



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 07:00 PM UTC

PDB ID : 7MJQ / pdb_00007mjq
EMDB ID : EMD-23882
Title : Vascular KATP channel: Kir6.1 SUR2B quatrefoil-like conformation 2
Authors : Sung, M.W.; Shyng, S.L.
Deposited on : 2021-04-20
Resolution : 4.20 Å(reported)
Based on initial model : 6BAA

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:

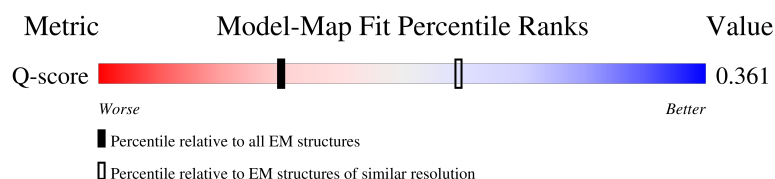
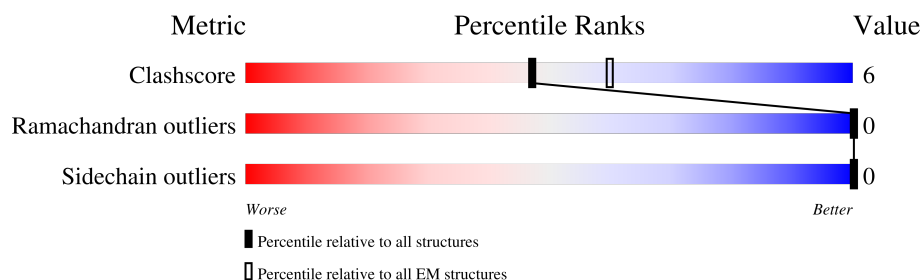
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.20 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.



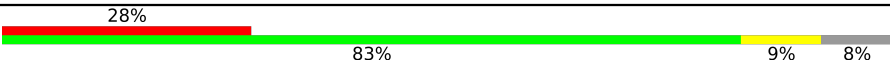
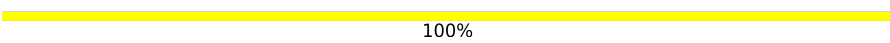
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	424	 79% 18%
1	B	424	 75% 5% 21%
1	C	424	 76% 20%
1	D	424	 71% 8% 21%

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Mol	Chain	Length	Quality of chain
2	E	1545	
2	G	1545	
3	F	2	
3	N	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	F	1	X	-	-	-
3	NAG	N	1	X	-	-	-
5	ATP	A	3002	-	-	X	-
5	ATP	B	501	-	-	X	-
5	ATP	E	1601	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14976 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 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	346	Total	C	N	O	0	0
			1714	1022	346	346		
1	B	337	Total	C	N	O	0	0
			1667	993	337	337		
1	C	338	Total	C	N	O	0	0
			1674	998	338	338		
1	D	337	Total	C	N	O	0	0
			1667	993	337	337		

- Molecule 2 is a protein called Isoform SUR2B of ATP-binding cassette sub-family C member 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	1426	Total	C	N	O	0	0
			7060	4206	1427	1427		
2	G	198	Total	C	N	O	0	0
			982	584	199	199		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

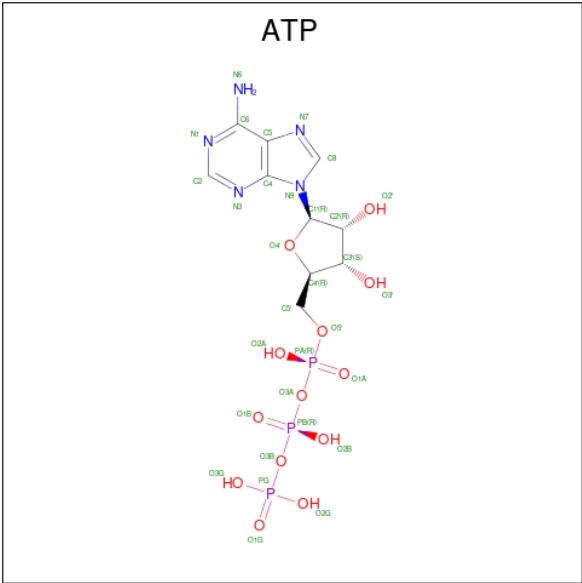


Mol	Chain	Residues	Atoms				AltConf	Trace
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	K	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

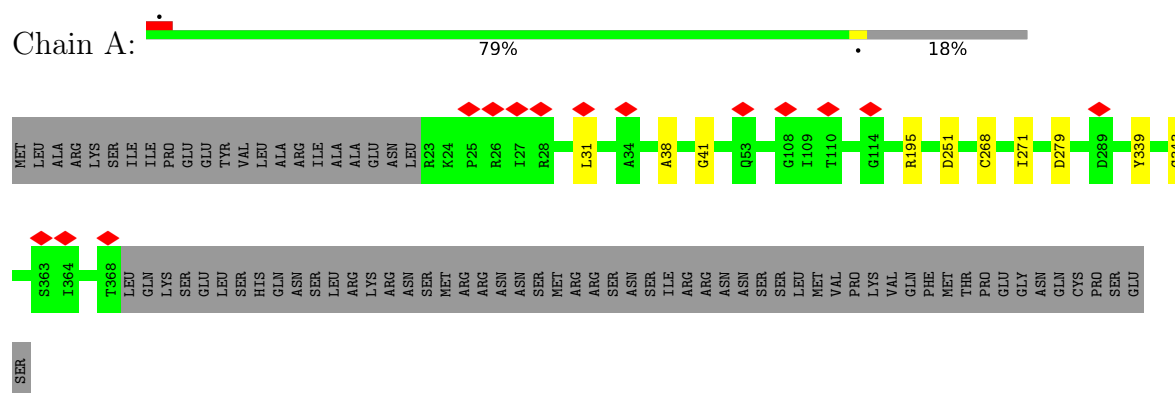


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

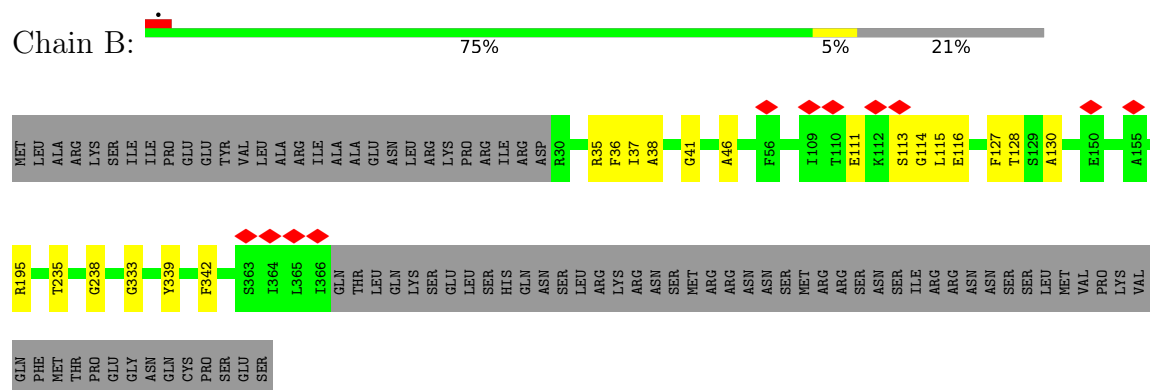
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

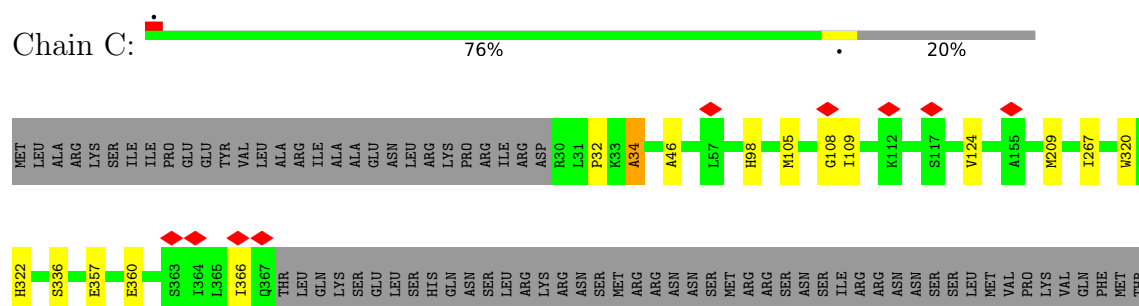
- Molecule 1: ATP-sensitive inward rectifier potassium channel 8



- Molecule 1: ATP-sensitive inward rectifier potassium channel 8



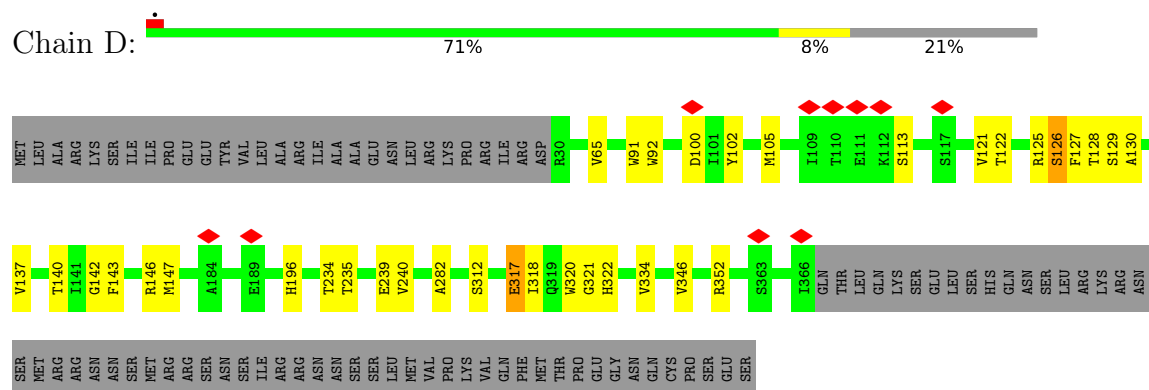
- Molecule 1: ATP-sensitive inward rectifier potassium channel 8



PRO
GLU
GLY
ASN
GLN
CYS
PRO
SER
GLU
SER

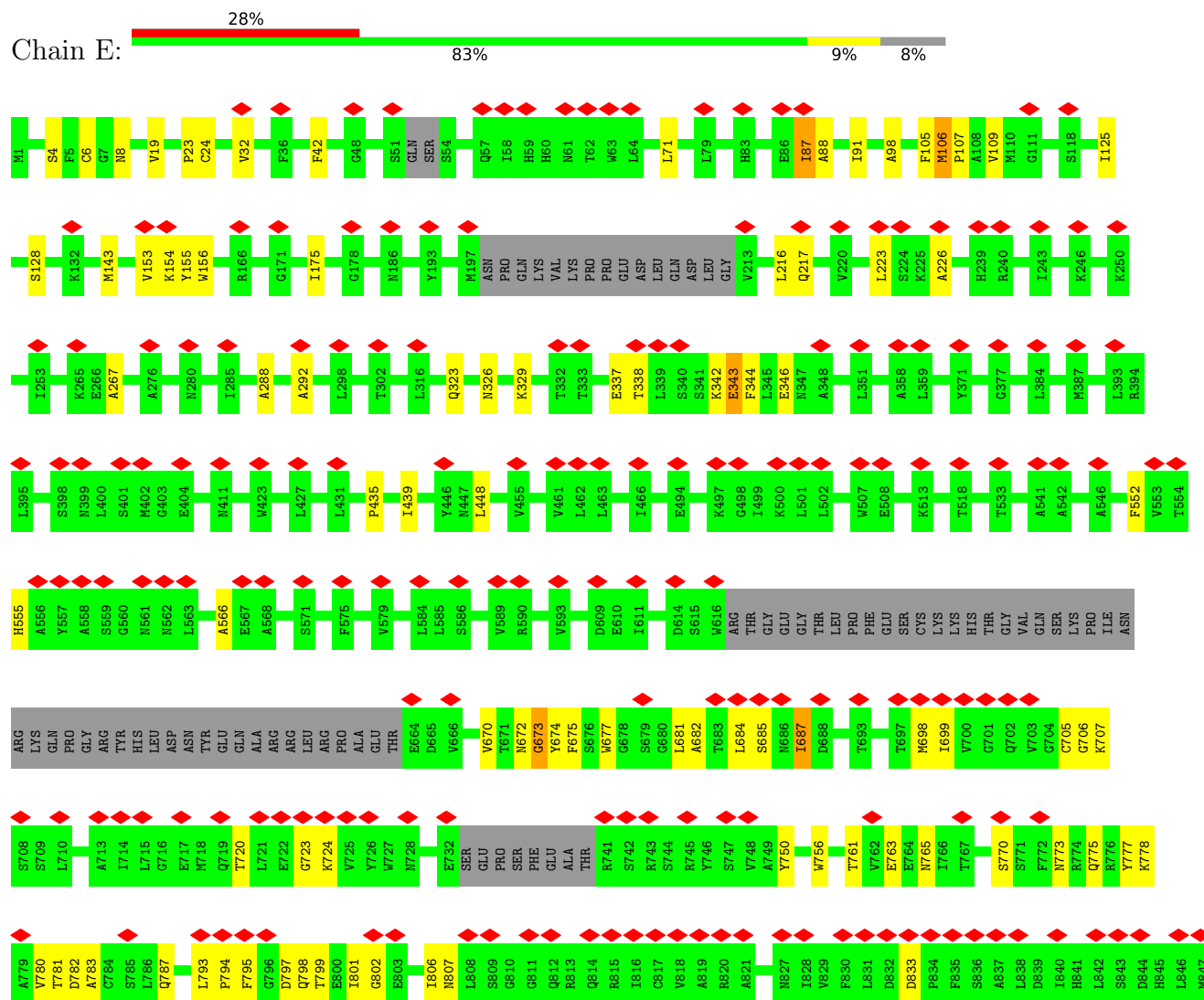
- Molecule 1: ATP-sensitive inward rectifier potassium channel 8

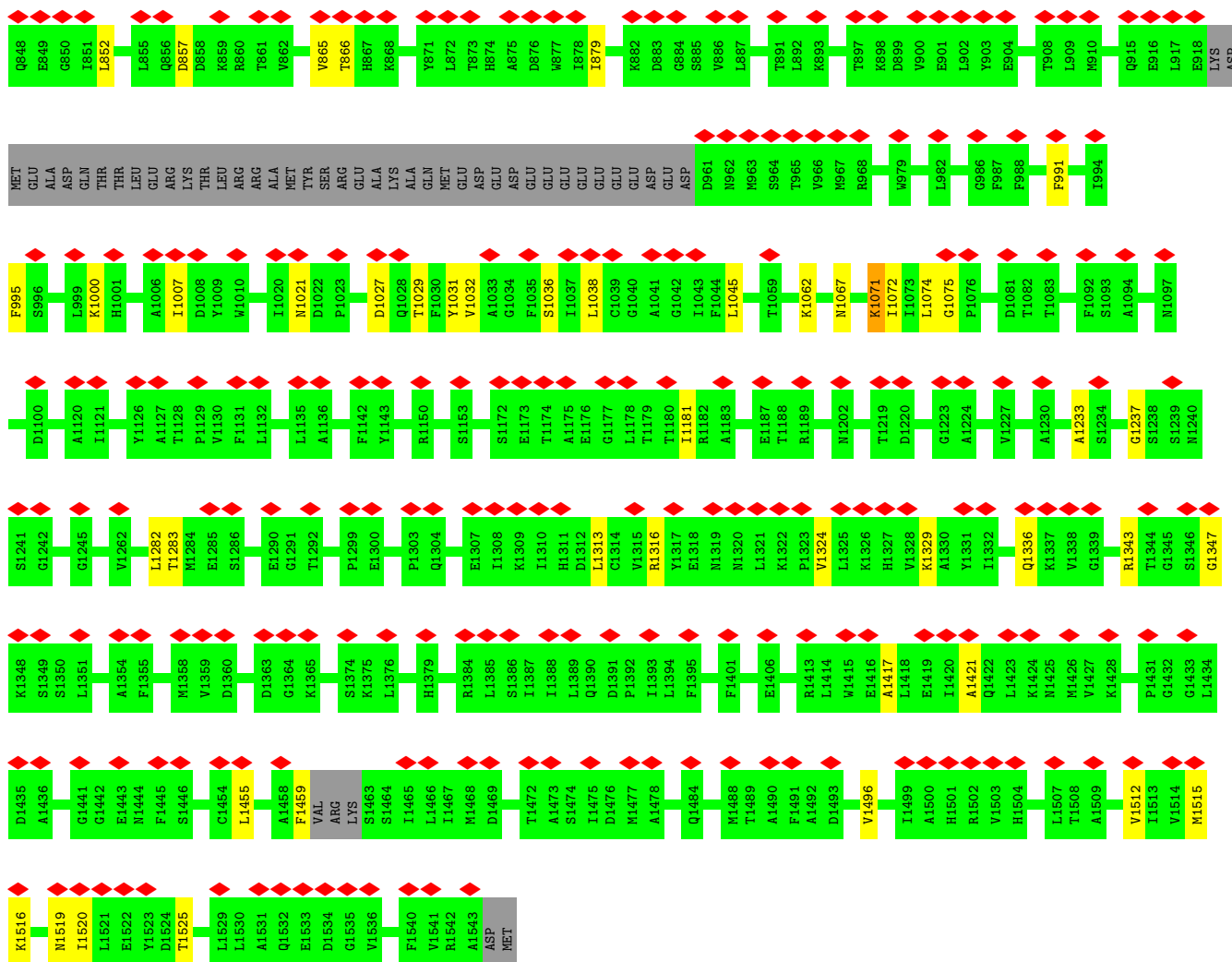
Chain D:



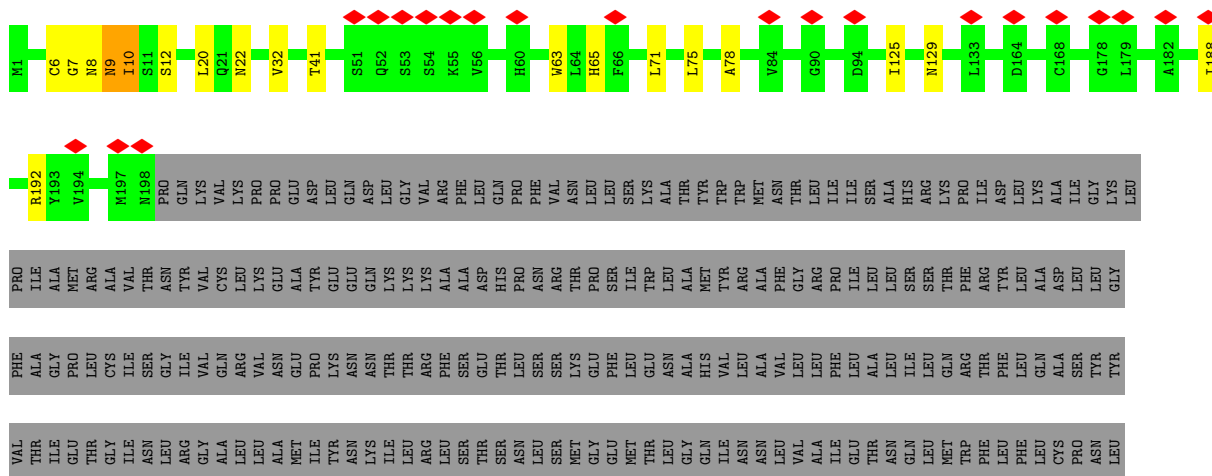
- Molecule 2: Isoform SUR2B of ATP-binding cassette sub-family C member 9

Chain E:





● Molecule 2: Isoform SUR2B of ATP-binding cassette sub-family C member 9

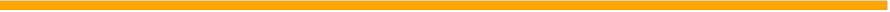


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22038	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	14.659	Depositor
Minimum map value	-11.933	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size ($\text{\AA}$)	125.628, 168.606, 166.953	wwPDB
Map dimensions	76, 102, 101	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.653, 1.653, 1.653	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.50	0/1714	0.81	4/2388 (0.2%)
1	B	0.50	0/1666	0.85	6/2320 (0.3%)
1	C	0.68	0/1674	0.93	9/2332 (0.4%)
1	D	0.86	3/1666 (0.2%)	1.17	17/2320 (0.7%)
2	E	0.69	1/7056 (0.0%)	1.12	69/9822 (0.7%)
2	G	0.90	1/981 (0.1%)	1.35	17/1365 (1.2%)
All	All	0.69	5/14757 (0.0%)	1.06	122/20547 (0.6%)

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	C	0	1
2	E	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	125	ARG	C-O	-5.69	1.17	1.24
1	D	318	ILE	C-O	-5.67	1.18	1.24
1	D	126	SER	C-O	-5.43	1.17	1.23
2	E	88	ALA	N-CA	-5.21	1.40	1.46
2	G	9	ASN	CG-ND2	5.20	1.44	1.33

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	98	ALA	N-CA-C	13.67	125.69	111.07
1	B	114	GLY	N-CA-C	13.11	128.35	112.49
2	G	6	CYS	N-CA-C	11.89	127.84	108.34
2	E	1075	GLY	CA-C-N	11.84	131.81	119.85
2	E	1075	GLY	C-N-CA	11.84	131.81	119.85
1	D	125	ARG	N-CA-C	11.50	123.89	111.36
1	D	312	SER	N-CA-C	10.49	121.67	108.45
2	G	22	ASN	CA-C-N	10.11	130.27	119.05
2	G	22	ASN	C-N-CA	10.11	130.27	119.05
2	E	346	GLU	N-CA-C	10.09	122.28	111.28
1	A	268	CYS	N-CA-C	9.66	124.85	108.23
2	E	673	GLY	N-CA-C	9.43	124.84	112.77
1	C	98	HIS	N-CA-C	-9.12	95.25	109.76
2	E	1072	ILE	N-CA-C	8.96	121.70	112.83
2	E	24	CYS	N-CA-C	8.83	124.19	113.41
2	E	750	TYR	N-CA-C	8.83	120.30	108.38
2	G	32	VAL	CB-CA-C	-8.81	102.46	114.00
2	G	7	GLY	N-CA-C	-8.64	92.70	113.18
2	E	806	ILE	N-CA-C	8.52	119.32	110.72
2	E	6	CYS	N-CA-C	-8.43	95.66	109.40
2	E	32	VAL	CB-CA-C	-8.37	103.03	114.00
2	E	71	LEU	N-CA-C	8.33	120.44	111.36
1	D	317	GLU	N-CA-C	8.29	122.96	113.01
2	E	87	ILE	O-C-N	8.28	130.02	121.91
2	E	798	GLN	N-CA-C	8.02	121.55	111.69
2	E	682	ALA	N-CA-C	7.97	120.43	108.31
1	D	65	VAL	N-CA-C	7.95	119.68	110.62
1	B	113	SER	N-CA-C	7.93	120.00	111.36
1	C	366	ILE	N-CA-C	7.91	118.69	110.62
2	E	756	TRP	N-CA-C	7.82	119.59	111.14
1	D	320	TRP	N-CA-C	7.81	120.97	110.35
2	G	63	TRP	N-CA-C	7.79	119.41	111.07
2	E	42	PHE	CA-C-N	-7.79	110.71	119.28
2	E	42	PHE	C-N-CA	-7.79	110.71	119.28
1	D	102	TYR	N-CA-C	7.69	119.66	111.28
1	D	143	PHE	N-CA-C	7.68	119.29	111.07
1	D	137	VAL	N-CA-C	7.66	117.78	110.42
2	E	106	MET	CA-C-N	7.62	128.31	119.47
2	E	106	MET	C-N-CA	7.62	128.31	119.47
2	G	8	ASN	N-CA-C	7.59	121.46	111.75
2	E	32	VAL	O-C-N	7.35	125.12	120.42
2	E	107	PRO	N-CA-C	-7.30	103.22	113.81
1	B	115	LEU	N-CA-C	7.21	119.22	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	775	GLN	N-CA-C	7.20	120.04	111.33
2	E	681	LEU	N-CA-C	7.08	120.78	109.24
1	D	321	GLY	N-CA-C	7.07	124.76	115.36
2	E	32	VAL	CA-C-N	-7.05	111.23	119.05
2	E	32	VAL	C-N-CA	-7.05	111.23	119.05
2	E	342	LYS	N-CA-C	6.88	121.52	112.72
1	B	111	GLU	N-CA-C	6.81	119.20	107.28
1	D	91	TRP	N-CA-C	6.80	121.91	112.45
1	A	279	ASP	N-CA-C	6.80	120.84	112.54
2	E	223	LEU	N-CA-C	6.77	118.73	111.36
2	E	1029	THR	N-CA-C	-6.71	103.89	111.07
1	D	126	SER	N-CA-C	6.70	119.91	109.52
1	D	105	MET	N-CA-C	6.70	118.66	111.36
2	E	217	GLN	N-CA-C	6.67	114.22	108.22
1	A	251	ASP	N-CA-C	6.63	120.56	111.54
1	C	105	MET	N-CA-C	6.57	118.24	111.14
2	E	326	ASN	N-CA-C	6.57	119.12	108.34
2	E	105	PHE	N-CA-C	6.54	119.39	111.40
2	E	1067	ASN	N-CA-C	6.47	118.42	111.36
2	E	1071	LYS	N-CA-C	6.46	118.32	111.28
1	A	271	ILE	N-CA-C	6.39	117.12	108.17
2	G	32	VAL	O-C-N	6.33	124.47	120.42
2	E	783	ALA	N-CA-C	6.32	122.90	114.12
2	E	329	LYS	N-CA-C	6.29	120.10	111.54
2	E	795	PHE	N-CA-C	6.24	118.08	110.41
1	D	140	THR	N-CA-C	6.23	120.15	111.74
2	E	687	ILE	N-CA-C	6.20	117.06	109.30
2	E	807	ASN	N-CA-C	6.15	118.30	109.14
2	E	226	ALA	N-CA-C	6.08	118.81	108.90
2	G	12	SER	N-CA-C	6.06	118.06	108.79
1	B	36	PHE	N-CA-C	-6.04	105.77	113.01
1	D	127	PHE	N-CA-C	-6.02	105.91	113.20
2	G	41	THR	N-CA-C	6.02	117.92	111.36
1	C	46	ALA	N-CA-C	5.99	118.95	109.96
2	E	797	ASP	CB-CA-C	-5.97	109.70	116.63
1	D	142	GLY	N-CA-C	5.95	127.28	113.18
2	E	216	LEU	N-CA-C	5.94	118.09	108.41
2	E	1074	LEU	N-CA-C	5.91	118.49	109.62
2	G	65	HIS	N-CA-C	5.89	117.70	111.28
2	E	677	TRP	N-CA-C	5.84	118.73	110.50
1	C	109	ILE	N-CA-C	5.83	116.02	110.42
1	D	100	ASP	N-CA-C	5.82	117.63	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	32	VAL	CA-C-N	-5.82	112.59	119.05
2	G	32	VAL	C-N-CA	-5.82	112.59	119.05
2	G	22	ASN	N-CA-C	-5.81	96.96	109.81
2	E	797	ASP	N-CA-C	5.80	117.89	108.08
2	E	675	PHE	N-CA-C	-5.77	98.94	109.56
2	E	684	LEU	N-CA-C	5.75	118.44	107.75
2	E	19	VAL	N-CA-C	5.69	116.43	110.62
2	E	770	SER	N-CA-C	5.67	119.75	107.49
1	B	116	GLU	N-CA-C	5.63	119.88	112.89
1	C	360	GLU	N-CA-C	5.58	117.17	111.14
2	E	1181	ILE	N-CA-C	-5.52	107.60	112.90
2	E	8	ASN	N-CA-C	5.52	119.49	112.87
1	C	124	VAL	N-CA-C	-5.48	100.50	108.17
2	E	337	GLU	N-CA-C	-5.47	101.95	110.10
2	E	780	VAL	N-CA-C	-5.45	104.28	111.09
2	E	175	ILE	N-CA-C	5.40	116.13	110.62
2	G	78	ALA	N-CA-C	-5.37	105.33	111.07
2	E	143	MET	CA-C-N	5.32	129.68	120.58
2	E	143	MET	C-N-CA	5.32	129.68	120.58
1	C	108	GLY	N-CA-C	5.30	119.55	112.77
2	E	773	ASN	N-CA-C	5.24	117.62	108.76
2	E	765	ASN	N-CA-C	-5.23	106.85	113.18
2	G	10	ILE	N-CA-C	5.22	117.61	111.09
2	E	4	SER	N-CA-C	5.16	116.82	108.41
1	C	34	ALA	N-CA-C	5.14	117.15	109.59
2	E	448	LEU	N-CA-C	5.14	120.42	114.04
2	E	42	PHE	O-C-N	5.14	125.54	120.71
2	E	787	GLN	N-CA-C	5.13	121.15	109.81
2	E	343	GLU	N-CA-C	5.10	116.84	111.28
2	E	344	PHE	N-CA-C	5.10	116.84	111.28
2	E	1062	LYS	N-CA-C	-5.07	105.75	111.28
2	G	20	LEU	N-CA-C	5.07	118.96	112.87
1	D	113	SER	N-CA-C	5.05	116.86	109.24
2	E	23	PRO	O-C-N	-5.04	115.49	122.24
2	E	1021	ASN	N-CA-C	5.03	116.76	111.28
2	E	682	ALA	CB-CA-C	-5.02	110.77	116.54
2	E	685	SER	N-CA-C	5.00	116.54	108.34

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	357	GLU	Mainchain
2	E	155	TYR	Mainchain

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	1714	0	779	14	0
1	B	1667	0	756	19	0
1	C	1674	0	764	5	0
1	D	1667	0	756	14	0
2	E	7060	0	3222	67	0
2	G	982	0	433	5	0
3	F	28	0	25	3	0
3	N	28	0	25	7	0
4	A	1	0	0	0	0
5	A	31	0	12	12	0
5	B	31	0	12	11	0
5	C	31	0	12	0	0
5	D	31	0	12	0	0
5	E	31	0	12	12	0
All	All	14976	0	6820	131	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 (131) 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:A:343:GLY:CA	5:A:3002:ATP:O1A	1.94	1.14
1:A:343:GLY:N	5:A:3002:ATP:O1A	1.83	1.09
1:B:339:TYR:O	5:B:501:ATP:N6	1.85	1.09
1:B:339:TYR:C	5:B:501:ATP:HN61	1.59	1.09
1:A:343:GLY:HA3	5:A:3002:ATP:O1A	1.55	1.05
2:E:1071:LYS:CB	2:E:1283:THR:HA	1.87	1.05
2:E:706:GLY:HA2	5:E:1601:ATP:H5'1	1.39	1.04
2:E:1000:LYS:HA	2:E:1045:LEU:CB	1.91	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:2:NAG:H3	3:N:2:NAG:H82	1.45	0.97
1:A:195:ARG:H	5:A:3002:ATP:H5'1	1.26	0.96
2:E:705:CYS:CB	5:E:1601:ATP:O2A	2.14	0.94
2:E:763:GLU:CB	2:E:802:GLY:H	1.82	0.93
2:E:777:TYR:O	2:E:781:THR:N	2.03	0.92
2:E:706:GLY:HA2	5:E:1601:ATP:C5'	2.02	0.90
1:B:339:TYR:C	5:B:501:ATP:N6	2.24	0.89
1:D:121:VAL:HA	1:D:147:MET:O	1.73	0.89
2:E:1000:LYS:CB	2:E:1045:LEU:CB	2.56	0.83
1:D:126:SER:H	1:D:129:SER:CB	1.93	0.82
2:E:1000:LYS:CA	2:E:1045:LEU:CB	2.59	0.81
2:E:153:VAL:O	2:E:156:TRP:CB	2.30	0.79
2:E:761:THR:CB	2:E:802:GLY:CA	2.62	0.77
2:E:267:ALA:HB2	2:E:292:ALA:HB3	1.66	0.76
2:E:763:GLU:CB	2:E:802:GLY:N	2.48	0.75
2:E:338:THR:CB	2:E:343:GLU:CB	2.65	0.75
2:E:706:GLY:H	5:E:1601:ATP:H5'2	1.52	0.75
2:E:267:ALA:HB2	2:E:292:ALA:CB	2.20	0.71
1:B:342:PHE:CB	5:B:501:ATP:C8	2.73	0.71
2:E:706:GLY:N	5:E:1601:ATP:H5'2	2.06	0.70
1:B:195:ARG:H	5:B:501:ATP:H5'1	1.57	0.70
2:E:707:LYS:N	5:E:1601:ATP:O1A	2.25	0.69
2:E:778:LYS:HA	2:E:781:THR:CB	2.24	0.67
2:E:1336:GLN:O	2:E:1496:VAL:N	2.22	0.66
3:F:2:NAG:O6	3:F:2:NAG:O4	2.10	0.65
1:B:195:ARG:CB	5:B:501:ATP:H5'2	2.27	0.64
1:A:195:ARG:N	5:A:3002:ATP:H5'1	2.05	0.64
2:E:1032:VAL:O	2:E:1036:SER:CB	2.45	0.64
2:E:699:ILE:HA	2:E:879:ILE:H	1.62	0.64
2:E:706:GLY:CA	5:E:1601:ATP:C5'	2.76	0.64
2:E:323:GLN:HA	2:E:566:ALA:HB2	1.81	0.63
1:A:195:ARG:CB	5:A:3002:ATP:H5'2	2.29	0.62
1:A:343:GLY:HA3	5:A:3002:ATP:PA	2.38	0.62
1:A:339:TYR:O	5:A:3002:ATP:N7	2.33	0.62
1:D:196:HIS:CB	1:D:317:GLU:O	2.47	0.62
2:E:761:THR:CB	2:E:802:GLY:HA2	2.29	0.61
2:E:1343:ARG:O	2:E:1347:GLY:N	2.32	0.61
2:E:1455:LEU:O	2:E:1459:PHE:N	2.32	0.61
1:D:126:SER:CB	1:D:129:SER:H	2.12	0.61
1:B:342:PHE:CB	5:B:501:ATP:N7	2.64	0.61
2:E:672:ASN:CB	2:E:723:GLY:HA3	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:991:PHE:O	2:E:995:PHE:CB	2.48	0.61
2:E:1071:LYS:CB	2:E:1282:LEU:O	2.49	0.61
2:E:1233:ALA:O	2:E:1237:GLY:N	2.30	0.59
2:G:9:ASN:C	2:G:9:ASN:OD1	2.46	0.58
2:E:1071:LYS:CB	2:E:1283:THR:CA	2.74	0.58
1:D:322:HIS:CB	1:D:346:VAL:O	2.51	0.57
1:B:195:ARG:N	5:B:501:ATP:H5'1	2.18	0.57
2:E:267:ALA:HB1	2:E:288:ALA:HB1	1.85	0.57
1:D:234:THR:HA	1:D:240:VAL:HA	1.87	0.56
2:G:9:ASN:OD1	2:G:10:ILE:N	2.38	0.56
1:D:126:SER:C	1:D:128:THR:H	2.13	0.56
1:C:209:MET:HA	1:C:267:ILE:O	2.05	0.56
2:E:706:GLY:N	5:E:1601:ATP:O2A	2.41	0.54
2:E:1007:ILE:HA	2:E:1038:LEU:CB	2.36	0.54
2:E:761:THR:CB	2:E:802:GLY:O	2.56	0.53
1:A:339:TYR:CB	5:A:3002:ATP:N6	2.71	0.53
2:E:991:PHE:HA	2:E:995:PHE:CB	2.38	0.53
1:D:126:SER:C	1:D:128:THR:N	2.65	0.53
3:N:2:NAG:H82	3:N:2:NAG:C3	2.28	0.53
1:D:126:SER:O	1:D:129:SER:N	2.42	0.53
2:E:706:GLY:CA	5:E:1601:ATP:H5'2	2.38	0.53
1:B:339:TYR:CB	5:B:501:ATP:N6	2.73	0.52
2:E:761:THR:CB	2:E:802:GLY:C	2.82	0.52
2:E:1515:MET:HA	2:E:1520:ILE:HA	1.92	0.51
2:E:698:MET:HA	2:E:865:VAL:HA	1.93	0.51
2:E:106:MET:O	2:E:109:VAL:N	2.44	0.51
2:E:833:ASP:HA	2:E:866:THR:HA	1.93	0.51
2:G:71:LEU:O	2:G:75:LEU:CB	2.59	0.51
1:B:127:PHE:O	1:B:130:ALA:N	2.44	0.50
2:E:761:THR:CB	2:E:802:GLY:HA3	2.41	0.50
2:G:188:ILE:O	2:G:192:ARG:N	2.45	0.50
1:C:34:ALA:CB	1:D:334:VAL:HA	2.42	0.50
1:D:235:THR:N	1:D:239:GLU:O	2.44	0.50
2:E:1417:ALA:O	2:E:1421:ALA:N	2.46	0.49
2:G:125:ILE:O	2:G:129:ASN:HA	2.13	0.49
2:E:125:ILE:O	2:E:128:SER:O	2.31	0.48
2:E:778:LYS:O	2:E:782:ASP:N	2.39	0.48
2:E:793:LEU:N	2:E:794:PRO:CD	2.76	0.48
3:N:1:NAG:N2	3:N:1:NAG:H5	2.27	0.48
2:E:1313:LEU:H	2:E:1329:LYS:HA	1.79	0.48
2:E:1516:LYS:N	2:E:1519:ASN:O	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:2:NAG:N2	3:N:2:NAG:H5	2.27	0.47
1:B:35:ARG:C	1:B:37:ILE:N	2.70	0.47
1:A:195:ARG:CB	5:A:3002:ATP:C5'	2.93	0.47
1:A:339:TYR:C	5:A:3002:ATP:HN61	2.23	0.46
2:E:706:GLY:H	5:E:1601:ATP:C5'	2.24	0.46
2:E:799:THR:C	2:E:801:ILE:N	2.72	0.46
2:E:1512:VAL:H	2:E:1525:THR:HA	1.80	0.46
3:N:2:NAG:H3	3:N:2:NAG:C8	2.25	0.46
2:E:1316:ARG:HA	2:E:1324:VAL:O	2.15	0.46
2:E:552:PHE:O	2:E:555:HIS:CB	2.64	0.45
2:E:1027:ASP:O	2:E:1031:TYR:N	2.46	0.45
2:E:706:GLY:H	5:E:1601:ATP:PA	2.39	0.45
1:B:235:THR:O	1:B:238:GLY:N	2.50	0.45
1:A:339:TYR:CB	5:A:3002:ATP:HN61	2.29	0.45
1:C:320:TRP:C	1:C:322:HIS:H	2.25	0.45
3:F:2:NAG:HO4	3:F:2:NAG:HO6	1.57	0.45
2:E:674:TYR:O	2:E:720:THR:CB	2.65	0.44
1:A:38:ALA:O	1:A:41:GLY:N	2.51	0.44
1:B:46:ALA:HB3	1:C:336:SER:HA	1.98	0.44
1:B:339:TYR:O	5:B:501:ATP:C6	2.65	0.44
2:E:673:GLY:HA2	2:E:687:ILE:CB	2.47	0.44
2:E:670:VAL:CB	2:E:724:LYS:O	2.66	0.44
2:E:87:ILE:O	2:E:91:ILE:N	2.40	0.44
3:N:2:NAG:N2	3:N:2:NAG:C5	2.81	0.43
1:B:35:ARG:C	1:B:37:ILE:H	2.27	0.43
3:F:1:NAG:O7	3:F:1:NAG:H3	2.17	0.43
2:E:267:ALA:CB	2:E:288:ALA:HB1	2.49	0.43
1:D:282:ALA:HB2	1:D:352:ARG:O	2.19	0.42
2:E:154:LYS:C	2:E:156:TRP:N	2.78	0.42
2:E:706:GLY:N	5:E:1601:ATP:C5'	2.78	0.42
1:B:38:ALA:HB3	1:B:41:GLY:O	2.20	0.41
2:E:435:PRO:O	2:E:439:ILE:CB	2.68	0.41
3:N:1:NAG:O4	3:N:1:NAG:O7	2.39	0.41
1:D:92:TRP:HA	1:D:130:ALA:CB	2.50	0.41
2:E:267:ALA:HB1	2:E:288:ALA:CB	2.50	0.41
1:A:31:LEU:O	1:B:333:GLY:HA2	2.21	0.41
1:D:122:THR:O	1:D:146:ARG:HA	2.21	0.41
2:E:852:LEU:O	2:E:857:ASP:N	2.53	0.41
1:B:127:PHE:O	1:B:128:THR:C	2.63	0.40
1:C:32:PRO:O	1:C:32:PRO:CG	2.70	0.40
1:B:195:ARG:N	5:B:501:ATP:C5'	2.84	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	344/424 (81%)	311 (90%)	33 (10%)	0	100	100
1	B	335/424 (79%)	296 (88%)	39 (12%)	0	100	100
1	C	336/424 (79%)	301 (90%)	35 (10%)	0	100	100
1	D	335/424 (79%)	301 (90%)	34 (10%)	0	100	100
2	E	1412/1545 (91%)	1286 (91%)	126 (9%)	0	100	100
2	G	196/1545 (13%)	184 (94%)	12 (6%)	0	100	100
All	All	2958/4786 (62%)	2679 (91%)	279 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	1/376 (0%)	1 (100%)	0	100	100
1	C	1/376 (0%)	1 (100%)	0	100	100
2	E	4/1348 (0%)	4 (100%)	0	100	100
2	G	1/1348 (0%)	1 (100%)	0	100	100
All	All	7/3448 (0%)	7 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	F	1	2,3	14,14,15	0.74	0	17,19,21	2.88	6 (35%)
3	NAG	F	2	3	14,14,15	0.44	0	17,19,21	1.32	2 (11%)
3	NAG	N	1	2,3	14,14,15	0.29	0	17,19,21	0.59	0
3	NAG	N	2	3	14,14,15	0.26	0	17,19,21	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	2,3	1/1/5/7	6/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	NAG	N	1	2,3	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	N	2	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C4-C3-C2	-7.00	100.76	111.02
3	F	1	NAG	O4-C4-C3	5.83	124.11	110.38
3	F	1	NAG	O5-C5-C4	-4.98	98.70	110.83
3	F	2	NAG	C2-N2-C7	-3.18	118.64	122.90
3	F	1	NAG	C1-O5-C5	2.92	116.10	112.19
3	F	1	NAG	C2-N2-C7	-2.83	119.10	122.90
3	F	2	NAG	C1-O5-C5	2.52	115.57	112.19
3	F	1	NAG	C3-C4-C5	-2.43	105.83	110.23

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	N	1	NAG	C1
3	F	1	NAG	C1

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
3	N	2	NAG	C3-C2-N2-C7
3	N	2	NAG	C8-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C3-C2-N2-C7
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	F	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C8-C7-N2-C2
3	F	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O7-C7-N2-C2
3	N	1	NAG	C3-C2-N2-C7
3	F	1	NAG	C1-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 10 short contacts:

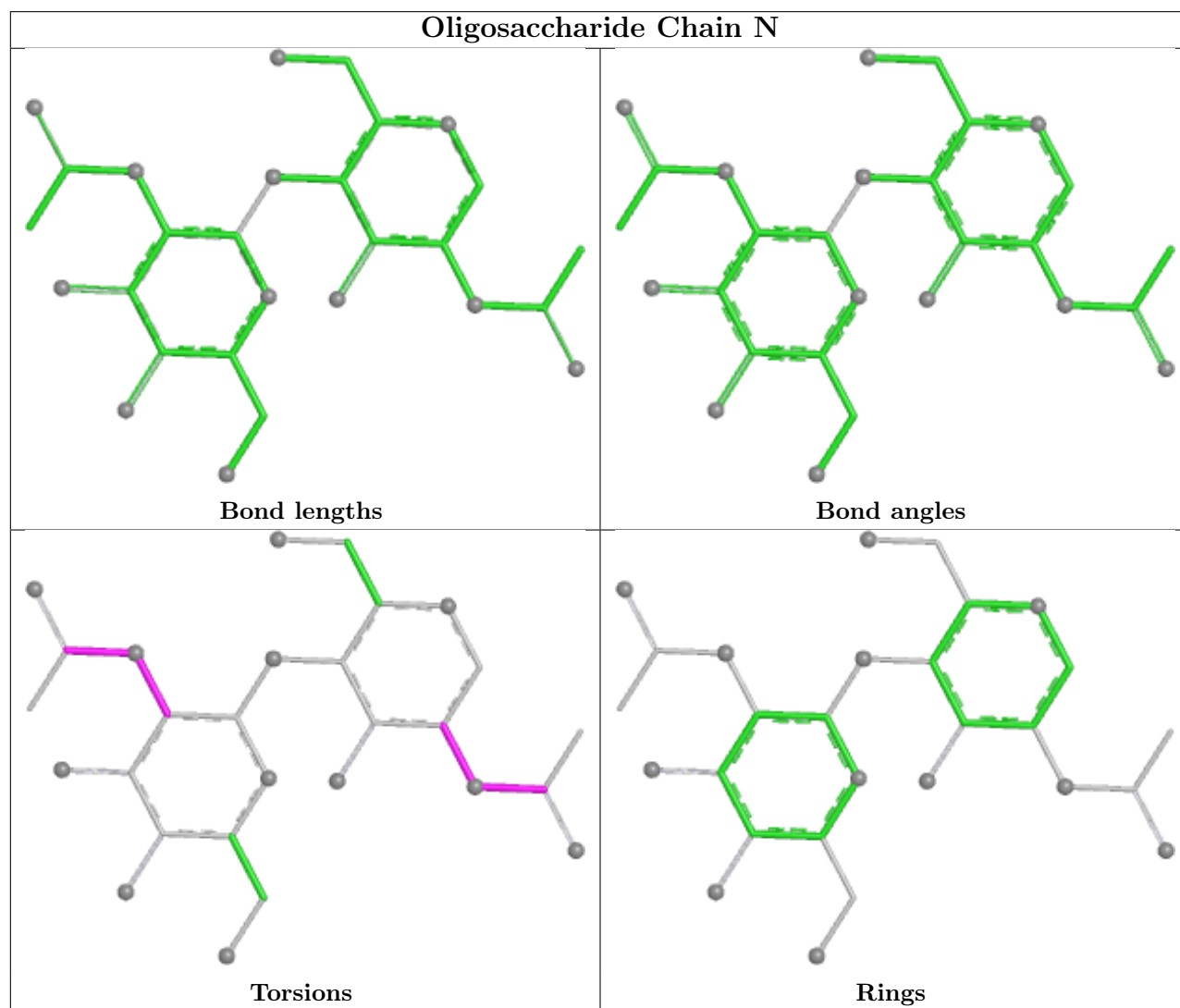
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	2	0

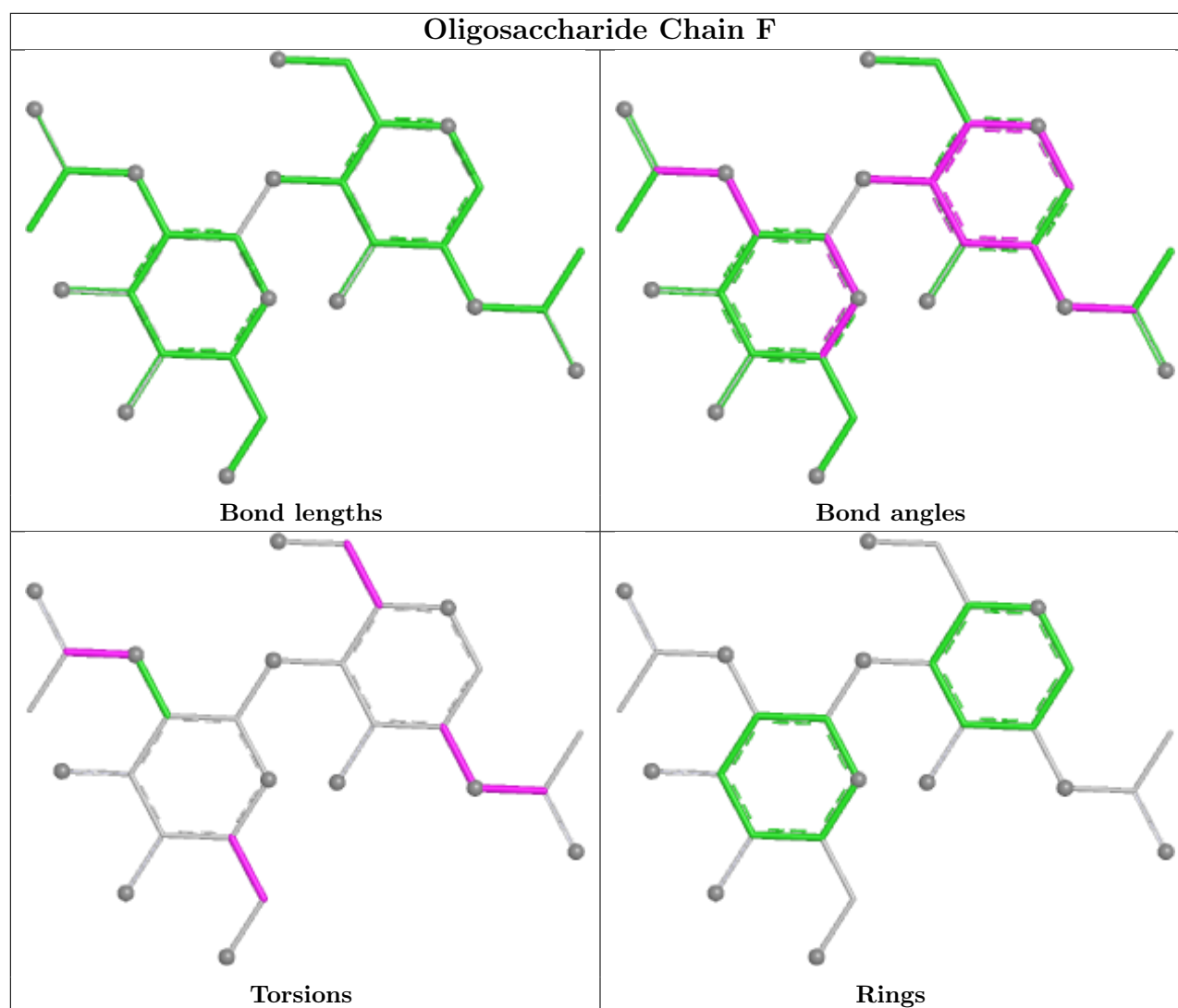
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	1	NAG	2	0
3	F	1	NAG	1	0
3	N	2	NAG	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	D	501	-	32,33,33	1.30	6 (18%)	48,52,52	1.71	8 (16%)
5	ATP	E	1601	-	32,33,33	1.40	4 (12%)	48,52,52	1.76	9 (18%)
5	ATP	B	501	-	32,33,33	1.29	5 (15%)	48,52,52	1.76	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ATP	A	3002	-	32,33,33	1.36	5 (15%)	48,52,52	1.79	11 (22%)
5	ATP	C	501	-	32,33,33	1.31	5 (15%)	48,52,52	1.79	12 (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	D	501	-	-	4/22/38/38	0/3/3/3
5	ATP	E	1601	-	-	1/22/38/38	0/3/3/3
5	ATP	B	501	-	-	4/22/38/38	0/3/3/3
5	ATP	A	3002	-	-	5/22/38/38	0/3/3/3
5	ATP	C	501	-	-	5/22/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1601	ATP	C5-C4	4.73	1.47	1.39
5	A	3002	ATP	C5-C4	4.37	1.46	1.39
5	B	501	ATP	C5-C4	4.31	1.46	1.39
5	C	501	ATP	C5-C4	4.15	1.46	1.39
5	D	501	ATP	C5-C4	4.14	1.46	1.39
5	D	501	ATP	C5-N7	-2.75	1.34	1.39
5	C	501	ATP	C5-N7	-2.71	1.34	1.39
5	A	3002	ATP	C5-C6	2.68	1.48	1.41
5	C	501	ATP	C4-N9	-2.54	1.32	1.37
5	D	501	ATP	C4-N9	-2.52	1.32	1.37
5	B	501	ATP	C5-N7	-2.52	1.34	1.39
5	E	1601	ATP	C5-C6	2.48	1.47	1.41
5	E	1601	ATP	C5-N7	-2.46	1.34	1.39
5	A	3002	ATP	C8-N7	2.38	1.36	1.31
5	B	501	ATP	C5-C6	2.38	1.47	1.41
5	B	501	ATP	C4-N9	-2.35	1.32	1.37
5	D	501	ATP	C5-C6	2.34	1.47	1.41
5	C	501	ATP	C5-C6	2.34	1.47	1.41
5	E	1601	ATP	C8-N7	2.29	1.36	1.31
5	A	3002	ATP	C5-N7	-2.29	1.34	1.39
5	B	501	ATP	C8-N7	2.29	1.36	1.31
5	A	3002	ATP	C4-N9	-2.10	1.33	1.37
5	C	501	ATP	C8-N7	2.08	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	ATP	C8-N7	2.05	1.35	1.31
5	D	501	ATP	C8-N9	-2.01	1.34	1.37

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1601	ATP	C5-C4-N3	-5.69	118.88	126.72
5	A	3002	ATP	C5-C4-N3	-5.68	118.89	126.72
5	C	501	ATP	C5-C4-N3	-5.60	119.01	126.72
5	B	501	ATP	C5-C4-N3	-5.57	119.05	126.72
5	D	501	ATP	C5-C4-N3	-5.48	119.17	126.72
5	E	1601	ATP	N3-C4-N9	4.61	135.00	127.17
5	C	501	ATP	N3-C4-N9	4.48	134.79	127.17
5	D	501	ATP	N3-C4-N9	4.31	134.50	127.17
5	B	501	ATP	N3-C4-N9	4.23	134.35	127.17
5	A	3002	ATP	N3-C4-N9	4.15	134.22	127.17
5	A	3002	ATP	C4-C5-N7	-3.80	106.24	110.58
5	C	501	ATP	C2-N3-C4	3.71	120.89	111.83
5	A	3002	ATP	C2-N3-C4	3.71	120.89	111.83
5	D	501	ATP	C2-N3-C4	3.59	120.60	111.83
5	B	501	ATP	C2-N3-C4	3.53	120.45	111.83
5	C	501	ATP	N3-C2-N1	-3.49	123.30	128.58
5	E	1601	ATP	C2-N3-C4	3.49	120.35	111.83
5	C	501	ATP	C4-C5-N7	-3.39	106.70	110.58
5	B	501	ATP	C4-C5-N7	-3.39	106.71	110.58
5	E	1601	ATP	C4-C5-N7	-3.36	106.74	110.58
5	A	3002	ATP	N3-C2-N1	-3.33	123.55	128.58
5	D	501	ATP	C4-C5-N7	-3.20	106.92	110.58
5	D	501	ATP	N3-C2-N1	-3.17	123.79	128.58
5	C	501	ATP	C4-N9-C8	3.11	109.00	105.74
5	E	1601	ATP	N3-C2-N1	-3.05	123.96	128.58
5	B	501	ATP	N3-C2-N1	-2.88	124.22	128.58
5	E	1601	ATP	C4-N9-C8	2.75	108.62	105.74
5	D	501	ATP	C4-N9-C8	2.64	108.51	105.74
5	A	3002	ATP	C5-N7-C8	2.61	107.55	103.45
5	B	501	ATP	C3'-C2'-C1'	2.55	106.28	101.46
5	B	501	ATP	C4-N9-C8	2.53	108.40	105.74
5	E	1601	ATP	C5-N7-C8	2.51	107.40	103.45
5	C	501	ATP	C5-N7-C8	2.49	107.37	103.45
5	A	3002	ATP	C4-N9-C8	2.47	108.33	105.74
5	A	3002	ATP	C6-C5-N7	2.41	136.74	132.09
5	B	501	ATP	C5-N7-C8	2.32	107.10	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	ATP	N9-C8-N7	-2.27	110.72	113.94
5	A	3002	ATP	C3'-C2'-C1'	2.21	105.64	101.46
5	D	501	ATP	C5-N7-C8	2.18	106.88	103.45
5	B	501	ATP	C6-C5-N7	2.17	136.27	132.09
5	E	1601	ATP	C3'-C2'-C1'	2.15	105.53	101.46
5	A	3002	ATP	N9-C8-N7	-2.08	110.99	113.94
5	C	501	ATP	O2A-PA-O1A	2.06	122.03	112.44
5	A	3002	ATP	O2A-PA-O1A	2.05	121.97	112.44
5	D	501	ATP	O4'-C1'-N9	2.04	112.00	108.09
5	E	1601	ATP	C2'-C1'-N9	-2.04	108.25	113.30
5	B	501	ATP	O2A-PA-O1A	2.03	121.91	112.44
5	C	501	ATP	C6-C5-N7	2.03	136.01	132.09
5	C	501	ATP	C3'-C2'-C1'	2.02	105.28	101.46
5	C	501	ATP	C2-N1-C6	2.00	122.02	118.73

There are no chirality outliers.

All (19) torsion outliers are listed below:

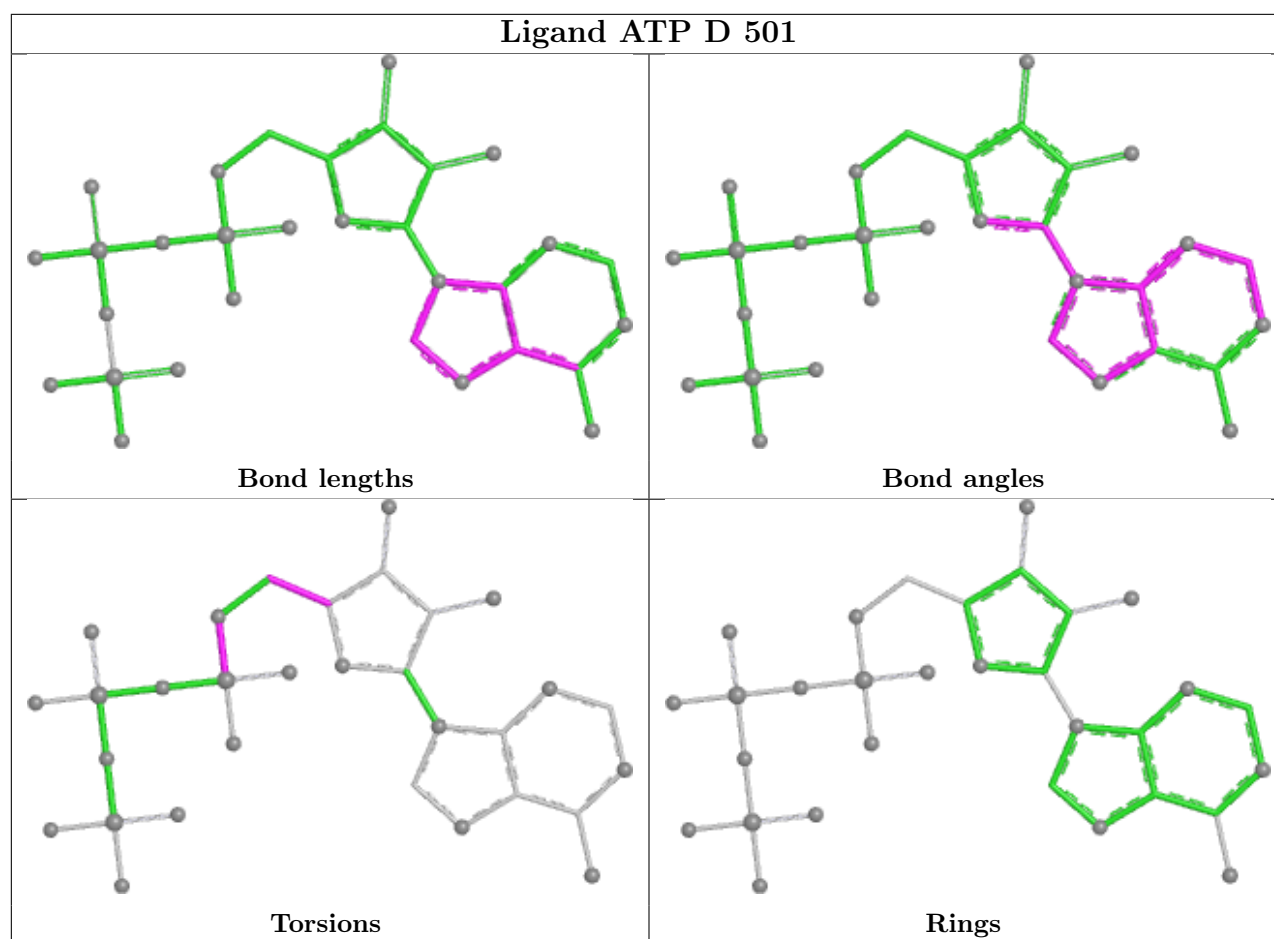
Mol	Chain	Res	Type	Atoms
5	A	3002	ATP	C5'-O5'-PA-O3A
5	B	501	ATP	C5'-O5'-PA-O3A
5	C	501	ATP	C5'-O5'-PA-O1A
5	C	501	ATP	C5'-O5'-PA-O2A
5	C	501	ATP	C5'-O5'-PA-O3A
5	C	501	ATP	O4'-C4'-C5'-O5'
5	D	501	ATP	C5'-O5'-PA-O2A
5	D	501	ATP	C5'-O5'-PA-O3A
5	C	501	ATP	C3'-C4'-C5'-O5'
5	D	501	ATP	O4'-C4'-C5'-O5'
5	A	3002	ATP	O4'-C4'-C5'-O5'
5	D	501	ATP	C3'-C4'-C5'-O5'
5	A	3002	ATP	C5'-O5'-PA-O1A
5	B	501	ATP	C5'-O5'-PA-O1A
5	E	1601	ATP	C5'-O5'-PA-O1A
5	B	501	ATP	PB-O3A-PA-O1A
5	A	3002	ATP	PB-O3A-PA-O2A
5	B	501	ATP	PB-O3A-PA-O2A
5	A	3002	ATP	C3'-C4'-C5'-O5'

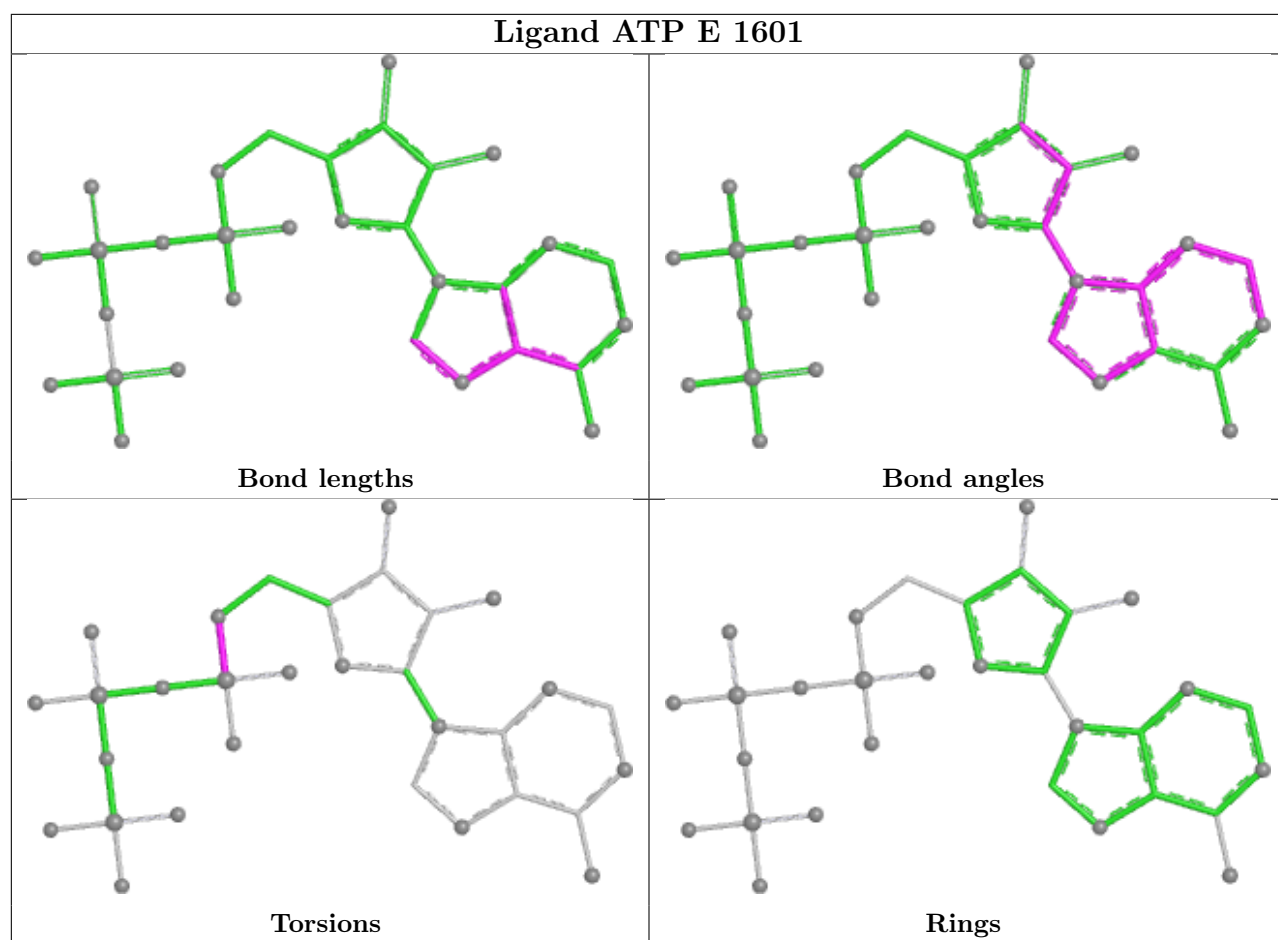
There are no ring outliers.

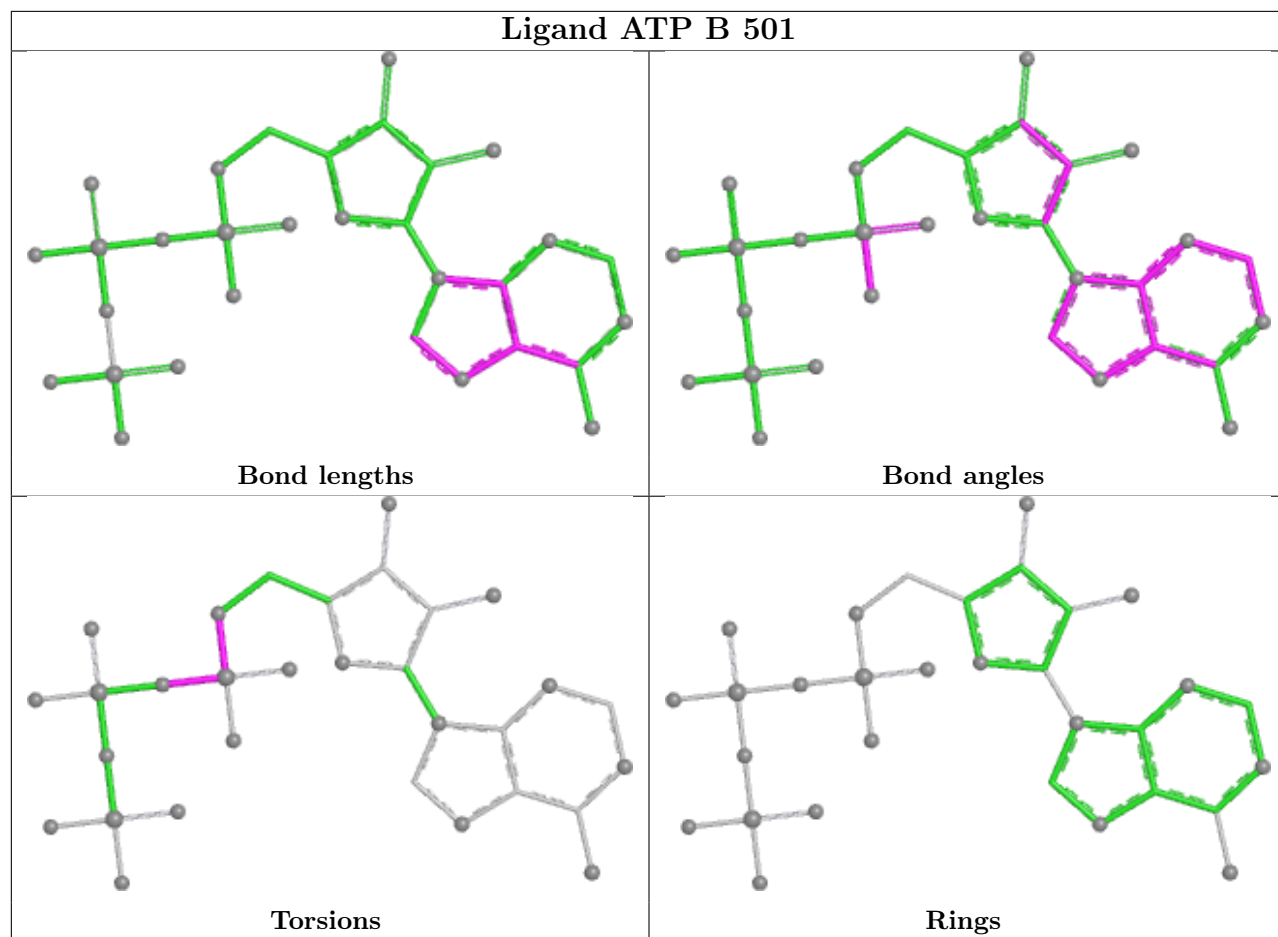
3 monomers are involved in 35 short contacts:

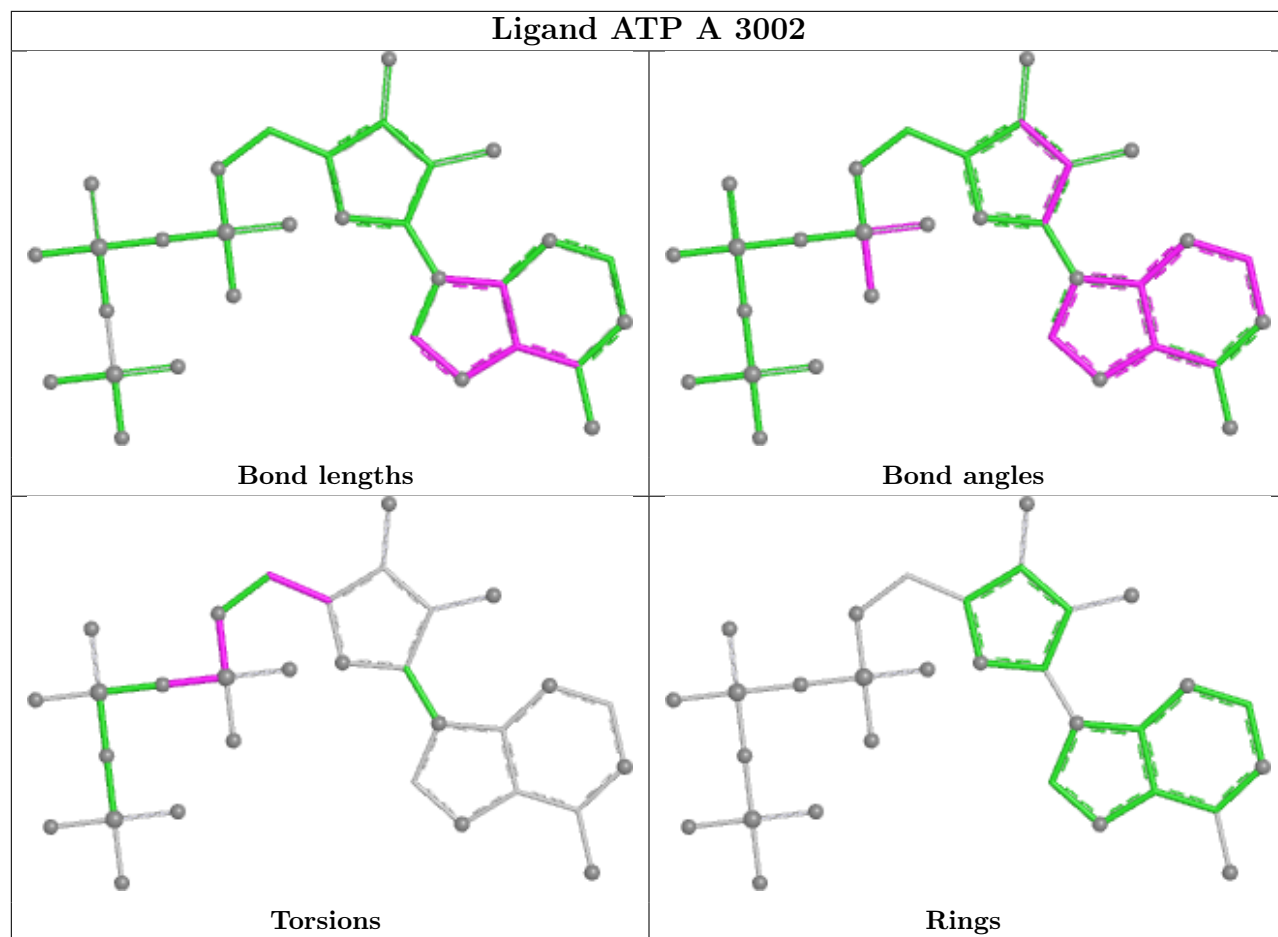
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1601	ATP	12	0
5	B	501	ATP	11	0
5	A	3002	ATP	12	0

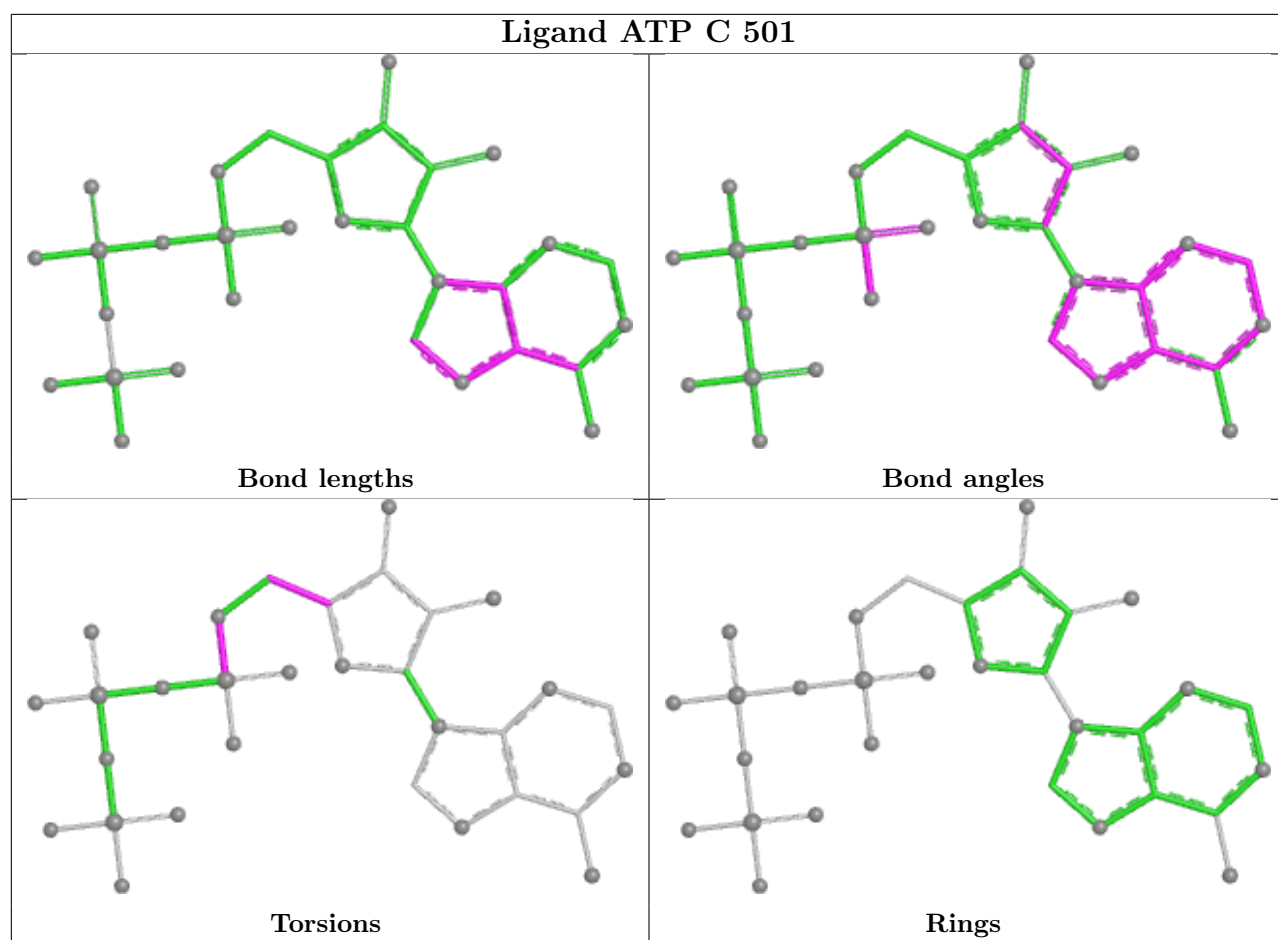
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

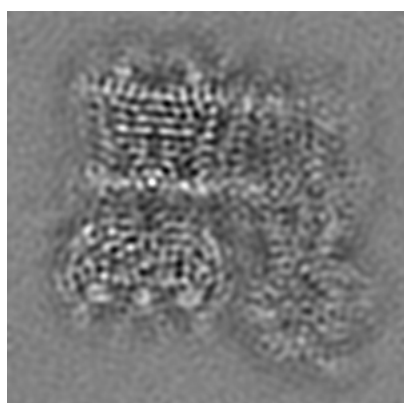
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23882. These allow visual inspection of the internal detail of the map and identification of artifacts.

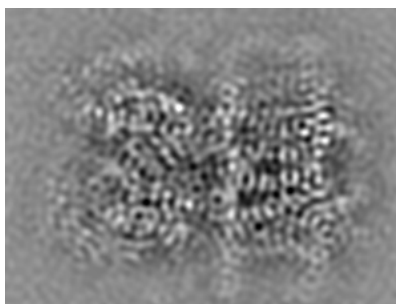
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

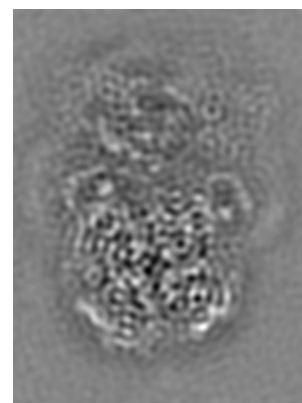
6.1.1 Primary map



X



Y

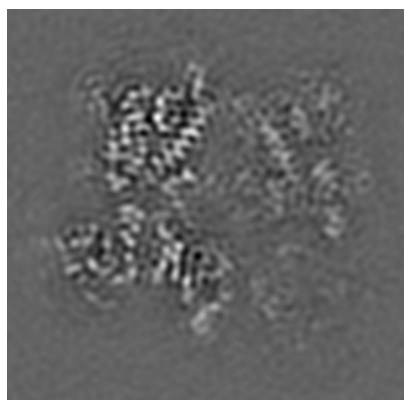


Z

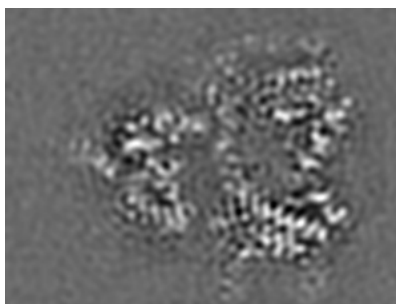
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

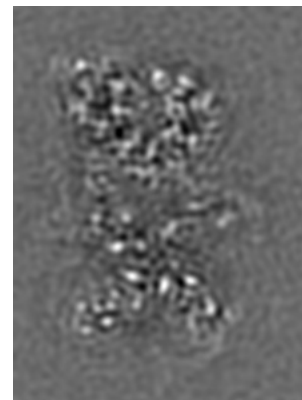
6.2.1 Primary map



X Index: 38



Y Index: 51

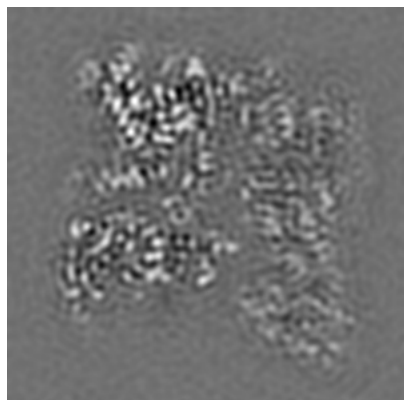


Z Index: 50

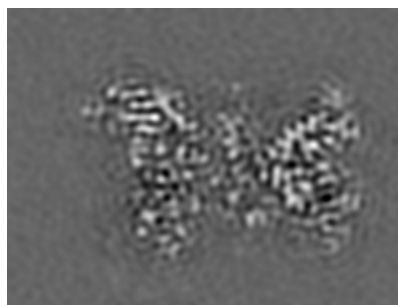
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

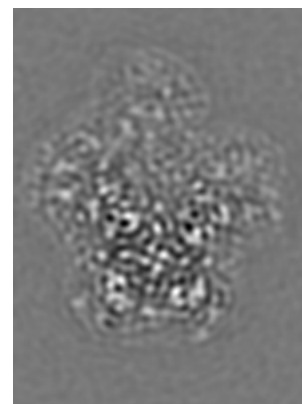
6.3.1 Primary map



X Index: 27



Y Index: 29

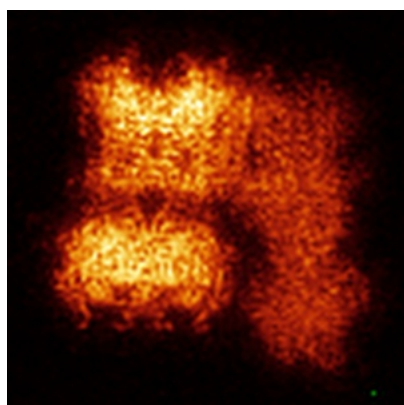


Z Index: 77

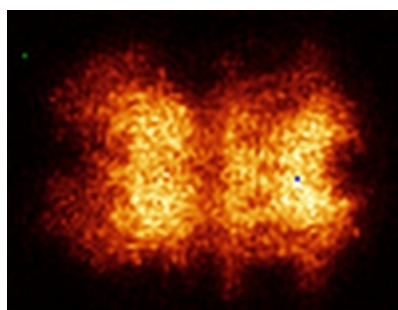
The images above show the largest variance slices of the map in three orthogonal directions.

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

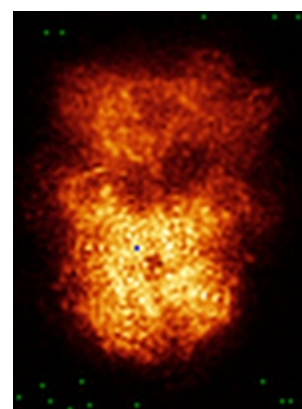
6.4.1 Primary map



X



Y

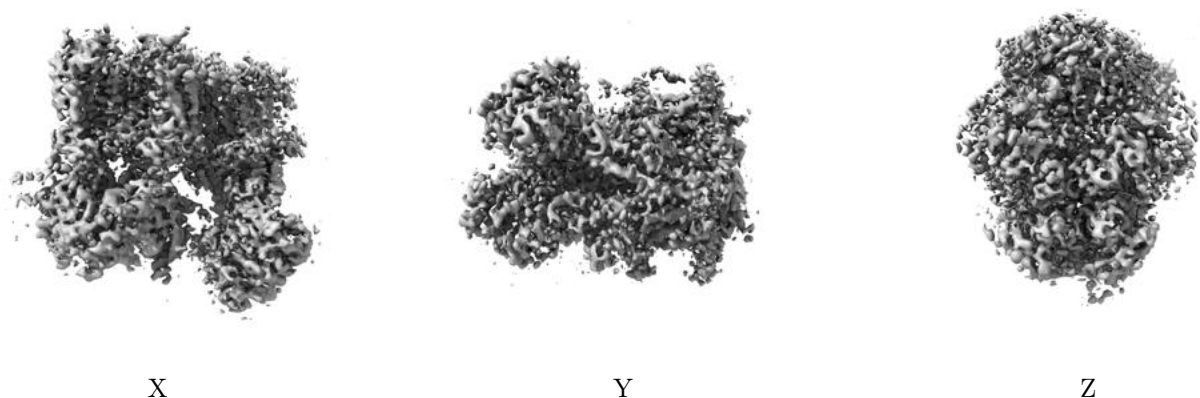


Z

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 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

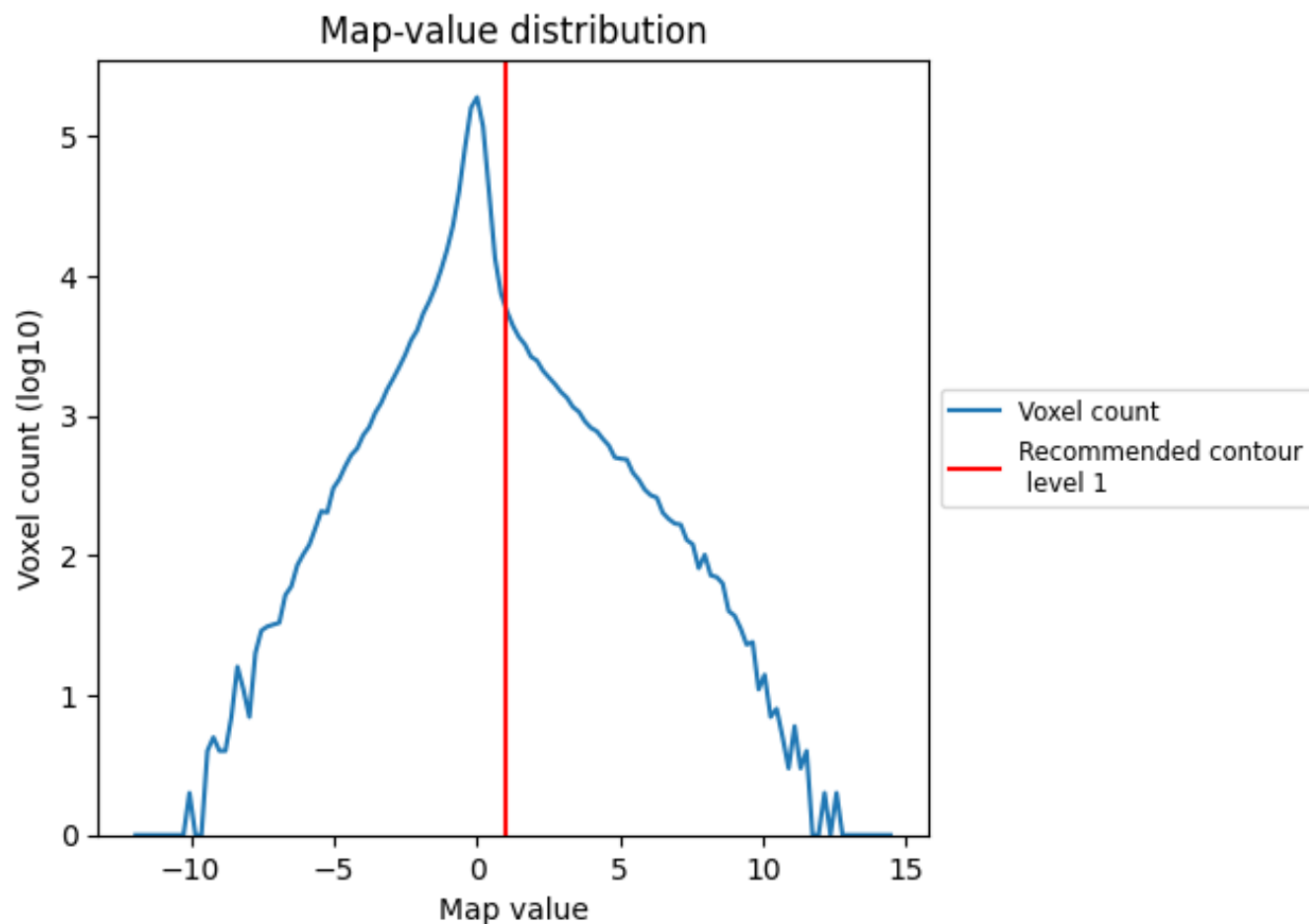
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

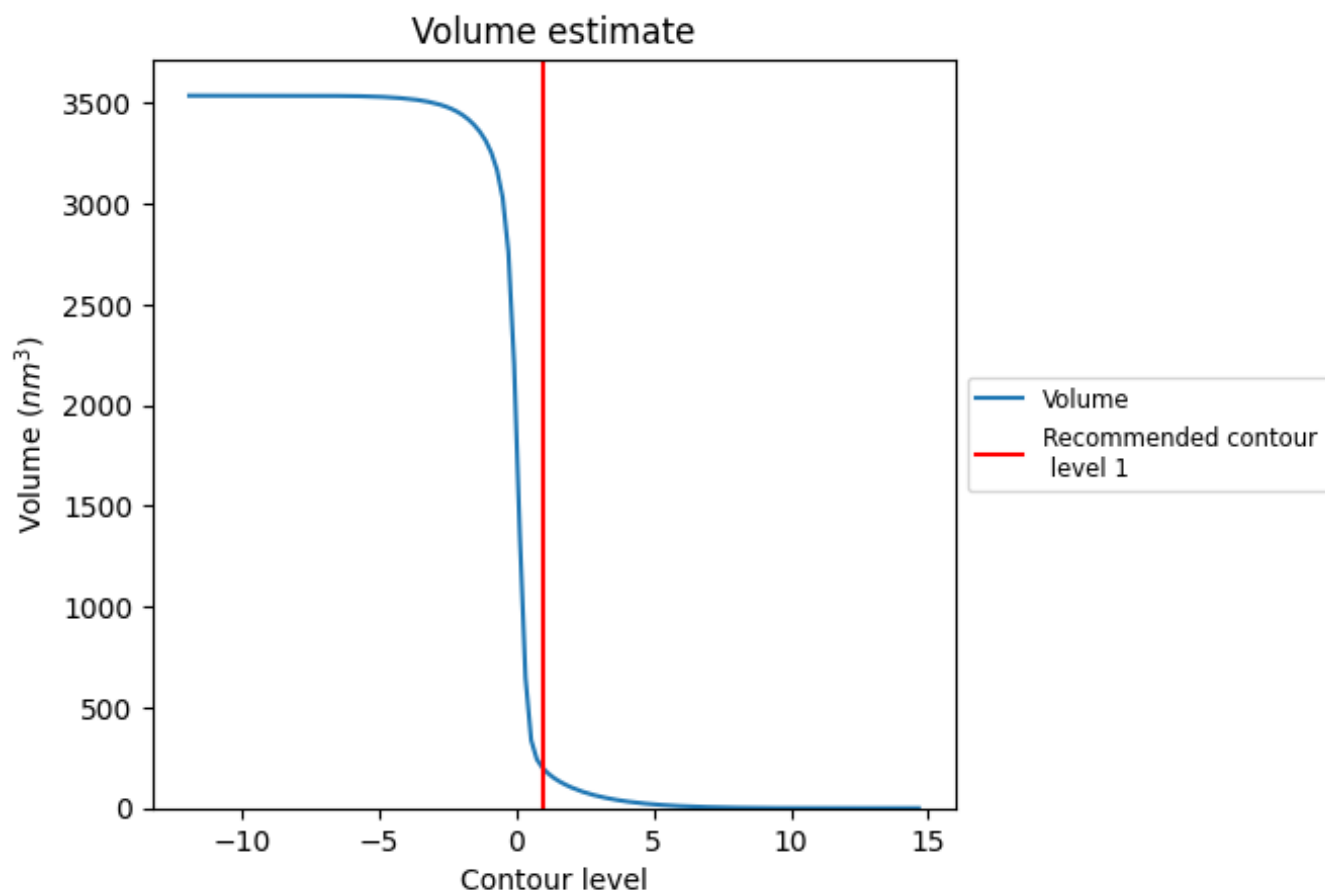
This section contains the results of statistical analysis of the map.

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 193 nm³; this corresponds to an approximate mass of 174 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

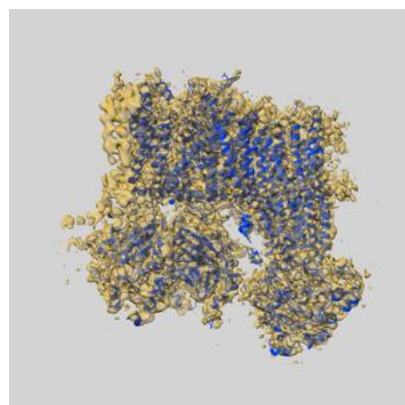
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

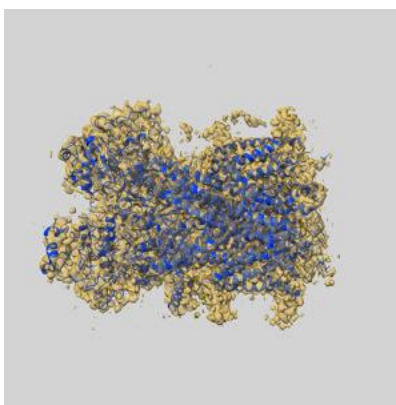
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23882 and PDB model 7MJQ. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

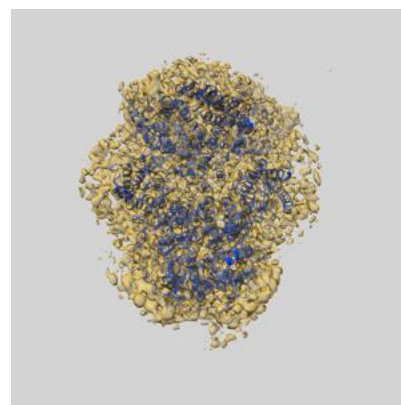
9.1 Map-model overlay [i](#)



X



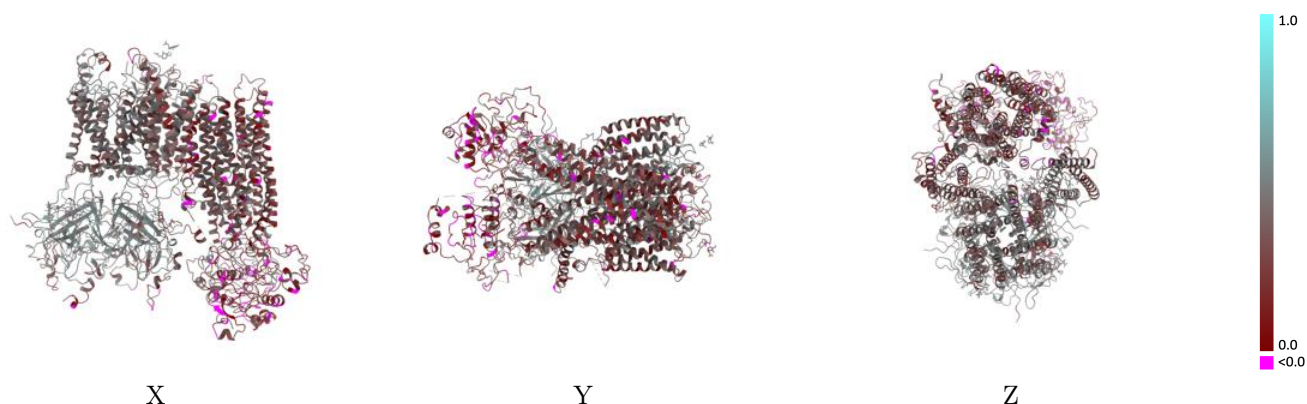
Y



Z

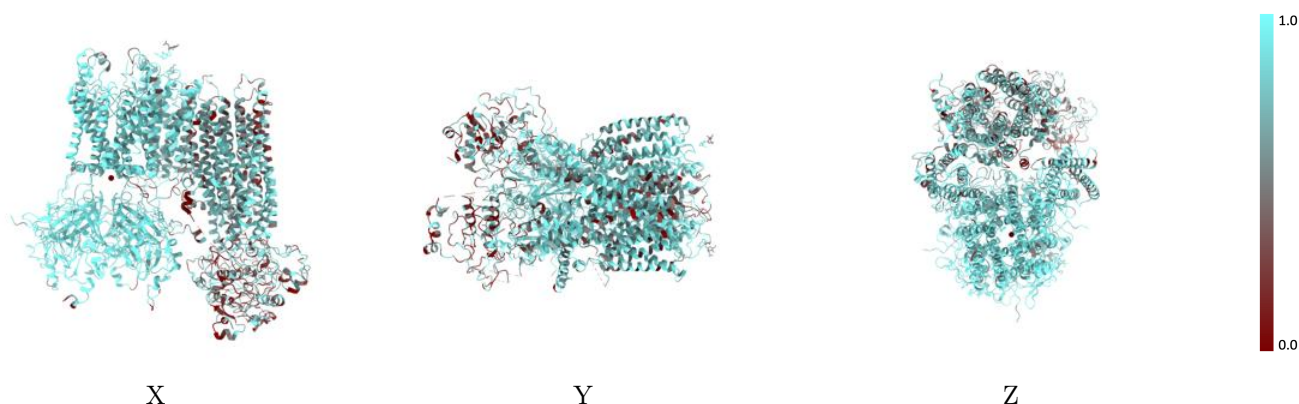
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



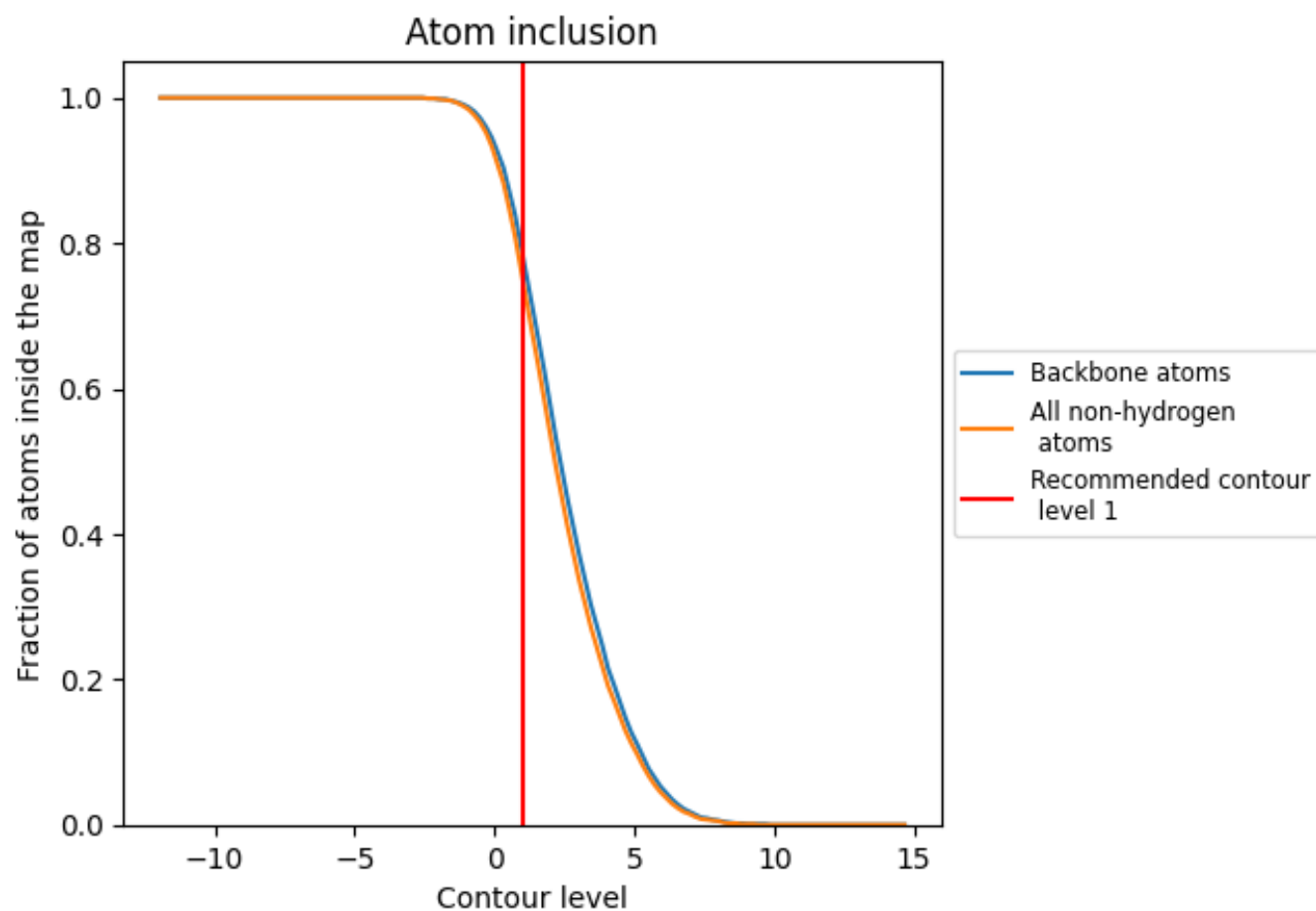
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 75% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7520	0.3610
A	0.8640	0.4340
B	0.8870	0.4480
C	0.9030	0.4460
D	0.8840	0.4310
E	0.6220	0.2810
F	0.6790	0.4680
G	0.7760	0.3810
N	0.7140	0.3130

