	3:C:344:ALA:HB1	2.50	0.46
3:C:108:ARG:HH22	3:C:161:ARG:HD2	1.80	0.46
1:A:54:MET:SD	1:A:58:ASN:HB2	2.55	0.46
1:A:499:ARG:HB2	1:A:507:PHE:CE2	2.50	0.46
3:C:239:SER:OG	3:C:301:GLN:HG2	2.15	0.46
1:A:13:ILE:CG1	1:A:287:ILE:HA	2.44	0.46
1:A:182:TYR:CD2	2:B:174:PRO:HG3	2.50	0.46
1:A:387:VAL:HG23	2:B:125:ILE:HD13	1.98	0.46
1:A:122:ASP:HA	1:A:125:LEU:HD21	1.97	0.46
1:A:205:ARG:HD3	5:A:602:F3S:S3	2.56	0.46
1:A:358:ARG:NE	1:A:410:GLU:OE1	2.43	0.46
1:A:369:ASN:OD1	1:A:371:THR:OG1	2.21	0.46
3:C:200:HIS:HB2	3:C:203:GLU:HG2	1.97	0.46
1:A:295:PRO:HB2	1:A:419:LEU:HD23	1.97	0.46
1:A:384:MET:SD	1:A:384:MET:N	2.85	0.46
1:A:500:THR:OG1	1:A:506:LEU:HB3	2.16	0.46
3:C:305:ASN:O	3:C:369:GLY:HA3	2.16	0.46
1:A:20:SER:HB3	1:A:238:ALA:N	2.30	0.46
1:A:115:SER:O	1:A:202:PRO:HG2	2.16	0.46
1:A:187:PHE:HD2	1:A:187:PHE:O	1.99	0.46
1:A:117:ARG:HA	1:A:146:TYR:OH	2.15	0.45
1:A:403:VAL:HG21	1:A:462:MET:HE1	1.97	0.45
1:A:382:LEU:HD13	2:B:126:ARG:HG2	1.97	0.45
1:A:47:ILE:HB	1:A:225:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:176:LYS:HD2	3:C:177:PRO:N	2.31	0.45
3:C:398:PHE:HZ	6:C:501:HEC:HMC2	1.82	0.45
1:A:418:ARG:HH11	1:A:419:LEU:C	2.20	0.45
3:C:130:ASP:OD2	3:C:193:TYR:OH	2.15	0.45
1:A:12:ILE:CD1	1:A:35:LEU:HD23	2.47	0.45
1:A:523:THR:HA	1:A:526:MET:HG2	1.98	0.45
3:C:91:ILE:HB	3:C:94:TYR:CD1	2.51	0.45
1:A:42:ARG:HA	3:C:328:THR:HB	1.98	0.44
1:A:251:ASN:HB3	1:A:273:PRO:HD3	1.98	0.44
3:C:185:ASN:HB2	3:C:187:ASP:OD2	2.17	0.44
3:C:283:ILE:O	3:C:287:VAL:HG12	2.17	0.44
3:C:445:VAL:HG22	3:C:446:PRO:HD2	1.99	0.44
7:C:504:U10:H272	7:C:504:U10:H251	1.54	0.44
1:A:185:ARG:O	1:A:189:GLU:HG2	2.17	0.44
3:C:247:GLN:OE1	3:C:247:GLN:HA	2.18	0.44
1:A:292:ILE:HG23	1:A:419:LEU:HD11	1.99	0.44
1:A:35:LEU:HD23	1:A:35:LEU:HA	1.85	0.44
1:A:77:THR:OG1	1:A:99:GLY:HA2	2.18	0.44
1:A:184:ASP:OD1	1:A:346:MET:HB2	2.17	0.44
1:A:157:GLY:HA3	1:A:173:TRP:CE3	2.53	0.44
1:A:196:PHE:HZ	1:A:454:ARG:HG2	1.83	0.44
1:A:228:ILE:HD13	1:A:228:ILE:HA	1.82	0.44
1:A:111:TRP:CZ3	1:A:523:THR:HG21	2.53	0.44
2:B:93:LEU:HD21	2:B:117:LEU:HB3	2.00	0.44
3:C:176:LYS:HD2	3:C:177:PRO:CD	2.47	0.44
3:C:336:ALA:HB2	3:C:418:TYR:HE2	1.82	0.44
1:A:69:PRO:HD2	3:C:327:SER:HB3	1.99	0.44
2:B:68:ASP:HB3	2:B:71:ILE:HD12	1.99	0.44
3:C:126:LEU:CD1	3:C:197:GLU:HB3	2.45	0.44
6:C:501:HEC:HMB1	6:C:501:HEC:HBB3	1.99	0.44
1:A:62:TYR:HB3	1:A:64:TYR:CZ	2.53	0.43
1:A:145:TYR:O	1:A:148:GLU:HG2	2.18	0.43
1:A:145:TYR:CE2	1:A:532:ARG:HG3	2.52	0.43
3:C:106:GLY:C	3:C:114:LEU:HD13	2.37	0.43
3:C:413:ALA:HA	3:C:430:VAL:HG12	2.00	0.43
1:A:311:ALA:H	1:A:503:HIS:HE1	1.66	0.43
1:A:480:THR:HA	1:A:511:GLY:O	2.19	0.43
2:B:144:PHE:C	2:B:146:LYS:H	2.22	0.43
3:C:186:ASP:OD1	3:C:186:ASP:N	2.51	0.43
2:B:130:SER:HA	2:B:149:MET:SD	2.59	0.43
3:C:160:ILE:O	3:C:160:ILE:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:TYR:HA	1:A:236:TYR:HE2	1.83	0.43
1:A:257:MET:HA	1:A:268:ILE:HA	2.00	0.43
3:C:315:TYR:CD1	3:C:340:GLU:HG3	2.54	0.43
3:C:326:ASN:O	3:C:331:LYS:NZ	2.48	0.43
1:A:10:VAL:HG12	1:A:12:ILE:HG23	2.01	0.43
1:A:14:GLY:HA3	1:A:288:ALA:O	2.19	0.43
3:C:63:GLN:CG	3:C:145:VAL:HG11	2.48	0.43
1:A:61:GLN:HB2	1:A:80:PHE:HZ	1.83	0.43
1:A:112:ALA:N	1:A:223:MET:HE1	2.34	0.43
1:A:256:ALA:HB3	1:A:269:SER:OG	2.19	0.43
1:A:322:MET:HB3	1:A:322:MET:HE2	1.74	0.43
1:A:514:MET:CE	1:A:529:LEU:HD11	2.49	0.43
3:C:129:GLU:O	3:C:132:LYS:HG2	2.18	0.43
1:A:219:ASN:HB2	5:A:602:F3S:S1	2.59	0.43
2:B:112:MET:HE3	2:B:115:ASP:OD1	2.18	0.43
3:C:95:THR:HA	3:C:135:TYR:OH	2.19	0.43
1:A:141:GLU:OE2	1:A:532:ARG:NH1	2.52	0.42
1:A:352:PHE:O	1:A:363:ALA:HB1	2.19	0.42
1:A:469:MET:HA	1:A:469:MET:CE	2.49	0.42
3:C:87:LYS:HD2	3:C:87:LYS:HA	1.81	0.42
3:C:207:PRO:HD2	3:C:218:ALA:O	2.18	0.42
3:C:331:LYS:H	3:C:331:LYS:HD2	1.83	0.42
1:A:254:VAL:HG12	1:A:297:LEU:HD11	2.01	0.42
2:B:165:ASN:HB3	3:C:355:LYS:HB3	2.01	0.42
3:C:79:TYR:H	3:C:152:THR:HB	1.83	0.42
3:C:326:ASN:HB3	3:C:331:LYS:NZ	2.34	0.42
1:A:87:ILE:O	1:A:435:GLU:HA	2.19	0.42
2:B:74:ALA:HB1	2:B:142:TYR:CD2	2.53	0.42
3:C:121:ASP:HB2	3:C:173:ILE:HG12	2.01	0.42
3:C:138:ILE:O	3:C:142:VAL:HG13	2.18	0.42
3:C:342:VAL:HG13	3:C:343:CYS:SG	2.59	0.42
1:A:34:LEU:HD23	1:A:34:LEU:O	2.20	0.42
2:B:54:PHE:HA	2:B:90:ILE:HD11	2.01	0.42
1:A:214:PRO:HG3	6:C:501:HEC:HAC	2.01	0.42
1:A:374:ASN:OD1	1:A:374:ASN:N	2.53	0.42
1:A:489:PRO:HA	1:A:501:HIS:ND1	2.35	0.42
1:A:52:ARG:NH1	3:C:340:GLU:O	2.51	0.42
1:A:211:ASP:OD1	1:A:211:ASP:O	2.37	0.42
1:A:285:PHE:O	1:A:506:LEU:HA	2.20	0.42
1:A:376:ARG:NH2	1:A:404:ASP:OD2	2.49	0.42
3:C:63:GLN:HE21	3:C:145:VAL:HB	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:ASP:HA	3:C:173:ILE:HG23	2.01	0.42
3:C:212:LEU:HD21	3:C:445:VAL:HG21	2.02	0.42
3:C:407:LEU:HD12	3:C:412:ILE:HD12	2.02	0.42
3:C:419:VAL:HG21	6:C:501:HEC:HMB3	2.01	0.42
1:A:535:ASP:HA	1:A:538:LEU:HD12	2.02	0.42
3:C:43:GLY:HA3	3:C:137:TYR:HB2	2.02	0.42
3:C:122:ALA:HB1	3:C:196:ASP:O	2.20	0.42
3:C:194:LEU:HD12	3:C:286:ILE:HG13	2.01	0.42
1:A:63:ASP:OD2	1:A:66:THR:HG22	2.20	0.41
1:A:362:ALA:H	1:A:447:SER:HB2	1.84	0.41
1:A:469:MET:HA	1:A:469:MET:HE3	2.02	0.41
3:C:403:LEU:HD23	3:C:403:LEU:HA	1.77	0.41
1:A:4:GLU:H	1:A:4:GLU:CD	2.24	0.41
1:A:54:MET:CE	1:A:59:LYS:HG3	2.50	0.41
1:A:95:ALA:HB2	1:A:473:PHE:HB2	2.02	0.41
1:A:105:GLY:HA3	1:A:109:TRP:CD1	2.55	0.41
1:A:333:SER:N	1:A:401:HIS:O	2.38	0.41
1:A:16:GLY:HA3	4:A:601:FAD:O1A	2.20	0.41
2:B:129:TYR:CG	2:B:148:LEU:HB2	2.55	0.41
3:C:338:LEU:HB3	3:C:415:ILE:HD11	2.03	0.41
3:C:409:ASP:HA	3:C:412:ILE:HD13	2.03	0.41
1:A:187:PHE:O	1:A:191:VAL:HG22	2.20	0.41
2:B:103:GLN:OE1	2:B:103:GLN:HA	2.21	0.41
3:C:89:HIS:HB3	3:C:148:PRO:HD3	2.03	0.41
3:C:339:TYR:CD2	3:C:343:CYS:HB2	2.56	0.41
1:A:110:HIS:ND1	1:A:110:HIS:C	2.73	0.41
2:B:55:MET:HA	2:B:58:SER:OG	2.21	0.41
3:C:156:PHE:CG	3:C:157:PRO:HA	2.56	0.41
3:C:407:LEU:HD13	3:C:411:GLN:CB	2.51	0.41
1:A:223:MET:HA	1:A:223:MET:CE	2.50	0.41
1:A:19:GLY:CA	1:A:35:LEU:HD21	2.51	0.41
1:A:53:ASN:OD1	3:C:320:ALA:HB3	2.21	0.41
1:A:226:CYS:HB3	1:A:231:MET:SD	2.61	0.41
2:B:129:TYR:O	2:B:147:ALA:HB1	2.21	0.41
3:C:108:ARG:HB2	3:C:110:ASP:OD1	2.21	0.41
3:C:267:MET:HE1	6:C:502:HEC:C1B	2.51	0.41
1:A:483:THR:O	1:A:513:THR:HA	2.21	0.41
3:C:278:LEU:HA	3:C:279:PRO:HD3	1.97	0.41
2:B:90:ILE:HG23	2:B:91:LYS:HD2	2.03	0.40
2:B:142:TYR:CD2	3:C:318:ALA:HB2	2.56	0.40
1:A:181:GLY:O	1:A:185:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:LEU:O	2:B:97:ILE:HG23	2.21	0.40
3:C:58:ASN:HA	3:C:69:TYR:HB2	2.02	0.40
3:C:395:MET:HB2	6:C:501:HEC:C1D	2.51	0.40
2:B:87:SER:HA	2:B:90:ILE:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	538/544 (99%)	508 (94%)	30 (6%)	0	100	100
2	B	134/183 (73%)	127 (95%)	7 (5%)	0	100	100
3	C	411/486 (85%)	389 (95%)	22 (5%)	0	100	100
All	All	1083/1213 (89%)	1024 (95%)	59 (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	442/445 (99%)	412 (93%)	30 (7%)	16	46
2	B	116/152 (76%)	103 (89%)	13 (11%)	6	23
3	C	327/384 (85%)	293 (90%)	34 (10%)	7	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	885/981 (90%)	808 (91%)	77 (9%)	14	35

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	MET
1	A	66	THR
1	A	93	ARG
1	A	96	TYR
1	A	110	HIS
1	A	124	LYS
1	A	133	ARG
1	A	146	TYR
1	A	163	ILE
1	A	171	ASN
1	A	173	TRP
1	A	184	ASP
1	A	187	PHE
1	A	210	TYR
1	A	231	MET
1	A	264	ARG
1	A	313	SER
1	A	319	ARG
1	A	321	MET
1	A	335	GLU
1	A	358	ARG
1	A	368	TYR
1	A	376	ARG
1	A	384	MET
1	A	390	LYS
1	A	397	ARG
1	A	436	VAL
1	A	469	MET
1	A	485	MET
1	A	503	HIS
2	B	65	LYS
2	B	80	GLU
2	B	83	LYS
2	B	84	HIS
2	B	115	ASP
2	B	120	THR
2	B	123	GLN

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Mol	Chain	Res	Type
2	B	142	TYR
2	B	149	MET
2	B	164	HIS
2	B	178	ASP
2	B	179	VAL
2	B	183	PHE
3	C	60	ARG
3	C	61	ASP
3	C	64	PHE
3	C	69	TYR
3	C	75	MET
3	C	82	ASN
3	C	87	LYS
3	C	89	HIS
3	C	94	TYR
3	C	95	THR
3	C	124	ASN
3	C	142	VAL
3	C	161	ARG
3	C	180	PHE
3	C	185	ASN
3	C	186	ASP
3	C	208	ARG
3	C	211	LEU
3	C	243	SER
3	C	257	LYS
3	C	267	MET
3	C	277	TYR
3	C	291	ARG
3	C	301	GLN
3	C	315	TYR
3	C	329	LEU
3	C	331	LYS
3	C	355	LYS
3	C	389	ASP
3	C	418	TYR
3	C	421	SER
3	C	443	LYS
3	C	445	VAL
3	C	449	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands 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	$\#\|Z\| > 2$
6	HEC	C	501	3	32,50,50	2.20	4 (12%)	24,82,82	1.53	5 (20%)
6	HEC	C	503	3	32,50,50	2.29	3 (9%)	24,82,82	1.40	3 (12%)
6	HEC	C	502	3	32,50,50	2.10	4 (12%)	24,82,82	1.94	3 (12%)
4	FAD	A	601	-	53,58,58	0.44	0	68,89,89	0.52	1 (1%)
5	F3S	A	602	1	0,9,9	-	-	-		
7	U10	C	504	-	38,38,63	2.71	12 (31%)	46,49,79	1.52	9 (19%)

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	HEC	C	501	3	-	3/10/54/54	-
6	HEC	C	503	3	-	1/10/54/54	-
6	HEC	C	502	3	-	1/10/54/54	-
4	FAD	A	601	-	-	13/30/50/50	0/6/6/6
5	F3S	A	602	1	-		0/3/3/3
7	U10	C	504	-	-	13/33/57/87	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	503	HEC	C2B-C3B	-6.93	1.33	1.40
6	C	503	HEC	C3C-C2C	-6.78	1.33	1.40
6	C	502	HEC	C2B-C3B	-6.52	1.33	1.40
6	C	501	HEC	C3C-C2C	-6.46	1.34	1.40
7	C	504	U10	C8-C9	6.09	1.47	1.33
6	C	501	HEC	C2B-C3B	-6.07	1.34	1.40
7	C	504	U10	C18-C19	6.06	1.47	1.33
7	C	504	U10	C23-C24	6.01	1.47	1.33
7	C	504	U10	C13-C14	6.00	1.47	1.33
6	C	501	HEC	C3D-C2D	5.64	1.54	1.37
6	C	503	HEC	C3D-C2D	5.43	1.53	1.37
7	C	504	U10	O3-C3	-5.39	1.23	1.36
7	C	504	U10	O4-C4	-5.38	1.23	1.36
6	C	502	HEC	C3D-C2D	5.38	1.53	1.37
7	C	504	U10	C28-C29	5.28	1.47	1.32
6	C	502	HEC	C3C-C2C	-4.90	1.35	1.40
7	C	504	U10	C4-C5	-3.28	1.39	1.48
7	C	504	U10	C3-C2	-3.28	1.39	1.48
7	C	504	U10	C6-C5	-2.65	1.39	1.46
7	C	504	U10	C6-C1	2.58	1.39	1.35
6	C	501	HEC	CAD-C3D	2.25	1.55	1.52
7	C	504	U10	C1-C2	-2.16	1.39	1.47
6	C	502	HEC	CAD-C3D	2.06	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	502	HEC	CMC-C2C-C1C	-6.96	117.77	128.46
7	C	504	U10	C25-C24-C26	3.25	120.74	115.27
7	C	504	U10	C20-C19-C21	3.10	120.48	115.27
7	C	504	U10	C12-C13-C14	-3.05	120.31	127.66
6	C	502	HEC	CBA-CAA-C2A	-2.92	107.68	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	501	HEC	CMB-C2B-C1B	-2.87	124.05	128.46
7	C	504	U10	C10-C9-C11	2.86	120.08	115.27
7	C	504	U10	C22-C23-C24	-2.75	121.04	127.66
7	C	504	U10	C17-C18-C19	-2.71	121.13	127.66
7	C	504	U10	C15-C14-C16	2.66	119.75	115.27
6	C	503	HEC	CBA-CAA-C2A	-2.59	108.24	112.60
6	C	503	HEC	CBD-CAD-C3D	-2.52	108.32	112.62
6	C	502	HEC	CMB-C2B-C1B	-2.45	124.70	128.46
7	C	504	U10	C31-C29-C30	2.42	119.94	114.60
6	C	501	HEC	CMC-C2C-C1C	-2.39	124.79	128.46
6	C	501	HEC	CMB-C2B-C3B	2.35	128.58	125.82
4	A	601	FAD	C5A-C6A-N6A	2.28	123.81	120.35
6	C	501	HEC	CAA-CBA-CGA	-2.27	107.40	113.76
6	C	501	HEC	C1D-C2D-C3D	-2.16	105.49	107.00
7	C	504	U10	C7-C8-C9	-2.15	123.22	126.79
6	C	503	HEC	C1D-C2D-C3D	-2.14	105.51	107.00

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	FAD	C1'-C2'-C3'-O3'
4	A	601	FAD	C1'-C2'-C3'-C4'
4	A	601	FAD	O3'-C3'-C4'-C5'
4	A	601	FAD	C3'-C4'-C5'-O5'
4	A	601	FAD	O4'-C4'-C5'-O5'
6	C	501	HEC	C2D-C3D-CAD-CBD
6	C	501	HEC	C4D-C3D-CAD-CBD
6	C	502	HEC	C2A-CAA-CBA-CGA
7	C	504	U10	C7-C8-C9-C10
7	C	504	U10	C7-C8-C9-C11
7	C	504	U10	C18-C19-C21-C22
7	C	504	U10	C20-C19-C21-C22
7	C	504	U10	C25-C24-C26-C27
7	C	504	U10	C23-C24-C26-C27
4	A	601	FAD	O2'-C2'-C3'-O3'
4	A	601	FAD	O2'-C2'-C3'-C4'
4	A	601	FAD	C2'-C3'-C4'-O4'
7	C	504	U10	C19-C21-C22-C23
6	C	501	HEC	C3D-CAD-CBD-CGD
6	C	503	HEC	C2A-CAA-CBA-CGA
4	A	601	FAD	O3'-C3'-C4'-O4'

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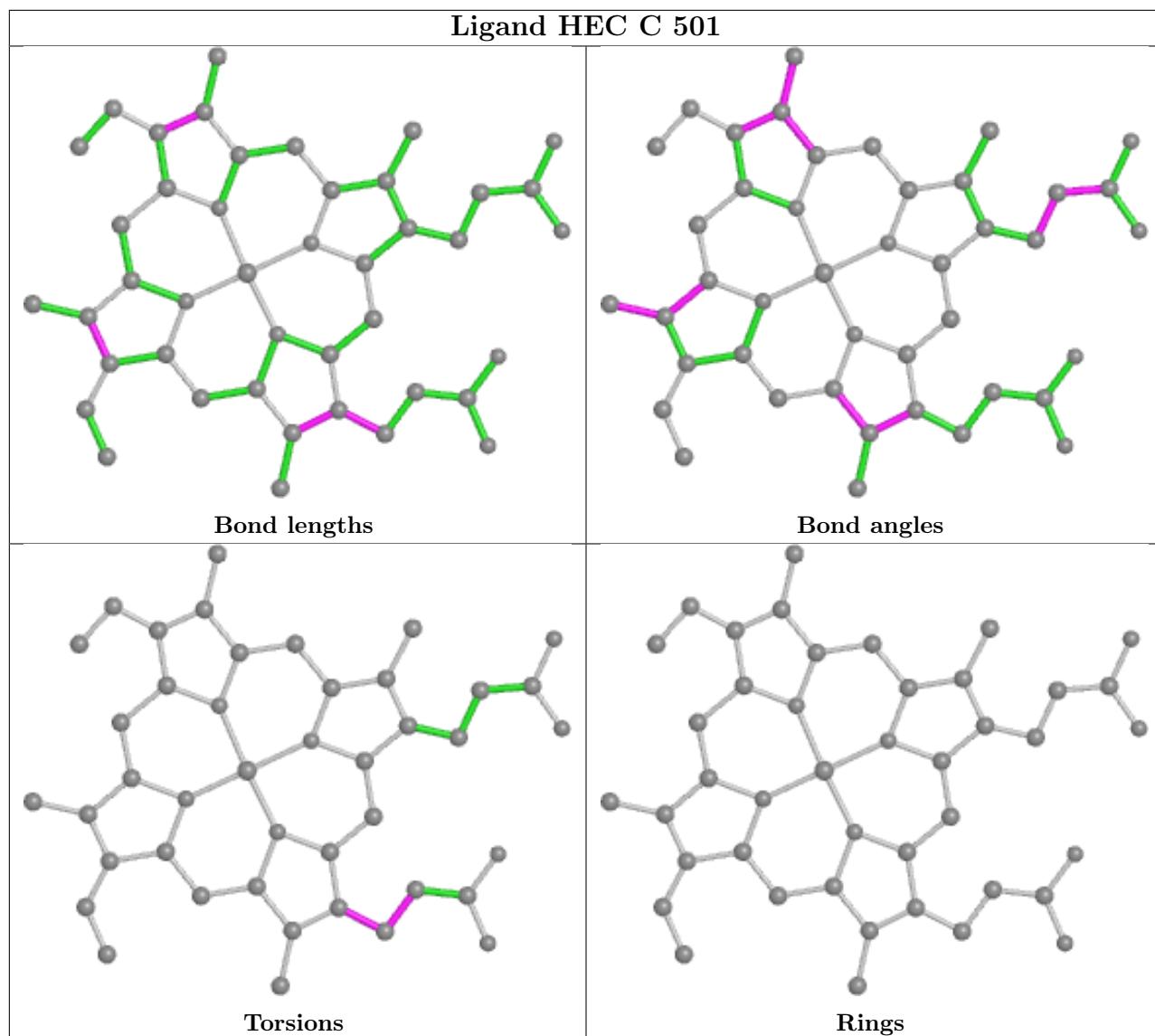
Mol	Chain	Res	Type	Atoms
4	A	601	FAD	O4B-C4B-C5B-O5B
4	A	601	FAD	C3B-C4B-C5B-O5B
7	C	504	U10	C24-C26-C27-C28
7	C	504	U10	C27-C28-C29-C31
4	A	601	FAD	C2'-C3'-C4'-C5'
7	C	504	U10	C27-C28-C29-C30
7	C	504	U10	C14-C16-C17-C18
7	C	504	U10	C5-C4-O4-C4M
7	C	504	U10	C6-C7-C8-C9
4	A	601	FAD	C5'-O5'-P-O1P
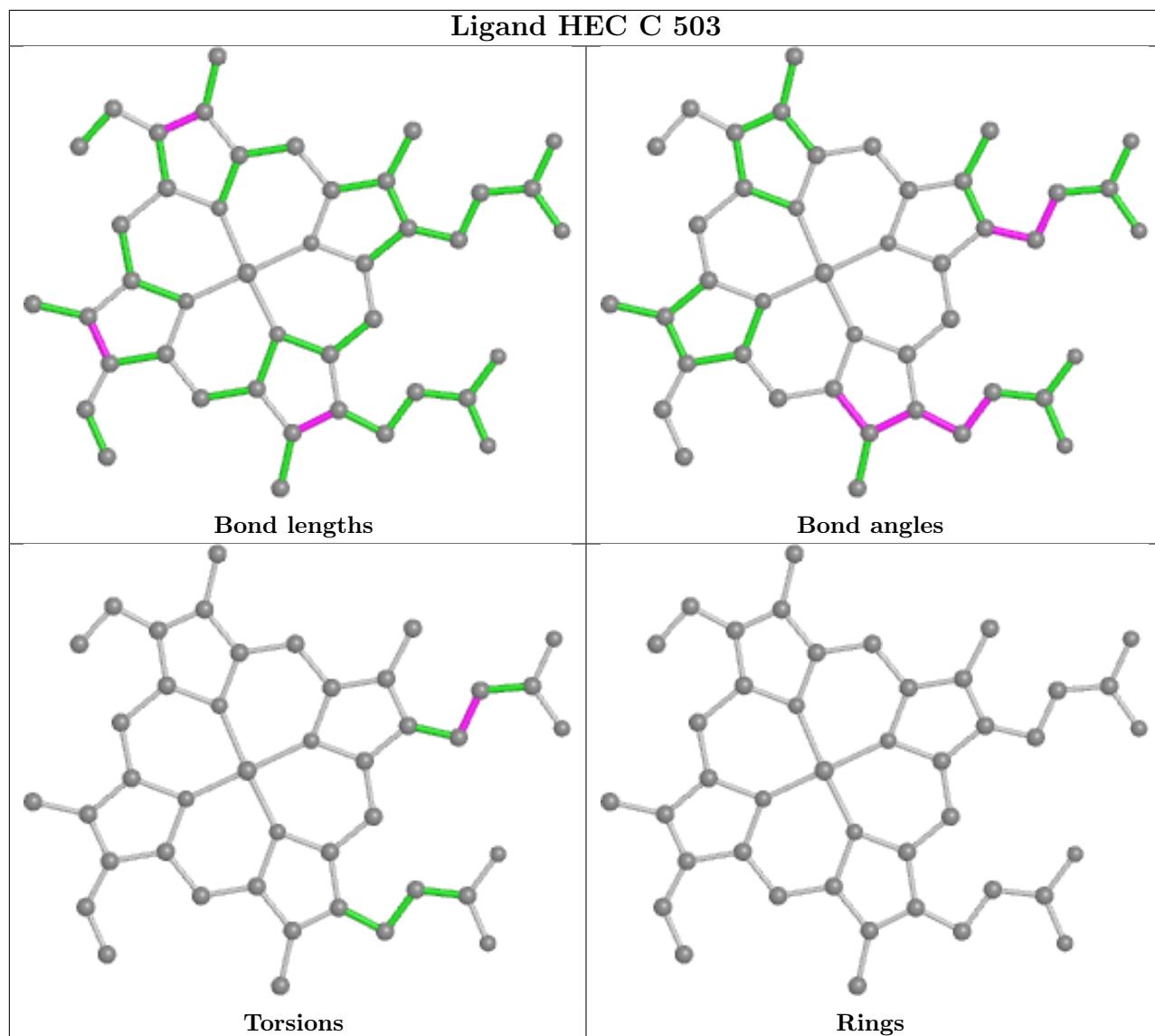
There are no ring outliers.
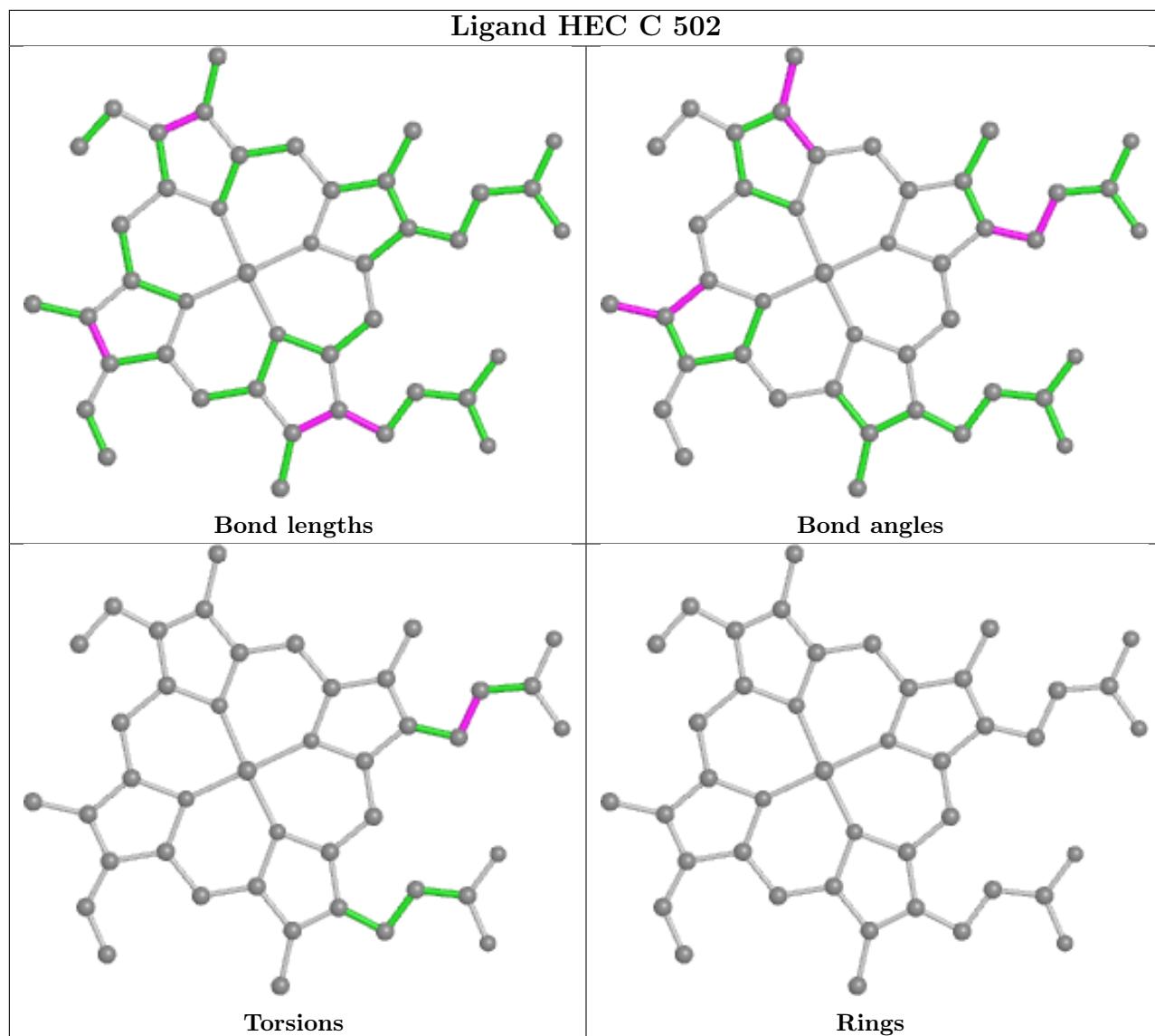
5 monomers are involved in 20 short contacts:
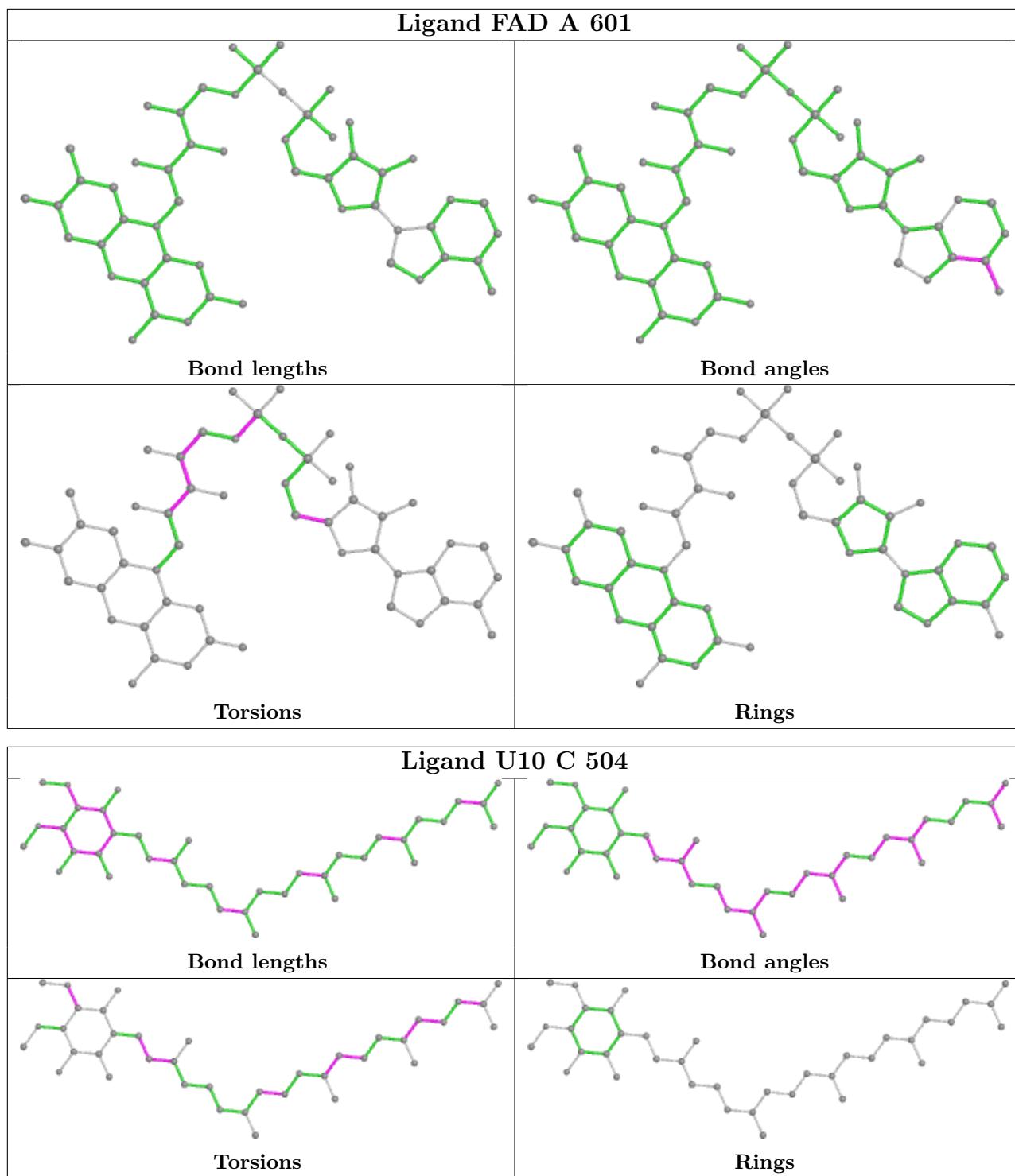
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	501	HEC	7	0
6	C	502	HEC	6	0
4	A	601	FAD	4	0
5	A	602	F3S	2	0
7	C	504	U10	2	0

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 then 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.

Ligand HEC C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC C 503

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC C 502

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 601

Bond lengths

Bond angles

Torsions

Rings

Ligand U10 C 504

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.
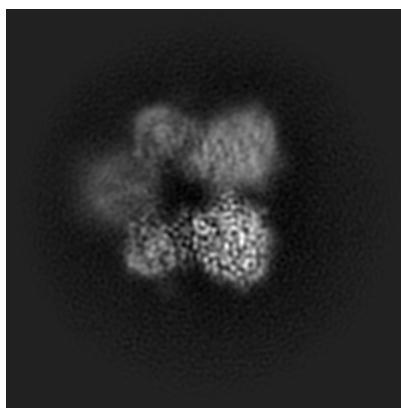
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-38248. These allow visual inspection of the internal detail of the map and identification of artifacts.
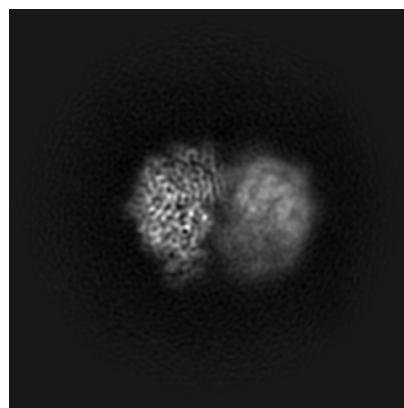
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ
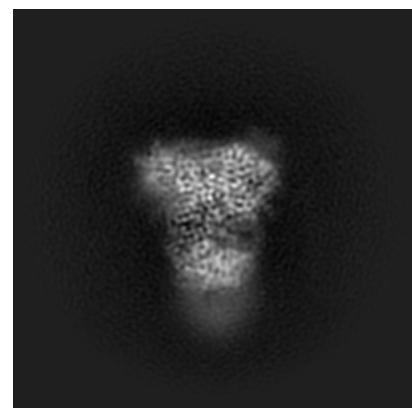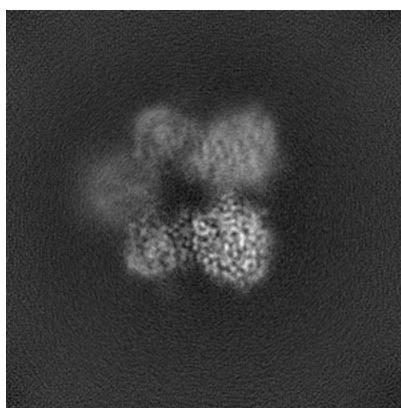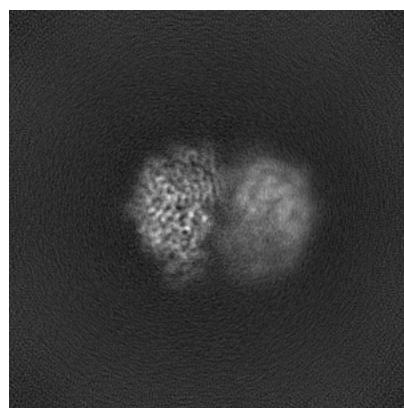
6.1.1 Primary map

| X | Y | Z |
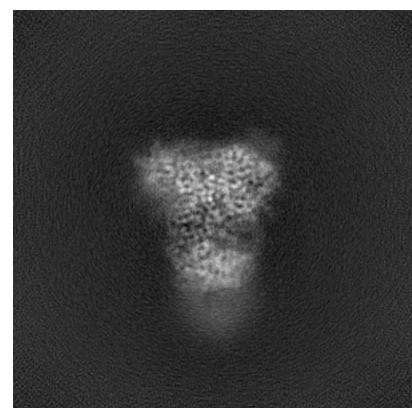
6.1.2 Raw map

| X | Y | Z |
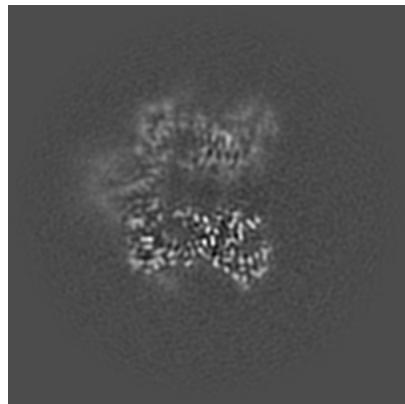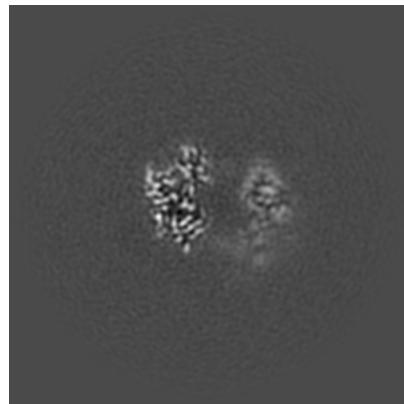
The images above show the map projected in three orthogonal directions.

6.2   Central slices   ⓘ
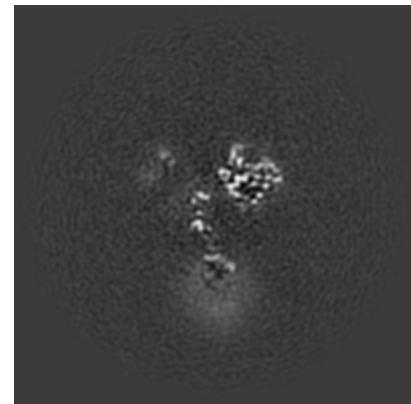
6.2.1   Primary map
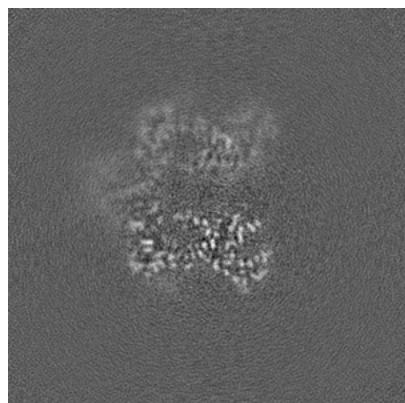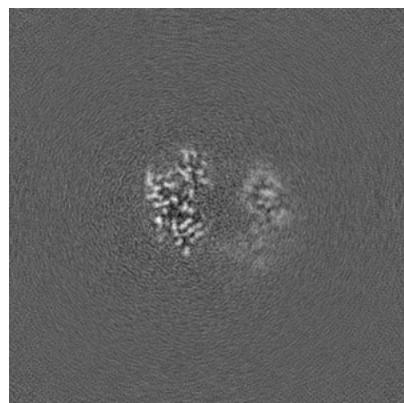
| X Index: 140 | Y Index: 140 | Z Index: 140 |
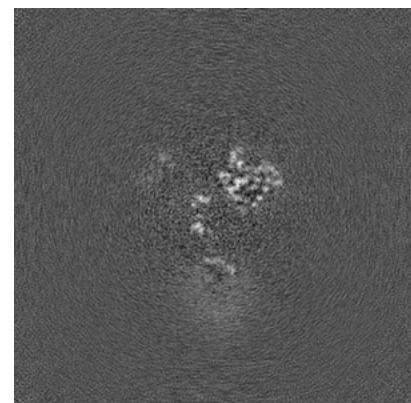
6.2.2   Raw map
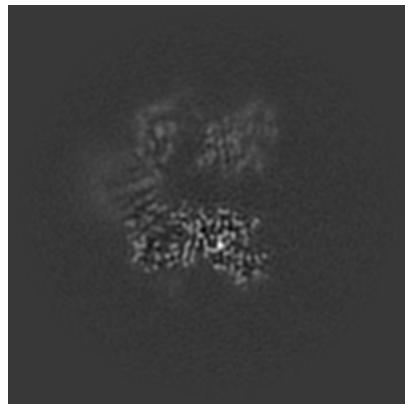
| X Index: 140 | Y Index: 140 | Z Index: 140 |
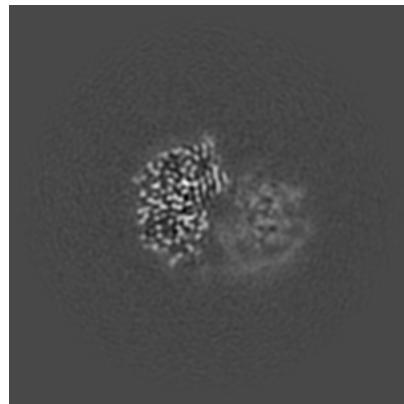
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices ⓘ
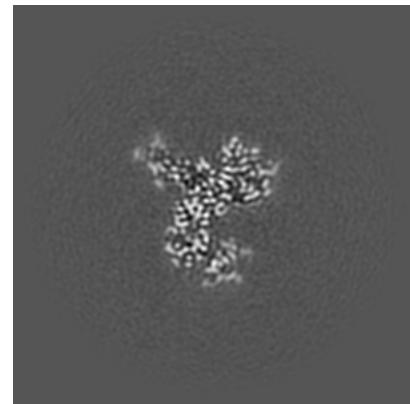
6.3.1   Primary map
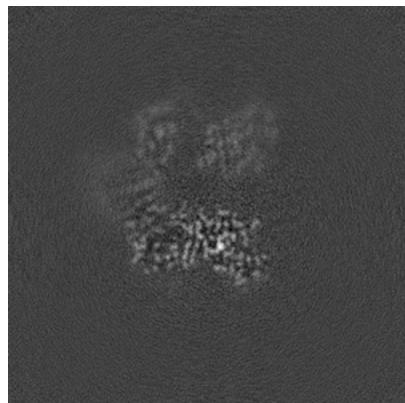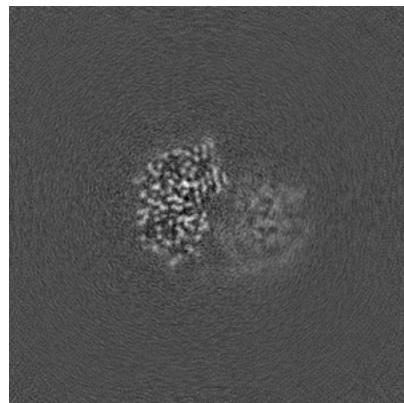
X Index: 137   Y Index: 156   Z Index: 116
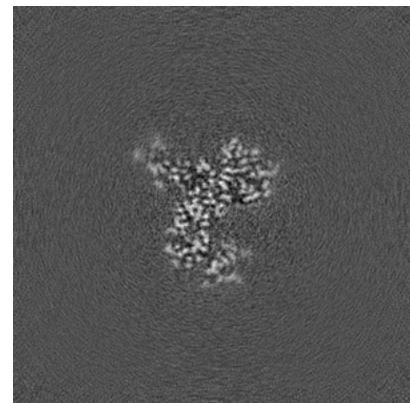
6.3.2   Raw map
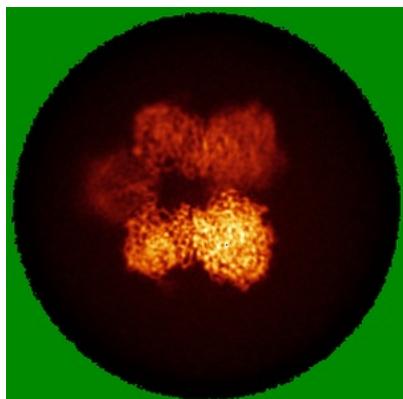
X Index: 137   Y Index: 156   Z Index: 116
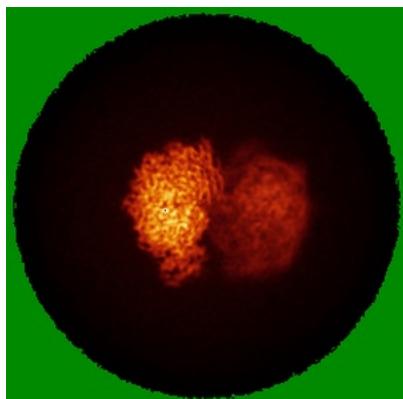
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ
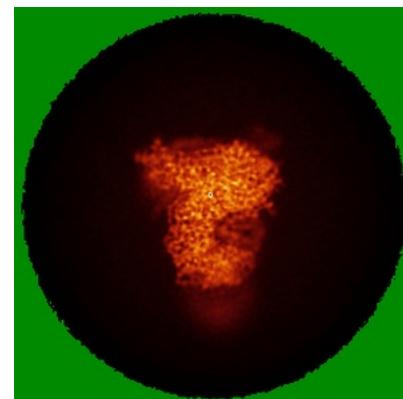
6.4.1 Primary map
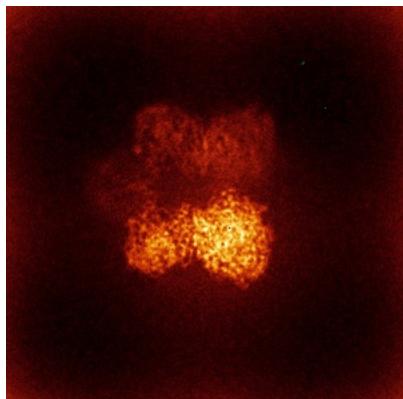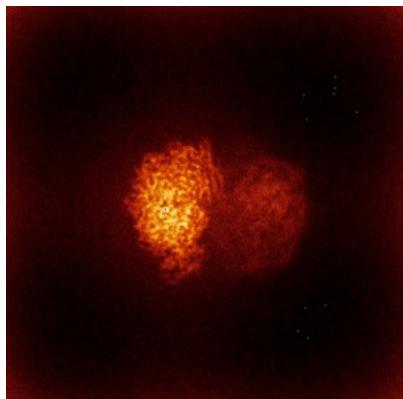
| X | Y | Z |
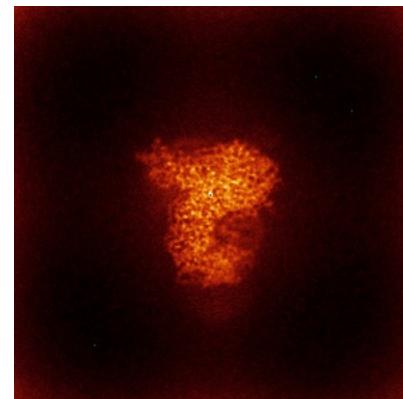
6.4.2 Raw map

| X | Y | Z |
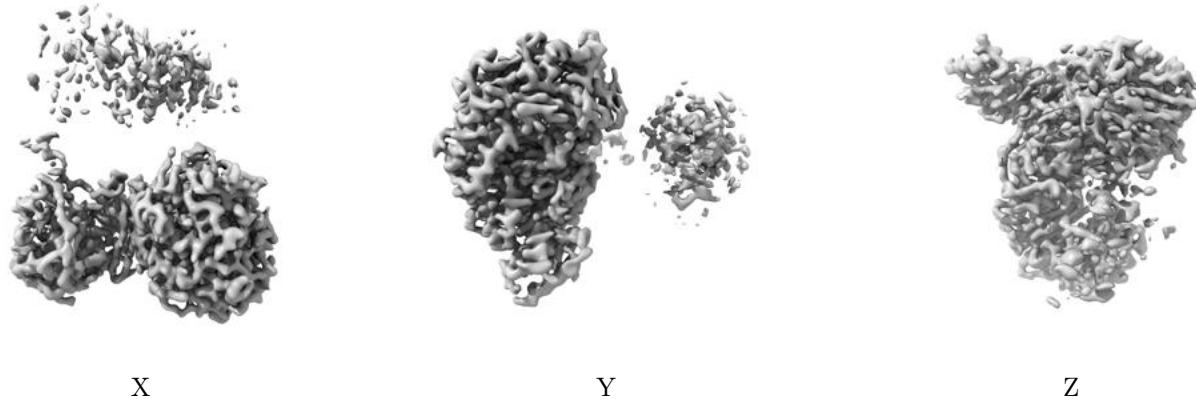
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.
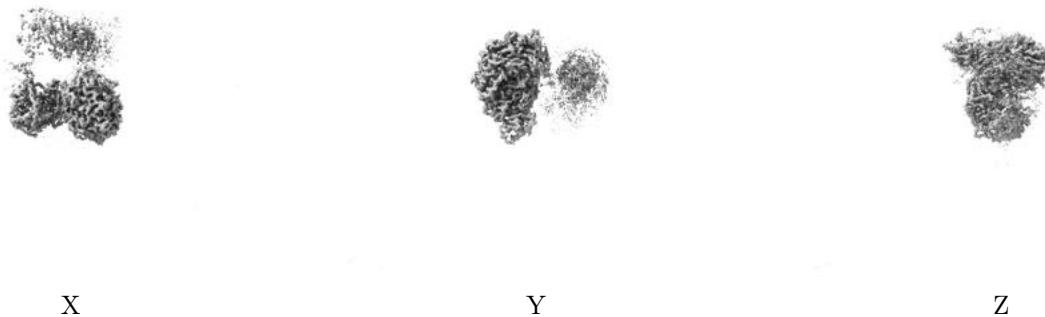
6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X	Y	Z

The images above show the 3D surface view of the map at the recommended contour level 0.127. 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

X	Y	Z

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.
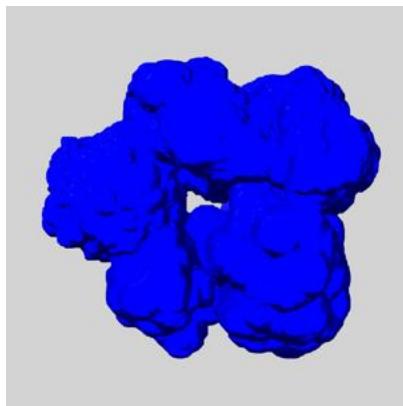
6.6　Mask visualisation　ⓘ

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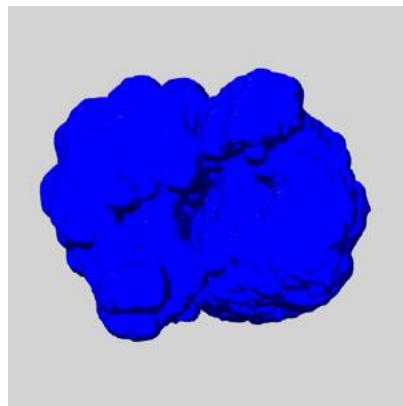
A mask typically either:

- Encompasses the whole structure

- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure
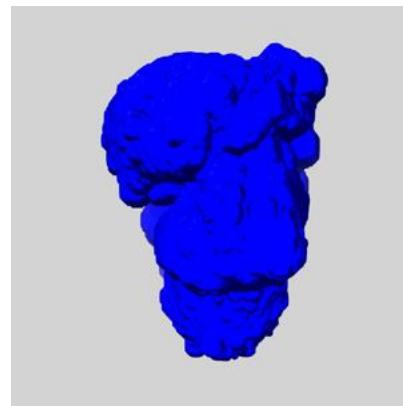
6.6.1　emd_38248_msk_1.map　ⓘ

X　　　　　　　　　　　Y　　　　　　　　　　　Z
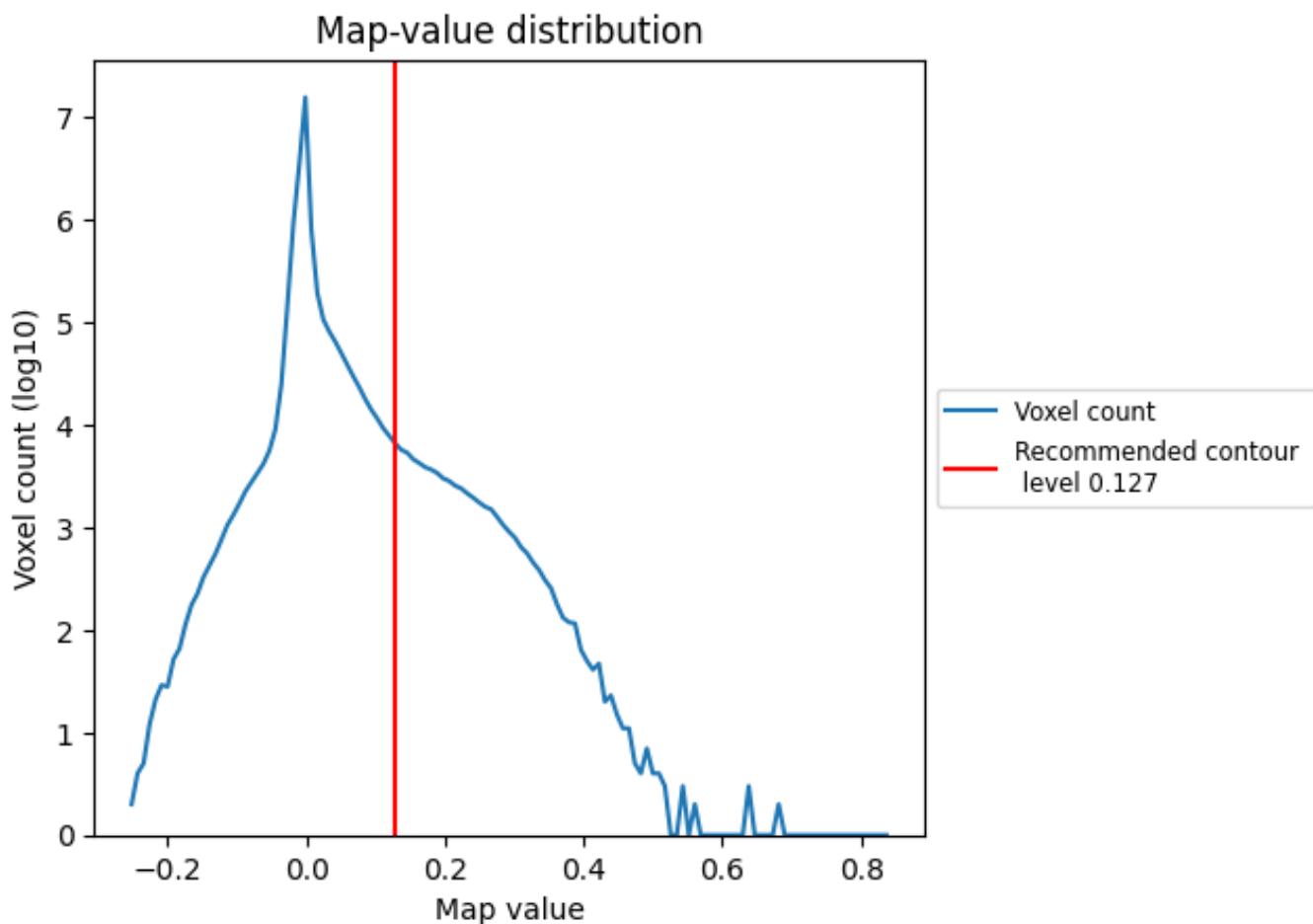
7 Map analysis ⓘ
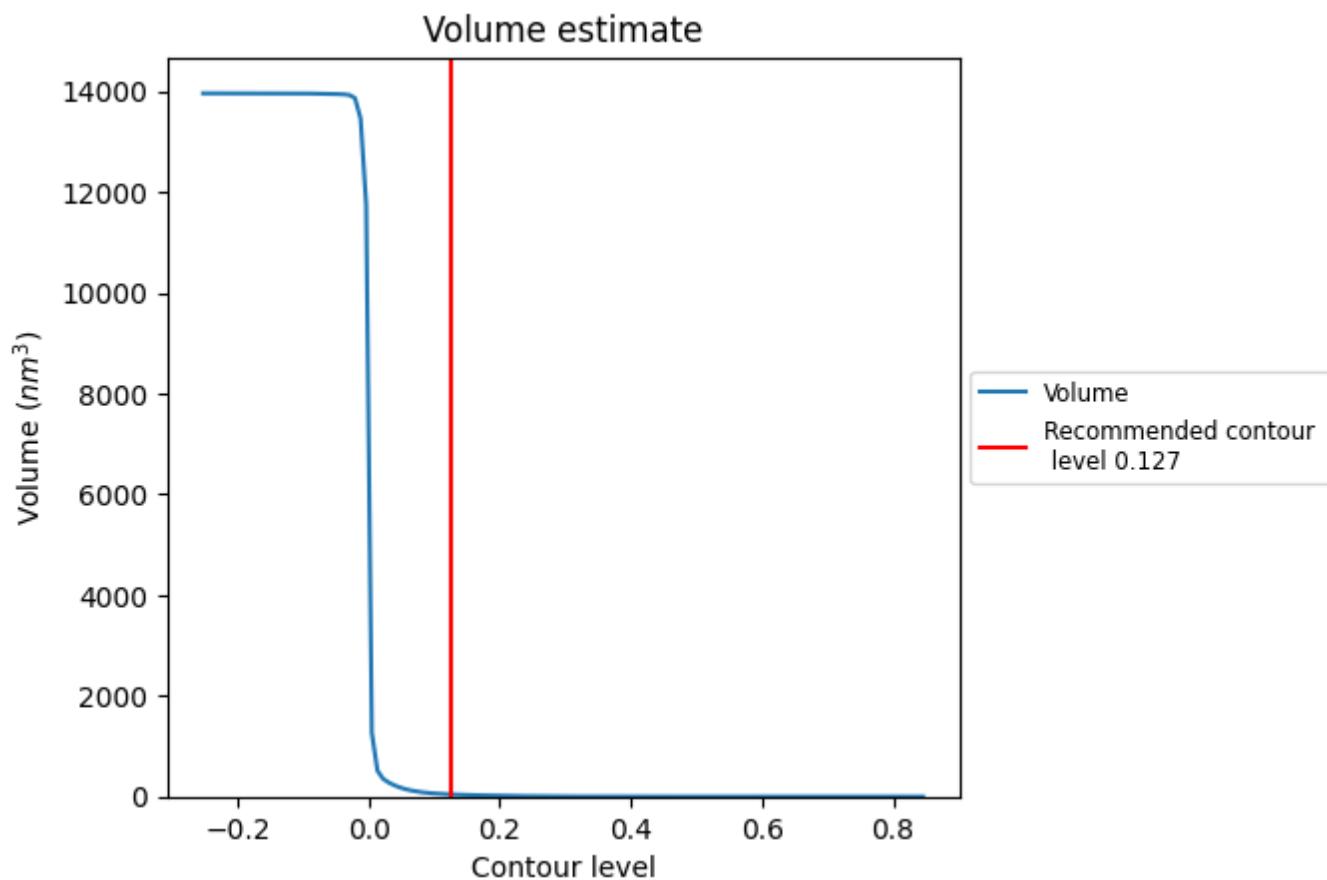
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

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.
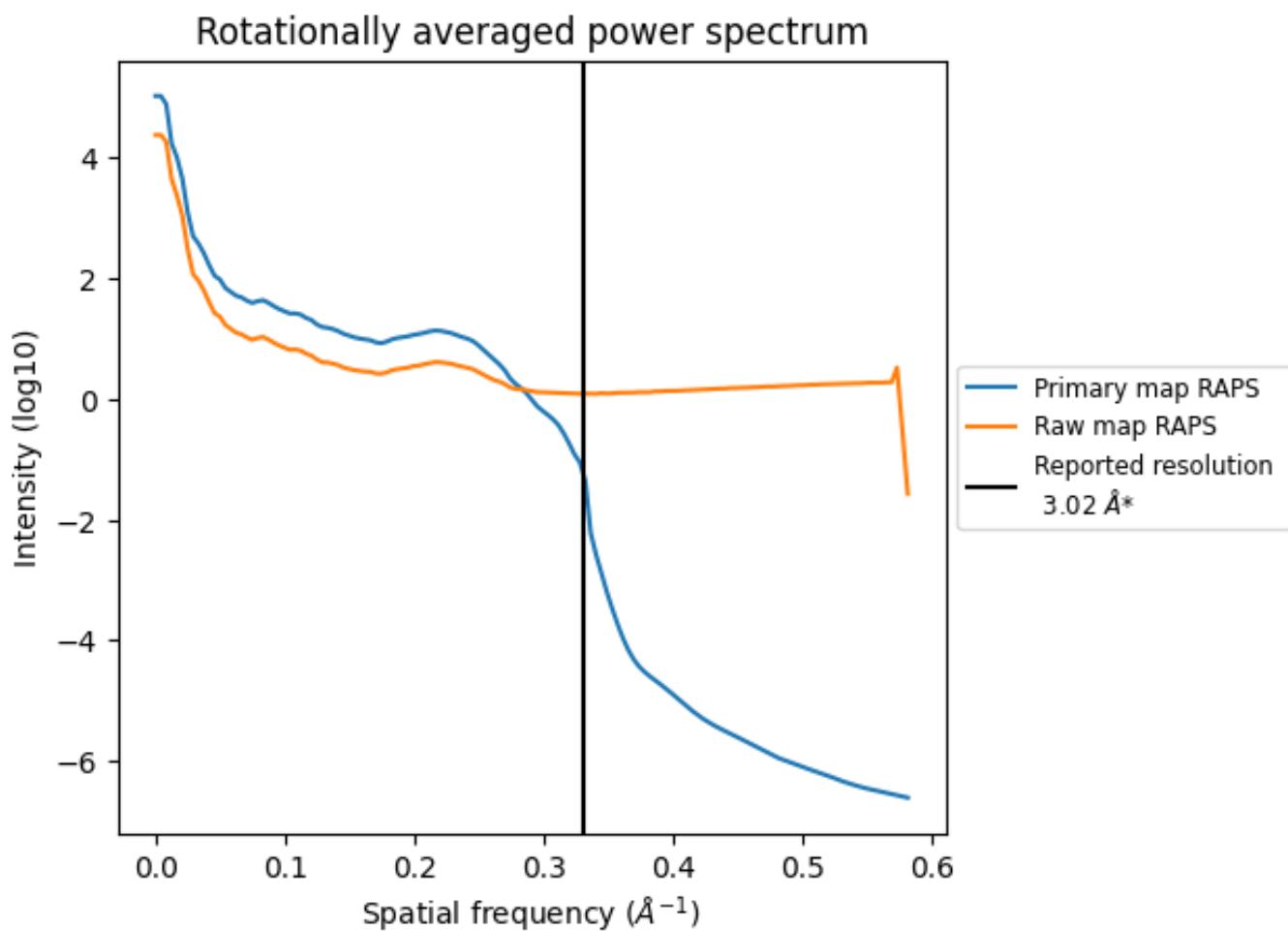
7.2 Volume estimate ⓘ

The volume at the recommended contour level is 42 nm^3; this corresponds to an approximate mass of 38 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 ⓘ
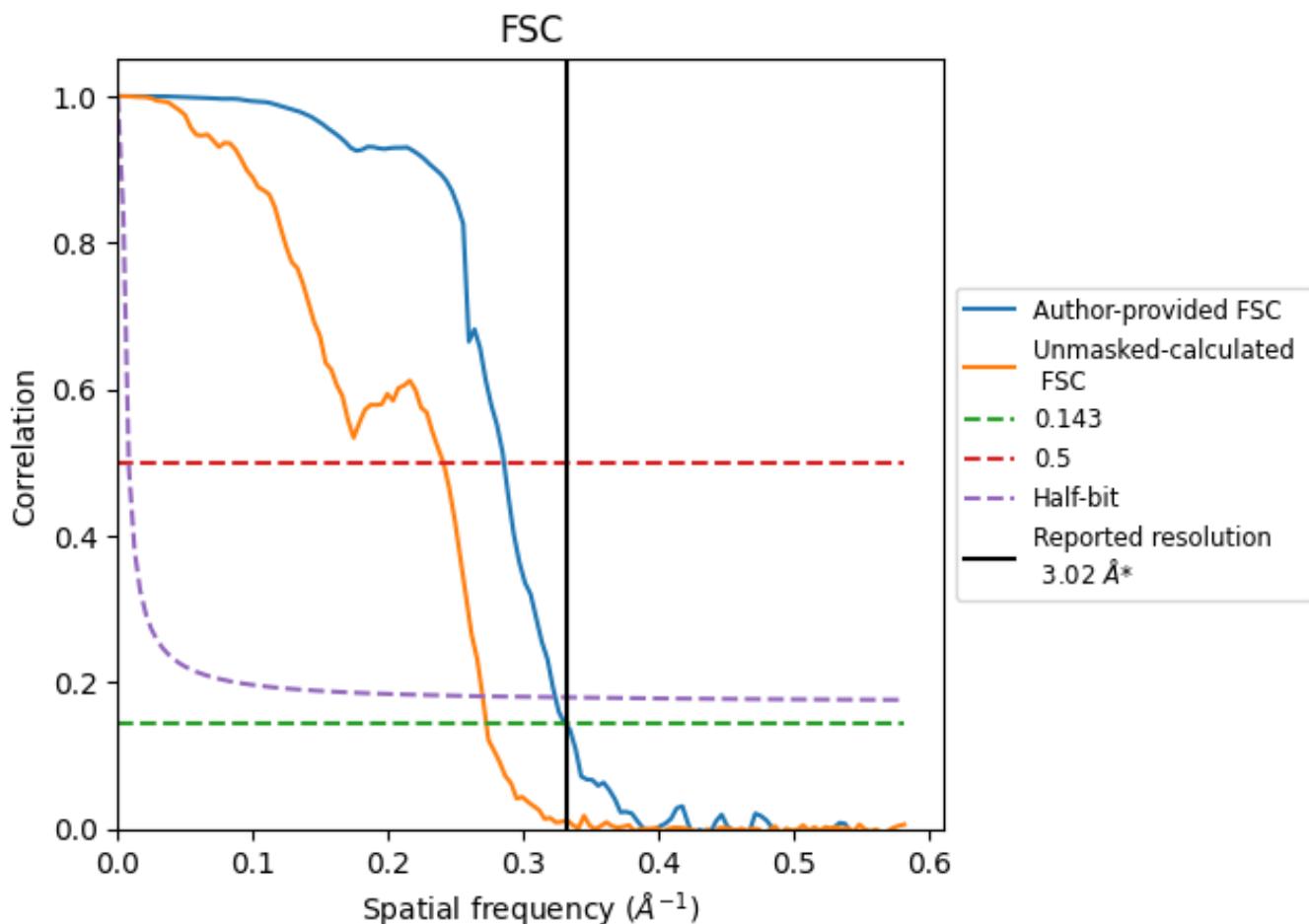
*Reported resolution corresponds to spatial frequency of 0.331 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ

*Reported resolution corresponds to spatial frequency of 0.331 Å^{-1}

8.2 Resolution estimates ⓘ
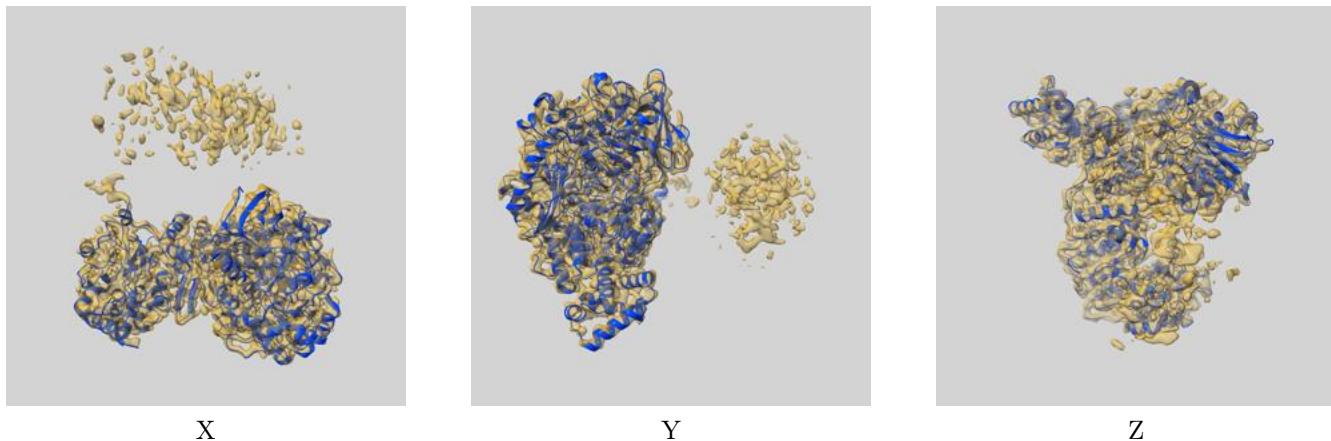
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.50	3.09
Unmasked-calculated*	3.67	4.15	3.71

*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 3.67 differs from the reported value 3.02 by more than 10 %

9 Map-model fit ⓘ
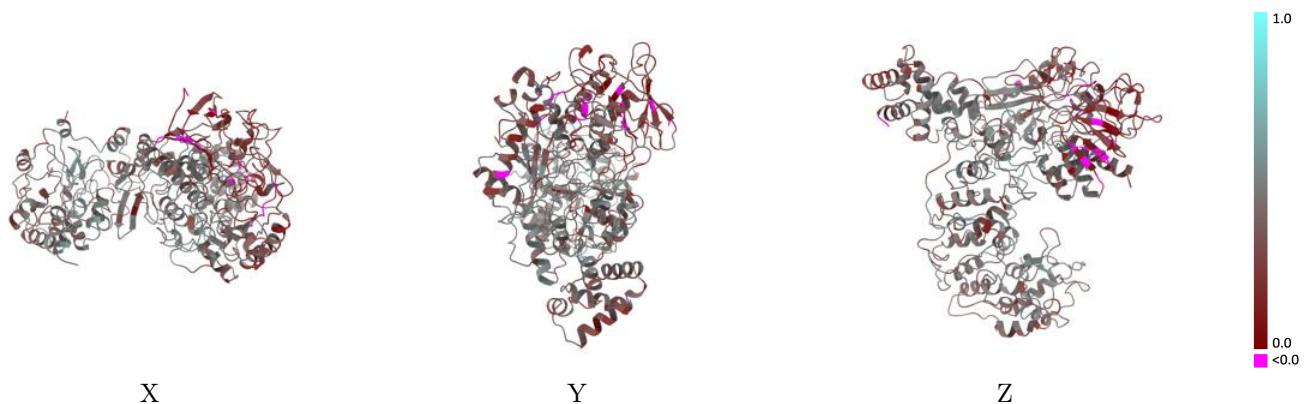
This section contains information regarding the fit between EMDB map EMD-38248 and PDB model 8XCN. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay ⓘ

X   Y   Z
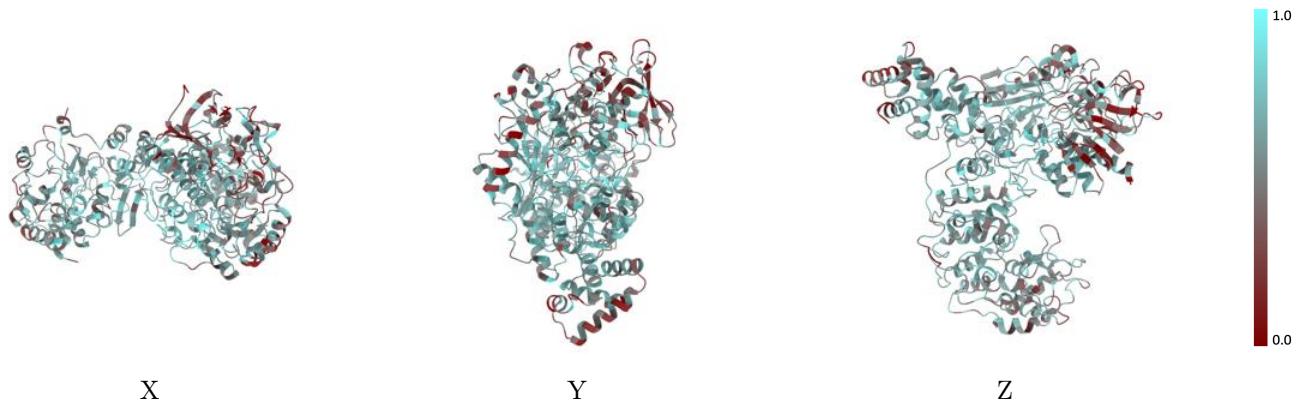
The images above show the 3D surface view of the map at the recommended contour level 0.127 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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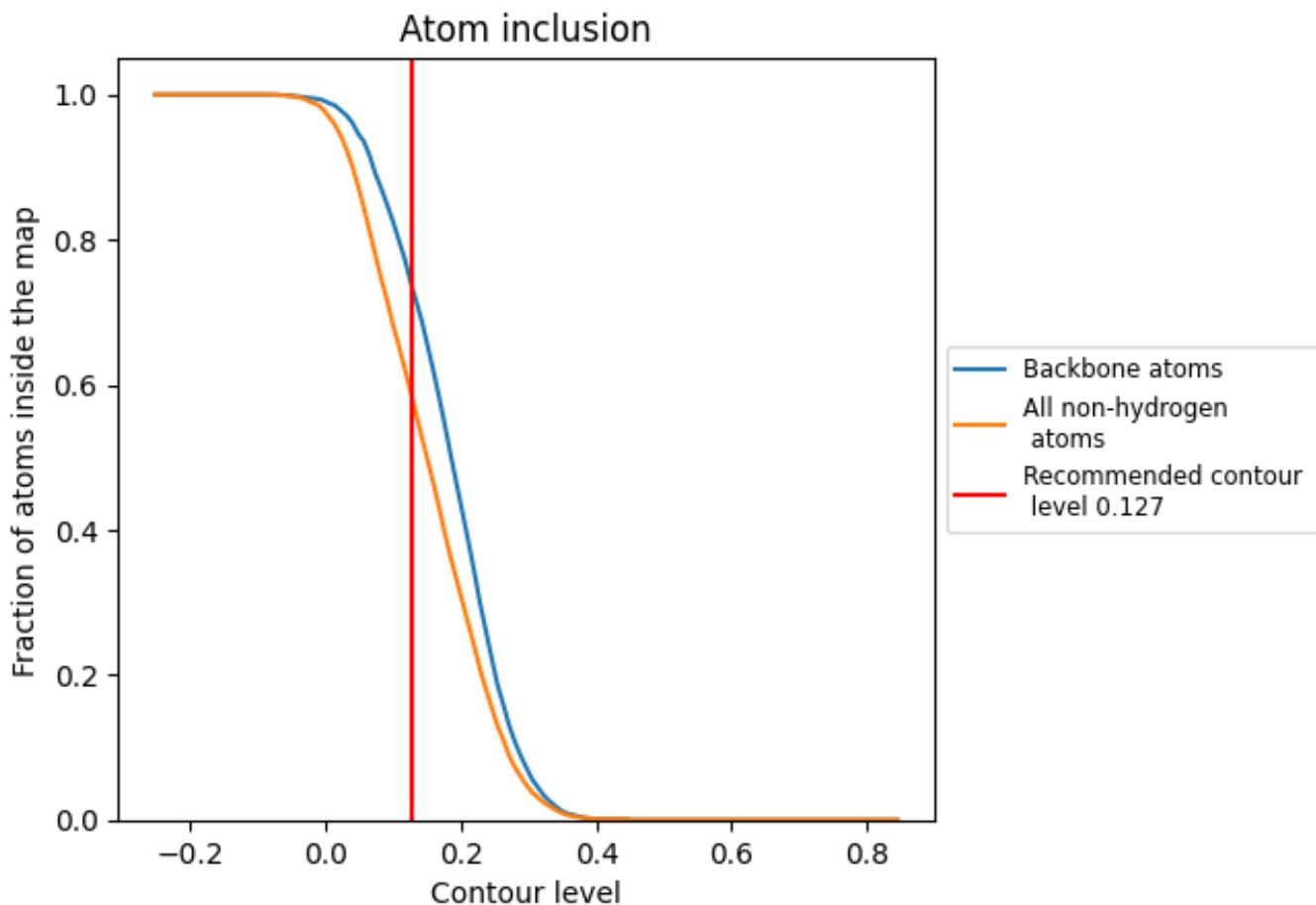
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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 (0.127).

9.4 Atom inclusion ⓘ

At the recommended contour level, 74% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.127) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5840	0.3780
A	0.5780	0.3480
B	0.5450	0.3850
C	0.6040	0.4130

1.0

0.0

<0.0