



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:28 PM UTC

PDB ID : 8APA / pdb_00008apa
EMDB ID : EMD-15563
Title : rotational state 1a of the Trypanosoma brucei mitochondrial ATP synthase dimer
Authors : Muehleip, A.; Gahura, O.; Zikova, A.; Amunts, A.
Deposited on : 2022-08-09
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

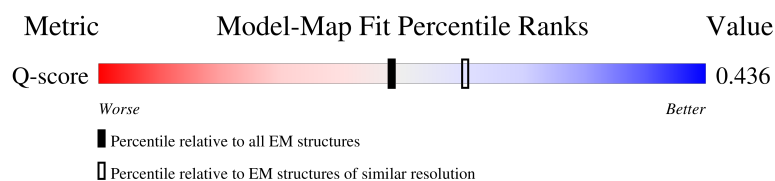
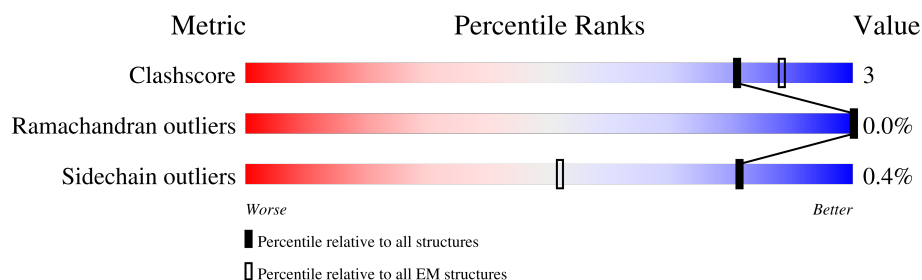
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.70 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	11569 (3.20 - 4.20)

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	A1	584	9% 82% 8% 9%
1	B1	584	8% 82% 8% 10%
1	C1	584	• 85% 5% 10%
2	D1	519	8% 86% 8% 6%

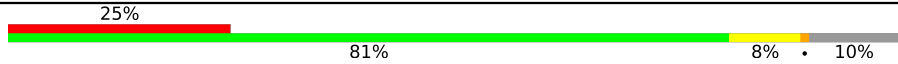
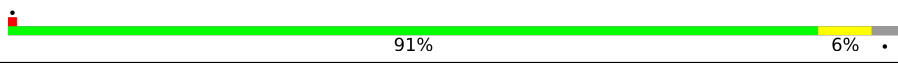
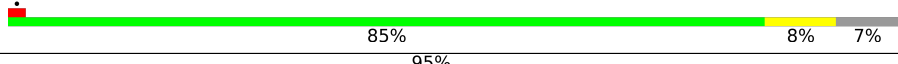
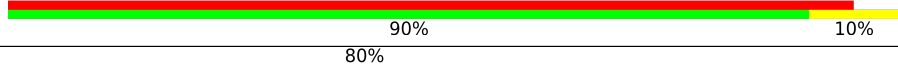
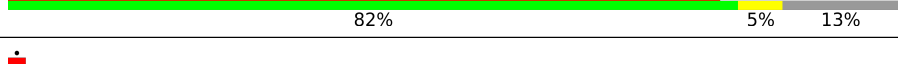
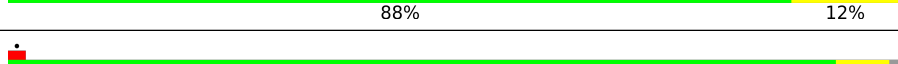
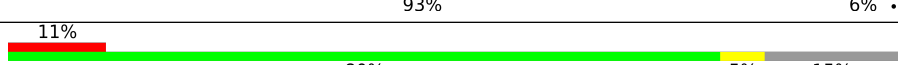
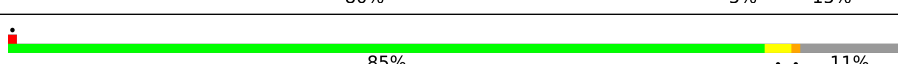
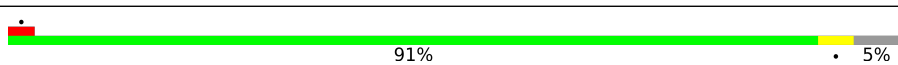
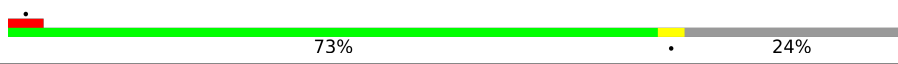
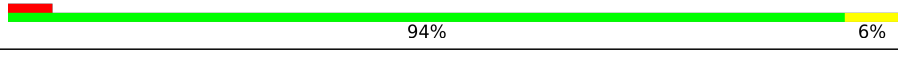
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Mol	Chain	Length	Quality of chain
2	E1	519	
2	F1	519	
3	G1	305	
4	H1	182	
5	I1	75	
6	J1	188	
6	K1	188	
6	L1	188	
7	L	92	
7	l	92	
8	M	144	
8	m	144	
9	M1	255	
10	O1	118	
10	P1	118	
10	Q1	118	
10	R1	118	
10	S1	118	
10	T1	118	
10	U1	118	
10	V1	118	
10	W1	118	
10	X1	118	
11	a	231	
12	c	114	

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Mol	Chain	Length	Quality of chain
13	d	370	
14	e	396	
15	f	145	
16	g	269	
17	h	157	
18	i	104	
19	j	169	
20	k	124	
21	n	156	
22	o	101	
23	p	105	
24	q	98	
25	r	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	Q7G	e	407	X	-	-	-
33	Q7G	n	201	X	-	-	-

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 129568 atoms, of which 65465 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, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A1	530	Total	C	H	N	O	S	0	0
			8281	2612	4197	710	742	20		
1	B1	523	Total	C	H	N	O	S	0	0
			8200	2585	4162	702	731	20		
1	C1	523	Total	C	H	N	O	S	0	0
			8194	2587	4155	701	731	20		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D1	487	Total	C	H	N	O	S	0	0
			7431	2329	3742	631	710	19		
2	E1	486	Total	C	H	N	O	S	0	0
			7415	2324	3733	630	709	19		
2	F1	489	Total	C	H	N	O	S	0	0
			7462	2339	3759	633	712	19		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G1	300	Total	C	H	N	O	S	0	0
			4774	1507	2387	423	448	9		

- Molecule 4 is a protein called ATP synthase, epsilon chain, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	H1	161	Total	C	H	N	O	S	0	0
			2483	788	1232	211	248	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	I1	65	Total	C	H	N	O	S	0	0
			1046	332	513	97	102	2		

- Molecule 6 is a protein called ATP synthase subunit p18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	J1	166	Total	C	H	N	O	S	0	0
			2591	822	1276	221	258	14		
6	K1	166	Total	C	H	N	O	S	0	0
			2591	822	1276	221	258	14		
6	L1	165	Total	C	H	N	O	S	0	0
			2581	819	1271	220	257	14		

- Molecule 7 is a protein called subunit-e.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	L	65	Total	C	H	N	O	S	0	0
			1082	340	545	104	92	1		
7	l	65	Total	C	H	N	O	S	0	0
			1082	340	545	104	92	1		

- Molecule 8 is a protein called subunit-g.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	M	129	Total	C	H	N	O	S	0	0
			2069	662	1042	177	186	2		
8	m	129	Total	C	H	N	O	S	0	0
			2069	662	1042	177	186	2		

- Molecule 9 is a protein called OSCP.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	M1	234	Total	C	H	N	O	S	0	0
			3750	1212	1873	302	360	3		

- Molecule 10 is a protein called ATPase subunit 9, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	O1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
10	P1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	Q1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
10	R1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
10	S1	78	Total	C	H	N	O	S	0	0
			1166	376	601	89	96	4		
10	T1	78	Total	C	H	N	O	S	0	0
			1166	376	601	89	96	4		
10	U1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
10	V1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
10	W1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
10	X1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	a	231	Total	C	H	N	O	S	0	0
			4076	1459	2044	261	284	28		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	23	TRP	-	insertion	UNP P24499
a	180	TRP	-	insertion	UNP P24499

- Molecule 12 is a protein called subunit-8.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	c	86	Total	C	H	N	O	S	0	0
			1460	494	715	116	130	5		

- Molecule 13 is a protein called subunit-d.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	d	332	Total	C	H	N	O	S	0	0
			5499	1710	2762	505	514	8		

- Molecule 14 is a protein called ATPTB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	e	383	Total	C	H	N	O	S	0	0
			6270	2060	3050	558	585	17		

- Molecule 15 is a protein called subunit-f.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	f	135	Total	C	H	N	O	S	0	0
			2256	744	1111	201	195	5		

- Molecule 16 is a protein called ATPTB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	g	268	Total	C	H	N	O	S	0	0
			3953	1211	2020	343	378	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	176	ALA	VAL	conflict	UNP A0A3L6KRX7

- Molecule 17 is a protein called ATPTB4.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	h	137	Total	C	H	N	O	S	0	0
			2158	680	1088	184	203	3		

- Molecule 18 is a protein called subunit-i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	i	103	Total	C	H	N	O	S	0	0
			1740	574	857	152	151	6		

- Molecule 19 is a protein called ATPTB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	j	168	Total	C	H	N	O	S	0	0
			2835	919	1411	249	249	7		

- Molecule 20 is a protein called subunit-k.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	k	105	Total	C	H	N	O	S	0	0
			1749	577	876	149	141	6		

- Molecule 21 is a protein called ATPTB11.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	n	139	Total	C	H	N	O	S	0	0
			2210	730	1082	183	208	7		

- Molecule 22 is a protein called ATPTB12.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	o	96	Total	C	H	N	O	S	0	0
			1556	506	767	140	140	3		

- Molecule 23 is a protein called subunit-b.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	p	80	Total	C	H	N	O	S	0	0
			1335	448	651	108	125	3		

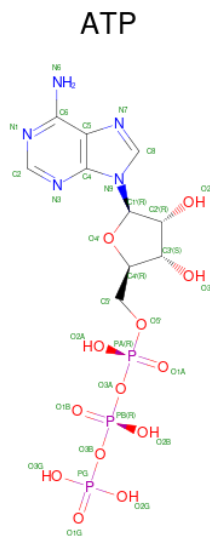
- Molecule 24 is a protein called ATPEG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	q	85	Total	C	H	N	O		0	0
			1486	499	720	142	125			

- Molecule 25 is a protein called ATPEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	r	62	Total	C	H	N	O	S	0	0
			1040	358	498	94	85	5		

- Molecule 26 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

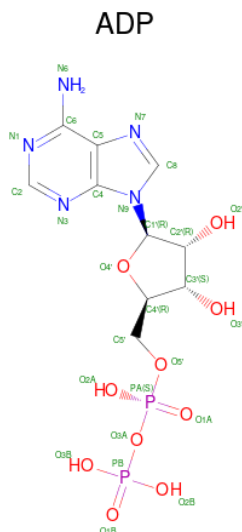


Mol	Chain	Residues	Atoms						AltConf
26	A1	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
26	B1	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
26	C1	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
26	F1	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

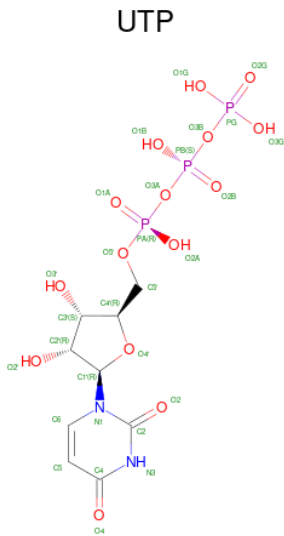
Mol	Chain	Residues	Atoms	AltConf
27	A1	1	Total Mg 1 1	0
27	B1	1	Total Mg 1 1	0
27	C1	1	Total Mg 1 1	0
27	D1	1	Total Mg 1 1	0
27	F1	1	Total Mg 1 1	0

- Molecule 28 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



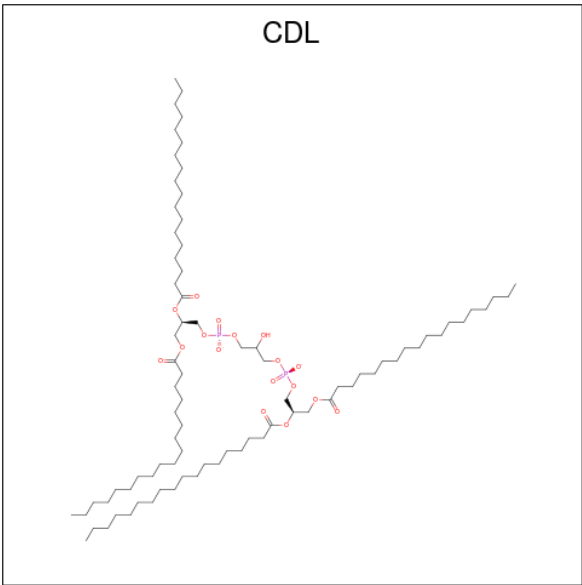
Mol	Chain	Residues	Atoms						AltConf
28	D1	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 29 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: $\text{C}_9\text{H}_{15}\text{N}_2\text{O}_{15}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



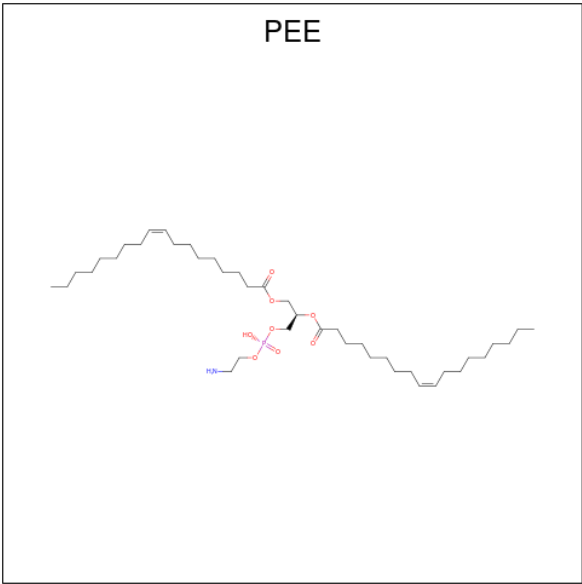
Mol	Chain	Residues	Atoms						AltConf
29	H1	1	Total	C	H	N	O	P	0
			40	9	11	2	15	3	

- Molecule 30 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



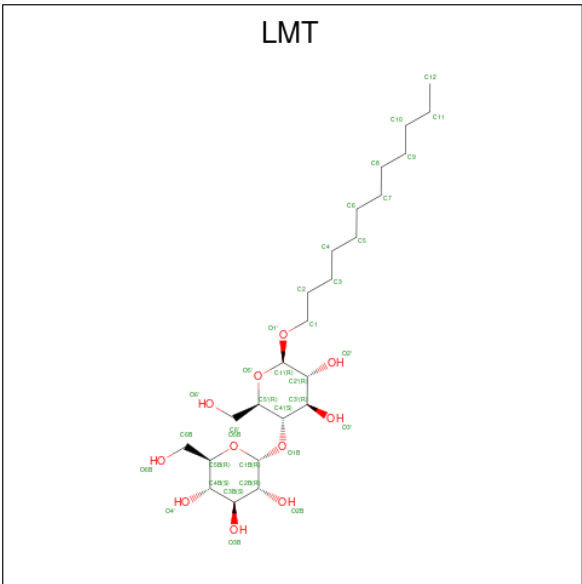
Mol	Chain	Residues	Atoms					AltConf
30	L	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	c	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	j	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	l	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	m	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	p	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	q	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	q	1	Total	C	H	O	P	0
			256	81	156	17	2	

- Molecule 31 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



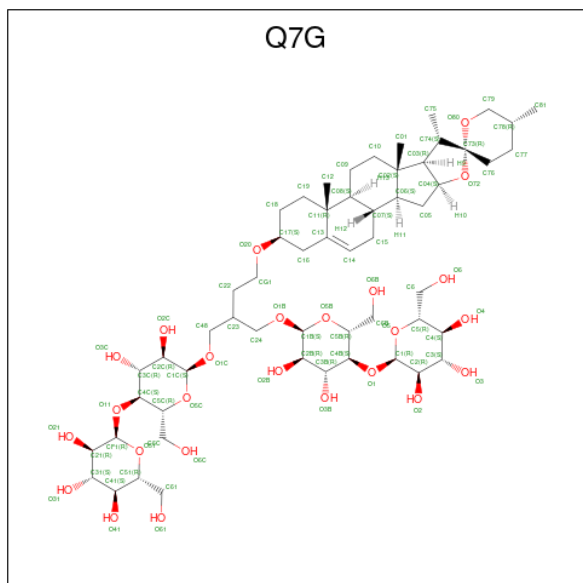
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
31	M	1	Total 133	41	82	1	8	1	0
31	f	1	Total 133	41	82	1	8	1	0
31	m	1	Total 133	41	82	1	8	1	0

- Molecule 32 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



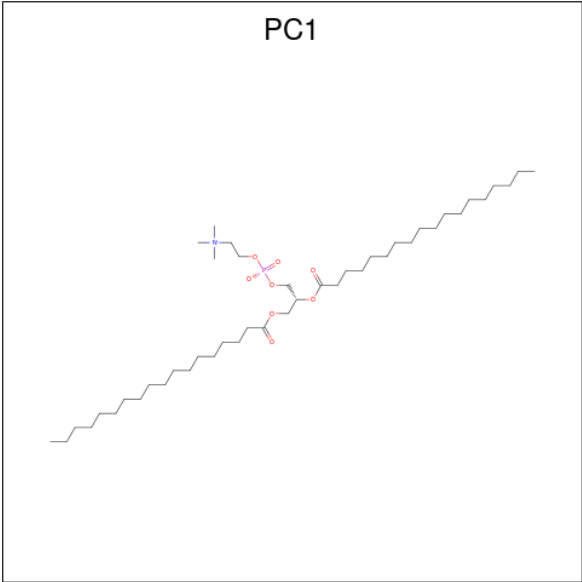
Mol	Chain	Residues	Atoms				AltConf
32	e	1	Total	C	H	O	0
			74	24	39	11	
32	j	1	Total	C	H	O	0
			74	24	39	11	

- Molecule 33 is 2-[[[(4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranosyl)oxy]methyl]-4-[[[(3 beta,9beta,14beta,17beta,25R)-spirost-5-en-3-yl]oxy]butyl 4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranoside (CCD ID: Q7G) (formula: C₅₆H₉₂O₂₅).



Mol	Chain	Residues	Atoms				AltConf
33	e	1	Total	C	H	O	0
			108	38	60	10	
33	n	1	Total	C	H	O	0
			129	44	70	15	

- Molecule 34 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P) (labeled as "Ligand of Interest" by depositor).

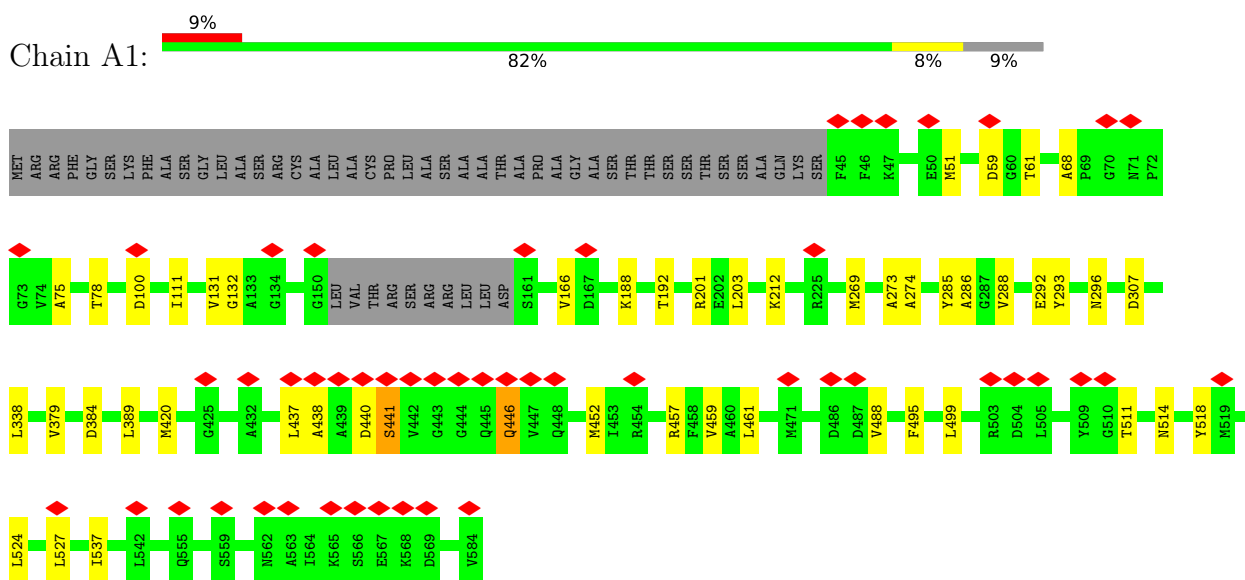


Mol	Chain	Residues	Atoms						AltConf
34	f	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
34	f	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
34	i	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
34	j	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

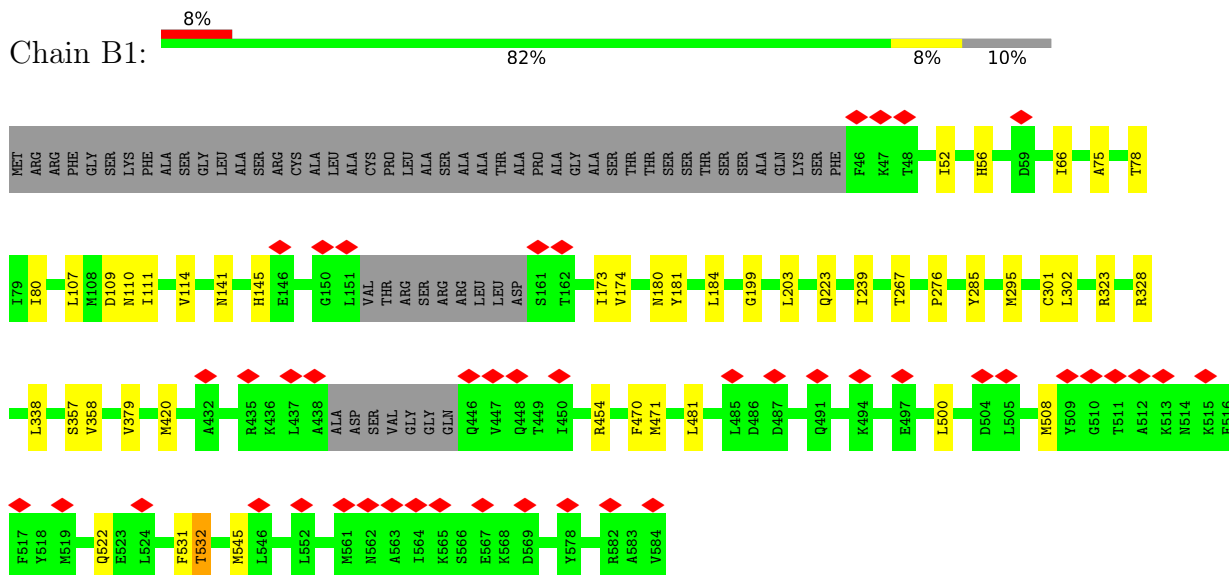
3 Residue-property plots

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.

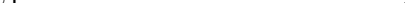
- Molecule 1: ATP synthase subunit alpha, mitochondrial

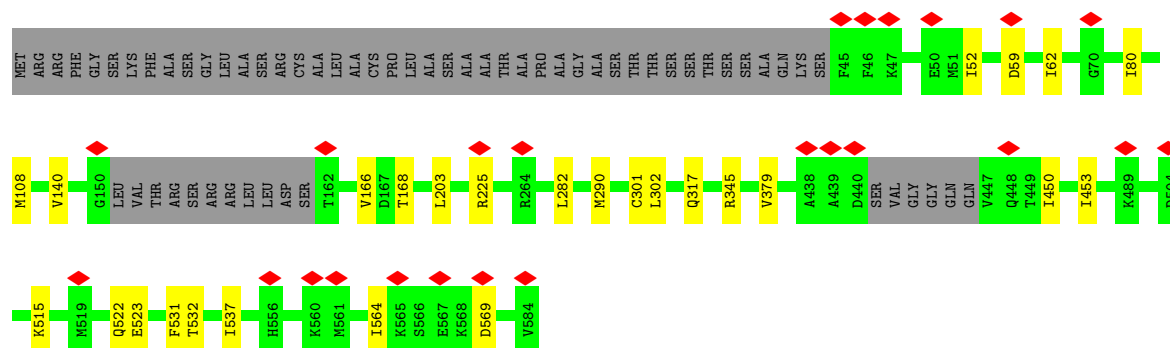


- Molecule 1: ATP synthase subunit alpha, mitochondrial

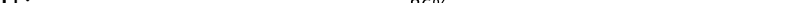


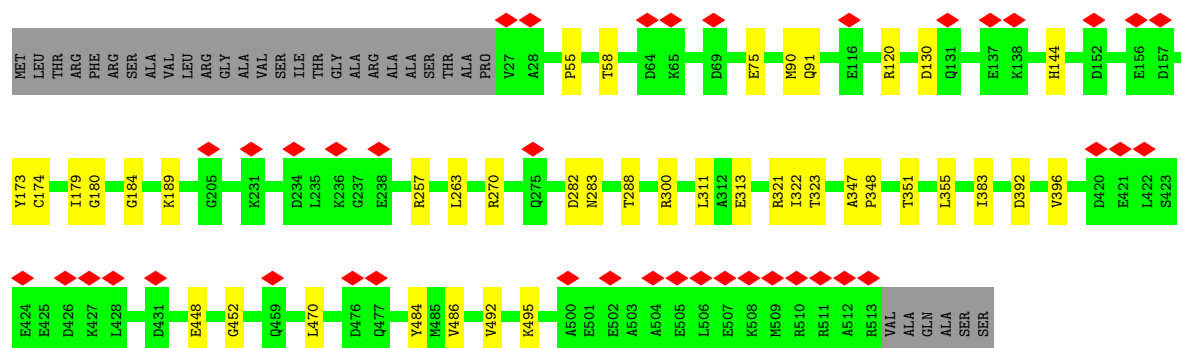
- Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain C1:  85% 5% 10%

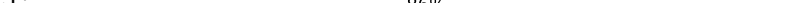


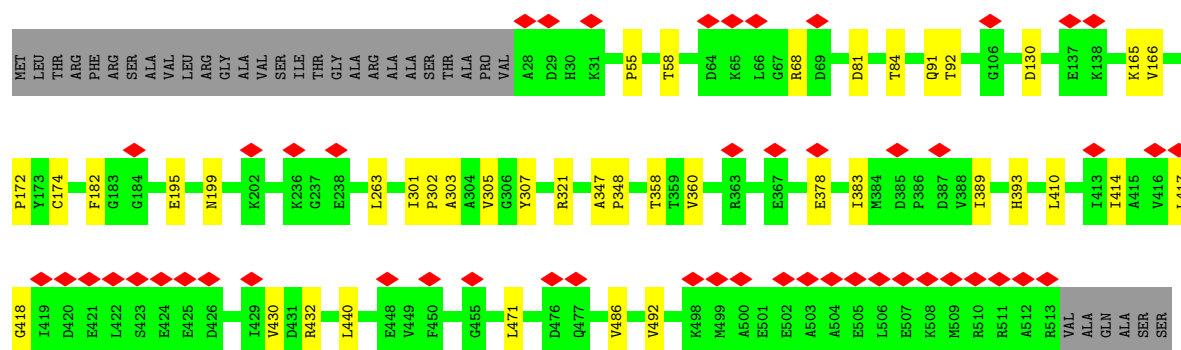
- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain D1: 

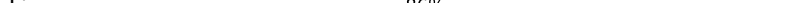


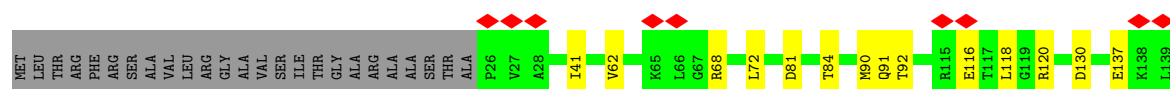
- Molecule 2: ATP synthase subunit beta, mitochondrial

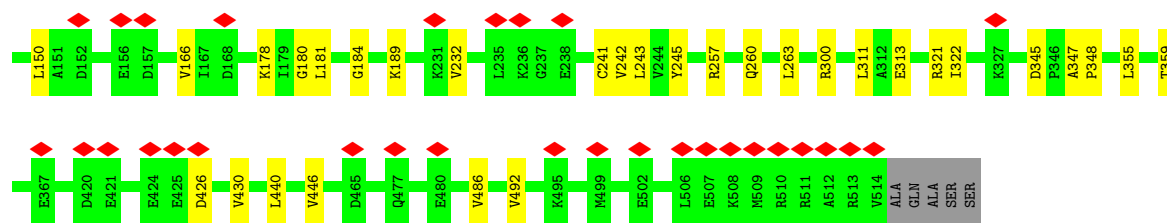
Chain E1: 



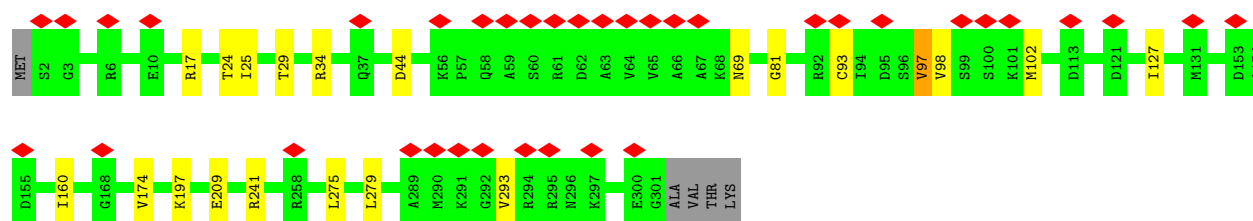
- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain F1: 

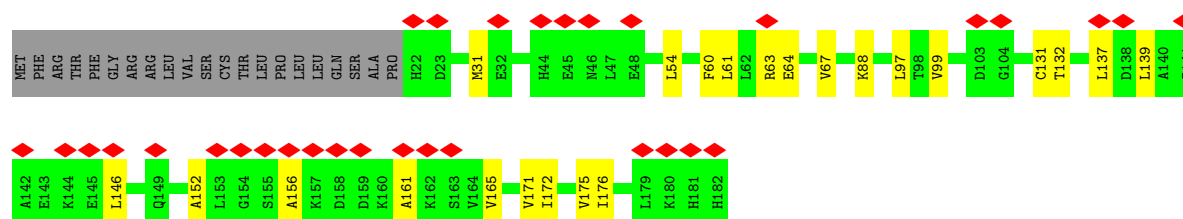
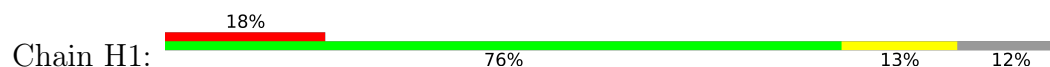




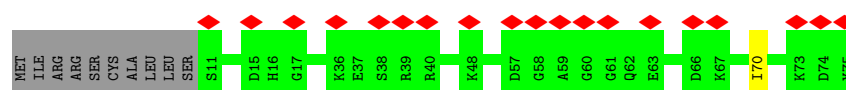
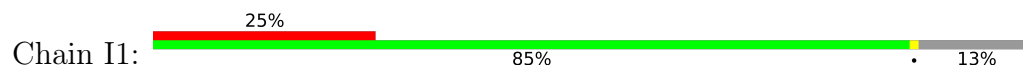
• Molecule 3: ATP synthase gamma subunit



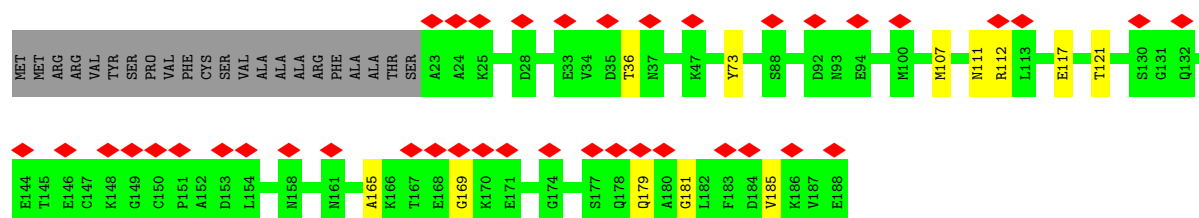
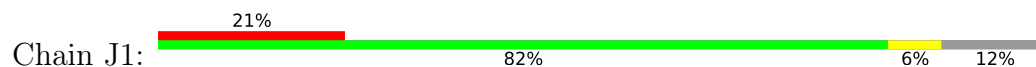
• Molecule 4: ATP synthase, epsilon chain, putative



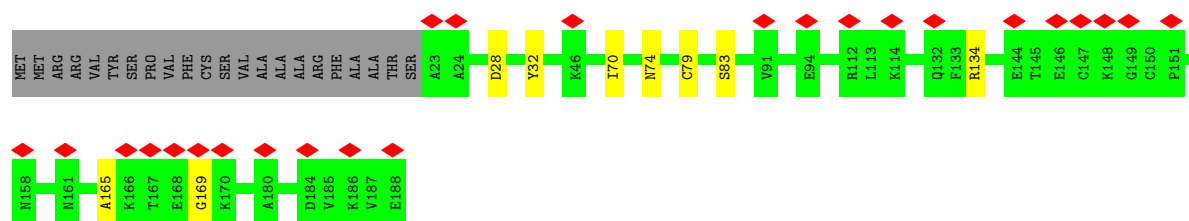
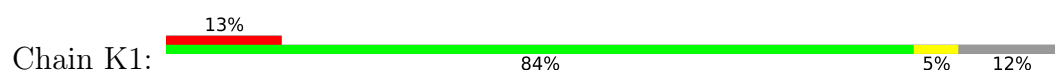
• Molecule 5: ATP synthase subunit epsilon, mitochondrial



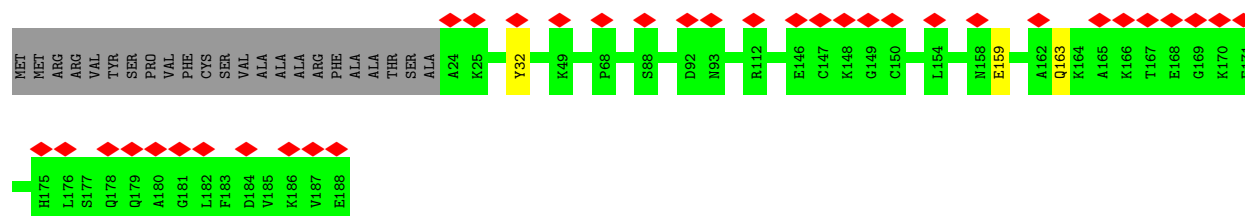
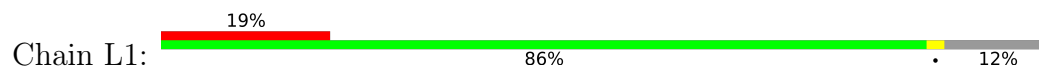
• Molecule 6: ATP synthase subunit p18, mitochondrial



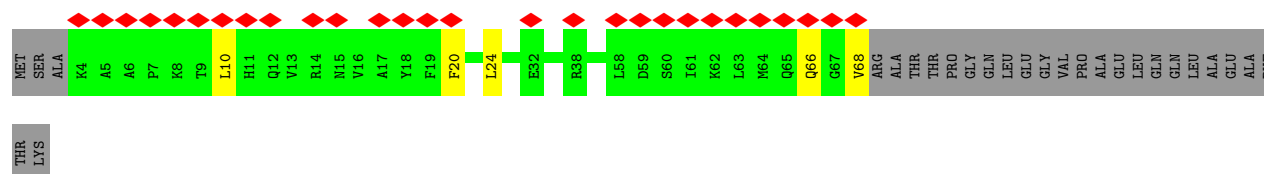
• Molecule 6: ATP synthase subunit p18, mitochondrial



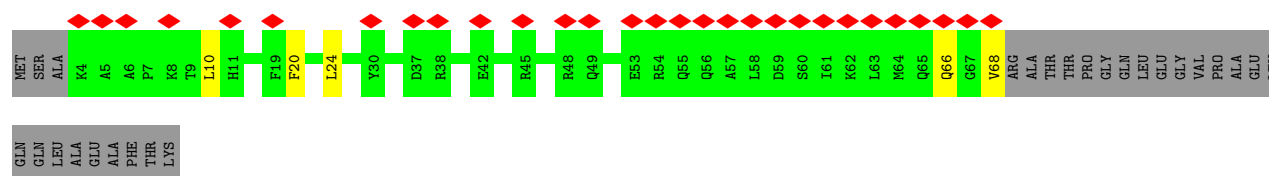
- Molecule 6: ATP synthase subunit p18, mitochondrial



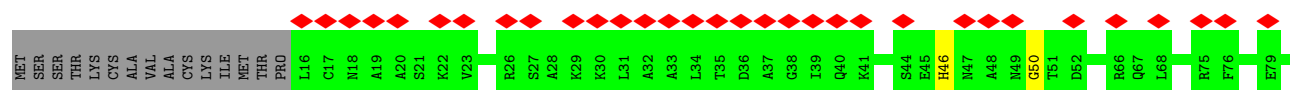
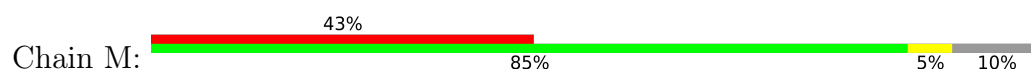
- Molecule 7: subunit-e

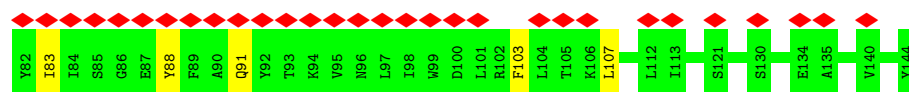


- Molecule 7: subunit-e

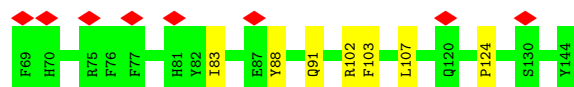
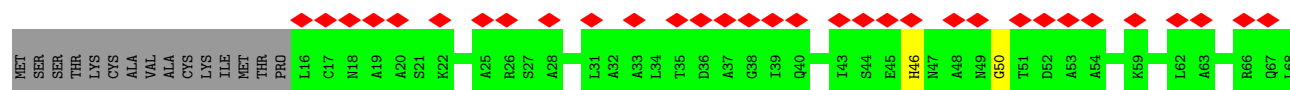
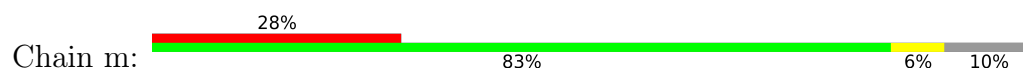


- Molecule 8: subunit-g

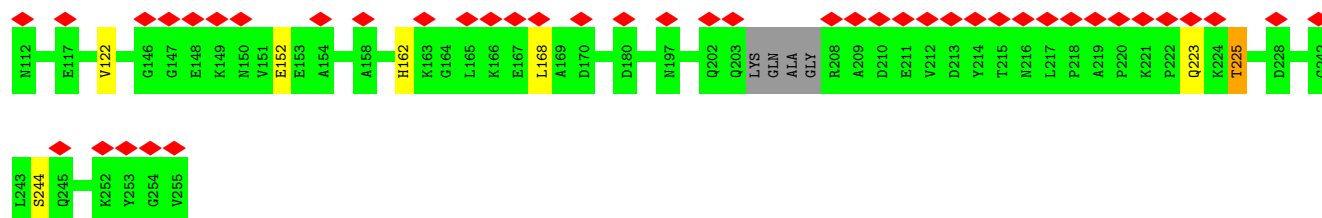
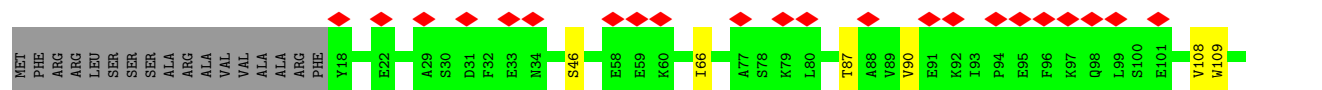
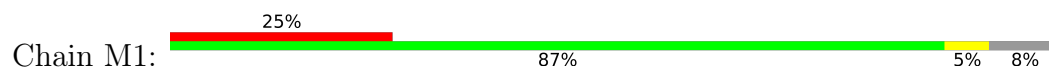




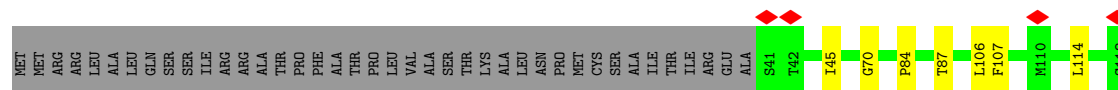
- Molecule 8: subunit-g



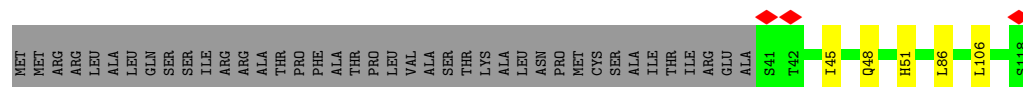
- Molecule 9: OSCP



- Molecule 10: ATPase subunit 9, putative

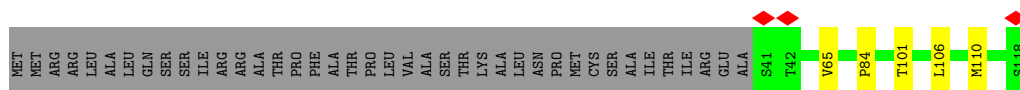


- Molecule 10: ATPase subunit 9, putative

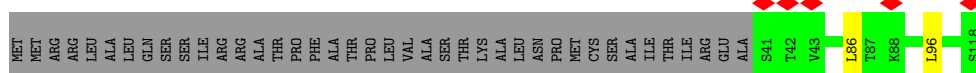


- Molecule 10: ATPase subunit 9, putative

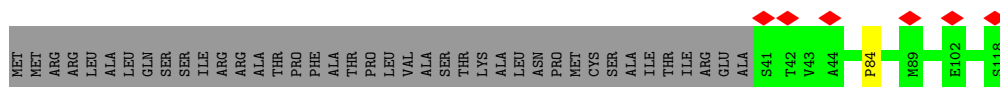




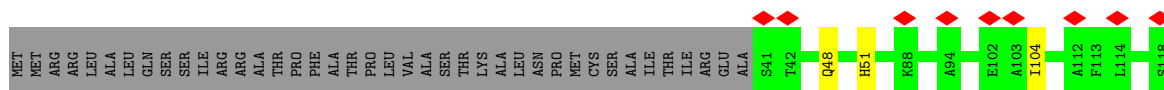
- Molecule 10: ATPase subunit 9, putative



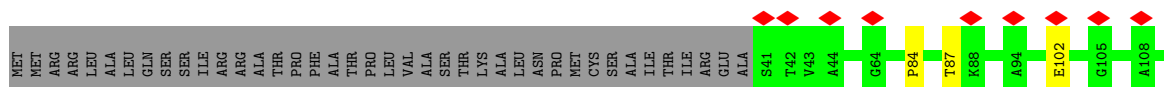
- Molecule 10: ATPase subunit 9, putative



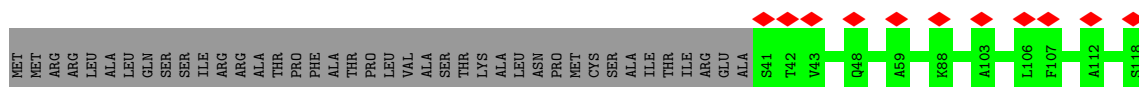
- Molecule 10: ATPase subunit 9, putative



- Molecule 10: ATPase subunit 9, putative

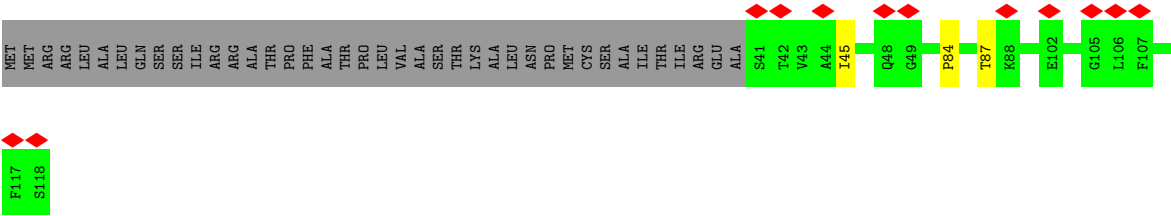


- Molecule 10: ATPase subunit 9, putative

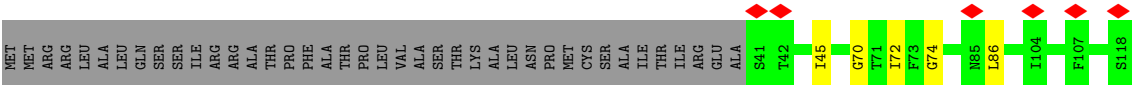


- Molecule 10: ATPase subunit 9, putative

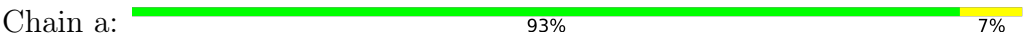




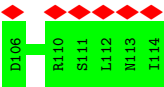
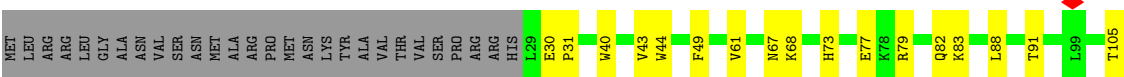
• Molecule 10: ATPase subunit 9, putative



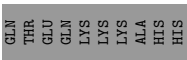
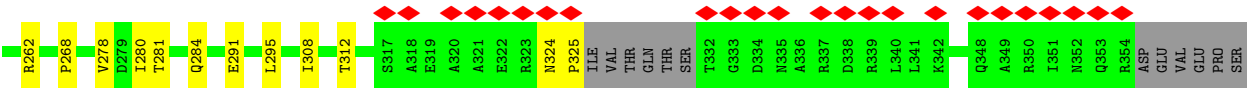
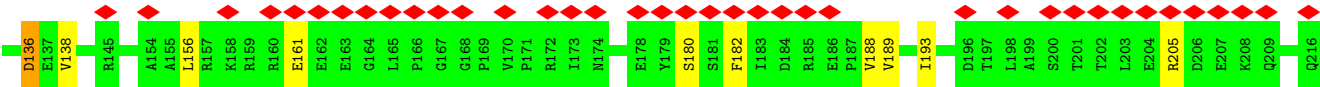
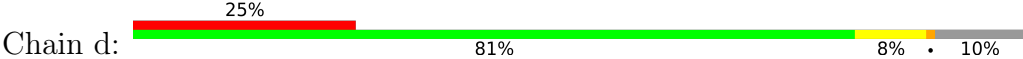
• Molecule 11: ATP synthase subunit a



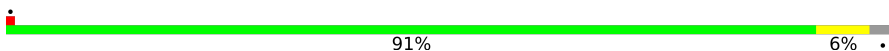
• Molecule 12: subunit-8

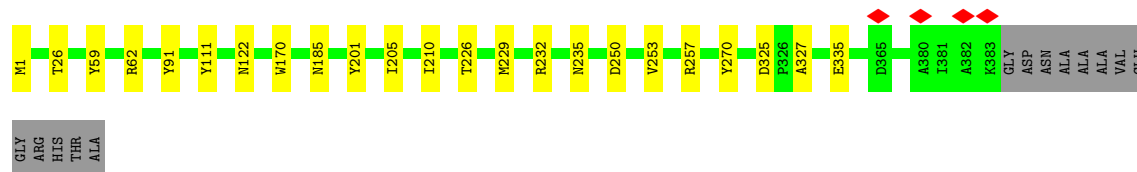


• Molecule 13: subunit-d



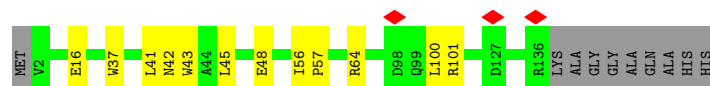
- Molecule 14: ATPTB1

Chain e:  91% 6%

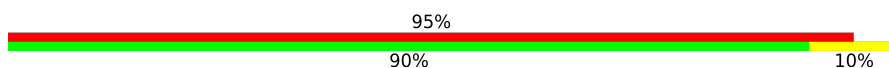


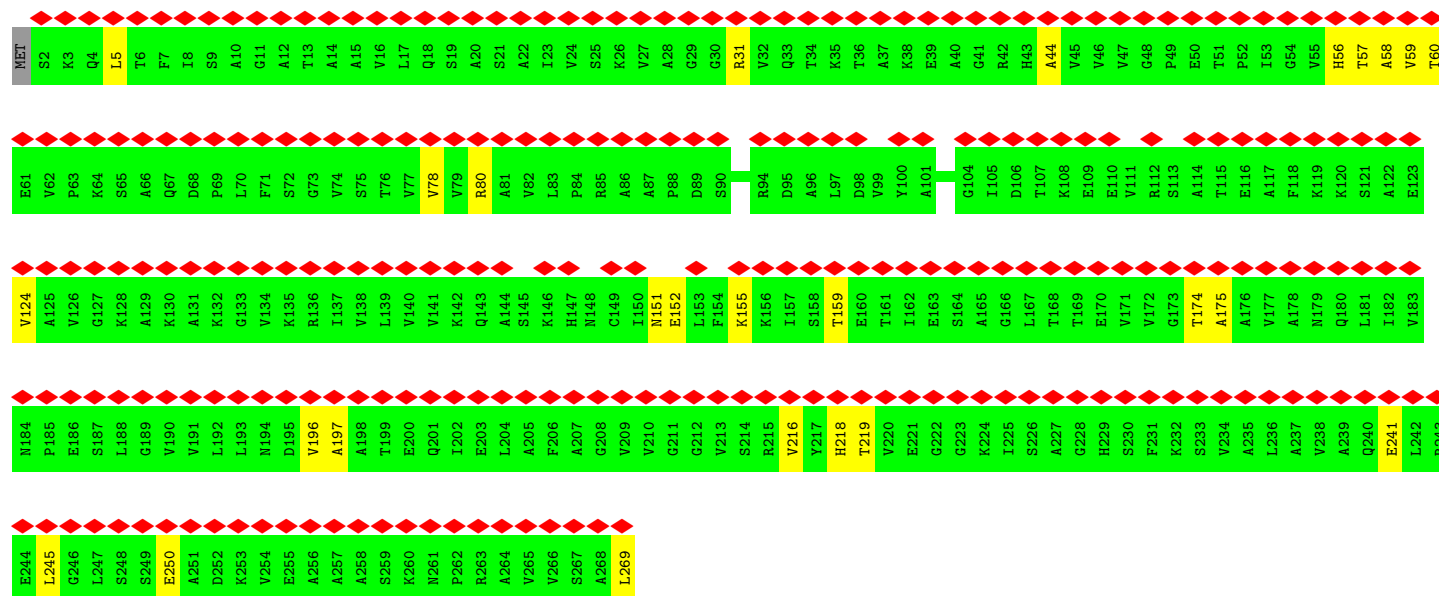
- Molecule 15: subunit-f

Chain f:  85% 8% 7%



- Molecule 16: ATPTB3

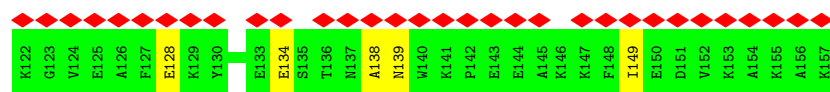
Chain g:  95% 90% 10%



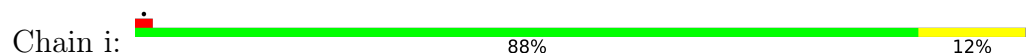
- Molecule 17: ATPTB4

Chain h:  80% 82% 5% 13%

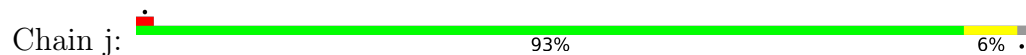




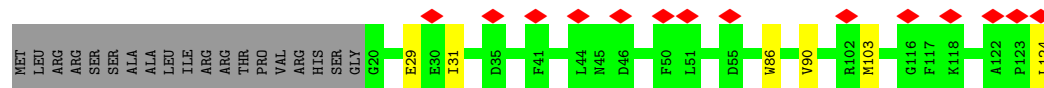
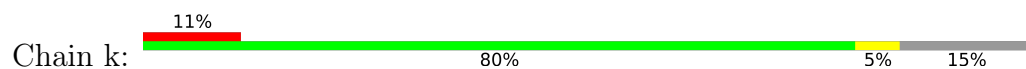
- Molecule 18: subunit-i/j



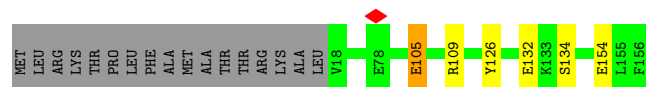
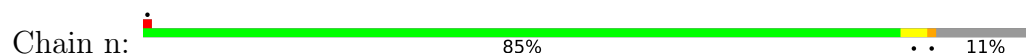
- Molecule 19: ATPTB6



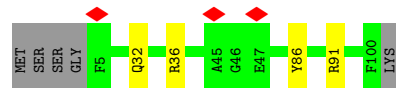
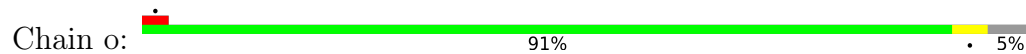
- Molecule 20: subunit-k



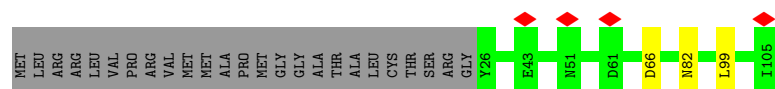
- Molecule 21: ATPTB11



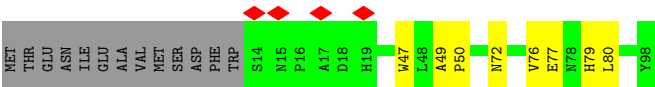
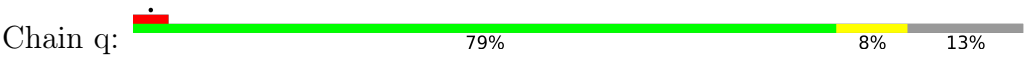
- Molecule 22: ATPTB12



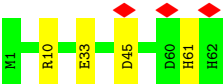
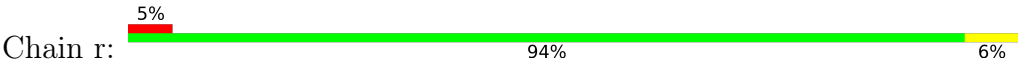
- Molecule 23: subunit-b



- Molecule 24: ATPEG3



● Molecule 25: ATPEG4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19764	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 ($e^-/\text{\AA}^2$)	33	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.091	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	464.8, 464.8, 464.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, UTP, PC1, LMT, AME, Q7G, PEE, CDL, ATP

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	A1	0.14	0/4159	0.22	0/5632
1	B1	0.13	0/4111	0.22	0/5566
1	C1	0.15	0/4113	0.22	0/5569
2	D1	0.14	0/3745	0.22	0/5077
2	E1	0.13	0/3738	0.22	0/5067
2	F1	0.14	0/3760	0.23	0/5098
3	G1	0.13	0/2427	0.24	0/3268
4	H1	0.17	0/1274	0.26	0/1728
5	I1	0.10	0/547	0.21	0/738
6	J1	0.08	0/1342	0.19	0/1810
6	K1	0.09	0/1342	0.20	0/1810
6	L1	0.08	0/1337	0.19	0/1803
7	L	0.09	0/547	0.16	0/735
7	l	0.09	0/547	0.16	0/735
8	M	0.09	0/1049	0.19	0/1423
8	m	0.09	0/1049	0.19	0/1423
9	M1	0.09	0/1916	0.20	0/2591
10	O1	0.14	0/574	0.21	0/777
10	P1	0.17	0/574	0.20	0/777
10	Q1	0.15	0/574	0.18	0/777
10	R1	0.14	0/574	0.20	0/777
10	S1	0.13	0/574	0.21	0/777
10	T1	0.13	0/574	0.18	0/777
10	U1	0.13	0/574	0.19	0/777
10	V1	0.12	0/574	0.17	0/777
10	W1	0.12	0/574	0.17	0/777
10	X1	0.12	0/574	0.19	0/777
11	a	0.23	0/2111	0.26	0/2861
12	c	0.23	0/772	0.36	0/1054
13	d	0.13	0/2786	0.24	0/3760
14	e	0.18	0/3305	0.23	0/4482
15	f	0.19	0/1183	0.27	0/1601

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	g	0.07	0/1953	0.19	0/2650
17	h	0.06	0/1088	0.16	0/1466
18	i	0.21	0/913	0.23	0/1240
19	j	0.15	0/1462	0.20	0/1973
20	k	0.14	0/904	0.22	0/1228
21	n	0.20	0/1166	0.24	0/1581
22	o	0.14	0/814	0.19	0/1100
23	p	0.15	0/707	0.22	0/957
24	q	0.19	0/799	0.25	0/1091
25	r	0.19	0/567	0.24	0/767
All	All	0.14	0/63273	0.22	0/85654

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	4084	4197	4196	34	0
1	B1	4038	4162	4160	28	0
1	C1	4039	4155	4154	18	0
2	D1	3689	3742	3741	25	0
2	E1	3682	3733	3733	26	0
2	F1	3703	3759	3758	29	0
3	G1	2387	2387	2387	12	0
4	H1	1251	1232	1231	15	0
5	I1	533	513	513	1	0
6	J1	1315	1276	1276	7	0
6	K1	1315	1276	1276	6	0
6	L1	1310	1271	1271	2	0
7	L	537	545	545	3	0
7	l	537	545	545	3	0
8	M	1027	1042	1042	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	m	1027	1042	1042	7	0
9	M1	1877	1873	1873	6	0
10	O1	565	600	599	9	0
10	P1	565	600	599	4	0
10	Q1	565	600	599	3	0
10	R1	565	600	599	2	0
10	S1	565	601	599	1	0
10	T1	565	601	599	2	0
10	U1	565	600	599	2	0
10	V1	565	600	599	0	0
10	W1	565	600	599	2	0
10	X1	565	600	599	4	0
11	a	2032	2044	2044	17	0
12	c	745	715	715	12	0
13	d	2737	2762	2763	24	0
14	e	3220	3050	3061	14	0
15	f	1145	1111	1111	12	0
16	g	1933	2020	2020	14	0
17	h	1070	1088	1088	6	0
18	i	883	857	857	9	0
19	j	1424	1411	1411	7	0
20	k	873	876	876	5	0
21	n	1128	1082	1082	4	0
22	o	789	767	767	3	0
23	p	684	651	651	3	0
24	q	766	720	720	7	0
25	r	542	498	498	5	0
26	A1	31	12	12	0	0
26	B1	31	12	12	0	0
26	C1	31	12	12	0	0
26	F1	31	12	12	0	0
27	A1	1	0	0	0	0
27	B1	1	0	0	0	0
27	C1	1	0	0	0	0
27	D1	1	0	0	0	0
27	F1	1	0	0	0	0
28	D1	27	12	12	0	0
29	H1	29	11	11	0	0
30	L	100	156	156	0	0
30	c	100	156	156	1	0
30	e	500	780	780	1	0
30	f	100	156	156	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	j	100	156	156	0	0
30	l	100	156	156	0	0
30	m	100	156	156	0	0
30	p	100	156	156	1	0
30	q	200	312	312	1	0
31	M	51	82	82	0	0
31	f	51	82	82	0	0
31	m	51	82	82	0	0
32	e	35	39	46	0	0
32	j	35	39	46	0	0
33	e	48	60	0	0	0
33	n	59	70	0	0	0
34	f	108	176	176	2	0
34	i	54	88	88	0	0
34	j	54	88	88	0	0
All	All	64103	65465	65342	339	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (339) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:531:PHE:O	1:B1:532:THR:OG1	1.98	0.81
19:j:19:ARG:NH2	24:q:77:GLU:O	2.15	0.80
13:d:17:ILE:N	13:d:182:PHE:O	2.16	0.79
14:e:250:ASP:OD1	14:e:270:TYR:OH	2.02	0.76
14:e:62:ARG:NH2	30:e:402:CDL:OB4	2.24	0.70
15:f:64:ARG:NH2	25:r:33:GLU:OE2	2.24	0.70
4:H1:152:ALA:O	4:H1:156:ALA:N	2.23	0.70
2:E1:165:LYS:NZ	2:E1:486:VAL:O	2.20	0.70
1:A1:75:ALA:HB3	1:A1:78:THR:HG21	1.75	0.69
2:F1:184:GLY:O	2:F1:189:LYS:NZ	2.25	0.68
12:c:49:PHE:O	18:i:15:GLN:NE2	2.27	0.67
1:B1:328:ARG:NH2	2:F1:345:ASP:OD1	2.30	0.64
19:j:128:LEU:HD21	19:j:142:LEU:HD12	1.79	0.64
10:O1:84:PRO:O	10:O1:87:THR:HG23	1.99	0.63
13:d:262:ARG:NH2	14:e:335:GLU:O	2.31	0.62
2:D1:184:GLY:O	2:D1:189:LYS:NZ	2.33	0.61
6:K1:79:CYS:O	6:K1:83:SER:OG	2.16	0.61
11:a:68:LEU:HD13	15:f:45:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:101:ARG:NH1	25:r:45:ASP:O	2.34	0.60
13:d:308:ILE:O	13:d:312:THR:HG23	2.02	0.59
14:e:185:ASN:ND2	14:e:325:ASP:OD1	2.35	0.59
1:B1:180:ASN:OD1	1:B1:181:TYR:N	2.36	0.59
7:l:10:LEU:HD13	8:m:83:ILE:HD11	1.84	0.59
17:h:128:GLU:HG2	17:h:149:ILE:HD11	1.85	0.59
10:T1:48:GLN:O	10:T1:51:HIS:ND1	2.35	0.58
10:P1:106:LEU:HD13	11:a:150:ASN:HA	1.86	0.58
1:C1:523:GLU:N	1:C1:523:GLU:OE1	2.37	0.58
7:L:10:LEU:HD13	8:M:83:ILE:HD11	1.85	0.58
7:l:66:GLN:HG3	7:l:68:VAL:HG23	1.86	0.57
10:R1:86:LEU:HD11	10:S1:84:PRO:HB3	1.86	0.57
7:L:66:GLN:HG3	7:L:68:VAL:HG23	1.86	0.57
11:a:8:ASP:OD1	21:n:126:TYR:OH	2.19	0.56
12:c:40:TRP:O	12:c:43:VAL:HG12	2.04	0.56
1:A1:437:LEU:HD13	1:A1:452:MET:HG3	1.88	0.56
1:B1:420:MET:HE2	1:B1:470:PHE:CE1	2.41	0.56
2:E1:130:ASP:O	6:L1:32:TYR:OH	2.23	0.56
2:F1:486:VAL:HG21	2:F1:492:VAL:HG22	1.86	0.56
15:f:101:ARG:NH2	8:m:124:PRO:O	2.34	0.56
2:E1:68:ARG:NH1	2:E1:92:THR:O	2.39	0.55
12:c:68:LYS:NZ	13:d:284:GLN:O	2.39	0.55
17:h:134:GLU:O	17:h:138:ALA:N	2.39	0.55
6:K1:28:ASP:OD1	6:K1:32:TYR:N	2.39	0.55
2:D1:347:ALA:HB3	2:D1:348:PRO:HD3	1.88	0.55
6:J1:117:GLU:O	6:J1:121:THR:HG23	2.06	0.55
13:d:291:GLU:O	13:d:295:LEU:N	2.39	0.55
14:e:201:TYR:O	14:e:205:ILE:N	2.36	0.55
2:E1:263:LEU:HD21	2:E1:321:ARG:HB2	1.88	0.54
12:c:73:HIS:NE2	12:c:77:GLU:OE2	2.40	0.54
13:d:131:VAL:HG13	13:d:136:ASP:OD1	2.07	0.54
11:a:26:LEU:HD22	15:f:43:TRP:CZ2	2.43	0.54
16:g:59:VAL:HG13	16:g:216:VAL:HB	1.90	0.54
1:A1:59:ASP:OD1	2:D1:300:ARG:NH2	2.41	0.54
10:T1:104:ILE:HD11	10:U1:102:GLU:OE1	2.09	0.53
16:g:5:LEU:HD21	16:g:245:LEU:HD11	1.89	0.53
2:F1:90:MET:HE1	2:F1:257:ARG:HG3	1.90	0.53
6:K1:70:ILE:O	6:K1:74:ASN:ND2	2.42	0.53
12:c:61:VAL:HG13	13:d:278:VAL:HG11	1.91	0.53
16:g:155:LYS:O	16:g:159:THR:HG22	2.09	0.53
19:j:37:ARG:NH2	30:q:101:CDL:OA3	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:457:ARG:NH2	1:A1:488:VAL:O	2.37	0.52
10:O1:106:LEU:HD13	11:a:194:PHE:CE1	2.44	0.52
8:M:103:PHE:CE2	8:M:107:LEU:HD11	2.45	0.52
1:B1:500:LEU:HD11	1:B1:545:MET:HE1	1.90	0.52
10:O1:70:GLY:HA2	10:X1:72:ILE:HD11	1.90	0.52
4:H1:132:THR:HG21	4:H1:137:LEU:HD21	1.91	0.52
8:m:103:PHE:CE2	8:m:107:LEU:HD11	2.45	0.52
4:H1:171:VAL:O	4:H1:175:VAL:HG23	2.10	0.52
6:K1:165:ALA:O	6:K1:169:GLY:N	2.43	0.52
4:H1:161:ALA:O	4:H1:165:VAL:HG23	2.10	0.52
1:A1:514:ASN:O	1:A1:518:TYR:OH	2.19	0.52
1:B1:173:ILE:HG23	1:B1:174:VAL:HG13	1.93	0.51
1:C1:168:THR:OG1	1:C1:345:ARG:NH2	2.43	0.51
10:O1:114:LEU:HD13	11:a:160:MET:HE2	1.92	0.51
9:M1:162:HIS:NE2	9:M1:168:LEU:O	2.38	0.51
22:o:86:TYR:O	22:o:91:ARG:NE	2.44	0.51
1:B1:301:CYS:SG	1:B1:302:LEU:N	2.84	0.51
11:a:166:TYR:OH	34:f:204:PC1:O12	2.24	0.51
11:a:26:LEU:O	12:c:67:ASN:ND2	2.42	0.51
18:i:88:LYS:O	22:o:32:GLN:NE2	2.44	0.51
20:k:29:GLU:N	20:k:29:GLU:OE1	2.44	0.51
1:B1:75:ALA:HB3	1:B1:78:THR:HG21	1.94	0.50
19:j:54:TYR:O	19:j:92:ARG:NH1	2.42	0.50
2:D1:90:MET:HE1	2:D1:257:ARG:HG3	1.94	0.50
2:E1:81:ASP:OD1	2:E1:84:THR:N	2.42	0.50
8:M:103:PHE:CZ	8:M:107:LEU:HD11	2.46	0.50
1:B1:141:ASN:OD1	1:B1:145:HIS:N	2.45	0.50
4:H1:54:LEU:HD21	4:H1:131:CYS:SG	2.51	0.50
10:Q1:106:LEU:O	10:Q1:110:MET:N	2.38	0.50
16:g:44:ALA:N	16:g:241:GLU:OE2	2.45	0.50
1:B1:239:ILE:HG23	1:B1:267:THR:HG23	1.94	0.50
1:C1:515:LYS:O	6:K1:134:ARG:NH1	2.43	0.50
13:d:131:VAL:HG22	13:d:136:ASP:OD1	2.12	0.50
8:m:103:PHE:CZ	8:m:107:LEU:HD11	2.46	0.50
11:a:231:VAL:O	14:e:170:TRP:NE1	2.42	0.50
10:O1:106:LEU:HD13	11:a:194:PHE:HE1	1.77	0.50
1:A1:212:LYS:HG2	1:A1:389:LEU:HD12	1.93	0.50
2:F1:118:LEU:HA	2:F1:242:VAL:HG22	1.93	0.49
1:A1:166:VAL:HG12	1:A1:166:VAL:O	2.12	0.49
1:B1:111:ILE:HD12	1:B1:276:PRO:HB3	1.93	0.49
2:F1:116:GLU:OE1	2:F1:116:GLU:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:j:120:GLU:OE2	19:j:123:ARG:NH2	2.45	0.49
1:A1:51:MET:HE3	1:A1:68:ALA:HB1	1.93	0.49
21:n:154:GLU:OE1	21:n:154:GLU:N	2.41	0.49
1:C1:59:ASP:OD1	2:F1:300:ARG:NH2	2.46	0.49
2:E1:301:ILE:HG23	3:G1:279:LEU:HD13	1.93	0.49
23:p:66:ASP:OD2	25:r:10:ARG:NH1	2.46	0.49
1:B1:52:ILE:C	1:B1:52:ILE:HD12	2.38	0.49
1:B1:508:MET:O	6:J1:179:GLN:NE2	2.46	0.49
3:G1:44:ASP:HA	4:H1:31:MET:HE2	1.95	0.48
8:m:102:ARG:NH2	23:p:82:ASN:OD1	2.45	0.48
13:d:28:PRO:HB3	13:d:193:ILE:HD12	1.95	0.48
14:e:111:TYR:OH	24:q:47:TRP:O	2.26	0.48
1:A1:285:TYR:OH	1:A1:338:LEU:HD12	2.14	0.48
1:C1:62:ILE:HD12	1:C1:62:ILE:C	2.38	0.48
13:d:17:ILE:O	17:h:139:ASN:ND2	2.46	0.48
2:D1:270:ARG:NH1	2:D1:323:THR:O	2.43	0.48
2:D1:484:TYR:O	2:D1:495:LYS:NZ	2.45	0.48
12:c:88:LEU:HD12	12:c:88:LEU:O	2.14	0.48
1:A1:524:LEU:HD23	1:A1:527:LEU:HD12	1.95	0.48
1:B1:285:TYR:OH	1:B1:338:LEU:O	2.28	0.48
1:C1:531:PHE:O	1:C1:532:THR:CB	2.62	0.48
15:f:41:LEU:HD23	15:f:45:LEU:HD12	1.95	0.48
2:F1:178:LYS:HG2	2:F1:355:LEU:HD23	1.95	0.48
10:Q1:65:VAL:HG13	10:Q1:101:THR:HG22	1.96	0.48
18:i:16:LEU:O	18:i:20:THR:HG22	2.13	0.48
1:B1:80:ILE:HD12	1:B1:80:ILE:C	2.39	0.48
2:E1:302:PRO:HB2	3:G1:275:LEU:HD21	1.95	0.48
14:e:253:VAL:O	14:e:257:ARG:N	2.47	0.48
2:F1:178:LYS:NZ	2:F1:322:ILE:O	2.38	0.48
13:d:22:PRO:O	13:d:23:LEU:HD23	2.14	0.48
1:A1:459:VAL:HG12	1:A1:459:VAL:O	2.14	0.47
2:D1:91:GLN:OE1	2:D1:91:GLN:N	2.47	0.47
4:H1:146:LEU:HB2	4:H1:172:ILE:HG21	1.97	0.47
13:d:156:LEU:HD23	13:d:156:LEU:O	2.14	0.47
13:d:130:VAL:HG12	13:d:130:VAL:O	2.13	0.47
18:i:87:PRO:O	18:i:91:GLY:N	2.35	0.47
6:J1:181:GLY:O	6:J1:185:VAL:HG23	2.15	0.47
10:O1:106:LEU:HD22	11:a:194:PHE:CE1	2.49	0.47
16:g:58:ALA:HB3	16:g:80:ARG:HB3	1.97	0.47
1:A1:292:GLU:O	1:A1:296:ASN:ND2	2.47	0.47
1:B1:110:ASN:O	1:B1:114:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:531:PHE:O	1:B1:532:THR:CB	2.63	0.47
2:D1:120:ARG:NE	2:D1:130:ASP:OD2	2.42	0.47
2:D1:486:VAL:HG21	2:D1:492:VAL:HG22	1.96	0.47
2:F1:41:ILE:HG23	2:F1:41:ILE:O	2.15	0.47
10:O1:45:ILE:HD12	10:P1:45:ILE:HG21	1.96	0.47
18:i:62:ARG:NH2	21:n:134:SER:O	2.46	0.47
30:p:201:CDL:H772	30:p:201:CDL:H812	1.95	0.47
10:O1:84:PRO:HB3	10:X1:86:LEU:HD11	1.97	0.47
24:q:49:ALA:N	24:q:50:PRO:CD	2.78	0.47
6:J1:165:ALA:O	6:J1:169:GLY:N	2.48	0.46
24:q:77:GLU:OE2	24:q:79:HIS:NE2	2.49	0.46
1:B1:107:LEU:HD12	1:B1:111:ILE:HG23	1.97	0.46
2:D1:263:LEU:HD21	2:D1:321:ARG:HB2	1.97	0.46
2:F1:166:VAL:HG12	2:F1:440:LEU:HD22	1.97	0.46
13:d:280:ILE:O	13:d:280:ILE:HD12	2.15	0.46
2:D1:351:THR:HG22	2:D1:351:THR:O	2.15	0.46
2:E1:347:ALA:HB3	2:E1:348:PRO:CD	2.46	0.46
2:F1:263:LEU:HD21	2:F1:321:ARG:HB2	1.97	0.46
10:P1:48:GLN:O	10:P1:51:HIS:ND1	2.48	0.46
12:c:43:VAL:HG13	12:c:44:TRP:N	2.30	0.46
2:D1:174:CYS:HB3	2:D1:383:ILE:HG21	1.97	0.46
17:h:67:LEU:O	17:h:72:GLN:NE2	2.49	0.46
1:B1:109:ASP:OD1	1:B1:109:ASP:N	2.48	0.46
8:M:88:TYR:O	8:M:91:GLN:NE2	2.49	0.46
1:A1:203:LEU:HD13	1:A1:379:VAL:CG1	2.46	0.46
1:A1:537:ILE:HD12	1:A1:537:ILE:N	2.31	0.46
12:c:30:GLU:N	12:c:31:PRO:CD	2.78	0.46
8:m:88:TYR:O	8:m:91:GLN:NE2	2.49	0.46
2:E1:55:PRO:O	2:E1:58:THR:OG1	2.20	0.46
10:P1:86:LEU:HD11	10:Q1:84:PRO:HB3	1.96	0.46
14:e:1:AME:O	14:e:122:ASN:ND2	2.43	0.46
20:k:103:MET:HE1	24:q:80:LEU:HA	1.97	0.46
1:B1:203:LEU:HD13	1:B1:379:VAL:HG11	1.98	0.46
1:C1:52:ILE:HD12	1:C1:52:ILE:C	2.41	0.46
14:e:26:THR:HG23	14:e:91:TYR:OH	2.16	0.46
2:E1:417:LEU:O	3:G1:34:ARG:NH2	2.48	0.46
2:F1:137:GLU:OE1	2:F1:137:GLU:N	2.42	0.46
4:H1:97:LEU:C	4:H1:97:LEU:HD23	2.41	0.46
1:B1:199:GLY:N	1:B1:357:SER:OG	2.48	0.45
1:A1:441:SER:HB2	1:A1:446:GLN:HB3	1.98	0.45
1:C1:140:VAL:HG21	1:C1:290:MET:HE1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M1:225:THR:HG23	9:M1:244:SER:OG	2.15	0.45
15:f:16:GLU:OE1	15:f:16:GLU:N	2.49	0.45
15:f:45:LEU:HD13	34:f:204:PC1:H3I3	1.99	0.45
1:C1:166:VAL:HG12	1:C1:166:VAL:O	2.16	0.45
2:D1:130:ASP:O	6:K1:32:TYR:OH	2.32	0.45
14:e:210:ILE:O	14:e:232:ARG:NH2	2.43	0.45
1:C1:225:ARG:NH2	1:C1:522:GLN:OE1	2.49	0.45
1:A1:61:THR:HG22	1:A1:111:ILE:CD1	2.47	0.45
2:F1:260:GLN:OE1	2:F1:260:GLN:N	2.49	0.45
2:E1:195:GLU:OE2	2:E1:199:ASN:ND2	2.49	0.45
3:G1:93:CYS:O	3:G1:97:VAL:HG23	2.17	0.45
1:A1:437:LEU:HD13	1:A1:452:MET:CG	2.47	0.45
2:F1:62:VAL:HG21	2:F1:72:LEU:HD23	1.99	0.45
18:i:2:VAL:HG22	18:i:3:TYR:H	1.82	0.45
2:F1:446:VAL:HG12	2:F1:446:VAL:O	2.17	0.45
13:d:24:LEU:HD22	17:h:134:GLU:HB3	1.99	0.45
13:d:92:THR:HG22	13:d:93:ASP:H	1.82	0.45
1:A1:188:LYS:NZ	1:A1:461:LEU:O	2.40	0.44
2:E1:410:LEU:O	2:E1:414:ILE:HG23	2.17	0.44
2:E1:305:VAL:HG12	2:E1:305:VAL:O	2.16	0.44
2:F1:232:VAL:HG11	2:F1:241:CYS:SG	2.57	0.44
2:F1:311:LEU:C	2:F1:311:LEU:HD23	2.42	0.44
1:A1:307:ASP:OD1	1:A1:307:ASP:N	2.50	0.44
1:C1:537:ILE:N	1:C1:537:ILE:HD12	2.33	0.44
2:F1:91:GLN:OE1	2:F1:91:GLN:N	2.51	0.44
2:F1:243:LEU:HD22	2:F1:245:TYR:HE2	1.82	0.44
2:F1:347:ALA:HB3	2:F1:348:PRO:CD	2.47	0.44
15:f:37:TRP:NE1	15:f:48:GLU:OE1	2.42	0.44
18:i:2:VAL:HG22	18:i:3:TYR:N	2.32	0.44
3:G1:98:VAL:HG22	3:G1:102:MET:HE1	1.98	0.44
4:H1:60:PHE:O	4:H1:60:PHE:CD1	2.71	0.44
1:C1:203:LEU:HD13	1:C1:379:VAL:CG1	2.47	0.44
30:c:201:CDL:H872	30:c:201:CDL:H832	1.99	0.44
14:e:229:MET:SD	14:e:235:ASN:ND2	2.87	0.44
15:f:100:LEU:HD21	23:p:99:LEU:HD23	1.99	0.44
2:E1:91:GLN:N	2:E1:91:GLN:OE1	2.51	0.44
3:G1:293:VAL:HG11	9:M1:109:TRP:CZ2	2.52	0.44
2:E1:410:LEU:HD13	2:E1:430:VAL:HG23	1.98	0.44
4:H1:146:LEU:HD12	4:H1:146:LEU:O	2.17	0.44
5:I1:70:ILE:N	5:I1:70:ILE:HD12	2.32	0.44
2:D1:448:GLU:O	2:D1:452:GLY:N	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E1:432:ARG:NH1	2:E1:471:LEU:O	2.51	0.44
1:B1:454:ARG:NH1	1:B1:481:LEU:O	2.50	0.44
2:F1:150:LEU:HD23	2:F1:150:LEU:O	2.18	0.44
4:H1:67:VAL:HG11	4:H1:99:VAL:CG1	2.48	0.43
1:C1:80:ILE:C	1:C1:80:ILE:HD12	2.43	0.43
10:W1:84:PRO:O	10:W1:87:THR:HG23	2.19	0.43
15:f:64:ARG:NH1	25:r:33:GLU:OE1	2.45	0.43
10:X1:70:GLY:O	10:X1:74:GLY:N	2.46	0.43
8:m:46:HIS:O	8:m:50:GLY:N	2.52	0.43
1:B1:184:LEU:O	1:B1:223:GLN:NE2	2.50	0.43
1:B1:295:MET:HB2	1:B1:358:VAL:HG23	2.00	0.43
2:D1:392:ASP:O	2:D1:396:VAL:HG23	2.18	0.43
2:F1:120:ARG:NE	2:F1:130:ASP:OD2	2.46	0.43
18:i:90:THR:O	22:o:36:ARG:NH2	2.50	0.43
2:D1:282:ASP:HA	2:D1:283:ASN:HA	1.82	0.43
2:E1:182:PHE:CD1	2:E1:358:THR:HG23	2.53	0.43
10:O1:107:PHE:CD1	11:a:157:LEU:HD22	2.54	0.43
13:d:268:PRO:HB2	14:e:327:ALA:HB3	1.99	0.43
15:f:56:ILE:HB	15:f:57:PRO:HD3	2.00	0.43
1:A1:131:VAL:HG11	1:A1:293:TYR:HB2	2.00	0.43
2:D1:75:GLU:OE2	2:D1:144:HIS:NE2	2.45	0.43
4:H1:61:LEU:HD12	4:H1:61:LEU:H	1.84	0.43
1:A1:495:PHE:CE2	1:A1:499:LEU:HD11	2.54	0.43
10:W1:45:ILE:HD12	10:X1:45:ILE:CG2	2.49	0.43
9:M1:46:SER:O	9:M1:122:VAL:HG22	2.18	0.43
2:E1:172:PRO:O	2:E1:383:ILE:HD11	2.19	0.42
2:E1:486:VAL:HG21	2:E1:492:VAL:HG22	2.00	0.42
6:J1:107:MET:O	6:J1:112:ARG:N	2.52	0.42
11:a:49:LEU:HD23	11:a:49:LEU:H	1.83	0.42
2:E1:166:VAL:HG22	2:E1:440:LEU:HB3	2.01	0.42
1:A1:441:SER:CB	1:A1:446:GLN:HB3	2.49	0.42
2:D1:470:LEU:HD23	2:D1:470:LEU:O	2.18	0.42
4:H1:139:LEU:HD11	4:H1:176:ILE:HG23	2.01	0.42
13:d:284:GLN:OE1	13:d:284:GLN:N	2.42	0.42
16:g:56:HIS:NE2	16:g:219:THR:O	2.52	0.42
16:g:269:LEU:HD12	16:g:269:LEU:C	2.44	0.42
1:A1:192:THR:HG22	1:A1:420:MET:SD	2.59	0.42
16:g:57:THR:HB	16:g:218:HIS:HB2	2.02	0.42
1:C1:317:GLN:NE2	2:F1:313:GLU:OE1	2.51	0.42
2:E1:303:ALA:N	2:E1:307:TYR:O	2.43	0.42
2:F1:180:GLY:HA3	2:F1:355:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G1:209:GLU:OE2	4:H1:88:LYS:NZ	2.53	0.42
1:A1:269:MET:SD	1:A1:286:ALA:HB3	2.60	0.42
13:d:324:ASN:HB2	13:d:325:PRO:CD	2.49	0.42
16:g:31:ARG:NH2	16:g:250:GLU:OE2	2.46	0.42
1:A1:288:VAL:O	1:A1:292:GLU:N	2.45	0.42
2:E1:174:CYS:HB3	2:E1:383:ILE:HD13	2.02	0.42
13:d:25:TYR:HD2	13:d:189:VAL:HG13	1.84	0.42
1:A1:61:THR:HG22	1:A1:111:ILE:HD13	2.01	0.42
1:A1:201:ARG:NH2	1:A1:384:ASP:OD1	2.52	0.42
1:A1:203:LEU:HD13	1:A1:379:VAL:HG11	2.02	0.42
11:a:93:TYR:CE2	11:a:220:LEU:HD22	2.54	0.42
1:A1:511:THR:HG22	1:A1:511:THR:O	2.19	0.42
2:D1:173:TYR:CD2	2:D1:179:ILE:HD13	2.55	0.42
2:D1:263:LEU:HD13	2:D1:322:ILE:HG12	2.00	0.42
1:B1:285:TYR:OH	1:B1:338:LEU:HD12	2.20	0.42
1:C1:203:LEU:HD13	1:C1:379:VAL:HG11	2.02	0.42
9:M1:66:ILE:HD12	9:M1:66:ILE:N	2.35	0.42
16:g:196:VAL:HG12	16:g:197:ALA:N	2.35	0.42
16:g:151:ASN:OD1	16:g:152:GLU:N	2.53	0.41
17:h:24:MET:SD	17:h:24:MET:N	2.93	0.41
1:B1:56:HIS:HB2	1:B1:66:ILE:HG23	2.02	0.41
1:B1:323:ARG:HA	2:E1:301:ILE:HD12	2.01	0.41
1:C1:108:MET:HE3	1:C1:282:LEU:HD11	2.02	0.41
3:G1:25:ILE:O	3:G1:29:THR:HG23	2.20	0.41
13:d:25:TYR:CD2	13:d:189:VAL:HG13	2.54	0.41
13:d:182:PHE:CG	13:d:188:VAL:HG22	2.55	0.41
7:l:20:PHE:CE2	7:l:24:LEU:HD11	2.55	0.41
2:E1:389:ILE:HD12	2:E1:393:HIS:ND1	2.35	0.41
2:E1:414:ILE:O	2:E1:418:GLY:N	2.52	0.41
2:F1:426:ASP:O	2:F1:430:VAL:HG23	2.20	0.41
6:L1:159:GLU:OE2	6:L1:163:GLN:NE2	2.54	0.41
8:M:46:HIS:O	8:M:50:GLY:N	2.52	0.41
19:j:30:GLU:OE1	24:q:72:ASN:ND2	2.50	0.41
1:A1:61:THR:HG21	2:D1:313:GLU:OE2	2.20	0.41
6:J1:36:THR:O	6:J1:36:THR:HG22	2.20	0.41
19:j:68:PRO:HG3	20:k:31:ILE:HD13	2.02	0.41
1:A1:100:ASP:OD1	1:A1:100:ASP:N	2.54	0.41
6:J1:73:TYR:OH	6:J1:111:ASN:OD1	2.38	0.41
24:q:76:VAL:O	24:q:76:VAL:HG12	2.20	0.41
2:D1:263:LEU:HD21	2:D1:321:ARG:CB	2.51	0.41
2:D1:288:THR:HG23	2:D1:311:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:R1:96:LEU:HD23	10:R1:96:LEU:O	2.20	0.41
1:A1:273:ALA:O	1:A1:274:ALA:HB3	2.20	0.41
2:D1:180:GLY:HA3	2:D1:355:LEU:HD13	2.03	0.41
13:d:35:ASN:OD1	13:d:35:ASN:N	2.54	0.41
1:A1:131:VAL:HG12	1:A1:132:GLY:N	2.36	0.41
2:D1:55:PRO:O	2:D1:58:THR:OG1	2.31	0.41
12:c:105:THR:OG1	13:d:205:ARG:NH2	2.54	0.41
1:B1:471:MET:HE1	1:B1:522:GLN:HA	2.03	0.41
7:L:20:PHE:CE2	7:L:24:LEU:HD11	2.55	0.41
10:U1:84:PRO:O	10:U1:87:THR:HG23	2.21	0.41
20:k:86:TRP:O	20:k:90:VAL:HG23	2.21	0.41
21:n:105:GLU:OE2	21:n:109:ARG:NH2	2.48	0.41
16:g:57:THR:HG21	16:g:124:VAL:HG11	2.03	0.41
16:g:60:THR:HG22	16:g:78:VAL:O	2.21	0.41
25:r:61:HIS:ND1	25:r:61:HIS:C	2.79	0.41
11:a:78:THR:O	12:c:40:TRP:NE1	2.39	0.40
1:C1:301:CYS:SG	1:C1:302:LEU:N	2.95	0.40
1:C1:564:ILE:HG23	1:C1:569:ASP:HB2	2.03	0.40
2:F1:81:ASP:OD1	2:F1:84:THR:N	2.53	0.40
2:F1:181:LEU:HD23	2:F1:359:THR:HB	2.02	0.40
4:H1:63:ARG:O	4:H1:64:GLU:C	2.64	0.40
11:a:103:LEU:HD21	14:e:59:TYR:CG	2.56	0.40
1:A1:438:ALA:HA	1:A1:441:SER:HB3	2.03	0.40
2:E1:360:VAL:HG21	2:E1:378:GLU:HG3	2.03	0.40
2:F1:68:ARG:NH2	2:F1:92:THR:O	2.54	0.40
3:G1:81:GLY:O	3:G1:241:ARG:NH1	2.55	0.40
3:G1:127:ILE:N	3:G1:127:ILE:HD12	2.36	0.40
3:G1:197:LYS:C	3:G1:197:LYS:CD	2.95	0.40
9:M1:90:VAL:CG2	9:M1:108:VAL:HG22	2.51	0.40
16:g:174:THR:HG23	16:g:175:ALA:N	2.36	0.40
20:k:124:LEU:N	20:k:124:LEU:HD23	2.36	0.40
18:i:99:GLU:O	18:i:103:VAL:HG23	2.22	0.40
11:a:147:LEU:HD22	11:a:213:PHE:CD2	2.56	0.40
12:c:79:ARG:NH1	12:c:82:GLN:OE1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	526/584 (90%)	519 (99%)	7 (1%)	0	100	100
1	B1	517/584 (88%)	508 (98%)	8 (2%)	1 (0%)	43	72
1	C1	517/584 (88%)	509 (98%)	8 (2%)	0	100	100
2	D1	485/519 (93%)	477 (98%)	8 (2%)	0	100	100
2	E1	484/519 (93%)	475 (98%)	9 (2%)	0	100	100
2	F1	487/519 (94%)	476 (98%)	11 (2%)	0	100	100
3	G1	298/305 (98%)	293 (98%)	5 (2%)	0	100	100
4	H1	159/182 (87%)	156 (98%)	3 (2%)	0	100	100
5	I1	63/75 (84%)	62 (98%)	1 (2%)	0	100	100
6	J1	164/188 (87%)	163 (99%)	1 (1%)	0	100	100
6	K1	164/188 (87%)	160 (98%)	4 (2%)	0	100	100
6	L1	163/188 (87%)	161 (99%)	2 (1%)	0	100	100
7	L	63/92 (68%)	63 (100%)	0	0	100	100
7	l	63/92 (68%)	63 (100%)	0	0	100	100
8	M	127/144 (88%)	127 (100%)	0	0	100	100
8	m	127/144 (88%)	127 (100%)	0	0	100	100
9	M1	230/255 (90%)	224 (97%)	6 (3%)	0	100	100
10	O1	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
10	P1	76/118 (64%)	76 (100%)	0	0	100	100
10	Q1	76/118 (64%)	76 (100%)	0	0	100	100
10	R1	76/118 (64%)	76 (100%)	0	0	100	100
10	S1	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
10	T1	76/118 (64%)	76 (100%)	0	0	100	100
10	U1	76/118 (64%)	76 (100%)	0	0	100	100
10	V1	76/118 (64%)	76 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	W1	76/118 (64%)	76 (100%)	0	0	100	100
10	X1	76/118 (64%)	76 (100%)	0	0	100	100
11	a	229/231 (99%)	225 (98%)	4 (2%)	0	100	100
12	c	84/114 (74%)	82 (98%)	2 (2%)	0	100	100
13	d	328/370 (89%)	321 (98%)	7 (2%)	0	100	100
14	e	381/396 (96%)	376 (99%)	5 (1%)	0	100	100
15	f	133/145 (92%)	129 (97%)	4 (3%)	0	100	100
16	g	266/269 (99%)	264 (99%)	2 (1%)	0	100	100
17	h	135/157 (86%)	133 (98%)	2 (2%)	0	100	100
18	i	101/104 (97%)	100 (99%)	1 (1%)	0	100	100
19	j	166/169 (98%)	163 (98%)	3 (2%)	0	100	100
20	k	103/124 (83%)	100 (97%)	3 (3%)	0	100	100
21	n	137/156 (88%)	132 (96%)	5 (4%)	0	100	100
22	o	94/101 (93%)	94 (100%)	0	0	100	100
23	p	78/105 (74%)	77 (99%)	1 (1%)	0	100	100
24	q	83/98 (85%)	81 (98%)	2 (2%)	0	100	100
25	r	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	7775/8943 (87%)	7656 (98%)	118 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B1	532	THR

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	A1	439/479 (92%)	436 (99%)	3 (1%)	76	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B1	435/479 (91%)	435 (100%)	0	100	100
1	C1	434/479 (91%)	432 (100%)	2 (0%)	81	80
2	D1	398/420 (95%)	398 (100%)	0	100	100
2	E1	397/420 (94%)	397 (100%)	0	100	100
2	F1	400/420 (95%)	400 (100%)	0	100	100
3	G1	253/257 (98%)	247 (98%)	6 (2%)	43	61
4	H1	137/156 (88%)	137 (100%)	0	100	100
5	I1	58/67 (87%)	58 (100%)	0	100	100
6	J1	145/162 (90%)	145 (100%)	0	100	100
6	K1	145/162 (90%)	145 (100%)	0	100	100
6	L1	145/162 (90%)	145 (100%)	0	100	100
7	L	55/75 (73%)	55 (100%)	0	100	100
7	l	55/75 (73%)	55 (100%)	0	100	100
8	M	111/124 (90%)	111 (100%)	0	100	100
8	m	111/124 (90%)	111 (100%)	0	100	100
9	M1	200/215 (93%)	196 (98%)	4 (2%)	48	64
10	O1	56/89 (63%)	56 (100%)	0	100	100
10	P1	56/89 (63%)	56 (100%)	0	100	100
10	Q1	56/89 (63%)	56 (100%)	0	100	100
10	R1	56/89 (63%)	56 (100%)	0	100	100
10	S1	56/89 (63%)	56 (100%)	0	100	100
10	T1	56/89 (63%)	56 (100%)	0	100	100
10	U1	56/89 (63%)	56 (100%)	0	100	100
10	V1	56/89 (63%)	56 (100%)	0	100	100
10	W1	56/89 (63%)	56 (100%)	0	100	100
10	X1	56/89 (63%)	56 (100%)	0	100	100
11	a	225/225 (100%)	224 (100%)	1 (0%)	84	81
12	c	80/104 (77%)	78 (98%)	2 (2%)	42	61
13	d	297/334 (89%)	291 (98%)	6 (2%)	48	64
14	e	334/341 (98%)	333 (100%)	1 (0%)	86	83
15	f	119/124 (96%)	118 (99%)	1 (1%)	73	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	g	205/206 (100%)	205 (100%)	0	100	100
17	h	110/123 (89%)	110 (100%)	0	100	100
18	i	95/96 (99%)	95 (100%)	0	100	100
19	j	149/150 (99%)	149 (100%)	0	100	100
20	k	91/107 (85%)	91 (100%)	0	100	100
21	n	123/137 (90%)	121 (98%)	2 (2%)	55	68
22	o	82/86 (95%)	82 (100%)	0	100	100
23	p	75/94 (80%)	75 (100%)	0	100	100
24	q	80/92 (87%)	80 (100%)	0	100	100
25	r	56/56 (100%)	56 (100%)	0	100	100
All	All	6599/7441 (89%)	6571 (100%)	28 (0%)	81	81

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	440	ASP
1	A1	441	SER
1	A1	446	GLN
1	C1	450	ILE
1	C1	453	ILE
3	G1	17	ARG
3	G1	24	THR
3	G1	69	ASN
3	G1	97	VAL
3	G1	160	ILE
3	G1	174	VAL
9	M1	87	THR
9	M1	152	GLU
9	M1	223	GLN
9	M1	225	THR
11	a	144	PHE
12	c	83	LYS
12	c	91	THR
13	d	92	THR
13	d	136	ASP
13	d	138	VAL
13	d	161	GLU
13	d	180	SER

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Mol	Chain	Res	Type
13	d	281	THR
14	e	226	THR
15	f	42	ASN
21	n	105	GLU
21	n	132	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	56	HIS
1	A1	339	HIS
1	A1	551	HIS
1	B1	56	HIS
1	B1	245	GLN
1	B1	296	ASN
1	B1	386	GLN
1	B1	463	ASN
1	C1	83	GLN
1	C1	339	HIS
1	C1	416	GLN
1	C1	551	HIS
1	C1	558	GLN
2	D1	39	GLN
2	D1	48	HIS
2	D1	395	ASN
2	E1	48	HIS
2	E1	275	GLN
2	E1	354	HIS
2	E1	398	GLN
2	F1	36	HIS
2	F1	48	HIS
2	F1	108	ASN
2	F1	354	HIS
4	H1	41	HIS
4	H1	149	GLN
4	H1	150	GLN
5	I1	71	HIS
6	J1	82	GLN
6	J1	111	ASN
6	K1	82	GLN
6	K1	109	HIS
6	L1	140	GLN

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Mol	Chain	Res	Type
6	L1	163	GLN
6	L1	175	HIS
9	M1	65	ASN
10	T1	85	ASN
10	V1	75	ASN
10	V1	85	ASN
11	a	155	HIS
12	c	113	ASN
13	d	115	HIS
14	e	41	GLN
14	e	166	HIS
15	f	19	HIS
15	f	69	HIS
16	g	143	GLN
16	g	218	HIS
17	h	39	ASN
21	n	89	GLN
21	n	91	HIS
21	n	144	HIS
22	o	25	HIS
23	p	95	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
14	AME	e	1	14	9,10,11	0.29	0	9,11,13	0.42	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
14	AME	e	1	14	-	4/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	e	1	AME	O-C-CA-CB
14	e	1	AME	N-CA-CB-CG
14	e	1	AME	C-CA-N-CT1
14	e	1	AME	CB-CA-N-CT1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	e	1	AME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 5 are monoatomic - leaving 31 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
30	CDL	c	201	-	99,99,99	0.29	0	105,111,111	0.27	0
30	CDL	e	404	-	99,99,99	0.29	0	105,111,111	0.26	0
30	CDL	e	405	-	99,99,99	0.29	0	105,111,111	0.26	0
30	CDL	e	402	-	99,99,99	0.29	0	105,111,111	0.26	0
30	CDL	f	201	-	99,99,99	0.29	0	105,111,111	0.27	0
31	PEE	m	202	-	50,50,50	0.76	2 (4%)	53,55,55	0.48	0
26	ATP	B1	601	27	32,33,33	0.29	0	48,52,52	0.28	0
30	CDL	q	101	-	99,99,99	0.28	0	105,111,111	0.26	0
34	PC1	f	204	-	53,53,53	0.27	0	59,61,61	0.29	0
30	CDL	l	101	-	99,99,99	0.29	0	105,111,111	0.26	0
32	LMT	e	406	-	36,36,36	0.10	0	47,47,47	0.16	0
26	ATP	C1	601	27	32,33,33	0.29	0	48,52,52	0.28	0
30	CDL	m	201	-	99,99,99	0.29	0	105,111,111	0.25	0
29	UTP	H1	201	-	29,30,30	0.50	0	43,47,47	0.68	0
26	ATP	F1	601	27	32,33,33	0.29	0	48,52,52	0.28	0
33	Q7G	n	201	-	66,66,90	0.13	0	98,102,138	0.30	0
30	CDL	q	102	-	99,99,99	0.29	0	105,111,111	0.30	0
30	CDL	j	201	-	99,99,99	0.29	0	105,111,111	0.26	0
30	CDL	e	401	-	99,99,99	0.29	0	105,111,111	0.26	0
34	PC1	j	202	-	53,53,53	0.28	0	59,61,61	0.28	0
31	PEE	f	202	-	50,50,50	0.78	2 (4%)	53,55,55	0.47	0
34	PC1	f	203	-	53,53,53	0.28	0	59,61,61	0.29	0
32	LMT	j	203	-	36,36,36	0.10	0	47,47,47	0.21	0
28	ADP	D1	601	27	28,29,29	0.41	0	43,45,45	0.48	0
30	CDL	L	101	-	99,99,99	0.29	0	105,111,111	0.26	0
31	PEE	M	201	-	50,50,50	0.76	2 (4%)	53,55,55	0.48	0
33	Q7G	e	407	-	54,54,90	0.13	0	80,84,138	0.25	0
34	PC1	i	201	-	53,53,53	0.28	0	59,61,61	0.28	0
30	CDL	e	403	-	99,99,99	0.28	0	105,111,111	0.26	0
26	ATP	A1	601	27	32,33,33	0.29	0	48,52,52	0.28	0
30	CDL	p	201	-	99,99,99	0.30	0	105,111,111	0.27	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
30	CDL	c	201	-	-	25/110/110/110	-
30	CDL	e	404	-	-	21/110/110/110	-
30	CDL	e	405	-	-	31/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CDL	e	402	-	-	25/110/110/110	-
30	CDL	f	201	-	-	20/110/110/110	-
31	PEE	m	202	-	-	19/54/54/54	-
26	ATP	B1	601	27	-	8/22/38/38	0/3/3/3
30	CDL	q	101	-	-	32/110/110/110	-
34	PC1	f	204	-	-	7/57/57/57	-
30	CDL	l	101	-	-	20/110/110/110	-
32	LMT	e	406	-	-	1/21/61/61	0/2/2/2
26	ATP	C1	601	27	-	6/22/38/38	0/3/3/3
30	CDL	m	201	-	-	27/110/110/110	-
29	UTP	H1	201	-	-	3/22/38/38	0/2/2/2
26	ATP	F1	601	27	-	4/22/38/38	0/3/3/3
33	Q7G	n	201	-	2/2/24/34	6/20/148/200	0/8/8/10
30	CDL	q	102	-	-	25/110/110/110	-
30	CDL	j	201	-	-	24/110/110/110	-
30	CDL	e	401	-	-	23/110/110/110	-
34	PC1	j	202	-	-	12/57/57/57	-
31	PEE	f	202	-	-	16/54/54/54	-
34	PC1	f	203	-	-	8/57/57/57	-
32	LMT	j	203	-	-	5/21/61/61	0/2/2/2
28	ADP	D1	601	27	-	2/16/32/32	0/3/3/3
30	CDL	L	101	-	-	17/110/110/110	-
31	PEE	M	201	-	-	22/54/54/54	-
33	Q7G	e	407	-	1/1/19/34	5/15/123/200	0/7/7/10
34	PC1	i	201	-	-	11/57/57/57	-
30	CDL	e	403	-	-	28/110/110/110	-
26	ATP	A1	601	27	-	4/22/38/38	0/3/3/3
30	CDL	p	201	-	-	48/110/110/110	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	f	202	PEE	C39-C38	3.66	1.52	1.31
31	f	202	PEE	C18-C19	3.65	1.52	1.31
31	M	201	PEE	C18-C19	3.63	1.52	1.31
31	m	202	PEE	C18-C19	3.60	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	M	201	PEE	C39-C38	3.57	1.52	1.31
31	m	202	PEE	C39-C38	3.54	1.51	1.31

There are no bond angle outliers.

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	e	407	Q7G	C1B
33	n	201	Q7G	C1B
33	n	201	Q7G	C1C

All (505) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A1	601	ATP	PB-O3B-PG-O2G
26	A1	601	ATP	C5'-O5'-PA-O1A
26	B1	601	ATP	PB-O3B-PG-O2G
26	C1	601	ATP	PB-O3B-PG-O2G
26	C1	601	ATP	C5'-O5'-PA-O1A
26	F1	601	ATP	PB-O3B-PG-O2G
29	H1	201	UTP	PB-O3A-PA-O5'
29	H1	201	UTP	C5'-O5'-PA-O2A
29	H1	201	UTP	C5'-O5'-PA-O3A
30	L	101	CDL	CA2-OA2-PA1-OA4
30	L	101	CDL	CA2-OA2-PA1-OA5
30	L	101	CDL	CA3-OA5-PA1-OA2
30	c	201	CDL	CB3-OB5-PB2-OB2
30	c	201	CDL	CB3-OB5-PB2-OB3
30	c	201	CDL	CB3-OB5-PB2-OB4
30	e	401	CDL	CB2-OB2-PB2-OB3
30	e	401	CDL	CB2-OB2-PB2-OB4
30	e	401	CDL	CB2-OB2-PB2-OB5
30	e	401	CDL	CB3-OB5-PB2-OB2
30	e	401	CDL	CB3-OB5-PB2-OB3
30	e	402	CDL	CA3-OA5-PA1-OA2
30	e	402	CDL	CA3-OA5-PA1-OA3
30	e	402	CDL	CA3-OA5-PA1-OA4
30	e	403	CDL	CB2-OB2-PB2-OB3
30	e	404	CDL	CA3-OA5-PA1-OA2
30	e	404	CDL	CA3-OA5-PA1-OA3
30	e	404	CDL	CA3-OA5-PA1-OA4
30	e	404	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
30	e	404	CDL	CB3-OB5-PB2-OB3
30	e	404	CDL	CB3-OB5-PB2-OB4
30	e	405	CDL	CA3-OA5-PA1-OA2
30	e	405	CDL	CA3-OA5-PA1-OA3
30	e	405	CDL	CA3-OA5-PA1-OA4
30	e	405	CDL	CB3-OB5-PB2-OB2
30	e	405	CDL	OB5-CB3-CB4-OB6
30	f	201	CDL	CA2-OA2-PA1-OA4
30	f	201	CDL	CA2-OA2-PA1-OA5
30	f	201	CDL	CB3-OB5-PB2-OB2
30	j	201	CDL	CA2-OA2-PA1-OA3
30	j	201	CDL	CA3-OA5-PA1-OA2
30	j	201	CDL	CA3-OA5-PA1-OA3
30	j	201	CDL	CA3-OA5-PA1-OA4
30	l	101	CDL	CA2-OA2-PA1-OA3
30	l	101	CDL	CA2-OA2-PA1-OA4
30	l	101	CDL	CA2-OA2-PA1-OA5
30	l	101	CDL	CA3-OA5-PA1-OA2
30	m	201	CDL	CA2-C1-CB2-OB2
30	m	201	CDL	CA3-OA5-PA1-OA2
30	m	201	CDL	CA3-OA5-PA1-OA3
30	m	201	CDL	OA6-CA4-CA6-OA8
30	m	201	CDL	CB2-OB2-PB2-OB4
30	m	201	CDL	CB2-OB2-PB2-OB5
30	m	201	CDL	C51-CB5-OB6-CB4
30	p	201	CDL	CA2-C1-CB2-OB2
30	p	201	CDL	CA3-OA5-PA1-OA3
30	p	201	CDL	OA6-CA4-CA6-OA8
30	p	201	CDL	CB2-OB2-PB2-OB3
30	p	201	CDL	CB2-OB2-PB2-OB5
30	p	201	CDL	CB3-OB5-PB2-OB2
30	p	201	CDL	CB3-OB5-PB2-OB3
30	p	201	CDL	CB3-OB5-PB2-OB4
30	q	101	CDL	CA2-OA2-PA1-OA4
30	q	101	CDL	CB3-OB5-PB2-OB2
30	q	101	CDL	CB3-OB5-PB2-OB4
30	q	102	CDL	CA2-C1-CB2-OB2
30	q	102	CDL	CA2-OA2-PA1-OA5
30	q	102	CDL	OA5-CA3-CA4-OA6
30	q	102	CDL	CB2-OB2-PB2-OB3
30	q	102	CDL	CB2-OB2-PB2-OB4
31	M	201	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
31	M	201	PEE	C4-O4P-P-O2P
31	M	201	PEE	C4-O4P-P-O1P
31	M	201	PEE	O4P-C4-C5-N
31	f	202	PEE	C1-O3P-P-O4P
31	f	202	PEE	C4-O4P-P-O3P
31	f	202	PEE	C4-O4P-P-O2P
31	f	202	PEE	C4-O4P-P-O1P
31	m	202	PEE	C1-O3P-P-O2P
32	j	203	LMT	C2'-C1'-O1'-C1
32	j	203	LMT	O5'-C1'-O1'-C1
32	j	203	LMT	C2-C1-O1'-C1'
33	n	201	Q7G	C2B-C1B-O1B-C24
34	f	203	PC1	C11-O13-P-O12
34	f	203	PC1	C11-O13-P-O11
34	f	203	PC1	C1-O11-P-O14
34	f	203	PC1	C1-O11-P-O13
34	f	204	PC1	C11-O13-P-O12
34	f	204	PC1	C11-O13-P-O11
34	f	204	PC1	O13-C11-C12-N
34	i	201	PC1	C11-O13-P-O12
34	i	201	PC1	C11-O13-P-O14
34	i	201	PC1	C11-O13-P-O11
34	i	201	PC1	O13-C11-C12-N
34	j	202	PC1	C11-O13-P-O14
34	j	202	PC1	C11-O13-P-O11
34	j	202	PC1	C1-O11-P-O12
34	j	202	PC1	C1-O11-P-O14
34	j	202	PC1	C1-O11-P-O13
30	m	201	CDL	OB7-CB5-OB6-CB4
30	e	404	CDL	O1-C1-CA2-OA2
30	j	201	CDL	O1-C1-CA2-OA2
30	m	201	CDL	O1-C1-CB2-OB2
30	p	201	CDL	O1-C1-CB2-OB2
30	e	403	CDL	C11-CA5-OA6-CA4
30	p	201	CDL	C51-CB5-OB6-CB4
30	p	201	CDL	OB7-CB5-OB6-CB4
30	p	201	CDL	CB4-CB3-OB5-PB2
33	e	407	Q7G	O5B-C1B-O1B-C24
33	n	201	Q7G	O5B-C1B-O1B-C24
30	e	403	CDL	OA7-CA5-OA6-CA4
30	e	402	CDL	C31-CA7-OA8-CA6
31	M	201	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
33	e	407	Q7G	C2B-C1B-O1B-C24
30	q	102	CDL	O1-C1-CB2-OB2
30	e	401	CDL	C77-C78-C79-C80
30	m	201	CDL	CA5-C11-C12-C13
30	e	402	CDL	OA9-CA7-OA8-CA6
31	M	201	PEE	O5-C30-O3-C3
30	e	405	CDL	CA7-C31-C32-C33
30	p	201	CDL	CA5-C11-C12-C13
30	q	102	CDL	C11-CA5-OA6-CA4
31	m	202	PEE	C31-C32-C33-C34
30	q	102	CDL	OA7-CA5-OA6-CA4
31	M	201	PEE	C31-C32-C33-C34
30	e	405	CDL	C11-CA5-OA6-CA4
30	e	405	CDL	OA7-CA5-OA6-CA4
31	m	202	PEE	C17-C18-C19-C20
33	e	407	Q7G	CG1-C22-C23-C48
30	c	201	CDL	O1-C1-CA2-OA2
30	e	403	CDL	O1-C1-CA2-OA2
30	e	404	CDL	O1-C1-CB2-OB2
30	p	201	CDL	C80-C81-C82-C83
30	q	101	CDL	C11-CA5-OA6-CA4
31	m	202	PEE	C31-C30-O3-C3
30	q	101	CDL	OA7-CA5-OA6-CA4
32	e	406	LMT	C2-C1-O1'-C1'
30	q	101	CDL	C74-C75-C76-C77
30	e	403	CDL	C71-C72-C73-C74
30	q	101	CDL	C78-C79-C80-C81
30	c	201	CDL	CB2-C1-CA2-OA2
30	e	404	CDL	CA2-C1-CB2-OB2
30	j	201	CDL	CB2-C1-CA2-OA2
30	j	201	CDL	C13-C14-C15-C16
31	f	202	PEE	C11-C10-O2-C2
30	j	201	CDL	CA7-C31-C32-C33
31	m	202	PEE	O5-C30-O3-C3
30	L	101	CDL	C31-CA7-OA8-CA6
30	L	101	CDL	C11-CA5-OA6-CA4
30	e	403	CDL	C51-CB5-OB6-CB4
30	e	404	CDL	C11-CA5-OA6-CA4
30	f	201	CDL	C11-CA5-OA6-CA4
30	q	101	CDL	C51-CB5-OB6-CB4
30	e	403	CDL	OB7-CB5-OB6-CB4
30	e	404	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
30	c	201	CDL	C55-C56-C57-C58
30	p	201	CDL	C12-C13-C14-C15
30	e	403	CDL	C14-C15-C16-C17
30	m	201	CDL	C12-C13-C14-C15
32	j	203	LMT	O5B-C5B-C6B-O6B
30	j	201	CDL	C81-C82-C83-C84
30	q	101	CDL	C15-C16-C17-C18
33	n	201	Q7G	O5C-C5C-C6C-O6C
30	m	201	CDL	C73-C74-C75-C76
30	j	201	CDL	CA4-CA3-OA5-PA1
30	q	101	CDL	OB7-CB5-OB6-CB4
30	e	404	CDL	CB2-C1-CA2-OA2
30	e	404	CDL	C17-C18-C19-C20
31	f	202	PEE	C42-C43-C44-C45
30	c	201	CDL	C34-C35-C36-C37
30	e	405	CDL	C57-C58-C59-C60
30	j	201	CDL	OB5-CB3-CB4-CB6
30	q	101	CDL	OA5-CA3-CA4-CA6
30	q	102	CDL	OA5-CA3-CA4-CA6
30	q	102	CDL	CB7-C71-C72-C73
30	L	101	CDL	OA9-CA7-OA8-CA6
30	c	201	CDL	CA4-CA6-OA8-CA7
30	q	102	CDL	CA5-C11-C12-C13
31	M	201	PEE	C17-C18-C19-C20
30	e	405	CDL	CB3-CB4-CB6-OB8
30	m	201	CDL	CA3-CA4-CA6-OA8
30	p	201	CDL	CA3-CA4-CA6-OA8
31	M	201	PEE	C1-C2-C3-O3
34	f	203	PC1	C1-C2-C3-O31
30	j	201	CDL	C62-C63-C64-C65
30	e	403	CDL	C78-C79-C80-C81
30	L	101	CDL	OA7-CA5-OA6-CA4
30	e	403	CDL	C17-C18-C19-C20
31	M	201	PEE	C22-C23-C24-C25
30	m	201	CDL	C78-C79-C80-C81
30	l	101	CDL	C31-CA7-OA8-CA6
30	q	102	CDL	CB3-CB4-OB6-CB5
30	e	404	CDL	OA5-CA3-CA4-OA6
30	m	201	CDL	OA5-CA3-CA4-OA6
30	e	405	CDL	C40-C41-C42-C43
30	j	201	CDL	C34-C35-C36-C37
30	e	402	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	f	201	CDL	C77-C78-C79-C80
30	L	101	CDL	OA6-CA4-CA6-OA8
30	f	201	CDL	OB6-CB4-CB6-OB8
30	L	101	CDL	C14-C15-C16-C17
30	c	201	CDL	C51-C52-C53-C54
30	p	201	CDL	C63-C64-C65-C66
30	p	201	CDL	C21-C22-C23-C24
30	f	201	CDL	OA7-CA5-OA6-CA4
31	f	202	PEE	O4-C10-O2-C2
30	e	402	CDL	C78-C79-C80-C81
30	c	201	CDL	CA4-CA3-OA5-PA1
30	e	401	CDL	C18-C19-C20-C21
30	l	101	CDL	C14-C15-C16-C17
30	q	101	CDL	C79-C80-C81-C82
30	c	201	CDL	OA5-CA3-CA4-CA6
30	e	405	CDL	OB5-CB3-CB4-CB6
30	e	402	CDL	C75-C76-C77-C78
30	q	101	CDL	O1-C1-CB2-OB2
30	q	101	CDL	C76-C77-C78-C79
31	M	201	PEE	C43-C44-C45-C46
30	l	101	CDL	OA9-CA7-OA8-CA6
30	e	402	CDL	C81-C82-C83-C84
30	p	201	CDL	C18-C19-C20-C21
31	m	202	PEE	C41-C42-C43-C44
30	e	403	CDL	CB3-CB4-CB6-OB8
30	e	404	CDL	CB3-CB4-CB6-OB8
31	f	202	PEE	C1-C2-C3-O3
31	m	202	PEE	C22-C23-C24-C25
30	c	201	CDL	C39-C40-C41-C42
30	e	401	CDL	C56-C57-C58-C59
30	c	201	CDL	OA5-CA3-CA4-OA6
30	f	201	CDL	OA5-CA3-CA4-OA6
30	j	201	CDL	OB5-CB3-CB4-OB6
30	p	201	CDL	OA5-CA3-CA4-OA6
30	e	405	CDL	C76-C77-C78-C79
30	l	101	CDL	CA4-CA3-OA5-PA1
33	n	201	Q7G	C24-C23-C48-O1C
34	i	201	PC1	C2C-C2D-C2E-C2F
30	e	403	CDL	OB6-CB4-CB6-OB8
30	e	405	CDL	OB6-CB4-CB6-OB8
30	l	101	CDL	OA6-CA4-CA6-OA8
34	f	203	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
30	p	201	CDL	C62-C63-C64-C65
30	e	405	CDL	C78-C79-C80-C81
30	e	401	CDL	C81-C82-C83-C84
30	e	402	CDL	C11-CA5-OA6-CA4
30	l	101	CDL	C31-C32-C33-C34
33	e	407	Q7G	CG1-C22-C23-C24
30	m	201	CDL	C21-C22-C23-C24
30	e	403	CDL	C62-C63-C64-C65
30	q	102	CDL	CB2-C1-CA2-OA2
34	f	204	PC1	C37-C38-C39-C3A
31	M	201	PEE	C39-C40-C41-C42
34	i	201	PC1	C32-C31-O31-C3
30	f	201	CDL	C13-C14-C15-C16
30	m	201	CDL	OA5-CA3-CA4-CA6
30	e	405	CDL	CA4-CA3-OA5-PA1
30	e	402	CDL	OA7-CA5-OA6-CA4
33	n	201	Q7G	C16-C17-O20-CG1
26	B1	601	ATP	PB-O3B-PG-O3G
30	e	402	CDL	CA6-CA4-OA6-CA5
30	l	101	CDL	O1-C1-CA2-OA2
30	p	201	CDL	C38-C39-C40-C41
30	q	101	CDL	OA5-CA3-CA4-OA6
30	p	201	CDL	C74-C75-C76-C77
30	l	101	CDL	C64-C65-C66-C67
30	e	404	CDL	OB6-CB4-CB6-OB8
30	p	201	CDL	OB6-CB4-CB6-OB8
30	f	201	CDL	C12-C13-C14-C15
34	i	201	PC1	O32-C31-O31-C3
30	e	405	CDL	C56-C57-C58-C59
30	e	405	CDL	C53-C54-C55-C56
30	j	201	CDL	C1-CB2-OB2-PB2
30	e	405	CDL	C71-C72-C73-C74
30	q	102	CDL	C77-C78-C79-C80
26	B1	601	ATP	PA-O3A-PB-O2B
34	f	203	PC1	O13-C11-C12-N
34	j	202	PC1	O13-C11-C12-N
30	L	101	CDL	C31-C32-C33-C34
30	j	201	CDL	C55-C56-C57-C58
30	c	201	CDL	C83-C84-C85-C86
30	e	403	CDL	C12-C13-C14-C15
30	p	201	CDL	OA5-CA3-CA4-CA6
30	p	201	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
30	p	201	CDL	C42-C43-C44-C45
32	j	203	LMT	C2-C3-C4-C5
34	j	202	PC1	C2-C1-O11-P
30	e	402	CDL	C74-C75-C76-C77
30	e	405	CDL	OA5-CA3-CA4-OA6
30	q	101	CDL	C61-C62-C63-C64
30	e	401	CDL	C13-C14-C15-C16
31	f	202	PEE	C16-C17-C18-C19
30	p	201	CDL	C56-C57-C58-C59
31	M	201	PEE	O2-C2-C3-O3
31	f	202	PEE	O2-C2-C3-O3
30	q	101	CDL	CA2-C1-CB2-OB2
30	p	201	CDL	C33-C34-C35-C36
30	c	201	CDL	CA3-CA4-CA6-OA8
30	p	201	CDL	CB3-CB4-CB6-OB8
30	q	101	CDL	CB3-CB4-CB6-OB8
33	e	407	Q7G	C23-C24-O1B-C1B
30	q	101	CDL	C72-C73-C74-C75
26	B1	601	ATP	C5'-O5'-PA-O1A
30	L	101	CDL	CA2-OA2-PA1-OA3
30	L	101	CDL	CA3-OA5-PA1-OA3
30	c	201	CDL	CA3-OA5-PA1-OA3
30	c	201	CDL	CB2-OB2-PB2-OB3
30	e	401	CDL	CB3-OB5-PB2-OB4
30	e	403	CDL	CB3-OB5-PB2-OB3
30	e	405	CDL	CB3-OB5-PB2-OB3
30	f	201	CDL	CB3-OB5-PB2-OB3
30	j	201	CDL	CA2-OA2-PA1-OA4
30	j	201	CDL	CA2-OA2-PA1-OA5
30	l	101	CDL	CA3-OA5-PA1-OA3
30	l	101	CDL	CA3-OA5-PA1-OA4
30	m	201	CDL	CA3-OA5-PA1-OA4
30	m	201	CDL	CB3-OB5-PB2-OB3
30	p	201	CDL	CB2-OB2-PB2-OB4
30	q	101	CDL	CA2-OA2-PA1-OA3
30	q	101	CDL	CA2-OA2-PA1-OA5
30	q	102	CDL	CA2-OA2-PA1-OA3
30	q	102	CDL	CA3-OA5-PA1-OA3
30	q	102	CDL	CB2-OB2-PB2-OB5
30	q	102	CDL	CB3-OB5-PB2-OB3
31	f	202	PEE	C1-O3P-P-O1P
31	m	202	PEE	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
31	m	202	PEE	C1-O3P-P-O4P
34	f	203	PC1	C1-O11-P-O12
30	L	101	CDL	CA4-CA3-OA5-PA1
30	e	402	CDL	CA4-CA3-OA5-PA1
30	e	402	CDL	C1-CB2-OB2-PB2
30	f	201	CDL	CB4-CB3-OB5-PB2
30	q	101	CDL	CB4-CB3-OB5-PB2
31	M	201	PEE	C2-C1-O3P-P
34	j	202	PC1	C3C-C3D-C3E-C3F
30	p	201	CDL	C81-C82-C83-C84
33	n	201	Q7G	C18-C17-O20-CG1
30	e	403	CDL	CB5-C51-C52-C53
30	e	404	CDL	CA6-CA4-OA6-CA5
30	q	101	CDL	CB3-CB4-OB6-CB5
30	j	201	CDL	C77-C78-C79-C80
30	e	404	CDL	OA5-CA3-CA4-CA6
31	M	201	PEE	C23-C24-C25-C26
31	m	202	PEE	C36-C37-C38-C39
31	m	202	PEE	C38-C39-C40-C41
30	e	402	CDL	OB5-CB3-CB4-OB6
30	e	402	CDL	C53-C54-C55-C56
30	j	201	CDL	C72-C73-C74-C75
30	l	101	CDL	OA7-CA5-OA6-CA4
30	c	201	CDL	OA6-CA4-CA6-OA8
30	e	403	CDL	OA6-CA4-CA6-OA8
30	L	101	CDL	O1-C1-CA2-OA2
30	l	101	CDL	C11-CA5-OA6-CA4
30	p	201	CDL	C11-CA5-OA6-CA4
30	p	201	CDL	OA7-CA5-OA6-CA4
30	f	201	CDL	CB3-CB4-CB6-OB8
26	A1	601	ATP	PG-O3B-PB-O2B
26	C1	601	ATP	PG-O3B-PB-O2B
26	F1	601	ATP	PG-O3B-PB-O1B
26	F1	601	ATP	PG-O3B-PB-O2B
31	M	201	PEE	C36-C37-C38-C39
30	e	401	CDL	C43-C44-C45-C46
30	e	403	CDL	C83-C84-C85-C86
31	m	202	PEE	C13-C14-C15-C16
34	i	201	PC1	C2A-C2B-C2C-C2D
30	e	405	CDL	C59-C60-C61-C62
30	e	401	CDL	OB5-CB3-CB4-OB6
30	e	402	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
30	e	405	CDL	OA5-CA3-CA4-CA6
30	e	405	CDL	C11-C12-C13-C14
30	m	201	CDL	C71-CB7-OB8-CB6
31	M	201	PEE	C38-C39-C40-C41
30	p	201	CDL	C55-C56-C57-C58
30	c	201	CDL	C38-C39-C40-C41
30	m	201	CDL	C42-C43-C44-C45
30	c	201	CDL	C40-C41-C42-C43
30	q	102	CDL	C1-CB2-OB2-PB2
31	m	202	PEE	C23-C24-C25-C26
34	f	204	PC1	O31-C31-C32-C33
31	m	202	PEE	C34-C35-C36-C37
30	e	403	CDL	CA3-CA4-CA6-OA8
30	q	101	CDL	CA3-CA4-CA6-OA8
30	j	201	CDL	CA3-CA4-OA6-CA5
30	p	201	CDL	C22-C23-C24-C25
30	f	201	CDL	C78-C79-C80-C81
30	c	201	CDL	C62-C63-C64-C65
30	L	101	CDL	C39-C40-C41-C42
30	m	201	CDL	C33-C34-C35-C36
30	c	201	CDL	C42-C43-C44-C45
30	e	401	CDL	C16-C17-C18-C19
30	c	201	CDL	C35-C36-C37-C38
30	m	201	CDL	OB9-CB7-OB8-CB6
30	p	201	CDL	C79-C80-C81-C82
30	l	101	CDL	C39-C40-C41-C42
30	p	201	CDL	C14-C15-C16-C17
30	e	401	CDL	C11-C12-C13-C14
30	e	405	CDL	C79-C80-C81-C82
34	j	202	PC1	O11-C1-C2-O21
30	e	402	CDL	C77-C78-C79-C80
30	e	402	CDL	C54-C55-C56-C57
30	e	402	CDL	C55-C56-C57-C58
31	M	201	PEE	C34-C35-C36-C37
31	M	201	PEE	C16-C17-C18-C19
31	f	202	PEE	C18-C19-C20-C21
31	f	202	PEE	C19-C20-C21-C22
30	p	201	CDL	OA9-CA7-OA8-CA6
30	e	404	CDL	C18-C19-C20-C21
30	e	401	CDL	OB5-CB3-CB4-CB6
30	f	201	CDL	OA5-CA3-CA4-CA6
34	j	202	PC1	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
31	m	202	PEE	C16-C17-C18-C19
30	e	401	CDL	CB4-CB3-OB5-PB2
30	e	404	CDL	C78-C79-C80-C81
30	q	102	CDL	O1-C1-CA2-OA2
30	c	201	CDL	C56-C57-C58-C59
31	f	202	PEE	C36-C37-C38-C39
26	A1	601	ATP	PB-O3B-PG-O1G
26	C1	601	ATP	PB-O3B-PG-O1G
30	e	402	CDL	C52-C51-CB5-OB6
30	e	405	CDL	C52-C53-C54-C55
31	M	201	PEE	C18-C19-C20-C21
30	e	403	CDL	C1-CA2-OA2-PA1
30	L	101	CDL	CA3-CA4-CA6-OA8
30	l	101	CDL	CA3-CA4-CA6-OA8
30	e	402	CDL	C79-C80-C81-C82
30	q	101	CDL	C37-C38-C39-C40
30	q	101	CDL	OA6-CA4-CA6-OA8
31	m	202	PEE	C18-C19-C20-C21
30	l	101	CDL	C60-C61-C62-C63
30	e	401	CDL	C32-C31-CA7-OA8
31	f	202	PEE	O2-C10-C11-C12
30	e	402	CDL	C34-C35-C36-C37
30	m	201	CDL	OA7-CA5-OA6-CA4
30	p	201	CDL	C31-CA7-OA8-CA6
31	M	201	PEE	O2-C10-C11-C12
30	e	401	CDL	C80-C81-C82-C83
34	f	204	PC1	C24-C25-C26-C27
26	B1	601	ATP	PG-O3B-PB-O1B
26	B1	601	ATP	PG-O3B-PB-O2B
26	B1	601	ATP	PA-O3A-PB-O1B
26	C1	601	ATP	PA-O3A-PB-O1B
28	D1	601	ADP	PB-O3A-PA-O1A
28	D1	601	ADP	PB-O3A-PA-O2A
30	e	403	CDL	C71-CB7-OB8-CB6
30	f	201	CDL	C72-C71-CB7-OB8
30	m	201	CDL	C12-C11-CA5-OA6
31	m	202	PEE	O2-C10-C11-C12
30	e	401	CDL	OB7-CB5-OB6-CB4
30	e	403	CDL	OB9-CB7-OB8-CB6
30	f	201	CDL	C12-C11-CA5-OA6
30	p	201	CDL	C52-C51-CB5-OB6
30	q	101	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
30	q	102	CDL	C75-C76-C77-C78
30	j	201	CDL	C52-C51-CB5-OB6
30	p	201	CDL	C12-C11-CA5-OA6
30	e	403	CDL	C18-C19-C20-C21
30	e	405	CDL	C12-C11-CA5-OA6
34	j	202	PC1	O31-C31-C32-C33
30	q	101	CDL	C71-C72-C73-C74
30	e	403	CDL	C52-C51-CB5-OB6
30	e	405	CDL	C32-C31-CA7-OA8
30	L	101	CDL	C60-C61-C62-C63
26	B1	601	ATP	PB-O3B-PG-O1G
26	F1	601	ATP	PB-O3B-PG-O1G
30	p	201	CDL	C72-C73-C74-C75
30	q	102	CDL	OB5-CB3-CB4-CB6
30	e	403	CDL	C32-C31-CA7-OA8
30	q	101	CDL	C38-C39-C40-C41
30	e	403	CDL	C51-C52-C53-C54
30	p	201	CDL	C51-C52-C53-C54
30	j	201	CDL	CA6-CA4-OA6-CA5
30	l	101	CDL	C36-C37-C38-C39
30	p	201	CDL	C17-C18-C19-C20
30	e	401	CDL	C53-C54-C55-C56
30	f	201	CDL	C37-C38-C39-C40
30	e	401	CDL	C32-C31-CA7-OA9
30	p	201	CDL	C41-C42-C43-C44
30	e	403	CDL	C32-C31-CA7-OA9
30	m	201	CDL	C12-C11-CA5-OA7
30	q	102	CDL	OB5-CB3-CB4-OB6
30	q	102	CDL	C72-C71-CB7-OB8
30	q	101	CDL	C12-C11-CA5-OA7
31	f	202	PEE	O4-C10-C11-C12
31	m	202	PEE	O4-C10-C11-C12
30	c	201	CDL	C53-C54-C55-C56
34	f	204	PC1	C2B-C2C-C2D-C2E
30	p	201	CDL	C12-C11-CA5-OA7
30	p	201	CDL	C52-C51-CB5-OB7
30	q	101	CDL	C59-C60-C61-C62
34	i	201	PC1	O21-C21-C22-C23
30	e	403	CDL	C52-C51-CB5-OB7
31	M	201	PEE	O4-C10-C11-C12
31	m	202	PEE	C42-C43-C44-C45
30	f	201	CDL	C12-C11-CA5-OA7

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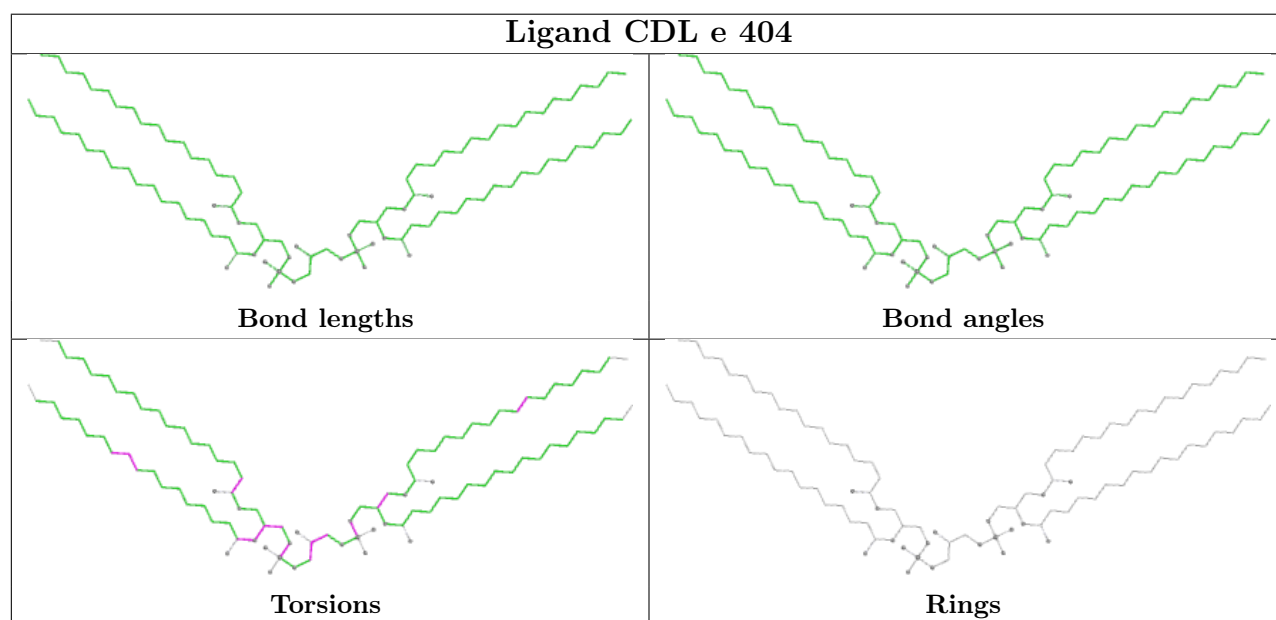
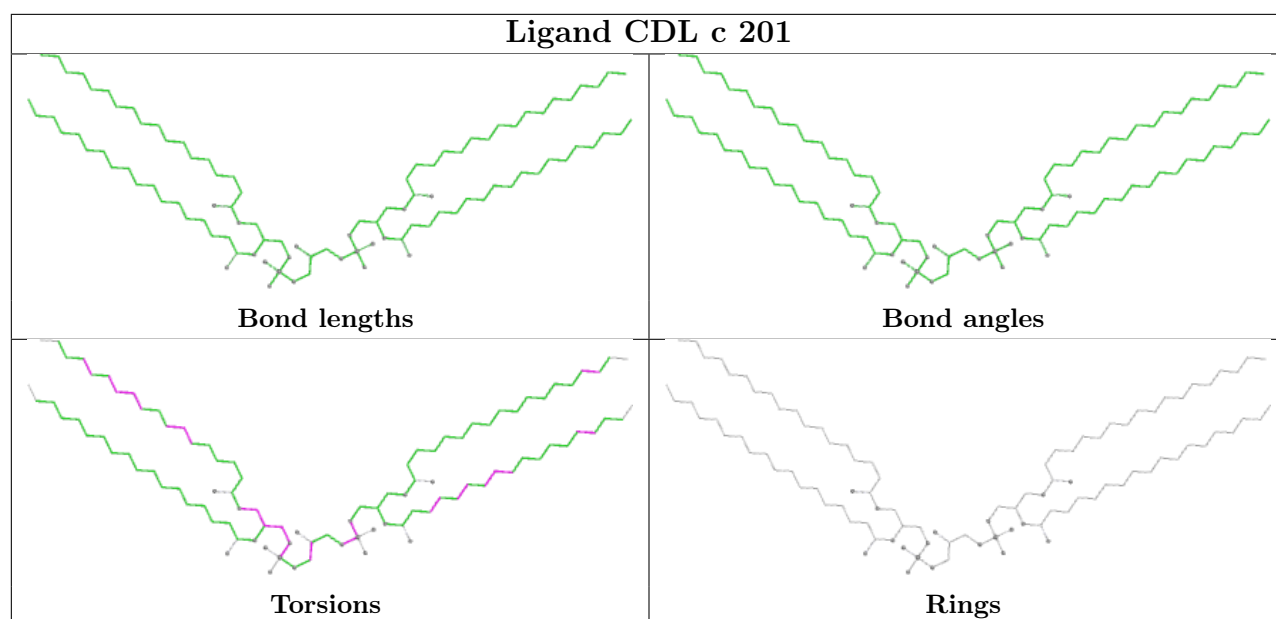
Mol	Chain	Res	Type	Atoms
30	e	405	CDL	C81-C82-C83-C84
30	q	101	CDL	OB6-CB4-CB6-OB8
30	e	405	CDL	C12-C11-CA5-OA7
30	f	201	CDL	C72-C71-CB7-OB9
30	e	405	CDL	C74-C75-C76-C77
30	e	402	CDL	C32-C31-CA7-OA8
30	e	404	CDL	C32-C31-CA7-OA8
30	e	401	CDL	C51-CB5-OB6-CB4
30	m	201	CDL	C11-CA5-OA6-CA4
26	C1	601	ATP	PA-O3A-PB-O2B
30	q	102	CDL	C72-C71-CB7-OB9
30	j	201	CDL	C52-C51-CB5-OB7
34	i	201	PC1	O22-C21-C22-C23
34	j	202	PC1	O32-C31-C32-C33
34	i	201	PC1	C3B-C3C-C3D-C3E

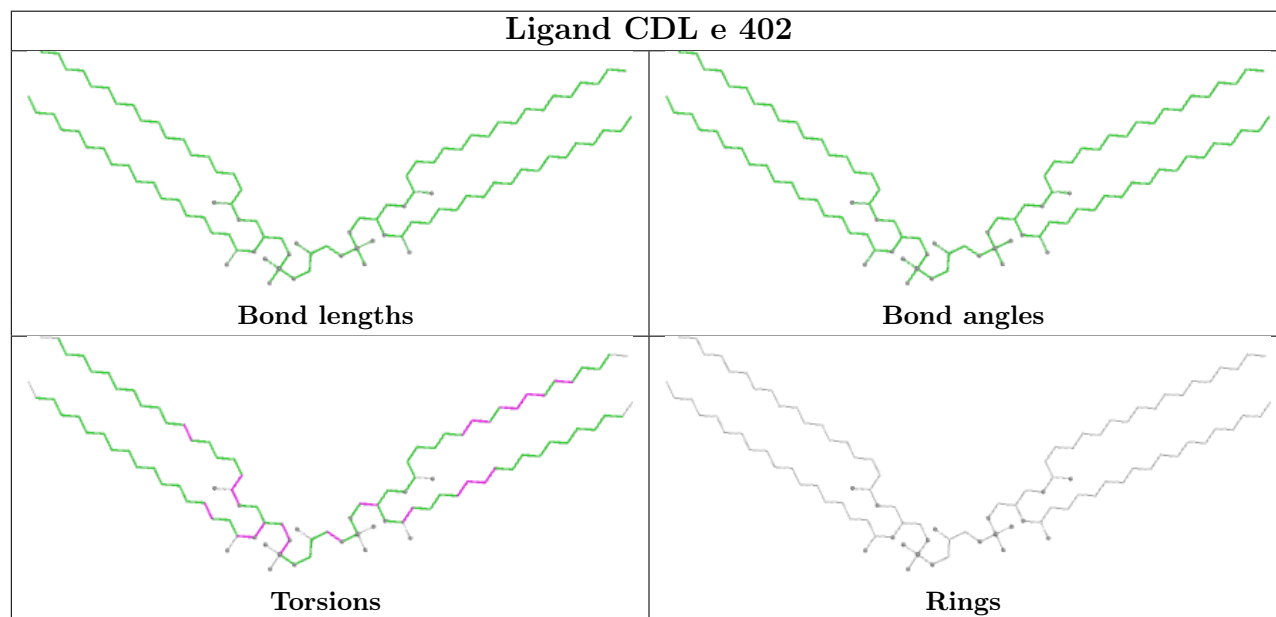
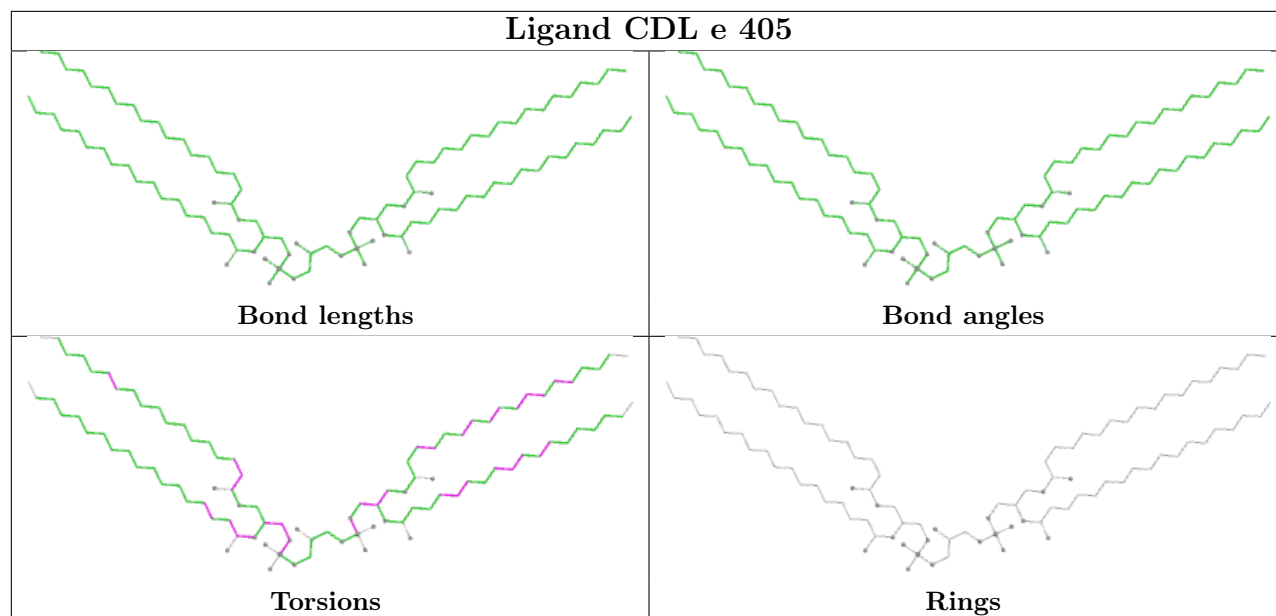
There are no ring outliers.

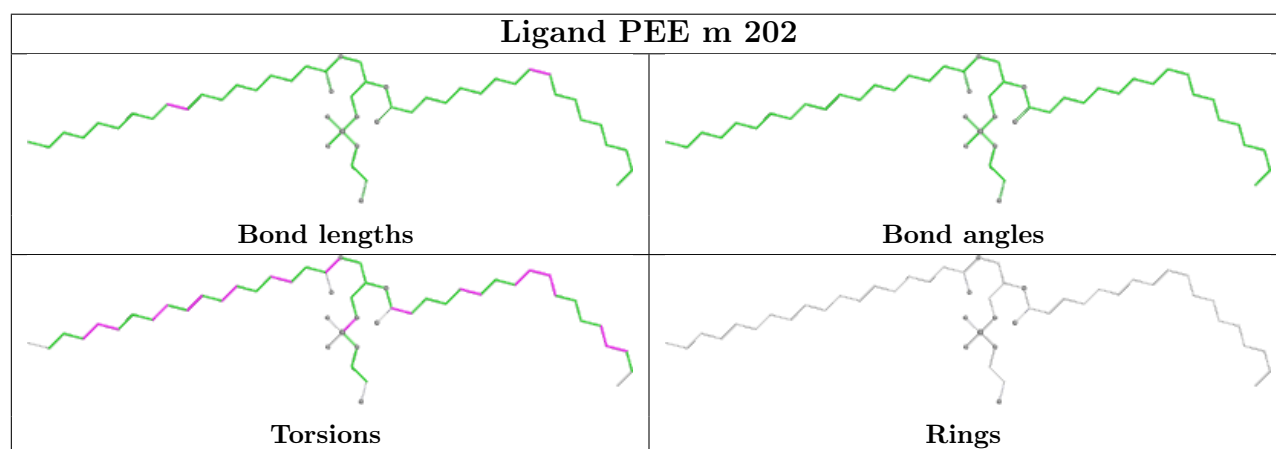
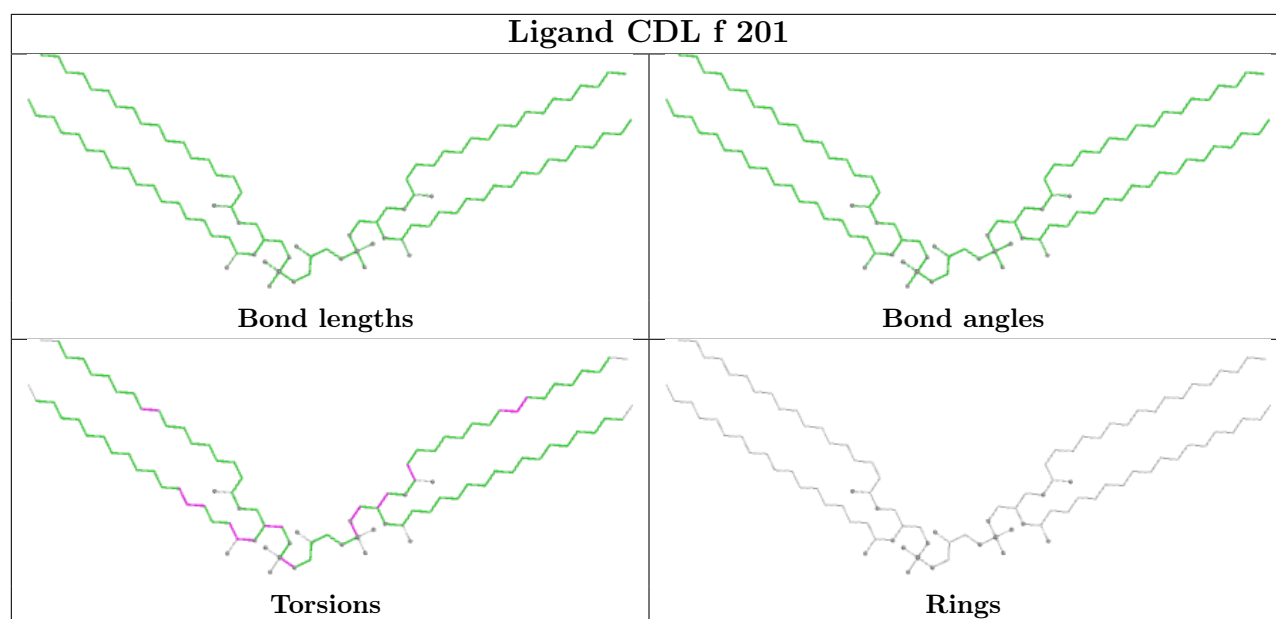
5 monomers are involved in 6 short contacts:

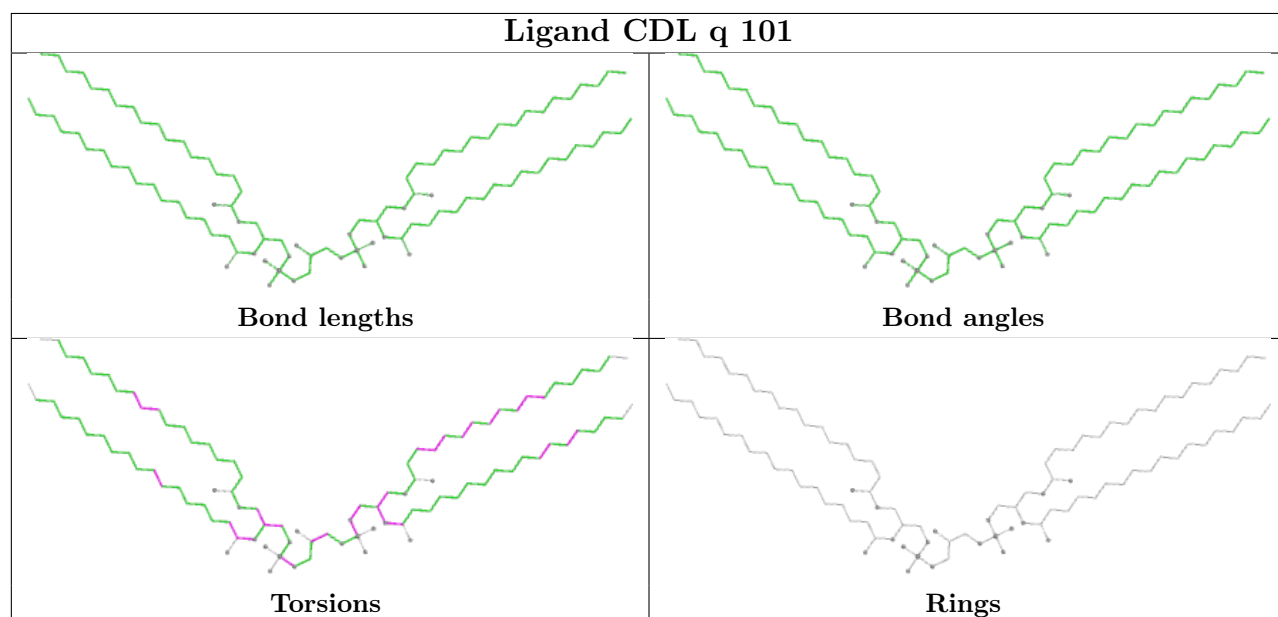
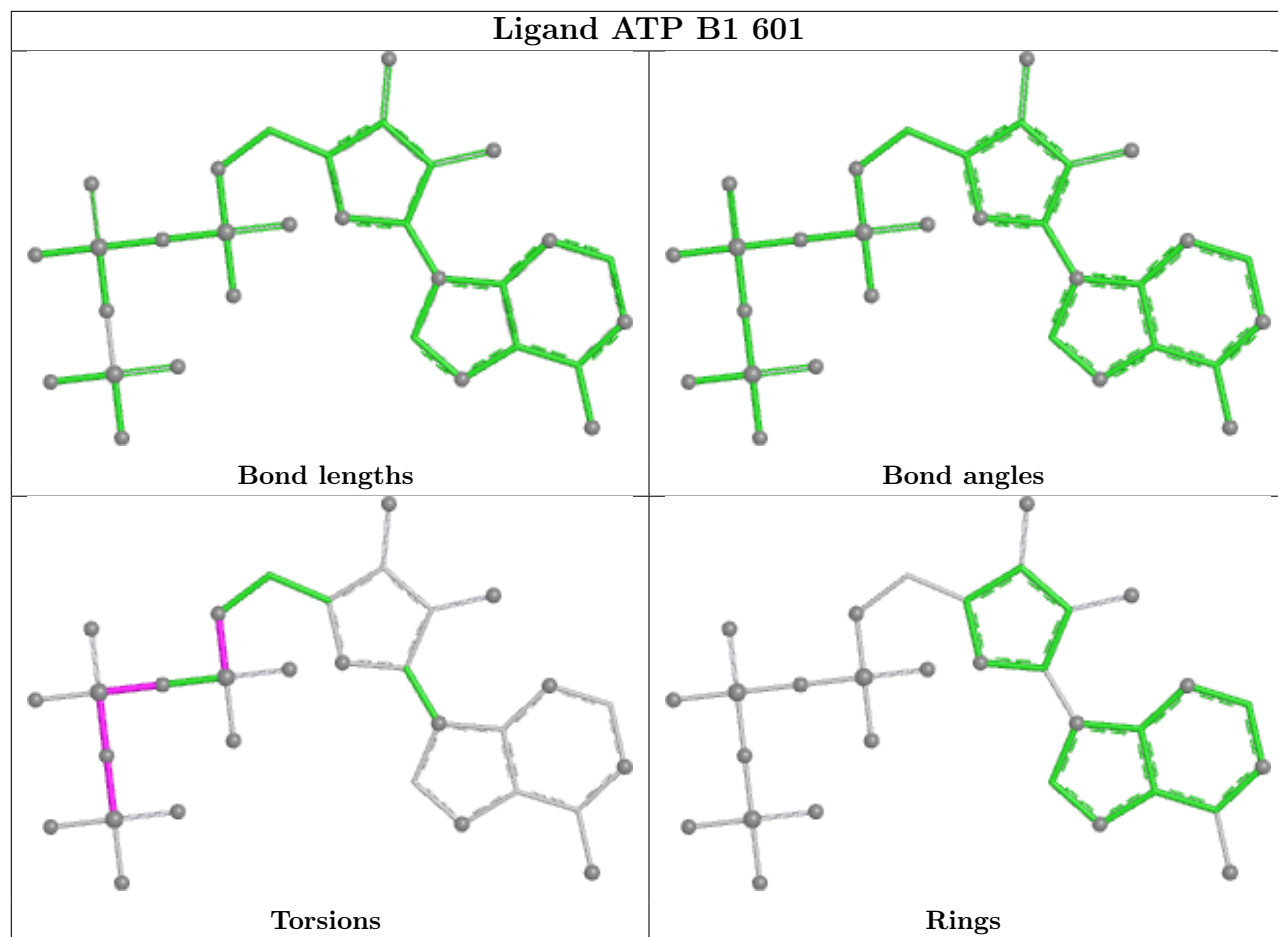
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	c	201	CDL	1	0
30	e	402	CDL	1	0
30	q	101	CDL	1	0
34	f	204	PC1	2	0
30	p	201	CDL	1	0

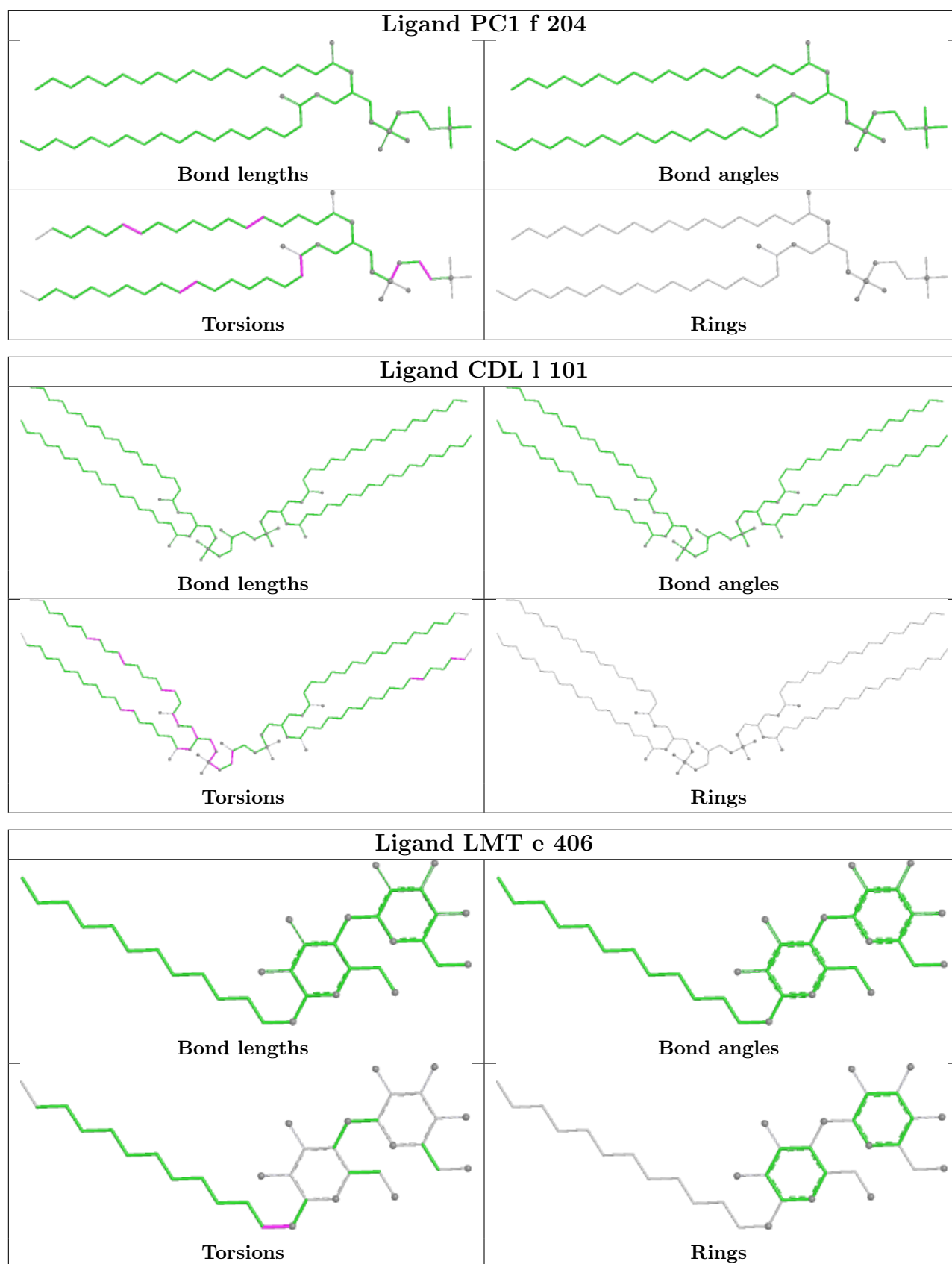
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

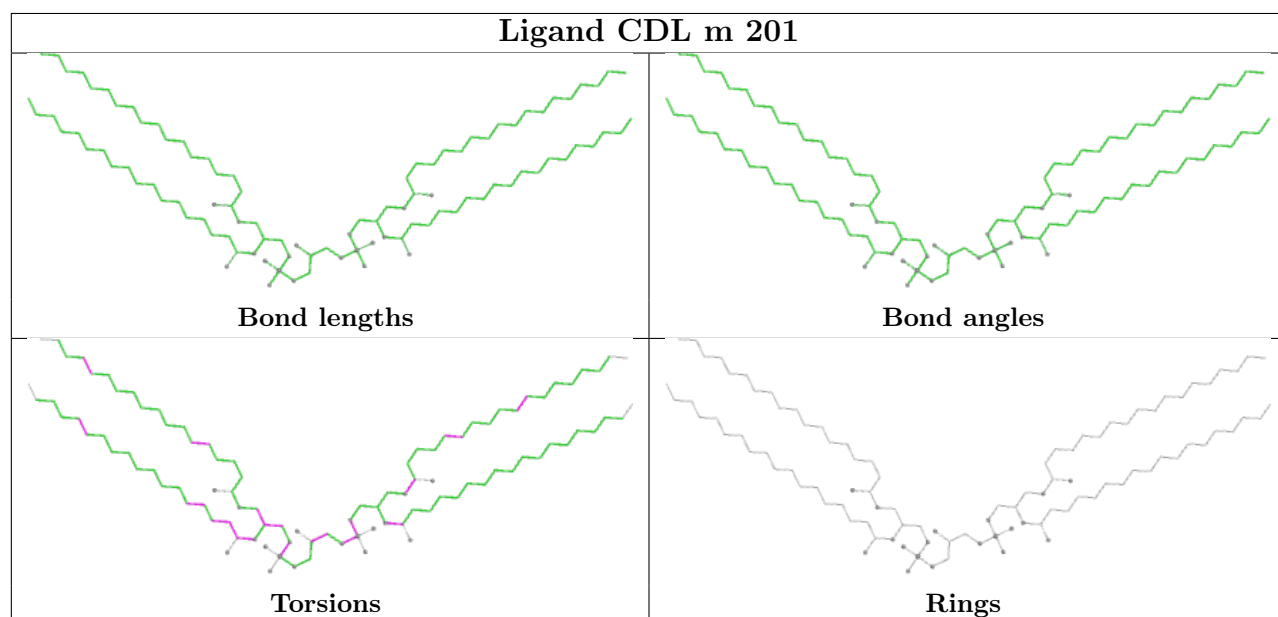
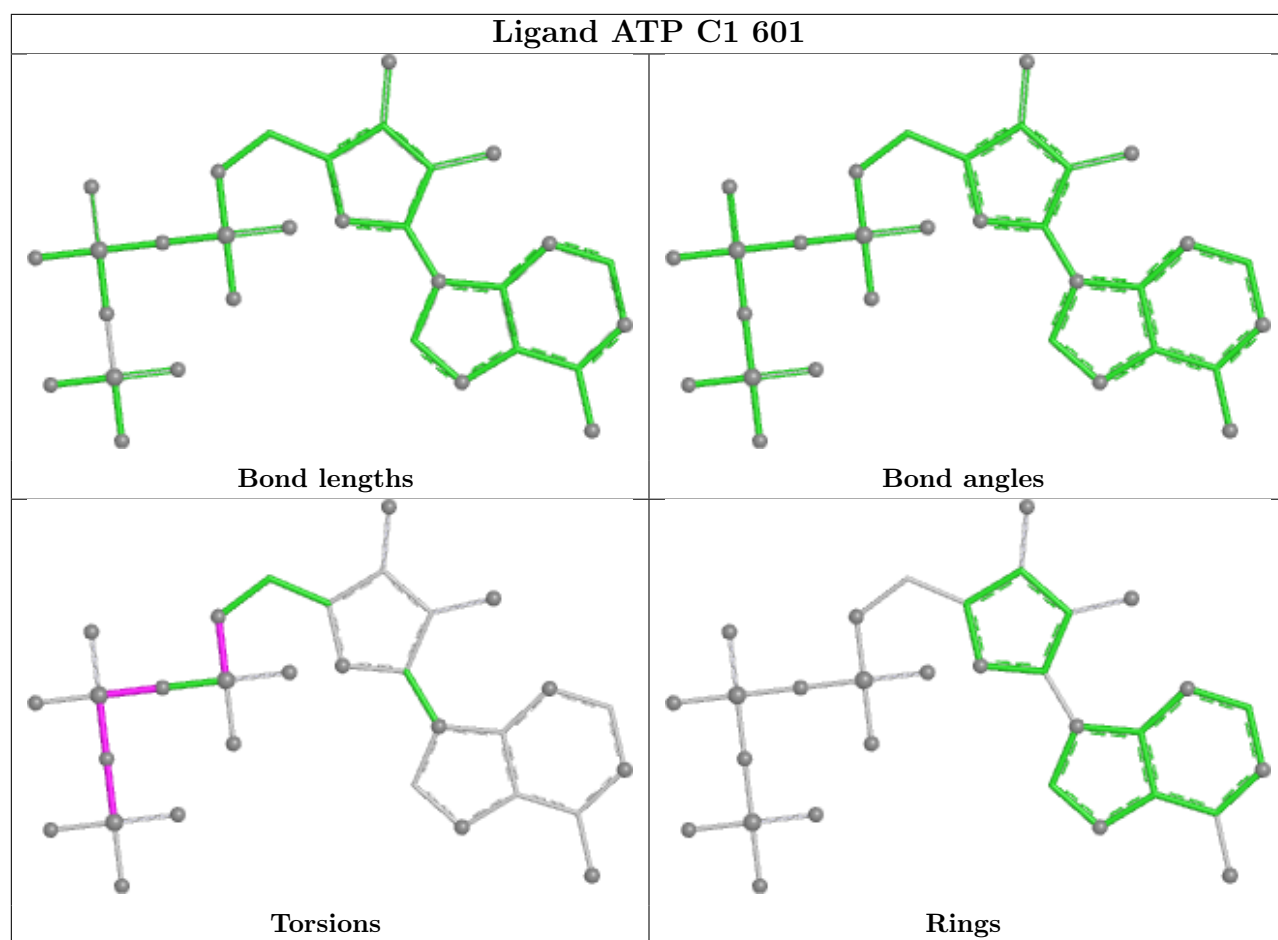


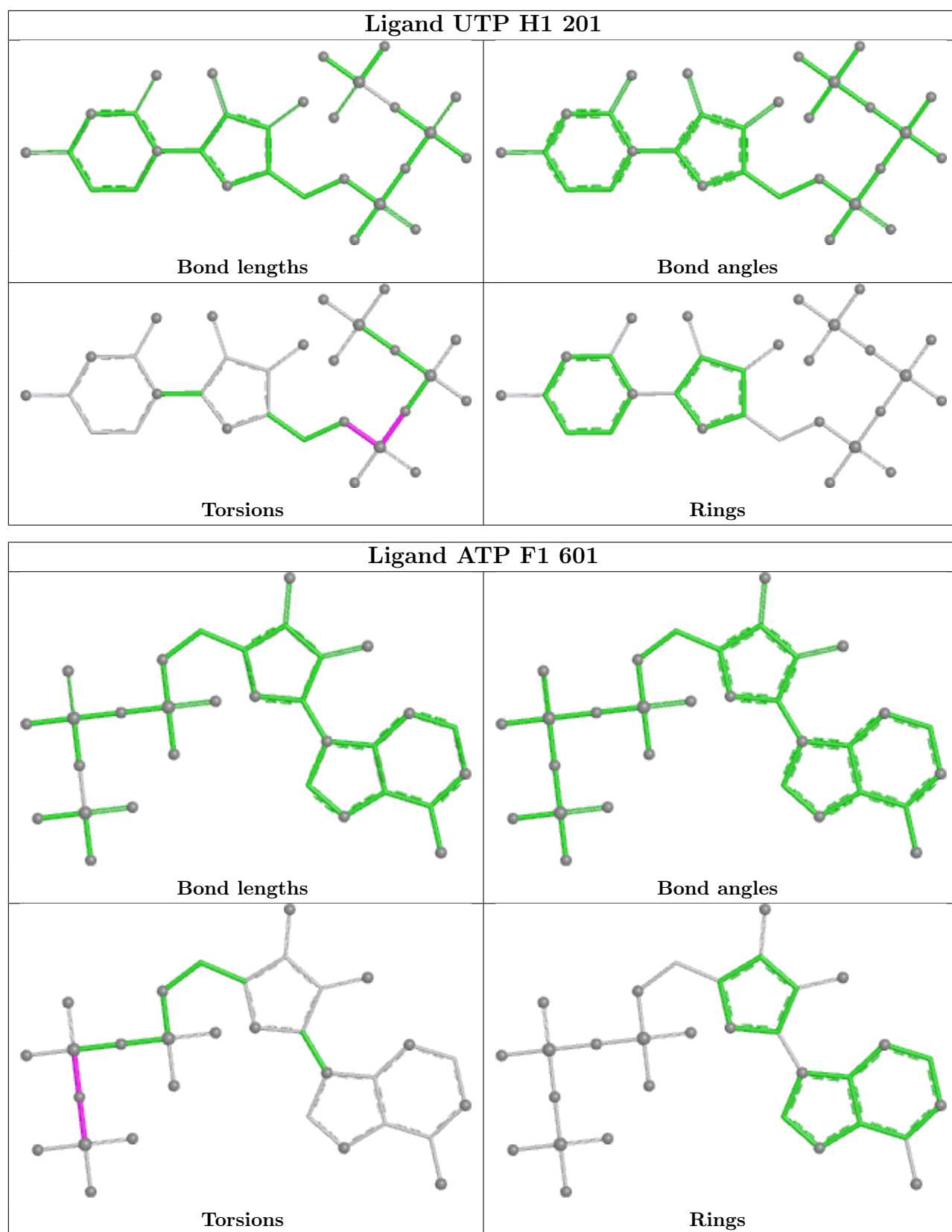


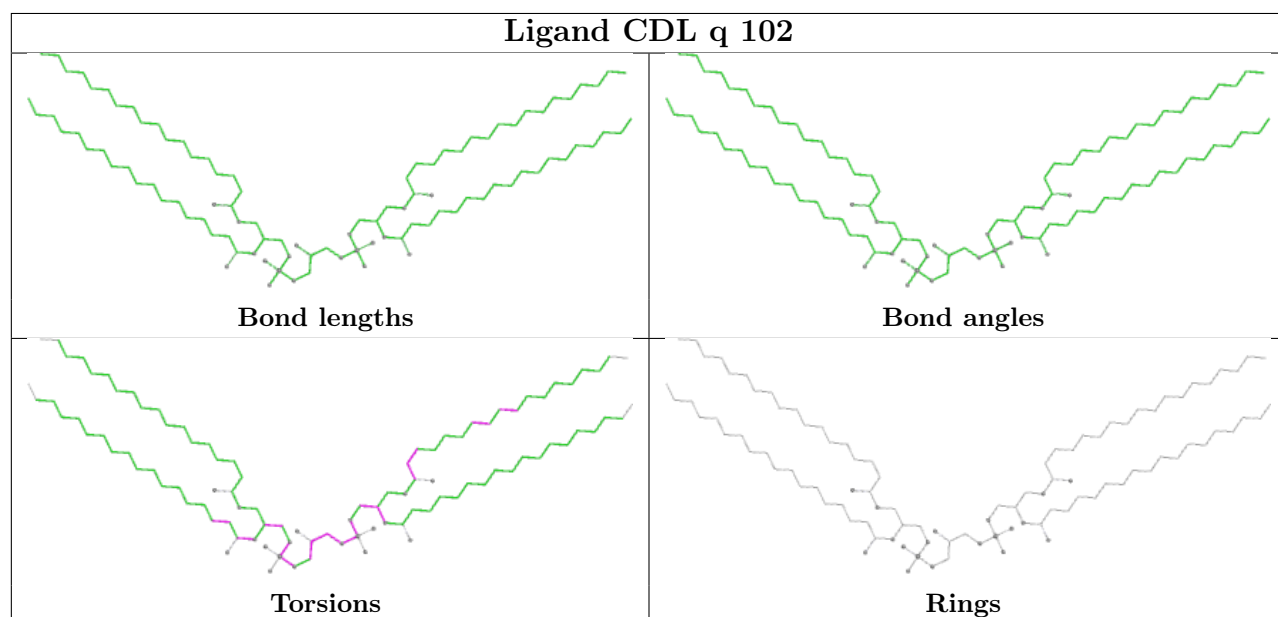
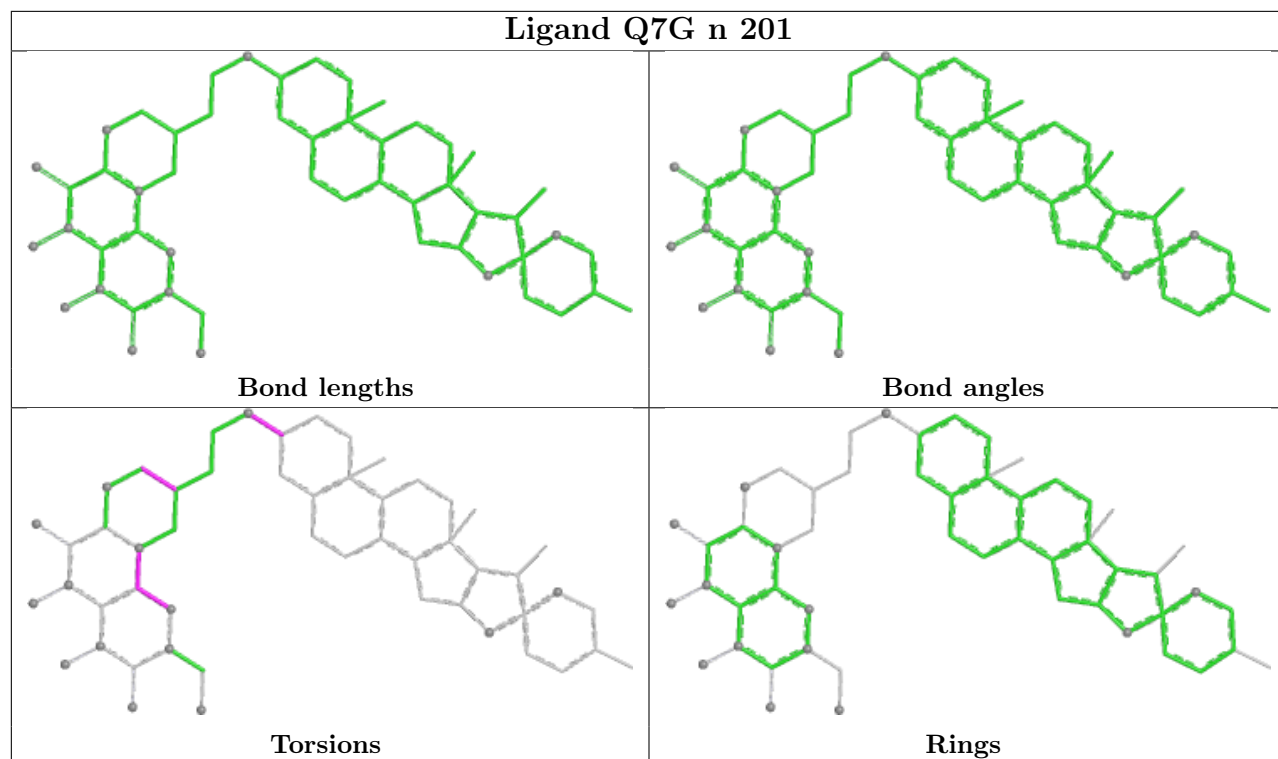


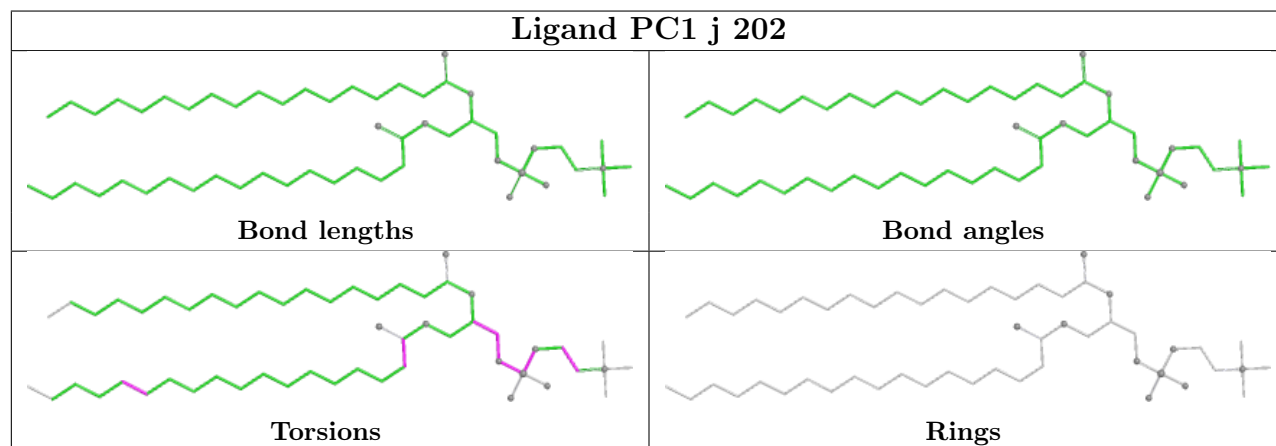
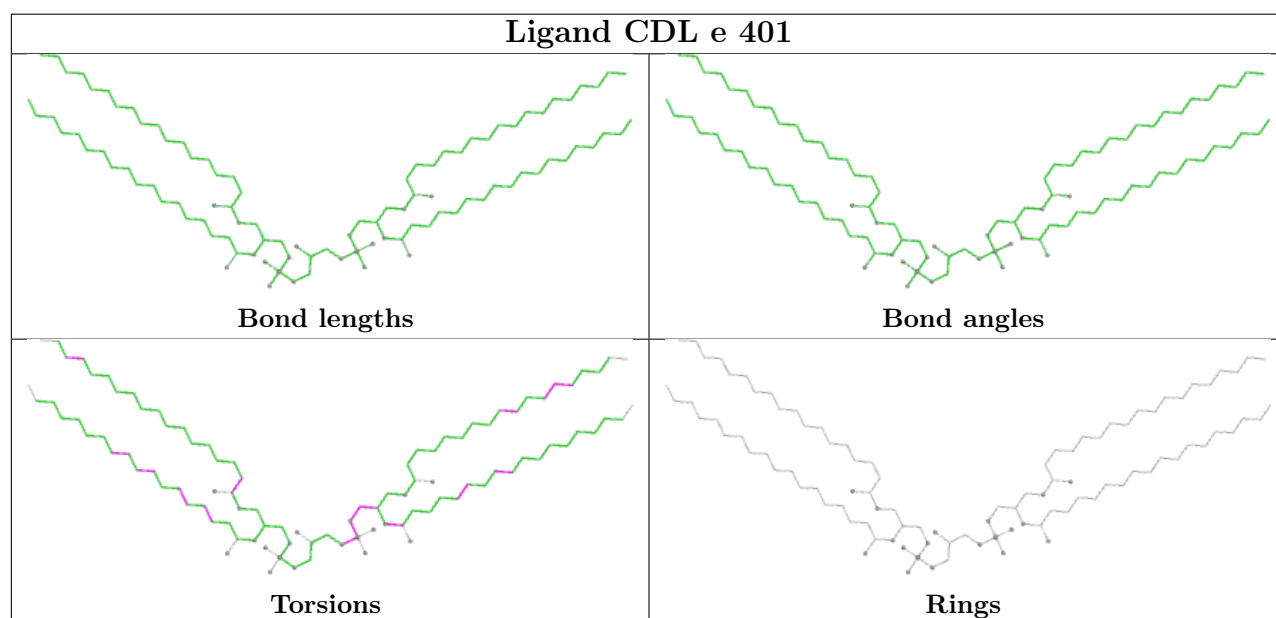
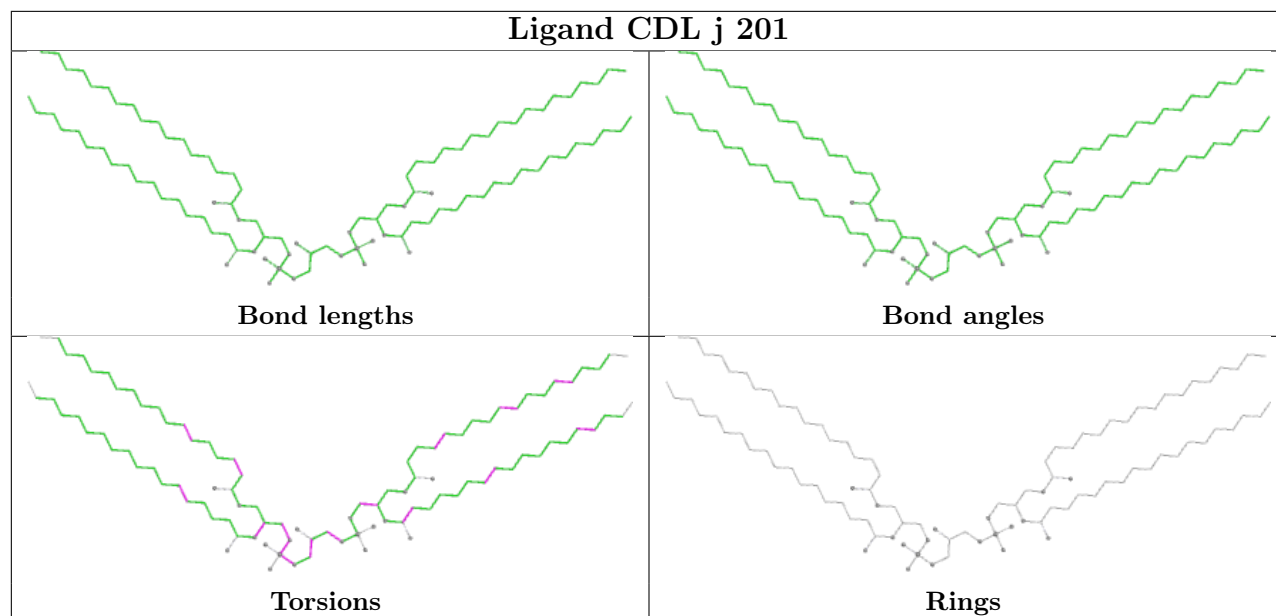


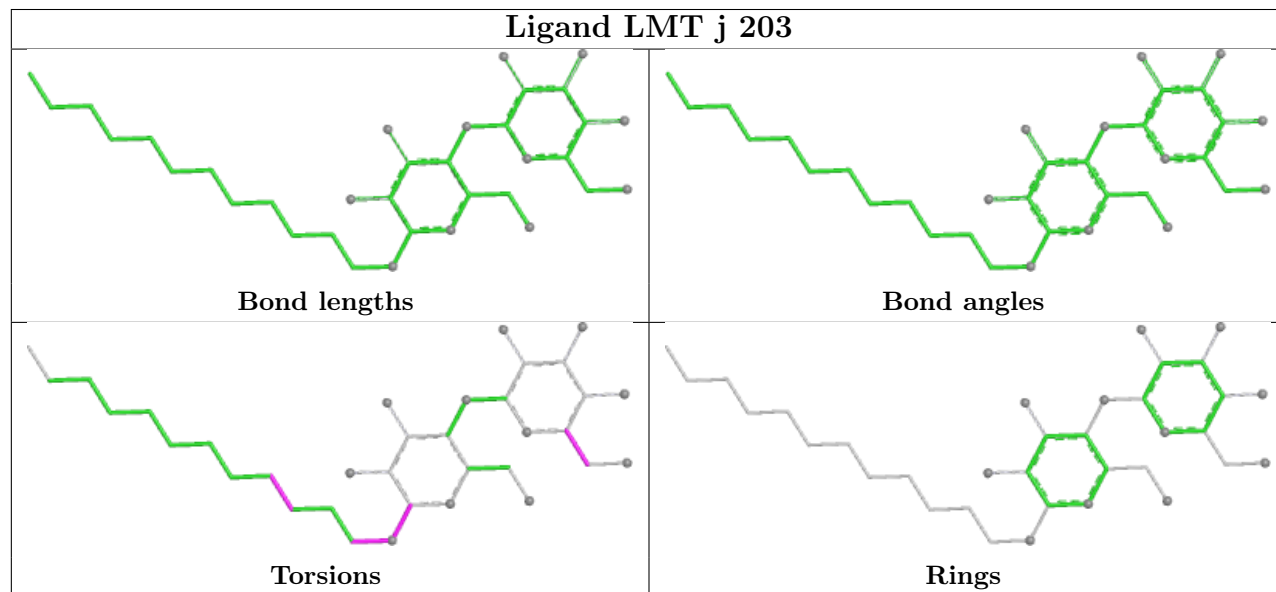
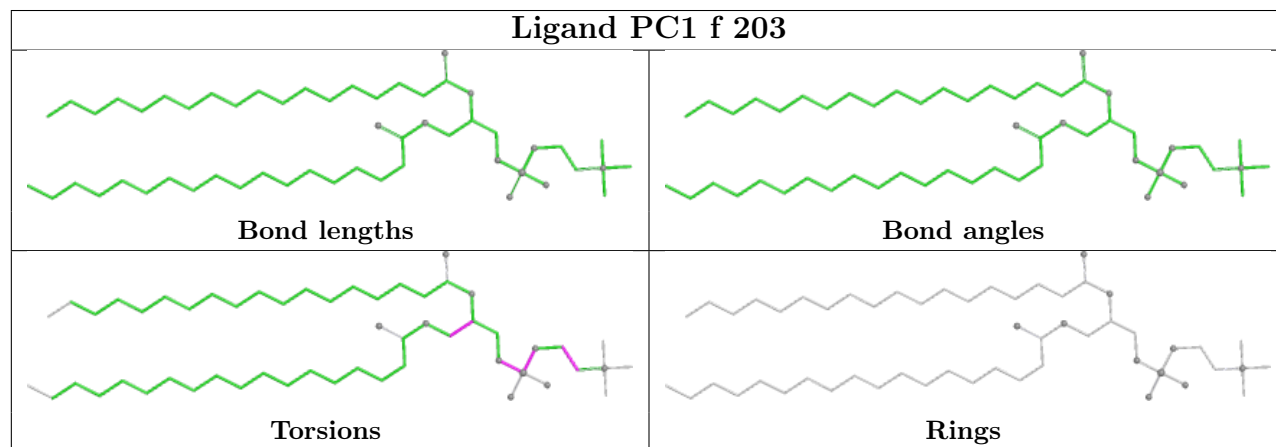
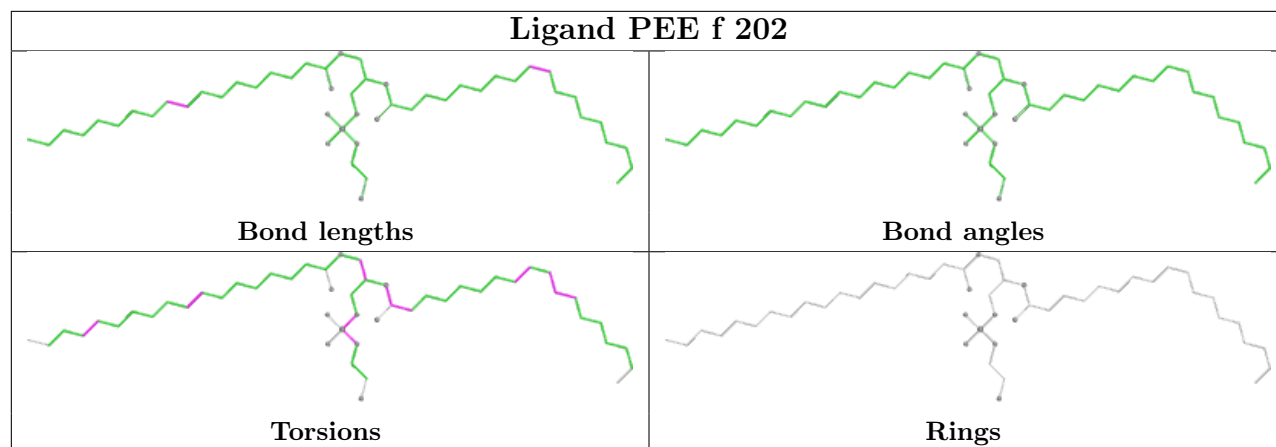


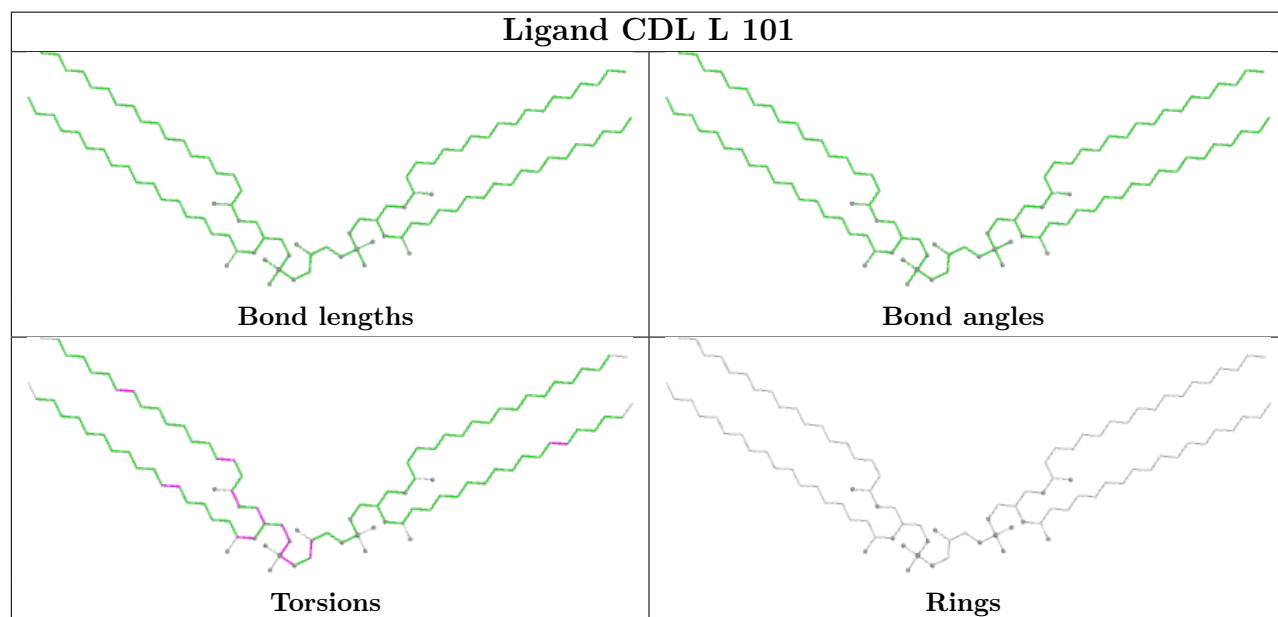
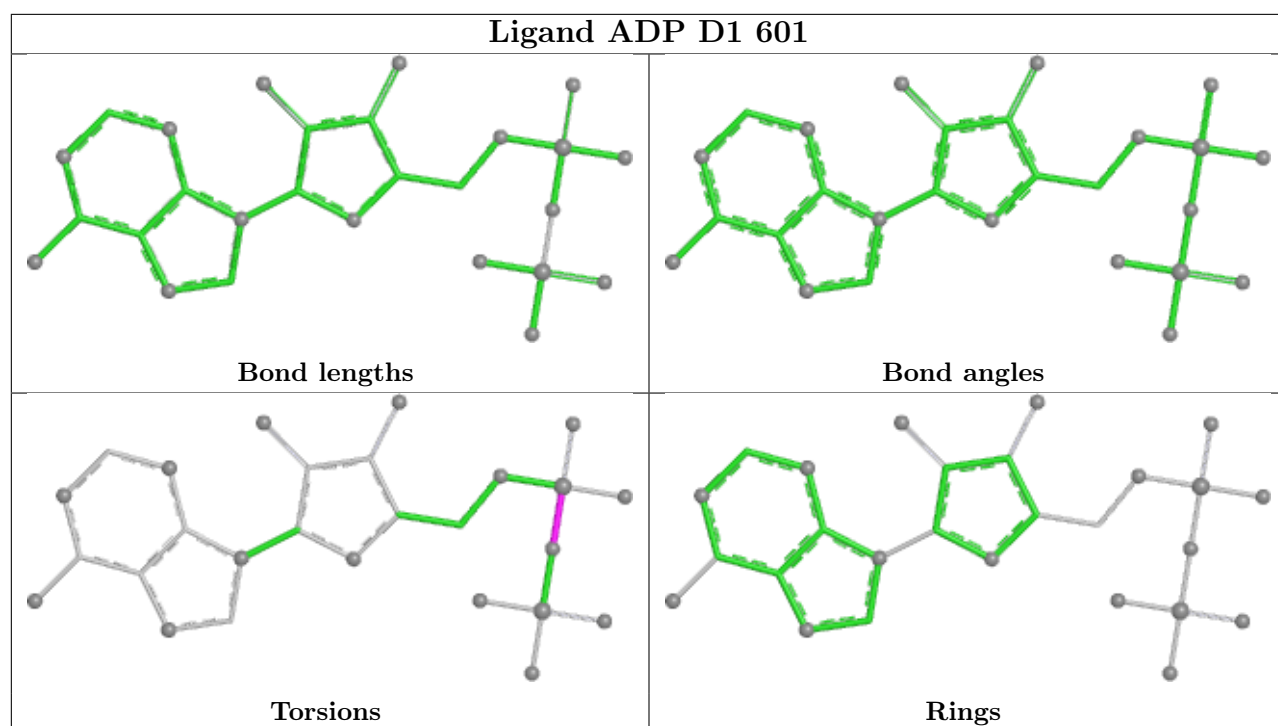


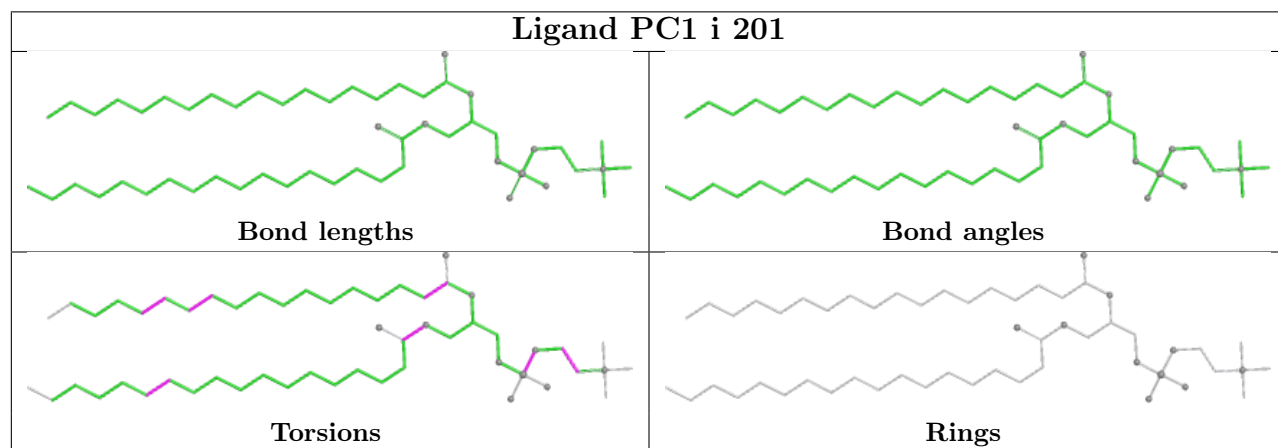
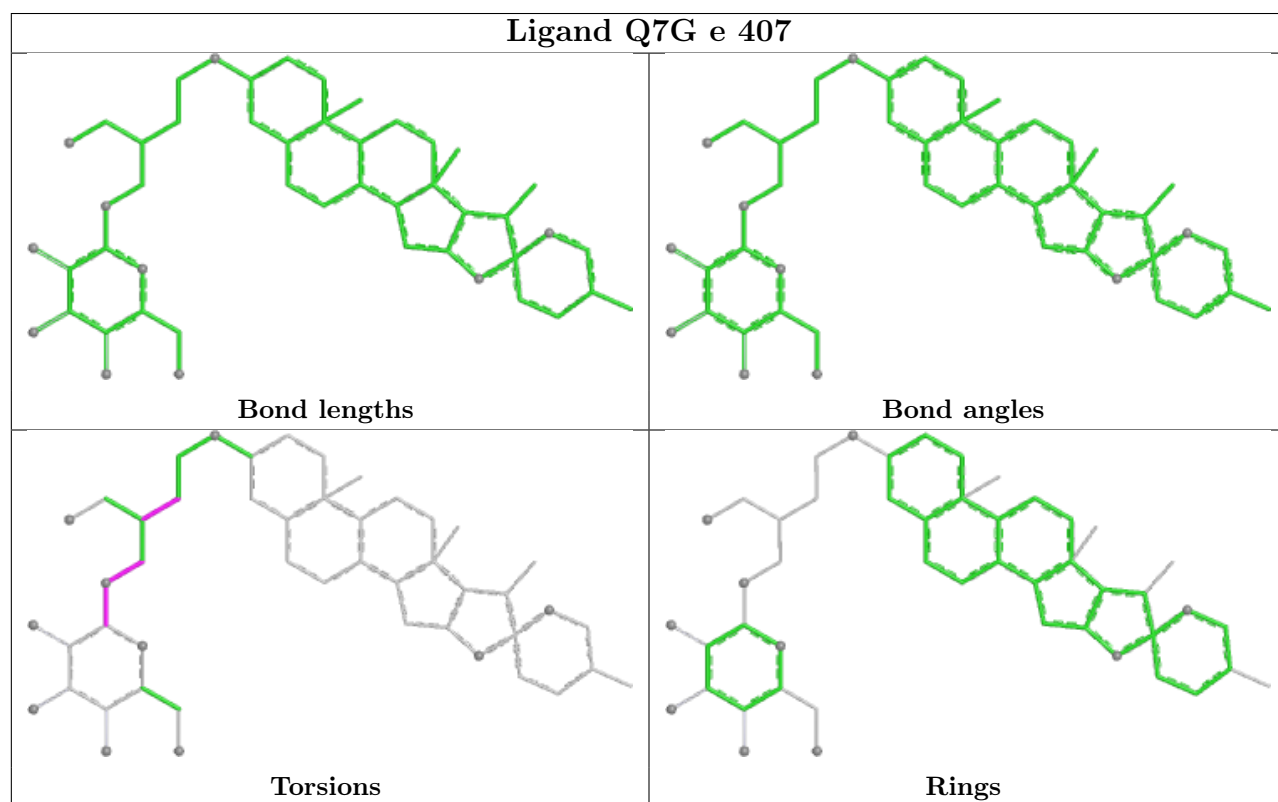
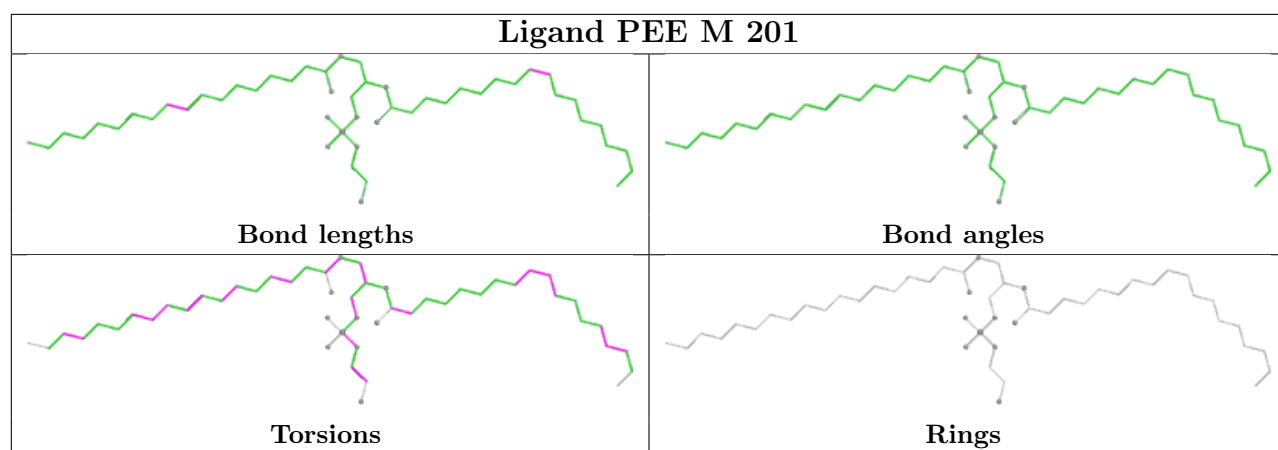


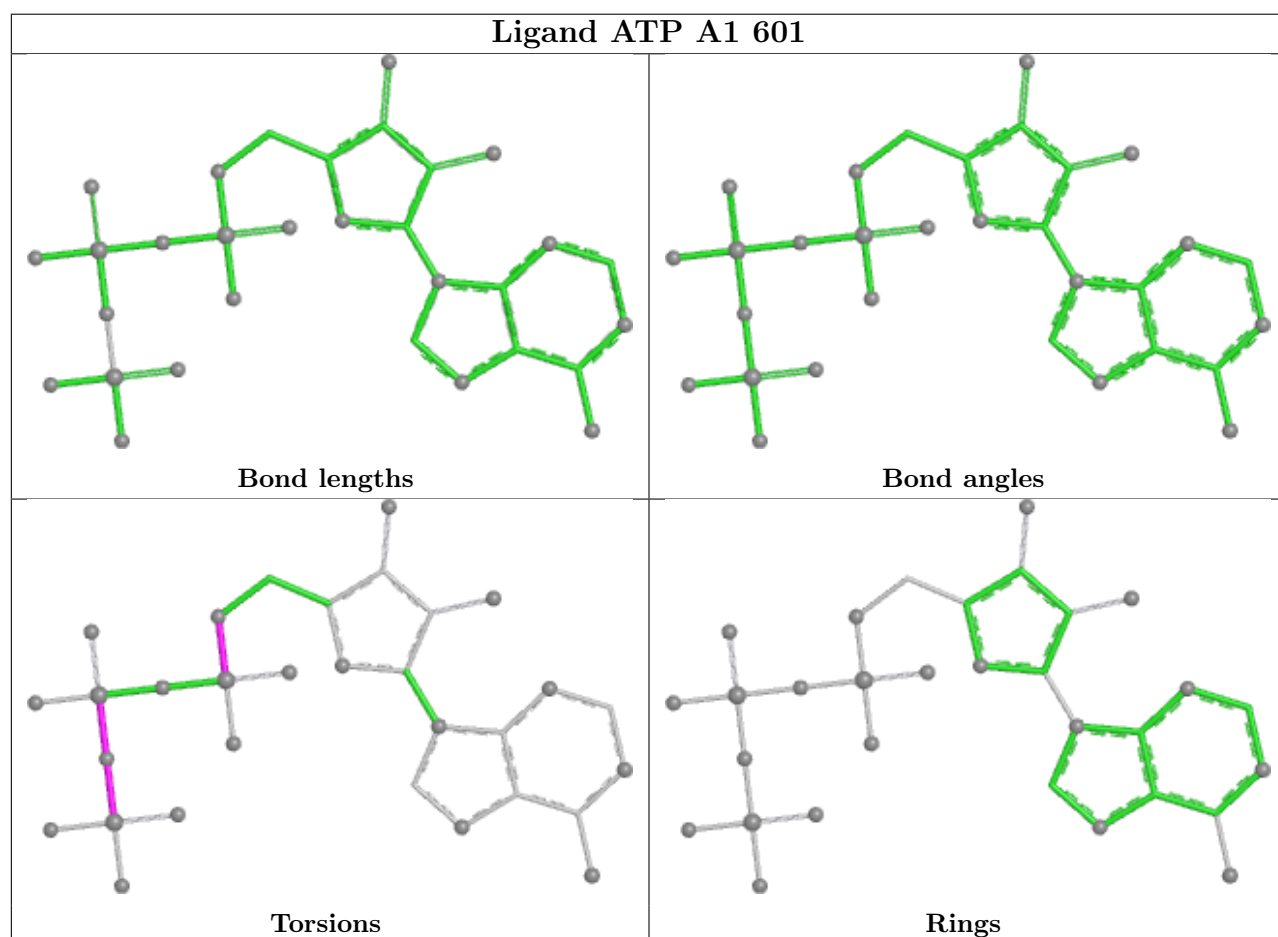
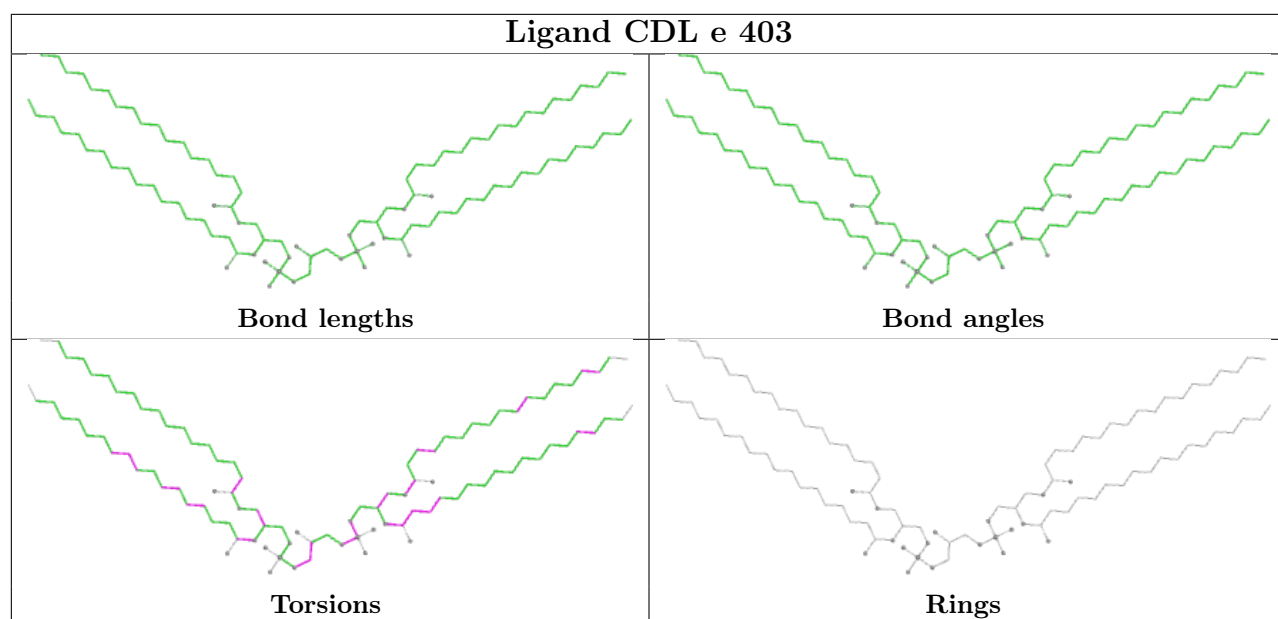


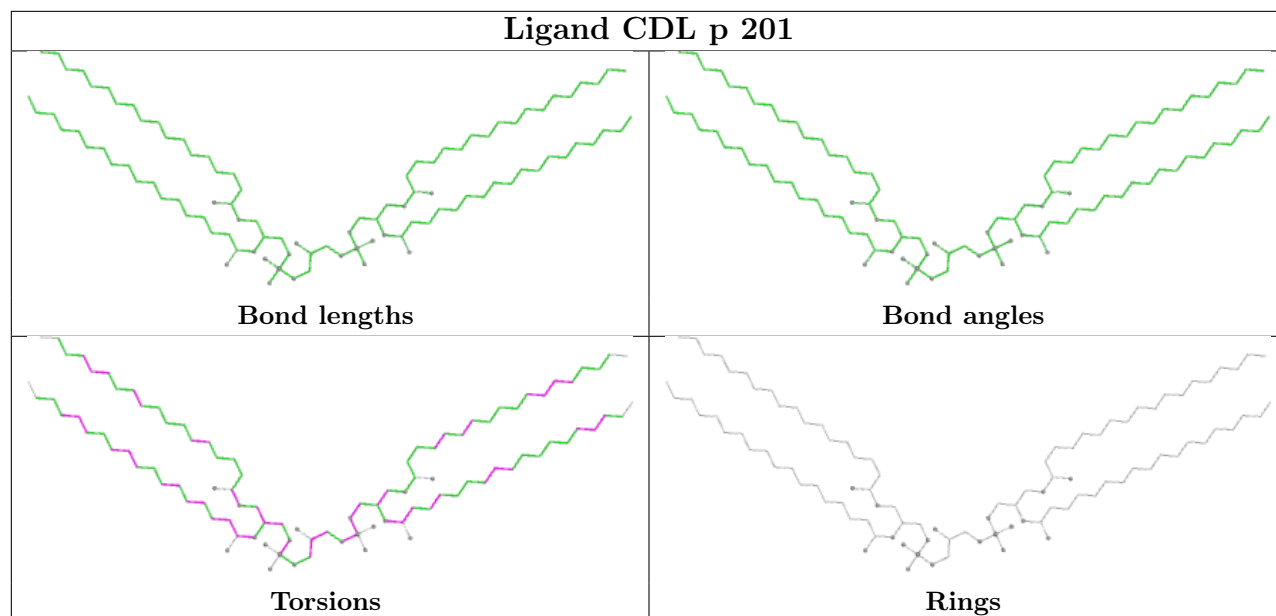












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

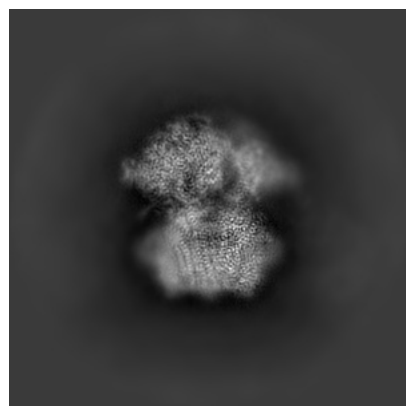
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15563. These allow visual inspection of the internal detail of the map and identification of artifacts.

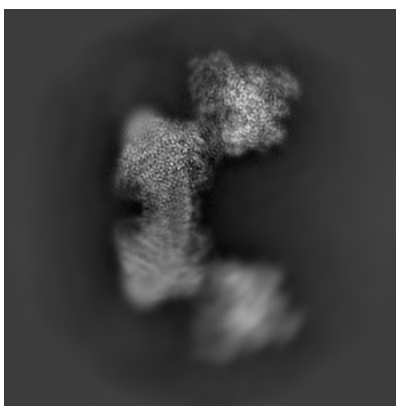
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

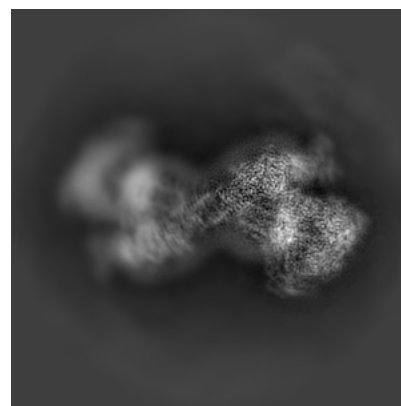
6.1.1 Primary map



X

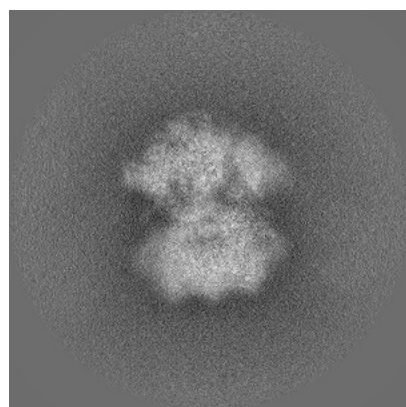


Y

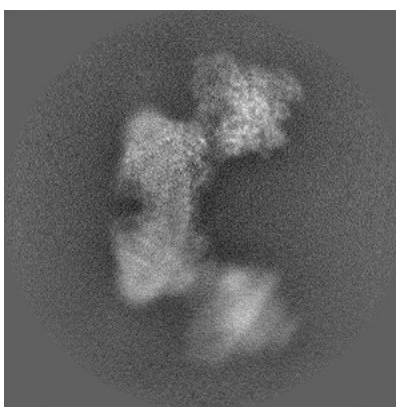


Z

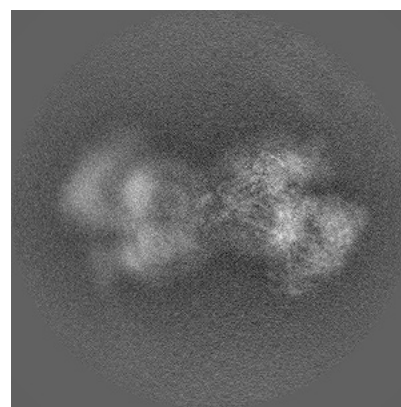
6.1.2 Raw map



X



Y

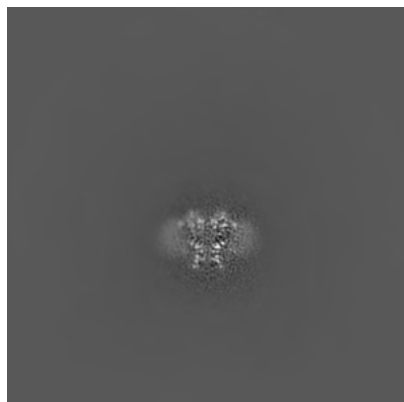


Z

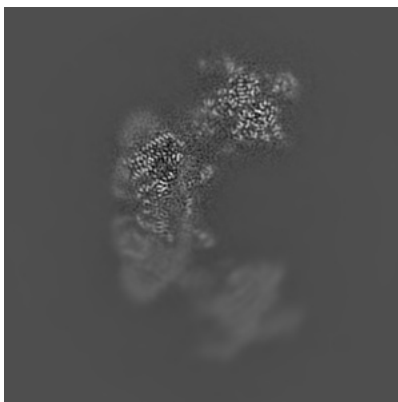
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

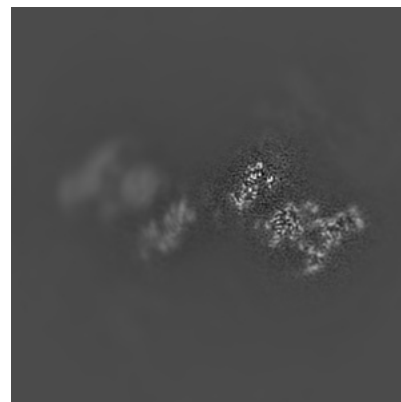
6.2.1 Primary map



X Index: 280

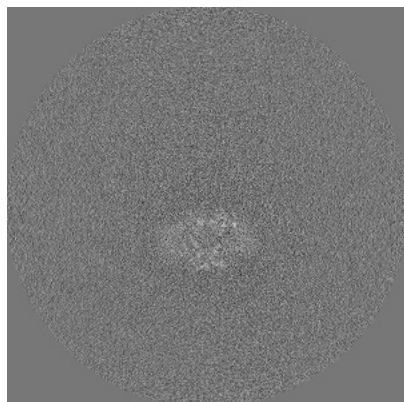


Y Index: 280

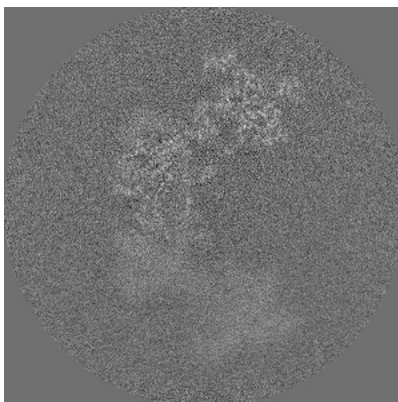


Z Index: 280

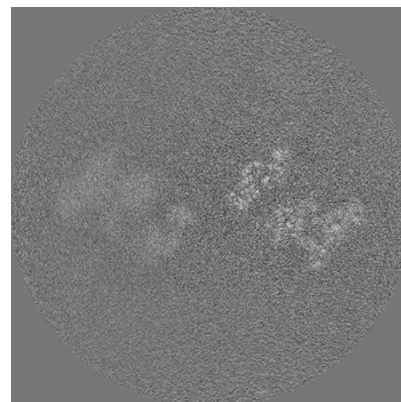
6.2.2 Raw map



X Index: 280



Y Index: 280

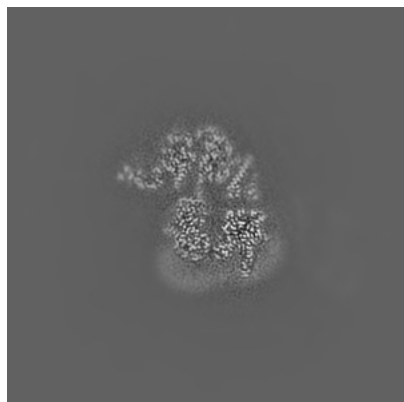


Z Index: 280

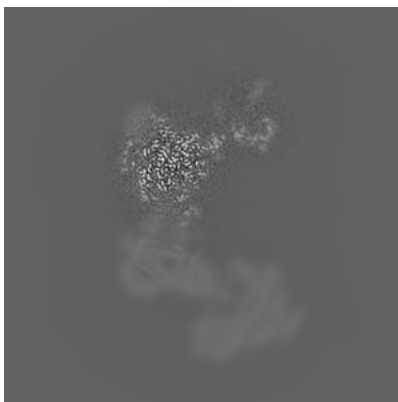
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

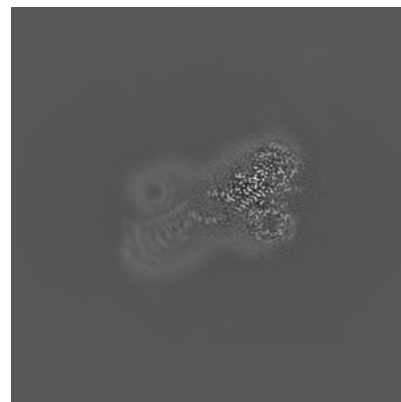
6.3.1 Primary map



X Index: 378

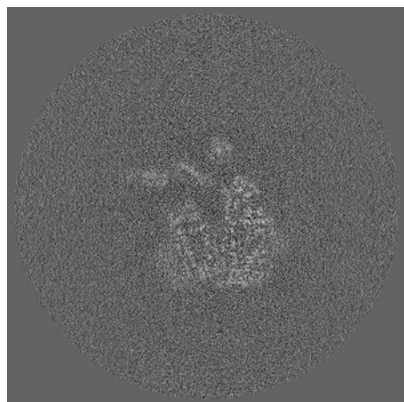


Y Index: 309

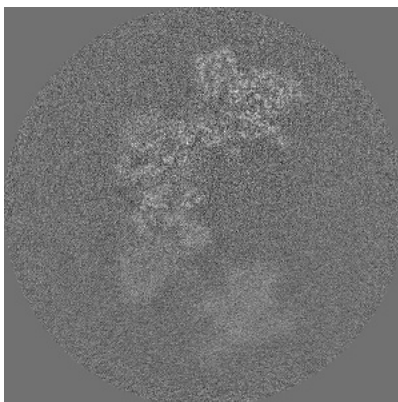


Z Index: 234

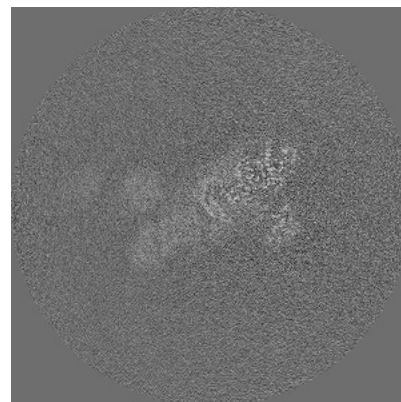
6.3.2 Raw map



X Index: 360



Y Index: 268

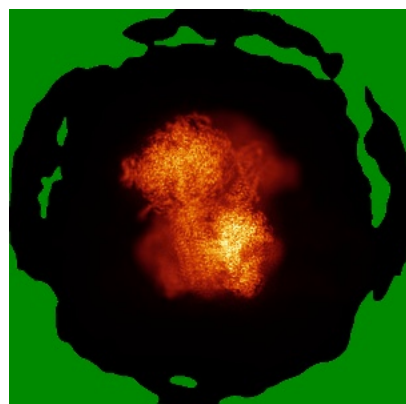


Z Index: 257

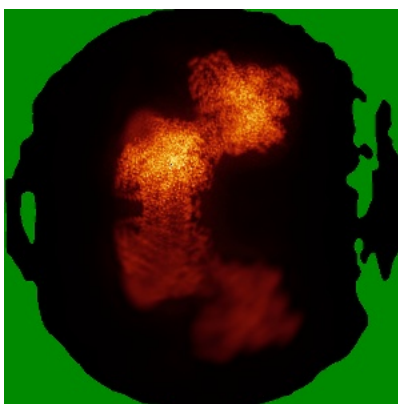
The images above show the largest variance slices of the map in three orthogonal directions.

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

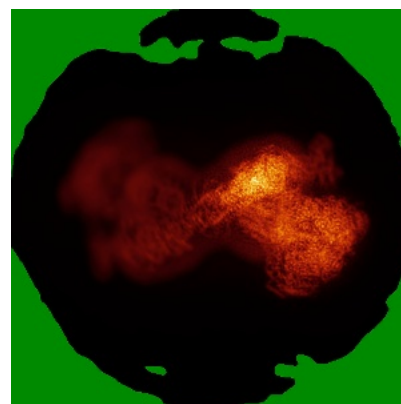
6.4.1 Primary map



X

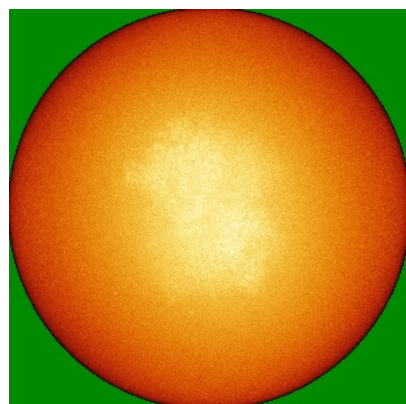


Y

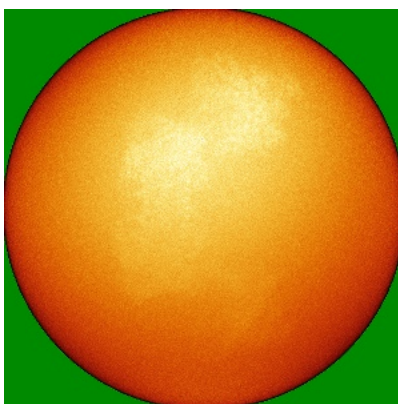


Z

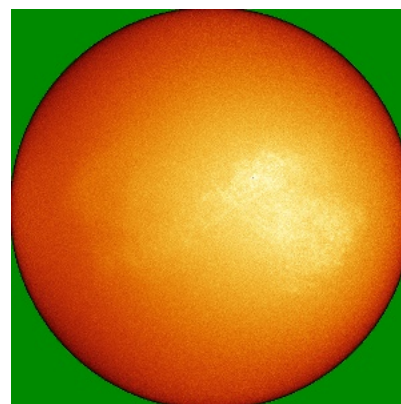
6.4.2 Raw map



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



X



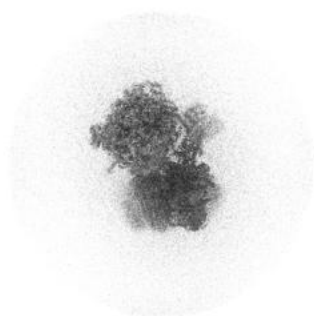
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

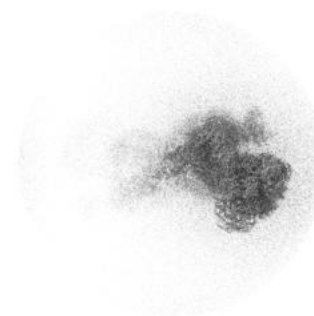
6.5.2 Raw map



X



Y



Z

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.

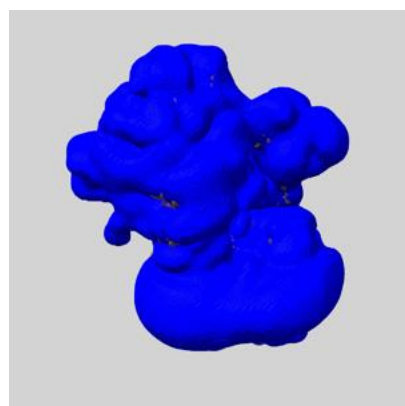
6.6 Mask visualisation [i](#)

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

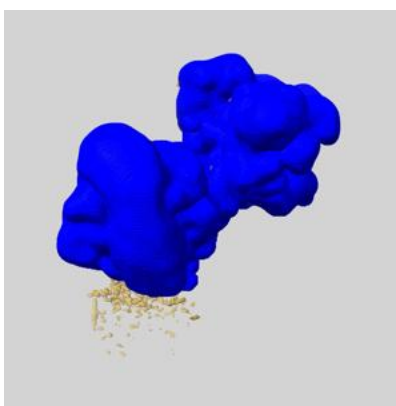
A mask typically either:

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

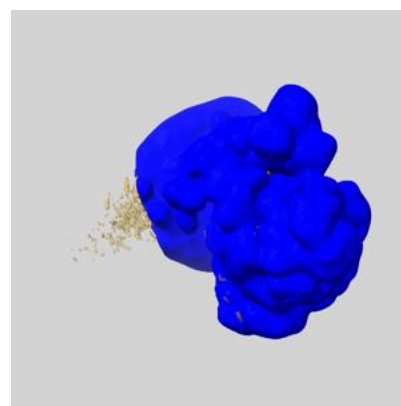
6.6.1 emd_15563_msk_1.map [i](#)



X



Y

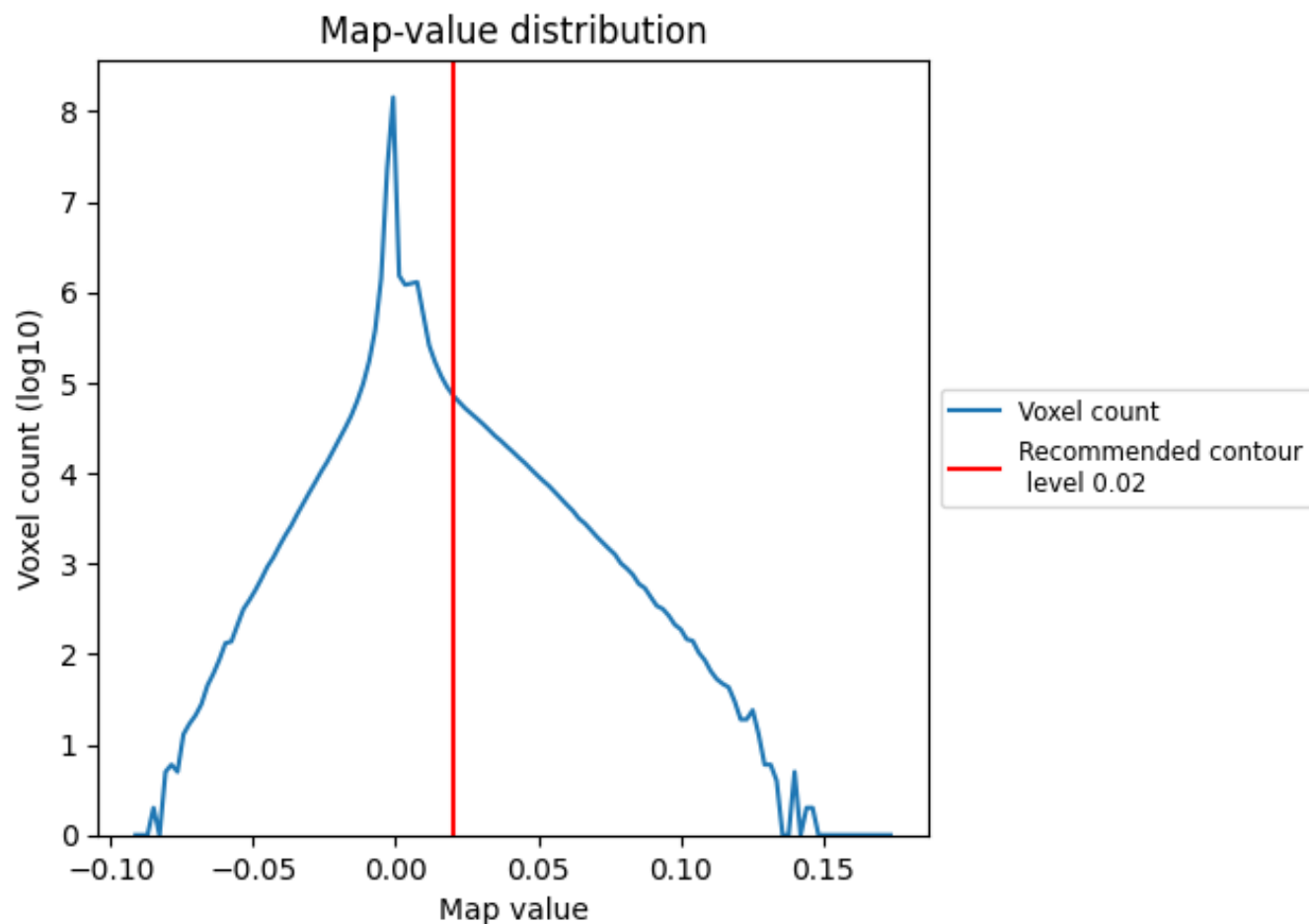


Z

7 Map analysis [i](#)

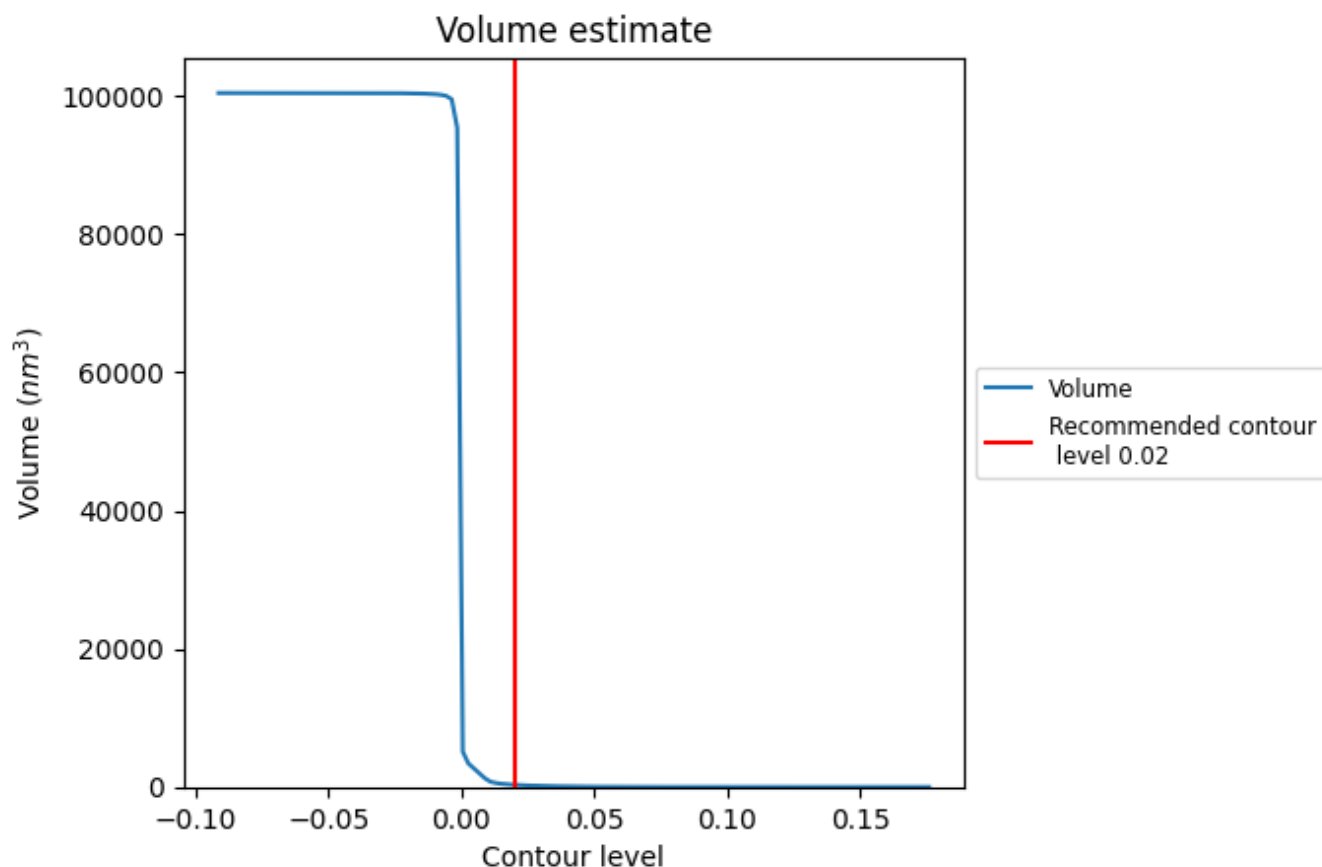
This section contains the results of statistical analysis of the map.

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.

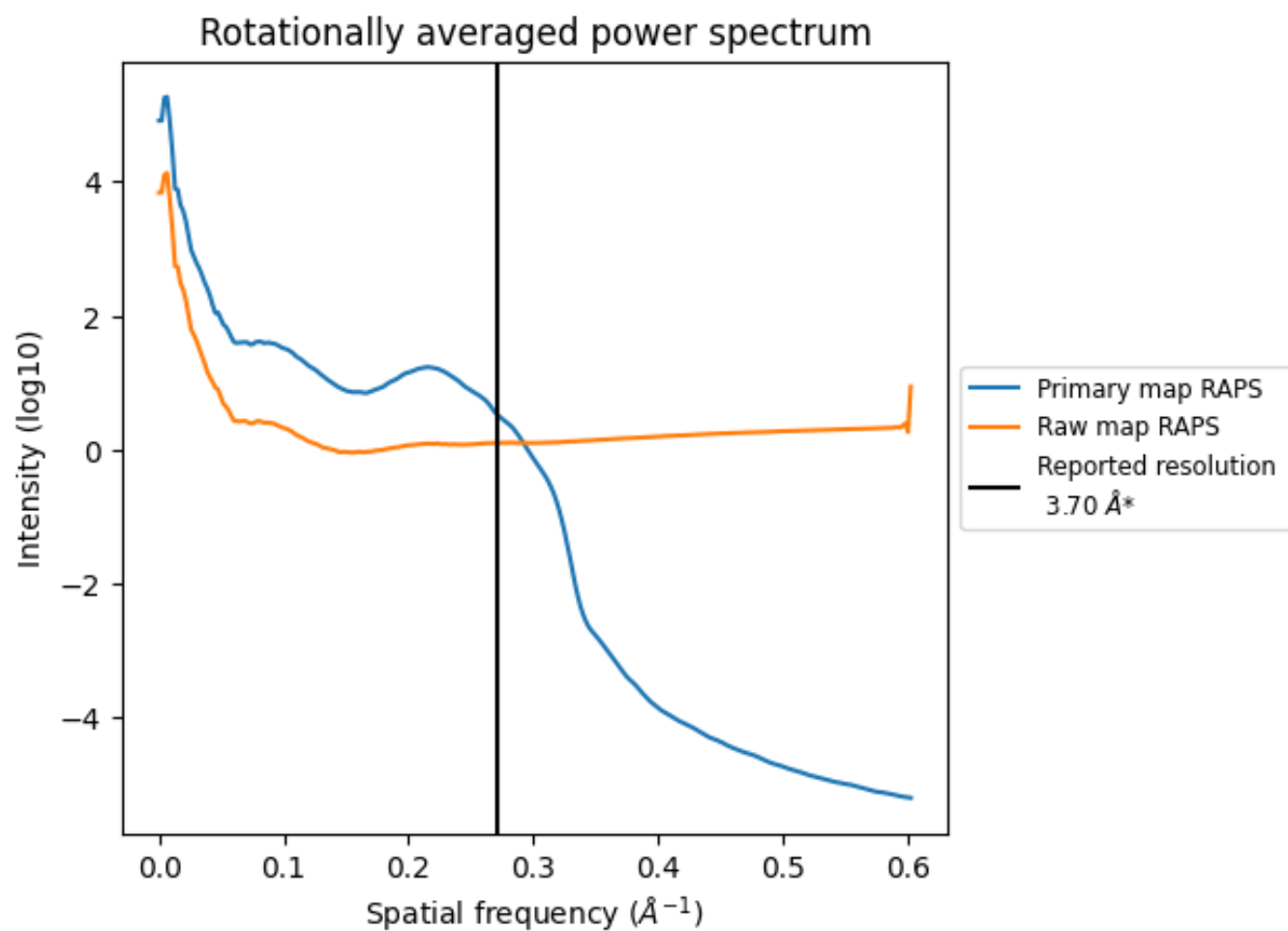
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 306 nm³; this corresponds to an approximate mass of 276 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

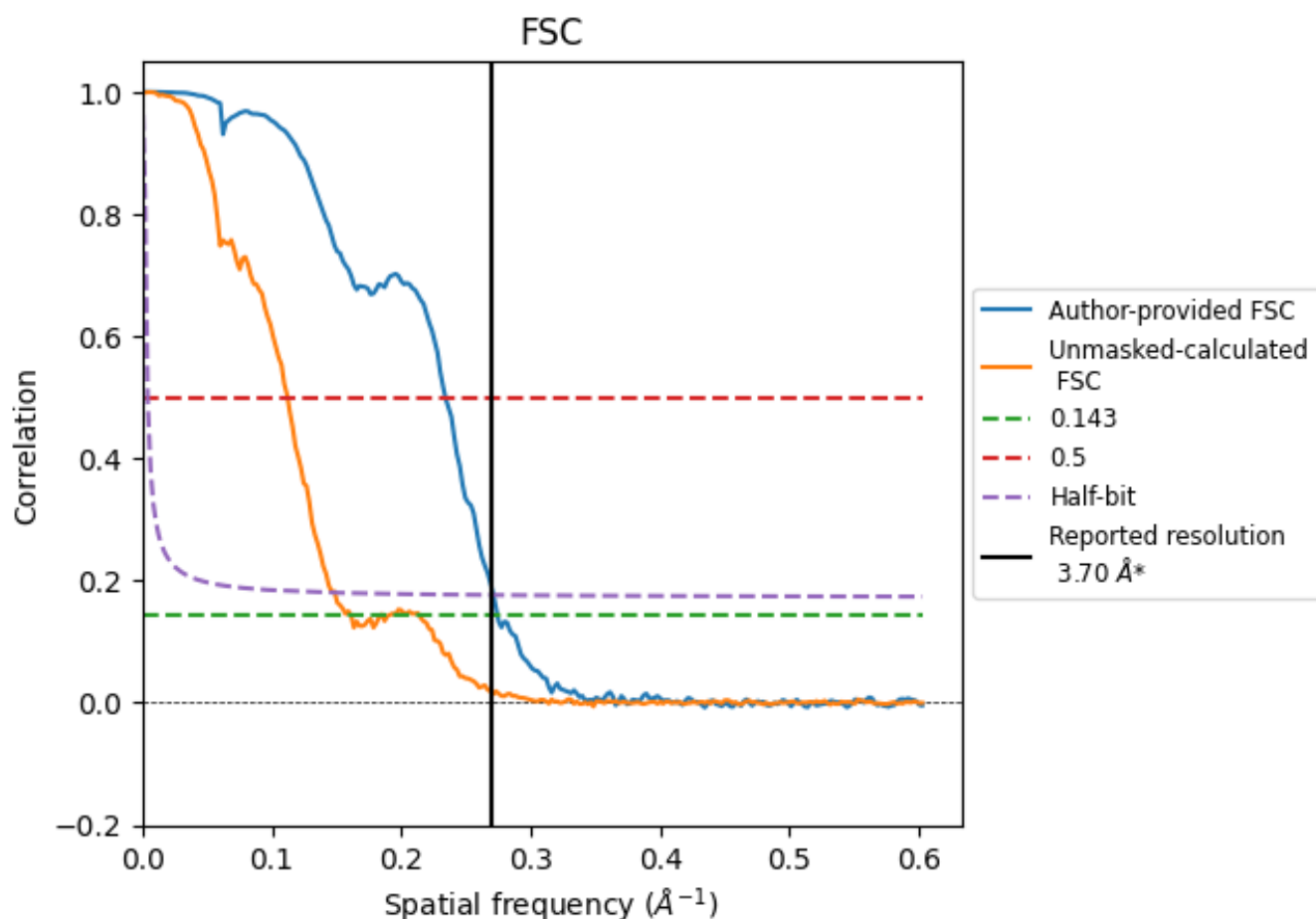


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

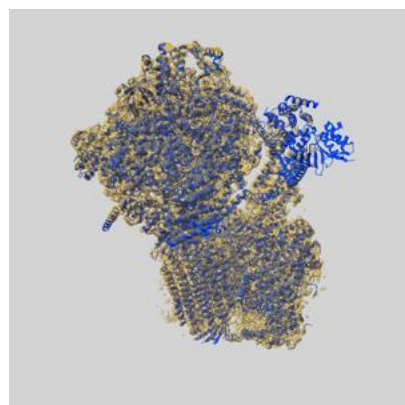
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.64	4.27	3.69
Unmasked-calculated*	6.20	8.91	6.72

*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 6.20 differs from the reported value 3.7 by more than 10 %

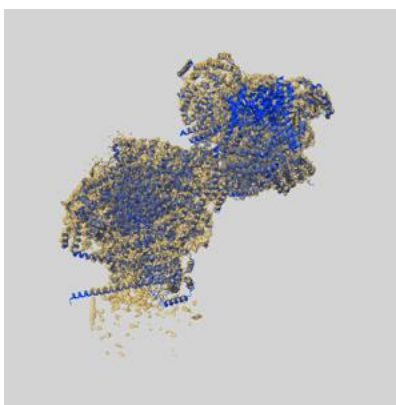
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15563 and PDB model 8APA. Per-residue inclusion information can be found in section 3 on page 16.

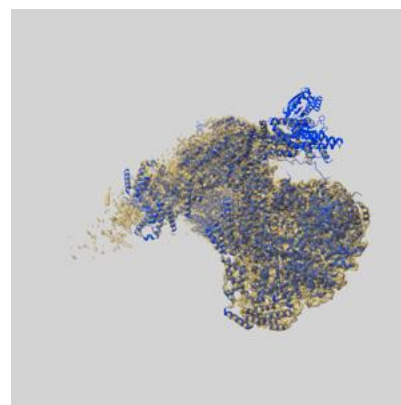
9.1 Map-model overlay [i](#)



X



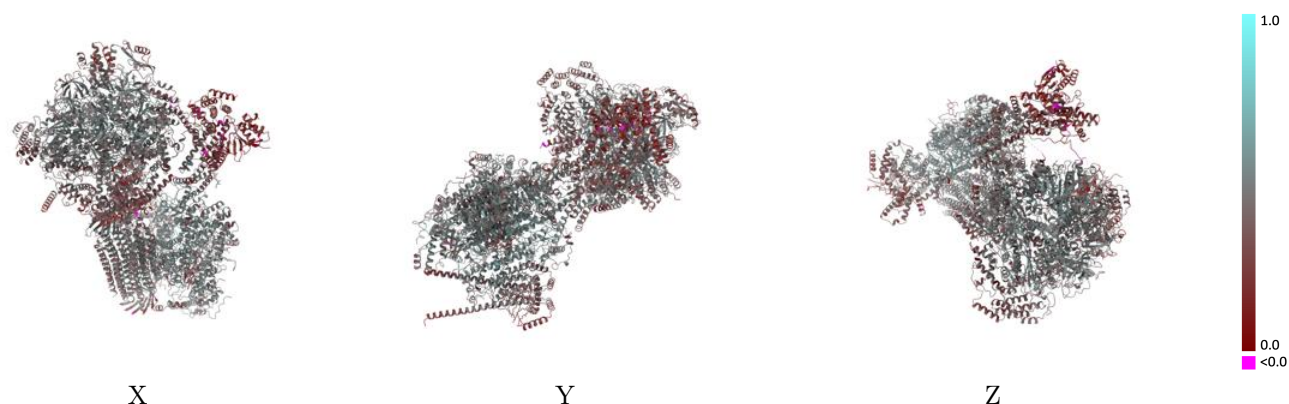
Y



Z

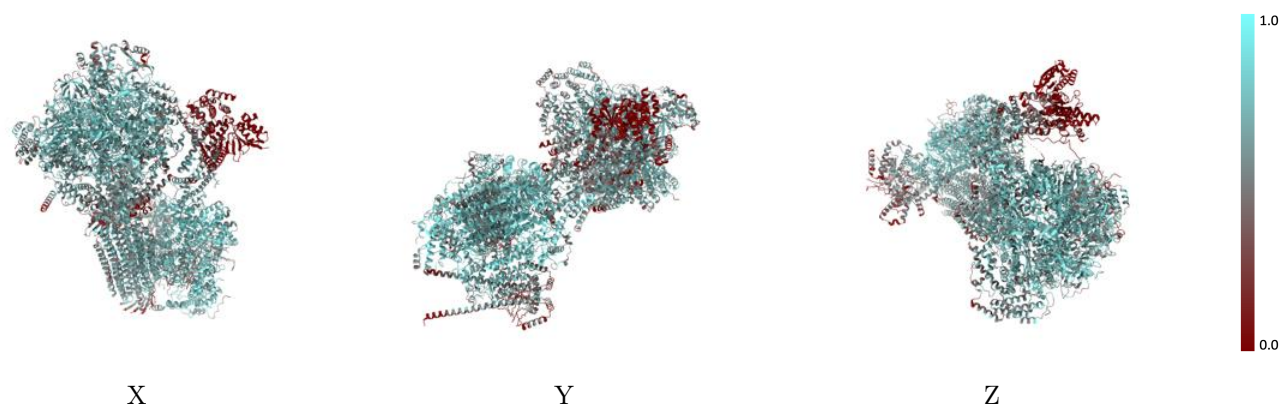
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



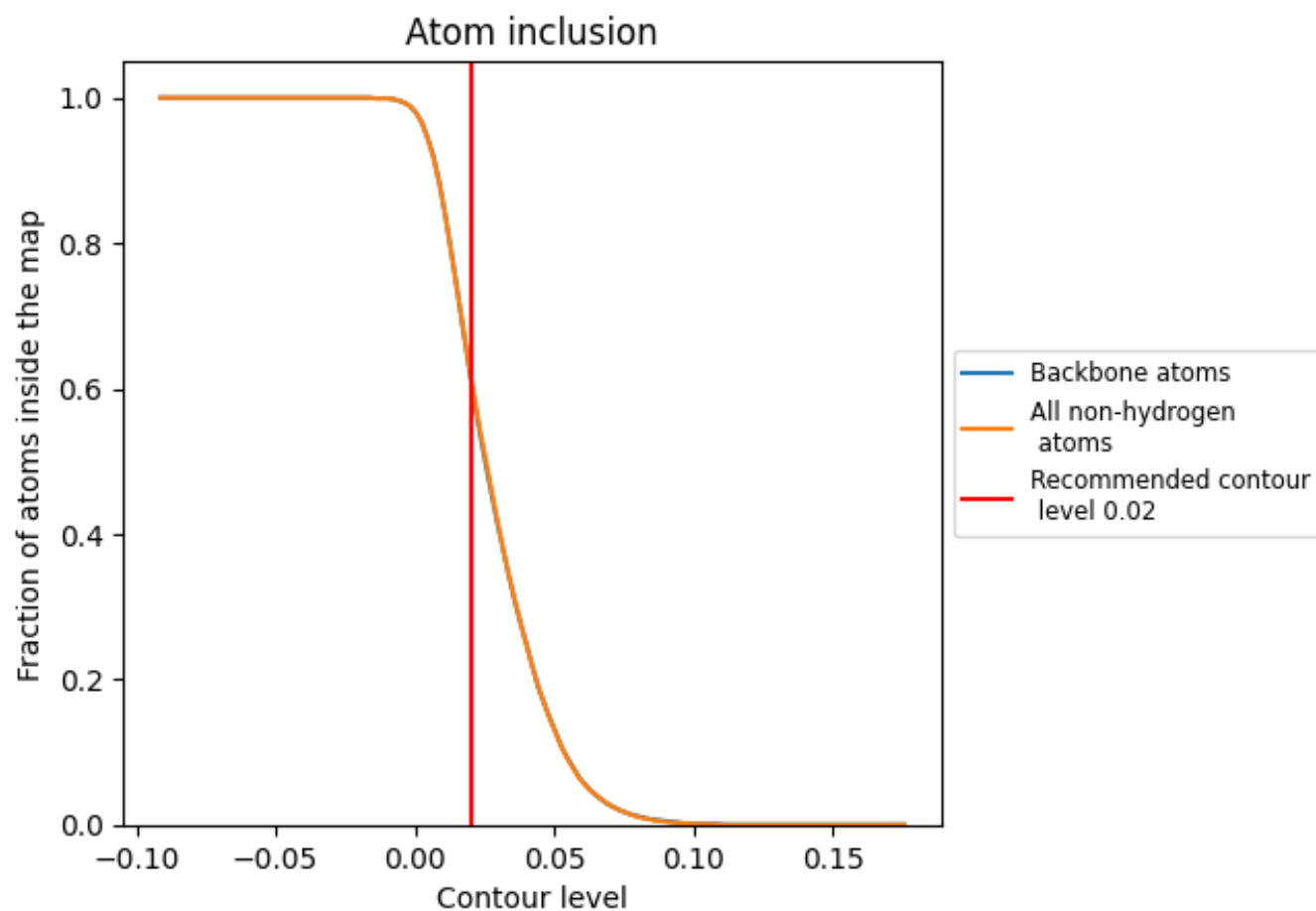
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 62% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6190	 0.4360
A1	 0.6780	 0.4550
B1	 0.6710	 0.4400
C1	 0.7140	 0.4830
D1	 0.6820	 0.4690
E1	 0.6500	 0.4440
F1	 0.6730	 0.4600
G1	 0.6450	 0.4370
H1	 0.5770	 0.4250
I1	 0.5660	 0.4330
J1	 0.5070	 0.3310
K1	 0.5840	 0.3860
L	 0.3630	 0.3340
L1	 0.5150	 0.3490
M	 0.3960	 0.3410
M1	 0.4990	 0.3470
O1	 0.6760	 0.4570
P1	 0.7150	 0.4730
Q1	 0.6990	 0.4740
R1	 0.6970	 0.4520
S1	 0.6220	 0.4450
T1	 0.6220	 0.4370
U1	 0.5940	 0.4240
V1	 0.5790	 0.4100
W1	 0.5940	 0.4240
X1	 0.6170	 0.4490
a	 0.8100	 0.5410
c	 0.7090	 0.5040
d	 0.5540	 0.4070
e	 0.7550	 0.4960
f	 0.7450	 0.4970
g	 0.0570	 0.2150
h	 0.1180	 0.1990
i	 0.8100	 0.5250
j	 0.7350	 0.4740



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.6870	 0.4730
l	 0.3800	 0.3520
m	 0.4390	 0.3500
n	 0.8200	 0.5400
o	 0.7300	 0.4620
p	 0.6480	 0.4500
q	 0.7390	 0.4960
r	 0.8090	 0.5260