



## wwPDB EM Validation Summary Report ⓘ

Oct 18, 2022 – 04:11 PM EDT

PDB ID : 7MJQ  
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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

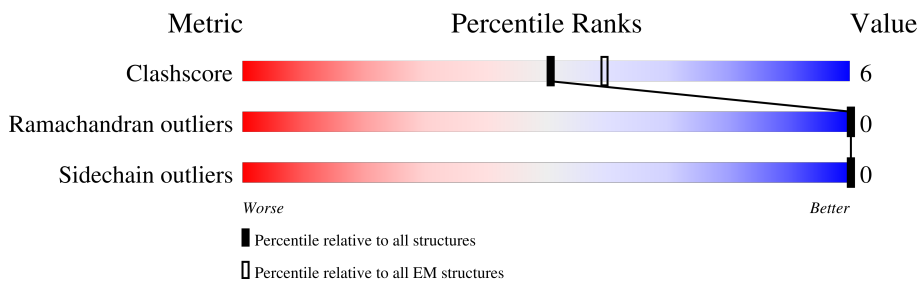
# 1 Overall quality at a glance

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	
1	B	424	
1	C	424	
1	D	424	
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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
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
			Total	C	N	O		
1	A	346	1714	1022	346	346	0	0
1	B	337	1667	993	337	337	0	0
1	C	338	1674	998	338	338	0	0
1	D	337	1667	993	337	337	0	0

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

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

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

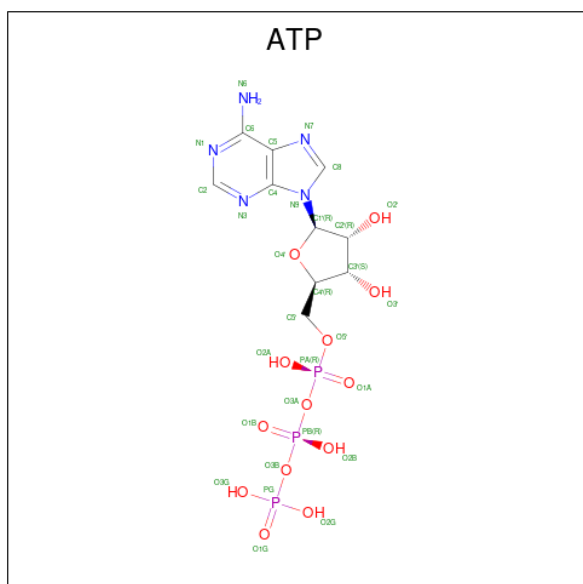


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	N	2	28	16	2	10	0	0
3	F	2	28	16	2	10	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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

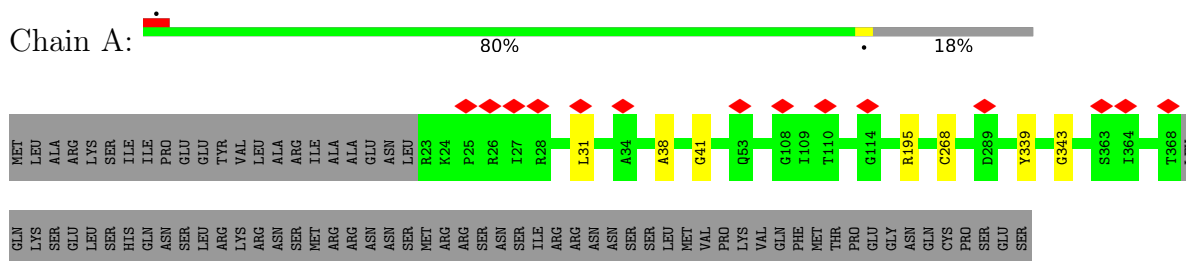


Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C N O P 31 10 5 13 3	0
5	B	1	Total C N O P 31 10 5 13 3	0
5	C	1	Total C N O P 31 10 5 13 3	0
5	D	1	Total C N O P 31 10 5 13 3	0
5	E	1	Total C N O P 31 10 5 13 3	0

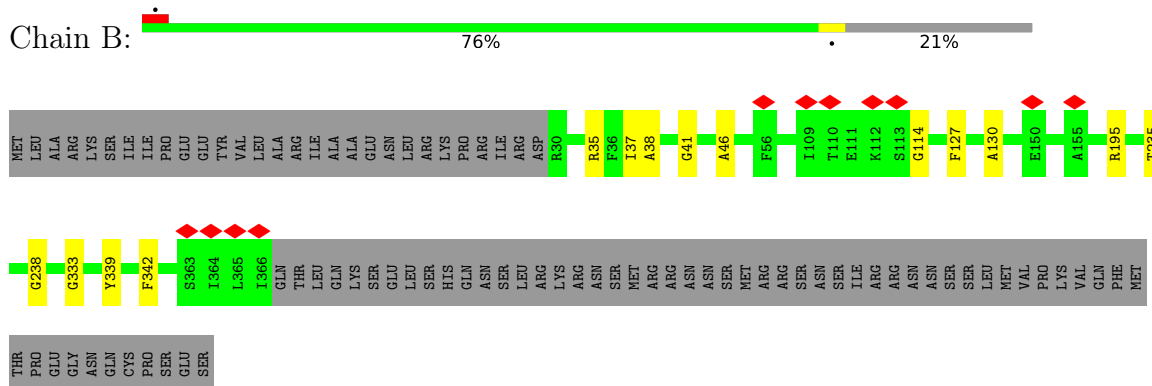
### 3 Residue-property plots [i](#)

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

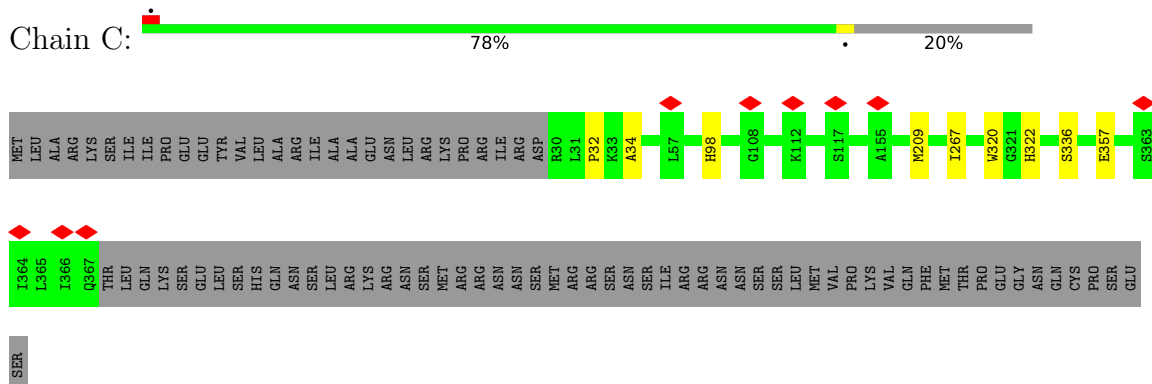
- Molecule 1: ATP-sensitive inward rectifier potassium channel 8



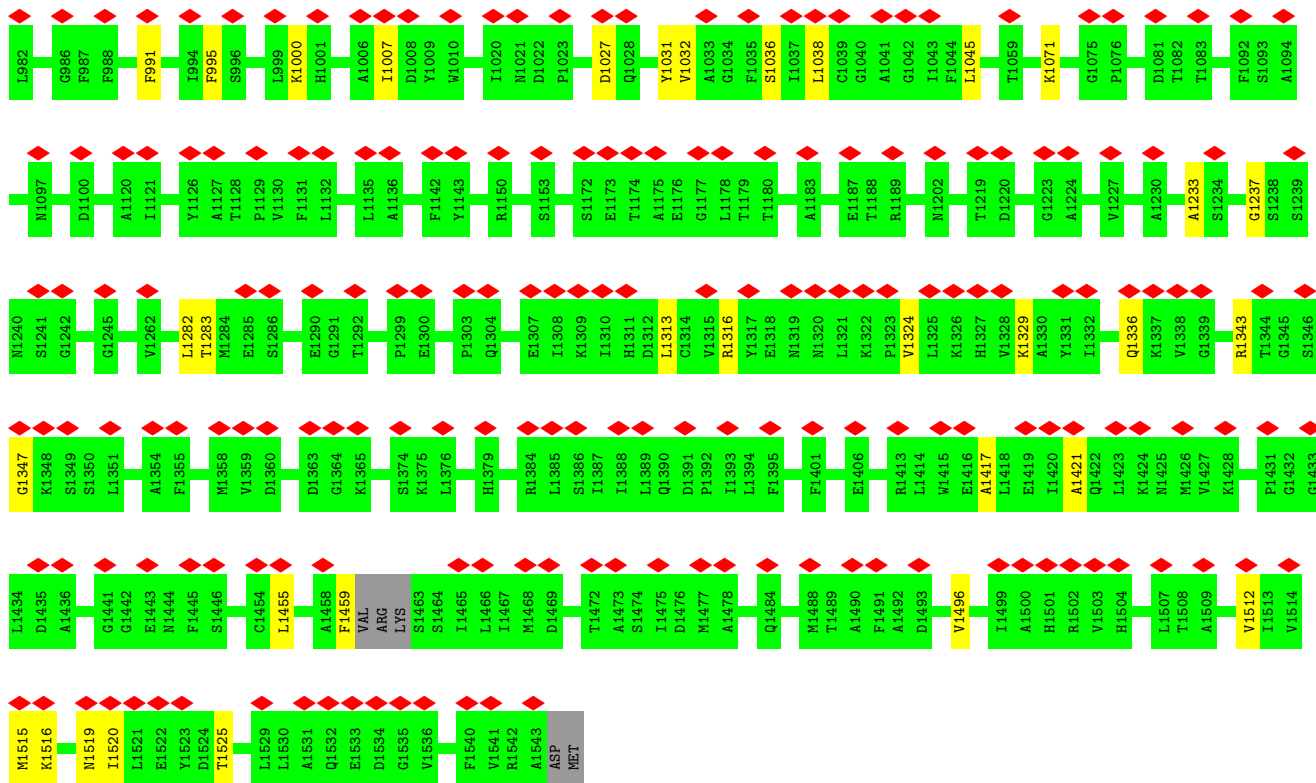
- Molecule 1: ATP-sensitive inward rectifier potassium channel 8



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







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



M1	M6	C7	N8	I10	M22	S81	Q82	S83	S84	K85	V86	H80	F86	L71	L75	V84	G90	D94	I125	M129	L133	D164	G168	G178	L179	A182	I188	R192	Y193	V194	M197	N198	PRO	GLN	LYS	VAL	LYS	PRO						
PRO	GLU	ASP	LEU	GLN	ASP	LEU	VAL	VAL	PHE	ALA	ARG	LEU	LEU	LEU	ALA	ALA	ASN	THR	THR	ALA	ALA	ILE	ILE	GLY	LYS	PRO	ILE	ALA	ARG	VAL	THR	ASN	VAL	LEU	LEU	PRO	GLN	LYS	VAL	LYS	PRO			
LYS	GLU	ALA	TYR	GLU	GLU	GLN	LYS	LYS	VAL	LYS	ARG	ASN	VAL	THR	LEU	THR	ALA	ALA	THR	THR	ALA	ALA	ARG	ILE	ILE	SER	ALA	ALA	VAL	VAL	VAL	THR	ASN	THR	THR	GLN	CYS	ALA	VAL	ARG	ARG			
VAL	ASN	PRO	LYS	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
LEU	ALA	ILE	TYR	ASN	LYS	ILE	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	
LEU	TYR	ASN	LEU	LEU	GLY	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	
TYR	ALA	TRP	GLU	HIS	ILE	PHE	CYS	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	
PRO	ALA	GLU	ALA	PHE	ALA	SER	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	
PHE	GLU	SER	CYS	LYS	LYS	HIS	THR	GLY	VAL	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE





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	1.0	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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, ATP, 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	0.38	0/1714	0.61	1/2388 (0.0%)
1	B	0.38	0/1666	0.62	1/2320 (0.0%)
1	C	0.45	0/1674	0.66	1/2332 (0.0%)
1	D	0.54	0/1666	0.78	1/2320 (0.0%)
2	E	0.44	0/7056	0.68	2/9822 (0.0%)
2	G	0.55	0/981	0.81	3/1365 (0.2%)
All	All	0.45	0/14757	0.69	9/20547 (0.0%)

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

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	7	GLY	N-CA-C	-8.16	92.70	113.10
2	G	6	CYS	N-CA-C	6.24	127.84	111.00
1	B	114	GLY	N-CA-C	6.10	128.35	113.10
1	C	98	HIS	N-CA-C	-5.83	95.25	111.00
2	E	6	CYS	N-CA-C	-5.68	95.66	111.00

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	17	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	129	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.

The worst 5 of 129 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: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

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	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 [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	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 [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

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	2.89	6 (35%)
3	NAG	F	2	3	14,14,15	0.44	0	17,19,21	1.35	3 (17%)
3	NAG	N	1	2,3	14,14,15	0.29	0	17,19,21	0.63	0
3	NAG	N	2	3	14,14,15	0.26	0	17,19,21	0.65	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	5/6/23/26	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	4/6/23/26	0/1/1/1
3	NAG	N	2	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 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	5.95	124.11	110.35
3	F	1	NAG	O5-C5-C4	-4.98	98.70	110.83
3	F	2	NAG	C2-N2-C7	-3.00	118.64	122.90
3	F	1	NAG	C1-O5-C5	2.89	116.10	112.19

All (2) chirality outliers are listed below:

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

5 of 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

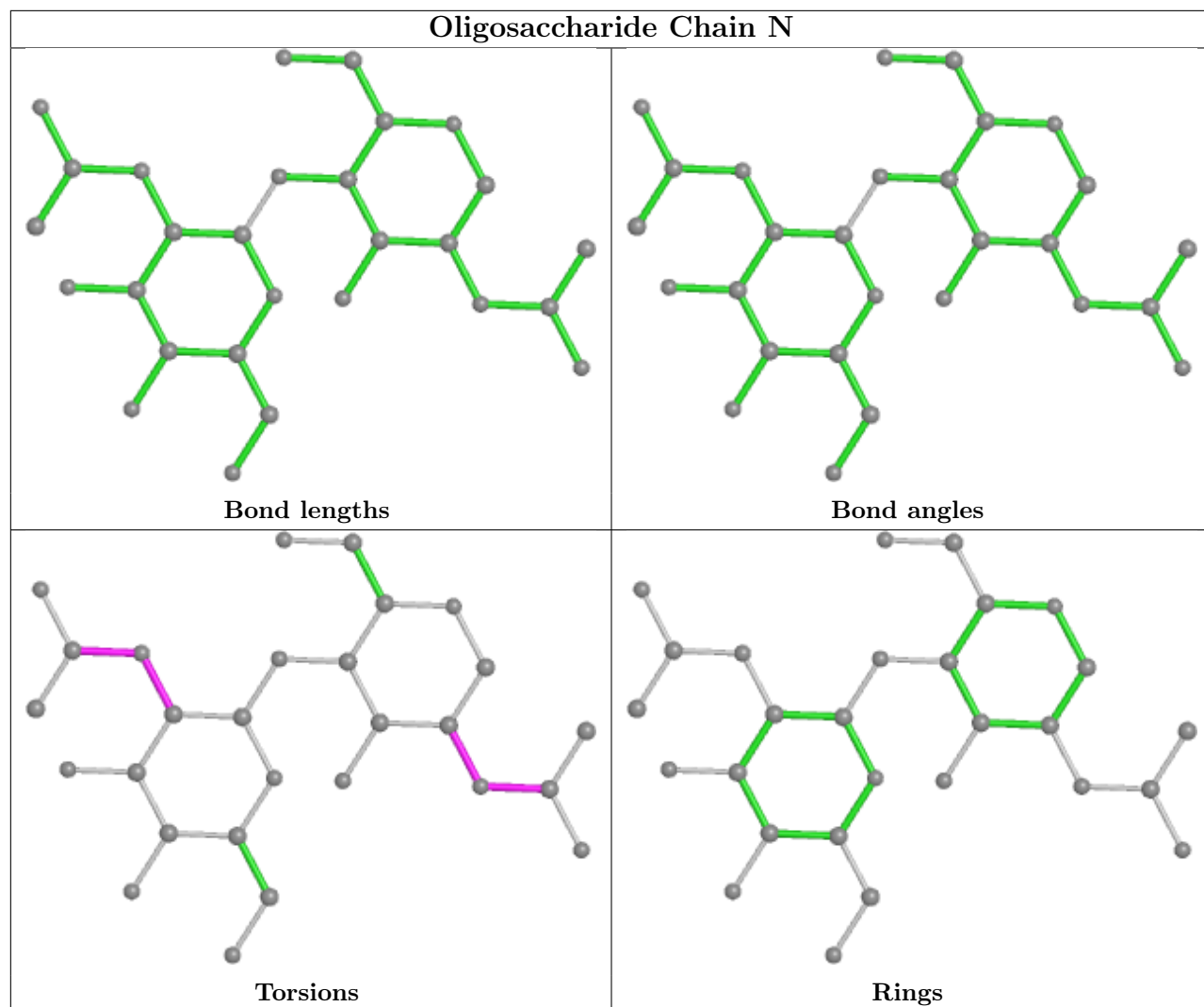
There are no ring outliers.

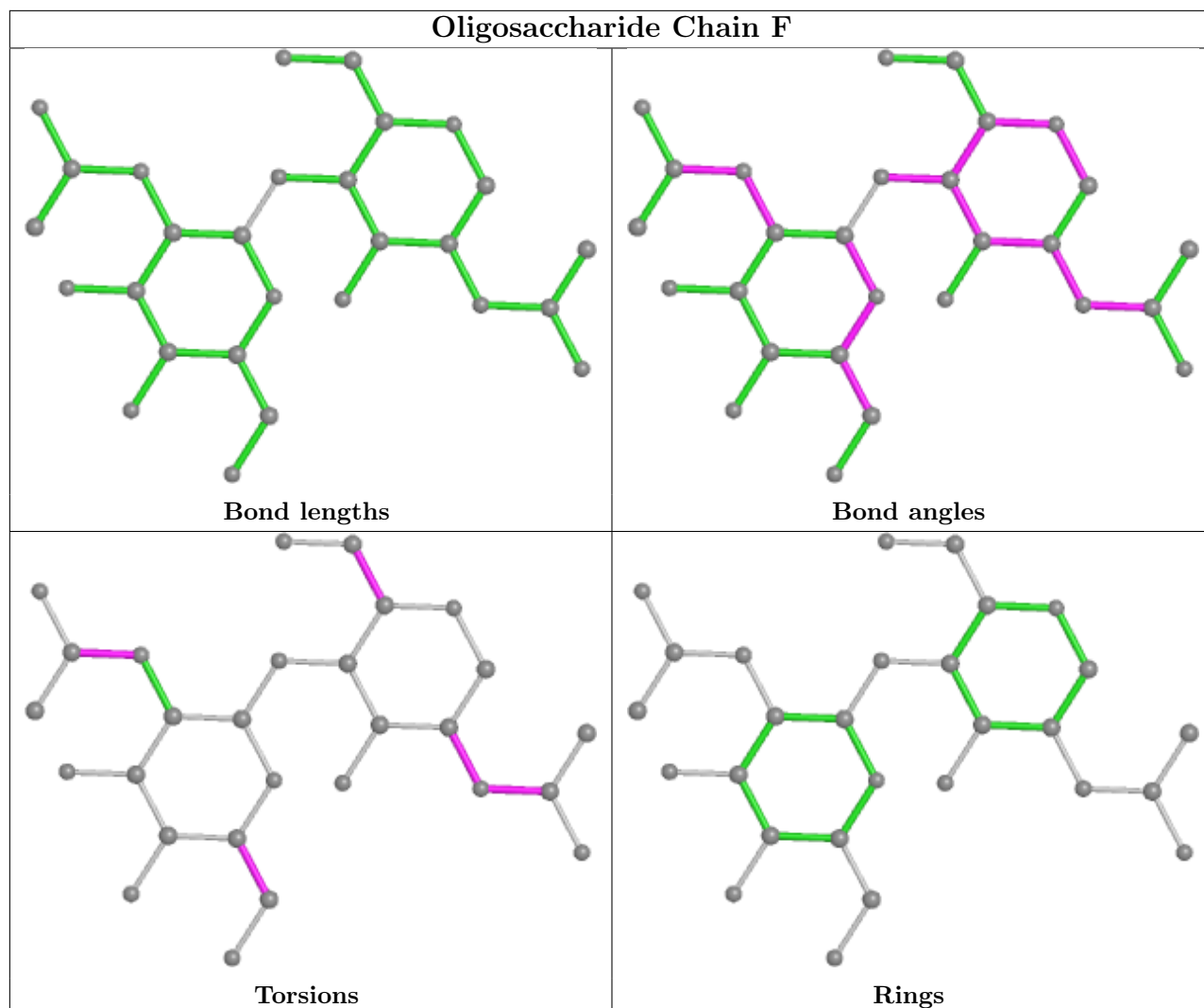
4 monomers are involved in 10 short contacts:

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
3	F	2	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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	E	1601	-	26,33,33	0.92	1 (3%)	31,52,52	1.65	5 (16%)
5	ATP	B	501	-	26,33,33	0.90	1 (3%)	31,52,52	1.85	5 (16%)
5	ATP	C	501	-	26,33,33	0.91	1 (3%)	31,52,52	1.73	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ATP	D	501	-	26,33,33	0.94	2 (7%)	31,52,52	1.73	5 (16%)
5	ATP	A	3002	-	26,33,33	0.94	1 (3%)	31,52,52	1.75	5 (16%)

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	1601	-	-	1/18/38/38	0/3/3/3
5	ATP	B	501	-	-	4/18/38/38	0/3/3/3
5	ATP	C	501	-	-	5/18/38/38	0/3/3/3
5	ATP	D	501	-	-	4/18/38/38	0/3/3/3
5	ATP	A	3002	-	-	5/18/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1601	ATP	C5-C4	2.49	1.47	1.40
5	A	3002	ATP	C5-C4	2.25	1.46	1.40
5	B	501	ATP	C5-C4	2.21	1.46	1.40
5	D	501	ATP	C2'-C1'	-2.16	1.50	1.53
5	C	501	ATP	C5-C4	2.10	1.46	1.40

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	ATP	PA-O3A-PB	-5.23	114.87	132.83
5	D	501	ATP	PA-O3A-PB	-4.69	116.72	132.83
5	D	501	ATP	PB-O3B-PG	-4.65	116.88	132.83
5	C	501	ATP	PA-O3A-PB	-4.48	117.46	132.83
5	B	501	ATP	PB-O3B-PG	-4.31	118.03	132.83

There are no chirality outliers.

5 of 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

*Continued on next page...*

*Continued from previous page...*

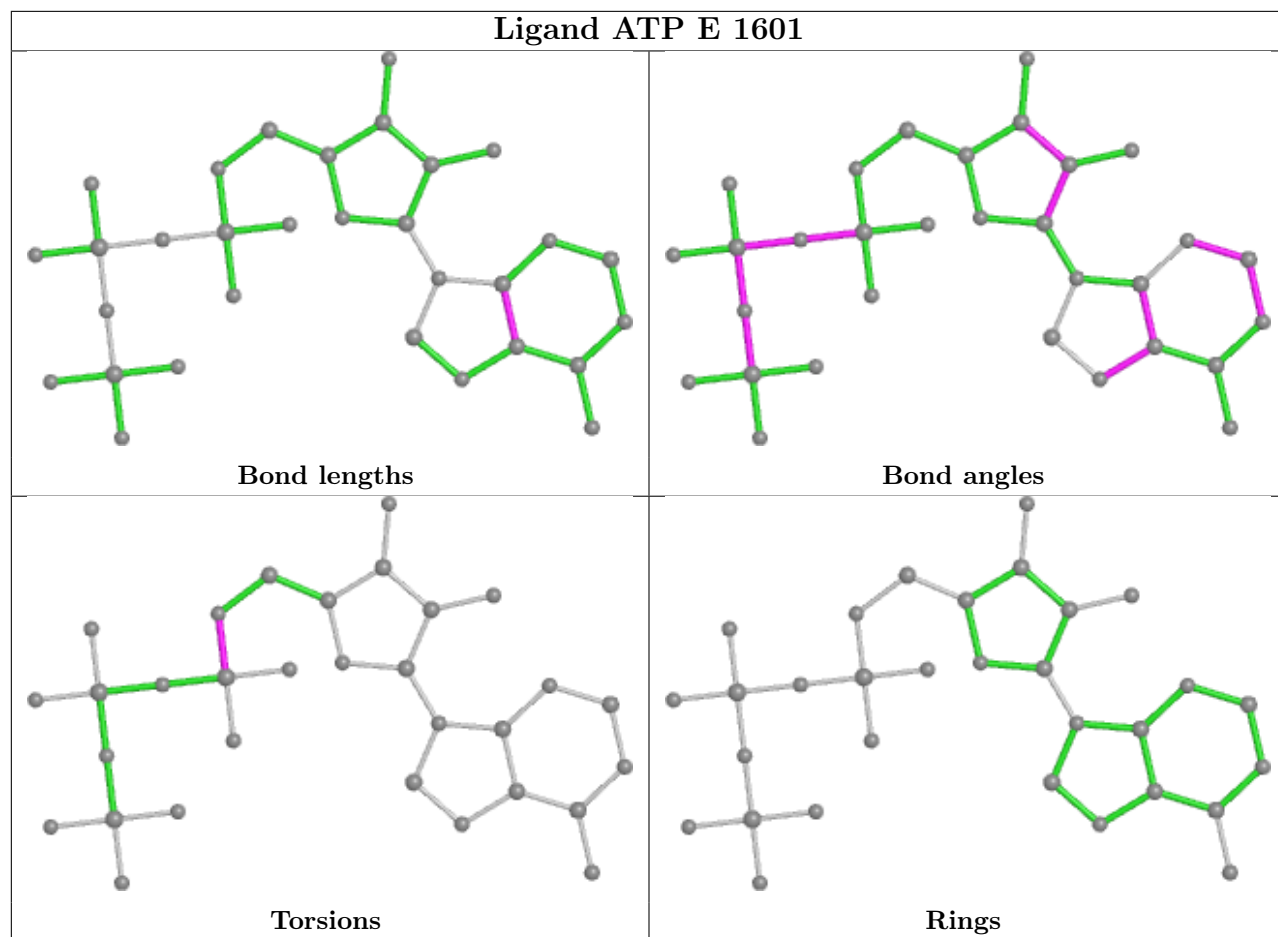
Mol	Chain	Res	Type	Atoms
5	C	501	ATP	C5'-O5'-PA-O2A
5	C	501	ATP	O4'-C4'-C5'-O5'

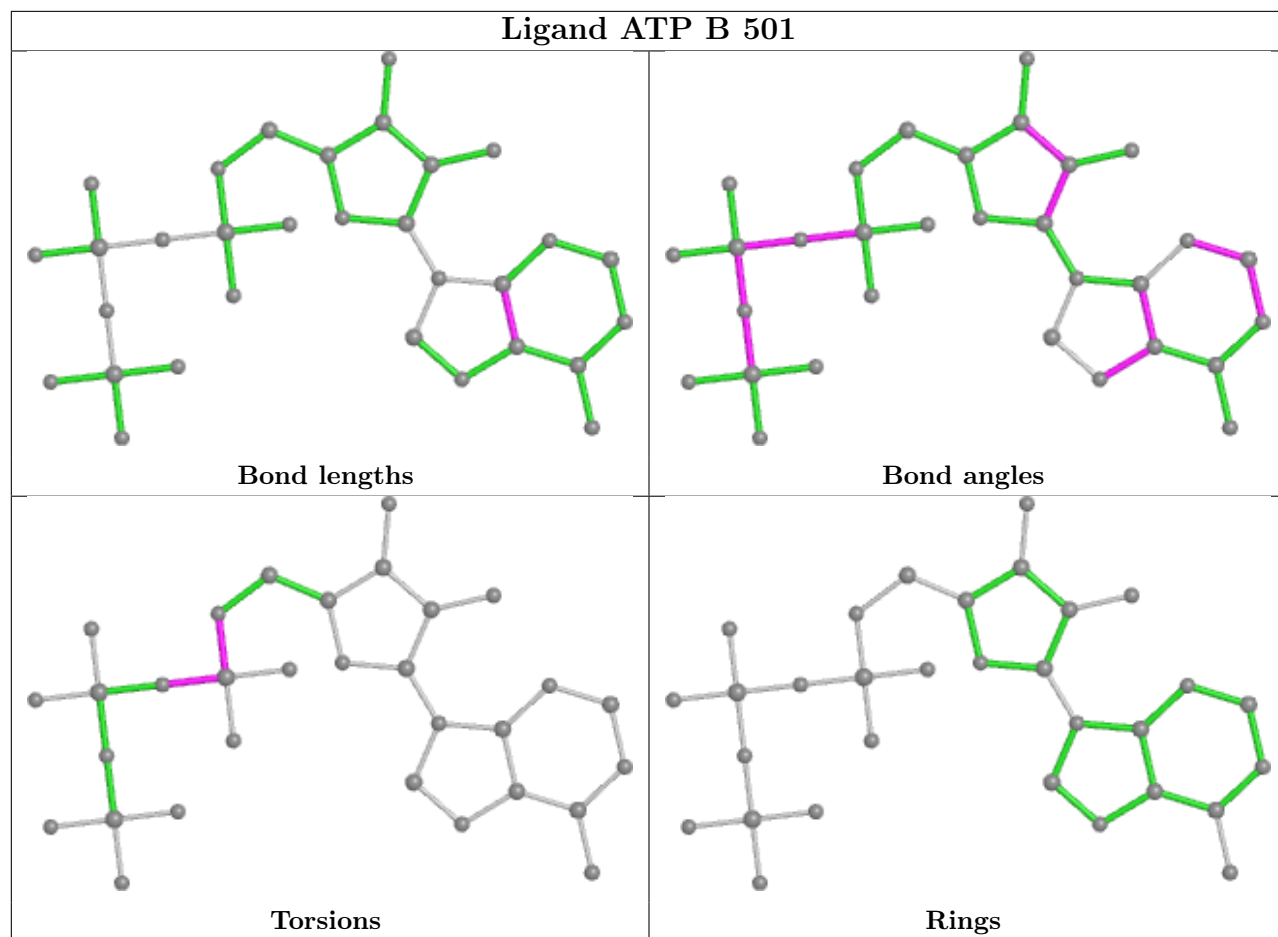
There are no ring outliers.

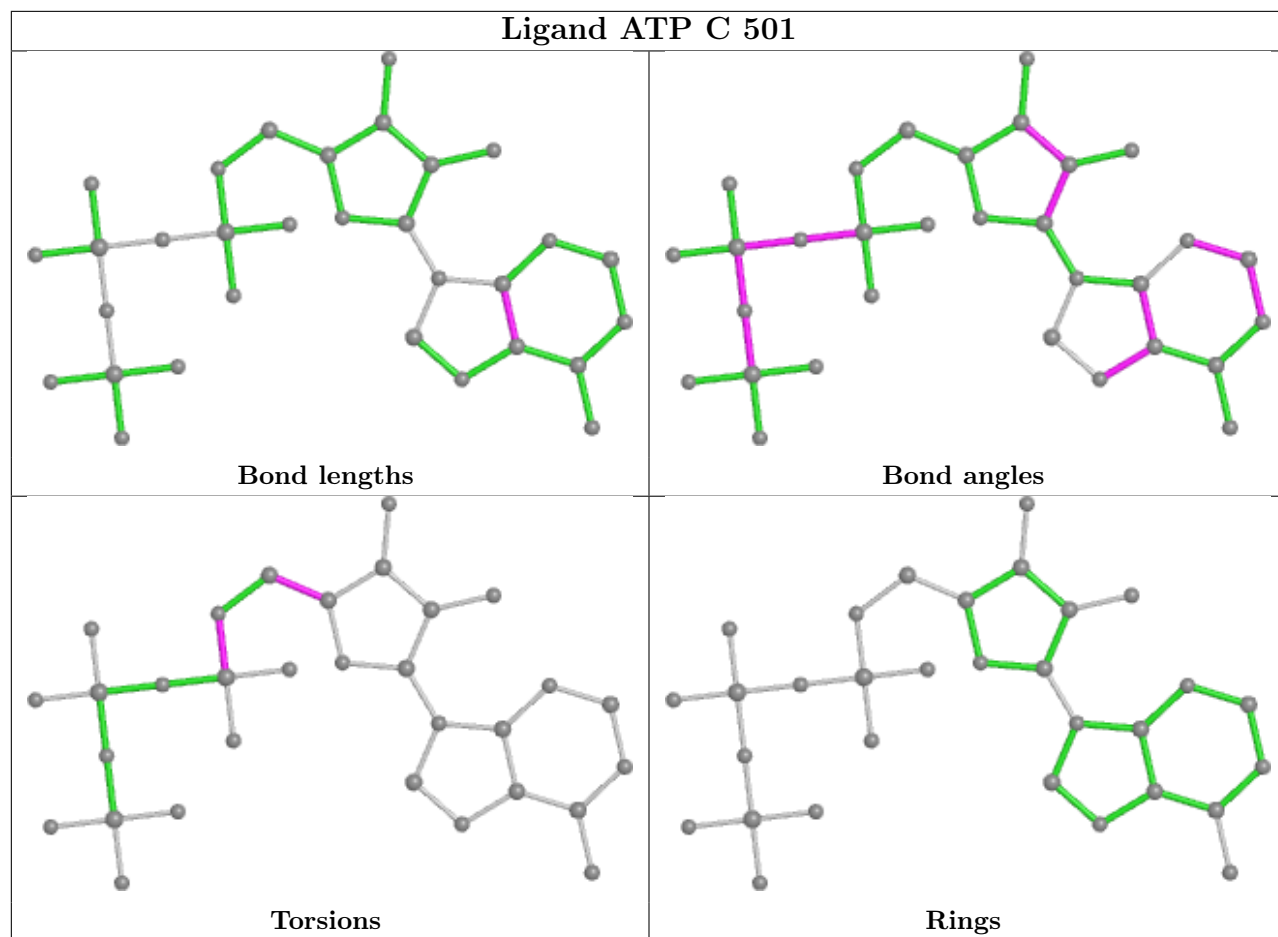
3 monomers are involved in 35 short contacts:

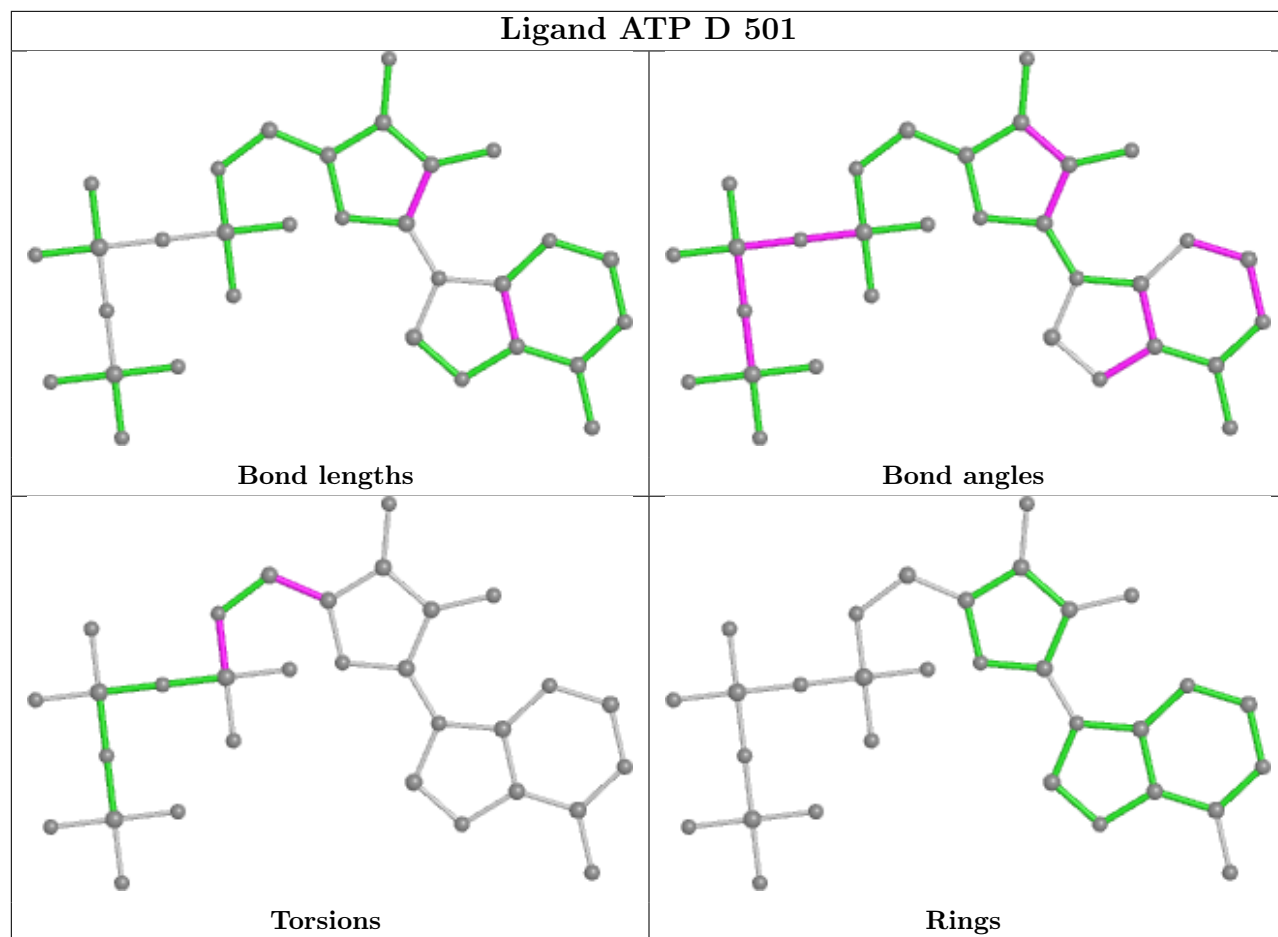
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1601	ATP	12	0
5	B	501	ATP	11	0
5	A	3002	ATP	12	0

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.

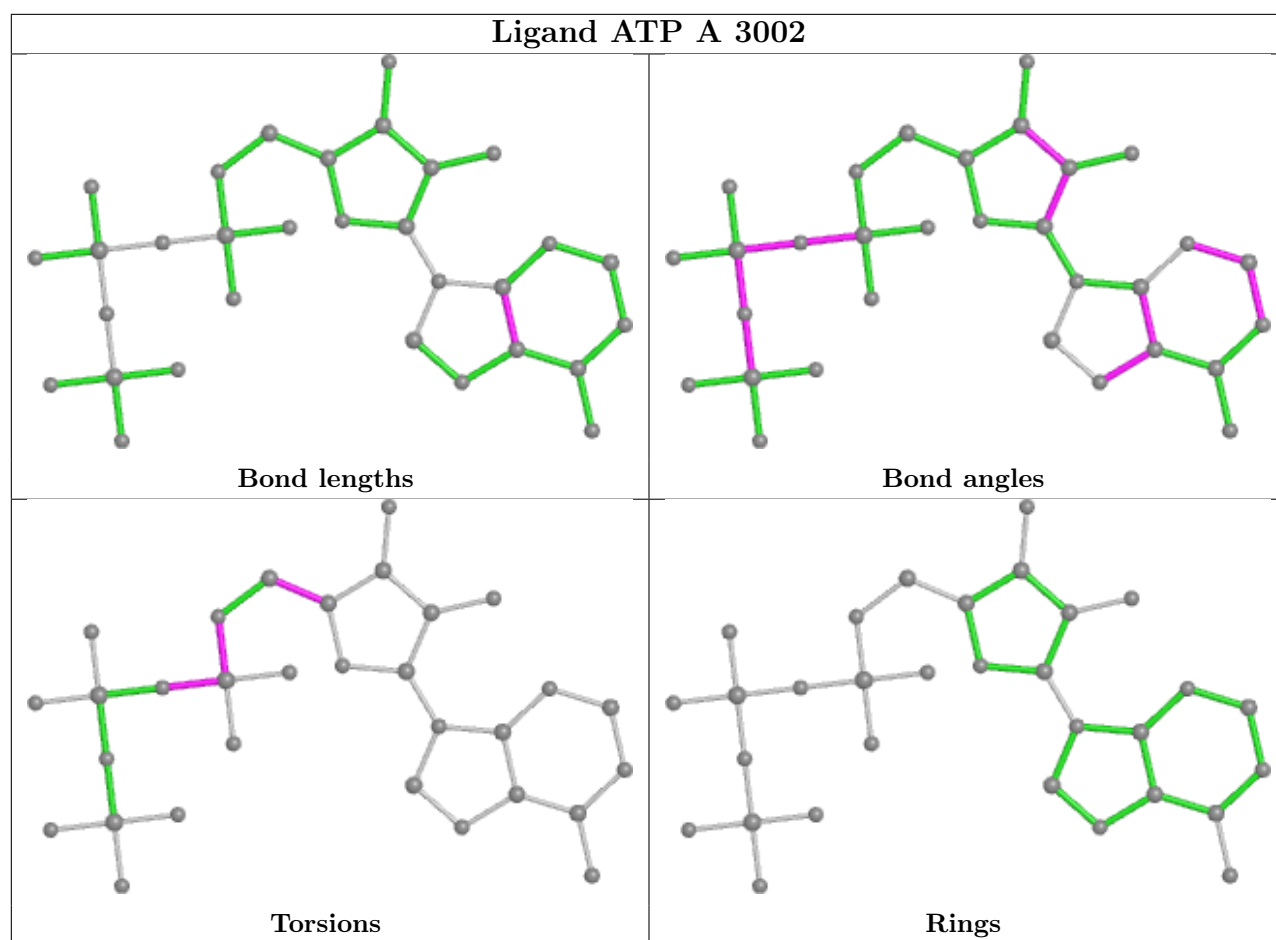












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

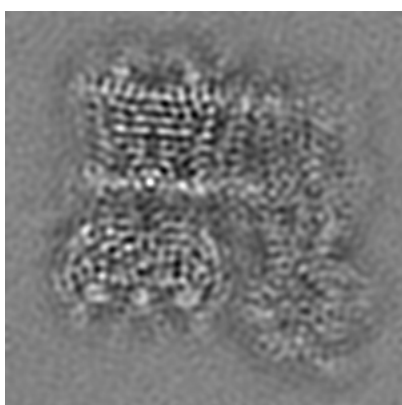
## 6 Map visualisation [i](#)

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.

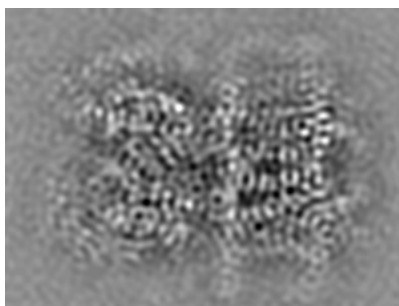
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

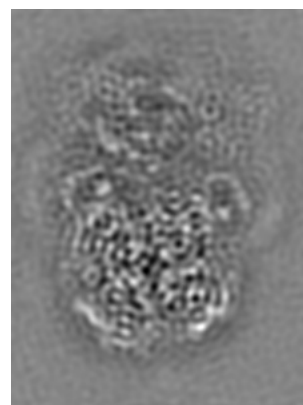
#### 6.1.1 Primary map



X



Y

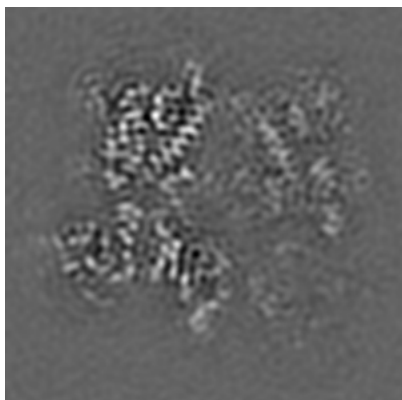


Z

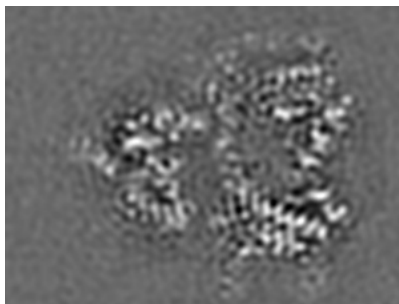
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

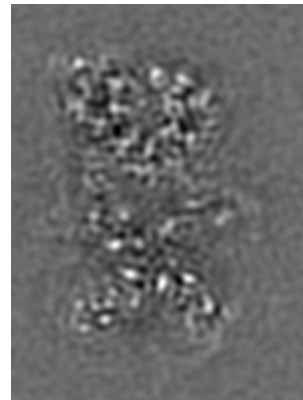
#### 6.2.1 Primary map



X Index: 38



Y Index: 51

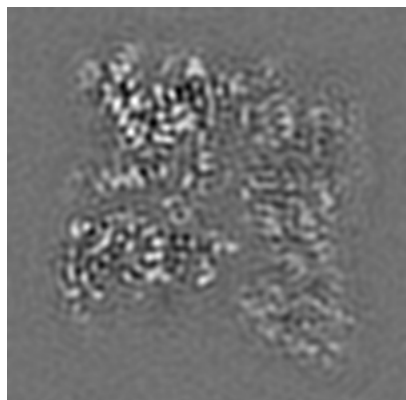


Z Index: 50

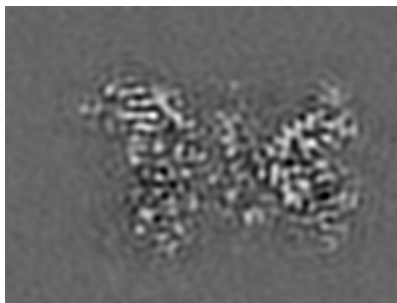
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

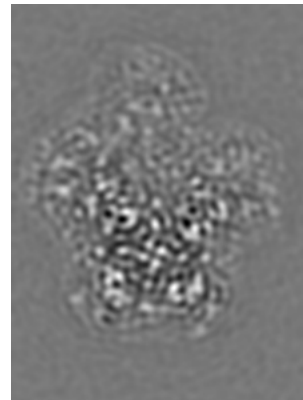
### 6.3.1 Primary map



X Index: 27



Y Index: 29

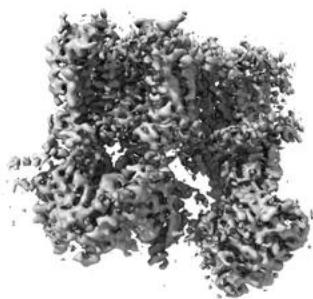


Z Index: 77

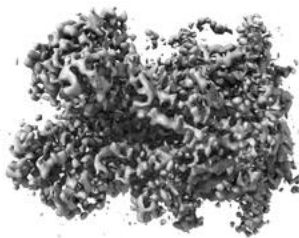
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

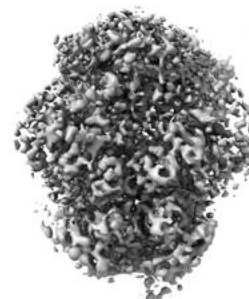
### 6.4.1 Primary map



X



Y



Z

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.

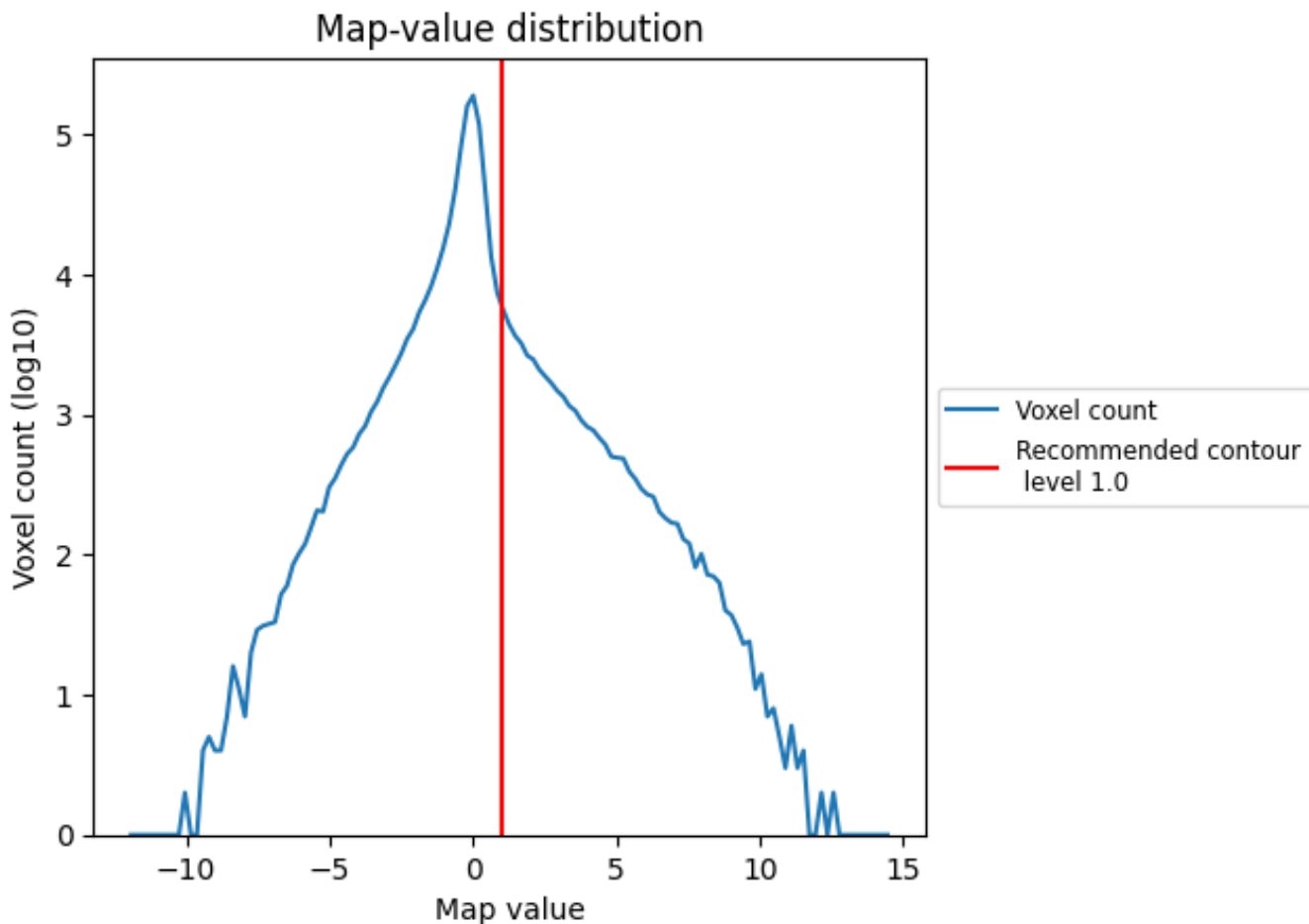
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

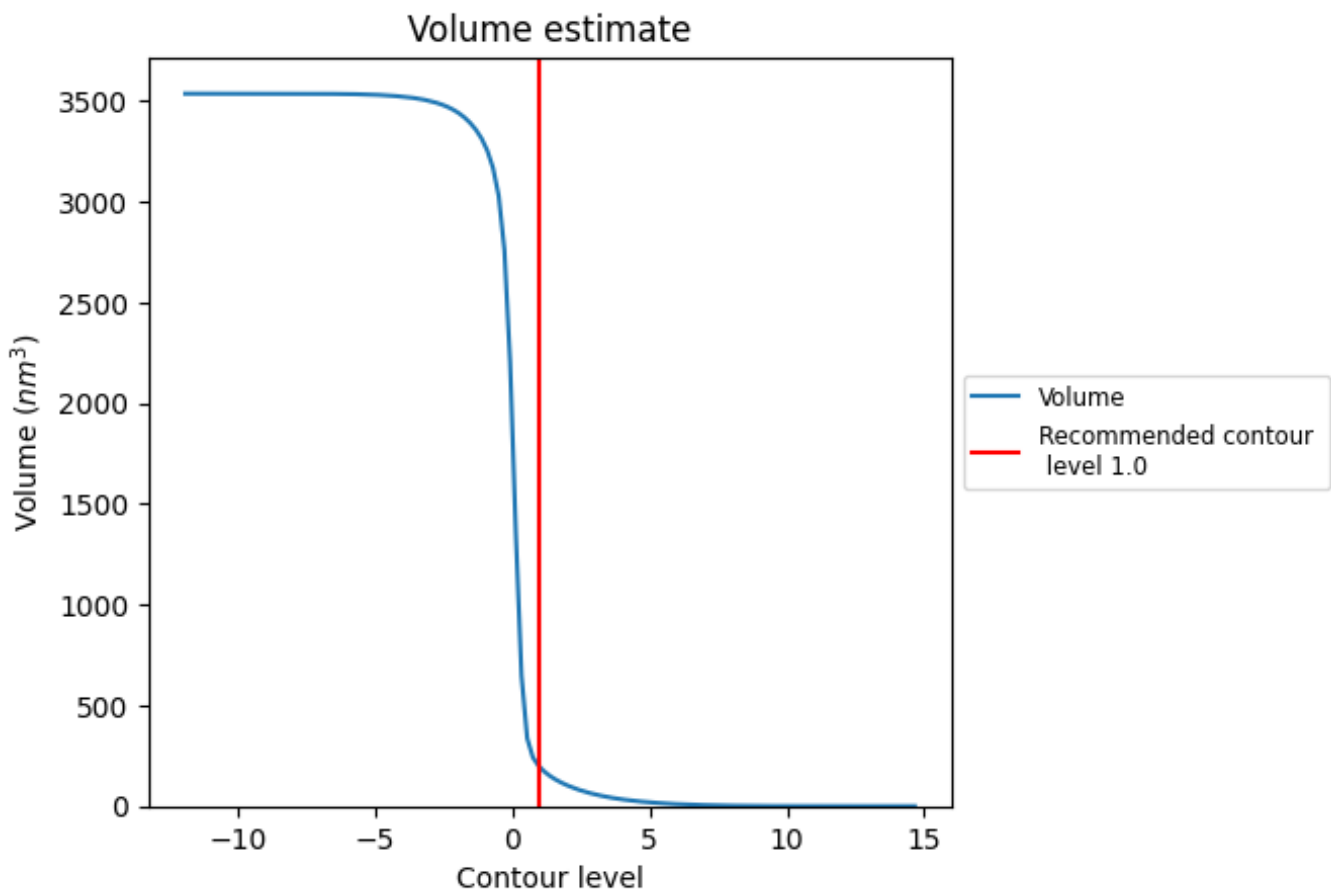
This section contains the results of statistical analysis of the map.

### 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  $\text{nm}^3$ ; 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.

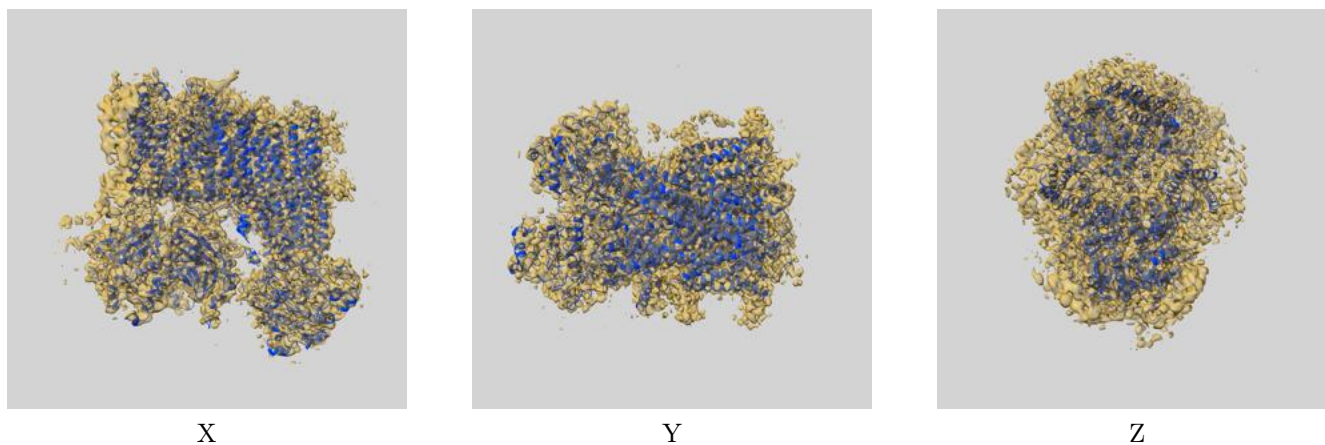
## 8 Fourier-Shell correlation

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.

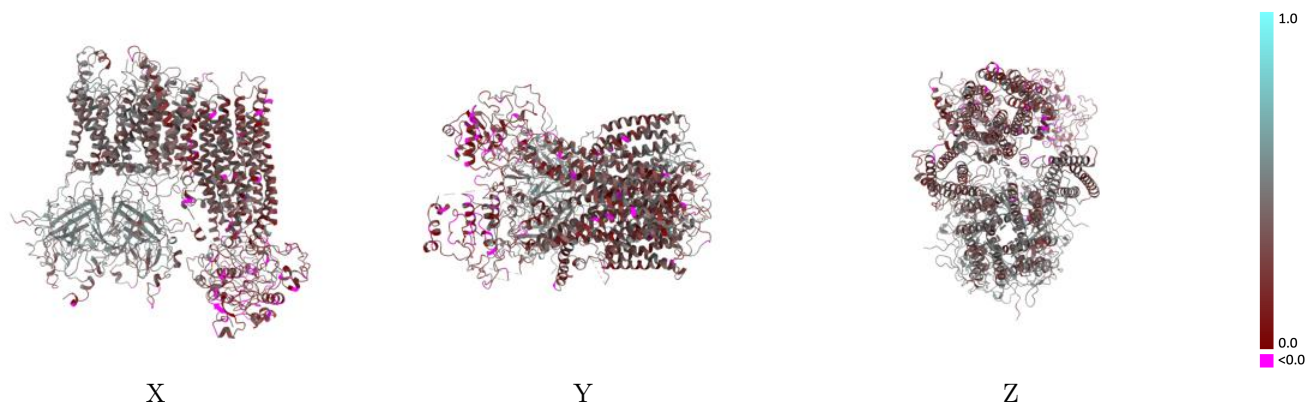
### 9.1 Map-model overlay [i](#)



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.

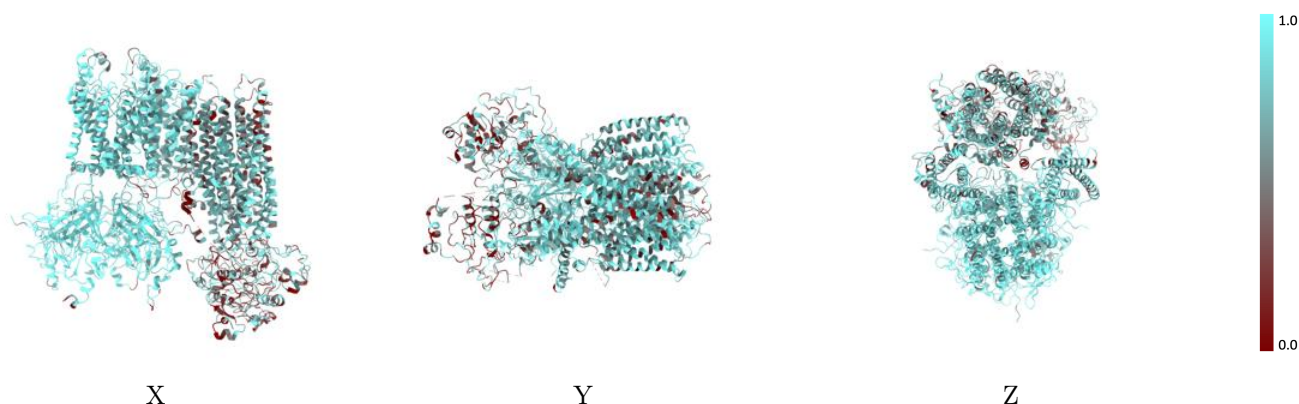


## 9.2 Q-score mapped to coordinate model [i](#)



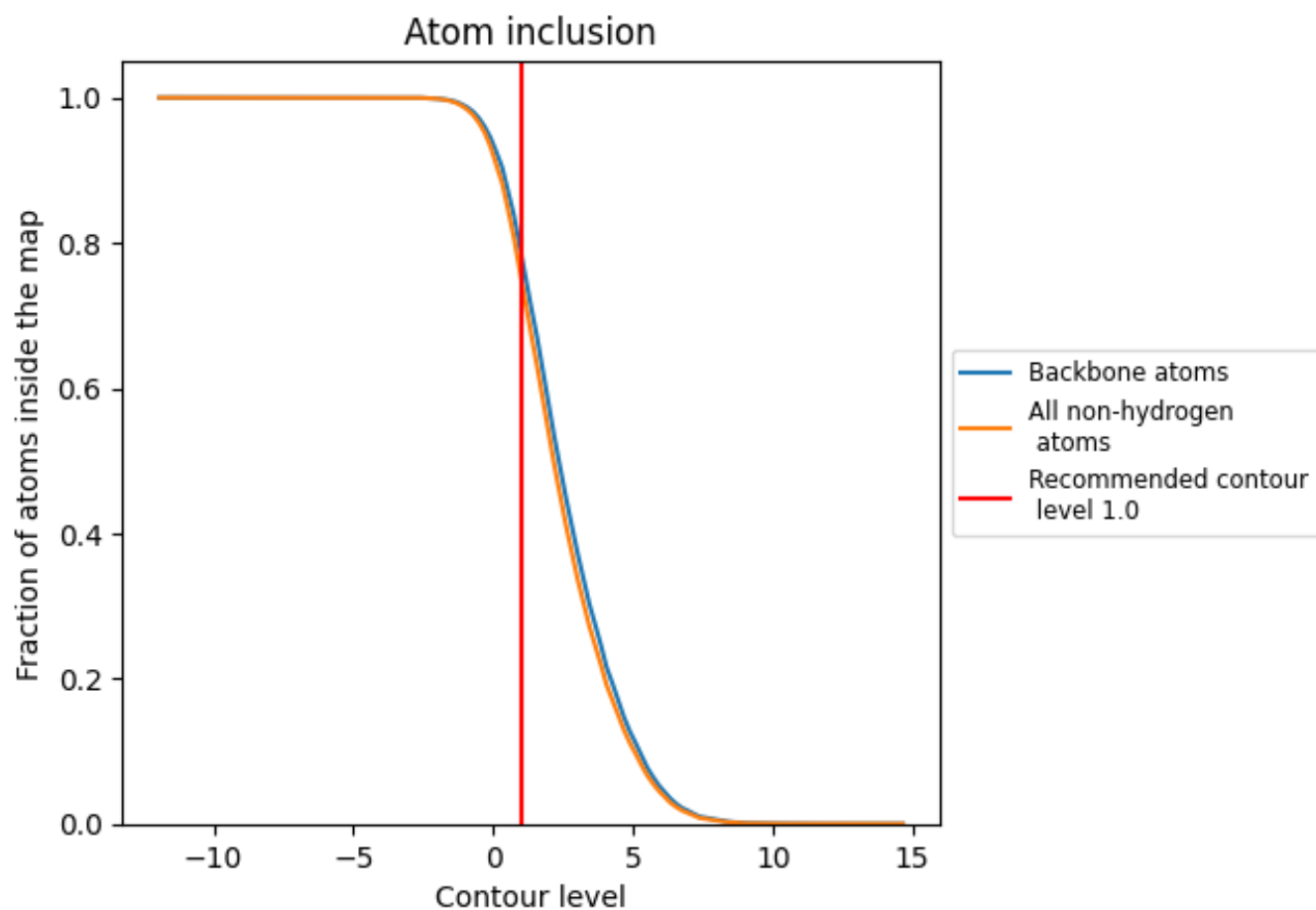
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.0).



















## 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 [i](#)

The table lists the average atom inclusion at the recommended contour level (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7525	 0.3610
A	 0.8637	 0.4340
B	 0.8869	 0.4480
C	 0.9032	 0.4460
D	 0.8840	 0.4310
E	 0.6223	 0.2810
F	 0.6786	 0.4680
G	 0.7760	 0.3810
N	 0.7143	 0.3130

