



Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 09:00 pm GMT

PDB ID : 6ZNA
EMDB ID : EMD-0667
Title : Porcine ATP synthase Fo domain
Authors : Spikes, T.E.; Montgomery, M.G.; Walker, J.E.
Deposited on : 2020-07-06
Resolution : 6.20 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:

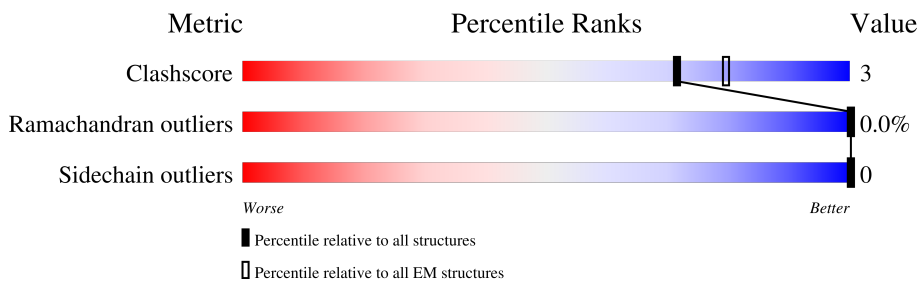
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 6.20 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 ≥ 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	8	67	
1	A8	67	
1	B8	67	
1	C8	67	
2	AK	75	
2	AL	75	
2	AM	75	
2	AN	75	


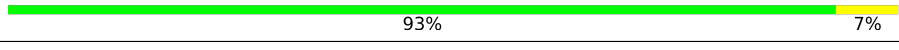
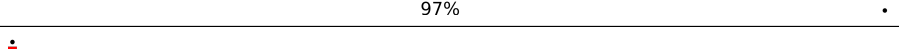
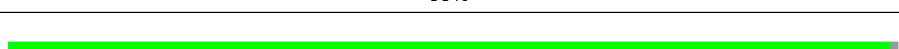
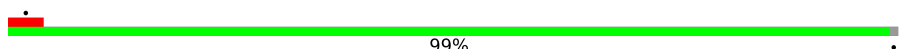
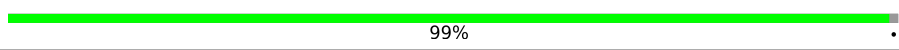

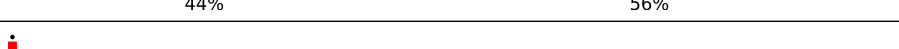





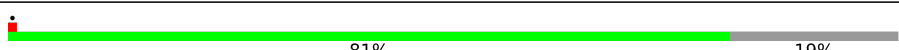


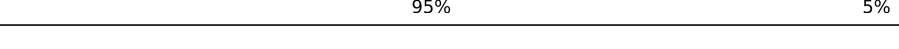

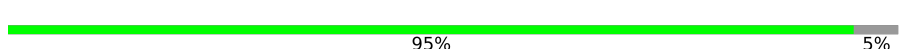





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Mol	Chain	Length	Quality of chain
2	AO	75	25% 84% 16%
2	AP	75	8% 95%
2	AQ	75	7% 95%
2	AR	75	96%
2	BK	75	95%
2	BL	75	93% 7%
2	BM	75	5% 89% 11%
2	BN	75	8% 88% 12%
2	BO	75	91% 8%
2	BP	75	96%
2	BQ	75	99%
2	BR	75	95%
2	CK	75	89% 11%
2	CL	75	9% 88% 12%
2	CM	75	7% 89% 9%
2	CN	75	24% 93% 7%
2	CO	75	23% 97%
2	CP	75	95%
2	CQ	75	9% 95%
2	CR	75	96%
2	K	75	95%
2	L	75	95%
2	M	75	93% 7%
2	N	75	9% 89% 11%
2	O	75	8% 88% 12%

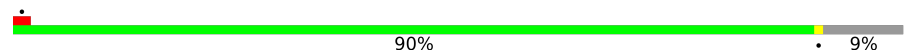



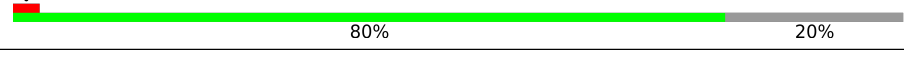



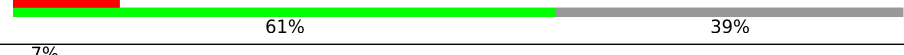

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Mol	Chain	Length	Quality of chain
2	P	75	 89% 9%
2	Q	75	 93% 7%
2	R	75	 97%
3	Aa	226	 99%
3	Ba	226	 99%
3	Ca	226	 99%
3	a	226	 99%
4	Ab	214	 44% 56%
4	Bb	214	 44% 56%
4	Cb	214	 44% 56%
4	b	214	 44% 56%
5	Ad	160	 21% 79%
5	Bd	160	 21% 79%
5	Cd	160	 21% 79%
5	d	160	 21% 79%
6	Ae	70	 80% 19%
6	Be	70	 81% 19%
6	Ce	70	 80% 19%
6	e	70	 81% 19%
7	Af	87	 95% 5%
7	Bf	87	 95% 5%
7	Cf	87	 95% 5%
7	f	87	 95% 5%
8	Ag	102	 90% 9%
8	Bg	102	73% 27%

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Mol	Chain	Length	Quality of chain
8	Cg	102	 90% 9%
8	g	102	 73% 27%
9	Aj	60	 5% 80% 20%
9	Bj	60	 5% 80% 20%
9	Cj	60	 5% 80% 20%
9	j	60	 80% 20%
10	Ak	57	 11% 61% 39%
10	Bk	57	 9% 61% 39%
10	Ck	57	 12% 61% 39%
10	k	57	 7% 61% 39%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 39195 atoms, of which 13428 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 synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
1	A8	34	238	102	68	34	34	0	0
1	B8	34	238	102	68	34	34	0	0
1	C8	34	238	102	68	34	34	0	0
1	8	34	238	102	68	34	34	0	0

- Molecule 2 is a protein called ATP synthase F(0) complex subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	AK	75	565	214	201	75	75	0	0	
2	AL	75	565	214	201	75	75	0	0	
2	AM	74	558	211	199	74	74	0	0	
2	AN	75	565	214	201	75	75	0	0	
2	AO	75	1096	356	559	83	94	4	0	
2	AP	74	558	211	199	74	74	0	0	
2	AQ	74	558	211	199	74	74	0	0	
2	AR	75	565	214	201	75	75	0	0	
2	BK	74	558	211	199	74	74	0	0	
2	BL	75	565	214	201	75	75	0	0	
2	BM	75	565	214	201	75	75	0	0	

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BN	75	Total	C	H	N	O	0	0
			565	214	201	75	75		
2	BO	74	Total	C	H	N	O	0	0
			558	211	199	74	74		
2	BP	75	Total	C	H	N	O	0	0
			565	214	201	75	75		
2	BQ	75	Total	C	H	N	O	0	0
			565	214	201	75	75		
2	BR	74	Total	C	H	N	O	0	0
			558	211	199	74	74		
2	CK	75	Total	C	H	N	O	0	0
			565	214	201	75	75		
2	CL	75	Total	C	H	N	O	0	0
			565	214	201	75	75		
2	CM	74	Total	C	H	N	O	0	0
			558	211	199	74	74		
2	CN	75	Total	C	H	N	O	0	0
			565	214	201	75	75		
2	CO	75	Total	C	H	N	O	0	0
			565	214	201	75	75		
2	CP	74	Total	C	H	N	O	0	0
			558	211	199	74	74		
2	CQ	74	Total	C	H	N	O	0	0
			558	211	199	74	74		
2	CR	75	Total	C	H	N	O	0	0
			565	214	201	75	75		
2	K	74	Total	C	H	N	O	0	0
			558	211	199	74	74		
2	L	74	Total	C	H	N	O	0	0
			558	211	199	74	74		
2	M	75	Total	C	H	N	O	0	0
			565	214	201	75	75		
2	N	75	Total	C	H	N	O	0	0
			565	214	201	75	75		
2	O	75	Total	C	H	N	O	0	0
			565	214	201	75	75		
2	P	74	Total	C	H	N	O	0	0
			558	211	199	74	74		
2	Q	75	Total	C	H	N	O	0	0
			565	214	201	75	75		
2	R	75	Total	C	H	N	O	0	0
			565	214	201	75	75		

- Molecule 3 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Aa	223	Total	C	H	N	O	0	0
			1599	659	494	223	223		
3	Ba	223	Total	C	H	N	O	0	0
			1599	659	494	223	223		
3	Ca	223	Total	C	H	N	O	0	0
			1599	659	494	223	223		
3	a	223	Total	C	H	N	O	0	0
			1599	659	494	223	223		

- Molecule 4 is a protein called ATP synthase peripheral stalk-membrane subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ab	94	Total	C	H	N	O	0	0
			669	272	209	94	94		
4	Bb	94	Total	C	H	N	O	0	0
			669	272	209	94	94		
4	Cb	94	Total	C	H	N	O	0	0
			669	272	209	94	94		
4	b	94	Total	C	H	N	O	0	0
			669	272	209	94	94		

- Molecule 5 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ad	33	Total	C	H	N	O	0	0
			226	99	61	33	33		
5	Bd	33	Total	C	H	N	O	0	0
			226	99	61	33	33		
5	Cd	33	Total	C	H	N	O	0	0
			226	99	61	33	33		
5	d	33	Total	C	H	N	O	0	0
			226	99	61	33	33		

- Molecule 6 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Ae	57	Total	C	H	N	O	0	0
			413	168	131	57	57		
6	Be	57	Total	C	H	N	O	0	0
			413	168	131	57	57		
6	Ce	57	Total	C	H	N	O	0	0
			413	168	131	57	57		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	e	57	Total	C	H	N	O	0	0
			413	168	131	57	57		

- Molecule 7 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Af	83	Total	C	H	N	O	0	0
			593	243	184	83	83		
7	Bf	83	Total	C	H	N	O	0	0
			593	243	184	83	83		
7	Cf	83	Total	C	H	N	O	0	0
			593	243	184	83	83		
7	f	83	Total	C	H	N	O	0	0
			593	243	184	83	83		

- Molecule 8 is a protein called ATP synthase g subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ag	93	Total	C	H	N	O	0	0
			708	275	247	93	93		
8	Bg	74	Total	C	H	N	O	0	0
			532	218	166	74	74		
8	Cg	93	Total	C	H	N	O	0	0
			708	275	247	93	93		
8	g	74	Total	C	H	N	O	0	0
			532	218	166	74	74		

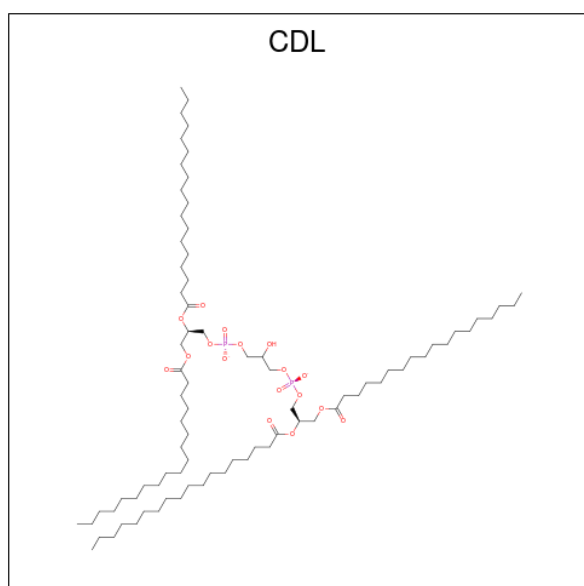
- Molecule 9 is a protein called ATP synthase j subunit (6.8PL).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Aj	48	Total	C	H	N	O	0	0
			339	141	102	48	48		
9	Bj	48	Total	C	H	N	O	0	0
			339	141	102	48	48		
9	Cj	48	Total	C	H	N	O	0	0
			339	141	102	48	48		
9	j	48	Total	C	H	N	O	0	0
			339	141	102	48	48		

- Molecule 10 is a protein called ATP synthase membrane subunit DAPIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
10	Ak	35	Total 250	C 101	H 79	N 35	O 35	0	0
10	Bk	35	Total 250	C 101	H 79	N 35	O 35	0	0
10	Ck	35	Total 250	C 101	H 79	N 35	O 35	0	0
10	k	35	Total 250	C 101	H 79	N 35	O 35	0	0

- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

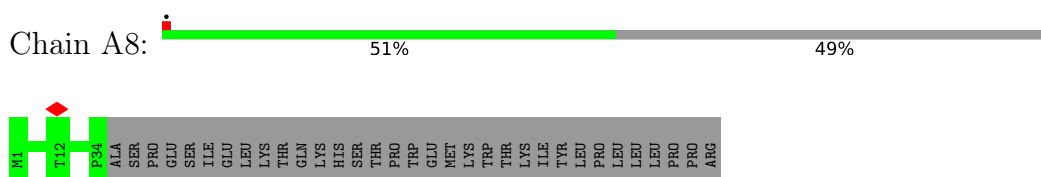


Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
11	Af	1	Total 220	C 70	H 131	O 17	P 2	0
11	Bf	1	Total 220	C 70	H 131	O 17	P 2	0
11	Cf	1	Total 220	C 70	H 131	O 17	P 2	0
11	f	1	Total 220	C 70	H 131	O 17	P 2	0

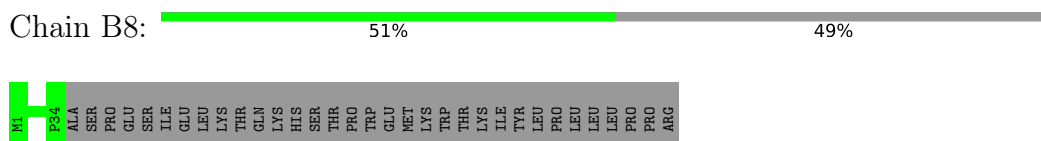
3 Residue-property plots [i](#)

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.

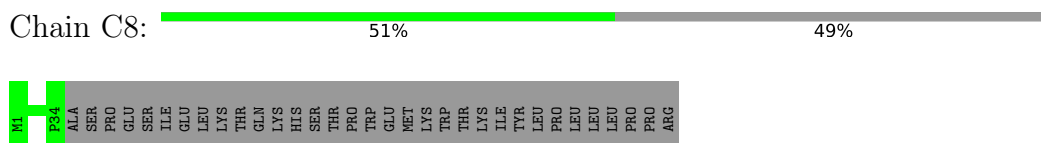
- Molecule 1: ATP synthase protein 8



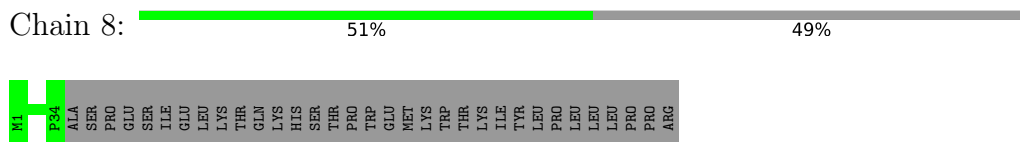
- Molecule 1: ATP synthase protein 8



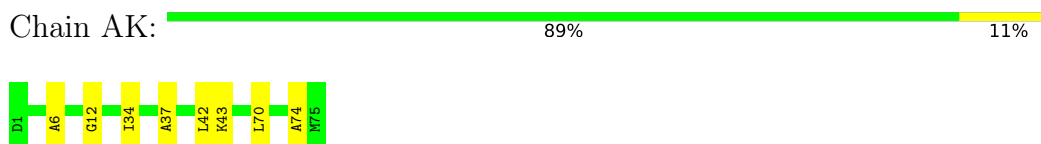
- Molecule 1: ATP synthase protein 8




- Molecule 1: ATP synthase protein 8



- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

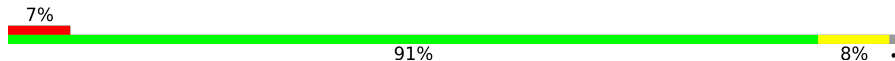


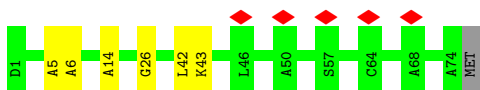
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain AL:  88% 12%



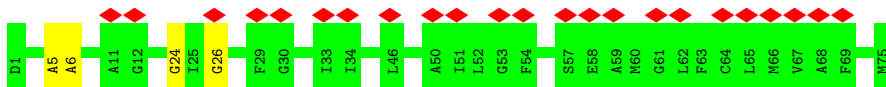
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain AM:  7% 91% 8%




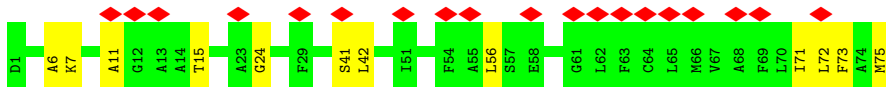
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain AN:  31% 95% 5%



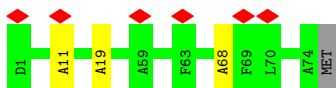
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain AO:  25% 84% 16%



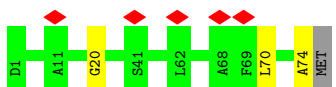
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain AP:  8% 95%



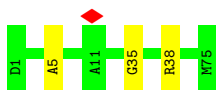
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain AQ:  7% 95%



- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain AR:  96%



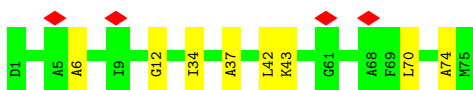
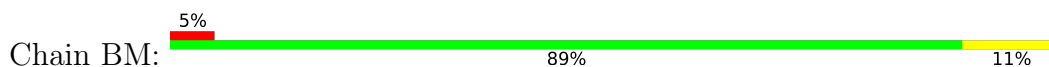
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial



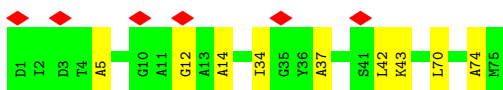
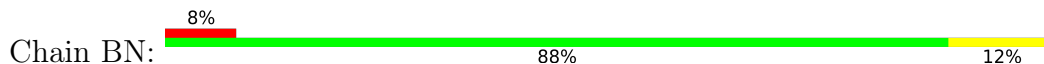
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial



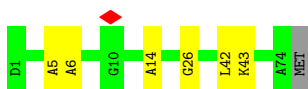
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial



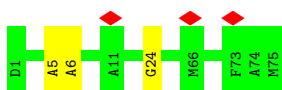
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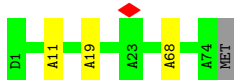
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain BQ:  99%



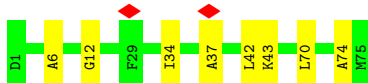
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain BR:  95%




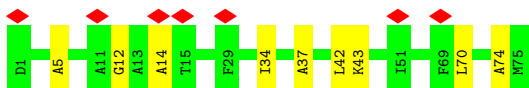
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain CK:  89% 11%



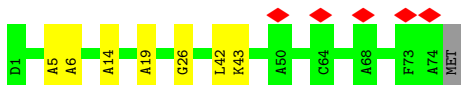
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain CL:  9% 88% 12%



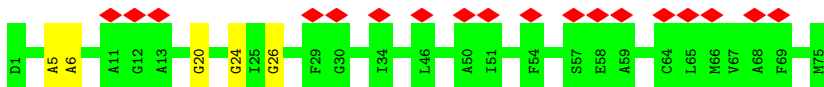
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain CM:  7% 89% 9%



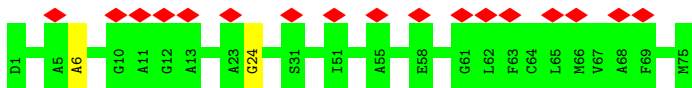
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain CN:  24% 93% 7%



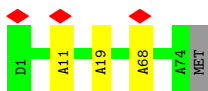
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain CO:  23% 97%



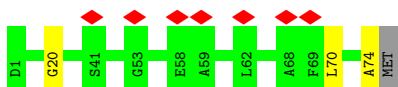
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain CP:  95%



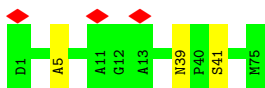
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain CQ:  95%



- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain CR:  96%



- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain K:  95%

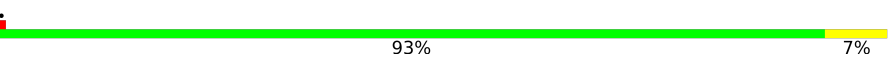


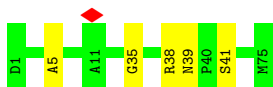
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain L:  95%




- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

Chain M:  93% 7%

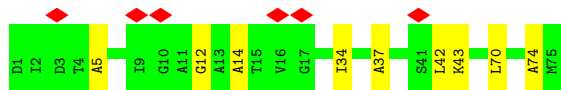
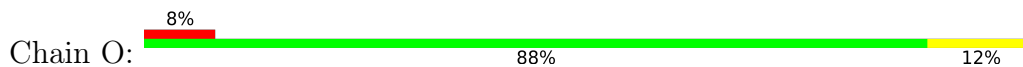


- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial

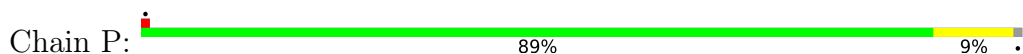
Chain N:  89% 11%



- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial



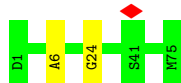
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial



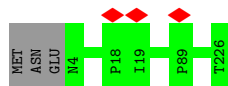
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial



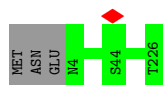
- Molecule 2: ATP synthase F(0) complex subunit C1, mitochondrial



- Molecule 3: ATP synthase subunit a

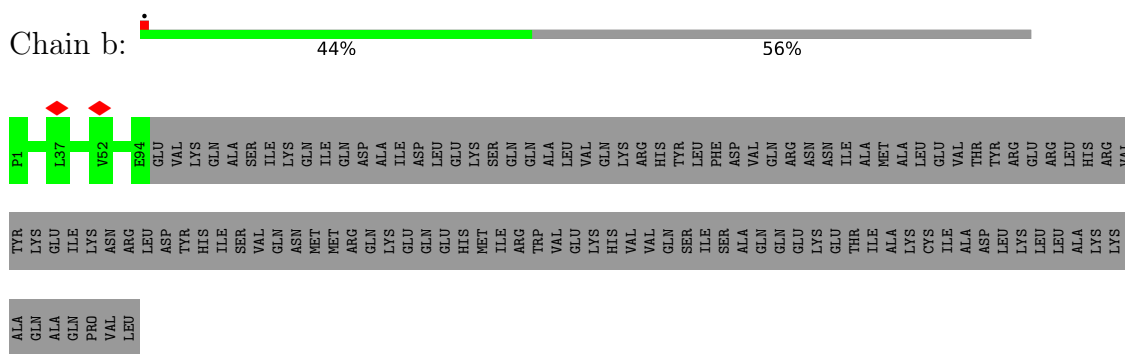


- Molecule 3: ATP synthase subunit a

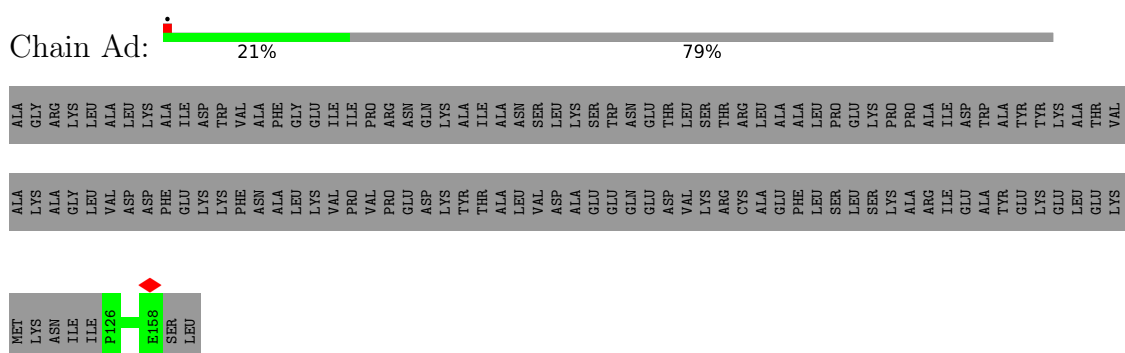


- Molecule 3: ATP synthase subunit a

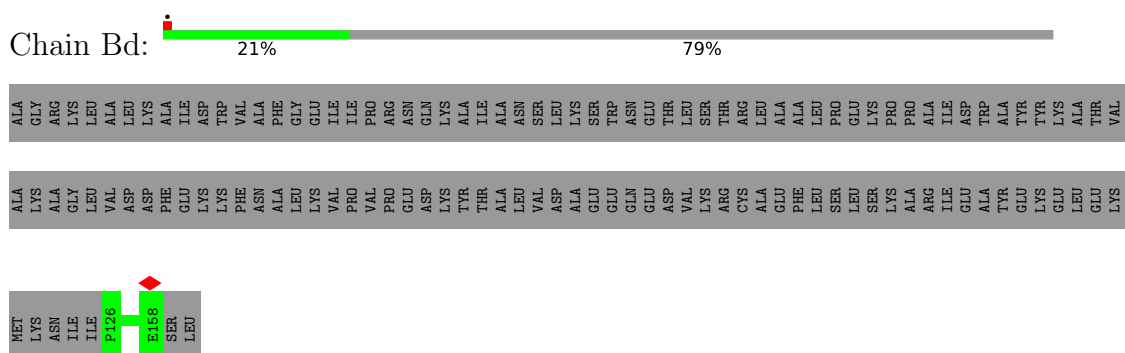
- Molecule 4: ATP synthase peripheral stalk-membrane subunit b



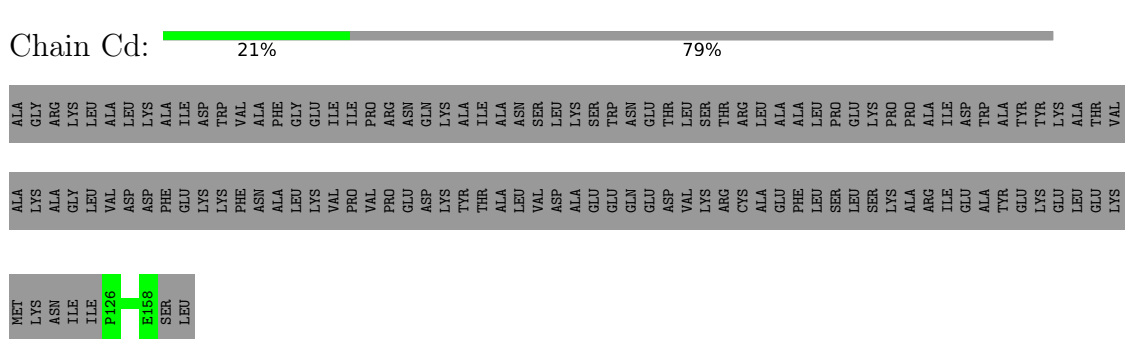
- Molecule 5: ATP synthase subunit d, mitochondrial



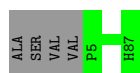
- Molecule 5: ATP synthase subunit d, mitochondrial



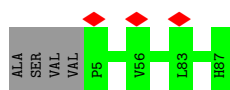
- Molecule 5: ATP synthase subunit d, mitochondrial



- Molecule 5: ATP synthase subunit d, mitochondrial



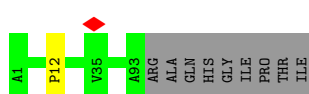
• Molecule 7: ATP synthase subunit f, mitochondrial



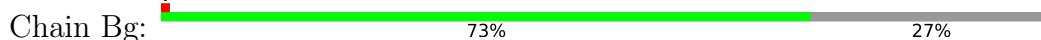
• Molecule 7: ATP synthase subunit f, mitochondrial



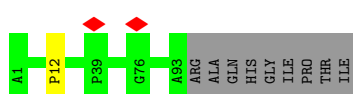
• Molecule 8: ATP synthase g subunit



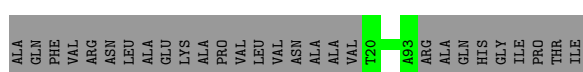
• Molecule 8: ATP synthase g subunit



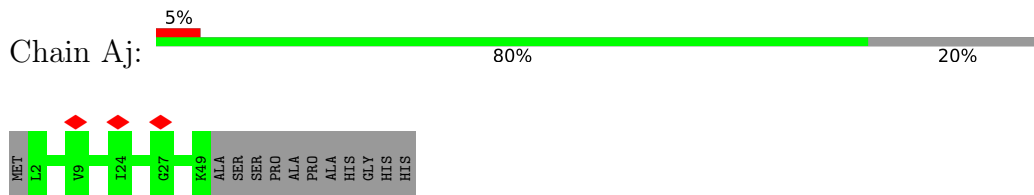
• Molecule 8: ATP synthase g subunit



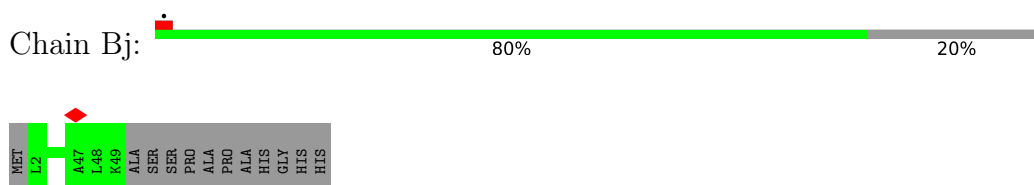
• Molecule 8: ATP synthase g subunit



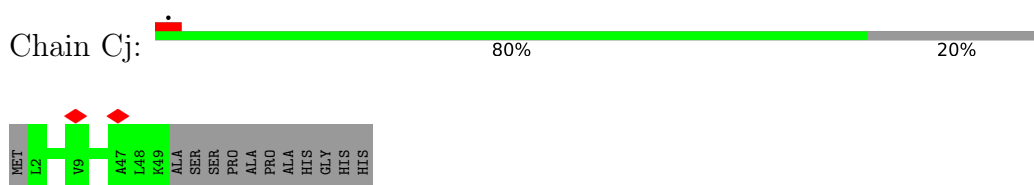
- Molecule 9: ATP synthase j subunit (6.8PL)



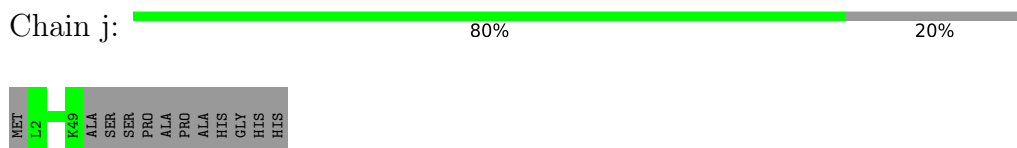
- Molecule 9: ATP synthase j subunit (6.8PL)



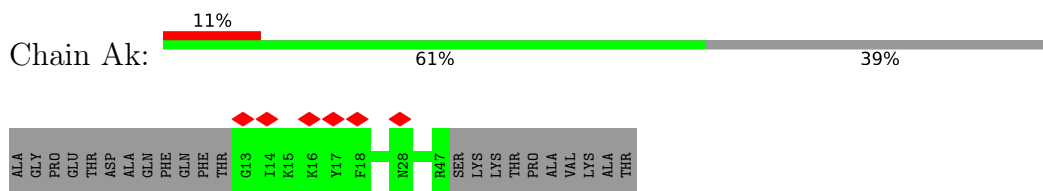
- Molecule 9: ATP synthase j subunit (6.8PL)



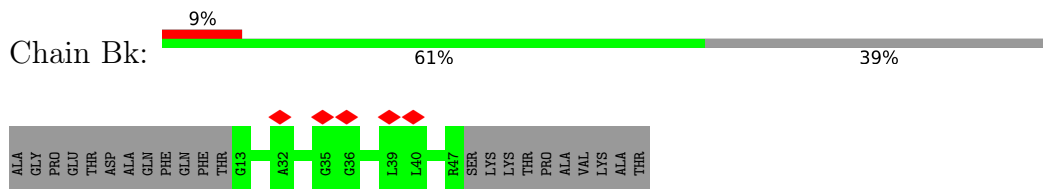
- Molecule 9: ATP synthase j subunit (6.8PL)



- Molecule 10: ATP synthase membrane subunit DAPIT

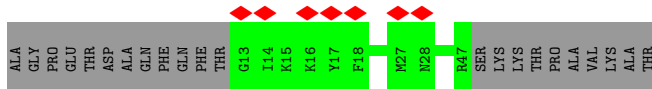


- Molecule 10: ATP synthase membrane subunit DAPIT

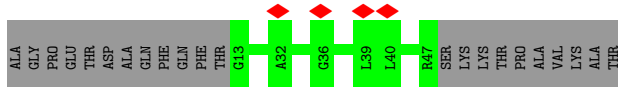


- Molecule 10: ATP synthase membrane subunit DAPIT





- Molecule 10: ATP synthase membrane subunit DAPIT



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170000	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 ($e^-/\text{\AA}^2$)	50	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	1.571	Depositor
Minimum map value	-0.528	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.315	Depositor
Map size (Å)	662.4, 662.4, 662.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	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: CDL, M3L

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	8	0.33	0/169	0.47	0/235
1	A8	0.33	0/169	0.47	0/235
1	B8	0.33	0/169	0.48	0/235
1	C8	0.32	0/169	0.48	0/235
2	AK	0.33	0/358	0.45	0/493
2	AL	0.32	0/358	0.50	0/493
2	AM	0.32	0/353	0.53	0/486
2	AN	0.32	0/358	0.49	0/493
2	AO	0.37	0/534	0.50	0/721
2	AP	0.31	0/353	0.44	0/486
2	AQ	0.31	0/353	0.45	0/486
2	AR	0.32	0/358	0.47	0/493
2	BK	0.31	0/353	0.45	0/486
2	BL	0.32	0/358	0.47	0/493
2	BM	0.33	0/358	0.45	0/493
2	BN	0.32	0/358	0.50	0/493
2	BO	0.33	0/353	0.54	0/486
2	BP	0.33	0/358	0.48	0/493
2	BQ	0.31	0/358	0.48	0/493
2	BR	0.30	0/353	0.44	0/486
2	CK	0.33	0/358	0.45	0/493
2	CL	0.32	0/358	0.50	0/493
2	CM	0.32	0/353	0.53	0/486
2	CN	0.33	0/358	0.48	0/493
2	CO	0.31	0/358	0.48	0/493
2	CP	0.31	0/353	0.44	0/486
2	CQ	0.30	0/353	0.45	0/486
2	CR	0.32	0/358	0.47	0/493
2	K	0.30	0/353	0.45	0/486
2	L	0.31	0/353	0.45	0/486
2	M	0.32	0/358	0.47	0/493
2	N	0.33	0/358	0.45	0/493

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	O	0.33	0/358	0.50	0/493
2	P	0.32	0/353	0.53	0/486
2	Q	0.33	0/358	0.48	0/493
2	R	0.31	0/358	0.48	0/493
3	Aa	0.33	0/1104	0.47	0/1538
3	Ba	0.33	0/1104	0.47	0/1538
3	Ca	0.33	0/1104	0.47	0/1538
3	a	0.33	0/1104	0.47	0/1538
4	Ab	0.31	0/459	0.44	0/635
4	Bb	0.31	0/459	0.44	0/635
4	Cb	0.31	0/459	0.44	0/635
4	b	0.31	0/459	0.44	0/635
5	Ad	0.30	0/164	0.41	0/228
5	Bd	0.30	0/164	0.41	0/228
5	Cd	0.29	0/164	0.41	0/228
5	d	0.30	0/164	0.41	0/228
6	Ae	0.31	0/281	0.50	0/390
6	Be	0.27	0/281	0.43	0/390
6	Ce	0.31	0/281	0.50	0/390
6	e	0.28	0/281	0.43	0/390
7	Af	0.29	0/408	0.44	0/566
7	Bf	0.29	0/408	0.45	0/566
7	Cf	0.29	0/408	0.44	0/566
7	f	0.29	0/408	0.45	0/566
8	Ag	0.56	0/460	0.71	1/640 (0.2%)
8	Bg	0.28	0/365	0.42	0/507
8	Cg	0.56	0/460	0.71	1/640 (0.2%)
8	g	0.28	0/365	0.42	0/507
9	Aj	0.29	0/236	0.45	0/327
9	Bj	0.29	0/236	0.45	0/327
9	Cj	0.30	0/236	0.45	0/327
9	j	0.29	0/236	0.45	0/327
10	Ak	0.26	0/170	0.43	0/234
10	Bk	0.26	0/170	0.43	0/234
10	Ck	0.25	0/170	0.43	0/234
10	k	0.25	0/170	0.43	0/234
All	All	0.33	0/25186	0.48	2/34826 (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
6	Ae	0	1
6	Ce	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Ag	12	PRO	N-CA-CB	5.22	109.56	103.30
8	Cg	12	PRO	N-CA-CB	5.22	109.56	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	Ae	7	SER	Mainchain
6	Ce	7	SER	Mainchain

5.2 Too-close contacts [i](#)

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	8	170	68	68	0	0
1	A8	170	68	68	0	0
1	B8	170	68	68	0	0
1	C8	170	68	68	0	0
2	AK	364	201	201	6	0
2	AL	364	201	200	7	0
2	AM	359	199	199	7	0
2	AN	364	201	200	5	0
2	AO	537	559	559	11	0
2	AP	359	199	199	2	0
2	AQ	359	199	199	2	0
2	AR	364	201	200	3	0
2	BK	359	199	199	2	0
2	BL	364	201	200	4	0
2	BM	364	201	201	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BN	364	201	200	7	0
2	BO	359	199	199	7	0
2	BP	364	201	200	4	0
2	BQ	364	201	201	1	0
2	BR	359	199	199	2	0
2	CK	364	201	201	6	0
2	CL	364	201	200	7	0
2	CM	359	199	198	8	0
2	CN	364	201	200	6	0
2	CO	364	201	201	2	0
2	CP	359	199	199	2	0
2	CQ	359	199	199	2	0
2	CR	364	201	200	3	0
2	K	359	199	199	2	0
2	L	359	199	199	2	0
2	M	364	201	200	4	0
2	N	364	201	201	6	0
2	O	364	201	200	7	0
2	P	359	199	199	8	0
2	Q	364	201	200	6	0
2	R	364	201	201	2	0
3	Aa	1105	494	494	0	0
3	Ba	1105	494	494	0	0
3	Ca	1105	494	494	0	0
3	a	1105	494	494	0	0
4	Ab	460	209	209	0	0
4	Bb	460	209	209	0	0
4	Cb	460	209	209	0	0
4	b	460	209	209	0	0
5	Ad	165	61	61	0	0
5	Bd	165	61	61	0	0
5	Cd	165	61	61	0	0
5	d	165	61	61	0	0
6	Ae	282	131	131	0	0
6	Be	282	131	131	0	0
6	Ce	282	131	131	0	0
6	e	282	131	131	0	0
7	Af	409	184	184	0	0
7	Bf	409	184	184	0	0
7	Cf	409	184	184	0	0
7	f	409	184	184	0	0
8	Ag	461	247	220	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	Bg	366	166	165	0	0
8	Cg	461	247	220	0	0
8	g	366	166	165	0	0
9	Aj	237	102	102	0	0
9	Bj	237	102	102	0	0
9	Cj	237	102	102	0	0
9	j	237	102	102	0	0
10	Ak	171	79	79	0	0
10	Bk	171	79	79	0	0
10	Ck	171	79	79	0	0
10	k	171	79	79	0	0
11	Af	89	131	125	0	0
11	Bf	89	131	125	0	0
11	Cf	89	131	125	0	0
11	f	89	131	125	0	0
All	All	25767	13428	13335	100	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 3.

All (100) 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:BP:5:ALA:HB1	2:BQ:6:ALA:HB2	1.73	0.71
2:AN:5:ALA:HB1	2:AO:6:ALA:HB2	1.73	0.69
2:Q:5:ALA:HB1	2:R:6:ALA:HB2	1.73	0.69
2:CN:5:ALA:HB1	2:CO:6:ALA:HB2	1.73	0.67
2:BL:5:ALA:HB1	2:BM:6:ALA:HB2	1.78	0.66
2:M:5:ALA:HB1	2:N:6:ALA:HB2	1.78	0.65
2:O:5:ALA:HB1	2:P:6:ALA:HB2	1.79	0.65
2:BN:5:ALA:HB1	2:BO:6:ALA:HB2	1.79	0.65
2:CK:6:ALA:HB2	2:CR:5:ALA:HB1	1.78	0.65
2:AL:5:ALA:HB1	2:AM:6:ALA:HB2	1.79	0.65
2:AO:71:ILE:HD12	2:AO:75:MET:HB2	1.79	0.65
2:CL:5:ALA:HB1	2:CM:6:ALA:HB2	1.78	0.64
2:AK:6:ALA:HB2	2:AR:5:ALA:HB1	1.78	0.64
2:CQ:70:LEU:O	2:CQ:74:ALA:N	2.31	0.64
2:BK:70:LEU:O	2:BK:74:ALA:N	2.31	0.63
2:CM:5:ALA:HB1	2:CN:6:ALA:HB2	1.80	0.63
2:AQ:70:LEU:O	2:AQ:74:ALA:N	2.31	0.63
2:AM:5:ALA:HB1	2:AN:6:ALA:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:70:LEU:O	2:L:74:ALA:N	2.31	0.63
2:P:5:ALA:HB1	2:Q:6:ALA:HB2	1.80	0.62
2:BO:5:ALA:HB1	2:BP:6:ALA:HB2	1.80	0.62
2:AO:56:LEU:O	2:AO:56:LEU:HD23	2.02	0.59
2:AO:42:LEU:HD12	2:AO:42:LEU:N	2.19	0.57
2:CM:5:ALA:HB1	2:CN:6:ALA:CB	2.36	0.55
2:AM:5:ALA:HB1	2:AN:6:ALA:CB	2.36	0.55
2:BO:5:ALA:HB1	2:BP:6:ALA:CB	2.36	0.55
2:AO:71:ILE:HD12	2:AO:75:MET:CB	2.36	0.55
2:P:5:ALA:HB1	2:Q:6:ALA:CB	2.36	0.55
2:BM:70:LEU:O	2:BM:74:ALA:N	2.41	0.53
2:AK:70:LEU:O	2:AK:74:ALA:N	2.42	0.53
2:N:70:LEU:O	2:N:74:ALA:N	2.42	0.52
2:CK:70:LEU:O	2:CK:74:ALA:N	2.42	0.52
2:BN:5:ALA:HB1	2:BO:6:ALA:CB	2.42	0.50
2:AL:5:ALA:HB1	2:AM:6:ALA:CB	2.42	0.49
2:AO:7:LYS:NZ	2:AO:73:PHE:O	2.44	0.49
2:BM:34:ILE:O	2:BM:37:ALA:N	2.46	0.49
2:CL:5:ALA:HB1	2:CM:6:ALA:CB	2.42	0.48
2:O:5:ALA:HB1	2:P:6:ALA:CB	2.42	0.48
2:AK:34:ILE:O	2:AK:37:ALA:N	2.46	0.48
2:CK:34:ILE:O	2:CK:37:ALA:N	2.46	0.47
2:AO:11:ALA:O	2:AO:15:THR:OG1	2.27	0.47
2:N:34:ILE:O	2:N:37:ALA:N	2.46	0.47
2:N:42:LEU:O	2:N:43:M3L:C	2.63	0.47
2:AK:42:LEU:O	2:AK:43:M3L:C	2.63	0.46
2:CK:42:LEU:O	2:CK:43:M3L:C	2.63	0.46
2:BL:5:ALA:HB1	2:BM:6:ALA:CB	2.46	0.46
2:CK:6:ALA:CB	2:CR:5:ALA:HB1	2.46	0.46
2:AK:6:ALA:CB	2:AR:5:ALA:HB1	2.46	0.46
2:M:5:ALA:HB1	2:N:6:ALA:CB	2.45	0.46
2:AP:19:ALA:HA	2:AQ:20:GLY:HA3	1.98	0.45
2:BK:20:GLY:HA3	2:BR:19:ALA:HA	1.98	0.45
2:AO:15:THR:HG22	2:AO:15:THR:O	2.17	0.45
2:CP:19:ALA:HA	2:CQ:20:GLY:HA3	1.98	0.45
2:K:19:ALA:HA	2:L:20:GLY:HA3	1.98	0.45
2:AP:11:ALA:O	2:AP:68:ALA:HB1	2.17	0.44
2:BM:42:LEU:O	2:BM:43:M3L:C	2.63	0.44
2:O:70:LEU:O	2:O:74:ALA:O	2.35	0.44
2:BN:70:LEU:O	2:BN:74:ALA:O	2.35	0.44
2:AO:41:SER:HB3	2:AO:42:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AL:70:LEU:O	2:AL:74:ALA:O	2.35	0.44
2:CP:11:ALA:O	2:CP:68:ALA:HB1	2.17	0.44
2:BR:11:ALA:O	2:BR:68:ALA:HB1	2.17	0.44
2:K:11:ALA:O	2:K:68:ALA:HB1	2.17	0.44
2:CL:70:LEU:O	2:CL:74:ALA:O	2.36	0.43
2:M:35:GLY:O	2:M:38:ARG:N	2.47	0.43
2:AM:26:GLY:HA3	2:AN:24:GLY:CA	2.49	0.42
2:O:12:GLY:O	2:P:14:ALA:HB2	2.19	0.42
2:P:26:GLY:HA3	2:Q:24:GLY:CA	2.49	0.42
2:AL:12:GLY:O	2:AM:14:ALA:HB2	2.19	0.42
2:AO:72:LEU:HD23	2:AO:73:PHE:CD1	2.54	0.42
2:CM:26:GLY:HA3	2:CN:24:GLY:CA	2.49	0.42
2:BN:12:GLY:O	2:BO:14:ALA:HB2	2.19	0.42
2:BM:12:GLY:CA	2:BN:14:ALA:HB2	2.50	0.42
2:P:42:LEU:O	2:P:43:M3L:C	2.68	0.42
2:N:12:GLY:CA	2:O:14:ALA:HB2	2.50	0.41
2:BO:26:GLY:HA3	2:BP:24:GLY:CA	2.49	0.41
2:BO:42:LEU:O	2:BO:43:M3L:C	2.68	0.41
2:CL:12:GLY:O	2:CM:14:ALA:HB2	2.19	0.41
2:BN:34:ILE:O	2:BN:37:ALA:N	2.54	0.41
2:AR:35:GLY:O	2:AR:38:ARG:N	2.47	0.41
2:CL:34:ILE:O	2:CL:37:ALA:N	2.54	0.41
2:O:42:LEU:O	2:O:43:M3L:C	2.68	0.41
2:CK:12:GLY:CA	2:CL:14:ALA:HB2	2.50	0.41
2:AM:42:LEU:O	2:AM:43:M3L:C	2.68	0.41
2:BL:35:GLY:O	2:BL:38:ARG:N	2.47	0.41
2:AK:12:GLY:CA	2:AL:14:ALA:HB2	2.50	0.41
2:AL:42:LEU:O	2:AL:43:M3L:C	2.69	0.41
2:Q:26:GLY:HA3	2:R:24:GLY:CA	2.51	0.41
2:CL:42:LEU:O	2:CL:43:M3L:C	2.69	0.41
2:O:34:ILE:O	2:O:37:ALA:N	2.54	0.41
2:AL:34:ILE:O	2:AL:37:ALA:N	2.54	0.40
2:AN:26:GLY:HA3	2:AO:24:GLY:CA	2.51	0.40
2:CN:26:GLY:HA3	2:CO:24:GLY:CA	2.51	0.40
2:P:19:ALA:O	2:Q:20:GLY:HA3	2.22	0.40
2:CM:19:ALA:O	2:CN:20:GLY:HA3	2.22	0.40
2:M:39:ASN:O	2:M:41:SER:N	2.55	0.40
2:BL:39:ASN:O	2:BL:41:SER:N	2.55	0.40
2:BN:42:LEU:O	2:BN:43:M3L:C	2.69	0.40
2:CM:42:LEU:O	2:CM:43:M3L:C	2.68	0.40
2:CR:39:ASN:O	2:CR:41:SER:N	2.55	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	8	32/67 (48%)	28 (88%)	4 (12%)	0	100	100
1	A8	32/67 (48%)	28 (88%)	4 (12%)	0	100	100
1	B8	32/67 (48%)	28 (88%)	4 (12%)	0	100	100
1	C8	32/67 (48%)	28 (88%)	4 (12%)	0	100	100
2	AK	72/75 (96%)	66 (92%)	6 (8%)	0	100	100
2	AL	72/75 (96%)	63 (88%)	9 (12%)	0	100	100
2	AM	71/75 (95%)	61 (86%)	10 (14%)	0	100	100
2	AN	72/75 (96%)	64 (89%)	8 (11%)	0	100	100
2	AO	72/75 (96%)	63 (88%)	9 (12%)	0	100	100
2	AP	71/75 (95%)	64 (90%)	7 (10%)	0	100	100
2	AQ	71/75 (95%)	67 (94%)	4 (6%)	0	100	100
2	AR	72/75 (96%)	66 (92%)	6 (8%)	0	100	100
2	BK	71/75 (95%)	67 (94%)	4 (6%)	0	100	100
2	BL	72/75 (96%)	66 (92%)	6 (8%)	0	100	100
2	BM	72/75 (96%)	66 (92%)	6 (8%)	0	100	100
2	BN	72/75 (96%)	63 (88%)	9 (12%)	0	100	100
2	BO	71/75 (95%)	61 (86%)	10 (14%)	0	100	100
2	BP	72/75 (96%)	64 (89%)	8 (11%)	0	100	100
2	BQ	72/75 (96%)	63 (88%)	9 (12%)	0	100	100
2	BR	71/75 (95%)	64 (90%)	7 (10%)	0	100	100
2	CK	72/75 (96%)	66 (92%)	6 (8%)	0	100	100
2	CL	72/75 (96%)	63 (88%)	9 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CM	71/75 (95%)	61 (86%)	10 (14%)	0	100	100
2	CN	72/75 (96%)	64 (89%)	8 (11%)	0	100	100
2	CO	72/75 (96%)	63 (88%)	9 (12%)	0	100	100
2	CP	71/75 (95%)	64 (90%)	7 (10%)	0	100	100
2	CQ	71/75 (95%)	67 (94%)	4 (6%)	0	100	100
2	CR	72/75 (96%)	66 (92%)	6 (8%)	0	100	100
2	K	71/75 (95%)	64 (90%)	7 (10%)	0	100	100
2	L	71/75 (95%)	67 (94%)	4 (6%)	0	100	100
2	M	72/75 (96%)	66 (92%)	6 (8%)	0	100	100
2	N	72/75 (96%)	66 (92%)	6 (8%)	0	100	100
2	O	72/75 (96%)	63 (88%)	9 (12%)	0	100	100
2	P	71/75 (95%)	61 (86%)	10 (14%)	0	100	100
2	Q	72/75 (96%)	64 (89%)	8 (11%)	0	100	100
2	R	72/75 (96%)	63 (88%)	9 (12%)	0	100	100
3	Aa	221/226 (98%)	193 (87%)	28 (13%)	0	100	100
3	Ba	221/226 (98%)	194 (88%)	27 (12%)	0	100	100
3	Ca	221/226 (98%)	194 (88%)	27 (12%)	0	100	100
3	a	221/226 (98%)	194 (88%)	27 (12%)	0	100	100
4	Ab	92/214 (43%)	83 (90%)	9 (10%)	0	100	100
4	Bb	92/214 (43%)	83 (90%)	9 (10%)	0	100	100
4	Cb	92/214 (43%)	83 (90%)	9 (10%)	0	100	100
4	b	92/214 (43%)	83 (90%)	9 (10%)	0	100	100
5	Ad	31/160 (19%)	28 (90%)	3 (10%)	0	100	100
5	Bd	31/160 (19%)	28 (90%)	3 (10%)	0	100	100
5	Cd	31/160 (19%)	28 (90%)	3 (10%)	0	100	100
5	d	31/160 (19%)	28 (90%)	3 (10%)	0	100	100
6	Ae	55/70 (79%)	52 (94%)	2 (4%)	1 (2%)	8	40
6	Be	55/70 (79%)	53 (96%)	2 (4%)	0	100	100
6	Ce	55/70 (79%)	52 (94%)	2 (4%)	1 (2%)	8	40
6	e	55/70 (79%)	53 (96%)	2 (4%)	0	100	100
7	Af	81/87 (93%)	74 (91%)	7 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Bf	81/87 (93%)	74 (91%)	7 (9%)	0	100	100
7	Cf	81/87 (93%)	74 (91%)	7 (9%)	0	100	100
7	f	81/87 (93%)	74 (91%)	7 (9%)	0	100	100
8	Ag	91/102 (89%)	88 (97%)	3 (3%)	0	100	100
8	Bg	72/102 (71%)	69 (96%)	3 (4%)	0	100	100
8	Cg	91/102 (89%)	89 (98%)	2 (2%)	0	100	100
8	g	72/102 (71%)	69 (96%)	3 (4%)	0	100	100
9	Aj	46/60 (77%)	42 (91%)	4 (9%)	0	100	100
9	Bj	46/60 (77%)	42 (91%)	4 (9%)	0	100	100
9	Cj	46/60 (77%)	42 (91%)	4 (9%)	0	100	100
9	j	46/60 (77%)	42 (91%)	4 (9%)	0	100	100
10	Ak	33/57 (58%)	30 (91%)	3 (9%)	0	100	100
10	Bk	33/57 (58%)	30 (91%)	3 (9%)	0	100	100
10	Ck	33/57 (58%)	30 (91%)	3 (9%)	0	100	100
10	k	33/57 (58%)	30 (91%)	3 (9%)	0	100	100
All	All	4982/6572 (76%)	4496 (90%)	484 (10%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	Ae	7	SER
6	Ce	7	SER

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	
2	AO	50/50 (100%)	50 (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](#)

32 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
2	M3L	BP	43	2	3,4,12	0.94	0	2,4,16	0.64	0
2	M3L	CK	43	2	3,4,12	0.78	0	2,4,16	0.48	0
2	M3L	AK	43	2	3,4,12	0.79	0	2,4,16	0.49	0
2	M3L	BN	43	2	3,4,12	0.91	0	2,4,16	0.55	0
2	M3L	AP	43	2	3,4,12	0.86	0	2,4,16	0.61	0
2	M3L	CL	43	2	3,4,12	0.90	0	2,4,16	0.58	0
2	M3L	CM	43	2	3,4,12	0.84	0	2,4,16	0.19	0
2	M3L	AR	43	2	3,4,12	0.93	0	2,4,16	0.20	0
2	M3L	AO	43	2	10,11,12	0.46	0	9,14,16	0.64	0
2	M3L	AL	43	2	3,4,12	0.91	0	2,4,16	0.58	0
2	M3L	AN	43	2	3,4,12	0.92	0	2,4,16	0.63	0
2	M3L	CP	43	2	3,4,12	0.87	0	2,4,16	0.64	0
2	M3L	K	43	2	3,4,12	0.88	0	2,4,16	0.65	0
2	M3L	CQ	43	2	3,4,12	1.10	0	2,4,16	0.24	0
2	M3L	BO	43	2	3,4,12	0.82	0	2,4,16	0.17	0
2	M3L	N	43	2	3,4,12	0.79	0	2,4,16	0.49	0
2	M3L	O	43	2	3,4,12	0.91	0	2,4,16	0.57	0
2	M3L	BL	43	2	3,4,12	0.96	0	2,4,16	0.19	0
2	M3L	P	43	2	3,4,12	0.85	0	2,4,16	0.17	0
2	M3L	CN	43	2	3,4,12	0.92	0	2,4,16	0.63	0
2	M3L	R	43	2	3,4,12	0.86	0	2,4,16	0.74	0
2	M3L	BK	43	2	3,4,12	1.09	0	2,4,16	0.24	0
2	M3L	BM	43	2	3,4,12	0.78	0	2,4,16	0.48	0
2	M3L	L	43	2	3,4,12	1.08	0	2,4,16	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	M3L	Q	43	2	3,4,12	0.92	0	2,4,16	0.63	0
2	M3L	AQ	43	2	3,4,12	1.10	0	2,4,16	0.24	0
2	M3L	AM	43	2	3,4,12	0.84	0	2,4,16	0.18	0
2	M3L	CR	43	2	3,4,12	0.96	0	2,4,16	0.22	0
2	M3L	CO	43	2	3,4,12	0.84	0	2,4,16	0.73	0
2	M3L	BR	43	2	3,4,12	0.84	0	2,4,16	0.65	0
2	M3L	M	43	2	3,4,12	0.94	0	2,4,16	0.19	0
2	M3L	BQ	43	2	3,4,12	0.85	0	2,4,16	0.73	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
2	M3L	BP	43	2	-	0/0/2/12	-
2	M3L	CK	43	2	-	0/0/2/12	-
2	M3L	AK	43	2	-	0/0/2/12	-
2	M3L	BN	43	2	-	0/0/2/12	-
2	M3L	AP	43	2	-	0/0/2/12	-
2	M3L	CL	43	2	-	0/0/2/12	-
2	M3L	CM	43	2	-	0/0/2/12	-
2	M3L	AR	43	2	-	0/0/2/12	-
2	M3L	AO	43	2	-	4/9/10/12	-
2	M3L	AL	43	2	-	0/0/2/12	-
2	M3L	AN	43	2	-	0/0/2/12	-
2	M3L	CP	43	2	-	0/0/2/12	-
2	M3L	K	43	2	-	0/0/2/12	-
2	M3L	CQ	43	2	-	0/0/2/12	-
2	M3L	BO	43	2	-	0/0/2/12	-
2	M3L	N	43	2	-	0/0/2/12	-
2	M3L	O	43	2	-	0/0/2/12	-
2	M3L	BL	43	2	-	0/0/2/12	-
2	M3L	P	43	2	-	0/0/2/12	-
2	M3L	CN	43	2	-	0/0/2/12	-
2	M3L	R	43	2	-	0/0/2/12	-
2	M3L	BK	43	2	-	0/0/2/12	-
2	M3L	BM	43	2	-	0/0/2/12	-
2	M3L	L	43	2	-	0/0/2/12	-
2	M3L	Q	43	2	-	0/0/2/12	-
2	M3L	AQ	43	2	-	0/0/2/12	-
2	M3L	AM	43	2	-	0/0/2/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	M3L	CR	43	2	-	0/0/2/12	-
2	M3L	CO	43	2	-	0/0/2/12	-
2	M3L	BR	43	2	-	0/0/2/12	-
2	M3L	M	43	2	-	0/0/2/12	-
2	M3L	BQ	43	2	-	0/0/2/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AO	43	M3L	CD-CE-NZ-CM2
2	AO	43	M3L	CD-CE-NZ-CM3
2	AO	43	M3L	CD-CE-NZ-CM1
2	AO	43	M3L	CE-CD-CG-CB

There are no ring outliers.

12 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CK	43	M3L	1	0
2	AK	43	M3L	1	0
2	BN	43	M3L	1	0
2	CL	43	M3L	1	0
2	CM	43	M3L	1	0
2	AL	43	M3L	1	0
2	BO	43	M3L	1	0
2	N	43	M3L	1	0
2	O	43	M3L	1	0
2	P	43	M3L	1	0
2	BM	43	M3L	1	0
2	AM	43	M3L	1	0

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 ligands 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
11	CDL	Cf	101	-	88,88,99	0.94	6 (6%)	94,100,111	1.06	5 (5%)
11	CDL	f	101	-	88,88,99	0.94	6 (6%)	94,100,111	1.06	5 (5%)
11	CDL	Af	101	-	88,88,99	0.94	6 (6%)	94,100,111	1.06	5 (5%)
11	CDL	Bf	101	-	88,88,99	0.95	6 (6%)	94,100,111	1.06	5 (5%)

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
11	CDL	Cf	101	-	-	42/99/99/110	-
11	CDL	f	101	-	-	42/99/99/110	-
11	CDL	Af	101	-	-	42/99/99/110	-
11	CDL	Bf	101	-	-	42/99/99/110	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Bf	101	CDL	OA6-CA4	-2.88	1.39	1.46
11	f	101	CDL	OA6-CA4	-2.87	1.39	1.46
11	Af	101	CDL	OA6-CA4	-2.81	1.39	1.46
11	Cf	101	CDL	OA6-CA4	-2.79	1.39	1.46
11	f	101	CDL	OA8-CA7	2.63	1.41	1.33
11	f	101	CDL	OB6-CB4	-2.61	1.40	1.46
11	Cf	101	CDL	OB6-CB4	-2.61	1.40	1.46
11	Bf	101	CDL	OB6-CB4	-2.59	1.40	1.46
11	Af	101	CDL	OB6-CB4	-2.58	1.40	1.46
11	Af	101	CDL	OA8-CA7	2.56	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Cf	101	CDL	OA8-CA7	2.52	1.40	1.33
11	Bf	101	CDL	OA8-CA7	2.52	1.40	1.33
11	Bf	101	CDL	OB8-CB7	2.43	1.40	1.33
11	Af	101	CDL	OB8-CB7	2.40	1.40	1.33
11	f	101	CDL	OB8-CB7	2.40	1.40	1.33
11	Cf	101	CDL	OB8-CB7	2.32	1.40	1.33
11	Bf	101	CDL	OB8-CB6	-2.16	1.40	1.45
11	Cf	101	CDL	OB8-CB6	-2.16	1.40	1.45
11	f	101	CDL	OB8-CB6	-2.13	1.40	1.45
11	Af	101	CDL	OB8-CB6	-2.12	1.40	1.45
11	f	101	CDL	OB6-CB5	2.08	1.40	1.34
11	Cf	101	CDL	OB6-CB5	2.06	1.40	1.34
11	Af	101	CDL	OB6-CB5	2.05	1.40	1.34
11	Bf	101	CDL	OB6-CB5	2.02	1.40	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Bf	101	CDL	OA6-CA5-C11	3.99	120.09	111.50
11	Af	101	CDL	OA6-CA5-C11	3.98	120.07	111.50
11	Cf	101	CDL	OA6-CA5-C11	3.96	120.03	111.50
11	f	101	CDL	OA6-CA5-C11	3.95	120.02	111.50
11	f	101	CDL	OB6-CB5-C51	3.64	119.34	111.50
11	Cf	101	CDL	OB6-CB5-C51	3.61	119.27	111.50
11	Bf	101	CDL	OB6-CB5-C51	3.59	119.23	111.50
11	Af	101	CDL	OB6-CB5-C51	3.57	119.20	111.50
11	Cf	101	CDL	CA4-OA6-CA5	-2.74	111.05	117.79
11	Af	101	CDL	CA4-OA6-CA5	-2.70	111.15	117.79
11	f	101	CDL	CA4-OA6-CA5	-2.69	111.16	117.79
11	Bf	101	CDL	CA4-OA6-CA5	-2.69	111.18	117.79
11	Cf	101	CDL	OB8-CB7-C71	2.48	119.69	111.91
11	Cf	101	CDL	OA8-CA7-C31	2.47	119.67	111.91
11	f	101	CDL	OB8-CB7-C71	2.46	119.61	111.91
11	Af	101	CDL	OA8-CA7-C31	2.45	119.59	111.91
11	Af	101	CDL	OB8-CB7-C71	2.44	119.55	111.91
11	Bf	101	CDL	OB8-CB7-C71	2.43	119.55	111.91
11	f	101	CDL	OA8-CA7-C31	2.43	119.54	111.91
11	Bf	101	CDL	OA8-CA7-C31	2.40	119.45	111.91

There are no chirality outliers.

All (168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	Af	101	CDL	OA5-CA3-CA4-OA6
11	Af	101	CDL	CB3-OB5-PB2-OB3
11	Af	101	CDL	CB3-OB5-PB2-OB4
11	Bf	101	CDL	OA5-CA3-CA4-OA6
11	Bf	101	CDL	CB3-OB5-PB2-OB3
11	Bf	101	CDL	CB3-OB5-PB2-OB4
11	Cf	101	CDL	OA5-CA3-CA4-OA6
11	Cf	101	CDL	CB3-OB5-PB2-OB3
11	Cf	101	CDL	CB3-OB5-PB2-OB4
11	f	101	CDL	OA5-CA3-CA4-OA6
11	f	101	CDL	CB3-OB5-PB2-OB3
11	f	101	CDL	CB3-OB5-PB2-OB4
11	Af	101	CDL	C31-CA7-OA8-CA6
11	Bf	101	CDL	C31-CA7-OA8-CA6
11	Cf	101	CDL	C31-CA7-OA8-CA6
11	f	101	CDL	C31-CA7-OA8-CA6
11	Af	101	CDL	OA9-CA7-OA8-CA6
11	Bf	101	CDL	OA9-CA7-OA8-CA6
11	Cf	101	CDL	OA9-CA7-OA8-CA6
11	f	101	CDL	OA9-CA7-OA8-CA6
11	Af	101	CDL	C51-CB5-OB6-CB4
11	Bf	101	CDL	C51-CB5-OB6-CB4
11	Cf	101	CDL	C51-CB5-OB6-CB4
11	f	101	CDL	C51-CB5-OB6-CB4
11	Cf	101	CDL	C71-CB7-OB8-CB6
11	f	101	CDL	C71-CB7-OB8-CB6
11	Af	101	CDL	OB7-CB5-OB6-CB4
11	Bf	101	CDL	OB7-CB5-OB6-CB4
11	Cf	101	CDL	OB7-CB5-OB6-CB4
11	f	101	CDL	OB7-CB5-OB6-CB4
11	Af	101	CDL	C71-CB7-OB8-CB6
11	Bf	101	CDL	C71-CB7-OB8-CB6
11	Af	101	CDL	CA7-C31-C32-C33
11	Bf	101	CDL	CA7-C31-C32-C33
11	Cf	101	CDL	CA7-C31-C32-C33
11	f	101	CDL	CA7-C31-C32-C33
11	Af	101	CDL	CB5-C51-C52-C53
11	Bf	101	CDL	CB5-C51-C52-C53
11	Cf	101	CDL	CB5-C51-C52-C53
11	f	101	CDL	CB5-C51-C52-C53
11	Af	101	CDL	OB9-CB7-OB8-CB6
11	Bf	101	CDL	OB9-CB7-OB8-CB6
11	Cf	101	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
11	f	101	CDL	OB9-CB7-OB8-CB6
11	Af	101	CDL	CB3-OB5-PB2-OB2
11	Bf	101	CDL	CB3-OB5-PB2-OB2
11	Cf	101	CDL	CB3-OB5-PB2-OB2
11	f	101	CDL	CB3-OB5-PB2-OB2
11	Af	101	CDL	C11-CA5-OA6-CA4
11	Bf	101	CDL	C11-CA5-OA6-CA4
11	Cf	101	CDL	C11-CA5-OA6-CA4
11	f	101	CDL	C11-CA5-OA6-CA4
11	Bf	101	CDL	C33-C34-C35-C36
11	Af	101	CDL	C33-C34-C35-C36
11	Cf	101	CDL	C33-C34-C35-C36
11	f	101	CDL	C33-C34-C35-C36
11	Af	101	CDL	C37-C38-C39-C40
11	Bf	101	CDL	C37-C38-C39-C40
11	Cf	101	CDL	C37-C38-C39-C40
11	f	101	CDL	C37-C38-C39-C40
11	Af	101	CDL	OA7-CA5-OA6-CA4
11	Bf	101	CDL	OA7-CA5-OA6-CA4
11	Cf	101	CDL	OA7-CA5-OA6-CA4
11	f	101	CDL	OA7-CA5-OA6-CA4
11	Af	101	CDL	C63-C64-C65-C66
11	Bf	101	CDL	C63-C64-C65-C66
11	Cf	101	CDL	C63-C64-C65-C66
11	f	101	CDL	C63-C64-C65-C66
11	f	101	CDL	C58-C59-C60-C61
11	Bf	101	CDL	CA5-C11-C12-C13
11	Cf	101	CDL	CA5-C11-C12-C13
11	f	101	CDL	CA5-C11-C12-C13
11	Af	101	CDL	C58-C59-C60-C61
11	Bf	101	CDL	C58-C59-C60-C61
11	Cf	101	CDL	C58-C59-C60-C61
11	Af	101	CDL	CA5-C11-C12-C13
11	Af	101	CDL	C31-C32-C33-C34
11	Bf	101	CDL	C31-C32-C33-C34
11	Cf	101	CDL	C31-C32-C33-C34
11	f	101	CDL	C31-C32-C33-C34
11	Af	101	CDL	OA5-CA3-CA4-CA6
11	Bf	101	CDL	OA5-CA3-CA4-CA6
11	Cf	101	CDL	OA5-CA3-CA4-CA6
11	f	101	CDL	OA5-CA3-CA4-CA6
11	Af	101	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
11	f	101	CDL	C55-C56-C57-C58
11	Bf	101	CDL	C55-C56-C57-C58
11	Cf	101	CDL	C55-C56-C57-C58
11	Af	101	CDL	OB6-CB4-CB6-OB8
11	Bf	101	CDL	OB6-CB4-CB6-OB8
11	Cf	101	CDL	OB6-CB4-CB6-OB8
11	f	101	CDL	OB6-CB4-CB6-OB8
11	Bf	101	CDL	C59-C60-C61-C62
11	Af	101	CDL	C59-C60-C61-C62
11	Cf	101	CDL	C59-C60-C61-C62
11	f	101	CDL	C59-C60-C61-C62
11	Af	101	CDL	C20-C21-C22-C23
11	Bf	101	CDL	C20-C21-C22-C23
11	Cf	101	CDL	C20-C21-C22-C23
11	f	101	CDL	C20-C21-C22-C23
11	Bf	101	CDL	C72-C73-C74-C75
11	Af	101	CDL	C72-C73-C74-C75
11	Bf	101	CDL	C53-C54-C55-C56
11	f	101	CDL	C72-C73-C74-C75
11	Af	101	CDL	C53-C54-C55-C56
11	Cf	101	CDL	C53-C54-C55-C56
11	Cf	101	CDL	C72-C73-C74-C75
11	f	101	CDL	C53-C54-C55-C56
11	Af	101	CDL	CA3-CA4-CA6-OA8
11	Bf	101	CDL	CA3-CA4-CA6-OA8
11	Cf	101	CDL	CA3-CA4-CA6-OA8
11	f	101	CDL	CA3-CA4-CA6-OA8
11	Bf	101	CDL	C78-C79-C80-C81
11	f	101	CDL	C78-C79-C80-C81
11	Af	101	CDL	OA6-CA4-CA6-OA8
11	Bf	101	CDL	OA6-CA4-CA6-OA8
11	Cf	101	CDL	OA6-CA4-CA6-OA8
11	f	101	CDL	OA6-CA4-CA6-OA8
11	Af	101	CDL	C78-C79-C80-C81
11	Cf	101	CDL	C78-C79-C80-C81
11	Bf	101	CDL	C12-C11-CA5-OA6
11	Af	101	CDL	C12-C11-CA5-OA6
11	Cf	101	CDL	C12-C11-CA5-OA6
11	f	101	CDL	C12-C11-CA5-OA6
11	Cf	101	CDL	C51-C52-C53-C54
11	Af	101	CDL	C51-C52-C53-C54
11	Bf	101	CDL	C51-C52-C53-C54

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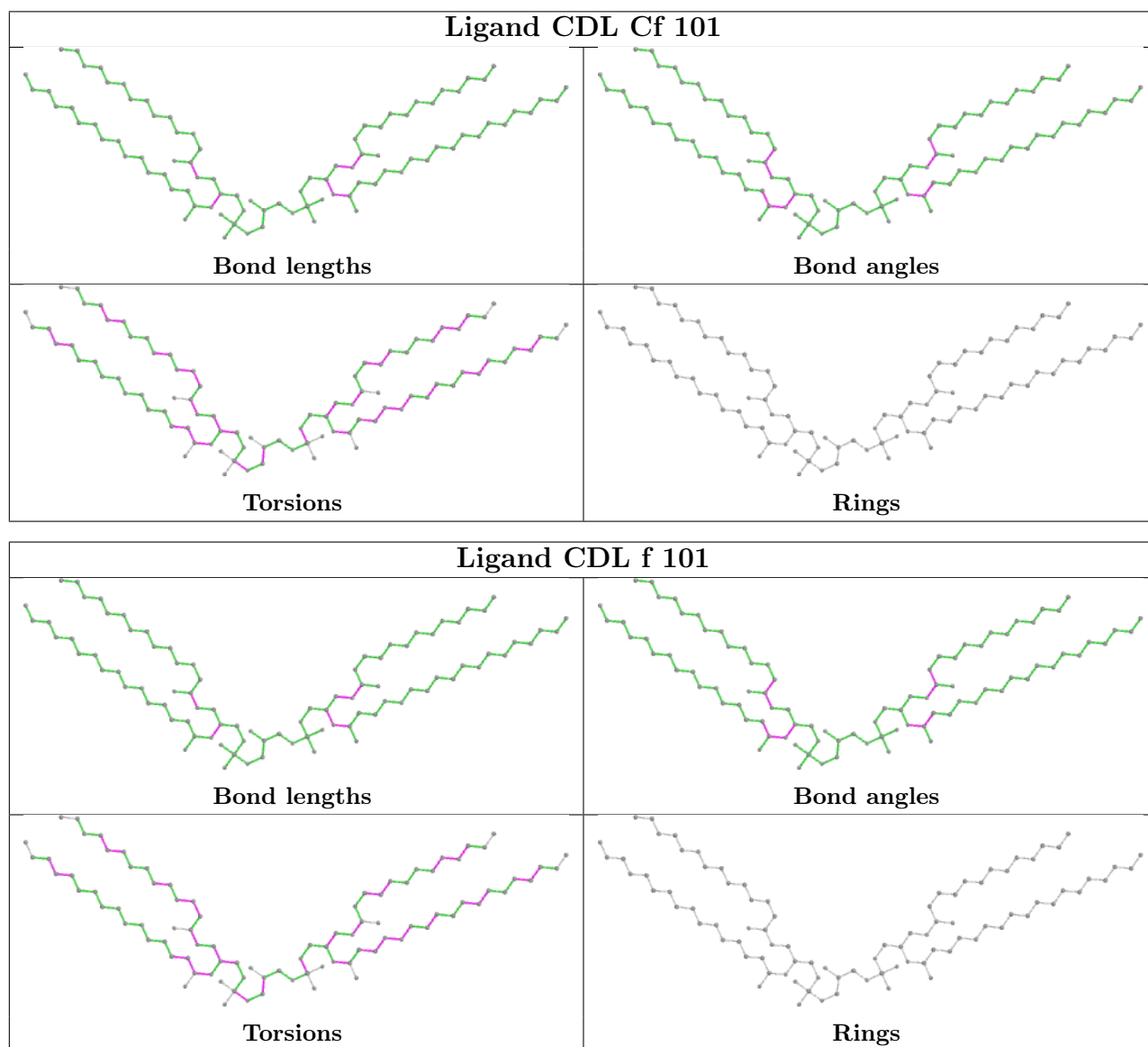
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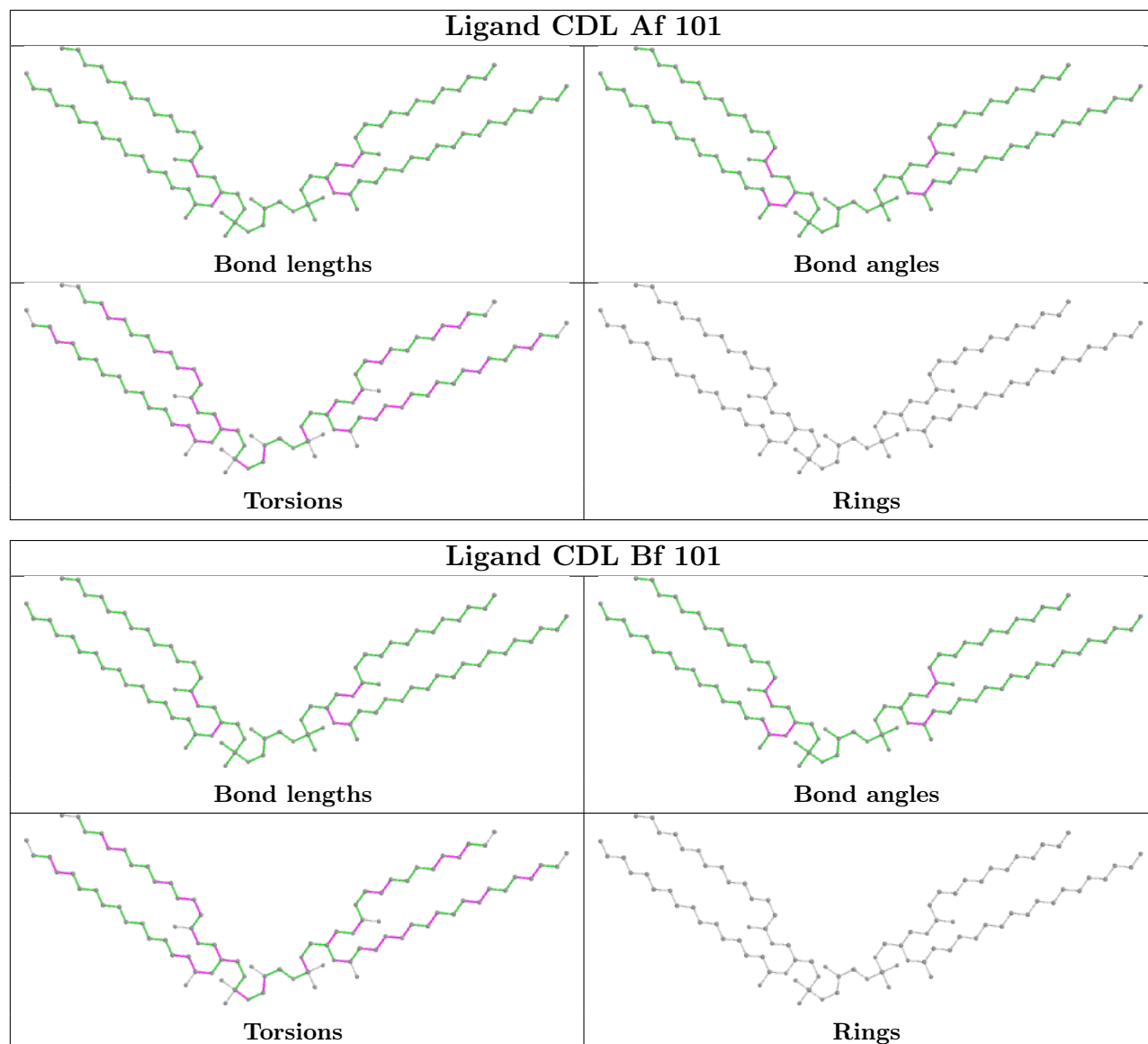
Mol	Chain	Res	Type	Atoms
11	f	101	CDL	C51-C52-C53-C54
11	Af	101	CDL	CB3-CB4-CB6-OB8
11	Bf	101	CDL	CB3-CB4-CB6-OB8
11	Cf	101	CDL	CB3-CB4-CB6-OB8
11	f	101	CDL	CB3-CB4-CB6-OB8
11	f	101	CDL	C71-C72-C73-C74
11	Bf	101	CDL	C76-C77-C78-C79
11	Af	101	CDL	C76-C77-C78-C79
11	Cf	101	CDL	C76-C77-C78-C79
11	f	101	CDL	C76-C77-C78-C79
11	Cf	101	CDL	C71-C72-C73-C74
11	Bf	101	CDL	C71-C72-C73-C74
11	Af	101	CDL	C71-C72-C73-C74
11	Cf	101	CDL	C52-C53-C54-C55
11	Af	101	CDL	C38-C39-C40-C41
11	Bf	101	CDL	C38-C39-C40-C41
11	Cf	101	CDL	C38-C39-C40-C41
11	Af	101	CDL	C52-C53-C54-C55
11	Af	101	CDL	C21-C22-C23-C24
11	Bf	101	CDL	C21-C22-C23-C24
11	f	101	CDL	C38-C39-C40-C41
11	f	101	CDL	C52-C53-C54-C55
11	Bf	101	CDL	C52-C53-C54-C55
11	Bf	101	CDL	C62-C63-C64-C65
11	Cf	101	CDL	C62-C63-C64-C65
11	f	101	CDL	C21-C22-C23-C24
11	Af	101	CDL	C62-C63-C64-C65
11	Cf	101	CDL	C21-C22-C23-C24
11	Cf	101	CDL	C77-C78-C79-C80
11	f	101	CDL	C62-C63-C64-C65
11	f	101	CDL	C77-C78-C79-C80
11	Bf	101	CDL	C77-C78-C79-C80
11	Af	101	CDL	C77-C78-C79-C80
11	Cf	101	CDL	CB2-C1-CA2-OA2
11	Af	101	CDL	CA2-OA2-PA1-OA3
11	Bf	101	CDL	CA2-OA2-PA1-OA3
11	Cf	101	CDL	CA2-OA2-PA1-OA3
11	f	101	CDL	CA2-OA2-PA1-OA3
11	Af	101	CDL	CB2-C1-CA2-OA2
11	Bf	101	CDL	CB2-C1-CA2-OA2
11	f	101	CDL	CB2-C1-CA2-OA2

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

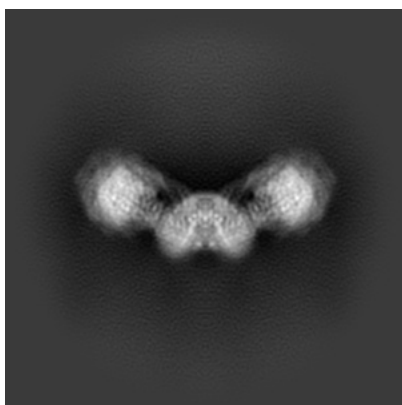
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0667. These allow visual inspection of the internal detail of the map and identification of artifacts.

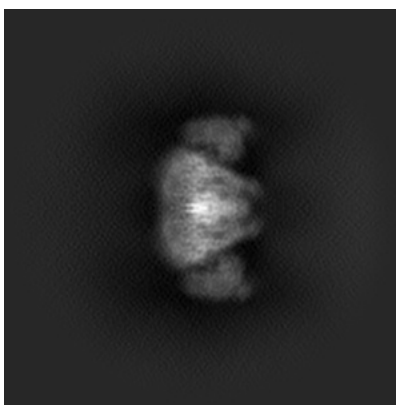
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

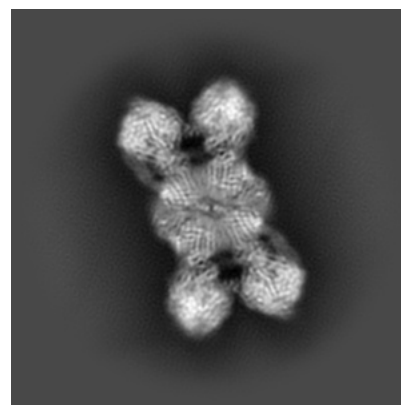
6.1.1 Primary map



X



Y

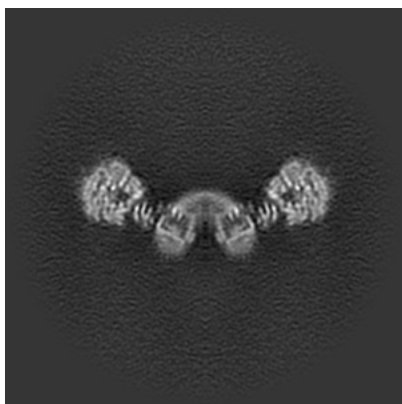


Z

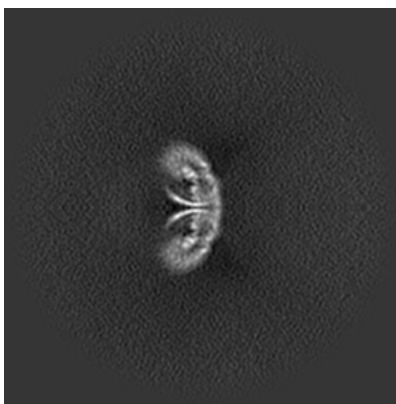
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

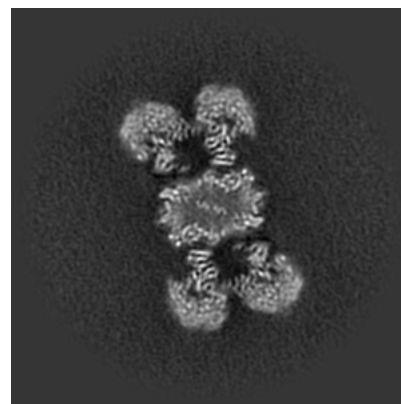
6.2.1 Primary map



X Index: 240



Y Index: 240

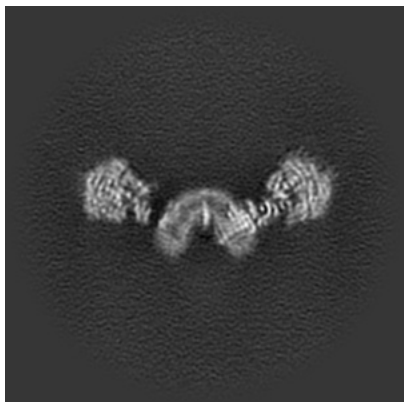


Z Index: 240

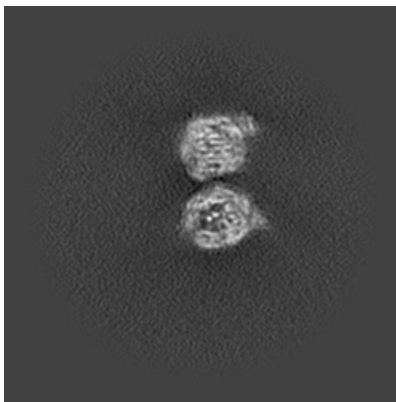
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

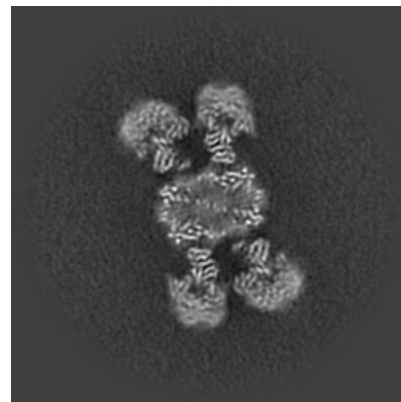
6.3.1 Primary map



X Index: 244



Y Index: 137



Z Index: 237

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

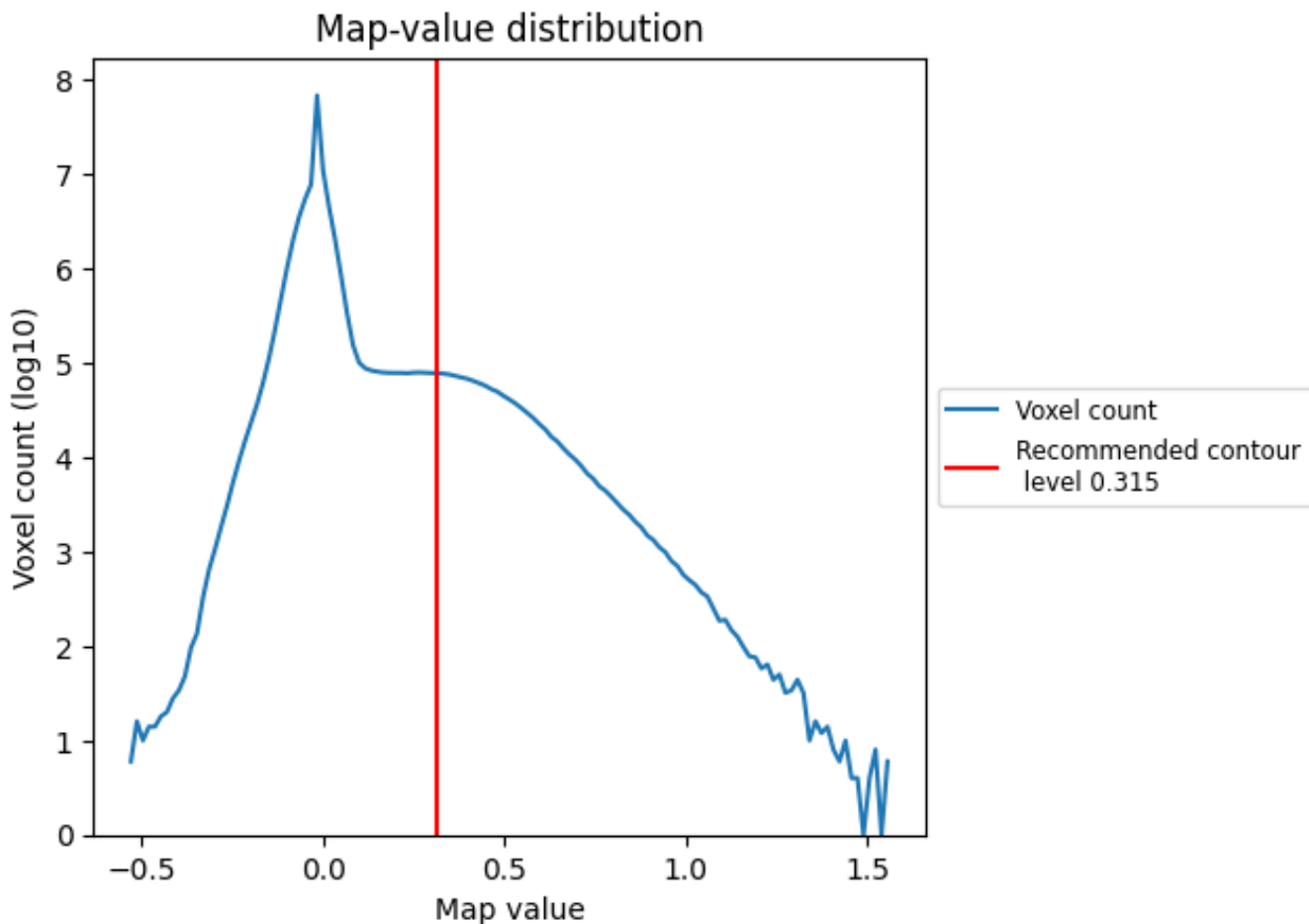
6.5 Mask visualisation

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

7 Map analysis [i](#)

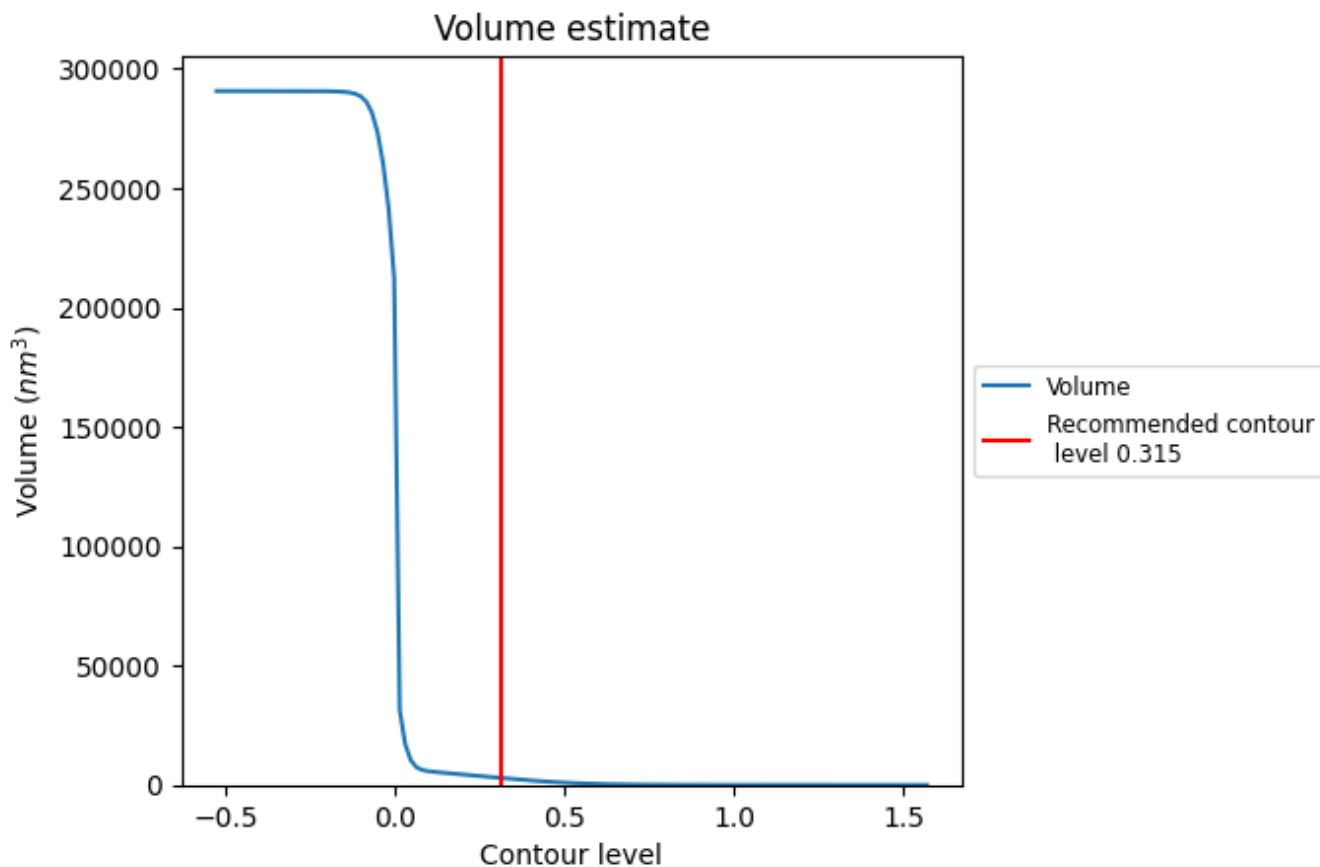
This section contains the results of statistical analysis of the map.

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.

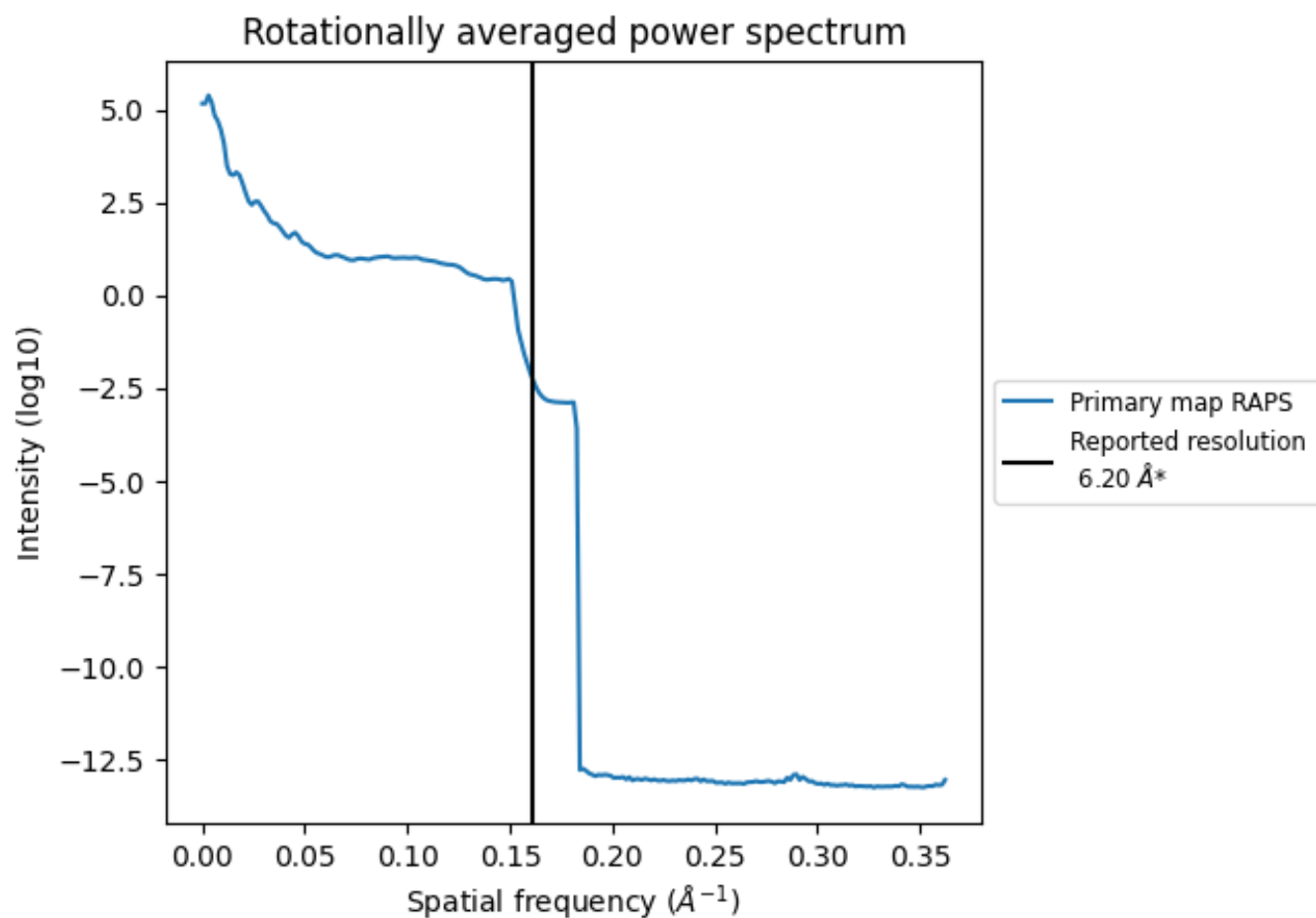
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2912 nm^3 ; this corresponds to an approximate mass of 2630 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](#)



*Reported resolution corresponds to spatial frequency of 0.161 Å⁻¹

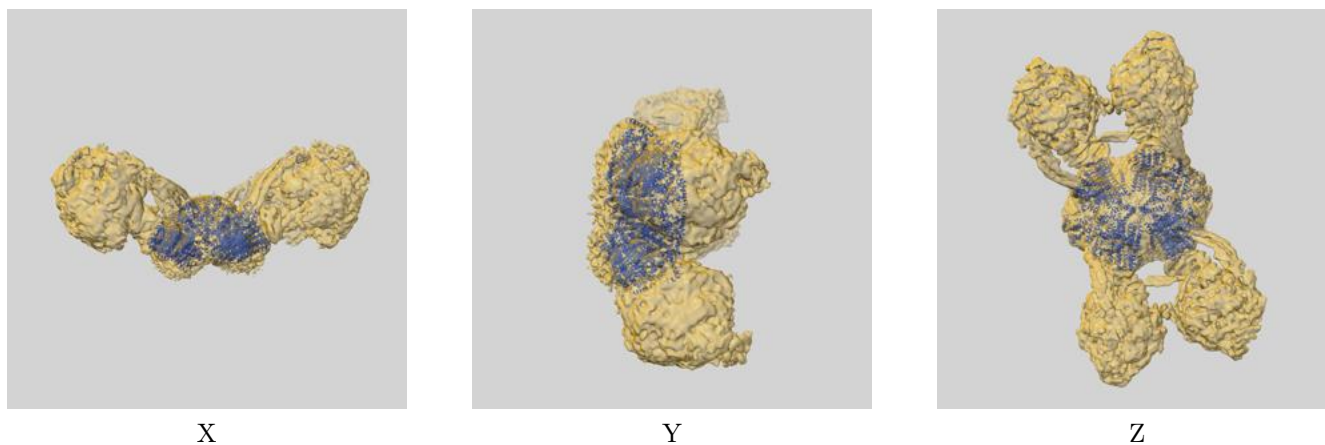
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

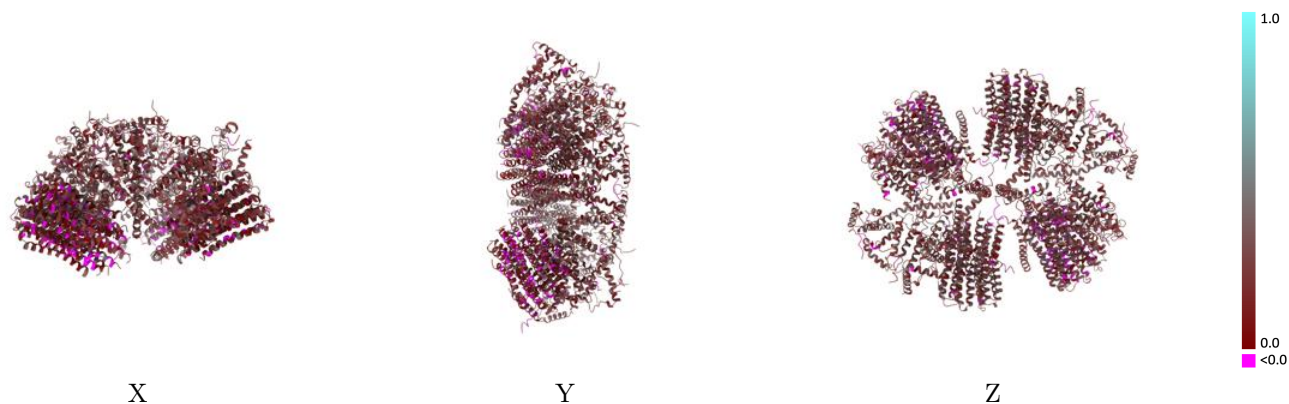
This section contains information regarding the fit between EMDB map EMD-0667 and PDB model 6ZNA. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



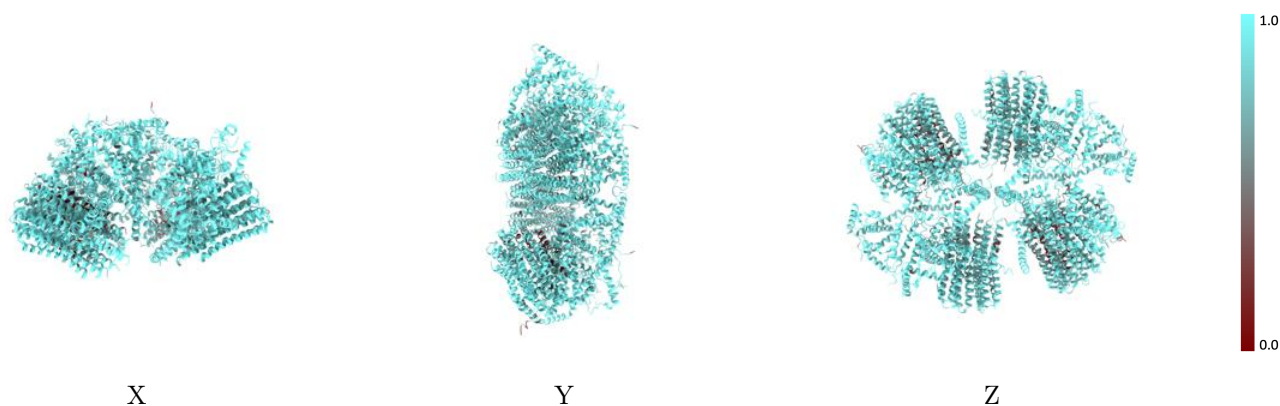
The images above show the 3D surface view of the map at the recommended contour level 0.315 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



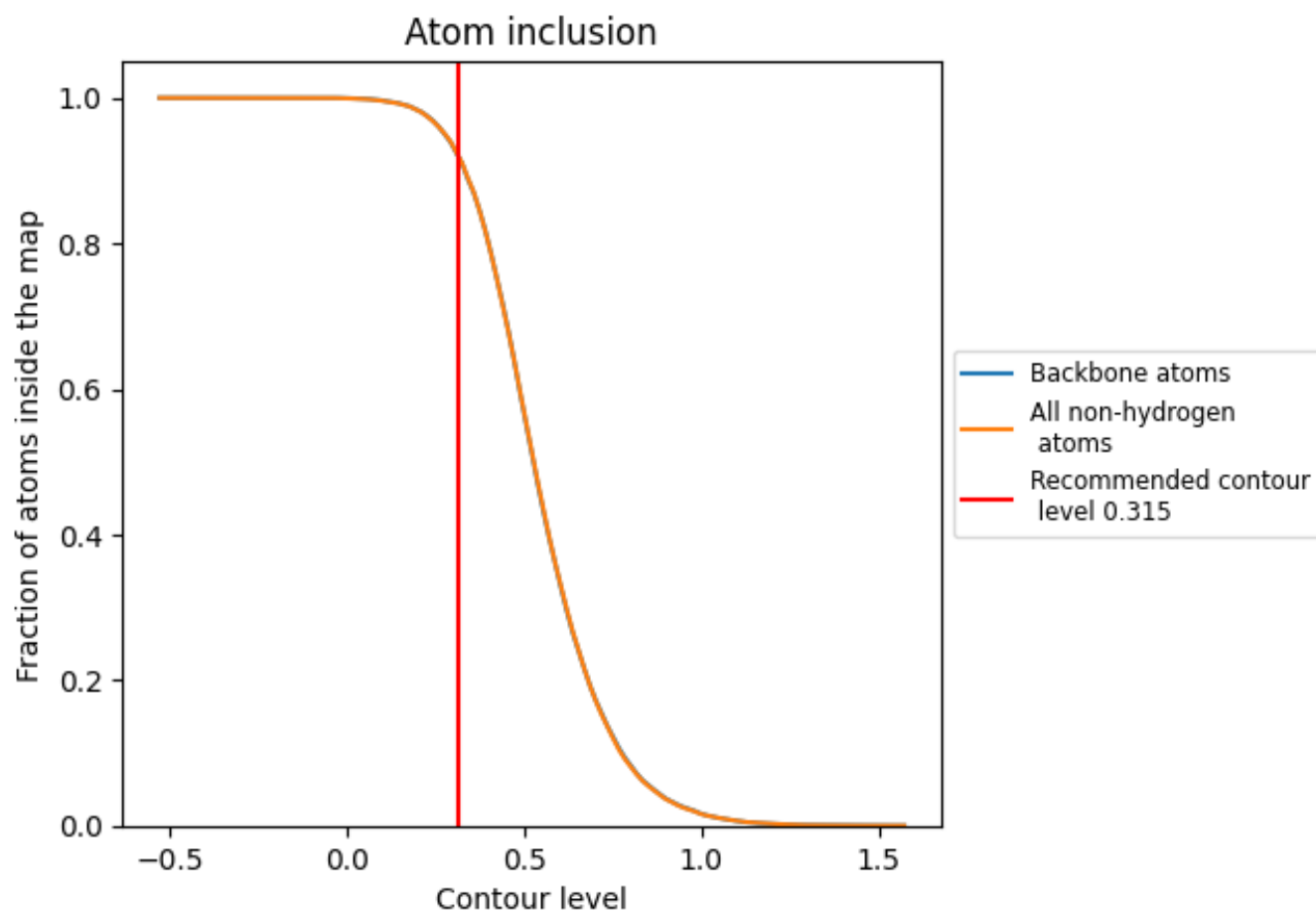
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.315).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.315) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9193	 0.2030
8	 0.9471	 0.2740
A8	 0.9412	 0.2510
AK	 0.9725	 0.1200
AL	 0.9176	 0.1390
AM	 0.8747	 0.1610
AN	 0.6703	 0.1170
AO	 0.6623	 0.0750
AP	 0.8886	 0.1930
AQ	 0.9276	 0.1420
AR	 0.9643	 0.1600
Aa	 0.9493	 0.2510
Ab	 0.9522	 0.2540
Ad	 0.9515	 0.2260
Ae	 0.9574	 0.2560
Af	 0.8675	 0.2040
Ag	 0.9761	 0.2370
Aj	 0.9198	 0.2210
Ak	 0.8012	 0.1840
B8	 0.9529	 0.2720
BK	 0.9861	 0.2150
BL	 0.9505	 0.2360
BM	 0.8736	 0.2060
BN	 0.8736	 0.2100
BO	 0.9276	 0.2330
BP	 0.9258	 0.2190
BQ	 0.9478	 0.1680
BR	 0.9777	 0.1690
Ba	 0.9656	 0.2570
Bb	 0.9717	 0.2420
Bd	 0.9636	 0.2490
Be	 0.9504	 0.2410
Bf	 0.9036	 0.2030
Bg	 0.9699	 0.2440
Bj	 0.9578	 0.2430



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Chain	Atom inclusion	Q-score
Bk	 0.8889	 0.1740
C8	 0.9588	 0.2500
CK	 0.9560	 0.0900
CL	 0.8654	 0.0840
CM	 0.8858	 0.1860
CN	 0.7363	 0.1420
CO	 0.7308	 0.1020
CP	 0.9109	 0.1800
CQ	 0.9109	 0.1080
CR	 0.9533	 0.1370
Ca	 0.9321	 0.2420
Cb	 0.9543	 0.2320
Cd	 0.9818	 0.2060
Ce	 0.9433	 0.2460
Cf	 0.8494	 0.2020
Cg	 0.9631	 0.2300
Cj	 0.9198	 0.2230
Ck	 0.7544	 0.1610
K	 0.9777	 0.1590
L	 0.9694	 0.2060
M	 0.9423	 0.2260
N	 0.8654	 0.1900
O	 0.8736	 0.1990
P	 0.9331	 0.2340
Q	 0.9368	 0.2150
R	 0.9313	 0.1450
a	 0.9584	 0.2490
b	 0.9587	 0.2400
d	 0.9697	 0.2580
e	 0.9504	 0.2410
f	 0.8936	 0.2010
g	 0.9781	 0.2340
j	 0.9662	 0.2350
k	 0.8889	 0.1660