



Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 08:37 AM EST

PDB ID : 7S60
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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

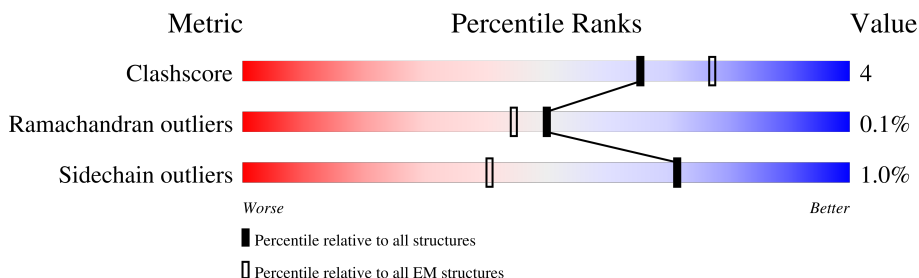
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	<div> <div>6%</div> <div>73%</div> <div>9%</div> <div>18%</div> </div>
1	B	390	<div> <div>6%</div> <div>75%</div> <div>7%</div> <div>18%</div> </div>
1	C	390	<div> <div>8%</div> <div>72%</div> <div>10%</div> <div>18%</div> </div>
1	D	390	<div> <div>7%</div> <div>76%</div> <div>6%</div> <div>18%</div> </div>
2	E	1582	<div> <div>14%</div> <div>76%</div> <div>12%</div> <div>12%</div> </div>

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:

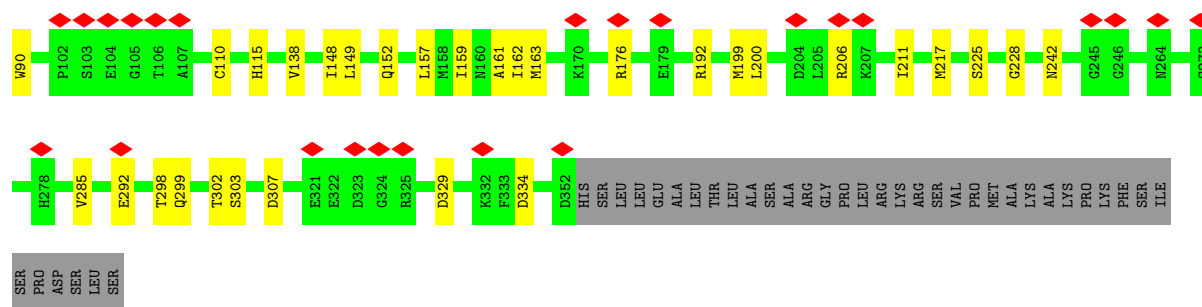
Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MET	-	expression tag	UNP Q09428
E	2	GLY	-	expression tag	UNP Q09428

- # ADP

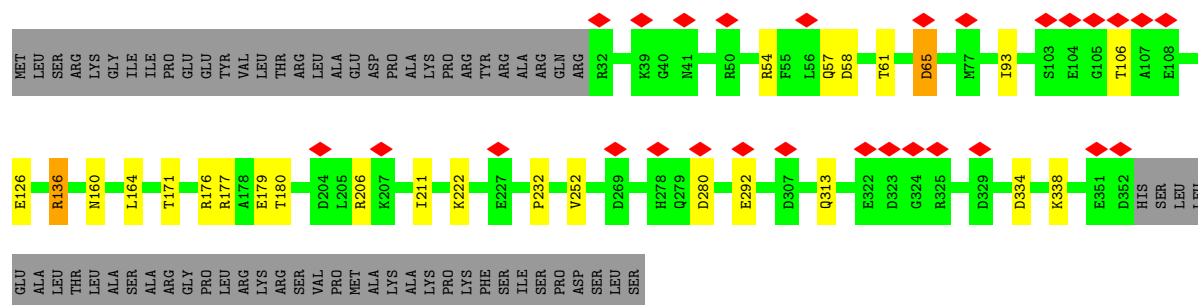
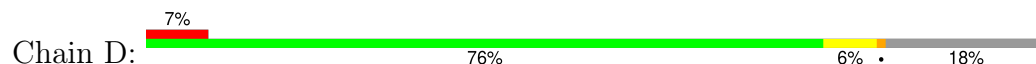
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

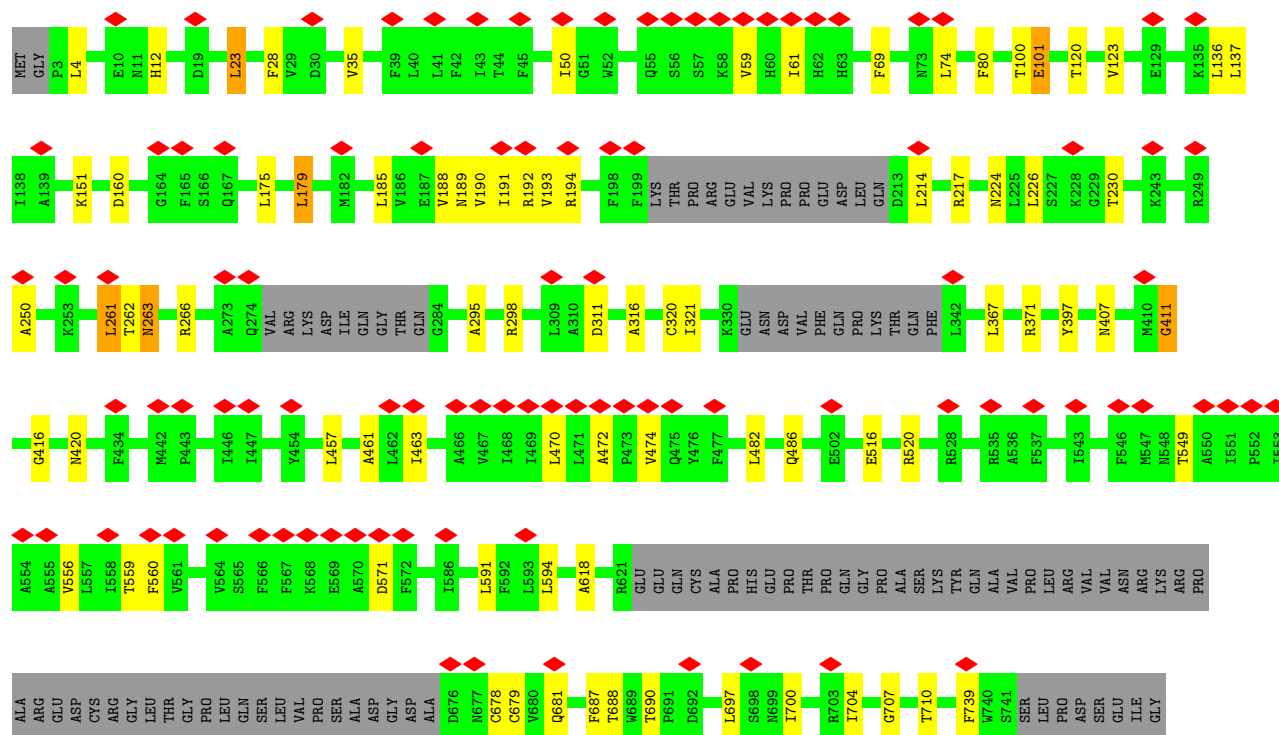


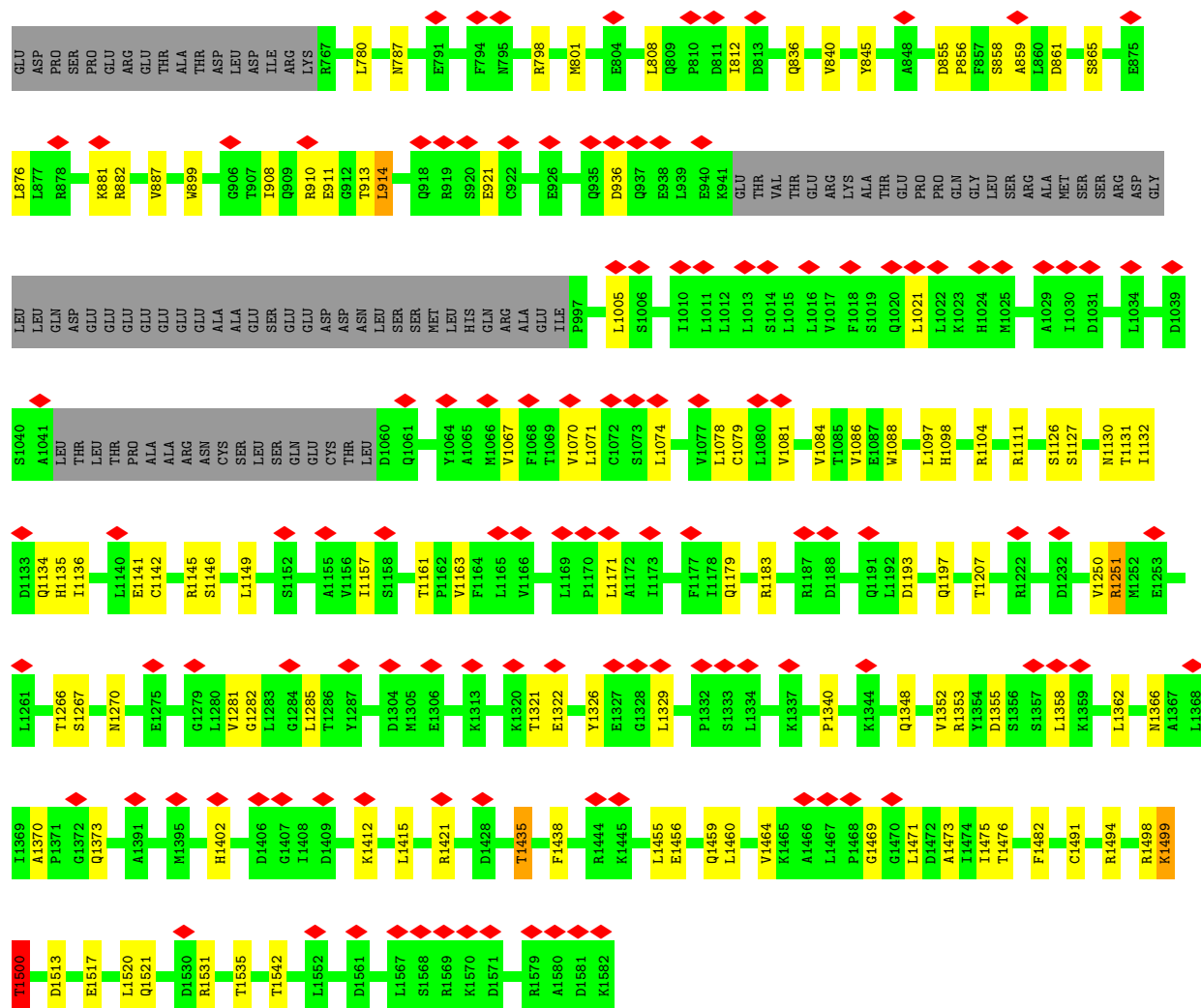


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



- 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, MG, ATP

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	0.46	0/2576	0.67	0/3502
1	B	0.48	0/2584	0.72	1/3512 (0.0%)
1	C	0.47	0/2576	0.67	1/3502 (0.0%)
1	D	0.47	1/2576 (0.0%)	0.68	0/3502
2	E	0.48	1/11175 (0.0%)	0.79	20/15167 (0.1%)
All	All	0.48	2/21487 (0.0%)	0.74	22/29185 (0.1%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	35	VAL	C-N	5.97	1.45	1.34
1	D	252	VAL	C-N	-5.13	1.22	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	261	LEU	CA-CB-CG	11.46	141.67	115.30
2	E	4	LEU	CA-CB-CG	9.67	137.55	115.30
2	E	23	LEU	CA-CB-CG	8.28	134.35	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1460	LEU	CA-CB-CG	7.14	131.72	115.30
2	E	185	LEU	CA-CB-CG	7.04	131.49	115.30
2	E	261	LEU	CB-CG-CD2	6.76	122.49	111.00
2	E	1074	LEU	CA-CB-CG	6.42	130.08	115.30
2	E	263	ASN	C-N-CA	6.36	137.59	121.70
2	E	571	ASP	CB-CG-OD2	6.15	123.83	118.30
2	E	1520	LEU	CA-CB-CG	6.07	129.25	115.30
2	E	1098	HIS	C-N-CA	5.93	136.52	121.70
2	E	1005	LEU	CA-CB-CG	5.75	128.53	115.30
2	E	160	ASP	CB-CG-OD1	5.36	123.13	118.30
2	E	137	LEU	CA-CB-CG	5.36	127.63	115.30
1	C	110	CYS	CA-CB-SG	5.33	123.60	114.00
2	E	1021	LEU	CA-CB-CG	5.33	127.56	115.30
2	E	1171	LEU	CA-CB-CG	5.22	127.31	115.30
1	B	220	VAL	CG1-CB-CG2	-5.20	102.59	110.90
2	E	1250	VAL	CG1-CB-CG2	-5.19	102.60	110.90
2	E	214	LEU	CA-CB-CG	5.12	127.08	115.30
2	E	914	LEU	CA-CB-CG	5.10	127.02	115.30
2	E	136	LEU	CA-CB-CG	-5.09	103.58	115.30

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	21	0
1	C	2519	0	2547	27	0
1	D	2519	0	2547	18	0
2	E	10942	0	11212	87	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	161	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 (161) 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
2:E:808:LEU:O	2:E:812:ILE:HB	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:58:ASP:N	1:A:58:ASP:OD1	2.49	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:224:ASN:N	2:E:224:ASN:OD1	2.46	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
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:1104:ARG:NH2	2:E:1321:THR:O	2.50	0.45
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
2:E:1348:GLN:HB3	2:E:1402:HIS:HB3	1.98	0.45
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:913:THR:OG1	2:E:914:LEU:N	2.50	0.43
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
1:C:302:THR:OG1	1:C:303:SER:N	2.52	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:798:ARG:HH22	2:E:882:ARG:HH11	1.67	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:549:THR:OG1	2:E:1079:CYS:SG	2.78	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
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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/390 (82%)	310 (97%)	9 (3%)	0	100	100
1	B	320/390 (82%)	306 (96%)	13 (4%)	1 (0%)	37	67
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2656/3142 (84%)	2513 (95%)	140 (5%)	3 (0%)	50 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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	278/337 (82%)	275 (99%)	3 (1%)	70 80
1	B	279/337 (83%)	279 (100%)	0	100 100
1	C	278/337 (82%)	275 (99%)	3 (1%)	70 80
1	D	278/337 (82%)	274 (99%)	4 (1%)	62 76
2	E	1182/1368 (86%)	1168 (99%)	14 (1%)	67 79
All	All	2295/2716 (84%)	2271 (99%)	24 (1%)	71 82

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

Mol	Chain	Res	Type
1	A	50	ARG
1	A	200	LEU
1	A	220	VAL
1	C	65	ASP
1	C	115	HIS
1	C	200	LEU
1	D	65	ASP
1	D	106	THR
1	D	136	ARG
1	D	280	ASP
2	E	59	VAL

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Mol	Chain	Res	Type
2	E	74	LEU
2	E	179	LEU
2	E	261	LEU
2	E	298	ARG
2	E	474	VAL
2	E	559	THR
2	E	704	ILE
2	E	887	VAL
2	E	1088	TRP
2	E	1251	ARG
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 (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	264	ASN
1	A	277	HIS
1	C	175	HIS
1	C	277	HIS
1	D	43	ASN
1	D	264	ASN
2	E	189	ASN
2	E	375	GLN
2	E	407	ASN
2	E	427	ASN
2	E	445	GLN
2	E	499	GLN
2	E	708	GLN
2	E	715	GLN
2	E	1346	GLN
2	E	1459	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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	28,33,33	0.84	0	34,52,52	1.36	5 (14%)
3	ADP	E	1601	4	24,29,29	0.87	0	29,45,45	1.41	3 (10%)

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	-	4/18/38/38	0/3/3/3
3	ADP	E	1601	4	-	2/12/32/32	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1604	ATP	N3-C2-N1	-4.57	122.47	128.67
3	E	1601	ADP	N3-C2-N1	-4.31	122.83	128.67
5	E	1604	ATP	C4'-O4'-C1'	2.55	112.26	109.92
3	E	1601	ADP	C4-C5-N7	-2.27	106.94	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1604	ATP	O4'-C1'-N9	-2.24	105.78	108.75
3	E	1601	ADP	O2A-PA-O3A	2.21	113.26	107.27
5	E	1604	ATP	N6-C6-N1	2.10	122.83	118.33
5	E	1604	ATP	C2'-C3'-C4'	2.06	106.58	102.61

There are no chirality outliers.

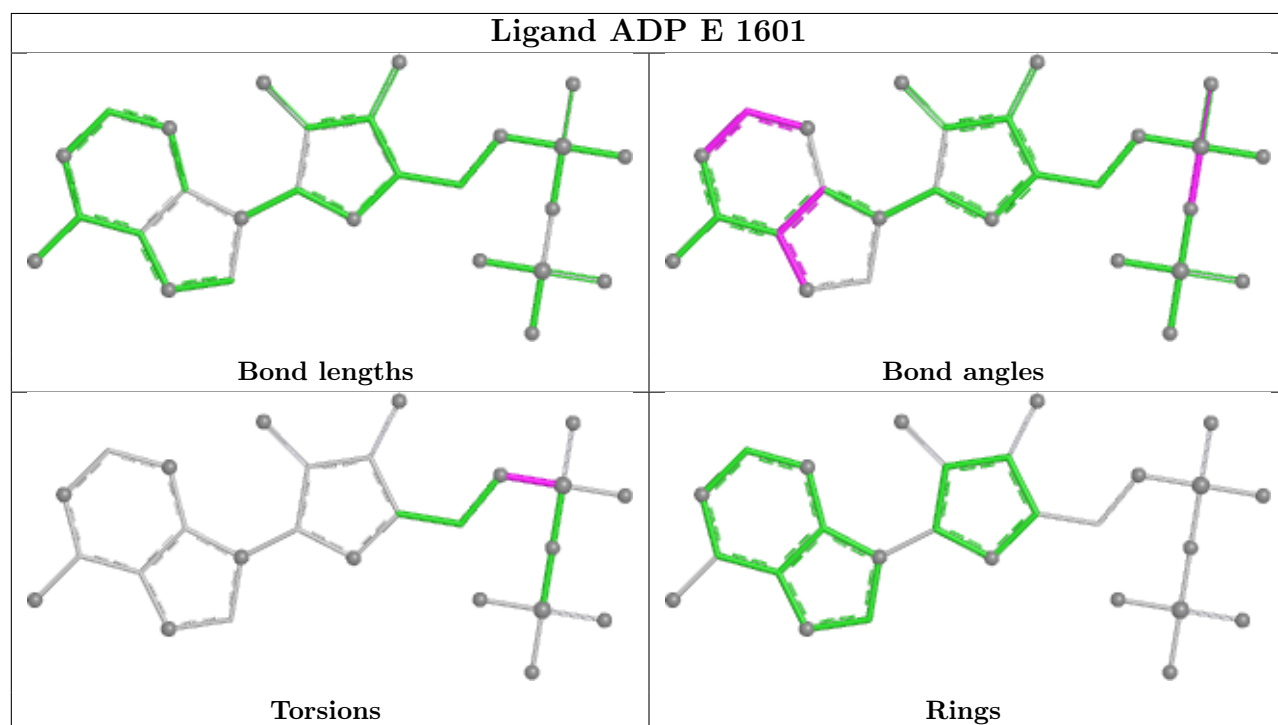
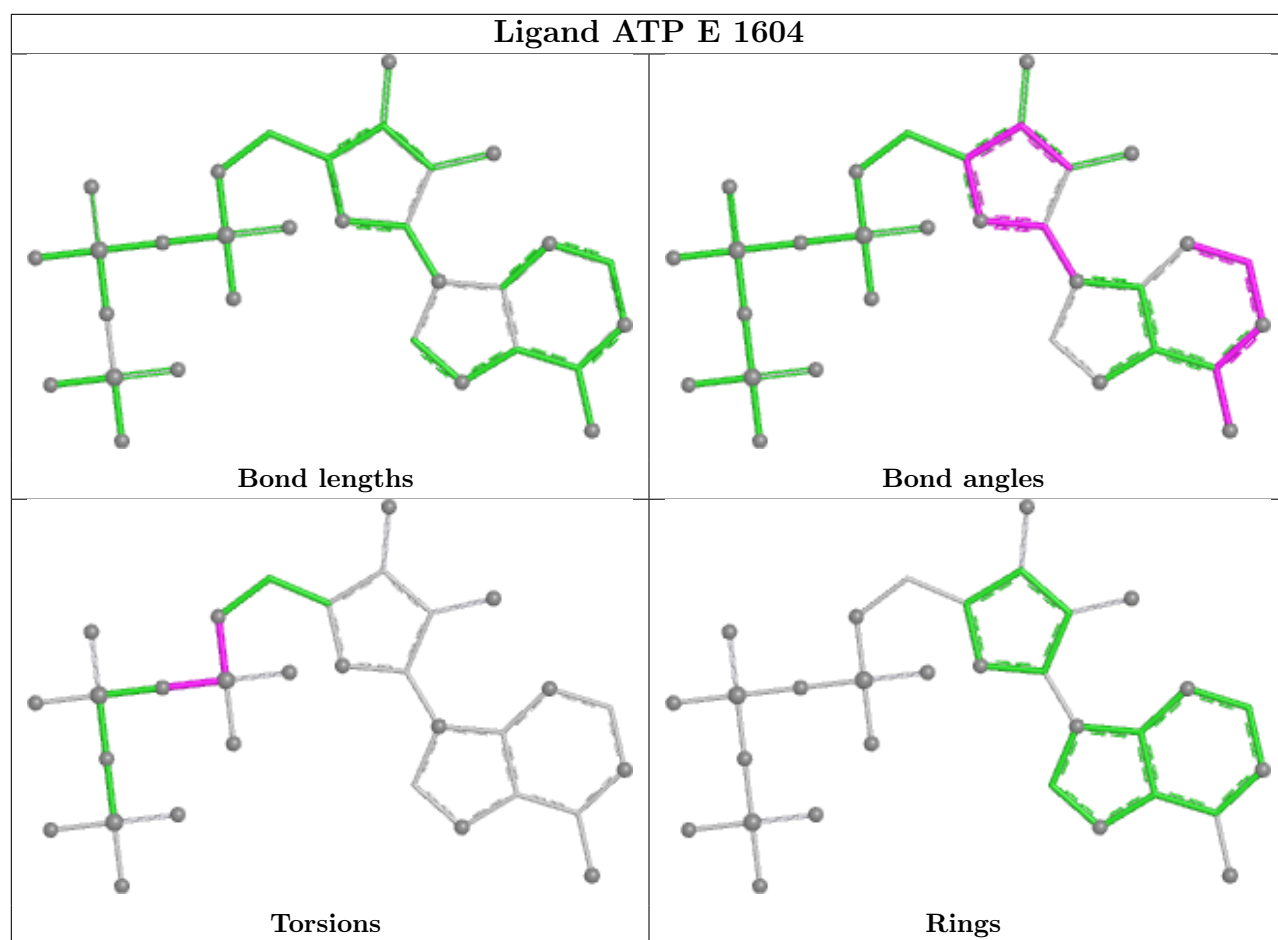
All (6) torsion outliers are listed below:

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
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.

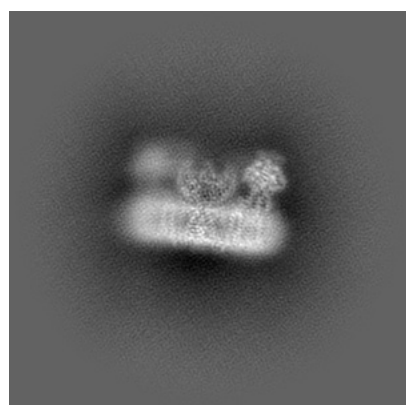
6 Map visualisation [i](#)

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.

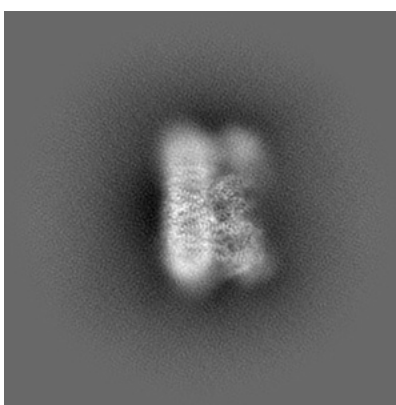
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

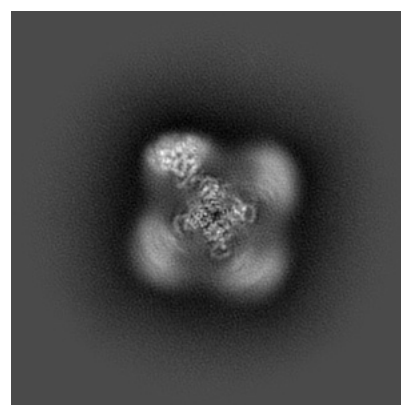
6.1.1 Primary map



X



Y

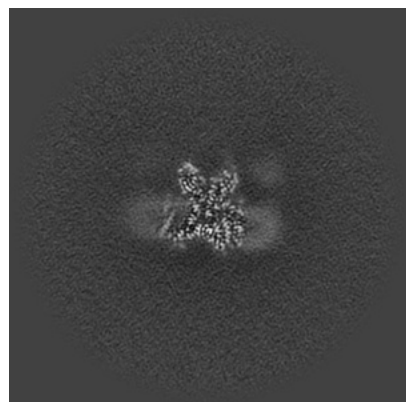


Z

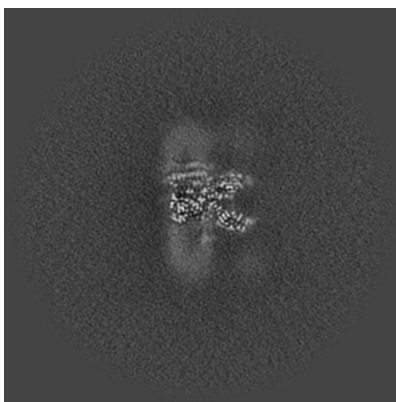
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

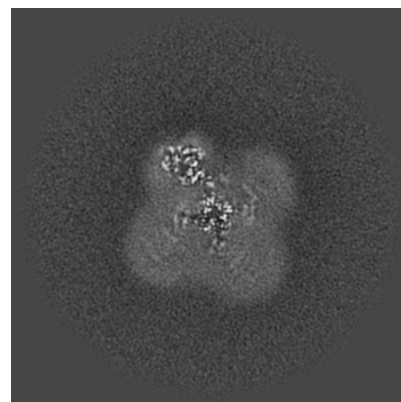
6.2.1 Primary map



X Index: 182



Y Index: 182

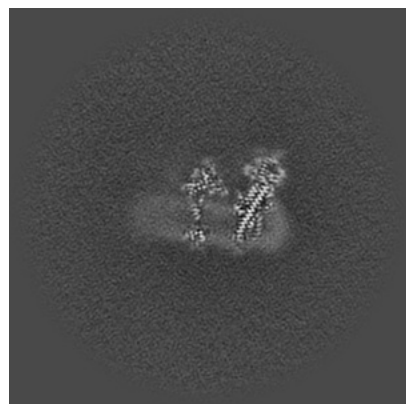


Z Index: 182

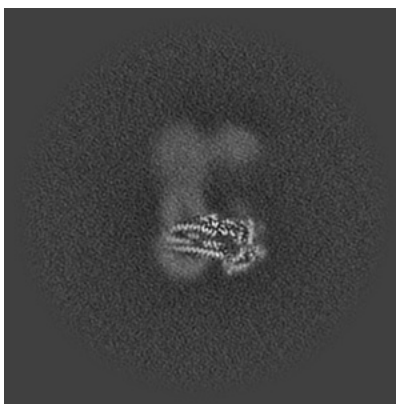
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

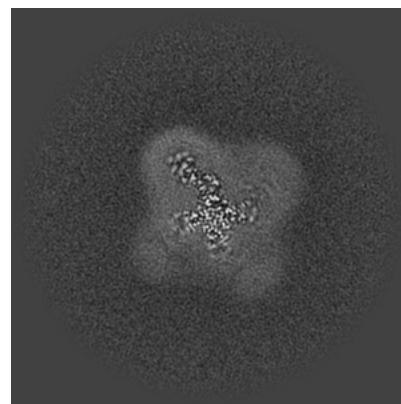
6.3.1 Primary map



X Index: 166



Y Index: 227

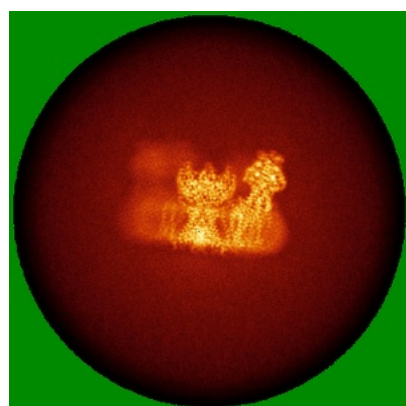


Z Index: 156

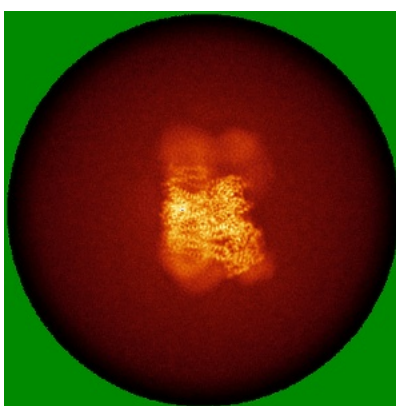
The images above show the largest variance slices of the map in three orthogonal directions.

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

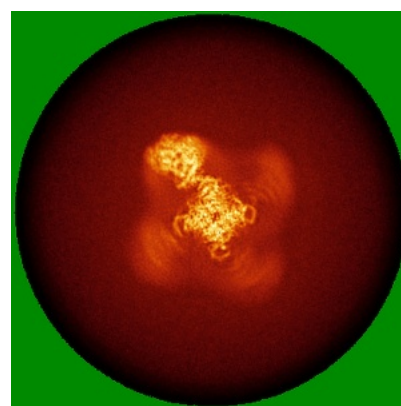
6.4.1 Primary map



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.

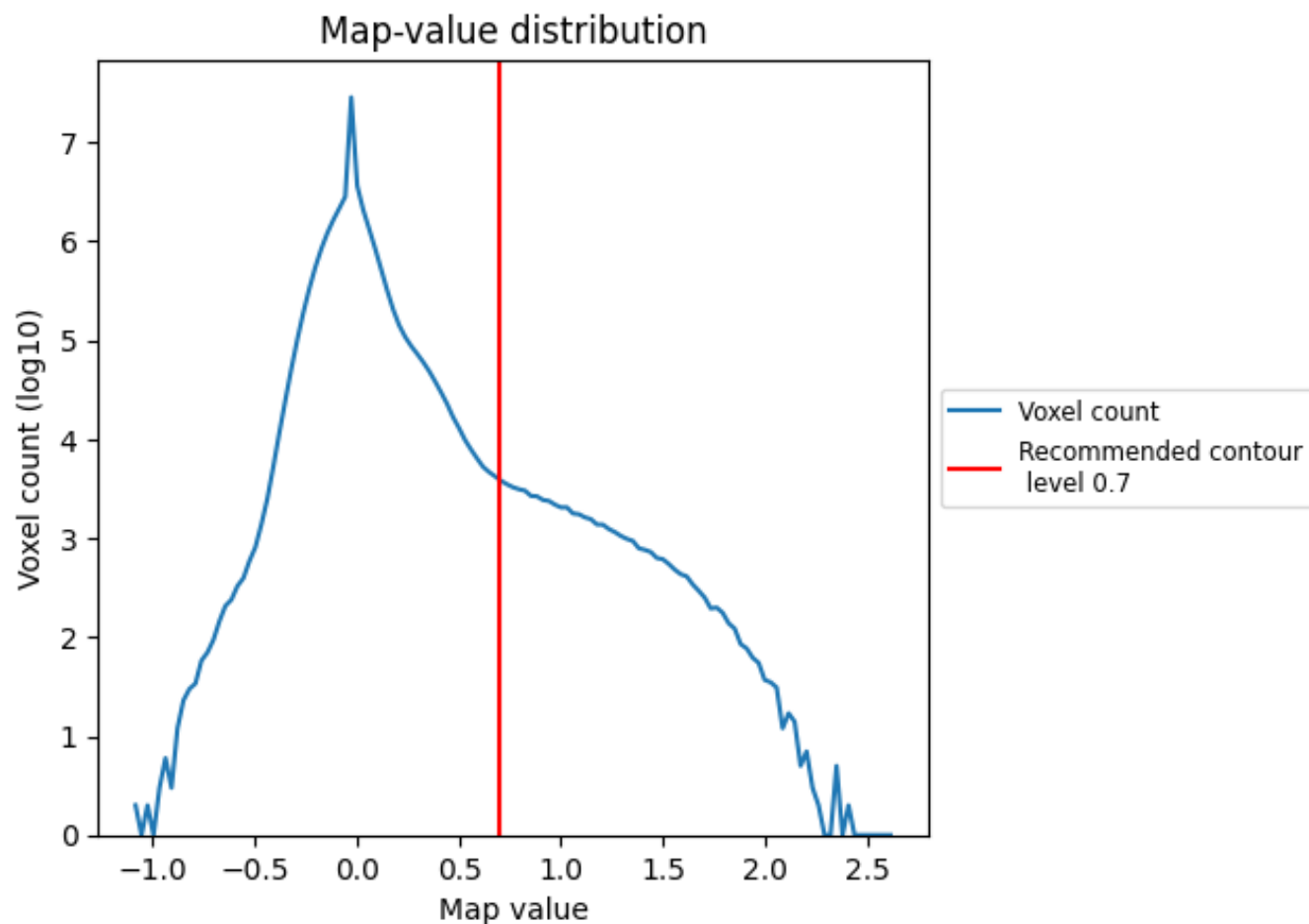
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

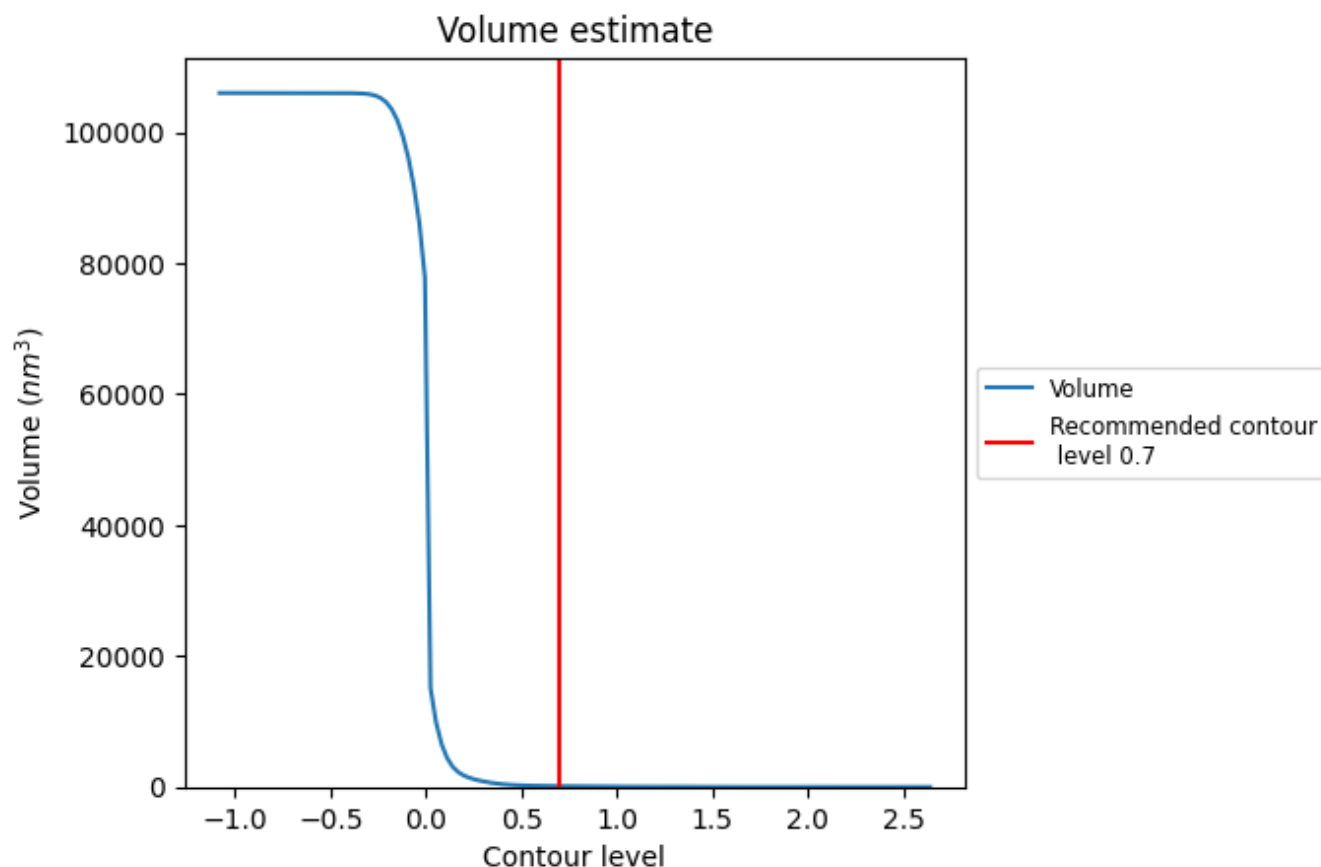
This section contains the results of statistical analysis of the map.

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.

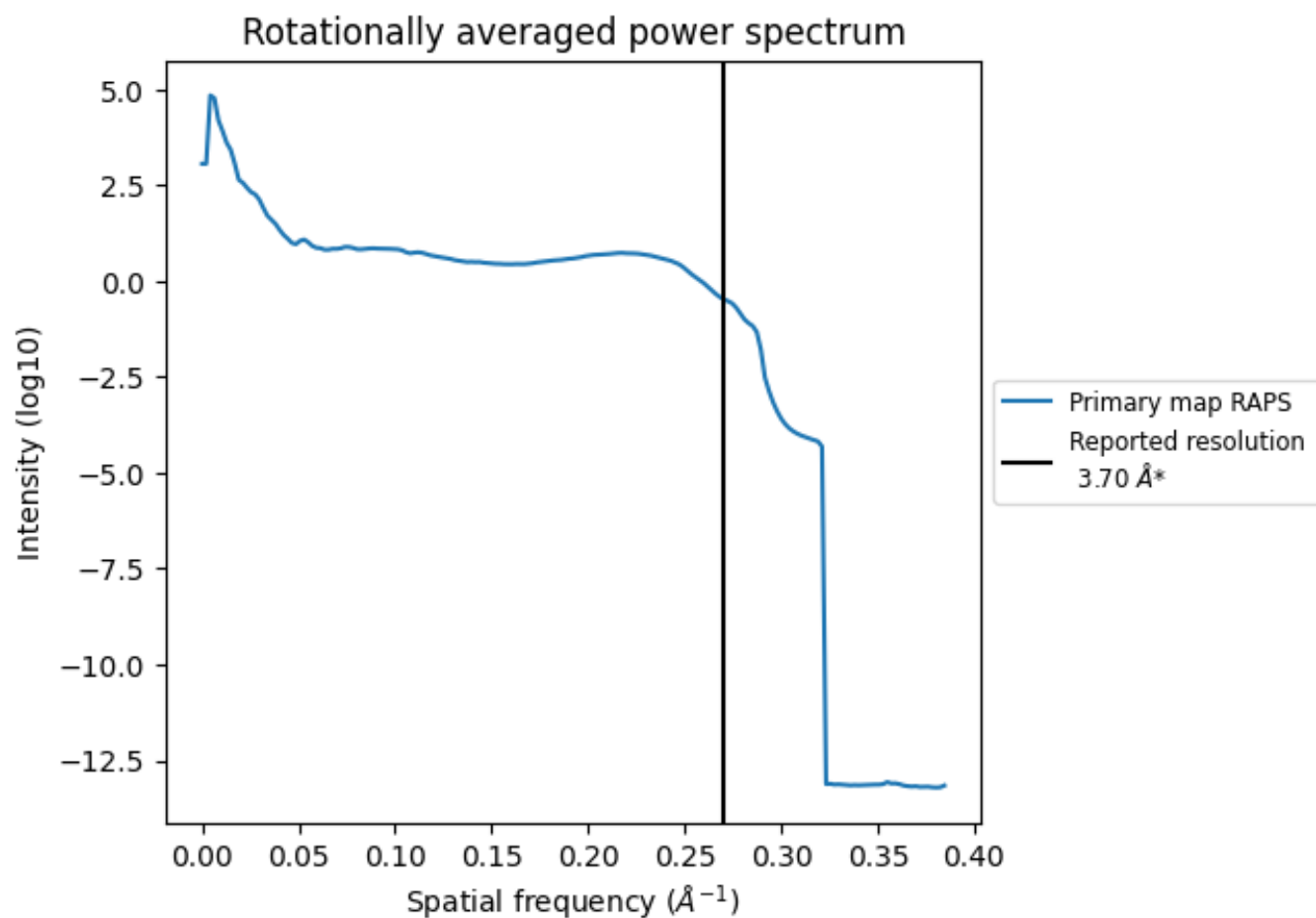
7.2 Volume estimate [i](#)



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 ⓘ

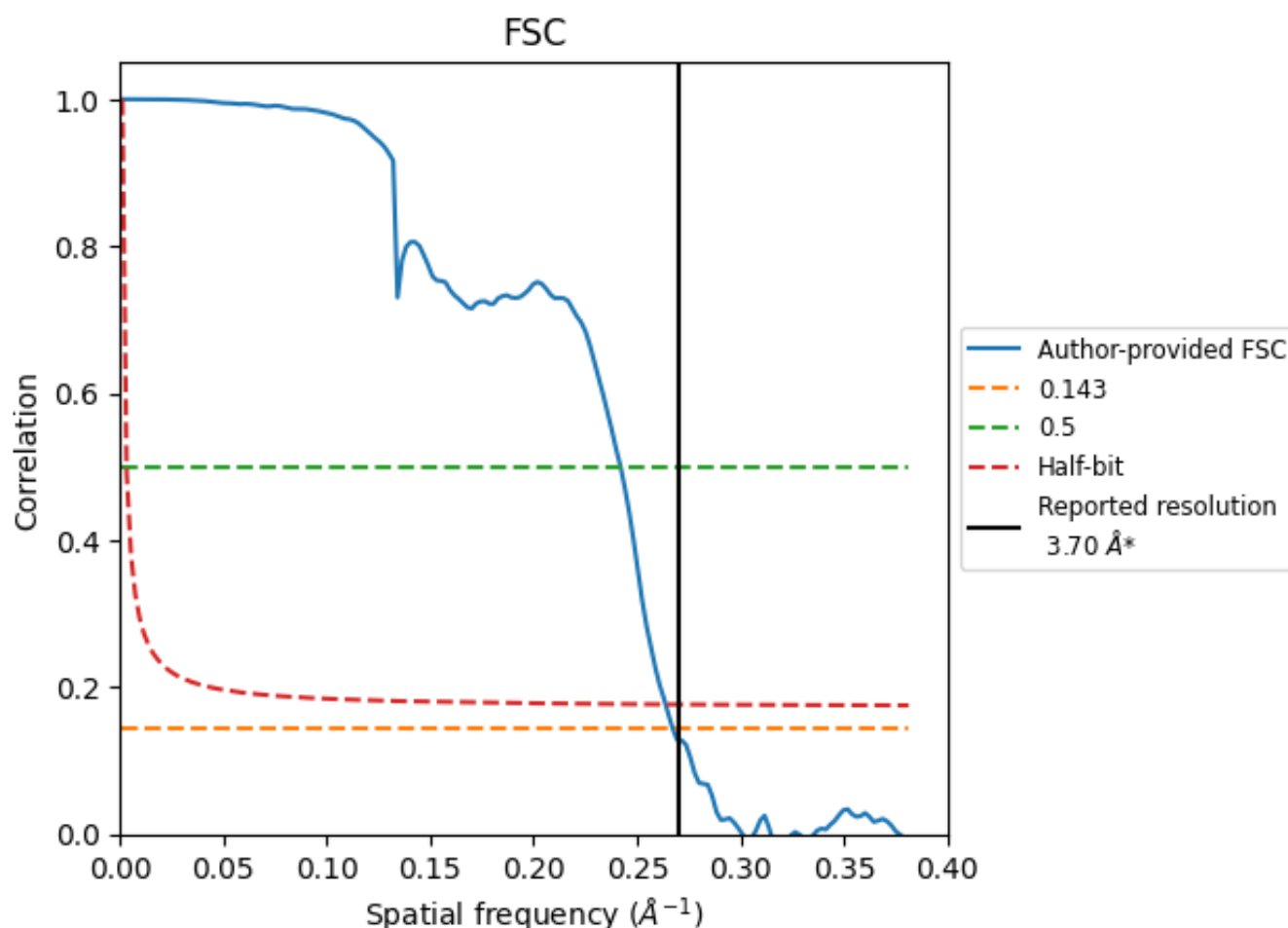


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

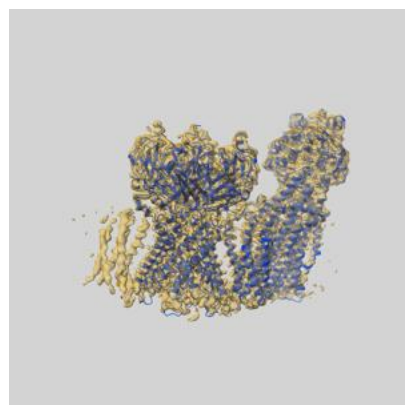
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.74	4.13	3.79
Unmasked-calculated*	-	-	-

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

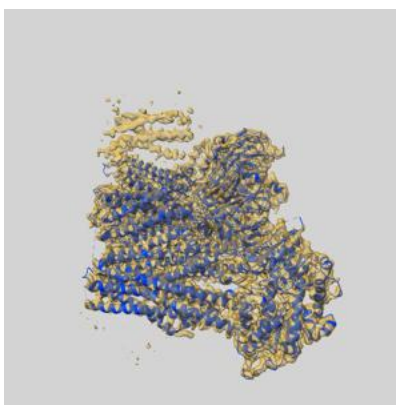
9 Map-model fit [i](#)

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 6.

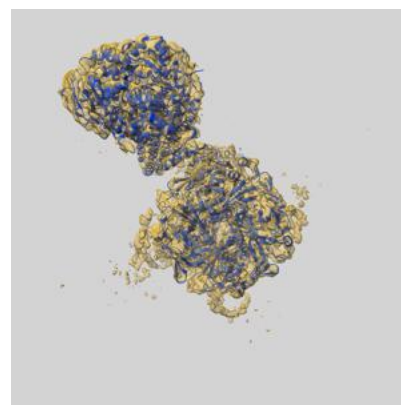
9.1 Map-model overlay [i](#)



X



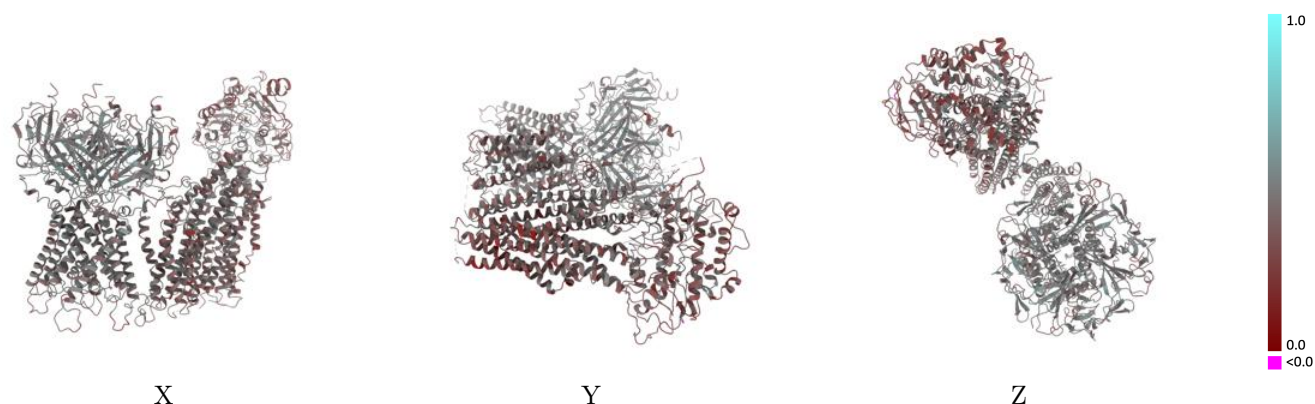
Y



Z

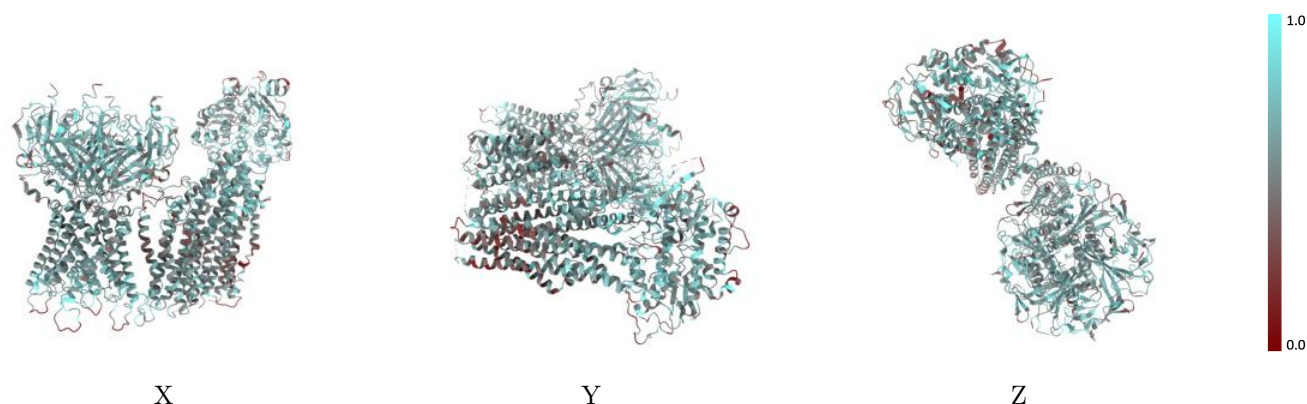
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



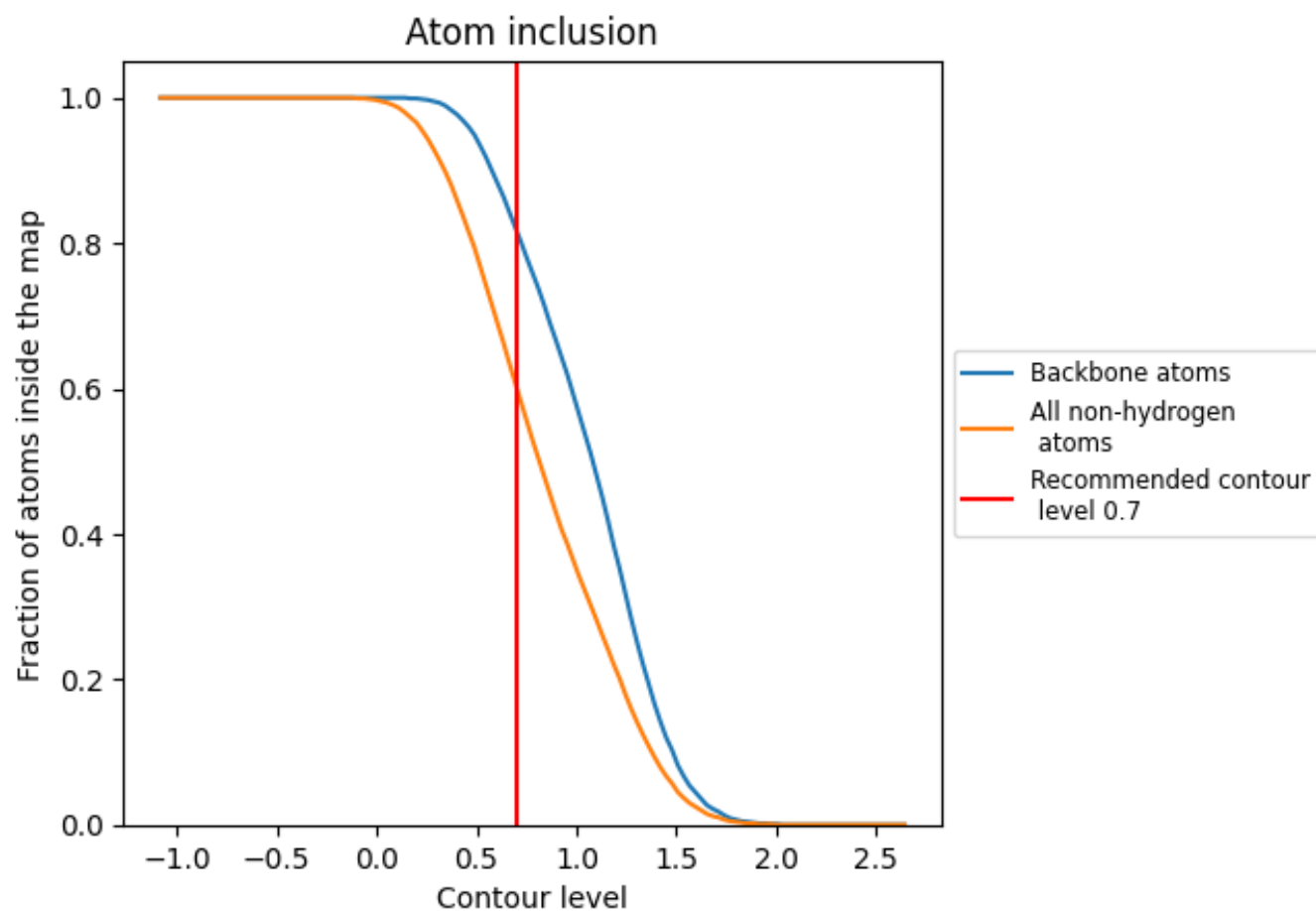
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.7).

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	<div></div> 0.6020	<div></div> 0.4190
A	<div></div> 0.6280	<div></div> 0.4580
B	<div></div> 0.6290	<div></div> 0.4590
C	<div></div> 0.6050	<div></div> 0.4550
D	<div></div> 0.6170	<div></div> 0.4550
E	<div></div> 0.5860	<div></div> 0.3840

