



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 09:16 PM UTC

PDB ID : 8IC4 / pdb_00008ic4
EMDB ID : EMD-35354
Title : Respiratory complex Membrane domain of CI, focus-refined of type I, PERK
-/- mouse under cold temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-10
Resolution : 3.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

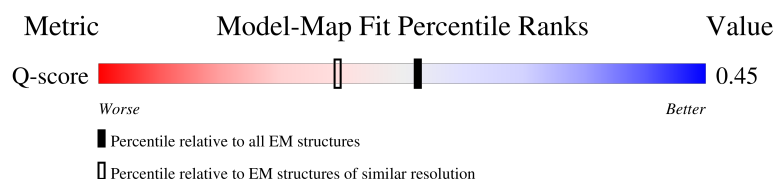
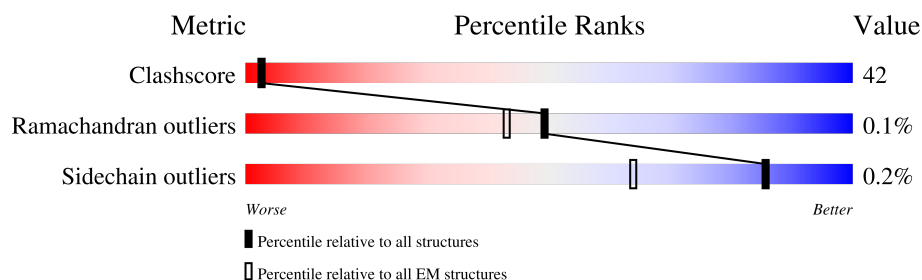
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



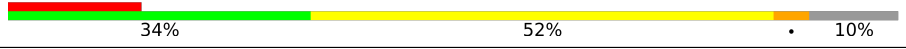
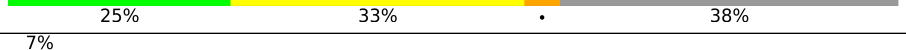
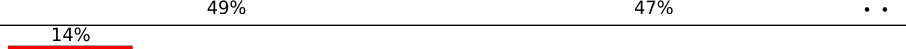
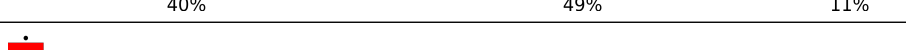
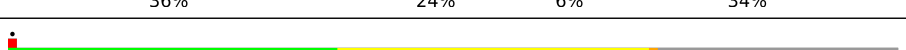
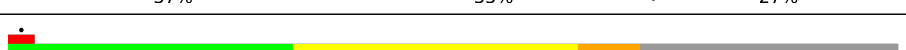
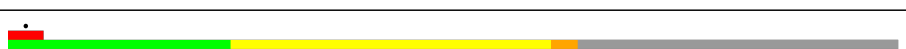
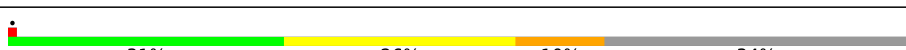
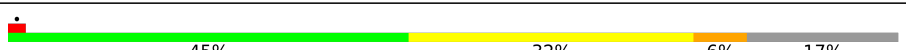
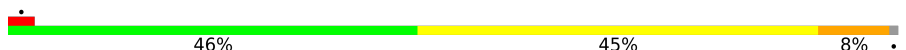
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	463	 5% 91%
2	J	172	 28% 30% 58% 10%
3	K	98	 7% 44% 52%
4	L	607	 34% 56% 10%

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Mol	Chain	Length	Quality of chain
5	M	459	
6	N	345	
7	O	355	
8	U	156	
9	X	172	
10	Y	143	
11	c	76	
12	d	120	
13	e	106	
14	f	57	
15	g	151	
16	h	189	
17	i	128	
18	j	105	
19	k	104	
20	l	186	
21	m	129	
22	n	179	
23	o	137	
24	p	176	

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 31638 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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	42	Total	C	N	O	S	0	0
			355	231	59	64	1		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	155	Total	C	N	O	S	0	0
			1178	797	167	199	15		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	96	Total	C	N	O	S	0	0
			721	468	110	134	9		

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	606	Total	C	N	O	S	0	0
			4798	3181	746	826	45		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	459	Total	C	N	O	S	0	0
			3630	2407	567	616	40		

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	344	Total	C	N	O	S	0	0
			2694	1790	416	451	37		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	318	Total	C	N	O	S	0	0
			2588	1662	426	490	10		

- Molecule 8 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	87	Total	C	N	O	S	0	0
			700	450	103	142	5		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	X	27	Total	C	N	O	0	0
			221	146	39	36		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Y	139	Total	C	N	O	S	0	0
			1030	657	174	191	8		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	47	Total	C	N	O	S	0	0
			389	255	67	66	1		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	103	Total	C	N	O	S	0	0
			859	544	157	150	8		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	51	Total	C	N	O	S	0	0
			439	284	79	74	2		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	99	Total	C	N	O	S	0	0
			835	541	134	156	4		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	138	Total	C	N	O	S	0	0
			1162	762	194	203	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	91	Total	C	N	O	S	0	0
			765	500	131	131	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	67	Total	C	N	O	S	0	0
			574	376	95	102	1		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	69	Total	C	N	O	S	0	0
			560	370	97	91	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	155	Total	C	N	O	S	0	0
			1304	840	218	235	11		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	126	Total	C	N	O	S	0	0
			1050	676	189	185			

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	177	Total	C	N	O	S	0	0
			1534	981	275	267	11		

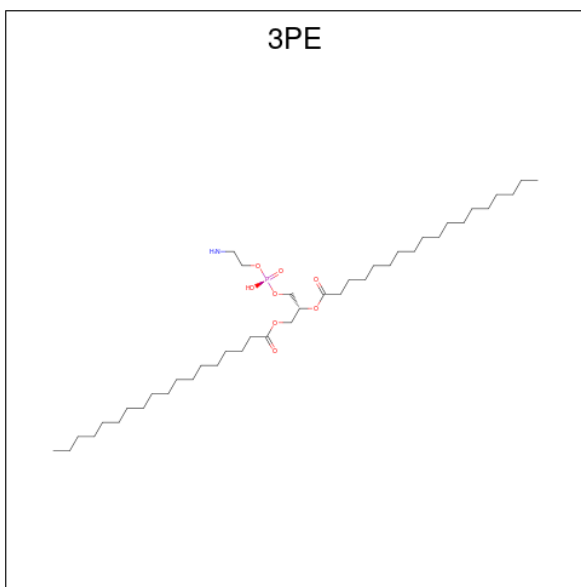
- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	121	Total	C	N	O	S	0	0
			1038	654	196	180	8		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

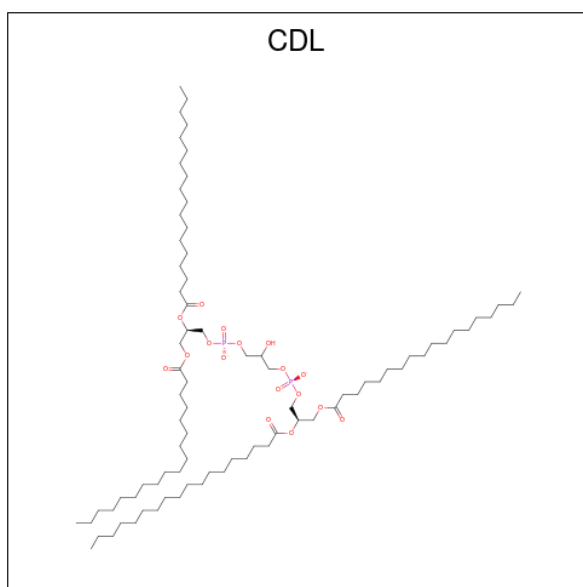
Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	167	Total	C	N	O	S	0	0
			1415	891	254	262	8		

- Molecule 25 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
25	D	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	J	1	Total	C	N	O	P	0
			46	36	1	8	1	
25	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
25	L	1	Total	C	N	O	P	0
			44	34	1	8	1	
25	M	1	Total	C	N	O	P	0
			37	27	1	8	1	
25	M	1	Total	C	N	O	P	0
			49	39	1	8	1	
25	i	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	m	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
26	L	1	Total	C	O	P	0
			73	54	17	2	
26	M	1	Total	C	O	P	0
			82	63	17	2	
26	Y	1	Total	C	O	P	0
			71	52	17	2	
26	d	1	Total	C	O	P	0
			65	46	17	2	
26	h	1	Total	C	O	P	0
			68	49	17	2	

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
27	L	1	Total	Zn	0
			1	1	

- Molecule 28 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltCon
28	O	1	Total	C	N	O	P	0
			27	10	5	10	2	

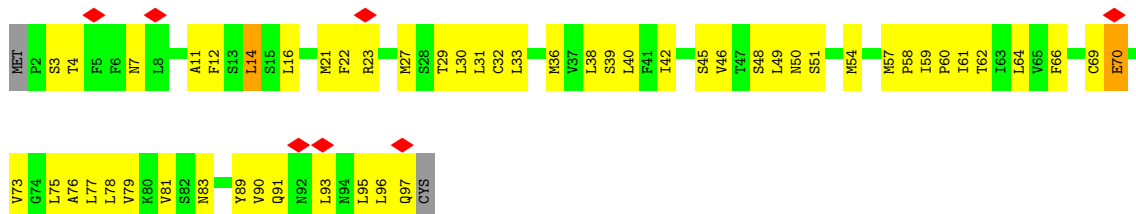
- Molecule 29 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS) (labeled as "Ligand of Interest" by depositor).



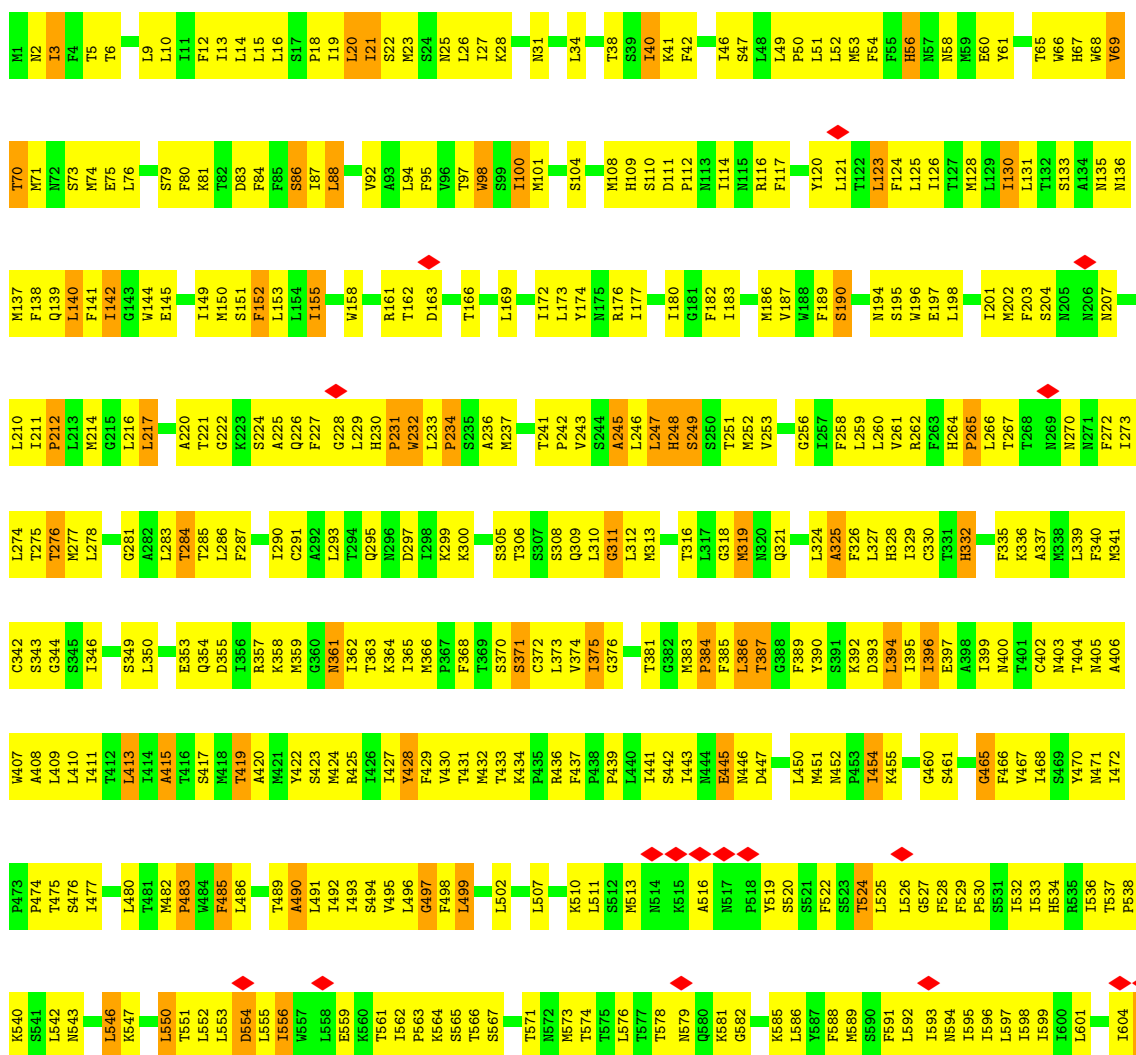
Mol	Chain	Residues	Atoms						AltCon
29	n	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	



• Molecule 3: NADH-ubiquinone oxidoreductase chain 4L

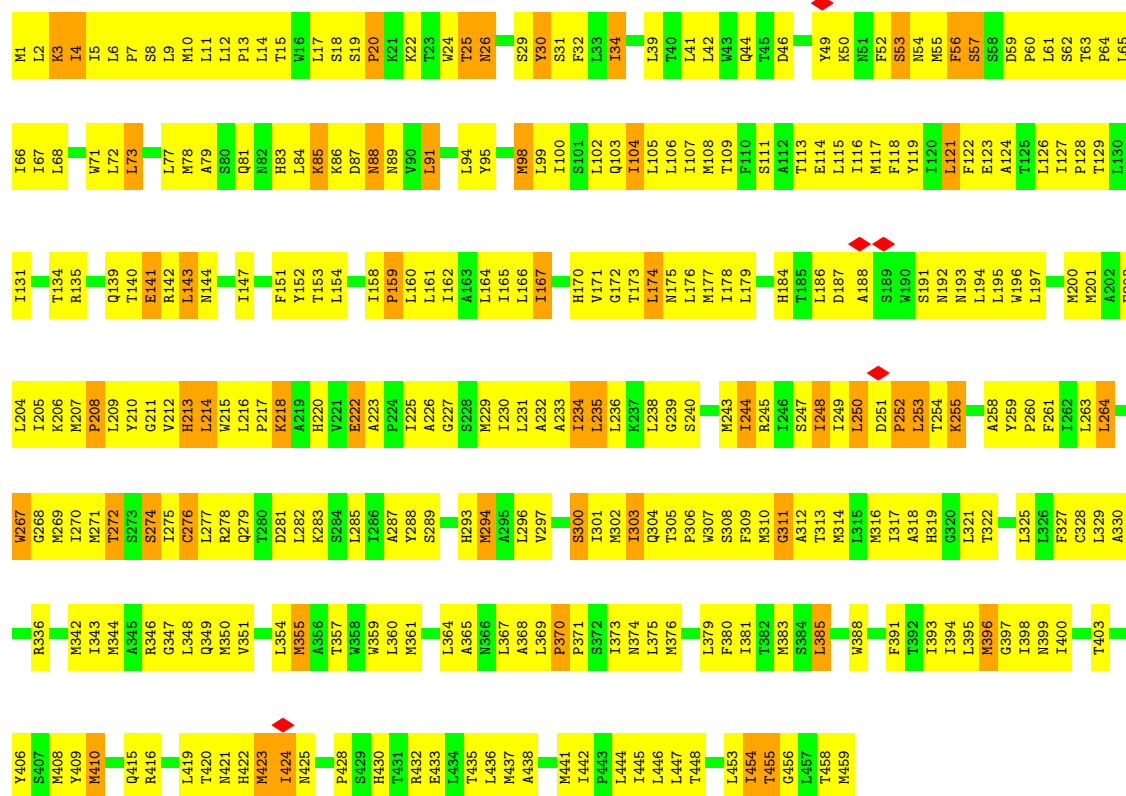
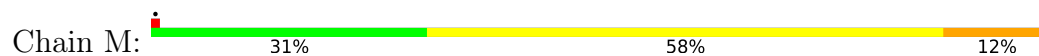


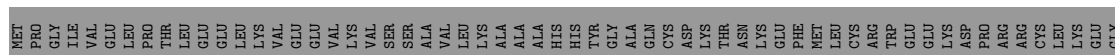
• Molecule 4: NADH-ubiquinone oxidoreductase chain 5





• Molecule 5: NADH-ubiquinone oxidoreductase chain 4





LYS LEU VAL GLY SER CYS ALA LEU ASN PHE ARG GLN ILE LYS SER HIS CYS ALA GLU PRO PHE THR GLU TVR TRP THR CYS ASP TVR SER ASN MET GLN LEU PHE ARG HIS CYS ARG GLN GLN LYS PHE ASP GLN CYS VAL LEU ASP LYS LEU TRP VAL ARG PRO

ASP LEU GLN VAL SER LYS VAL THR VAL LYS THR ASP ARG PRO LEU PRO GLU ASN PRO TVR HIS SER ARG A146 A147 P148 V153 I154 E155 L158 K159 P160 A161 K162 H163 G164 T165 R166 F167 F168 W170 T171 V172

- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y: 25% 50% 47% ..

MET ALA MET VAL K5 R6 F7 F8 E9 S10 Y11 H12 E13 P14 P15 D16 G17 T18 Q19 C20 H21 R22 K23 T24 Y25 I26 A29 L30 I37 G38 S39 A40 Y41 L45 M46 P47 A48 D49 S50 T51 L52 E53 A54 R57 V58 G59 R60 F63 T64 A65 I68 M71 F72

- Molecule 11: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c: 12% 25% 33% 38%

MET ALA PRO SER VAL LEU ARG SER PHE ARG LEU LEU ALA PRO ARG ALA LEU PRO LEU PRO CYS SER THR ARG LYS F29 Y30 V31 R32 E33 P34 V35 N36 A37 K38 P39 M40 N41 A43 V44 G45 L46 S47 A50 W55 Q60 T61 H62 M63 E64 V66 Y69 K70 R71 N73 G74 L75 G11J

- Molecule 12: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d: 7% 48% 49%

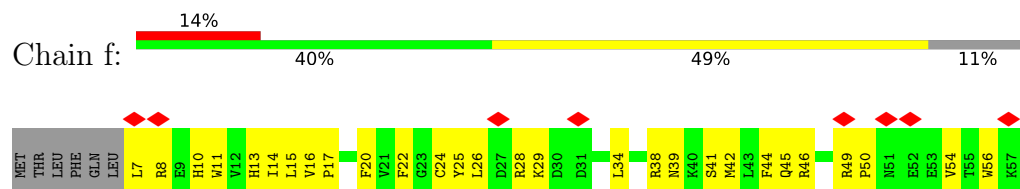
M1 M2 N3 G4 R5 P6 G7 H8 E9 P10 L11 K12 F13 L14 P15 D16 E17 A18 R19 S20 L21 P22 P23 P24 K25 L26 N27 D28 P29 R30 L37 Y39 L43 M44 D45 N46 M47 L48 R49 M50 R51 P52 V53 M54 G57 L58 H59 R60 Q61 L62 F63 L64 T65 T66 G72 Y73 F74 K77 R78 Q79 R80 Y81 L82 D87 H88 R89 R90 G92 Y93 D100 F101 P102 E103 A104 E105 Y109 I112 L113 E114 H117 P118 V119 R120

- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

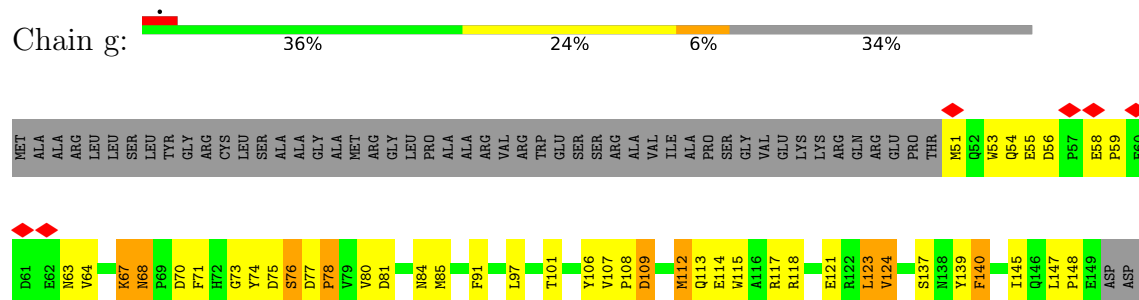
Chain e: 11% 49% 47%

MET F2 F3 I6 K9 L14 D15 R16 H17 F18 M19 F20 S22 A30 A31 R32 C33 H34 K38 E39 W40 I41 E42 C43 A44 H45 C46 G47 C49 T50 R51 A52 E64 E65 C66 L67 L68 R69 Y70 K71 T72 M73 R74 R75 M76 K81 Q82 R83 E84 K85 L86 M87 K88 E89 G90 K91 Y92 T93 F94 P95 H97 H98 S99 G100 R101 E102 E103 P104 ARG PRO

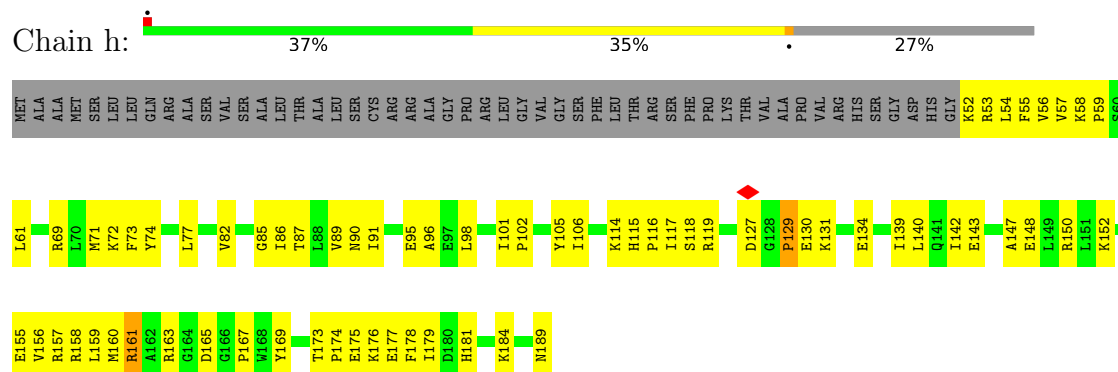
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



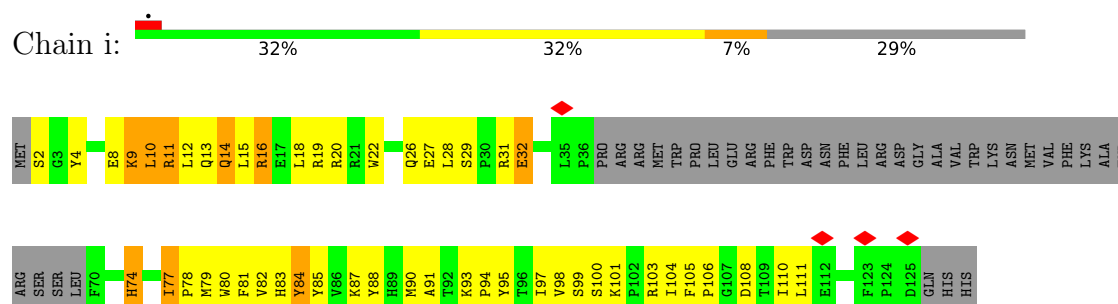
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



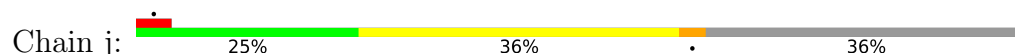
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

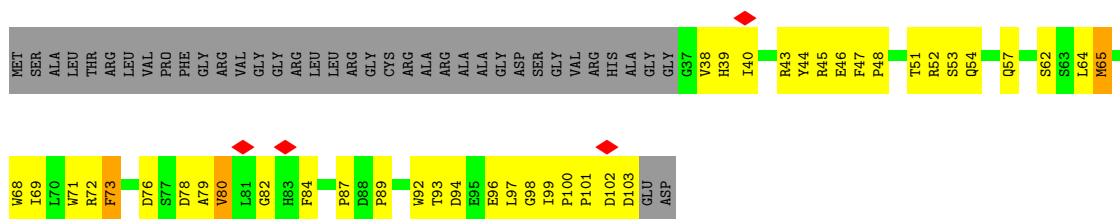


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

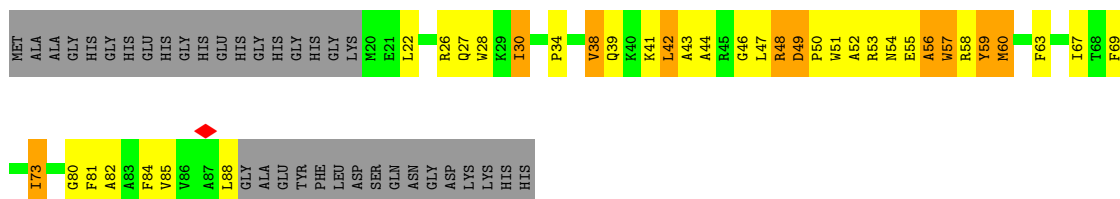
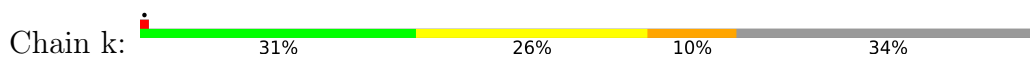


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

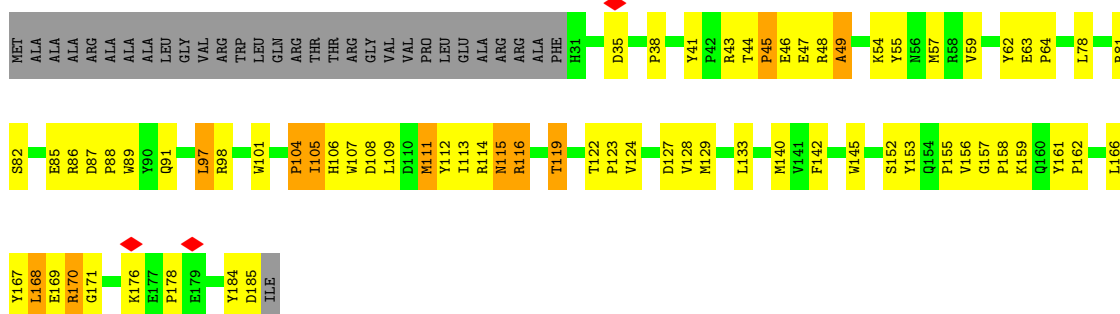




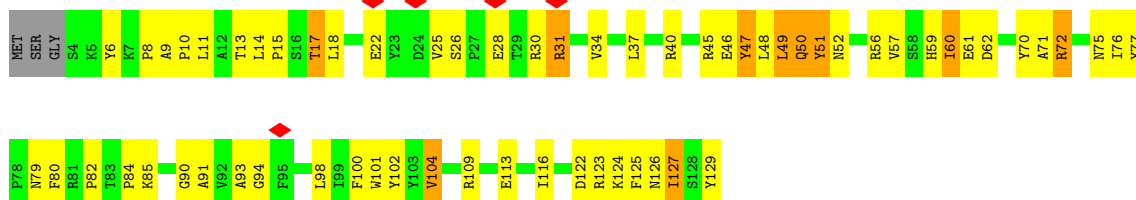
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



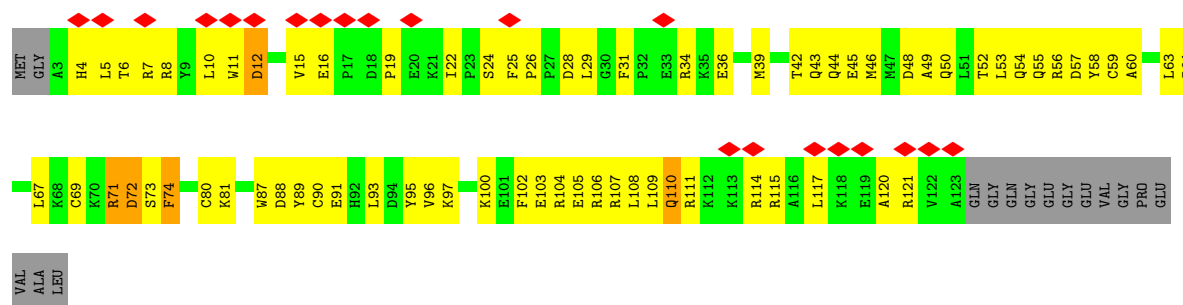
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



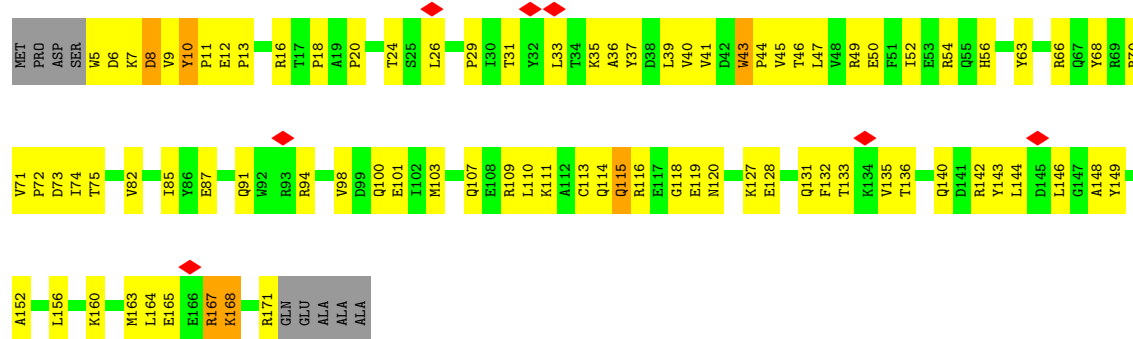
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45095	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 ($e^-/\text{\AA}^2$)	50.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.147	Depositor
Minimum map value	-1.164	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.45	Depositor
Map size ($\text{\AA}$)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EH2, CDL, ADP, 3PE

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	D	0.62	0/370	1.06	3/506 (0.6%)
2	J	0.55	1/1205 (0.1%)	0.92	6/1633 (0.4%)
3	K	0.85	0/732	1.44	11/994 (1.1%)
4	L	0.97	6/4921 (0.1%)	1.56	108/6696 (1.6%)
5	M	1.01	7/3717 (0.2%)	1.56	85/5062 (1.7%)
6	N	1.00	3/2756 (0.1%)	1.43	50/3751 (1.3%)
7	O	0.86	6/2655 (0.2%)	1.21	27/3601 (0.7%)
8	U	0.96	1/712 (0.1%)	1.35	12/962 (1.2%)
9	X	0.81	0/230	1.16	1/313 (0.3%)
10	Y	0.85	0/1054	0.96	3/1429 (0.2%)
11	c	0.69	0/400	1.24	8/544 (1.5%)
12	d	0.88	1/1028 (0.1%)	1.01	8/1387 (0.6%)
13	e	0.77	1/881 (0.1%)	1.01	4/1173 (0.3%)
14	f	0.59	0/451	0.75	0/607
15	g	0.87	3/863 (0.3%)	1.36	18/1175 (1.5%)
16	h	0.76	0/1197	1.22	7/1621 (0.4%)
17	i	0.85	0/790	1.38	16/1074 (1.5%)
18	j	0.75	0/599	1.23	8/820 (1.0%)
19	k	1.05	1/578 (0.2%)	1.56	18/782 (2.3%)
20	l	1.02	4/1359 (0.3%)	1.25	9/1855 (0.5%)
21	m	0.82	1/1079 (0.1%)	1.21	17/1463 (1.2%)
22	n	0.93	1/1589 (0.1%)	1.22	17/2152 (0.8%)
23	o	0.78	0/1063	1.14	7/1427 (0.5%)
24	p	0.72	1/1448 (0.1%)	1.01	13/1957 (0.7%)
All	All	0.89	37/31677 (0.1%)	1.32	456/42984 (1.1%)

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	265	PRO	N-CD	13.82	1.67	1.47
19	k	50	PRO	N-CD	-13.63	1.28	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	255	PRO	N-CD	-13.45	1.28	1.47
13	e	91	LYS	C-N	12.91	1.51	1.33
7	O	315	PRO	N-CD	-12.15	1.30	1.47

The worst 5 of 456 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	370	PRO	N-CA-C	14.56	128.46	110.70
6	N	255	PRO	N-CA-C	14.41	128.28	110.70
7	O	118	TYR	N-CA-C	13.89	125.94	111.07
5	M	424	ILE	N-CA-C	-11.65	94.03	109.30
5	M	104	ILE	N-CA-C	-11.57	99.08	110.30

There are no chirality outliers.

There are no planarity outliers.

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	D	355	0	330	43	0
2	J	1178	0	1204	158	0
3	K	721	0	753	83	0
4	L	4798	0	4986	584	0
5	M	3630	0	3854	500	0
6	N	2694	0	2896	345	0
7	O	2588	0	2539	246	0
8	U	700	0	691	70	0
9	X	221	0	215	29	0
10	Y	1030	0	1015	80	0
11	c	389	0	385	34	0
12	d	996	0	1001	71	0
13	e	859	0	849	87	0
14	f	439	0	433	35	0
15	g	835	0	772	67	0
16	h	1162	0	1163	119	0
17	i	765	0	769	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	j	574	0	522	91	0
19	k	560	0	560	47	0
20	l	1304	0	1193	95	0
21	m	1050	0	1061	114	0
22	n	1534	0	1463	135	0
23	o	1038	0	1030	105	0
24	p	1415	0	1385	106	0
25	D	38	0	50	6	0
25	J	46	0	66	1	0
25	L	133	0	194	18	0
25	M	86	0	123	15	0
25	i	40	0	54	11	0
25	m	41	0	56	9	0
26	L	73	0	90	12	0
26	M	82	0	114	12	0
26	Y	71	0	86	5	0
26	d	65	0	74	8	0
26	h	68	0	83	13	0
27	L	1	0	0	0	0
28	O	27	0	12	3	0
29	n	32	0	0	1	0
All	All	31638	0	32071	2683	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 42.

The worst 5 of 2683 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)
4:L:141:PHE:CE2	5:M:370:PRO:HG3	1.75	1.21
3:K:66:PHE:HZ	6:N:35:PHE:CZ	1.56	1.21
8:U:90:TYR:CE2	8:U:92:LYS:HB2	1.76	1.20
4:L:437:PHE:CE1	4:L:441:ILE:HG12	1.77	1.19
4:L:358:LYS:HG3	22:n:80:TYR:CZ	1.79	1.17

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	40/463 (9%)	36 (90%)	4 (10%)	0	100	100
2	J	149/172 (87%)	136 (91%)	13 (9%)	0	100	100
3	K	94/98 (96%)	92 (98%)	2 (2%)	0	100	100
4	L	604/607 (100%)	576 (95%)	28 (5%)	0	100	100
5	M	457/459 (100%)	439 (96%)	18 (4%)	0	100	100
6	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	36	68
7	O	316/355 (89%)	302 (96%)	14 (4%)	0	100	100
8	U	85/156 (54%)	83 (98%)	2 (2%)	0	100	100
9	X	25/172 (14%)	23 (92%)	2 (8%)	0	100	100
10	Y	137/143 (96%)	133 (97%)	4 (3%)	0	100	100
11	c	45/76 (59%)	44 (98%)	1 (2%)	0	100	100
12	d	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
13	e	101/106 (95%)	95 (94%)	6 (6%)	0	100	100
14	f	49/57 (86%)	49 (100%)	0	0	100	100
15	g	97/151 (64%)	91 (94%)	6 (6%)	0	100	100
16	h	136/189 (72%)	130 (96%)	6 (4%)	0	100	100
17	i	87/128 (68%)	80 (92%)	7 (8%)	0	100	100
18	j	65/105 (62%)	61 (94%)	4 (6%)	0	100	100
19	k	67/104 (64%)	64 (96%)	3 (4%)	0	100	100
20	l	153/186 (82%)	141 (92%)	12 (8%)	0	100	100
21	m	124/129 (96%)	117 (94%)	7 (6%)	0	100	100
22	n	175/179 (98%)	165 (94%)	9 (5%)	1 (1%)	21	56
23	o	119/137 (87%)	116 (98%)	3 (2%)	0	100	100
24	p	165/176 (94%)	148 (90%)	17 (10%)	0	100	100
All	All	3750/4813 (78%)	3569 (95%)	179 (5%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	N	109	ALA
22	n	156	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	37/395 (9%)	37 (100%)	0	100	100
2	J	124/138 (90%)	123 (99%)	1 (1%)	73	82
3	K	86/88 (98%)	86 (100%)	0	100	100
4	L	549/550 (100%)	547 (100%)	2 (0%)	84	86
5	M	415/415 (100%)	414 (100%)	1 (0%)	87	89
6	N	307/308 (100%)	306 (100%)	1 (0%)	86	88
7	O	282/309 (91%)	282 (100%)	0	100	100
8	U	80/135 (59%)	80 (100%)	0	100	100
9	X	23/154 (15%)	23 (100%)	0	100	100
10	Y	104/107 (97%)	104 (100%)	0	100	100
11	c	41/67 (61%)	41 (100%)	0	100	100
12	d	107/107 (100%)	107 (100%)	0	100	100
13	e	91/94 (97%)	91 (100%)	0	100	100
14	f	47/53 (89%)	47 (100%)	0	100	100
15	g	90/129 (70%)	90 (100%)	0	100	100
16	h	123/162 (76%)	123 (100%)	0	100	100
17	i	86/120 (72%)	86 (100%)	0	100	100
18	j	62/87 (71%)	62 (100%)	0	100	100
19	k	54/78 (69%)	54 (100%)	0	100	100
20	l	140/161 (87%)	140 (100%)	0	100	100
21	m	112/114 (98%)	111 (99%)	1 (1%)	70	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	n	162/164 (99%)	161 (99%)	1 (1%)	78	84
23	o	111/121 (92%)	111 (100%)	0	100	100
24	p	152/158 (96%)	152 (100%)	0	100	100
All	All	3385/4214 (80%)	3378 (100%)	7 (0%)	85	89

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	M	218	LYS
6	N	159	ILE
22	n	98	LYS
21	m	49	LEU
4	L	69	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
15	g	113	GLN
22	n	13	GLN
16	h	170	GLN
20	l	83	GLN
22	n	74	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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
26	CDL	Y	201	-	70,70,99	1.08	4 (5%)	76,82,111	1.17	7 (9%)
28	ADP	O	401	-	28,29,29	1.39	5 (17%)	43,45,45	1.81	10 (23%)
25	3PE	i	201	-	39,39,50	1.04	2 (5%)	42,44,55	1.15	3 (7%)
25	3PE	L	701	-	39,39,50	1.03	2 (5%)	42,44,55	1.07	2 (4%)
25	3PE	M	501	-	36,36,50	1.09	2 (5%)	39,41,55	1.06	3 (7%)
25	3PE	L	705	-	43,43,50	0.99	2 (4%)	46,48,55	1.09	3 (6%)
25	3PE	m	201	-	40,40,50	1.02	2 (5%)	43,45,55	1.16	3 (6%)
26	CDL	d	201	-	64,64,99	1.13	4 (6%)	70,76,111	1.22	7 (10%)
26	CDL	h	201	-	67,67,99	1.10	4 (5%)	73,79,111	1.16	6 (8%)
25	3PE	J	201	-	45,45,50	0.98	2 (4%)	48,50,55	1.07	3 (6%)
26	CDL	L	703	-	72,72,99	1.06	4 (5%)	78,84,111	1.15	6 (7%)
26	CDL	M	503	-	81,81,99	1.01	4 (4%)	87,93,111	1.15	7 (8%)
29	EHZ	n	201	-	29,31,37	1.82	7 (24%)	37,41,47	1.65	5 (13%)
25	3PE	D	501	-	37,37,50	1.07	2 (5%)	40,42,55	1.09	3 (7%)
25	3PE	L	702	-	48,48,50	0.93	2 (4%)	51,53,55	1.11	3 (5%)
25	3PE	M	502	-	48,48,50	0.93	2 (4%)	51,53,55	1.15	4 (7%)

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
26	CDL	Y	201	-	-	15/81/81/110	-
28	ADP	O	401	-	-	2/16/32/32	0/3/3/3
25	3PE	i	201	-	-	9/43/43/54	-
25	3PE	L	701	-	-	10/43/43/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	3PE	M	501	-	-	10/40/40/54	-
25	3PE	L	705	-	-	13/47/47/54	-
25	3PE	m	201	-	-	10/44/44/54	-
26	CDL	d	201	-	-	27/75/75/110	-
26	CDL	h	201	-	-	19/78/78/110	-
25	3PE	J	201	-	-	13/49/49/54	-
26	CDL	L	703	-	-	20/83/83/110	-
26	CDL	M	503	-	-	24/92/92/110	-
29	EHZ	n	201	-	-	22/39/39/45	-
25	3PE	D	501	-	-	8/41/41/54	-
25	3PE	L	702	-	-	13/52/52/54	-
25	3PE	M	502	-	-	14/52/52/54	-

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	n	201	EHZ	C12-N1	5.28	1.45	1.33
29	n	201	EHZ	C15-N2	4.93	1.45	1.33
28	O	401	ADP	C5-C4	4.50	1.47	1.39
26	Y	201	CDL	OA8-CA7	4.31	1.45	1.33
25	M	501	3PE	O31-C31	4.31	1.45	1.33

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	O	401	ADP	C5-C4-N3	-5.66	118.92	126.72
29	n	201	EHZ	C8-C9-S1	5.50	120.50	113.56
26	M	503	CDL	OA6-CA5-C11	4.62	121.47	111.48
28	O	401	ADP	N3-C4-N9	4.57	134.94	127.17
26	L	703	CDL	OB6-CB5-C51	4.22	120.61	111.48

There are no chirality outliers.

5 of 229 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	D	501	3PE	C1-O11-P-O14
25	J	201	3PE	C1-O11-P-O12
25	J	201	3PE	C1-O11-P-O13
25	J	201	3PE	C1-O11-P-O14

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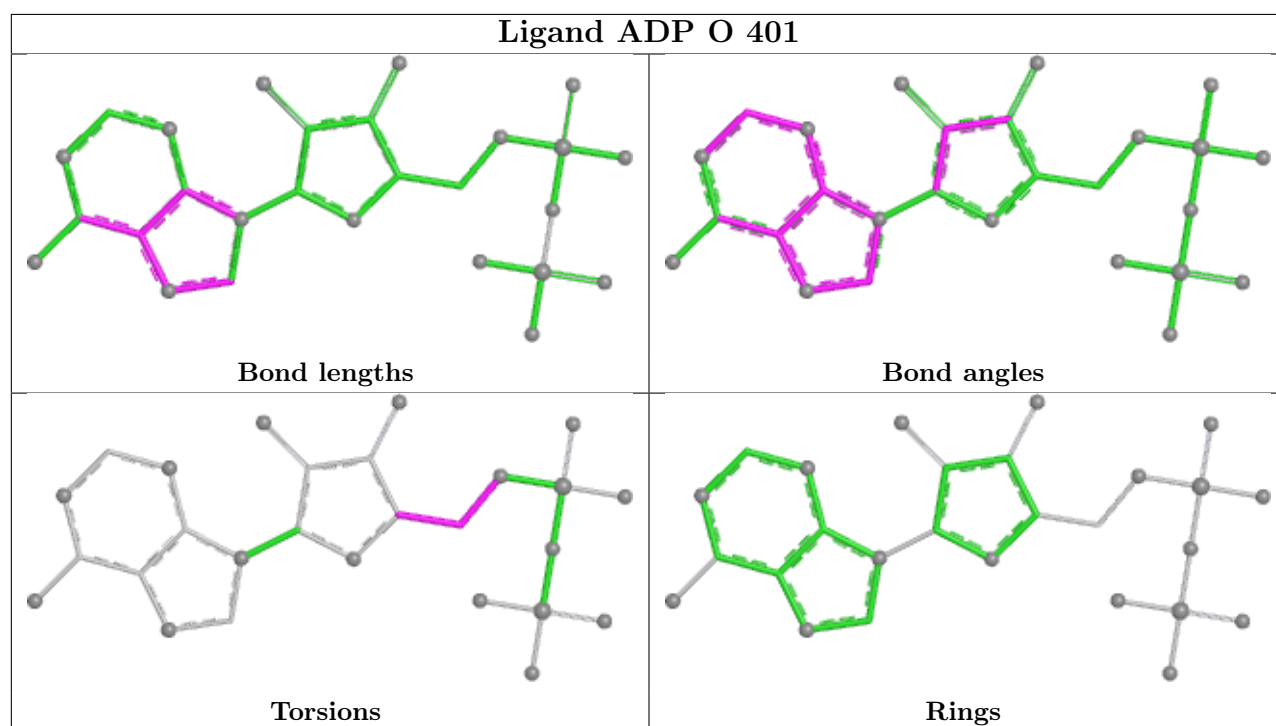
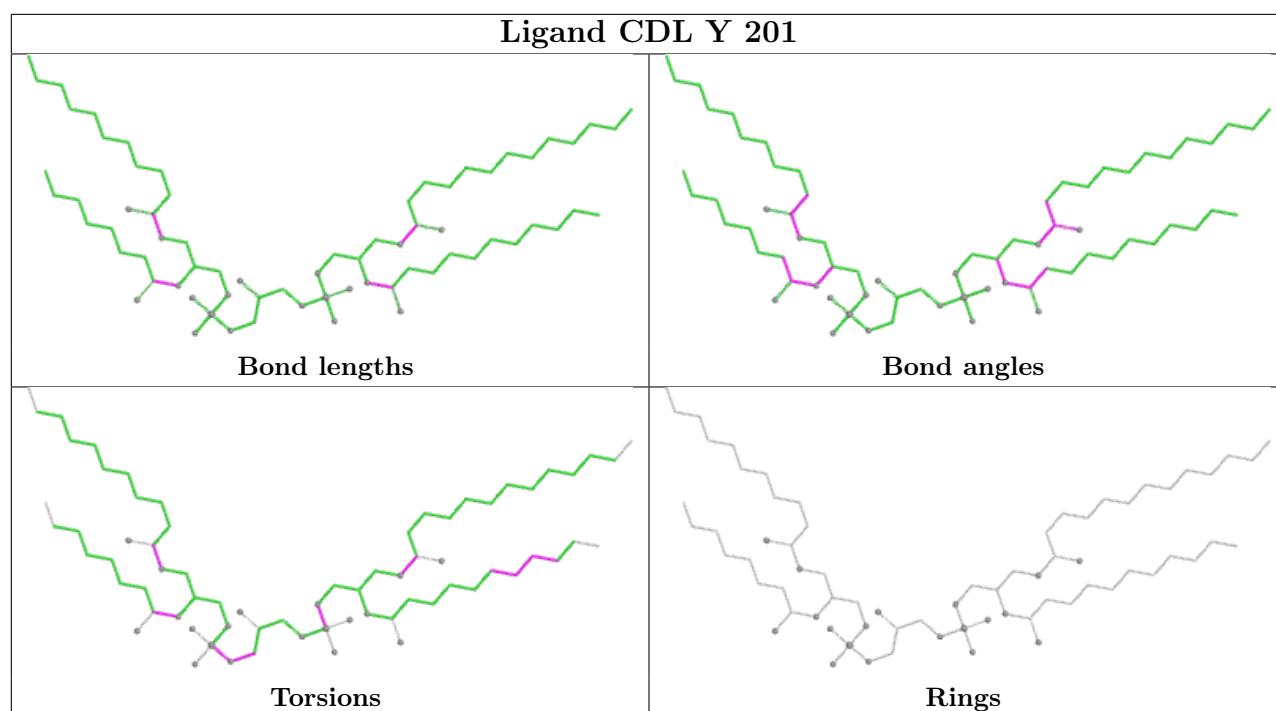
Mol	Chain	Res	Type	Atoms
25	L	701	3PE	C1-O11-P-O12

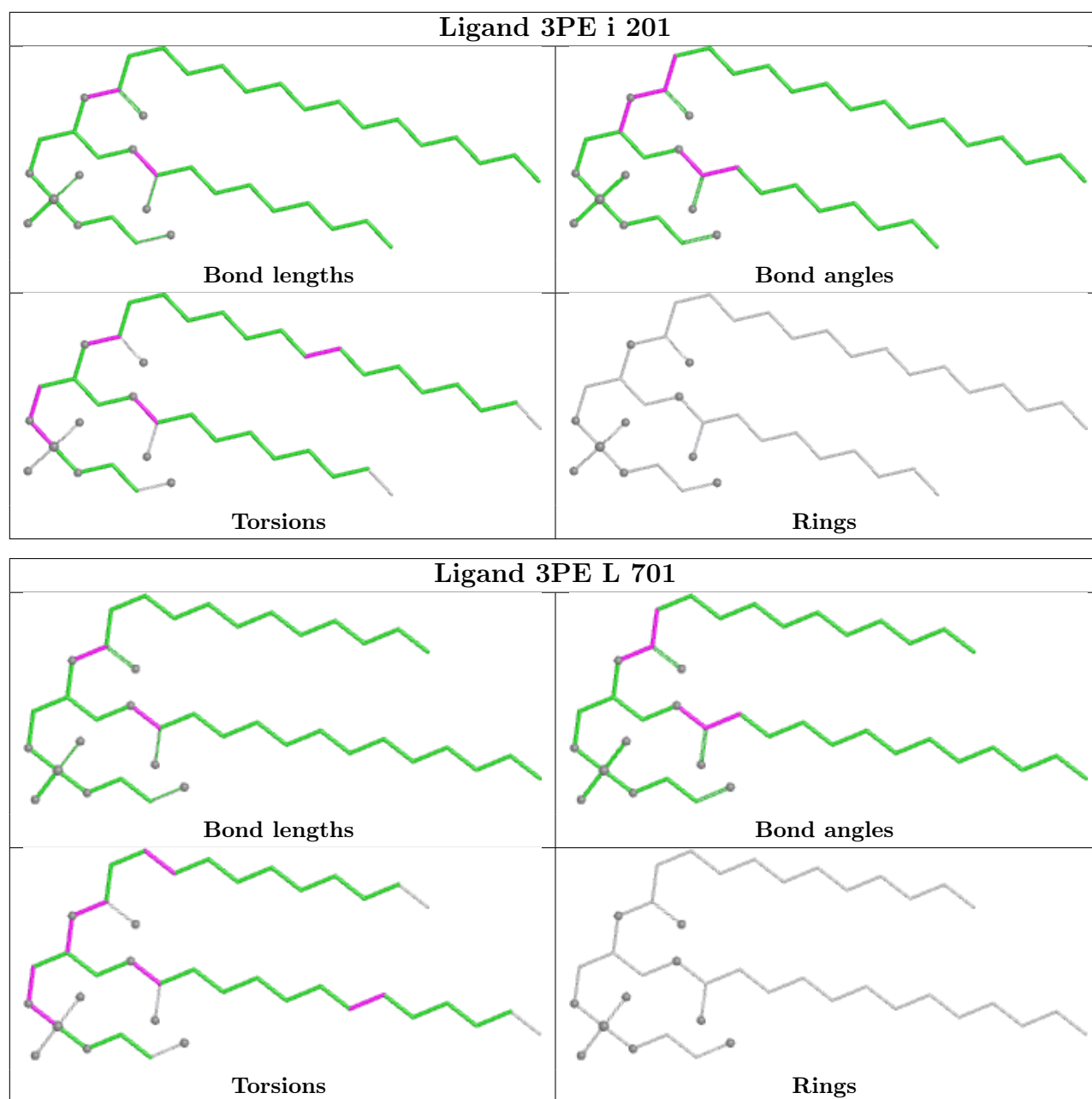
There are no ring outliers.

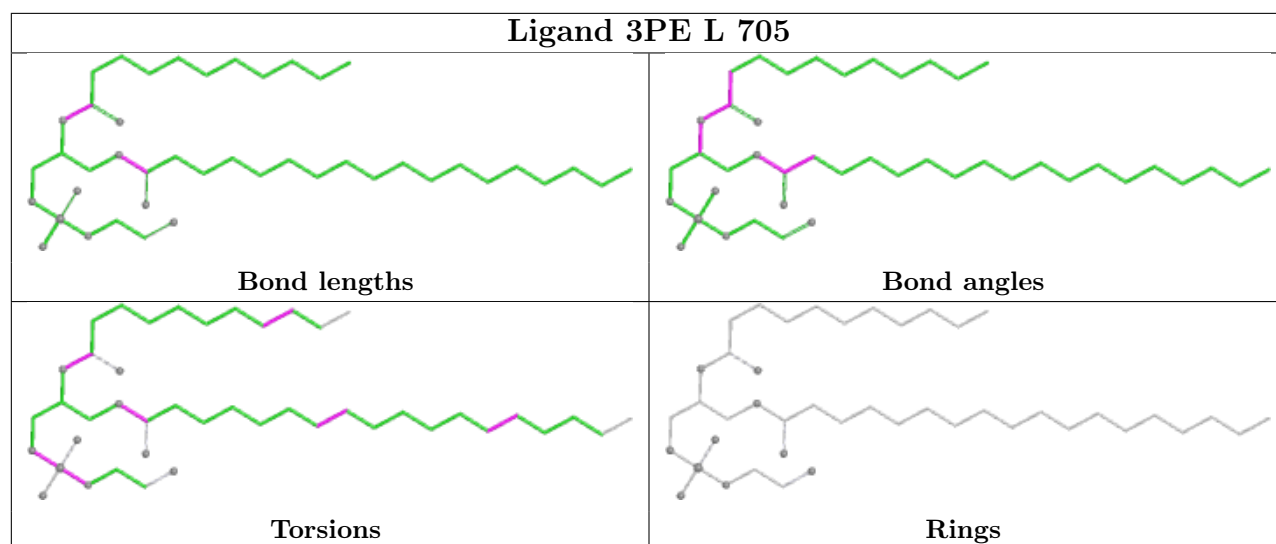
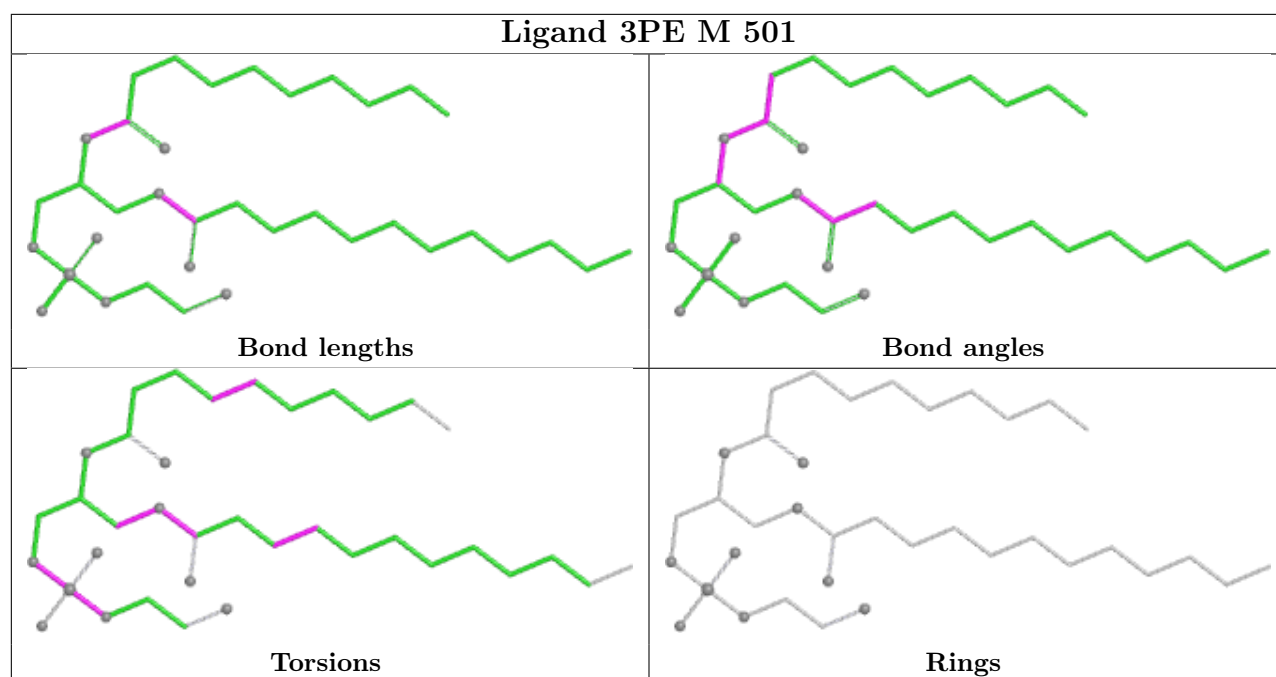
16 monomers are involved in 111 short contacts:

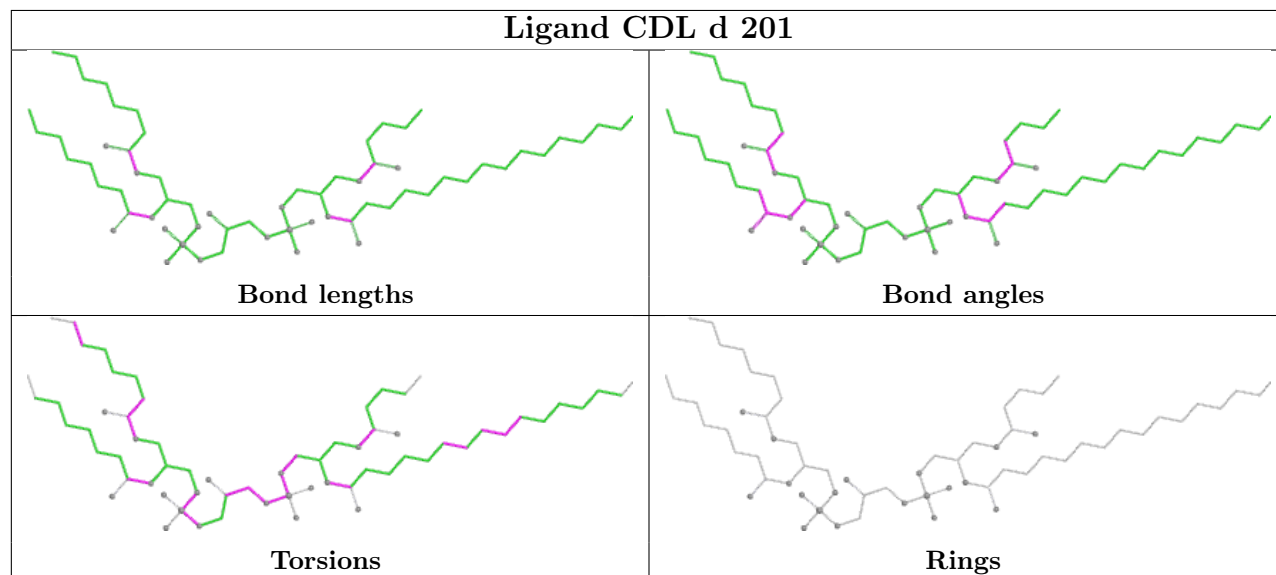
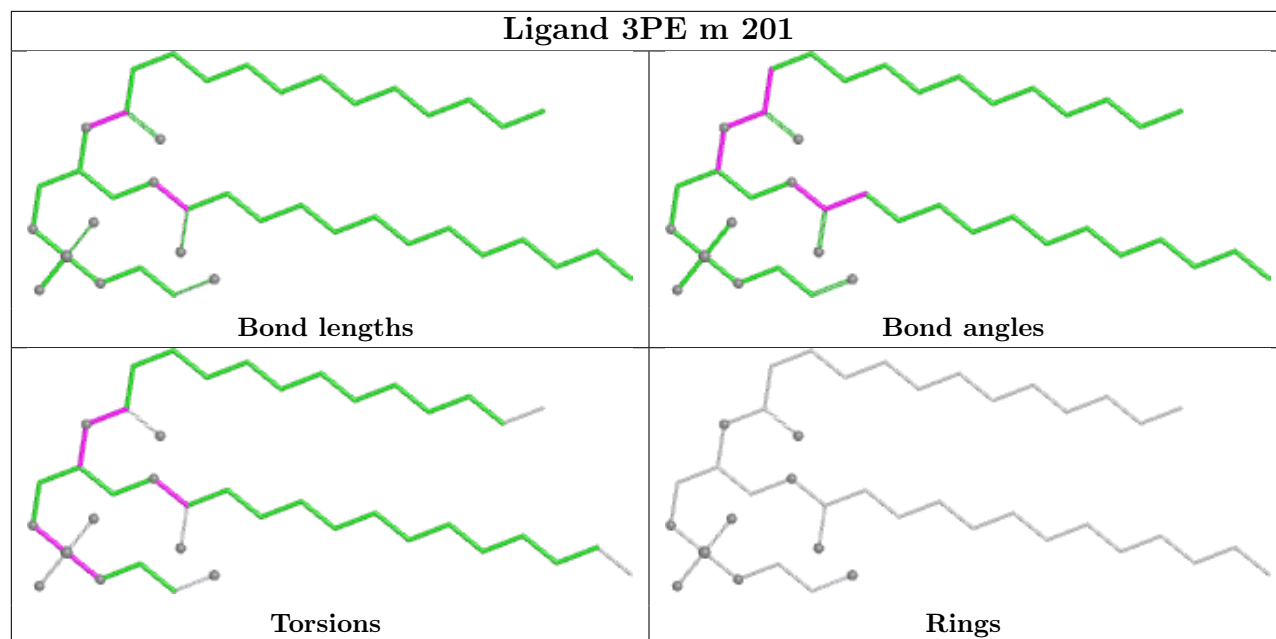
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	Y	201	CDL	5	0
28	O	401	ADP	3	0
25	i	201	3PE	11	0
25	L	701	3PE	5	0
25	M	501	3PE	10	0
25	L	705	3PE	4	0
25	m	201	3PE	9	0
26	d	201	CDL	8	0
26	h	201	CDL	13	0
25	J	201	3PE	1	0
26	L	703	CDL	12	0
26	M	503	CDL	12	0
29	n	201	EHZ	1	0
25	D	501	3PE	6	0
25	L	702	3PE	9	0
25	M	502	3PE	5	0

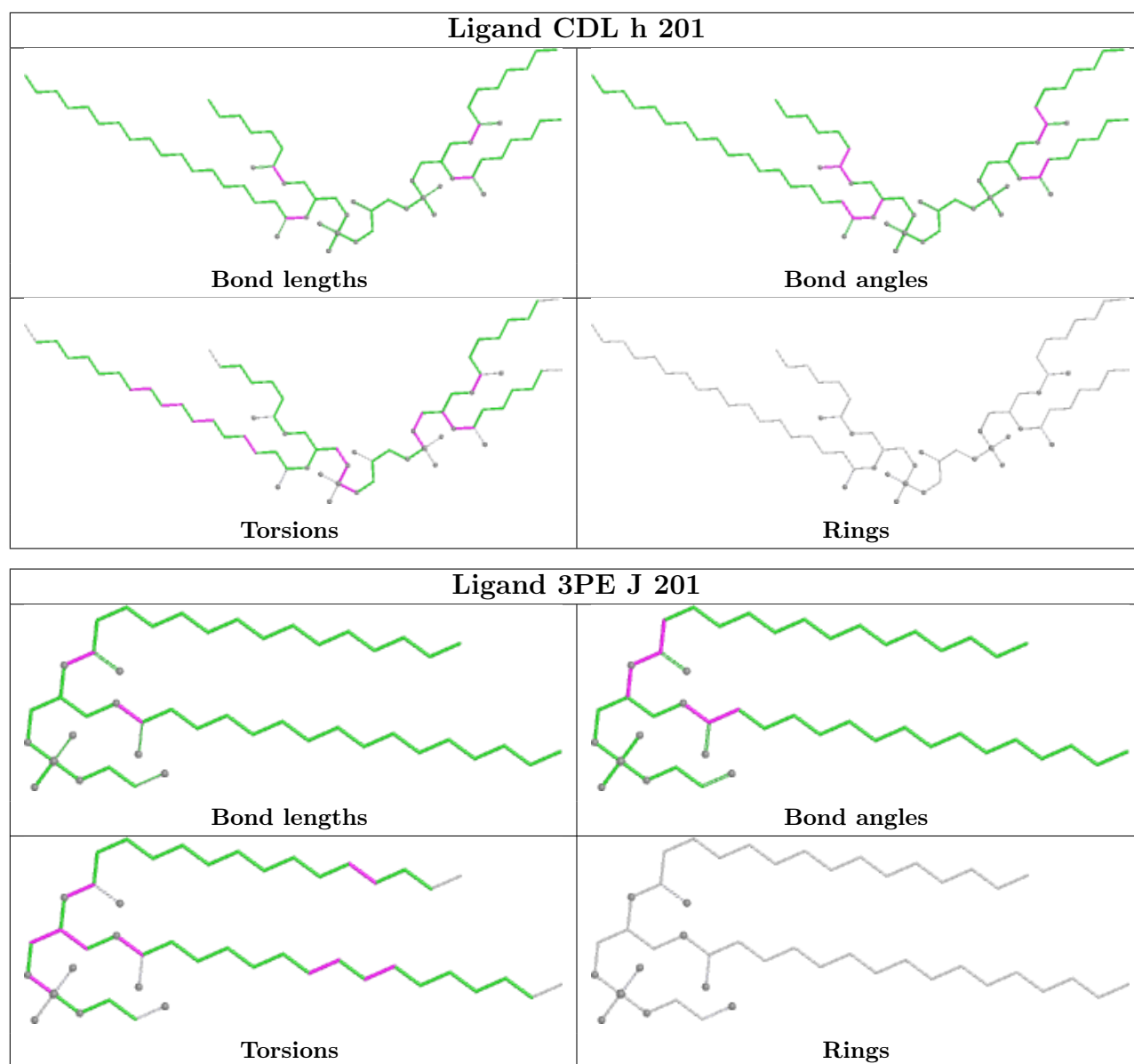
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

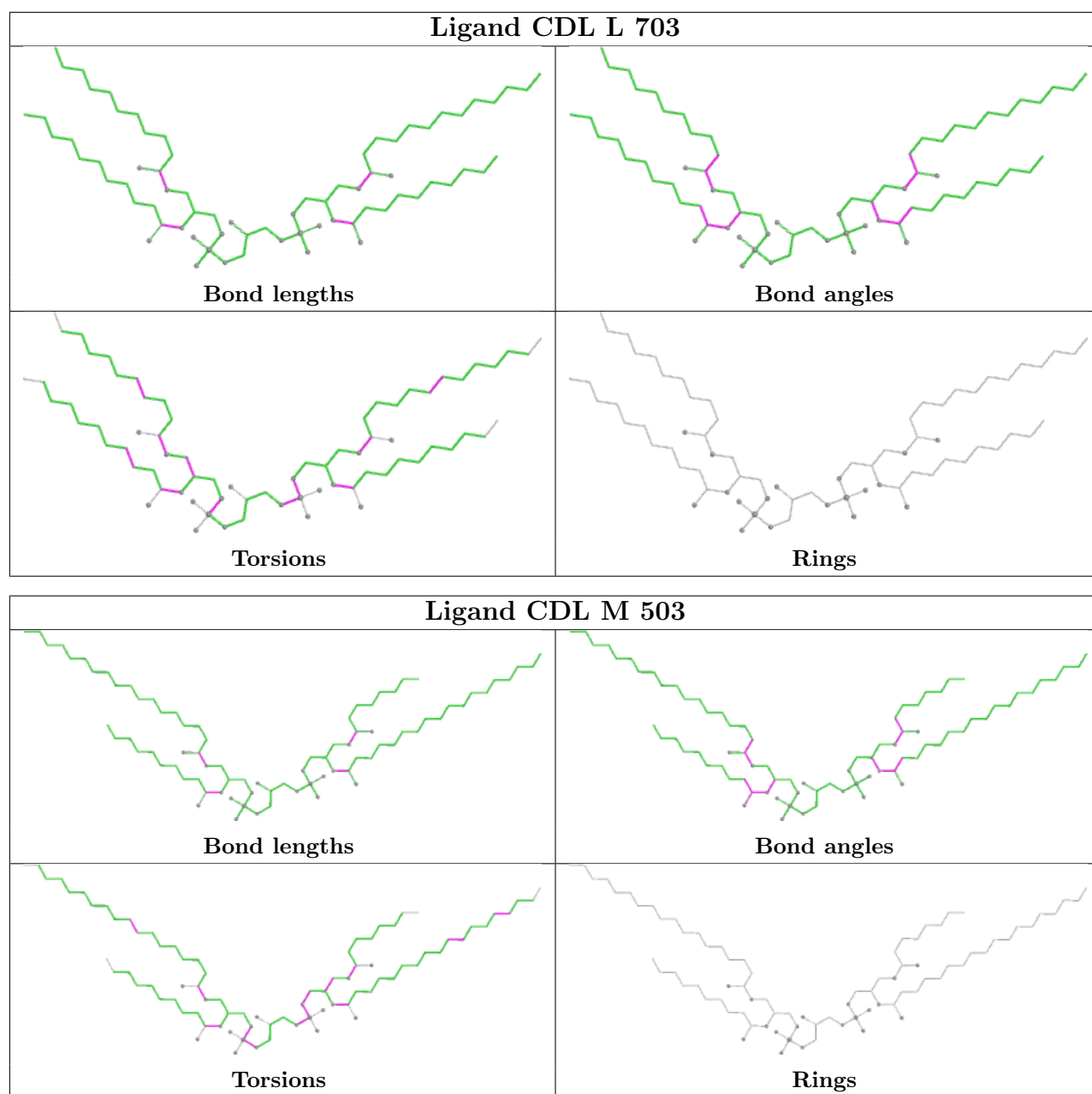


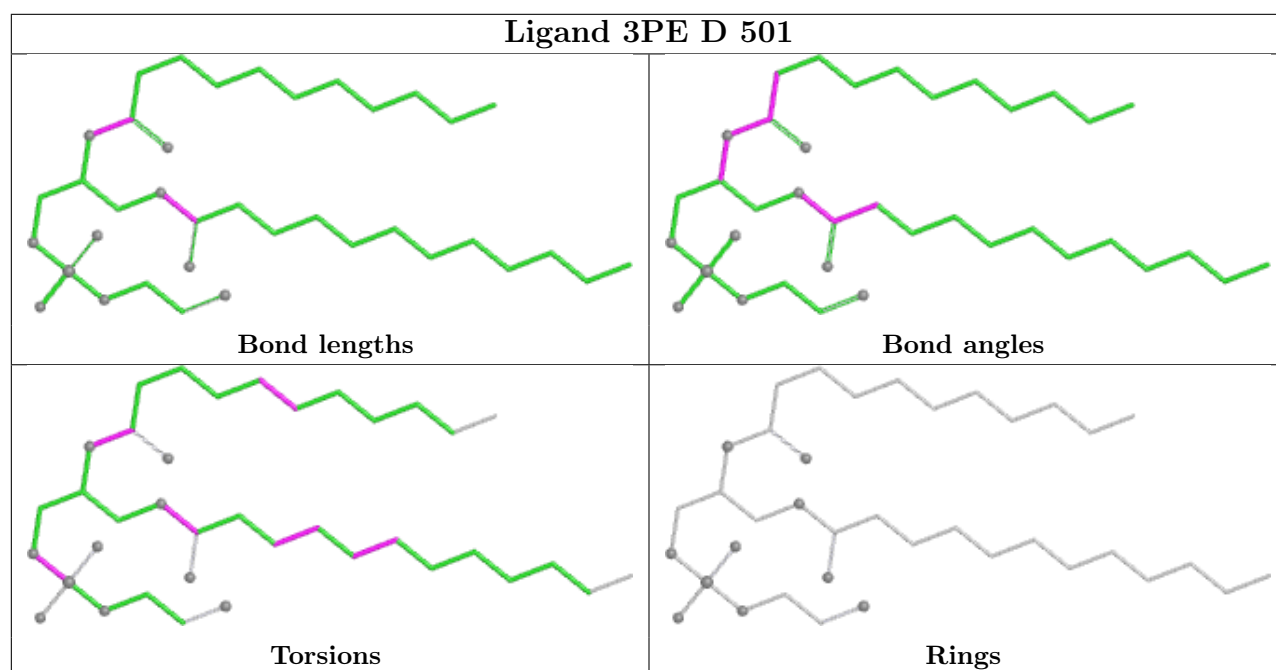
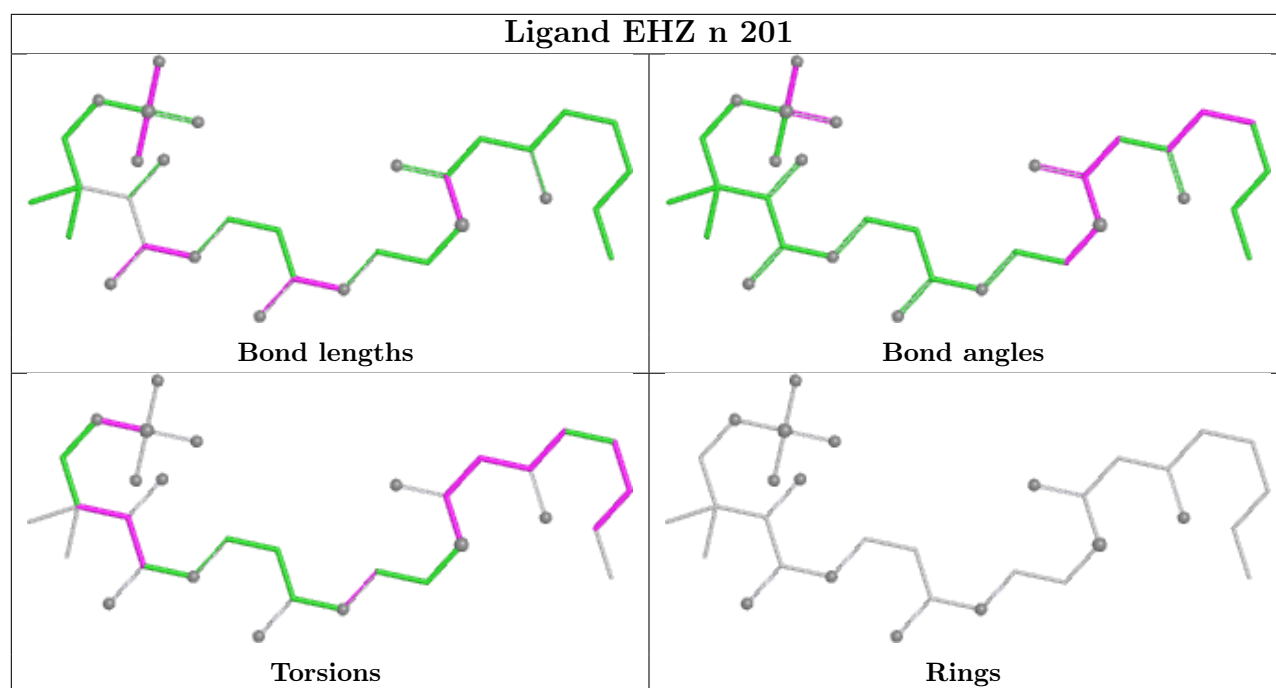


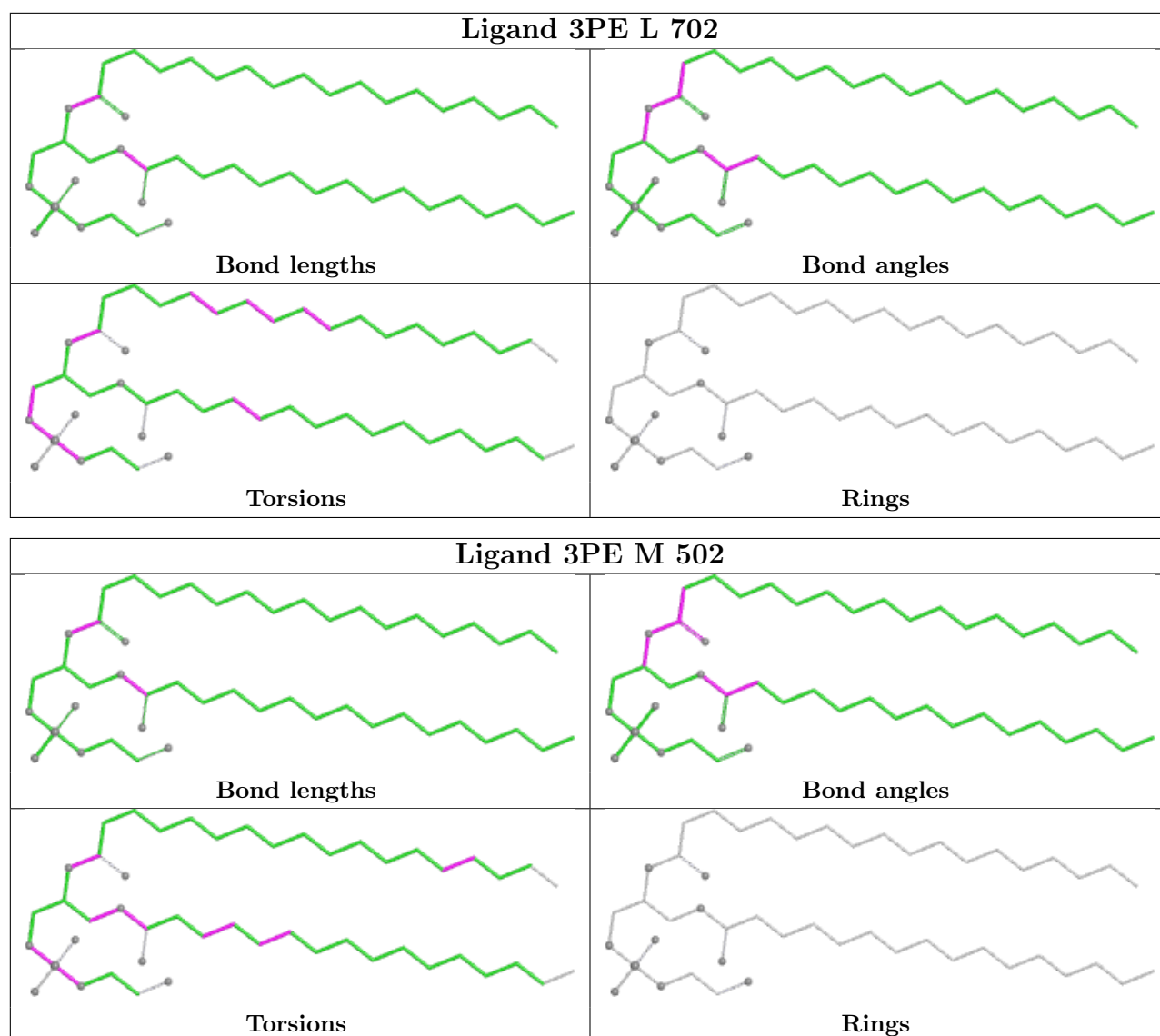












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

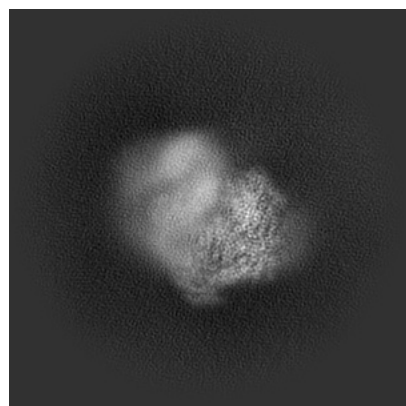
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35354. These allow visual inspection of the internal detail of the map and identification of artifacts.

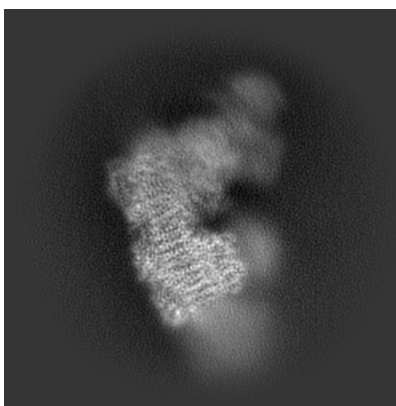
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

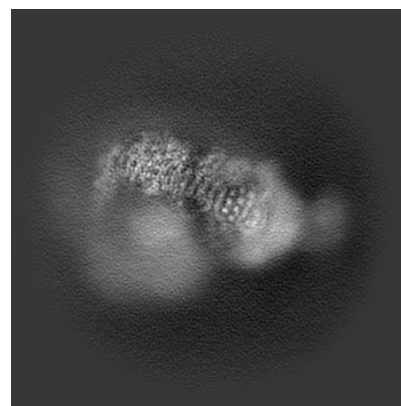
6.1.1 Primary map



X

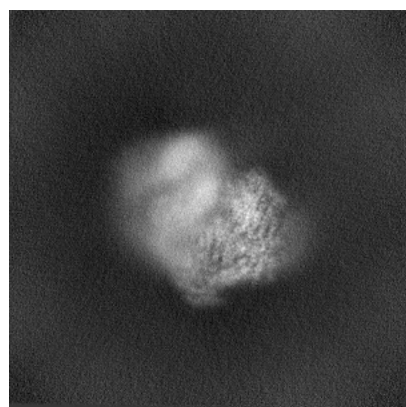


Y



Z

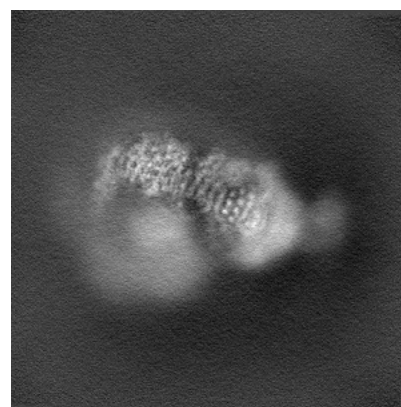
6.1.2 Raw map



X



Y

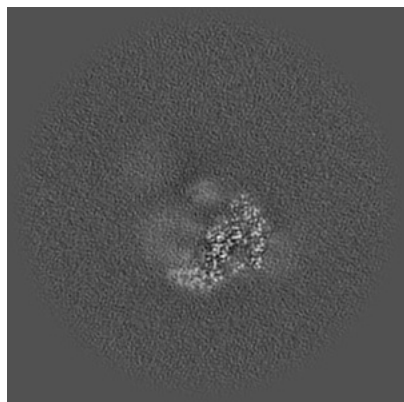


Z

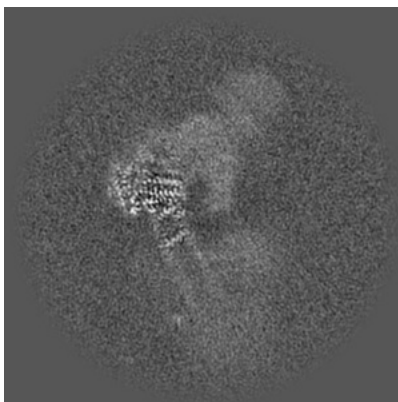
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

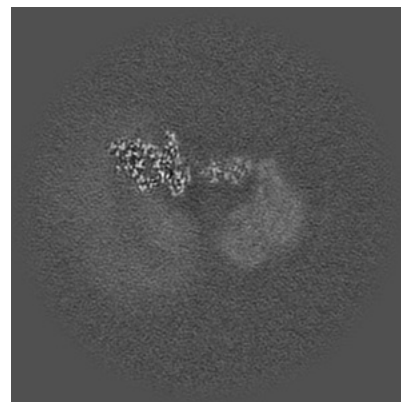
6.2.1 Primary map



X Index: 256

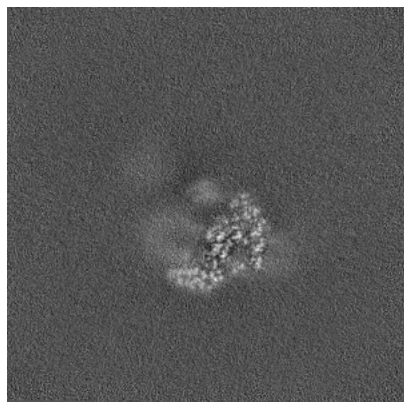


Y Index: 256

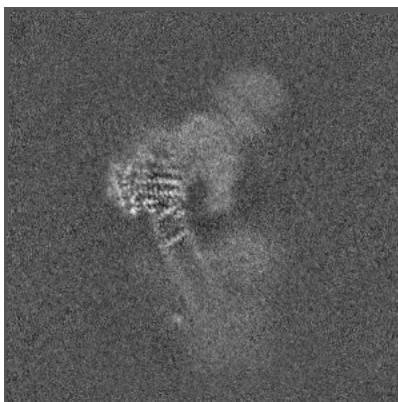


Z Index: 256

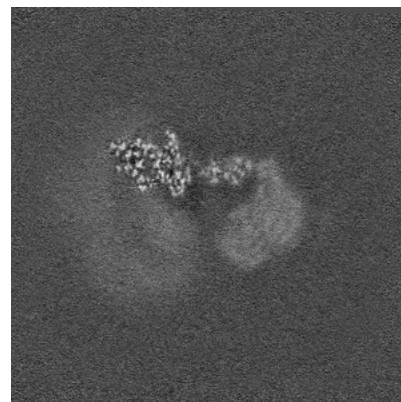
6.2.2 Raw map



X Index: 256



Y Index: 256

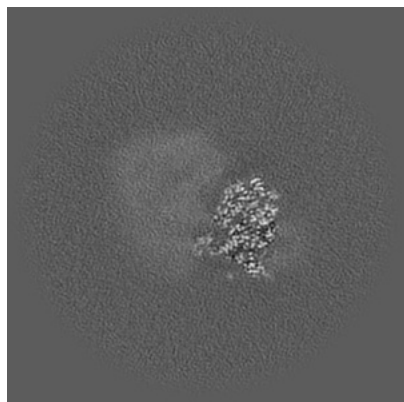


Z Index: 256

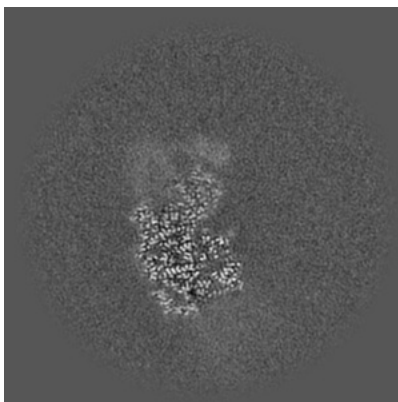
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

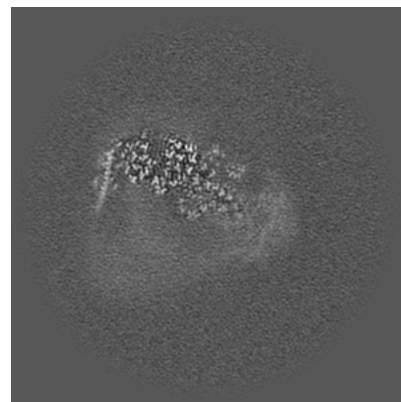
6.3.1 Primary map



X Index: 211

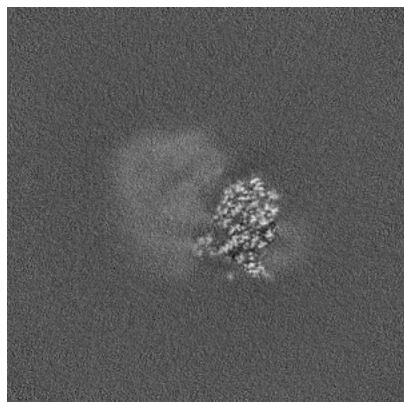


Y Index: 300

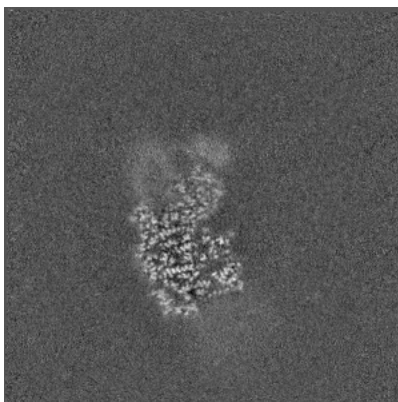


Z Index: 224

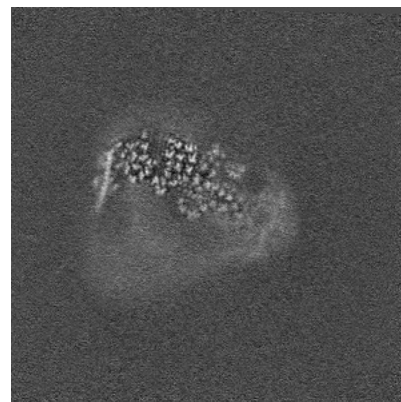
6.3.2 Raw map



X Index: 211



Y Index: 300

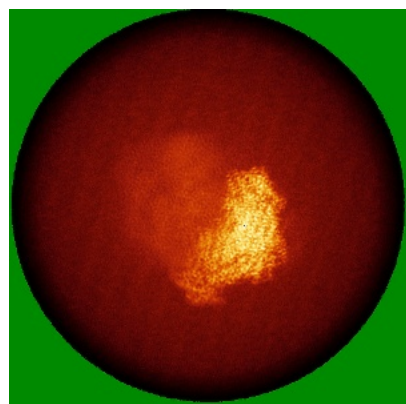


Z Index: 224

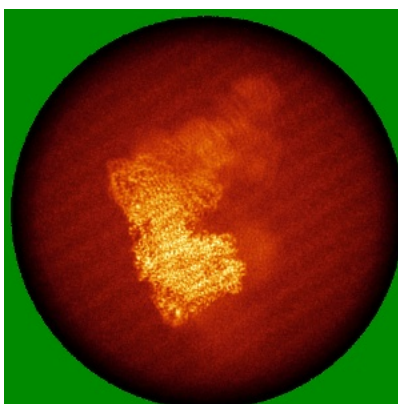
The images above show the largest variance slices of the map in three orthogonal directions.

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

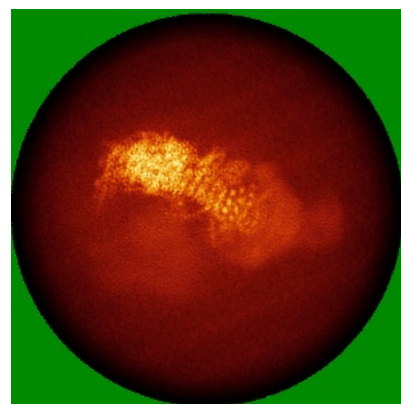
6.4.1 Primary map



X

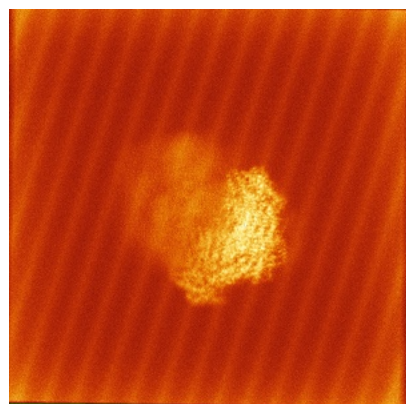


Y

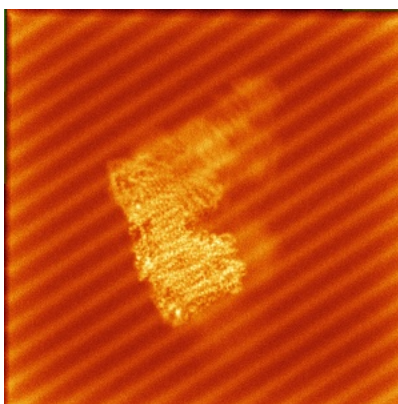


Z

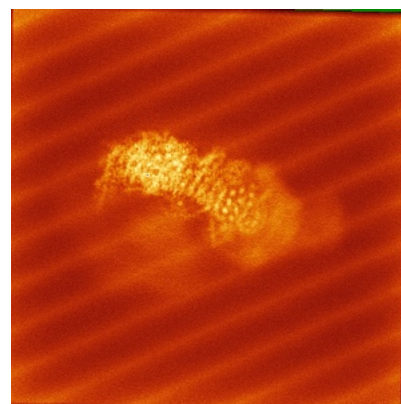
6.4.2 Raw map



X



Y

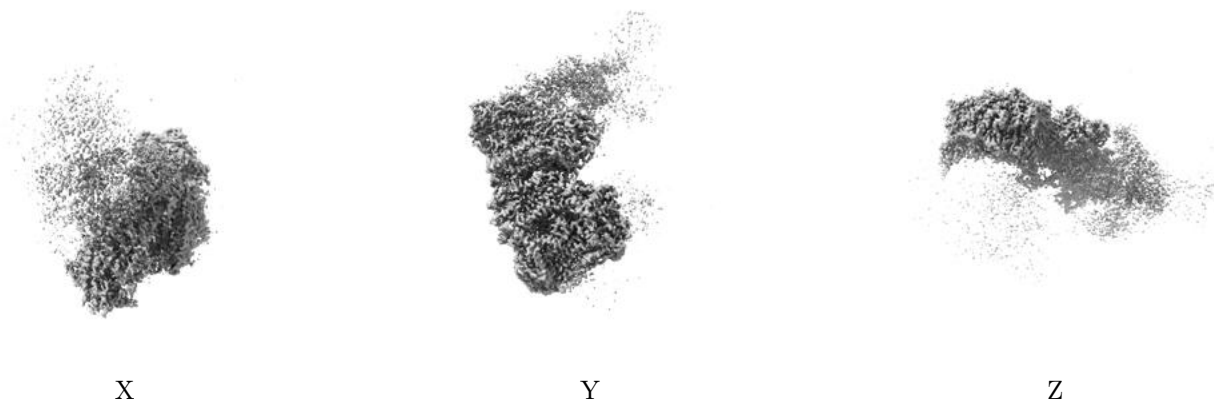


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

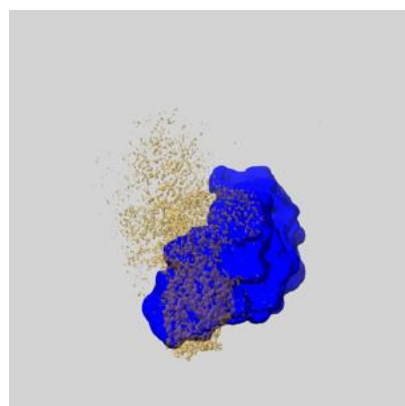
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

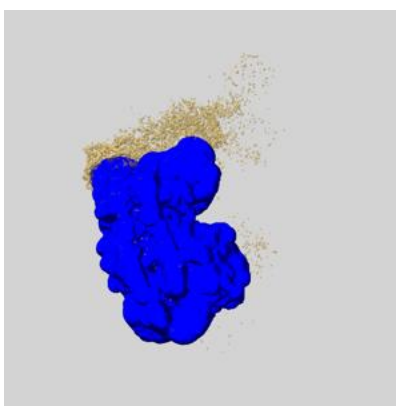
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_35354_msk_1.map [i](#)



X



Y

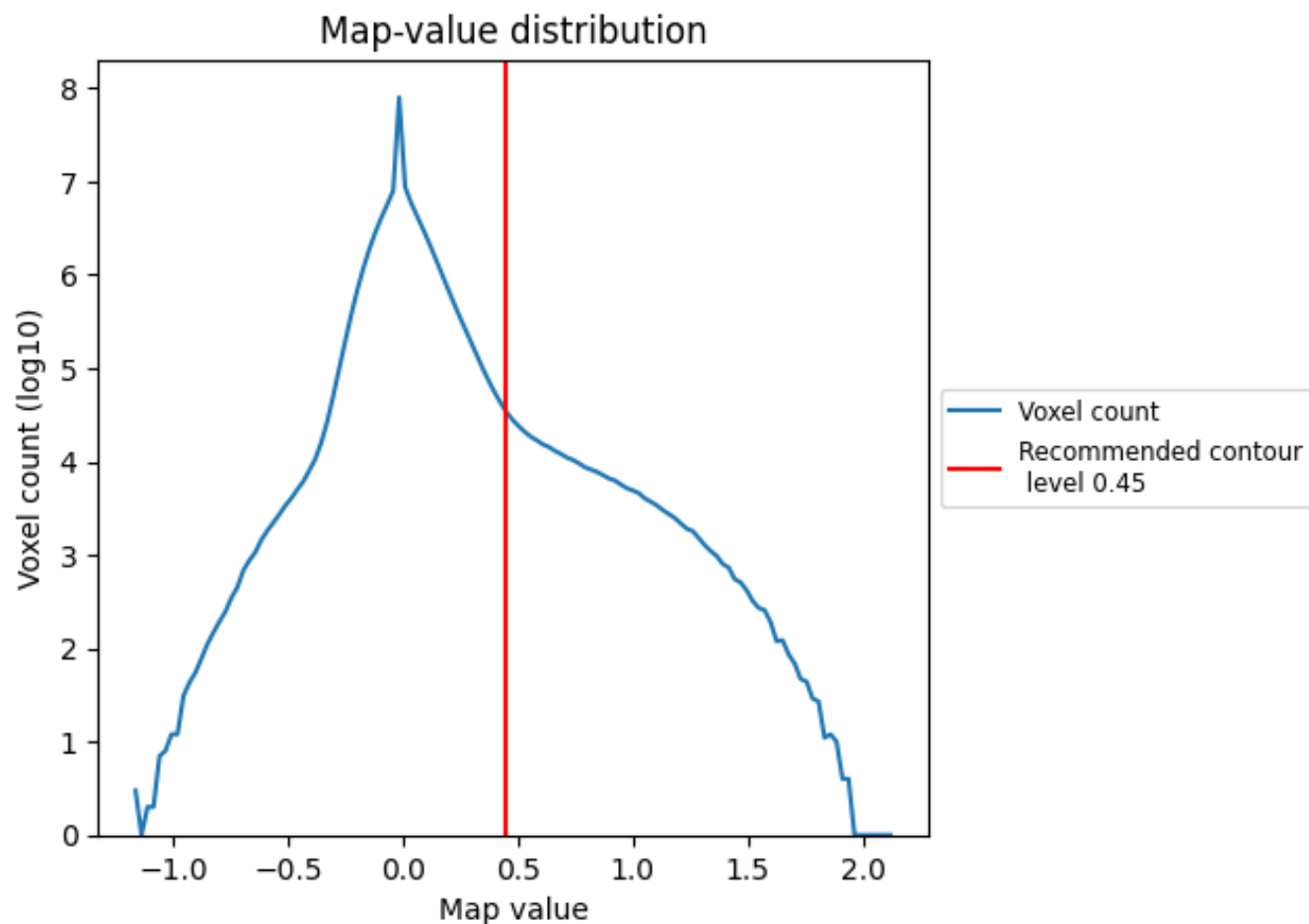


Z

7 Map analysis [i](#)

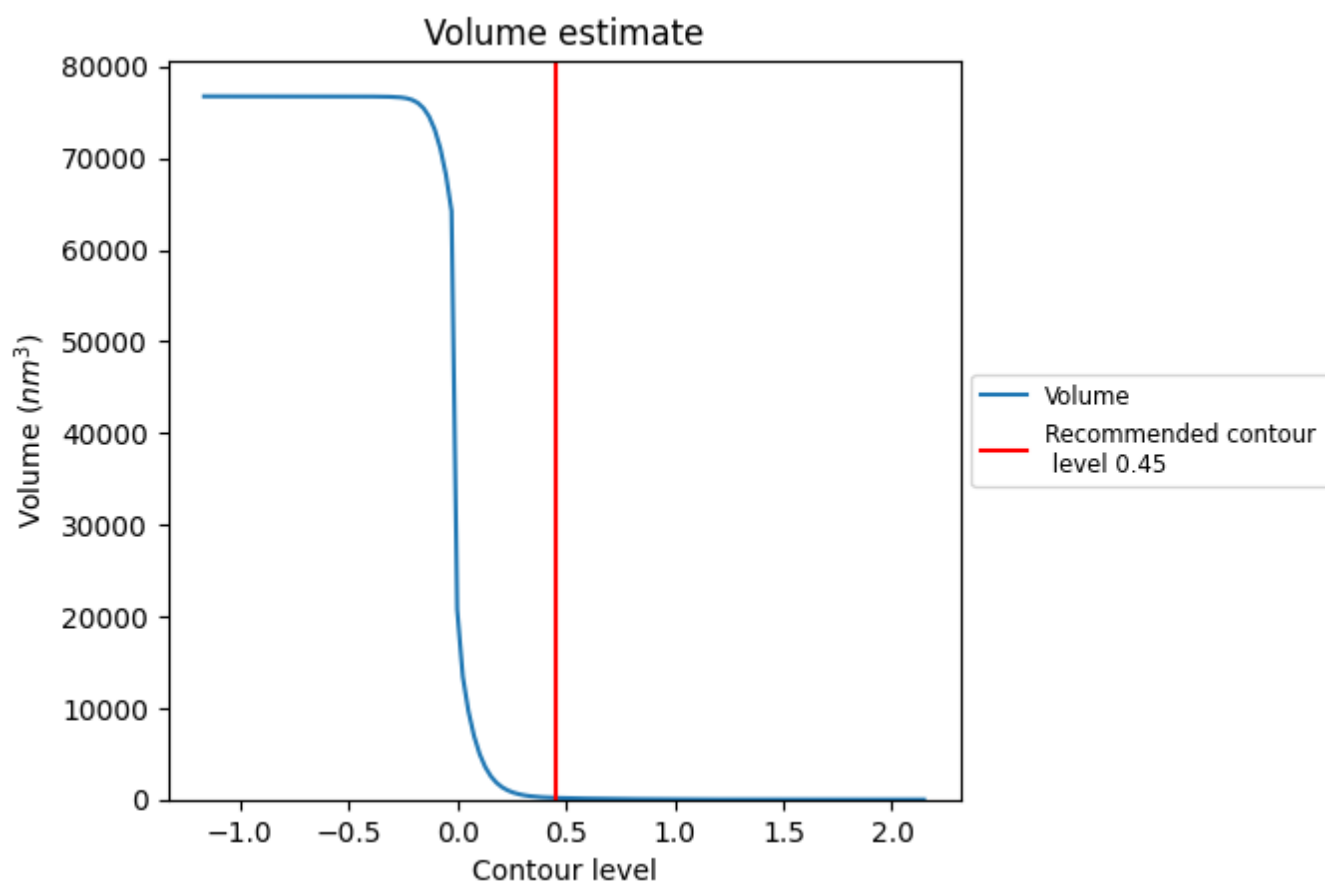
This section contains the results of statistical analysis of the map.

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.

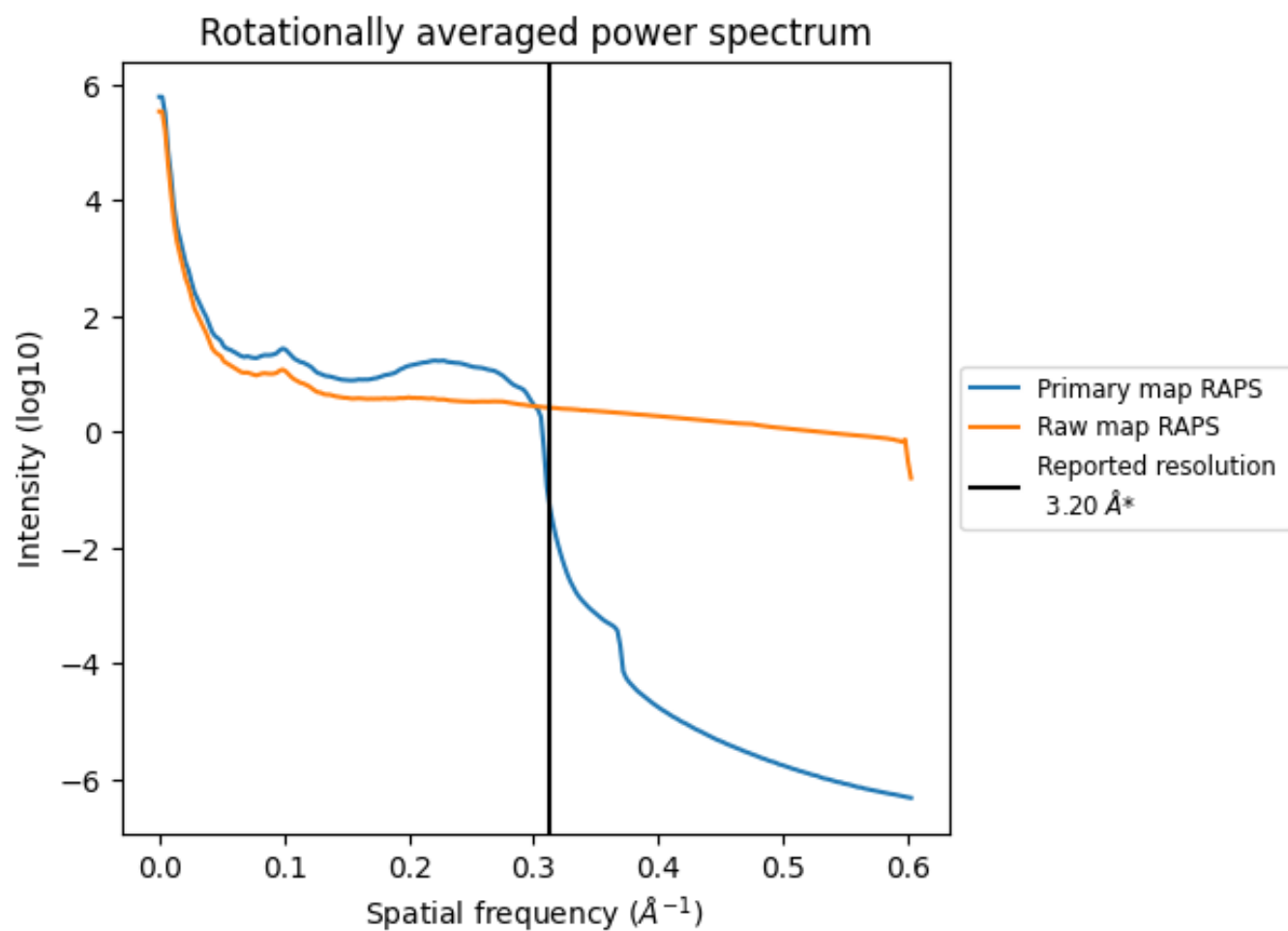
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 189 nm³; this corresponds to an approximate mass of 171 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

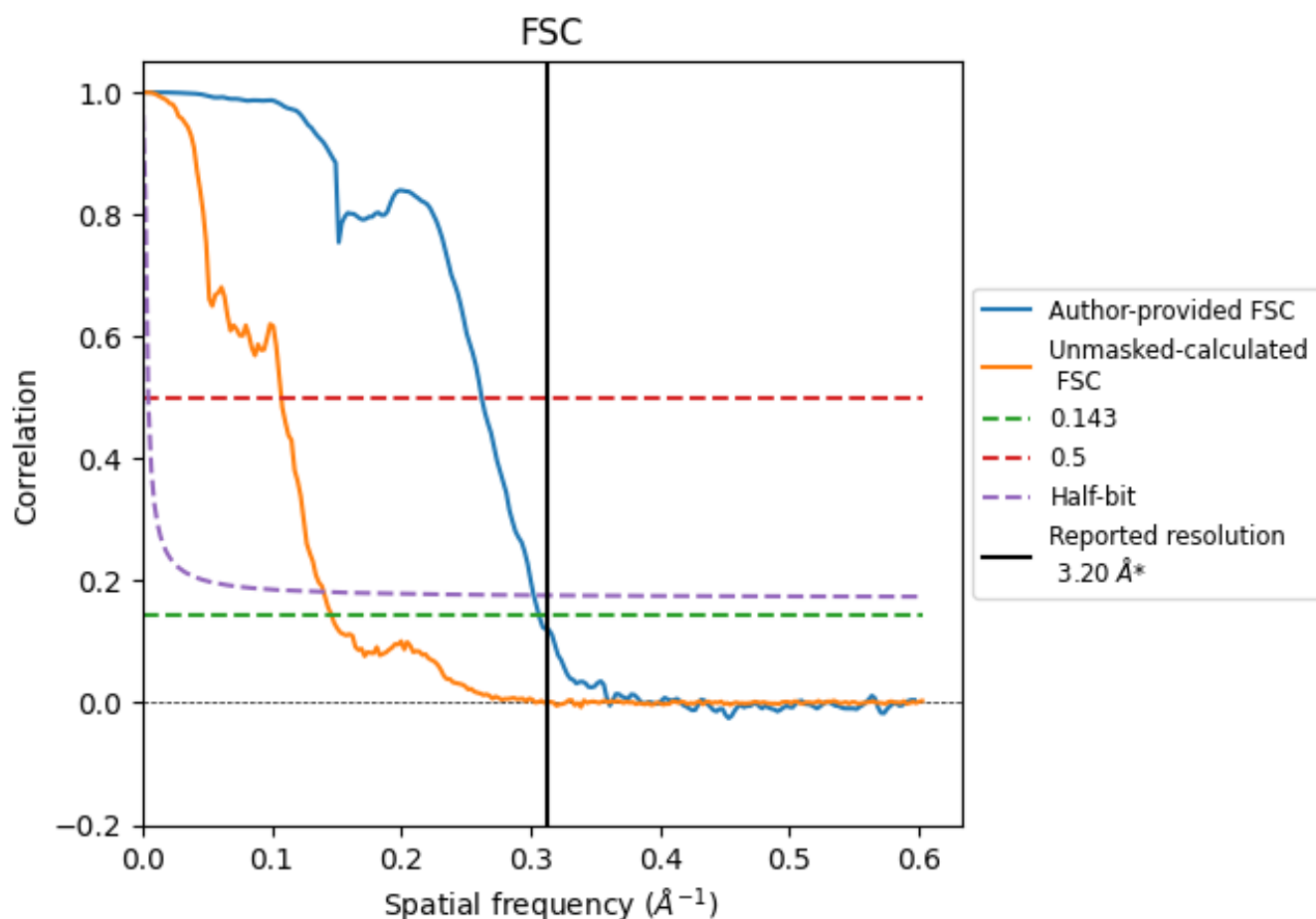


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

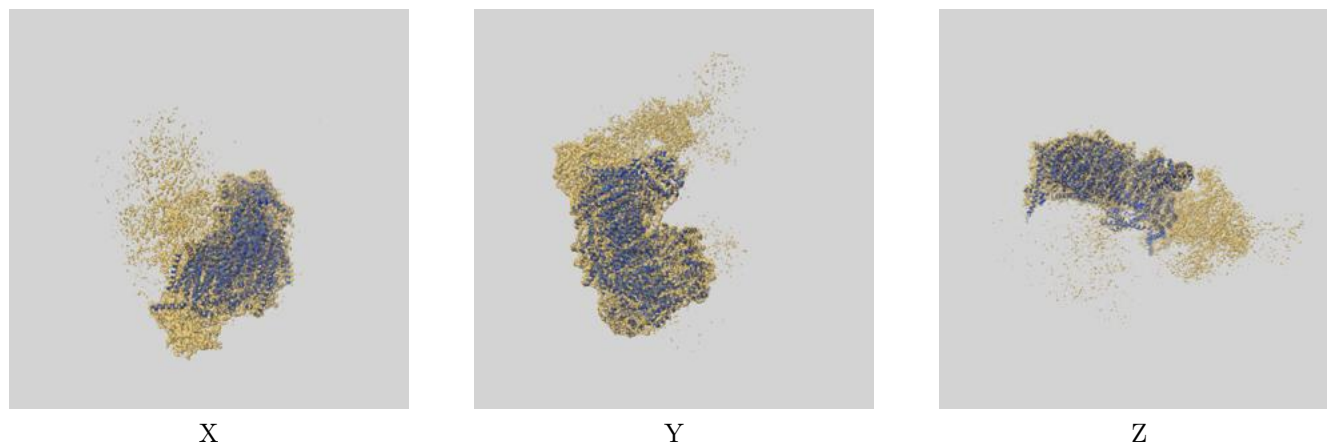
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.26	3.81	3.31
Unmasked-calculated*	6.84	9.31	7.14

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.84 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

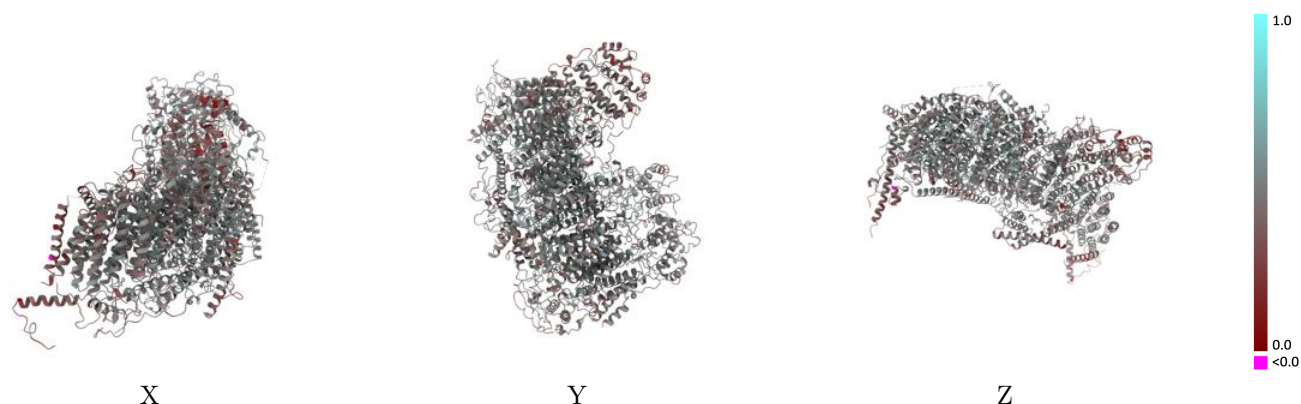
This section contains information regarding the fit between EMDB map EMD-35354 and PDB model 8IC4. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.45 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](#)

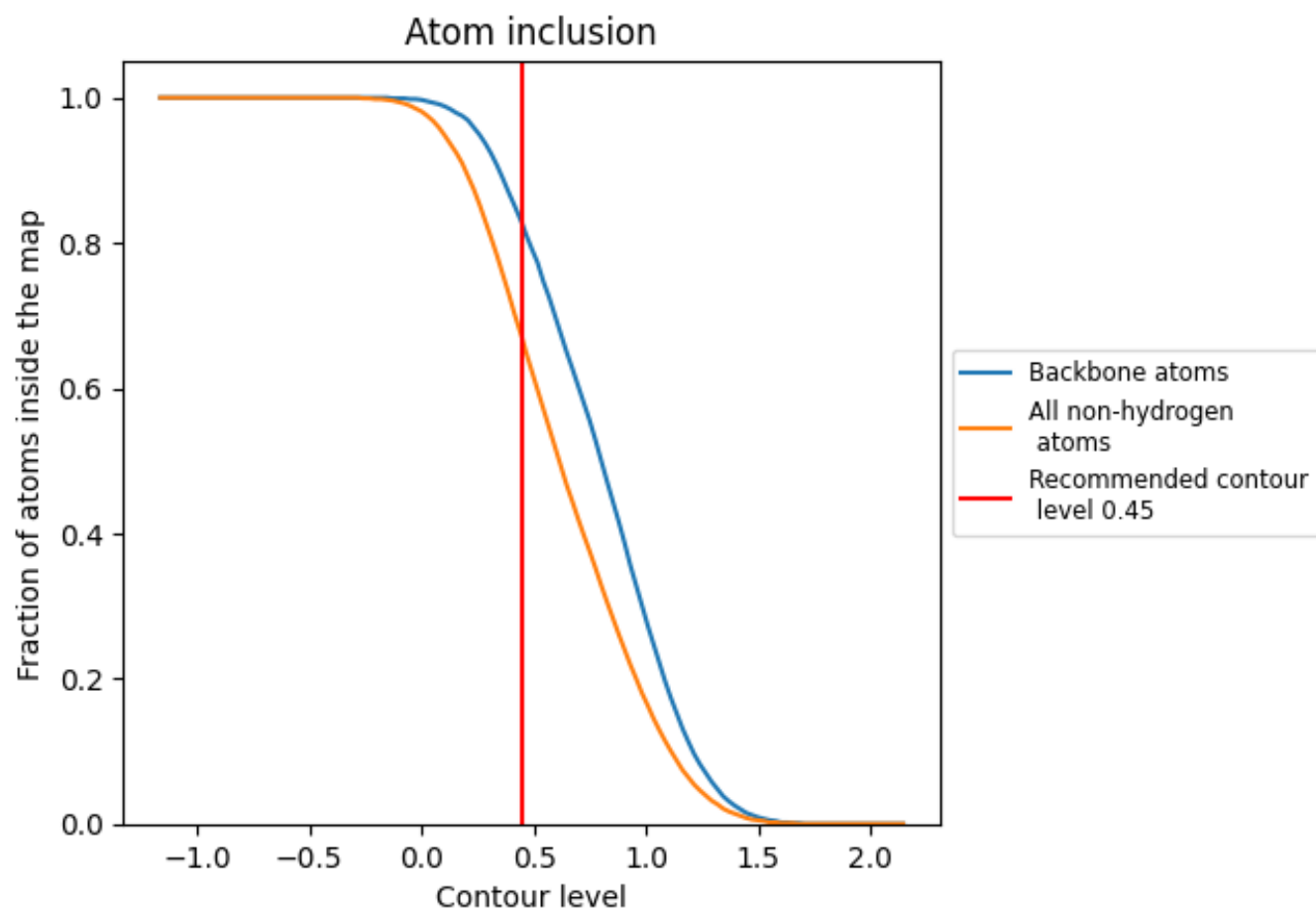


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 67% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6680	 0.4500
D	 0.4170	 0.4180
J	 0.4460	 0.4010
K	 0.6210	 0.4630
L	 0.6960	 0.4680
M	 0.7040	 0.4860
N	 0.6940	 0.4770
O	 0.5680	 0.3830
U	 0.7420	 0.4720
X	 0.7450	 0.4480
Y	 0.4880	 0.4150
c	 0.5820	 0.4040
d	 0.7030	 0.4670
e	 0.6030	 0.3850
f	 0.6640	 0.4600
g	 0.7100	 0.4560
h	 0.7180	 0.4630
i	 0.7060	 0.4560
j	 0.6920	 0.4160
k	 0.7520	 0.4620
l	 0.7480	 0.4710
m	 0.6850	 0.4550
n	 0.7610	 0.4750
o	 0.6540	 0.4080
p	 0.7070	 0.4380

