Full wwPDB EM Validation Report (i)

Sep 22, 2026 – 10:10 AM EDT

PDB ID	:	9DPI / pdb_00009dpi
EMDB ID	:	EMD-47105
Title	:	Cryo-EM structure of SerRS dimer in complex with two SIRT2
Authors	:	Yang, J.; Zhang, Q.; Zhang, H.; Lander, G.; Yang, X.
Deposited on	:	2024-09-21
Resolution	:	3.90 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.

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

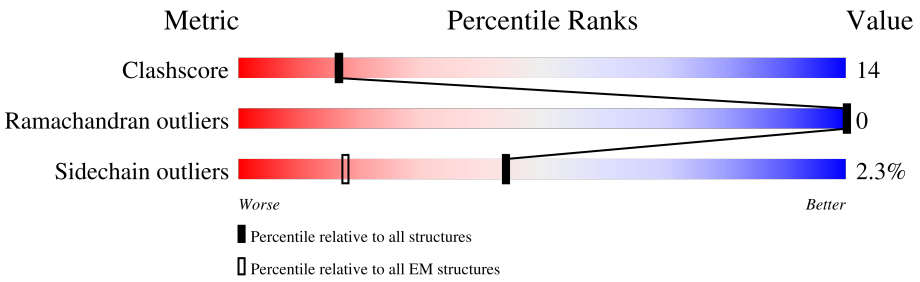
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

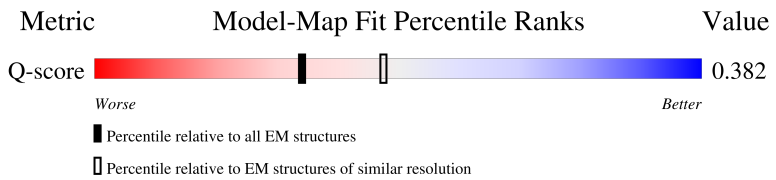
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	D	514	• 34% 15% 51%
1	F	514	• 35% 15% 49%
2	C	389	24% 32% 19% • 48%
2	E	389	31% 42% 20% • 38%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7651 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.

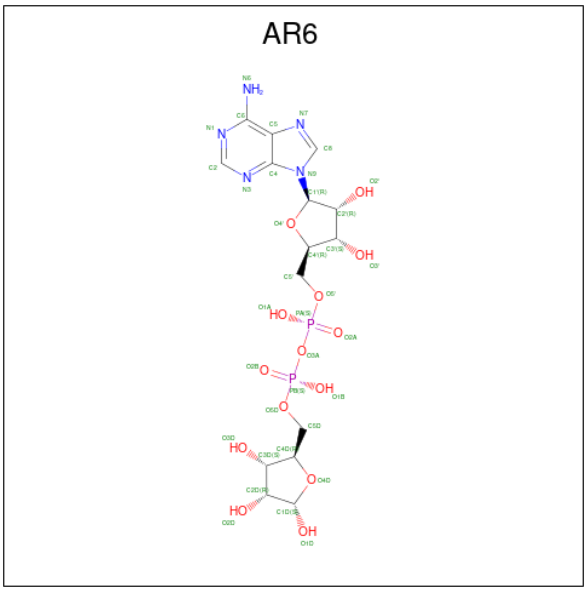
- Molecule 1 is a protein called Serine–tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	253	2030	1309	334	373	14	0	0
1	F	260	2079	1338	344	383	14	0	0

- Molecule 2 is a protein called NAD-dependent protein deacetylase sirtuin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	203	1573	1015	261	289	8	2	0
2	E	243	1897	1220	313	351	13	2	0

- Molecule 3 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL[HYDROXY-[[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (CCD ID: AR6) (formula: $C_{15}H_{23}N_5O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



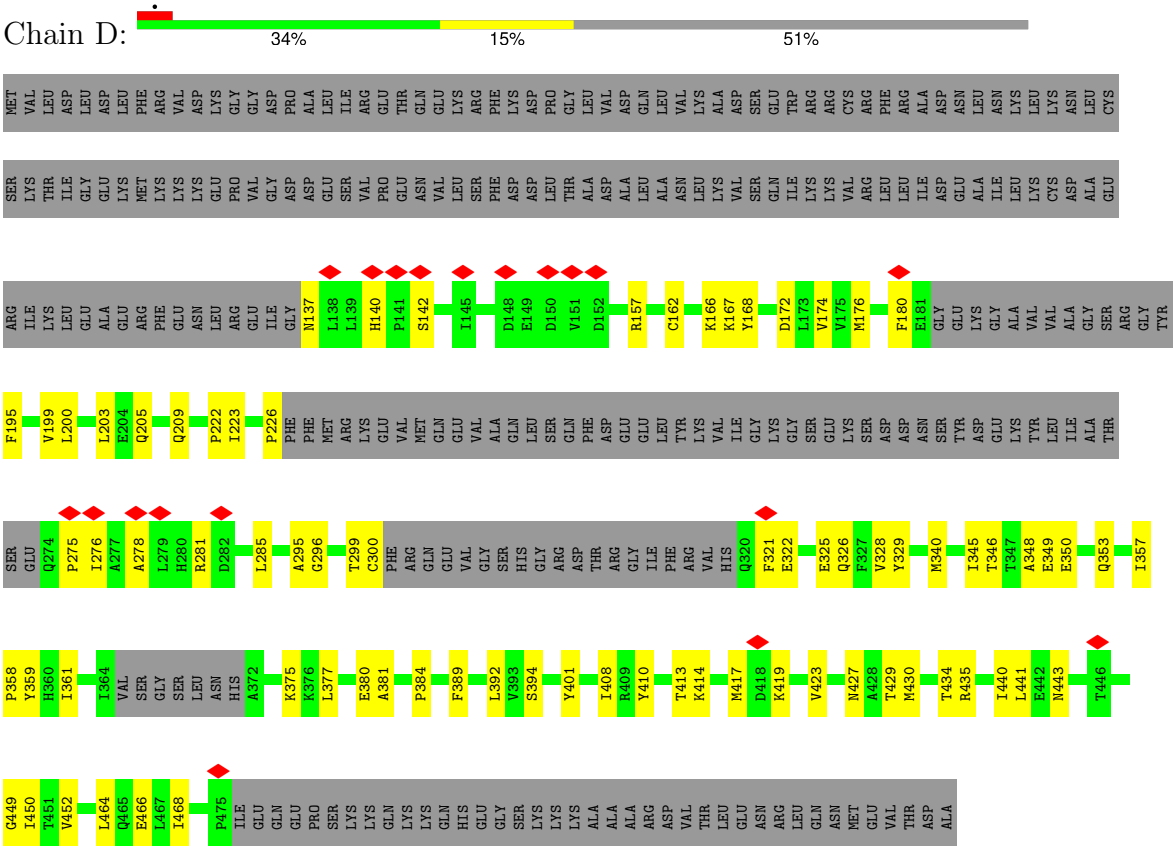
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	C	1	36	15	5	14	2	0
			Total	C	N	O	P	
3	E	1	36	15	5	14	2	0

3 Residue-property plots (i)

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.

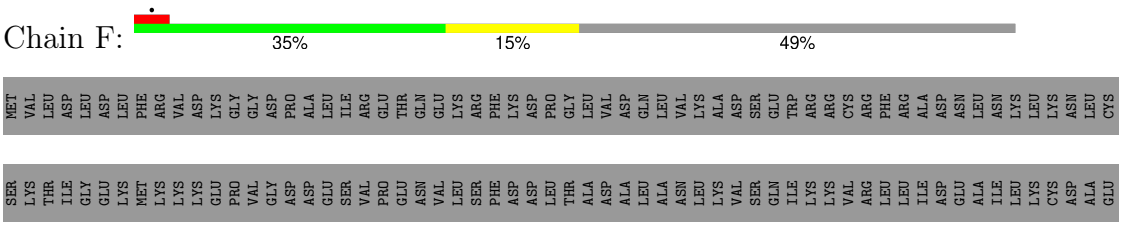
• Molecule 1: Serine–tRNA ligase, cytoplasmic

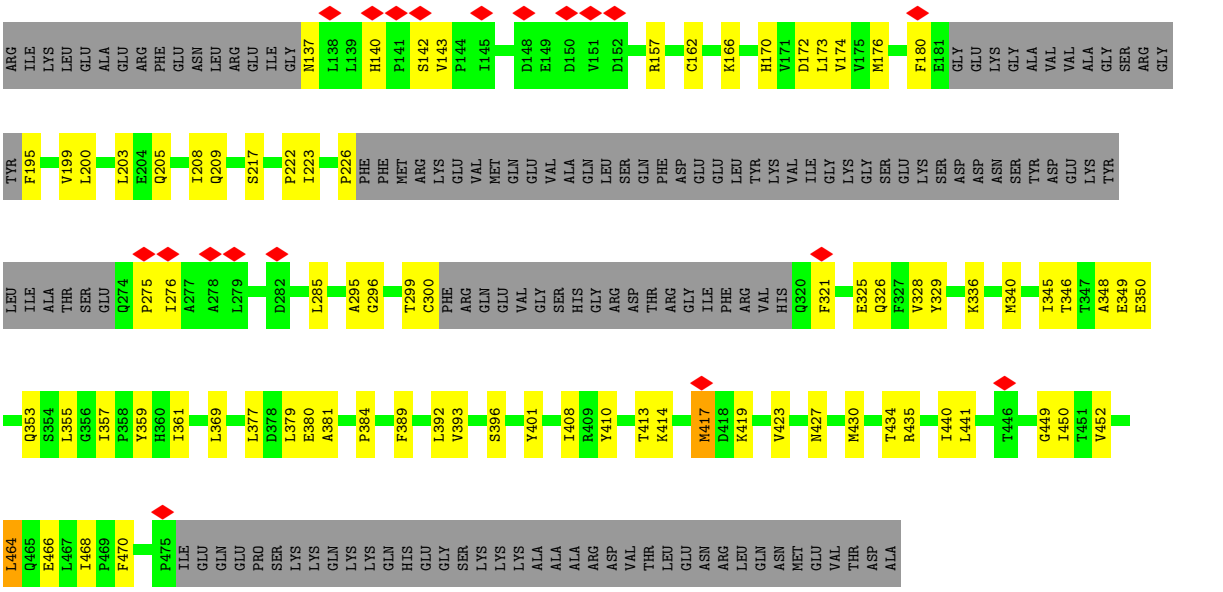
Chain D:



• Molecule 1: Serine–tRNA ligase, cytoplasmic

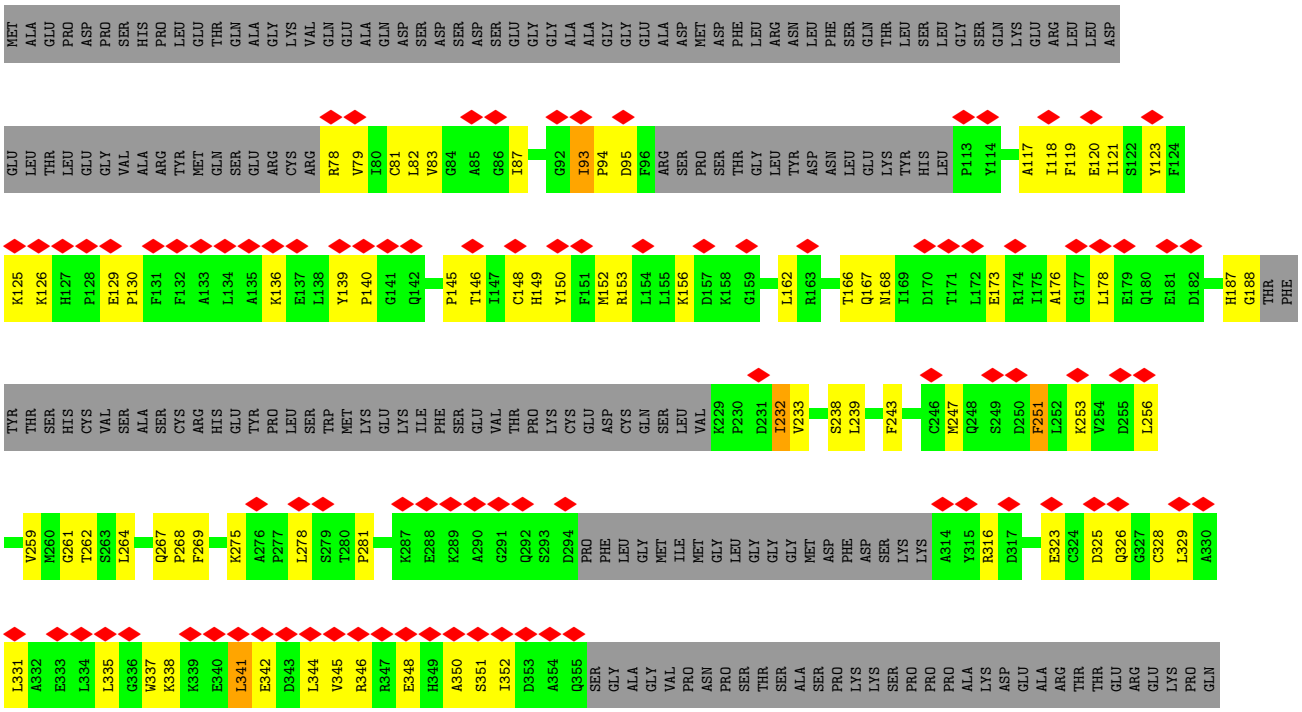
Chain F:





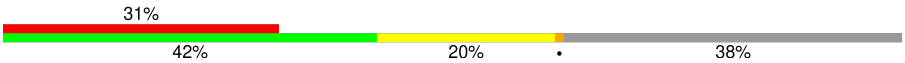
- Molecule 2: NAD-dependent protein deacetylase sirtuin-2

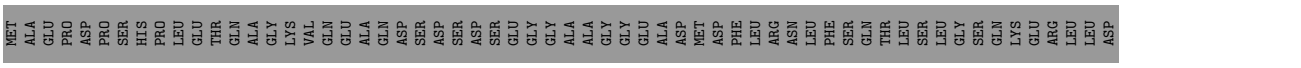
Chain C:

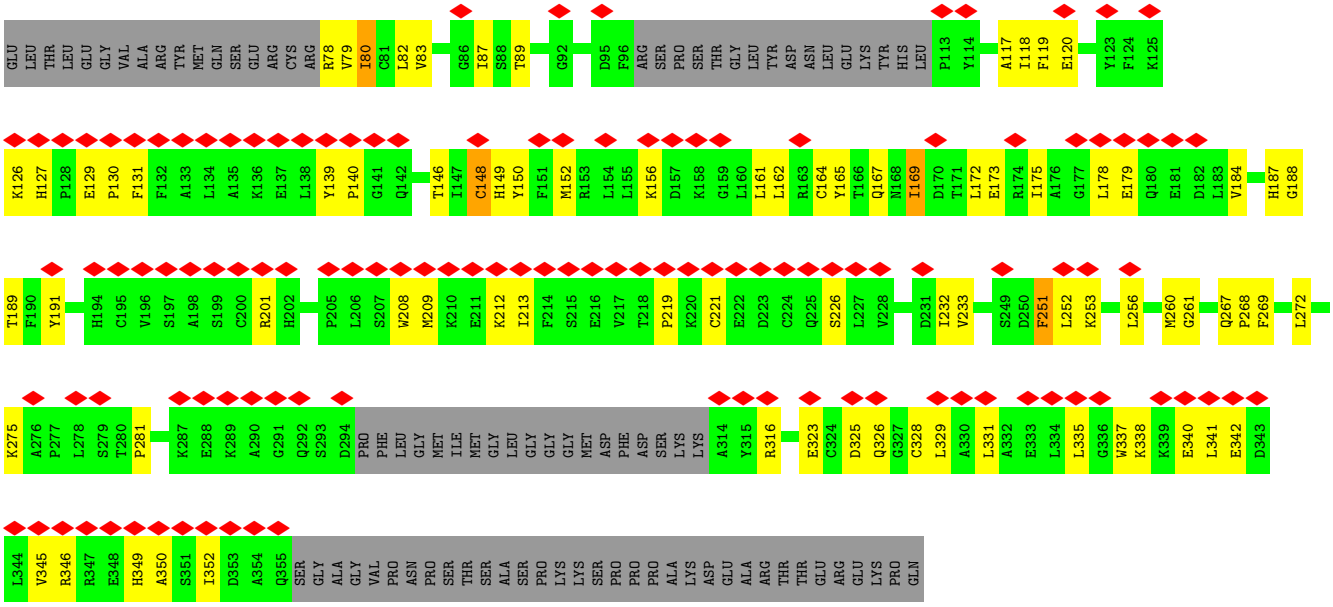


- Molecule 2: NAD-dependent protein deacetylase sirtuin-2

Chain E:






GLU LEU THR LEU GLU GLY VAL ALA ARG TYR MET GLN SER GLU ARG CYS ARG R78 V79 I80 C81 L82 V83 G86 I87 S88 T89 G92 D95 F96 ARG SER PRO SER THR GLY LEU TYR ASP ASN LEU GLU LYS TYR HIS LEU P113 Y114 A117 I118 F119 E120 Y123 F124 K125
K126 H127 P128 E129 P130 F131 F132 A133 L134 A135 K136 E137 L138 Y139 P140 G141 Q142 T146 I147 C148 H149 Y150 F151 M152 R153 L154 L155 K156 D157 K158 G159 L160 L161 L162 R163 C164 Y165 T166 Q167 N168 I169 D170 T171 L172 E173 R174 I175 A176 G177 L178 E179 Q180 E181 D182 L183 V184 H187 G188
T189 F190 Y191 H194 C195 V196 S197 A198 S199 C200 R201 H202 P205 L206 S207 W208 M209 K210 E211 K212 I213 F214 S215 E216 V217 T218 P219 K220 C221 E222 D223 C224 Q225 S226 L227 V228 D231 I232 V233 S249 D250 F251 L252 K253 L256 M260 G261 Q267 P268 F269 L272
K275 A276 P277 L278 S279 T280 P281 K287 E288 K289 A290 G291 Q292 S293 D294 PRO PHE LEU GLY MET ILE MET GLY LEU GLY GLY GLY MET ASP PHE ASP SER LYS LYS A314 Y315 R316 E323 C324 D325 Q326 G327 C328 L329 A330 L331 A332 E333 L334 L335 G336 W337 K338 K339 E340 L341 E342 D343
L344 V345 R346 R347 E348 H349 A350 S351 I352 D353 A354 Q355 SER GLY ALA GLY VAL PRO ASN PRO SER THR SER ALA SER PRO LYS LYS SER PRO PRO PRO ALA LYS ASP GLU ALA ARG THR THR GLU ARG GLU LYS PRO GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	523089	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	10.037	Depositor
Minimum map value	-7.745	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.134	Depositor
Recommended contour level	0.962	Depositor
Map size (Å)	294.4, 294.4, 294.4	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: AR6

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	D	0.15	0/2077	0.36	0/2812
1	F	0.14	0/2128	0.34	0/2883
2	C	0.17	0/1611	0.49	0/2176
2	E	0.16	0/1946	0.45	0/2632
All	All	0.15	0/7762	0.41	0/10503

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	D	2030	0	2011	52	0
1	F	2079	0	2058	52	0
2	C	1573	0	1550	60	0
2	E	1897	0	1858	58	0
3	C	36	0	21	0	0
3	E	36	0	21	2	0
All	All	7651	0	7519	214	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 14.

All (214) 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:E:188:GLY:HA3	2:E:232:ILE:HA	1.57	0.86
2:E:146:THR:HG22	2:E:148:CYS:H	1.43	0.82
2:E:267:GLN:HG3	2:E:268:PRO:HA	1.63	0.81
2:C:267:GLN:HG3	2:C:268:PRO:HA	1.63	0.79
2:C:146:THR:HG22	2:C:148:CYS:H	1.50	0.76
2:C:78:ARG:HE	2:C:253:LYS:HG3	1.54	0.71
1:D:357:ILE:HD11	1:D:440:ILE:HG12	1.73	0.71
2:C:79:VAL:HG22	2:C:256:LEU:HB3	1.73	0.70
2:E:209:MET:O	2:E:213:ILE:HG12	1.92	0.70
2:E:117:ALA:HA	2:E:120:GLU:HG3	1.74	0.70
2:C:118:ILE:HG22	2:C:119:PHE:HD1	1.58	0.69
2:E:79:VAL:HG22	2:E:256:LEU:HB3	1.75	0.68
2:C:188:GLY:HA3	2:C:232:ILE:HA	1.76	0.68
1:F:222:PRO:HA	1:F:295:ALA:HB3	1.75	0.68
1:D:222:PRO:HA	1:D:295:ALA:HB3	1.75	0.68
1:F:417:MET:HB2	1:F:419:LYS:HG2	1.76	0.67
2:E:323:GLU:HB2	2:E:326:GLN:HE22	1.59	0.67
1:D:140:HIS:HD2	1:D:142:SER:H	1.43	0.66
1:F:140:HIS:HD2	1:F:142:SER:H	1.41	0.66
2:C:251:PHE:HD1	2:C:275:LYS:HB3	1.61	0.65
2:E:78:ARG:HE	2:E:253:LYS:HG3	1.61	0.65
2:E:221:CYS:HB3	2:E:226:SER:H	1.60	0.65
2:C:251:PHE:CD1	2:C:275:LYS:HB3	2.33	0.63
2:C:344:LEU:HD12	2:C:348:GLU:OE1	1.97	0.63
2:C:173:GLU:HB2	2:C:178:LEU:HD12	1.80	0.63
1:F:226:PRO:HG3	1:F:275:PRO:HB2	1.80	0.63
1:D:328:VAL:HG11	1:D:340:MET:HG2	1.80	0.63
1:D:226:PRO:HG3	1:D:275:PRO:HB2	1.80	0.62
2:E:208:TRP:O	2:E:212:LYS:HG2	1.99	0.62
1:F:346:THR:O	1:F:350:GLU:HG2	2.00	0.61
1:D:166:LYS:HG3	1:D:384:PRO:HB2	1.82	0.61
1:F:325:GLU:HA	1:F:430:MET:H	1.65	0.61
1:D:346:THR:O	1:D:350:GLU:HG2	1.99	0.60
1:F:285:LEU:HD12	1:F:423:VAL:HG21	1.83	0.60
1:D:410:TYR:HB2	1:D:423:VAL:HG22	1.83	0.59
1:D:417:MET:HG3	1:D:419:LYS:HG2	1.83	0.59
1:D:285:LEU:HD12	1:D:423:VAL:HG21	1.83	0.59
2:E:80:ILE:HD13	2:E:251:PHE:HE2	1.67	0.59
2:E:189:THR:HG22	2:E:191:TYR:H	1.68	0.59
1:F:410:TYR:HB2	1:F:423:VAL:HG22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:VAL:HG12	1:D:180:PHE:HB2	1.85	0.59
1:D:414:LYS:HE2	2:C:187:HIS:HD2	1.68	0.59
2:C:117:ALA:HA	2:C:120:GLU:HG3	1.84	0.58
2:C:233:VAL:HG21	2:C:238:SER:O	2.03	0.58
2:C:341:LEU:HD13	2:C:344:LEU:HD23	1.84	0.58
2:E:156:LYS:HZ2	2:E:179:GLU:H	1.51	0.58
2:C:325:ASP:O	2:C:329:LEU:HG	2.04	0.58
1:D:413:THR:HG22	1:D:414:LYS:H	1.69	0.57
1:F:379:LEU:HD22	1:F:393:VAL:HG23	1.87	0.57
1:F:174:VAL:HG12	1:F:180:PHE:HB2	1.87	0.56
1:F:413:THR:HG22	1:F:414:LYS:H	1.70	0.56
2:E:172:LEU:HA	2:E:175:ILE:HG13	1.85	0.56
1:D:325:GLU:HA	1:D:430:MET:H	1.69	0.56
2:E:118:ILE:HG22	2:E:119:PHE:CD1	2.41	0.56
2:C:93:ILE:HD12	2:C:94:PRO:HD2	1.86	0.56
1:F:414:LYS:HD2	2:E:187:HIS:CD2	2.40	0.55
2:C:323:GLU:HB2	2:C:326:GLN:HE22	1.72	0.55
2:C:139:TYR:HD1	2:C:140:PRO:HD2	1.71	0.55
1:F:328:VAL:HG11	1:F:340:MET:HG2	1.87	0.55
1:D:199:VAL:HG13	1:D:464:LEU:HD21	1.89	0.55
2:E:126:LYS:HE3	2:E:127:HIS:HB2	1.88	0.55
2:E:139:TYR:HD1	2:E:140:PRO:HD2	1.71	0.55
1:F:166:LYS:HG3	1:F:384:PRO:HB2	1.89	0.54
1:D:157:ARG:HG2	1:D:361:ILE:HB	1.89	0.54
1:F:359:TYR:HA	1:F:381:ALA:HA	1.89	0.54
1:D:359:TYR:HA	1:D:381:ALA:HA	1.90	0.54
1:F:137:ASN:HD22	1:F:401:TYR:HB2	1.71	0.54
2:E:129:GLU:HG2	2:E:130:PRO:HD3	1.90	0.54
2:C:145:PRO:HD2	2:C:352:ILE:HD12	1.89	0.53
2:C:150:TYR:CE2	2:C:345:VAL:HA	2.42	0.53
2:C:331:LEU:O	2:C:335:LEU:HB3	2.08	0.53
1:F:226:PRO:HD2	1:F:276:ILE:HG12	1.91	0.53
1:F:329:TYR:HB3	1:F:423:VAL:HG11	1.89	0.53
1:D:226:PRO:HD2	1:D:276:ILE:HG12	1.91	0.53
1:F:348:ALA:HA	1:F:430:MET:HE1	1.91	0.53
1:F:157:ARG:HG2	1:F:361:ILE:HB	1.91	0.53
2:C:156:LYS:HD3	2:C:178:LEU:HD23	1.90	0.52
1:D:296:GLY:HA3	1:D:325:GLU:HG2	1.91	0.52
2:C:346:ARG:HH21	2:C:350:ALA:HB2	1.74	0.52
1:D:414:LYS:HE2	2:C:187:HIS:CD2	2.45	0.52
1:D:329:TYR:HB3	1:D:423:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:83:VAL:HG21	2:E:152:MET:HE2	1.92	0.51
1:D:137:ASN:HD22	1:D:401:TYR:HB2	1.74	0.51
2:E:173:GLU:HB3	2:E:178:LEU:HD12	1.93	0.51
2:E:325:ASP:O	2:E:329:LEU:HG	2.10	0.51
1:F:296:GLY:HA3	1:F:325:GLU:HG2	1.92	0.51
1:F:172:ASP:O	1:F:176:MET:HG3	2.11	0.51
2:C:278:LEU:HD12	2:C:278:LEU:H	1.76	0.50
2:C:123:TYR:HA	2:C:126:LYS:HE3	1.93	0.50
1:D:348:ALA:HA	1:D:430:MET:HE1	1.94	0.50
2:C:81:CYS:HB2	2:C:152:MET:HE1	1.93	0.50
2:C:338:LYS:HD2	2:C:338:LYS:O	2.12	0.49
1:D:392:LEU:HD23	1:D:435:ARG:HB3	1.95	0.49
2:C:129:GLU:H	2:C:129:GLU:CD	2.20	0.49
2:C:259:VAL:HG11	2:C:264:LEU:HD21	1.94	0.49
1:D:408:ILE:O	1:D:423:VAL:HG23	2.13	0.49
2:E:82:LEU:HD22	2:E:269:PHE:HE1	1.78	0.49
2:E:167:GLN:NE2	3:E:401:AR6:H5D	2.28	0.49
1:D:349:GLU:O	1:D:353:GLN:HG2	2.13	0.49
1:D:414:LYS:HA	2:C:268:PRO:HD3	1.95	0.49
2:E:165:TYR:HA	2:E:184:VAL:HG23	1.95	0.49
2:C:121:ILE:O	2:C:125:LYS:HG3	2.13	0.48
2:C:262:THR:HG23	2:C:264:LEU:HD22	1.94	0.48
1:F:408:ILE:O	1:F:423:VAL:HG23	2.12	0.48
2:E:150:TYR:CE2	2:E:345:VAL:HA	2.49	0.48
1:F:199:VAL:HG13	1:F:464:LEU:HD21	1.96	0.48
2:E:338:LYS:HD2	2:E:338:LYS:O	2.14	0.48
2:E:342:GLU:HA	2:E:345:VAL:HG12	1.96	0.48
2:E:131:PHE:CZ	2:E:232:ILE:HD11	2.49	0.48
1:D:172:ASP:O	1:D:176:MET:HG3	2.14	0.48
2:C:78:ARG:HG2	2:C:78:ARG:HH11	1.79	0.48
2:C:166:THR:HG22	2:C:168:ASN:H	1.78	0.48
1:F:349:GLU:O	1:F:353:GLN:HG2	2.14	0.47
1:D:299:THR:HG21	1:F:299:THR:HG21	1.96	0.47
2:E:87:ILE:HG22	2:E:261:GLY:HA3	1.96	0.47
1:D:167:LYS:HG2	1:D:168:TYR:CD1	2.50	0.47
1:F:414:LYS:HD2	2:E:187:HIS:HD2	1.78	0.47
2:C:238:SER:O	2:C:239:LEU:HD12	2.14	0.47
2:E:78:ARG:NE	2:E:253:LYS:HG3	2.29	0.47
2:E:349:HIS:HA	2:E:352:ILE:HG12	1.96	0.46
1:D:328:VAL:HG11	1:D:340:MET:CG	2.45	0.46
2:C:173:GLU:H	2:C:173:GLU:HG2	1.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:251:PHE:CD1	2:E:275:LYS:HB3	2.50	0.46
2:E:212:LYS:NZ	2:E:219:PRO:HA	2.31	0.46
2:E:346:ARG:HH21	2:E:350:ALA:HB2	1.81	0.46
1:F:200:LEU:HD21	1:F:441:LEU:HD11	1.98	0.46
1:D:380:GLU:HB3	1:D:389:PHE:HB3	1.96	0.46
1:D:441:LEU:HD22	1:D:450:ILE:HG12	1.97	0.46
1:F:143:VAL:HG11	1:F:369:LEU:HD11	1.97	0.46
2:C:78:ARG:HB2	2:C:162:LEU:HB2	1.97	0.46
2:C:153:ARG:HH21	2:C:176:ALA:HB1	1.80	0.46
1:F:336:LYS:HB2	1:F:336:LYS:HE3	1.76	0.46
1:D:195:PHE:CZ	1:F:226:PRO:HD3	2.51	0.45
2:C:331:LEU:O	2:C:335:LEU:CB	2.64	0.45
1:F:392:LEU:HD23	1:F:435:ARG:HB3	1.99	0.45
2:E:187:HIS:HA	2:E:233:VAL:HG22	1.98	0.45
2:C:87:ILE:HD11	2:C:149:HIS:CE1	2.52	0.45
2:C:136:LYS:HA	2:C:136:LYS:HD3	1.68	0.45
1:F:380:GLU:HB3	1:F:389:PHE:HB3	1.99	0.45
1:D:321:PHE:HD1	1:D:434:THR:HG21	1.82	0.45
2:E:83:VAL:HG22	2:E:260:MET:HB3	1.98	0.45
2:E:82:LEU:HB3	2:E:269:PHE:CZ	2.52	0.45
1:D:226:PRO:HD3	1:F:195:PHE:CZ	2.53	0.44
2:C:150:TYR:HE2	2:C:345:VAL:HA	1.81	0.44
1:F:449:GLY:HA3	1:F:468:ILE:O	2.17	0.44
2:E:345:VAL:HG22	2:E:349:HIS:HD2	1.83	0.44
1:F:450:ILE:N	1:F:450:ILE:HD12	2.32	0.44
2:E:78:ARG:HB2	2:E:162:LEU:HB2	2.00	0.44
1:F:321:PHE:HD1	1:F:434:THR:HG21	1.82	0.44
2:C:342:GLU:HA	2:C:345:VAL:HG12	1.98	0.44
1:D:345:ILE:HG12	1:D:377:LEU:HD23	1.98	0.44
1:D:394:SER:H	1:D:429:THR:HG22	1.82	0.44
1:D:450:ILE:N	1:D:450:ILE:HD12	2.33	0.44
1:D:358:PRO:HD2	1:D:443:ASN:ND2	2.33	0.43
2:E:150:TYR:HE2	2:E:345:VAL:HA	1.81	0.43
2:C:152:MET:HE3	2:C:152:MET:HB3	1.70	0.43
1:F:205:GLN:O	1:F:209:GLN:HG2	2.18	0.43
2:E:80:ILE:HD13	2:E:251:PHE:CE2	2.50	0.43
2:C:335:LEU:HG	2:C:337:TRP:CZ3	2.53	0.43
2:E:326:GLN:H	2:E:326:GLN:CD	2.27	0.43
2:C:82:LEU:HD22	2:C:269:PHE:CE2	2.53	0.43
2:C:167:GLN:HG2	2:C:187:HIS:CE1	2.53	0.43
1:F:357:ILE:HD11	1:F:440:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:ASN:HB2	1:D:401:TYR:HD1	1.84	0.43
2:E:169:ILE:HD13	2:E:169:ILE:H	1.83	0.43
1:D:464:LEU:HD23	1:D:464:LEU:O	2.18	0.43
1:F:345:ILE:HD12	1:F:345:ILE:HA	1.85	0.43
2:E:82:LEU:HB3	2:E:269:PHE:HZ	1.83	0.43
2:E:201:ARG:O	2:E:201:ARG:HG3	2.18	0.43
1:F:326:GLN:O	1:F:427:ASN:HA	2.18	0.43
2:C:153:ARG:HG3	2:C:156:LYS:HZ2	1.84	0.42
1:F:328:VAL:HG11	1:F:340:MET:CG	2.48	0.42
1:F:345:ILE:HG12	1:F:377:LEU:HD23	2.01	0.42
1:D:452:VAL:HG22	1:D:466:GLU:O	2.20	0.42
1:F:223:ILE:HD11	1:F:276:ILE:HD12	2.01	0.42
1:F:441:LEU:HD22	1:F:450:ILE:HG12	2.00	0.42
2:E:172:LEU:HD12	2:E:172:LEU:H	1.83	0.42
1:D:449:GLY:HA3	1:D:468:ILE:O	2.20	0.42
2:C:95:ASP:OD2	2:C:95:ASP:C	2.62	0.42
1:D:205:GLN:O	1:D:209:GLN:HG2	2.20	0.42
1:D:326:GLN:O	1:D:427:ASN:HA	2.19	0.42
2:C:247:MET:O	2:C:251:PHE:HB2	2.20	0.42
2:E:87:ILE:HD11	2:E:149:HIS:CE1	2.55	0.42
1:F:452:VAL:HG22	1:F:466:GLU:O	2.19	0.42
1:D:345:ILE:HD12	1:D:345:ILE:HA	1.85	0.42
2:C:129:GLU:N	2:C:130:PRO:HD2	2.33	0.42
2:E:131:PHE:HZ	2:E:232:ILE:HD11	1.84	0.42
1:D:223:ILE:HD11	1:D:276:ILE:HD12	2.01	0.42
1:F:137:ASN:ND2	1:F:401:TYR:HB2	2.34	0.42
1:D:375:LYS:HB2	1:D:375:LYS:HE3	1.73	0.41
2:C:87:ILE:HG22	2:C:261:GLY:HA3	2.01	0.41
2:E:335:LEU:HG	2:E:337:TRP:CE3	2.55	0.41
2:C:83:VAL:HG12	2:C:166:THR:HG23	2.03	0.41
2:C:328:CYS:HA	2:C:331:LEU:HG	2.03	0.41
2:C:281:PRO:HA	2:C:316:ARG:HB2	2.02	0.41
1:F:208:ILE:HD13	1:F:208:ILE:HA	1.93	0.41
1:F:355:LEU:HD12	1:F:355:LEU:HA	1.87	0.41
2:E:161:LEU:HD21	2:E:164:CYS:HB2	2.02	0.41
1:D:200:LEU:HD21	1:D:441:LEU:HD11	2.03	0.41
1:D:299:THR:HG22	1:D:322:GLU:HG3	2.03	0.41
2:C:326:GLN:H	2:C:326:GLN:CD	2.29	0.41
2:E:328:CYS:HA	2:E:331:LEU:HG	2.02	0.41
2:C:348:GLU:HA	2:C:351:SER:OG	2.21	0.41
1:F:170:HIS:HA	1:F:173:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:156:LYS:HD2	2:E:178:LEU:HD23	2.03	0.41
1:F:396:SER:HB2	1:F:427:ASN:OD1	2.21	0.40
1:D:278:ALA:HA	1:D:281:ARG:HG2	2.04	0.40
1:F:449:GLY:HA2	1:F:470:PHE:CZ	2.56	0.40
2:E:269:PHE:O	2:E:272:LEU:HB2	2.22	0.40
2:E:337:TRP:HD1	2:E:340[B]:GLU:OE1	2.04	0.40
2:C:87:ILE:HB	2:C:148:CYS:SG	2.61	0.40
2:E:89:THR:HG21	3:E:401:AR6:N6	2.37	0.40
2:C:239:LEU:HD23	2:C:243:PHE:CD2	2.57	0.40
2:E:281:PRO:HA	2:E:316:ARG:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	243/514 (47%)	229 (94%)	14 (6%)	0	100	100
1	F	252/514 (49%)	239 (95%)	13 (5%)	0	100	100
2	C	197/389 (51%)	183 (93%)	14 (7%)	0	100	100
2	E	239/389 (61%)	219 (92%)	20 (8%)	0	100	100
All	All	931/1806 (52%)	870 (93%)	61 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	223/453 (49%)	220 (99%)	3 (1%)	61	71
1	F	229/453 (51%)	223 (97%)	6 (3%)	40	60
2	C	165/332 (50%)	161 (98%)	4 (2%)	43	63
2	E	204/332 (61%)	198 (97%)	6 (3%)	37	58
All	All	821/1570 (52%)	802 (98%)	19 (2%)	44	63

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	162	CYS
1	D	203	LEU
1	D	300	CYS
2	C	93	ILE
2	C	232	ILE
2	C	251	PHE
2	C	341	LEU
1	F	162	CYS
1	F	203	LEU
1	F	217	SER
1	F	300	CYS
1	F	417	MET
1	F	464	LEU
2	E	80	ILE
2	E	148	CYS
2	E	169	ILE
2	E	251	PHE
2	E	252	LEU
2	E	341	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	137	ASN
2	C	187	HIS
2	C	326	GLN
1	F	443	ASN
2	E	326	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
3	AR6	C	401	-	39,39,39	1.29	2 (5%)	56,60,60	0.72	0
3	AR6	E	401	-	39,39,39	1.31	2 (5%)	56,60,60	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AR6	C	401	-	-	2/22/54/54	0/4/4/4
3	AR6	E	401	-	-	0/22/54/54	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	AR6	PB-O3A	4.94	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	AR6	PB-O3A	4.87	1.64	1.59
3	E	401	AR6	PA-O3A	4.72	1.64	1.59
3	C	401	AR6	PA-O3A	4.57	1.64	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	401	AR6	C5'-O5'-PA-O2A
3	C	401	AR6	PB-O3A-PA-O1A

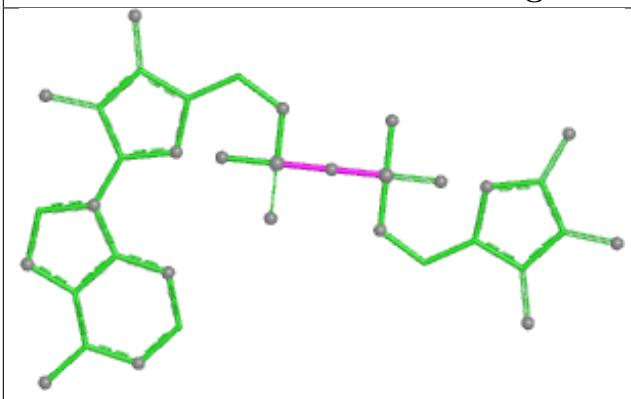
There are no ring outliers.

1 monomer is involved in 2 short contacts:

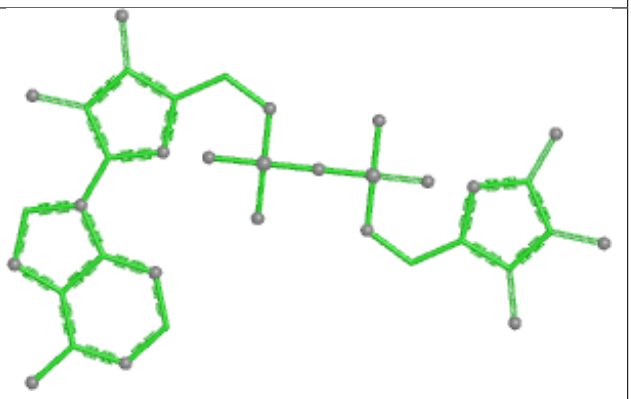
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	401	AR6	2	0

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.

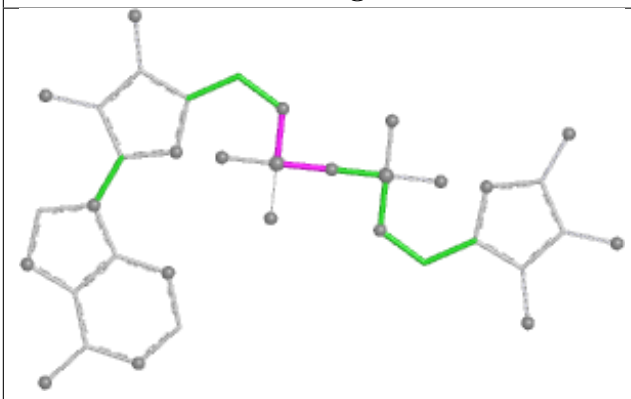
Ligand AR6 C 401



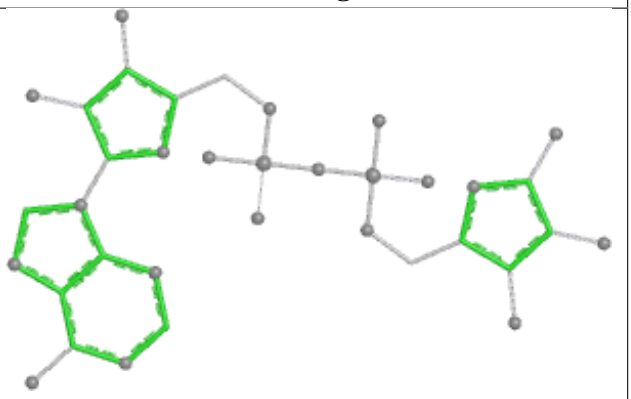
Bond lengths



Bond angles

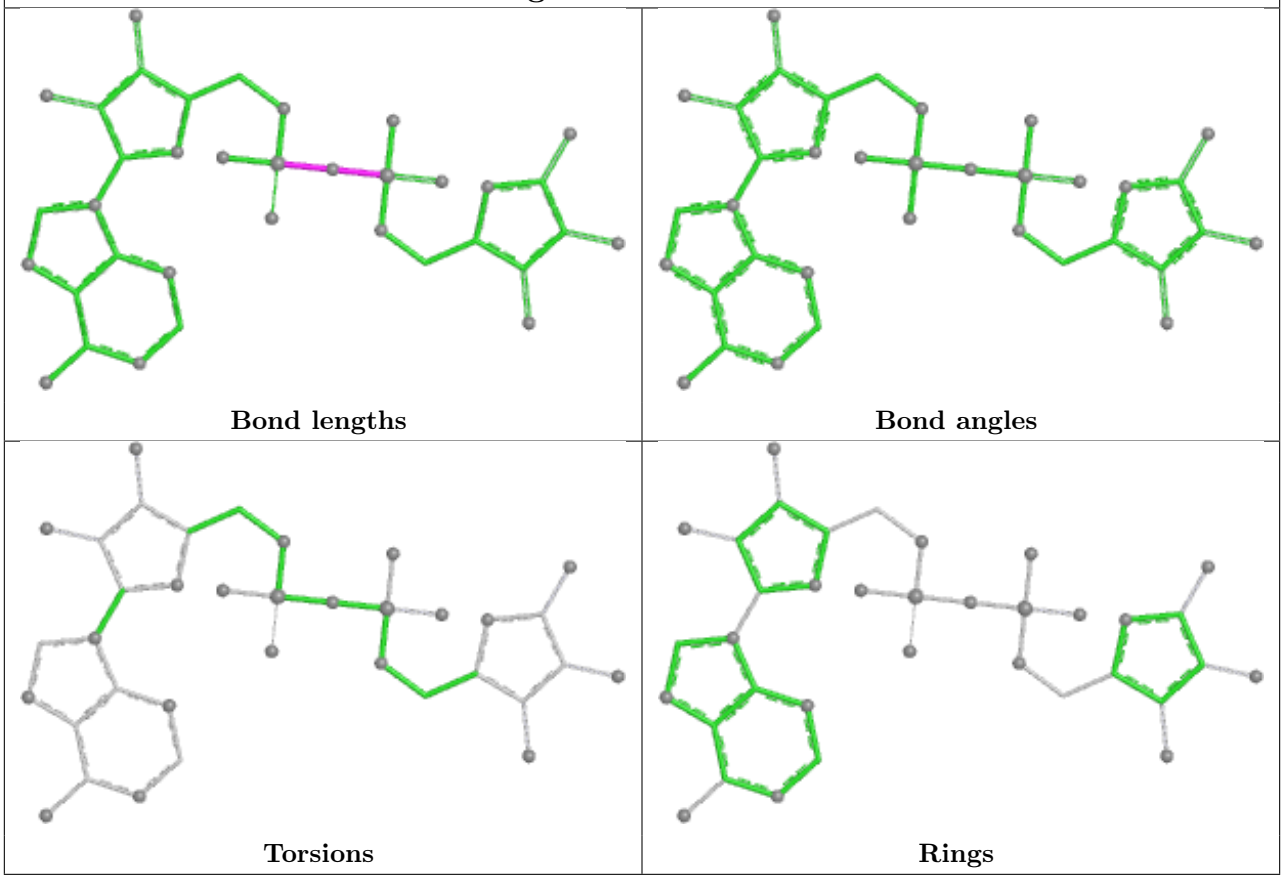


Torsions



Rings

Ligand AR6 E 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

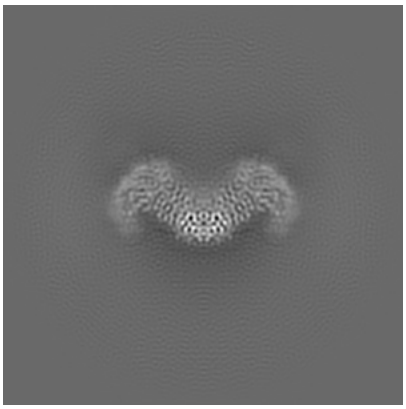
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-47105. These allow visual inspection of the internal detail of the map and identification of artifacts.

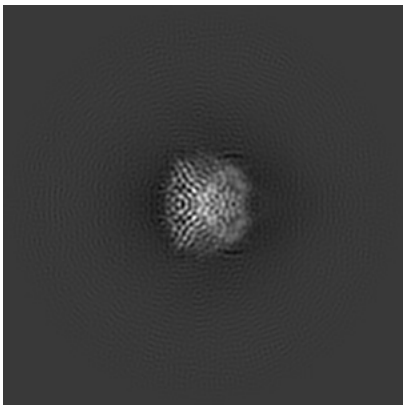
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

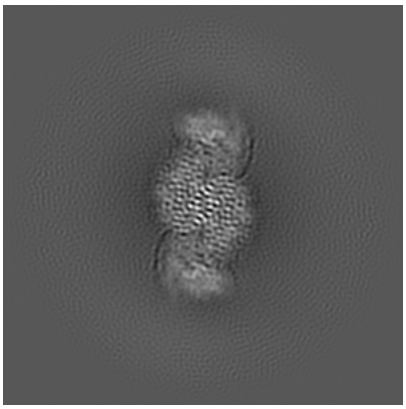
6.1.1 Primary map



X

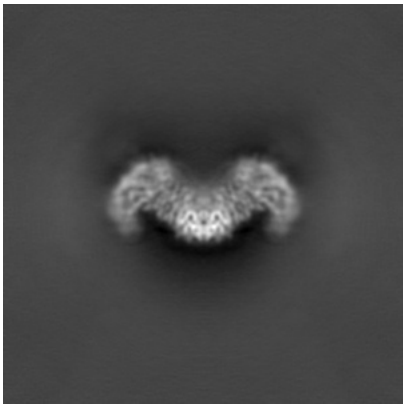


Y

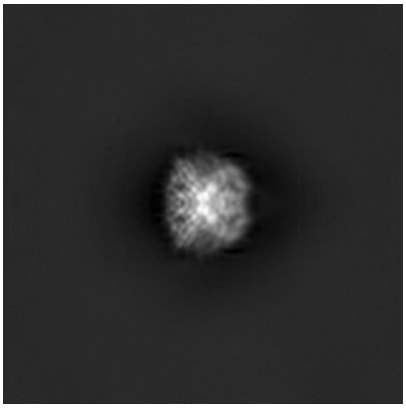


Z

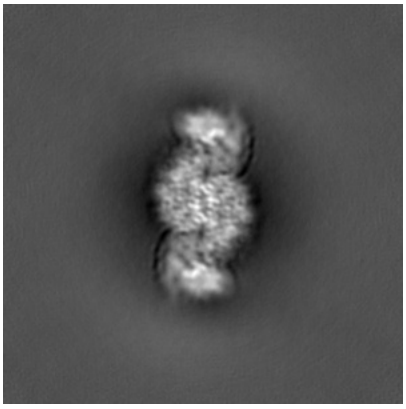
6.1.2 Raw map



X



Y

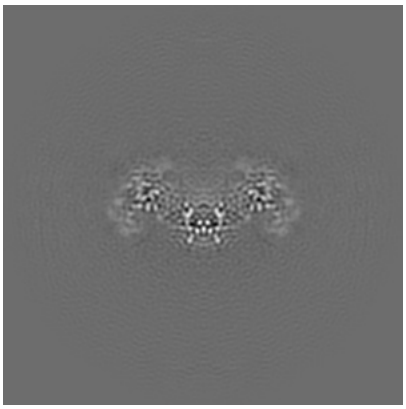


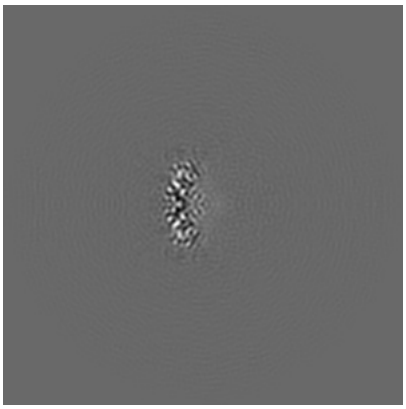
Z

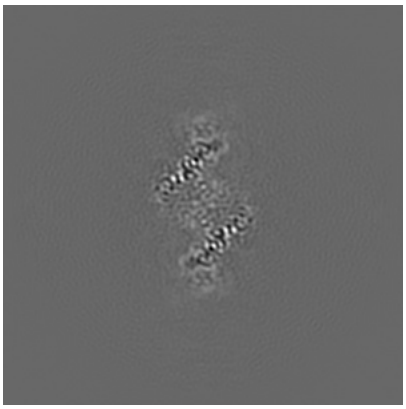
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

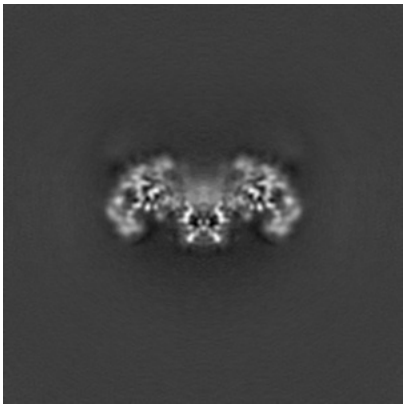
6.2.1 Primary map

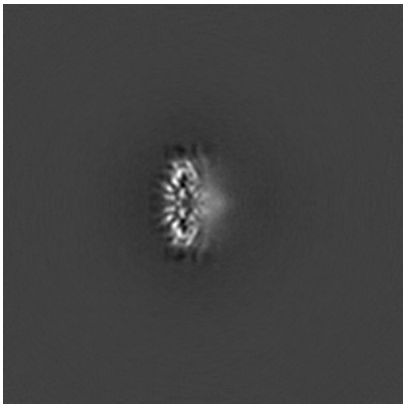

X Index: 128

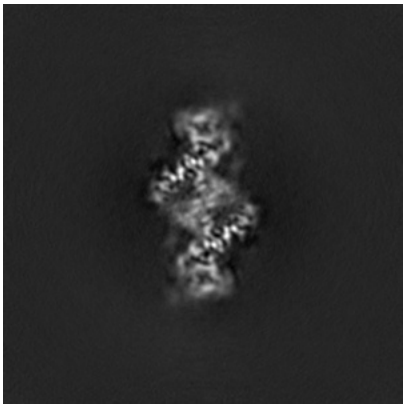

Y Index: 128


Z Index: 128

6.2.2 Raw map


X Index: 128

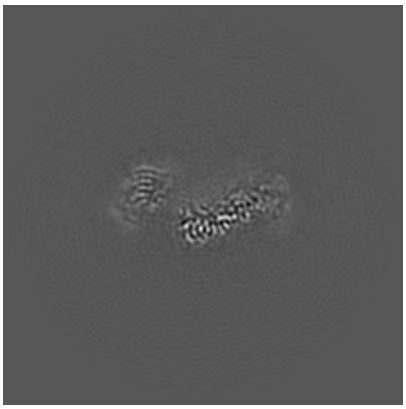

Y Index: 128


Z Index: 128

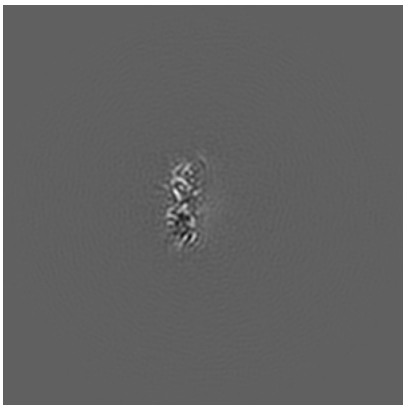
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

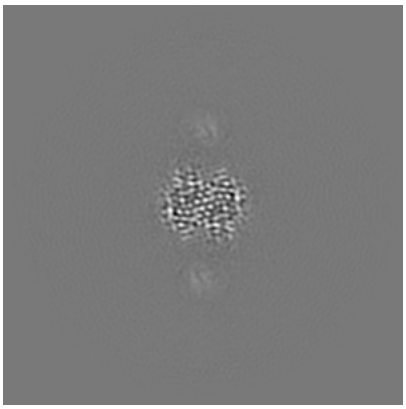
6.3.1 Primary map



X Index: 123

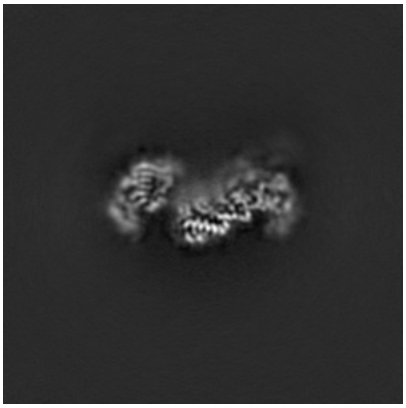


Y Index: 125

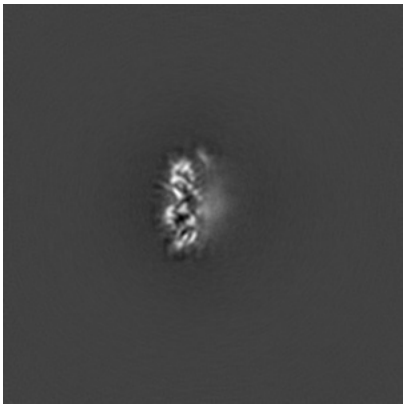


Z Index: 116

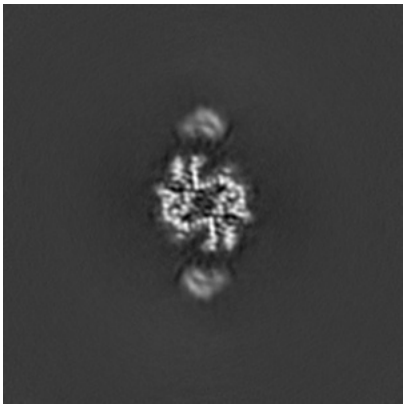
6.3.2 Raw map



X Index: 123



Y Index: 125

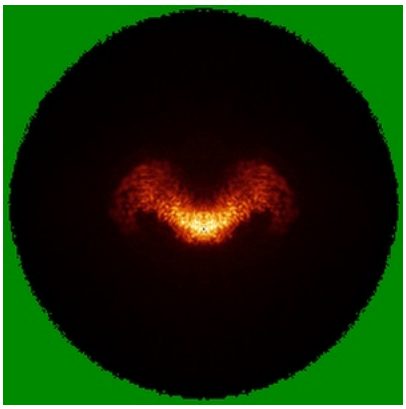


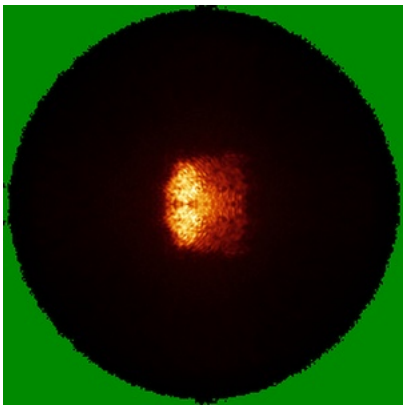
Z Index: 119

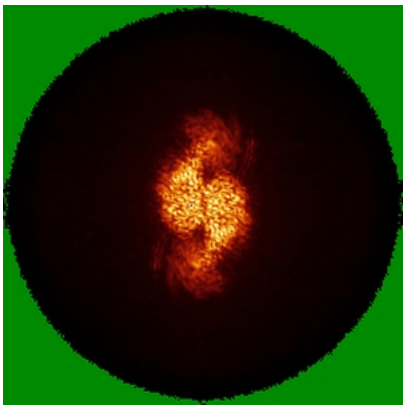
The images above show the largest variance slices of the map in three orthogonal directions.

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

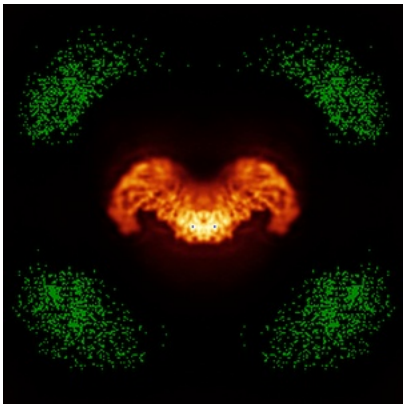
6.4.1 Primary map

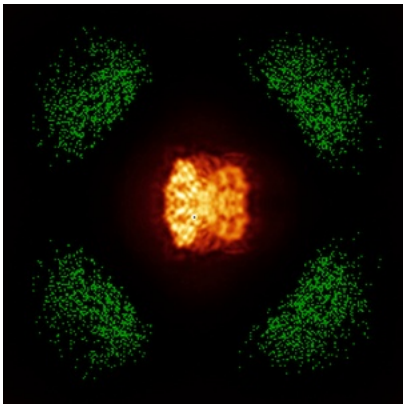

X

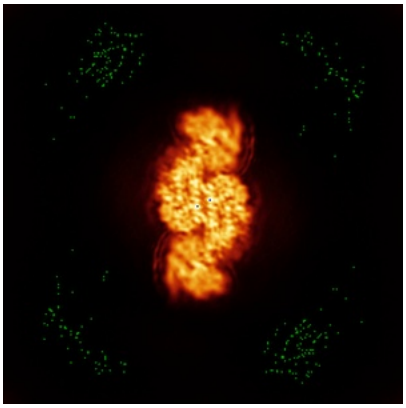

Y


Z

6.4.2 Raw map


X


Y


Z

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

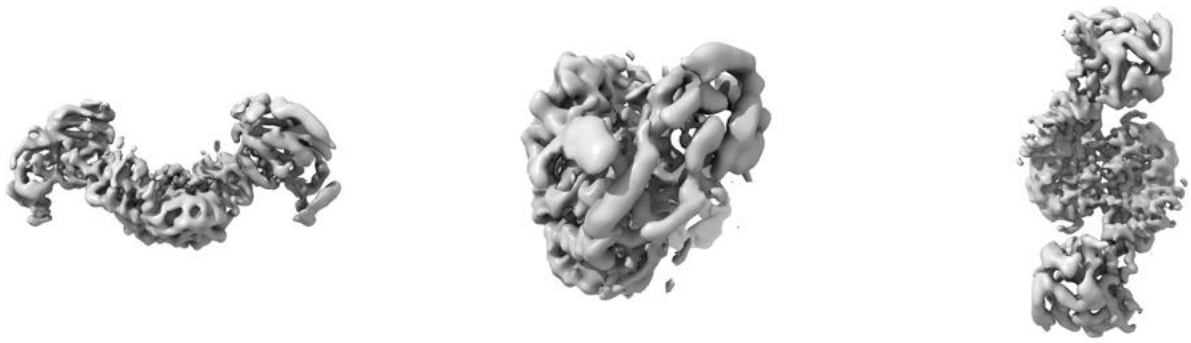
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.962. 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.

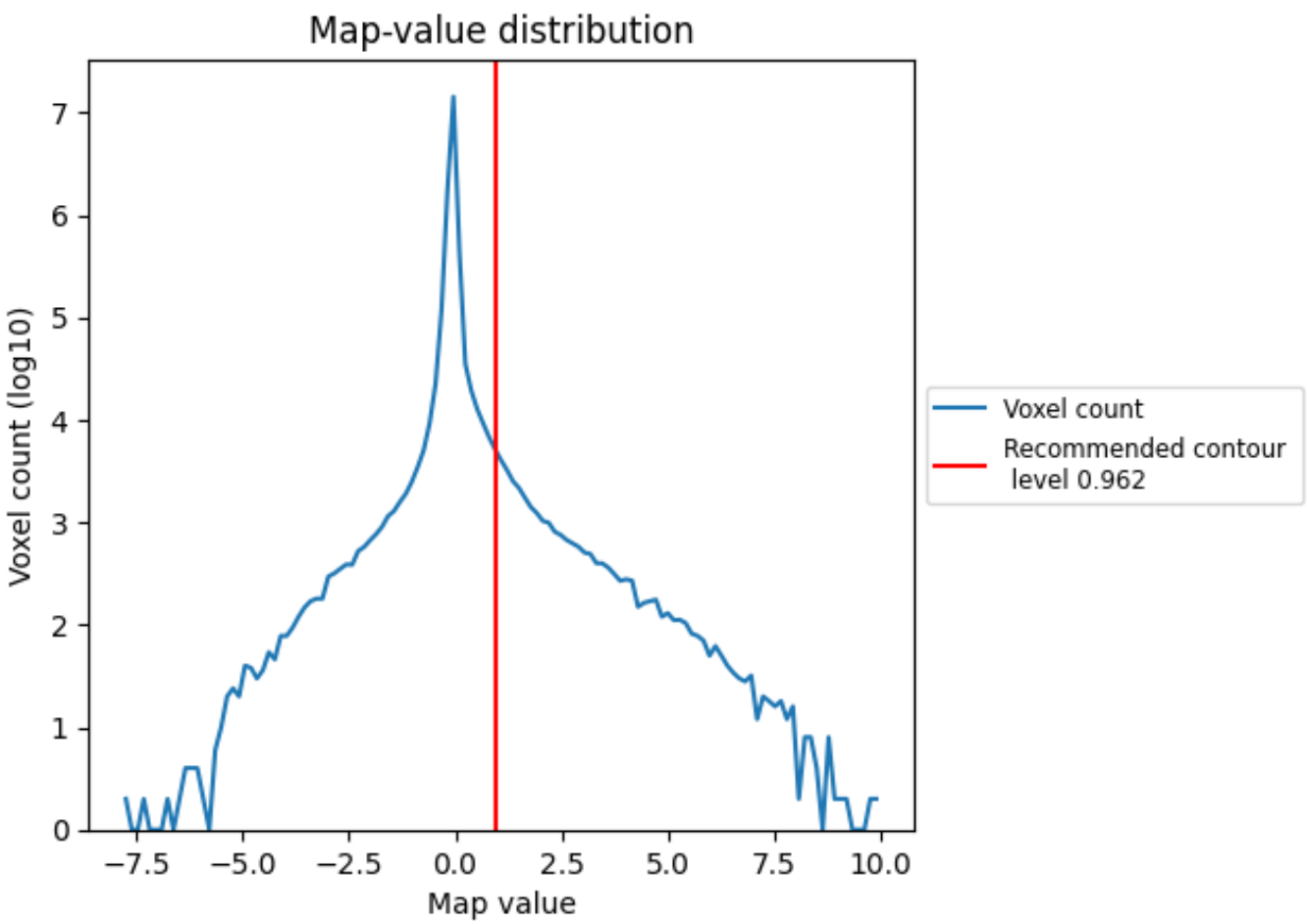
6.6 Mask visualisation (i)

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

7 Map analysis (i)

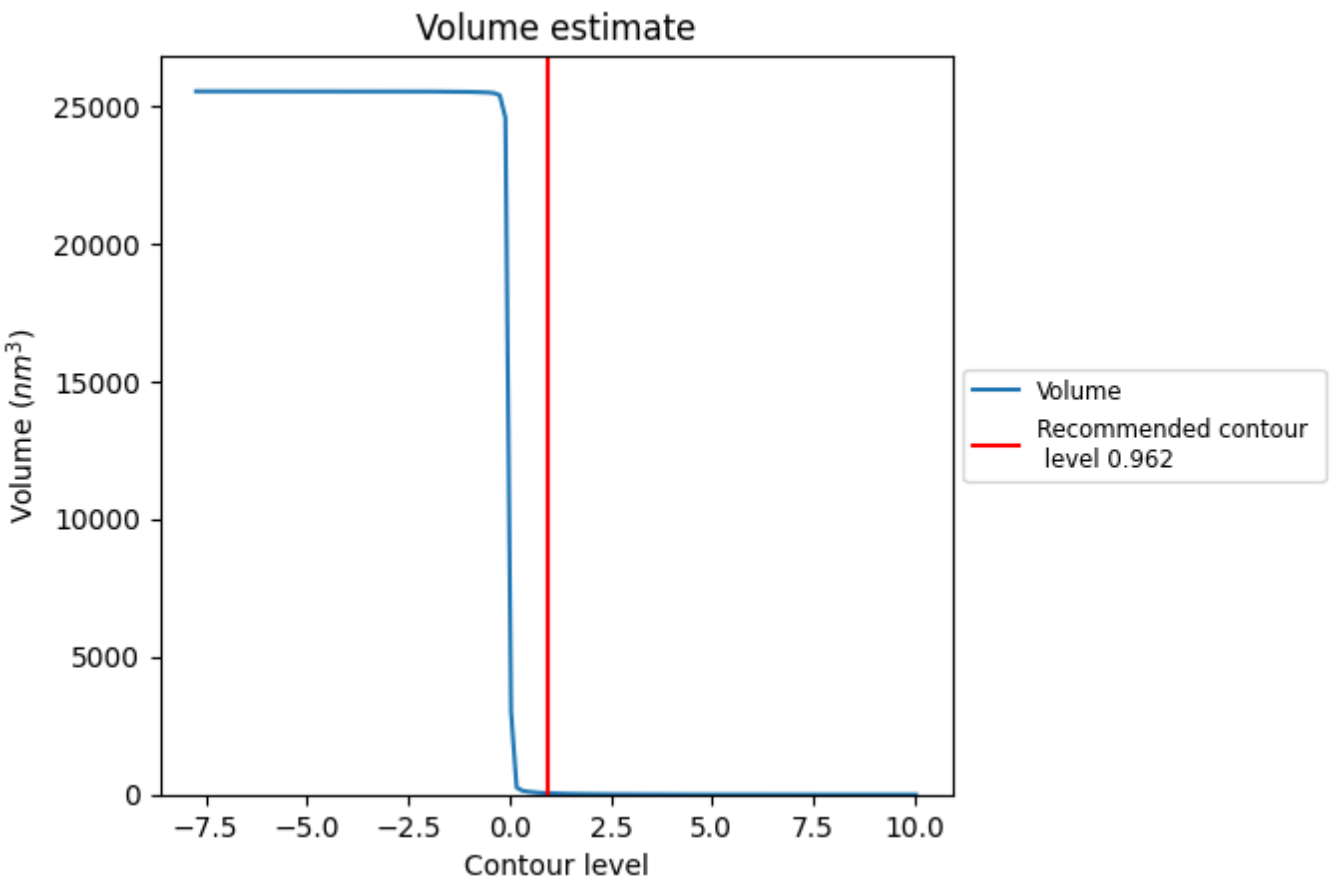
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

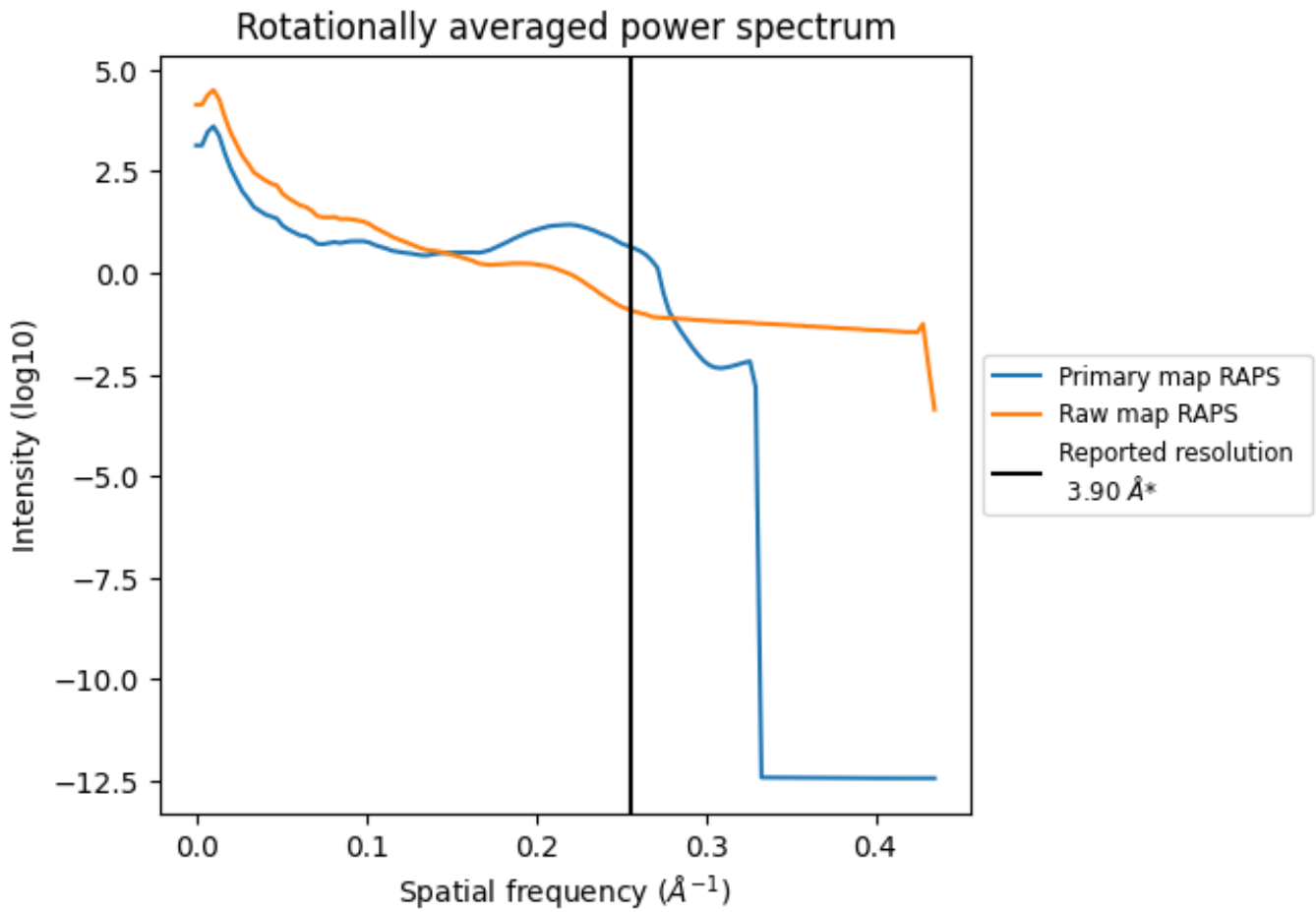
7.2 Volume estimate (i)



The volume at the recommended contour level is 48 nm^3; this corresponds to an approximate mass of 43 kDa.

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

7.3 Rotationally averaged power spectrum (i)

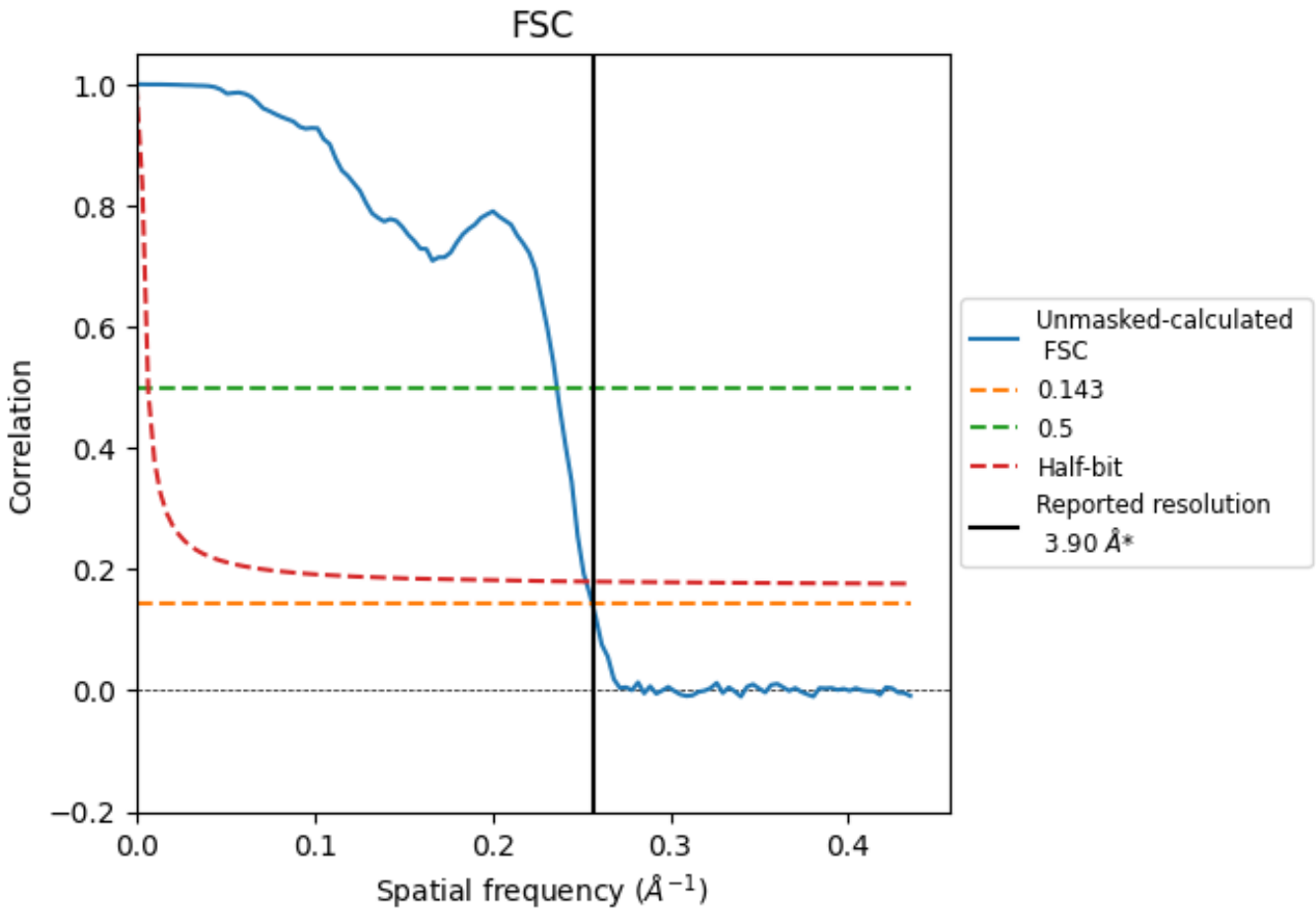


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

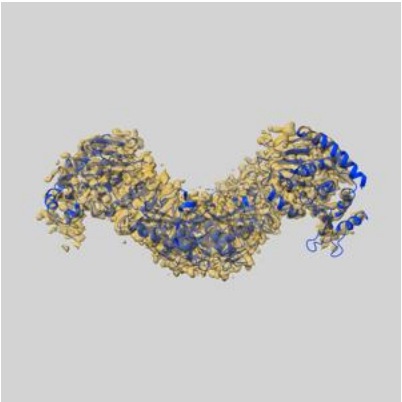
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.90	4.23	3.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

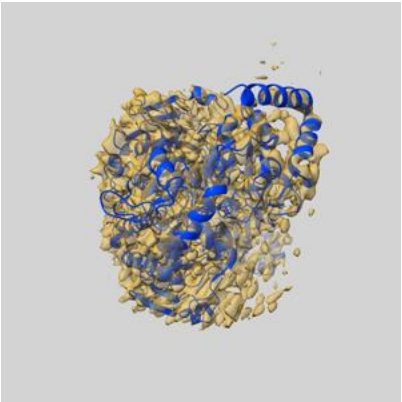
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-47105 and PDB model 9DPI. Per-residue inclusion information can be found in section 3 on page 5.

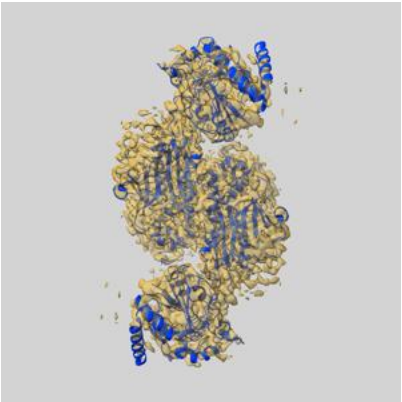
9.1 Map-model overlay (i)



X



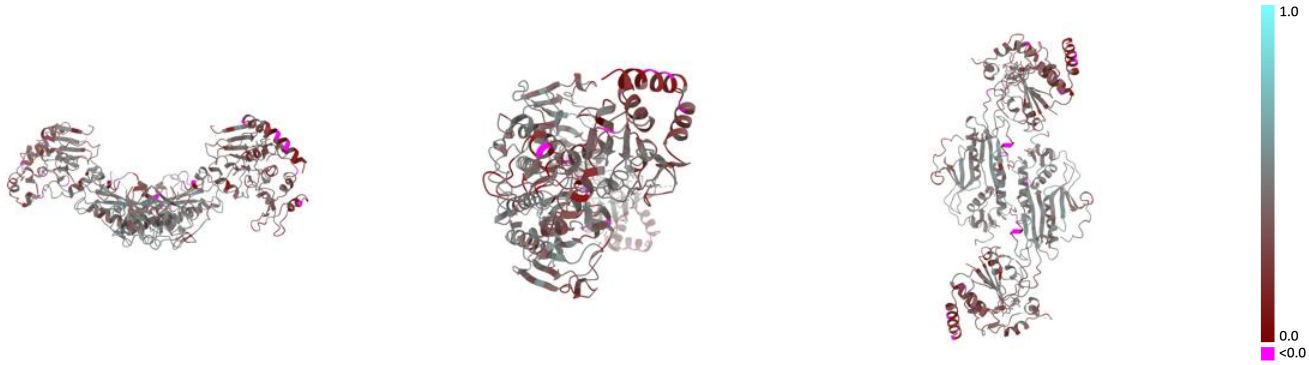
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.962 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

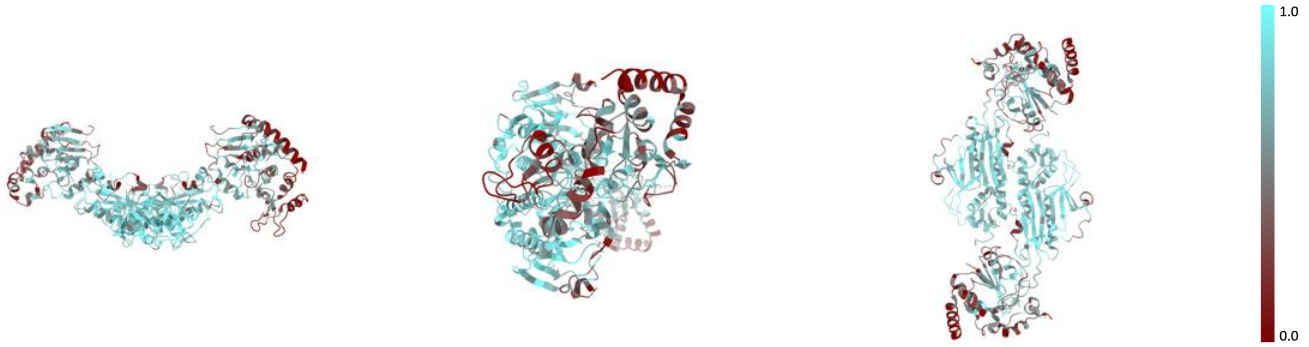
9.2 Q-score mapped to coordinate model (i)



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.

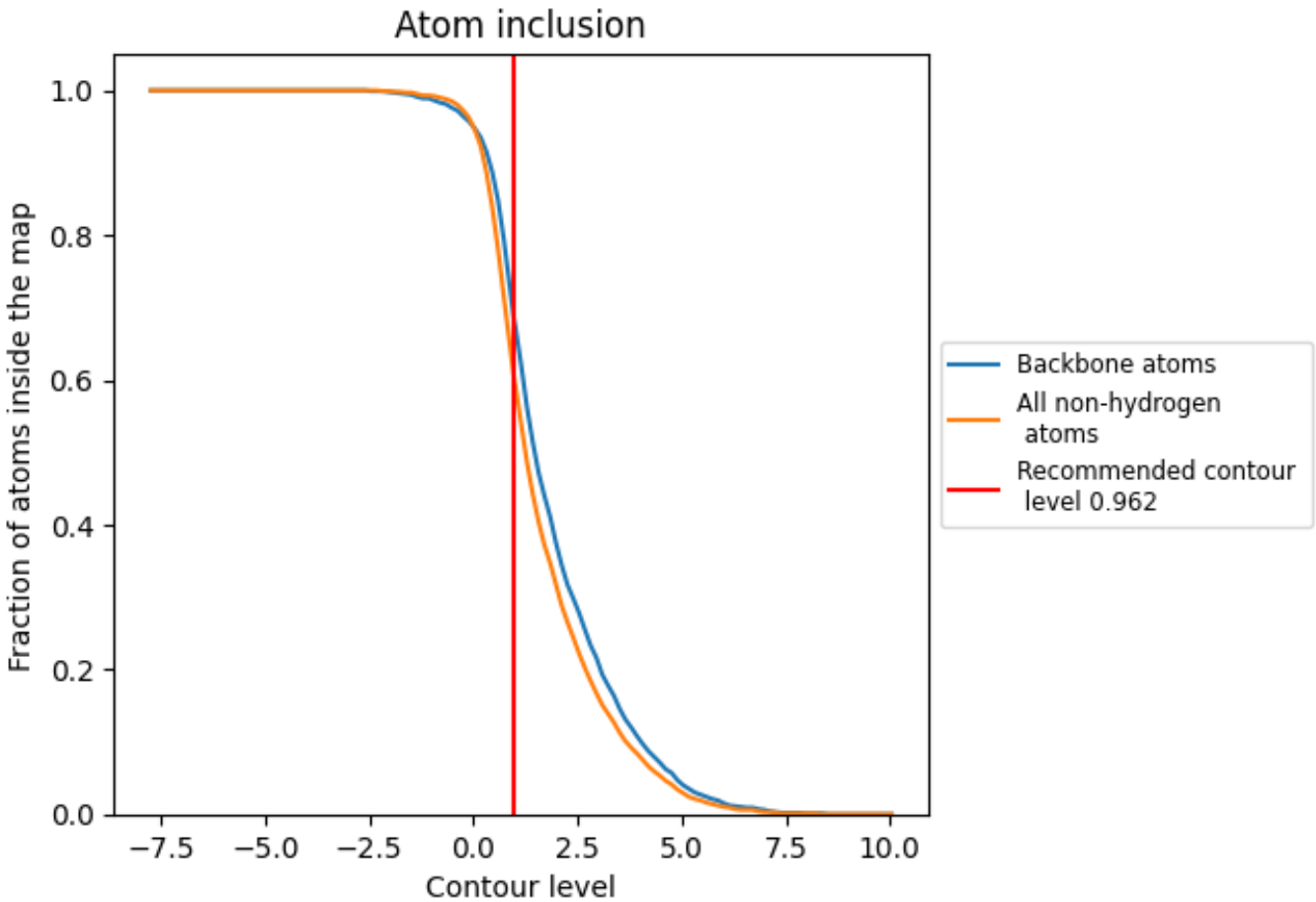
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.962).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 61% 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 (0.962) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6070	0.3820
C	0.4500	0.3340
D	0.7650	0.4340
E	0.4080	0.3180
F	0.7600	0.4280