



wwPDB EM Validation Summary Report ⓘ

Nov 9, 2024 – 10:45 am GMT

PDB ID : 6Q9B
EMDB ID : EMD-4479
Title : CI Membrane Arm focused refinement from Ovine respiratory SC I+III2
Authors : Letts, J.A.; Sazanov, L.A.
Deposited on : 2018-12-17
Resolution : 3.90 Å(reported)
Based on initial model : 1LNK

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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

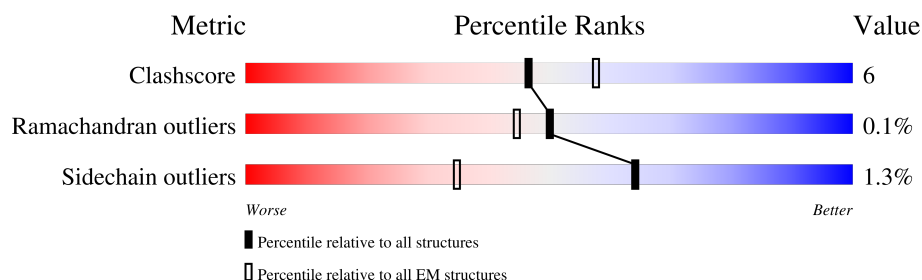
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	S2	430	
2	D3	115	
3	D1	318	
4	D6	175	
5	4L	98	
6	D5	606	
7	D4	459	
8	D2	347	

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Mol	Chain	Length	Quality of chain
9	AK	140	
10	B5	143	
11	AB	88	
12	A8	171	
13	BJ	175	
14	AJ	320	
15	S5	105	
16	A3	83	
17	B3	97	
18	C2	120	
19	B4	128	
20	AM	143	
21	B6	127	
22	B7	136	
23	B9	178	
24	B2	72	
25	B8	158	
26	BK	125	
27	C1	49	
28	B1	57	
29	A1	70	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 38012 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:ubiquinone oxidoreductase core subunit S2,NADH:ubiquinone oxidoreductase core subunit S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S2	39	Total	C	N	O	S	0	0
			325	211	54	59	1		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S2	1	ALA	-	insertion	UNP W5PJ73
S2	2	ARG	-	insertion	UNP W5PJ73
S2	3	GLN	-	expression tag	UNP W5PJ73
S2	4	TRP	-	expression tag	UNP W5PJ73
S2	5	GLN	-	expression tag	UNP W5PJ73
S2	6	PRO	-	expression tag	UNP W5PJ73
S2	7	ASP	-	expression tag	UNP W5PJ73
S2	8	VAL	-	expression tag	UNP W5PJ73
S2	9	GLU	-	expression tag	UNP W5PJ73
S2	10	TRP	-	expression tag	UNP W5PJ73
S2	11	ALA	-	expression tag	UNP W5PJ73
S2	12	GLU	-	expression tag	UNP W5PJ73
S2	13	GLN	-	expression tag	UNP W5PJ73
S2	14	TYR	-	expression tag	UNP W5PJ73
S2	15	GLY	-	expression tag	UNP W5PJ73
S2	16	GLY	-	expression tag	UNP W5PJ73
S2	17	ALA	-	expression tag	UNP W5PJ73
S2	18	VAL	-	expression tag	UNP W5PJ73

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D3	90	Total	C	N	O	S	0	0
			728	500	103	120	5		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D1	301	Total	C	N	O	S	0	0
			2400	1623	366	392	19		

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D6	171	Total	C	N	O	S	0	0
			1308	878	187	230	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4L	98	Total	C	N	O	S	0	0
			748	489	112	132	15		

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D5	606	Total	C	N	O	S	0	0
			4805	3187	746	828	44		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D4	459	Total	C	N	O	S	0	0
			3646	2428	571	607	40		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D2	347	Total	C	N	O	S	0	0
			2724	1808	416	460	40		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AK	140	Total	C	N	O	S	0	0
			1025	654	175	190	6		

- Molecule 10 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B5	139	Total	C	N	O	S	0	0
			1156	761	194	199	2		

- Molecule 11 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AB	87	Total	C	N	O	S	0	0
			702	451	103	143	5		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A8	171	Total	C	N	O	S	0	0
			1404	889	253	252	10		

- Molecule 13 is a protein called NADH:ubiquinone oxidoreductase subunit B10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BJ	171	Total	C	N	O	S	0	0
			1441	905	266	262	8		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AJ	319	Total	C	N	O	S	0	0
			2583	1653	430	490	10		

- Molecule 15 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S5	99	Total	C	N	O	S	0	0
			822	520	154	142	6		

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A3	74	Total	C	N	O	S	0	0
			582	379	96	105	2		

- Molecule 17 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B3	73	Total	C	N	O	S	0	0
			578	378	100	98	2		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	C2	119	Total	C	N	O	S	0	0
			997	647	174	172	4		

- Molecule 19 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	B4	128	Total	C	N	O	S	0	0
			1059	675	189	194	1		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AM	114	Total	C	N	O	S	0	0
			945	607	162	168	8		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B6	95	Total	C	N	O	S	0	0
			804	530	135	138	1		

- Molecule 22 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B7	119	Total	C	N	O	S	0	0
			1026	641	196	181	8		

- Molecule 23 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B9	176	Total	C	N	O	S	0	0
			1515	970	278	261	6		

- Molecule 24 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B2	65	Total	C	N	O	S	0	0
			563	372	93	97	1		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B8	157	Total	C	N	O	S	0	0
			1324	855	217	243	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BK	102	Total	C	N	O	S	0	0
			853	547	141	161	4		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	C1	46	Total	C	N	O	0	0
			391	258	67	66		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	B1	52	Total	C	N	O	0	0
			449	296	79	74		

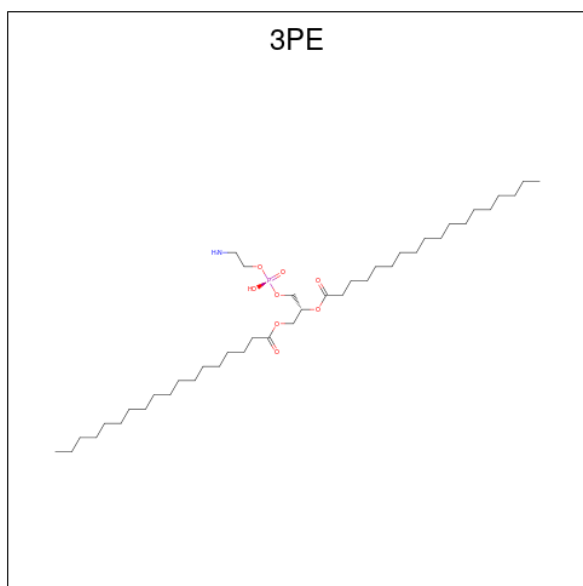
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	16	VAL	GLY	conflict	UNP W5QG39
B1	35	ALA	THR	conflict	UNP W5QG39
B1	38	ARG	TRP	conflict	UNP W5QG39

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

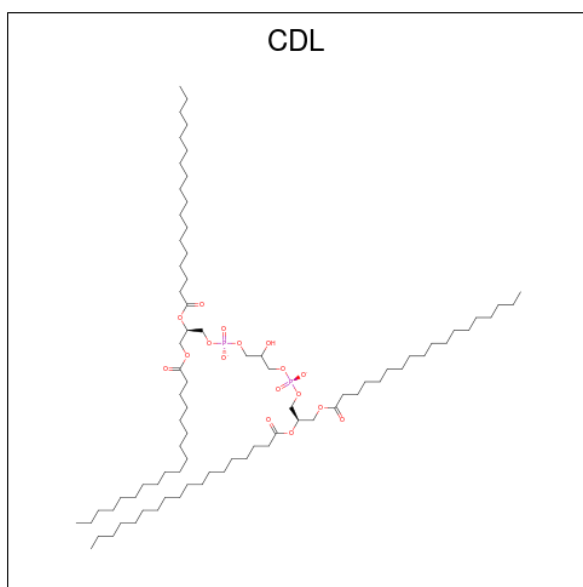
Mol	Chain	Residues	Atoms					AltConf	Trace
29	A1	70	Total	C	N	O	S	0	0
			577	369	106	97	5		

- Molecule 30 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



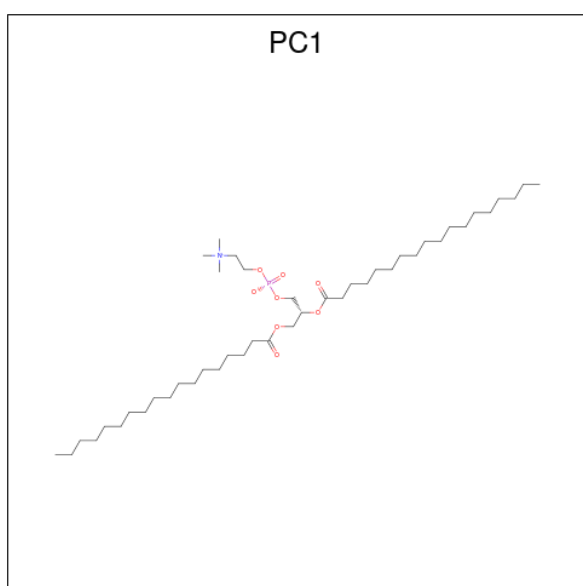
Mol	Chain	Residues	Atoms					AltConf
30	D6	1	Total	C	N	O	P	0
			32	22	1	8	1	
30	D5	1	Total	C	N	O	P	0
			38	28	1	8	1	
30	D5	1	Total	C	N	O	P	0
			40	30	1	8	1	
30	D4	1	Total	C	N	O	P	0
			25	15	1	8	1	
30	A8	1	Total	C	N	O	P	0
			25	15	1	8	1	
30	B4	1	Total	C	O	P		0
			27	18	8	1		

- Molecule 31 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



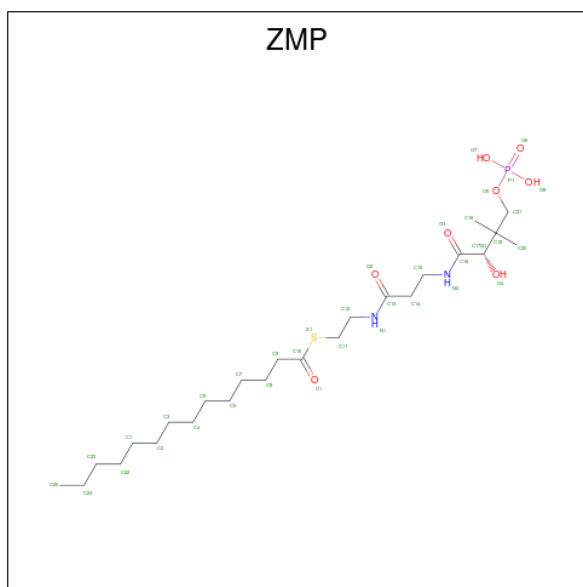
Mol	Chain	Residues	Atoms				AltConf
31	D5	1	Total	C	O	P	0
			60	41	17	2	
31	D5	1	Total	C	O	P	0
			62	43	17	2	
31	AK	1	Total	C	O	P	0
			64	45	17	2	
31	B5	1	Total	C	O	P	0
			65	46	17	2	

- Molecule 32 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).

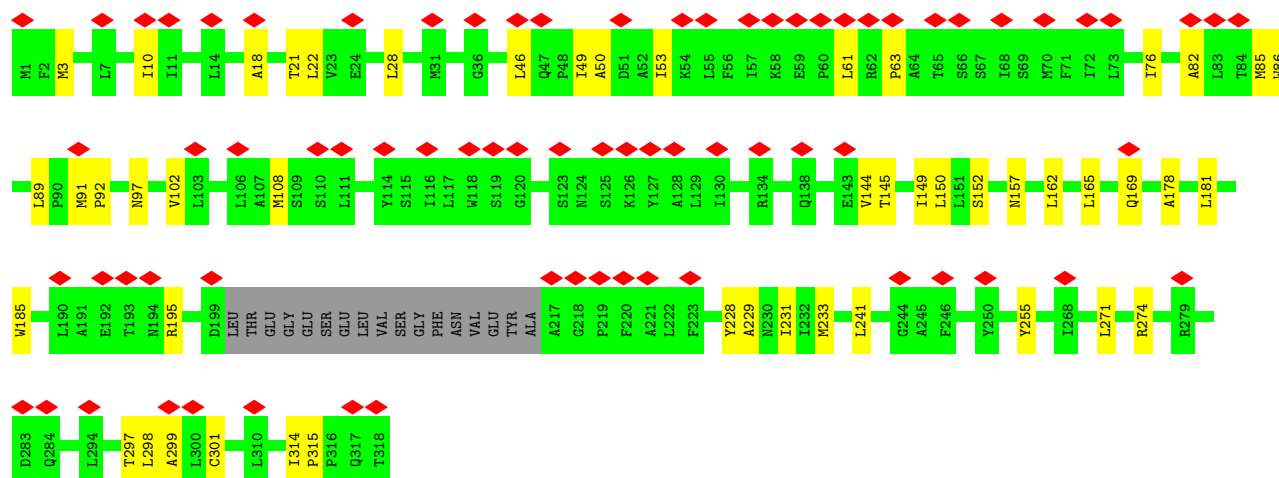


Mol	Chain	Residues	Atoms					AltConf
32	D4	1	Total	C	N	O	P	0
			35	25	1	8	1	
32	D4	1	Total	C	N	O	P	0
			28	18	1	8	1	

- Molecule 33 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C₂₅H₄₉N₂O₈PS).

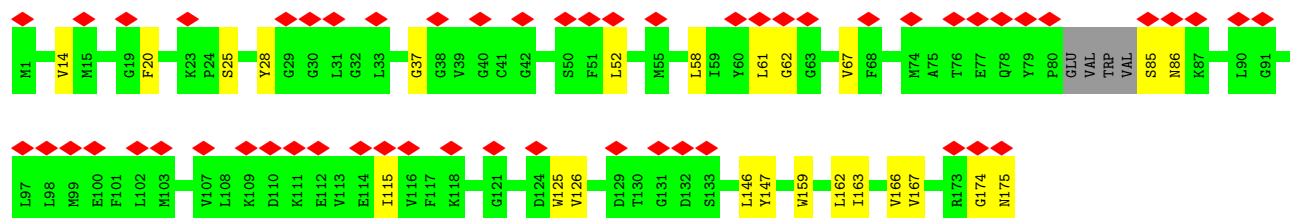


Mol	Chain	Residues	Atoms						AltConf
33	AB	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	



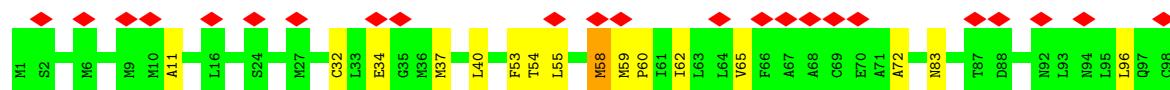
• Molecule 4: NADH-ubiquinone oxidoreductase chain 6

Chain D6: 31% 84% 14%



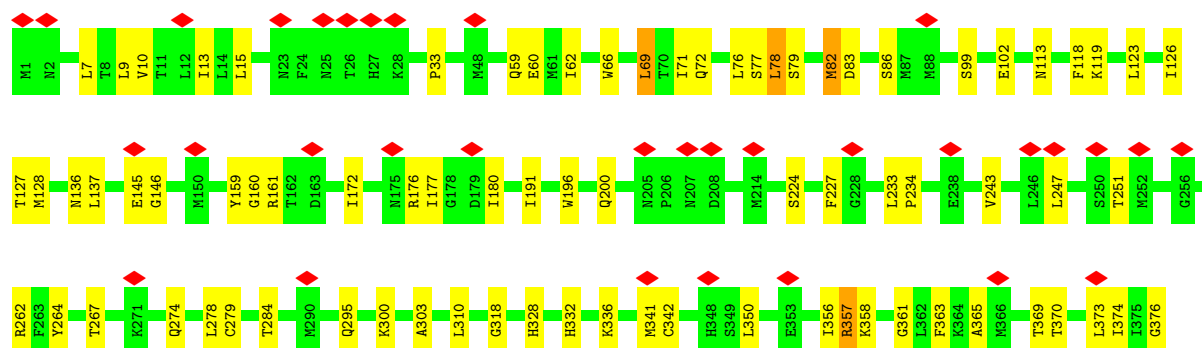
• Molecule 5: NADH-ubiquinone oxidoreductase chain 4L

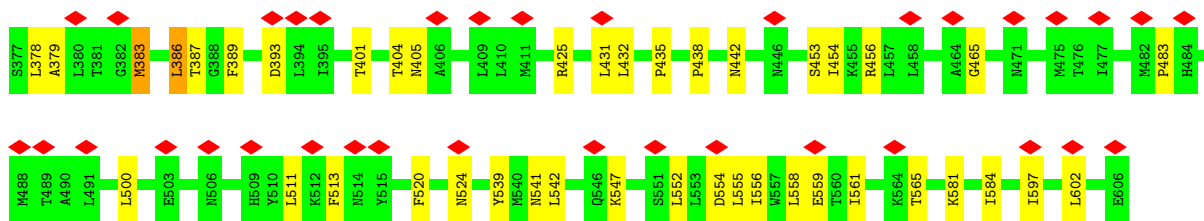
Chain 4L: 23% 84% 15%



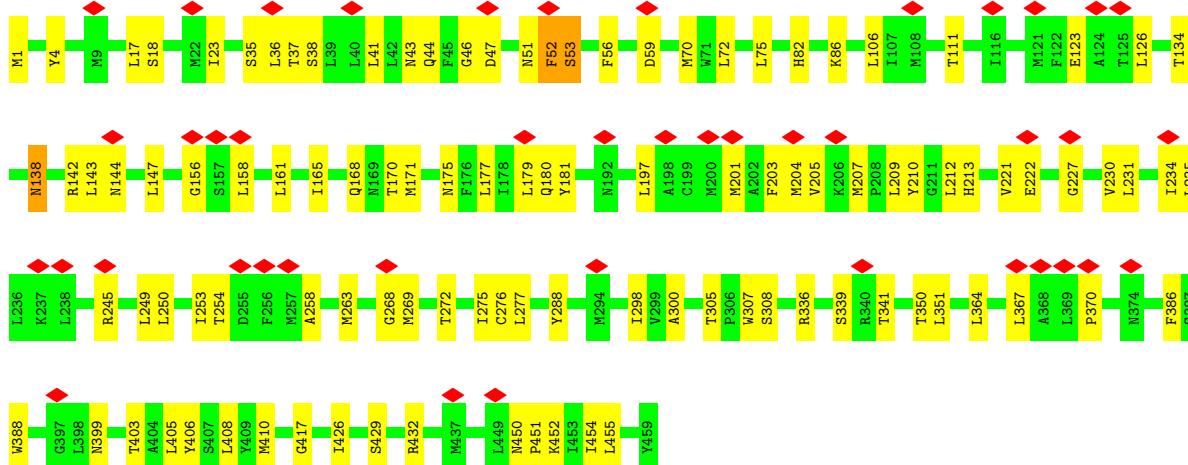
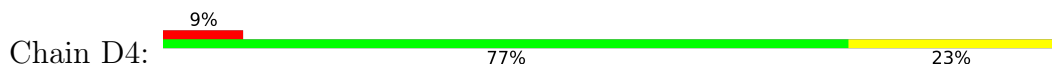
• Molecule 6: NADH-ubiquinone oxidoreductase chain 5

Chain D5: 11% 80% 19%

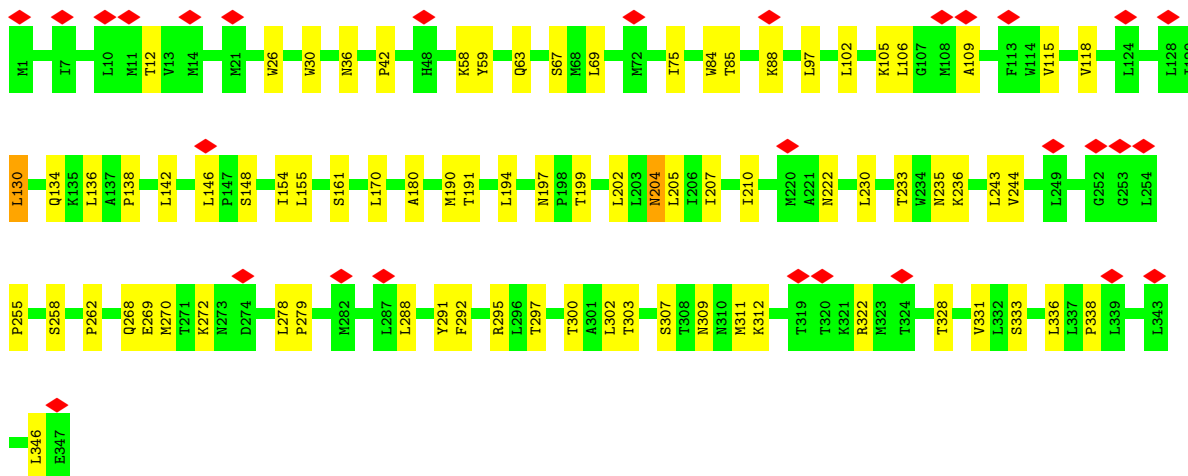
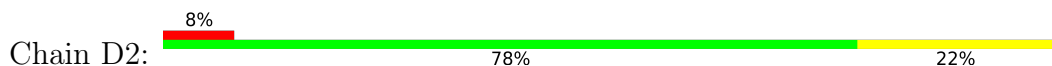




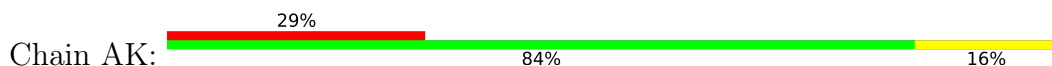
• Molecule 7: NADH-ubiquinone oxidoreductase chain 4

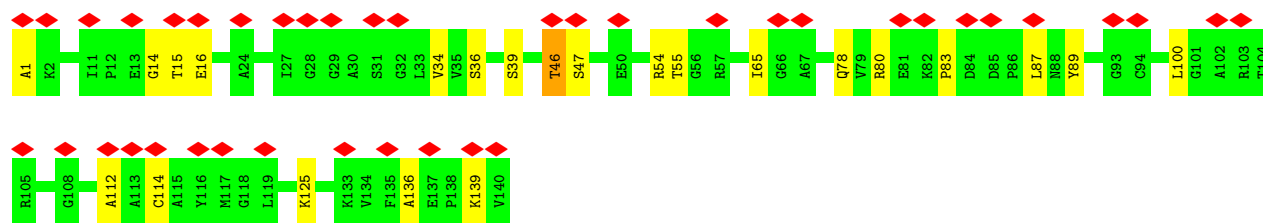


• Molecule 8: NADH-ubiquinone oxidoreductase chain 2

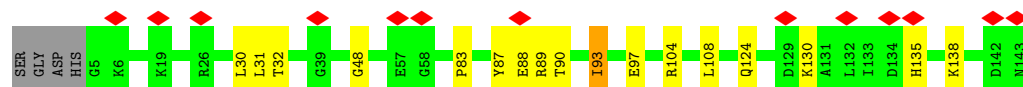
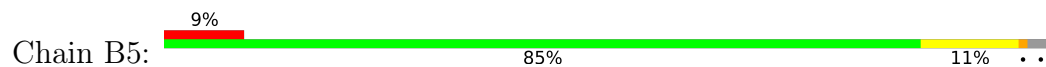


• Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

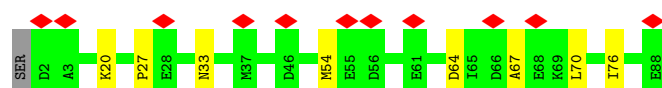




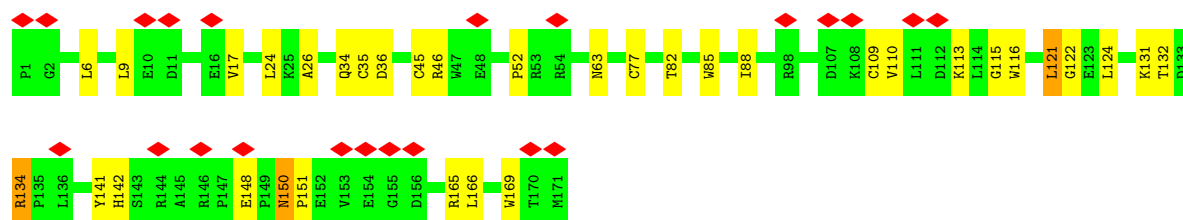
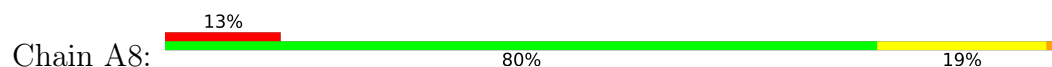
- Molecule 10: NADH:ubiquinone oxidoreductase subunit B5



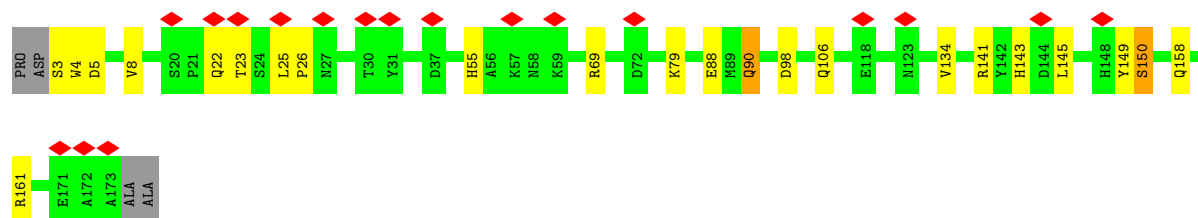
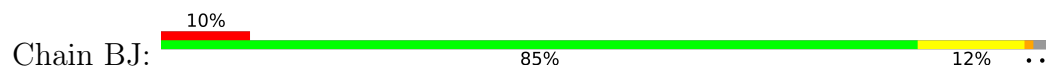
- Molecule 11: Acyl carrier protein



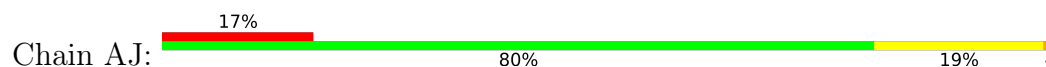
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

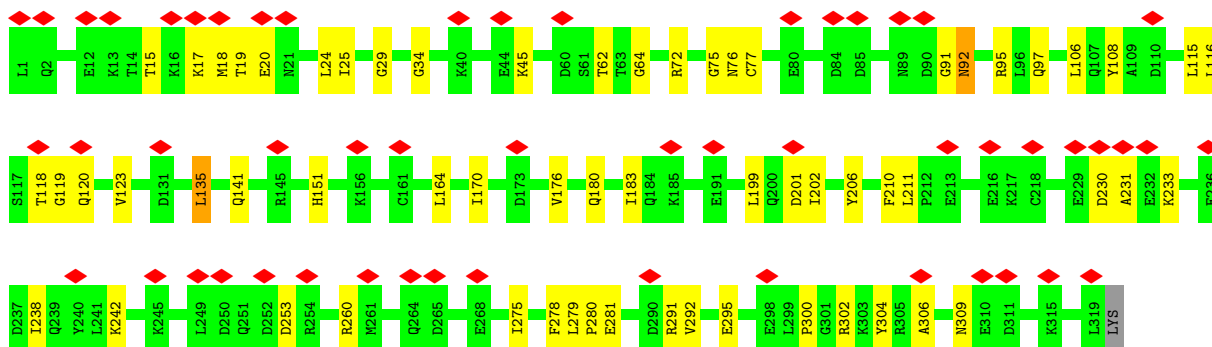


- Molecule 13: NADH:ubiquinone oxidoreductase subunit B10

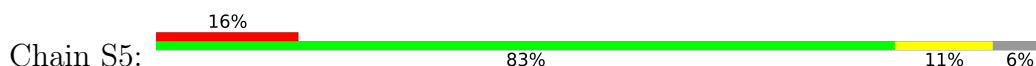


- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

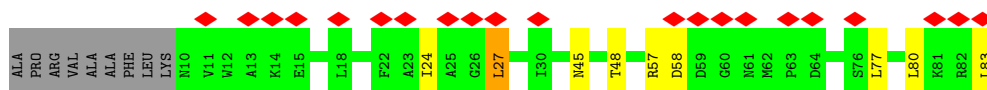
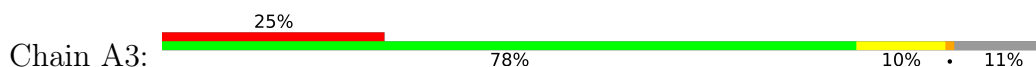




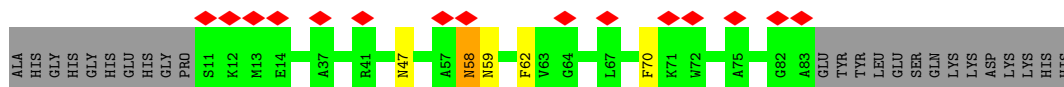
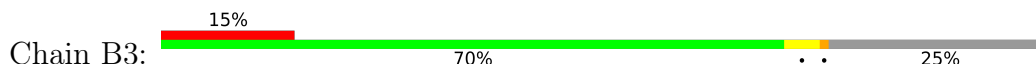
- Molecule 15: NADH:ubiquinone oxidoreductase subunit S5



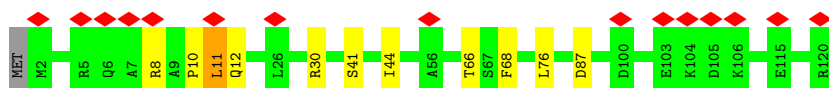
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A3



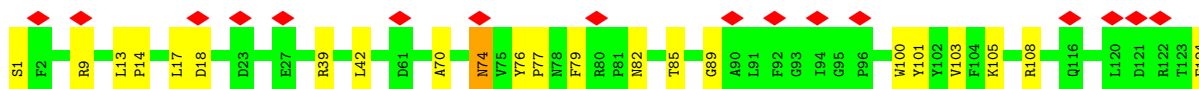
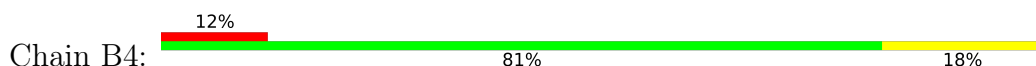
- Molecule 17: NADH:ubiquinone oxidoreductase subunit B3



- Molecule 18: NADH dehydrogenase [ubiquinone] 1 subunit C2

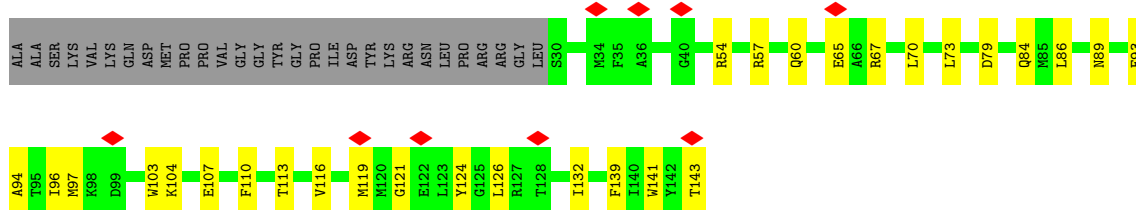


- Molecule 19: NADH:ubiquinone oxidoreductase subunit B4

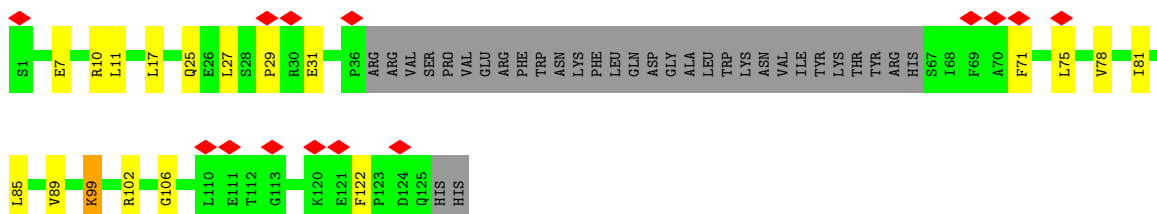




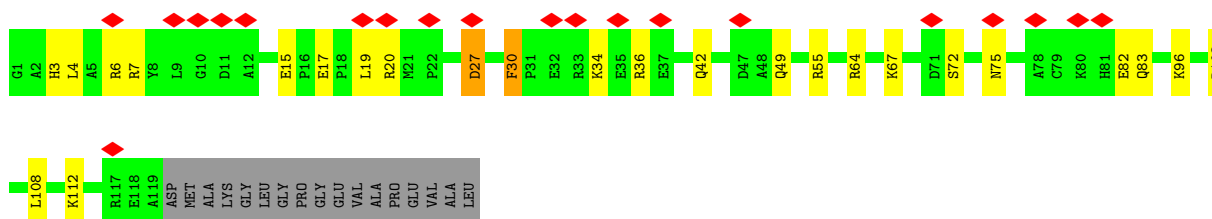
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



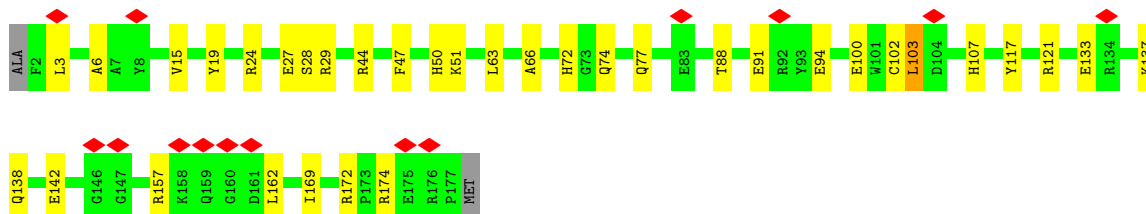
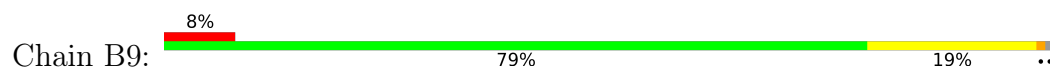
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6




- Molecule 22: NADH:ubiquinone oxidoreductase subunit B7

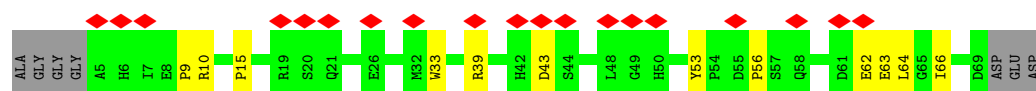


- Molecule 23: NADH:ubiquinone oxidoreductase subunit B9




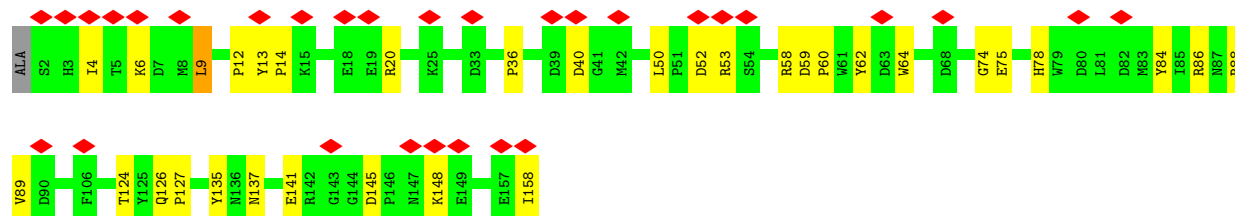
- Molecule 24: NADH:ubiquinone oxidoreductase subunit B2

Chain B2: 



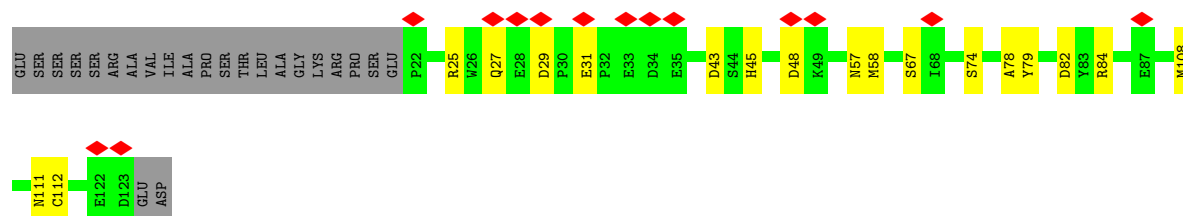
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain B8: 




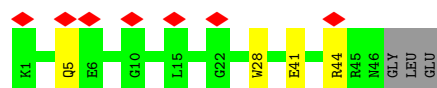
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain BK: 




- Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain C1: 



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain B1: 



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain A1: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	174334	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 ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.584	Depositor
Minimum map value	-0.318	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	716.8, 716.8, 716.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, PC1, CDL, ZMP

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	S2	0.32	0/342	0.46	0/474
2	D3	0.31	0/747	0.66	0/1022
3	D1	0.38	0/2472	0.68	2/3380 (0.1%)
4	D6	0.36	0/1339	0.66	1/1810 (0.1%)
5	4L	0.36	0/758	0.74	1/1024 (0.1%)
6	D5	0.38	0/4933	0.72	5/6710 (0.1%)
7	D4	0.38	0/3740	0.71	4/5095 (0.1%)
8	D2	0.38	0/2788	0.67	2/3795 (0.1%)
9	AK	0.32	0/1046	0.66	0/1419
10	B5	0.35	0/1189	0.59	2/1607 (0.1%)
11	AB	0.37	0/714	0.62	0/963
12	A8	0.35	0/1441	0.65	1/1942 (0.1%)
13	BJ	0.35	0/1475	0.57	1/1989 (0.1%)
14	AJ	0.36	0/2644	0.63	4/3579 (0.1%)
15	S5	0.36	0/843	0.62	0/1128
16	A3	0.32	0/602	0.70	1/828 (0.1%)
17	B3	0.36	0/595	0.65	0/803
18	C2	0.36	0/1028	0.61	1/1388 (0.1%)
19	B4	0.35	0/1085	0.64	1/1467 (0.1%)
20	AM	0.36	0/968	0.63	1/1303 (0.1%)
21	B6	0.37	0/830	0.72	2/1130 (0.2%)
22	B7	0.36	0/1051	0.64	2/1408 (0.1%)
23	B9	0.36	0/1568	0.60	1/2123 (0.0%)
24	B2	0.34	0/590	0.61	0/810
25	B8	0.38	0/1379	0.65	1/1884 (0.1%)
26	BK	0.37	0/880	0.61	0/1196
27	C1	0.32	0/404	0.57	0/548
28	B1	0.32	0/462	0.58	0/624
29	A1	0.32	0/592	0.64	1/795 (0.1%)
All	All	0.36	0/38505	0.66	34/52244 (0.1%)

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
3	D1	0	3
4	D6	0	1
6	D5	0	3
7	D4	0	3
9	AK	0	3
12	A8	0	1
13	BJ	0	2
14	AJ	0	1
15	S5	0	1
18	C2	0	2
19	B4	0	1
20	AM	0	1
21	B6	0	1
22	B7	0	1
24	B2	0	1
26	BK	0	1
28	B1	0	1
29	A1	0	1
All	All	0	28

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D5	69	LEU	CA-CB-CG	7.78	133.19	115.30
7	D4	36	LEU	CA-CB-CG	7.42	132.36	115.30
22	B7	27	ASP	CB-CG-OD1	7.40	124.96	118.30
22	B7	19	LEU	CA-CB-CG	6.93	131.24	115.30
3	D1	162	LEU	CA-CB-CG	6.78	130.88	115.30

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D1	61	LEU	Peptide
3	D1	63	PRO	Peptide
3	D1	91	MET	Peptide

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Mol	Chain	Res	Type	Group
6	D5	159	TYR	Peptide
4	D6	115	ILE	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S2	325	0	291	4	0
2	D3	728	0	773	14	0
3	D1	2400	0	2524	29	0
4	D6	1308	0	1329	17	0
5	4L	748	0	794	14	0
6	D5	4805	0	4950	82	0
7	D4	3646	0	3850	71	0
8	D2	2724	0	2930	53	0
9	AK	1025	0	1033	11	0
10	B5	1156	0	1177	14	0
11	AB	702	0	692	3	0
12	A8	1404	0	1384	25	0
13	BJ	1441	0	1417	15	0
14	AJ	2583	0	2547	37	0
15	S5	822	0	820	9	0
16	A3	582	0	583	11	0
17	B3	578	0	570	3	0
18	C2	997	0	983	8	0
19	B4	1059	0	1062	18	0
20	AM	945	0	932	19	0
21	B6	804	0	824	12	0
22	B7	1026	0	995	16	0
23	B9	1515	0	1469	29	0
24	B2	563	0	509	7	0
25	B8	1324	0	1219	23	0
26	BK	853	0	800	15	0
27	C1	391	0	391	4	0
28	B1	449	0	453	3	0
29	A1	577	0	570	2	0
30	A8	25	0	24	0	0
30	B4	27	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	D4	25	0	24	0	0
30	D5	78	0	104	2	0
30	D6	32	0	38	1	0
31	AK	64	0	72	0	0
31	B5	65	0	74	1	0
31	D5	122	0	132	4	0
32	D4	63	0	74	2	0
33	AB	31	0	34	9	0
All	All	38012	0	38474	448	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 448 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)
33:AB:101:ZMP:O1	23:B9:50:HIS:CE1	1.98	1.16
33:AB:101:ZMP:O1	23:B9:50:HIS:HE1	1.32	1.08
7:D4:52:PHE:O	7:D4:56:PHE:HB2	1.64	0.98
33:AB:101:ZMP:C10	23:B9:50:HIS:HE1	1.87	0.87
33:AB:101:ZMP:H20	23:B9:51:LYS:HD3	1.71	0.73

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	S2	37/430 (9%)	32 (86%)	5 (14%)	0	100	100
2	D3	86/115 (75%)	81 (94%)	5 (6%)	0	100	100
3	D1	297/318 (93%)	270 (91%)	27 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D6	167/175 (95%)	143 (86%)	24 (14%)	0	100	100
5	4L	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
6	D5	604/606 (100%)	544 (90%)	60 (10%)	0	100	100
7	D4	457/459 (100%)	418 (92%)	37 (8%)	2 (0%)	30	65
8	D2	345/347 (99%)	320 (93%)	25 (7%)	0	100	100
9	AK	138/140 (99%)	127 (92%)	11 (8%)	0	100	100
10	B5	137/143 (96%)	126 (92%)	11 (8%)	0	100	100
11	AB	85/88 (97%)	75 (88%)	10 (12%)	0	100	100
12	A8	169/171 (99%)	142 (84%)	27 (16%)	0	100	100
13	BJ	169/175 (97%)	158 (94%)	11 (6%)	0	100	100
14	AJ	317/320 (99%)	280 (88%)	37 (12%)	0	100	100
15	S5	97/105 (92%)	78 (80%)	19 (20%)	0	100	100
16	A3	72/83 (87%)	61 (85%)	11 (15%)	0	100	100
17	B3	71/97 (73%)	59 (83%)	11 (16%)	1 (1%)	9	39
18	C2	117/120 (98%)	104 (89%)	13 (11%)	0	100	100
19	B4	126/128 (98%)	110 (87%)	16 (13%)	0	100	100
20	AM	112/143 (78%)	104 (93%)	8 (7%)	0	100	100
21	B6	91/127 (72%)	77 (85%)	14 (15%)	0	100	100
22	B7	117/136 (86%)	99 (85%)	18 (15%)	0	100	100
23	B9	174/178 (98%)	145 (83%)	29 (17%)	0	100	100
24	B2	63/72 (88%)	52 (82%)	11 (18%)	0	100	100
25	B8	155/158 (98%)	119 (77%)	36 (23%)	0	100	100
26	BK	100/125 (80%)	81 (81%)	19 (19%)	0	100	100
27	C1	44/49 (90%)	41 (93%)	3 (7%)	0	100	100
28	B1	50/57 (88%)	42 (84%)	8 (16%)	0	100	100
29	A1	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
All	All	4561/5233 (87%)	4042 (89%)	516 (11%)	3 (0%)	50	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	D4	53	SER
17	B3	58	ASN

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Mol	Chain	Res	Type
7	D4	181	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S2	33/371 (9%)	32 (97%)	1 (3%)	36	58
2	D3	81/103 (79%)	80 (99%)	1 (1%)	67	78
3	D1	264/278 (95%)	263 (100%)	1 (0%)	89	91
4	D6	140/144 (97%)	140 (100%)	0	100	100
5	4L	87/87 (100%)	85 (98%)	2 (2%)	45	64
6	D5	539/539 (100%)	532 (99%)	7 (1%)	65	76
7	D4	412/412 (100%)	408 (99%)	4 (1%)	73	81
8	D2	315/315 (100%)	311 (99%)	4 (1%)	65	76
9	AK	101/101 (100%)	99 (98%)	2 (2%)	50	68
10	B5	122/125 (98%)	120 (98%)	2 (2%)	58	73
11	AB	80/81 (99%)	78 (98%)	2 (2%)	42	62
12	A8	154/154 (100%)	150 (97%)	4 (3%)	41	61
13	BJ	155/157 (99%)	153 (99%)	2 (1%)	65	76
14	AJ	283/284 (100%)	281 (99%)	2 (1%)	81	86
15	S5	88/94 (94%)	88 (100%)	0	100	100
16	A3	65/71 (92%)	65 (100%)	0	100	100
17	B3	55/75 (73%)	53 (96%)	2 (4%)	30	54
18	C2	106/107 (99%)	106 (100%)	0	100	100
19	B4	114/114 (100%)	113 (99%)	1 (1%)	75	83
20	AM	98/121 (81%)	95 (97%)	3 (3%)	35	56
21	B6	91/121 (75%)	90 (99%)	1 (1%)	70	79
22	B7	108/119 (91%)	105 (97%)	3 (3%)	38	59
23	B9	159/160 (99%)	156 (98%)	3 (2%)	52	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	B2	59/62 (95%)	59 (100%)	0	100	100
25	B8	142/142 (100%)	140 (99%)	2 (1%)	62	75
26	BK	93/112 (83%)	91 (98%)	2 (2%)	47	65
27	C1	42/44 (96%)	42 (100%)	0	100	100
28	B1	48/53 (91%)	48 (100%)	0	100	100
29	A1	59/59 (100%)	56 (95%)	3 (5%)	20	45
All	All	4093/4605 (89%)	4039 (99%)	54 (1%)	64	76

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	A8	134	ARG
17	B3	58	ASN
26	BK	27	GLN
12	A8	150	ASN
14	AJ	92	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
13	BJ	113	GLN
29	A1	68	ASN
17	B3	47	ASN
29	A1	58	ASN
25	B8	104	HIS

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

13 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
31	CDL	D5	901	-	59,59,99	0.38	0	65,71,111	0.53	1 (1%)
30	3PE	D5	903	-	39,39,50	0.33	0	42,44,55	0.31	0
30	3PE	D4	702	-	24,24,50	0.42	0	27,29,55	0.42	0
30	3PE	D6	501	-	31,31,50	0.37	0	34,36,55	0.40	0
30	3PE	B4	201	-	26,26,50	0.48	0	30,31,55	0.54	1 (3%)
31	CDL	D5	904	-	61,61,99	0.38	0	67,73,111	0.49	1 (1%)
31	CDL	B5	201	-	64,64,99	0.38	0	70,76,111	0.51	1 (1%)
32	PC1	D4	701	-	34,34,53	0.35	0	40,42,61	0.38	0
33	ZMP	AB	101	11	24,30,36	0.70	0	29,37,45	1.02	2 (6%)
32	PC1	D4	703	-	27,27,53	0.39	0	33,35,61	0.40	0
30	3PE	A8	301	-	24,24,50	0.43	0	27,29,55	0.34	0
31	CDL	AK	501	-	63,63,99	0.36	0	69,75,111	0.30	0
30	3PE	D5	902	-	37,37,50	0.34	0	40,42,55	0.36	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
31	CDL	D5	901	-	-	18/70/70/110	-
30	3PE	D5	903	-	-	9/43/43/54	-
30	3PE	D4	702	-	-	9/28/28/54	-
30	3PE	D6	501	-	-	8/35/35/54	-
30	3PE	B4	201	-	-	2/27/27/54	-
31	CDL	D5	904	-	-	21/72/72/110	-
31	CDL	B5	201	-	-	19/75/75/110	-
32	PC1	D4	701	-	-	7/38/38/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	ZMP	AB	101	11	-	11/35/37/43	-
32	PC1	D4	703	-	-	12/31/31/57	-
30	3PE	A8	301	-	-	4/28/28/54	-
31	CDL	AK	501	-	-	22/74/74/110	-
30	3PE	D5	902	-	-	9/41/41/54	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	AB	101	ZMP	O1-C10-C9	-2.45	121.10	123.99
33	AB	101	ZMP	C11-C12-N1	-2.35	107.48	112.42
31	D5	904	CDL	CA4-OA6-CA5	2.26	123.35	117.79
31	D5	901	CDL	CB4-OB6-CB5	2.19	123.19	117.79
31	B5	201	CDL	CB4-OB6-CB5	2.18	123.16	117.79

There are no chirality outliers.

5 of 151 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	D6	501	3PE	C1-O11-P-O12
30	D6	501	3PE	C11-O13-P-O12
30	D6	501	3PE	O13-C11-C12-N
30	D5	902	3PE	C11-O13-P-O12
30	D5	902	3PE	C11-O13-P-O14

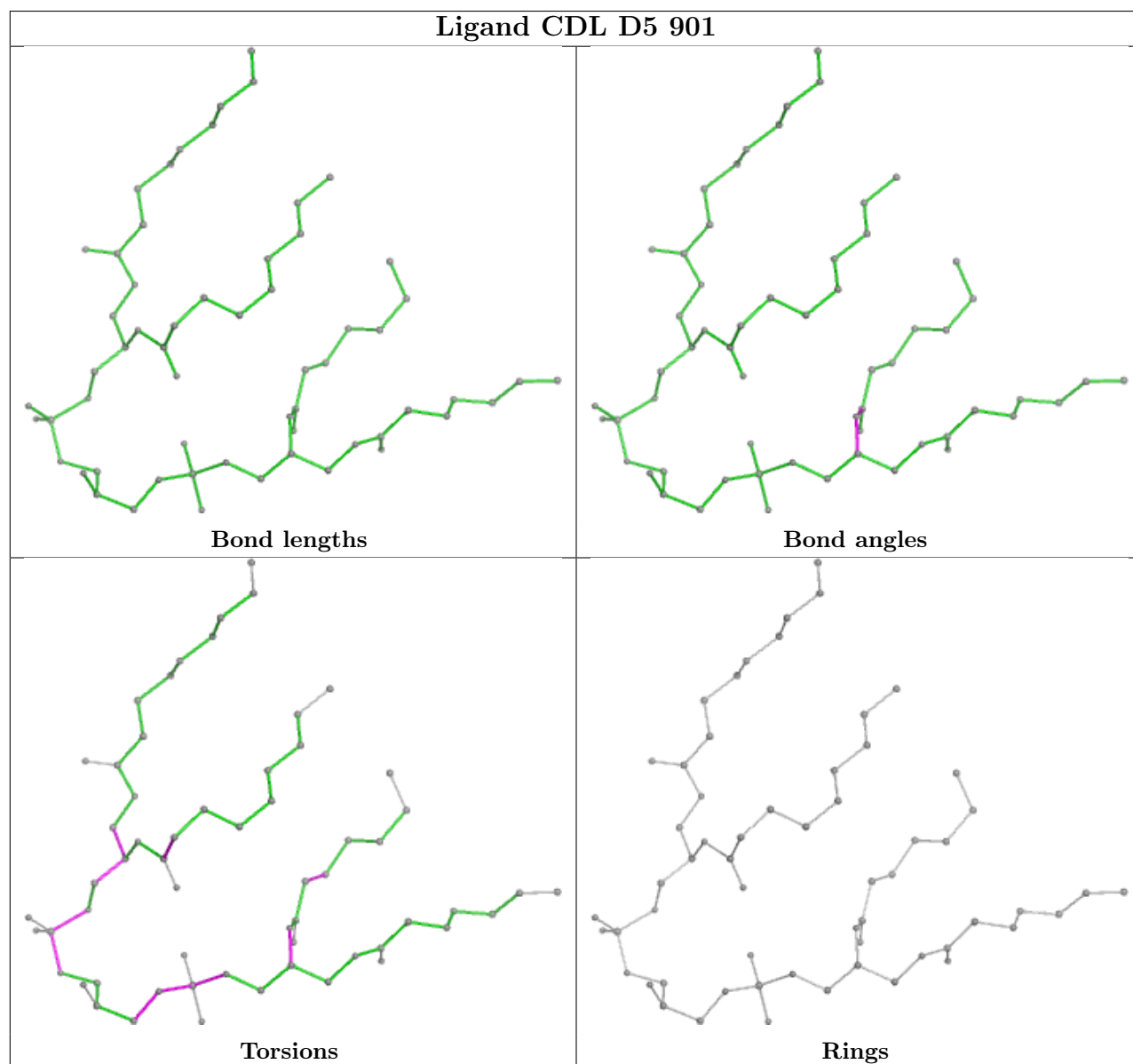
There are no ring outliers.

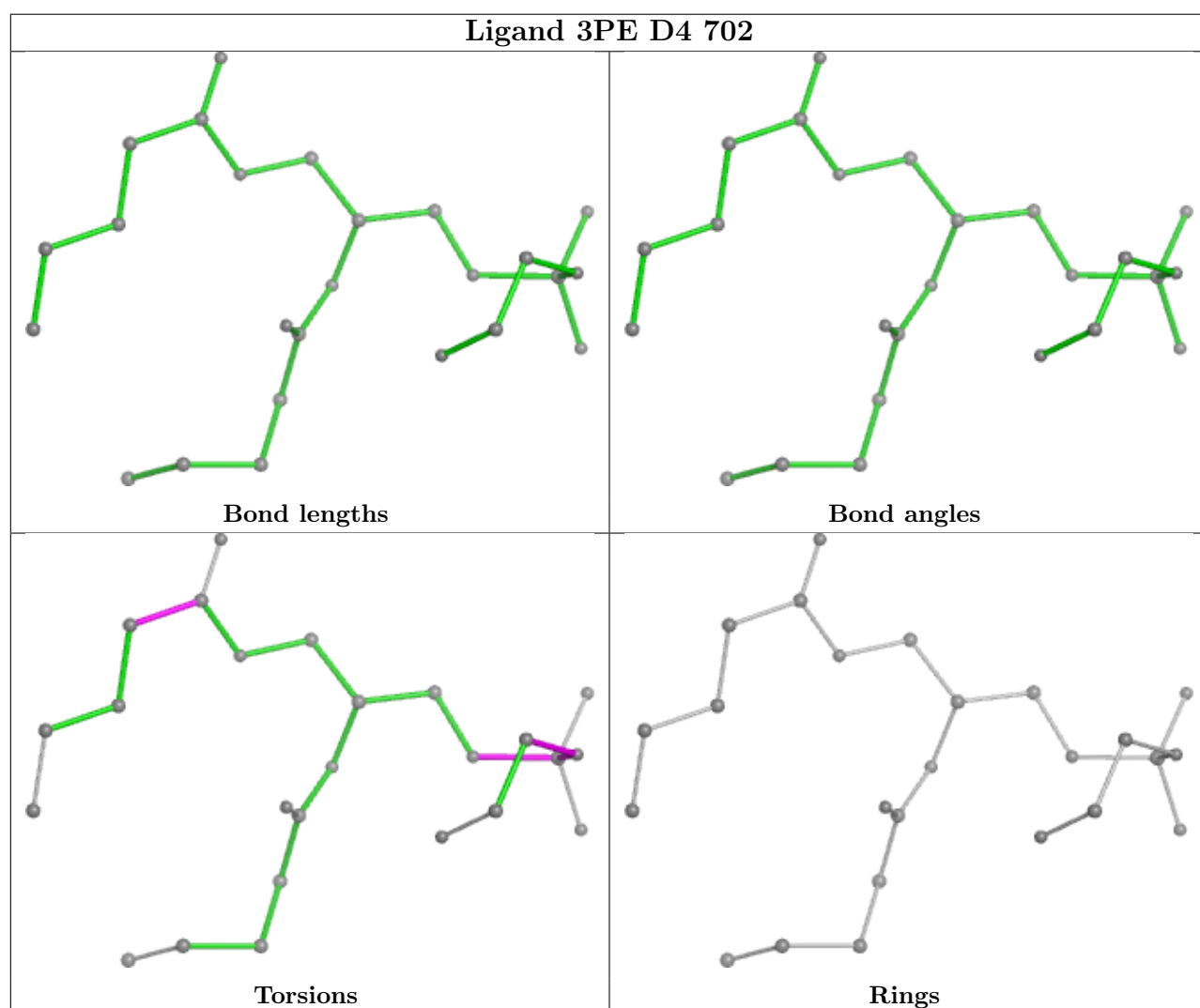
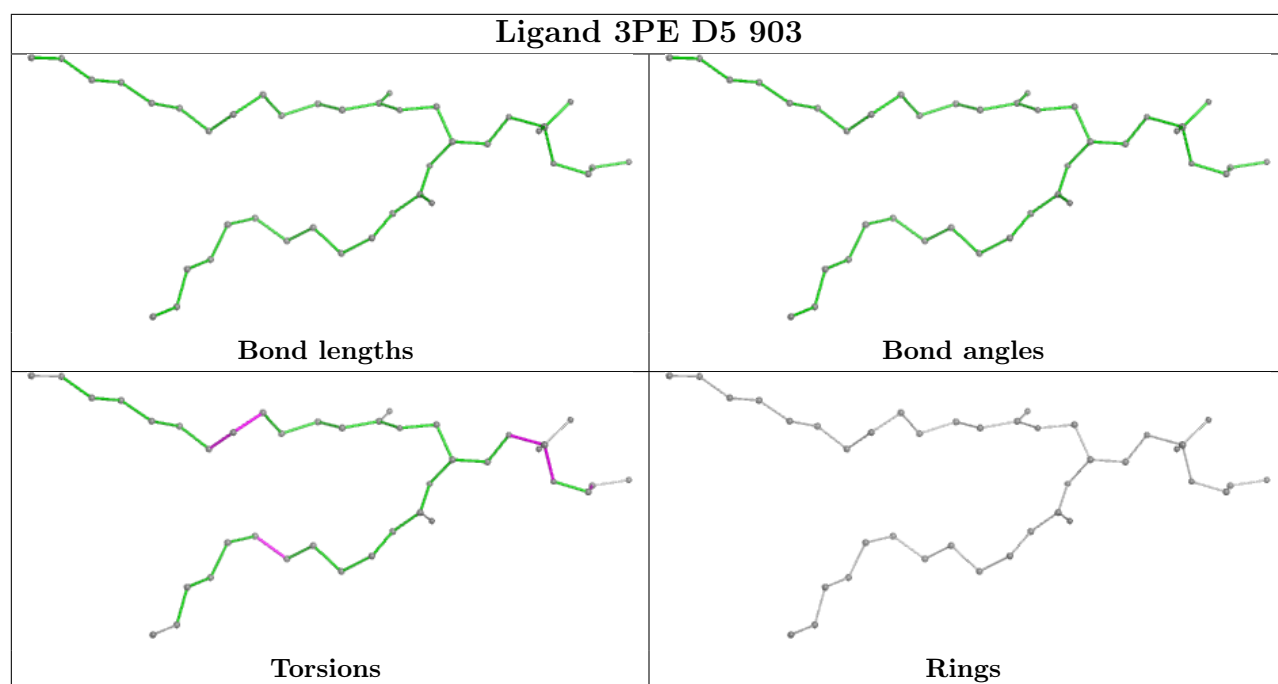
8 monomers are involved in 19 short contacts:

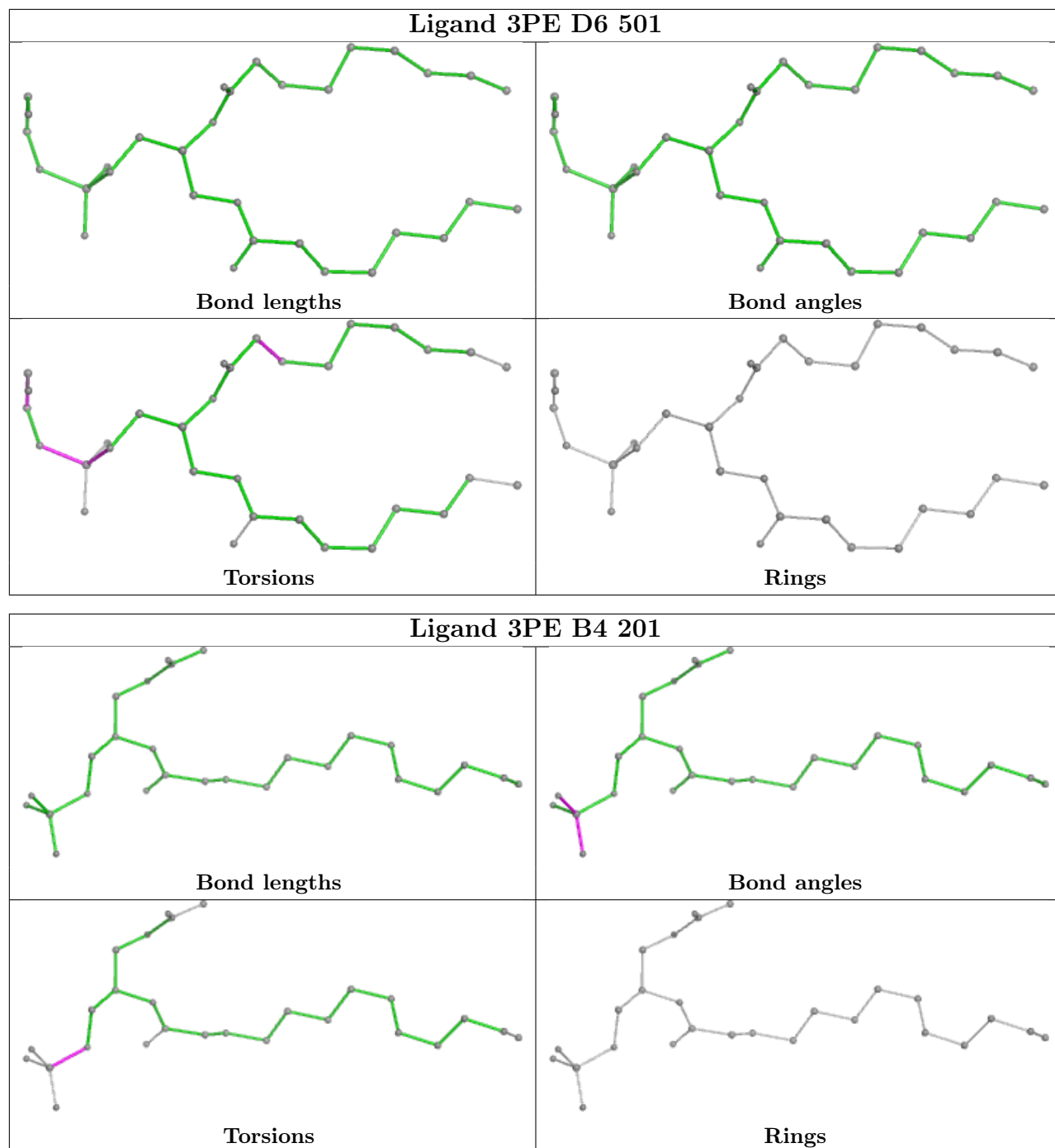
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	D5	901	CDL	2	0
30	D5	903	3PE	1	0
30	D6	501	3PE	1	0
31	D5	904	CDL	2	0
31	B5	201	CDL	1	0
32	D4	701	PC1	2	0
33	AB	101	ZMP	9	0
30	D5	902	3PE	1	0

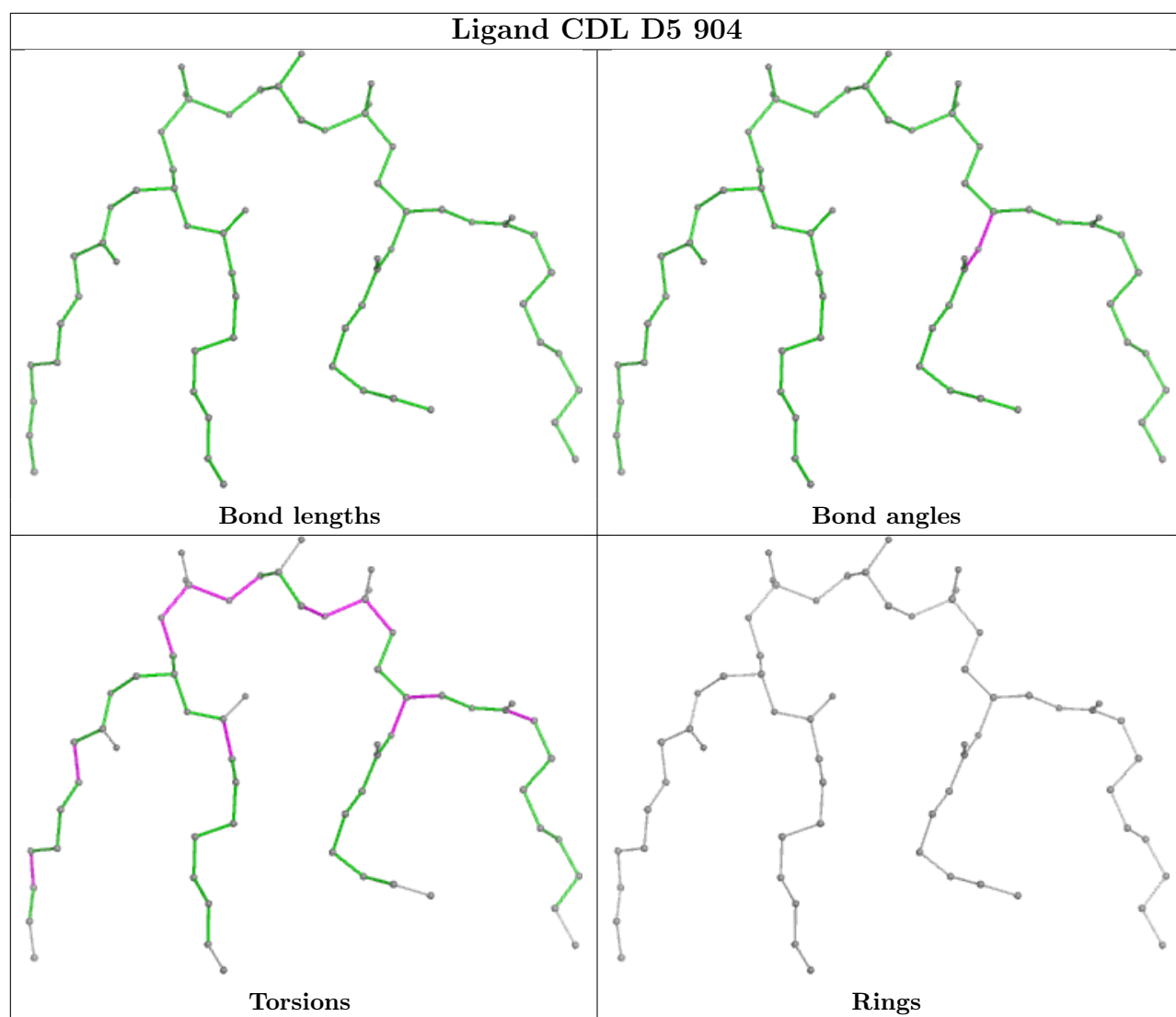
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

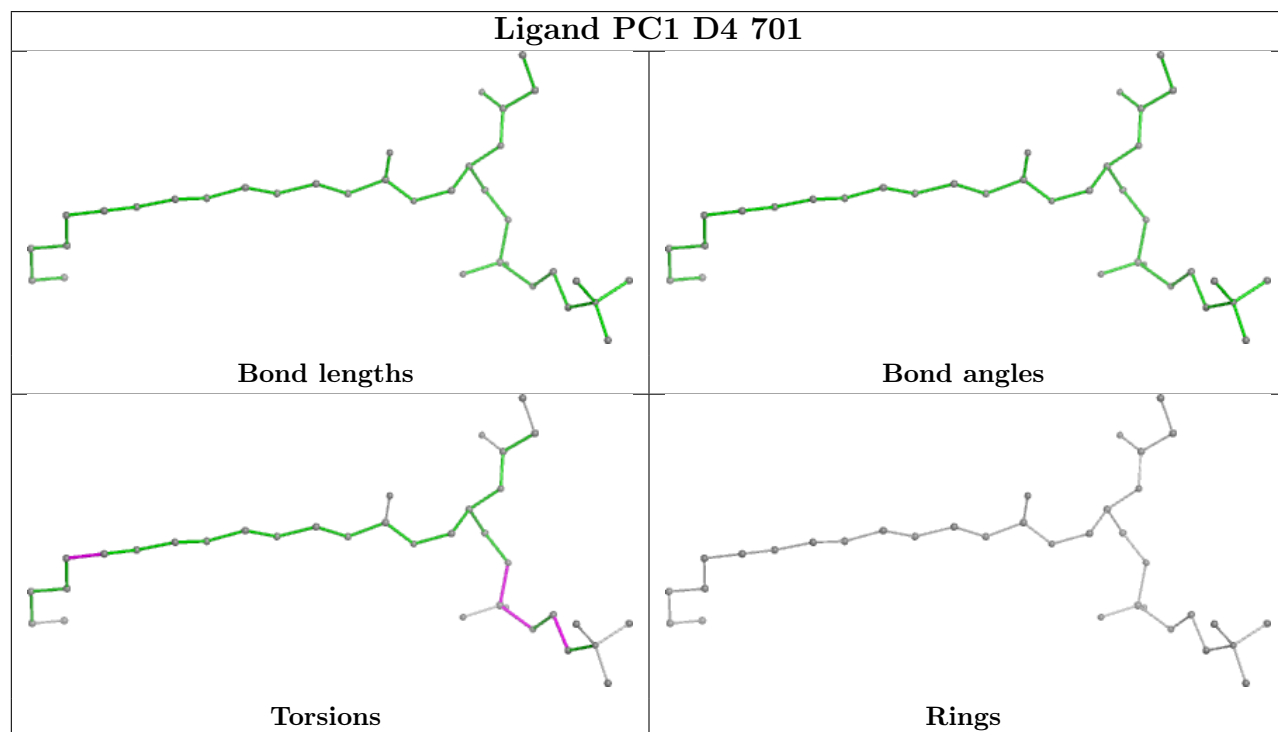
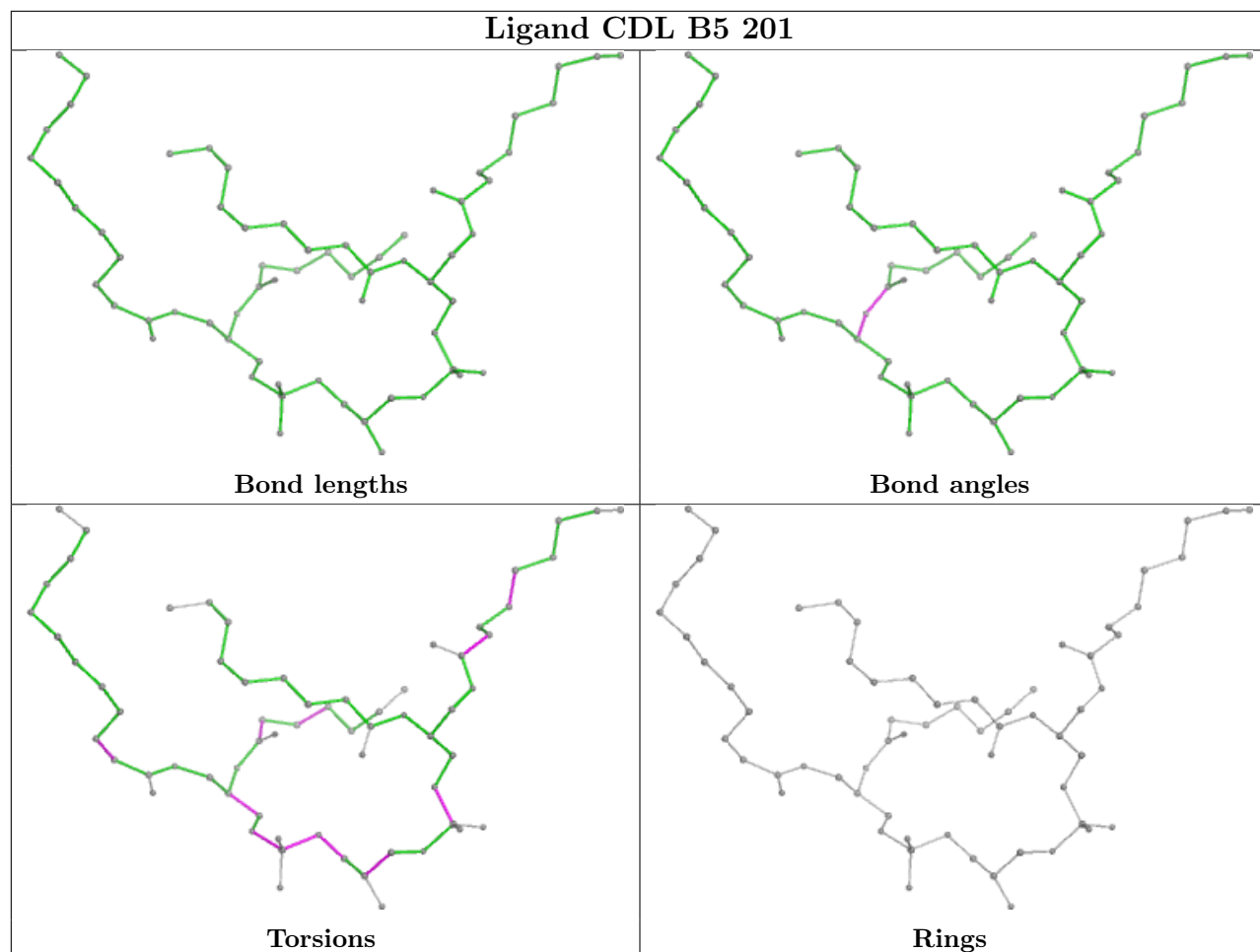
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

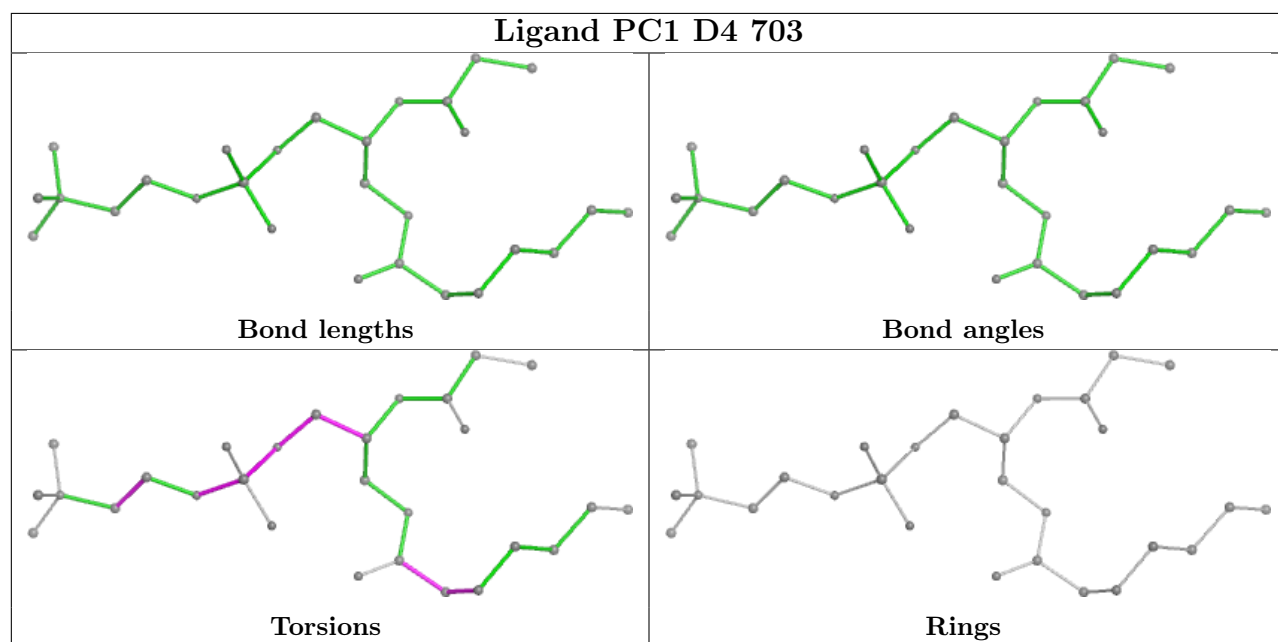
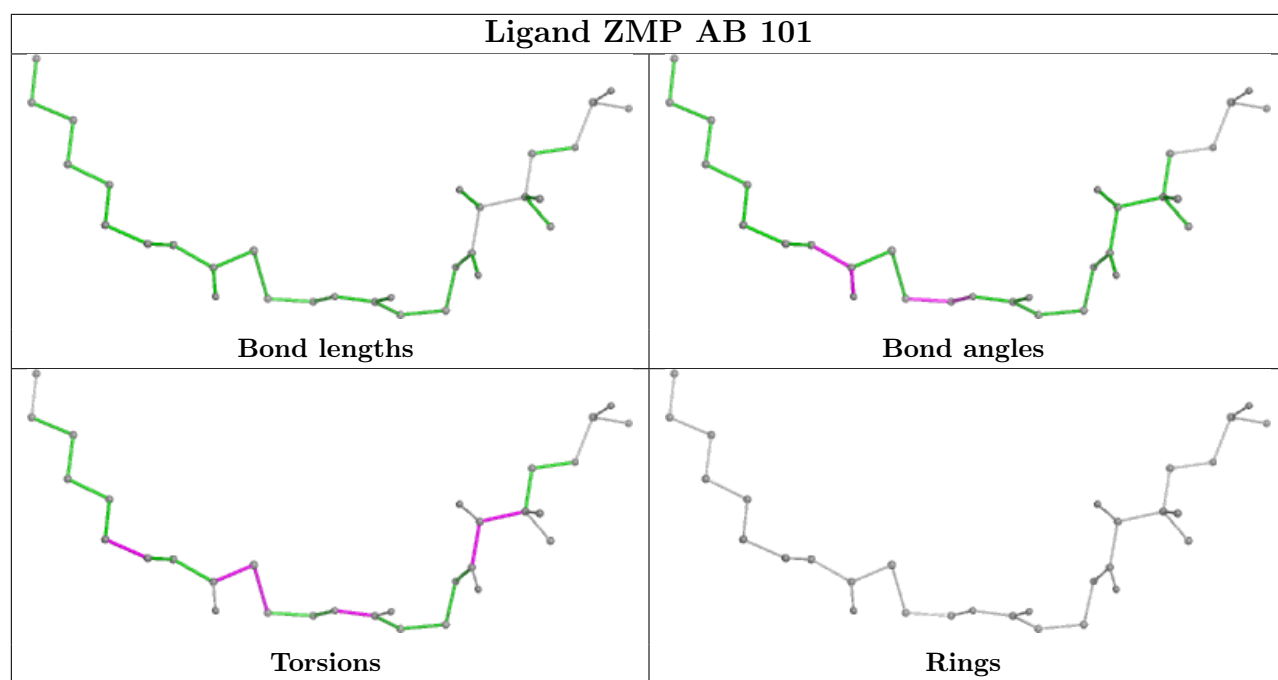


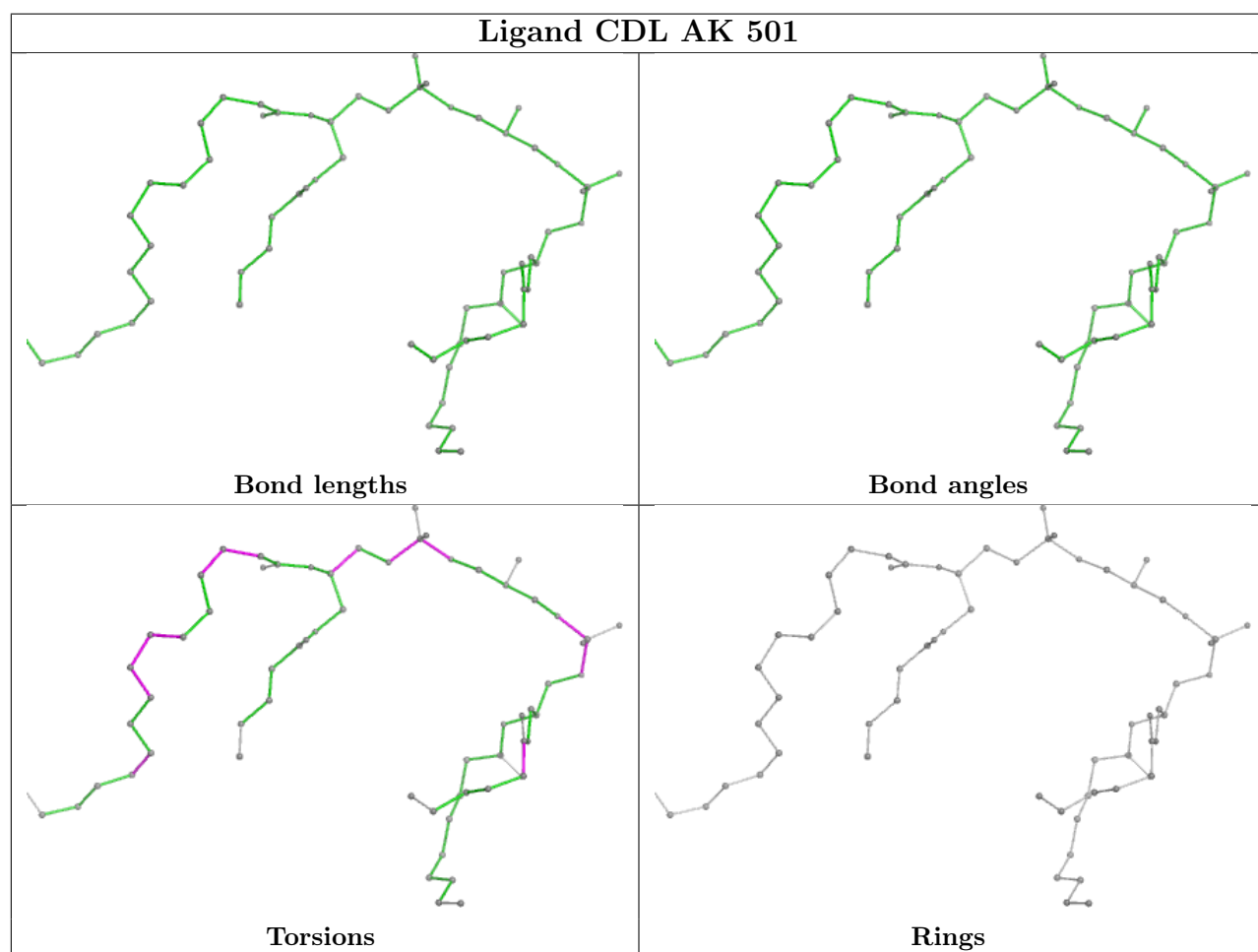
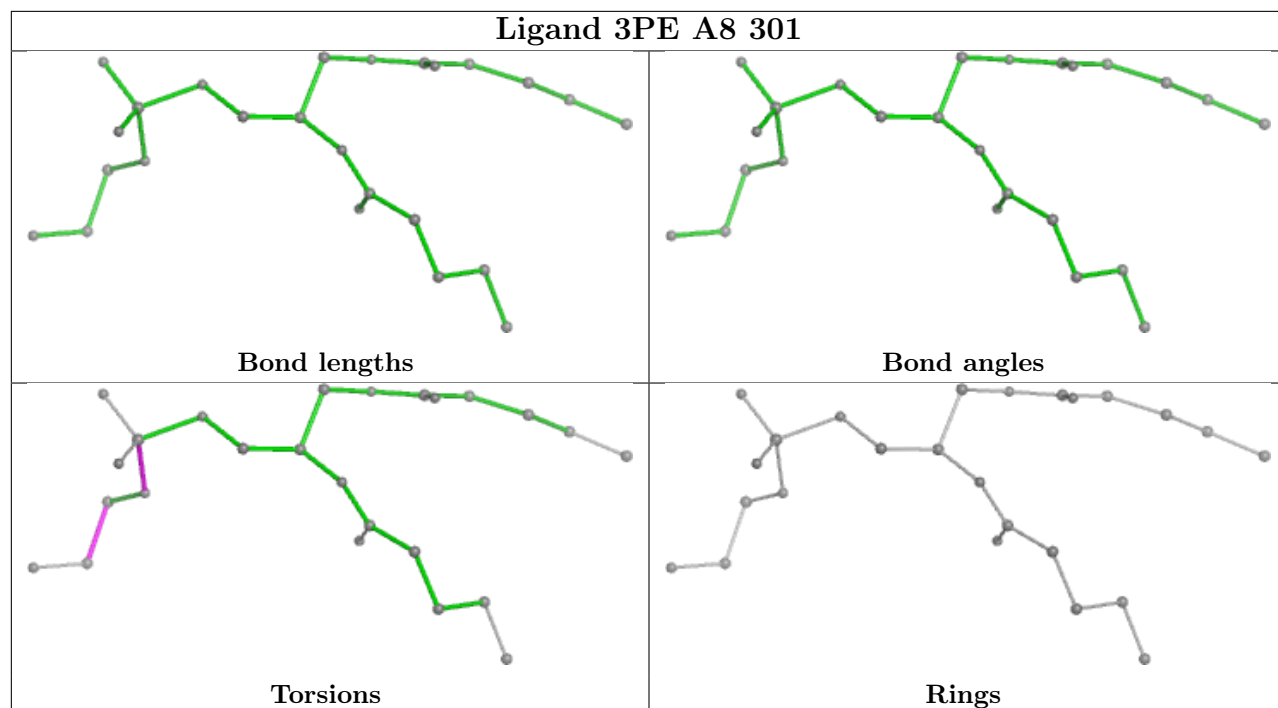


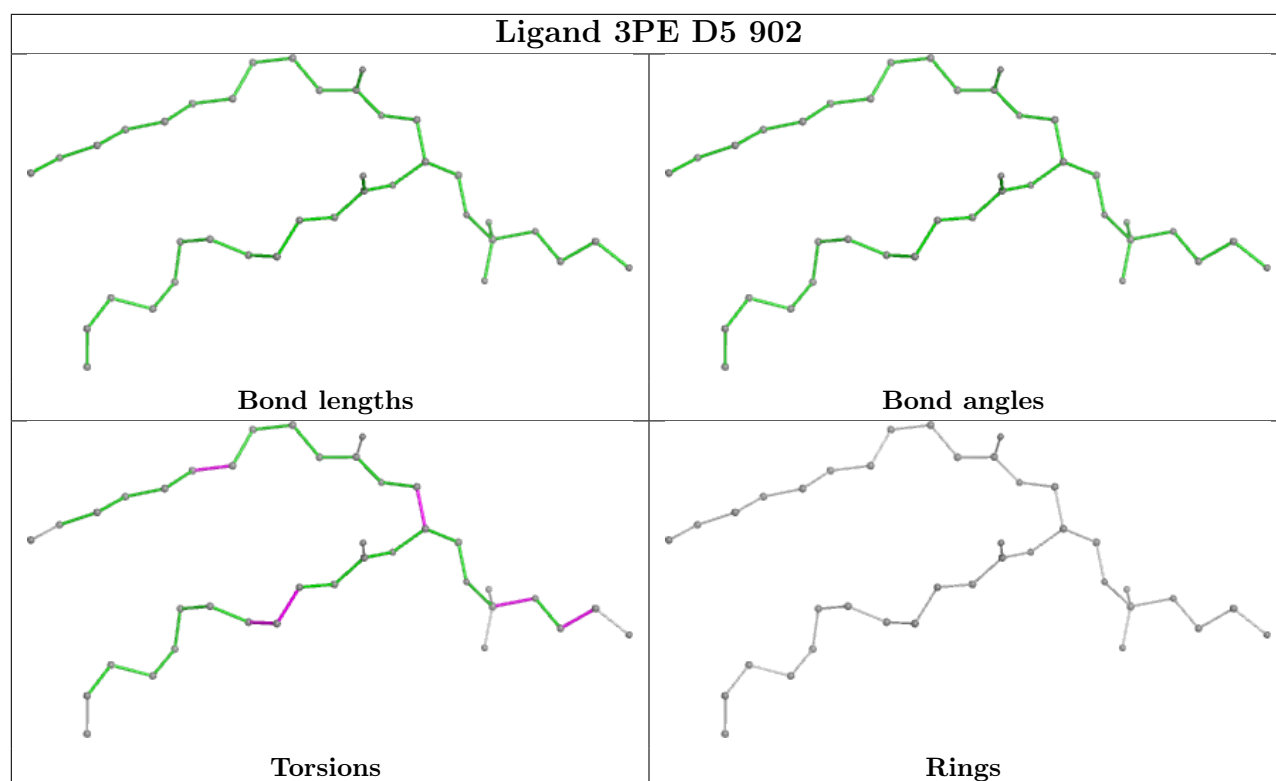












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

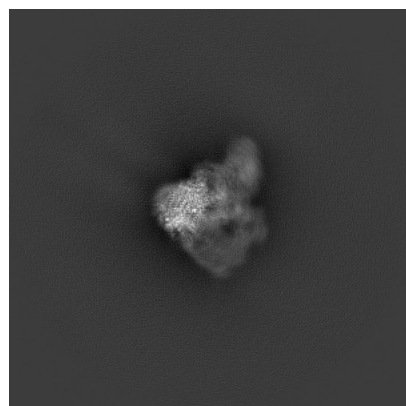
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4479. These allow visual inspection of the internal detail of the map and identification of artifacts.

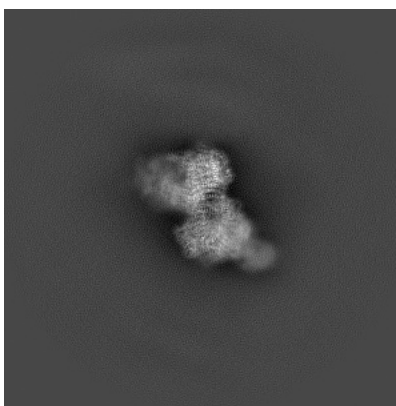
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

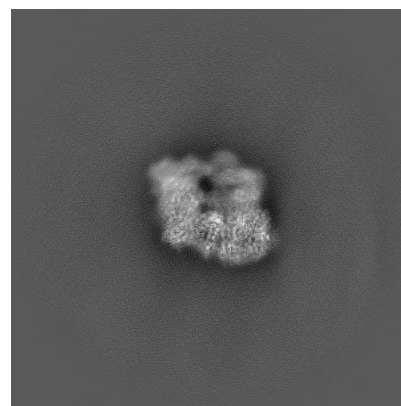
6.1.1 Primary map



X

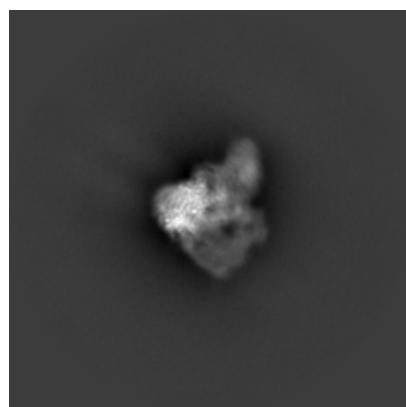


Y

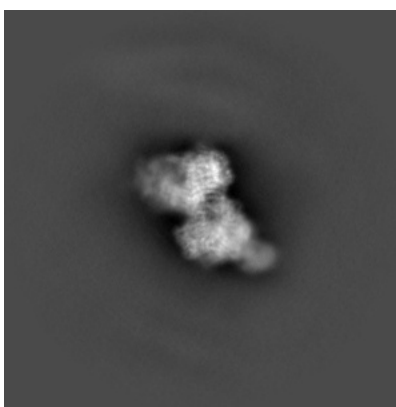


Z

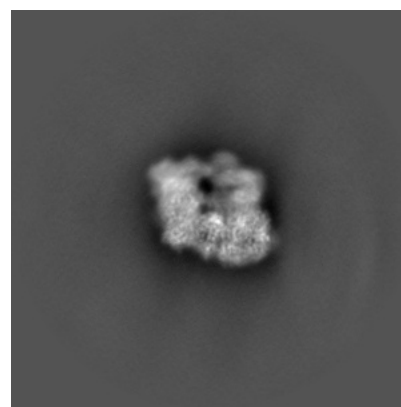
6.1.2 Raw map



X



Y

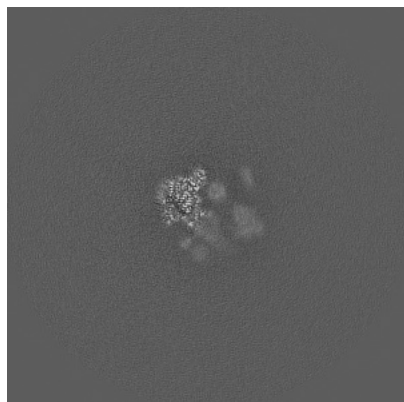


Z

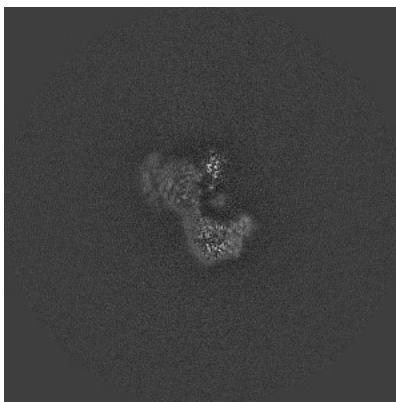
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

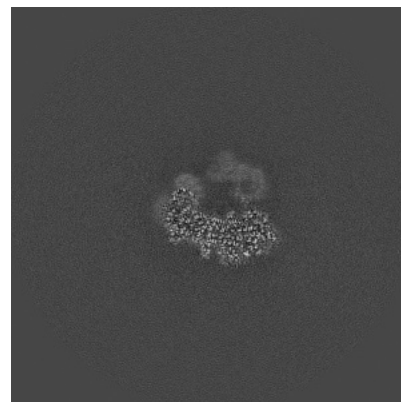
6.2.1 Primary map



X Index: 256

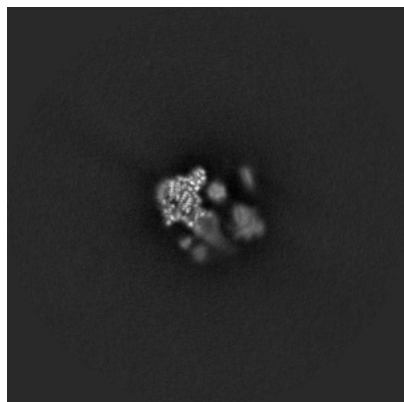


Y Index: 256

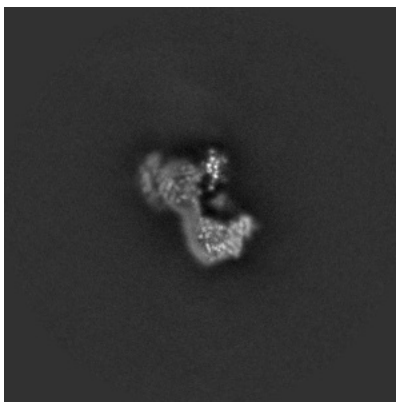


Z Index: 256

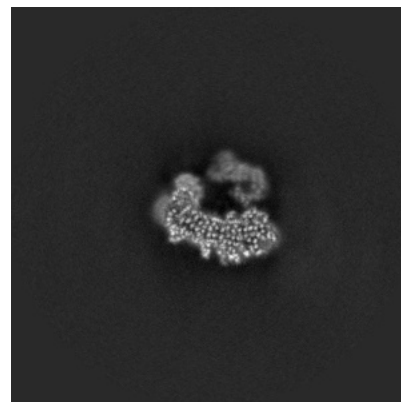
6.2.2 Raw map



X Index: 256



Y Index: 256

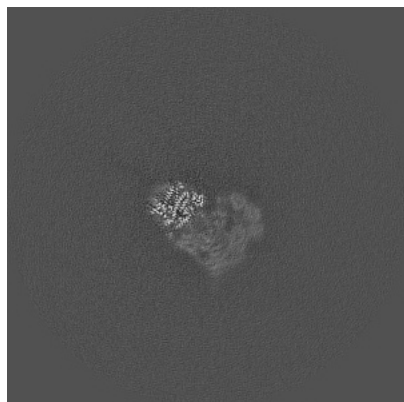


Z Index: 256

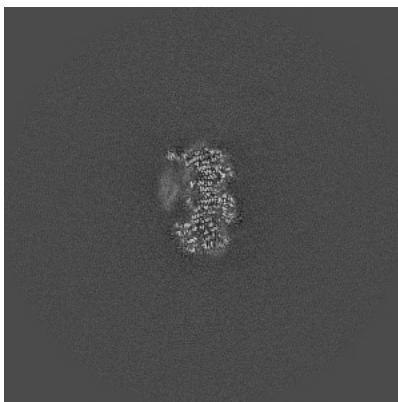
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

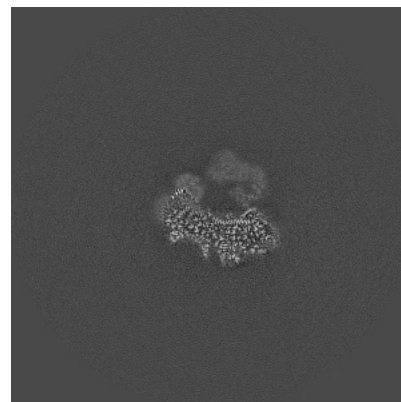
6.3.1 Primary map



X Index: 285

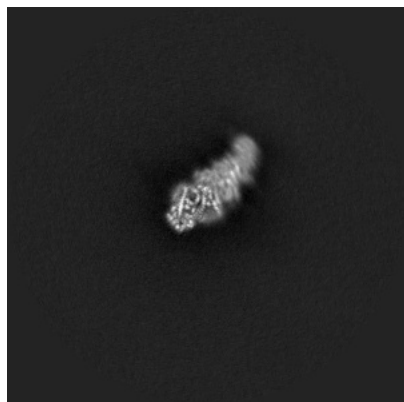


Y Index: 229

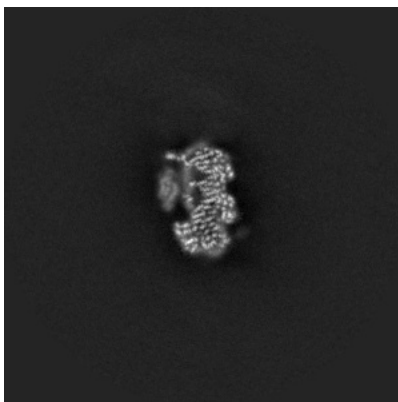


Z Index: 254

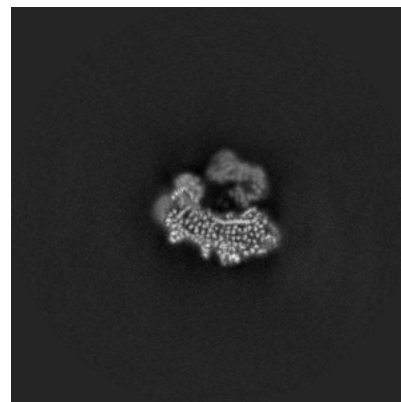
6.3.2 Raw map



X Index: 207



Y Index: 230

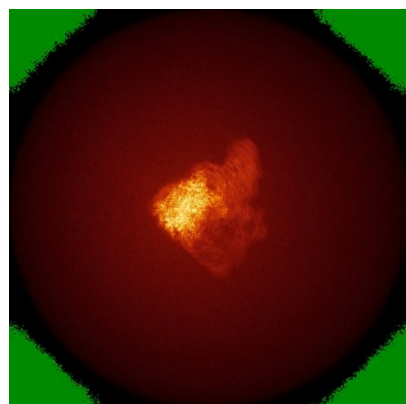


Z Index: 254

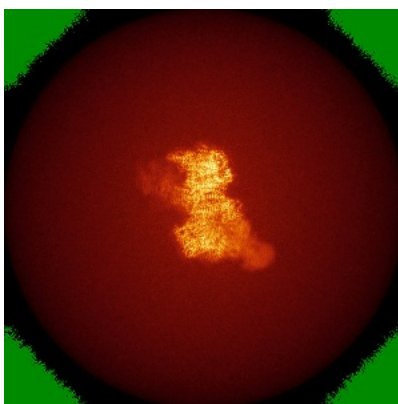
The images above show the largest variance slices of the map in three orthogonal directions.

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

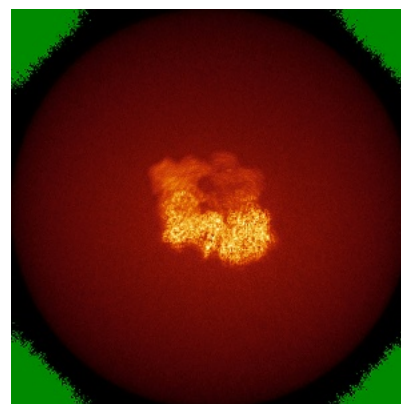
6.4.1 Primary map



X

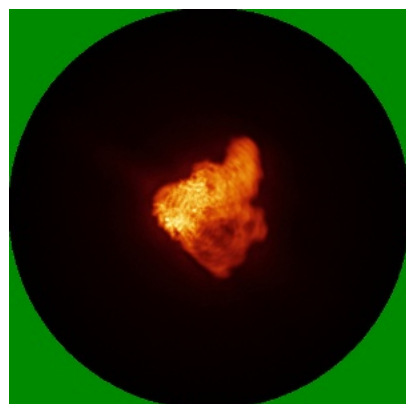


Y

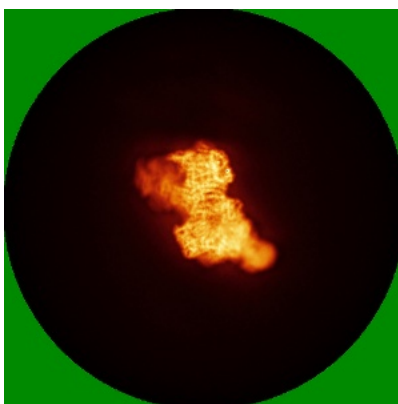


Z

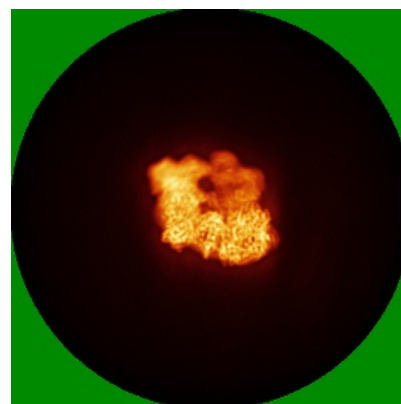
6.4.2 Raw map



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

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

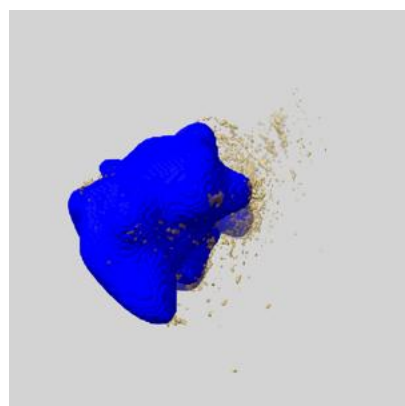
6.6 Mask visualisation [i](#)

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

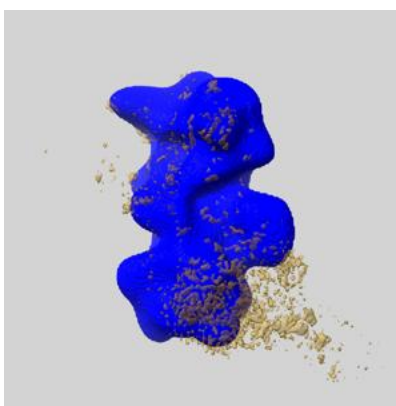
A mask typically either:

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

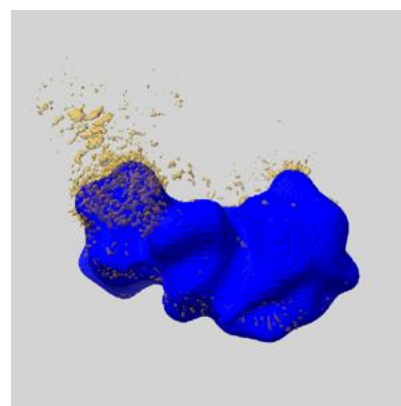
6.6.1 emd_4479_msk_1.map [i](#)



X



Y

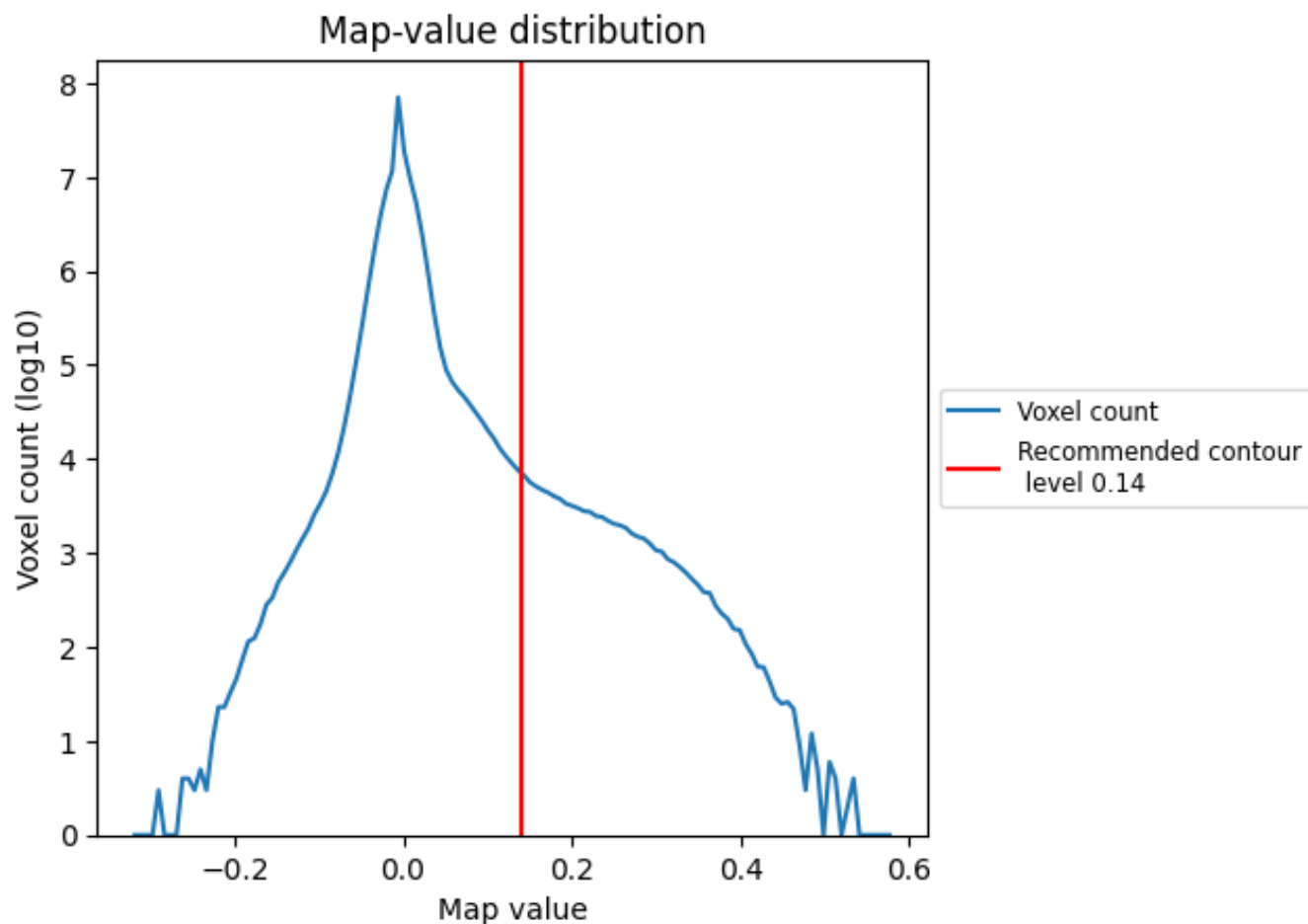


Z

7 Map analysis [i](#)

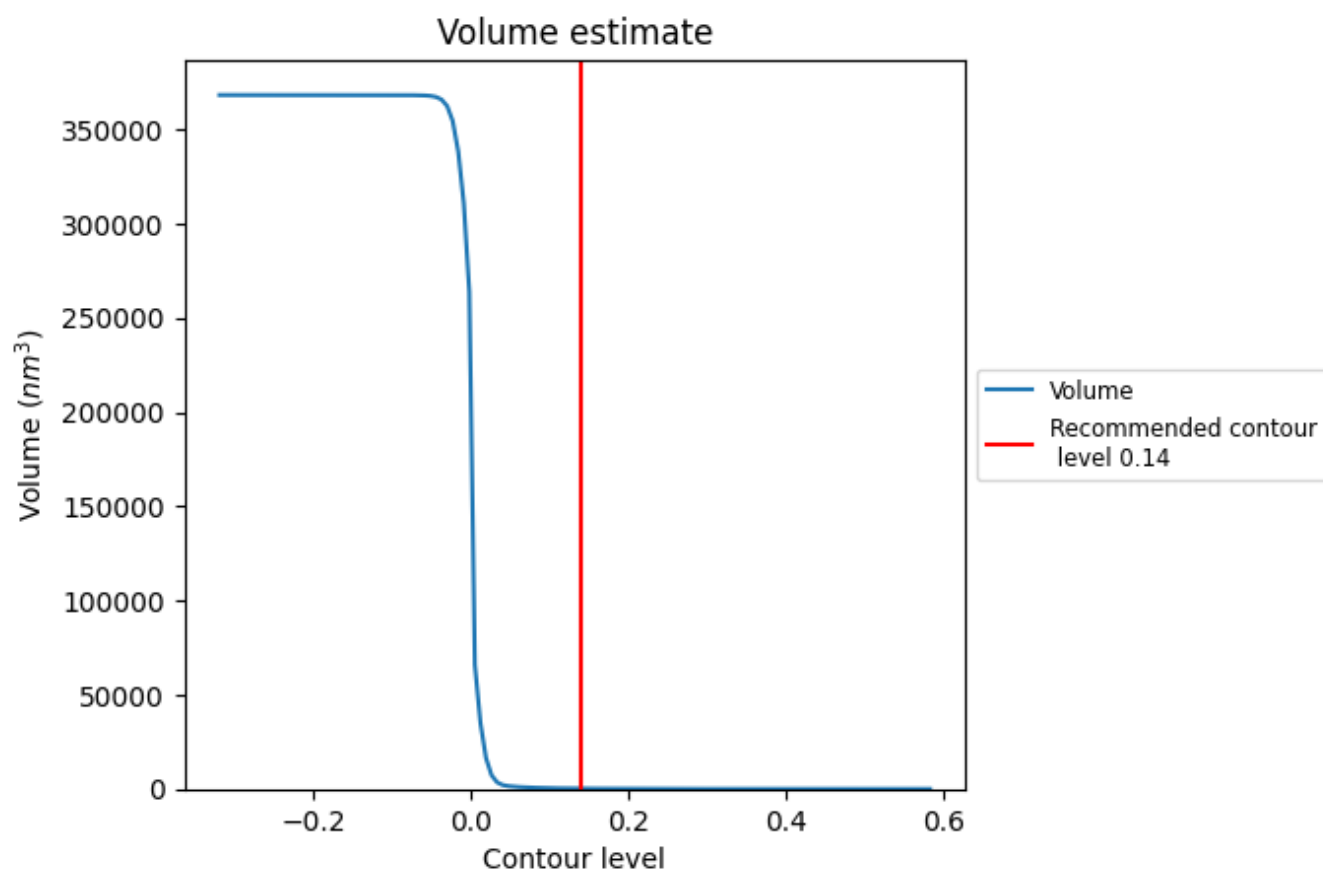
This section contains the results of statistical analysis of the map.

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.

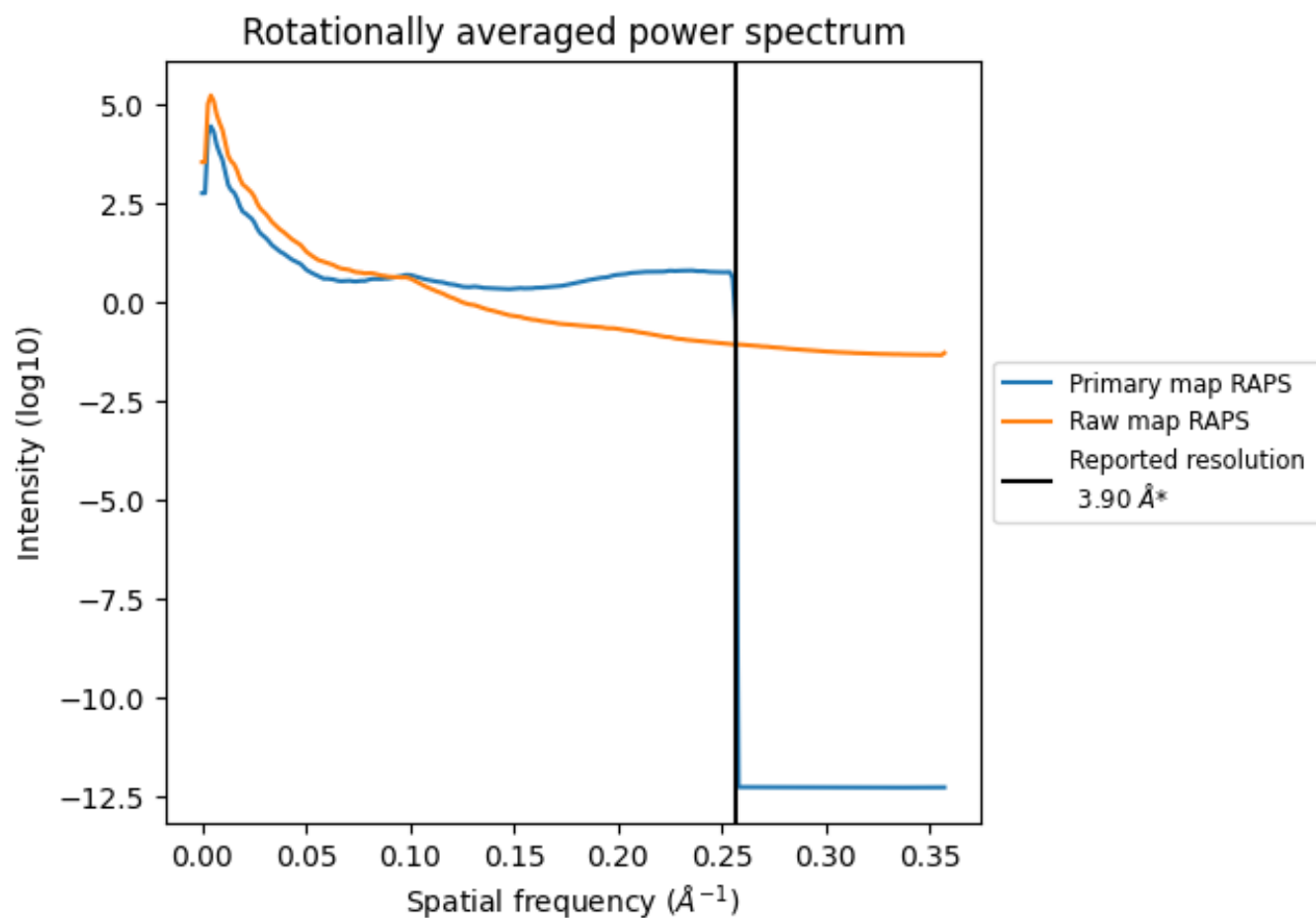
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 220 nm³; this corresponds to an approximate mass of 199 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

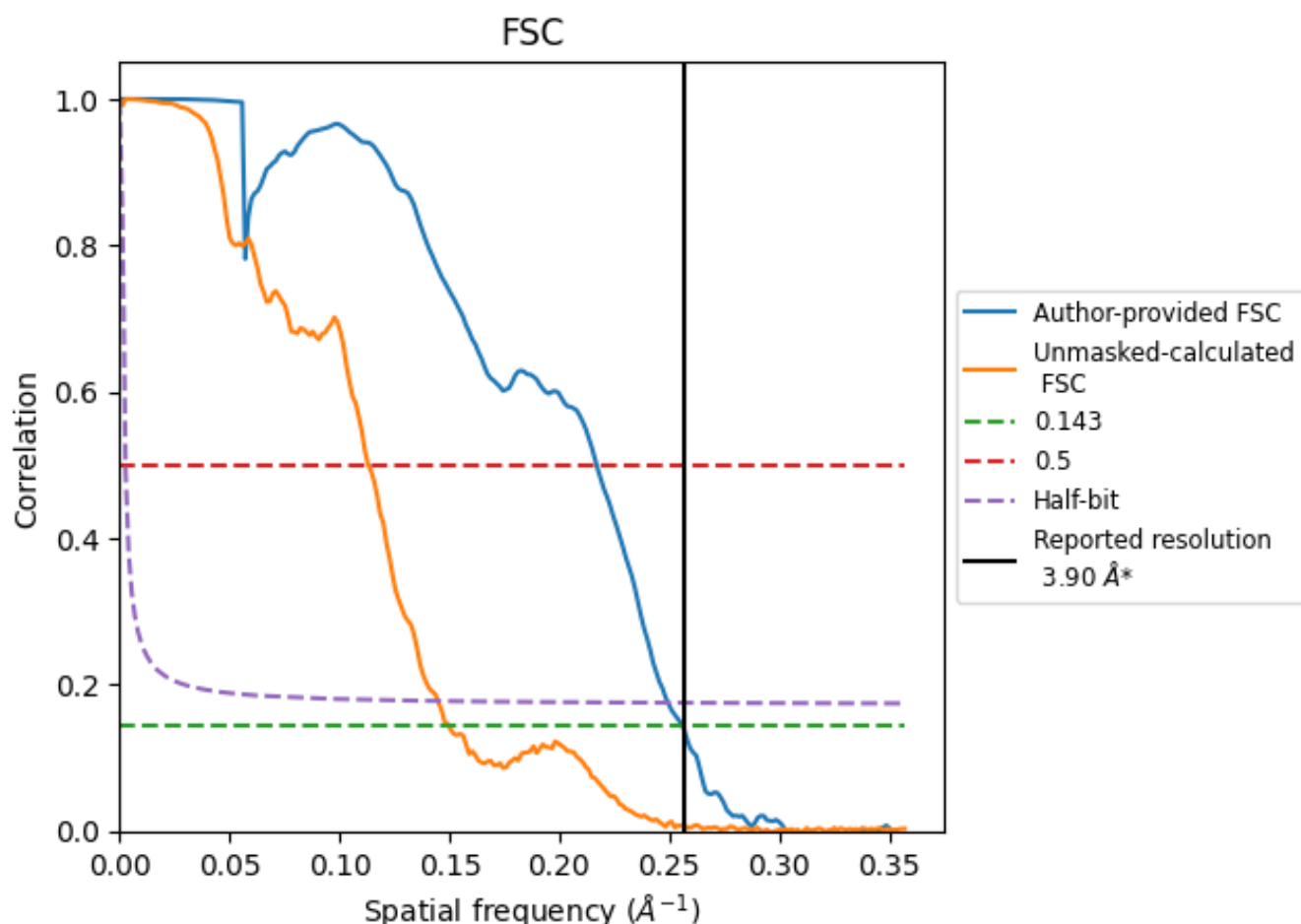


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 \AA^{-1}

8.2 Resolution estimates [i](#)

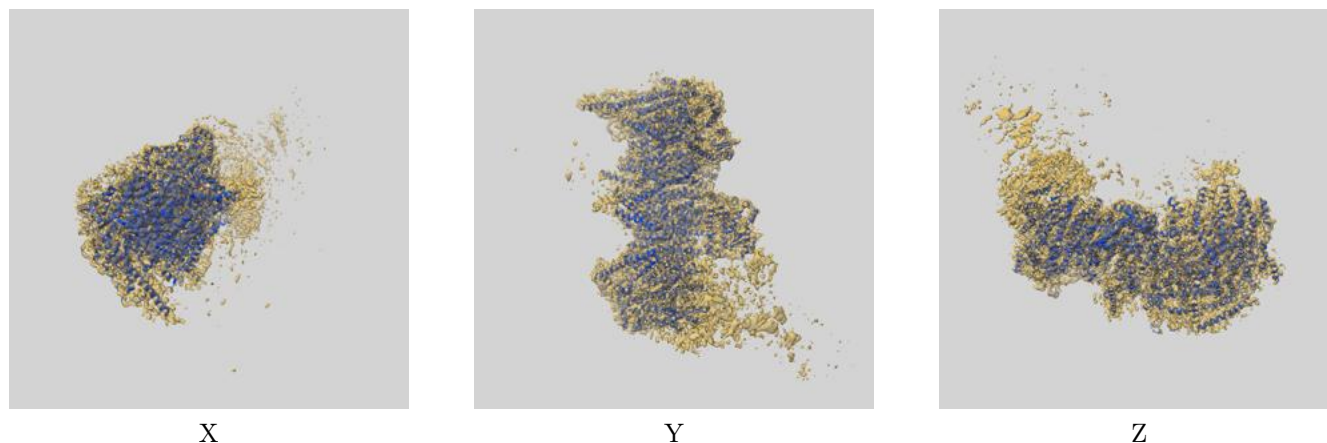
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.91	4.61	4.01
Unmasked-calculated*	6.68	8.84	6.91

*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 6.68 differs from the reported value 3.9 by more than 10 %

9 Map-model fit ⓘ

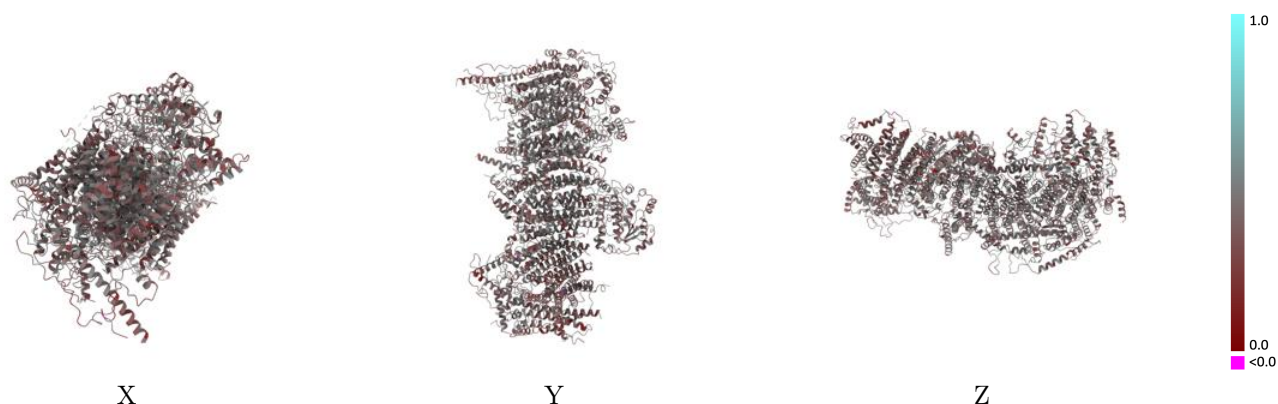
This section contains information regarding the fit between EMDB map EMD-4479 and PDB model 6Q9B. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay ⓘ



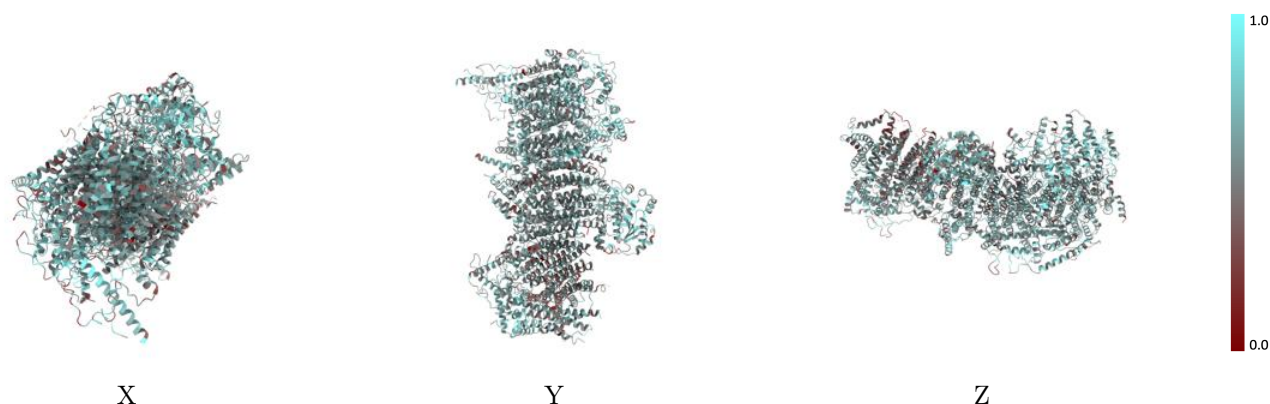
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



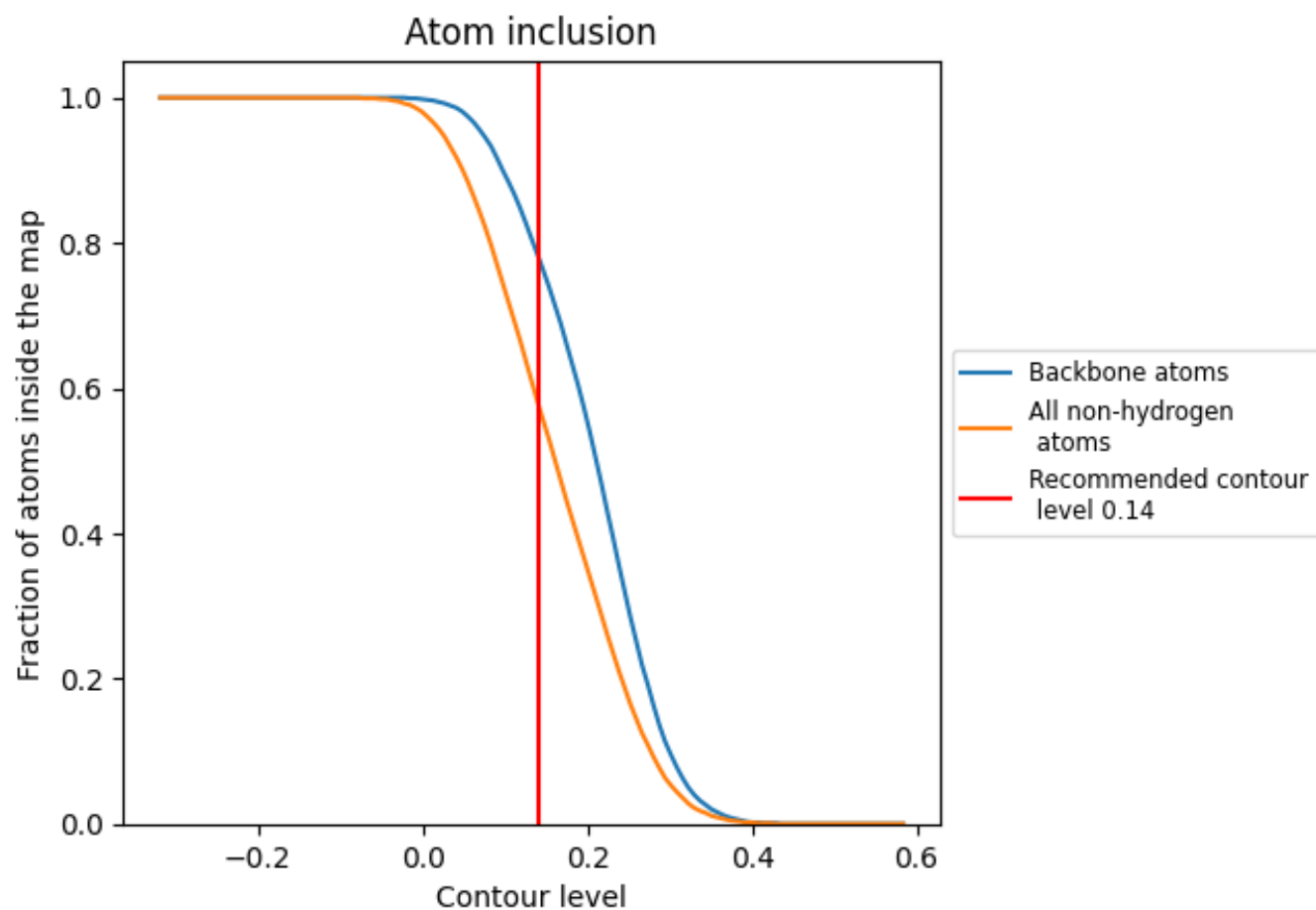
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.14).





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 58% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5800	 0.4030
4L	 0.5120	 0.3970
A1	 0.6260	 0.4180
A3	 0.5350	 0.3850
A8	 0.6190	 0.4020
AB	 0.6180	 0.3880
AJ	 0.6060	 0.3990
AK	 0.4780	 0.3970
AM	 0.6250	 0.3910
B1	 0.5270	 0.3780
B2	 0.5840	 0.3750
B3	 0.5940	 0.3840
B4	 0.5900	 0.4140
B5	 0.6200	 0.4210
B6	 0.6210	 0.3980
B7	 0.6320	 0.3700
B8	 0.6090	 0.4110
B9	 0.6720	 0.4110
BJ	 0.6450	 0.4060
BK	 0.5980	 0.3960
C1	 0.6070	 0.4100
C2	 0.6140	 0.4060
D1	 0.5260	 0.3730
D2	 0.5700	 0.4200
D3	 0.4700	 0.3790
D4	 0.5820	 0.4290
D5	 0.5610	 0.4160
D6	 0.4690	 0.3780
S2	 0.5110	 0.4090
S5	 0.6080	 0.3920

