WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Feb 4, 2024 – 12:21 PM EST

PDB ID	:	8CVZ
EMDB ID	:	EMD-27022
Title	:	Human glycogenin-1 and glycogen synthase-1 complex in the apo ordered state
Authors	:	Liu, Y.; Fastman, N.M.; Tzitzilonis, C.
Deposited on	:	2022-05-18
Resolution	:	3.52 Å(reported)
Based on initial models	:	4QLB, 3Q4S

The following versions of software and data (see references ⓘ) were used in the production of this report:
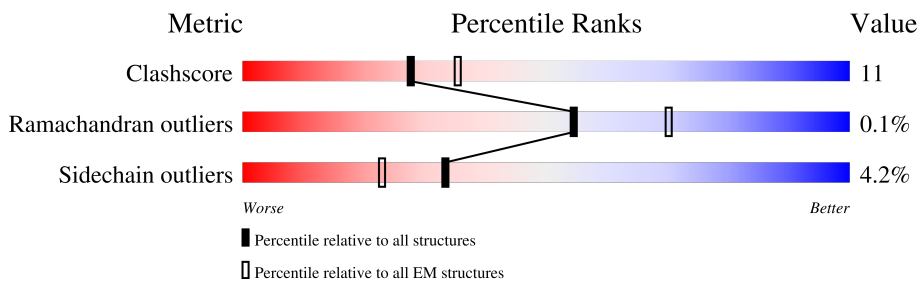
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.52 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		11
Ramachandran outliers		0.1%
Sidechain outliers		4.2%

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	E	352	9% · 90%
1	F	352	9% 8% · 90%
1	G	352	5% 8% · 90%
1	H	352	8% ·· 90%
1	I	352	60% 15% · 24%
1	J	352	21% 61% 13% · 26%
2	A	634	69% 24% · 5%
2	B	634	41% 70% 24% · 5%

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Mol	Chain	Length	Quality of chain
2	C	634	67% 27% 5%
2	D	634	72% 22% 5%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 24517 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 Glycogenin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	261	Total	C	N	O	S	0	0
			2057	1334	333	381	9		
1	E	35	Total	C	N	O	S	0	0
			295	180	52	62	1		
1	I	267	Total	C	N	O	S	0	0
			2100	1360	342	389	9		
1	F	35	Total	C	N	O	S	0	0
			295	180	52	62	1		
1	G	34	Total	C	N	O	S	0	0
			285	175	50	59	1		
1	H	34	Total	C	N	O	S	0	0
			285	175	50	59	1		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-1	GLY	-	expression tag	UNP P46976
J	0	PRO	-	expression tag	UNP P46976
J	195	PHE	TYR	engineered mutation	UNP P46976
E	-1	GLY	-	expression tag	UNP P46976
E	0	PRO	-	expression tag	UNP P46976
E	195	PHE	TYR	engineered mutation	UNP P46976
I	-1	GLY	-	expression tag	UNP P46976
I	0	PRO	-	expression tag	UNP P46976
I	195	PHE	TYR	engineered mutation	UNP P46976
F	-1	GLY	-	expression tag	UNP P46976
F	0	PRO	-	expression tag	UNP P46976
F	195	PHE	TYR	engineered mutation	UNP P46976
G	-1	GLY	-	expression tag	UNP P46976
G	0	PRO	-	expression tag	UNP P46976
G	195	PHE	TYR	engineered mutation	UNP P46976
H	-1	GLY	-	expression tag	UNP P46976
H	0	PRO	-	expression tag	UNP P46976
H	195	PHE	TYR	engineered mutation	UNP P46976

- Molecule 2 is a protein called Glycogen [starch] synthase, muscle.

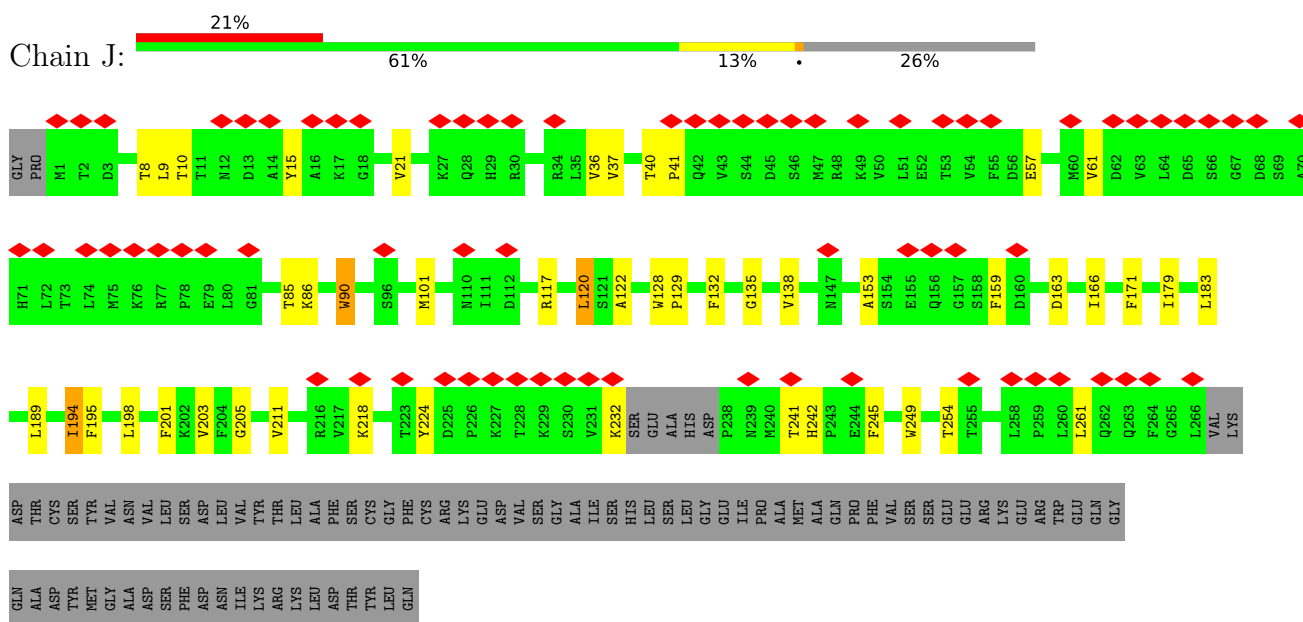| Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	602	Total	C	N	O	S	0	0
			4808	3095	822	867	24		
2	C	600	Total	C	N	O	S	0	0
			4781	3075	824	857	25		
2	D	601	Total	C	N	O	S	0	0
			4777	3078	814	860	25		
2	A	601	Total	C	N	O	S	0	0
			4834	3108	834	869	23		

There are 8 discrepancies between the modelled and reference sequences:

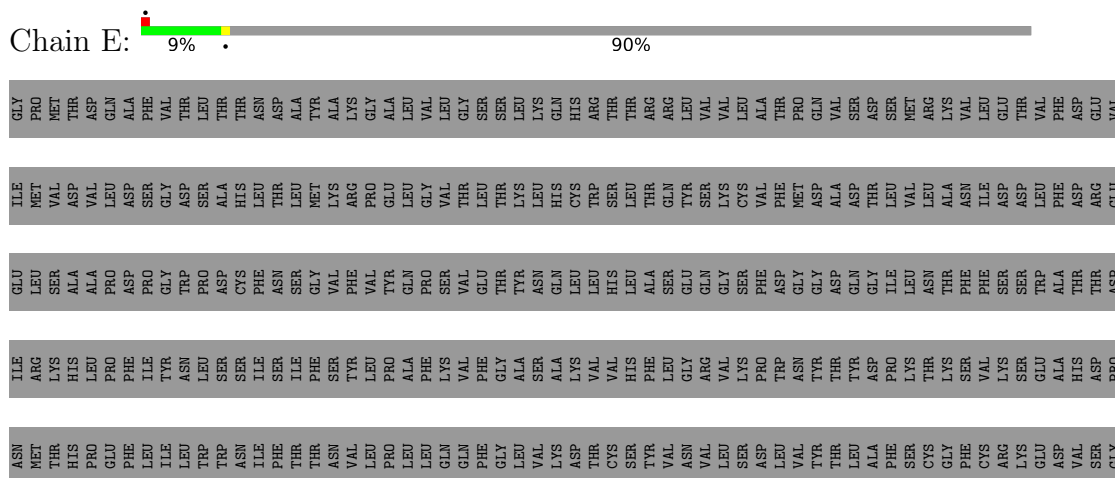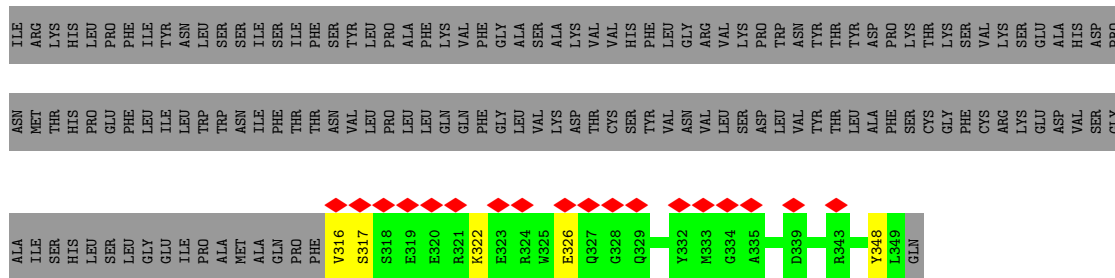| Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLU	SER	engineered mutation	UNP P13807
B	11	GLU	SER	engineered mutation	UNP P13807
C	8	GLU	SER	engineered mutation	UNP P13807
C	11	GLU	SER	engineered mutation	UNP P13807
D	8	GLU	SER	engineered mutation	UNP P13807
D	11	GLU	SER	engineered mutation	UNP P13807
A	8	GLU	SER	engineered mutation	UNP P13807
A	11	GLU	SER	engineered mutation	UNP P13807

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.
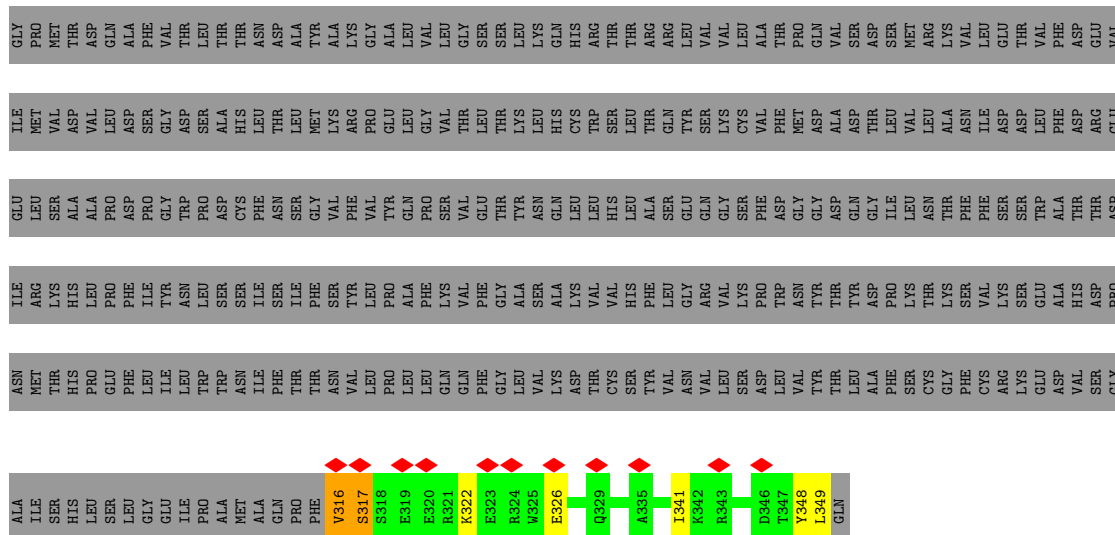
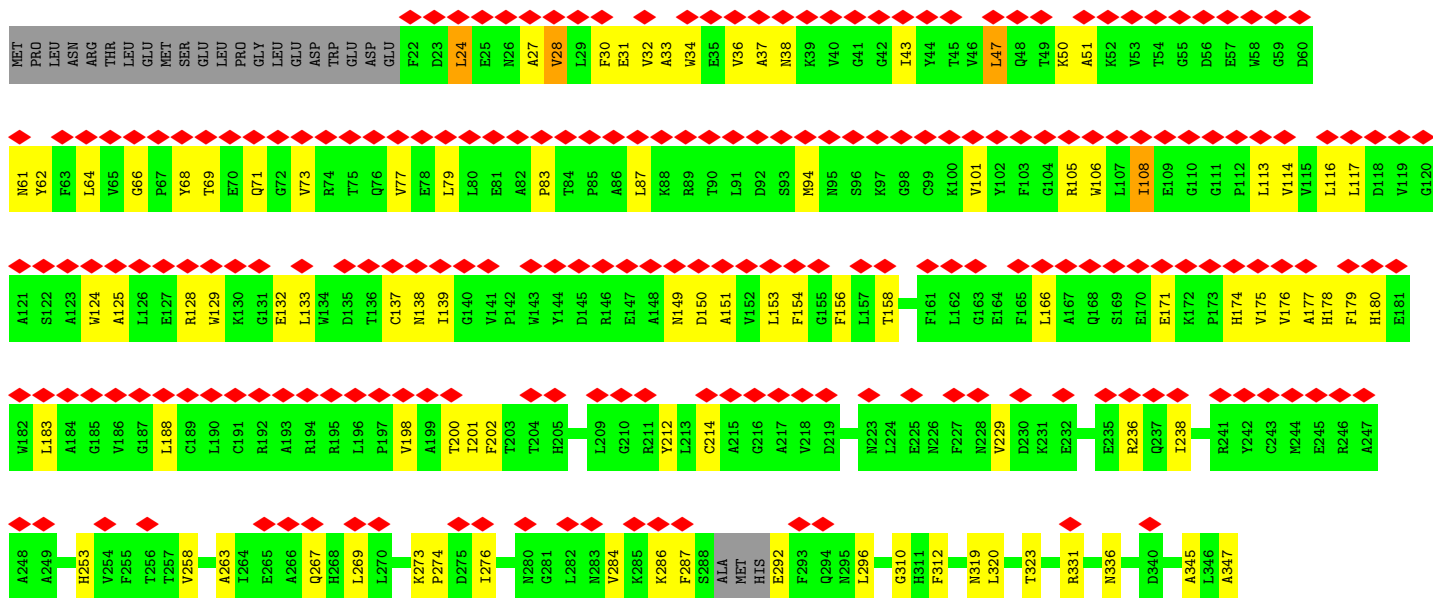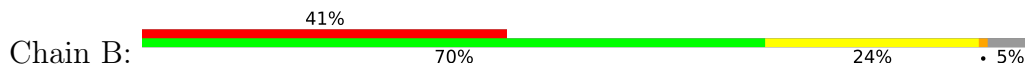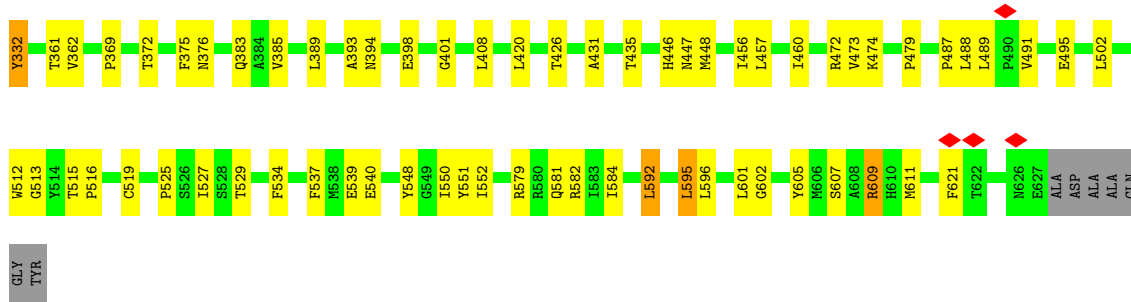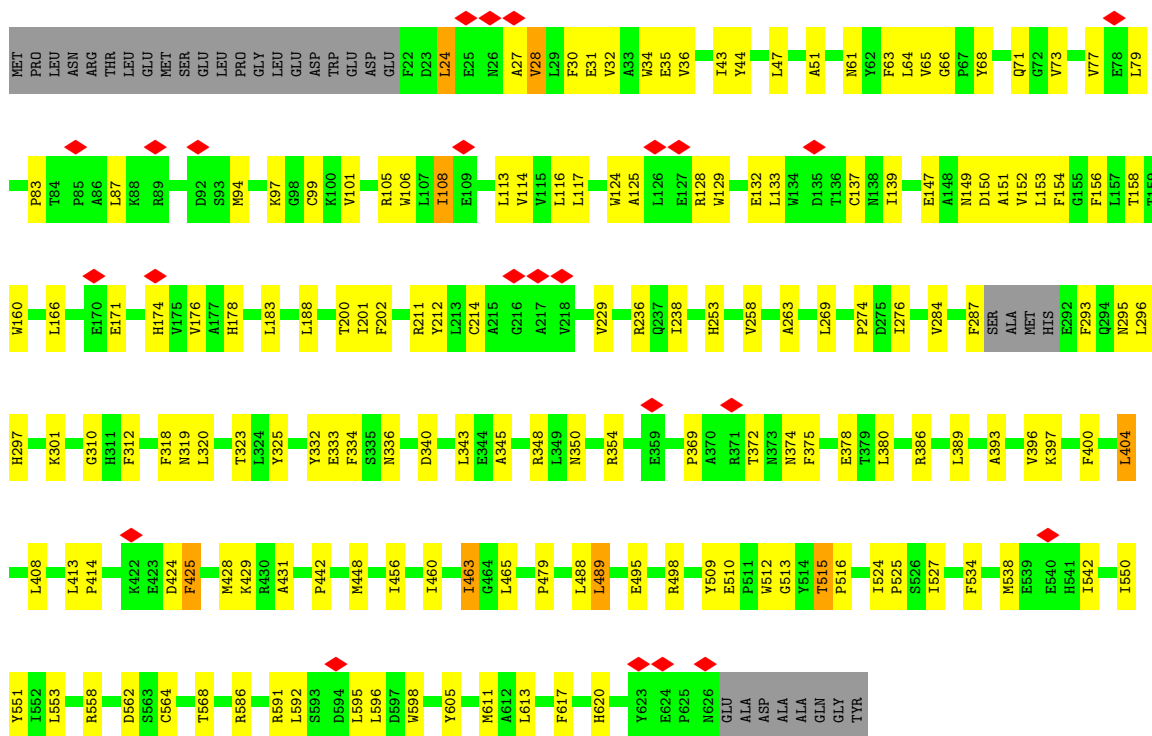- Molecule 1: Glycogenin-1

- Molecule 1: Glycogenin-1

• Molecule 1: Glycogenin-1

Chain I:

60%　　　　15%　　24%

• Molecule 1: Glycogenin-1

Chain F:

9%

8%　　　90%

• Molecule 1: Glycogenin-1

Chain G:

5%

8%　　　90%

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

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

ALA ILE SER HIS SER LEU SER LEU GLY GLU ILE PRO ALA MET ALA GLN GLN PRO PHE **V316 S317 S318 E319 E320 R321 K322 E323 R324 W325 E326 Q327 G328 Q329 Y332 M333 G334 A335 D339 R343 Y348 L349** GLN

• Molecule 1: Glycogenin-1

Chain H: 8% 90%

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

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

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

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

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

ALA ILE SER HIS SER LEU SER LEU GLY GLU ILE PRO ALA MET ALA GLN GLN PRO PHE **V316 S317 S318 E319 E320 R321 K322 E323 R324 W325 E326 Q329 A335 I341 K342 R343 D346 T347 Y348 L349** GLN

• Molecule 2: Glycogen [starch] synthase, muscle

Chain B: 41% 70% 24% 5%

MET PRO LEU ASN ARG THR LEU LEU MET SER GLU LEU PRO GLY LEU GLU ASP TRP GLU ASP GLU **F22 D23 L24 E25 N26 A27 V28 L29 F30 E31 V32 A33 W34 E35 V36 A37 N38 K39 V40 G41 G42 I43 Y44 T45 V46 L47 Q48 T49 K50 A51 K52 V53 T54 G55 D56 E57 W58 G59 D60**

N61 Y62 F63 L64 V65 G66 P67 Y68 T69 E70 Q71 G72 V73 R74 T75 Q76 V77 E78 L79 L80 E81 A82 P83 T84 P85 A86 L87 K88 R89 T90 L91 D92 S93 M94 N95 S96 K97 G98 C99 K100 V101 Y102 F103 G104 R105 W106 L107 I108 E109 G110 G111 P112 L113 V114 V115 L116 L117 D118 V119 G120

A121 S122 A123 W124 A125 L126 E127 R128 W129 K130 G131 E132 L133 W134 D135 T136 C137 N138 I139 G140 V141 P142 W143 Y144 D145 R146 E147 A148 N149 D150 A151 V152 L153 F154 G155 F156 L157 T158 F161 L162 G163 E164 F165 L166 A167 Q168 S169 E170 E171 K172 P173 H174 V175 V176 A177 H178 F179 H180 E181

W182 L183 A184 G185 V186 G187 L188 C189 L190 C191 R192 A193 R194 R195 L196 P197 V198 A199 T200 I201 F202 T203 T204 H205 L209 G210 R211 Y212 L213 C214 A215 G216 A217 V218 D219 N223 L224 E225 N226 F227 N228 V229 D230 K231 E232 E235 R236 Q237 I238 R241 Y242 C243 M244 E245 R246 A247

A248 A249 H253 V254 F255 T256 T257 V258 A263 I264 E265 A266 Q267 H268 L269 L270 K273 P274 D275 I276 N280 G281 L282 N283 V284 K285 K286 F287 S288 ALA MET HIS **E292 F293 Q294 N295 L296 G310 H311 F312 N319 L320 T323 R331 N336 D340 A345 L346 A347**

• Molecule 2: Glycogen [starch] synthase, muscle

Chain C:

67% 27% • 5%

• Molecule 2: Glycogen [starch] synthase, muscle

Chain D:

72% 22% • 5%

• Molecule 2: Glycogen [starch] synthase, muscle

Chain A:

69%   24%   • 5%

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	322214	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was performed in batch in early steps. CTF correction was performed on per particle bases in the last iterations	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	45	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	4.469	Depositor
Minimum map value	-3.439	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.101	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	296.2008, 296.2008, 296.2008	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9142, 0.9142, 0.9142	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	E	0.44	0/299	0.76	0/397
1	F	0.33	0/299	0.69	0/397
1	G	0.34	0/289	0.69	0/385
1	H	0.37	0/289	0.73	0/385
1	I	0.31	0/2158	0.68	0/2945
1	J	0.31	0/2112	0.67	0/2880
2	A	0.33	0/4963	0.71	0/6733
2	B	0.34	0/4937	0.73	0/6701
2	C	0.39	0/4907	0.78	0/6661
2	D	0.39	0/4905	0.76	0/6663
All	All	0.36	0/25158	0.73	0/34147

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	295	0	273	1	0
1	F	295	0	273	2	0
1	G	285	0	265	2	0
1	H	285	0	265	4	0
1	I	2100	0	2057	37	0
1	J	2057	0	2021	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4834	0	4705	118	0
2	B	4808	0	4653	120	0
2	C	4781	0	4641	124	0
2	D	4777	0	4611	106	0
All	All	24517	0	23764	517	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (517) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:313:TYR:HD1	2:C:382:GLY:HA2	1.49	0.75
1:I:194:ILE:HG13	1:I:241:THR:HB	1.68	0.74
2:B:105:ARG:HD3	2:B:113:LEU:HD23	1.72	0.72
2:A:105:ARG:HD3	2:A:113:LEU:HD23	1.71	0.72
2:C:295:ASN:HD21	2:A:293:PHE:H	1.38	0.71
2:B:229:VAL:HG11	2:B:269:LEU:HA	1.73	0.71
2:A:229:VAL:HG11	2:A:269:LEU:HA	1.71	0.71
2:C:90:THR:HG21	2:C:165:PHE:HA	1.73	0.70
2:A:296:LEU:HD13	2:A:498:ARG:HH21	1.56	0.70
1:I:122:ALA:HB3	1:I:132:PHE:HB2	1.74	0.69
2:D:31:GLU:HB2	2:D:64:LEU:HD23	1.73	0.69
2:D:389:LEU:HD23	2:D:431:ALA:HB1	1.74	0.69
2:A:301:LYS:HG3	2:A:325:TYR:HE2	1.57	0.69
2:C:36:VAL:HB	2:C:66:GLY:HA3	1.74	0.68
2:B:397:LYS:HG3	2:C:397:LYS:HG3	1.74	0.68
2:C:107:LEU:O	2:D:426:THR:HB	1.93	0.68
2:A:389:LEU:HD23	2:A:431:ALA:HB1	1.76	0.67
2:D:389:LEU:HD22	2:A:408:LEU:HB3	1.77	0.67
2:D:446:HIS:HB2	2:D:479:PRO:HG2	1.77	0.67
2:A:65:VAL:HG11	2:A:158:THR:HG22	1.75	0.67
2:A:99:CYS:HG	2:A:160:TRP:HZ3	1.43	0.67
2:D:408:LEU:HB3	2:A:389:LEU:HD22	1.78	0.66
1:J:179:ILE:HB	1:I:179:ILE:HB	1.76	0.66
2:A:36:VAL:HB	2:A:66:GLY:HA3	1.77	0.66
2:D:36:VAL:HB	2:D:66:GLY:HA3	1.77	0.66
2:B:175:VAL:HB	2:B:198:VAL:CG1	2.27	0.65
2:B:312:PHE:HE1	2:B:476:ILE:HD11	1.61	0.64
2:D:229:VAL:HG11	2:D:269:LEU:HA	1.78	0.64
2:C:538:MET:HG3	2:C:550:ILE:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:LEU:HD13	2:C:101:VAL:HG13	1.80	0.64
2:A:151:ALA:HB2	2:A:183:LEU:HB2	1.79	0.64
2:B:151:ALA:HB2	2:B:183:LEU:HB2	1.79	0.63
2:D:305:GLN:HE21	2:D:320:LEU:HB3	1.62	0.63
2:B:331:ARG:HH21	2:B:336:ASN:HD22	1.47	0.63
2:A:524:ILE:HD12	2:A:586:ARG:HH22	1.63	0.63
1:I:61:VAL:HG12	1:I:85:THR:HG23	1.81	0.63
2:D:51:ALA:HB1	2:D:112:PRO:HG3	1.79	0.63
2:D:141:VAL:HG21	2:D:152:VAL:HG21	1.81	0.63
2:D:550:ILE:HD13	2:D:592:LEU:HD23	1.80	0.63
2:C:301:LYS:HG3	2:C:325:TYR:HE2	1.64	0.62
2:D:201:ILE:HD11	2:D:609:ARG:HA	1.81	0.62
2:C:125:ALA:HA	2:C:129:TRP:HB2	1.79	0.62
2:B:32:VAL:N	2:B:178:HIS:O	2.32	0.62
2:B:377:VAL:HG21	1:I:145:THR:OG1	1.99	0.61
2:B:524:ILE:HD12	2:B:586:ARG:HH22	1.65	0.61
2:C:208:LEU:HG	2:C:238:ILE:HD11	1.82	0.61
1:J:9:LEU:HD11	1:J:85:THR:HG22	1.83	0.61
2:C:596:LEU:HA	2:C:601:LEU:HD11	1.82	0.61
2:A:106:TRP:HB2	2:A:114:VAL:HG21	1.83	0.61
1:I:9:LEU:HD11	1:I:85:THR:HG22	1.83	0.60
2:C:379:THR:HG21	2:C:445:THR:HA	1.84	0.60
2:A:236:ARG:O	2:A:238:ILE:HG12	2.01	0.60
2:A:396:VAL:HG22	2:A:424:ASP:HB2	1.84	0.60
2:B:236:ARG:O	2:B:238:ILE:HG12	2.01	0.60
2:B:83:PRO:HD2	2:B:87:LEU:HD23	1.83	0.60
1:J:122:ALA:HB3	1:J:132:PHE:HB2	1.83	0.59
2:B:50:LYS:HE2	2:B:180:HIS:HE1	1.66	0.59
2:A:83:PRO:HD2	2:A:87:LEU:HD23	1.83	0.59
2:C:279:PRO:HG2	2:C:601:LEU:HD22	1.84	0.59
2:D:34:TRP:HH2	2:D:150:ASP:HB3	1.67	0.59
2:C:201:ILE:HD11	2:C:609:ARG:HA	1.85	0.59
2:B:175:VAL:HB	2:B:198:VAL:HG11	1.84	0.59
2:B:263:ALA:HB1	2:B:274:PRO:HG3	1.85	0.59
2:A:124:TRP:O	2:A:128:ARG:HB3	2.03	0.59
2:C:538:MET:HE1	2:C:592:LEU:HD13	1.85	0.58
2:B:558:ARG:HG2	2:B:562:ASP:HB2	1.86	0.58
2:A:263:ALA:HB1	2:A:274:PRO:HG3	1.85	0.58
2:A:558:ARG:HG2	2:A:562:ASP:HB2	1.86	0.58
2:C:347:ALA:HB2	2:C:463:ILE:HB	1.86	0.58
2:B:550:ILE:HD13	2:B:592:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:550:ILE:HD13	2:A:592:LEU:HD12	1.85	0.57
2:B:31:GLU:HB2	2:B:64:LEU:HD23	1.86	0.57
2:B:106:TRP:HB2	2:B:114:VAL:HG21	1.86	0.57
2:C:51:ALA:HB1	2:C:112:PRO:HG3	1.85	0.57
2:A:276:ILE:HD11	2:A:611:MET:HG3	1.86	0.57
2:D:166:LEU:HD13	2:D:197:PRO:HD2	1.87	0.57
1:I:40:THR:HB	1:I:41:PRO:HD2	1.85	0.57
2:C:208:LEU:HD21	2:C:241:ARG:HB3	1.86	0.57
2:B:564:CYS:O	2:B:568:THR:HG23	2.05	0.56
2:A:34:TRP:CH2	2:A:150:ASP:HB3	2.39	0.56
2:A:564:CYS:O	2:A:568:THR:HG23	2.05	0.56
2:B:117:LEU:HD11	2:B:154:PHE:HD1	1.70	0.56
2:A:372:THR:HG21	2:A:479:PRO:HG2	1.87	0.56
2:D:307:PHE:CD1	2:D:488:LEU:HD21	2.40	0.56
2:B:174:HIS:CE1	2:B:620:HIS:HB3	2.41	0.56
2:A:174:HIS:CE1	2:A:620:HIS:HB3	2.40	0.56
2:B:132:GLU:CD	2:B:156:PHE:HE1	2.09	0.56
2:B:188:LEU:HD13	2:B:202:PHE:HB2	1.87	0.56
2:C:34:TRP:HH2	2:C:150:ASP:HB3	1.71	0.56
2:A:132:GLU:CD	2:A:156:PHE:HE1	2.09	0.56
2:A:456:ILE:O	2:A:460:ILE:HG13	2.06	0.56
2:D:65:VAL:HG11	2:D:158:THR:HG22	1.87	0.56
2:D:312:PHE:HE1	2:D:474:LYS:HE3	1.71	0.56
2:C:263:ALA:HB1	2:C:274:PRO:HG3	1.88	0.56
2:C:46:VAL:HG11	2:C:205:HIS:HE1	1.69	0.55
2:A:174:HIS:CD2	2:A:617:PHE:HE2	2.24	0.55
2:C:204:THR:O	2:C:204:THR:OG1	2.12	0.55
2:C:527:ILE:HG23	2:C:551:TYR:HB2	1.87	0.55
2:A:188:LEU:HD13	2:A:202:PHE:HB2	1.89	0.55
1:J:159:PHE:HB2	1:I:203:VAL:HG21	1.88	0.55
2:C:564:CYS:O	2:C:568:THR:HG23	2.06	0.55
2:B:50:LYS:NZ	2:B:180:HIS:CE1	2.74	0.55
2:B:149:ASN:O	2:B:153:LEU:HG	2.07	0.55
2:B:212:TYR:HB3	2:B:236:ARG:HD3	1.89	0.55
2:B:534:PHE:CE1	2:B:596:LEU:HD11	2.42	0.55
2:C:28:VAL:HA	2:C:61:ASN:HB3	1.88	0.55
2:C:538:MET:O	2:C:542:ILE:HG22	2.07	0.55
2:B:174:HIS:CD2	2:B:617:PHE:HE2	2.25	0.55
2:D:539:GLU:HG3	2:D:552:ILE:HG13	1.88	0.55
2:A:460:ILE:HG22	2:A:465:LEU:O	2.07	0.55
2:A:534:PHE:CE1	2:A:596:LEU:HD11	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:62:TYR:CE2	2:C:64:LEU:HD11	2.42	0.54
2:C:367:ILE:HD11	2:C:496:PHE:CE1	2.43	0.54
1:J:40:THR:HB	1:J:41:PRO:HD2	1.89	0.54
2:B:37:ALA:HB2	2:B:116:LEU:HD23	1.88	0.54
2:D:27:ALA:HA	2:D:174:HIS:O	2.07	0.54
2:A:149:ASN:O	2:A:153:LEU:HG	2.08	0.54
2:C:26:ASN:HB3	2:C:173:PRO:HB3	1.90	0.54
2:C:295:ASN:ND2	2:A:293:PHE:H	2.03	0.54
2:C:238:ILE:HG13	2:C:241:ARG:HH11	1.72	0.54
2:C:376:ASN:HB3	2:C:379:THR:HG23	1.89	0.54
2:D:307:PHE:HA	2:D:383:GLN:HE21	1.71	0.54
2:B:258:VAL:HG21	2:B:512:TRP:HB2	1.90	0.54
2:D:251:CYS:HA	1:H:349:LEU:HD11	1.90	0.54
2:B:34:TRP:CH2	2:B:150:ASP:HB3	2.43	0.54
2:C:219:ASP:OD2	2:C:222:ASN:HB2	2.07	0.54
2:C:307:PHE:HE2	2:C:476:ILE:HG21	1.73	0.54
2:A:538:MET:O	2:A:542:ILE:HG22	2.07	0.54
2:C:463:ILE:HD11	2:C:465:LEU:HD12	1.88	0.54
1:E:322:LYS:O	1:E:326:GLU:HG2	2.07	0.54
1:I:36:VAL:HG21	1:I:95:TYR:CZ	2.42	0.54
2:B:538:MET:O	2:B:542:ILE:HG22	2.07	0.54
2:C:507:SER:H	2:C:529:THR:HG21	1.72	0.54
2:D:361:THR:HG1	2:D:472:ARG:HH11	1.55	0.54
2:D:33:ALA:HB3	2:D:36:VAL:HG23	1.91	0.53
2:D:141:VAL:HG21	2:D:152:VAL:CG2	2.39	0.53
2:D:64:LEU:HB2	2:D:114:VAL:HG22	1.90	0.53
1:I:212:HIS:CE1	1:I:214:LEU:HD21	2.43	0.53
2:D:420:LEU:HD11	2:A:400:PHE:HZ	1.74	0.53
2:C:62:TYR:CZ	2:C:64:LEU:HD11	2.44	0.53
1:I:117:ARG:HG3	1:I:183:LEU:HD21	1.91	0.53
2:D:376:ASN:HA	2:D:447:ASN:HD22	1.74	0.53
2:B:263:ALA:CB	2:B:274:PRO:HG3	2.39	0.53
2:D:34:TRP:CH2	2:D:150:ASP:HB3	2.44	0.53
2:D:389:LEU:HD11	2:D:435:THR:HG22	1.91	0.53
2:A:211:ARG:HG3	2:A:509:TYR:CE2	2.44	0.53
2:A:498:ARG:HA	2:A:524:ILE:HD11	1.91	0.53
2:A:65:VAL:CG1	2:A:158:THR:HG22	2.39	0.52
2:C:142:PRO:HA	1:G:326:GLU:HA	1.92	0.52
2:C:519:CYS:SG	2:C:526:SER:HB3	2.48	0.52
2:D:263:ALA:CB	2:D:274:PRO:HG2	2.39	0.52
2:A:31:GLU:HB2	2:A:64:LEU:HD23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:129:PRO:HB2	1:I:124:PRO:HB2	1.91	0.52
2:B:331:ARG:NH2	2:B:336:ASN:HD22	2.07	0.52
2:A:524:ILE:HD12	2:A:586:ARG:NH2	2.24	0.52
1:H:322:LYS:O	1:H:326:GLU:HG2	2.10	0.52
2:C:22:PHE:HB2	2:C:623:TYR:HB3	1.90	0.52
2:A:350:ASN:O	2:A:354:ARG:HG2	2.10	0.52
2:D:114:VAL:HG12	2:D:116:LEU:HG	1.92	0.52
2:A:456:ILE:HG22	2:A:460:ILE:HD11	1.92	0.52
2:B:524:ILE:HD12	2:B:586:ARG:NH2	2.25	0.52
2:C:263:ALA:CB	2:C:274:PRO:HG3	2.40	0.52
2:A:35:GLU:HB3	2:A:44:TYR:HB2	1.90	0.52
2:A:99:CYS:SG	2:A:160:TRP:HZ3	2.32	0.52
2:A:332:TYR:HB2	2:A:369:PRO:O	2.10	0.52
1:F:322:LYS:O	1:F:326:GLU:HG2	2.10	0.52
2:B:138:ASN:HD21	1:F:321:ARG:HH22	1.56	0.52
2:B:284:VAL:HG23	2:B:597:ASP:OD1	2.09	0.52
2:C:312:PHE:HD1	2:C:441:PRO:HG2	1.75	0.52
1:G:322:LYS:O	1:G:326:GLU:HG2	2.10	0.52
2:D:106:TRP:HB2	2:D:114:VAL:HG21	1.92	0.52
2:D:456:ILE:O	2:D:460:ILE:HG13	2.09	0.51
2:C:33:ALA:HB3	2:C:36:VAL:HG23	1.93	0.51
2:C:267:GLN:HG2	2:C:273:LYS:HD2	1.91	0.51
2:D:362:VAL:HG12	2:D:473:VAL:HG13	1.92	0.51
2:A:425:PHE:HA	2:A:428:MET:HE2	1.91	0.51
2:B:350:ASN:O	2:B:354:ARG:HG2	2.10	0.51
2:C:484:SER:HA	2:C:490:PRO:O	2.10	0.51
2:C:404:LEU:HD12	2:C:414:PRO:HB3	1.91	0.51
2:C:456:ILE:O	2:C:460:ILE:HG13	2.10	0.51
2:B:183:LEU:HD23	2:B:183:LEU:H	1.75	0.51
2:A:94:MET:HB3	2:A:101:VAL:HG11	1.93	0.51
2:A:183:LEU:HD23	2:A:183:LEU:H	1.74	0.51
1:I:61:VAL:CG1	1:I:85:THR:HG23	2.40	0.51
2:B:498:ARG:HA	2:B:524:ILE:HD11	1.92	0.51
2:A:238:ILE:O	2:A:238:ILE:HG22	2.11	0.51
2:B:456:ILE:O	2:B:460:ILE:HG13	2.11	0.51
2:D:534:PHE:HE1	2:D:596:LEU:HD11	1.76	0.51
1:J:101:MET:HA	1:J:135:GLY:O	2.11	0.51
1:J:211:VAL:HG11	1:J:245:PHE:HB3	1.93	0.51
2:B:178:HIS:CD2	2:B:201:ILE:HB	2.46	0.51
2:C:507:SER:O	2:C:529:THR:HG21	2.11	0.51
2:D:534:PHE:CE1	2:D:596:LEU:HD11	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:263:ALA:CB	2:A:274:PRO:HG3	2.40	0.50
2:B:369:PRO:HA	2:B:479:PRO:O	2.12	0.50
2:A:97:LYS:HB3	2:A:160:TRP:HH2	1.76	0.50
2:A:117:LEU:HD11	2:A:154:PHE:HD1	1.76	0.50
2:A:133:LEU:HB2	2:A:156:PHE:HE2	1.76	0.50
2:B:94:MET:HB3	2:B:101:VAL:HG11	1.92	0.50
2:D:513:GLY:C	2:D:516:PRO:HD2	2.32	0.50
2:C:312:PHE:CE1	2:C:474:LYS:HD2	2.47	0.50
2:D:527:ILE:HG12	2:D:551:TYR:HB2	1.94	0.50
2:B:276:ILE:HD12	2:B:608:ALA:HA	1.94	0.50
2:C:34:TRP:CH2	2:C:150:ASP:HB3	2.46	0.50
2:D:313:TYR:CE1	2:D:385:VAL:HG11	2.46	0.50
2:C:389:LEU:HD22	2:C:431:ALA:HB1	1.94	0.49
2:D:602:GLY:HA2	2:D:605:TYR:CE2	2.48	0.49
1:I:222:TYR:HB2	1:I:250:TRP:HE1	1.77	0.49
2:B:389:LEU:HD11	2:B:435:THR:HG22	1.95	0.49
2:B:527:ILE:HG13	2:B:551:TYR:HB2	1.95	0.49
2:C:375:PHE:CD1	2:C:488:LEU:HD12	2.48	0.49
2:A:124:TRP:CB	2:A:128:ARG:HE	2.26	0.49
1:I:101:MET:HA	1:I:135:GLY:O	2.11	0.49
1:I:8:THR:HG23	1:I:37:VAL:HG23	1.94	0.49
2:B:238:ILE:HG22	2:B:238:ILE:O	2.12	0.49
2:A:106:TRP:HB2	2:A:114:VAL:CG2	2.41	0.49
2:B:389:LEU:HD23	2:B:431:ALA:HB1	1.94	0.49
1:J:36:VAL:HG13	1:J:57:GLU:HB2	1.95	0.49
2:A:200:THR:H	2:A:253:HIS:CD2	2.31	0.49
2:B:133:LEU:HB2	2:B:156:PHE:HE2	1.76	0.49
2:C:385:VAL:HG22	2:C:434:ALA:HB1	1.95	0.49
2:B:534:PHE:HE1	2:B:596:LEU:HD11	1.77	0.49
2:C:352:LEU:HD23	2:C:572:TYR:CG	2.48	0.49
2:A:527:ILE:HG13	2:A:551:TYR:HB2	1.95	0.49
2:B:50:LYS:HE2	2:B:180:HIS:CE1	2.47	0.49
2:D:73:VAL:HA	2:D:77:VAL:HB	1.95	0.49
2:A:258:VAL:HG21	2:A:512:TRP:HB2	1.95	0.49
2:A:345:ALA:HA	2:A:568:THR:HG22	1.95	0.48
2:D:48:GLN:HA	2:D:108:ILE:HD13	1.94	0.48
2:B:393:ALA:O	2:B:397:LYS:HB3	2.13	0.48
1:I:36:VAL:HG21	1:I:95:TYR:OH	2.12	0.48
1:J:153:ALA:HB2	1:J:166:ILE:CD1	2.43	0.48
2:B:106:TRP:HB2	2:B:114:VAL:CG2	2.42	0.48
2:B:345:ALA:HA	2:B:568:THR:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:369:PRO:HA	2:D:479:PRO:O	2.13	0.48
2:B:175:VAL:HB	2:B:198:VAL:HG13	1.96	0.48
2:D:137:CYS:SG	2:D:189:CYS:HB3	2.53	0.48
2:A:297:HIS:HB2	2:A:586:ARG:NH1	2.28	0.48
2:B:38:ASN:HB3	2:B:69:THR:HG21	1.95	0.48
2:C:30:PHE:HE2	2:C:162:LEU:HB3	1.79	0.48
2:B:24:LEU:HB2	2:B:27:ALA:HB3	1.95	0.48
2:C:27:ALA:HA	2:C:174:HIS:O	2.12	0.48
2:D:601:LEU:HA	2:D:601:LEU:HD23	1.68	0.48
2:A:534:PHE:HE1	2:A:596:LEU:HD11	1.79	0.48
2:A:174:HIS:HD2	2:A:617:PHE:HE2	1.60	0.48
2:B:276:ILE:HD11	2:B:611:MET:HG3	1.95	0.48
2:D:258:VAL:HG21	2:D:512:TRP:HB2	1.96	0.48
2:D:375:PHE:CE1	2:D:487:PRO:HD2	2.49	0.47
2:A:413:LEU:HD23	2:A:414:PRO:HD2	1.94	0.47
2:A:598:TRP:CZ3	2:A:605:TYR:CE2	3.02	0.47
2:B:32:VAL:O	2:B:179:PHE:HA	2.14	0.47
2:B:598:TRP:CZ3	2:B:605:TYR:CE2	3.02	0.47
2:C:513:GLY:C	2:C:516:PRO:HD2	2.35	0.47
2:D:65:VAL:CG1	2:D:158:THR:HG22	2.44	0.47
2:D:209:LEU:HD23	2:D:229:VAL:HG12	1.96	0.47
2:D:307:PHE:HD1	2:D:488:LEU:HD21	1.77	0.47
2:A:513:GLY:C	2:A:516:PRO:HD2	2.34	0.47
1:I:50:VAL:HG21	1:I:261:LEU:HD23	1.95	0.47
2:B:28:VAL:HA	2:B:61:ASN:HB3	1.97	0.47
2:C:313:TYR:HD2	2:C:437:ARG:HB3	1.78	0.47
2:D:188:LEU:HD11	2:D:252:ALA:HA	1.96	0.47
2:D:332:TYR:HB2	2:D:369:PRO:O	2.13	0.47
2:A:211:ARG:HG3	2:A:509:TYR:HE2	1.78	0.47
2:C:258:VAL:HG21	2:C:512:TRP:HB2	1.96	0.47
2:D:375:PHE:CE2	2:D:488:LEU:HB2	2.50	0.47
1:J:10:THR:HG22	1:J:15:TYR:O	2.14	0.47
2:C:313:TYR:CD1	2:C:382:GLY:HA2	2.40	0.47
2:C:345:ALA:HA	2:C:568:THR:HG22	1.96	0.47
2:D:238:ILE:HG13	2:D:241:ARG:HD2	1.96	0.47
2:C:86:ALA:O	2:C:90:THR:HG23	2.13	0.47
2:B:24:LEU:CB	2:B:27:ALA:HB3	2.45	0.47
2:B:36:VAL:HB	2:B:66:GLY:HA3	1.96	0.47
2:B:114:VAL:HG12	2:B:116:LEU:HG	1.97	0.47
2:B:124:TRP:CB	2:B:128:ARG:HE	2.27	0.47
2:B:365:PHE:HB3	2:B:367:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:178:HIS:CD2	2:A:201:ILE:HB	2.50	0.47
2:A:509:TYR:O	2:A:510:GLU:C	2.53	0.47
2:D:209:LEU:HD12	2:D:209:LEU:HA	1.79	0.47
2:A:369:PRO:HA	2:A:479:PRO:O	2.14	0.47
2:B:30:PHE:N	2:B:176:VAL:O	2.41	0.47
2:B:495:GLU:HA	2:B:495:GLU:OE1	2.15	0.47
2:B:513:GLY:C	2:B:516:PRO:HD2	2.36	0.47
1:J:9:LEU:HD22	1:J:86:LYS:HB2	1.97	0.47
2:C:394:ASN:HA	2:C:397:LYS:HE2	1.96	0.47
1:I:31:THR:HG21	1:I:35:LEU:HD21	1.97	0.47
2:C:30:PHE:CE2	2:C:162:LEU:HB3	2.50	0.46
2:C:332:TYR:HE1	2:C:477:PHE:CZ	2.34	0.46
2:A:114:VAL:HG12	2:A:116:LEU:HG	1.97	0.46
1:I:36:VAL:HG13	1:I:57:GLU:HB2	1.97	0.46
2:A:27:ALA:HA	2:A:174:HIS:O	2.14	0.46
1:I:117:ARG:HG3	1:I:183:LEU:CD2	2.45	0.46
2:A:378:GLU:HG2	2:A:442:PRO:HD3	1.98	0.46
2:B:174:HIS:HD2	2:B:617:PHE:HE2	1.62	0.46
2:C:202:PHE:O	2:C:202:PHE:CG	2.68	0.46
2:D:106:TRP:HB2	2:D:114:VAL:CG2	2.45	0.46
2:A:495:GLU:OE1	2:A:495:GLU:HA	2.16	0.46
2:B:36:VAL:HG11	2:B:64:LEU:HB3	1.97	0.46
2:D:28:VAL:HA	2:D:61:ASN:HB3	1.97	0.46
2:D:152:VAL:HA	2:D:186:VAL:HG21	1.98	0.46
2:D:548:TYR:HB3	2:D:592:LEU:HD22	1.98	0.46
1:I:10:THR:HG22	1:I:15:TYR:O	2.16	0.46
2:B:125:ALA:HA	2:B:129:TRP:HB2	1.96	0.46
2:B:177:ALA:HB3	2:B:200:THR:HG22	1.98	0.46
1:I:63:VAL:HG12	1:I:70:ALA:HB3	1.97	0.46
2:B:200:THR:H	2:B:253:HIS:HD2	1.62	0.46
2:B:310:GLY:HA2	2:B:386:ARG:HB2	1.98	0.46
2:C:188:LEU:CD1	2:C:202:PHE:HB2	2.46	0.46
2:D:38:ASN:HB3	2:D:69:THR:HG21	1.98	0.46
2:B:416:MET:HG2	2:C:417:ASN:H	1.81	0.45
2:C:307:PHE:CE2	2:C:476:ILE:HG21	2.51	0.45
2:D:51:ALA:HB1	2:D:112:PRO:CG	2.46	0.45
2:A:68:TYR:HD1	2:A:73:VAL:HG21	1.82	0.45
2:B:124:TRP:HB3	2:B:128:ARG:HE	1.81	0.45
2:A:125:ALA:HA	2:A:129:TRP:HB2	1.97	0.45
2:A:343:LEU:HD11	2:A:456:ILE:HG23	1.98	0.45
2:A:372:THR:HG22	2:A:448:MET:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:258:VAL:HA	2:C:278:THR:O	2.16	0.45
2:C:327:PHE:CZ	2:C:505:PHE:HZ	2.34	0.45
2:D:308:VAL:O	2:D:312:PHE:HD2	2.00	0.45
2:A:28:VAL:HA	2:A:61:ASN:HB3	1.97	0.45
2:A:212:TYR:HB3	2:A:236:ARG:HD3	1.98	0.45
2:A:348:ARG:HD2	2:A:568:THR:HG21	1.98	0.45
2:B:27:ALA:HA	2:B:174:HIS:O	2.16	0.45
2:B:77:VAL:HG11	2:B:116:LEU:HD11	1.98	0.45
2:C:313:TYR:CD2	2:C:437:ARG:HB3	2.51	0.45
2:C:368:MET:HB2	2:C:477:PHE:HE1	1.82	0.45
2:D:115:VAL:HG21	2:D:161:PHE:CE2	2.51	0.45
2:D:231:LYS:O	2:D:235:GLU:HG2	2.17	0.45
2:B:50:LYS:HZ1	2:B:180:HIS:CE1	2.35	0.45
2:C:519:CYS:SG	2:C:524:ILE:HB	2.56	0.45
2:D:607:SER:O	2:D:611:MET:HG2	2.17	0.45
2:B:286:LYS:HG3	2:B:521:VAL:HG12	1.99	0.45
2:C:117:LEU:HD11	2:C:154:PHE:CD1	2.51	0.45
2:B:68:TYR:HD1	2:B:73:VAL:HG21	1.82	0.45
2:C:119:VAL:HG12	2:C:119:VAL:O	2.16	0.45
2:A:312:PHE:HD2	2:A:318:PHE:CZ	2.34	0.45
2:D:401:GLY:HA3	2:A:397:LYS:HD2	1.99	0.45
2:D:489:LEU:HD12	2:D:489:LEU:HA	1.88	0.45
2:B:117:LEU:HD11	2:B:154:PHE:CD1	2.51	0.45
2:C:467:ASN:HB3	2:C:474:LYS:HD3	1.99	0.45
2:A:310:GLY:HA2	2:A:386:ARG:HB2	1.99	0.45
2:C:446:HIS:HB2	2:C:479:PRO:HD2	1.99	0.45
2:A:525:PRO:HD3	2:A:586:ARG:HD2	1.99	0.45
1:I:9:LEU:HD22	1:I:86:LYS:HB2	1.98	0.45
2:D:327:PHE:HZ	2:D:519:CYS:HG	1.65	0.44
2:C:574:PHE:O	2:C:577:GLN:HB2	2.17	0.44
2:A:147:GLU:HG3	2:A:183:LEU:HD13	1.98	0.44
1:J:159:PHE:CB	1:I:203:VAL:HG21	2.48	0.44
2:C:416:MET:O	2:C:417:ASN:HB2	2.18	0.44
2:A:132:GLU:CD	2:A:156:PHE:CE1	2.91	0.44
2:D:23:ASP:OD2	2:D:621:PHE:HB3	2.18	0.44
2:B:68:TYR:CD1	2:B:73:VAL:HG21	2.52	0.44
2:C:509:TYR:O	2:C:510:GLU:C	2.56	0.44
1:I:151:HIS:CE1	1:I:155:GLU:HG3	2.52	0.44
1:J:8:THR:HG23	1:J:37:VAL:HG23	1.98	0.44
2:D:33:ALA:O	2:D:67:PRO:HD3	2.18	0.44
2:D:332:TYR:CE2	2:D:456:ILE:HG12	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:489:LEU:HD23	2:A:489:LEU:HA	1.87	0.44
1:J:117:ARG:HG3	1:J:183:LEU:CD2	2.48	0.44
2:D:502:LEU:HD12	2:D:525:PRO:HB2	2.00	0.44
2:A:393:ALA:O	2:A:397:LYS:HB3	2.17	0.44
1:J:194:ILE:HB	1:J:201:PHE:HB2	2.00	0.44
2:C:296:LEU:HD13	2:C:296:LEU:HA	1.81	0.44
2:D:258:VAL:O	2:D:279:PRO:HA	2.17	0.44
2:B:348:ARG:HD2	2:B:568:THR:HG21	2.00	0.43
2:C:273:LYS:HE3	2:C:273:LYS:HB3	1.75	0.43
2:D:138:ASN:HB3	1:H:341:ILE:HD12	2.00	0.43
2:D:488:LEU:HD22	2:D:489:LEU:HB2	2.00	0.43
2:A:68:TYR:CD1	2:A:73:VAL:HG21	2.53	0.43
2:A:77:VAL:HG11	2:A:116:LEU:HD11	2.00	0.43
2:D:47:LEU:HD23	2:D:64:LEU:HD22	2.00	0.43
2:D:176:VAL:HA	2:D:199:ALA:O	2.19	0.43
2:A:334:PHE:CE2	2:A:340:ASP:HB3	2.53	0.43
2:C:224:LEU:HD21	2:C:265:GLU:HA	2.00	0.43
2:C:343:LEU:HG	2:C:366:PHE:CZ	2.54	0.43
1:J:120:LEU:HD23	1:J:171:PHE:CZ	2.53	0.43
2:B:200:THR:H	2:B:253:HIS:CD2	2.35	0.43
2:A:400:PHE:CE2	2:A:404:LEU:HD13	2.53	0.43
2:A:515:THR:HG23	2:A:516:PRO:HD3	1.99	0.43
2:B:404:LEU:HD12	2:B:408:LEU:HD13	2.00	0.43
2:D:43:ILE:HD12	2:D:43:ILE:H	1.83	0.43
2:A:375:PHE:CE2	2:A:488:LEU:HB2	2.53	0.43
2:B:509:TYR:O	2:B:510:GLU:C	2.57	0.43
2:C:84:THR:HB	2:C:87:LEU:HB3	2.00	0.43
2:D:117:LEU:HG	2:D:157:LEU:HB3	2.01	0.43
2:D:119:VAL:O	2:D:153:LEU:HD13	2.19	0.43
2:C:573:SER:O	2:C:577:GLN:HG3	2.19	0.43
1:I:37:VAL:HG13	1:I:58:VAL:HG13	2.00	0.43
2:B:151:ALA:HB1	2:B:183:LEU:O	2.19	0.42
2:B:404:LEU:HD13	2:B:414:PRO:HG3	2.01	0.42
2:C:28:VAL:O	2:C:175:VAL:HG13	2.19	0.42
2:C:366:PHE:HD1	2:C:366:PHE:H	1.67	0.42
2:D:394:ASN:O	2:D:398:GLU:HG3	2.19	0.42
1:H:316:VAL:HB	1:H:317:SER:H	1.71	0.42
2:B:258:VAL:CG2	2:B:512:TRP:HB2	2.49	0.42
2:B:525:PRO:HD3	2:B:586:ARG:HD2	2.01	0.42
2:D:581:GLN:HA	2:D:584:ILE:HD12	2.01	0.42
1:J:90:TRP:CZ2	1:J:120:LEU:HD21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:ALA:HA	2:C:404:LEU:HD23	2.02	0.42
2:C:209:LEU:HD21	2:C:232:GLU:HB2	2.01	0.42
2:C:301:LYS:HG3	2:C:325:TYR:CE2	2.51	0.42
2:C:329:ALA:HA	2:C:367:ILE:O	2.19	0.42
2:C:348:ARG:HD2	2:C:568:THR:HG21	2.01	0.42
2:C:393:ALA:O	2:C:397:LYS:HB3	2.18	0.42
2:C:554:ASP:O	2:C:558:ARG:HD2	2.19	0.42
1:I:185:PHE:HZ	1:I:193:SER:HB3	1.84	0.42
2:B:296:LEU:HD22	2:B:498:ARG:NH2	2.34	0.42
2:C:29:LEU:HD12	2:C:176:VAL:O	2.19	0.42
2:C:498:ARG:HA	2:C:524:ILE:HD11	2.01	0.42
2:C:595:LEU:HD13	2:C:595:LEU:HA	1.93	0.42
2:A:132:GLU:OE2	2:A:156:PHE:HE1	2.03	0.42
2:A:174:HIS:CD2	2:A:613:LEU:HG	2.55	0.42
1:J:128:TRP:CH2	1:I:189:LEU:HD11	2.54	0.42
1:J:40:THR:HA	1:J:61:VAL:O	2.20	0.42
1:J:218:LYS:HD3	1:J:218:LYS:HA	1.78	0.42
2:B:511:PRO:HB2	2:B:512:TRP:H	1.58	0.42
2:C:372:THR:OG1	2:C:446:HIS:HB3	2.20	0.42
2:D:263:ALA:HB1	2:D:274:PRO:HG2	2.00	0.42
1:I:21:VAL:HG11	1:I:249:TRP:CD1	2.55	0.42
1:J:21:VAL:HG11	1:J:249:TRP:CD1	2.55	0.42
2:D:224:LEU:HD12	2:D:224:LEU:HA	1.79	0.42
2:D:246:ARG:HG3	2:D:270:LEU:O	2.19	0.42
2:D:301:LYS:HG3	2:D:325:TYR:HE2	1.84	0.42
2:A:24:LEU:H	2:A:24:LEU:HG	1.69	0.42
2:A:137:CYS:HB2	2:A:139:ILE:HG22	2.02	0.42
2:B:43:ILE:HD12	2:B:43:ILE:H	1.85	0.42
2:C:343:LEU:HD23	2:C:343:LEU:HA	1.96	0.42
2:D:279:PRO:HD2	2:D:601:LEU:HD22	2.02	0.42
2:B:33:ALA:HB2	2:B:180:HIS:HB2	2.01	0.42
2:C:362:VAL:HB	2:C:473:VAL:HG22	2.02	0.42
2:C:580:ARG:HA	2:C:583:ILE:HD12	2.01	0.42
1:I:34:ARG:HE	1:I:34:ARG:HB3	1.65	0.42
1:J:120:LEU:N	1:J:138:VAL:O	2.52	0.41
2:B:375:PHE:HB3	2:B:380:LEU:HG	2.02	0.41
2:C:368:MET:O	2:C:369:PRO:C	2.59	0.41
2:A:154:PHE:O	2:A:158:THR:HG23	2.20	0.41
2:A:258:VAL:CG2	2:A:512:TRP:HB2	2.49	0.41
2:A:598:TRP:HZ3	2:A:605:TYR:CE2	2.38	0.41
1:I:50:VAL:HG22	1:I:264:PHE:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:LEU:H	2:B:24:LEU:HG	1.72	0.41
2:B:31:GLU:HG3	2:B:62:TYR:HE1	1.85	0.41
2:B:132:GLU:OE2	2:B:156:PHE:HE1	2.02	0.41
2:B:137:CYS:HB2	2:B:139:ILE:HG22	2.02	0.41
2:B:151:ALA:CB	2:B:183:LEU:HB2	2.47	0.41
2:C:166:LEU:HD21	2:C:175:VAL:HG23	2.02	0.41
2:C:507:SER:H	2:C:529:THR:CG2	2.32	0.41
1:I:133:ASN:HB3	1:I:188:ASN:ND2	2.35	0.41
2:C:332:TYR:CE1	2:C:456:ILE:HD13	2.55	0.41
2:C:472:ARG:HE	2:C:472:ARG:HA	1.85	0.41
2:C:538:MET:HE1	2:C:592:LEU:CD1	2.49	0.41
2:C:588:ARG:HH21	2:A:591:ARG:NH2	2.18	0.41
2:D:579:ARG:HD2	2:D:582:ARG:HH21	1.85	0.41
2:B:347:ALA:HB2	2:B:463:ILE:HG13	2.02	0.41
2:B:379:THR:HG22	2:B:488:LEU:HD22	2.01	0.41
2:C:106:TRP:CD2	2:C:108:ILE:HG12	2.55	0.41
2:A:43:ILE:HD12	2:A:43:ILE:H	1.85	0.41
2:A:51:ALA:HB3	2:A:108:ILE:CD1	2.51	0.41
2:A:595:LEU:HD13	2:A:595:LEU:HA	1.92	0.41
1:I:218:LYS:HB3	1:I:219:PRO:HD2	2.02	0.41
1:J:194:ILE:HG12	1:J:195:PHE:N	2.35	0.41
2:B:51:ALA:HB3	2:B:108:ILE:CD1	2.50	0.41
2:B:284:VAL:HG12	2:B:287:PHE:CD2	2.56	0.41
2:C:258:VAL:CG2	2:C:512:TRP:HB2	2.50	0.41
2:C:276:ILE:HD13	2:C:608:ALA:HA	2.02	0.41
2:D:258:VAL:CG2	2:D:512:TRP:HB2	2.51	0.41
2:B:36:VAL:HG22	2:B:47:LEU:HD22	2.03	0.41
2:B:132:GLU:CD	2:B:156:PHE:CE1	2.91	0.41
2:D:375:PHE:CE2	2:D:488:LEU:CB	3.04	0.41
2:D:537:PHE:CE2	2:D:595:LEU:HD23	2.56	0.41
2:A:200:THR:H	2:A:253:HIS:HD2	1.68	0.41
1:I:257:VAL:O	1:I:260:LEU:N	2.54	0.41
2:D:313:TYR:CD1	2:D:385:VAL:HG21	2.55	0.41
2:B:489:LEU:HD12	2:B:489:LEU:HA	1.94	0.41
2:C:122:SER:HA	2:C:153:LEU:HD11	2.03	0.41
2:C:343:LEU:HD13	2:C:459:THR:HB	2.02	0.41
2:D:36:VAL:HG11	2:D:64:LEU:O	2.21	0.41
2:D:448:MET:HB3	2:D:448:MET:HE3	1.88	0.41
2:D:592:LEU:HD12	2:D:592:LEU:HA	1.69	0.41
2:B:30:PHE:O	2:B:178:HIS:N	2.37	0.41
2:B:106:TRP:CD2	2:B:108:ILE:HG12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:LEU:HD23	2:B:323:THR:HG21	2.02	0.41
2:C:34:TRP:CD2	2:C:67:PRO:HG3	2.55	0.41
2:C:70:GLU:HG3	2:C:71:GLN:N	2.35	0.41
2:D:78:GLU:HB2	2:D:107:LEU:HD21	2.02	0.41
2:D:515:THR:OG1	2:D:516:PRO:HD3	2.20	0.41
2:A:31:GLU:HG2	2:A:178:HIS:HB3	2.03	0.41
2:A:117:LEU:HD11	2:A:154:PHE:CD1	2.54	0.41
2:B:174:HIS:CD2	2:B:613:LEU:HG	2.56	0.41
2:C:99:CYS:SG	2:C:160:TRP:HZ3	2.44	0.41
2:D:361:THR:HG23	2:D:472:ARG:O	2.21	0.41
2:D:488:LEU:C	2:D:488:LEU:HD23	2.41	0.41
2:A:106:TRP:CD2	2:A:108:ILE:HG12	2.56	0.41
2:D:313:TYR:HD1	2:D:385:VAL:HG21	1.86	0.40
1:I:194:ILE:HD12	1:I:242:HIS:HB2	2.02	0.40
1:J:224:TYR:CE1	1:J:254:THR:HG21	2.56	0.40
2:B:267:GLN:HG2	2:B:273:LYS:HG2	2.03	0.40
2:C:580:ARG:HH22	2:A:284:VAL:HG21	1.86	0.40
2:A:32:VAL:N	2:A:178:HIS:O	2.50	0.40
2:A:149:ASN:O	2:A:152:VAL:HG22	2.21	0.40
2:A:333:GLU:HG2	2:A:336:ASN:HB2	2.02	0.40
2:C:64:LEU:HD12	2:C:64:LEU:N	2.36	0.40
2:C:258:VAL:O	2:C:279:PRO:HA	2.21	0.40
2:D:35:GLU:HB3	2:D:44:TYR:HB2	2.04	0.40
2:A:30:PHE:HA	2:A:63:PHE:O	2.22	0.40
2:A:463:ILE:CG2	2:A:465:LEU:HG	2.51	0.40
1:J:201:PHE:O	1:J:205:GLY:N	2.54	0.40
1:J:203:VAL:HG21	1:I:159:PHE:HB3	2.03	0.40
2:B:154:PHE:O	2:B:158:THR:HG23	2.22	0.40
2:B:595:LEU:HD13	2:B:595:LEU:HA	1.93	0.40
2:D:106:TRP:CD2	2:D:108:ILE:HG12	2.56	0.40
2:D:155:GLY:HA3	2:D:186:VAL:HB	2.03	0.40
2:D:393:ALA:HA	2:A:404:LEU:HD23	2.03	0.40
2:A:320:LEU:HD23	2:A:323:THR:HG21	2.03	0.40
2:B:296:LEU:HD22	2:B:498:ARG:HH21	1.85	0.40
2:C:43:ILE:HD12	2:C:43:ILE:H	1.86	0.40
2:C:192:ARG:HD2	2:C:192:ARG:HA	1.77	0.40
2:D:154:PHE:O	2:D:158:THR:HG23	2.21	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	E	33/352 (9%)	31 (94%)	2 (6%)	0	100	100
1	F	33/352 (9%)	30 (91%)	3 (9%)	0	100	100
1	G	32/352 (9%)	29 (91%)	3 (9%)	0	100	100
1	H	32/352 (9%)	28 (88%)	4 (12%)	0	100	100
1	I	265/352 (75%)	253 (96%)	12 (4%)	0	100	100
1	J	257/352 (73%)	247 (96%)	10 (4%)	0	100	100
2	A	597/634 (94%)	587 (98%)	10 (2%)	0	100	100
2	B	598/634 (94%)	583 (98%)	14 (2%)	1 (0%)	47	80
2	C	596/634 (94%)	572 (96%)	23 (4%)	1 (0%)	47	80
2	D	597/634 (94%)	587 (98%)	10 (2%)	0	100	100
All	All	3040/4648 (65%)	2947 (97%)	91 (3%)	2 (0%)	54	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	511	PRO
2	C	369	PRO

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	E	31/311 (10%)	28 (90%)	3 (10%)	8	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	31/311 (10%)	28 (90%)	3 (10%)	8	34
1	G	30/311 (10%)	27 (90%)	3 (10%)	7	33
1	H	30/311 (10%)	27 (90%)	3 (10%)	7	33
1	I	233/311 (75%)	227 (97%)	6 (3%)	46	74
1	J	229/311 (74%)	219 (96%)	10 (4%)	28	62
2	A	511/545 (94%)	489 (96%)	22 (4%)	29	62
2	B	505/545 (93%)	485 (96%)	20 (4%)	31	64
2	C	501/545 (92%)	482 (96%)	19 (4%)	33	65
2	D	499/545 (92%)	478 (96%)	21 (4%)	30	63
All	All	2600/4046 (64%)	2490 (96%)	110 (4%)	33	63

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	90	TRP
1	J	120	LEU
1	J	163	ASP
1	J	189	LEU
1	J	194	ILE
1	J	198	LEU
1	J	232	LYS
1	J	241	THR
1	J	242	HIS
1	J	261	LEU
2	B	24	LEU
2	B	28	VAL
2	B	47	LEU
2	B	71	GLN
2	B	79	LEU
2	B	108	ILE
2	B	166	LEU
2	B	171	GLU
2	B	214	CYS
2	B	292	GLU
2	B	319	ASN
2	B	367	ILE
2	B	408	LEU
2	B	432	ILE
2	B	445	THR

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Mol	Chain	Res	Type
2	B	463	ILE
2	B	479	PRO
2	B	492	ASP
2	B	515	THR
2	B	553	LEU
2	C	24	LEU
2	C	47	LEU
2	C	87	LEU
2	C	91	LEU
2	C	108	ILE
2	C	143	TRP
2	C	214	CYS
2	C	242	TYR
2	C	296	LEU
2	C	315	HIS
2	C	316	LEU
2	C	323	THR
2	C	372	THR
2	C	420	LEU
2	C	457	LEU
2	C	491	VAL
2	C	561	ASP
2	C	617	PHE
2	C	619	GLU
2	D	28	VAL
2	D	36	VAL
2	D	47	LEU
2	D	58	TRP
2	D	108	ILE
2	D	138	ASN
2	D	188	LEU
2	D	204	THR
2	D	208	LEU
2	D	230	ASP
2	D	272	ARG
2	D	332	TYR
2	D	372	THR
2	D	457	LEU
2	D	491	VAL
2	D	495	GLU
2	D	529	THR
2	D	540	GLU

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Mol	Chain	Res	Type
2	D	592	LEU
2	D	595	LEU
2	D	609	ARG
2	A	24	LEU
2	A	28	VAL
2	A	47	LEU
2	A	71	GLN
2	A	79	LEU
2	A	108	ILE
2	A	166	LEU
2	A	171	GLU
2	A	176	VAL
2	A	214	CYS
2	A	287	PHE
2	A	295	ASN
2	A	319	ASN
2	A	374	ASN
2	A	380	LEU
2	A	404	LEU
2	A	425	PHE
2	A	429	LYS
2	A	463	ILE
2	A	489	LEU
2	A	515	THR
2	A	553	LEU
1	E	316	VAL
1	E	317	SER
1	E	348	TYR
1	I	90	TRP
1	I	120	LEU
1	I	189	LEU
1	I	193	SER
1	I	194	ILE
1	I	233	SER
1	F	316	VAL
1	F	317	SER
1	F	348	TYR
1	G	316	VAL
1	G	317	SER
1	G	348	TYR
1	H	316	VAL
1	H	317	SER

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Mol	Chain	Res	Type
1	H	348	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	140	GLN
2	B	95	ASN
2	B	138	ASN
2	B	174	HIS
2	B	180	HIS
2	B	205	HIS
2	B	253	HIS
2	B	260	GLN
2	B	336	ASN
2	B	388	GLN
2	B	438	GLN
2	B	530	ASN
2	B	576	GLN
2	B	587	ASN
2	C	95	ASN
2	C	138	ASN
2	C	205	HIS
2	C	240	HIS
2	C	280	ASN
2	C	283	ASN
2	C	295	ASN
2	C	299	GLN
2	C	388	GLN
2	C	436	GLN
2	D	138	ASN
2	D	280	ASN
2	D	305	GLN
2	D	336	ASN
2	D	360	GLN
2	D	436	GLN
2	D	447	ASN
2	D	581	GLN
2	D	620	HIS
2	A	174	HIS
2	A	178	HIS
2	A	205	HIS
2	A	253	HIS

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Mol	Chain	Res	Type
2	A	260	GLN
2	A	299	GLN
2	A	388	GLN
2	A	417	ASN
2	A	530	ASN
2	A	576	GLN
2	A	587	ASN
2	A	620	HIS
1	E	350	GLN
1	I	140	GLN
1	I	164	GLN
1	F	350	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 ⓘ

There are no ligands in this entry.

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-27022. 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 ⓘ
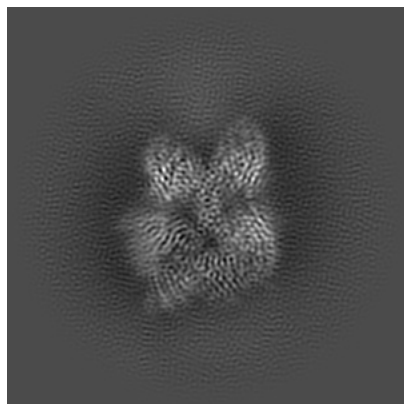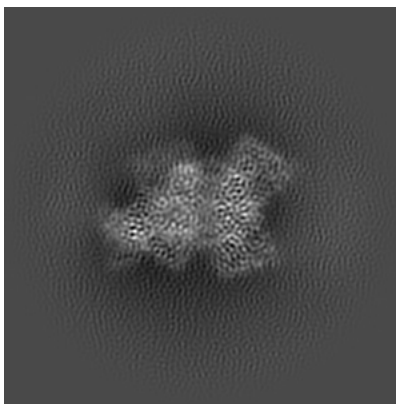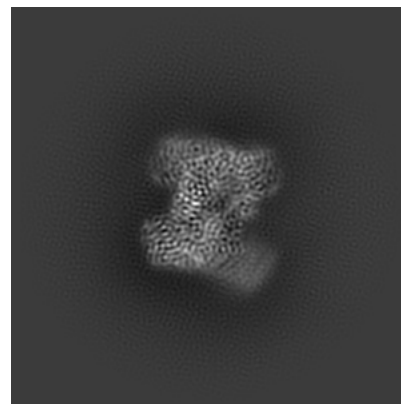
6.1.1 Primary map

| X | Y | Z |

6.1.2 Raw map

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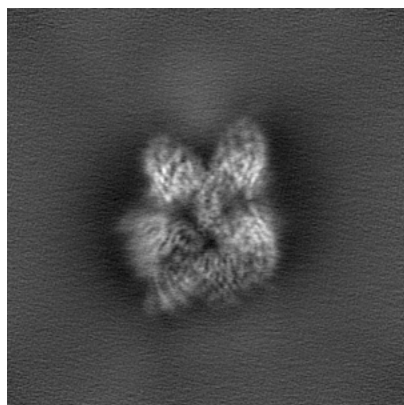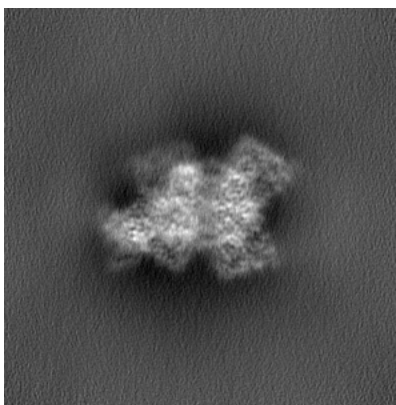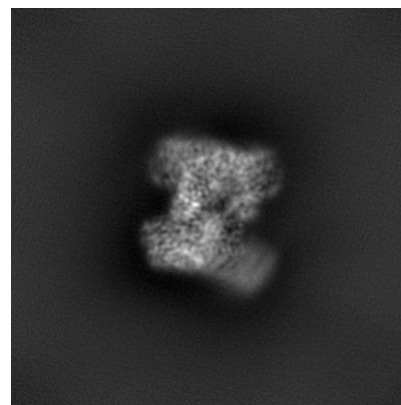
The images above show the map projected in three orthogonal directions.

6.2　Central slices ⓘ
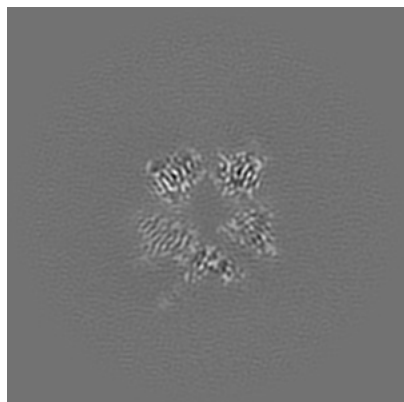
6.2.1　Primary map
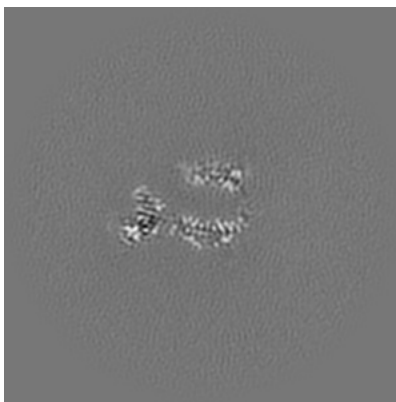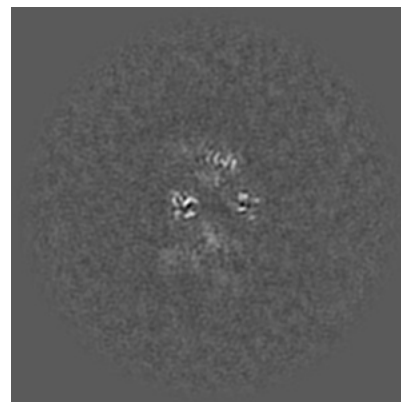
X Index: 162　　　　Y Index: 162　　　　Z Index: 162

6.2.2　Raw map
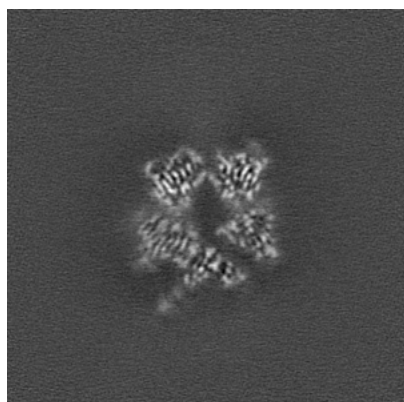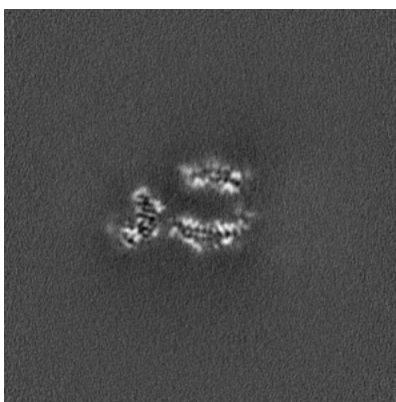
X Index: 162　　　　Y Index: 162　　　　Z Index: 162

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

6.3 Largest variance slices (i)

6.3.1 Primary map
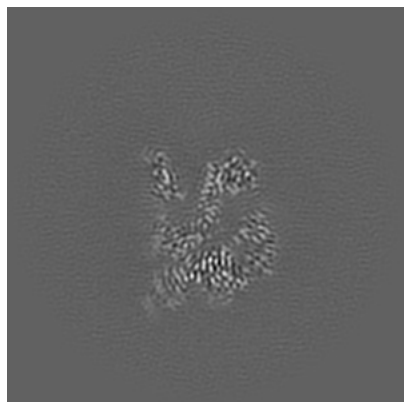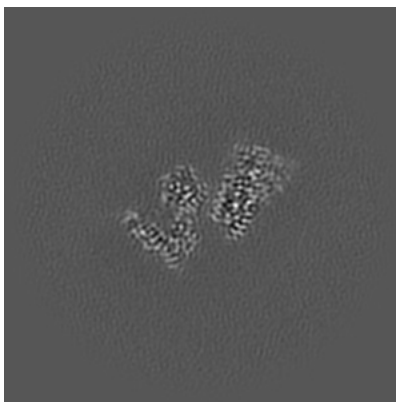
| X Index: 147 | Y Index: 195 | Z Index: 186 |
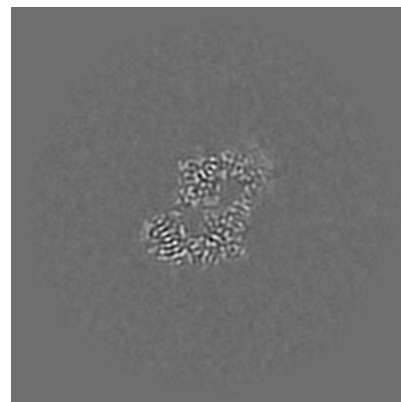
6.3.2 Raw map
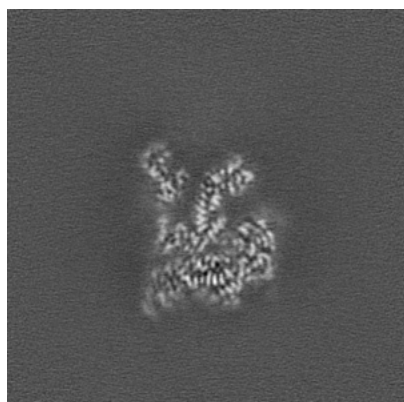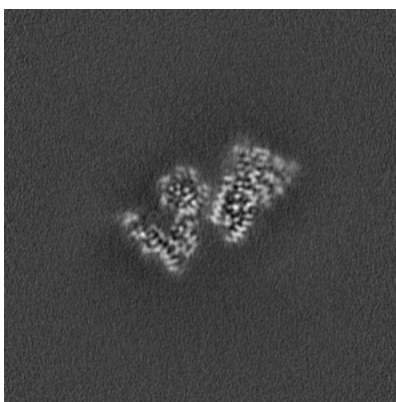
| X Index: 142 | Y Index: 195 | Z Index: 187 |
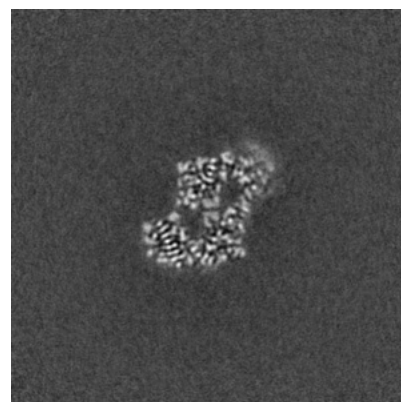
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map
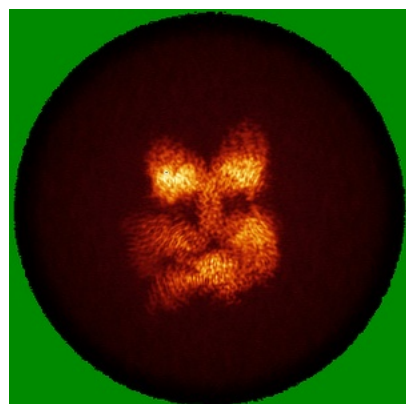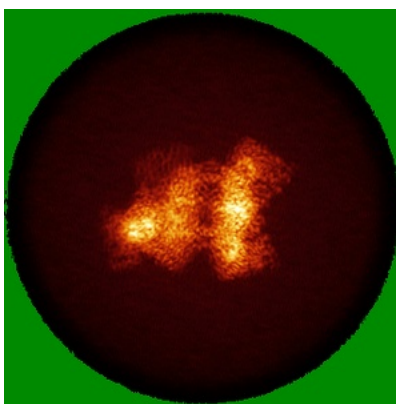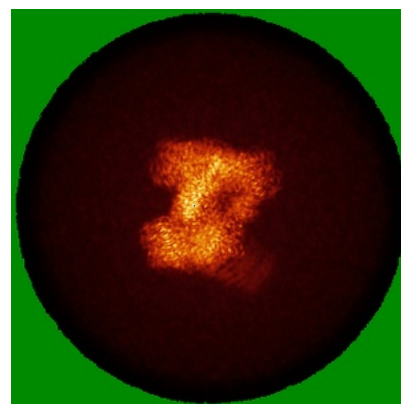
X   Y   Z

6.4.2 Raw map

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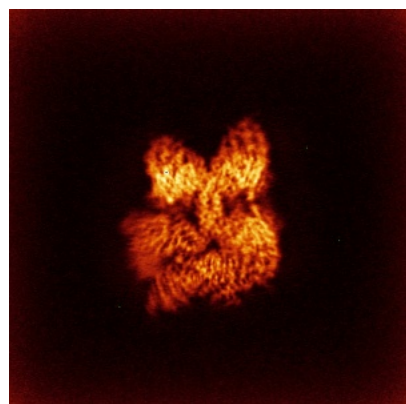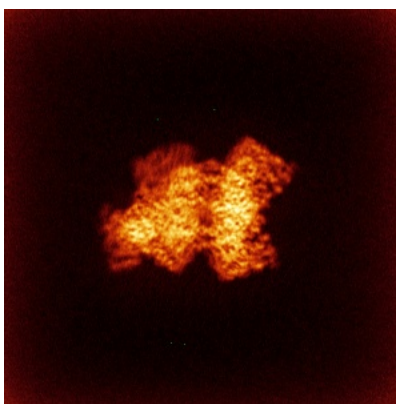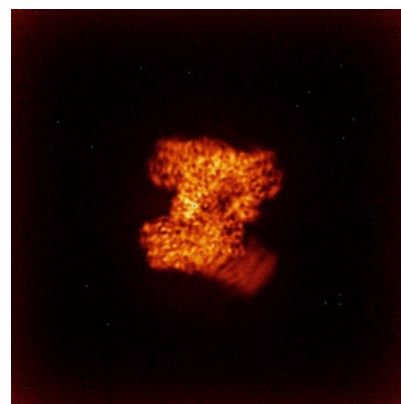
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X   Y   Z
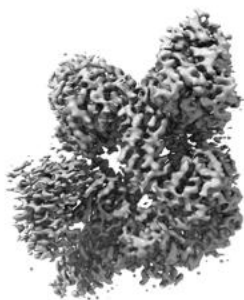
The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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_27022_msk_1.map ⓘ

X　　　　　　　　　　　　　　Y　　　　　　　　　　　　　　Z
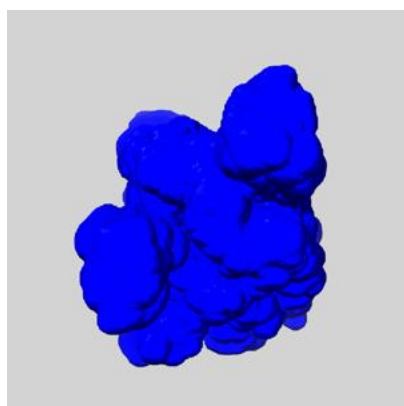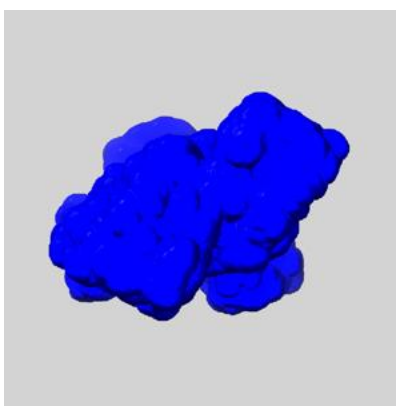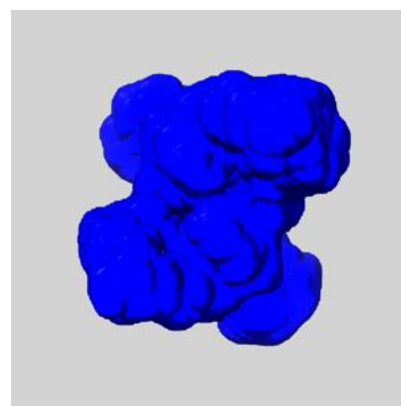
7 Map analysis ⓘ

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 ⓘ
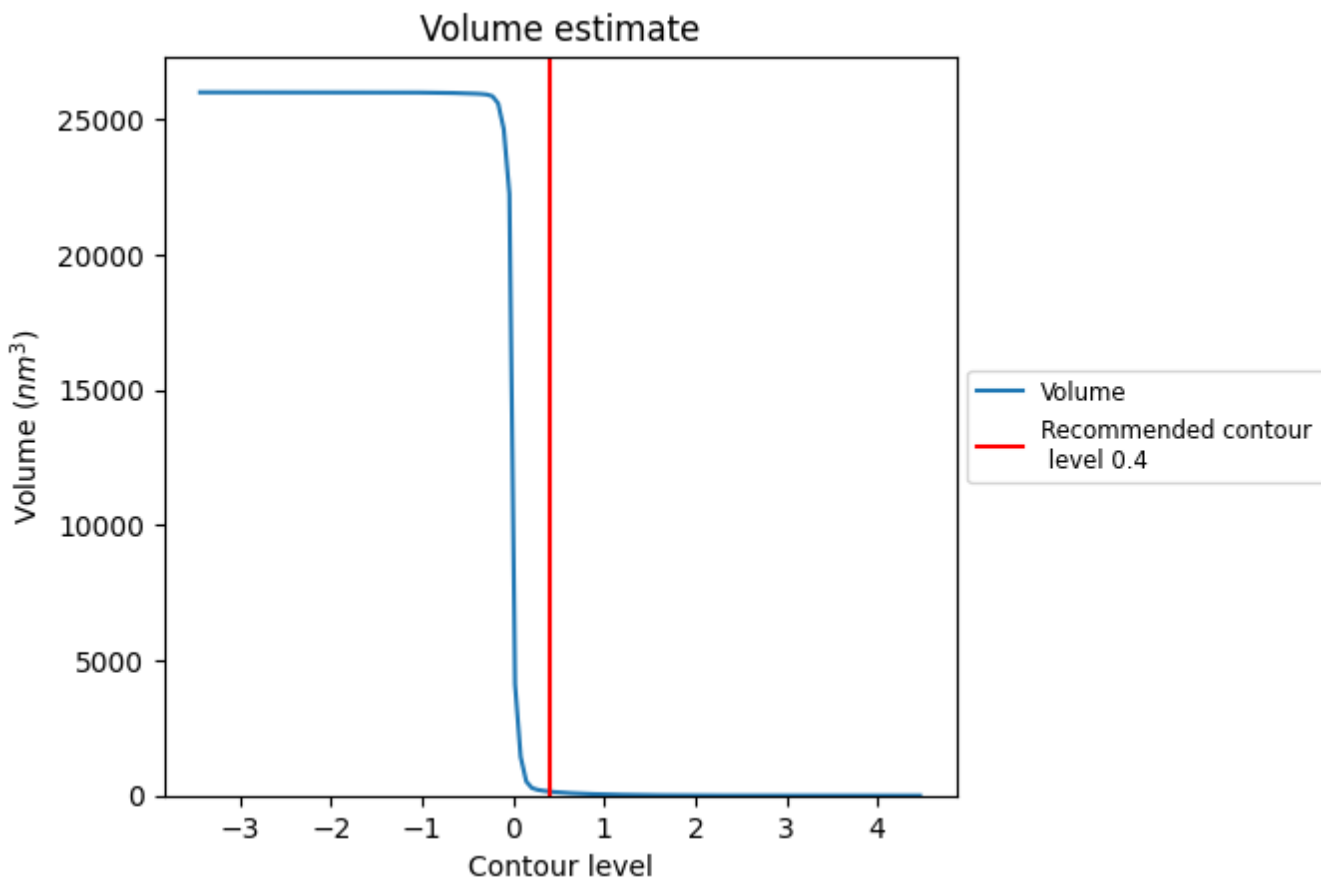
The volume at the recommended contour level is 149 nm^3; this corresponds to an approximate mass of 134 kDa.

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 ⓘ
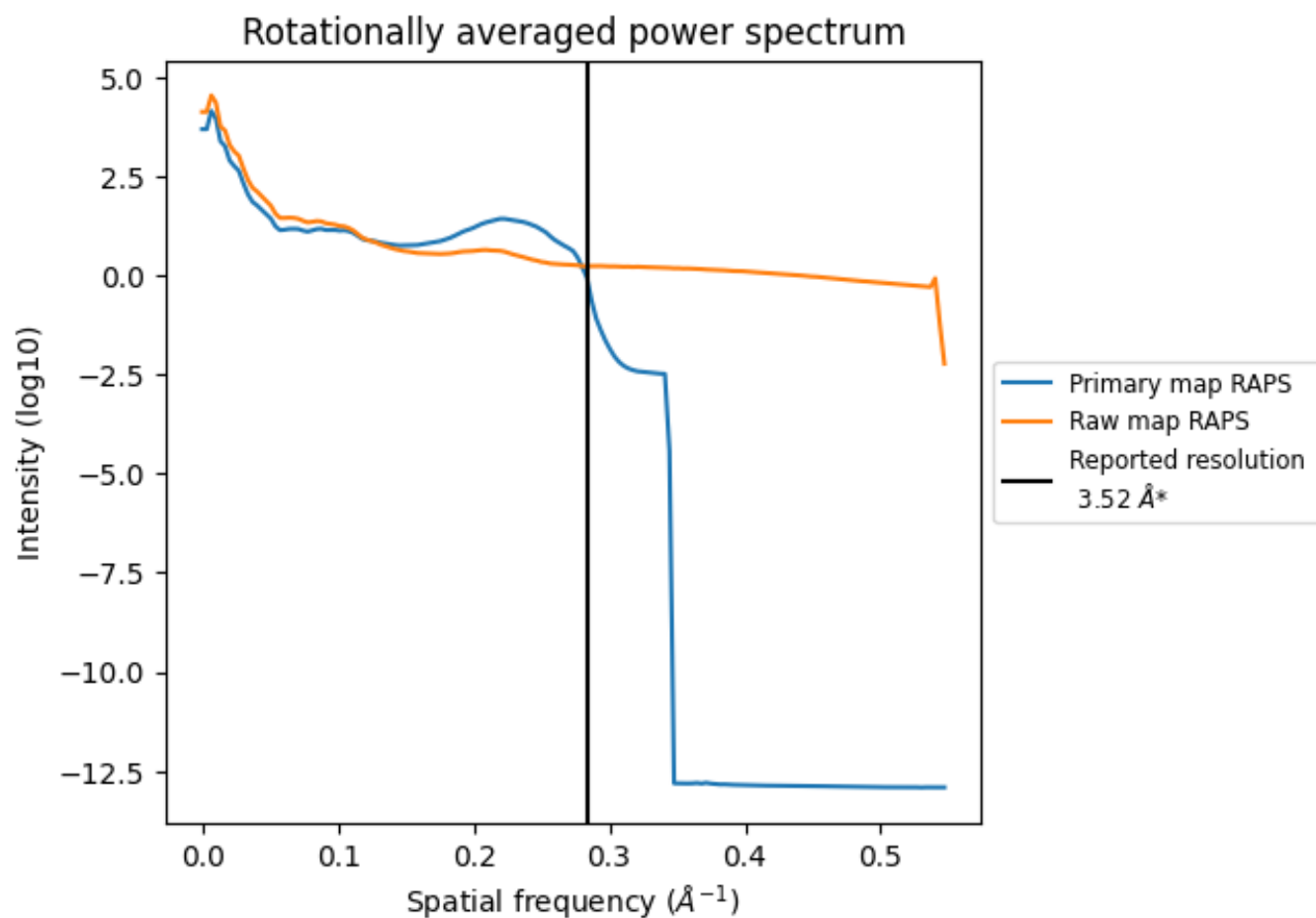
*Reported resolution corresponds to spatial frequency of 0.284 Å^{-1}

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 ⓘ
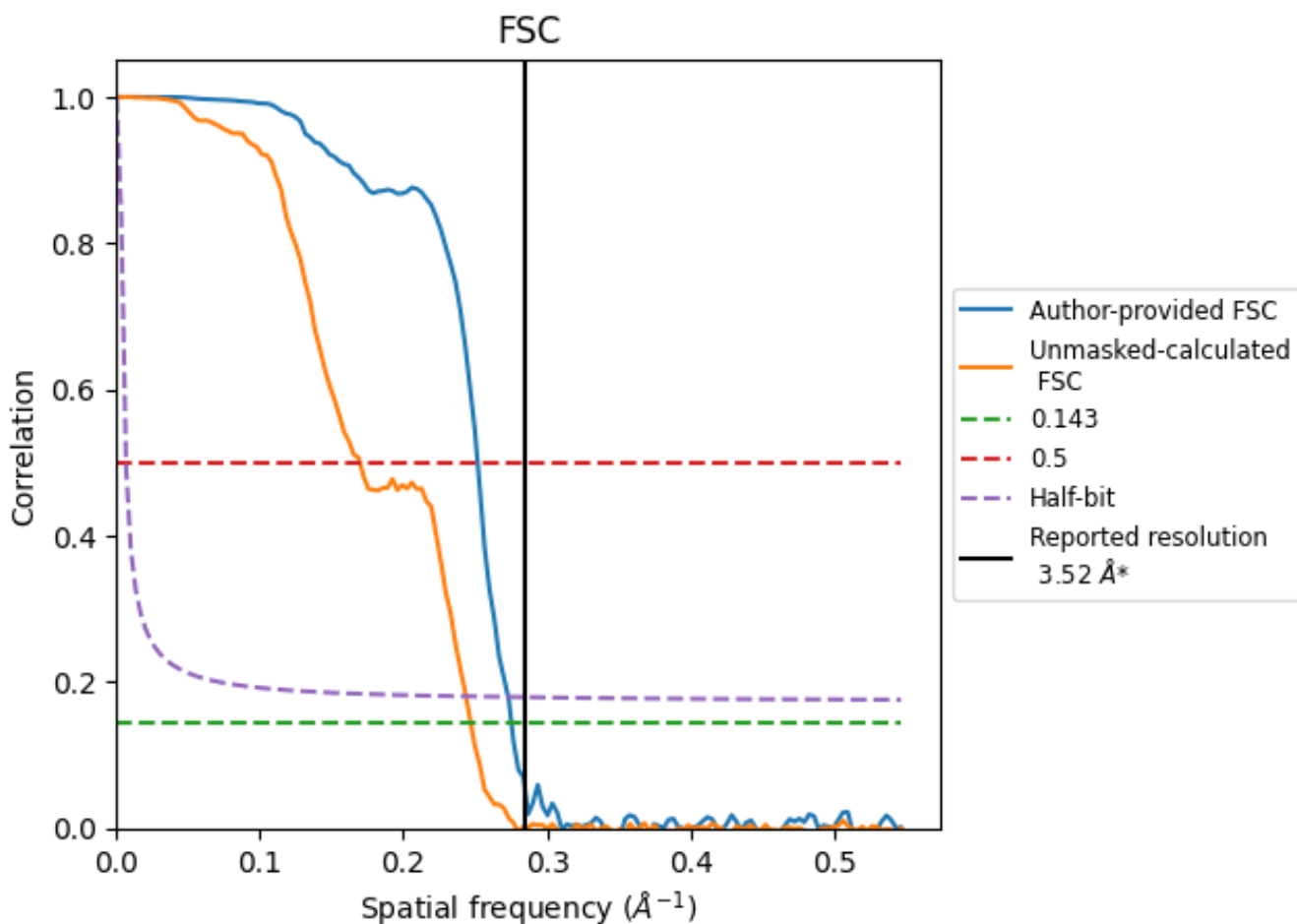
*Reported resolution corresponds to spatial frequency of 0.284 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.52	-	-
Author-provided FSC curve	3.63	3.97	3.66
Unmasked-calculated*	4.05	5.89	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 3.52 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-27022 and PDB model 8CVZ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay ⓘ

X   Y   Z
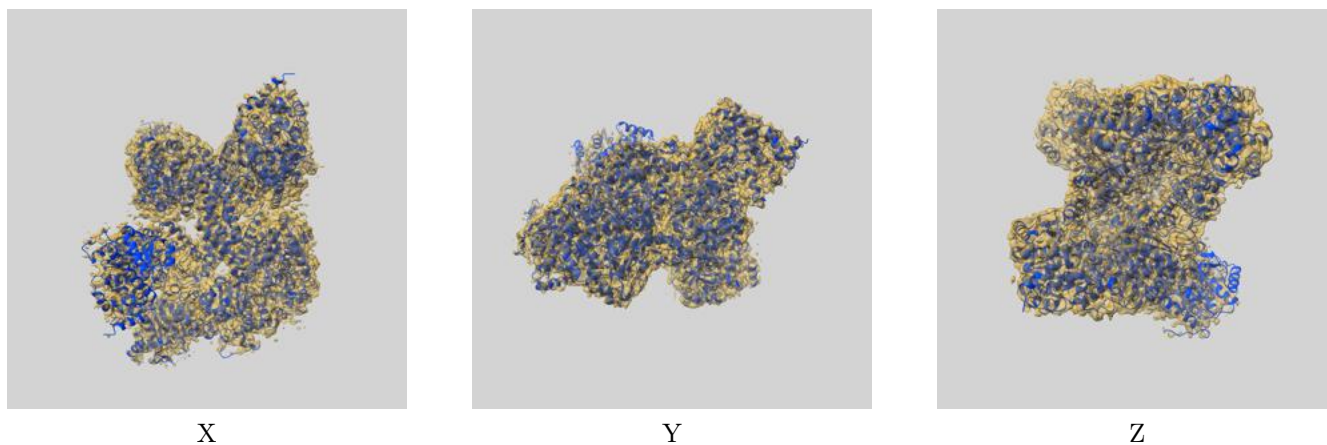
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

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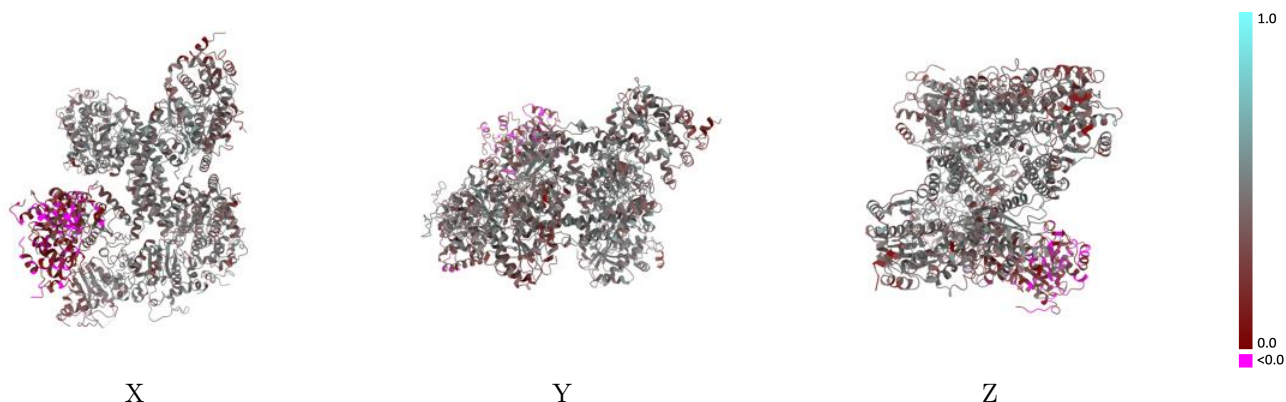
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
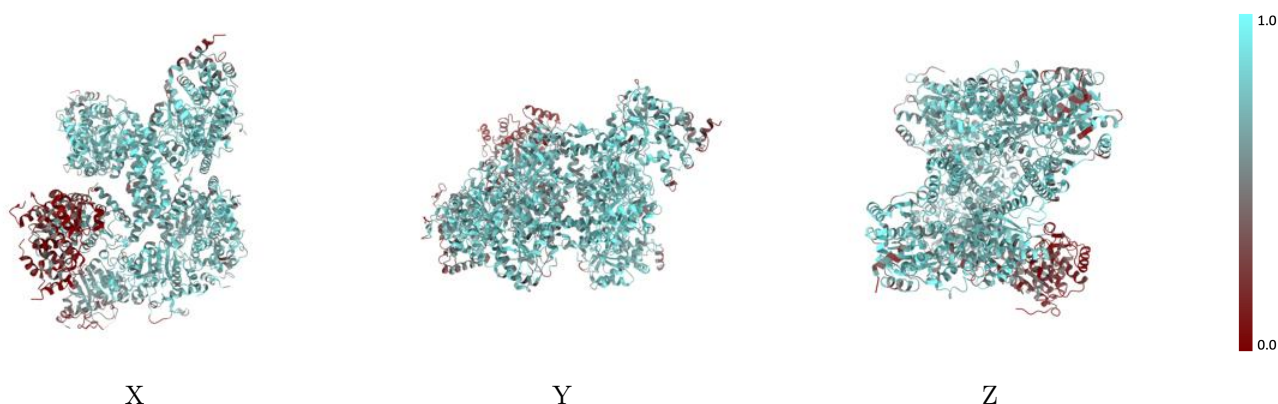
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4   Atom inclusion ⓘ
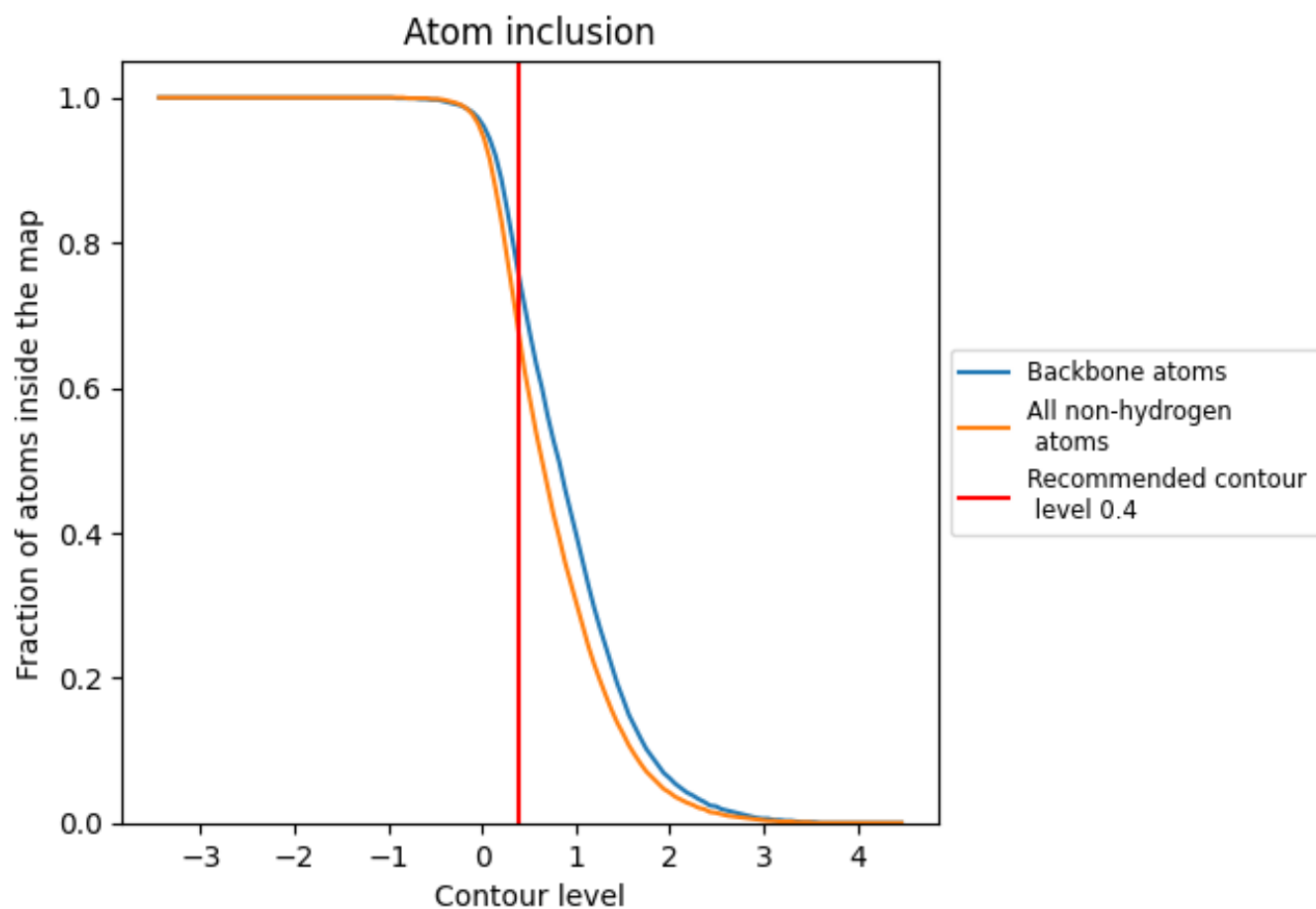
At the recommended contour level, 75% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6670	0.3830
A	0.7330	0.4090
B	0.4570	0.2430
C	0.7590	0.4390
D	0.7820	0.4470
E	0.6850	0.4090
F	0.1500	0.0810
G	0.4310	0.2730
H	0.5430	0.3190
I	0.7510	0.4560
J	0.5580	0.3550

1.0

0.0
<0.0