



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:31 AM UTC

PDB ID : 7S60 / pdb_00007s60
EMDB ID : EMD-24845
Title : Human KATP channel in open conformation, focused on Kir and one SUR, position 4
Authors : Zhao, C.; MacKinnon, R.
Deposited on : 2021-09-12
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

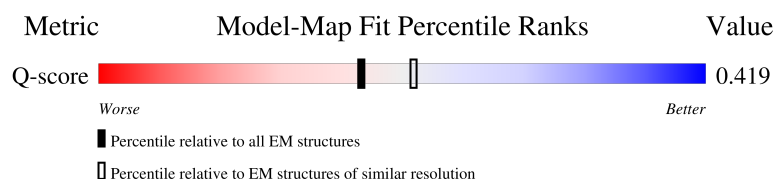
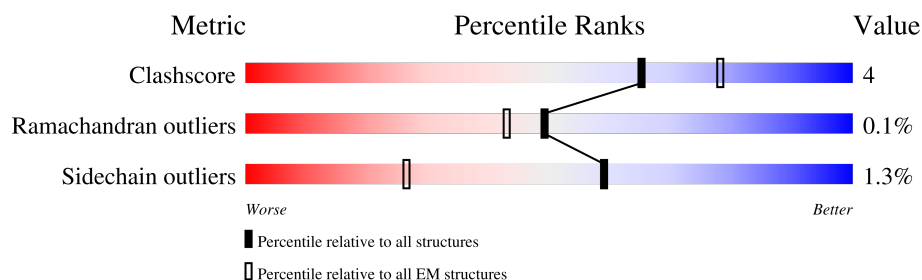
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	390	6% 73% 9% 18%
1	B	390	6% 74% 8% 18%
1	C	390	8% 71% 11% 18%
1	D	390	7% 75% 7% 18%

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Mol	Chain	Length	Quality of chain
2	E	1582	14% 75% 13% • 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21086 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 ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	321	Total	C	N	O	S	0	0
			2519	1622	430	451	16		
1	B	321	Total	C	N	O	S	1	0
			2527	1627	431	452	17		
1	C	321	Total	C	N	O	S	0	0
			2519	1622	430	451	16		
1	D	321	Total	C	N	O	S	0	0
			2519	1622	430	451	16		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	SER	CYS	engineered mutation	UNP B2RC52
A	334	ASP	GLY	engineered mutation	UNP B2RC52
B	166	SER	CYS	engineered mutation	UNP B2RC52
B	334	ASP	GLY	engineered mutation	UNP B2RC52
C	166	SER	CYS	engineered mutation	UNP B2RC52
C	334	ASP	GLY	engineered mutation	UNP B2RC52
D	166	SER	CYS	engineered mutation	UNP B2RC52
D	334	ASP	GLY	engineered mutation	UNP B2RC52

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	1395	Total	C	N	O	S	0	0
			10942	7122	1854	1909	57		

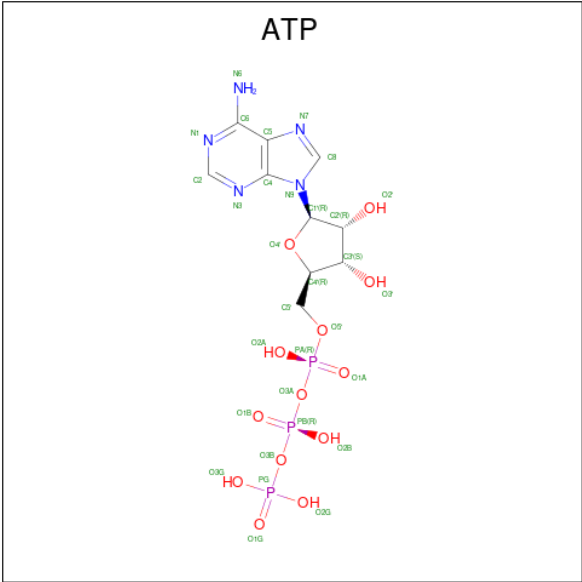
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MET	-	expression tag	UNP Q09428
E	2	GLY	-	expression tag	UNP Q09428

- # ADP

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).

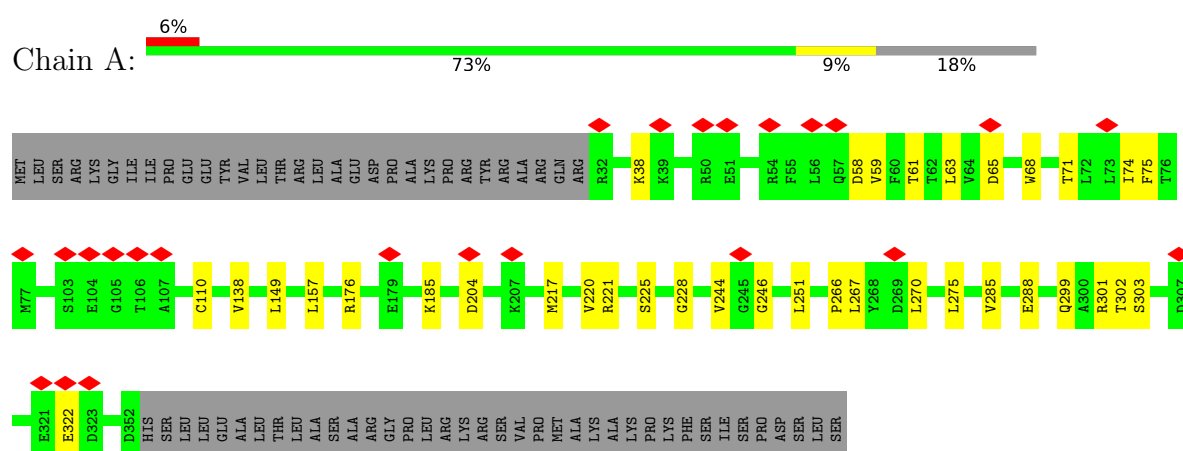


Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

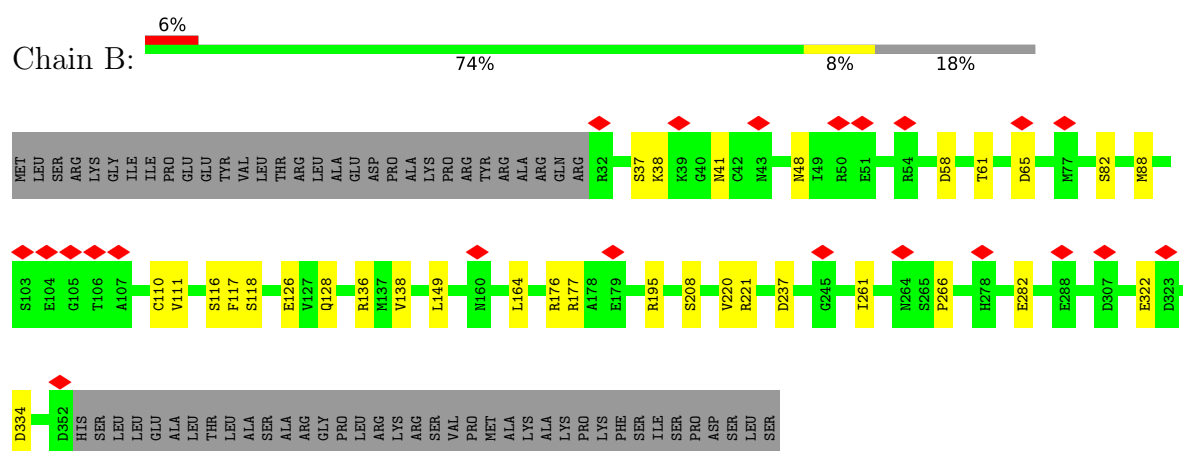
3 Residue-property plots

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.

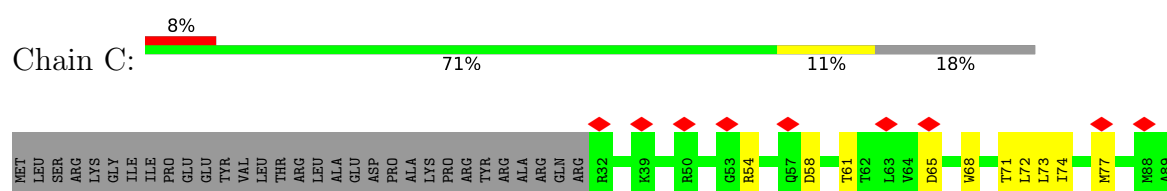
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

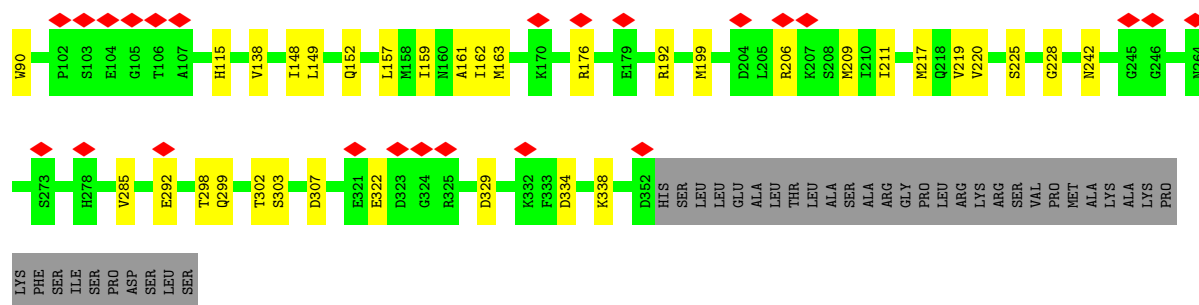


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

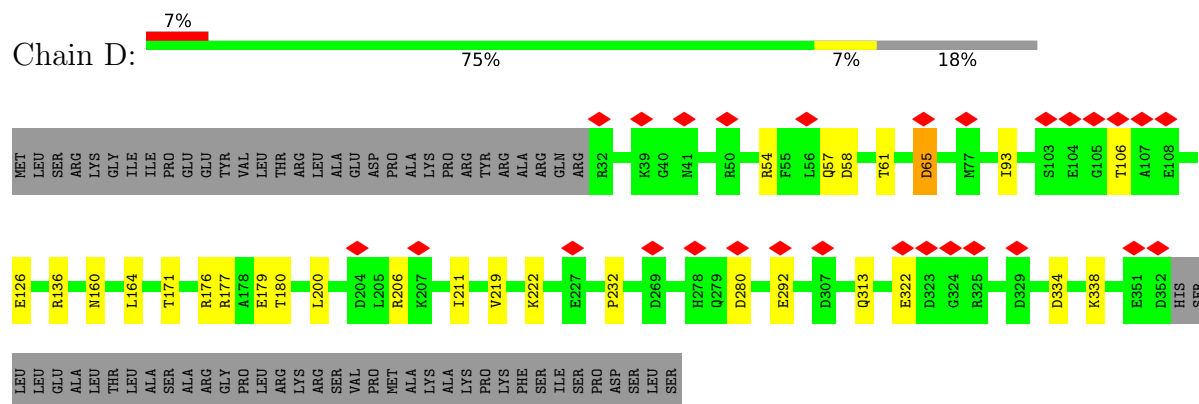


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

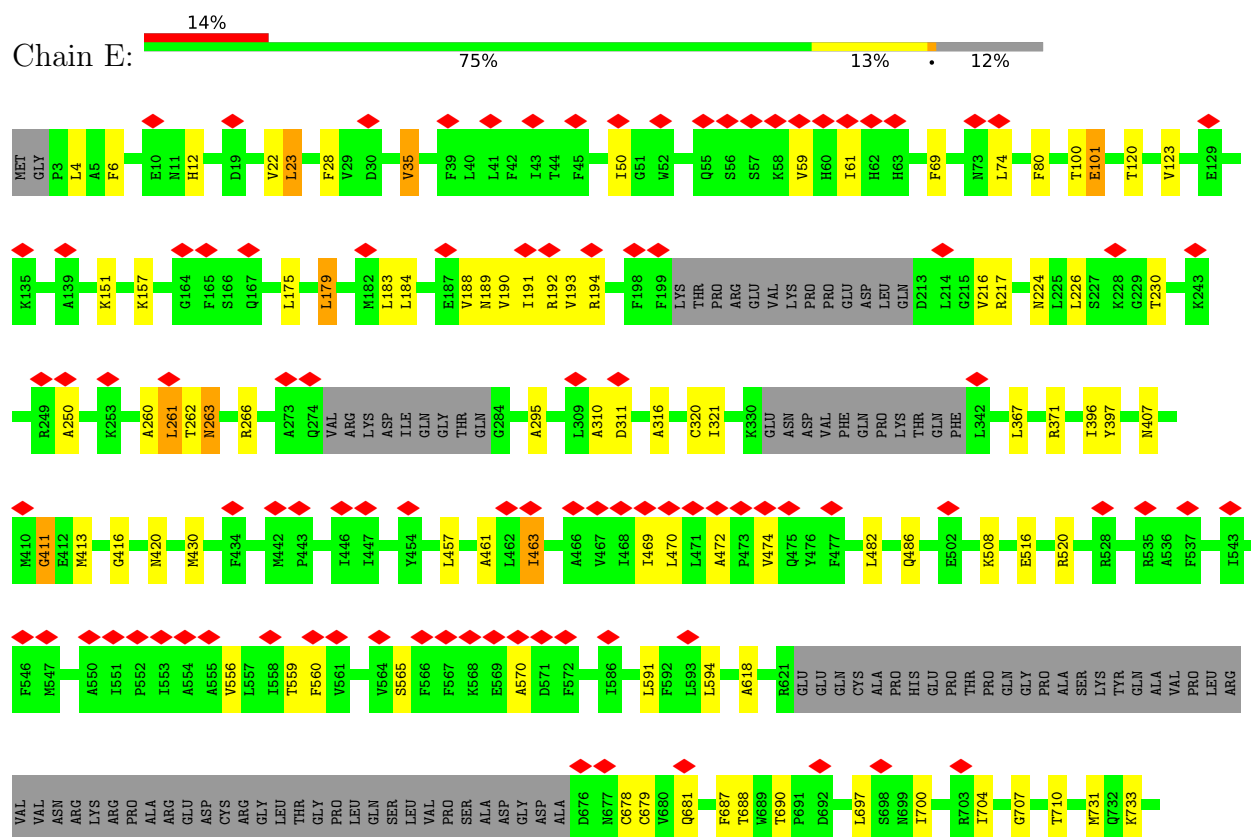


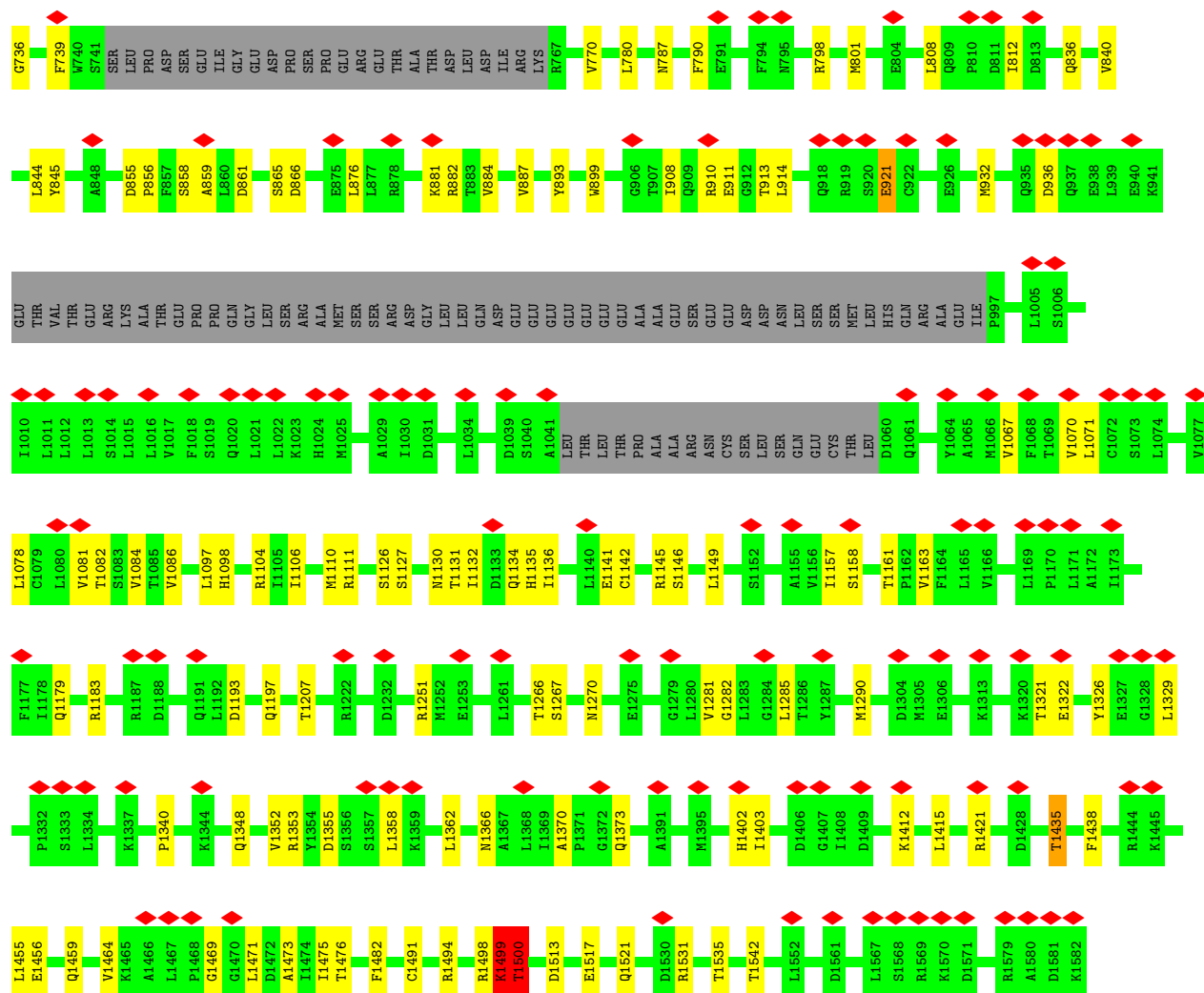


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



- Molecule 2: ATP-binding cassette sub-family C member 8





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28719	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.642	Depositor
Minimum map value	-1.081	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	473.19998, 473.19998, 473.19998	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.40	0/2576	0.73	2/3502 (0.1%)
1	B	0.42	0/2584	0.81	2/3512 (0.1%)
1	C	0.40	0/2576	0.75	3/3502 (0.1%)
1	D	0.41	0/2576	0.75	2/3502 (0.1%)
2	E	0.45	1/11175 (0.0%)	0.91	35/15167 (0.2%)
All	All	0.43	1/21487 (0.0%)	0.84	44/29185 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
2	E	0	16
All	All	0	18

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	35	VAL	C-N	9.25	1.45	1.34

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1158	SER	N-CA-C	-8.87	104.51	114.62
2	E	263	ASN	CA-C-N	8.40	137.59	121.54
2	E	263	ASN	C-N-CA	8.40	137.59	121.54
2	E	261	LEU	CA-CB-CG	7.25	141.67	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	570	ALA	CA-C-N	6.25	133.48	121.54
2	E	570	ALA	C-N-CA	6.25	133.48	121.54
2	E	932	MET	CA-C-N	6.24	130.99	122.19
2	E	932	MET	C-N-CA	6.24	130.99	122.19
2	E	4	LEU	CA-CB-CG	6.07	137.55	116.30
2	E	260	ALA	CA-C-N	5.92	132.34	123.05
2	E	260	ALA	C-N-CA	5.92	132.34	123.05
2	E	921	GLU	CA-C-N	5.90	132.80	121.54
2	E	921	GLU	C-N-CA	5.90	132.80	121.54
2	E	1098	HIS	CA-C-N	5.87	136.52	125.66
2	E	1098	HIS	C-N-CA	5.87	136.52	125.66
2	E	1499	LYS	CA-C-N	5.85	132.71	121.54
2	E	1499	LYS	C-N-CA	5.85	132.71	121.54
2	E	469	ILE	CA-C-N	5.82	132.65	121.54
2	E	469	ILE	C-N-CA	5.82	132.65	121.54
2	E	6	PHE	CA-C-N	5.74	132.50	121.54
2	E	6	PHE	C-N-CA	5.74	132.50	121.54
2	E	1403	ILE	CA-C-N	5.61	128.95	120.77
2	E	1403	ILE	C-N-CA	5.61	128.95	120.77
1	D	322	GLU	CA-C-N	5.52	132.08	121.54
1	D	322	GLU	C-N-CA	5.52	132.08	121.54
1	B	322	GLU	CA-C-N	5.51	129.95	122.07
1	B	322	GLU	C-N-CA	5.51	129.95	122.07
1	A	322	GLU	CA-C-N	5.34	129.93	122.08
1	A	322	GLU	C-N-CA	5.34	129.93	122.08
2	E	565	SER	CA-C-N	5.33	131.73	121.54
2	E	565	SER	C-N-CA	5.33	131.73	121.54
2	E	1500	THR	N-CA-CB	5.33	119.49	110.49
2	E	22	VAL	CA-C-N	5.32	129.90	122.08
2	E	22	VAL	C-N-CA	5.32	129.90	122.08
1	C	338	LYS	N-CA-C	5.25	117.05	110.91
1	C	322	GLU	CA-C-N	5.24	129.78	122.08
1	C	322	GLU	C-N-CA	5.24	129.78	122.08
2	E	790	PHE	CA-C-N	5.16	129.88	122.40
2	E	790	PHE	C-N-CA	5.16	129.88	122.40
2	E	23	LEU	CA-CB-CG	5.16	134.35	116.30
2	E	310	ALA	CA-C-N	5.15	131.37	121.54
2	E	310	ALA	C-N-CA	5.15	131.37	121.54
2	E	184	LEU	CA-C-N	5.14	131.35	121.18
2	E	184	LEU	C-N-CA	5.14	131.35	121.18

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	CYS	Peptide
1	B	110	CYS	Peptide
2	E	101	GLU	Peptide
2	E	1097	LEU	Peptide
2	E	1157	ILE	Peptide
2	E	12	HIS	Peptide
2	E	1498	ARG	Peptide
2	E	1499	LYS	Peptide
2	E	1500	THR	Peptide
2	E	193	VAL	Peptide
2	E	194	ARG	Peptide
2	E	262	THR	Peptide
2	E	263	ASN	Peptide
2	E	311	ASP	Peptide
2	E	411	GLY	Peptide
2	E	463	ILE	Peptide
2	E	470	LEU	Peptide
2	E	472	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2519	0	2547	22	0
1	B	2527	0	2557	23	0
1	C	2519	0	2547	28	0
1	D	2519	0	2547	18	0
2	E	10942	0	11212	95	0
3	E	27	0	12	0	0
4	E	2	0	0	0	0
5	E	31	0	12	0	0
All	All	21086	0	21434	171	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 4.

All (171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:THR:O	1:C:65:ASP:HB2	1.76	0.83
1:B:61:THR:O	1:B:65:ASP:HB2	1.88	0.74
1:D:61:THR:O	1:D:65:ASP:HB2	1.93	0.68
2:E:1179:GLN:O	2:E:1183:ARG:HB2	1.96	0.66
2:E:1067:VAL:O	2:E:1071:LEU:HB2	1.97	0.65
2:E:416:GLY:O	2:E:420:ASN:HB2	1.96	0.64
2:E:175:LEU:O	2:E:179:LEU:HB2	1.99	0.63
1:C:73:LEU:O	1:C:77:MET:HB2	2.01	0.61
1:A:61:THR:O	1:A:65:ASP:HB2	2.01	0.59
1:C:58:ASP:HB3	1:D:176:ARG:HB3	1.87	0.57
2:E:190:VAL:HG23	2:E:191:ILE:HG13	1.87	0.56
1:A:244:VAL:HG23	1:A:246:GLY:H	1.72	0.55
1:A:176:ARG:HB3	1:D:58:ASP:HB3	1.89	0.55
2:E:681:GLN:HB2	2:E:739:PHE:HB2	1.88	0.55
2:E:457:LEU:HB2	2:E:461:ALA:HB2	1.89	0.54
2:E:516:GLU:O	2:E:520:ARG:HB2	2.08	0.54
2:E:1491:CYS:SG	2:E:1494:ARG:NH1	2.81	0.54
2:E:1329:LEU:HB2	2:E:1412:LYS:HG2	1.89	0.53
1:B:88[B]:MET:HE1	2:E:35:VAL:HG23	1.91	0.53
2:E:808:LEU:O	2:E:812:ILE:HB	2.09	0.53
2:E:1266:THR:O	2:E:1270:ASN:HB2	2.08	0.52
1:C:192:ARG:NH2	1:C:199:MET:SD	2.83	0.51
2:E:1086:VAL:HG21	2:E:1141:GLU:HB3	1.92	0.51
2:E:1326:TYR:HA	2:E:1415:LEU:HD12	1.93	0.51
2:E:861:ASP:O	2:E:865:SER:HB3	2.11	0.50
2:E:1469:GLY:HA3	2:E:1473:ALA:HB2	1.93	0.50
1:B:61:THR:OG1	1:C:206:ARG:NH1	2.45	0.50
2:E:840:VAL:HG11	2:E:856:PRO:HB3	1.94	0.50
2:E:100:THR:OG1	2:E:101:GLU:N	2.44	0.49
2:E:1370:ALA:HB3	2:E:1373:GLN:HB2	1.94	0.49
1:B:220:VAL:HG23	1:B:282:GLU:HB3	1.95	0.49
1:B:334:ASP:OD1	1:B:334:ASP:N	2.46	0.49
2:E:1126:SER:OG	2:E:1127:SER:N	2.46	0.49
2:E:1282:GLY:HA2	2:E:1285:LEU:HD12	1.94	0.49
1:C:334:ASP:OD1	1:C:334:ASP:N	2.45	0.49
1:B:221:ARG:NH2	1:B:266:PRO:O	2.46	0.49
2:E:266:ARG:NH2	2:E:295:ALA:O	2.46	0.48
1:D:222:LYS:HG3	1:D:232:PRO:HA	1.95	0.48
2:E:688:THR:HG22	2:E:690:THR:H	1.79	0.48
1:C:58:ASP:N	1:C:58:ASP:OD1	2.47	0.48
2:E:482:LEU:O	2:E:486:GLN:HB2	2.13	0.48
1:A:221:ARG:NH2	1:A:266:PRO:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:SER:OG	1:B:38:LYS:N	2.46	0.48
2:E:397:TYR:HE1	2:E:1207:THR:HG21	1.79	0.48
2:E:1456:GLU:O	2:E:1459:GLN:NE2	2.47	0.48
1:A:157:LEU:HD22	1:B:164:LEU:HD11	1.96	0.48
1:A:299:GLN:OE1	1:A:301:ARG:NH1	2.46	0.48
1:D:160:ASN:O	1:D:164:LEU:HB2	2.14	0.48
2:E:1500:THR:O	2:E:1531:ARG:NH1	2.47	0.48
1:A:217:MET:HG2	1:A:285:VAL:HG22	1.94	0.47
2:E:836:GLN:NE2	2:E:855:ASP:O	2.47	0.47
2:E:798:ARG:NH1	2:E:845:TYR:O	2.48	0.47
1:D:126:GLU:OE2	1:D:136:ARG:NH2	2.48	0.47
2:E:1132:ILE:HA	2:E:1136:ILE:HD12	1.96	0.47
2:E:1455:LEU:HD13	2:E:1464:VAL:HG11	1.97	0.47
2:E:556:VAL:O	2:E:560:PHE:HB2	2.14	0.47
1:C:157:LEU:HD22	1:D:164:LEU:HD11	1.97	0.47
2:E:316:ALA:O	2:E:320:CYS:HB2	2.15	0.46
2:E:936:ASP:OD1	2:E:936:ASP:N	2.43	0.46
2:E:1161:THR:HG22	2:E:1163:VAL:H	1.81	0.46
2:E:910:ARG:NH1	2:E:921:GLU:OE1	2.49	0.46
1:A:288:GLU:HB3	1:A:299:GLN:HG3	1.98	0.46
1:B:58:ASP:OD2	1:B:58:ASP:N	2.48	0.46
2:E:1513:ASP:O	2:E:1517:GLU:HB2	2.16	0.46
2:E:188:VAL:HA	2:E:192:ARG:HB2	1.98	0.46
1:D:58:ASP:OD1	1:D:58:ASP:N	2.49	0.46
2:E:1366:ASN:N	2:E:1366:ASN:OD1	2.48	0.46
1:B:195:ARG:NH1	1:B:261:ILE:O	2.49	0.46
1:B:237:ASP:OD1	1:C:242:ASN:ND2	2.49	0.46
1:A:68:TRP:HA	1:A:71:THR:HG22	1.98	0.46
1:A:71:THR:O	1:A:75:PHE:HB2	2.16	0.45
1:B:88[B]:MET:HE2	1:B:88[B]:MET:HB3	1.80	0.45
2:E:1067:VAL:HA	2:E:1070:VAL:HG12	1.97	0.45
1:B:58:ASP:HB3	1:C:176:ARG:HB3	1.97	0.45
1:D:211:ILE:HD11	1:D:292:GLU:HG3	1.98	0.45
2:E:899:TRP:HE1	2:E:911:GLU:HB2	1.81	0.45
1:A:59:VAL:O	1:A:63:LEU:HB2	2.16	0.45
2:E:700:ILE:HG22	2:E:908:ILE:HG12	1.97	0.45
2:E:1521:GLN:NE2	2:E:1542:THR:O	2.49	0.45
2:E:69:PHE:HB3	2:E:189:ASN:HD21	1.82	0.45
1:B:126:GLU:OE2	1:B:136:ARG:NH1	2.50	0.45
2:E:224:ASN:OD1	2:E:224:ASN:N	2.46	0.45
2:E:1104:ARG:NH2	2:E:1321:THR:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:SER:OG	1:A:228:GLY:N	2.49	0.45
2:E:858:SER:OG	2:E:859:ALA:N	2.50	0.45
1:D:177:ARG:NH1	1:D:180:THR:OG1	2.49	0.45
1:A:270:LEU:HD21	1:A:275:LEU:HD21	1.99	0.45
1:B:82:SER:OG	1:B:128:GLN:NE2	2.47	0.45
1:B:177:ARG:NH2	1:B:208:SER:O	2.50	0.45
1:A:38:LYS:NZ	1:A:185:LYS:O	2.50	0.45
1:B:116:SER:OG	1:B:117:PHE:N	2.49	0.45
1:A:58:ASP:N	1:A:58:ASP:OD1	2.49	0.45
2:E:1348:GLN:HB3	2:E:1402:HIS:HB3	1.98	0.45
2:E:733:LYS:NZ	2:E:736:GLY:O	2.49	0.44
1:A:267:LEU:HD22	1:A:270:LEU:HD22	1.99	0.44
1:C:162:ILE:HG12	1:D:171:THR:HG21	1.99	0.44
2:E:1353:ARG:NH1	2:E:1355:ASP:O	2.48	0.44
1:C:61:THR:OG1	1:D:206:ARG:NH1	2.51	0.44
1:C:211:ILE:HD11	1:C:292:GLU:HG3	2.00	0.44
2:E:430:MET:HE2	2:E:430:MET:HB3	1.85	0.44
2:E:707:GLY:HA3	2:E:881:LYS:HG2	1.98	0.44
1:A:204:ASP:HB2	1:A:251:LEU:HG	2.00	0.44
1:C:217:MET:HG2	1:C:285:VAL:HG22	1.98	0.44
2:E:217:ARG:HH21	2:E:250:ALA:HA	1.82	0.44
1:A:138:VAL:HG21	1:A:149:LEU:HD22	1.99	0.44
1:C:68:TRP:HA	1:C:71:THR:HG22	1.99	0.44
2:E:230:THR:O	2:E:1251:ARG:NH1	2.50	0.44
2:E:801:MET:HG2	2:E:876:LEU:HD11	1.99	0.43
2:E:1130:ASN:OD1	2:E:1134:GLN:NE2	2.51	0.43
2:E:120:THR:HA	2:E:123:VAL:HG12	2.00	0.43
2:E:780:LEU:O	2:E:787:ASN:ND2	2.51	0.43
1:C:71:THR:HA	1:C:74:ILE:HG22	2.01	0.43
1:D:54:ARG:HA	1:D:57:GLN:HG3	2.00	0.43
2:E:1078:LEU:HA	2:E:1081:VAL:HG22	2.01	0.43
1:C:138:VAL:HG21	1:C:149:LEU:HD22	2.01	0.43
2:E:23:LEU:H	2:E:28:PHE:HD2	1.67	0.43
2:E:1111:ARG:HH12	2:E:1358:LEU:HD11	1.82	0.43
2:E:1131:THR:HA	2:E:1135:HIS:HB2	2.01	0.43
2:E:1267:SER:HB2	2:E:1281:VAL:HG13	2.01	0.43
1:A:138:VAL:O	1:B:136:ARG:NH2	2.47	0.43
1:B:116:SER:OG	1:B:118:SER:N	2.47	0.43
1:C:225:SER:OG	1:C:228:GLY:N	2.52	0.43
1:A:71:THR:HA	1:A:74:ILE:HG22	2.00	0.43
1:B:48:ASN:ND2	1:C:329:ASP:OD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:23:LEU:O	2:E:157:LYS:NZ	2.49	0.43
1:C:302:THR:OG1	1:C:303:SER:N	2.52	0.43
2:E:731:MET:HE3	2:E:731:MET:HB3	1.86	0.43
2:E:407:ASN:HD21	2:E:618:ALA:H	1.67	0.42
2:E:710:THR:HG23	2:E:899:TRP:HB3	2.00	0.42
2:E:407:ASN:HB3	2:E:413:MET:HE3	2.02	0.42
2:E:798:ARG:HH22	2:E:882:ARG:HH11	1.67	0.42
1:C:209:MET:HE2	1:C:209:MET:HB2	1.84	0.42
2:E:1352:VAL:HG22	2:E:1362:LEU:HB2	2.01	0.42
2:E:1475:ILE:HG12	2:E:1482:PHE:HE2	1.84	0.42
2:E:678:CYS:SG	2:E:679:CYS:N	2.93	0.42
2:E:1321:THR:OG1	2:E:1322:GLU:N	2.52	0.42
1:A:58:ASP:HB3	1:B:176:ARG:HB3	2.02	0.42
1:C:159:ILE:O	1:C:163:MET:HB2	2.19	0.42
2:E:866:ASP:OD1	2:E:893:TYR:OH	2.37	0.42
2:E:913:THR:OG1	2:E:914:LEU:N	2.50	0.42
2:E:1290:MET:HE3	2:E:1290:MET:HB2	1.96	0.42
1:A:302:THR:OG1	1:A:303:SER:N	2.53	0.42
2:E:80:PHE:HZ	2:E:226:LEU:HD12	1.85	0.42
2:E:321:ILE:HG12	2:E:1285:LEU:HD13	2.02	0.42
2:E:411:GLY:H	2:E:1476:THR:HG21	1.84	0.42
1:C:90:TRP:NE1	1:C:152:GLN:OE1	2.48	0.41
2:E:61:ILE:HD12	2:E:61:ILE:HA	1.98	0.41
1:B:138:VAL:HG21	1:B:149:LEU:HD22	2.01	0.41
1:D:93:ILE:HD13	1:D:93:ILE:HA	1.96	0.41
2:E:230:THR:OG1	2:E:1251:ARG:NH1	2.50	0.41
2:E:508:LYS:HD2	2:E:1110:MET:HE2	2.02	0.41
2:E:151:LYS:HD2	2:E:151:LYS:HA	1.87	0.41
1:C:148:ILE:HD13	1:C:148:ILE:HA	1.97	0.41
2:E:697:LEU:HD23	2:E:697:LEU:HA	1.98	0.41
2:E:1145:ARG:O	2:E:1149:LEU:HB2	2.20	0.41
2:E:1435:THR:HG23	2:E:1438:PHE:HB3	2.02	0.41
1:C:161:ALA:HB2	1:D:164:LEU:HG	2.03	0.41
1:C:298:THR:OG1	1:C:299:GLN:N	2.54	0.41
2:E:367:LEU:O	2:E:371:ARG:HB2	2.20	0.41
2:E:591:LEU:HA	2:E:594:LEU:HD23	2.02	0.41
2:E:687:PHE:HB2	2:E:697:LEU:HB2	2.03	0.41
2:E:1340:PRO:HG3	2:E:1421:ARG:HB3	2.03	0.41
1:C:307:ASP:OD1	1:C:307:ASP:N	2.49	0.40
1:B:41:ASN:OD1	1:B:41:ASN:N	2.50	0.40
2:E:1081:VAL:HA	2:E:1084:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ARG:NE	1:D:179:GLU:O	2.48	0.40
2:E:1142:CYS:O	2:E:1146:SER:HB3	2.21	0.40
1:D:313:GLN:HG2	1:D:338:LYS:HG2	2.02	0.40
1:D:334:ASP:OD1	1:D:334:ASP:N	2.45	0.40
2:E:50:ILE:HD13	2:E:50:ILE:HA	1.97	0.40
2:E:1193:ASP:O	2:E:1197:GLN:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/390 (82%)	310 (97%)	9 (3%)	0	100	100
1	B	320/390 (82%)	306 (96%)	13 (4%)	1 (0%)	36	65
1	C	319/390 (82%)	309 (97%)	10 (3%)	0	100	100
1	D	319/390 (82%)	307 (96%)	12 (4%)	0	100	100
2	E	1379/1582 (87%)	1281 (93%)	96 (7%)	2 (0%)	48	78
All	All	2656/3142 (84%)	2513 (95%)	140 (5%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	1500	THR
2	E	1499	LYS
1	B	111	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/337 (82%)	277 (100%)	1 (0%)	84	81
1	B	279/337 (83%)	279 (100%)	0	100	100
1	C	278/337 (82%)	274 (99%)	4 (1%)	59	70
1	D	278/337 (82%)	273 (98%)	5 (2%)	51	67
2	E	1182/1368 (86%)	1162 (98%)	20 (2%)	53	67
All	All	2295/2716 (84%)	2265 (99%)	30 (1%)	59	71

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	VAL
1	C	72	LEU
1	C	115	HIS
1	C	219	VAL
1	C	220	VAL
1	D	65	ASP
1	D	106	THR
1	D	200	LEU
1	D	219	VAL
1	D	280	ASP
2	E	59	VAL
2	E	74	LEU
2	E	179	LEU
2	E	183	LEU
2	E	216	VAL
2	E	261	LEU
2	E	396	ILE
2	E	463	ILE
2	E	474	VAL
2	E	559	THR
2	E	704	ILE
2	E	770	VAL
2	E	844	LEU

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Mol	Chain	Res	Type
2	E	884	VAL
2	E	887	VAL
2	E	1082	THR
2	E	1106	ILE
2	E	1435	THR
2	E	1471	LEU
2	E	1535	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	ASN
1	B	235	GLN
1	C	52	GLN
1	C	57	GLN
1	C	175	HIS
1	D	43	ASN
1	D	160	ASN
1	D	216	HIS
1	D	235	GLN
1	D	264	ASN
2	E	189	ASN
2	E	263	ASN
2	E	355	ASN
2	E	375	GLN
2	E	407	ASN
2	E	475	GLN
2	E	609	GLN
2	E	715	GLN
2	E	817	HIS
2	E	918	GLN
2	E	927	HIS
2	E	1190	GLN
2	E	1225	GLN
2	E	1270	ASN
2	E	1301	ASN
2	E	1416	HIS
2	E	1459	GLN
2	E	1488	GLN
2	E	1518	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	ATP	E	1604	4	32,33,33	1.31	4 (12%)	48,52,52	1.77	9 (18%)
3	ADP	E	1601	4	28,29,29	1.40	5 (17%)	43,45,45	1.86	11 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	E	1604	4	-	4/22/38/38	0/3/3/3
3	ADP	E	1601	4	-	2/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1601	ADP	C5-C4	4.44	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1604	ATP	C5-C4	4.31	1.46	1.39
5	E	1604	ATP	C5-N7	-3.07	1.33	1.39
3	E	1601	ADP	C5-C6	2.69	1.48	1.41
3	E	1601	ADP	C5-N7	-2.46	1.34	1.39
3	E	1601	ADP	C4-N9	-2.25	1.33	1.37
5	E	1604	ATP	C4-N9	-2.25	1.33	1.37
3	E	1601	ADP	C8-N7	2.23	1.36	1.31
5	E	1604	ATP	C5-C6	2.00	1.46	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1604	ATP	C5-C4-N3	-5.44	119.23	126.72
3	E	1601	ADP	C5-C4-N3	-5.09	119.71	126.72
5	E	1604	ATP	N3-C4-N9	4.91	135.52	127.17
3	E	1601	ADP	N3-C4-N9	4.15	134.23	127.17
5	E	1604	ATP	N3-C2-N1	-4.04	122.47	128.58
3	E	1601	ADP	N3-C2-N1	-3.80	122.83	128.58
5	E	1604	ATP	C2-N3-C4	3.77	121.04	111.83
3	E	1601	ADP	C2-N3-C4	3.73	120.93	111.83
3	E	1601	ADP	C4-C5-N7	-3.19	106.94	110.58
3	E	1601	ADP	C4-N9-C8	3.00	108.89	105.74
5	E	1604	ATP	C4-N9-C8	2.55	108.42	105.74
5	E	1604	ATP	C3'-C2'-C1'	2.51	106.21	101.46
3	E	1601	ADP	C6-C5-N7	2.45	136.81	132.09
3	E	1601	ADP	C5-N7-C8	2.35	107.15	103.45
3	E	1601	ADP	O2A-PA-O3A	2.21	113.26	107.27
3	E	1601	ADP	C2-N1-C6	2.14	122.25	118.73
5	E	1604	ATP	C2-N1-C6	2.13	122.24	118.73
5	E	1604	ATP	C4-C5-N7	-2.12	108.16	110.58
3	E	1601	ADP	N9-C8-N7	-2.09	110.97	113.94
5	E	1604	ATP	C2'-C3'-C4'	2.06	106.58	102.61

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1601	ADP	C5'-O5'-PA-O2A
3	E	1601	ADP	C5'-O5'-PA-O3A
5	E	1604	ATP	C5'-O5'-PA-O3A
5	E	1604	ATP	C5'-O5'-PA-O1A
5	E	1604	ATP	PB-O3A-PA-O1A

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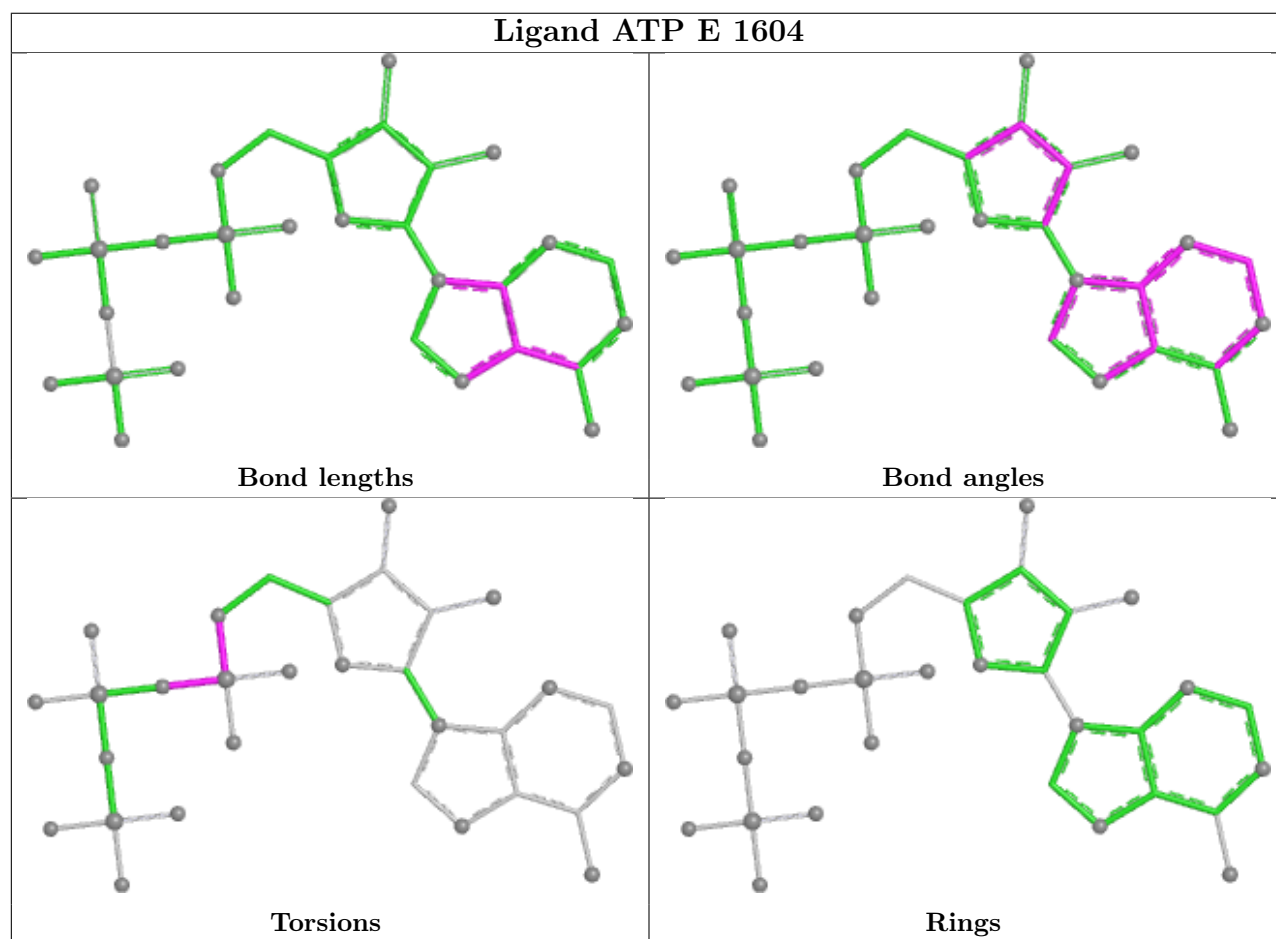
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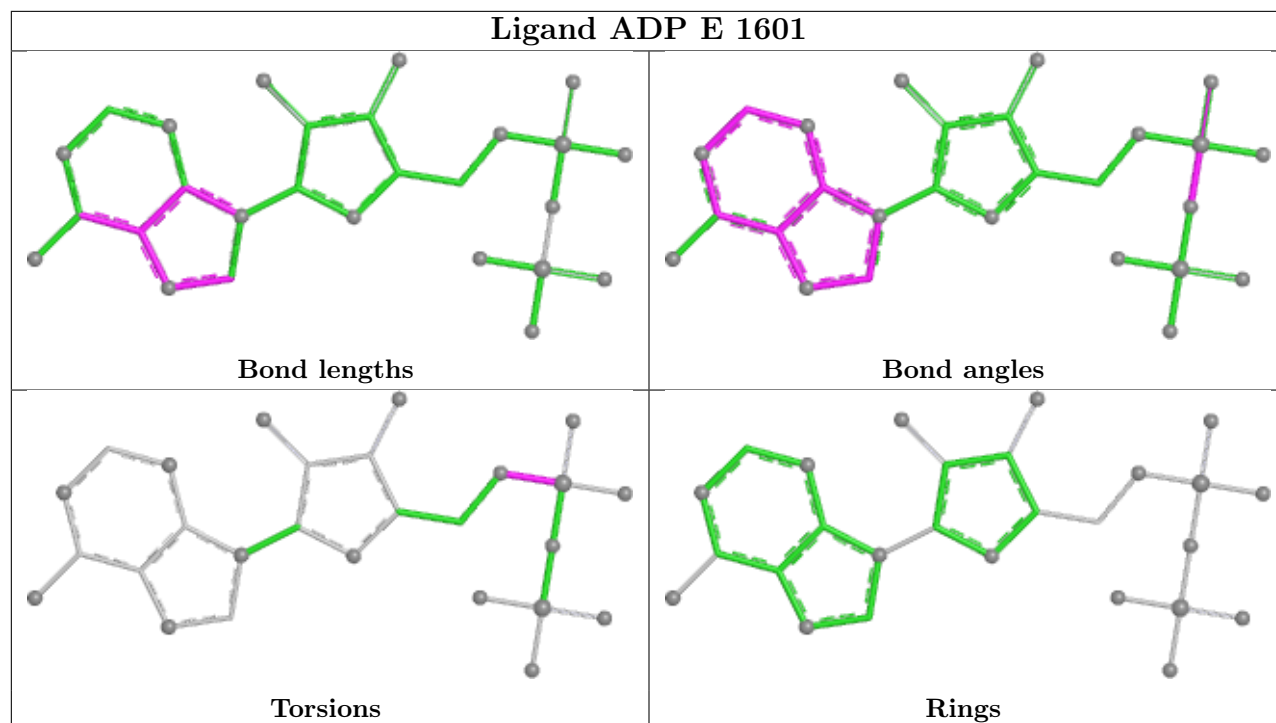
Mol	Chain	Res	Type	Atoms
5	E	1604	ATP	PB-O3A-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

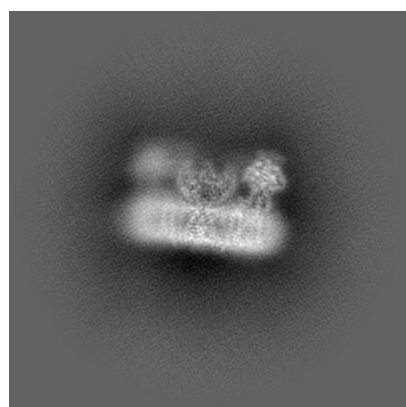
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24845. These allow visual inspection of the internal detail of the map and identification of artifacts.

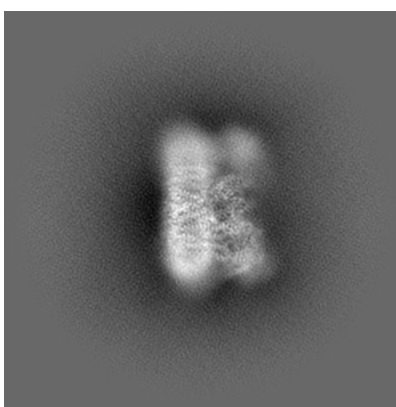
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

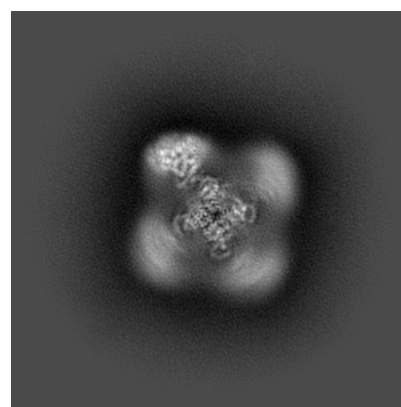
6.1.1 Primary map



X



Y

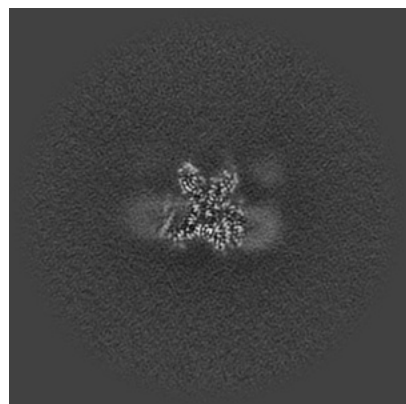


Z

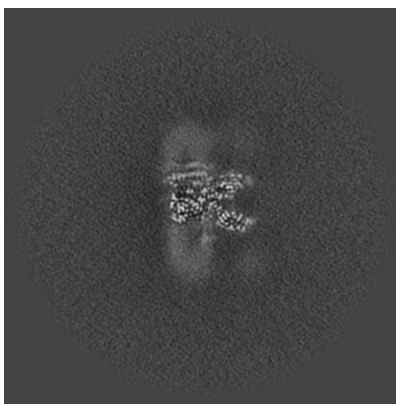
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

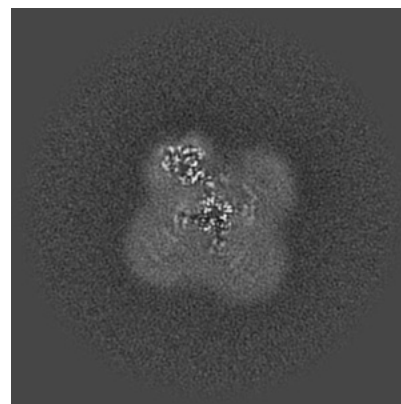
6.2.1 Primary map



X Index: 182



Y Index: 182

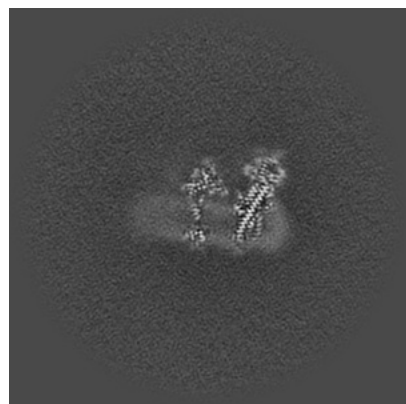


Z Index: 182

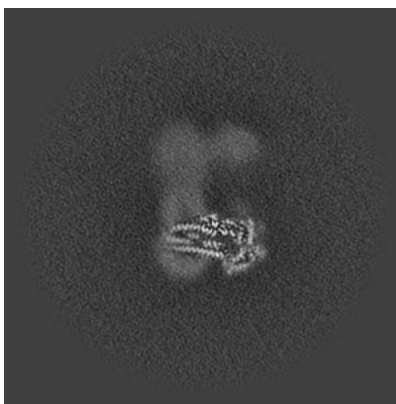
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

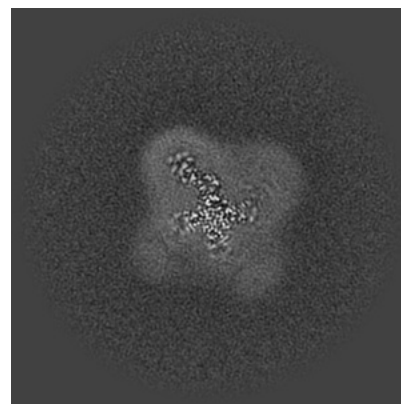
6.3.1 Primary map



X Index: 166



Y Index: 227

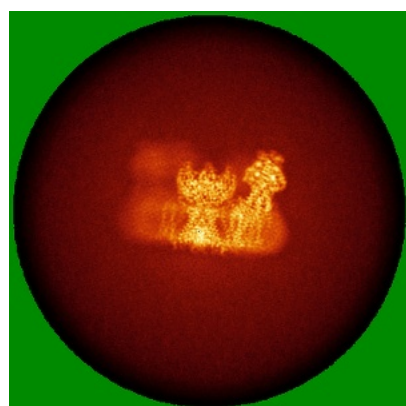


Z Index: 156

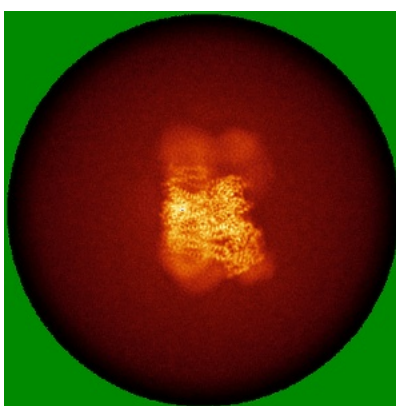
The images above show the largest variance slices of the map in three orthogonal directions.

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

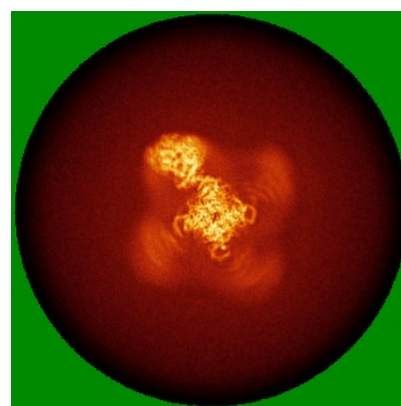
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

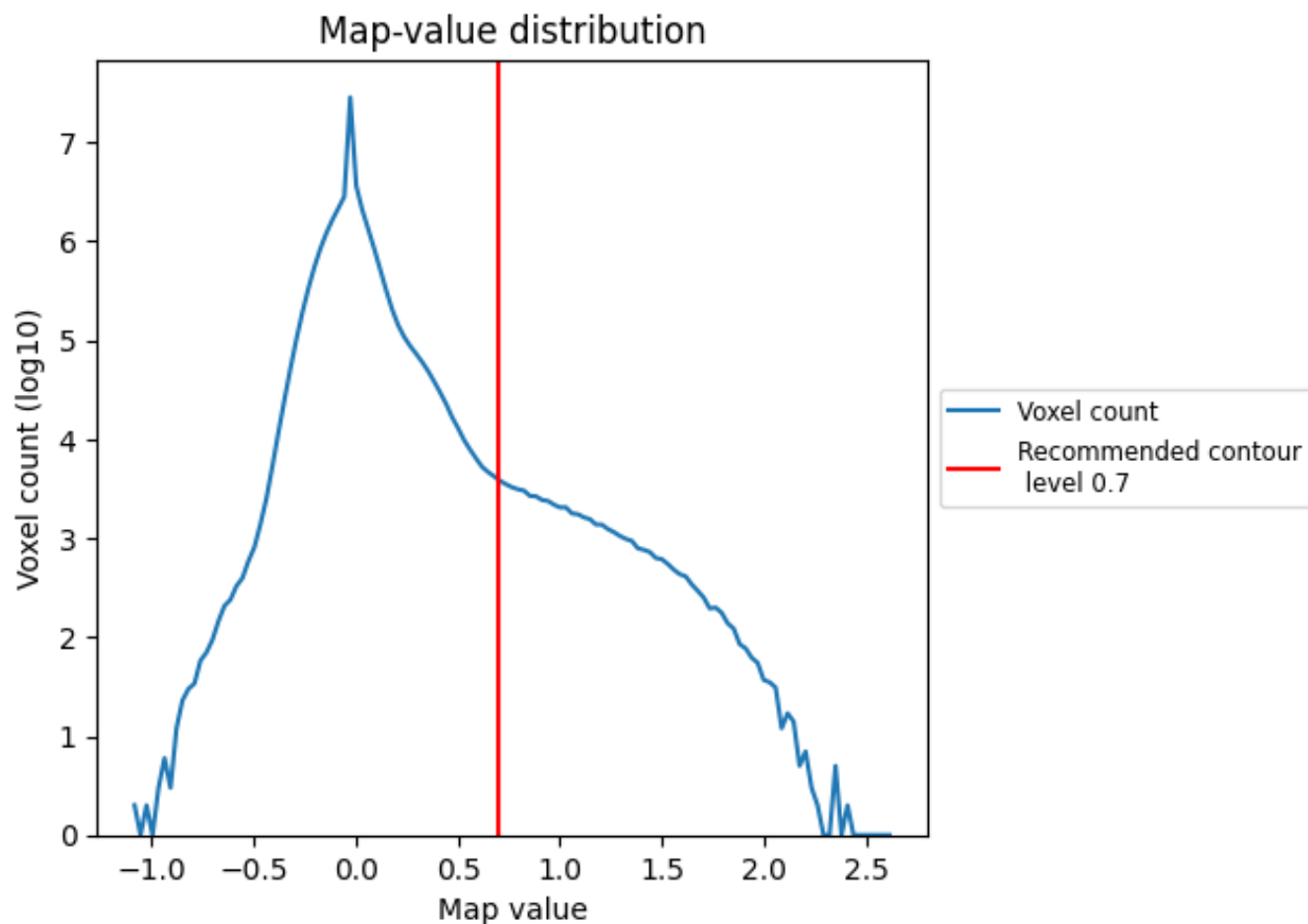
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

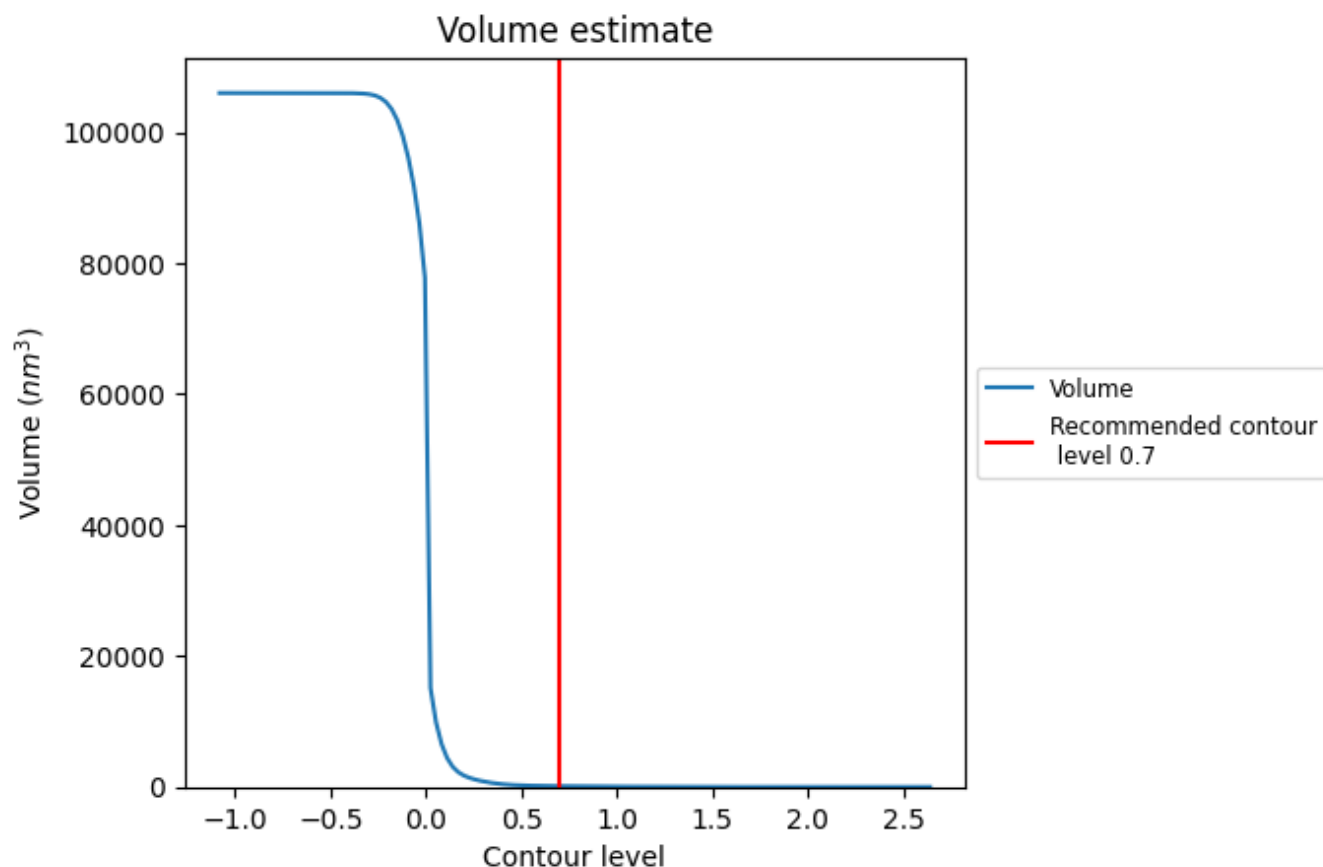
This section contains the results of statistical analysis of the map.

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.

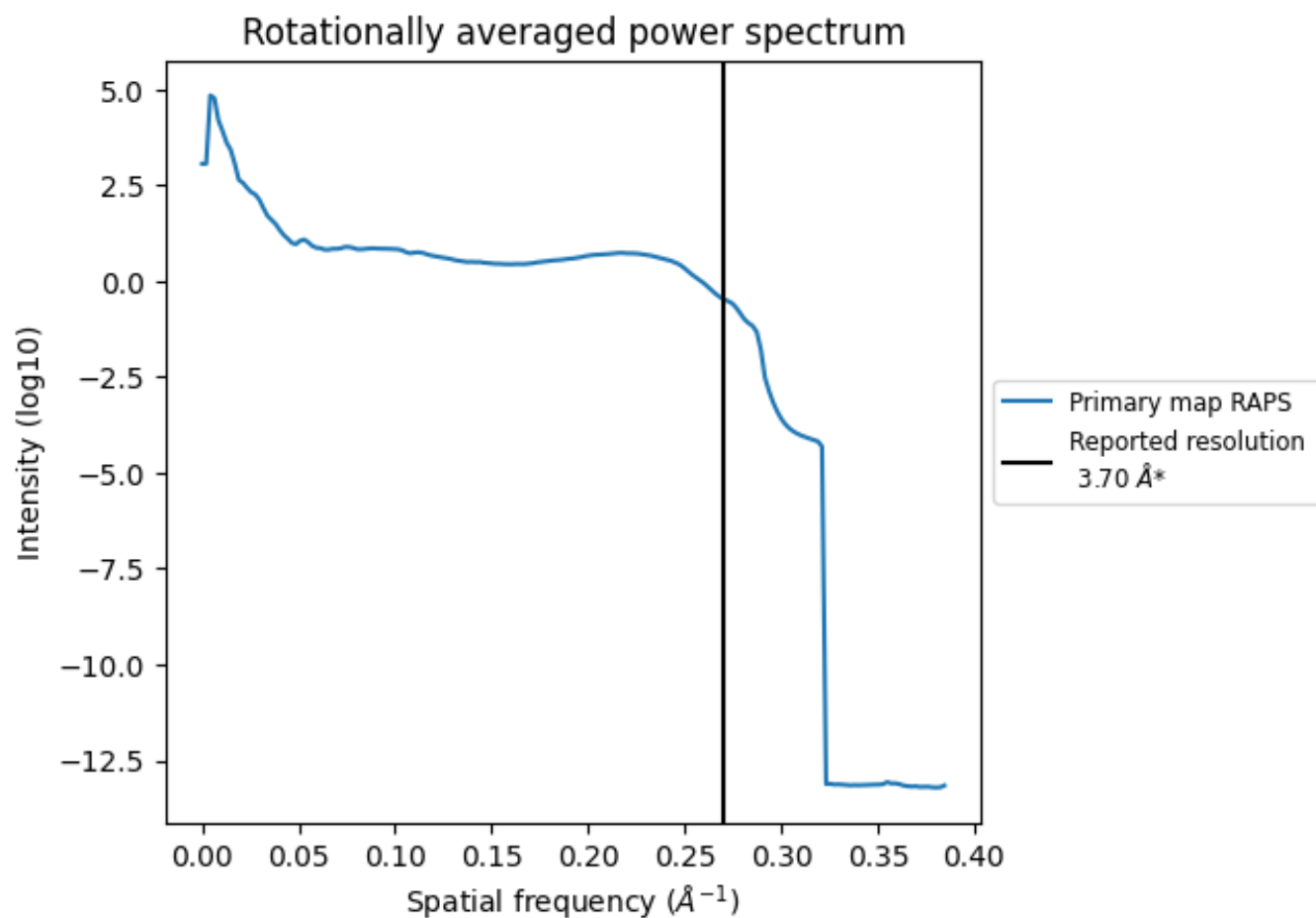
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 124 nm^3 ; this corresponds to an approximate mass of 112 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 ⓘ

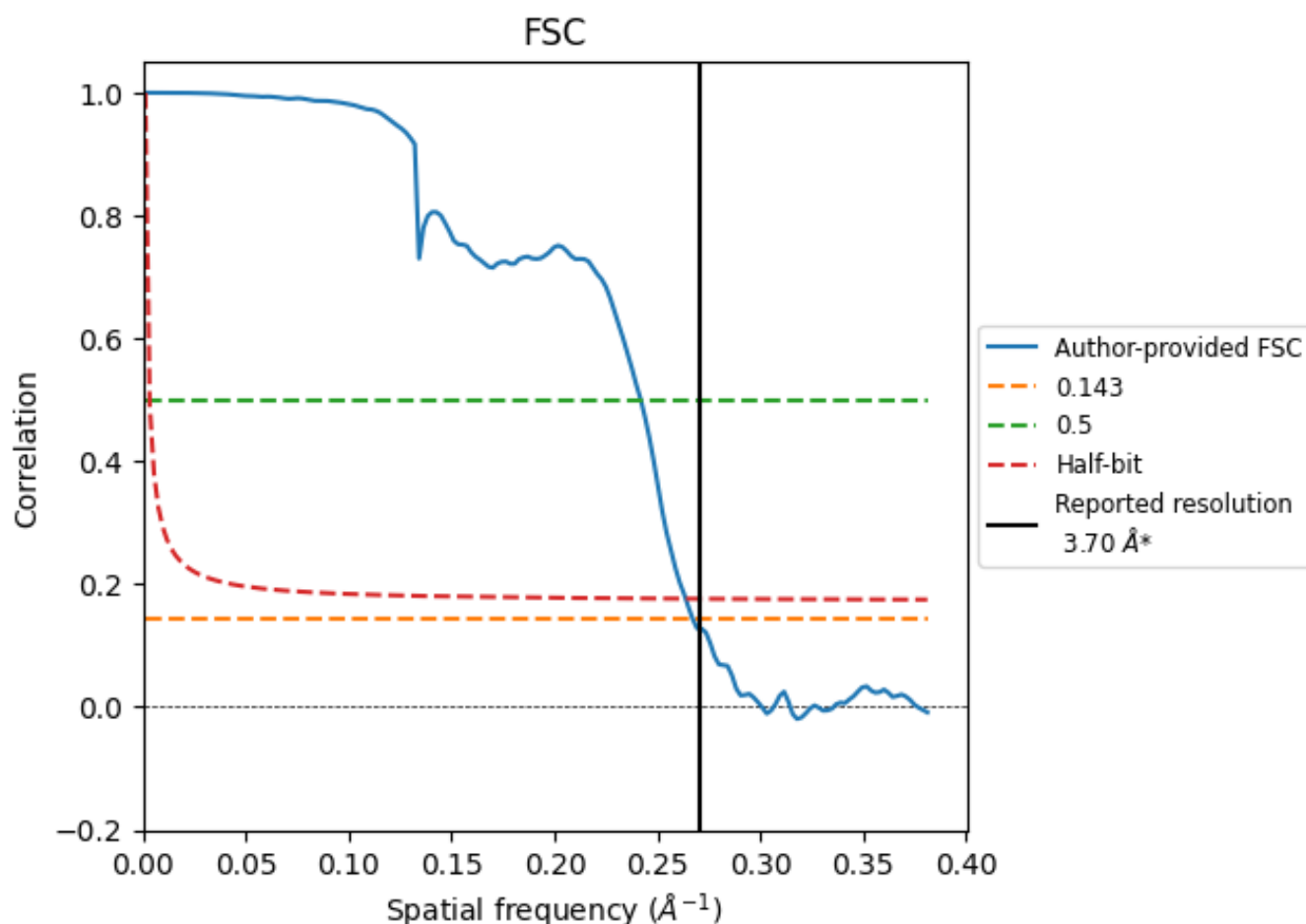


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

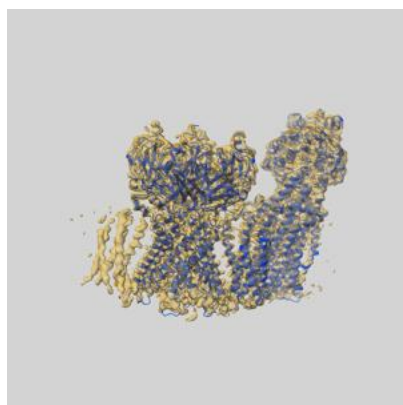
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.74	4.13	3.79
Unmasked-calculated*	-	-	-

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

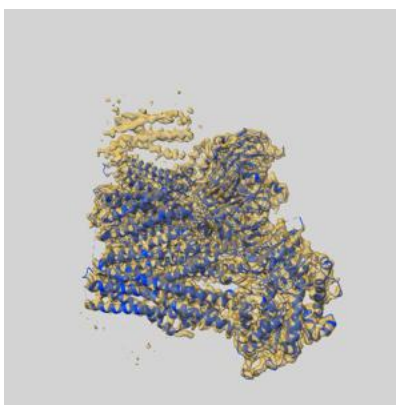
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24845 and PDB model 7S60. Per-residue inclusion information can be found in section 3 on page 7.

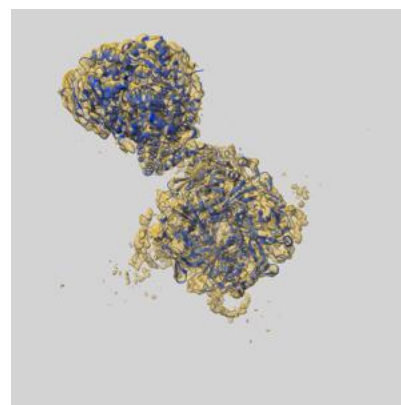
9.1 Map-model overlay [i](#)



X



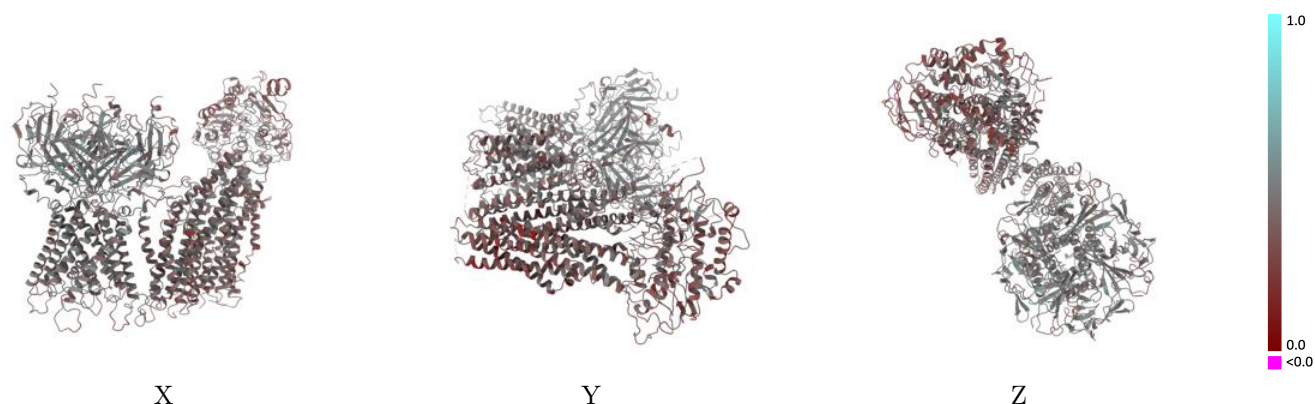
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

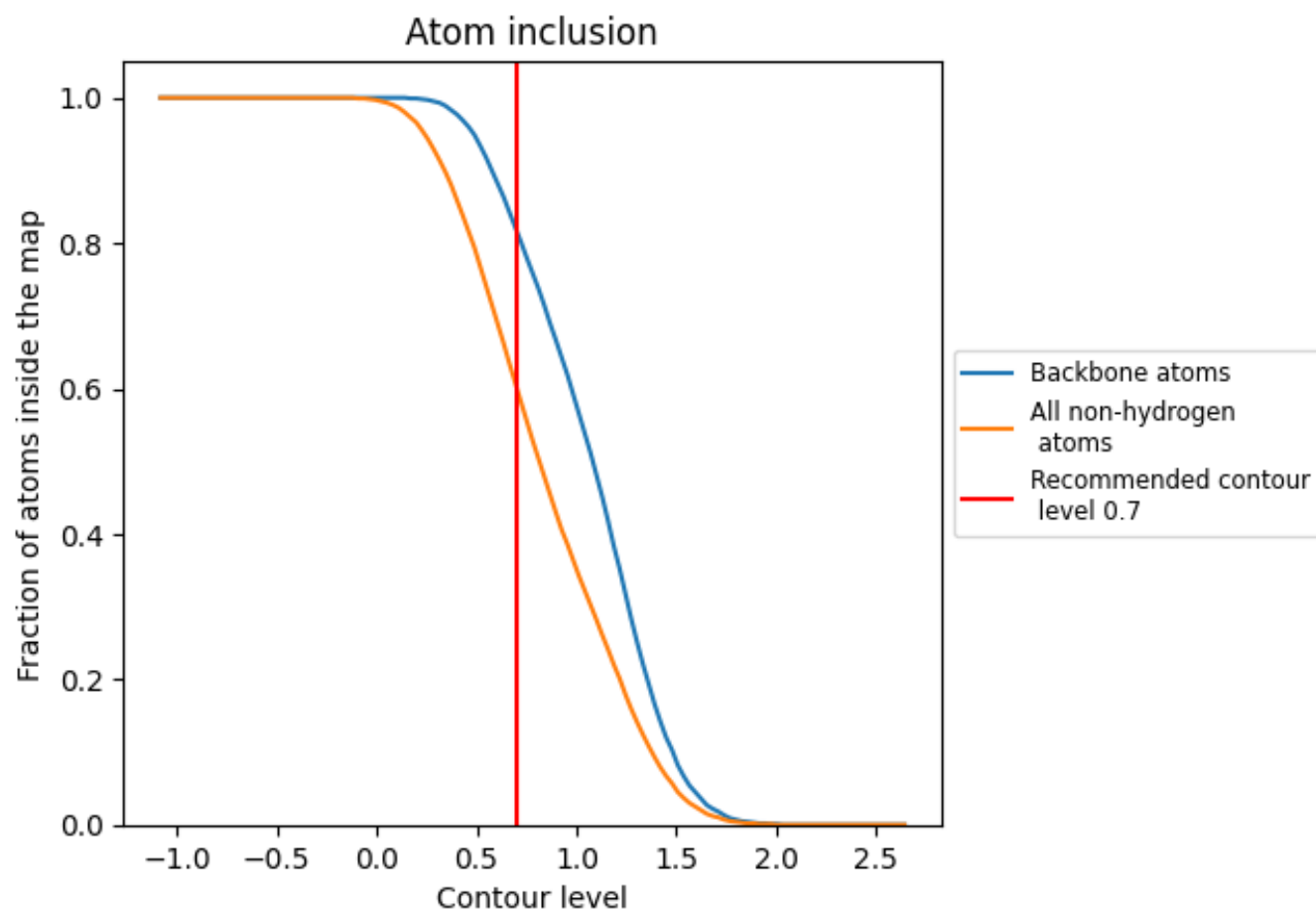


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 60% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6020	0.4190
A	0.6280	0.4580
B	0.6290	0.4590
C	0.6050	0.4550
D	0.6170	0.4550
E	0.5860	0.3840

