



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 10:22 AM UTC

PDB ID : 7S5Y / pdb_00007s5y
EMDB ID : EMD-24843
Title : Human KATP channel in open conformation, focused on Kir and one SUR, position 2
Authors : Zhao, C.; MacKinnon, R.
Deposited on : 2021-09-12
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 ⓘ 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:

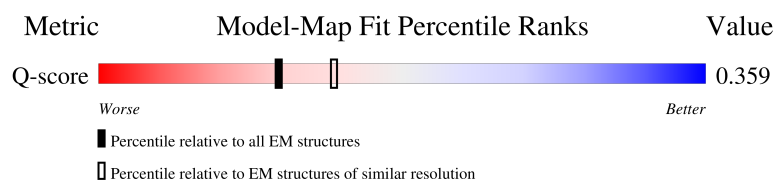
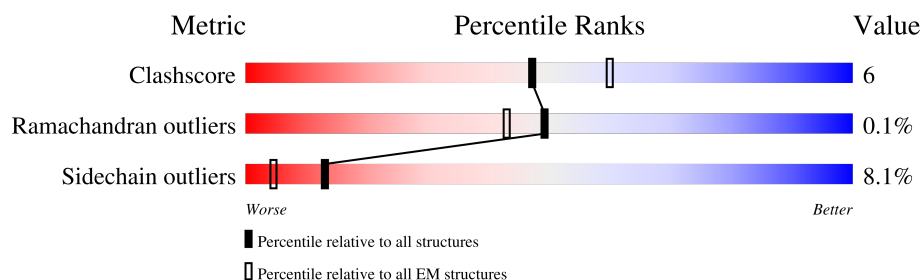
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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 $\leq 5\%$. 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	14% 59% 21% • 18%
1	B	390	20% 59% 22% • 18%
1	C	390	17% 59% 21% • 18%
1	D	390	18% 60% 21% • 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	1582	26% 73% 15% • 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21106 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	0	0
			2519	1622	430	451	16		
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

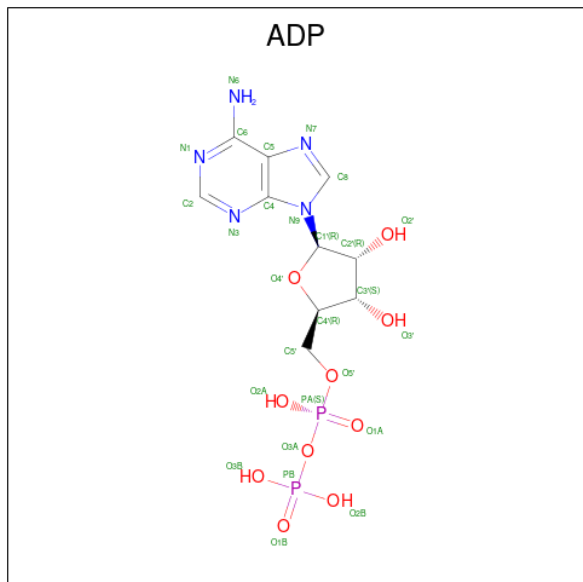
- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	1402	Total	C	N	O	S	0	0
			10970	7131	1864	1920	55		

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

Mol	Chain	Residues	Atoms		AltConf
4	E	2	Total	Mg	0
			2	2	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

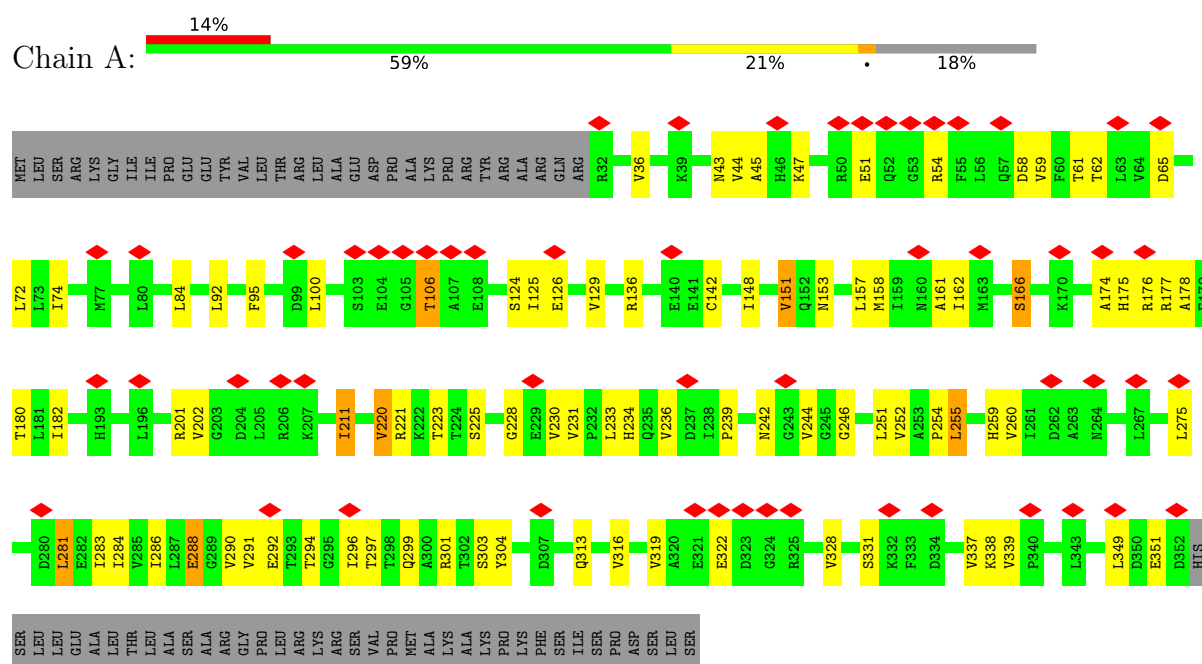


Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

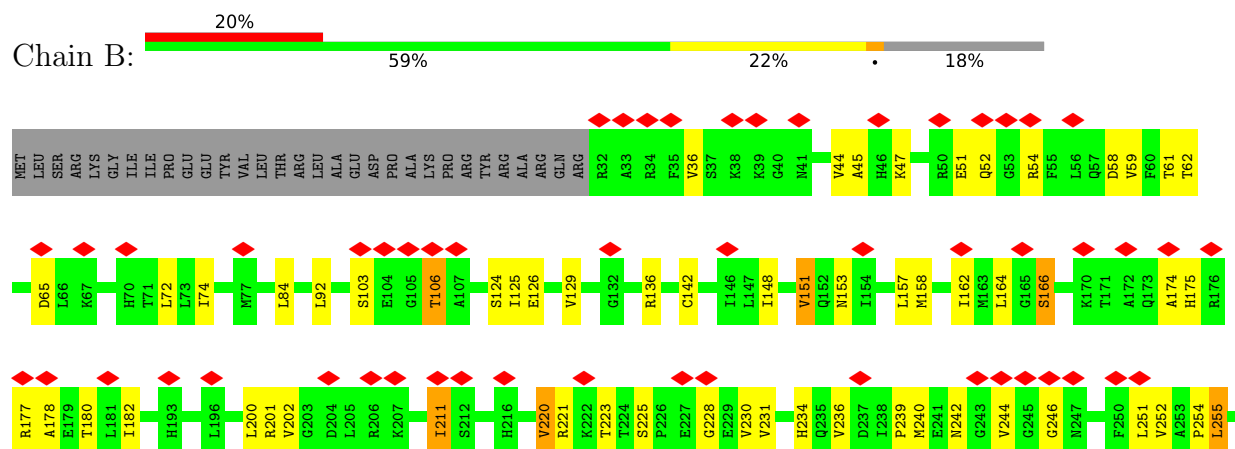
3 Residue-property plots

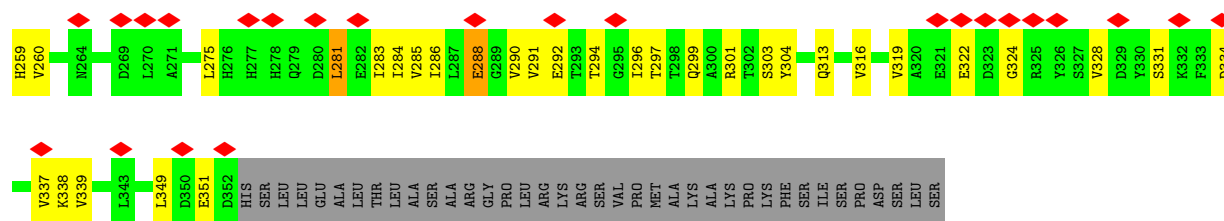
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

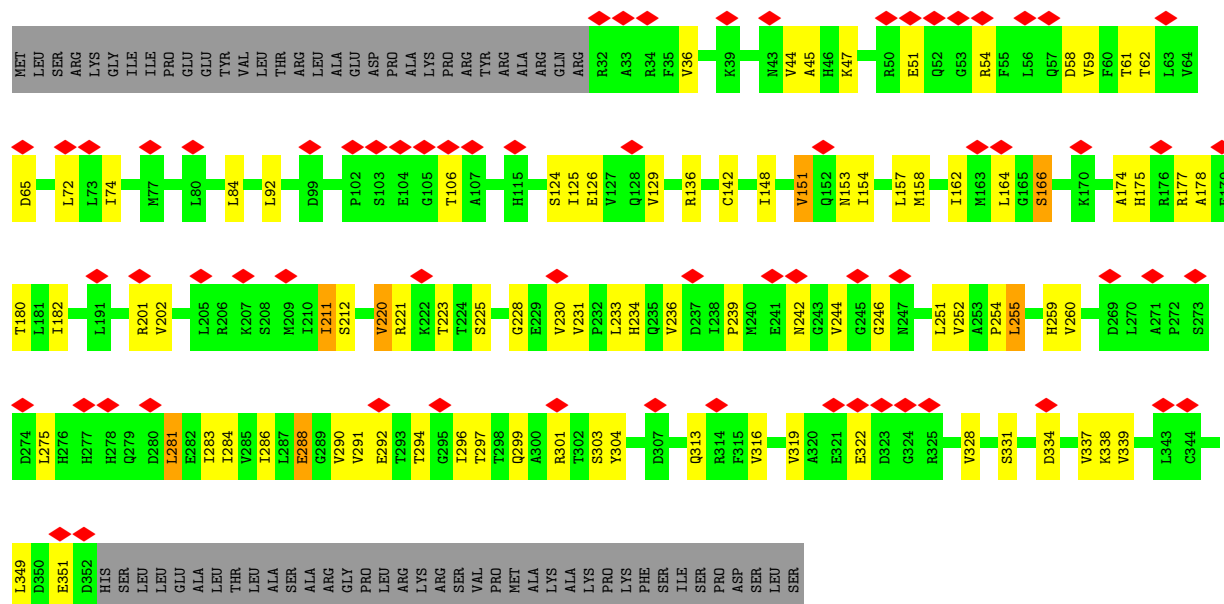


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

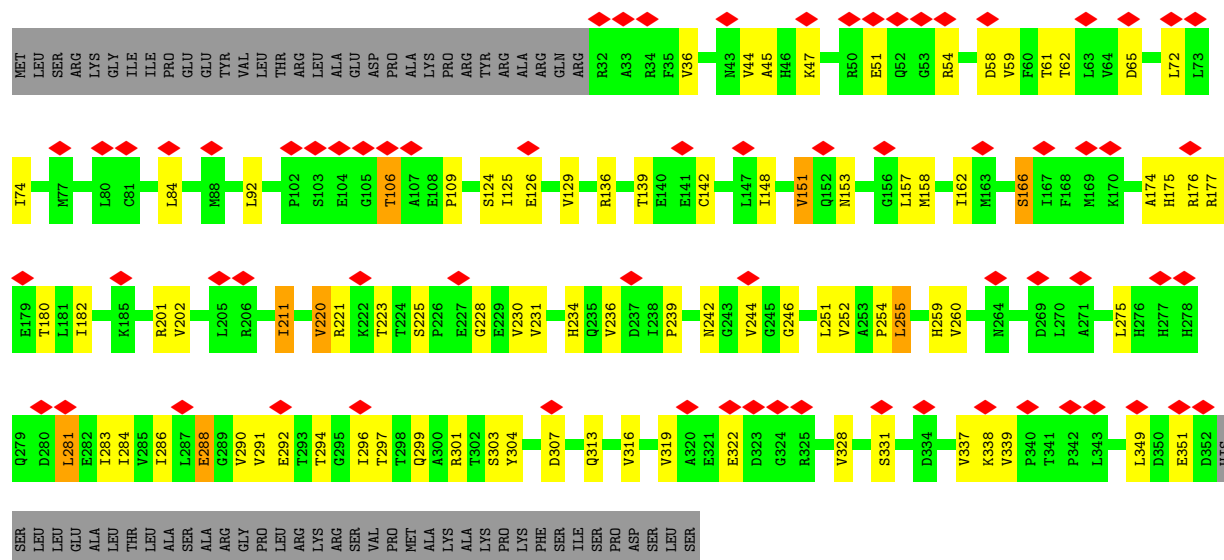




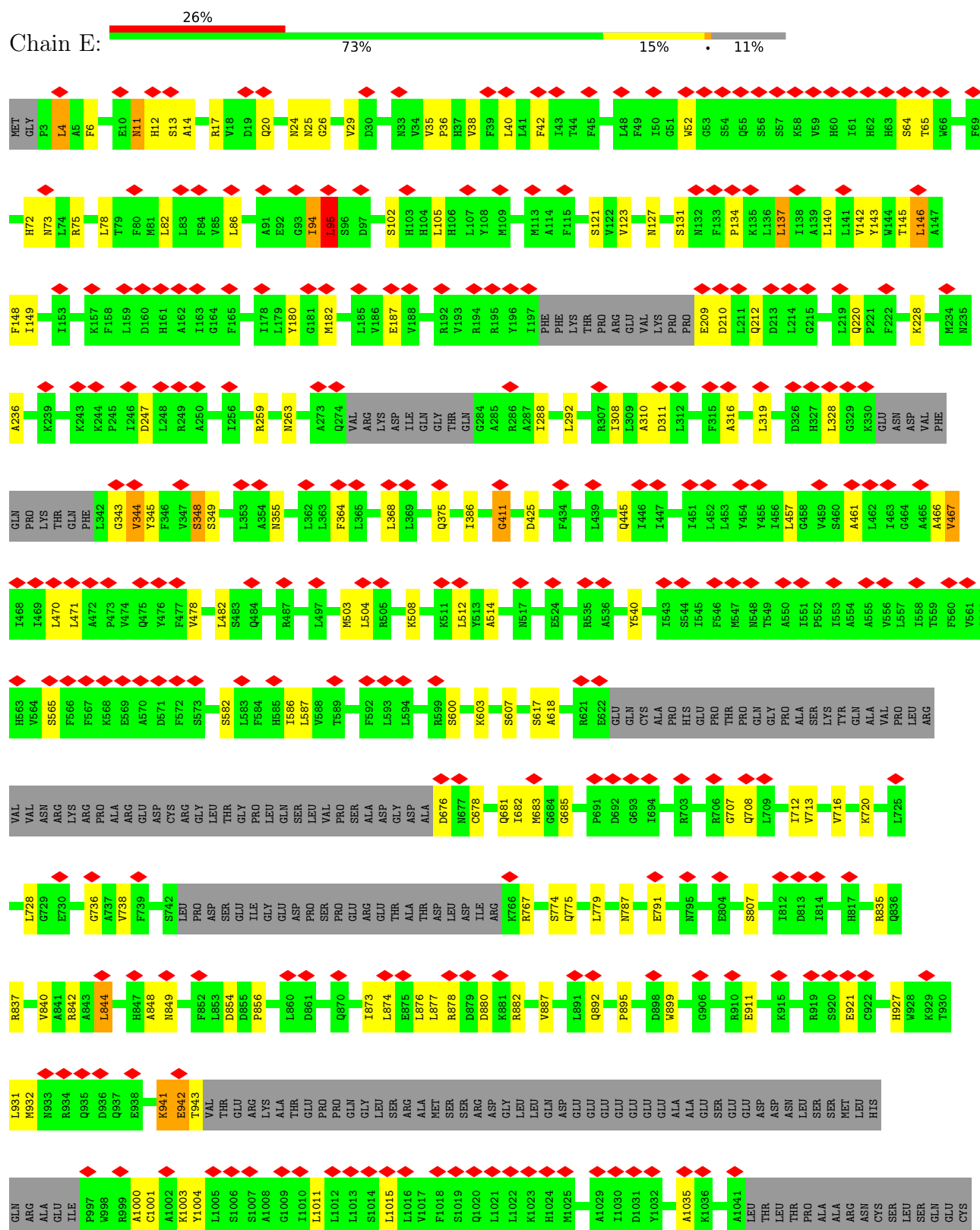
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

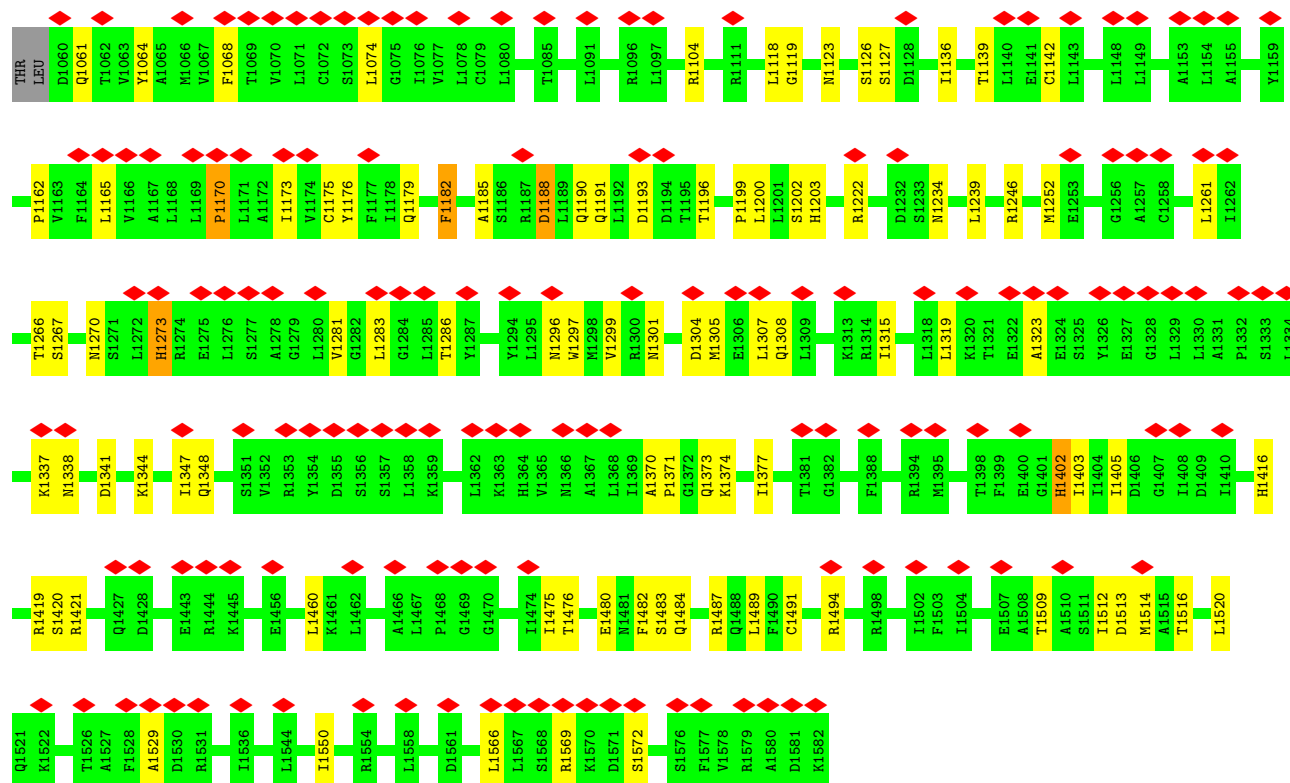


• Molecule 1: ATP-sensitive inward rectifier potassium channel 11



• 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	24689	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	2.090	Depositor
Minimum map value	-0.791	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.075	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 [i](#)

5.1 Standard geometry [i](#)

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	0.44	0/2576	0.79	6/3502 (0.2%)
1	B	0.44	0/2576	0.79	6/3502 (0.2%)
1	C	0.44	0/2576	0.79	6/3502 (0.2%)
1	D	0.44	0/2576	0.80	6/3502 (0.2%)
2	E	0.45	1/11201 (0.0%)	0.93	45/15205 (0.3%)
All	All	0.44	1/21505 (0.0%)	0.87	69/29213 (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
2	E	0	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1136	ILE	C-N	5.09	1.45	1.33

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	310	ALA	CA-C-N	7.38	135.64	121.54
2	E	310	ALA	C-N-CA	7.38	135.64	121.54
2	E	1061	GLN	CA-C-N	6.71	134.35	121.54
2	E	1061	GLN	C-N-CA	6.71	134.35	121.54
2	E	600	SER	CA-C-N	6.69	134.32	121.54
2	E	600	SER	C-N-CA	6.69	134.32	121.54
2	E	348	SER	CA-C-N	6.47	130.52	120.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	348	SER	C-N-CA	6.47	130.52	120.82
2	E	565	SER	CA-C-N	6.40	133.76	121.54
2	E	565	SER	C-N-CA	6.40	133.76	121.54
2	E	72	HIS	CA-C-N	6.32	137.34	125.66
2	E	72	HIS	C-N-CA	6.32	137.34	125.66
2	E	1273	HIS	CA-C-N	6.26	134.17	122.84
2	E	1273	HIS	C-N-CA	6.26	134.17	122.84
2	E	94	ILE	CA-C-N	6.00	133.01	121.54
2	E	94	ILE	C-N-CA	6.00	133.01	121.54
2	E	11	ASN	CA-C-N	5.91	132.84	121.54
2	E	11	ASN	C-N-CA	5.91	132.84	121.54
2	E	209	GLU	CA-C-N	5.86	132.74	121.54
2	E	209	GLU	C-N-CA	5.86	132.74	121.54
1	D	337	VAL	CA-C-N	5.71	132.45	121.54
1	D	337	VAL	C-N-CA	5.71	132.45	121.54
1	A	337	VAL	CA-C-N	5.70	132.43	121.54
1	A	337	VAL	C-N-CA	5.70	132.43	121.54
1	B	337	VAL	CA-C-N	5.70	132.42	121.54
1	B	337	VAL	C-N-CA	5.70	132.42	121.54
1	C	337	VAL	CA-C-N	5.70	132.42	121.54
1	C	337	VAL	C-N-CA	5.70	132.42	121.54
2	E	1569	ARG	CA-C-N	5.69	132.41	121.54
2	E	1569	ARG	C-N-CA	5.69	132.41	121.54
2	E	349	SER	N-CA-C	5.64	120.68	111.37
1	B	351	GLU	CA-C-N	5.64	131.85	121.70
1	B	351	GLU	C-N-CA	5.64	131.85	121.70
1	C	351	GLU	CA-C-N	5.63	131.83	121.70
1	C	351	GLU	C-N-CA	5.63	131.83	121.70
2	E	874	LEU	CA-CB-CG	5.61	135.94	116.30
2	E	64	SER	CA-C-N	5.61	130.78	122.82
2	E	64	SER	C-N-CA	5.61	130.78	122.82
1	D	351	GLU	CA-C-N	5.61	131.79	121.70
1	D	351	GLU	C-N-CA	5.61	131.79	121.70
2	E	73	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	351	GLU	CA-C-N	5.59	131.75	121.70
1	A	351	GLU	C-N-CA	5.59	131.75	121.70
2	E	1405	ILE	CA-C-N	5.59	130.29	122.08
2	E	1405	ILE	C-N-CA	5.59	130.29	122.08
2	E	311	ASP	CA-CB-CG	5.50	118.10	112.60
2	E	844	LEU	CA-CB-CG	5.46	135.40	116.30
1	D	322	GLU	CA-C-N	5.44	131.93	121.54
1	D	322	GLU	C-N-CA	5.44	131.93	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	GLU	CA-C-N	5.43	131.91	121.54
1	B	322	GLU	C-N-CA	5.43	131.91	121.54
1	C	322	GLU	CA-C-N	5.42	131.90	121.54
1	C	322	GLU	C-N-CA	5.42	131.90	121.54
2	E	921	GLU	CA-C-N	5.41	131.55	123.05
2	E	921	GLU	C-N-CA	5.41	131.55	123.05
1	A	322	GLU	CA-C-N	5.41	131.88	121.54
1	A	322	GLU	C-N-CA	5.41	131.88	121.54
2	E	14	ALA	CA-C-N	5.32	131.71	121.54
2	E	14	ALA	C-N-CA	5.32	131.71	121.54
2	E	95	LEU	CA-CB-CG	5.30	134.84	116.30
2	E	6	PHE	CA-C-N	5.28	131.91	122.09
2	E	6	PHE	C-N-CA	5.28	131.91	122.09
2	E	344	VAL	N-CA-C	5.25	120.27	109.34
2	E	932	MET	CA-C-N	5.25	131.30	123.05
2	E	932	MET	C-N-CA	5.25	131.30	123.05
2	E	848	ALA	CA-C-N	5.19	131.45	121.54
2	E	848	ALA	C-N-CA	5.19	131.45	121.54
2	E	236	ALA	CA-C-N	5.02	132.24	123.91
2	E	236	ALA	C-N-CA	5.02	132.24	123.91

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	102	SER	Peptide
2	E	1170	PRO	Peptide
2	E	1182	PHE	Peptide
2	E	1188	ASP	Peptide
2	E	1273	HIS	Peptide
2	E	131	SER	Peptide
2	E	137	LEU	Peptide
2	E	1402	HIS	Peptide
2	E	145	THR	Peptide
2	E	146	LEU	Peptide
2	E	343	GLY	Peptide
2	E	348	SER	Peptide
2	E	4	LEU	Peptide
2	E	411	GLY	Peptide
2	E	854	ASP	Peptide
2	E	95	LEU	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	2549	33	0
1	B	2519	0	2549	36	0
1	C	2519	0	2549	33	0
1	D	2519	0	2549	32	0
2	E	10970	0	11215	128	0
3	E	27	0	12	0	0
4	E	2	0	0	0	0
5	E	31	0	12	1	0
All	All	21106	0	21435	255	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 6.

All (255) 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:942:GLU:OE1	2:E:942:GLU:HA	1.73	0.88
2:E:466:ALA:O	2:E:470:LEU:HB2	1.79	0.83
1:C:61:THR:O	1:C:65:ASP:HB2	1.81	0.81
1:B:61:THR:O	1:B:65:ASP:HB2	1.81	0.81
1:A:61:THR:O	1:A:65:ASP:HB2	1.81	0.80
2:E:941:LYS:HE3	2:E:941:LYS:O	1.80	0.80
1:D:61:THR:O	1:D:65:ASP:HB2	1.81	0.79
1:C:220:VAL:HA	1:C:234:HIS:O	1.91	0.71
1:A:220:VAL:HA	1:A:234:HIS:O	1.91	0.71
1:D:220:VAL:HA	1:D:234:HIS:O	1.91	0.71
1:B:220:VAL:HA	1:B:234:HIS:O	1.91	0.70
2:E:1000:ALA:O	2:E:1003:LYS:HB3	1.93	0.68
1:A:202:VAL:O	1:A:254:PRO:HA	1.96	0.66
1:B:202:VAL:O	1:B:254:PRO:HA	1.96	0.66
1:D:202:VAL:O	1:D:254:PRO:HA	1.96	0.65
1:C:202:VAL:O	1:C:254:PRO:HA	1.96	0.65
2:E:942:GLU:OE1	2:E:942:GLU:CA	2.46	0.64
2:E:1119:GLY:O	2:E:1123:ASN:HB2	1.97	0.64
2:E:1516:THR:O	2:E:1520:LEU:HB2	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1301:ASN:O	2:E:1305:MET:HB2	1.99	0.62
2:E:478:VAL:O	2:E:482:LEU:HB2	1.99	0.62
2:E:603:LYS:O	2:E:607:SER:HB2	2.01	0.61
2:E:787:ASN:HD22	2:E:842:ARG:HH22	1.49	0.61
2:E:140:LEU:O	2:E:143:TYR:HB3	2.01	0.60
2:E:1001:CYS:O	2:E:1004:TYR:HB3	2.02	0.60
2:E:134:PRO:O	2:E:137:LEU:HB3	2.01	0.60
1:B:157:LEU:HG	1:C:164:LEU:HD21	1.84	0.60
2:E:941:LYS:O	2:E:941:LYS:CE	2.48	0.59
2:E:1170:PRO:O	2:E:1173:ILE:HB	2.04	0.57
1:B:103:SER:HB3	2:E:13:SER:HB3	1.87	0.56
2:E:514:ALA:HB2	2:E:1419:ARG:HG3	1.86	0.56
1:A:290:VAL:HG22	1:A:297:THR:HG22	1.89	0.55
1:B:290:VAL:HG22	1:B:297:THR:HG22	1.89	0.55
2:E:82:LEU:O	2:E:86:LEU:HB2	2.06	0.55
2:E:508:LYS:O	2:E:512:LEU:HB2	2.07	0.55
2:E:682:ILE:HG12	2:E:738:VAL:HG13	1.88	0.55
1:A:211:ILE:HB	1:A:290:VAL:HB	1.89	0.55
2:E:895:PRO:CB	2:E:942:GLU:HG2	2.37	0.54
1:C:290:VAL:HG22	1:C:297:THR:HG22	1.89	0.54
2:E:288:ILE:O	2:E:292:LEU:HB2	2.08	0.54
2:E:78:LEU:HD21	2:E:182:MET:HG3	1.90	0.54
1:C:211:ILE:HB	1:C:290:VAL:HB	1.90	0.54
1:B:211:ILE:HB	1:B:290:VAL:HB	1.90	0.53
2:E:457:LEU:HB3	2:E:461:ALA:HB2	1.91	0.53
2:E:712:ILE:HB	2:E:887:VAL:HG12	1.90	0.53
2:E:467:VAL:HA	2:E:471:LEU:HD23	1.91	0.53
2:E:840:VAL:HG11	2:E:856:PRO:HB3	1.90	0.53
2:E:1162:PRO:O	2:E:1165:LEU:HB2	2.08	0.53
1:B:283:ILE:HB	1:B:304:TYR:HB2	1.91	0.53
1:D:283:ILE:HB	1:D:304:TYR:HB2	1.91	0.53
1:C:283:ILE:HB	1:C:304:TYR:HB2	1.91	0.53
1:D:290:VAL:HG22	1:D:297:THR:HG22	1.89	0.53
1:A:283:ILE:HB	1:A:304:TYR:HB2	1.91	0.52
1:B:175:HIS:O	1:B:178:ALA:HB3	2.10	0.52
1:A:175:HIS:O	1:A:178:ALA:HB3	2.10	0.52
2:E:678:CYS:HB3	2:E:681:GLN:HE21	1.75	0.52
1:D:211:ILE:HB	1:D:290:VAL:HB	1.89	0.52
2:E:210:ASP:HB3	2:E:212:GLN:HG3	1.92	0.52
2:E:375:GLN:HE22	2:E:1246:ARG:HE	1.57	0.52
2:E:582:SER:HB3	2:E:1286:THR:HG22	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:873:ILE:HA	2:E:877:LEU:HD12	1.92	0.51
1:D:175:HIS:O	1:D:178:ALA:HB3	2.10	0.51
2:E:1460:LEU:HD13	2:E:1489:LEU:HD23	1.92	0.51
1:C:175:HIS:O	1:C:178:ALA:HB3	2.10	0.51
2:E:681:GLN:HB3	2:E:683:MET:HE3	1.92	0.51
2:E:895:PRO:HB3	2:E:942:GLU:HG2	1.92	0.50
2:E:941:LYS:HE3	2:E:941:LYS:C	2.35	0.50
1:A:43:ASN:ND2	1:B:324:GLY:O	2.44	0.50
1:B:174:ALA:O	1:B:177:ARG:HB3	2.12	0.50
1:D:174:ALA:O	1:D:177:ARG:HB3	2.11	0.50
1:C:174:ALA:O	1:C:177:ARG:HB3	2.11	0.50
1:A:176:ARG:HB3	1:D:58:ASP:HB3	1.94	0.49
2:E:713:VAL:HA	2:E:720:LYS:HZ1	1.77	0.49
2:E:791:GLU:O	2:E:1222:ARG:NH2	2.45	0.49
2:E:1347:ILE:HA	2:E:1403:ILE:HG22	1.94	0.49
2:E:75:ARG:NH2	2:E:187:GLU:OE2	2.45	0.49
1:A:174:ALA:O	1:A:177:ARG:HB3	2.11	0.49
1:D:162:ILE:O	1:D:166:SER:HB3	2.13	0.49
2:E:4:LEU:HD22	2:E:105:LEU:HD11	1.95	0.49
2:E:927:HIS:O	2:E:931:LEU:HB2	2.13	0.49
1:A:162:ILE:O	1:A:166:SER:HB3	2.13	0.49
1:C:153:ASN:O	1:C:157:LEU:HB2	2.13	0.49
1:C:242:ASN:ND2	1:C:246:GLY:O	2.46	0.49
1:A:242:ASN:ND2	1:A:246:GLY:O	2.46	0.48
1:B:162:ILE:O	1:B:166:SER:HB3	2.13	0.48
1:D:242:ASN:ND2	1:D:246:GLY:O	2.46	0.48
2:E:728:LEU:O	2:E:767:ARG:NH1	2.46	0.48
1:B:153:ASN:O	1:B:157:LEU:HB2	2.13	0.48
2:E:685:GLY:HA2	2:E:736:GLY:HA3	1.95	0.48
1:B:242:ASN:ND2	1:B:246:GLY:O	2.46	0.48
1:A:153:ASN:O	1:A:157:LEU:HB2	2.13	0.48
1:B:126:GLU:OE2	1:B:136:ARG:NH2	2.47	0.48
1:C:162:ILE:O	1:C:166:SER:HB3	2.13	0.48
1:D:126:GLU:OE2	1:D:136:ARG:NH2	2.47	0.48
1:D:153:ASN:O	1:D:157:LEU:HB2	2.13	0.48
2:E:35:VAL:HA	2:E:38:VAL:HG12	1.96	0.48
2:E:1252:MET:HE1	2:E:1299:VAL:HG21	1.96	0.48
2:E:38:VAL:O	2:E:42:PHE:HB2	2.14	0.48
2:E:774:SER:OG	2:E:775:GLN:N	2.45	0.48
1:C:221:ARG:HD3	1:C:281:LEU:HD12	1.96	0.47
2:E:504:LEU:HB3	2:E:1118:LEU:HD11	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:899:TRP:NE1	2:E:911:GLU:OE1	2.47	0.47
1:A:126:GLU:OE2	1:A:136:ARG:NH2	2.47	0.47
1:B:221:ARG:HD3	1:B:281:LEU:HD12	1.96	0.47
2:E:1142:CYS:SG	2:E:1301:ASN:ND2	2.86	0.47
1:D:45:ALA:HB1	1:D:47:LYS:HE3	1.96	0.47
1:D:58:ASP:N	1:D:58:ASP:OD1	2.48	0.47
2:E:247:ASP:OD1	2:E:247:ASP:N	2.46	0.47
2:E:807:SER:O	2:E:837:ARG:NH2	2.47	0.47
1:B:45:ALA:HB1	1:B:47:LYS:HE3	1.96	0.47
2:E:1139:THR:HG21	2:E:1308:GLN:HE22	1.79	0.47
2:E:1185:ALA:O	2:E:1188:ASP:HB2	2.15	0.47
2:E:1338:ASN:HB3	2:E:1341:ASP:HB3	1.96	0.47
2:E:1416:HIS:O	2:E:1420:SER:HB3	2.14	0.47
2:E:1200:LEU:O	2:E:1203:HIS:HB3	2.15	0.47
1:C:58:ASP:OD1	1:C:58:ASP:N	2.48	0.46
2:E:123:VAL:O	2:E:127:ASN:ND2	2.47	0.46
2:E:1491:CYS:SG	2:E:1494:ARG:NH2	2.87	0.46
1:C:126:GLU:OE2	1:C:136:ARG:NH2	2.47	0.46
1:C:201:ARG:HA	1:C:255:LEU:O	2.16	0.46
2:E:1188:ASP:O	2:E:1191:GLN:HB3	2.15	0.46
1:A:58:ASP:OD1	1:A:58:ASP:N	2.48	0.46
1:A:221:ARG:HD3	1:A:281:LEU:HD12	1.96	0.46
1:C:45:ALA:HB1	1:C:47:LYS:HE3	1.96	0.46
1:A:45:ALA:HB1	1:A:47:LYS:HE3	1.96	0.46
1:A:283:ILE:O	1:A:303:SER:HA	2.16	0.46
1:B:58:ASP:N	1:B:58:ASP:OD1	2.48	0.46
1:D:201:ARG:HA	1:D:255:LEU:O	2.16	0.46
2:E:1480:GLU:OE2	2:E:1487:ARG:NH2	2.48	0.46
1:B:201:ARG:HA	1:B:255:LEU:O	2.16	0.46
1:D:221:ARG:HD3	1:D:281:LEU:HD12	1.96	0.46
1:B:299:GLN:OE1	1:B:301:ARG:NH1	2.49	0.46
2:E:36:PRO:HB3	2:E:146:LEU:HB3	1.98	0.46
2:E:779:LEU:HD22	2:E:835:ARG:HD3	1.98	0.46
2:E:1064:TYR:O	2:E:1068:PHE:HB2	2.16	0.46
2:E:1337:LYS:O	2:E:1421:ARG:NH1	2.49	0.46
2:E:259:ARG:O	2:E:263:ASN:ND2	2.46	0.46
1:A:299:GLN:OE1	1:A:301:ARG:NH1	2.49	0.46
2:E:1104:ARG:HH12	2:E:1323:ALA:HB2	1.81	0.45
2:E:1190:GLN:O	2:E:1193:ASP:HB3	2.16	0.45
2:E:1344:LYS:HE2	2:E:1371:PRO:HD3	1.97	0.45
1:A:201:ARG:HA	1:A:255:LEU:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ILE:O	1:B:303:SER:HA	2.16	0.45
1:B:51:GLU:OE2	1:B:54:ARG:NH1	2.49	0.45
2:E:386:ILE:HG21	2:E:1239:LEU:HG	1.99	0.45
1:C:58:ASP:HB3	1:D:176:ARG:HB3	1.99	0.45
1:C:286:ILE:HG22	1:C:288:GLU:HG2	1.99	0.45
1:C:299:GLN:OE1	1:C:301:ARG:NH1	2.49	0.45
1:D:299:GLN:OE1	1:D:301:ARG:NH1	2.49	0.45
1:C:283:ILE:O	1:C:303:SER:HA	2.16	0.45
2:E:328:LEU:HD23	2:E:1281:VAL:HG11	1.99	0.45
2:E:445:GLN:NE2	2:E:586:ILE:O	2.50	0.45
2:E:1266:THR:O	2:E:1270:ASN:HB2	2.17	0.45
2:E:1377:ILE:HG12	2:E:1550:ILE:HB	1.99	0.45
1:D:106:THR:O	1:D:106:THR:OG1	2.35	0.45
1:A:106:THR:O	1:A:106:THR:OG1	2.35	0.45
1:D:51:GLU:OE2	1:D:54:ARG:NH1	2.49	0.45
1:D:283:ILE:O	1:D:303:SER:HA	2.16	0.45
1:D:286:ILE:HG22	1:D:288:GLU:HG2	1.99	0.45
2:E:707:GLY:O	2:E:878:ARG:NH1	2.49	0.45
2:E:1348:GLN:HB3	2:E:1402:HIS:HB3	1.99	0.45
1:B:106:THR:O	1:B:106:THR:OG1	2.35	0.45
2:E:17:ARG:O	2:E:25:ASN:ND2	2.50	0.44
2:E:1296:ASN:N	2:E:1296:ASN:OD1	2.49	0.44
1:A:313:GLN:HA	1:A:338:LYS:HA	2.00	0.44
1:D:313:GLN:HA	1:D:338:LYS:HA	2.00	0.44
2:E:445:GLN:HE22	2:E:587:LEU:HA	1.83	0.44
2:E:1126:SER:OG	2:E:1127:SER:N	2.49	0.44
1:A:286:ILE:HG22	1:A:288:GLU:HG2	1.99	0.44
1:A:303:SER:OG	1:A:304:TYR:N	2.51	0.44
1:C:51:GLU:OE2	1:C:54:ARG:NH1	2.49	0.44
2:E:1035:ALA:HB2	2:E:1283:LEU:HD21	1.99	0.44
1:A:51:GLU:OE2	1:A:54:ARG:NH1	2.49	0.44
1:C:313:GLN:HA	1:C:338:LYS:HA	2.00	0.44
2:E:1196:THR:O	2:E:1234:ASN:ND2	2.47	0.44
2:E:1374:LYS:NZ	2:E:1529:ALA:O	2.51	0.44
2:E:1341:ASP:OD1	2:E:1341:ASP:N	2.46	0.43
1:B:239:PRO:O	1:B:259:HIS:ND1	2.45	0.43
2:E:11:ASN:O	2:E:12:HIS:ND1	2.48	0.43
1:D:319:VAL:HG22	1:D:328:VAL:HG22	2.00	0.43
2:E:142:VAL:O	2:E:146:LEU:N	2.51	0.43
1:B:313:GLN:HA	1:B:338:LYS:HA	2.00	0.43
1:C:319:VAL:HG22	1:C:328:VAL:HG22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ILE:HG22	1:B:288:GLU:HG2	1.99	0.43
1:B:319:VAL:HG22	1:B:328:VAL:HG22	2.00	0.43
2:E:316:ALA:HA	2:E:319:LEU:HD12	2.00	0.43
2:E:425:ASP:O	2:E:607:SER:OG	2.36	0.43
2:E:95:LEU:HD22	2:E:355:ASN:HD22	1.83	0.43
2:E:716:VAL:HG11	2:E:1512:ILE:HG23	2.01	0.43
2:E:1370:ALA:HB3	2:E:1373:GLN:HB2	2.01	0.43
1:A:319:VAL:HG22	1:A:328:VAL:HG22	2.00	0.42
2:E:1176:TYR:O	2:E:1179:GLN:HB3	2.18	0.42
1:C:212:SER:O	1:C:212:SER:OG	2.38	0.42
2:E:1297:TRP:O	2:E:1301:ASN:HB2	2.19	0.42
1:B:303:SER:OG	1:B:304:TYR:N	2.51	0.42
1:D:307:ASP:OD1	1:D:307:ASP:N	2.52	0.42
2:E:40:LEU:HD21	2:E:121:SER:HB3	2.00	0.42
1:A:239:PRO:O	1:A:259:HIS:ND1	2.45	0.42
1:D:158:MET:HE2	1:D:158:MET:HB3	1.93	0.42
2:E:482:LEU:HD22	2:E:540:TYR:HB3	2.00	0.42
1:C:158:MET:HE2	1:C:158:MET:HB3	1.93	0.42
2:E:617:SER:OG	2:E:618:ALA:N	2.51	0.42
2:E:1513:ASP:OD1	2:E:1516:THR:OG1	2.35	0.42
2:E:1566:LEU:O	2:E:1572:SER:OG	2.36	0.42
1:B:158:MET:HE2	1:B:158:MET:HB3	1.93	0.42
1:C:303:SER:OG	1:C:304:TYR:N	2.51	0.42
2:E:411:GLY:H	2:E:1476:THR:HG21	1.85	0.42
1:A:148:ILE:HA	1:A:151:VAL:HG12	2.01	0.42
1:D:303:SER:OG	1:D:304:TYR:N	2.51	0.42
2:E:844:LEU:HD12	2:E:876:LEU:HD11	2.01	0.42
1:C:148:ILE:HA	1:C:151:VAL:HG12	2.01	0.42
2:E:503:MET:HE2	2:E:503:MET:HB2	1.91	0.42
2:E:1011:LEU:O	2:E:1015:LEU:HB2	2.20	0.41
2:E:1267:SER:HB2	2:E:1281:VAL:HG23	2.01	0.41
1:A:161:ALA:HB2	1:B:164:LEU:HD22	2.03	0.41
1:B:240:MET:HE3	1:B:240:MET:HB2	1.95	0.41
1:C:239:PRO:O	1:C:259:HIS:ND1	2.45	0.41
2:E:676:ASP:OD2	2:E:681:GLN:NE2	2.52	0.41
2:E:775:GLN:NE2	5:E:1604:ATP:O2G	2.53	0.41
1:A:225:SER:OG	1:A:228:GLY:N	2.54	0.41
1:B:334:ASP:OD1	1:B:334:ASP:N	2.45	0.41
1:A:158:MET:HE2	1:A:158:MET:HB3	1.93	0.41
2:E:65:THR:HB	2:E:212:GLN:HB2	2.03	0.41
2:E:148:PHE:HB2	2:E:180:TYR:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:26:GLY:HA2	2:E:29:VAL:HG22	2.03	0.41
1:C:334:ASP:OD1	1:C:334:ASP:N	2.45	0.41
2:E:94:ILE:HD12	2:E:94:ILE:HA	1.98	0.41
2:E:1484:GLN:HA	2:E:1487:ARG:HE	1.85	0.41
1:B:148:ILE:HA	1:B:151:VAL:HG12	2.01	0.41
1:C:154:ILE:HD13	1:C:154:ILE:HA	1.97	0.41
1:D:239:PRO:O	1:D:259:HIS:ND1	2.45	0.41
2:E:364:PHE:HB2	2:E:1261:LEU:HD13	2.02	0.41
1:A:233:LEU:HD12	1:A:233:LEU:HA	1.98	0.41
1:B:225:SER:OG	1:B:228:GLY:N	2.54	0.41
1:C:225:SER:OG	1:C:228:GLY:N	2.54	0.41
1:D:148:ILE:HA	1:D:151:VAL:HG12	2.01	0.41
2:E:892:GLN:HE21	2:E:1514:MET:HE1	1.86	0.41
2:E:1182:PHE:O	2:E:1185:ALA:HB3	2.21	0.41
2:E:1304:ASP:HA	2:E:1307:LEU:HB3	2.02	0.41
2:E:1483:SER:OG	2:E:1484:GLN:N	2.52	0.41
1:C:233:LEU:HD12	1:C:233:LEU:HA	1.98	0.41
2:E:708:GLN:HA	2:E:878:ARG:HH12	1.86	0.41
2:E:895:PRO:HB2	2:E:942:GLU:HG2	2.01	0.41
2:E:1315:ILE:O	2:E:1319:LEU:HB2	2.21	0.41
1:B:52:GLN:OE1	2:E:52:TRP:NE1	2.54	0.40
2:E:1199:PRO:O	2:E:1202:SER:HB2	2.21	0.40
2:E:1475:ILE:HG12	2:E:1482:PHE:HE2	1.87	0.40
1:A:95:PHE:HD1	1:A:100:LEU:HD12	1.86	0.40
1:D:109:PRO:O	1:D:139:THR:OG1	2.40	0.40
2:E:849:ASN:HA	2:E:882:ARG:HG2	2.04	0.40
1:B:200:LEU:HD21	1:B:285:VAL:HG11	2.03	0.40
1:D:225:SER:OG	1:D:228:GLY:N	2.54	0.40
2:E:20:GLN:OE1	2:E:24:ASN:ND2	2.54	0.40
2:E:220:GLN:HE22	2:E:228:LYS:HA	1.86	0.40
2:E:880:ASP:OD1	2:E:880:ASP:N	2.48	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%)	306 (96%)	13 (4%)	0	100	100
1	B	319/390 (82%)	306 (96%)	13 (4%)	0	100	100
1	C	319/390 (82%)	306 (96%)	13 (4%)	0	100	100
1	D	319/390 (82%)	306 (96%)	13 (4%)	0	100	100
2	E	1386/1582 (88%)	1296 (94%)	88 (6%)	2 (0%)	48	80
All	All	2662/3142 (85%)	2520 (95%)	140 (5%)	2 (0%)	49	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	344	VAL
2	E	345	TYR

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%)	238 (86%)	40 (14%)	3	17
1	B	278/337 (82%)	238 (86%)	40 (14%)	3	17
1	C	278/337 (82%)	238 (86%)	40 (14%)	3	17
1	D	278/337 (82%)	238 (86%)	40 (14%)	3	17
2	E	992/1368 (72%)	982 (99%)	10 (1%)	68	75
All	All	2104/2716 (78%)	1934 (92%)	170 (8%)	13	35

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	44	VAL
1	A	59	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	62	THR
1	A	72	LEU
1	A	74	ILE
1	A	84	LEU
1	A	92	LEU
1	A	106	THR
1	A	124	SER
1	A	125	ILE
1	A	129	VAL
1	A	142	CYS
1	A	151	VAL
1	A	166	SER
1	A	180	THR
1	A	182	ILE
1	A	211	ILE
1	A	220	VAL
1	A	223	THR
1	A	230	VAL
1	A	231	VAL
1	A	236	VAL
1	A	244	VAL
1	A	251	LEU
1	A	252	VAL
1	A	255	LEU
1	A	260	VAL
1	A	275	LEU
1	A	281	LEU
1	A	284	ILE
1	A	288	GLU
1	A	291	VAL
1	A	292	GLU
1	A	294	THR
1	A	296	ILE
1	A	316	VAL
1	A	331	SER
1	A	339	VAL
1	A	349	LEU
1	B	36	VAL
1	B	44	VAL
1	B	59	VAL
1	B	62	THR
1	B	72	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	74	ILE
1	B	84	LEU
1	B	92	LEU
1	B	106	THR
1	B	124	SER
1	B	125	ILE
1	B	129	VAL
1	B	142	CYS
1	B	151	VAL
1	B	166	SER
1	B	180	THR
1	B	182	ILE
1	B	211	ILE
1	B	220	VAL
1	B	223	THR
1	B	230	VAL
1	B	231	VAL
1	B	236	VAL
1	B	244	VAL
1	B	251	LEU
1	B	252	VAL
1	B	255	LEU
1	B	260	VAL
1	B	275	LEU
1	B	281	LEU
1	B	284	ILE
1	B	288	GLU
1	B	291	VAL
1	B	292	GLU
1	B	294	THR
1	B	296	ILE
1	B	316	VAL
1	B	331	SER
1	B	339	VAL
1	B	349	LEU
1	C	36	VAL
1	C	44	VAL
1	C	59	VAL
1	C	62	THR
1	C	72	LEU
1	C	74	ILE
1	C	84	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	92	LEU
1	C	106	THR
1	C	124	SER
1	C	125	ILE
1	C	129	VAL
1	C	142	CYS
1	C	151	VAL
1	C	166	SER
1	C	180	THR
1	C	182	ILE
1	C	211	ILE
1	C	220	VAL
1	C	223	THR
1	C	230	VAL
1	C	231	VAL
1	C	236	VAL
1	C	244	VAL
1	C	251	LEU
1	C	252	VAL
1	C	255	LEU
1	C	260	VAL
1	C	275	LEU
1	C	281	LEU
1	C	284	ILE
1	C	288	GLU
1	C	291	VAL
1	C	292	GLU
1	C	294	THR
1	C	296	ILE
1	C	316	VAL
1	C	331	SER
1	C	339	VAL
1	C	349	LEU
1	D	36	VAL
1	D	44	VAL
1	D	59	VAL
1	D	62	THR
1	D	72	LEU
1	D	74	ILE
1	D	84	LEU
1	D	92	LEU
1	D	106	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	124	SER
1	D	125	ILE
1	D	129	VAL
1	D	142	CYS
1	D	151	VAL
1	D	166	SER
1	D	180	THR
1	D	182	ILE
1	D	211	ILE
1	D	220	VAL
1	D	223	THR
1	D	230	VAL
1	D	231	VAL
1	D	236	VAL
1	D	244	VAL
1	D	251	LEU
1	D	252	VAL
1	D	255	LEU
1	D	260	VAL
1	D	275	LEU
1	D	281	LEU
1	D	284	ILE
1	D	288	GLU
1	D	291	VAL
1	D	292	GLU
1	D	294	THR
1	D	296	ILE
1	D	316	VAL
1	D	331	SER
1	D	339	VAL
1	D	349	LEU
2	E	149	ILE
2	E	308	ILE
2	E	368	LEU
2	E	467	VAL
2	E	941	LYS
2	E	942	GLU
2	E	943	THR
2	E	1074	LEU
2	E	1175	CYS
2	E	1509	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	277	HIS
1	B	70	HIS
1	B	97	HIS
1	B	277	HIS
1	C	97	HIS
1	C	277	HIS
1	D	46	HIS
1	D	97	HIS
1	D	277	HIS
2	E	24	ASN
2	E	25	ASN
2	E	33	ASN
2	E	55	GLN
2	E	73	ASN
2	E	127	ASN
2	E	220	GLN
2	E	355	ASN
2	E	375	GLN
2	E	445	GLN
2	E	486	GLN
2	E	501	ASN
2	E	681	GLN
2	E	715	GLN
2	E	787	ASN
2	E	817	HIS
2	E	867	HIS
2	E	892	GLN
2	E	1123	ASN
2	E	1135	HIS
2	E	1179	GLN
2	E	1301	ASN
2	E	1308	GLN
2	E	1518	ASN
2	E	1521	GLN

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	32,33,33	1.28	4 (12%)	48,52,52	1.77	10 (20%)
3	ADP	E	1601	4	28,29,29	1.41	5 (17%)	43,45,45	1.85	10 (23%)

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	-	7/22/38/38	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	4.45	1.47	1.39
5	E	1604	ATP	C5-C4	4.12	1.46	1.39
5	E	1604	ATP	C5-N7	-2.91	1.33	1.39
3	E	1601	ADP	C5-C6	2.60	1.48	1.41
3	E	1601	ADP	C5-N7	-2.58	1.34	1.39
5	E	1604	ATP	C4-N9	-2.57	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1601	ADP	C8-N7	2.14	1.35	1.31
3	E	1601	ADP	C4-N9	-2.12	1.33	1.37
5	E	1604	ATP	C5-C6	2.05	1.46	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1601	ADP	C5-C4-N3	-5.29	119.43	126.72
5	E	1604	ATP	C5-C4-N3	-5.07	119.74	126.72
5	E	1604	ATP	N3-C4-N9	4.52	134.86	127.17
3	E	1601	ADP	N3-C4-N9	4.40	134.65	127.17
5	E	1604	ATP	N3-C2-N1	-4.08	122.40	128.58
3	E	1601	ADP	N3-C2-N1	-3.94	122.62	128.58
3	E	1601	ADP	C2-N3-C4	3.84	121.21	111.83
5	E	1604	ATP	C2-N3-C4	3.74	120.95	111.83
3	E	1601	ADP	C4-C5-N7	-3.06	107.08	110.58
5	E	1604	ATP	C4-N9-C8	2.93	108.81	105.74
3	E	1601	ADP	C4-N9-C8	2.86	108.74	105.74
3	E	1601	ADP	C5-N7-C8	2.32	107.09	103.45
3	E	1601	ADP	C6-C5-N7	2.31	136.54	132.09
5	E	1604	ATP	C2'-C3'-C4'	2.27	107.00	102.61
3	E	1601	ADP	C3'-C2'-C1'	2.24	105.70	101.46
5	E	1604	ATP	C4-C5-N7	-2.24	108.02	110.58
3	E	1601	ADP	C2-N1-C6	2.11	122.20	118.73
5	E	1604	ATP	C2-N1-C6	2.07	122.13	118.73
5	E	1604	ATP	O2B-PB-O1B	2.04	121.92	112.44
5	E	1604	ATP	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (9) torsion outliers are listed below:

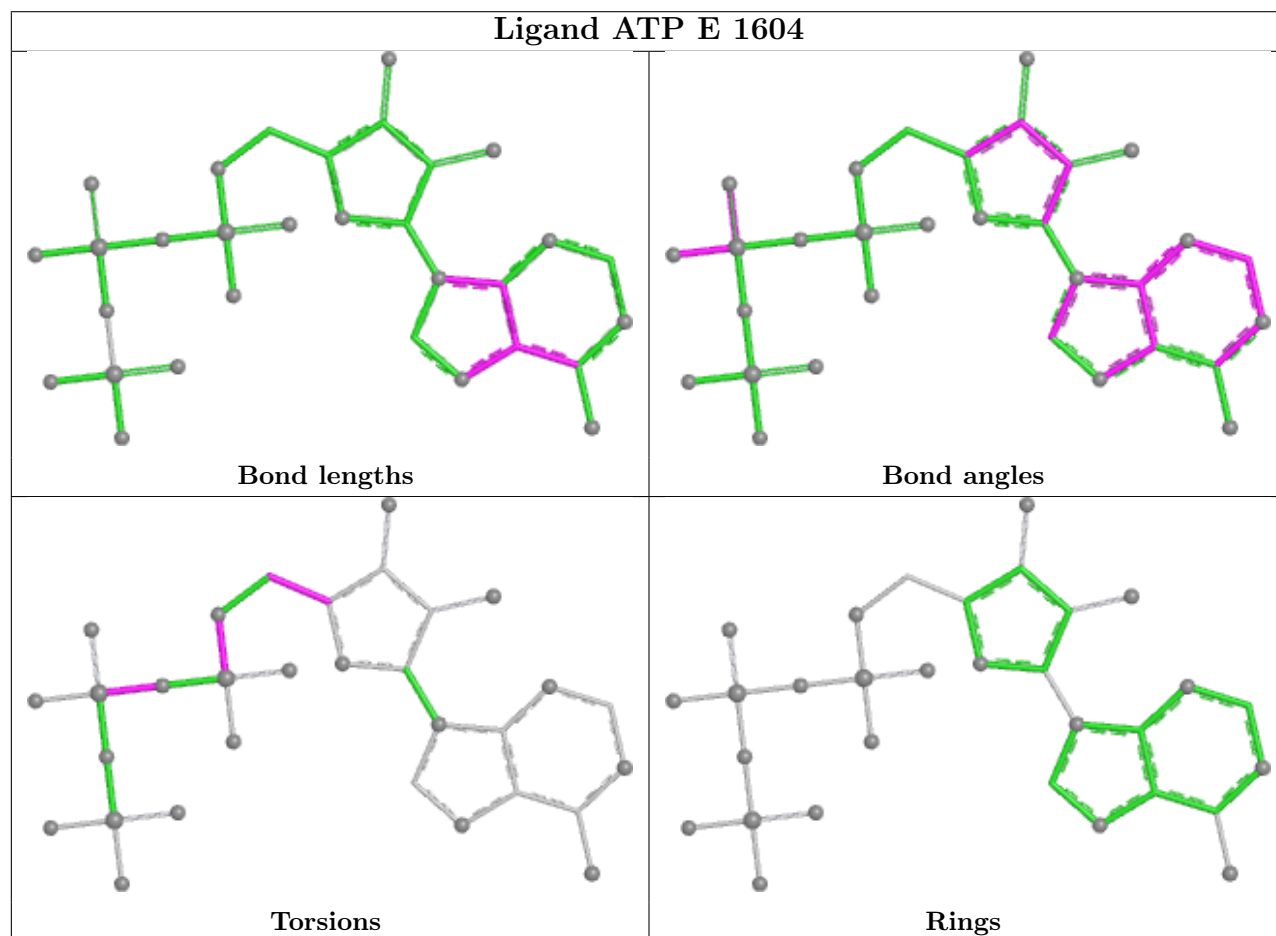
Mol	Chain	Res	Type	Atoms
5	E	1604	ATP	C5'-O5'-PA-O1A
5	E	1604	ATP	C5'-O5'-PA-O2A
5	E	1604	ATP	C5'-O5'-PA-O3A
3	E	1601	ADP	PB-O3A-PA-O1A
5	E	1604	ATP	O4'-C4'-C5'-O5'
5	E	1604	ATP	C3'-C4'-C5'-O5'
5	E	1604	ATP	PA-O3A-PB-O2B
3	E	1601	ADP	PB-O3A-PA-O2A
5	E	1604	ATP	PA-O3A-PB-O1B

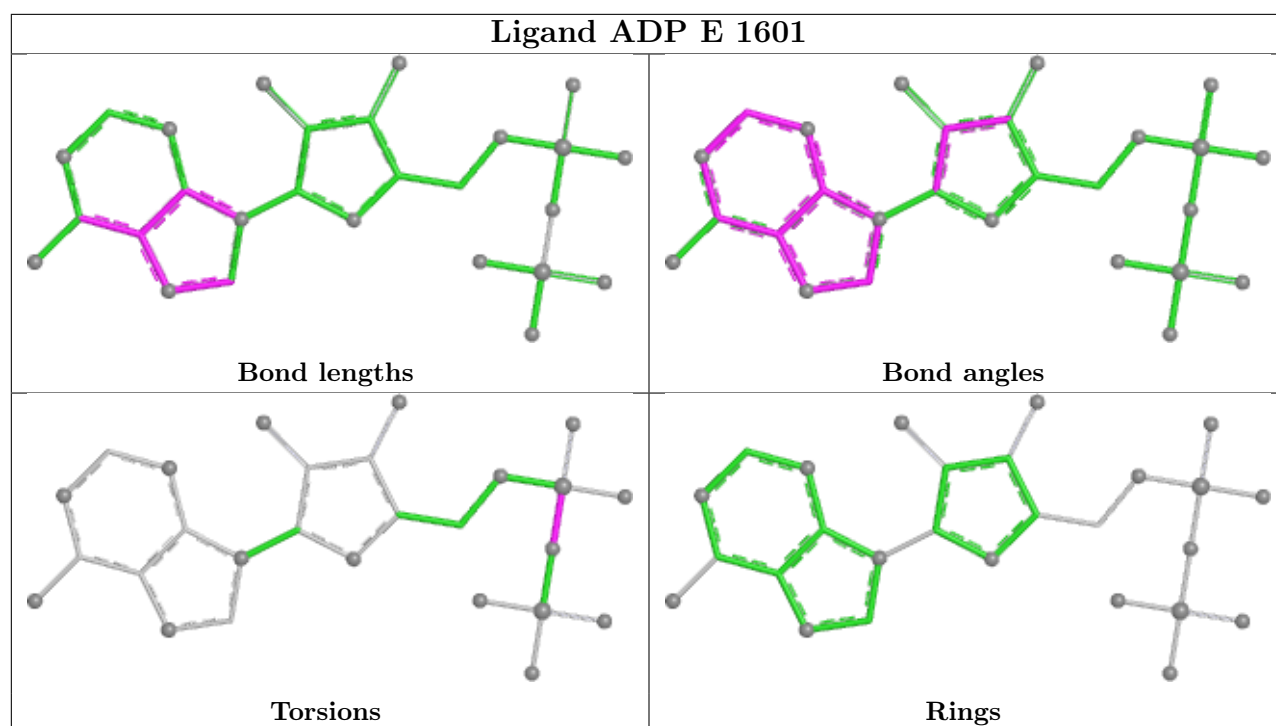
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1604	ATP	1	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 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.

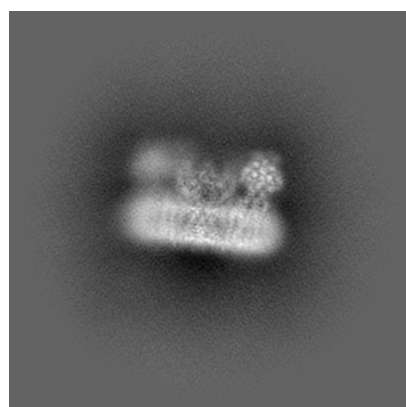
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24843. These allow visual inspection of the internal detail of the map and identification of artifacts.

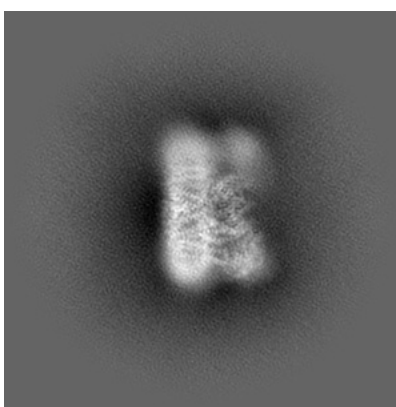
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

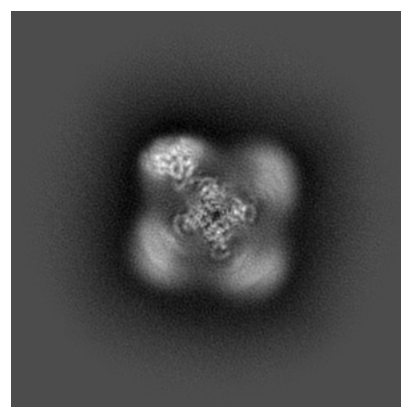
6.1.1 Primary map



X



Y

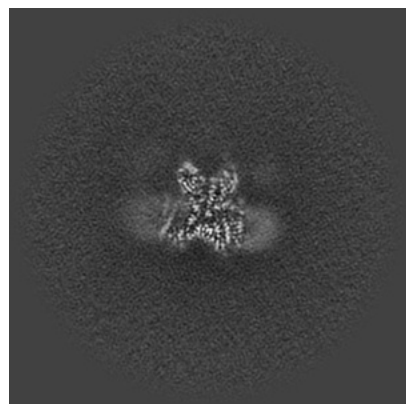


Z

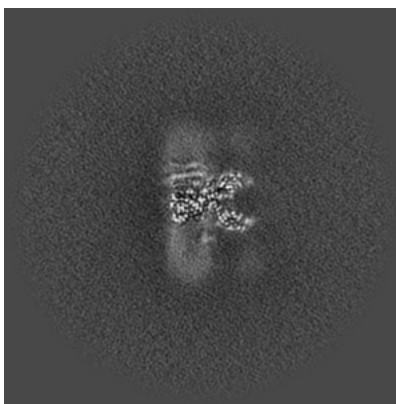
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

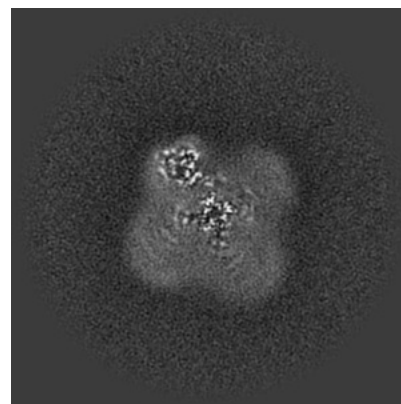
6.2.1 Primary map



X Index: 182



Y Index: 182

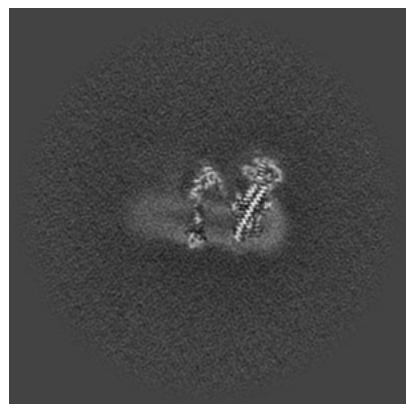


Z Index: 182

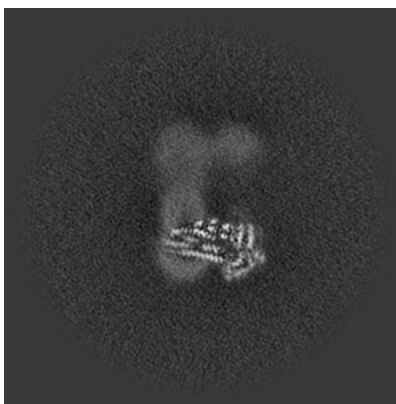
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

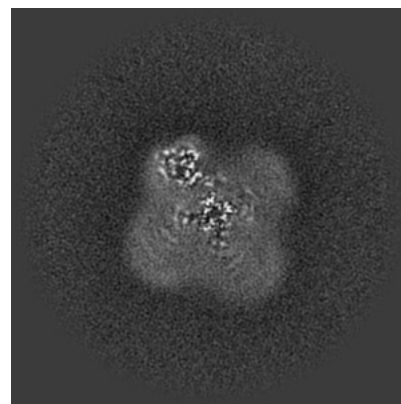
6.3.1 Primary map



X Index: 163



Y Index: 224

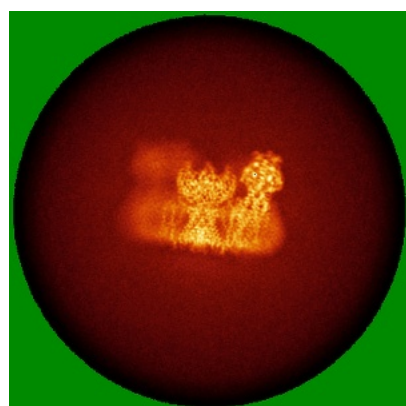


Z Index: 182

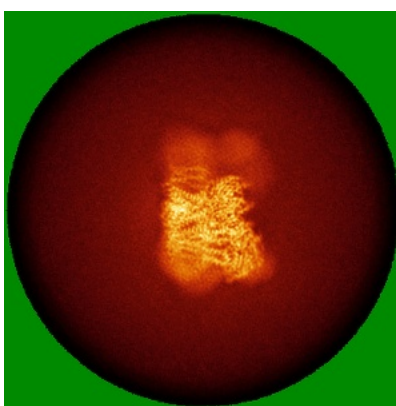
The images above show the largest variance slices of the map in three orthogonal directions.

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

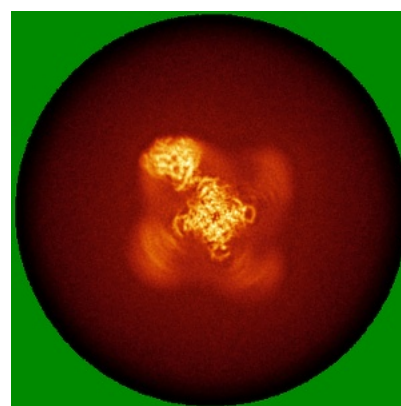
6.4.1 Primary map



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.

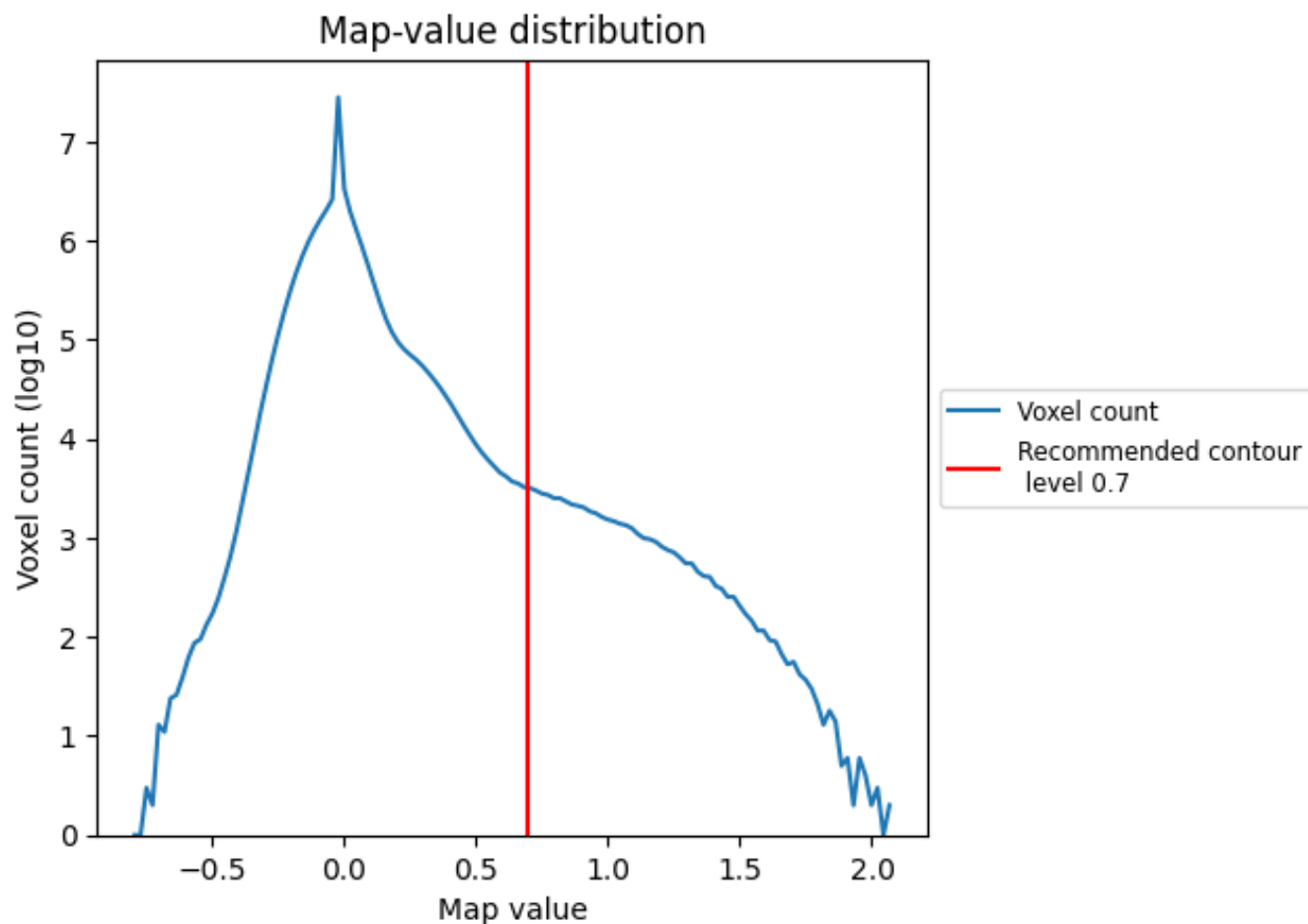
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

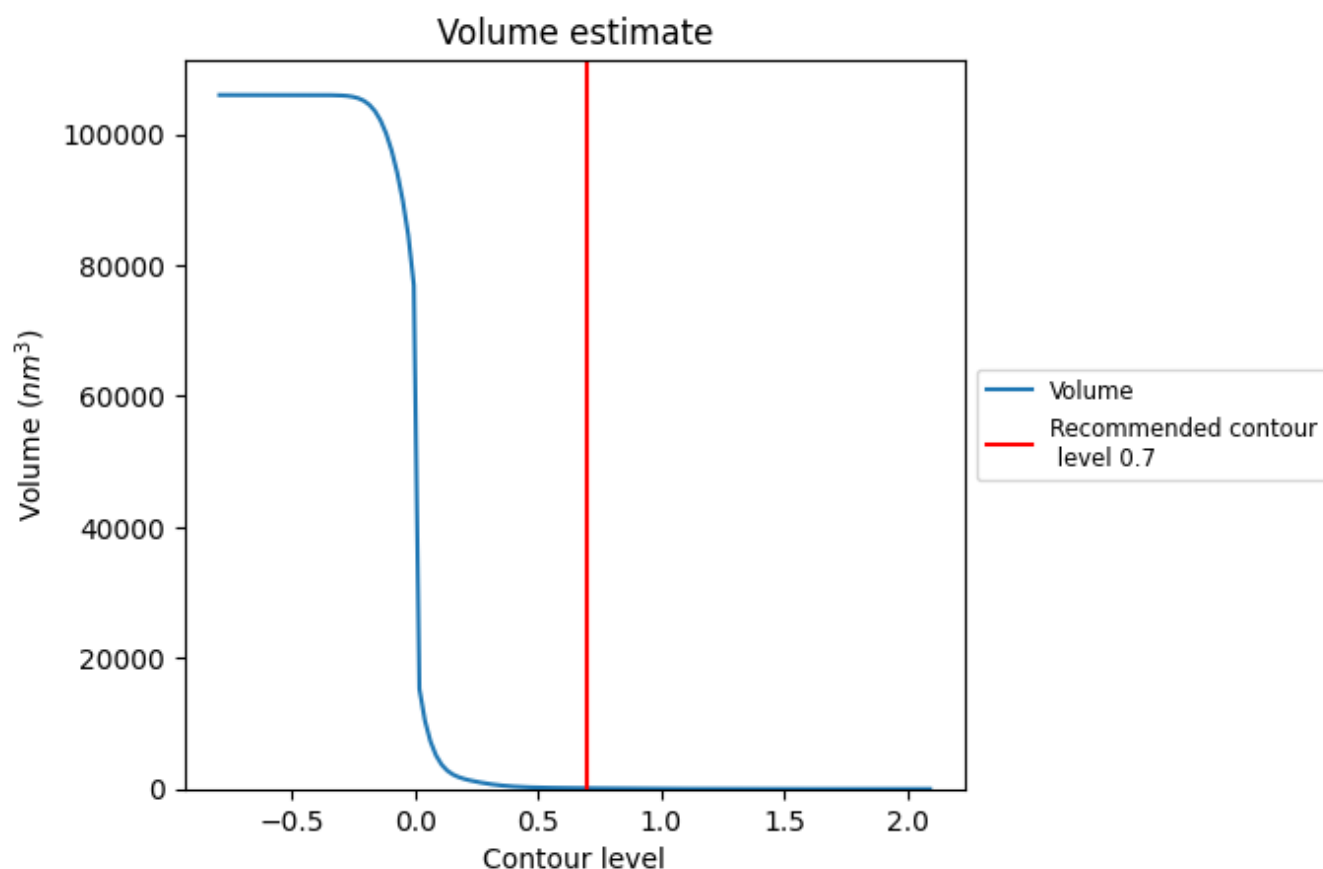
This section contains the results of statistical analysis of the map.

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.

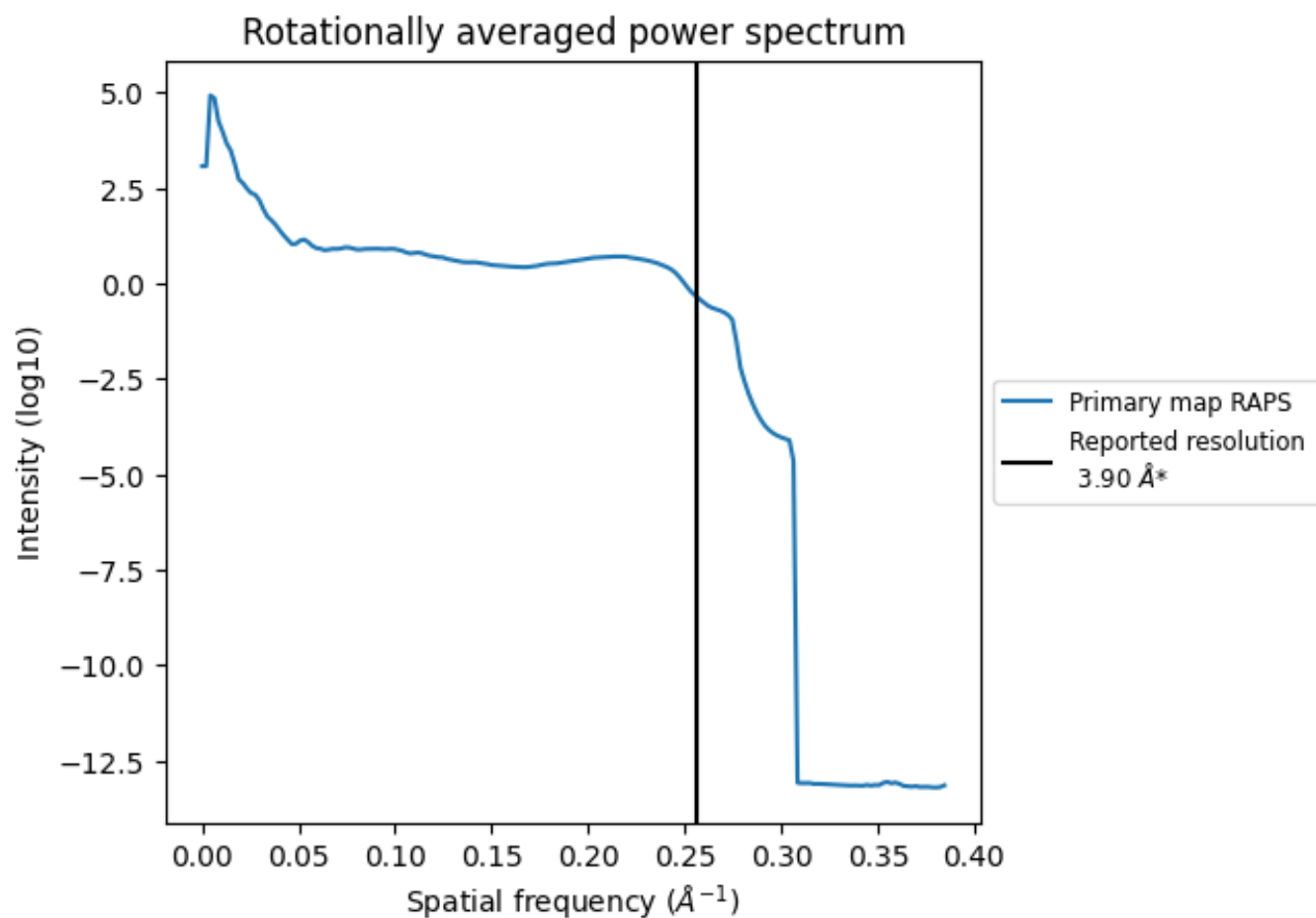
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 110 nm^3 ; this corresponds to an approximate mass of 100 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 ⓘ

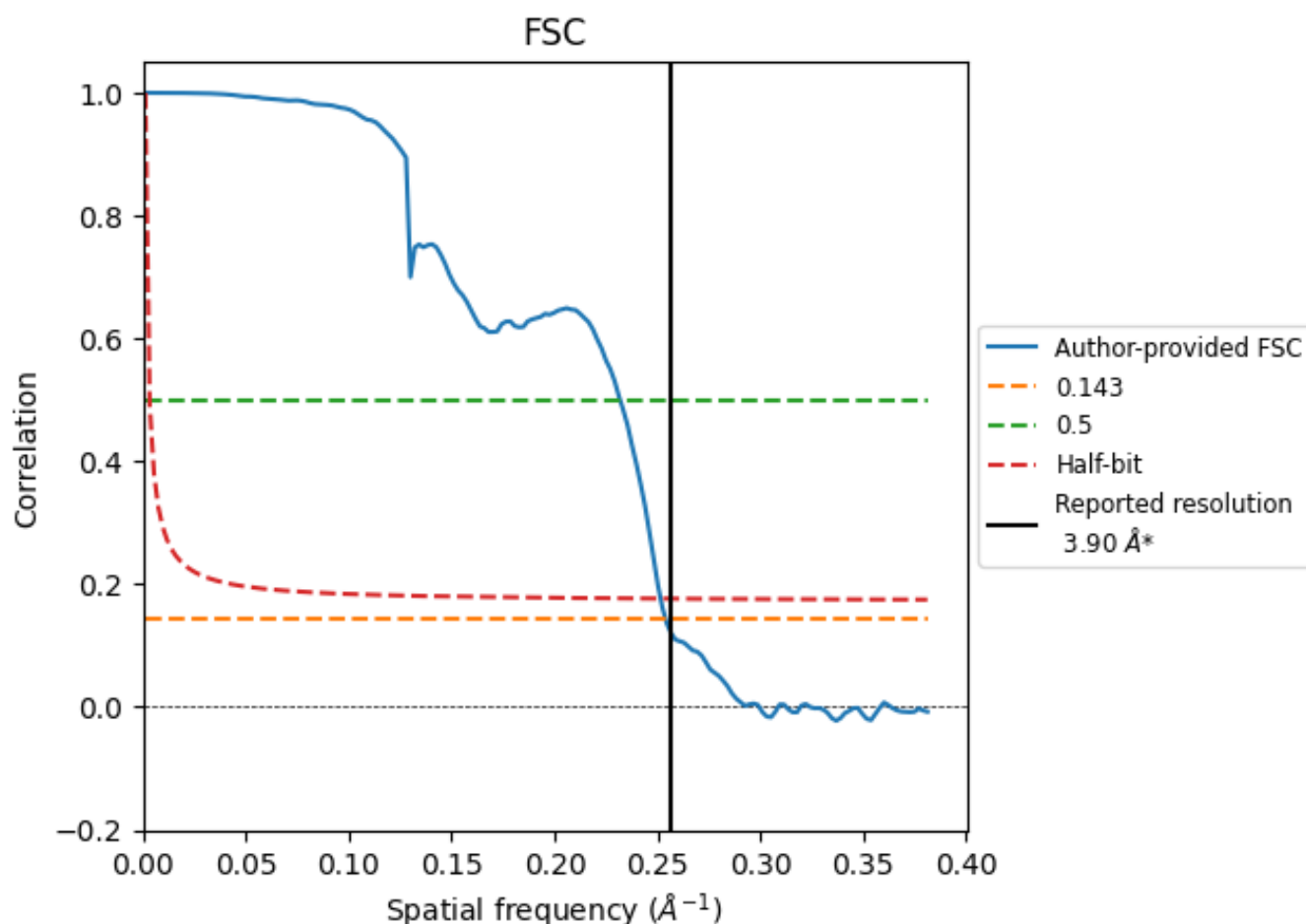


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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](#)

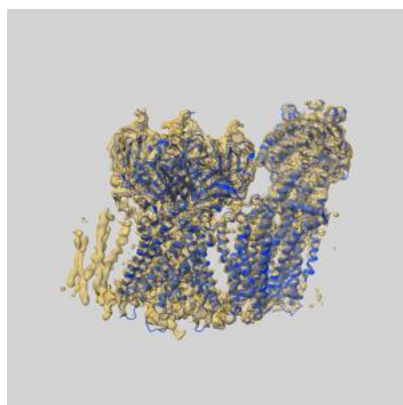
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.94	4.31	3.97
Unmasked-calculated*	-	-	-

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

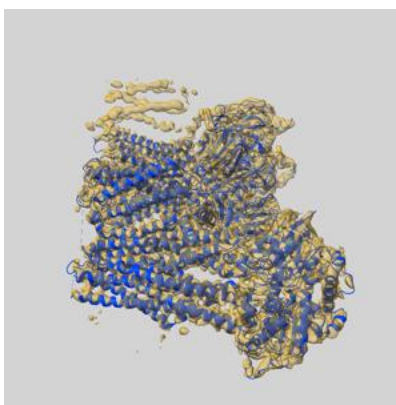
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24843 and PDB model 7S5Y. Per-residue inclusion information can be found in section [3](#) on page [7](#).

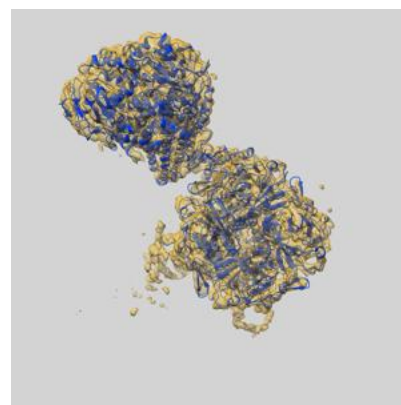
9.1 Map-model overlay [i](#)



X



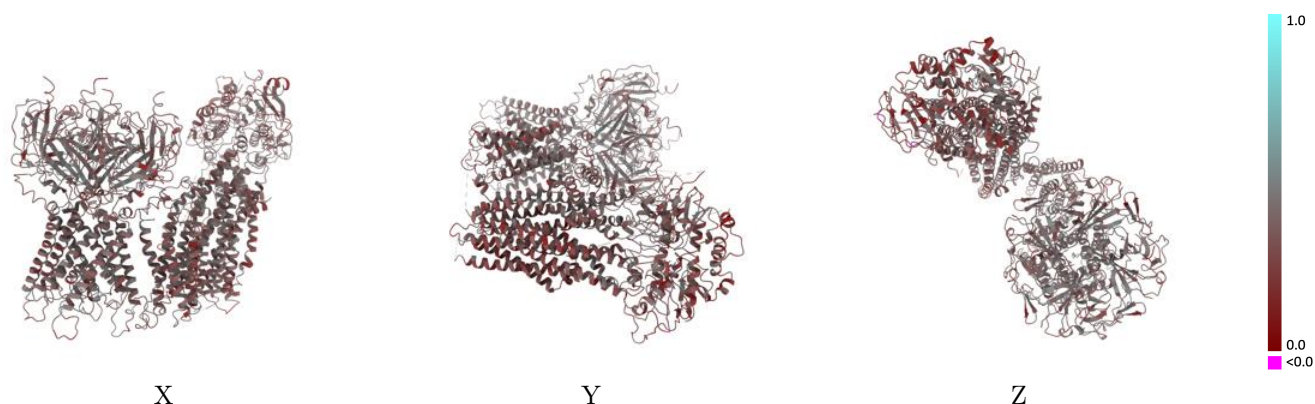
Y



Z

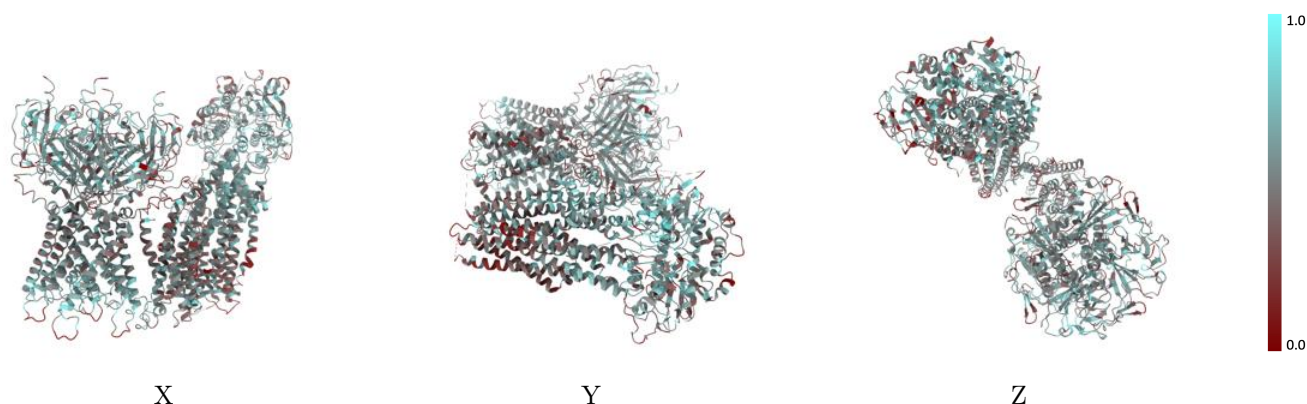
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



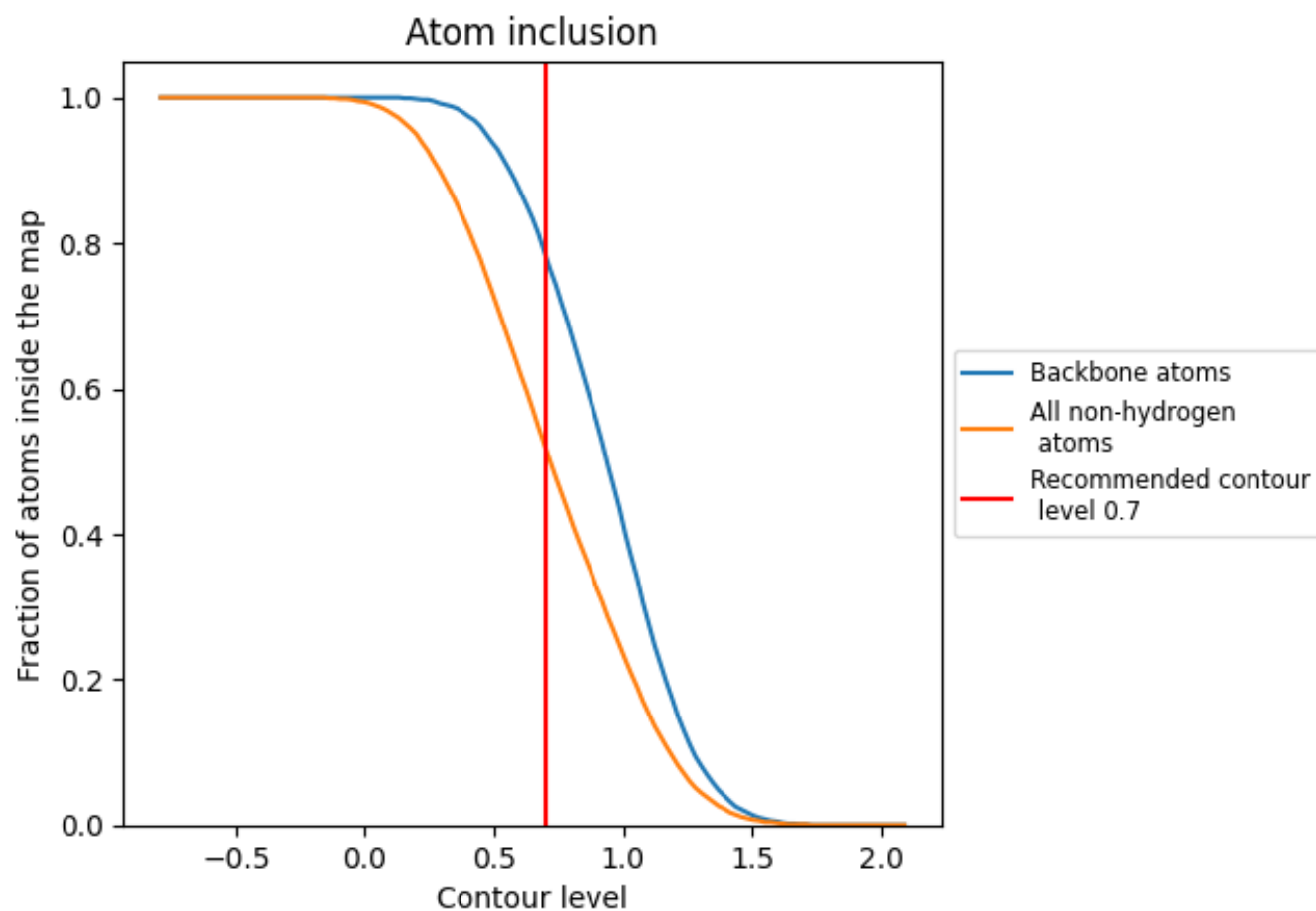
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 78% of all backbone atoms, 52% 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	0.5170	0.3590
A	0.5450	0.3960
B	0.5300	0.3810
C	0.5230	0.3880
D	0.5350	0.3780
E	0.5020	0.3340

