



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 10:04 AM UTC

PDB ID : 6TT7 / pdb_00006tt7
EMDB ID : EMD-10573
Title : Ovine ATP synthase 1a state
Authors : Pinke, G.; Zhou, L.; Sazanov, L.A.
Deposited on : 2019-12-23
Resolution : 3.50 Å (reported)
Based on initial model : 5ARA

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:

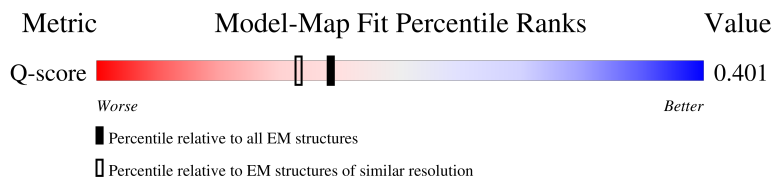
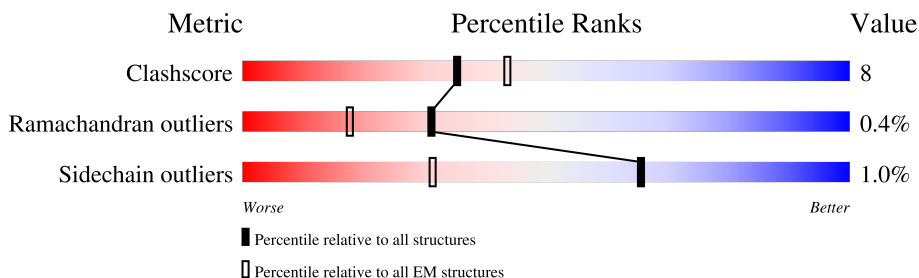
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.50 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.



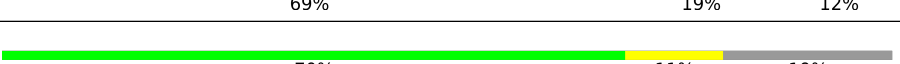
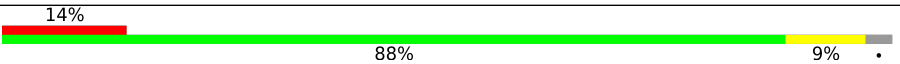
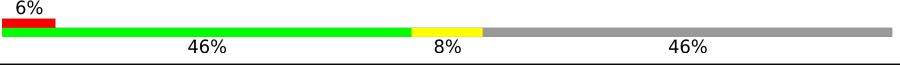
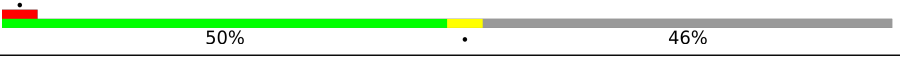
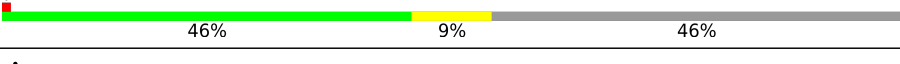
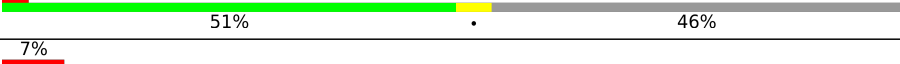
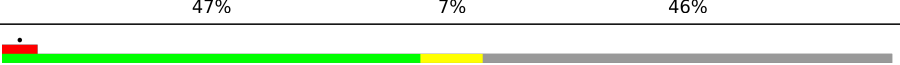
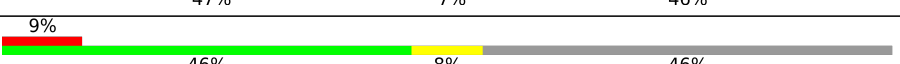
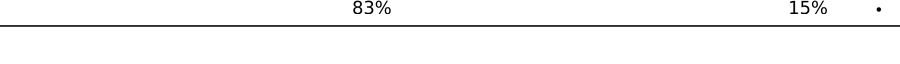
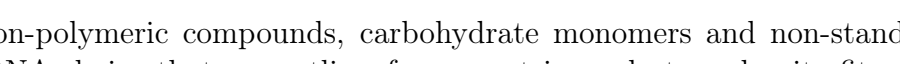
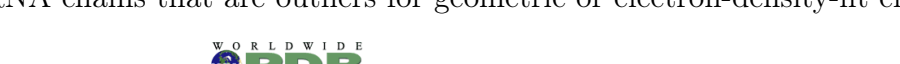
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	A	553	
1	B	553	
1	C	553	
2	D	528	

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Mol	Chain	Length	Quality of chain
2	E	528	
2	F	528	
3	G	298	
4	H	168	
5	I	51	
6	J	213	
7	K	256	
8	L	108	
9	M	161	
10	1	136	
10	2	136	
10	3	136	
10	4	136	
10	5	136	
10	6	136	
10	7	136	
10	8	136	
11	N	226	
12	O	58	
13	P	60	
14	Q	66	
15	R	88	
16	S	103	
17	T	71	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CDL	R	301	X	-	-	-
22	CDL	R	302	X	-	-	-
22	CDL	R	303	X	-	-	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 40337 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	488	Total	C	N	O	S	0	0
			3724	2347	657	708	12		
1	C	503	Total	C	N	O	S	0	0
			3834	2414	675	733	12		
1	A	507	Total	C	N	O	S	0	0
			3860	2429	679	740	12		

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	467	Total	C	N	O	S	0	0
			3536	2242	601	682	11		
2	D	469	Total	C	N	O	S	0	0
			3544	2246	603	684	11		
2	F	472	Total	C	N	O	S	0	0
			3570	2260	608	691	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	272	Total	C	N	O	S	0	0
			2115	1330	368	409	8		

- Molecule 4 is a protein called ATP synthase F1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	132	Total	C	N	O	S	0	0
			978	613	165	198	2		

- Molecule 5 is a protein called ATP synthase F1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	47	Total	C	N	O	S	0	0
			368	236	66	64	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	10	LEU	VAL	conflict	UNP W5Q3H8

- Molecule 6 is a protein called ATP synthase peripheral stalk subunit OSCP.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	188	Total	C	N	O	S	0	0
			1452	922	251	269	10		

- Molecule 7 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	208	Total	C	N	O	S	0	0
			1689	1089	289	305	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	58	PHE	ALA	conflict	UNP W5QEA9

- Molecule 8 is a protein called ATP synthase-coupling factor 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	69	Total	C	N	O	S	0	0
			576	366	97	111	2		

- Molecule 9 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	156	Total	C	N	O	S	0	0
			1284	829	209	243	3		

- Molecule 10 is a protein called ATP synthase F(0) complex subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1	74	Total	C	N	O	S	0	0
			526	348	82	93	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	2	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
10	3	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
10	4	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
10	5	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
10	6	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
10	7	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
10	8	74	Total	C	N	O	S	0	0
			526	348	82	93	3		

- Molecule 11 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	225	Total	C	N	O	S	0	0
			1734	1150	277	295	12		

- Molecule 12 is a protein called Subunit DAPIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	40	Total	C	N	O	S	0	0
			327	219	53	53	2		

- Molecule 13 is a protein called ATP synthase membrane subunit 6.8PL.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	52	Total	C	N	O	S	0	0
			425	281	70	71	3		

- Molecule 14 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	47	Total	C	N	O	S	0	0
			371	248	58	62	3		

- Molecule 15 is a protein called ATP synthase membrane subunit f.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	84	Total	C	N	O	S	0	0
			701	461	121	116	3		

- Molecule 16 is a protein called ATP synthase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	85	Total	C	N	O	S	0	0
			673	448	106	118	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	96	ARG	HIS	conflict	UNP W5Q5U7
S	99	ILE	THR	conflict	UNP W5Q5U7

- Molecule 17 is a protein called Subunit e.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	70	Total	C	N	O	S	0	0
			577	364	106	106	1		

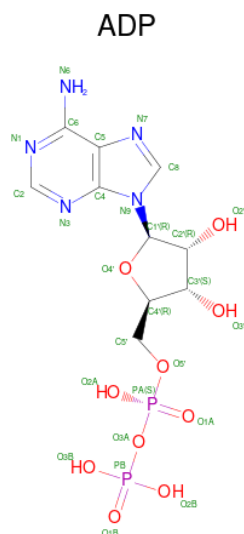
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	23	MET	VAL	conflict	UNP W5PF18
T	26	GLY	SER	conflict	UNP W5PF18
T	38	GLU	-	insertion	UNP W5PF18

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

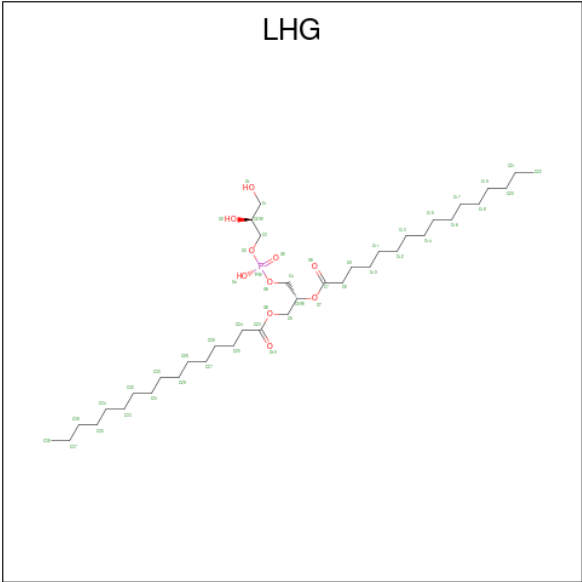
Mol	Chain	Residues	Atoms		AltConf
18	B	1	Total	Mg	0
			1	1	
18	C	1	Total	Mg	0
			1	1	
18	A	1	Total	Mg	0
			1	1	

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



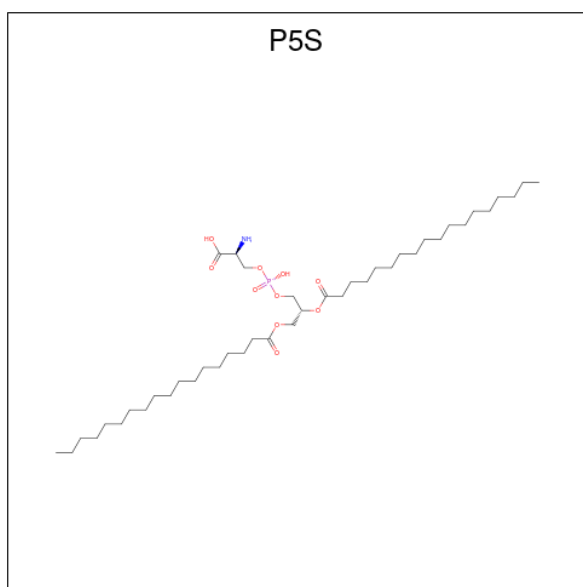
Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total 27	C 10	N 5	O 10	P 2	0
19	C	1	Total 27	C 10	N 5	O 10	P 2	0
19	A	1	Total 27	C 10	N 5	O 10	P 2	0
19	D	1	Total 27	C 10	N 5	O 10	P 2	0
19	F	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



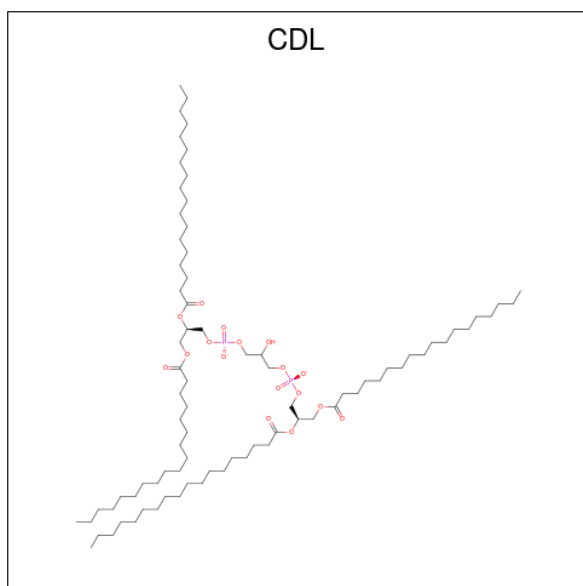
Mol	Chain	Residues	Atoms				AltConf
20	K	1	Total	C	O	P	0
			43	32	10	1	
20	K	1	Total	C	O	P	0
			49	38	10	1	
20	2	1	Total	C	O	P	0
			45	34	10	1	
20	R	1	Total	C	O	P	0
			49	38	10	1	
20	S	1	Total	C	O	P	0
			49	38	10	1	
20	S	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 21 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).



Mol	Chain	Residues	Atoms					AltConf
21	2	1	Total	C	N	O	P	0
			54	42	1	10	1	

- Molecule 22 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
22	R	1	Total	C	O	P	0
			100	81	17	2	
22	R	1	Total	C	O	P	0
			92	73	17	2	
22	R	1	Total	C	O	P	0
			88	69	17	2	

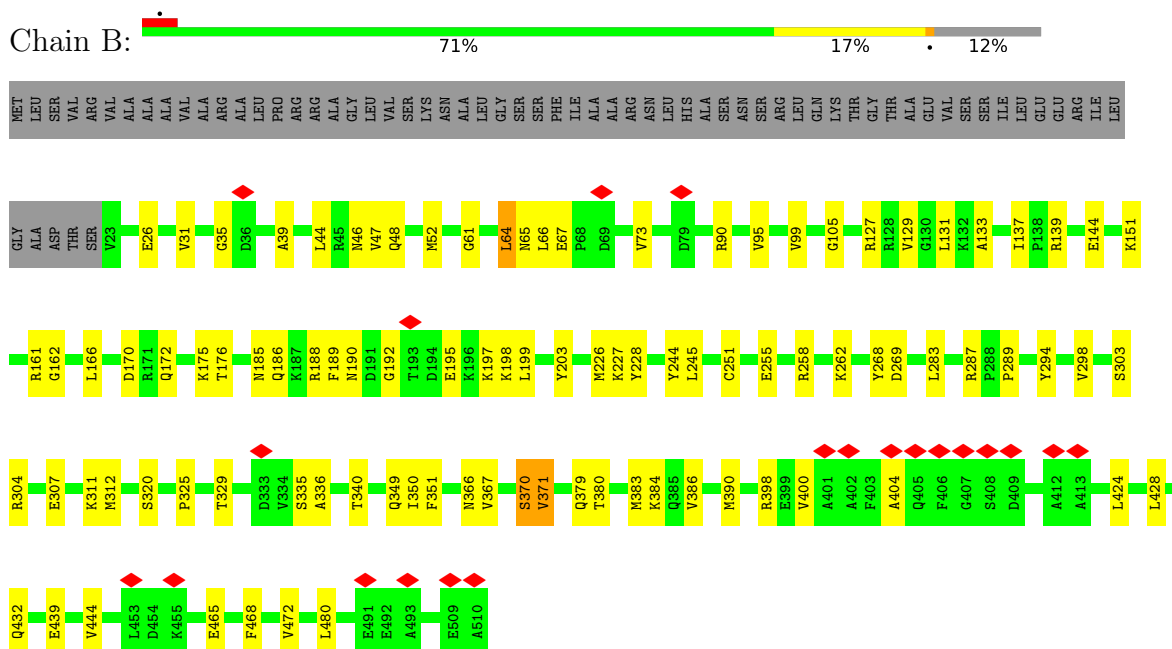
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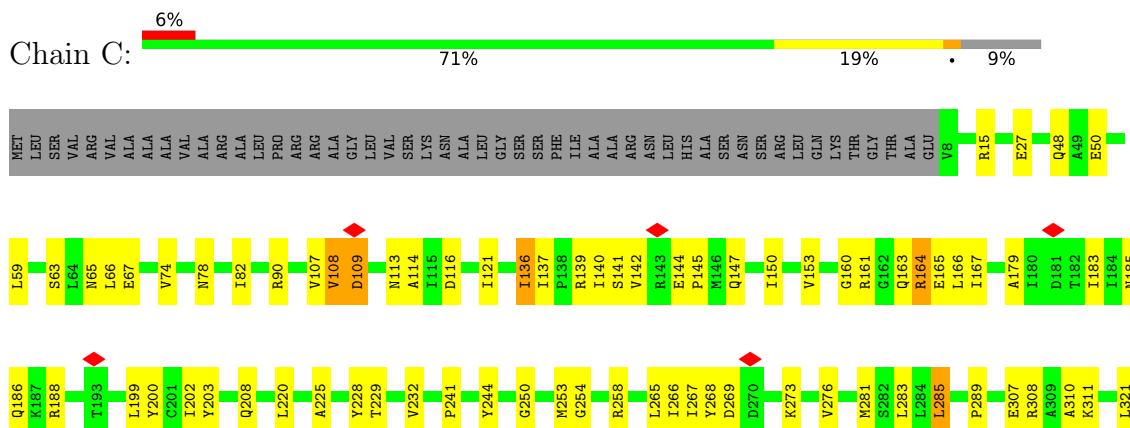
3 Residue-property plots [i](#)

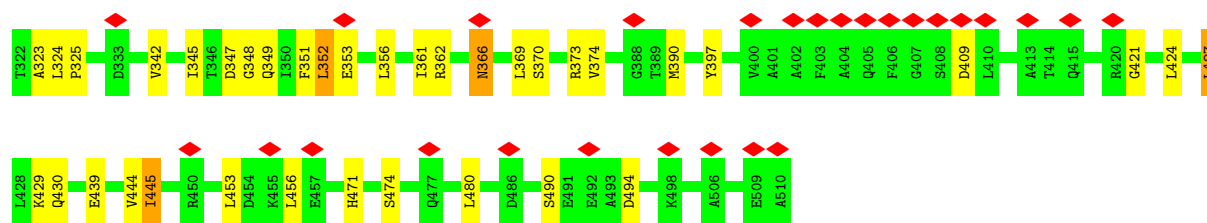
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: ATP synthase subunit alpha



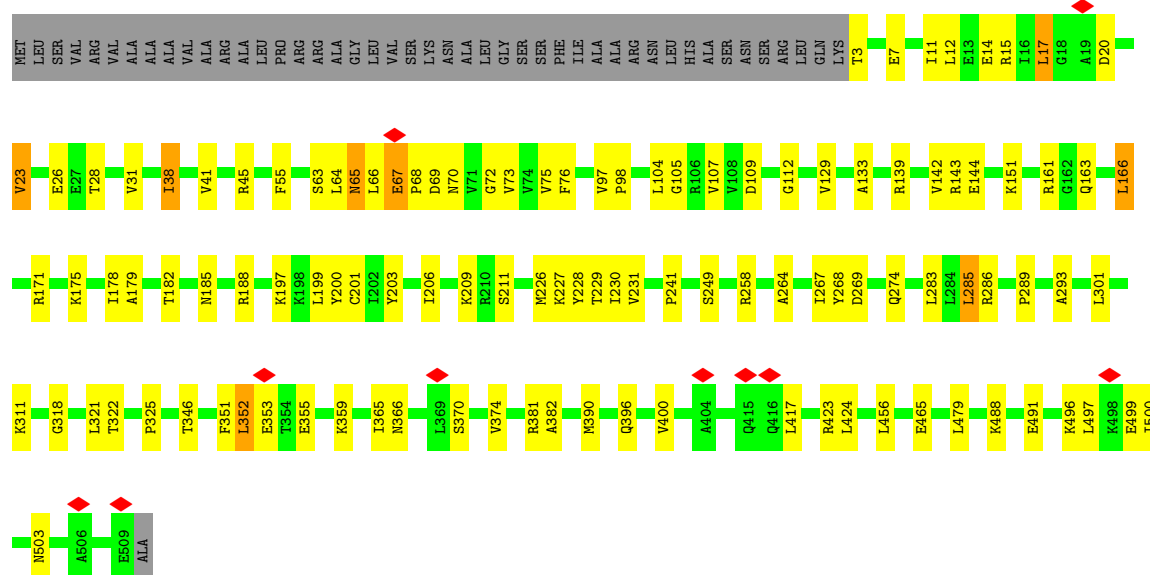
• Molecule 1: ATP synthase subunit alpha





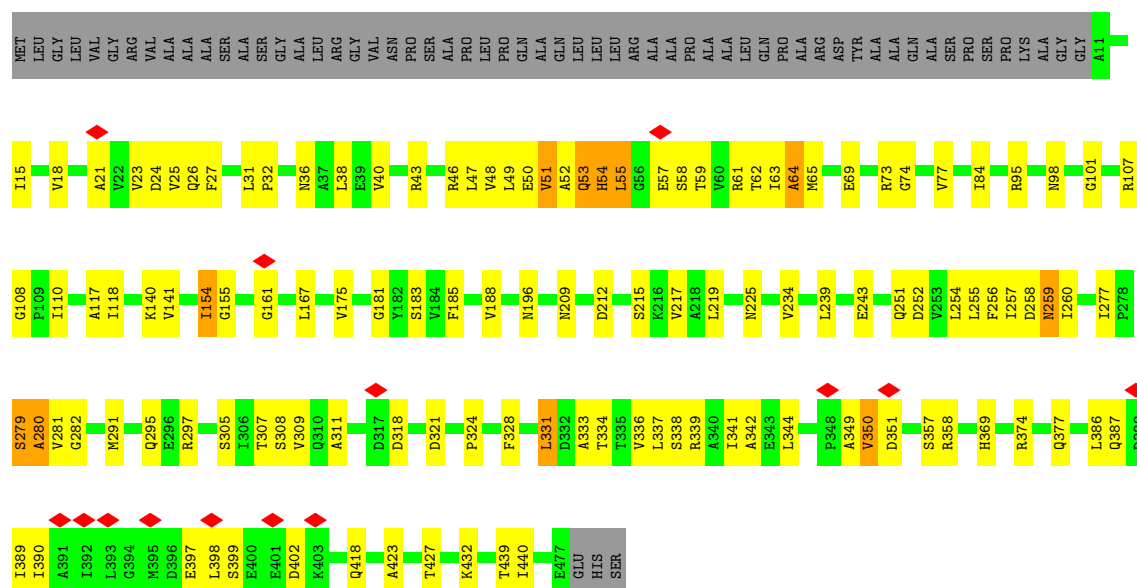
• Molecule 1: ATP synthase subunit alpha

Chain A: 71% 19% 8%

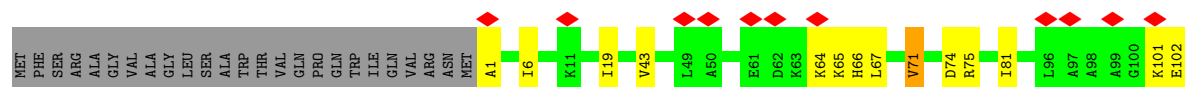
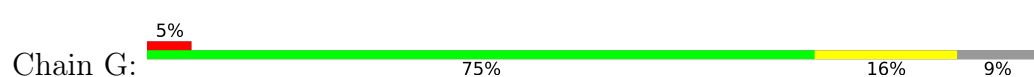


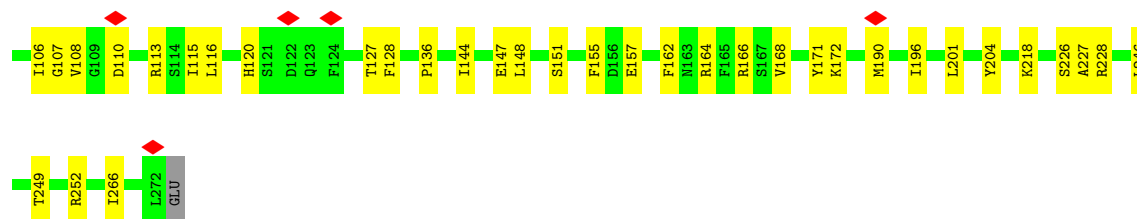
• Molecule 2: ATP synthase subunit beta

Chain E: 65% 21% 12%

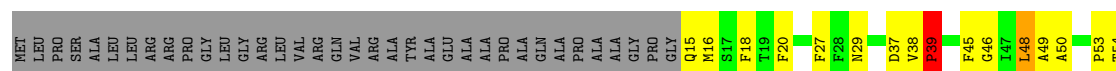


Chain D: 66% 21% 11%

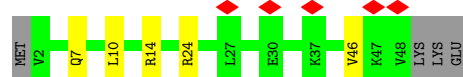
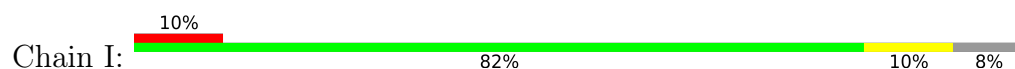




• Molecule 4: ATP synthase F1 subunit delta



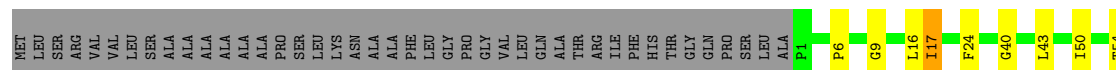
• Molecule 5: ATP synthase F1 subunit epsilon



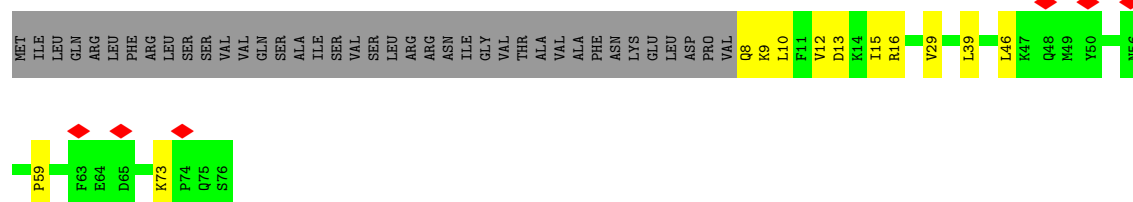
• Molecule 6: ATP synthase peripheral stalk subunit OSCP



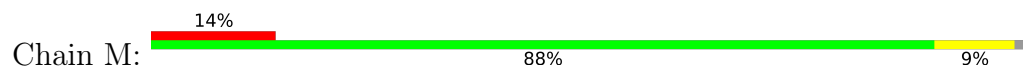
• Molecule 7: ATP synthase subunit b



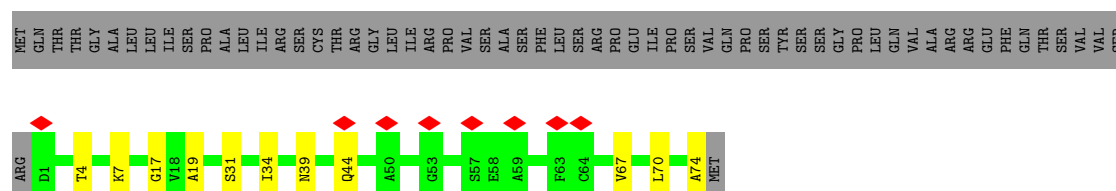
• Molecule 8: ATP synthase-coupling factor 6, mitochondrial



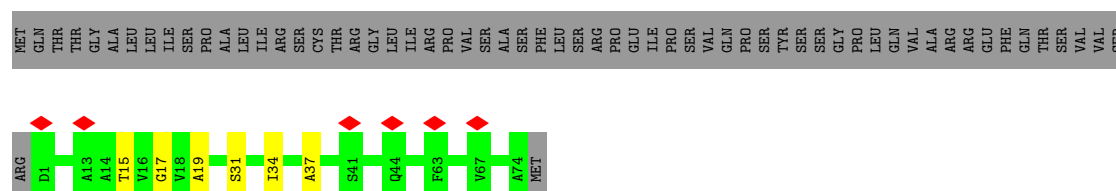
- Molecule 9: ATP synthase subunit d, mitochondrial



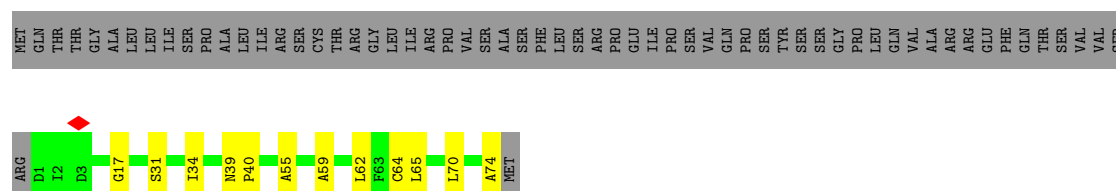
- Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial



- Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial



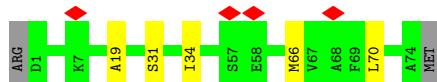
- Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial



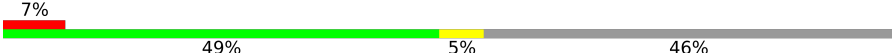
- Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 4:  51% 46%

MET GLN THR THR GLY ALA LEU LEU ILE SER PRO PRO ARG ALA LEU LEU ILE ARG SER CYS THR THR ARG GLY LEU ILE ARG PRO VAL SER ALA SER PHE SER LEU SER ARG PRO PRO GLU ILE ILE PRO PRO VAL VAL GLN VAL ALA ARG ARG ARG PHE THR SER VAL VAL SER



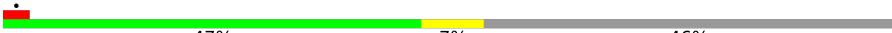
- Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 5:  7% 49% 5% 46%

MET GLN THR THR GLY ALA LEU LEU ILE SER PRO PRO ARG ALA LEU LEU ILE ARG SER CYS THR THR ARG GLY LEU ILE ARG PRO VAL SER ALA SER PHE SER LEU SER ARG PRO PRO GLU ILE ILE PRO PRO VAL VAL GLN VAL ALA ARG ARG ARG PHE THR SER VAL VAL SER



- Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 6:  47% 7% 46%

MET GLN THR THR GLY ALA LEU LEU ILE SER PRO PRO ARG ALA LEU LEU ILE ARG SER CYS THR THR ARG GLY LEU ILE ARG PRO VAL SER ALA SER PHE SER LEU SER ARG PRO PRO GLU ILE ILE PRO PRO VAL VAL GLN VAL ALA ARG ARG ARG PHE THR SER VAL VAL SER



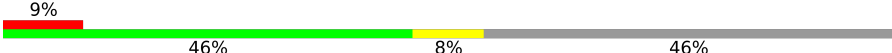
- Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 7:  47% 7% 46%

MET GLN THR THR GLY ALA LEU LEU ILE SER PRO PRO ARG ALA LEU LEU ILE ARG SER CYS THR THR ARG GLY LEU ILE ARG PRO VAL SER ALA SER PHE SER LEU SER ARG PRO PRO GLU ILE ILE PRO PRO VAL VAL GLN VAL ALA ARG ARG ARG PHE THR SER VAL VAL SER



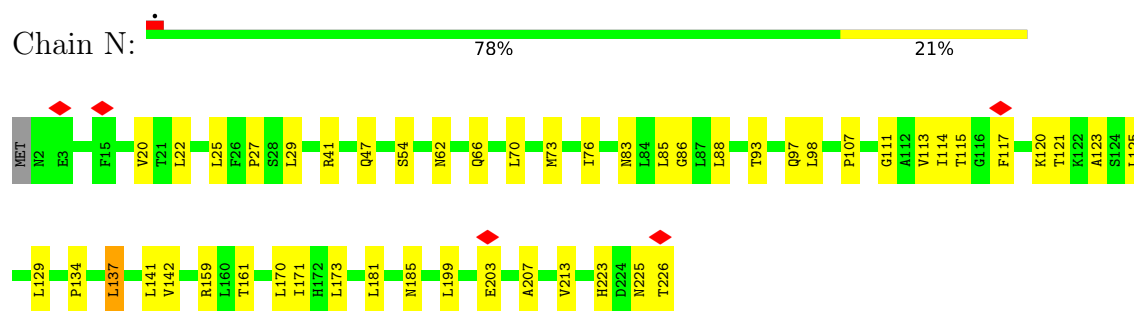
- Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 8:  9% 46% 8% 46%

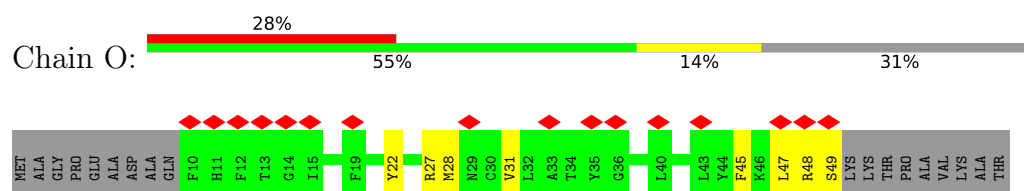
MET GLN THR THR GLY ALA LEU LEU ILE SER PRO PRO ARG ALA LEU LEU ILE ARG SER CYS THR THR ARG GLY LEU ILE ARG PRO VAL SER ALA SER PHE SER LEU SER ARG PRO PRO GLU ILE ILE PRO PRO VAL VAL GLN VAL ALA ARG ARG ARG PHE THR SER VAL VAL SER



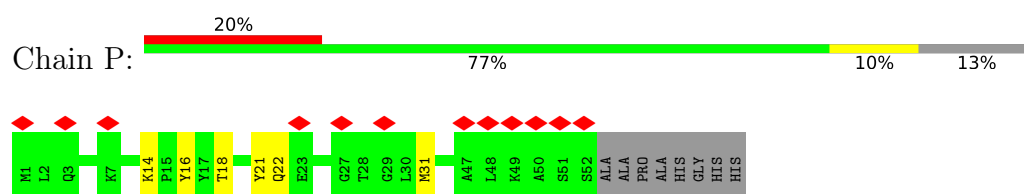
- Molecule 11: ATP synthase subunit a



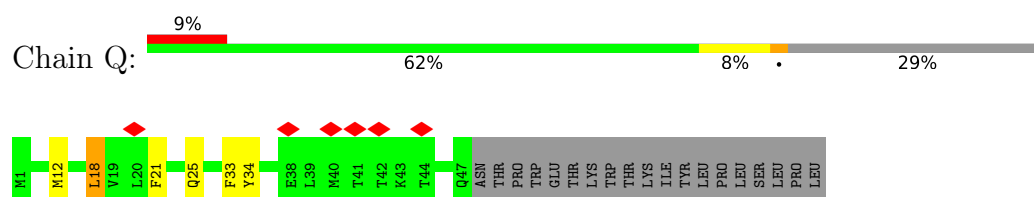
- Molecule 12: Subunit DAPIT



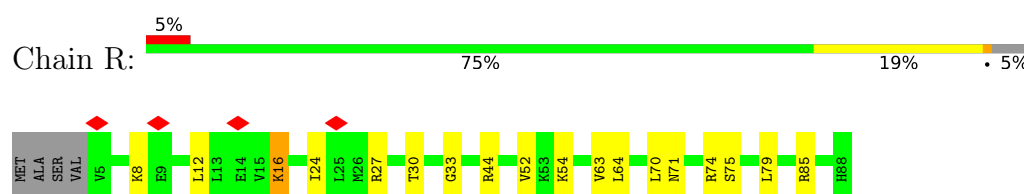
- Molecule 13: ATP synthase membrane subunit 6.8PL



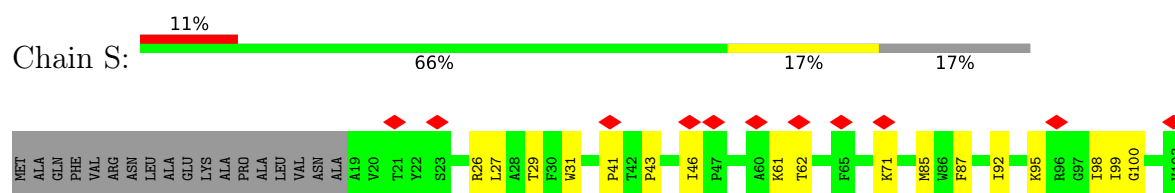
- Molecule 14: ATP synthase protein 8



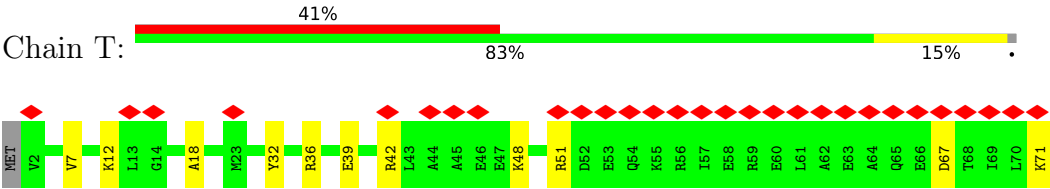
- Molecule 15: ATP synthase membrane subunit f



- Molecule 16: ATP synthase subunit



- Molecule 17: Subunit e



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	35000	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 ($e^-/\text{\AA}^2$)	106	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	131951	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	0.000	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	146.418, 147.479, 244.03	wwPDB
Map dimensions	230, 139, 138	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, S12, CDL, ADP, P5S, LHG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.36	0/3911	0.77	6/5278 (0.1%)
1	B	0.38	0/3775	0.72	4/5092 (0.1%)
1	C	0.37	0/3885	0.75	2/5241 (0.0%)
2	D	0.35	0/3601	0.75	6/4884 (0.1%)
2	E	0.37	0/3593	0.74	2/4874 (0.0%)
2	F	0.37	0/3628	0.77	9/4919 (0.2%)
3	G	0.28	0/2141	0.68	1/2876 (0.0%)
4	H	0.31	0/990	0.75	1/1346 (0.1%)
5	I	0.23	0/373	0.54	0/499
6	J	0.29	0/1470	0.65	0/1977
7	K	0.26	0/1722	0.61	0/2321
8	L	0.27	0/589	0.72	1/788 (0.1%)
9	M	0.23	0/1315	0.53	0/1781
10	1	0.28	0/535	0.59	0/722
10	2	0.29	0/535	0.60	0/722
10	3	0.31	0/535	0.63	0/722
10	4	0.28	0/535	0.60	0/722
10	5	0.27	0/535	0.55	0/722
10	6	0.29	0/535	0.59	0/722
10	7	0.27	0/535	0.57	0/722
10	8	0.29	0/535	0.59	0/722
11	N	0.30	0/1772	0.62	2/2421 (0.1%)
12	O	0.19	0/335	0.50	0/450
13	P	0.23	0/435	0.51	0/585
14	Q	0.25	0/381	0.61	0/518
15	R	0.29	0/719	0.58	0/963
16	S	0.27	0/691	0.61	0/940
17	T	0.25	0/585	0.60	0/780
All	All	0.33	0/40191	0.70	34/54309 (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
1	A	0	5
1	B	0	4
1	C	0	3
2	D	0	7
2	E	0	6
2	F	0	6
4	H	0	1
All	All	0	32

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(°)
2	D	64	ALA	CA-C-N	8.40	134.95	120.58
2	D	64	ALA	C-N-CA	8.40	134.95	120.58
2	F	258	ASP	CA-C-N	8.20	136.45	121.70
2	F	258	ASP	C-N-CA	8.20	136.45	121.70
2	D	258	ASP	CA-C-N	7.48	135.17	121.70

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	162	GLY	Peptide
1	B	227	LYS	Peptide
1	B	371	VAL	Peptide
1	B	64	LEU	Peptide
1	C	109	ASP	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	A	3860	0	3961	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3724	0	3825	58	0
1	C	3834	0	3937	76	0
2	D	3544	0	3597	80	0
2	E	3536	0	3591	84	0
2	F	3570	0	3615	75	0
3	G	2115	0	2185	33	0
4	H	978	0	976	28	0
5	I	368	0	390	4	0
6	J	1452	0	1557	28	0
7	K	1689	0	1739	23	0
8	L	576	0	560	10	0
9	M	1284	0	1292	13	0
10	1	526	0	544	8	0
10	2	526	0	544	5	0
10	3	526	0	544	10	0
10	4	526	0	544	6	0
10	5	526	0	544	6	0
10	6	526	0	544	9	0
10	7	526	0	544	8	0
10	8	526	0	544	9	0
11	N	1734	0	1856	36	0
12	O	327	0	337	6	0
13	P	425	0	455	6	0
14	Q	371	0	357	8	0
15	R	701	0	726	15	0
16	S	673	0	701	13	0
17	T	577	0	601	7	0
18	A	1	0	0	0	0
18	B	1	0	0	0	0
18	C	1	0	0	0	0
19	A	27	0	12	0	0
19	B	27	0	12	2	0
19	C	27	0	12	1	0
19	D	27	0	12	0	0
19	F	27	0	12	1	0
20	2	45	0	63	0	0
20	K	92	0	133	3	0
20	R	49	0	74	2	0
20	S	98	0	148	5	0
21	2	54	0	80	2	0
22	R	280	0	422	13	0
23	T	35	0	44	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	40337	0	41634	650	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 8.

The worst 5 of 650 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:259:ASN:HA	2:D:311:ALA:O	1.38	1.22
2:F:259:ASN:HA	2:F:311:ALA:O	1.52	1.07
2:D:338:SER:O	2:D:349:ALA:HB3	1.54	1.05
2:F:338:SER:O	2:F:349:ALA:HB3	1.54	1.04
1:B:199:LEU:O	1:B:228:TYR:HB3	1.59	1.02

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	505/553 (91%)	457 (90%)	46 (9%)	2 (0%)	30	62
1	B	486/553 (88%)	448 (92%)	37 (8%)	1 (0%)	43	74
1	C	501/553 (91%)	456 (91%)	45 (9%)	0	100	100
2	D	467/528 (88%)	420 (90%)	42 (9%)	5 (1%)	11	43
2	E	465/528 (88%)	425 (91%)	33 (7%)	7 (2%)	8	37
2	F	470/528 (89%)	433 (92%)	34 (7%)	3 (1%)	21	54
3	G	270/298 (91%)	256 (95%)	14 (5%)	0	100	100
4	H	130/168 (77%)	119 (92%)	10 (8%)	1 (1%)	16	49
5	I	45/51 (88%)	43 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	J	186/213 (87%)	175 (94%)	10 (5%)	1 (0%)	24	57
7	K	206/256 (80%)	193 (94%)	13 (6%)	0	100	100
8	L	67/108 (62%)	60 (90%)	7 (10%)	0	100	100
9	M	154/161 (96%)	150 (97%)	4 (3%)	0	100	100
10	1	72/136 (53%)	71 (99%)	1 (1%)	0	100	100
10	2	72/136 (53%)	72 (100%)	0	0	100	100
10	3	72/136 (53%)	71 (99%)	1 (1%)	0	100	100
10	4	72/136 (53%)	70 (97%)	2 (3%)	0	100	100
10	5	72/136 (53%)	70 (97%)	2 (3%)	0	100	100
10	6	72/136 (53%)	71 (99%)	1 (1%)	0	100	100
10	7	72/136 (53%)	71 (99%)	1 (1%)	0	100	100
10	8	72/136 (53%)	70 (97%)	2 (3%)	0	100	100
11	N	223/226 (99%)	212 (95%)	11 (5%)	0	100	100
12	O	38/58 (66%)	37 (97%)	1 (3%)	0	100	100
13	P	50/60 (83%)	49 (98%)	1 (2%)	0	100	100
14	Q	45/66 (68%)	42 (93%)	3 (7%)	0	100	100
15	R	82/88 (93%)	81 (99%)	1 (1%)	0	100	100
16	S	83/103 (81%)	78 (94%)	5 (6%)	0	100	100
17	T	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
All	All	5117/6258 (82%)	4767 (93%)	330 (6%)	20 (0%)	31	62

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	53	GLN
2	E	259	ASN
2	E	280	ALA
2	E	281	VAL
2	D	281	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/443 (93%)	403 (98%)	7 (2%)	53	70
1	B	394/443 (89%)	390 (99%)	4 (1%)	68	75
1	C	407/443 (92%)	400 (98%)	7 (2%)	53	70
2	D	376/415 (91%)	372 (99%)	4 (1%)	65	74
2	E	376/415 (91%)	372 (99%)	4 (1%)	65	74
2	F	379/415 (91%)	374 (99%)	5 (1%)	61	72
3	G	230/251 (92%)	227 (99%)	3 (1%)	61	72
4	H	104/127 (82%)	102 (98%)	2 (2%)	50	68
5	I	38/42 (90%)	38 (100%)	0	100	100
6	J	164/185 (89%)	164 (100%)	0	100	100
7	K	184/218 (84%)	182 (99%)	2 (1%)	65	74
8	L	63/98 (64%)	63 (100%)	0	100	100
9	M	141/144 (98%)	141 (100%)	0	100	100
10	1	50/105 (48%)	50 (100%)	0	100	100
10	2	50/105 (48%)	50 (100%)	0	100	100
10	3	50/105 (48%)	50 (100%)	0	100	100
10	4	50/105 (48%)	50 (100%)	0	100	100
10	5	50/105 (48%)	50 (100%)	0	100	100
10	6	50/105 (48%)	50 (100%)	0	100	100
10	7	50/105 (48%)	50 (100%)	0	100	100
10	8	50/105 (48%)	50 (100%)	0	100	100
11	N	197/198 (100%)	195 (99%)	2 (1%)	68	75
12	O	35/47 (74%)	35 (100%)	0	100	100
13	P	45/49 (92%)	45 (100%)	0	100	100
14	Q	39/66 (59%)	38 (97%)	1 (3%)	40	62
15	R	73/76 (96%)	71 (97%)	2 (3%)	39	62
16	S	71/84 (84%)	71 (100%)	0	100	100
17	T	59/60 (98%)	59 (100%)	0	100	100
All	All	4185/5059 (83%)	4142 (99%)	43 (1%)	65	75

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	389	ILE
4	H	103	LEU
2	F	416	LEU
3	G	144	ILE
7	K	86	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
4	H	15	GLN
7	K	145	HIS
4	H	32	ASN
6	J	10	GLN
10	1	44	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 3 are 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
19	ADP	B	602	18	28,29,29	1.38	4 (14%)	43,45,45	1.88	12 (27%)
20	LHG	K	301	-	42,42,48	0.65	0	45,48,54	1.24	4 (8%)
22	CDL	R	303	-	87,87,99	1.06	6 (6%)	93,99,111	1.03	14 (15%)
22	CDL	R	302	-	91,91,99	1.08	7 (7%)	97,103,111	0.98	12 (12%)
19	ADP	F	600	-	28,29,29	1.37	5 (17%)	43,45,45	1.79	7 (16%)
20	LHG	S	202	-	48,48,48	0.63	1 (2%)	51,54,54	1.25	6 (11%)
19	ADP	A	602	18	28,29,29	1.38	4 (14%)	43,45,45	1.98	8 (18%)
22	CDL	R	301	-	99,99,99	1.15	8 (8%)	105,111,111	1.00	16 (15%)
23	S12	T	201	-	33,34,34	0.68	1 (3%)	34,40,40	0.45	0
21	P5S	2	201	-	52,53,53	0.33	0	54,60,60	0.55	1 (1%)
20	LHG	R	304	-	48,48,48	0.66	1 (2%)	51,54,54	1.26	6 (11%)
20	LHG	2	202	-	44,44,48	0.69	1 (2%)	47,50,54	1.35	6 (12%)
20	LHG	S	201	-	48,48,48	0.67	1 (2%)	51,54,54	1.27	6 (11%)
20	LHG	K	302	-	48,48,48	0.70	1 (2%)	51,54,54	1.33	7 (13%)
19	ADP	C	602	18	28,29,29	1.37	4 (14%)	43,45,45	1.84	8 (18%)
19	ADP	D	600	-	28,29,29	1.38	4 (14%)	43,45,45	1.85	7 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	ADP	B	602	18	-	10/16/32/32	0/3/3/3
20	LHG	K	301	-	-	27/47/47/53	-
22	CDL	R	303	-	2/2/9/9	29/98/98/110	-
22	CDL	R	302	-	1/1/9/9	39/102/102/110	-
19	ADP	F	600	-	-	2/16/32/32	0/3/3/3
22	CDL	R	301	-	1/1/9/9	39/110/110/110	-
19	ADP	A	602	18	-	10/16/32/32	0/3/3/3
20	LHG	S	202	-	-	30/53/53/53	-
23	S12	T	201	-	-	14/38/38/38	-
21	P5S	2	201	-	-	14/59/59/59	-
20	LHG	R	304	-	-	32/53/53/53	-
20	LHG	2	202	-	-	26/49/49/53	-
20	LHG	S	201	-	-	27/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LHG	K	302	-	-	26/53/53/53	-
19	ADP	C	602	18	-	3/16/32/32	0/3/3/3
19	ADP	D	600	-	-	3/16/32/32	0/3/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	600	ADP	C5-C4	4.47	1.47	1.39
19	C	602	ADP	C5-C4	4.44	1.47	1.39
19	A	602	ADP	C5-C4	4.43	1.47	1.39
19	B	602	ADP	C5-C4	4.38	1.46	1.39
19	F	600	ADP	C5-C4	4.27	1.46	1.39

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	602	ADP	C5-C4-N3	-6.46	117.82	126.72
19	D	600	ADP	C5-C4-N3	-6.04	118.40	126.72
19	C	602	ADP	C5-C4-N3	-5.96	118.51	126.72
19	B	602	ADP	C5-C4-N3	-5.89	118.60	126.72
19	F	600	ADP	C5-C4-N3	-5.77	118.77	126.72

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	R	301	CDL	CB4
22	R	302	CDL	CB4
22	R	303	CDL	CA4
22	R	303	CDL	CB4

5 of 331 torsion outliers are listed below:

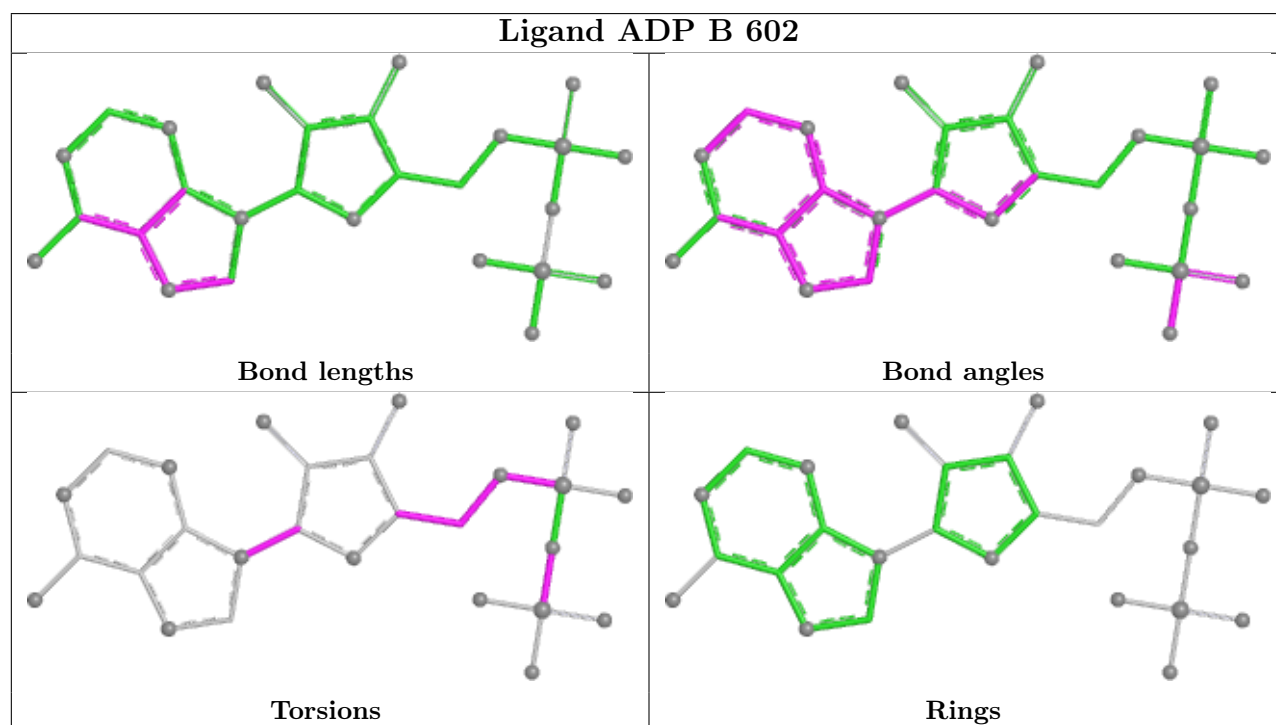
Mol	Chain	Res	Type	Atoms
19	B	602	ADP	C5'-O5'-PA-O3A
19	B	602	ADP	C2'-C1'-N9-C8
19	C	602	ADP	C5'-O5'-PA-O1A
19	A	602	ADP	PA-O3A-PB-O2B
19	A	602	ADP	PA-O3A-PB-O3B

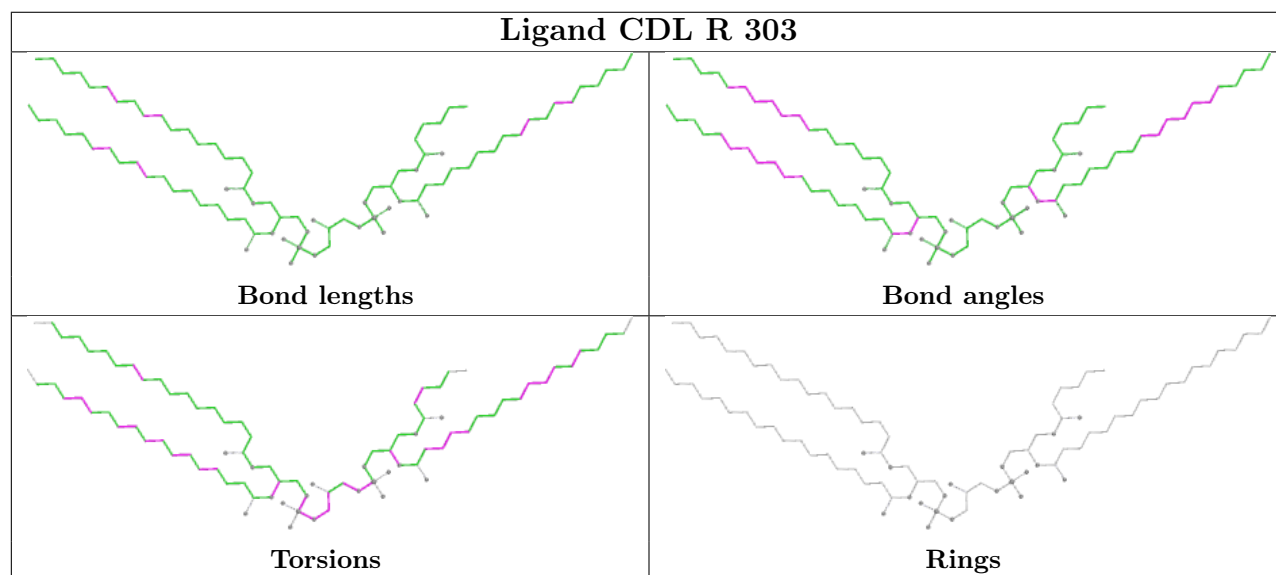
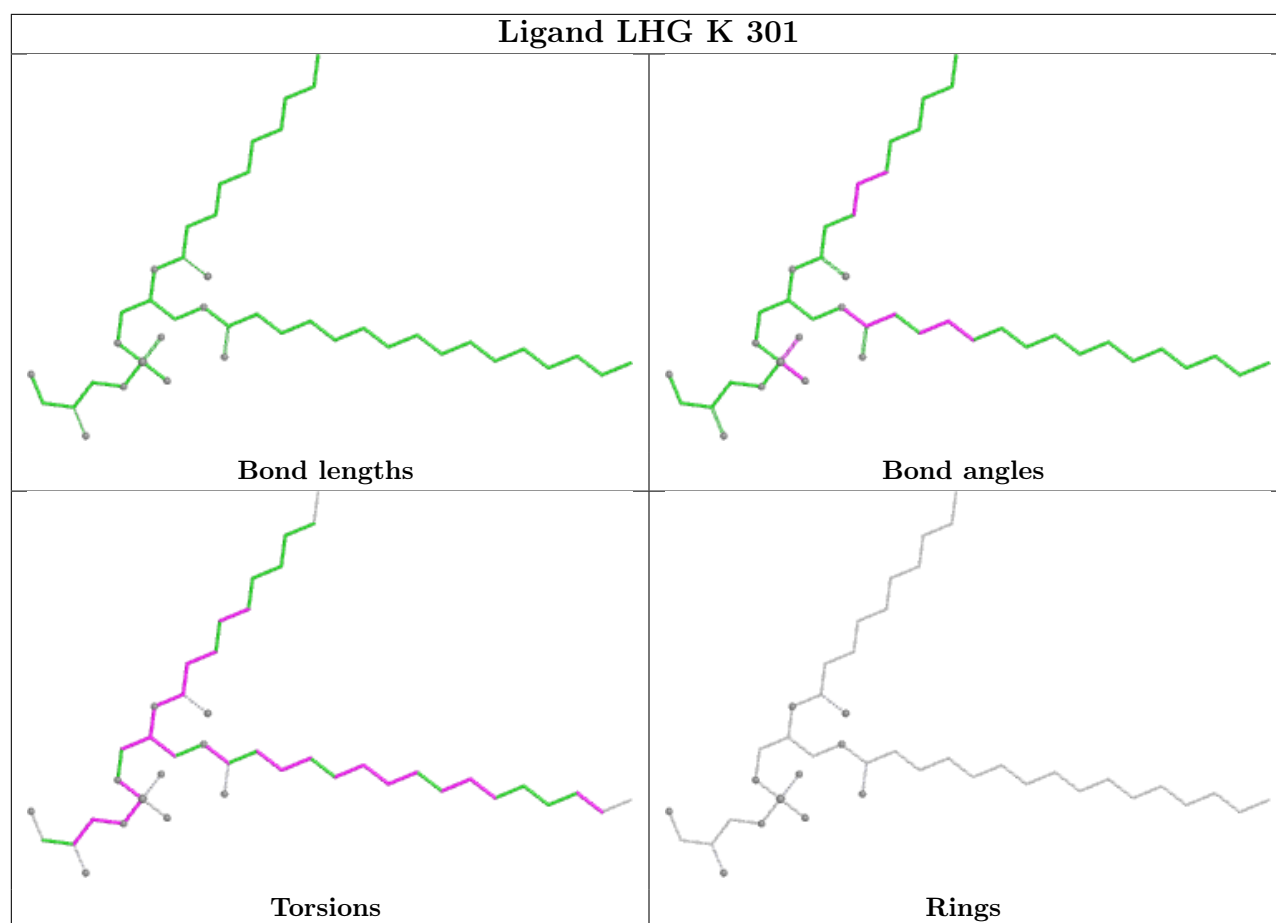
There are no ring outliers.

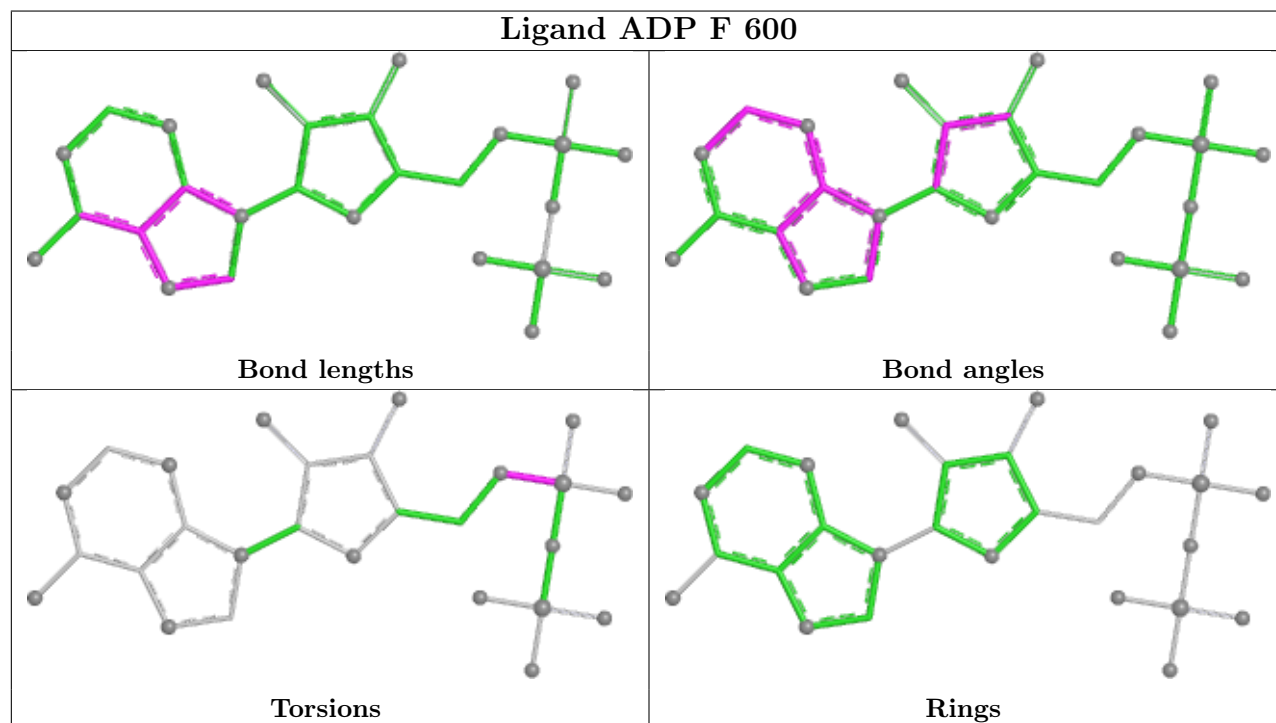
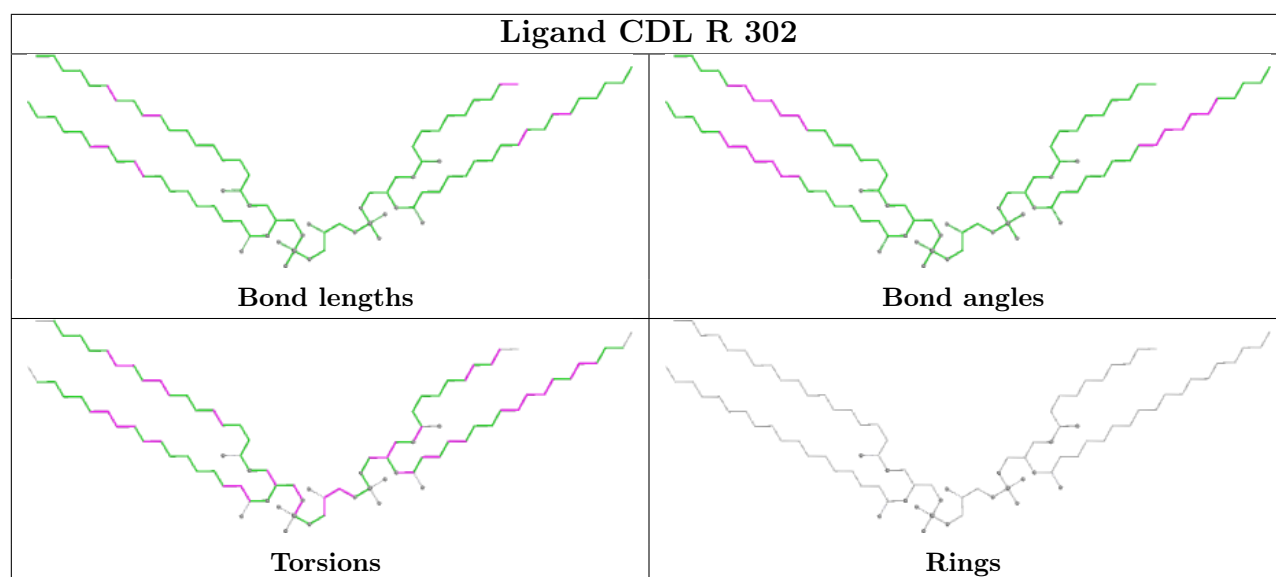
12 monomers are involved in 29 short contacts:

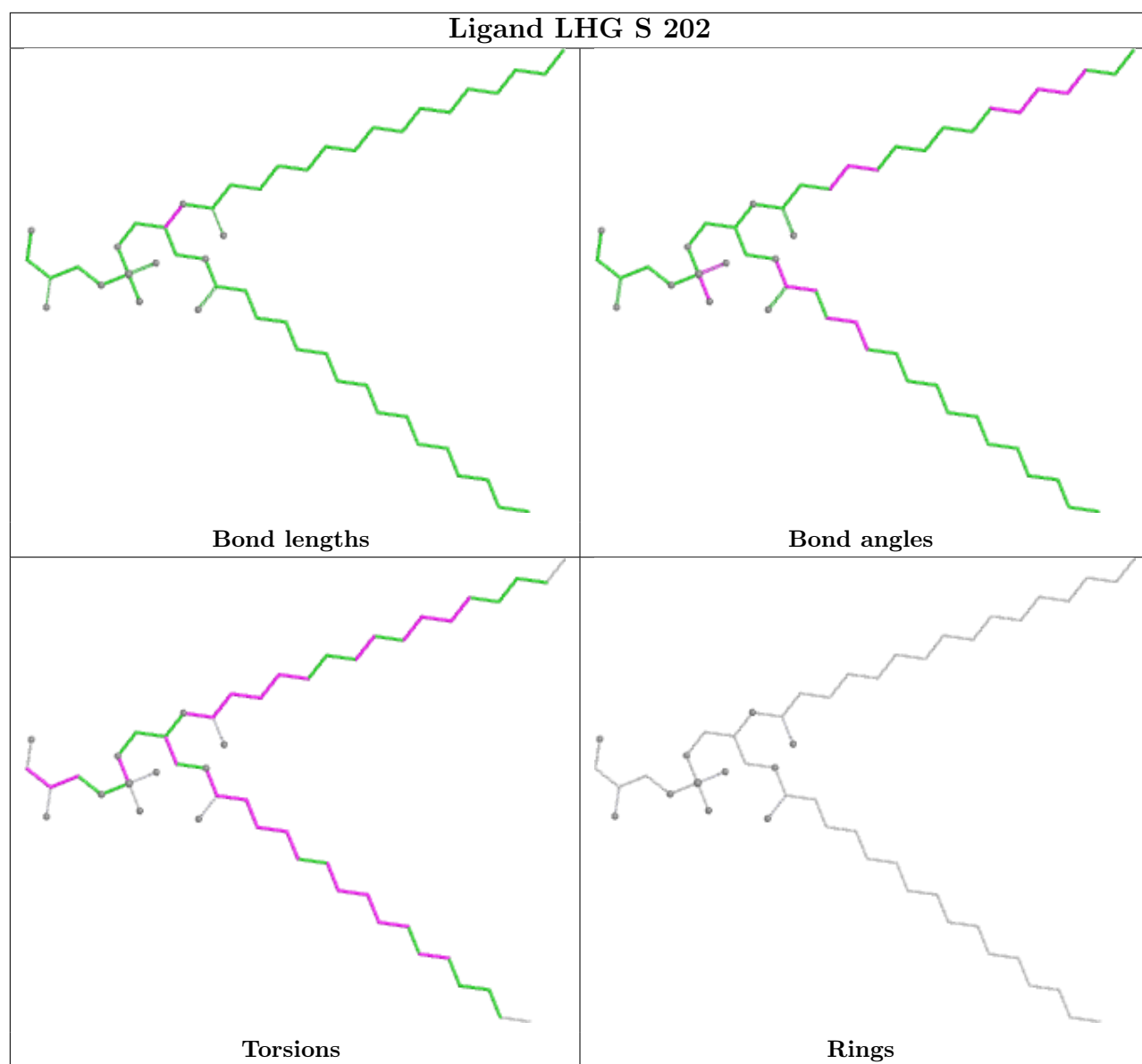
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	602	ADP	2	0
22	R	303	CDL	6	0
22	R	302	CDL	7	0
19	F	600	ADP	1	0
20	S	202	LHG	1	0
22	R	301	CDL	2	0
23	T	201	S12	1	0
21	2	201	P5S	2	0
20	R	304	LHG	2	0
20	S	201	LHG	4	0
20	K	302	LHG	3	0
19	C	602	ADP	1	0

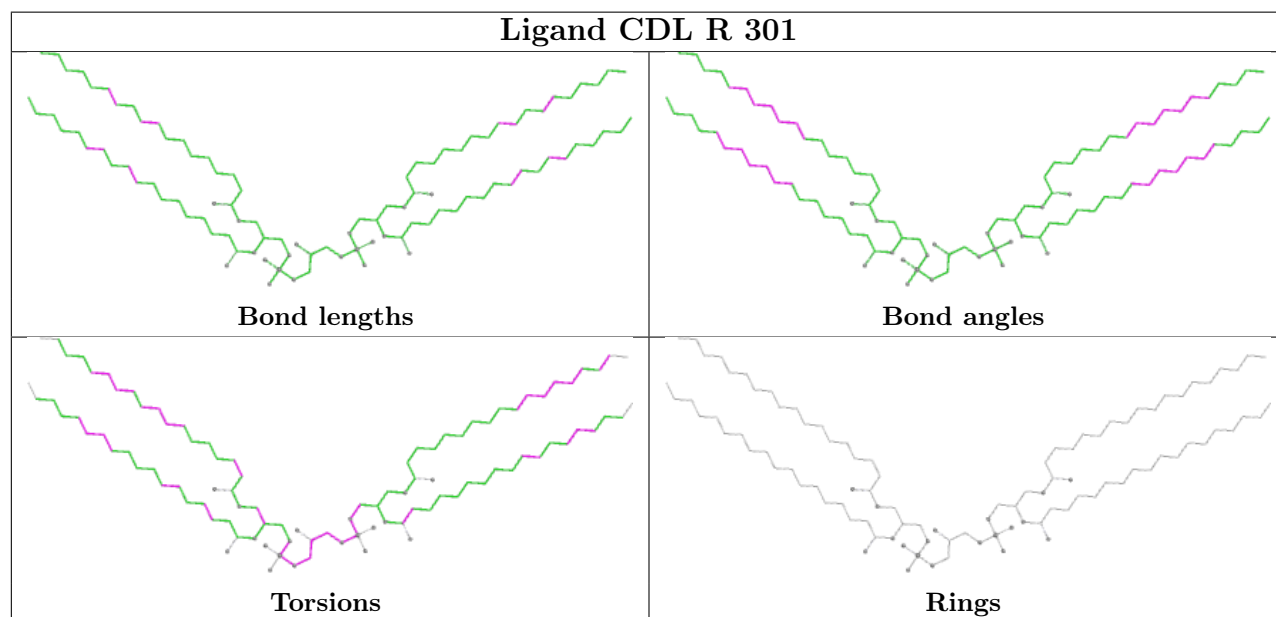
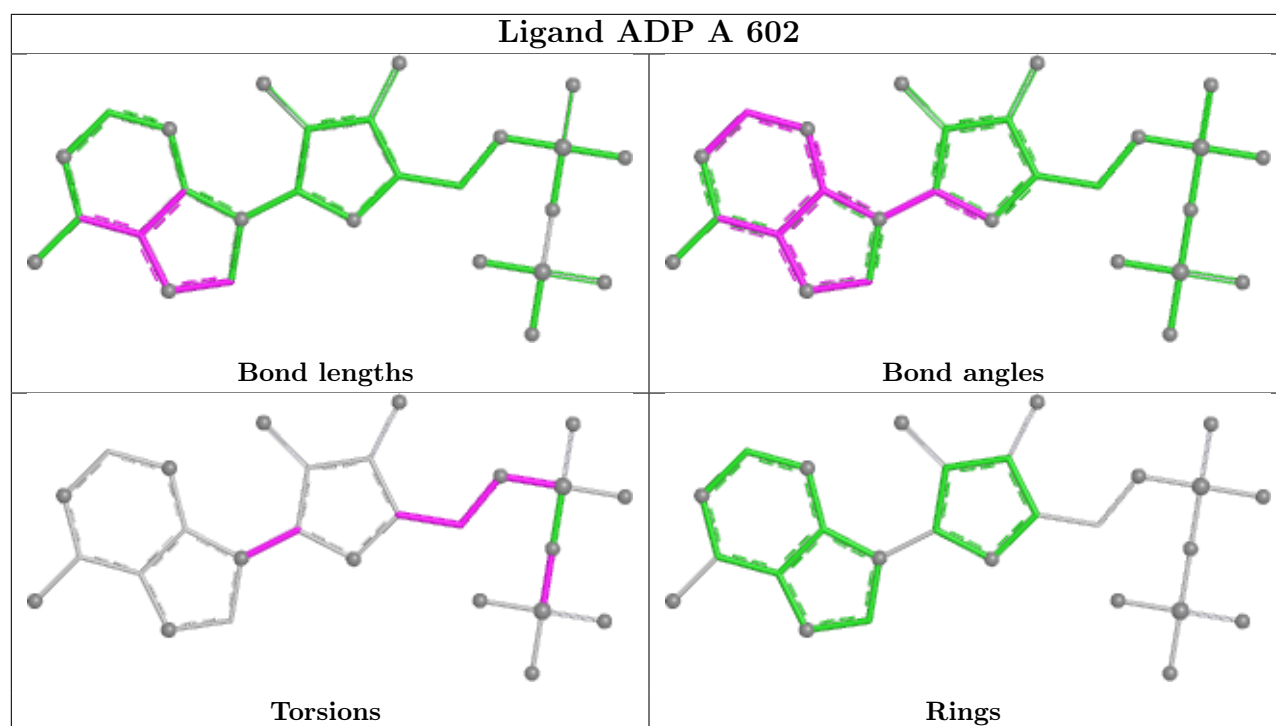
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

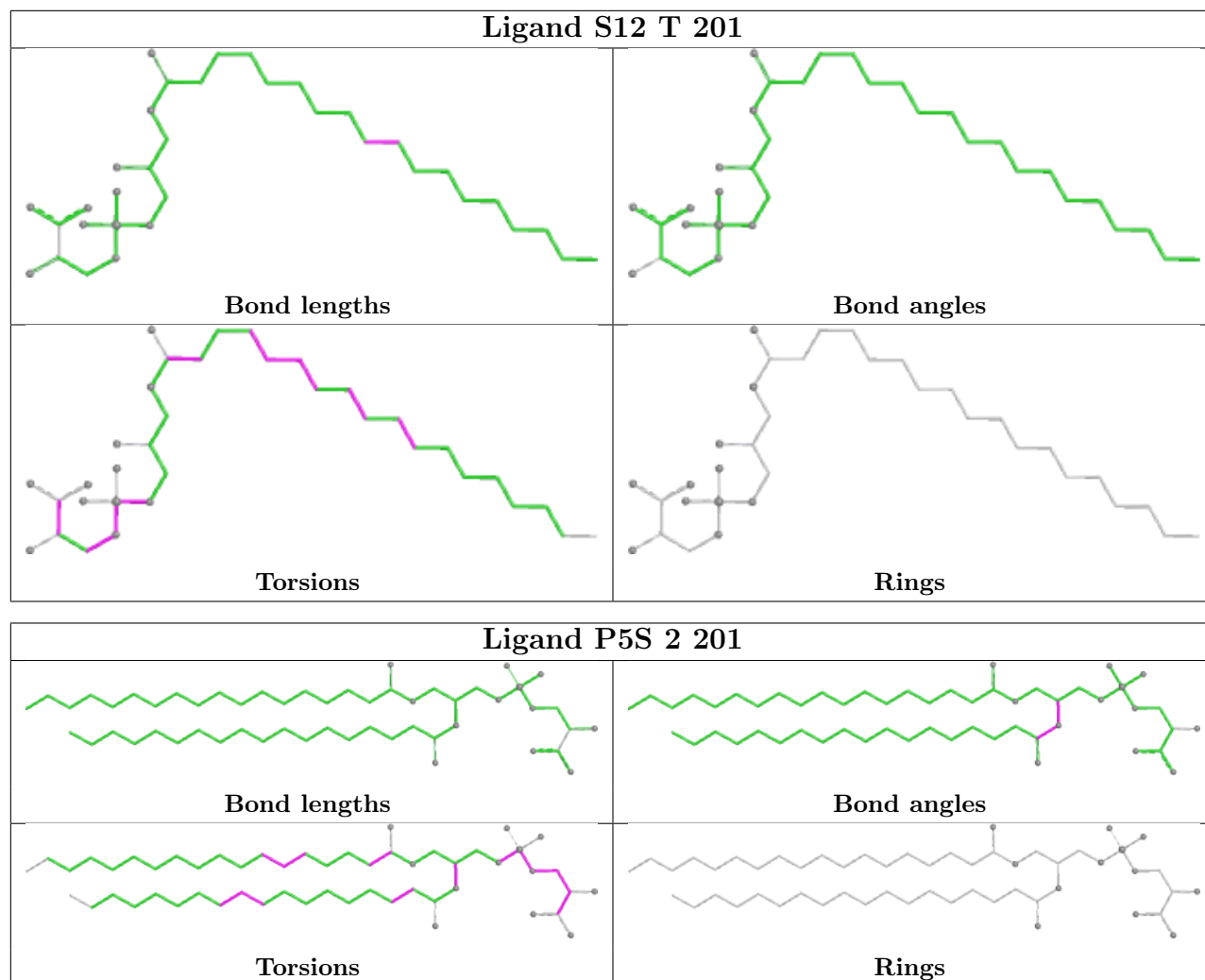


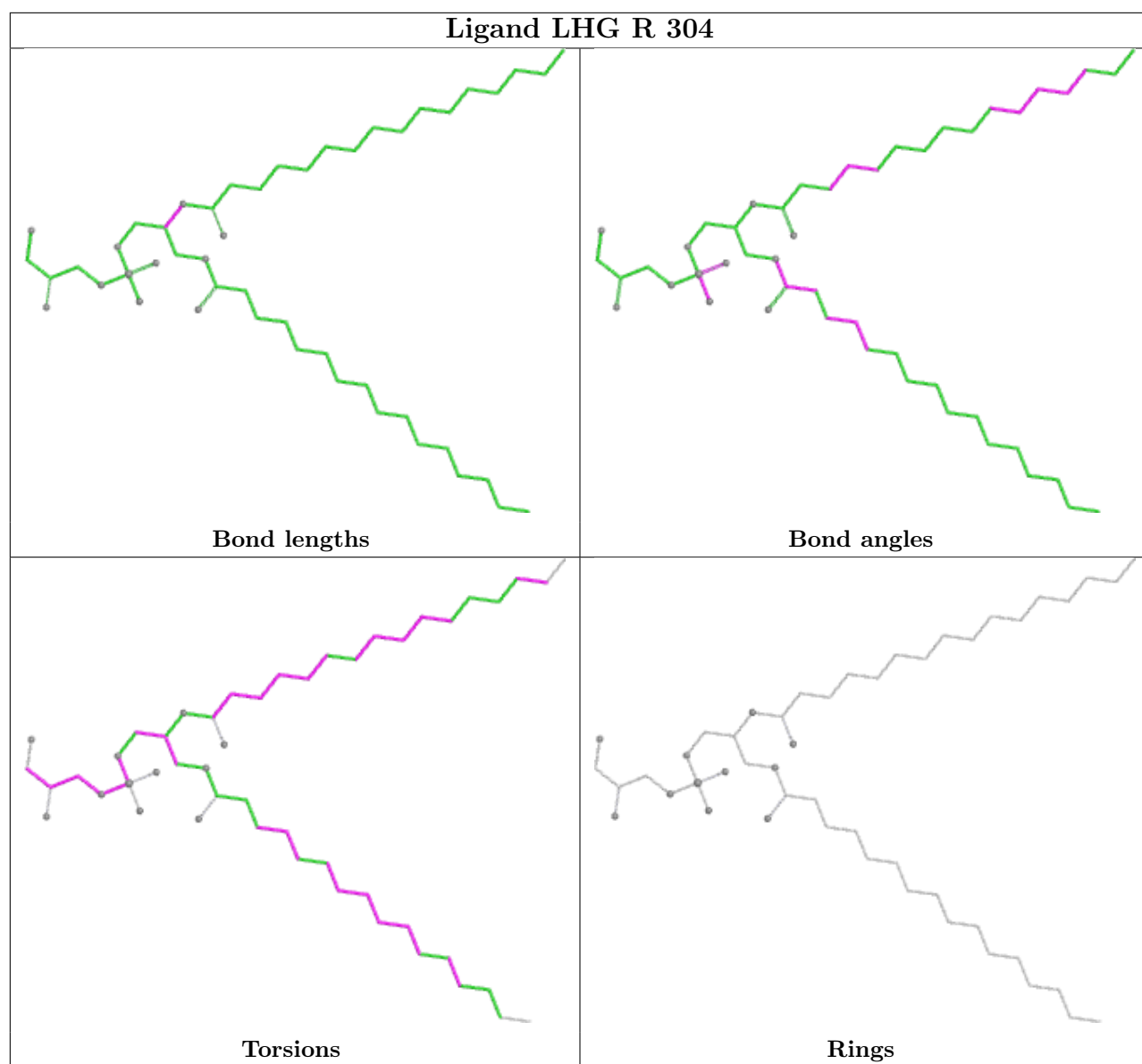


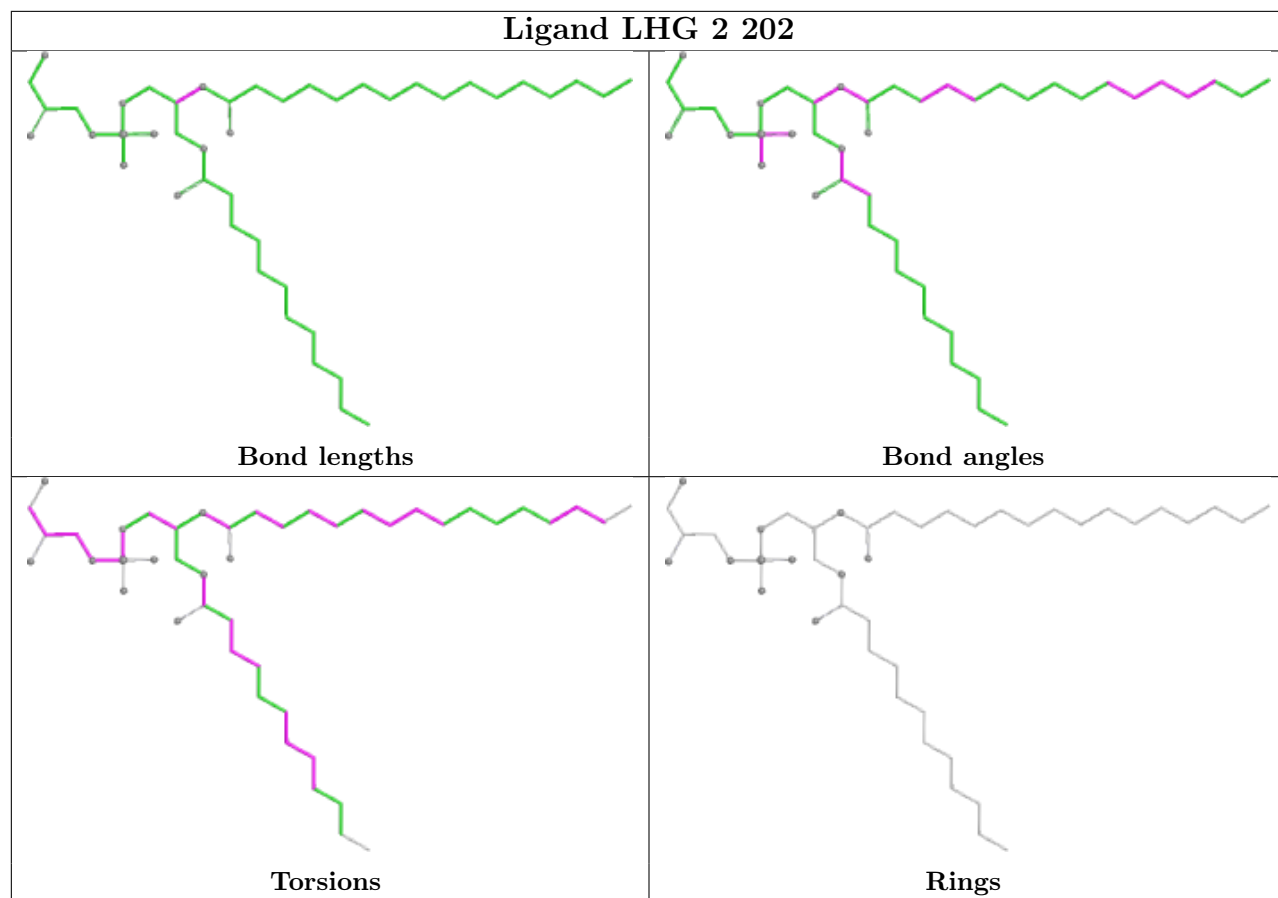


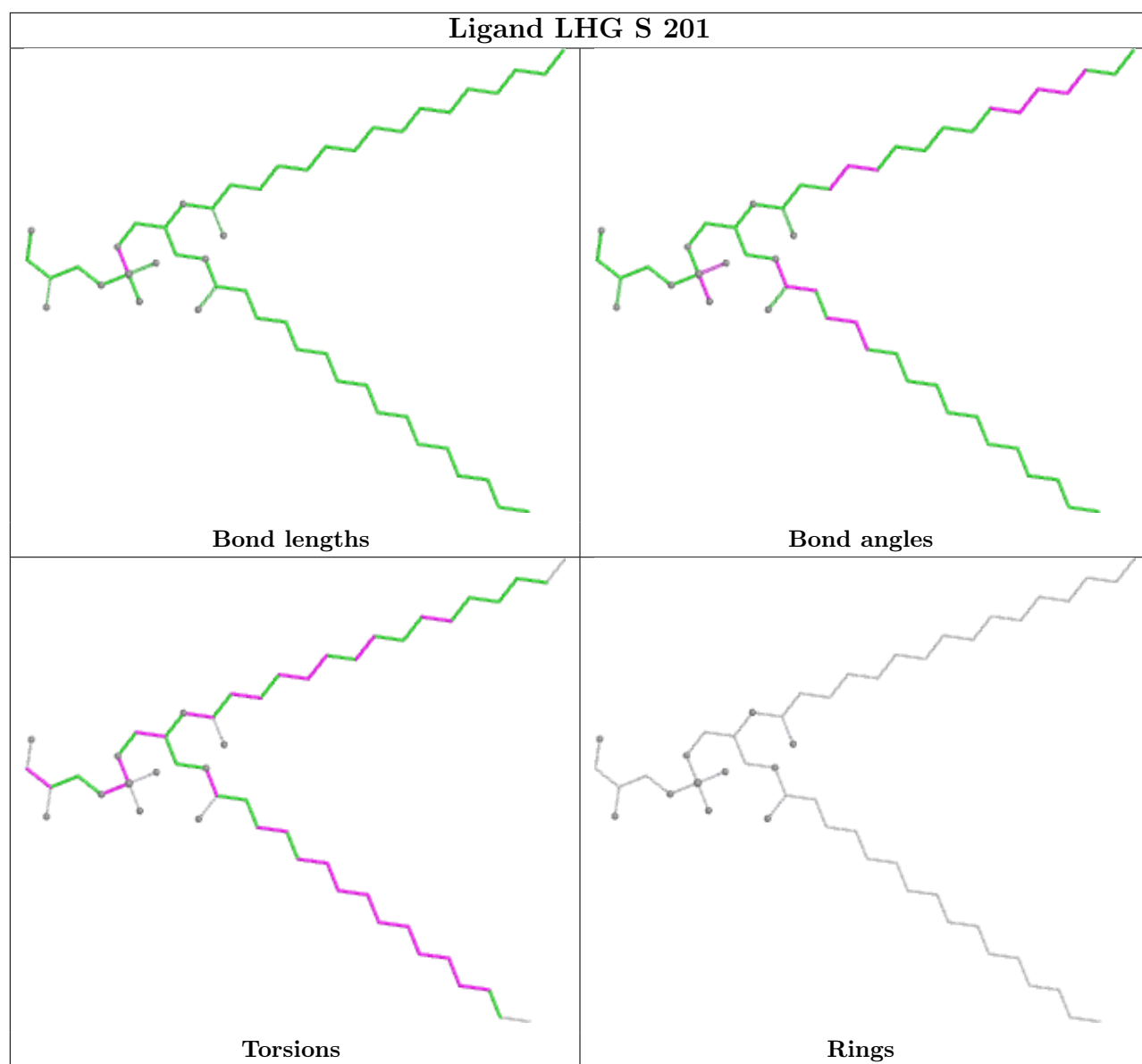


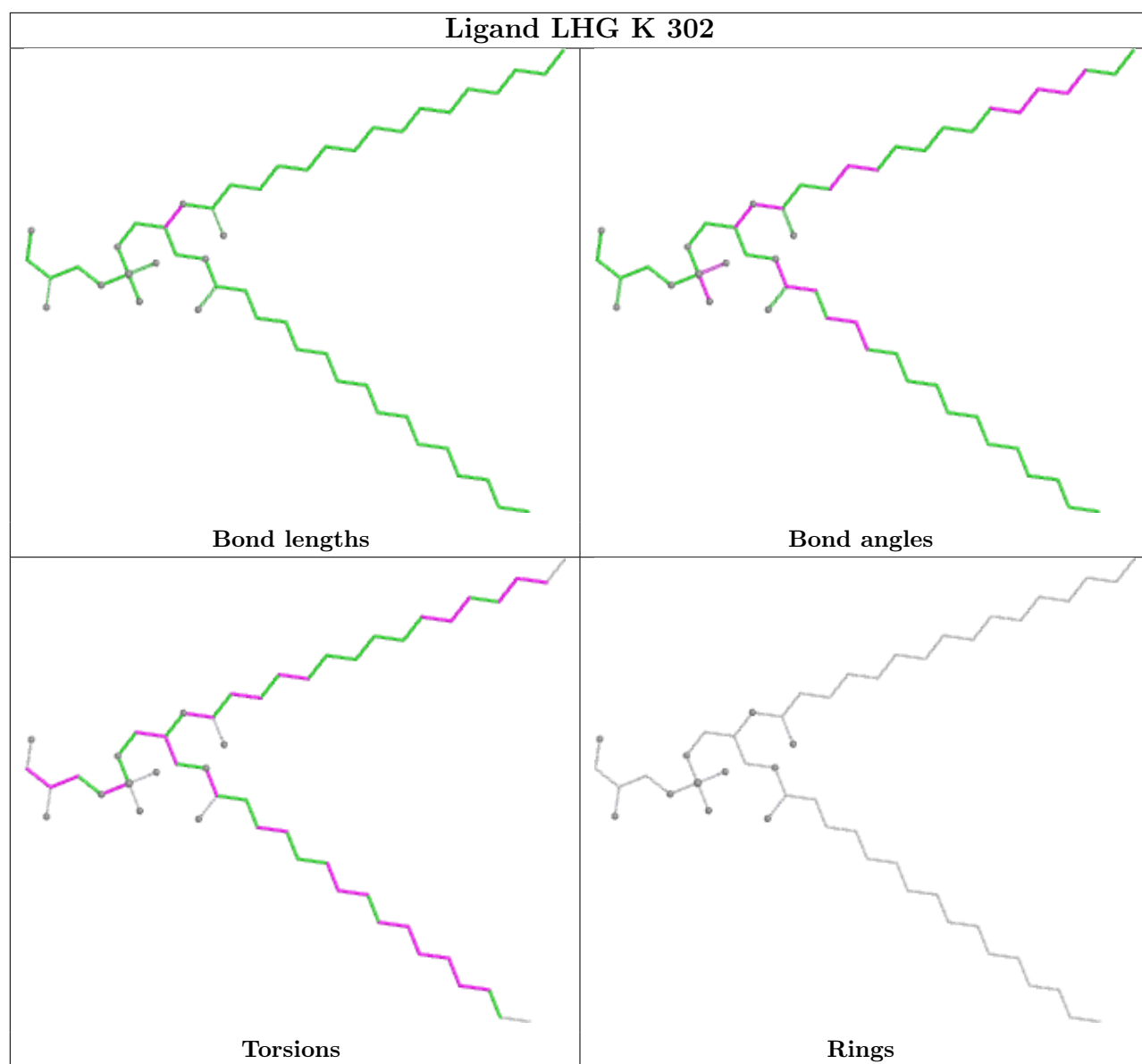


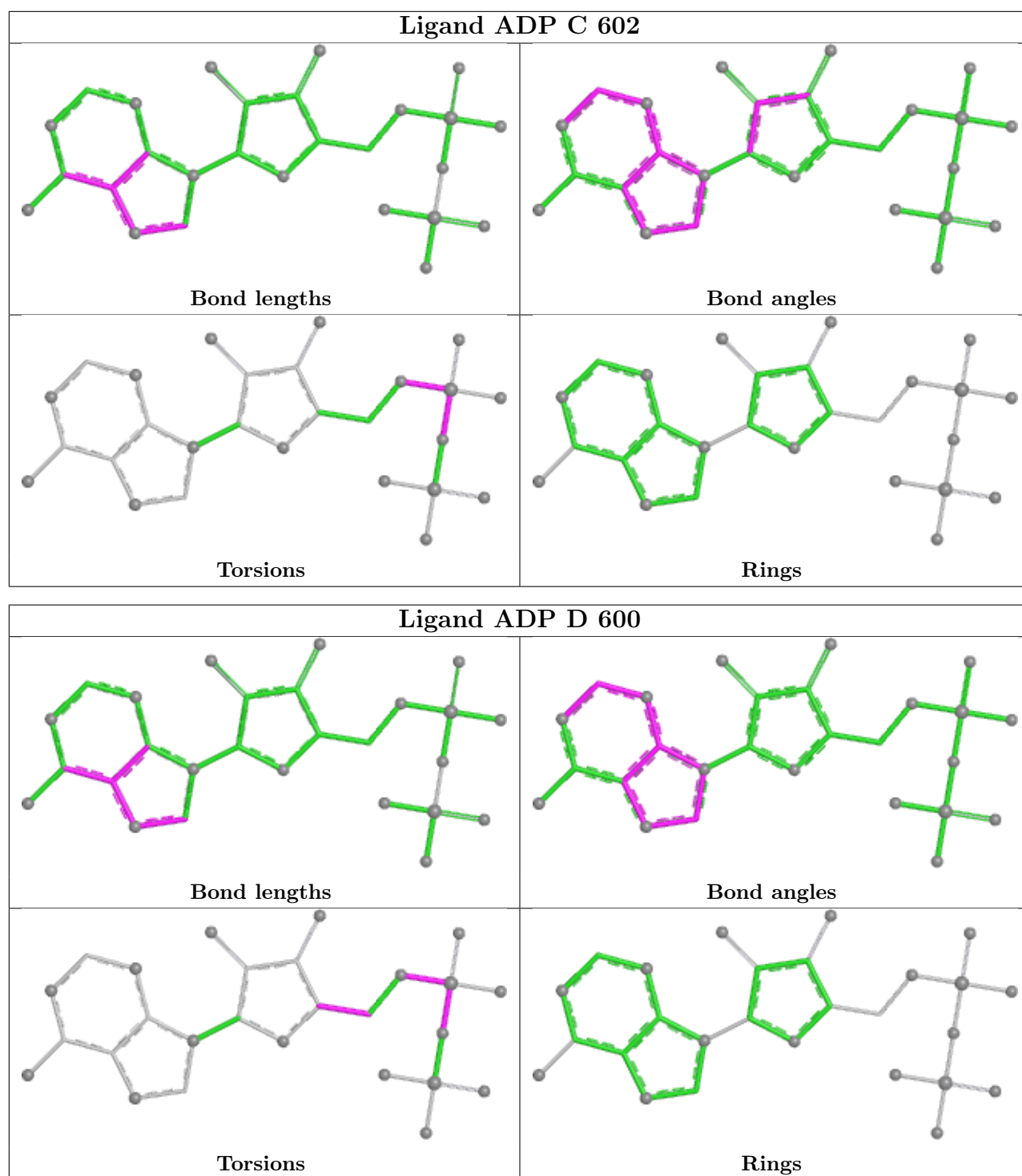












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	143:ARG	C	144:GLU	N	1.61

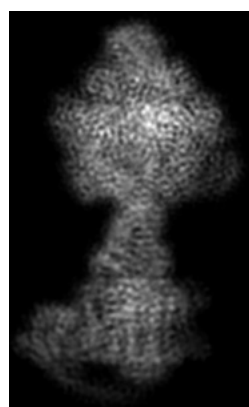
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10573. These allow visual inspection of the internal detail of the map and identification of artifacts.

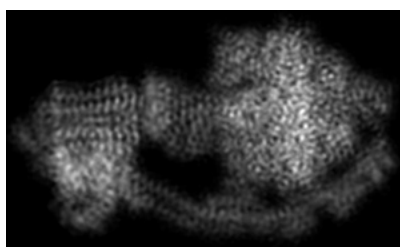
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

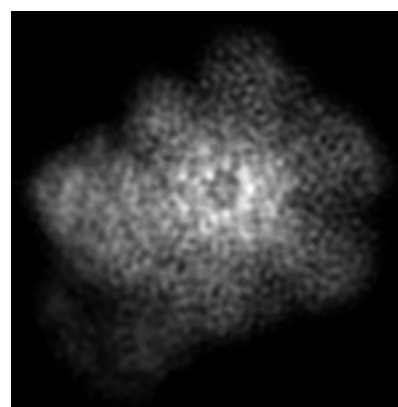
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

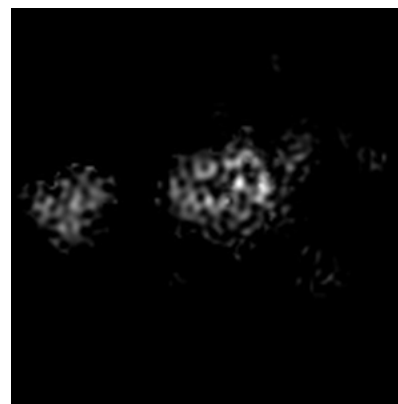
6.2.1 Primary map



X Index: 69



Y Index: 69



Z Index: 115

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

6.3 Largest variance slices [i](#)

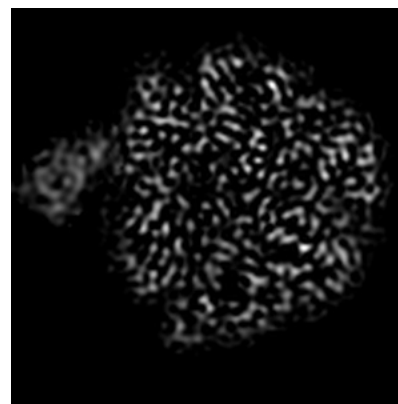
6.3.1 Primary map



X Index: 81



Y Index: 69

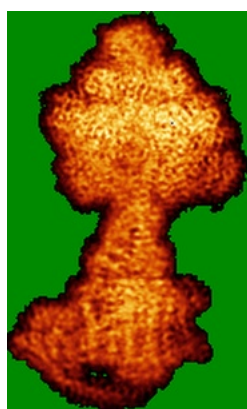


Z Index: 167

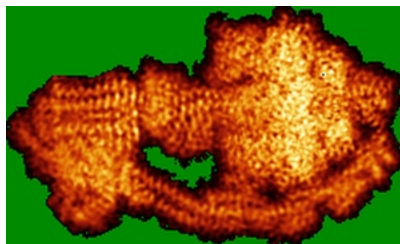
The images above show the largest variance slices of the map in three orthogonal directions.

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

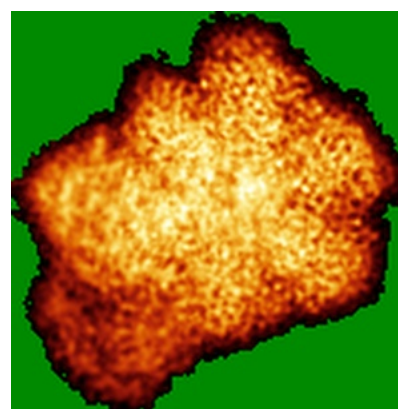
6.4.1 Primary map



X



Y

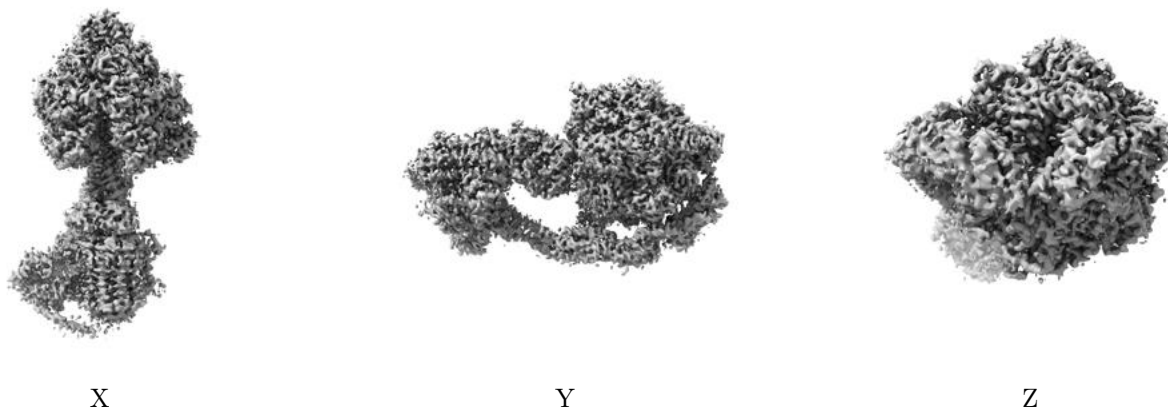


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

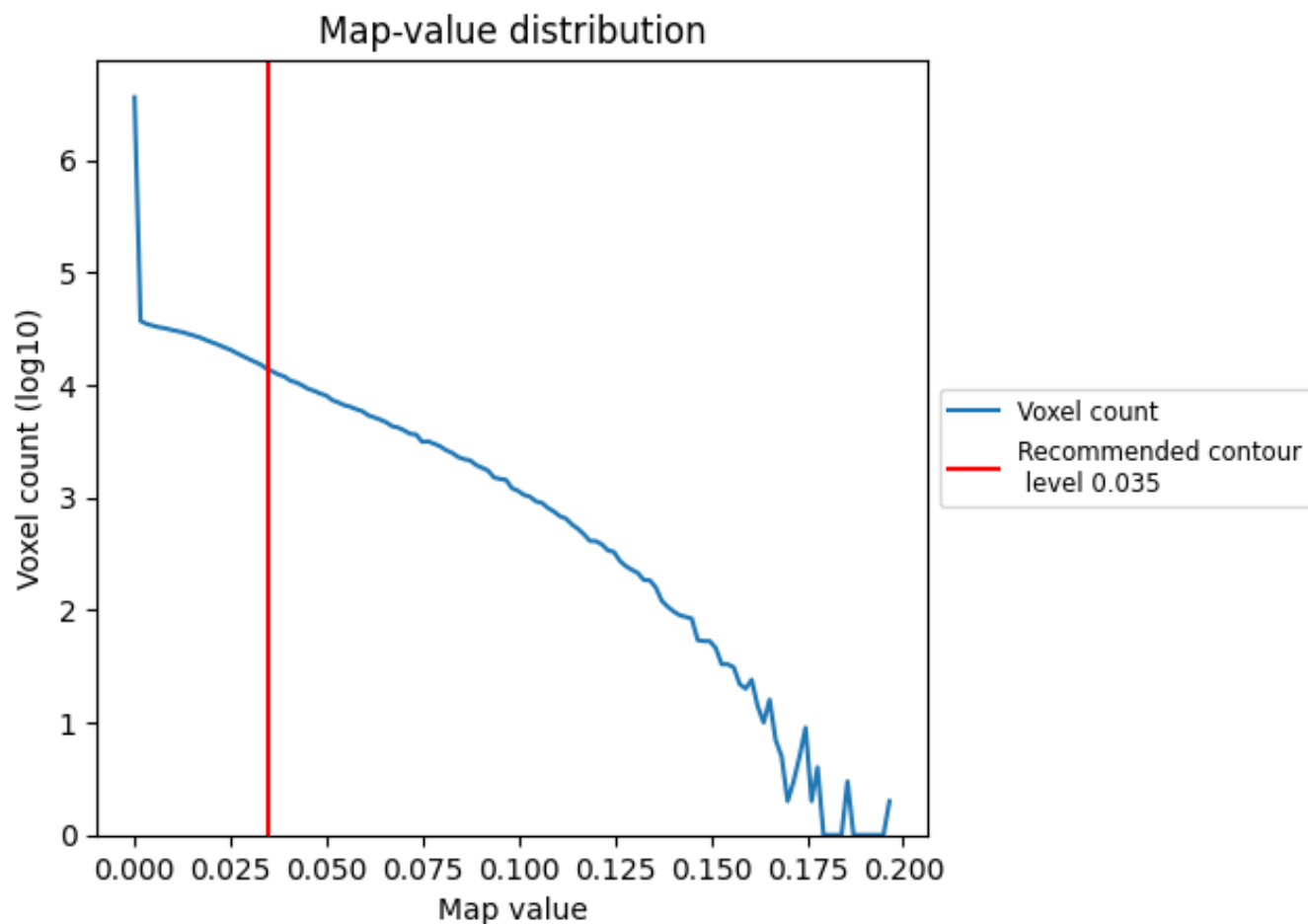
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

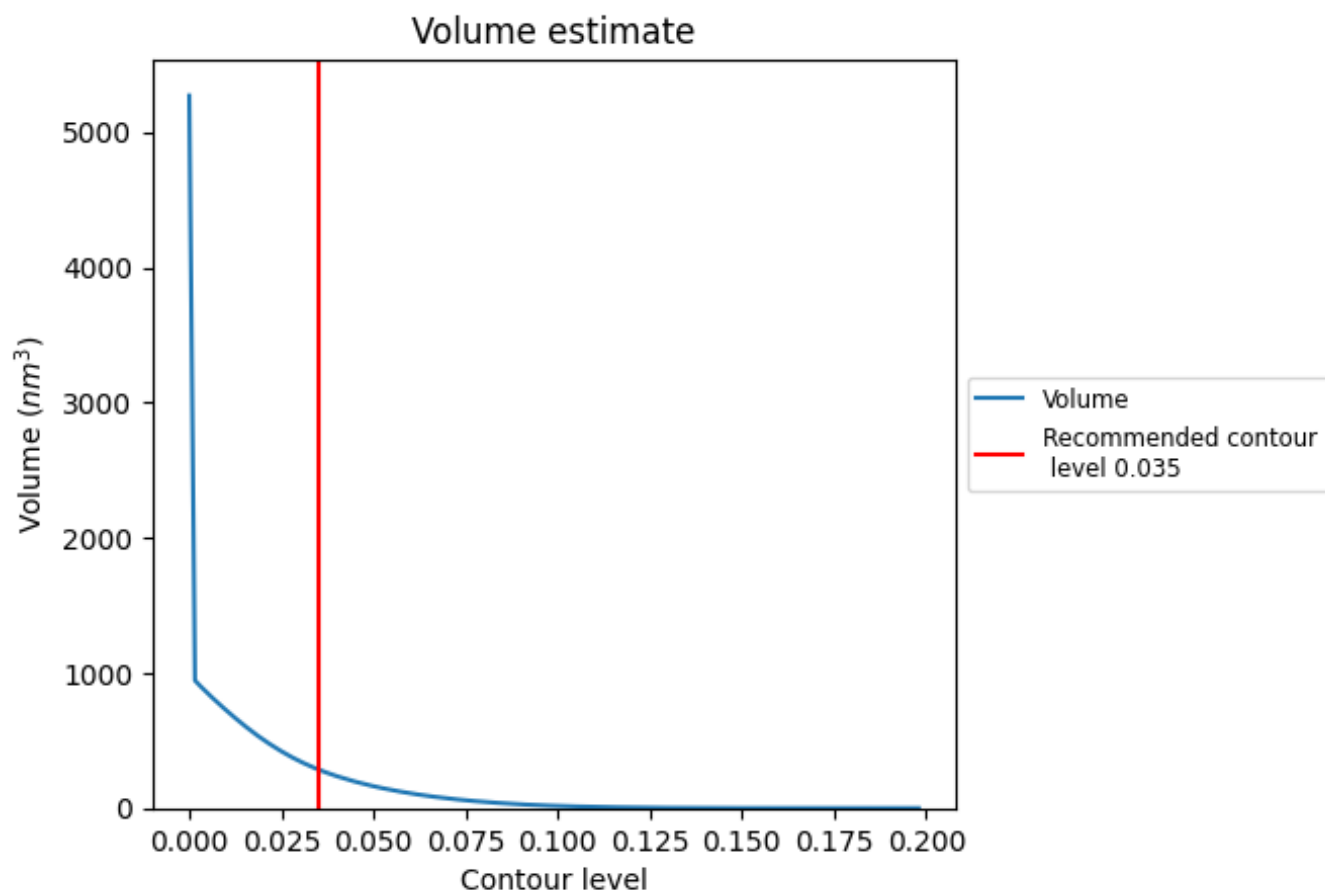
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 286 nm³; this corresponds to an approximate mass of 259 kDa.

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

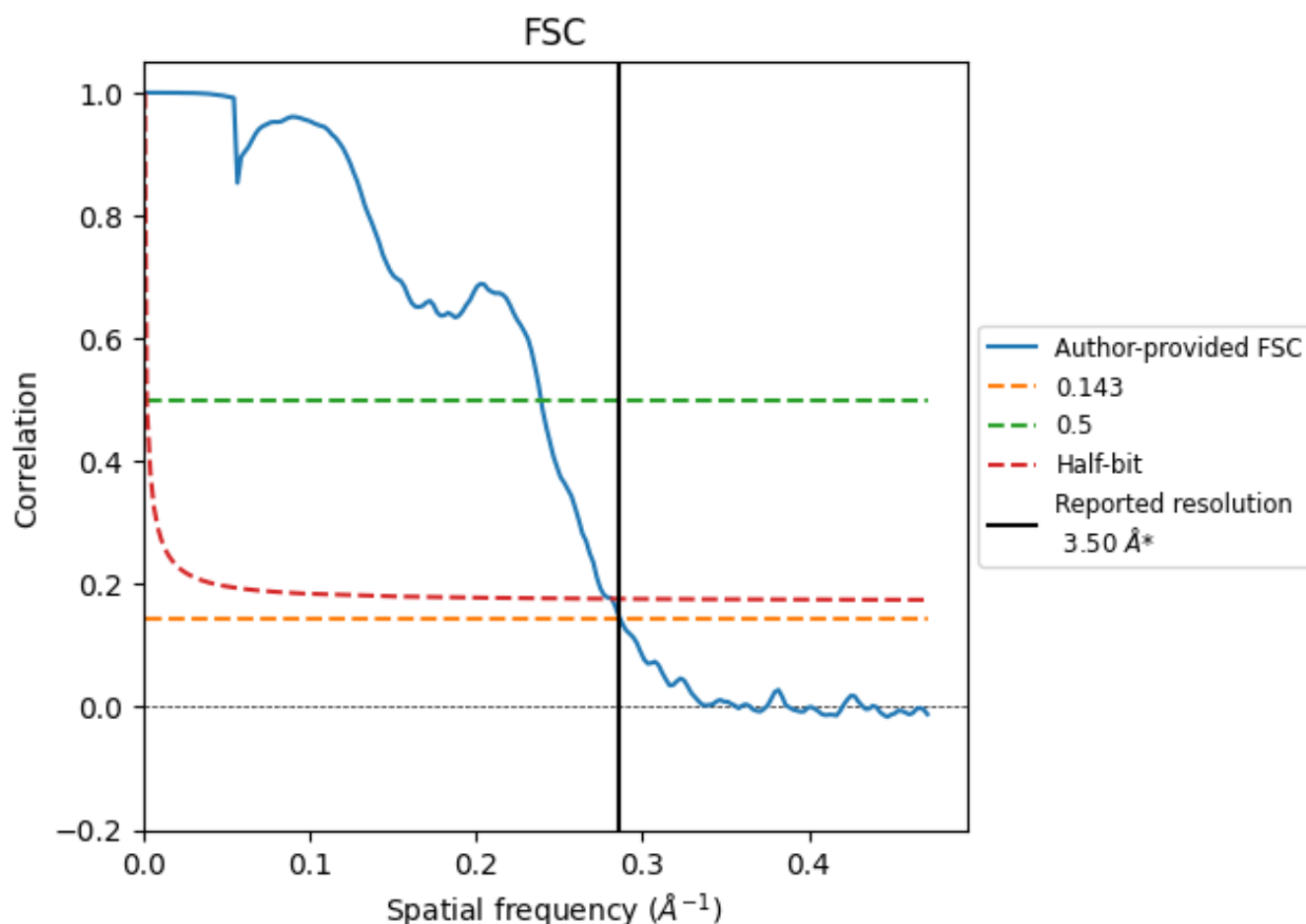
7.3 Rotationally averaged power spectrum [i](#)

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

8 Fourier-Shell correlation [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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

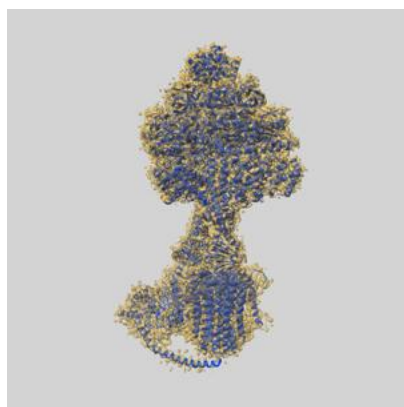
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	4.18	3.55
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

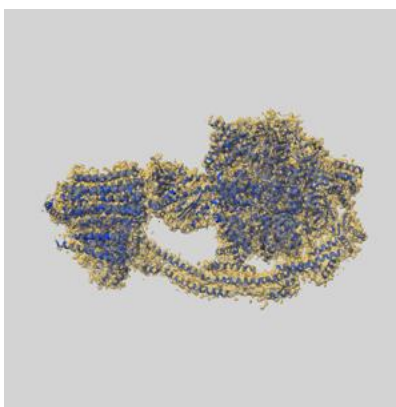
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10573 and PDB model 6TT7. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

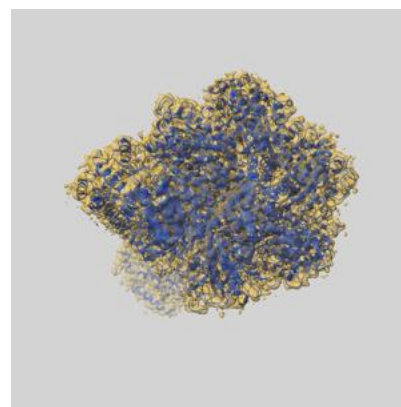
9.1 Map-model overlay [i](#)



X



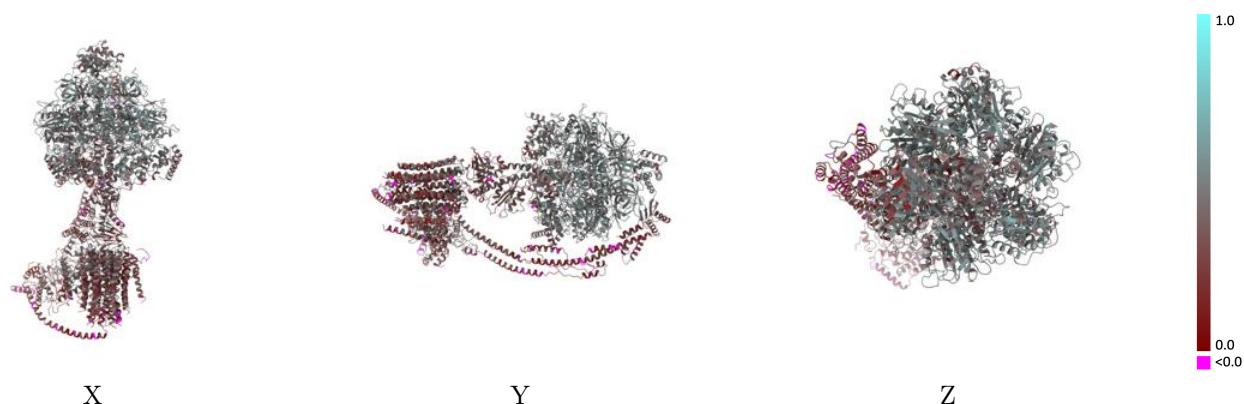
Y



Z

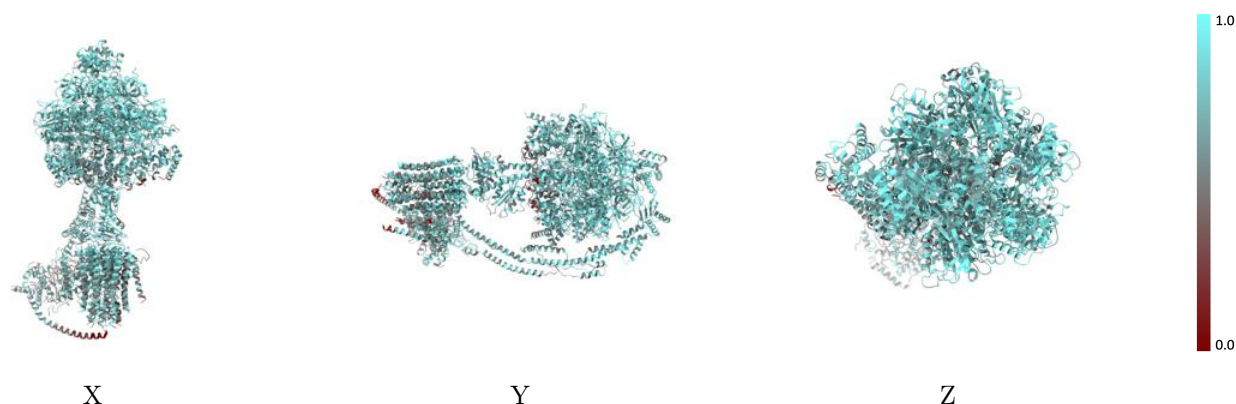
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



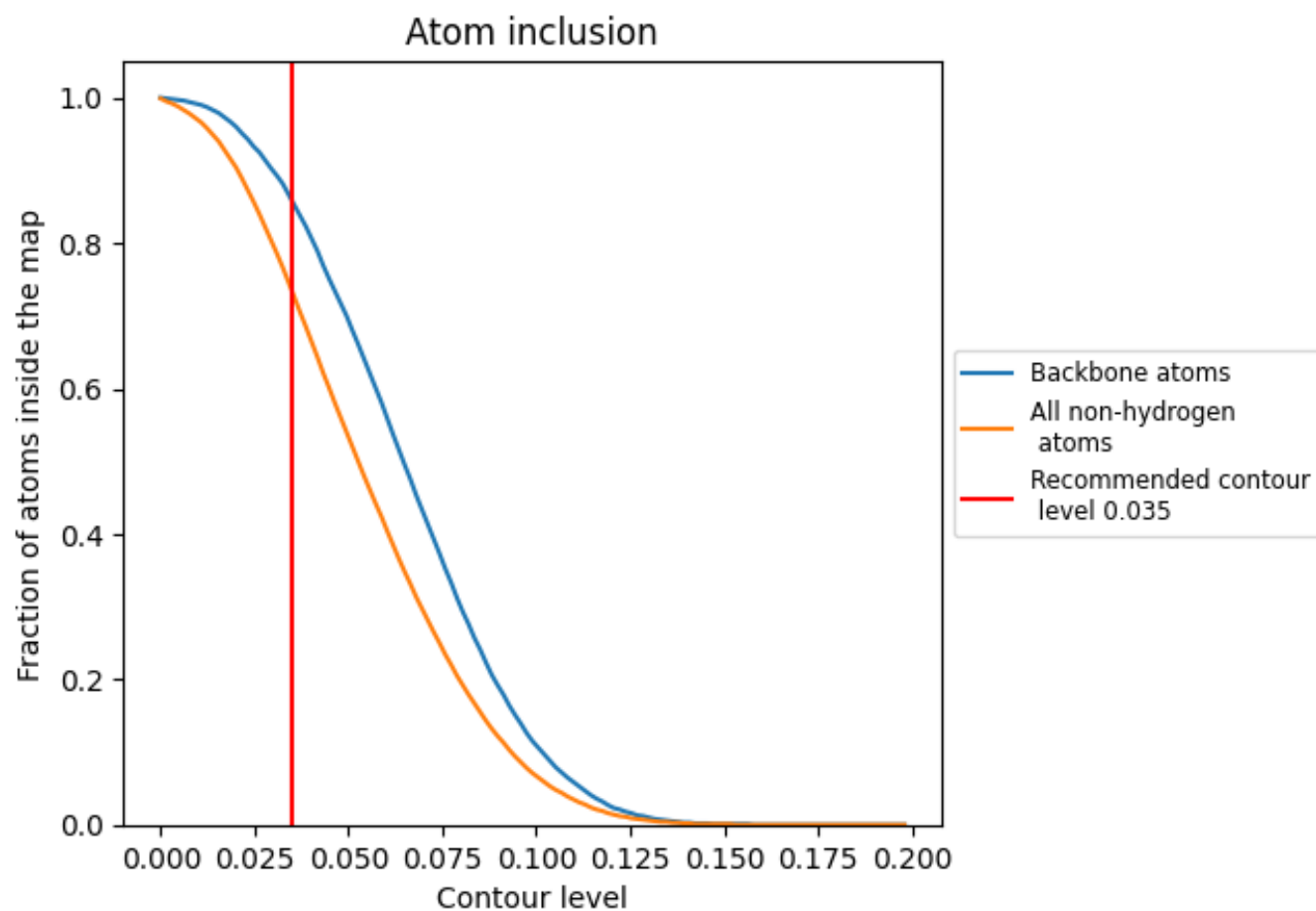
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 73% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7340	 0.4010
1	 0.6700	 0.3020
2	 0.6220	 0.3180
3	 0.7180	 0.3370
4	 0.6800	 0.3380
5	 0.6670	 0.3030
6	 0.7110	 0.3270
7	 0.7110	 0.3430
8	 0.6740	 0.3060
A	 0.7750	 0.4720
B	 0.7800	 0.4810
C	 0.7480	 0.4500
D	 0.7480	 0.4660
E	 0.7750	 0.4770
F	 0.7920	 0.4940
G	 0.7530	 0.3780
H	 0.7180	 0.3100
I	 0.7430	 0.3210
J	 0.7740	 0.4110
K	 0.7440	 0.2870
L	 0.7310	 0.2230
M	 0.6640	 0.2340
N	 0.7300	 0.3570
O	 0.4550	 0.1830
P	 0.6420	 0.2780
Q	 0.7180	 0.3620
R	 0.5790	 0.2890
S	 0.5800	 0.2090
T	 0.5070	 0.2110

