



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 10:58 AM UTC

PDB ID : 6TMG / pdb_00006tmg
EMDB ID : EMD-10520
Title : Cryo-EM structure of Toxoplasma gondii mitochondrial ATP synthase dimer, membrane region model
Authors : Muhleip, A.; Kock Flygaard, R.; Amunts, A.
Deposited on : 2019-12-04
Resolution : 2.80 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:

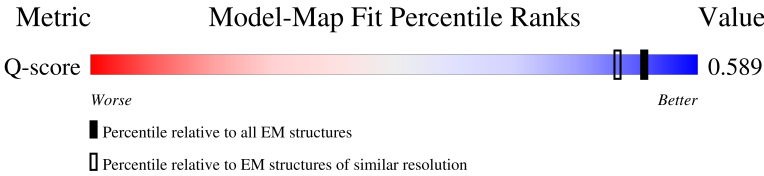
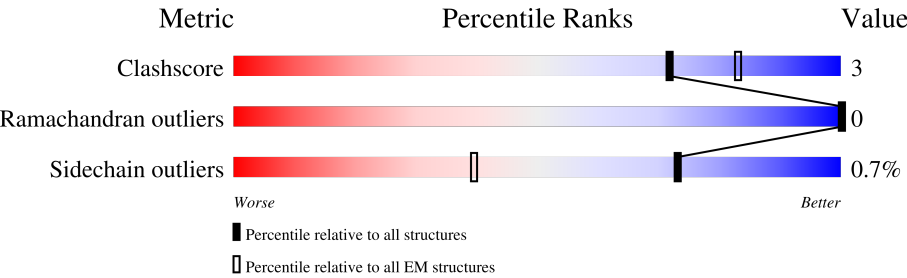
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 2.80 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.



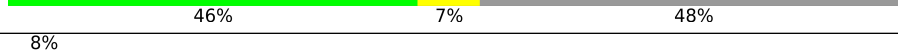
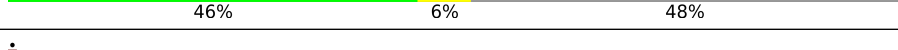
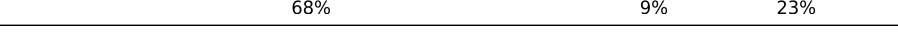
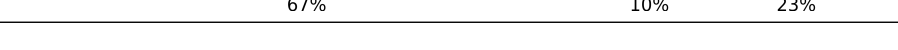
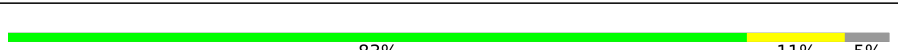
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	Q	134	7% 83% 16% ..
1	q	134	6% 85% 13% ..
2	I	236	35% 62%
2	i	236	34% 62%

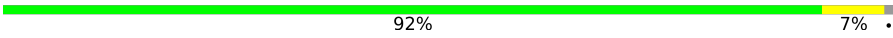
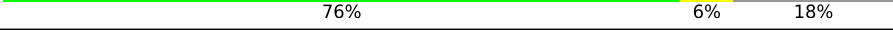
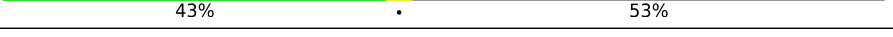
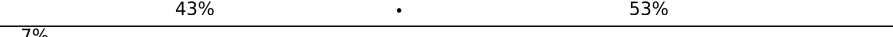
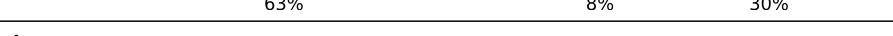
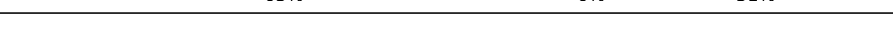
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Mol	Chain	Length	Quality of chain
3	T	133	
3	t	133	
4	G	252	
4	g	252	
5	O	157	
5	o	157	
6	K	224	
6	k	224	
7	J	229	
7	j	229	
8	S	128	
8	s	128	
9	U	126	
9	u	126	
10	H	239	
10	h	239	
11	E	325	
11	e	325	
12	X	83	
12	x	83	
13	B	571	
13	b	571	
14	R	134	
14	r	134	
15	P	138	

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Mol	Chain	Length	Quality of chain
15	p	138	
16	V	111	
16	v	111	
17	L	208	
17	l	208	
18	C	398	
18	c	398	
19	D	310	
19	d	310	
20	M	205	
20	m	205	
21	N	166	
21	n	166	
22	F	267	
22	f	267	
23	W	106	
23	w	106	
24	A	536	
24	a	536	

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 121066 atoms, of which 60518 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 ATPTG11.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	q	133	Total	C	H	N	O	S	0	0
			2119	674	1044	194	202	5		
1	Q	133	Total	C	H	N	O	S	0	0
			2119	674	1044	194	202	5		

- Molecule 2 is a protein called ATPTG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	i	90	Total	C	H	N	O	S	0	0
			1386	433	678	136	129	10		
2	I	90	Total	C	H	N	O	S	0	0
			1386	433	678	136	129	10		

- Molecule 3 is a protein called ATPTG14.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	t	92	Total	C	H	N	O	S	0	0
			1439	463	716	127	129	4		
3	T	92	Total	C	H	N	O	S	0	0
			1439	463	716	127	129	4		

- Molecule 4 is a protein called ATPTG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	g	112	Total	C	H	N	O	S	0	0
			1732	548	856	152	168	8		
4	G	112	Total	C	H	N	O	S	0	0
			1732	548	856	152	168	8		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	51	VAL	PHE	conflict	UNP S7WD71

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Chain	Residue	Modelled	Actual	Comment	Reference
g	73	CYS	SER	conflict	UNP S7WD71
g	110	LYS	GLU	conflict	UNP S7WD71
g	233	THR	MET	conflict	UNP S7WD71
G	51	VAL	PHE	conflict	UNP S7WD71
G	73	CYS	SER	conflict	UNP S7WD71
G	110	LYS	GLU	conflict	UNP S7WD71
G	233	THR	MET	conflict	UNP S7WD71

- Molecule 5 is a protein called subunit k.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	o	149	Total	C	H	N	O	S	0	0
			2415	786	1195	210	219	5		
5	O	149	Total	C	H	N	O	S	0	0
			2415	786	1195	210	219	5		

- Molecule 6 is a protein called subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	k	117	Total	C	H	N	O	S	0	0
			1904	645	952	145	155	7		
6	K	117	Total	C	H	N	O	S	0	0
			1904	645	952	145	155	7		

- Molecule 7 is a protein called subunit i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	j	176	Total	C	H	N	O	S	0	0
			2981	1003	1469	261	244	4		
7	J	176	Total	C	H	N	O	S	0	0
			2981	1003	1469	261	244	4		

- Molecule 8 is a protein called ATPTG13.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	s	95	Total	C	H	N	O	S	0	0
			1570	526	770	130	142	2		
8	S	95	Total	C	H	N	O	S	0	0
			1570	526	770	130	142	2		

- Molecule 9 is a protein called ATPTG15.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	u	94	Total	C	H	N	O	S	0	0
			1492	482	741	132	133	4		
9	U	94	Total	C	H	N	O	S	0	0
			1492	482	741	132	133	4		

- Molecule 10 is a protein called ATPTG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	h	226	Total	C	H	N	O	S	0	0
			3589	1157	1741	334	348	9		
10	H	226	Total	C	H	N	O	S	0	0
			3589	1157	1741	334	348	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	89	ASN	HIS	conflict	UNP A0A125YLR0
H	89	ASN	HIS	conflict	UNP A0A125YLR0

- Molecule 11 is a protein called ATPTG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	e	140	Total	C	H	N	O	S	0	0
			2179	719	1064	187	204	5		
11	E	140	Total	C	H	N	O	S	0	0
			2179	719	1064	187	204	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	?	-	LYS	deletion	UNP A0A125YLR0
e	63	PRO	SER	conflict	UNP A0A125YLR0
e	99	LEU	PRO	conflict	UNP A0A125YLR0
e	312	ALA	THR	conflict	UNP A0A125YLR0
E	?	-	LYS	deletion	UNP A0A125YLR0
E	63	PRO	SER	conflict	UNP A0A125YLR0
E	99	LEU	PRO	conflict	UNP A0A125YLR0
E	312	ALA	THR	conflict	UNP A0A125YLR0

- Molecule 12 is a protein called ATPTG17.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	x	82	Total	C	H	N	O	S	0	0
			1298	420	639	116	120	3		
12	X	82	Total	C	H	N	O	S	0	0
			1298	420	639	116	120	3		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	77	TRP	-	expression tag	UNP S7W180
x	78	MET	-	expression tag	UNP S7W180
x	79	PHE	-	expression tag	UNP S7W180
x	80	GLY	-	expression tag	UNP S7W180
x	81	ASN	-	expression tag	UNP S7W180
x	82	SER	-	expression tag	UNP S7W180
x	83	TYR	-	expression tag	UNP S7W180
X	77	TRP	-	expression tag	UNP S7W180
X	78	MET	-	expression tag	UNP S7W180
X	79	PHE	-	expression tag	UNP S7W180
X	80	GLY	-	expression tag	UNP S7W180
X	81	ASN	-	expression tag	UNP S7W180
X	82	SER	-	expression tag	UNP S7W180
X	83	TYR	-	expression tag	UNP S7W180

- Molecule 13 is a protein called subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	b	253	Total	C	H	N	O	S	0	0
			4157	1374	2056	328	390	9		
13	B	253	Total	C	H	N	O	S	0	0
			4157	1374	2056	328	390	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	50	LEU	SER	conflict	UNP S7V2T0
b	474	THR	ALA	conflict	UNP S7V2T0
B	50	LEU	SER	conflict	UNP S7V2T0
B	474	THR	ALA	conflict	UNP S7V2T0

- Molecule 14 is a protein called ATPTG12.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	r	90	Total	C	H	N	O	S	0	0
			1485	470	750	128	133	4		
14	R	90	Total	C	H	N	O	S	0	0
			1485	470	750	128	133	4		

- Molecule 15 is a protein called ATPTG10.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	p	108	Total	C	H	N	O	S	0	0
			1711	553	847	148	157	6		
15	P	108	Total	C	H	N	O	S	0	0
			1711	553	847	148	157	6		

- Molecule 16 is a protein called subunit f.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	v	110	Total	C	H	N	O	S	0	0
			1801	590	888	170	148	5		
16	V	110	Total	C	H	N	O	S	0	0
			1801	590	888	170	148	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	54	ALA	VAL	conflict	UNP S7UQT7
V	54	ALA	VAL	conflict	UNP S7UQT7

- Molecule 17 is a protein called ATPTG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	l	207	Total	C	H	N	O	S	0	0
			3273	1013	1647	298	305	10		
17	L	207	Total	C	H	N	O	S	0	0
			3273	1013	1647	298	305	10		

- Molecule 18 is a protein called ATPTG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	c	122	Total	C	H	N	O	S	0	0
			2029	656	999	189	184	1		
18	C	122	Total	C	H	N	O	S	0	0
			2029	656	999	189	184	1		

- Molecule 19 is a protein called ATPTG2.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	d	254	Total	C	H	N	O	S	0	0
			4046	1323	1970	365	380	8		
19	D	254	Total	C	H	N	O	S	0	0
			4046	1323	1970	365	380	8		

- Molecule 20 is a protein called subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	m	96	Total	C	H	N	O	S	0	0
			1509	501	744	126	131	7		
20	M	96	Total	C	H	N	O	S	0	0
			1509	501	744	126	131	7		

- Molecule 21 is a protein called ATPTG9.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	n	160	Total	C	H	N	O	S	0	0
			2451	774	1204	227	235	11		
21	N	160	Total	C	H	N	O	S	0	0
			2451	774	1204	227	235	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	140	SER	ALA	conflict	UNP A0A125YUZ2
N	140	SER	ALA	conflict	UNP A0A125YUZ2

- Molecule 22 is a protein called ATPTG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	f	188	Total	C	H	N	O	S	0	0
			2867	919	1425	245	274	4		
22	F	188	Total	C	H	N	O	S	0	0
			2867	919	1425	245	274	4		

- Molecule 23 is a protein called ATPTG16.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	w	96	Total	C	H	N	O	S	0	0
			1509	494	755	127	129	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	96	Total	C	H	N	O	S	0	0
			1509	494	755	127	129	4		

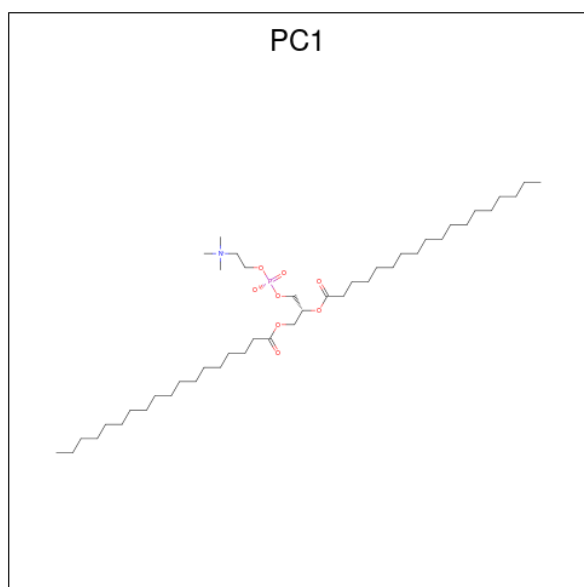
- Molecule 24 is a protein called subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	a	371	Total	C	H	N	O	S	0	0
			5895	1923	2873	523	558	18		
24	A	371	Total	C	H	N	O	S	0	0
			5895	1923	2873	523	558	18		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	351	THR	ALA	conflict	UNP S7V493
A	351	THR	ALA	conflict	UNP S7V493

- Molecule 25 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P) (labeled as "Ligand of Interest" by depositor).



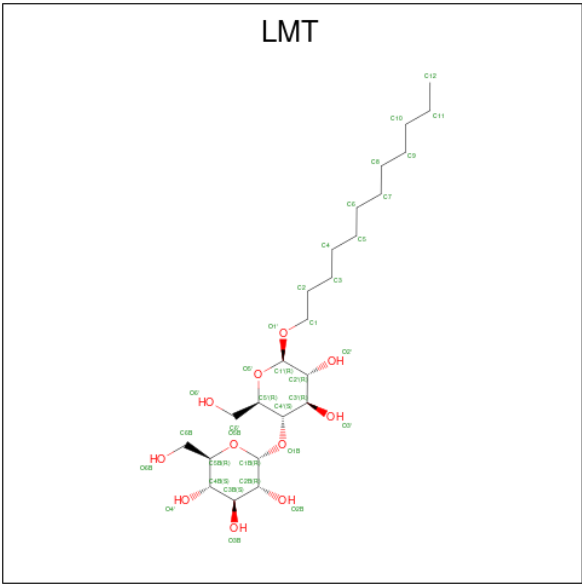
Mol	Chain	Residues	Atoms						AltConf
25	o	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
25	o	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
25	v	1	Total	C	H	N	O	P
			142	44	88	1	8	1
25	O	1	Total	C	H	N	O	P
			142	44	88	1	8	1
25	O	1	Total	C	H	N	O	P
			142	44	88	1	8	1
25	V	1	Total	C	H	N	O	P
			142	44	88	1	8	1

- Molecule 26 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



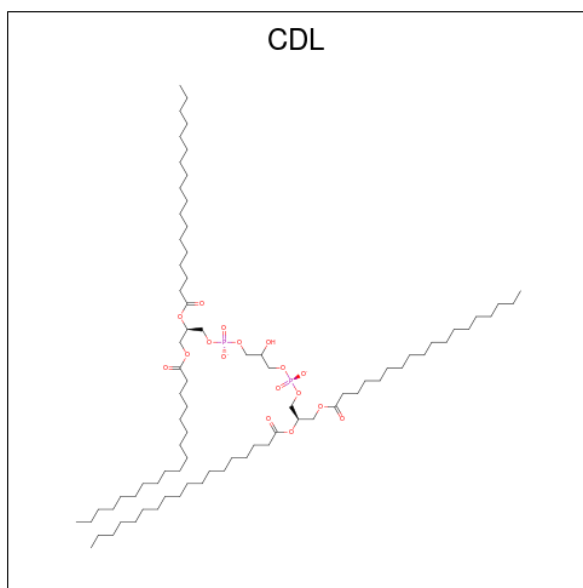
Mol	Chain	Residues	Atoms				AltConf
26	o	1	Total	C	H	O	0
			81	24	46	11	
26	h	1	Total	C	H	O	0
			81	24	46	11	
26	x	1	Total	C	H	O	0
			81	24	46	11	
26	c	1	Total	C	H	O	0
			81	24	46	11	
26	c	1	Total	C	H	O	0
			81	24	46	11	
26	d	1	Total	C	H	O	0
			81	24	46	11	
26	d	1	Total	C	H	O	0
			81	24	46	11	

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Mol	Chain	Residues	Atoms				AltConf
26	O	1	Total	C	H	O	0
			81	24	46	11	
26	H	1	Total	C	H	O	0
			81	24	46	11	
26	X	1	Total	C	H	O	0
			81	24	46	11	
26	C	1	Total	C	H	O	0
			81	24	46	11	
26	C	1	Total	C	H	O	0
			81	24	46	11	
26	D	1	Total	C	H	O	0
			81	24	46	11	
26	D	1	Total	C	H	O	0
			81	24	46	11	

- Molecule 27 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



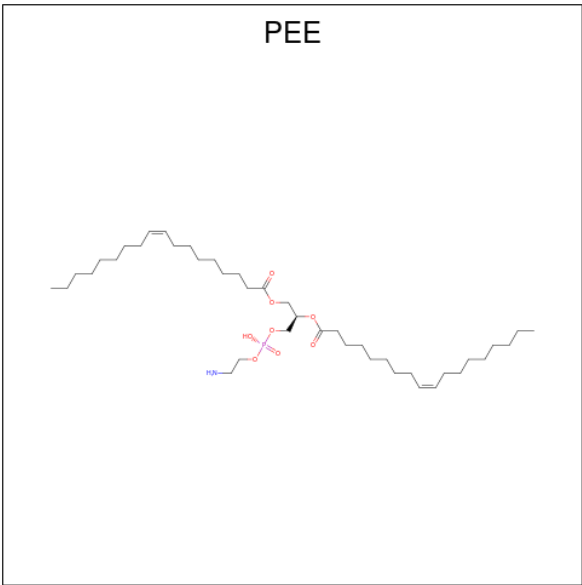
Mol	Chain	Residues	Atoms					AltConf
27	o	1	Total	C	H	O	P	0
			256	81	156	17	2	
27	u	1	Total	C	H	O	P	0
			256	81	156	17	2	
27	h	1	Total	C	H	O	P	0
			256	81	156	17	2	
27	e	1	Total	C	H	O	P	0
			256	81	156	17	2	

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Mol	Chain	Residues	Atoms					AltConf
27	b	1	Total 256	C 81	H 156	O 17	P 2	0
27	v	1	Total 256	C 81	H 156	O 17	P 2	0
27	c	1	Total 256	C 81	H 156	O 17	P 2	0
27	d	1	Total 256	C 81	H 156	O 17	P 2	0
27	O	1	Total 256	C 81	H 156	O 17	P 2	0
27	U	1	Total 256	C 81	H 156	O 17	P 2	0
27	H	1	Total 256	C 81	H 156	O 17	P 2	0
27	E	1	Total 256	C 81	H 156	O 17	P 2	0
27	B	1	Total 256	C 81	H 156	O 17	P 2	0
27	B	1	Total 256	C 81	H 156	O 17	P 2	0
27	V	1	Total 256	C 81	H 156	O 17	P 2	0
27	V	1	Total 256	C 81	H 156	O 17	P 2	0
27	C	1	Total 256	C 81	H 156	O 17	P 2	0
27	D	1	Total 256	C 81	H 156	O 17	P 2	0

- Molecule 28 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).

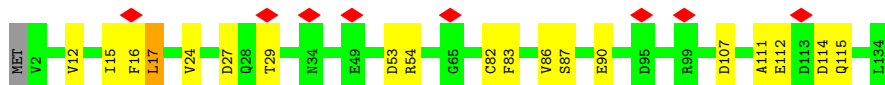
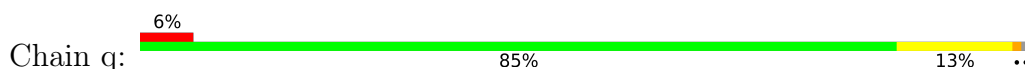


Mol	Chain	Residues	Atoms						AltConf
28	j	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	j	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	c	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	J	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	J	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	C	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

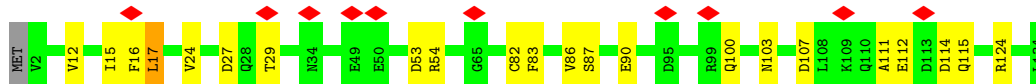
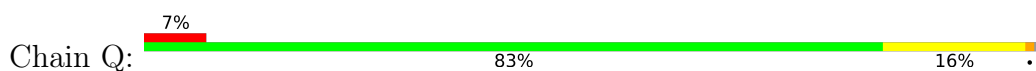
3 Residue-property plots [i](#)

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

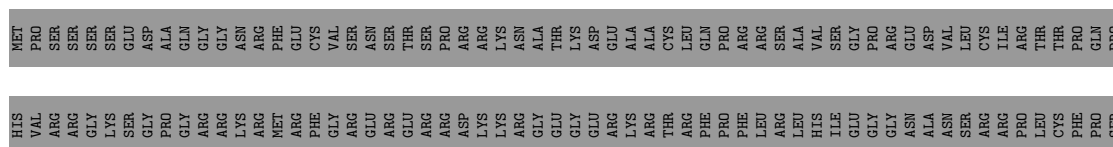
- Molecule 1: ATPTG11



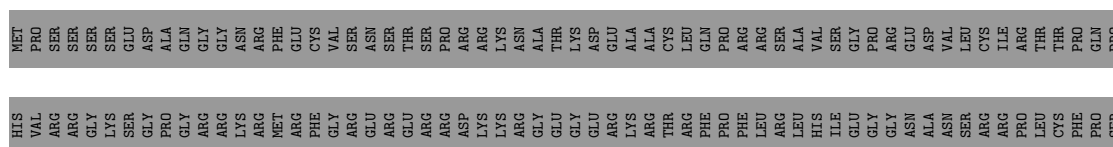
- Molecule 1: ATPTG11

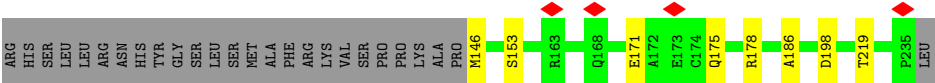


- Molecule 2: ATPTG7



- Molecule 2: ATPTG7





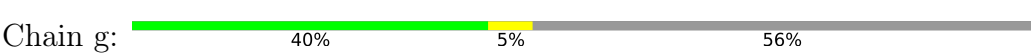
• Molecule 3: ATPTG14



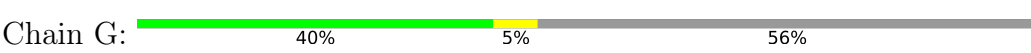
• Molecule 3: ATPTG14



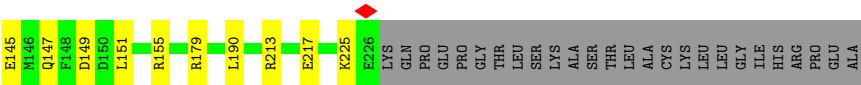
• Molecule 4: ATPTG5



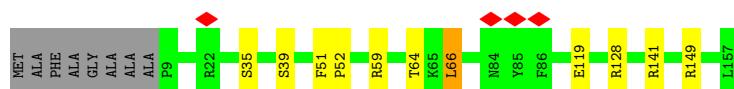
• Molecule 4: ATPTG5



• Molecule 5: subunit k



Chain o:  88% 6% • 5%

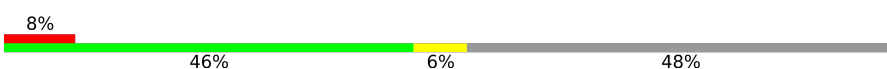


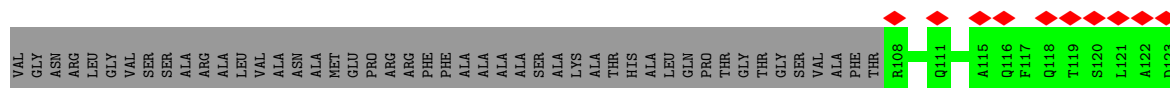
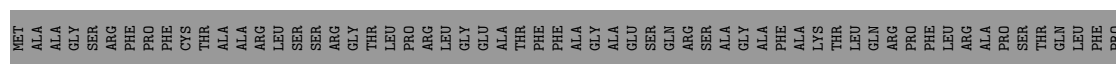
• Molecule 5: subunit k

Chain O:  85% 9% • 5%

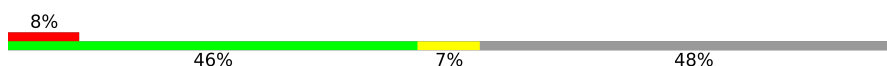


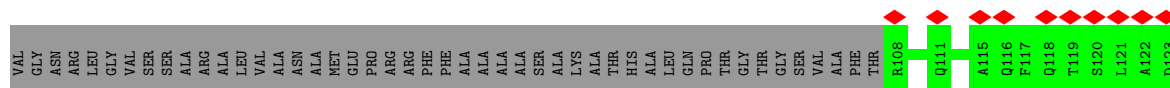
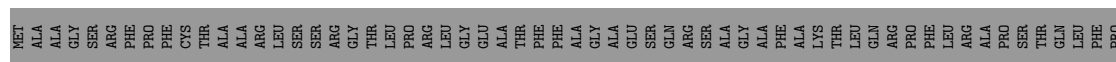
• Molecule 6: subunit a

Chain k:  8% 46% 6% 48%



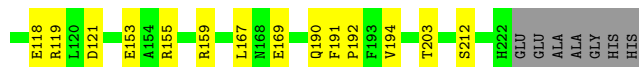
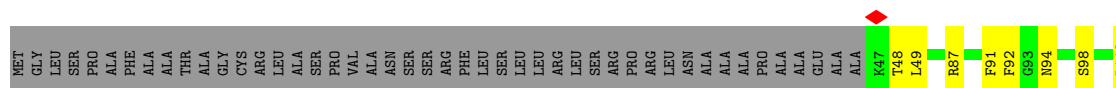
• Molecule 6: subunit a

Chain K:  8% 46% 7% 48%

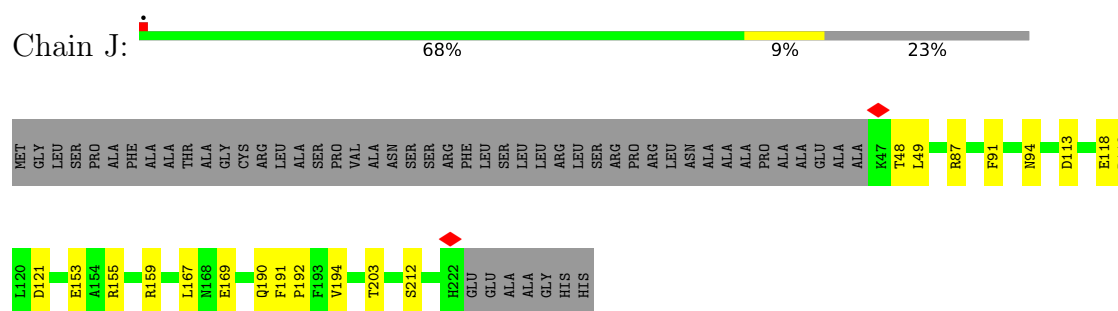


• Molecule 7: subunit i/j

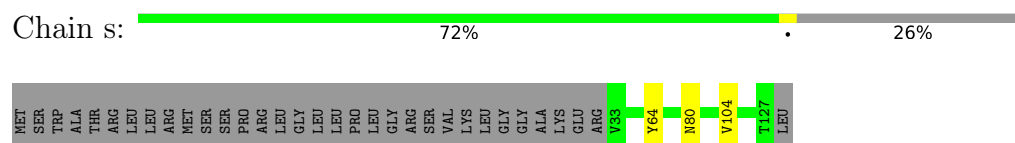
Chain j:  67% 10% 23%



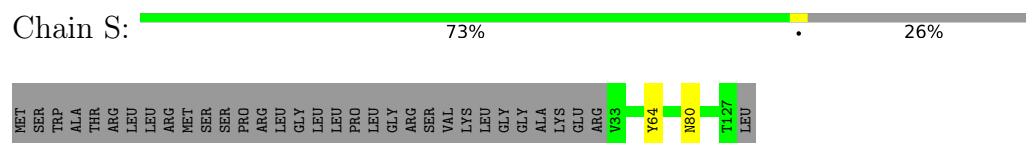
- Molecule 7: subunit i/j



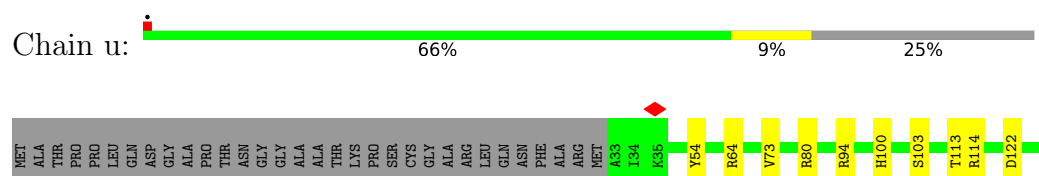
- Molecule 8: ATPTG13



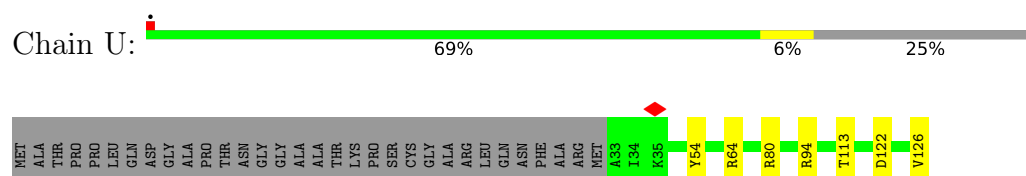
- Molecule 8: ATPTG13



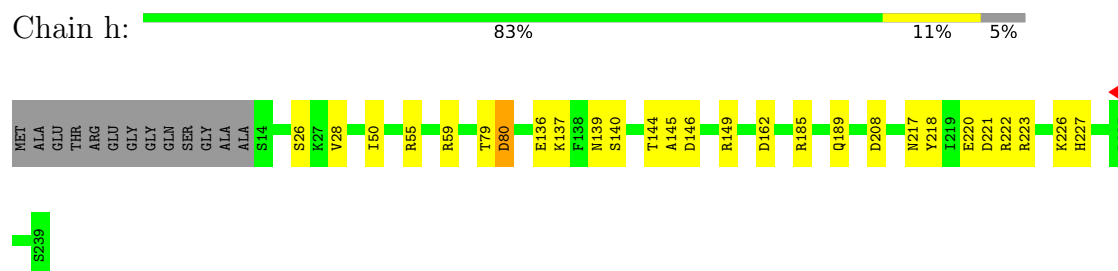
- Molecule 9: ATPTG15



- Molecule 9: ATPTG15



- Molecule 10: ATPTG6



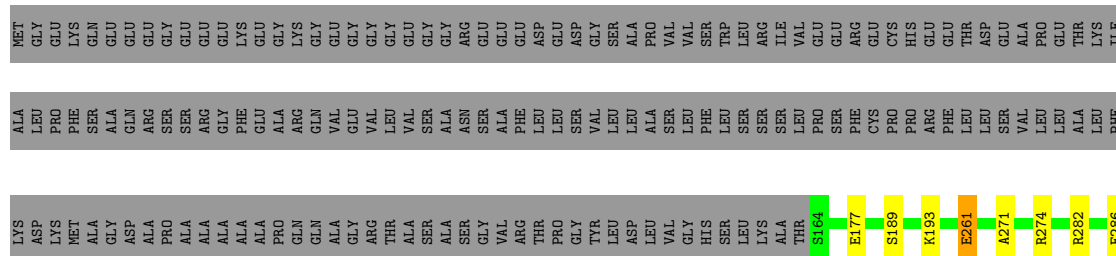
- Molecule 10: ATPTG6

Chain H:  85% 9% 5%



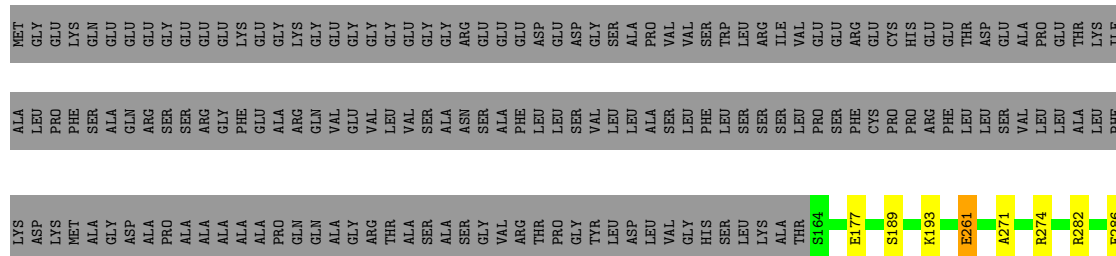
- Molecule 11: ATPTG3

Chain e:  40% 57%



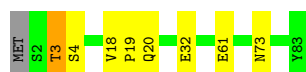
- Molecule 11: ATPTG3

Chain E:  40% 57%



- Molecule 12: ATPTG17

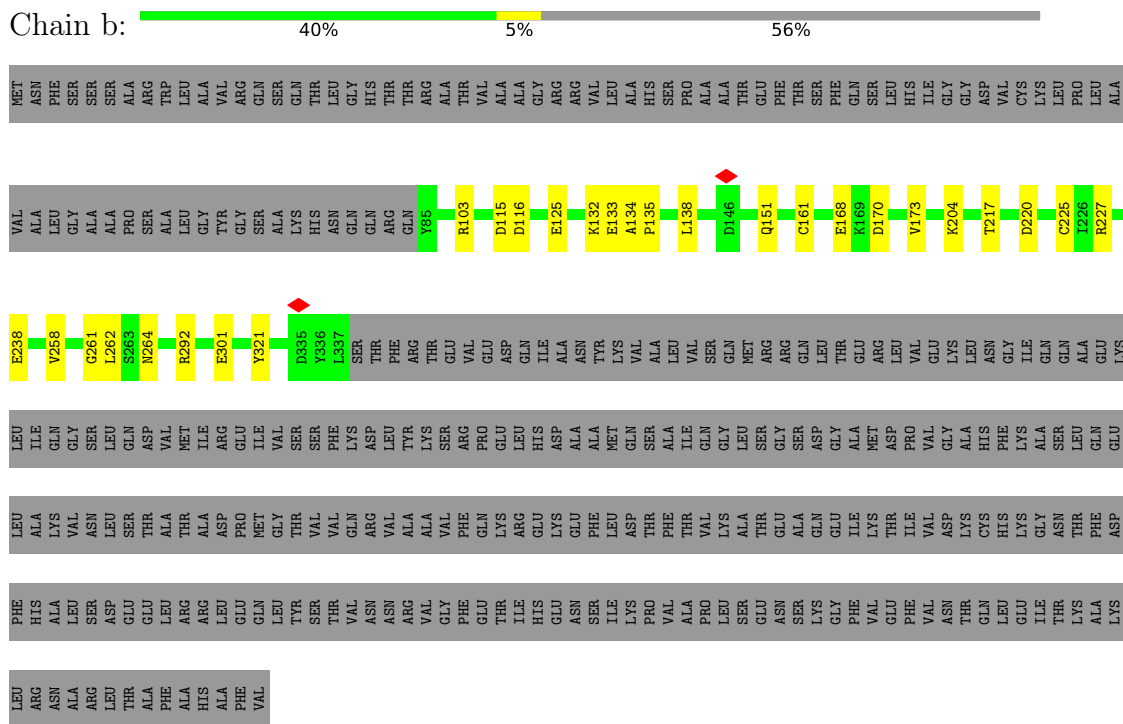
Chain x:  89% 8% ..



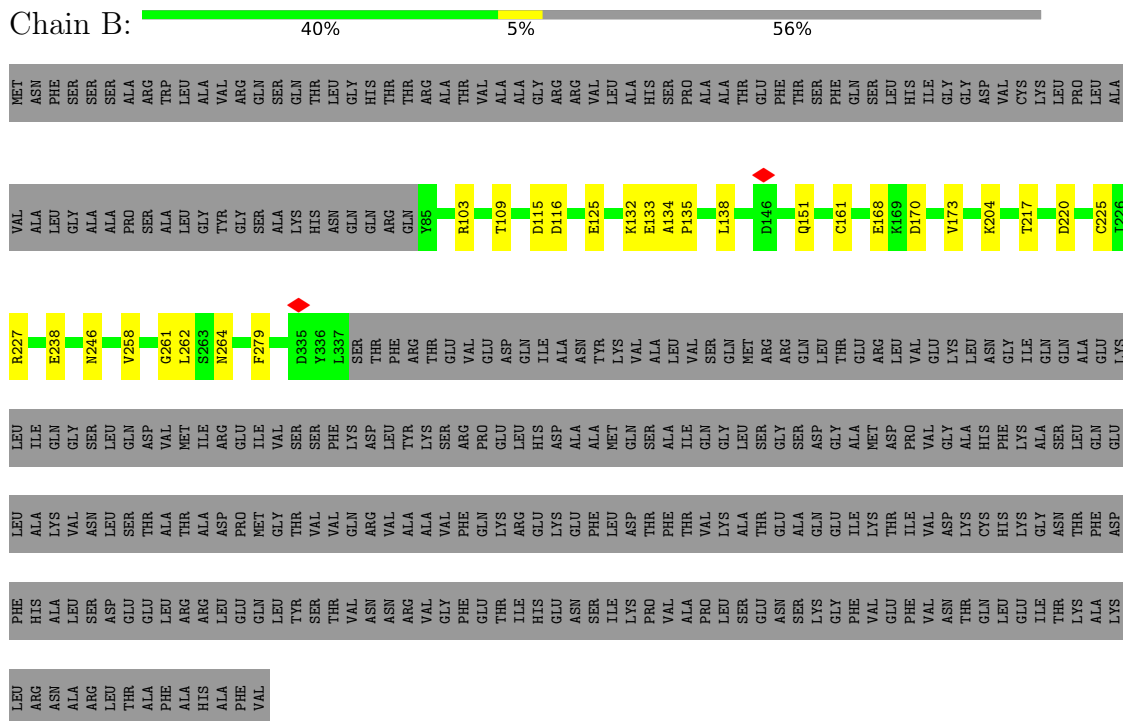
- Molecule 12: ATPTG17

Chain X:  89% 8% ..

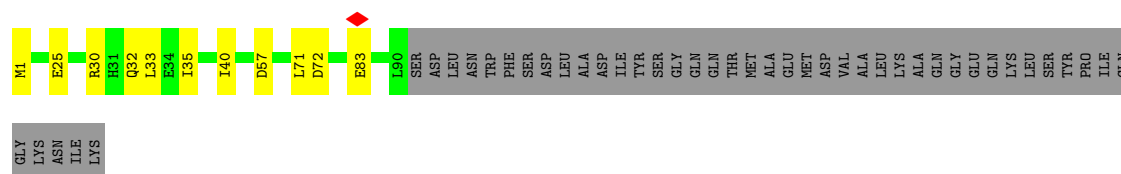
- Molecule 13: subunit b



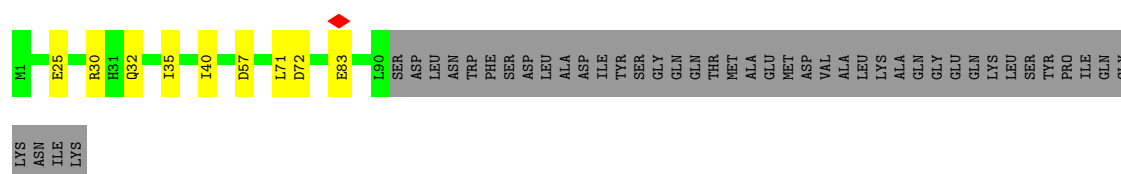
- Molecule 13: subunit b



- Molecule 14: ATPTG12



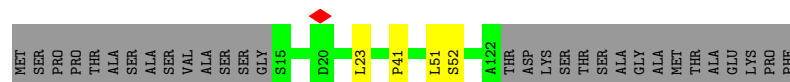
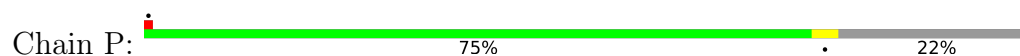
• Molecule 14: ATPTG12



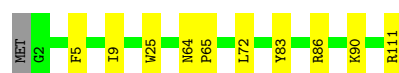
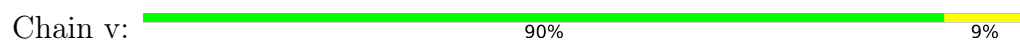
• Molecule 15: ATPTG10



• Molecule 15: ATPTG10



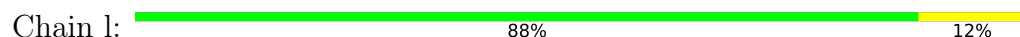
• Molecule 16: subunit f



• Molecule 16: subunit f



• Molecule 17: ATPTG8

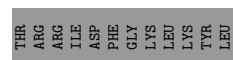
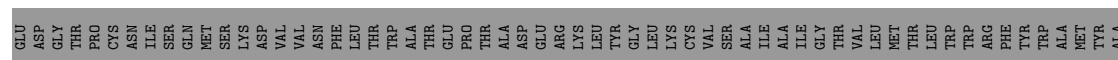
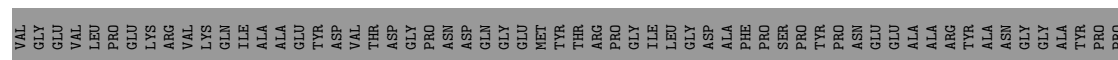
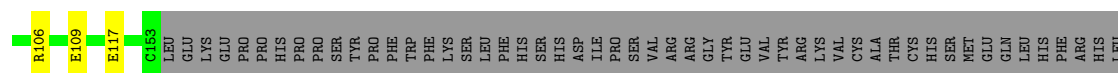
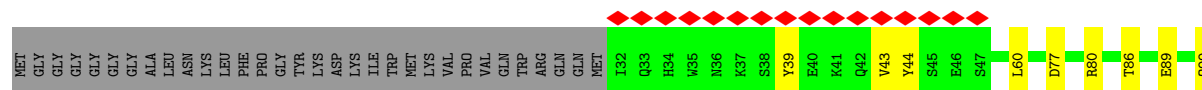




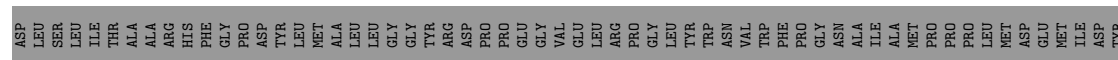
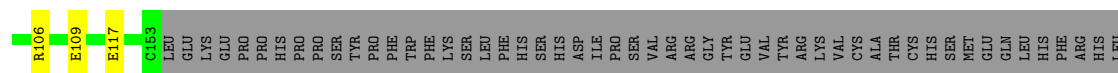
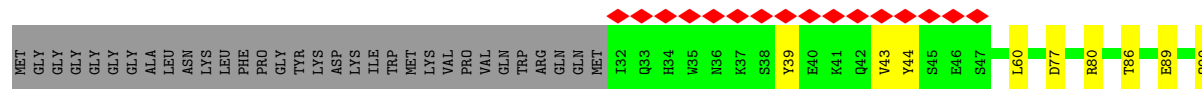
• Molecule 17: ATPTG8



• Molecule 18: ATPTG1

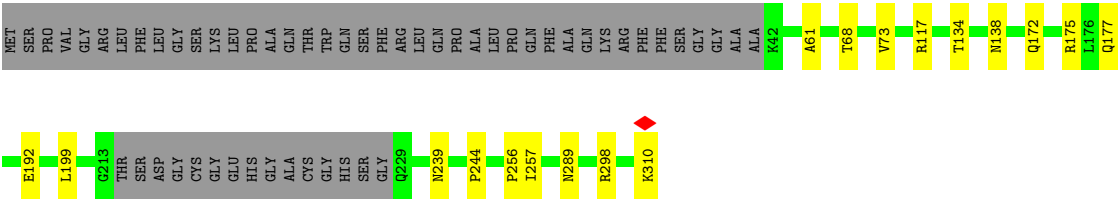


• Molecule 18: ATPTG1

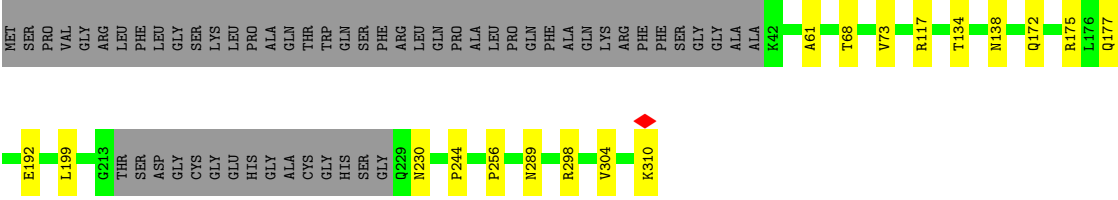


THR
ARG
TLE
ASP
PHE
GLY
LYS
LEU
TYR
LEU

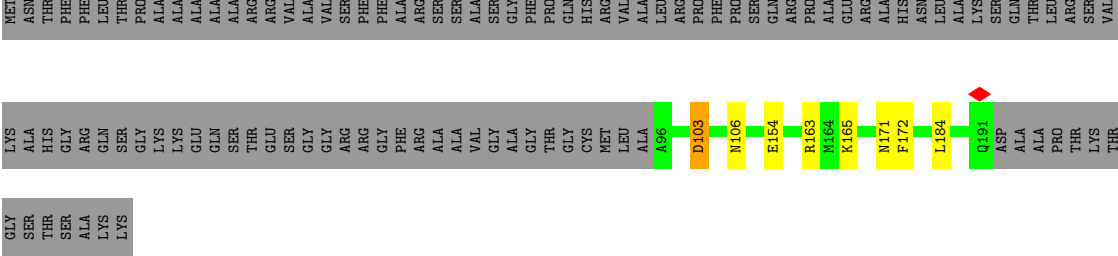
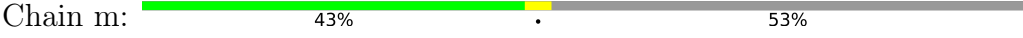
• Molecule 19: ATPTG2



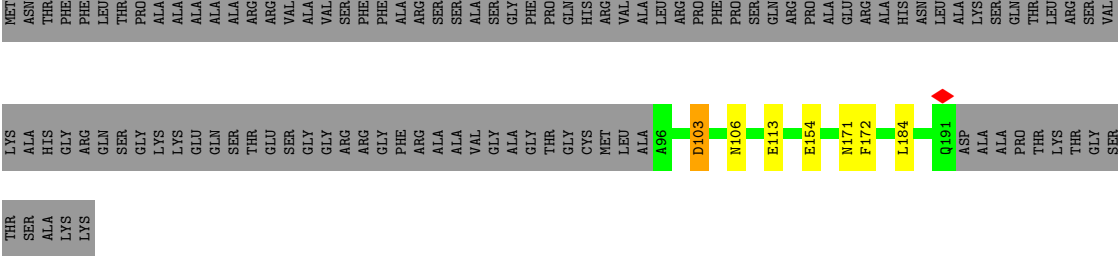
• Molecule 19: ATPTG2



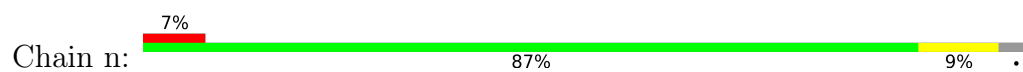
• Molecule 20: subunit 8



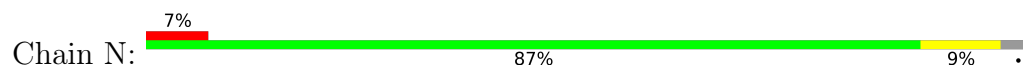
• Molecule 20: subunit 8



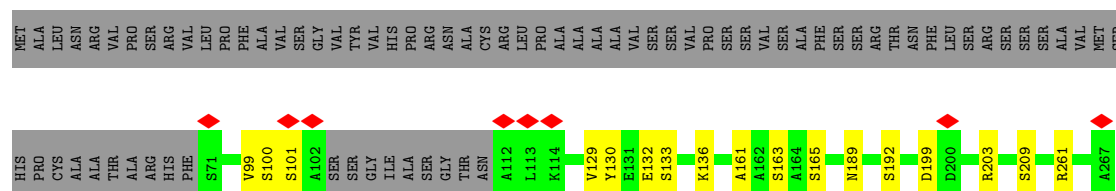
• Molecule 21: ATPTG9



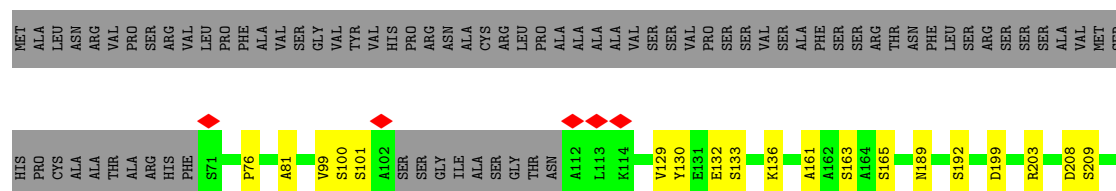
• Molecule 21: ATPTG9



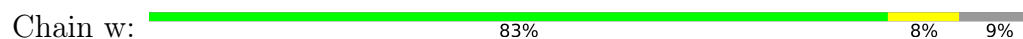
• Molecule 22: ATPTG4



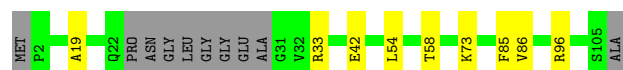
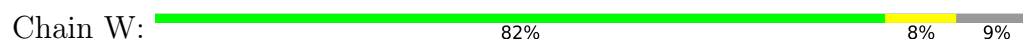
• Molecule 22: ATPTG4



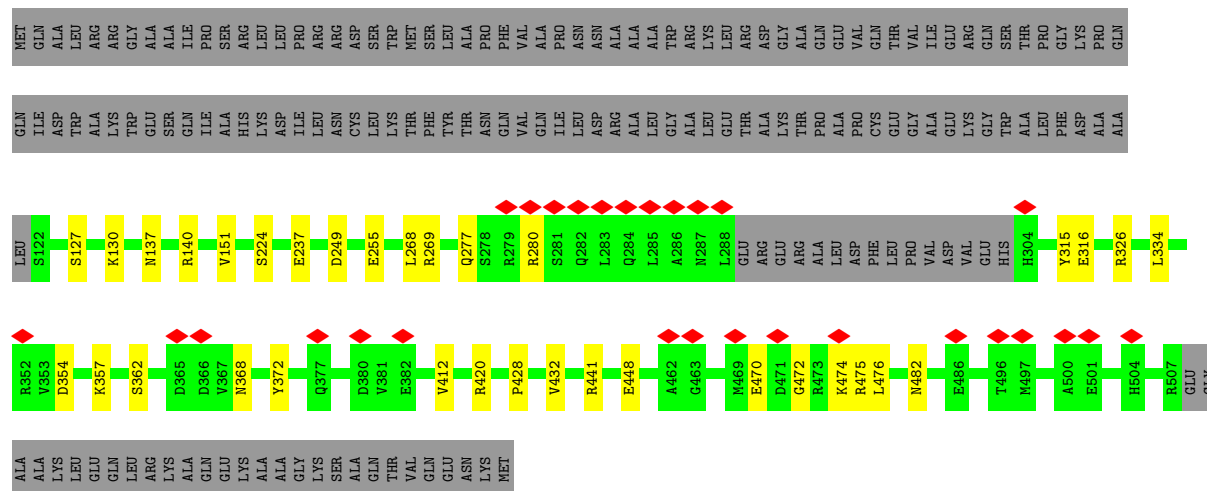
• Molecule 23: ATPTG16



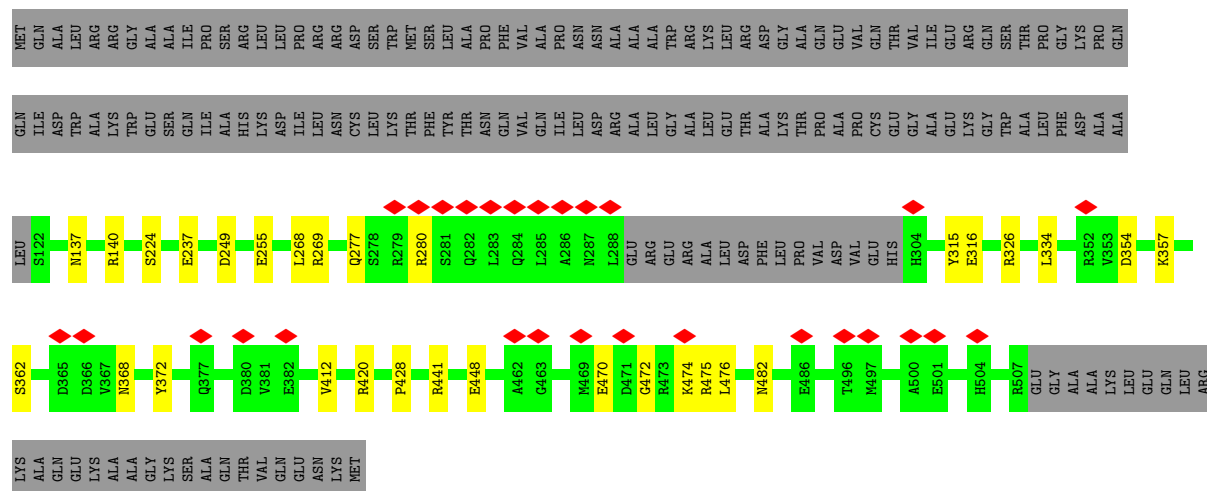
• Molecule 23: ATPTG16



Chain a: 5% 63% 6% 26%



Chain A: 5% 64% 6% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	101505	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.346	Depositor
Minimum map value	-0.157	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	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: PC1, CDL, LMT, PEE

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	Q	0.15	0/1103	0.28	0/1496
1	q	0.15	0/1103	0.28	0/1496
2	I	0.17	0/719	0.28	0/962
2	i	0.17	0/719	0.28	0/962
3	T	0.17	0/741	0.29	0/1007
3	t	0.17	0/741	0.29	0/1007
4	G	0.19	0/896	0.27	0/1216
4	g	0.18	0/896	0.27	0/1216
5	O	0.20	0/1250	0.28	0/1682
5	o	0.20	0/1250	0.28	0/1682
6	K	0.18	0/981	0.25	0/1321
6	k	0.18	0/981	0.25	0/1321
7	J	0.26	0/1573	0.33	0/2137
7	j	0.26	0/1573	0.33	0/2137
8	S	0.20	0/826	0.26	0/1119
8	s	0.20	0/826	0.26	0/1119
9	U	0.22	0/770	0.31	0/1040
9	u	0.22	0/770	0.31	0/1040
10	H	0.23	0/1902	0.30	0/2575
10	h	0.23	0/1902	0.30	0/2575
11	E	0.22	0/1154	0.29	0/1572
11	e	0.22	0/1154	0.29	0/1572
12	X	0.19	0/678	0.26	0/923
12	x	0.19	0/678	0.27	0/923
13	B	0.20	0/2159	0.26	0/2920
13	b	0.20	0/2159	0.26	0/2920
14	R	0.20	0/750	0.31	0/1008
14	r	0.21	0/750	0.31	0/1008
15	P	0.20	0/888	0.28	0/1202
15	p	0.20	0/888	0.28	0/1202
16	V	0.24	0/944	0.31	0/1280
16	v	0.24	0/944	0.31	0/1280

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	L	0.22	0/1651	0.27	0/2227
17	l	0.22	0/1651	0.27	0/2227
18	C	0.21	0/1057	0.31	0/1428
18	c	0.21	0/1057	0.31	0/1428
19	D	0.23	0/2138	0.28	0/2905
19	d	0.23	0/2138	0.28	0/2905
20	M	0.21	0/789	0.28	0/1065
20	m	0.21	0/789	0.28	0/1065
21	N	0.16	0/1280	0.27	0/1734
21	n	0.16	0/1280	0.27	0/1734
22	F	0.18	0/1475	0.30	0/2009
22	f	0.18	0/1475	0.30	0/2009
23	W	0.21	0/778	0.25	0/1057
23	w	0.21	0/778	0.25	0/1057
24	A	0.17	0/3107	0.26	0/4207
24	a	0.17	0/3107	0.26	0/4207
All	All	0.20	0/59218	0.28	0/80184

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 ⓘ

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	Q	1075	1044	1044	14	0
1	q	1075	1044	1044	12	0
2	I	708	678	678	7	0
2	i	708	678	678	8	0
3	T	723	716	728	12	0
3	t	723	716	728	10	0
4	G	876	856	856	9	0
4	g	876	856	856	10	0
5	O	1220	1195	1195	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	o	1220	1195	1195	11	0
6	K	952	952	952	10	0
6	k	952	952	952	9	0
7	J	1512	1469	1469	15	0
7	j	1512	1469	1469	16	0
8	S	800	770	770	2	0
8	s	800	770	770	4	0
9	U	751	741	741	6	0
9	u	751	741	741	9	0
10	H	1848	1741	1741	15	0
10	h	1848	1741	1741	18	0
11	E	1115	1064	1064	10	0
11	e	1115	1064	1064	9	0
12	X	659	639	639	6	0
12	x	659	639	639	7	0
13	B	2101	2056	2056	20	0
13	b	2101	2056	2056	20	0
14	R	735	750	750	7	0
14	r	735	750	750	9	0
15	P	864	847	847	3	0
15	p	864	847	847	5	0
16	V	913	888	888	7	0
16	v	913	888	888	8	0
17	L	1626	1647	1647	14	0
17	l	1626	1647	1647	17	0
18	C	1030	999	999	7	0
18	c	1030	999	999	7	0
19	D	2076	1970	1970	16	0
19	d	2076	1970	1970	16	0
20	M	765	744	744	5	0
20	m	765	744	744	7	0
21	N	1247	1204	1202	12	0
21	n	1247	1204	1202	12	0
22	F	1442	1425	1425	12	0
22	f	1442	1425	1425	9	0
23	W	754	755	755	9	0
23	w	754	755	755	8	0
24	A	3022	2873	2872	20	0
24	a	3022	2873	2872	23	0
25	O	108	176	176	2	0
25	V	54	88	88	0	0
25	o	108	176	176	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	v	54	88	88	0	0
26	C	70	92	92	1	0
26	D	70	92	92	0	0
26	H	35	46	46	2	0
26	O	35	46	46	3	0
26	X	35	46	46	0	0
26	c	70	92	92	1	0
26	d	70	92	92	0	0
26	h	35	46	46	2	0
26	o	35	46	46	3	0
26	x	35	46	46	0	0
27	B	200	312	312	7	0
27	C	100	156	156	1	0
27	D	100	156	156	0	0
27	E	100	156	156	9	0
27	H	100	156	156	0	0
27	O	100	156	156	0	0
27	U	100	156	156	1	0
27	V	200	312	312	7	0
27	b	100	156	156	0	0
27	c	100	156	156	1	0
27	d	100	156	156	1	0
27	e	100	156	156	5	0
27	h	100	156	156	0	0
27	o	100	156	156	0	0
27	u	100	156	156	1	0
27	v	100	156	156	1	0
28	C	51	82	82	0	0
28	J	102	164	164	3	0
28	c	51	82	82	0	0
28	j	102	164	164	3	0
All	All	60548	60518	60536	412	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 (412) 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)
27:E:401:CDL:OB5	27:E:401:CDL:O1	1.90	0.88
27:E:401:CDL:OB3	16:V:90:LYS:NZ	2.09	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:50:ILE:O	10:H:55:ARG:NH1	2.09	0.85
1:Q:27:ASP:OD2	1:Q:29:THR:OG1	1.94	0.85
10:h:50:ILE:O	10:h:55:ARG:NH1	2.09	0.85
19:d:61:ALA:O	23:w:96:ARG:NH2	2.09	0.85
18:C:77:ASP:OD2	18:C:80:ARG:NH1	2.10	0.85
19:D:61:ALA:O	23:W:96:ARG:NH2	2.11	0.84
5:O:128:ARG:NH1	10:H:208:ASP:OD2	2.09	0.84
27:E:401:CDL:OA4	21:N:159:SER:OG	1.93	0.84
5:o:128:ARG:NH1	10:h:208:ASP:OD2	2.11	0.84
8:s:80:ASN:OD1	9:u:80:ARG:NH2	2.11	0.84
18:c:77:ASP:OD2	18:c:80:ARG:NH1	2.10	0.84
16:v:86:ARG:NH2	21:n:158:GLU:OE1	2.12	0.83
1:q:27:ASP:OD2	1:q:29:THR:OG1	1.94	0.82
24:a:357:LYS:O	24:a:372:TYR:OH	1.98	0.81
16:V:86:ARG:NH2	21:N:158:GLU:OE1	2.14	0.81
3:t:73:ASP:OD1	24:a:441:ARG:NH1	2.15	0.80
22:f:129:VAL:O	22:f:133:SER:OG	1.99	0.80
24:A:357:LYS:O	24:A:372:TYR:OH	1.98	0.80
14:r:25:GLU:OE1	14:r:30:ARG:NH2	2.15	0.80
22:F:129:VAL:O	22:F:133:SER:OG	1.99	0.79
14:R:25:GLU:OE1	14:R:30:ARG:NH2	2.15	0.79
10:h:136:GLU:OE2	10:h:185:ARG:NH1	2.16	0.79
22:F:101:SER:OG	24:A:428:PRO:O	1.99	0.79
8:S:80:ASN:OD1	9:U:80:ARG:NH2	2.15	0.79
10:H:136:GLU:OE2	10:H:185:ARG:NH1	2.16	0.79
5:O:39:SER:OG	25:O:201:PC1:O22	2.00	0.79
3:T:73:ASP:OD1	24:A:441:ARG:NH1	2.17	0.77
17:l:40:ASN:OD1	17:l:43:ARG:NH2	2.18	0.77
19:d:298:ARG:NH2	19:D:310:LYS:O	2.19	0.76
3:t:82:ARG:NH1	24:a:316:GLU:OE2	2.19	0.76
7:j:153:GLU:OE1	23:w:58:THR:OG1	2.02	0.76
17:L:40:ASN:OD1	17:L:43:ARG:NH2	2.18	0.76
7:j:121:ASP:OD1	7:j:159:ARG:NH2	2.19	0.76
13:b:132:LYS:NZ	13:b:204:LYS:O	2.20	0.75
19:d:310:LYS:O	19:D:298:ARG:NH2	2.20	0.75
7:J:153:GLU:OE1	23:W:58:THR:OG1	2.04	0.75
7:J:121:ASP:OD1	7:J:159:ARG:NH2	2.19	0.74
9:U:113:THR:O	17:L:56:ARG:NH1	2.20	0.74
13:B:132:LYS:NZ	13:B:204:LYS:O	2.20	0.74
2:I:186:ALA:HB1	11:E:286:GLU:HG3	1.68	0.74
24:A:268:LEU:HD22	24:A:412:VAL:HG23	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:82:ARG:NH1	24:A:316:GLU:OE2	2.21	0.73
10:H:223:ARG:O	26:H:301:LMT:O3B	2.03	0.73
1:Q:111:ALA:O	4:G:225:LYS:NZ	2.22	0.72
3:T:19:ARG:O	3:T:22:ARG:NH1	2.22	0.72
4:g:213:ARG:NH2	4:g:217:GLU:OE1	2.22	0.72
5:o:39:SER:OG	25:o:201:PC1:O22	2.05	0.72
20:M:154:GLU:OE2	23:W:73:LYS:NZ	2.19	0.72
16:v:25:TRP:O	19:d:117:ARG:NH1	2.21	0.72
3:T:104:LEU:O	24:A:315:TYR:OH	2.07	0.72
22:F:161:ALA:O	22:F:165:SER:OG	2.04	0.72
4:G:213:ARG:NH2	4:G:217:GLU:OE1	2.22	0.72
3:t:19:ARG:O	3:t:22:ARG:NH1	2.22	0.71
2:i:186:ALA:HB1	11:e:286:GLU:HG3	1.70	0.71
4:g:147:GLN:OE1	4:g:179:ARG:NH2	2.24	0.71
24:a:268:LEU:HD22	24:a:412:VAL:HG23	1.70	0.71
19:D:172:GLN:OE1	19:D:175:ARG:NH1	2.24	0.71
22:f:161:ALA:O	22:f:165:SER:OG	2.04	0.71
22:f:101:SER:OG	24:a:428:PRO:O	2.04	0.70
17:l:113:ASP:OD1	17:l:141:ARG:NH1	2.24	0.70
17:L:113:ASP:OD1	17:L:141:ARG:NH1	2.24	0.70
27:e:401:CDL:OA4	21:n:159:SER:OG	2.08	0.70
17:L:100:GLU:N	17:L:100:GLU:OE1	2.25	0.70
27:e:401:CDL:H671	27:B:601:CDL:H811	1.73	0.70
17:l:100:GLU:OE1	17:l:100:GLU:N	2.25	0.70
4:G:147:GLN:OE1	4:G:179:ARG:NH2	2.24	0.70
19:d:172:GLN:OE1	19:d:175:ARG:NH1	2.24	0.69
22:f:199:ASP:OD2	22:f:203:ARG:NH2	2.26	0.69
1:Q:53:ASP:OD1	1:Q:54:ARG:N	2.26	0.69
13:B:262:LEU:HD21	27:V:201:CDL:H832	1.75	0.69
1:q:53:ASP:OD1	1:q:54:ARG:N	2.26	0.68
9:u:113:THR:O	17:l:56:ARG:NH1	2.26	0.68
22:F:199:ASP:OD2	22:F:203:ARG:NH2	2.26	0.68
13:B:133:GLU:N	13:B:133:GLU:OE1	2.28	0.66
13:b:133:GLU:N	13:b:133:GLU:OE1	2.28	0.66
3:t:104:LEU:O	24:a:315:TYR:OH	2.14	0.65
1:q:111:ALA:O	4:G:225:LYS:NZ	2.30	0.65
13:B:217:THR:OG1	13:B:220:ASP:OD1	2.15	0.65
27:e:401:CDL:OB3	16:v:90:LYS:NZ	2.24	0.64
12:x:3:THR:OG1	12:x:4:SER:N	2.30	0.64
3:T:84:CYS:HB3	24:A:334:LEU:HD21	1.78	0.64
7:j:192:PRO:O	7:J:212:SER:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:64:TYR:OH	12:X:32:GLU:OE1	2.14	0.64
8:s:64:TYR:OH	12:x:32:GLU:OE1	2.15	0.64
24:a:237:GLU:OE1	24:a:269:ARG:NH1	2.31	0.64
4:G:134:SER:O	4:G:137:ASN:ND2	2.31	0.64
13:b:217:THR:OG1	13:b:220:ASP:OD1	2.15	0.64
12:X:3:THR:OG1	12:X:4:SER:N	2.30	0.64
4:g:134:SER:O	4:g:137:ASN:ND2	2.31	0.63
7:j:212:SER:N	7:J:192:PRO:O	2.31	0.63
9:U:64:ARG:NH1	27:U:201:CDL:OA4	2.31	0.63
24:A:237:GLU:OE1	24:A:269:ARG:NH1	2.31	0.63
22:F:130:TYR:OH	22:F:261:ARG:NH1	2.32	0.63
13:b:292:ARG:NH1	13:B:109:THR:O	2.31	0.63
3:T:83:GLU:OE2	24:A:420:ARG:NH2	2.30	0.63
3:t:84:CYS:HB3	24:a:334:LEU:HD21	1.81	0.63
21:n:115:ASN:OD1	23:w:33:ARG:NH2	2.32	0.63
20:m:154:GLU:OE2	23:w:73:LYS:NZ	2.26	0.62
22:f:130:TYR:OH	22:f:261:ARG:NH1	2.31	0.62
2:I:186:ALA:HB1	11:E:286:GLU:CG	2.30	0.62
2:i:186:ALA:HB1	11:e:286:GLU:CG	2.29	0.62
7:j:155:ARG:NH1	7:j:169:GLU:OE2	2.31	0.62
27:B:601:CDL:H472	27:V:201:CDL:H472	1.82	0.62
24:A:472:GLY:O	24:A:476:LEU:N	2.30	0.62
10:H:162:ASP:O	17:L:138:ARG:NH2	2.32	0.61
3:t:83:GLU:OE2	24:a:420:ARG:NH2	2.33	0.61
9:U:94:ARG:NH2	23:W:42:GLU:OE2	2.27	0.61
3:T:76:GLN:NE2	24:A:249:ASP:OD1	2.33	0.61
24:a:472:GLY:O	24:a:476:LEU:N	2.30	0.60
21:n:83:GLU:OE1	21:n:86:ARG:NH1	2.35	0.60
3:T:95:LEU:O	24:A:326:ARG:NH2	2.35	0.60
20:M:103:ASP:OD2	20:M:106:ASN:ND2	2.35	0.60
7:J:155:ARG:NH1	7:J:169:GLU:OE2	2.31	0.60
27:E:401:CDL:H671	27:V:201:CDL:H811	1.83	0.60
13:B:246:ASN:OD1	16:V:14:ARG:NH2	2.33	0.60
20:m:103:ASP:OD2	20:m:106:ASN:ND2	2.35	0.60
13:B:103:ARG:NH1	27:V:201:CDL:OA3	2.32	0.60
21:N:83:GLU:OE1	21:N:86:ARG:NH1	2.35	0.59
21:N:115:ASN:OD1	23:W:33:ARG:NH2	2.35	0.59
9:u:54:TYR:HH	19:d:134:THR:HG1	1.50	0.59
26:O:202:LMT:O6B	26:O:202:LMT:O3B	2.17	0.59
26:o:202:LMT:O6B	26:o:202:LMT:O3B	2.17	0.58
28:J:301:PEE:H46	23:W:85:PHE:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:113:ASP:OD1	28:J:302:PEE:N	2.35	0.58
1:Q:16:PHE:CE2	1:Q:17:LEU:HD23	2.39	0.58
13:b:262:LEU:HD21	27:B:601:CDL:H832	1.86	0.58
13:B:125:GLU:N	13:B:125:GLU:OE1	2.36	0.58
1:q:16:PHE:CE2	1:q:17:LEU:HD23	2.39	0.57
24:a:137:ASN:OD1	24:a:140:ARG:NH1	2.37	0.57
13:b:103:ARG:NH1	27:B:601:CDL:OA3	2.37	0.57
14:R:72:ASP:OD2	24:A:137:ASN:ND2	2.38	0.57
13:B:151:GLN:OE1	13:B:151:GLN:N	2.37	0.57
24:A:137:ASN:OD1	24:A:140:ARG:NH1	2.37	0.57
13:b:125:GLU:N	13:b:125:GLU:OE1	2.36	0.57
13:b:151:GLN:OE1	13:b:151:GLN:N	2.37	0.57
10:h:162:ASP:O	17:l:138:ARG:NH2	2.37	0.56
13:b:115:ASP:OD1	13:b:116:ASP:N	2.39	0.56
7:j:191:PHE:HA	7:j:194:VAL:O	2.06	0.56
7:J:119:ARG:NH2	10:H:226:LYS:O	2.39	0.56
21:n:58:GLU:N	21:n:58:GLU:OE1	2.37	0.56
3:t:76:GLN:NE2	24:a:249:ASP:OD1	2.38	0.56
21:N:58:GLU:OE1	21:N:58:GLU:N	2.38	0.55
5:o:64:THR:HG21	26:o:202:LMT:C6'	2.36	0.55
28:j:301:PEE:H46	23:w:85:PHE:HB3	1.88	0.55
7:j:119:ARG:NH2	10:h:226:LYS:O	2.40	0.55
1:Q:24:VAL:HG12	15:P:41:PRO:HB3	1.89	0.55
13:b:134:ALA:HB2	13:b:161:CYS:SG	2.47	0.55
13:B:227:ARG:NH1	14:R:57:ASP:OD2	2.40	0.55
1:q:24:VAL:HG12	15:p:41:PRO:HB3	1.89	0.54
7:J:191:PHE:HA	7:J:194:VAL:O	2.06	0.54
10:h:223:ARG:O	26:h:301:LMT:O3B	2.18	0.54
13:b:168:GLU:N	13:b:168:GLU:OE2	2.39	0.54
11:e:189:SER:O	21:n:161:ARG:NH1	2.38	0.54
13:B:134:ALA:HB2	13:B:161:CYS:SG	2.47	0.54
3:t:30:VAL:O	3:t:30:VAL:HG23	2.08	0.53
18:c:99:GLN:O	18:c:106:ARG:NH2	2.42	0.53
4:G:149:ASP:OD2	4:G:155:ARG:NH2	2.39	0.53
3:T:30:VAL:HG23	3:T:30:VAL:O	2.08	0.53
16:V:25:TRP:O	19:D:117:ARG:NH1	2.42	0.53
9:u:94:ARG:NH2	23:w:42:GLU:OE2	2.31	0.53
5:O:66:LEU:HD23	5:O:66:LEU:H	1.74	0.52
4:g:149:ASP:OD2	4:g:155:ARG:NH2	2.39	0.52
14:r:35:ILE:HG21	14:r:40:ILE:HD11	1.92	0.52
23:w:54:LEU:O	23:w:58:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:54:LEU:O	23:W:58:THR:HG23	2.09	0.52
5:O:35:SER:O	5:O:39:SER:OG	2.28	0.52
14:R:35:ILE:HG21	14:R:40:ILE:HD11	1.92	0.52
18:C:39:TYR:O	18:C:43:VAL:HG23	2.10	0.52
18:C:99:GLN:O	18:C:106:ARG:NH2	2.42	0.52
5:o:66:LEU:HD23	5:o:66:LEU:H	1.74	0.52
6:K:124:LYS:HB2	18:C:60:LEU:HD11	1.91	0.52
5:o:35:SER:O	5:o:39:SER:OG	2.28	0.52
13:b:170:ASP:OD2	13:b:238:GLU:N	2.41	0.52
18:c:39:TYR:O	18:c:43:VAL:HG23	2.10	0.52
13:B:115:ASP:OD1	13:B:116:ASP:N	2.39	0.52
3:t:95:LEU:O	24:a:326:ARG:NH2	2.43	0.51
6:k:217:THR:O	6:k:221:THR:OG1	2.27	0.51
13:B:170:ASP:OD2	13:B:238:GLU:N	2.41	0.51
13:B:168:GLU:OE2	13:B:168:GLU:N	2.39	0.51
24:A:277:GLN:OE1	24:A:280:ARG:NH2	2.39	0.51
12:x:18:VAL:HG22	12:x:19:PRO:HD3	1.93	0.51
2:I:171:GLU:O	2:I:175:GLN:NE2	2.42	0.51
12:X:18:VAL:HG22	12:X:19:PRO:HD3	1.93	0.51
11:E:189:SER:O	21:N:161:ARG:NH1	2.40	0.51
6:k:124:LYS:HB2	18:c:60:LEU:HD11	1.93	0.50
21:n:161:ARG:NH2	21:n:166:ALA:OXT	2.44	0.50
24:a:224:SER:OG	24:a:255:GLU:O	2.29	0.50
19:d:177:GLN:NE2	10:H:80:ASP:OD1	2.37	0.50
24:a:277:GLN:OE1	24:a:280:ARG:NH2	2.39	0.50
1:Q:16:PHE:HE2	1:Q:17:LEU:HD23	1.77	0.50
9:u:114:ARG:NE	17:l:184:GLN:OE1	2.43	0.50
26:c:401:LMT:O2'	26:c:403:LMT:O6B	2.14	0.50
17:L:123:ALA:O	17:L:130:ARG:NH1	2.45	0.50
11:e:261:GLU:N	11:e:261:GLU:OE2	2.44	0.50
11:E:261:GLU:OE2	11:E:261:GLU:N	2.44	0.50
1:q:16:PHE:HE2	1:q:17:LEU:HD23	1.77	0.50
10:h:26:SER:O	10:h:28:VAL:N	2.45	0.50
2:I:219:THR:HG23	15:P:23:LEU:HD13	1.93	0.50
10:h:222:ARG:NH1	26:h:301:LMT:O4'	2.45	0.49
14:r:71:LEU:HD21	20:m:184:LEU:HD22	1.94	0.49
7:j:113:ASP:OD1	28:j:302:PEE:N	2.44	0.49
10:H:26:SER:O	10:H:28:VAL:N	2.45	0.49
17:l:123:ALA:O	17:l:130:ARG:NH1	2.45	0.49
11:E:177:GLU:OE2	19:D:289:ASN:ND2	2.46	0.49
13:b:227:ARG:NH1	14:r:57:ASP:OD2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:64:THR:HG21	26:O:202:LMT:C6'	2.43	0.49
21:N:161:ARG:NH2	21:N:166:ALA:OXT	2.44	0.49
11:e:193:LYS:O	19:d:138:ASN:ND2	2.40	0.49
7:J:191:PHE:CD1	7:J:191:PHE:C	2.91	0.49
14:R:83:GLU:OE1	14:R:83:GLU:N	2.46	0.49
14:r:83:GLU:OE1	14:r:83:GLU:N	2.46	0.49
19:D:199:LEU:C	19:D:199:LEU:HD12	2.38	0.49
22:F:199:ASP:O	22:F:203:ARG:NH2	2.45	0.49
17:l:206:GLU:HG2	2:I:146:MET:HE3	1.95	0.49
19:d:199:LEU:C	19:d:199:LEU:HD12	2.38	0.49
7:j:191:PHE:CD1	7:j:191:PHE:C	2.91	0.48
24:A:448:GLU:OE2	24:A:448:GLU:N	2.42	0.48
1:q:83:PHE:O	1:q:86:VAL:HG22	2.13	0.48
28:j:302:PEE:H64	27:c:404:CDL:H272	1.95	0.48
14:R:32:GLN:N	14:R:32:GLN:OE1	2.46	0.48
13:b:301:GLU:OE2	20:m:163:ARG:NE	2.37	0.48
1:Q:83:PHE:O	1:Q:86:VAL:HG22	2.13	0.48
13:B:261:GLY:O	13:B:264:ASN:ND2	2.42	0.48
12:x:18:VAL:N	12:x:19:PRO:CD	2.77	0.48
14:r:32:GLN:N	14:r:32:GLN:OE1	2.46	0.48
22:f:189:ASN:O	22:f:192:SER:OG	2.31	0.48
6:k:148:LEU:O	6:k:151:ARG:NH2	2.47	0.48
22:f:199:ASP:O	22:f:203:ARG:NH2	2.45	0.48
26:C:401:LMT:O2'	26:C:403:LMT:O6B	2.14	0.48
13:b:321:TYR:HE1	14:r:33:LEU:HD13	1.76	0.48
6:K:182:LEU:HD23	6:K:185:MET:HE2	1.95	0.48
9:U:54:TYR:HH	19:D:134:THR:HG1	1.56	0.48
11:E:193:LYS:O	19:D:138:ASN:ND2	2.39	0.48
12:X:18:VAL:N	12:X:19:PRO:CD	2.77	0.48
6:k:182:LEU:HD23	6:k:185:MET:HE2	1.95	0.48
24:a:368:ASN:ND2	24:a:482:ASN:OD1	2.46	0.48
9:u:64:ARG:NH1	27:u:201:CDL:OA4	2.47	0.47
17:L:14:VAL:HG23	17:L:14:VAL:O	2.14	0.47
24:A:368:ASN:ND2	24:A:482:ASN:OD1	2.46	0.47
11:e:177:GLU:OE2	19:d:289:ASN:ND2	2.47	0.47
2:i:171:GLU:O	2:i:175:GLN:NE2	2.42	0.47
6:k:224:PHE:OXT	7:j:87:ARG:NE	2.48	0.47
21:n:28:ASN:ND2	21:n:36:CYS:SG	2.88	0.47
21:n:77:GLU:OE1	21:n:77:GLU:N	2.45	0.47
21:N:28:ASN:ND2	21:N:36:CYS:SG	2.88	0.47
22:F:189:ASN:O	22:F:192:SER:OG	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:q:107:ASP:OD1	1:q:107:ASP:N	2.48	0.47
17:l:14:VAL:O	17:l:14:VAL:HG23	2.14	0.47
24:a:448:GLU:OE2	24:a:448:GLU:N	2.42	0.47
28:J:302:PEE:H64	27:C:404:CDL:H272	1.95	0.47
7:J:118:GLU:OE2	10:H:227:HIS:ND1	2.48	0.47
10:h:80:ASP:OD1	19:D:177:GLN:NE2	2.38	0.46
6:K:148:LEU:O	6:K:151:ARG:NH2	2.47	0.46
17:L:2:THR:N	19:D:192:GLU:OE1	2.49	0.46
7:j:118:GLU:OE2	10:h:227:HIS:ND1	2.48	0.46
5:o:149:ARG:NH2	19:d:256:PRO:O	2.42	0.46
1:Q:107:ASP:OD1	1:Q:107:ASP:N	2.48	0.46
10:H:222:ARG:NH1	26:H:301:LMT:O4'	2.49	0.46
21:N:92:LEU:CD1	21:N:121:LEU:HD12	2.46	0.46
1:q:112:GLU:C	4:g:225:LYS:HZ2	2.24	0.46
7:j:94:ASN:HB3	23:w:86:VAL:HG22	1.97	0.46
24:A:224:SER:OG	24:A:255:GLU:O	2.29	0.46
21:n:92:LEU:CD1	21:n:121:LEU:HD12	2.46	0.46
27:E:401:CDL:H673	27:V:201:CDL:H762	1.97	0.46
2:i:219:THR:HG23	15:p:23:LEU:HD13	1.99	0.46
11:e:294:ASP:OD2	11:e:298:LYS:NZ	2.49	0.46
6:K:224:PHE:OXT	7:J:87:ARG:NE	2.49	0.45
7:J:94:ASN:HB3	23:W:86:VAL:HG22	1.97	0.45
13:b:261:GLY:O	13:b:264:ASN:ND2	2.42	0.45
27:E:401:CDL:H1O1	27:E:401:CDL:PB2	2.37	0.45
8:s:80:ASN:HB2	9:u:73:VAL:HG13	1.97	0.45
3:T:99:GLU:OE1	3:T:99:GLU:N	2.46	0.45
16:v:111:ARG:HB3	19:d:257:ILE:HD13	1.99	0.45
1:q:15:ILE:HD12	1:q:15:ILE:N	2.32	0.45
2:i:191:ARG:NH1	17:L:207:GLY:O	2.45	0.45
6:k:144:ALA:O	6:k:148:LEU:HD23	2.17	0.45
17:l:202:LEU:O	17:l:205:VAL:HG12	2.17	0.45
21:N:77:GLU:OE1	21:N:77:GLU:N	2.45	0.45
1:Q:15:ILE:HD12	1:Q:15:ILE:N	2.32	0.45
14:R:71:LEU:HD21	20:M:184:LEU:HD22	1.99	0.45
24:A:470:GLU:O	24:A:474:LYS:NZ	2.49	0.45
10:h:59:ARG:NH2	10:h:137:LYS:O	2.50	0.45
11:E:294:ASP:OD2	11:E:298:LYS:NZ	2.49	0.45
1:q:114:ASP:OD1	1:q:115:GLN:N	2.47	0.44
24:a:470:GLU:O	24:a:474:LYS:NZ	2.49	0.44
5:O:43:THR:OG1	25:O:201:PC1:O14	2.35	0.44
2:i:198:ASP:OD1	11:e:282:ARG:NH2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:x:61:GLU:O	12:x:73:ASN:ND2	2.51	0.44
9:U:122:ASP:HA	9:U:126:VAL:HG23	2.00	0.44
10:H:59:ARG:NH2	10:H:137:LYS:O	2.50	0.44
3:T:59:ARG:NH1	22:F:81:ALA:O	2.51	0.44
7:J:48:THR:HG22	7:J:49:LEU:N	2.33	0.44
6:k:214:THR:O	6:k:217:THR:HG22	2.18	0.44
1:Q:114:ASP:OD1	1:Q:115:GLN:N	2.47	0.44
24:A:362:SER:OG	24:A:475:ARG:NH1	2.51	0.44
6:K:214:THR:O	6:K:217:THR:HG22	2.18	0.44
24:a:362:SER:OG	24:a:475:ARG:NH1	2.51	0.43
17:L:202:LEU:O	17:L:205:VAL:HG12	2.17	0.43
5:o:119:GLU:OE1	5:o:119:GLU:N	2.49	0.43
22:f:99:VAL:HG12	22:f:100:SER:N	2.33	0.43
20:M:171:ASN:O	20:M:172:PHE:HB2	2.19	0.43
13:b:173:VAL:HG23	13:b:225:CYS:SG	2.59	0.43
20:m:171:ASN:O	20:m:172:PHE:HB2	2.18	0.43
5:o:59:ARG:NH2	12:x:20:GLN:OE1	2.51	0.43
6:k:154:PHE:HA	6:k:157:MET:HG2	2.00	0.43
10:H:217:ASN:OD1	10:H:218:TYR:N	2.46	0.43
7:j:48:THR:HG22	7:j:49:LEU:N	2.33	0.43
9:u:122:ASP:HA	9:u:126:VAL:HG23	1.99	0.43
17:l:98:ASP:OD1	17:l:99:VAL:N	2.52	0.43
1:Q:124:ARG:NH2	5:O:156:ASN:OD1	2.51	0.43
6:K:144:ALA:O	6:K:148:LEU:HD23	2.17	0.43
17:l:112:VAL:HG11	17:l:141:ARG:HG2	2.01	0.43
18:c:106:ARG:NH1	18:c:109:GLU:O	2.52	0.43
27:E:401:CDL:H672	16:V:78:ALA:HB2	2.00	0.43
17:L:98:ASP:OD1	17:L:99:VAL:N	2.52	0.43
16:v:72:LEU:HB3	27:d:402:CDL:H371	2.01	0.43
21:n:52:THR:HG22	21:n:53:SER:N	2.33	0.43
1:Q:12:VAL:HG12	1:Q:16:PHE:CE1	2.54	0.43
6:K:154:PHE:HA	6:K:157:MET:HG2	2.00	0.43
13:B:173:VAL:HG23	13:B:225:CYS:SG	2.59	0.43
27:B:601:CDL:H273	27:V:201:CDL:H802	2.00	0.43
17:L:197:ARG:O	17:L:200:VAL:HG22	2.19	0.43
18:C:89:GLU:O	19:D:68:THR:HG21	2.19	0.43
4:g:145:GLU:N	4:g:145:GLU:OE1	2.52	0.43
4:G:145:GLU:OE1	4:G:145:GLU:N	2.52	0.43
6:K:217:THR:O	6:K:221:THR:OG1	2.27	0.43
16:V:5:PHE:O	16:V:9:ILE:HG12	2.19	0.43
18:C:106:ARG:NH1	18:C:109:GLU:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:52:THR:HG22	21:N:53:SER:N	2.33	0.43
21:n:92:LEU:HD11	21:n:121:LEU:HD12	2.01	0.42
1:q:12:VAL:HG12	1:q:16:PHE:CE1	2.54	0.42
11:e:271:ALA:O	11:e:274:ARG:C	2.62	0.42
14:r:1:MET:HE2	20:m:172:PHE:CE1	2.54	0.42
16:v:83:TYR:OH	27:v:201:CDL:OB4	2.28	0.42
5:O:59:ARG:NH2	12:X:20:GLN:OE1	2.52	0.42
5:O:97:TYR:OH	20:M:113:GLU:OE2	2.36	0.42
5:O:100:ASP:OD2	26:O:202:LMT:O6B	2.38	0.42
10:H:139:ASN:O	10:H:140:SER:OG	2.32	0.42
17:L:112:VAL:HG11	17:L:141:ARG:HG2	2.01	0.42
27:e:401:CDL:H673	27:B:601:CDL:H762	2.01	0.42
5:O:119:GLU:N	5:O:119:GLU:OE1	2.49	0.42
15:P:51:LEU:O	15:P:52:SER:C	2.62	0.42
3:t:99:GLU:OE1	3:t:99:GLU:N	2.46	0.42
22:F:99:VAL:HG12	22:F:100:SER:N	2.33	0.42
17:l:2:THR:N	19:d:192:GLU:OE1	2.52	0.42
18:c:89:GLU:O	19:d:68:THR:HG21	2.20	0.42
21:N:92:LEU:HD11	21:N:121:LEU:HD12	2.01	0.42
7:j:191:PHE:O	7:j:192:PRO:C	2.63	0.42
15:p:51:LEU:O	15:p:52:SER:C	2.62	0.42
3:T:40:ALA:HB3	22:F:76:PRO:O	2.19	0.42
13:B:134:ALA:HB1	13:B:138:LEU:CD1	2.50	0.42
2:i:226:GLN:HE22	15:p:19:MET:HE3	1.85	0.42
27:e:401:CDL:H622	13:b:258:VAL:HG13	2.02	0.42
17:l:197:ARG:O	17:l:200:VAL:HG22	2.19	0.42
20:m:165:LYS:HG2	24:a:151:VAL:HG22	2.02	0.42
27:V:201:CDL:H171	27:V:201:CDL:H211	2.02	0.42
14:r:72:ASP:OD2	24:a:137:ASN:ND2	2.49	0.42
16:v:5:PHE:O	16:v:9:ILE:HG12	2.19	0.42
18:c:44:TYR:N	18:c:44:TYR:CD2	2.87	0.42
11:E:271:ALA:O	11:E:274:ARG:C	2.62	0.42
19:D:230:ASN:ND2	23:W:19:ALA:O	2.52	0.42
4:g:134:SER:N	4:g:137:ASN:OD1	2.52	0.41
4:g:190:LEU:HD12	4:g:190:LEU:N	2.35	0.41
10:h:217:ASN:OD1	10:h:218:TYR:N	2.46	0.41
6:k:166:ARG:HB3	6:k:167:PRO:HD3	2.03	0.41
6:K:202:VAL:HG22	13:B:279:PHE:CE2	2.56	0.41
22:F:132:GLU:O	22:F:136:LYS:O	2.39	0.41
10:h:139:ASN:O	10:h:140:SER:OG	2.32	0.41
17:l:36:LEU:O	17:l:39:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:149:ARG:NH2	19:D:256:PRO:O	2.41	0.41
27:E:401:CDL:H622	13:B:258:VAL:HG13	2.02	0.41
2:i:205:ARG:NH2	15:p:82:ALA:O	2.54	0.41
4:G:190:LEU:N	4:G:190:LEU:HD12	2.35	0.41
6:K:166:ARG:HB3	6:K:167:PRO:HD3	2.03	0.41
10:H:221:ASP:OD1	10:H:222:ARG:N	2.50	0.41
13:b:134:ALA:HB1	13:b:138:LEU:CD1	2.50	0.41
2:I:198:ASP:OD1	11:E:282:ARG:NH2	2.49	0.41
18:C:44:TYR:N	18:C:44:TYR:CD2	2.87	0.41
7:J:167:LEU:HD23	19:D:244:PRO:HG2	2.02	0.41
8:s:104:VAL:HG21	17:l:103:LEU:HD21	2.03	0.41
9:u:100:HIS:O	9:u:103:SER:OG	2.32	0.41
12:x:61:GLU:OE1	12:x:61:GLU:N	2.48	0.41
1:Q:112:GLU:C	4:G:225:LYS:HZ2	2.29	0.41
5:O:51:PHE:HB2	5:O:52:PRO:HD3	2.02	0.41
5:O:141:ARG:NH2	10:H:220:GLU:OE2	2.46	0.41
7:J:191:PHE:O	7:J:192:PRO:C	2.63	0.41
13:B:134:ALA:N	13:B:135:PRO:CD	2.84	0.41
5:o:141:ARG:NH2	10:h:220:GLU:OE2	2.44	0.41
10:h:144:THR:HG22	10:h:145:ALA:N	2.36	0.41
10:h:146:ASP:OD1	10:h:149:ARG:NH2	2.54	0.41
10:h:221:ASP:OD1	10:h:222:ARG:N	2.50	0.41
1:Q:100:GLN:HA	1:Q:103:ASN:OD1	2.21	0.41
27:B:601:CDL:H171	27:B:601:CDL:H211	2.02	0.41
22:F:208:ASP:OD2	22:F:213:LYS:N	2.54	0.41
5:o:51:PHE:HB2	5:o:52:PRO:HD3	2.02	0.40
13:b:134:ALA:N	13:b:135:PRO:CD	2.84	0.40
24:a:334:LEU:HD22	24:a:432:VAL:HG12	2.03	0.40
7:j:167:LEU:HD23	19:d:244:PRO:HG2	2.03	0.40
22:f:132:GLU:O	22:f:136:LYS:O	2.39	0.40
4:g:151:LEU:HD23	17:L:14:VAL:HG12	2.03	0.40
10:h:189:GLN:NE2	19:d:239:ASN:OD1	2.54	0.40
16:v:64:ASN:HB2	16:v:65:PRO:HD2	2.03	0.40
5:o:64:THR:HG21	26:o:202:LMT:H6E	2.02	0.40
24:a:127:SER:O	24:a:130:LYS:HG3	2.22	0.40
12:X:61:GLU:O	12:X:73:ASN:ND2	2.51	0.40
7:j:92:PHE:O	7:j:98:SER:OG	2.31	0.40
17:l:14:VAL:HG12	4:G:151:LEU:CD2	2.51	0.40
2:I:178:ARG:NE	11:E:294:ASP:OD1	2.55	0.40
27:E:401:CDL:O1	27:E:401:CDL:PB2	2.78	0.40
16:V:89:LYS:HA	19:D:304:VAL:HG21	2.03	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	Q	131/134 (98%)	128 (98%)	3 (2%)	0	100	100
1	q	131/134 (98%)	128 (98%)	3 (2%)	0	100	100
2	I	88/236 (37%)	85 (97%)	3 (3%)	0	100	100
2	i	88/236 (37%)	85 (97%)	3 (3%)	0	100	100
3	T	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
3	t	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
4	G	110/252 (44%)	107 (97%)	3 (3%)	0	100	100
4	g	110/252 (44%)	107 (97%)	3 (3%)	0	100	100
5	O	147/157 (94%)	141 (96%)	6 (4%)	0	100	100
5	o	147/157 (94%)	140 (95%)	7 (5%)	0	100	100
6	K	115/224 (51%)	111 (96%)	4 (4%)	0	100	100
6	k	115/224 (51%)	112 (97%)	3 (3%)	0	100	100
7	J	174/229 (76%)	171 (98%)	3 (2%)	0	100	100
7	j	174/229 (76%)	171 (98%)	3 (2%)	0	100	100
8	S	93/128 (73%)	92 (99%)	1 (1%)	0	100	100
8	s	93/128 (73%)	92 (99%)	1 (1%)	0	100	100
9	U	92/126 (73%)	90 (98%)	2 (2%)	0	100	100
9	u	92/126 (73%)	90 (98%)	2 (2%)	0	100	100
10	H	224/239 (94%)	215 (96%)	9 (4%)	0	100	100
10	h	224/239 (94%)	214 (96%)	10 (4%)	0	100	100
11	E	138/325 (42%)	135 (98%)	3 (2%)	0	100	100
11	e	138/325 (42%)	135 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	X	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
12	x	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
13	B	251/571 (44%)	247 (98%)	4 (2%)	0	100	100
13	b	251/571 (44%)	247 (98%)	4 (2%)	0	100	100
14	R	88/134 (66%)	84 (96%)	4 (4%)	0	100	100
14	r	88/134 (66%)	84 (96%)	4 (4%)	0	100	100
15	P	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
15	p	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
16	V	108/111 (97%)	108 (100%)	0	0	100	100
16	v	108/111 (97%)	108 (100%)	0	0	100	100
17	L	205/208 (99%)	200 (98%)	5 (2%)	0	100	100
17	l	205/208 (99%)	200 (98%)	5 (2%)	0	100	100
18	C	120/398 (30%)	114 (95%)	6 (5%)	0	100	100
18	c	120/398 (30%)	114 (95%)	6 (5%)	0	100	100
19	D	250/310 (81%)	247 (99%)	3 (1%)	0	100	100
19	d	250/310 (81%)	247 (99%)	3 (1%)	0	100	100
20	M	94/205 (46%)	88 (94%)	6 (6%)	0	100	100
20	m	94/205 (46%)	89 (95%)	5 (5%)	0	100	100
21	N	158/166 (95%)	154 (98%)	4 (2%)	0	100	100
21	n	158/166 (95%)	154 (98%)	4 (2%)	0	100	100
22	F	184/267 (69%)	176 (96%)	8 (4%)	0	100	100
22	f	184/267 (69%)	176 (96%)	8 (4%)	0	100	100
23	W	92/106 (87%)	88 (96%)	4 (4%)	0	100	100
23	w	92/106 (87%)	88 (96%)	4 (4%)	0	100	100
24	A	367/536 (68%)	356 (97%)	11 (3%)	0	100	100
24	a	367/536 (68%)	356 (97%)	11 (3%)	0	100	100
All	All	7010/10832 (65%)	6808 (97%)	202 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	Q	119/120 (99%)	115 (97%)	4 (3%)	32	68
1	q	119/120 (99%)	115 (97%)	4 (3%)	32	68
2	I	71/197 (36%)	70 (99%)	1 (1%)	59	85
2	i	71/197 (36%)	70 (99%)	1 (1%)	59	85
3	T	77/106 (73%)	77 (100%)	0	100	100
3	t	77/106 (73%)	77 (100%)	0	100	100
4	G	93/214 (44%)	93 (100%)	0	100	100
4	g	93/214 (44%)	93 (100%)	0	100	100
5	O	127/129 (98%)	126 (99%)	1 (1%)	73	90
5	o	127/129 (98%)	126 (99%)	1 (1%)	73	90
6	K	100/175 (57%)	100 (100%)	0	100	100
6	k	100/175 (57%)	100 (100%)	0	100	100
7	J	160/195 (82%)	157 (98%)	3 (2%)	50	81
7	j	160/195 (82%)	157 (98%)	3 (2%)	50	81
8	S	86/113 (76%)	86 (100%)	0	100	100
8	s	86/113 (76%)	86 (100%)	0	100	100
9	U	76/98 (78%)	76 (100%)	0	100	100
9	u	76/98 (78%)	76 (100%)	0	100	100
10	H	197/204 (97%)	195 (99%)	2 (1%)	68	88
10	h	197/204 (97%)	195 (99%)	2 (1%)	68	88
11	E	118/258 (46%)	117 (99%)	1 (1%)	73	90
11	e	118/258 (46%)	117 (99%)	1 (1%)	73	90
12	X	70/71 (99%)	69 (99%)	1 (1%)	59	85
12	x	70/71 (99%)	69 (99%)	1 (1%)	59	85
13	B	227/491 (46%)	227 (100%)	0	100	100
13	b	227/491 (46%)	227 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	R	80/117 (68%)	80 (100%)	0	100	100
14	r	80/117 (68%)	80 (100%)	0	100	100
15	P	91/113 (80%)	91 (100%)	0	100	100
15	p	91/113 (80%)	91 (100%)	0	100	100
16	V	86/87 (99%)	86 (100%)	0	100	100
16	v	86/87 (99%)	86 (100%)	0	100	100
17	L	177/178 (99%)	176 (99%)	1 (1%)	78	92
17	l	177/178 (99%)	176 (99%)	1 (1%)	78	92
18	C	107/338 (32%)	105 (98%)	2 (2%)	50	81
18	c	107/338 (32%)	105 (98%)	2 (2%)	50	81
19	D	218/259 (84%)	217 (100%)	1 (0%)	81	93
19	d	218/259 (84%)	217 (100%)	1 (0%)	81	93
20	M	77/156 (49%)	76 (99%)	1 (1%)	61	86
20	m	77/156 (49%)	76 (99%)	1 (1%)	61	86
21	N	138/144 (96%)	138 (100%)	0	100	100
21	n	138/144 (96%)	138 (100%)	0	100	100
22	F	155/218 (71%)	153 (99%)	2 (1%)	61	86
22	f	155/218 (71%)	153 (99%)	2 (1%)	61	86
23	W	84/89 (94%)	84 (100%)	0	100	100
23	w	84/89 (94%)	84 (100%)	0	100	100
24	A	315/447 (70%)	314 (100%)	1 (0%)	86	95
24	a	315/447 (70%)	314 (100%)	1 (0%)	86	95
All	All	6098/9034 (68%)	6056 (99%)	42 (1%)	73	91

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	q	17	LEU
1	q	82	CYS
1	q	87	SER
1	q	90	GLU
2	i	153	SER
5	o	66	LEU
7	j	91	PHE

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Mol	Chain	Res	Type
7	j	190	GLN
7	j	203	THR
10	h	79	THR
10	h	80	ASP
11	e	261	GLU
12	x	3	THR
17	l	47	ASP
18	c	86	THR
18	c	117	GLU
19	d	73	VAL
20	m	103	ASP
22	f	163	SER
22	f	209	SER
24	a	354	ASP
1	Q	17	LEU
1	Q	82	CYS
1	Q	87	SER
1	Q	90	GLU
2	I	153	SER
5	O	66	LEU
7	J	91	PHE
7	J	190	GLN
7	J	203	THR
10	H	79	THR
10	H	80	ASP
11	E	261	GLU
12	X	3	THR
17	L	47	ASP
18	C	86	THR
18	C	117	GLU
19	D	73	VAL
20	M	103	ASP
22	F	163	SER
22	F	209	SER
24	A	354	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	q	25	GLN
1	q	133	HIS
2	i	206	HIS

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Mol	Chain	Res	Type
3	t	88	GLN
4	g	156	GLN
4	g	169	GLN
5	o	69	HIS
7	j	86	ASN
7	j	137	HIS
7	j	199	ASN
7	j	210	HIS
7	j	217	GLN
10	h	33	GLN
10	h	39	HIS
14	r	54	HIS
17	l	172	GLN
18	c	42	GLN
19	d	46	HIS
20	m	132	ASN
21	n	10	GLN
22	f	115	ASN
22	f	167	ASN
22	f	251	HIS
23	w	49	GLN
24	a	155	ASN
24	a	321	GLN
24	a	411	HIS
1	Q	25	GLN
1	Q	133	HIS
2	I	206	HIS
3	T	88	GLN
4	G	156	GLN
4	G	169	GLN
5	O	69	HIS
7	J	86	ASN
7	J	137	HIS
7	J	199	ASN
7	J	210	HIS
10	H	39	HIS
12	X	28	ASN
14	R	54	HIS
16	V	80	HIS
16	V	88	GLN
17	L	172	GLN
19	D	46	HIS

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Mol	Chain	Res	Type
22	F	115	ASN
22	F	250	HIS
22	F	251	HIS
23	W	49	GLN
24	A	155	ASN
24	A	180	GLN
24	A	321	GLN
24	A	411	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

44 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
27	CDL	O	203	-	99,99,99	0.89	7 (7%)	105,111,111	1.06	5 (4%)
28	PEE	j	302	-	50,50,50	1.16	6 (12%)	53,55,55	1.17	3 (5%)
28	PEE	c	402	-	50,50,50	1.17	6 (12%)	53,55,55	1.06	3 (5%)
28	PEE	J	301	-	50,50,50	1.15	6 (12%)	53,55,55	1.14	3 (5%)
27	CDL	V	202	-	99,99,99	0.90	7 (7%)	105,111,111	1.00	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CDL	d	402	-	99,99,99	0.89	8 (8%)	105,111,111	1.04	4 (3%)
26	LMT	d	401	-	36,36,36	1.14	2 (5%)	47,47,47	0.96	1 (2%)
26	LMT	D	401	-	36,36,36	1.14	2 (5%)	47,47,47	0.96	1 (2%)
27	CDL	h	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.04	4 (3%)
25	PC1	o	201	-	53,53,53	0.96	3 (5%)	59,61,61	1.04	3 (5%)
27	CDL	E	401	-	99,99,99	0.88	8 (8%)	105,111,111	1.03	4 (3%)
25	PC1	O	204	-	53,53,53	0.96	4 (7%)	59,61,61	1.00	2 (3%)
26	LMT	h	301	-	36,36,36	1.13	2 (5%)	47,47,47	0.99	1 (2%)
27	CDL	u	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.06	4 (3%)
27	CDL	U	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.06	4 (3%)
27	CDL	D	402	-	99,99,99	0.88	8 (8%)	105,111,111	1.04	4 (3%)
25	PC1	v	202	-	53,53,53	0.98	4 (7%)	59,61,61	0.96	2 (3%)
27	CDL	H	302	-	99,99,99	0.89	7 (7%)	105,111,111	1.04	4 (3%)
28	PEE	j	301	-	50,50,50	1.15	6 (12%)	53,55,55	1.14	3 (5%)
28	PEE	J	302	-	50,50,50	1.16	6 (12%)	53,55,55	1.17	3 (5%)
25	PC1	o	204	-	53,53,53	0.96	4 (7%)	59,61,61	1.01	2 (3%)
27	CDL	o	203	-	99,99,99	0.89	7 (7%)	105,111,111	1.06	5 (4%)
27	CDL	B	602	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	4 (3%)
26	LMT	C	401	-	36,36,36	1.08	2 (5%)	47,47,47	1.14	2 (4%)
26	LMT	H	301	-	36,36,36	1.13	2 (5%)	47,47,47	0.99	2 (4%)
27	CDL	B	601	-	99,99,99	0.89	8 (8%)	105,111,111	1.06	4 (3%)
27	CDL	v	201	-	99,99,99	0.90	7 (7%)	105,111,111	1.00	4 (3%)
26	LMT	x	101	-	36,36,36	1.16	3 (8%)	47,47,47	1.06	2 (4%)
27	CDL	V	201	-	99,99,99	0.89	7 (7%)	105,111,111	1.06	4 (3%)
26	LMT	D	403	-	36,36,36	1.12	2 (5%)	47,47,47	0.91	0
27	CDL	b	601	-	99,99,99	0.90	8 (8%)	105,111,111	1.03	4 (3%)
26	LMT	o	202	-	36,36,36	1.11	2 (5%)	47,47,47	0.94	1 (2%)
27	CDL	C	404	-	99,99,99	0.89	8 (8%)	105,111,111	1.05	4 (3%)
25	PC1	O	201	-	53,53,53	0.96	3 (5%)	59,61,61	1.04	3 (5%)
27	CDL	e	401	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	4 (3%)
25	PC1	V	203	-	53,53,53	0.98	4 (7%)	59,61,61	0.96	2 (3%)
26	LMT	O	202	-	36,36,36	1.12	2 (5%)	47,47,47	0.94	1 (2%)
26	LMT	C	403	-	36,36,36	1.11	2 (5%)	47,47,47	1.04	1 (2%)
27	CDL	c	404	-	99,99,99	0.88	7 (7%)	105,111,111	1.05	4 (3%)
26	LMT	c	403	-	36,36,36	1.11	2 (5%)	47,47,47	1.04	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LMT	c	401	-	36,36,36	1.08	2 (5%)	47,47,47	1.14	2 (4%)
26	LMT	d	403	-	36,36,36	1.12	2 (5%)	47,47,47	0.92	0
26	LMT	X	101	-	36,36,36	1.16	3 (8%)	47,47,47	1.06	2 (4%)
28	PEE	C	402	-	50,50,50	1.16	6 (12%)	53,55,55	1.06	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CDL	O	203	-	-	47/110/110/110	-
28	PEE	j	302	-	-	22/54/54/54	-
28	PEE	c	402	-	-	17/54/54/54	-
28	PEE	J	301	-	-	18/54/54/54	-
27	CDL	V	202	-	-	36/110/110/110	-
27	CDL	d	402	-	-	34/110/110/110	-
26	LMT	d	401	-	-	12/21/61/61	0/2/2/2
26	LMT	D	401	-	-	12/21/61/61	0/2/2/2
27	CDL	h	302	-	-	46/110/110/110	-
25	PC1	o	201	-	-	18/57/57/57	-
27	CDL	E	401	-	-	35/110/110/110	-
25	PC1	O	204	-	-	26/57/57/57	-
26	LMT	h	301	-	-	7/21/61/61	0/2/2/2
27	CDL	u	201	-	-	35/110/110/110	-
27	CDL	U	201	-	-	35/110/110/110	-
27	CDL	D	402	-	-	34/110/110/110	-
25	PC1	v	202	-	-	24/57/57/57	-
27	CDL	H	302	-	-	46/110/110/110	-
28	PEE	j	301	-	-	18/54/54/54	-
28	PEE	J	302	-	-	22/54/54/54	-
25	PC1	o	204	-	-	26/57/57/57	-
27	CDL	o	203	-	-	47/110/110/110	-
27	CDL	B	602	-	-	42/110/110/110	-
26	LMT	C	401	-	-	6/21/61/61	0/2/2/2
26	LMT	H	301	-	-	7/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CDL	B	601	-	-	43/110/110/110	-
27	CDL	v	201	-	-	36/110/110/110	-
26	LMT	x	101	-	-	12/21/61/61	0/2/2/2
27	CDL	V	201	-	-	43/110/110/110	-
26	LMT	D	403	-	-	5/21/61/61	0/2/2/2
27	CDL	b	601	-	-	42/110/110/110	-
26	LMT	o	202	-	-	3/21/61/61	0/2/2/2
27	CDL	C	404	-	-	41/110/110/110	-
25	PC1	O	201	-	-	18/57/57/57	-
27	CDL	e	401	-	-	35/110/110/110	-
25	PC1	V	203	-	-	24/57/57/57	-
26	LMT	O	202	-	-	3/21/61/61	0/2/2/2
26	LMT	C	403	-	-	4/21/61/61	0/2/2/2
27	CDL	c	404	-	-	41/110/110/110	-
26	LMT	c	403	-	-	4/21/61/61	0/2/2/2
26	LMT	c	401	-	-	6/21/61/61	0/2/2/2
26	LMT	d	403	-	-	5/21/61/61	0/2/2/2
26	LMT	X	101	-	-	12/21/61/61	0/2/2/2
28	PEE	C	402	-	-	17/54/54/54	-

All (225) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	402	PEE	C18-C19	3.82	1.53	1.31
28	J	302	PEE	C39-C38	3.82	1.53	1.31
28	j	302	PEE	C39-C38	3.82	1.53	1.31
28	C	402	PEE	C18-C19	3.82	1.53	1.31
28	c	402	PEE	C39-C38	3.81	1.53	1.31
28	C	402	PEE	C39-C38	3.81	1.53	1.31
28	j	301	PEE	C39-C38	3.80	1.53	1.31
28	J	301	PEE	C39-C38	3.80	1.53	1.31
28	J	302	PEE	C18-C19	3.78	1.53	1.31
28	j	302	PEE	C18-C19	3.77	1.53	1.31
28	j	301	PEE	C18-C19	3.70	1.52	1.31
28	J	301	PEE	C18-C19	3.70	1.52	1.31
26	O	202	LMT	O5B-C1B	3.42	1.50	1.41
26	d	401	LMT	O5B-C1B	3.41	1.50	1.41
26	D	401	LMT	O5B-C1B	3.40	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	o	202	LMT	O5B-C1B	3.40	1.50	1.41
26	X	101	LMT	O5B-C1B	3.37	1.50	1.41
26	x	101	LMT	O5B-C1B	3.35	1.50	1.41
26	H	301	LMT	O5'-C1'	3.33	1.50	1.41
26	H	301	LMT	O5B-C1B	3.33	1.50	1.41
26	h	301	LMT	O5'-C1'	3.33	1.50	1.41
26	X	101	LMT	O5'-C1'	3.32	1.50	1.41
26	d	403	LMT	O5B-C1B	3.31	1.50	1.41
26	h	301	LMT	O5B-C1B	3.30	1.50	1.41
26	C	401	LMT	O5B-C1B	3.30	1.50	1.41
26	c	401	LMT	O5B-C1B	3.30	1.50	1.41
26	D	403	LMT	O5B-C1B	3.29	1.50	1.41
26	x	101	LMT	O5'-C1'	3.29	1.50	1.41
26	c	403	LMT	O5B-C1B	3.25	1.50	1.41
26	C	403	LMT	O5B-C1B	3.22	1.50	1.41
26	d	401	LMT	O5'-C1'	3.20	1.50	1.41
26	D	401	LMT	O5'-C1'	3.16	1.50	1.41
26	d	403	LMT	O5'-C1'	3.03	1.49	1.41
26	D	403	LMT	O5'-C1'	3.02	1.49	1.41
26	c	403	LMT	O5'-C1'	3.01	1.49	1.41
26	C	403	LMT	O5'-C1'	3.01	1.49	1.41
26	o	202	LMT	O5'-C1'	2.96	1.49	1.41
26	O	202	LMT	O5'-C1'	2.96	1.49	1.41
26	c	401	LMT	O5'-C1'	2.92	1.49	1.41
27	o	203	CDL	OA6-CA4	-2.91	1.39	1.46
25	o	201	PC1	O21-C2	-2.90	1.39	1.46
25	O	201	PC1	O21-C2	-2.90	1.39	1.46
27	u	201	CDL	OA6-CA4	-2.89	1.39	1.46
26	C	401	LMT	O5'-C1'	2.89	1.49	1.41
27	U	201	CDL	OA6-CA4	-2.88	1.39	1.46
27	O	203	CDL	OA6-CA4	-2.87	1.39	1.46
27	e	401	CDL	OB6-CB4	-2.86	1.39	1.46
27	B	601	CDL	OA6-CA4	-2.86	1.39	1.46
27	V	201	CDL	OB6-CB4	-2.86	1.39	1.46
27	E	401	CDL	OB6-CB4	-2.85	1.39	1.46
27	V	201	CDL	OA6-CA4	-2.84	1.39	1.46
27	B	601	CDL	OB6-CB4	-2.83	1.40	1.46
27	h	302	CDL	OB6-CB4	-2.81	1.40	1.46
27	H	302	CDL	OB6-CB4	-2.81	1.40	1.46
27	B	602	CDL	OB6-CB4	-2.79	1.40	1.46
27	C	404	CDL	OB6-CB4	-2.79	1.40	1.46
27	b	601	CDL	OB6-CB4	-2.79	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	h	302	CDL	OA6-CA4	-2.77	1.40	1.46
27	U	201	CDL	OB6-CB4	-2.76	1.40	1.46
27	c	404	CDL	OB6-CB4	-2.76	1.40	1.46
27	O	203	CDL	OB6-CB4	-2.75	1.40	1.46
27	H	302	CDL	OA6-CA4	-2.75	1.40	1.46
27	o	203	CDL	OB6-CB4	-2.75	1.40	1.46
27	D	402	CDL	OB6-CB4	-2.75	1.40	1.46
27	d	402	CDL	OB6-CB4	-2.73	1.40	1.46
27	u	201	CDL	OB6-CB4	-2.71	1.40	1.46
27	v	201	CDL	OA6-CA4	-2.69	1.40	1.46
27	V	202	CDL	OA6-CA4	-2.69	1.40	1.46
27	V	202	CDL	OB6-CB4	-2.69	1.40	1.46
28	j	301	PEE	O2-C2	-2.67	1.40	1.46
27	v	201	CDL	OB6-CB4	-2.67	1.40	1.46
28	J	301	PEE	O2-C2	-2.66	1.40	1.46
25	O	204	PC1	O21-C2	-2.66	1.40	1.46
27	E	401	CDL	OA6-CA4	-2.65	1.40	1.46
25	o	204	PC1	O21-C2	-2.64	1.40	1.46
28	j	302	PEE	O2-C2	-2.63	1.40	1.46
27	e	401	CDL	OA6-CA4	-2.62	1.40	1.46
27	C	404	CDL	OA6-CA4	-2.62	1.40	1.46
28	J	302	PEE	O2-C2	-2.62	1.40	1.46
27	V	202	CDL	OB8-CB7	2.61	1.41	1.33
27	v	201	CDL	OB8-CB7	2.60	1.40	1.33
27	c	404	CDL	OA6-CA4	-2.60	1.40	1.46
27	b	601	CDL	OA6-CA4	-2.58	1.40	1.46
27	B	602	CDL	OA6-CA4	-2.56	1.40	1.46
25	V	203	PC1	O21-C2	-2.56	1.40	1.46
27	C	404	CDL	OA8-CA7	2.55	1.40	1.33
25	v	202	PC1	O21-C2	-2.54	1.40	1.46
28	c	402	PEE	O2-C2	-2.54	1.40	1.46
28	C	402	PEE	O2-C2	-2.53	1.40	1.46
27	u	201	CDL	OB8-CB7	2.53	1.40	1.33
27	c	404	CDL	OA8-CA7	2.53	1.40	1.33
27	U	201	CDL	OB8-CB7	2.51	1.40	1.33
27	B	602	CDL	OA8-CA7	2.51	1.40	1.33
27	u	201	CDL	OA8-CA7	2.51	1.40	1.33
27	U	201	CDL	OA8-CA7	2.50	1.40	1.33
27	e	401	CDL	OA8-CA7	2.49	1.40	1.33
27	b	601	CDL	OA8-CA7	2.49	1.40	1.33
27	B	601	CDL	OA8-CA7	2.47	1.40	1.33
27	E	401	CDL	OA8-CA7	2.47	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	V	202	CDL	OA8-CA7	2.47	1.40	1.33
27	v	201	CDL	OA8-CA7	2.46	1.40	1.33
27	D	402	CDL	OA6-CA4	-2.45	1.40	1.46
28	j	302	PEE	O3-C30	2.44	1.40	1.33
25	v	202	PC1	O31-C31	2.44	1.40	1.33
27	C	404	CDL	OB8-CB7	2.44	1.40	1.33
27	d	402	CDL	OA6-CA4	-2.43	1.40	1.46
27	c	404	CDL	OB8-CB7	2.43	1.40	1.33
25	V	203	PC1	O31-C31	2.42	1.40	1.33
27	O	203	CDL	OB8-CB7	2.42	1.40	1.33
27	b	601	CDL	OB8-CB7	2.42	1.40	1.33
27	V	201	CDL	OA8-CA7	2.42	1.40	1.33
27	O	203	CDL	OA8-CA7	2.42	1.40	1.33
27	d	402	CDL	OB8-CB7	2.42	1.40	1.33
27	o	203	CDL	OB8-CB7	2.41	1.40	1.33
28	J	302	PEE	O3-C30	2.41	1.40	1.33
28	C	402	PEE	O3-C30	2.41	1.40	1.33
28	c	402	PEE	O3-C30	2.41	1.40	1.33
27	B	602	CDL	OB8-CB7	2.40	1.40	1.33
27	H	302	CDL	OB8-CB7	2.40	1.40	1.33
27	h	302	CDL	OB8-CB7	2.40	1.40	1.33
25	O	204	PC1	O31-C31	2.39	1.40	1.33
25	o	201	PC1	O31-C3	-2.38	1.39	1.45
27	o	203	CDL	OA8-CA7	2.38	1.40	1.33
27	h	302	CDL	OA8-CA7	2.38	1.40	1.33
25	o	204	PC1	O31-C31	2.37	1.40	1.33
27	H	302	CDL	OA8-CA7	2.37	1.40	1.33
27	D	402	CDL	OB8-CB7	2.36	1.40	1.33
27	e	401	CDL	OB8-CB7	2.36	1.40	1.33
27	V	201	CDL	OB8-CB7	2.35	1.40	1.33
27	d	402	CDL	OA8-CA7	2.34	1.40	1.33
27	E	401	CDL	OB8-CB7	2.34	1.40	1.33
27	B	601	CDL	OB8-CB7	2.34	1.40	1.33
25	O	201	PC1	O31-C3	-2.33	1.40	1.45
28	J	301	PEE	O3-C30	2.31	1.40	1.33
27	D	402	CDL	OA8-CA7	2.30	1.40	1.33
28	j	301	PEE	O3-C30	2.29	1.40	1.33
28	J	301	PEE	O3-C3	-2.29	1.40	1.45
25	o	201	PC1	O31-C31	2.28	1.40	1.33
25	O	201	PC1	O31-C31	2.28	1.40	1.33
27	b	601	CDL	OA6-CA5	2.27	1.40	1.34
28	j	301	PEE	O3-C3	-2.26	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	402	CDL	OA8-CA6	-2.25	1.40	1.45
27	B	602	CDL	OA6-CA5	2.25	1.40	1.34
27	e	401	CDL	OB8-CB6	-2.25	1.40	1.45
27	d	402	CDL	OB8-CB6	-2.25	1.40	1.45
27	D	402	CDL	OA8-CA6	-2.25	1.40	1.45
27	B	601	CDL	OB8-CB6	-2.25	1.40	1.45
27	b	601	CDL	OB8-CB6	-2.24	1.40	1.45
27	C	404	CDL	OB8-CB6	-2.24	1.40	1.45
27	V	202	CDL	OA6-CA5	2.24	1.40	1.34
27	O	203	CDL	OB8-CB6	-2.23	1.40	1.45
27	V	202	CDL	OB6-CB5	2.23	1.40	1.34
27	V	201	CDL	OB8-CB6	-2.23	1.40	1.45
27	D	402	CDL	OB8-CB6	-2.22	1.40	1.45
27	c	404	CDL	OB8-CB6	-2.22	1.40	1.45
27	O	203	CDL	OA8-CA6	-2.22	1.40	1.45
27	B	602	CDL	OB8-CB6	-2.22	1.40	1.45
27	v	201	CDL	OA6-CA5	2.22	1.40	1.34
27	E	401	CDL	OB8-CB6	-2.22	1.40	1.45
27	o	203	CDL	OB8-CB6	-2.21	1.40	1.45
27	o	203	CDL	OA8-CA6	-2.21	1.40	1.45
25	O	204	PC1	O21-C21	2.20	1.40	1.34
27	B	601	CDL	OA8-CA6	-2.20	1.40	1.45
25	o	204	PC1	O21-C21	2.20	1.40	1.34
28	c	402	PEE	O3-C3	-2.19	1.40	1.45
27	d	402	CDL	OB6-CB5	2.19	1.40	1.34
27	v	201	CDL	OB6-CB5	2.19	1.40	1.34
27	V	201	CDL	OA8-CA6	-2.19	1.40	1.45
27	h	302	CDL	OB8-CB6	-2.19	1.40	1.45
25	V	203	PC1	O21-C21	2.18	1.40	1.34
27	D	402	CDL	OB6-CB5	2.18	1.40	1.34
27	H	302	CDL	OB8-CB6	-2.18	1.40	1.45
27	h	302	CDL	OA8-CA6	-2.17	1.40	1.45
25	v	202	PC1	O21-C21	2.17	1.40	1.34
28	J	302	PEE	O2-C10	2.17	1.40	1.34
27	b	601	CDL	OA8-CA6	-2.17	1.40	1.45
27	D	402	CDL	OA6-CA5	2.16	1.40	1.34
27	U	201	CDL	OA6-CA5	2.16	1.40	1.34
27	d	402	CDL	OA6-CA5	2.15	1.40	1.34
27	u	201	CDL	OA6-CA5	2.15	1.40	1.34
28	C	402	PEE	O3-C3	-2.15	1.40	1.45
27	C	404	CDL	OA6-CA5	2.14	1.40	1.34
27	O	203	CDL	OB6-CB5	2.14	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	j	302	PEE	O2-C10	2.14	1.40	1.34
27	C	404	CDL	OB6-CB5	2.13	1.40	1.34
27	B	602	CDL	OA8-CA6	-2.13	1.40	1.45
27	U	201	CDL	OA8-CA6	-2.13	1.40	1.45
28	c	402	PEE	O2-C10	2.12	1.40	1.34
27	H	302	CDL	OA8-CA6	-2.12	1.40	1.45
27	h	302	CDL	OA6-CA5	2.12	1.40	1.34
27	H	302	CDL	OA6-CA5	2.11	1.40	1.34
28	j	301	PEE	O2-C10	2.11	1.40	1.34
28	C	402	PEE	O2-C10	2.11	1.40	1.34
27	V	202	CDL	OA8-CA6	-2.11	1.40	1.45
27	c	404	CDL	OB6-CB5	2.10	1.40	1.34
28	J	301	PEE	O2-C10	2.10	1.40	1.34
27	o	203	CDL	OB6-CB5	2.10	1.40	1.34
25	o	204	PC1	O31-C3	-2.10	1.40	1.45
27	u	201	CDL	OA8-CA6	-2.10	1.40	1.45
25	O	204	PC1	O31-C3	-2.09	1.40	1.45
27	c	404	CDL	OA6-CA5	2.09	1.40	1.34
25	V	203	PC1	O31-C3	-2.09	1.40	1.45
25	v	202	PC1	O31-C3	-2.09	1.40	1.45
27	V	201	CDL	OB6-CB5	2.08	1.40	1.34
27	v	201	CDL	OA8-CA6	-2.08	1.40	1.45
27	E	401	CDL	OA8-CA6	-2.08	1.40	1.45
27	b	601	CDL	OB6-CB5	2.08	1.40	1.34
27	e	401	CDL	OA8-CA6	-2.07	1.40	1.45
27	B	602	CDL	OB6-CB5	2.07	1.40	1.34
28	j	302	PEE	O3-C3	-2.07	1.40	1.45
27	e	401	CDL	OB6-CB5	2.07	1.40	1.34
27	U	201	CDL	OB6-CB5	2.07	1.40	1.34
28	J	302	PEE	O3-C3	-2.07	1.40	1.45
27	B	601	CDL	OB6-CB5	2.06	1.40	1.34
27	e	401	CDL	OA6-CA5	2.06	1.40	1.34
26	x	101	LMT	O5'-C5'	2.06	1.49	1.44
27	E	401	CDL	OB6-CB5	2.06	1.40	1.34
27	E	401	CDL	OA6-CA5	2.05	1.40	1.34
27	u	201	CDL	OB6-CB5	2.04	1.40	1.34
26	X	101	LMT	O5'-C5'	2.03	1.49	1.44
27	U	201	CDL	OB8-CB6	-2.03	1.40	1.45
27	h	302	CDL	OB6-CB5	2.03	1.40	1.34
27	C	404	CDL	OA8-CA6	-2.01	1.40	1.45
27	u	201	CDL	OB8-CB6	-2.01	1.40	1.45
27	B	601	CDL	OA6-CA5	2.00	1.39	1.34

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	402	CDL	OB6-CB5-C51	4.17	120.50	111.48
27	d	402	CDL	OB6-CB5-C51	4.16	120.47	111.48
27	B	602	CDL	OB6-CB5-C51	4.11	120.37	111.48
25	o	204	PC1	O21-C21-C22	4.09	120.34	111.48
27	b	601	CDL	OB6-CB5-C51	4.09	120.33	111.48
27	c	404	CDL	OB6-CB5-C51	4.08	120.30	111.48
25	O	204	PC1	O21-C21-C22	4.07	120.29	111.48
27	C	404	CDL	OB6-CB5-C51	4.07	120.29	111.48
25	O	201	PC1	O21-C21-C22	4.07	120.29	111.48
25	o	201	PC1	O21-C21-C22	4.06	120.27	111.48
27	U	201	CDL	OB6-CB5-C51	4.05	120.24	111.48
27	u	201	CDL	OB6-CB5-C51	4.04	120.23	111.48
27	v	201	CDL	OB6-CB5-C51	4.00	120.13	111.48
27	V	202	CDL	OB6-CB5-C51	3.97	120.07	111.48
27	B	601	CDL	OB6-CB5-C51	3.94	120.00	111.48
28	J	301	PEE	O2-C10-C11	3.94	120.00	111.48
28	j	301	PEE	O2-C10-C11	3.94	120.00	111.48
27	V	201	CDL	OB6-CB5-C51	3.94	119.99	111.48
27	h	302	CDL	OB6-CB5-C51	3.89	119.89	111.48
27	H	302	CDL	OB6-CB5-C51	3.86	119.82	111.48
28	j	302	PEE	O2-C10-C11	3.80	119.69	111.48
27	o	203	CDL	OA6-CA5-C11	3.78	119.67	111.48
27	O	203	CDL	OA6-CA5-C11	3.77	119.64	111.48
27	d	402	CDL	OA6-CA5-C11	3.77	119.63	111.48
27	D	402	CDL	OA6-CA5-C11	3.77	119.63	111.48
25	v	202	PC1	O21-C21-C22	3.76	119.62	111.48
28	J	302	PEE	O2-C10-C11	3.76	119.62	111.48
27	O	203	CDL	OB6-CB5-C51	3.76	119.61	111.48
25	V	203	PC1	O21-C21-C22	3.76	119.61	111.48
27	o	203	CDL	OB6-CB5-C51	3.76	119.61	111.48
27	e	401	CDL	OA6-CA5-C11	3.67	119.41	111.48
27	E	401	CDL	OA6-CA5-C11	3.66	119.40	111.48
27	B	602	CDL	OA6-CA5-C11	3.61	119.28	111.48
27	B	601	CDL	OA6-CA5-C11	3.60	119.27	111.48
27	V	201	CDL	OA6-CA5-C11	3.60	119.26	111.48
26	x	101	LMT	O5'-C5'-C4'	3.59	117.14	109.72
27	b	601	CDL	OA6-CA5-C11	3.58	119.22	111.48
26	X	101	LMT	O5'-C5'-C4'	3.56	117.07	109.72
28	c	402	PEE	O2-C10-C11	3.47	118.98	111.48
27	v	201	CDL	OA6-CA5-C11	3.45	118.95	111.48
27	V	202	CDL	OA6-CA5-C11	3.45	118.94	111.48
28	C	402	PEE	O2-C10-C11	3.45	118.94	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	404	CDL	OA8-CA7-C31	3.37	122.11	111.83
27	h	302	CDL	OA6-CA5-C11	3.37	118.77	111.48
27	H	302	CDL	OA6-CA5-C11	3.37	118.76	111.48
27	C	404	CDL	OA8-CA7-C31	3.36	122.06	111.83
27	c	404	CDL	OA6-CA5-C11	3.33	118.69	111.48
27	C	404	CDL	OA6-CA5-C11	3.31	118.64	111.48
27	u	201	CDL	OA6-CA5-C11	3.27	118.55	111.48
27	U	201	CDL	OA6-CA5-C11	3.24	118.49	111.48
27	U	201	CDL	OA8-CA7-C31	3.04	121.11	111.83
27	u	201	CDL	OA8-CA7-C31	3.03	121.07	111.83
27	e	401	CDL	OB6-CB5-C51	2.95	117.86	111.48
27	E	401	CDL	OB6-CB5-C51	2.95	117.85	111.48
26	d	401	LMT	C1B-O1B-C4'	-2.92	111.06	117.98
26	D	401	LMT	C1B-O1B-C4'	-2.91	111.09	117.98
27	B	601	CDL	OA8-CA7-C31	2.88	120.62	111.83
27	V	201	CDL	OA8-CA7-C31	2.87	120.59	111.83
27	h	302	CDL	OA8-CA7-C31	2.78	120.32	111.83
27	H	302	CDL	OA8-CA7-C31	2.77	120.27	111.83
27	E	401	CDL	OB8-CB7-C71	2.76	120.24	111.83
27	e	401	CDL	OB8-CB7-C71	2.76	120.24	111.83
25	v	202	PC1	O31-C31-C32	2.74	120.20	111.83
25	V	203	PC1	O31-C31-C32	2.73	120.16	111.83
28	J	302	PEE	O3-C30-C31	2.69	120.05	111.83
27	D	402	CDL	OB8-CB7-C71	2.69	120.03	111.83
27	d	402	CDL	OB8-CB7-C71	2.68	120.00	111.83
25	O	204	PC1	O31-C31-C32	2.68	120.00	111.83
25	o	204	PC1	O31-C31-C32	2.68	120.00	111.83
28	j	302	PEE	O3-C30-C31	2.67	119.99	111.83
27	b	601	CDL	OA8-CA7-C31	2.64	119.88	111.83
27	B	602	CDL	OA8-CA7-C31	2.64	119.87	111.83
27	v	201	CDL	OB8-CB7-C71	2.63	119.85	111.83
27	E	401	CDL	OA8-CA7-C31	2.63	119.84	111.83
27	e	401	CDL	OA8-CA7-C31	2.62	119.83	111.83
25	O	201	PC1	O31-C31-C32	2.61	119.81	111.83
27	V	202	CDL	OB8-CB7-C71	2.61	119.80	111.83
25	o	201	PC1	O31-C31-C32	2.61	119.79	111.83
27	U	201	CDL	OB8-CB7-C71	2.57	119.68	111.83
26	C	403	LMT	C1B-O1B-C4'	-2.56	111.91	117.98
26	c	403	LMT	C1B-O1B-C4'	-2.56	111.91	117.98
27	u	201	CDL	OB8-CB7-C71	2.56	119.63	111.83
27	O	203	CDL	OB8-CB7-C71	2.55	119.61	111.83
27	o	203	CDL	OB8-CB7-C71	2.54	119.58	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	h	302	CDL	OB8-CB7-C71	2.52	119.53	111.83
27	B	601	CDL	OB8-CB7-C71	2.52	119.51	111.83
27	V	201	CDL	OB8-CB7-C71	2.52	119.51	111.83
27	H	302	CDL	OB8-CB7-C71	2.50	119.46	111.83
25	o	201	PC1	C2-O21-C21	-2.48	111.86	117.80
28	c	402	PEE	O3-C30-C31	2.47	119.38	111.83
25	O	201	PC1	C2-O21-C21	-2.47	111.88	117.80
28	j	301	PEE	O3-C30-C31	2.46	119.33	111.83
27	b	601	CDL	OB8-CB7-C71	2.45	119.31	111.83
27	C	404	CDL	OB8-CB7-C71	2.45	119.31	111.83
28	C	402	PEE	O3-C30-C31	2.45	119.30	111.83
27	c	404	CDL	OB8-CB7-C71	2.45	119.29	111.83
27	o	203	CDL	OA8-CA7-C31	2.44	119.29	111.83
28	J	301	PEE	O3-C30-C31	2.44	119.28	111.83
27	O	203	CDL	OA8-CA7-C31	2.44	119.27	111.83
27	o	203	CDL	CA4-OA6-CA5	-2.44	111.96	117.80
27	O	203	CDL	CA4-OA6-CA5	-2.44	111.96	117.80
27	B	602	CDL	OB8-CB7-C71	2.43	119.25	111.83
27	V	202	CDL	OA8-CA7-C31	2.38	119.10	111.83
27	v	201	CDL	OA8-CA7-C31	2.38	119.10	111.83
27	D	402	CDL	OA8-CA7-C31	2.38	119.09	111.83
26	X	101	LMT	C1B-O1B-C4'	-2.38	112.34	117.98
26	x	101	LMT	C1B-O1B-C4'	-2.37	112.36	117.98
27	d	402	CDL	OA8-CA7-C31	2.36	119.05	111.83
26	c	401	LMT	C1'-O5'-C5'	-2.34	109.15	113.72
26	C	401	LMT	C1'-O5'-C5'	-2.31	109.20	113.72
26	O	202	LMT	O5'-C5'-C4'	2.21	114.30	109.72
26	o	202	LMT	O5'-C5'-C4'	2.21	114.30	109.72
28	j	301	PEE	C17-C18-C19	-2.12	108.92	124.83
26	h	301	LMT	O1B-C4'-C3'	2.12	112.63	107.23
28	J	301	PEE	C17-C18-C19	-2.12	108.96	124.83
26	C	401	LMT	C2'-C3'-C4'	2.11	114.48	109.68
26	H	301	LMT	O1B-C4'-C3'	2.10	112.58	107.23
28	j	302	PEE	C40-C39-C38	-2.10	109.07	124.83
28	J	302	PEE	C40-C39-C38	-2.10	109.09	124.83
26	c	401	LMT	C2'-C3'-C4'	2.09	114.43	109.68
28	C	402	PEE	C37-C38-C39	-2.06	109.44	124.83
28	c	402	PEE	C37-C38-C39	-2.05	109.44	124.83
26	H	301	LMT	C3B-C4B-C5B	2.01	113.87	110.23

There are no chirality outliers.

All (1066) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	o	201	PC1	O13-C11-C12-N
25	o	201	PC1	C22-C21-O21-C2
25	o	204	PC1	C22-C21-O21-C2
25	v	202	PC1	C1-O11-P-O13
25	v	202	PC1	C12-C11-O13-P
25	v	202	PC1	O13-C11-C12-N
25	v	202	PC1	O22-C21-O21-C2
25	v	202	PC1	C22-C21-O21-C2
25	O	201	PC1	O13-C11-C12-N
25	O	201	PC1	C22-C21-O21-C2
25	O	204	PC1	C22-C21-O21-C2
25	V	203	PC1	C1-O11-P-O13
25	V	203	PC1	C12-C11-O13-P
25	V	203	PC1	O13-C11-C12-N
25	V	203	PC1	O22-C21-O21-C2
26	h	301	LMT	O5'-C1'-O1'-C1
26	x	101	LMT	C2'-C1'-O1'-C1
26	c	403	LMT	O5'-C1'-O1'-C1
26	H	301	LMT	O5'-C1'-O1'-C1
26	X	101	LMT	C2'-C1'-O1'-C1
26	C	403	LMT	O5'-C1'-O1'-C1
27	o	203	CDL	CA2-OA2-PA1-OA5
27	o	203	CDL	CA3-OA5-PA1-OA2
27	o	203	CDL	CA3-OA5-PA1-OA4
27	o	203	CDL	C11-CA5-OA6-CA4
27	o	203	CDL	CB2-OB2-PB2-OB3
27	o	203	CDL	CB3-OB5-PB2-OB2
27	o	203	CDL	CB3-OB5-PB2-OB3
27	o	203	CDL	CB3-OB5-PB2-OB4
27	u	201	CDL	CA3-OA5-PA1-OA4
27	h	302	CDL	CA2-OA2-PA1-OA5
27	h	302	CDL	OA6-CA4-CA6-OA8
27	e	401	CDL	CA3-OA5-PA1-OA2
27	e	401	CDL	C1-CB2-OB2-PB2
27	e	401	CDL	CB2-OB2-PB2-OB3
27	e	401	CDL	CB3-OB5-PB2-OB2
27	e	401	CDL	CB3-OB5-PB2-OB4
27	b	601	CDL	CA2-OA2-PA1-OA3
27	b	601	CDL	CA2-OA2-PA1-OA4
27	b	601	CDL	CA2-OA2-PA1-OA5
27	b	601	CDL	CA3-OA5-PA1-OA3
27	b	601	CDL	C51-CB5-OB6-CB4
27	v	201	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
27	v	201	CDL	CA3-OA5-PA1-OA3
27	v	201	CDL	CA3-OA5-PA1-OA4
27	v	201	CDL	CB3-OB5-PB2-OB2
27	v	201	CDL	CB3-OB5-PB2-OB3
27	v	201	CDL	CB3-OB5-PB2-OB4
27	c	404	CDL	CB3-OB5-PB2-OB4
27	c	404	CDL	C51-CB5-OB6-CB4
27	d	402	CDL	CA2-OA2-PA1-OA3
27	d	402	CDL	C1-CB2-OB2-PB2
27	d	402	CDL	CB2-OB2-PB2-OB5
27	d	402	CDL	OB6-CB4-CB6-OB8
27	d	402	CDL	C51-CB5-OB6-CB4
27	O	203	CDL	CA2-OA2-PA1-OA5
27	O	203	CDL	CA3-OA5-PA1-OA2
27	O	203	CDL	CA3-OA5-PA1-OA4
27	O	203	CDL	C11-CA5-OA6-CA4
27	O	203	CDL	CB2-OB2-PB2-OB3
27	O	203	CDL	CB3-OB5-PB2-OB2
27	O	203	CDL	CB3-OB5-PB2-OB3
27	O	203	CDL	CB3-OB5-PB2-OB4
27	U	201	CDL	CA3-OA5-PA1-OA4
27	H	302	CDL	CA2-OA2-PA1-OA5
27	H	302	CDL	OA6-CA4-CA6-OA8
27	E	401	CDL	CA3-OA5-PA1-OA2
27	E	401	CDL	C1-CB2-OB2-PB2
27	E	401	CDL	CB2-OB2-PB2-OB3
27	E	401	CDL	CB3-OB5-PB2-OB2
27	E	401	CDL	CB3-OB5-PB2-OB4
27	B	601	CDL	CB3-OB5-PB2-OB2
27	B	601	CDL	CB3-OB5-PB2-OB3
27	B	601	CDL	OB7-CB5-OB6-CB4
27	B	602	CDL	CA2-OA2-PA1-OA3
27	B	602	CDL	CA2-OA2-PA1-OA4
27	B	602	CDL	CA2-OA2-PA1-OA5
27	B	602	CDL	CA3-OA5-PA1-OA3
27	B	602	CDL	C51-CB5-OB6-CB4
27	V	201	CDL	CB3-OB5-PB2-OB2
27	V	201	CDL	CB3-OB5-PB2-OB3
27	V	201	CDL	OB7-CB5-OB6-CB4
27	V	202	CDL	CA3-OA5-PA1-OA2
27	V	202	CDL	CA3-OA5-PA1-OA3
27	V	202	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
27	V	202	CDL	CB3-OB5-PB2-OB2
27	V	202	CDL	CB3-OB5-PB2-OB3
27	V	202	CDL	CB3-OB5-PB2-OB4
27	C	404	CDL	CB3-OB5-PB2-OB4
27	C	404	CDL	C51-CB5-OB6-CB4
27	D	402	CDL	CA2-OA2-PA1-OA3
27	D	402	CDL	C1-CB2-OB2-PB2
27	D	402	CDL	CB2-OB2-PB2-OB5
27	D	402	CDL	OB6-CB4-CB6-OB8
27	D	402	CDL	C51-CB5-OB6-CB4
28	j	301	PEE	O4P-C4-C5-N
28	j	302	PEE	C4-O4P-P-O3P
28	j	302	PEE	C4-O4P-P-O1P
28	j	302	PEE	O4P-C4-C5-N
28	J	301	PEE	O4P-C4-C5-N
28	J	302	PEE	C4-O4P-P-O3P
28	J	302	PEE	C4-O4P-P-O1P
28	J	302	PEE	O4P-C4-C5-N
27	v	201	CDL	OA9-CA7-OA8-CA6
27	c	404	CDL	OA9-CA7-OA8-CA6
27	V	202	CDL	OA9-CA7-OA8-CA6
27	C	404	CDL	OA9-CA7-OA8-CA6
27	v	201	CDL	C31-CA7-OA8-CA6
27	c	404	CDL	C31-CA7-OA8-CA6
27	V	202	CDL	C31-CA7-OA8-CA6
27	C	404	CDL	C31-CA7-OA8-CA6
27	h	302	CDL	OB9-CB7-OB8-CB6
27	b	601	CDL	OA9-CA7-OA8-CA6
27	H	302	CDL	OB9-CB7-OB8-CB6
27	B	601	CDL	OB9-CB7-OB8-CB6
27	B	602	CDL	OA9-CA7-OA8-CA6
27	V	201	CDL	OB9-CB7-OB8-CB6
25	o	201	PC1	O22-C21-O21-C2
25	O	201	PC1	O22-C21-O21-C2
27	o	203	CDL	OA7-CA5-OA6-CA4
27	b	601	CDL	OB7-CB5-OB6-CB4
27	c	404	CDL	OA7-CA5-OA6-CA4
27	c	404	CDL	OB7-CB5-OB6-CB4
27	d	402	CDL	OB7-CB5-OB6-CB4
27	O	203	CDL	OA7-CA5-OA6-CA4
27	B	602	CDL	OB7-CB5-OB6-CB4
27	C	404	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
27	C	404	CDL	OB7-CB5-OB6-CB4
27	D	402	CDL	OB7-CB5-OB6-CB4
27	h	302	CDL	C71-CB7-OB8-CB6
27	c	404	CDL	C71-CB7-OB8-CB6
27	H	302	CDL	C71-CB7-OB8-CB6
27	B	601	CDL	C71-CB7-OB8-CB6
27	V	201	CDL	C71-CB7-OB8-CB6
27	C	404	CDL	C71-CB7-OB8-CB6
25	V	203	PC1	C22-C21-O21-C2
27	c	404	CDL	C11-CA5-OA6-CA4
27	B	601	CDL	C51-CB5-OB6-CB4
27	V	201	CDL	C51-CB5-OB6-CB4
27	C	404	CDL	C11-CA5-OA6-CA4
26	x	101	LMT	O5B-C5B-C6B-O6B
26	X	101	LMT	O5B-C5B-C6B-O6B
26	h	301	LMT	C3'-C4'-O1B-C1B
26	H	301	LMT	C3'-C4'-O1B-C1B
27	b	601	CDL	C31-CA7-OA8-CA6
27	B	602	CDL	C31-CA7-OA8-CA6
28	j	301	PEE	C37-C38-C39-C40
28	J	301	PEE	C37-C38-C39-C40
26	h	301	LMT	O5'-C5'-C6'-O6'
26	d	403	LMT	O5B-C5B-C6B-O6B
26	H	301	LMT	O5'-C5'-C6'-O6'
26	D	403	LMT	O5B-C5B-C6B-O6B
27	c	404	CDL	OB9-CB7-OB8-CB6
27	C	404	CDL	OB9-CB7-OB8-CB6
25	o	204	PC1	O22-C21-O21-C2
25	O	204	PC1	O22-C21-O21-C2
27	h	302	CDL	O1-C1-CA2-OA2
27	d	402	CDL	O1-C1-CB2-OB2
27	H	302	CDL	O1-C1-CA2-OA2
27	D	402	CDL	O1-C1-CB2-OB2
26	D	403	LMT	C4B-C5B-C6B-O6B
26	d	403	LMT	C4B-C5B-C6B-O6B
27	o	203	CDL	C31-CA7-OA8-CA6
27	O	203	CDL	C31-CA7-OA8-CA6
26	h	301	LMT	C4'-C5'-C6'-O6'
26	H	301	LMT	C4'-C5'-C6'-O6'
27	h	302	CDL	CA4-CA3-OA5-PA1
27	H	302	CDL	CA4-CA3-OA5-PA1
26	x	101	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
26	X	101	LMT	C4B-C5B-C6B-O6B
26	x	101	LMT	O5'-C1'-O1'-C1
26	X	101	LMT	O5'-C1'-O1'-C1
26	d	401	LMT	O5B-C5B-C6B-O6B
26	D	401	LMT	O5B-C5B-C6B-O6B
26	h	301	LMT	O5B-C5B-C6B-O6B
26	H	301	LMT	O5B-C5B-C6B-O6B
28	c	402	PEE	C17-C18-C19-C20
28	C	402	PEE	C17-C18-C19-C20
27	o	203	CDL	OA9-CA7-OA8-CA6
27	O	203	CDL	OA9-CA7-OA8-CA6
26	d	401	LMT	O5'-C5'-C6'-O6'
26	D	401	LMT	O5'-C5'-C6'-O6'
27	h	302	CDL	CB2-C1-CA2-OA2
27	H	302	CDL	CB2-C1-CA2-OA2
25	o	201	PC1	C32-C31-O31-C3
25	O	201	PC1	C32-C31-O31-C3
27	e	401	CDL	C71-CB7-OB8-CB6
27	d	402	CDL	C71-CB7-OB8-CB6
27	E	401	CDL	C71-CB7-OB8-CB6
27	B	601	CDL	C31-CA7-OA8-CA6
27	V	201	CDL	C31-CA7-OA8-CA6
27	D	402	CDL	C71-CB7-OB8-CB6
26	d	401	LMT	C4B-C5B-C6B-O6B
26	D	401	LMT	C4B-C5B-C6B-O6B
25	o	201	PC1	O32-C31-O31-C3
25	O	201	PC1	O32-C31-O31-C3
27	d	402	CDL	OB9-CB7-OB8-CB6
27	D	402	CDL	OB9-CB7-OB8-CB6
27	v	201	CDL	OA6-CA4-CA6-OA8
27	V	202	CDL	OA6-CA4-CA6-OA8
28	C	402	PEE	C31-C30-O3-C3
27	c	404	CDL	CA5-C11-C12-C13
28	c	402	PEE	C31-C30-O3-C3
27	C	404	CDL	CA5-C11-C12-C13
25	o	201	PC1	C31-C32-C33-C34
25	O	201	PC1	C31-C32-C33-C34
27	v	201	CDL	CB5-C51-C52-C53
27	V	202	CDL	CB5-C51-C52-C53
27	u	201	CDL	CB5-C51-C52-C53
27	h	302	CDL	CA5-C11-C12-C13
27	U	201	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
27	H	302	CDL	CA5-C11-C12-C13
27	e	401	CDL	OB9-CB7-OB8-CB6
27	E	401	CDL	OB9-CB7-OB8-CB6
27	B	601	CDL	OA9-CA7-OA8-CA6
27	V	201	CDL	OA9-CA7-OA8-CA6
27	d	402	CDL	C11-CA5-OA6-CA4
27	D	402	CDL	C11-CA5-OA6-CA4
27	d	402	CDL	OA7-CA5-OA6-CA4
27	D	402	CDL	OA7-CA5-OA6-CA4
27	e	401	CDL	C11-CA5-OA6-CA4
27	E	401	CDL	C11-CA5-OA6-CA4
27	e	401	CDL	OA7-CA5-OA6-CA4
27	E	401	CDL	OA7-CA5-OA6-CA4
27	o	203	CDL	C33-C34-C35-C36
27	O	203	CDL	C33-C34-C35-C36
27	u	201	CDL	CA7-C31-C32-C33
27	U	201	CDL	CA7-C31-C32-C33
26	h	301	LMT	C4B-C5B-C6B-O6B
26	H	301	LMT	C4B-C5B-C6B-O6B
28	c	402	PEE	O5-C30-O3-C3
28	C	402	PEE	O5-C30-O3-C3
27	h	302	CDL	C20-C21-C22-C23
27	H	302	CDL	C20-C21-C22-C23
27	e	401	CDL	CB7-C71-C72-C73
27	E	401	CDL	CB7-C71-C72-C73
27	d	402	CDL	C52-C53-C54-C55
26	d	401	LMT	C3-C4-C5-C6
26	D	401	LMT	C3-C4-C5-C6
27	h	302	CDL	C59-C60-C61-C62
27	h	302	CDL	C63-C64-C65-C66
27	e	401	CDL	C59-C60-C61-C62
27	H	302	CDL	C59-C60-C61-C62
27	H	302	CDL	C63-C64-C65-C66
27	E	401	CDL	C59-C60-C61-C62
27	D	402	CDL	C52-C53-C54-C55
25	o	204	PC1	C32-C33-C34-C35
25	O	204	PC1	C32-C33-C34-C35
27	b	601	CDL	C58-C59-C60-C61
27	v	201	CDL	C58-C59-C60-C61
27	V	202	CDL	C58-C59-C60-C61
26	x	101	LMT	O5B-C1B-O1B-C4'
26	X	101	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
25	V	203	PC1	C25-C26-C27-C28
26	c	401	LMT	C11-C10-C9-C8
26	C	401	LMT	C11-C10-C9-C8
27	B	602	CDL	C58-C59-C60-C61
28	c	402	PEE	C40-C41-C42-C43
28	C	402	PEE	C40-C41-C42-C43
26	d	403	LMT	C2-C1-O1'-C1'
26	D	403	LMT	C2-C1-O1'-C1'
25	v	202	PC1	C25-C26-C27-C28
27	B	601	CDL	C41-C42-C43-C44
27	B	601	CDL	C72-C73-C74-C75
27	V	201	CDL	C41-C42-C43-C44
27	V	201	CDL	C72-C73-C74-C75
27	C	404	CDL	C63-C64-C65-C66
27	B	601	CDL	C11-CA5-OA6-CA4
27	V	201	CDL	C11-CA5-OA6-CA4
27	c	404	CDL	C63-C64-C65-C66
27	O	203	CDL	C37-C38-C39-C40
27	o	203	CDL	C37-C38-C39-C40
27	B	601	CDL	C74-C75-C76-C77
27	V	201	CDL	C74-C75-C76-C77
27	h	302	CDL	CB5-C51-C52-C53
27	H	302	CDL	CB5-C51-C52-C53
26	C	403	LMT	C1-C2-C3-C4
27	o	203	CDL	C16-C17-C18-C19
27	e	401	CDL	C74-C75-C76-C77
27	b	601	CDL	C52-C53-C54-C55
27	v	201	CDL	C23-C24-C25-C26
27	O	203	CDL	C16-C17-C18-C19
27	E	401	CDL	C74-C75-C76-C77
27	C	404	CDL	C39-C40-C41-C42
27	c	404	CDL	C39-C40-C41-C42
27	B	602	CDL	C52-C53-C54-C55
27	V	202	CDL	C23-C24-C25-C26
28	c	402	PEE	C23-C24-C25-C26
26	c	403	LMT	C1-C2-C3-C4
25	o	204	PC1	C3A-C3B-C3C-C3D
25	O	204	PC1	C3A-C3B-C3C-C3D
28	C	402	PEE	C23-C24-C25-C26
25	o	201	PC1	C37-C38-C39-C3A
27	h	302	CDL	C71-C72-C73-C74
27	v	201	CDL	C81-C82-C83-C84

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Mol	Chain	Res	Type	Atoms
27	H	302	CDL	C71-C72-C73-C74
27	B	602	CDL	C56-C57-C58-C59
27	V	202	CDL	C81-C82-C83-C84
25	O	201	PC1	C37-C38-C39-C3A
27	C	404	CDL	C82-C83-C84-C85
27	c	404	CDL	C82-C83-C84-C85
27	o	203	CDL	C31-C32-C33-C34
27	o	203	CDL	C61-C62-C63-C64
27	b	601	CDL	C56-C57-C58-C59
27	O	203	CDL	C31-C32-C33-C34
27	O	203	CDL	C61-C62-C63-C64
27	u	201	CDL	C35-C36-C37-C38
27	d	402	CDL	C63-C64-C65-C66
27	U	201	CDL	C35-C36-C37-C38
27	D	402	CDL	C63-C64-C65-C66
27	e	401	CDL	C76-C77-C78-C79
27	E	401	CDL	C76-C77-C78-C79
27	u	201	CDL	C11-CA5-OA6-CA4
28	c	402	PEE	C11-C10-O2-C2
28	C	402	PEE	C11-C10-O2-C2
27	b	601	CDL	C40-C41-C42-C43
27	v	201	CDL	C78-C79-C80-C81
27	B	602	CDL	C40-C41-C42-C43
27	V	202	CDL	C78-C79-C80-C81
27	b	601	CDL	C62-C63-C64-C65
27	H	302	CDL	C76-C77-C78-C79
27	B	602	CDL	C62-C63-C64-C65
28	j	301	PEE	C23-C24-C25-C26
28	J	301	PEE	C23-C24-C25-C26
27	h	302	CDL	C76-C77-C78-C79
27	E	401	CDL	C31-C32-C33-C34
27	B	601	CDL	C16-C17-C18-C19
27	B	601	CDL	C61-C62-C63-C64
27	V	201	CDL	C16-C17-C18-C19
27	V	201	CDL	C61-C62-C63-C64
27	e	401	CDL	C31-C32-C33-C34
27	B	601	CDL	OA7-CA5-OA6-CA4
27	V	201	CDL	OA7-CA5-OA6-CA4
25	o	201	PC1	C3E-C3F-C3G-C3H
25	O	201	PC1	C3E-C3F-C3G-C3H
27	b	601	CDL	C41-C42-C43-C44
27	B	602	CDL	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
27	u	201	CDL	C14-C15-C16-C17
27	h	302	CDL	C22-C23-C24-C25
27	e	401	CDL	C15-C16-C17-C18
27	e	401	CDL	C62-C63-C64-C65
27	U	201	CDL	C14-C15-C16-C17
27	H	302	CDL	C22-C23-C24-C25
27	E	401	CDL	C15-C16-C17-C18
27	E	401	CDL	C62-C63-C64-C65
27	B	602	CDL	C77-C78-C79-C80
27	v	201	CDL	CB7-C71-C72-C73
27	V	202	CDL	CB7-C71-C72-C73
27	b	601	CDL	C77-C78-C79-C80
27	c	404	CDL	C53-C54-C55-C56
27	C	404	CDL	C53-C54-C55-C56
28	j	301	PEE	C34-C35-C36-C37
28	c	402	PEE	C13-C14-C15-C16
27	o	203	CDL	C83-C84-C85-C86
27	u	201	CDL	C79-C80-C81-C82
27	d	402	CDL	C71-C72-C73-C74
27	O	203	CDL	C83-C84-C85-C86
27	U	201	CDL	C79-C80-C81-C82
27	D	402	CDL	C71-C72-C73-C74
28	J	301	PEE	C34-C35-C36-C37
28	C	402	PEE	C13-C14-C15-C16
27	d	402	CDL	C36-C37-C38-C39
27	D	402	CDL	C36-C37-C38-C39
28	j	302	PEE	C23-C24-C25-C26
28	J	302	PEE	C23-C24-C25-C26
27	U	201	CDL	C11-CA5-OA6-CA4
25	o	204	PC1	C23-C24-C25-C26
25	O	204	PC1	C23-C24-C25-C26
27	b	601	CDL	C51-C52-C53-C54
27	B	601	CDL	C18-C19-C20-C21
27	B	602	CDL	C51-C52-C53-C54
27	V	201	CDL	C18-C19-C20-C21
27	h	302	CDL	C56-C57-C58-C59
27	v	201	CDL	C14-C15-C16-C17
27	H	302	CDL	C56-C57-C58-C59
27	V	202	CDL	C14-C15-C16-C17
25	v	202	PC1	C35-C36-C37-C38
25	V	203	PC1	C35-C36-C37-C38
27	h	302	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
27	h	302	CDL	C77-C78-C79-C80
25	o	201	PC1	C29-C2A-C2B-C2C
25	O	201	PC1	C29-C2A-C2B-C2C
27	B	602	CDL	C22-C23-C24-C25
28	j	302	PEE	C14-C15-C16-C17
28	J	302	PEE	C14-C15-C16-C17
27	o	203	CDL	C59-C60-C61-C62
27	b	601	CDL	C22-C23-C24-C25
27	O	203	CDL	C59-C60-C61-C62
27	H	302	CDL	C77-C78-C79-C80
27	u	201	CDL	C41-C42-C43-C44
27	v	201	CDL	C37-C38-C39-C40
27	U	201	CDL	C41-C42-C43-C44
27	V	202	CDL	C37-C38-C39-C40
26	c	403	LMT	C2-C3-C4-C5
26	C	403	LMT	C2-C3-C4-C5
27	H	302	CDL	C31-CA7-OA8-CA6
27	u	201	CDL	C23-C24-C25-C26
27	U	201	CDL	C23-C24-C25-C26
27	b	601	CDL	OB5-CB3-CB4-OB6
27	B	602	CDL	OB5-CB3-CB4-OB6
27	v	201	CDL	C74-C75-C76-C77
27	V	202	CDL	C74-C75-C76-C77
27	V	201	CDL	C63-C64-C65-C66
27	B	601	CDL	C63-C64-C65-C66
28	j	301	PEE	C19-C20-C21-C22
28	J	301	PEE	C19-C20-C21-C22
27	e	401	CDL	C35-C36-C37-C38
27	e	401	CDL	C72-C73-C74-C75
27	E	401	CDL	C35-C36-C37-C38
27	E	401	CDL	C72-C73-C74-C75
25	v	202	PC1	C3B-C3C-C3D-C3E
25	O	201	PC1	C3D-C3E-C3F-C3G
27	c	404	CDL	C14-C15-C16-C17
27	C	404	CDL	C14-C15-C16-C17
25	o	201	PC1	C3D-C3E-C3F-C3G
25	V	203	PC1	C3B-C3C-C3D-C3E
27	v	201	CDL	C42-C43-C44-C45
27	V	202	CDL	C42-C43-C44-C45
27	h	302	CDL	C74-C75-C76-C77
27	H	302	CDL	C74-C75-C76-C77
27	u	201	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
27	U	201	CDL	OA7-CA5-OA6-CA4
25	o	204	PC1	C27-C28-C29-C2A
25	O	204	PC1	C27-C28-C29-C2A
27	h	302	CDL	C61-C62-C63-C64
27	H	302	CDL	C61-C62-C63-C64
27	B	601	CDL	C32-C33-C34-C35
27	V	201	CDL	C32-C33-C34-C35
26	C	401	LMT	C3-C4-C5-C6
26	c	401	LMT	C3-C4-C5-C6
27	b	601	CDL	C38-C39-C40-C41
27	B	602	CDL	C38-C39-C40-C41
25	o	204	PC1	C25-C26-C27-C28
25	O	204	PC1	C25-C26-C27-C28
27	B	601	CDL	OB5-CB3-CB4-CB6
27	V	201	CDL	OB5-CB3-CB4-CB6
26	x	101	LMT	C3-C4-C5-C6
26	X	101	LMT	C3-C4-C5-C6
27	d	402	CDL	C75-C76-C77-C78
27	D	402	CDL	C75-C76-C77-C78
28	j	301	PEE	C22-C23-C24-C25
28	J	301	PEE	C22-C23-C24-C25
27	B	602	CDL	C82-C83-C84-C85
28	j	301	PEE	C14-C15-C16-C17
28	J	301	PEE	C14-C15-C16-C17
27	b	601	CDL	C82-C83-C84-C85
27	b	601	CDL	C71-CB7-OB8-CB6
27	B	602	CDL	C71-CB7-OB8-CB6
28	c	402	PEE	O4-C10-O2-C2
28	C	402	PEE	O4-C10-O2-C2
27	v	201	CDL	CA3-CA4-CA6-OA8
27	V	202	CDL	CA3-CA4-CA6-OA8
28	j	301	PEE	C1-C2-C3-O3
28	J	301	PEE	C1-C2-C3-O3
25	O	201	PC1	C26-C27-C28-C29
27	b	601	CDL	C73-C74-C75-C76
27	B	602	CDL	C73-C74-C75-C76
25	o	201	PC1	C26-C27-C28-C29
26	o	202	LMT	C5-C6-C7-C8
26	O	202	LMT	C5-C6-C7-C8
26	D	401	LMT	C4-C5-C6-C7
25	o	204	PC1	C39-C3A-C3B-C3C
26	d	401	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	O	204	PC1	C39-C3A-C3B-C3C
27	v	201	CDL	C31-C32-C33-C34
27	V	202	CDL	C31-C32-C33-C34
26	x	101	LMT	C2-C3-C4-C5
26	X	101	LMT	C2-C3-C4-C5
27	C	404	CDL	C81-C82-C83-C84
27	h	302	CDL	OA9-CA7-OA8-CA6
27	H	302	CDL	OA9-CA7-OA8-CA6
27	o	203	CDL	C12-C13-C14-C15
27	c	404	CDL	C81-C82-C83-C84
27	O	203	CDL	C12-C13-C14-C15
27	o	203	CDL	C72-C73-C74-C75
27	O	203	CDL	C38-C39-C40-C41
27	O	203	CDL	C72-C73-C74-C75
28	j	301	PEE	C42-C43-C44-C45
28	J	301	PEE	C42-C43-C44-C45
27	c	404	CDL	CA6-CA4-OA6-CA5
27	C	404	CDL	CA6-CA4-OA6-CA5
28	c	402	PEE	C1-C2-O2-C10
28	C	402	PEE	C1-C2-O2-C10
27	o	203	CDL	C38-C39-C40-C41
27	h	302	CDL	C16-C17-C18-C19
27	c	404	CDL	C74-C75-C76-C77
27	C	404	CDL	C74-C75-C76-C77
27	c	404	CDL	C42-C43-C44-C45
27	d	402	CDL	C60-C61-C62-C63
27	H	302	CDL	C16-C17-C18-C19
27	C	404	CDL	C42-C43-C44-C45
27	D	402	CDL	C60-C61-C62-C63
27	B	602	CDL	OB9-CB7-OB8-CB6
27	b	601	CDL	C76-C77-C78-C79
27	B	602	CDL	C76-C77-C78-C79
25	v	202	PC1	C23-C24-C25-C26
27	b	601	CDL	OB9-CB7-OB8-CB6
25	V	203	PC1	C23-C24-C25-C26
25	o	204	PC1	C37-C38-C39-C3A
25	O	204	PC1	C37-C38-C39-C3A
27	E	401	CDL	C78-C79-C80-C81
25	o	204	PC1	C26-C27-C28-C29
25	O	204	PC1	C26-C27-C28-C29
27	e	401	CDL	C78-C79-C80-C81
27	u	201	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	U	201	CDL	C11-C12-C13-C14
25	o	204	PC1	C3E-C3F-C3G-C3H
25	O	204	PC1	C3E-C3F-C3G-C3H
27	h	302	CDL	C64-C65-C66-C67
27	H	302	CDL	C64-C65-C66-C67
27	e	401	CDL	C61-C62-C63-C64
27	E	401	CDL	C61-C62-C63-C64
27	u	201	CDL	C51-CB5-OB6-CB4
27	U	201	CDL	C51-CB5-OB6-CB4
25	v	202	PC1	C33-C34-C35-C36
25	V	203	PC1	C33-C34-C35-C36
27	h	302	CDL	C53-C54-C55-C56
27	H	302	CDL	C53-C54-C55-C56
27	u	201	CDL	C58-C59-C60-C61
27	U	201	CDL	C58-C59-C60-C61
27	o	203	CDL	C44-C45-C46-C47
27	O	203	CDL	C44-C45-C46-C47
26	c	401	LMT	C3'-C4'-O1B-C1B
26	C	401	LMT	C3'-C4'-O1B-C1B
26	H	301	LMT	C5'-C4'-O1B-C1B
27	b	601	CDL	OB5-CB3-CB4-CB6
27	v	201	CDL	OB5-CB3-CB4-CB6
27	c	404	CDL	OB5-CB3-CB4-CB6
27	d	402	CDL	OA5-CA3-CA4-CA6
27	B	602	CDL	OB5-CB3-CB4-CB6
27	V	202	CDL	OB5-CB3-CB4-CB6
27	C	404	CDL	OB5-CB3-CB4-CB6
27	D	402	CDL	OA5-CA3-CA4-CA6
26	h	301	LMT	C5'-C4'-O1B-C1B
27	D	402	CDL	C33-C34-C35-C36
27	d	402	CDL	C33-C34-C35-C36
27	U	201	CDL	C78-C79-C80-C81
27	V	201	CDL	C56-C57-C58-C59
27	u	201	CDL	C75-C76-C77-C78
27	u	201	CDL	C78-C79-C80-C81
27	B	601	CDL	C56-C57-C58-C59
27	H	302	CDL	C13-C14-C15-C16
27	h	302	CDL	C13-C14-C15-C16
27	U	201	CDL	C75-C76-C77-C78
27	h	302	CDL	C24-C25-C26-C27
27	H	302	CDL	C24-C25-C26-C27
26	d	401	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
26	D	401	LMT	C4'-C5'-C6'-O6'
26	c	403	LMT	C5-C6-C7-C8
27	C	404	CDL	C22-C23-C24-C25
26	c	401	LMT	C4'-C5'-C6'-O6'
26	C	401	LMT	C4'-C5'-C6'-O6'
27	c	404	CDL	C22-C23-C24-C25
28	c	402	PEE	C12-C13-C14-C15
28	C	402	PEE	C12-C13-C14-C15
27	v	201	CDL	C19-C20-C21-C22
27	o	203	CDL	CA3-CA4-CA6-OA8
27	h	302	CDL	CA3-CA4-CA6-OA8
27	c	404	CDL	CB3-CB4-CB6-OB8
27	O	203	CDL	CA3-CA4-CA6-OA8
27	H	302	CDL	CA3-CA4-CA6-OA8
27	C	404	CDL	CB3-CB4-CB6-OB8
26	C	403	LMT	C5-C6-C7-C8
27	b	601	CDL	C44-C45-C46-C47
27	B	602	CDL	C44-C45-C46-C47
27	V	202	CDL	C19-C20-C21-C22
27	b	601	CDL	C83-C84-C85-C86
27	B	602	CDL	C83-C84-C85-C86
27	d	402	CDL	C42-C43-C44-C45
26	d	401	LMT	C1-C2-C3-C4
26	D	401	LMT	C1-C2-C3-C4
28	j	301	PEE	C10-C11-C12-C13
28	J	301	PEE	C10-C11-C12-C13
25	o	204	PC1	O11-C1-C2-O21
25	O	204	PC1	O11-C1-C2-O21
27	D	402	CDL	C42-C43-C44-C45
27	v	201	CDL	C17-C18-C19-C20
27	V	202	CDL	C17-C18-C19-C20
27	v	201	CDL	C51-CB5-OB6-CB4
27	V	202	CDL	C51-CB5-OB6-CB4
28	c	402	PEE	C21-C22-C23-C24
27	c	404	CDL	OB6-CB4-CB6-OB8
27	C	404	CDL	OB6-CB4-CB6-OB8
28	j	302	PEE	O2-C2-C3-O3
28	J	302	PEE	O2-C2-C3-O3
28	j	301	PEE	C41-C42-C43-C44
28	J	301	PEE	C41-C42-C43-C44
28	C	402	PEE	C21-C22-C23-C24
27	b	601	CDL	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
25	v	202	PC1	C38-C39-C3A-C3B
27	h	302	CDL	C80-C81-C82-C83
27	H	302	CDL	C80-C81-C82-C83
25	V	203	PC1	C38-C39-C3A-C3B
27	B	602	CDL	C43-C44-C45-C46
28	c	402	PEE	C36-C37-C38-C39
28	C	402	PEE	C36-C37-C38-C39
27	b	601	CDL	C11-C12-C13-C14
27	B	602	CDL	C11-C12-C13-C14
27	B	601	CDL	CA7-C31-C32-C33
27	V	201	CDL	CA7-C31-C32-C33
26	D	403	LMT	O1'-C1-C2-C3
27	O	203	CDL	C14-C15-C16-C17
27	o	203	CDL	C14-C15-C16-C17
26	d	403	LMT	O1'-C1-C2-C3
26	c	401	LMT	C5'-C4'-O1B-C1B
26	C	401	LMT	C5'-C4'-O1B-C1B
27	d	402	CDL	CA2-C1-CB2-OB2
27	D	402	CDL	CA2-C1-CB2-OB2
27	e	401	CDL	C32-C31-CA7-OA8
27	E	401	CDL	C32-C31-CA7-OA8
27	u	201	CDL	C36-C37-C38-C39
27	b	601	CDL	C71-C72-C73-C74
27	B	602	CDL	C71-C72-C73-C74
27	e	401	CDL	OA5-CA3-CA4-CA6
27	E	401	CDL	OA5-CA3-CA4-CA6
27	U	201	CDL	C36-C37-C38-C39
27	v	201	CDL	C53-C54-C55-C56
27	V	202	CDL	C53-C54-C55-C56
28	j	301	PEE	C31-C30-O3-C3
28	J	301	PEE	C31-C30-O3-C3
27	e	401	CDL	C81-C82-C83-C84
27	E	401	CDL	C81-C82-C83-C84
27	e	401	CDL	C80-C81-C82-C83
27	d	402	CDL	CA6-CA4-OA6-CA5
27	D	402	CDL	CA6-CA4-OA6-CA5
27	E	401	CDL	C80-C81-C82-C83
27	B	601	CDL	C78-C79-C80-C81
27	V	201	CDL	C78-C79-C80-C81
27	u	201	CDL	C13-C14-C15-C16
27	U	201	CDL	C13-C14-C15-C16
27	v	201	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
27	V	202	CDL	OB7-CB5-OB6-CB4
27	o	203	CDL	C32-C31-CA7-OA8
27	O	203	CDL	C32-C31-CA7-OA8
27	v	201	CDL	OB5-CB3-CB4-OB6
27	c	404	CDL	OB5-CB3-CB4-OB6
27	V	202	CDL	OB5-CB3-CB4-OB6
27	C	404	CDL	OB5-CB3-CB4-OB6
27	d	402	CDL	CB3-CB4-CB6-OB8
27	D	402	CDL	CB3-CB4-CB6-OB8
27	u	201	CDL	C80-C81-C82-C83
27	U	201	CDL	C80-C81-C82-C83
27	o	203	CDL	C51-C52-C53-C54
27	O	203	CDL	C51-C52-C53-C54
25	o	204	PC1	C12-C11-O13-P
25	O	204	PC1	C12-C11-O13-P
27	U	201	CDL	C55-C56-C57-C58
28	j	302	PEE	C31-C32-C33-C34
28	J	302	PEE	C31-C32-C33-C34
27	B	601	CDL	OB6-CB4-CB6-OB8
27	V	201	CDL	OB6-CB4-CB6-OB8
26	D	403	LMT	C3-C4-C5-C6
27	u	201	CDL	C55-C56-C57-C58
27	u	201	CDL	C56-C57-C58-C59
27	u	201	CDL	OB7-CB5-OB6-CB4
27	U	201	CDL	OB7-CB5-OB6-CB4
26	d	403	LMT	C3-C4-C5-C6
27	U	201	CDL	C56-C57-C58-C59
28	c	402	PEE	C34-C35-C36-C37
28	C	402	PEE	C34-C35-C36-C37
25	o	204	PC1	O13-C11-C12-N
25	O	204	PC1	O13-C11-C12-N
26	o	202	LMT	C2-C1-O1'-C1'
26	O	202	LMT	C2-C1-O1'-C1'
27	b	601	CDL	C60-C61-C62-C63
27	B	602	CDL	C60-C61-C62-C63
28	j	301	PEE	O5-C30-O3-C3
27	v	201	CDL	C71-CB7-OB8-CB6
27	d	402	CDL	C41-C42-C43-C44
27	H	302	CDL	C58-C59-C60-C61
27	D	402	CDL	C41-C42-C43-C44
27	o	203	CDL	C21-C22-C23-C24
27	h	302	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
27	O	203	CDL	C21-C22-C23-C24
28	J	301	PEE	O5-C30-O3-C3
27	o	203	CDL	CA4-CA3-OA5-PA1
27	O	203	CDL	CA4-CA3-OA5-PA1
27	e	401	CDL	OA5-CA3-CA4-OA6
27	d	402	CDL	OA5-CA3-CA4-OA6
27	E	401	CDL	OA5-CA3-CA4-OA6
27	D	402	CDL	OA5-CA3-CA4-OA6
27	e	401	CDL	C44-C45-C46-C47
27	E	401	CDL	C44-C45-C46-C47
27	V	202	CDL	C71-CB7-OB8-CB6
27	H	302	CDL	C51-C52-C53-C54
27	h	302	CDL	C51-C52-C53-C54
25	v	202	PC1	O21-C2-C3-O31
25	V	203	PC1	O21-C2-C3-O31
27	o	203	CDL	OA6-CA4-CA6-OA8
27	O	203	CDL	OA6-CA4-CA6-OA8
28	j	301	PEE	O2-C2-C3-O3
28	J	301	PEE	O2-C2-C3-O3
25	o	204	PC1	C22-C23-C24-C25
27	B	601	CDL	C57-C58-C59-C60
27	V	201	CDL	C57-C58-C59-C60
27	V	202	CDL	OB9-CB7-OB8-CB6
27	V	202	CDL	C33-C34-C35-C36
25	O	204	PC1	C22-C23-C24-C25
27	v	201	CDL	C33-C34-C35-C36
27	v	201	CDL	OB9-CB7-OB8-CB6
27	B	601	CDL	CA5-C11-C12-C13
25	o	201	PC1	C11-O13-P-O14
25	o	204	PC1	C11-O13-P-O14
25	v	202	PC1	C11-O13-P-O12
25	v	202	PC1	C11-O13-P-O14
25	v	202	PC1	C11-O13-P-O11
25	O	201	PC1	C11-O13-P-O14
25	O	204	PC1	C11-O13-P-O14
25	V	203	PC1	C11-O13-P-O12
25	V	203	PC1	C11-O13-P-O14
25	V	203	PC1	C11-O13-P-O11
27	u	201	CDL	CA3-OA5-PA1-OA2
27	u	201	CDL	CA3-OA5-PA1-OA3
27	u	201	CDL	CB2-OB2-PB2-OB3
27	u	201	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
27	u	201	CDL	CB2-OB2-PB2-OB5
27	h	302	CDL	CA2-OA2-PA1-OA3
27	h	302	CDL	CB2-OB2-PB2-OB4
27	h	302	CDL	CB2-OB2-PB2-OB5
27	h	302	CDL	CB3-OB5-PB2-OB4
27	e	401	CDL	CA2-OA2-PA1-OA3
27	e	401	CDL	CB3-OB5-PB2-OB3
27	b	601	CDL	CB3-OB5-PB2-OB3
27	c	404	CDL	CB3-OB5-PB2-OB2
27	c	404	CDL	CB3-OB5-PB2-OB3
27	d	402	CDL	CB2-OB2-PB2-OB3
27	d	402	CDL	CB3-OB5-PB2-OB2
27	U	201	CDL	CA3-OA5-PA1-OA2
27	U	201	CDL	CA3-OA5-PA1-OA3
27	U	201	CDL	CB2-OB2-PB2-OB3
27	U	201	CDL	CB2-OB2-PB2-OB4
27	U	201	CDL	CB2-OB2-PB2-OB5
27	H	302	CDL	CA2-OA2-PA1-OA3
27	H	302	CDL	CB2-OB2-PB2-OB4
27	H	302	CDL	CB2-OB2-PB2-OB5
27	H	302	CDL	CB3-OB5-PB2-OB4
27	E	401	CDL	CA2-OA2-PA1-OA3
27	E	401	CDL	CB3-OB5-PB2-OB3
27	B	601	CDL	CA3-OA5-PA1-OA3
27	B	601	CDL	CB3-OB5-PB2-OB4
27	B	602	CDL	CB3-OB5-PB2-OB3
27	V	201	CDL	CA3-OA5-PA1-OA3
27	V	201	CDL	CB3-OB5-PB2-OB4
27	C	404	CDL	CB3-OB5-PB2-OB2
27	C	404	CDL	CB3-OB5-PB2-OB3
27	D	402	CDL	CB2-OB2-PB2-OB3
27	D	402	CDL	CB3-OB5-PB2-OB2
28	j	302	PEE	C4-O4P-P-O2P
28	J	302	PEE	C4-O4P-P-O2P
27	V	201	CDL	C54-C55-C56-C57
27	O	203	CDL	C20-C21-C22-C23
27	B	601	CDL	C54-C55-C56-C57
27	o	203	CDL	C20-C21-C22-C23
27	o	203	CDL	C1-CB2-OB2-PB2
27	h	302	CDL	C1-CA2-OA2-PA1
27	b	601	CDL	C1-CB2-OB2-PB2
27	O	203	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
27	H	302	CDL	C1-CA2-OA2-PA1
27	B	602	CDL	C1-CB2-OB2-PB2
27	d	402	CDL	C24-C25-C26-C27
28	c	402	PEE	C37-C38-C39-C40
28	C	402	PEE	C37-C38-C39-C40
27	D	402	CDL	C80-C81-C82-C83
27	D	402	CDL	C24-C25-C26-C27
27	V	201	CDL	CA5-C11-C12-C13
27	d	402	CDL	C80-C81-C82-C83
25	o	201	PC1	C3A-C3B-C3C-C3D
25	O	201	PC1	C3A-C3B-C3C-C3D
28	c	402	PEE	C38-C39-C40-C41
28	C	402	PEE	C38-C39-C40-C41
27	h	302	CDL	CB3-CB4-OB6-CB5
27	e	401	CDL	CA6-CA4-OA6-CA5
27	b	601	CDL	CA3-CA4-OA6-CA5
27	H	302	CDL	CB3-CB4-OB6-CB5
27	E	401	CDL	CA6-CA4-OA6-CA5
27	B	602	CDL	CA3-CA4-OA6-CA5
28	j	302	PEE	C3-C2-O2-C10
28	J	302	PEE	C3-C2-O2-C10
25	o	201	PC1	C34-C35-C36-C37
25	O	201	PC1	C34-C35-C36-C37
25	o	204	PC1	O11-C1-C2-C3
25	O	204	PC1	O11-C1-C2-C3
27	V	201	CDL	C36-C37-C38-C39
25	o	201	PC1	C32-C33-C34-C35
25	O	201	PC1	C32-C33-C34-C35
27	B	601	CDL	OB5-CB3-CB4-OB6
27	V	201	CDL	OB5-CB3-CB4-OB6
27	B	601	CDL	C36-C37-C38-C39
25	o	204	PC1	O31-C31-C32-C33
25	O	204	PC1	O31-C31-C32-C33
27	u	201	CDL	C84-C85-C86-C87
27	U	201	CDL	C84-C85-C86-C87
28	J	302	PEE	C40-C41-C42-C43
28	j	302	PEE	C40-C41-C42-C43
27	C	404	CDL	C16-C17-C18-C19
27	c	404	CDL	C16-C17-C18-C19
27	c	404	CDL	OA6-CA4-CA6-OA8
27	C	404	CDL	OA6-CA4-CA6-OA8
27	u	201	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
27	U	201	CDL	C32-C31-CA7-OA8
27	U	201	CDL	C44-C45-C46-C47
27	u	201	CDL	C44-C45-C46-C47
27	H	302	CDL	C14-C15-C16-C17
27	h	302	CDL	C14-C15-C16-C17
25	O	204	PC1	C2A-C2B-C2C-C2D
28	j	302	PEE	C41-C42-C43-C44
28	J	302	PEE	C41-C42-C43-C44
25	o	204	PC1	C2A-C2B-C2C-C2D
25	o	204	PC1	C3B-C3C-C3D-C3E
25	o	204	PC1	C3C-C3D-C3E-C3F
25	O	204	PC1	C3B-C3C-C3D-C3E
25	O	204	PC1	C3C-C3D-C3E-C3F
27	e	401	CDL	CA4-CA6-OA8-CA7
27	E	401	CDL	CA4-CA6-OA8-CA7
25	o	201	PC1	C38-C39-C3A-C3B
28	j	302	PEE	C31-C30-O3-C3
28	J	302	PEE	C31-C30-O3-C3
25	O	201	PC1	C38-C39-C3A-C3B
26	D	401	LMT	C2'-C1'-O1'-C1
27	c	404	CDL	C15-C16-C17-C18
27	C	404	CDL	C15-C16-C17-C18
28	J	301	PEE	C12-C13-C14-C15
28	j	301	PEE	C12-C13-C14-C15
27	B	601	CDL	O1-C1-CA2-OA2
27	V	201	CDL	O1-C1-CA2-OA2
25	V	203	PC1	C26-C27-C28-C29
27	v	201	CDL	C32-C33-C34-C35
27	V	202	CDL	C32-C33-C34-C35
25	v	202	PC1	C26-C27-C28-C29
27	u	201	CDL	C77-C78-C79-C80
27	h	302	CDL	C39-C40-C41-C42
27	H	302	CDL	C39-C40-C41-C42
27	U	201	CDL	C77-C78-C79-C80
27	e	401	CDL	C1-CA2-OA2-PA1
27	E	401	CDL	C1-CA2-OA2-PA1
27	o	203	CDL	C53-C54-C55-C56
27	O	203	CDL	C53-C54-C55-C56
27	O	203	CDL	C63-C64-C65-C66
25	v	202	PC1	C27-C28-C29-C2A
26	c	401	LMT	C5-C6-C7-C8
27	o	203	CDL	C63-C64-C65-C66

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Mol	Chain	Res	Type	Atoms
27	B	602	CDL	C15-C16-C17-C18
26	x	101	LMT	C4-C5-C6-C7
26	X	101	LMT	C4-C5-C6-C7
26	C	401	LMT	C5-C6-C7-C8
27	B	601	CDL	C35-C36-C37-C38
27	u	201	CDL	C33-C34-C35-C36
27	U	201	CDL	C33-C34-C35-C36
25	V	203	PC1	C27-C28-C29-C2A
27	b	601	CDL	C15-C16-C17-C18
28	c	402	PEE	C11-C12-C13-C14
28	j	301	PEE	C36-C37-C38-C39
28	j	302	PEE	C1-C2-C3-O3
28	J	301	PEE	C36-C37-C38-C39
28	J	302	PEE	C1-C2-C3-O3
27	V	201	CDL	C35-C36-C37-C38
28	C	402	PEE	C11-C12-C13-C14
27	v	201	CDL	C40-C41-C42-C43
27	V	202	CDL	C40-C41-C42-C43
26	x	101	LMT	O5'-C5'-C6'-O6'
27	h	302	CDL	CA3-CA4-OA6-CA5
27	b	601	CDL	CB3-CB4-OB6-CB5
27	b	601	CDL	CB6-CB4-OB6-CB5
27	d	402	CDL	CB3-CB4-OB6-CB5
27	d	402	CDL	CB6-CB4-OB6-CB5
27	H	302	CDL	CA3-CA4-OA6-CA5
27	B	602	CDL	CB3-CB4-OB6-CB5
27	B	602	CDL	CB6-CB4-OB6-CB5
27	D	402	CDL	CB3-CB4-OB6-CB5
27	D	402	CDL	CB6-CB4-OB6-CB5
28	j	302	PEE	C1-C2-O2-C10
28	J	302	PEE	C1-C2-O2-C10
26	X	101	LMT	O5'-C5'-C6'-O6'
27	V	201	CDL	C21-C22-C23-C24
27	B	601	CDL	C21-C22-C23-C24
28	J	302	PEE	C18-C19-C20-C21
25	o	204	PC1	C28-C29-C2A-C2B
25	v	202	PC1	C2A-C2B-C2C-C2D
25	V	203	PC1	C2A-C2B-C2C-C2D
25	O	204	PC1	C28-C29-C2A-C2B
26	d	401	LMT	C2'-C1'-O1'-C1
27	v	201	CDL	OA5-CA3-CA4-OA6
27	V	202	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
27	O	203	CDL	C79-C80-C81-C82
27	o	203	CDL	C79-C80-C81-C82
28	j	302	PEE	C18-C19-C20-C21
27	c	404	CDL	C36-C37-C38-C39
27	V	201	CDL	C84-C85-C86-C87
27	C	404	CDL	C36-C37-C38-C39
27	B	601	CDL	C84-C85-C86-C87
27	B	601	CDL	C37-C38-C39-C40
27	o	203	CDL	C75-C76-C77-C78
27	O	203	CDL	C75-C76-C77-C78
27	V	201	CDL	C80-C81-C82-C83
27	B	601	CDL	C80-C81-C82-C83
27	V	201	CDL	C37-C38-C39-C40
27	d	402	CDL	C73-C74-C75-C76
27	D	402	CDL	C73-C74-C75-C76
27	h	302	CDL	OB7-CB5-OB6-CB4
27	H	302	CDL	OB7-CB5-OB6-CB4
28	j	301	PEE	C32-C33-C34-C35
28	J	301	PEE	C32-C33-C34-C35
25	v	202	PC1	C21-C22-C23-C24
27	c	404	CDL	C52-C53-C54-C55
27	C	404	CDL	C52-C53-C54-C55
27	B	601	CDL	C81-C82-C83-C84
25	V	203	PC1	C21-C22-C23-C24
27	V	201	CDL	C81-C82-C83-C84
27	o	203	CDL	C72-C71-CB7-OB8
27	O	203	CDL	C72-C71-CB7-OB8
27	u	201	CDL	C38-C39-C40-C41
27	U	201	CDL	C38-C39-C40-C41
28	j	302	PEE	C21-C22-C23-C24
27	c	404	CDL	C40-C41-C42-C43
27	B	602	CDL	C21-C22-C23-C24
28	J	302	PEE	C21-C22-C23-C24
25	v	202	PC1	C39-C3A-C3B-C3C
25	V	203	PC1	C39-C3A-C3B-C3C
27	c	404	CDL	CA3-CA4-CA6-OA8
27	C	404	CDL	CA3-CA4-CA6-OA8
27	C	404	CDL	C40-C41-C42-C43
27	b	601	CDL	C21-C22-C23-C24
27	b	601	CDL	OA5-CA3-CA4-OA6
27	B	602	CDL	OA5-CA3-CA4-OA6
27	c	404	CDL	C59-C60-C61-C62

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Mol	Chain	Res	Type	Atoms
27	d	402	CDL	C11-C12-C13-C14
28	J	302	PEE	O5-C30-O3-C3
27	c	404	CDL	C17-C18-C19-C20
27	C	404	CDL	C17-C18-C19-C20
27	C	404	CDL	C59-C60-C61-C62
27	D	402	CDL	C11-C12-C13-C14
28	j	302	PEE	O5-C30-O3-C3
27	h	302	CDL	C79-C80-C81-C82
27	H	302	CDL	C79-C80-C81-C82
27	v	201	CDL	OA5-CA3-CA4-CA6
27	V	202	CDL	OA5-CA3-CA4-CA6
27	h	302	CDL	C34-C35-C36-C37
27	H	302	CDL	C34-C35-C36-C37
27	h	302	CDL	C51-CB5-OB6-CB4
27	h	302	CDL	C36-C37-C38-C39
27	H	302	CDL	C36-C37-C38-C39
27	O	203	CDL	OB9-CB7-OB8-CB6
27	o	203	CDL	C71-C72-C73-C74
27	O	203	CDL	C71-C72-C73-C74
26	X	101	LMT	C3'-C4'-O1B-C1B
27	H	302	CDL	C51-CB5-OB6-CB4
25	o	201	PC1	C35-C36-C37-C38
25	O	201	PC1	C35-C36-C37-C38
28	j	302	PEE	C44-C45-C46-C47
27	e	401	CDL	C34-C35-C36-C37
27	o	203	CDL	OB9-CB7-OB8-CB6
28	J	302	PEE	C44-C45-C46-C47
26	x	101	LMT	C3'-C4'-O1B-C1B
27	E	401	CDL	C34-C35-C36-C37
27	o	203	CDL	CA5-C11-C12-C13
27	O	203	CDL	CA5-C11-C12-C13
28	C	402	PEE	C41-C42-C43-C44
28	c	402	PEE	C41-C42-C43-C44
28	j	302	PEE	C17-C18-C19-C20
28	J	302	PEE	C17-C18-C19-C20
27	o	203	CDL	C71-CB7-OB8-CB6
27	O	203	CDL	C71-CB7-OB8-CB6
25	v	202	PC1	C1-C2-C3-O31
25	V	203	PC1	C1-C2-C3-O31
27	V	201	CDL	CB3-CB4-CB6-OB8
27	u	201	CDL	C52-C53-C54-C55
27	O	203	CDL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
27	o	203	CDL	C17-C18-C19-C20
27	U	201	CDL	C52-C53-C54-C55
27	c	404	CDL	C12-C13-C14-C15
25	o	204	PC1	C3D-C3E-C3F-C3G
25	O	204	PC1	C3D-C3E-C3F-C3G
27	C	404	CDL	C12-C13-C14-C15
27	B	602	CDL	C17-C18-C19-C20
26	D	401	LMT	C5-C6-C7-C8
27	b	601	CDL	C17-C18-C19-C20
27	c	404	CDL	C52-C51-CB5-OB6
27	C	404	CDL	C52-C51-CB5-OB6
27	b	601	CDL	OA5-CA3-CA4-CA6
27	B	602	CDL	OA5-CA3-CA4-CA6
26	d	401	LMT	C5-C6-C7-C8
27	o	203	CDL	C52-C51-CB5-OB6
27	O	203	CDL	C52-C51-CB5-OB6
26	x	101	LMT	C7-C8-C9-C10
27	e	401	CDL	C32-C31-CA7-OA9
27	E	401	CDL	C32-C31-CA7-OA9
26	X	101	LMT	C7-C8-C9-C10
26	D	401	LMT	C11-C10-C9-C8
26	d	401	LMT	C11-C10-C9-C8
28	j	302	PEE	O4-C10-O2-C2
25	o	204	PC1	C2C-C2D-C2E-C2F
27	o	203	CDL	C12-C11-CA5-OA6
27	O	203	CDL	C12-C11-CA5-OA6
25	O	204	PC1	C2C-C2D-C2E-C2F
28	J	302	PEE	O4-C10-O2-C2
27	c	404	CDL	C24-C25-C26-C27
25	O	201	PC1	C23-C24-C25-C26
25	o	201	PC1	C23-C24-C25-C26
27	C	404	CDL	C24-C25-C26-C27
27	B	601	CDL	C11-C12-C13-C14
25	V	203	PC1	C32-C31-O31-C3
27	V	201	CDL	C11-C12-C13-C14
27	e	401	CDL	C57-C58-C59-C60
27	E	401	CDL	C57-C58-C59-C60
27	B	601	CDL	CB3-CB4-CB6-OB8
25	v	202	PC1	C32-C31-O31-C3
26	d	401	LMT	O5'-C1'-O1'-C1
26	D	401	LMT	O5'-C1'-O1'-C1
27	u	201	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
27	U	201	CDL	C72-C71-CB7-OB8
27	B	601	CDL	C40-C41-C42-C43
27	V	201	CDL	C40-C41-C42-C43
27	B	601	CDL	C15-C16-C17-C18
27	o	203	CDL	C74-C75-C76-C77
27	O	203	CDL	C74-C75-C76-C77
27	V	201	CDL	C15-C16-C17-C18
28	j	302	PEE	C11-C10-O2-C2
27	H	302	CDL	C12-C13-C14-C15
27	h	302	CDL	C12-C13-C14-C15
27	E	401	CDL	CA5-C11-C12-C13
26	X	101	LMT	C2B-C1B-O1B-C4'
27	e	401	CDL	CA5-C11-C12-C13
25	o	204	PC1	O21-C21-C22-C23
25	O	204	PC1	O21-C21-C22-C23
27	V	201	CDL	C32-C31-CA7-OA8
26	o	202	LMT	C7-C8-C9-C10
27	c	404	CDL	C61-C62-C63-C64
26	O	202	LMT	C7-C8-C9-C10
27	C	404	CDL	C13-C14-C15-C16
26	x	101	LMT	C2B-C1B-O1B-C4'
27	h	302	CDL	C52-C53-C54-C55
27	c	404	CDL	C13-C14-C15-C16
27	B	601	CDL	C32-C31-CA7-OA8
27	H	302	CDL	C52-C53-C54-C55
25	v	202	PC1	O32-C31-O31-C3
27	O	203	CDL	C77-C78-C79-C80
27	C	404	CDL	C61-C62-C63-C64
27	D	402	CDL	C22-C23-C24-C25
27	o	203	CDL	C77-C78-C79-C80
27	o	203	CDL	C32-C31-CA7-OA9
27	O	203	CDL	C32-C31-CA7-OA9
25	V	203	PC1	O32-C31-O31-C3
27	d	402	CDL	C22-C23-C24-C25
27	B	601	CDL	C44-C45-C46-C47
27	v	201	CDL	C55-C56-C57-C58
27	V	201	CDL	C44-C45-C46-C47
28	J	302	PEE	C11-C10-O2-C2
26	d	401	LMT	C7-C8-C9-C10
27	o	203	CDL	C12-C11-CA5-OA7
27	O	203	CDL	C12-C11-CA5-OA7
26	D	401	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
27	V	202	CDL	C55-C56-C57-C58
28	J	302	PEE	C13-C14-C15-C16
28	j	302	PEE	C13-C14-C15-C16
27	c	404	CDL	C52-C51-CB5-OB7
27	C	404	CDL	C52-C51-CB5-OB7
25	o	204	PC1	O22-C21-C22-C23
25	O	204	PC1	O22-C21-C22-C23
27	u	201	CDL	C72-C71-CB7-OB9
27	U	201	CDL	C72-C71-CB7-OB9
28	J	301	PEE	C13-C14-C15-C16
27	B	602	CDL	C74-C75-C76-C77
27	b	601	CDL	C74-C75-C76-C77
28	j	301	PEE	C13-C14-C15-C16
25	v	202	PC1	O31-C31-C32-C33
25	V	203	PC1	O31-C31-C32-C33

There are no ring outliers.

24 monomers are involved in 47 short contacts:

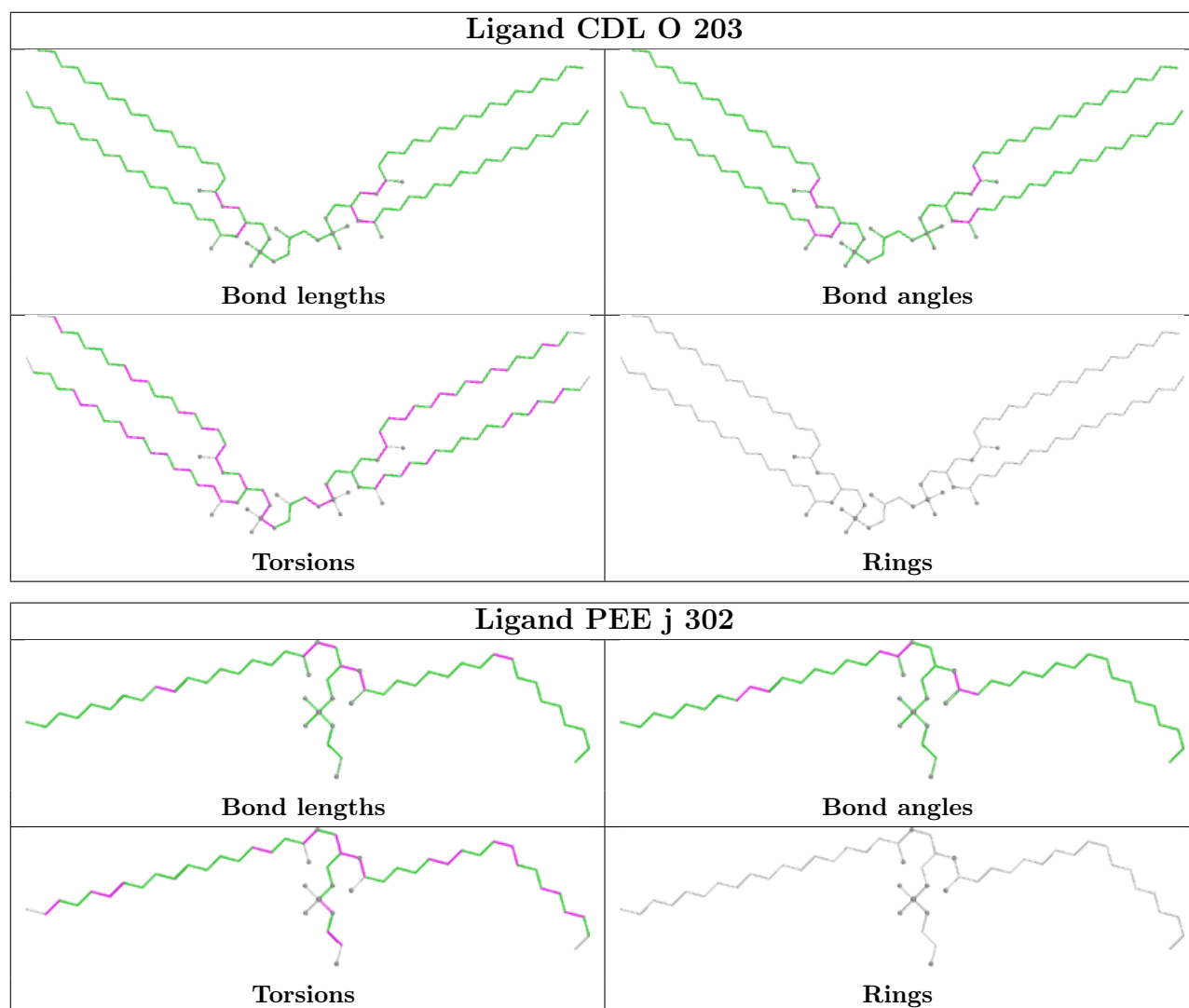
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	j	302	PEE	2	0
28	J	301	PEE	1	0
27	d	402	CDL	1	0
25	o	201	PC1	1	0
27	E	401	CDL	9	0
26	h	301	LMT	2	0
27	u	201	CDL	1	0
27	U	201	CDL	1	0
28	j	301	PEE	1	0
28	J	302	PEE	2	0
26	C	401	LMT	1	0
26	H	301	LMT	2	0
27	B	601	CDL	7	0
27	v	201	CDL	1	0
27	V	201	CDL	7	0
26	o	202	LMT	3	0
27	C	404	CDL	1	0
25	O	201	PC1	2	0
27	e	401	CDL	5	0
26	O	202	LMT	3	0
26	C	403	LMT	1	0
27	c	404	CDL	1	0

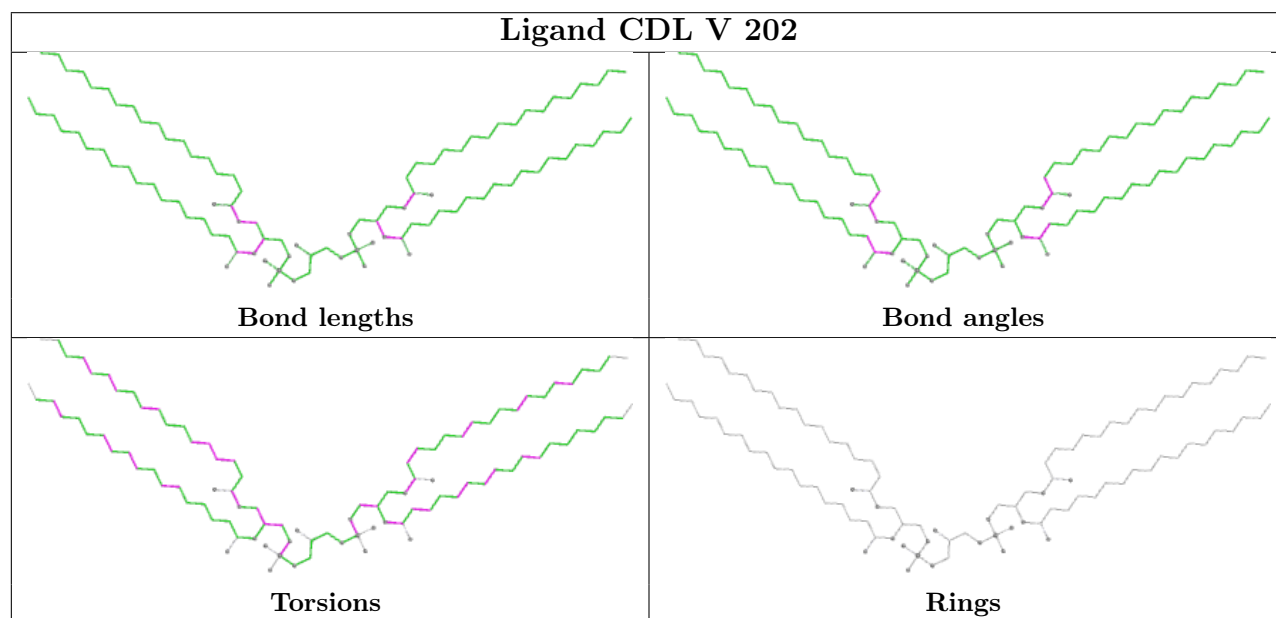
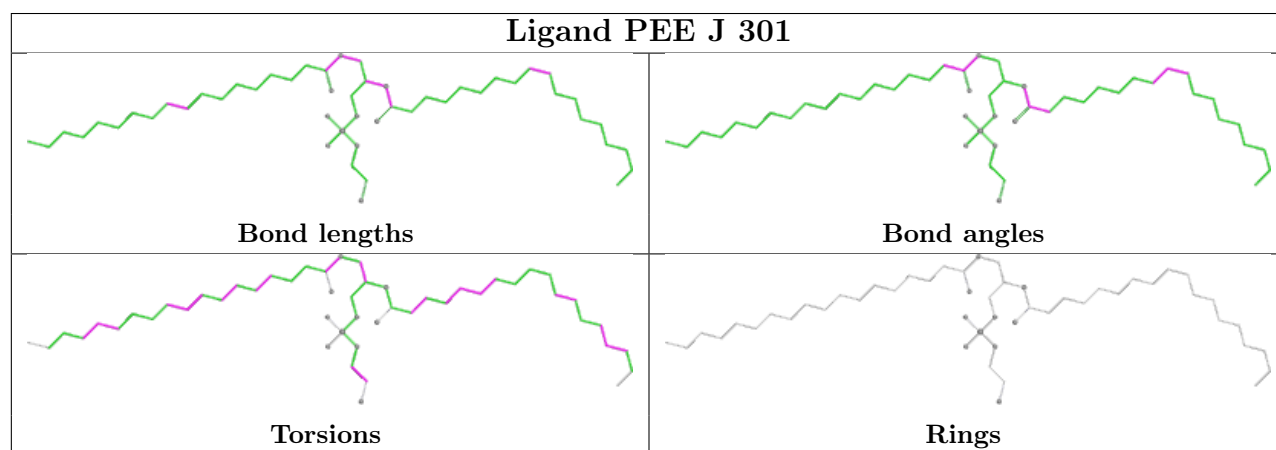
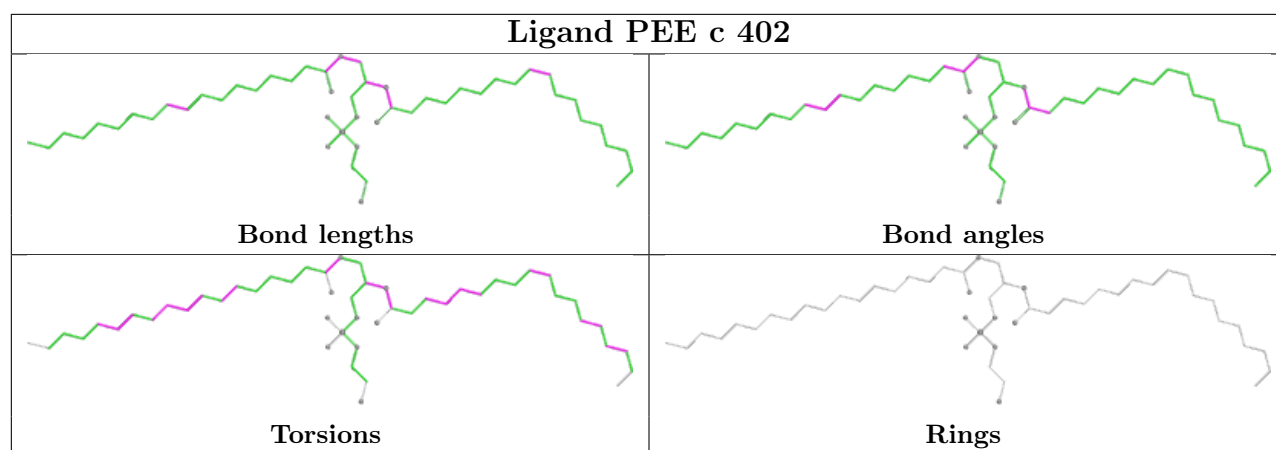
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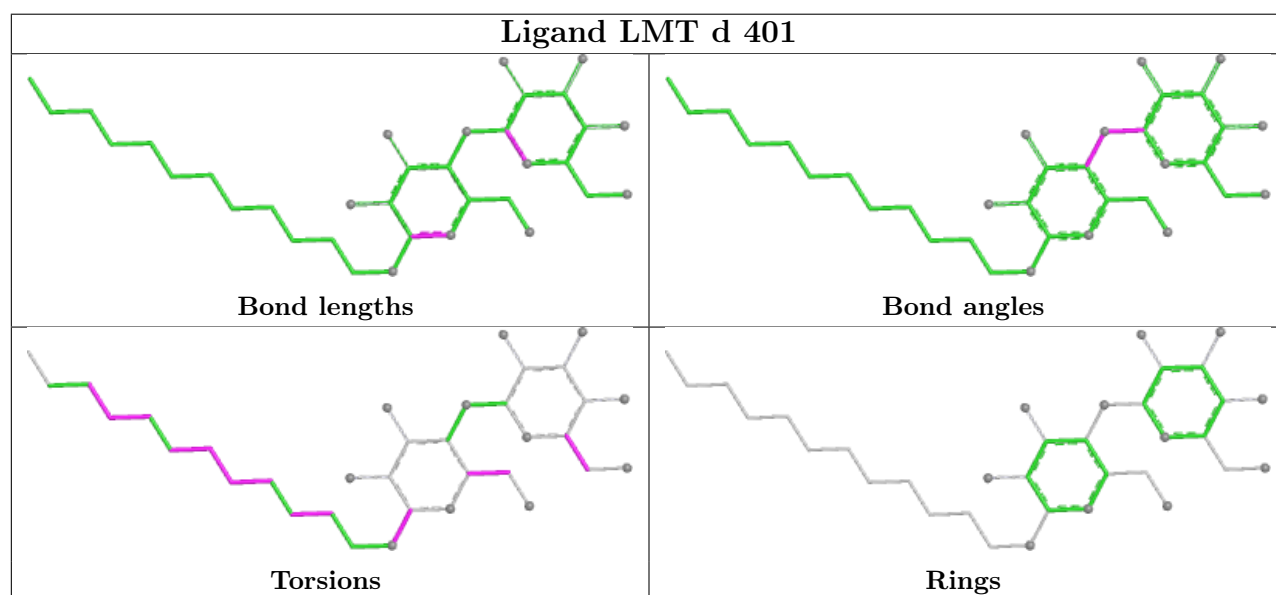
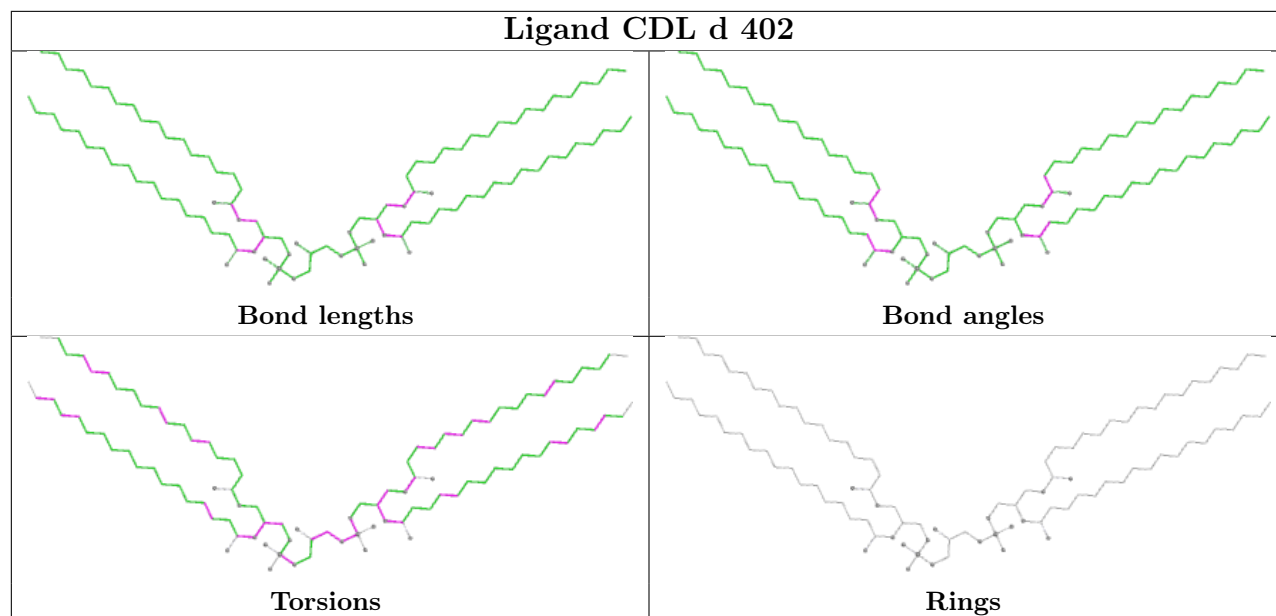
Continued from previous page...

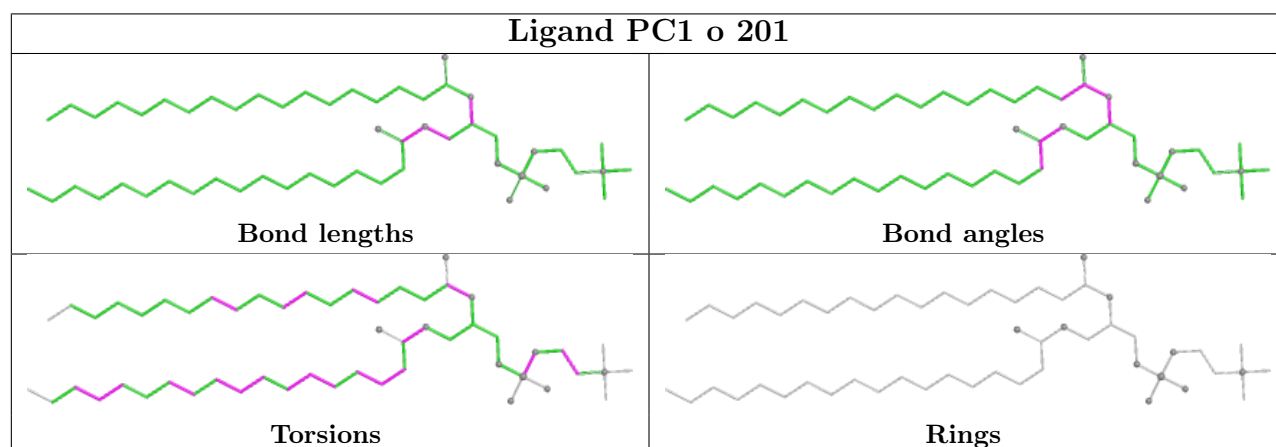
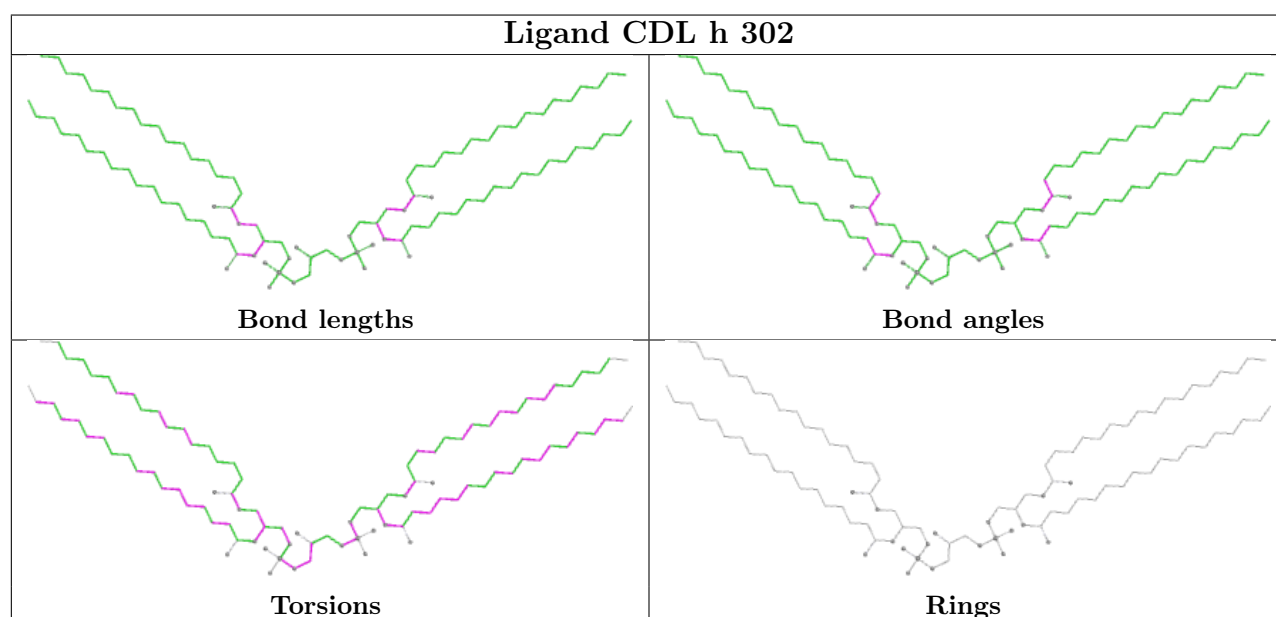
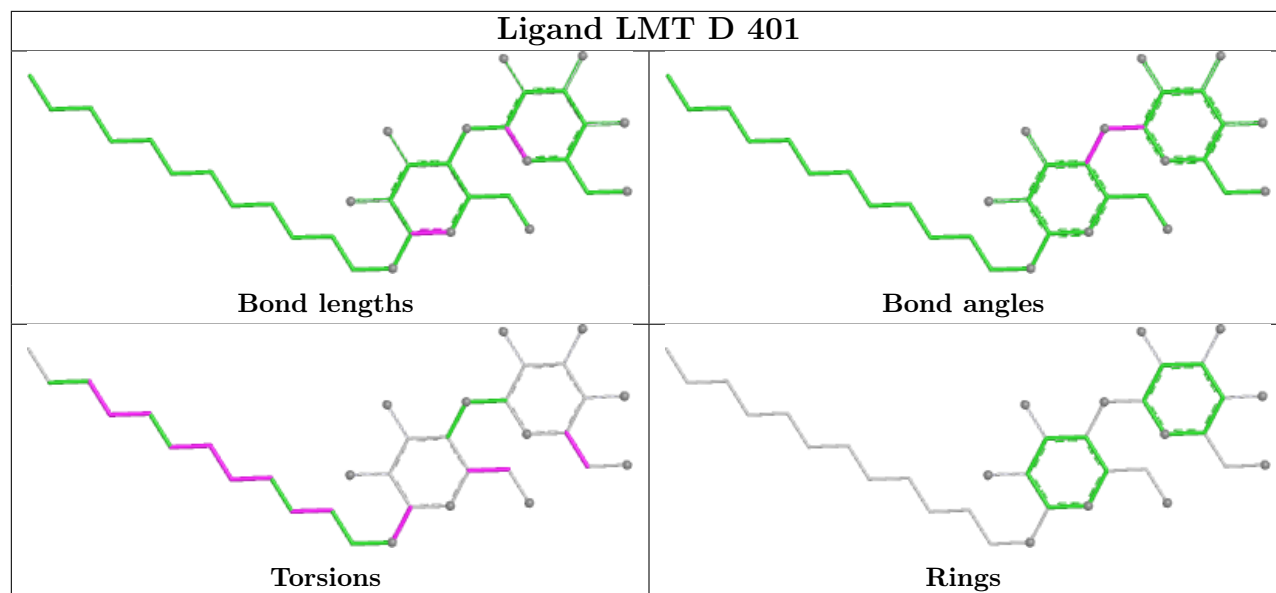
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	c	403	LMT	1	0
26	c	401	LMT	1	0

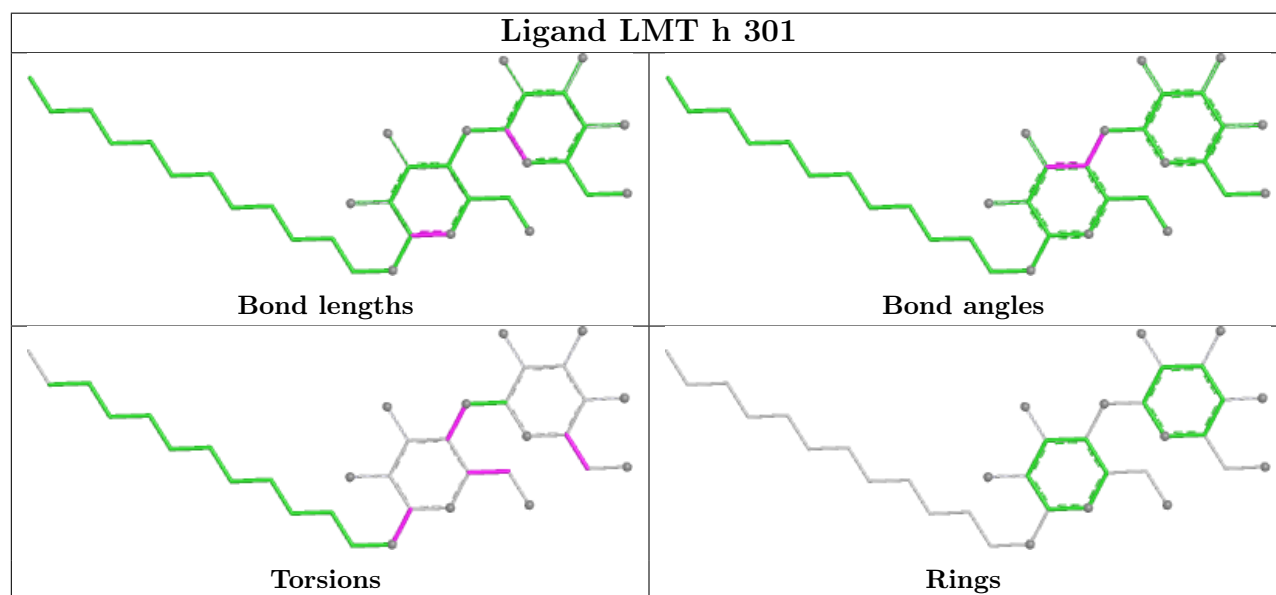
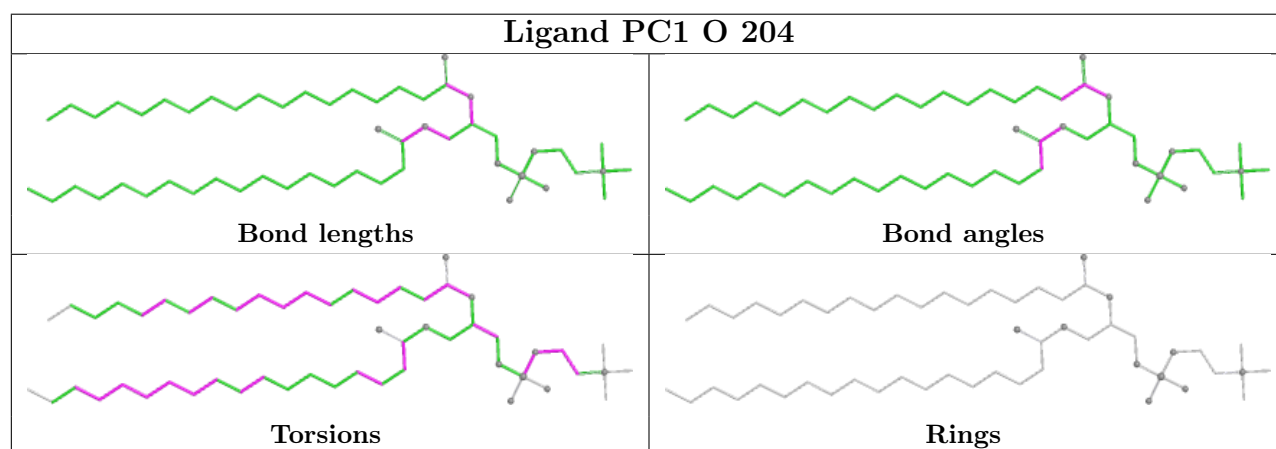
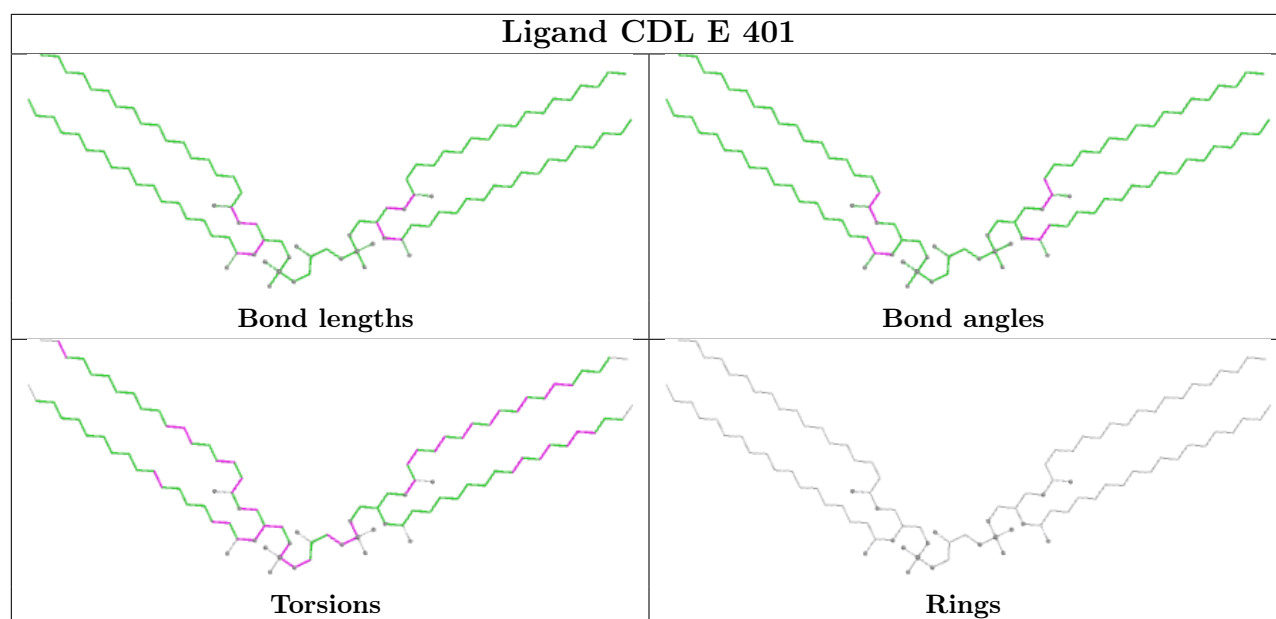
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

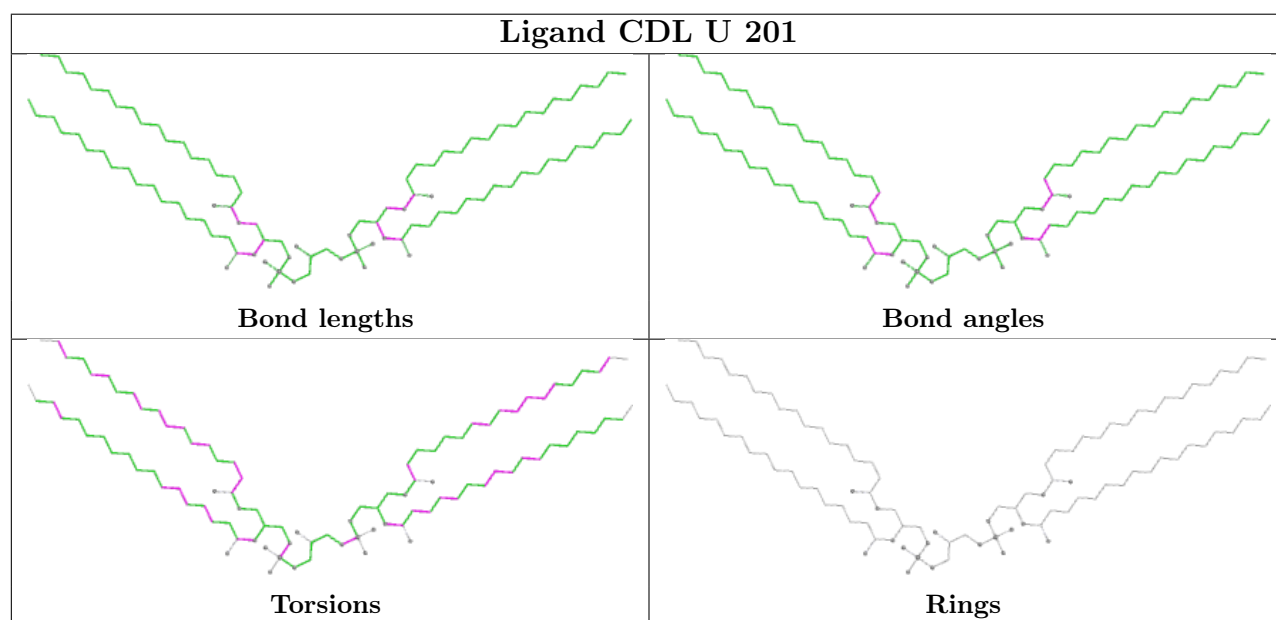
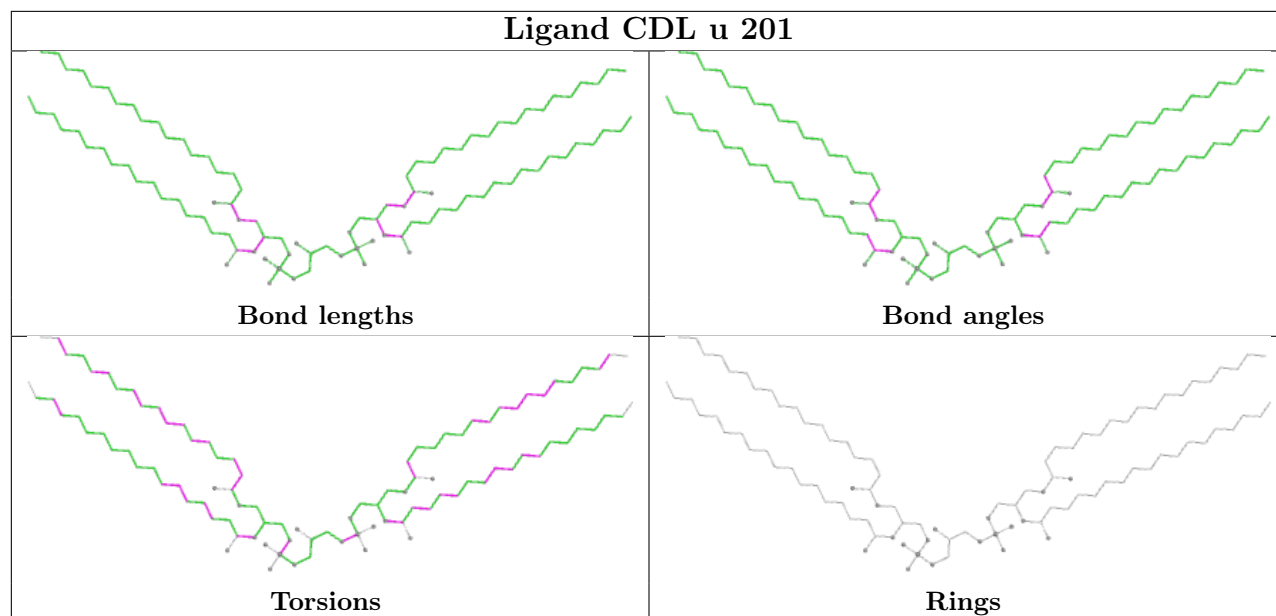


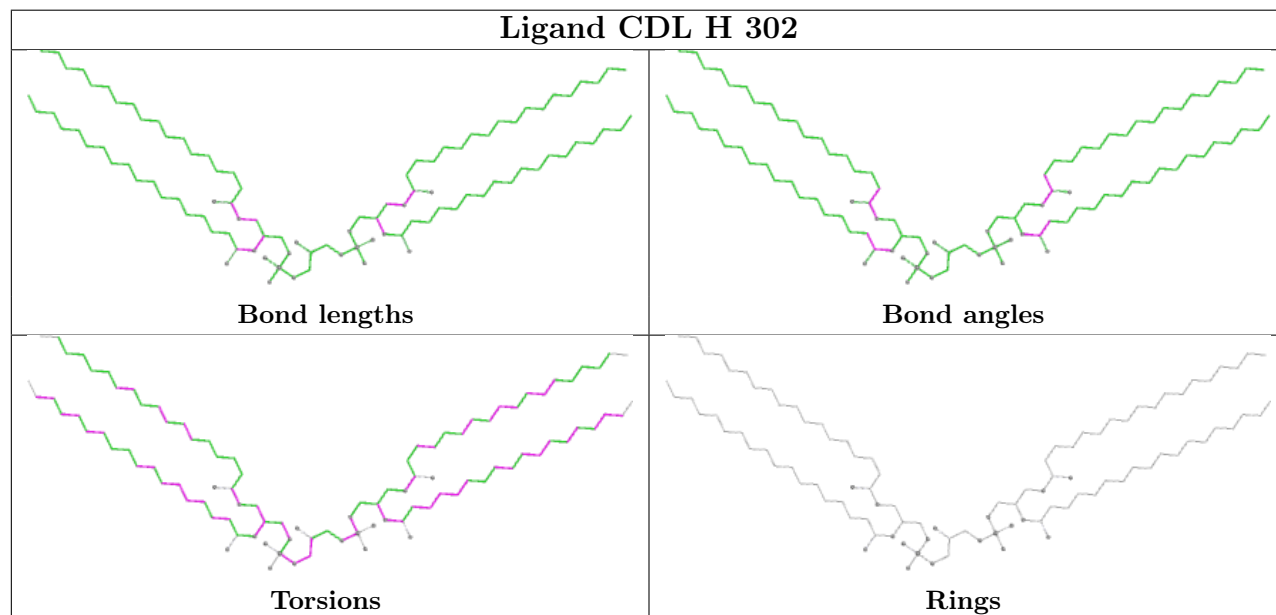
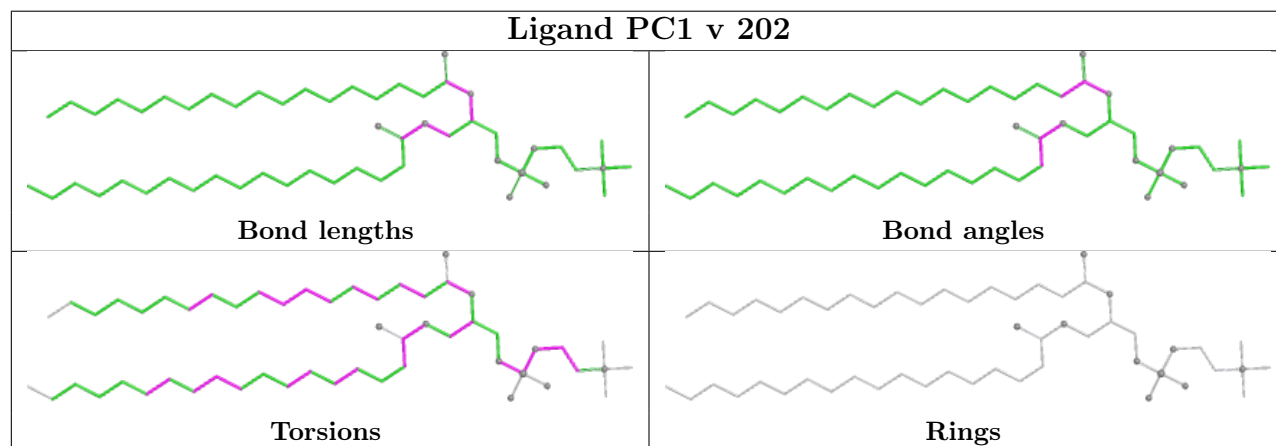
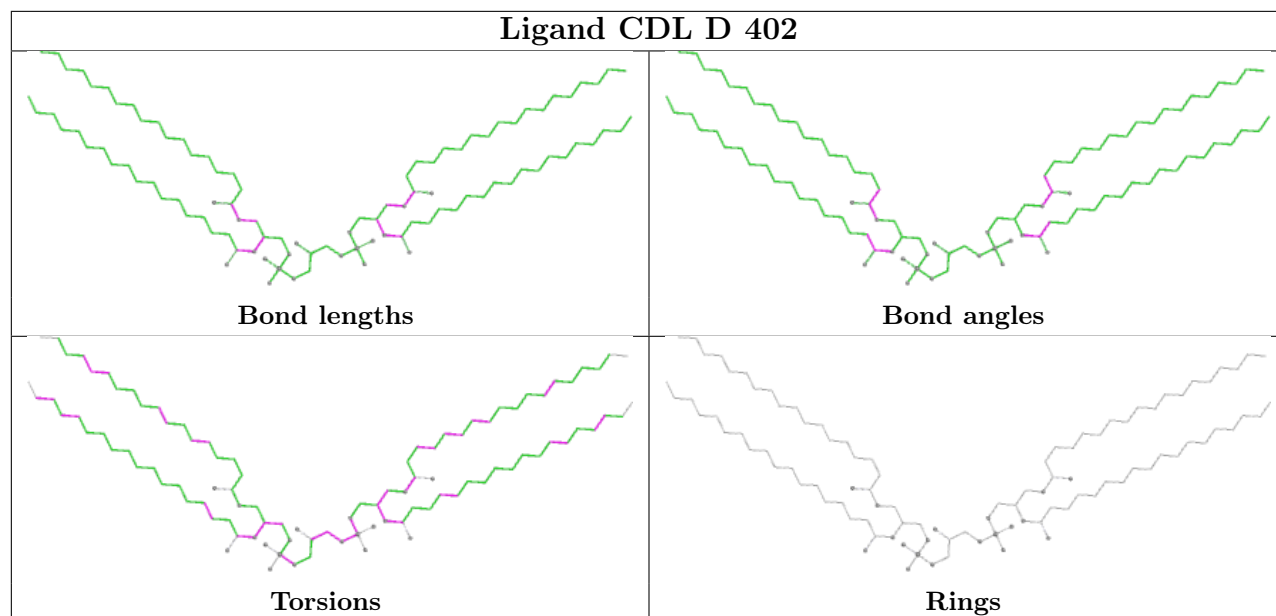


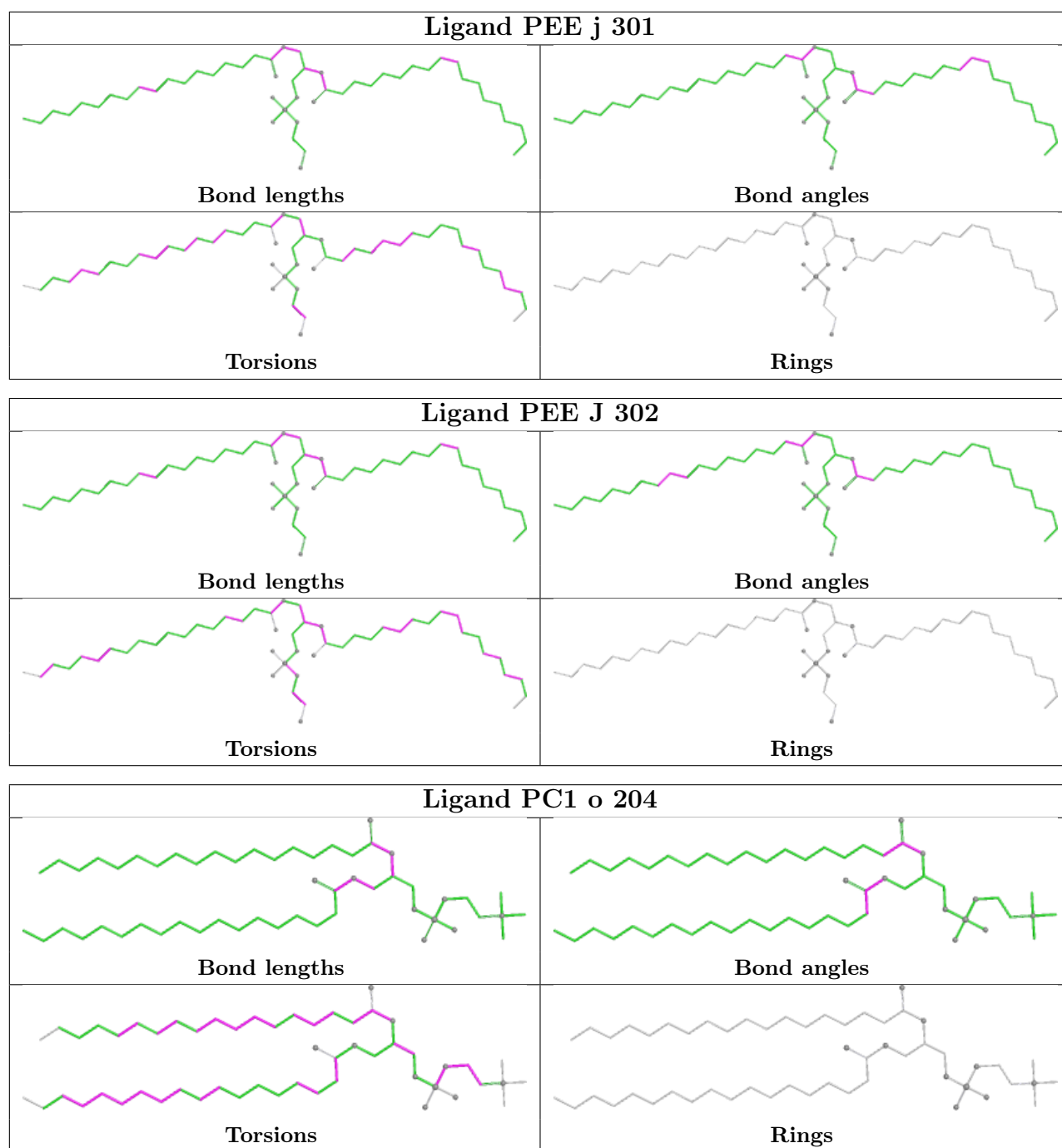


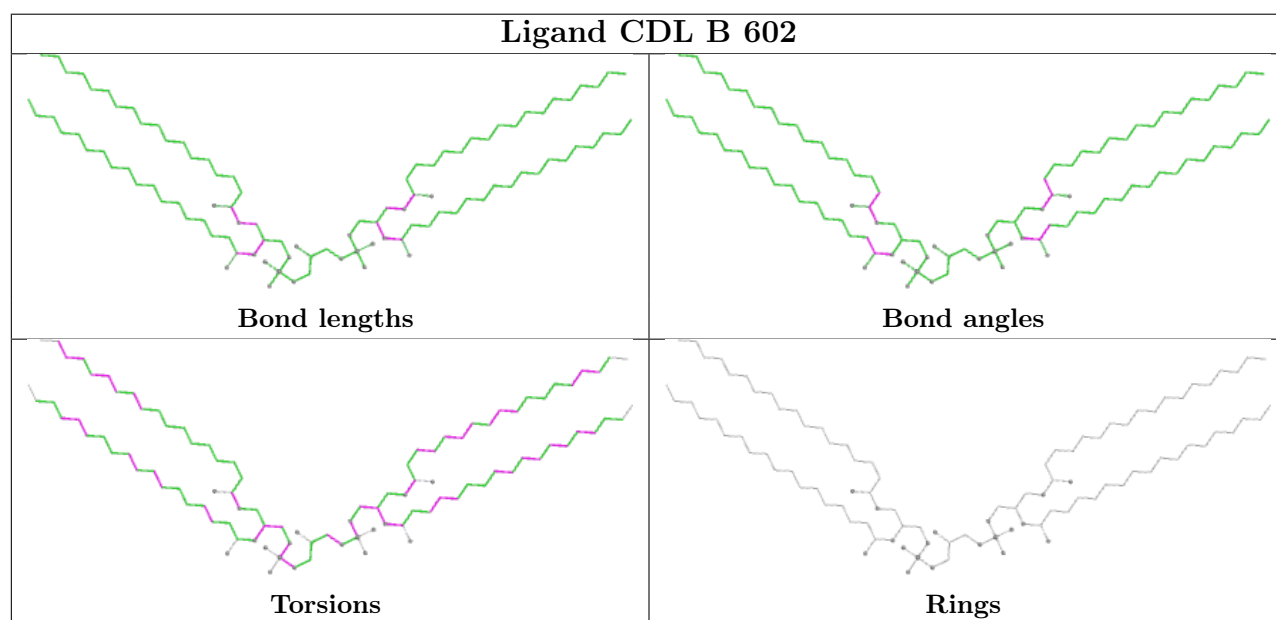
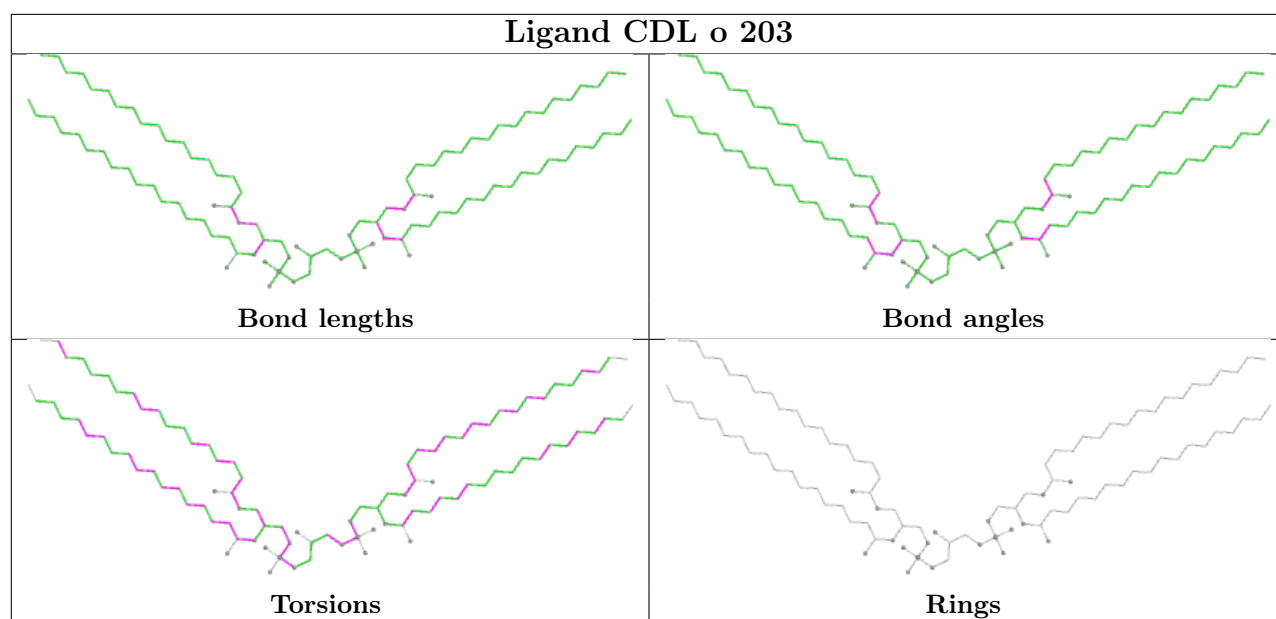


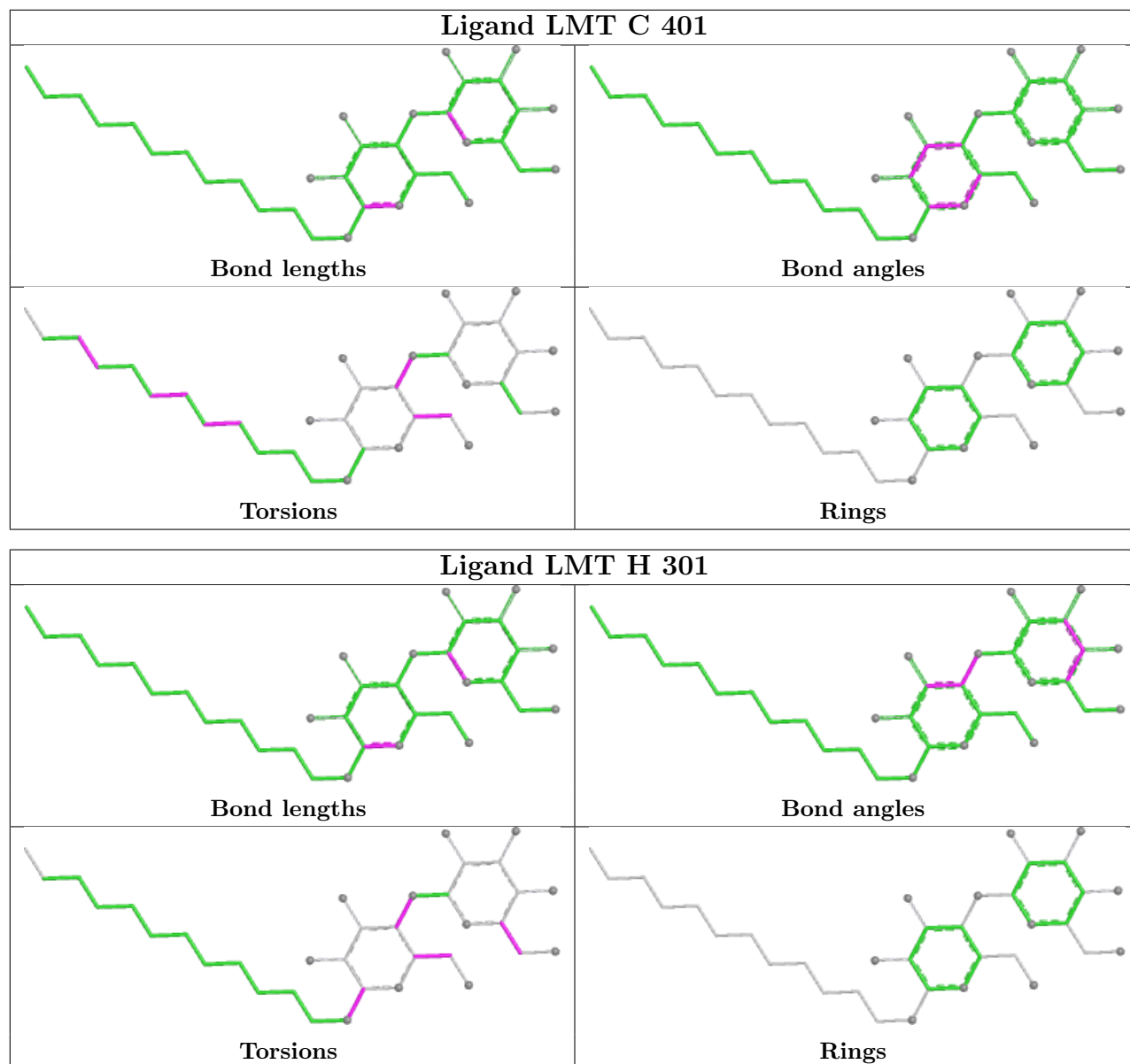


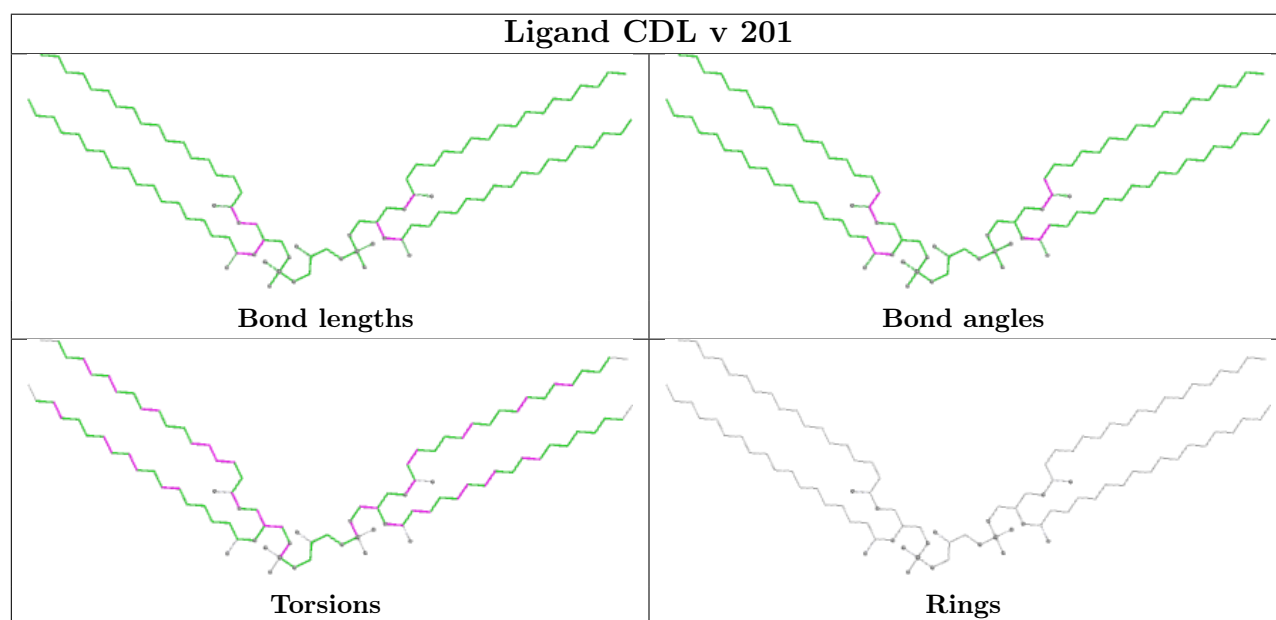
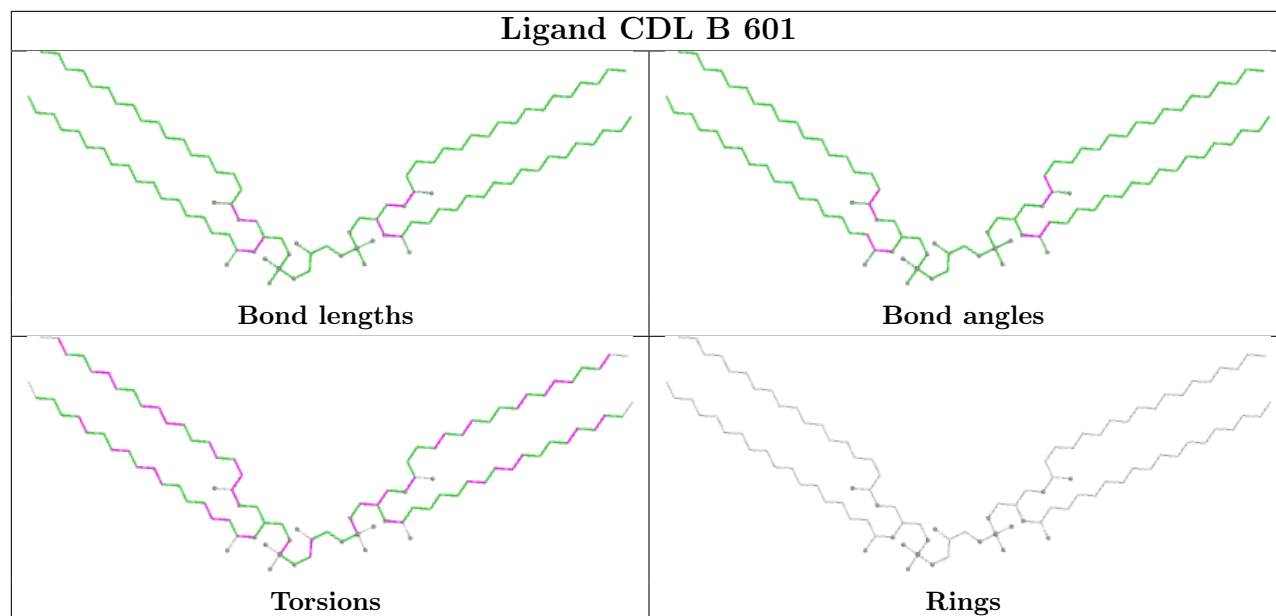


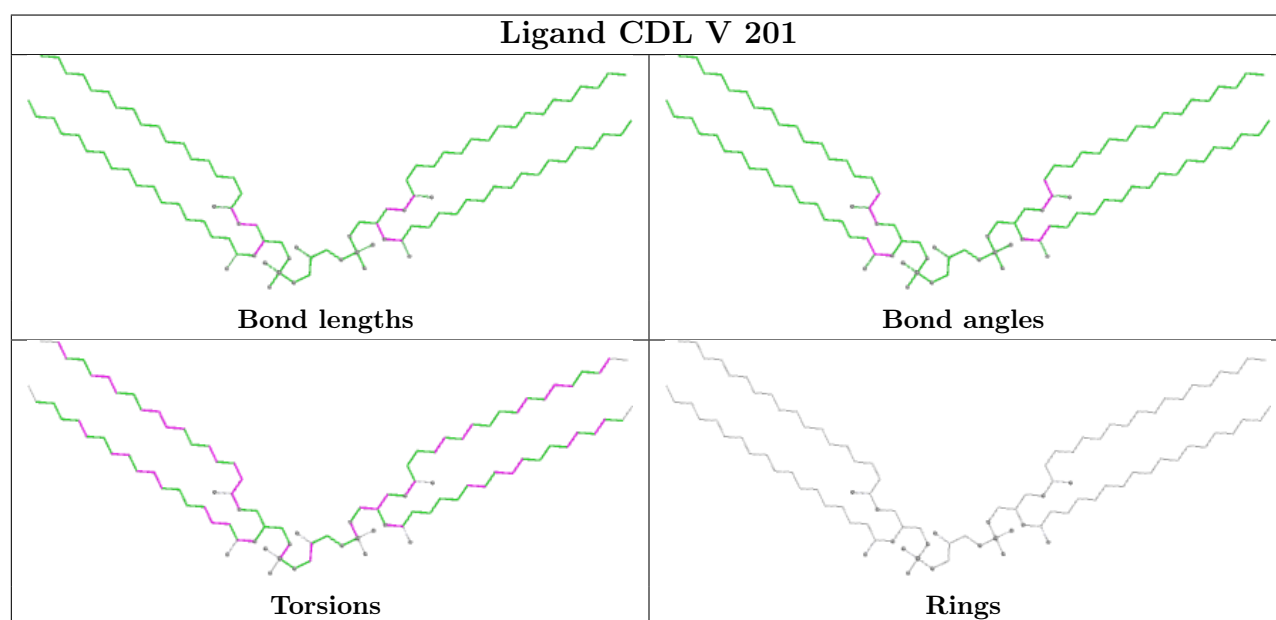
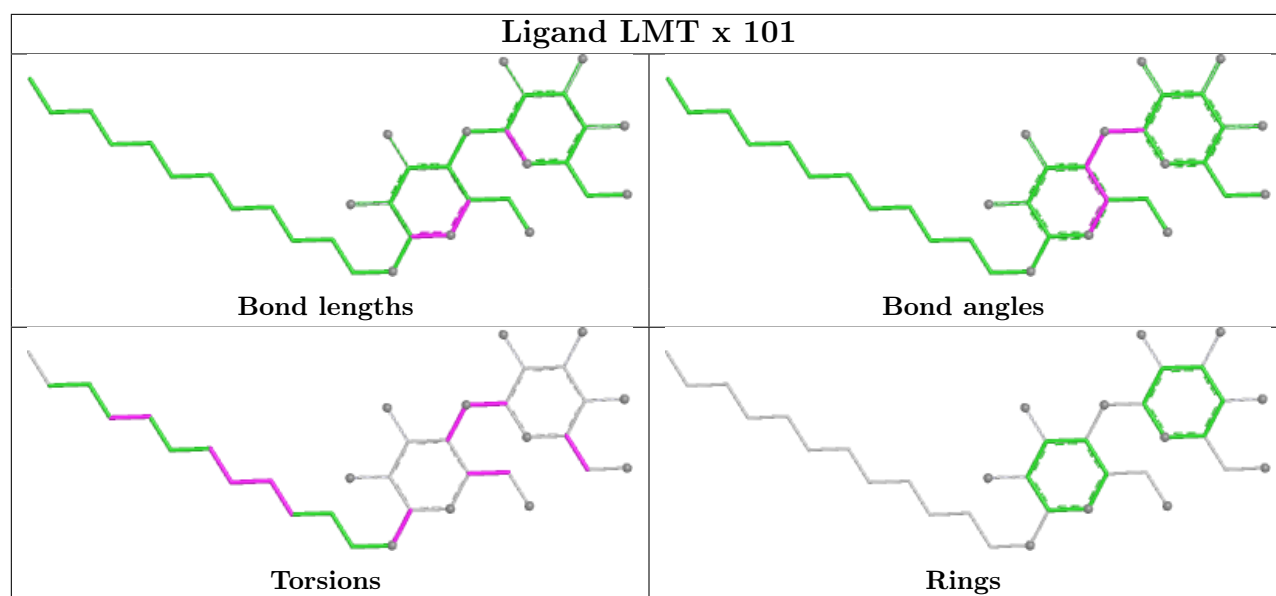


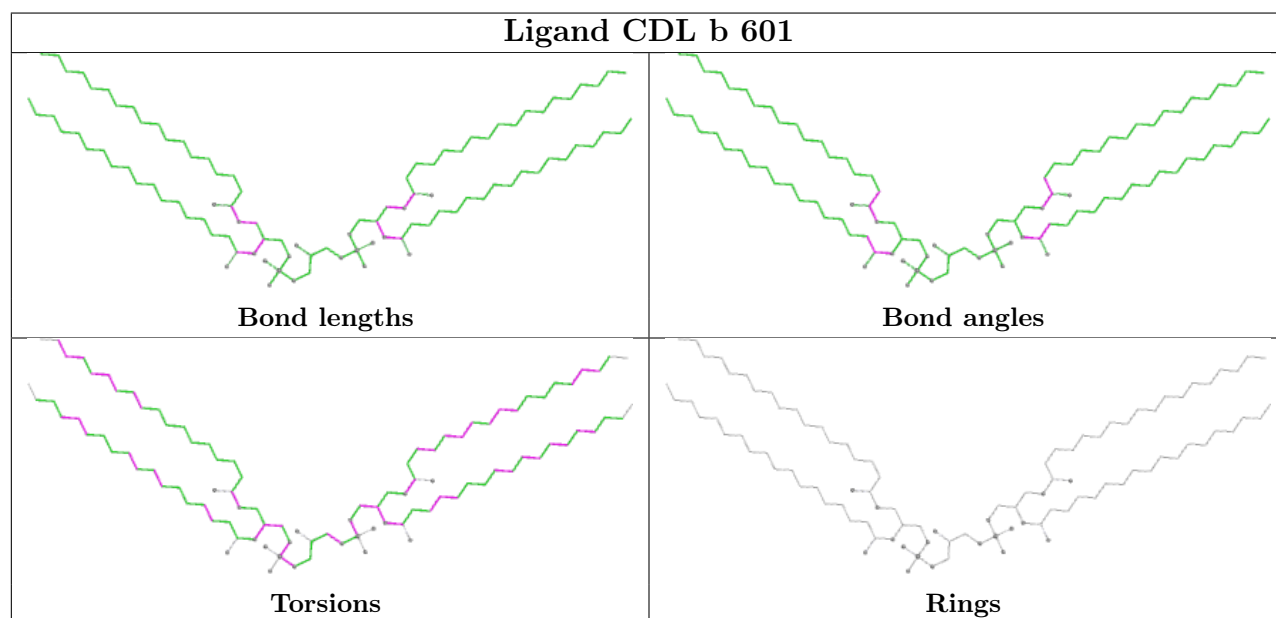
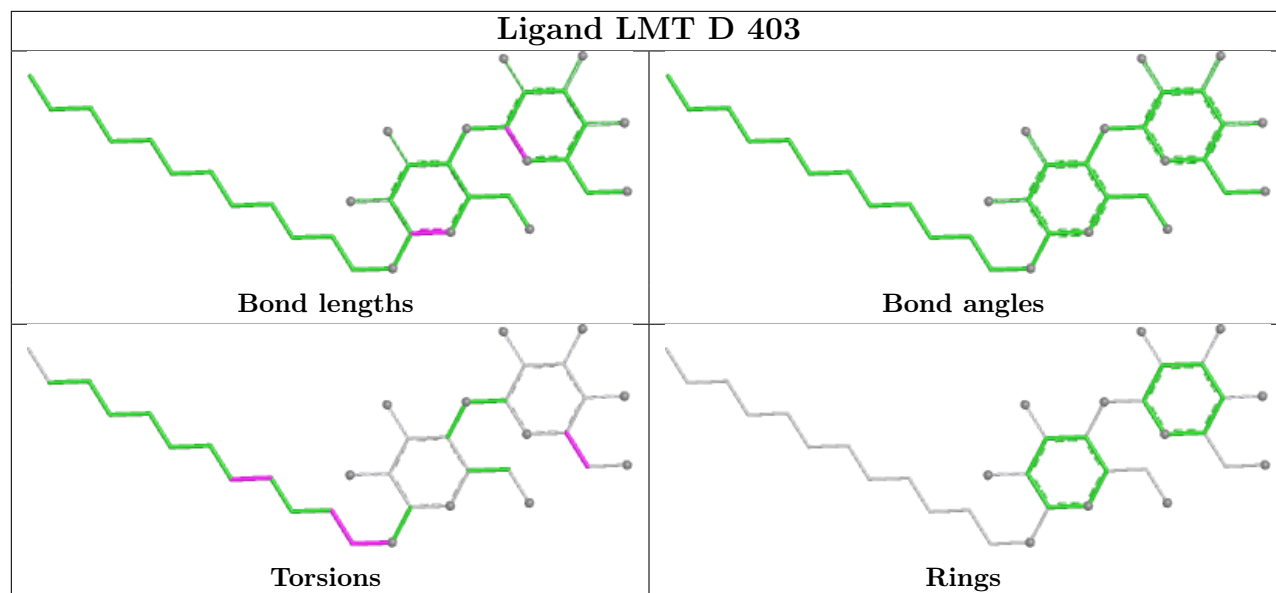


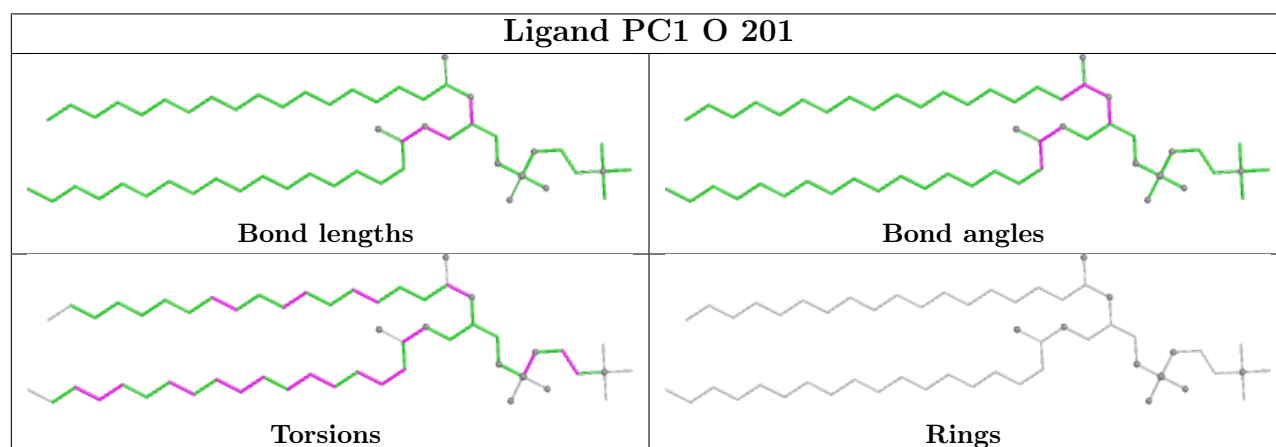
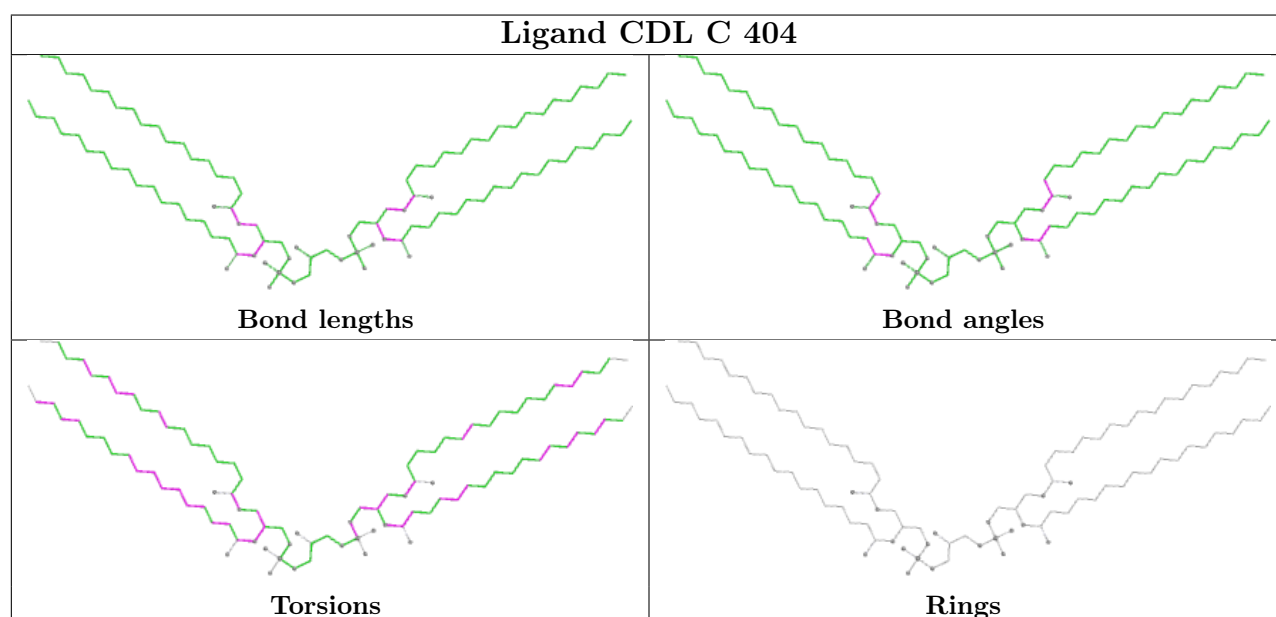
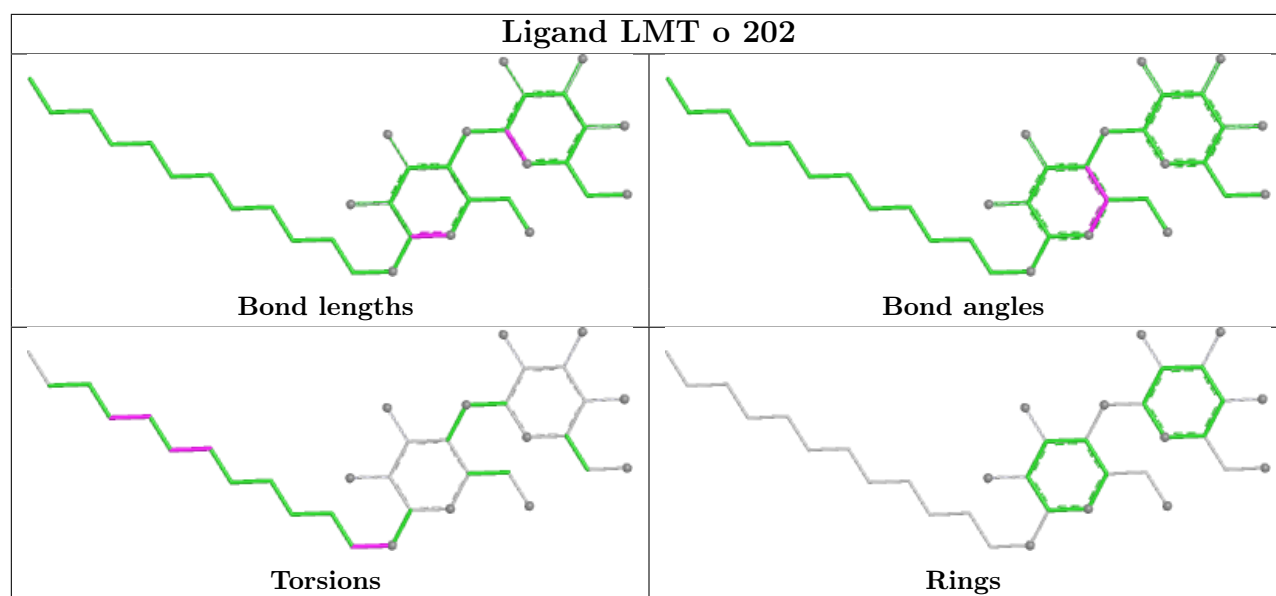


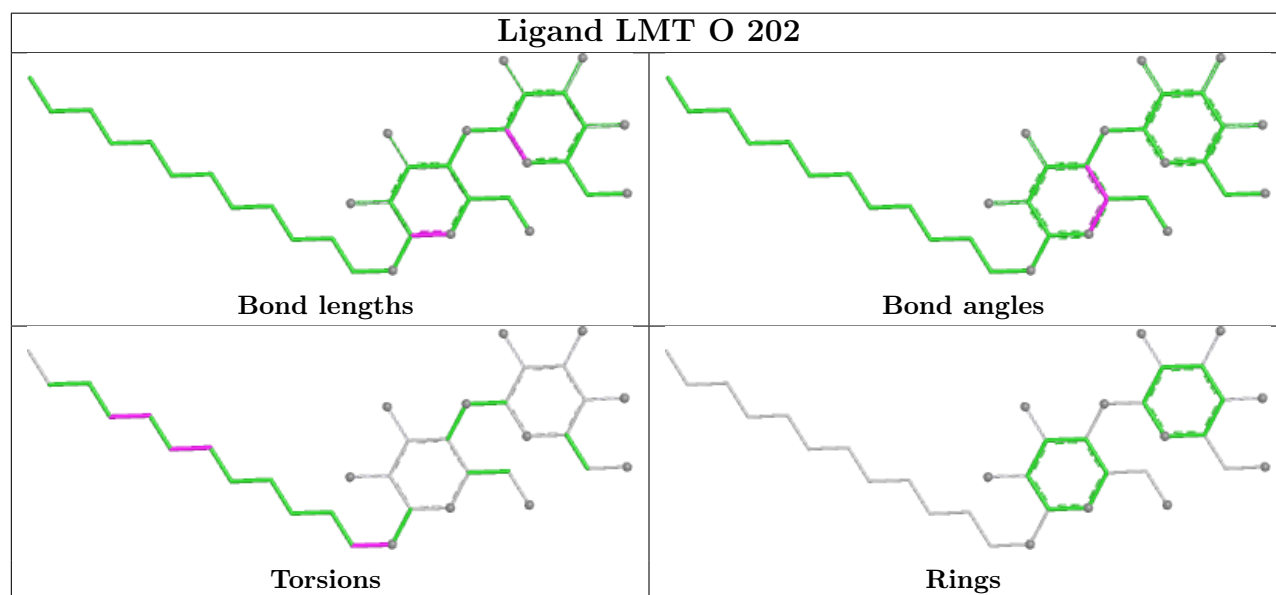
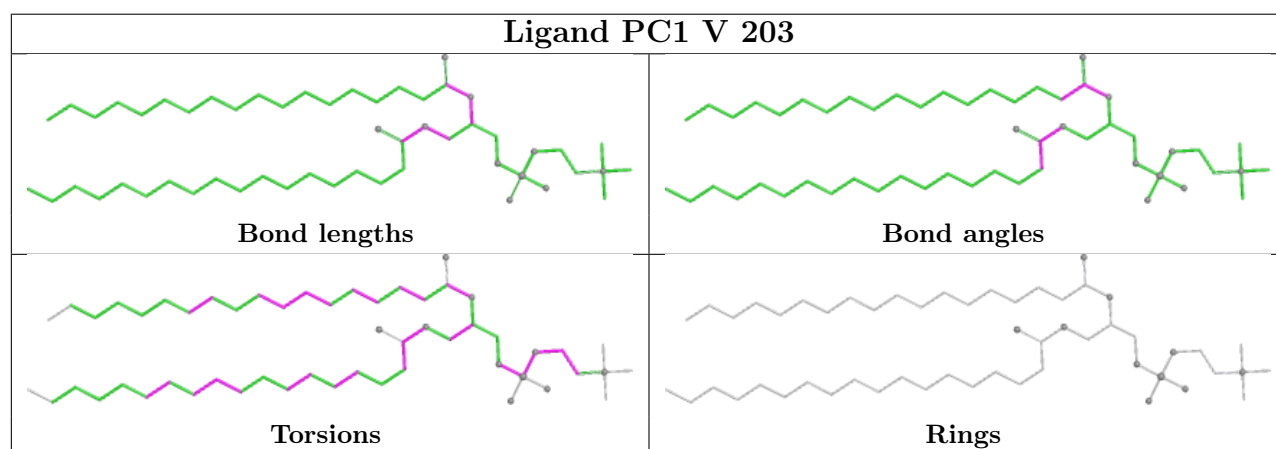
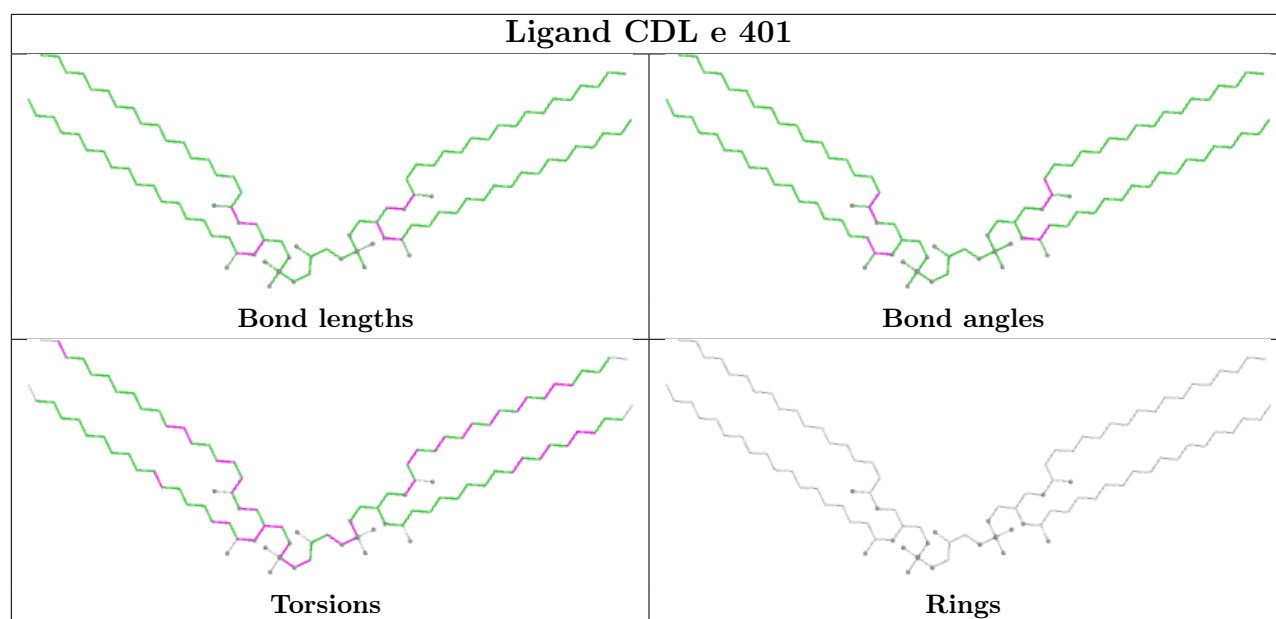


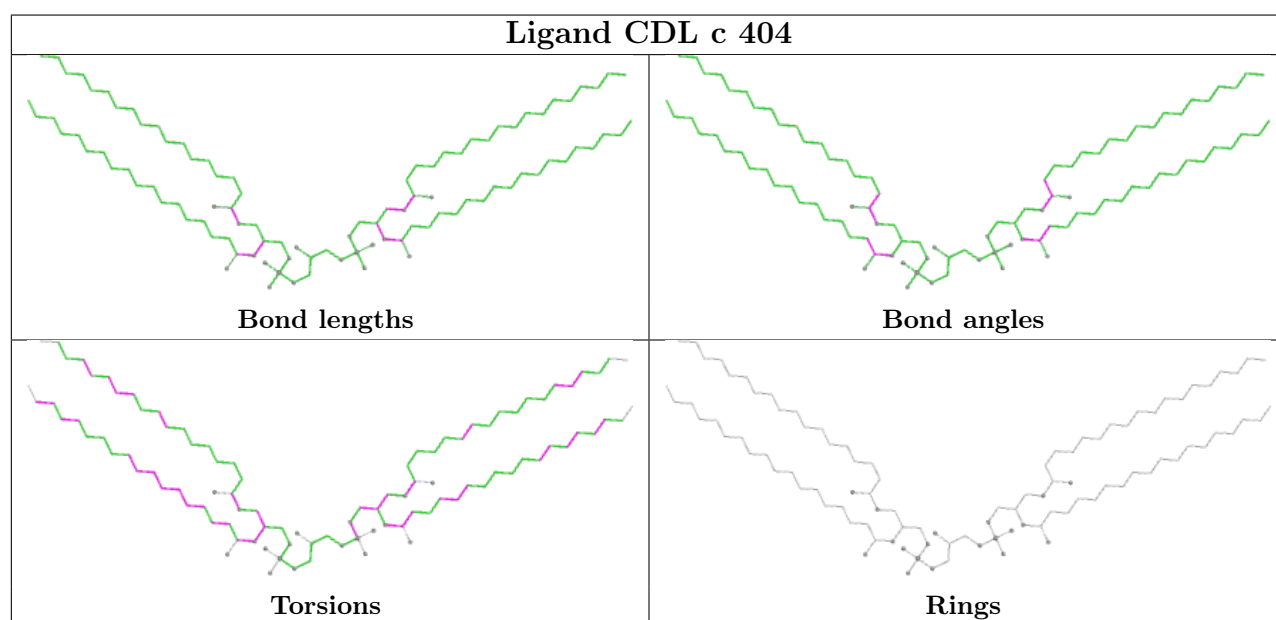
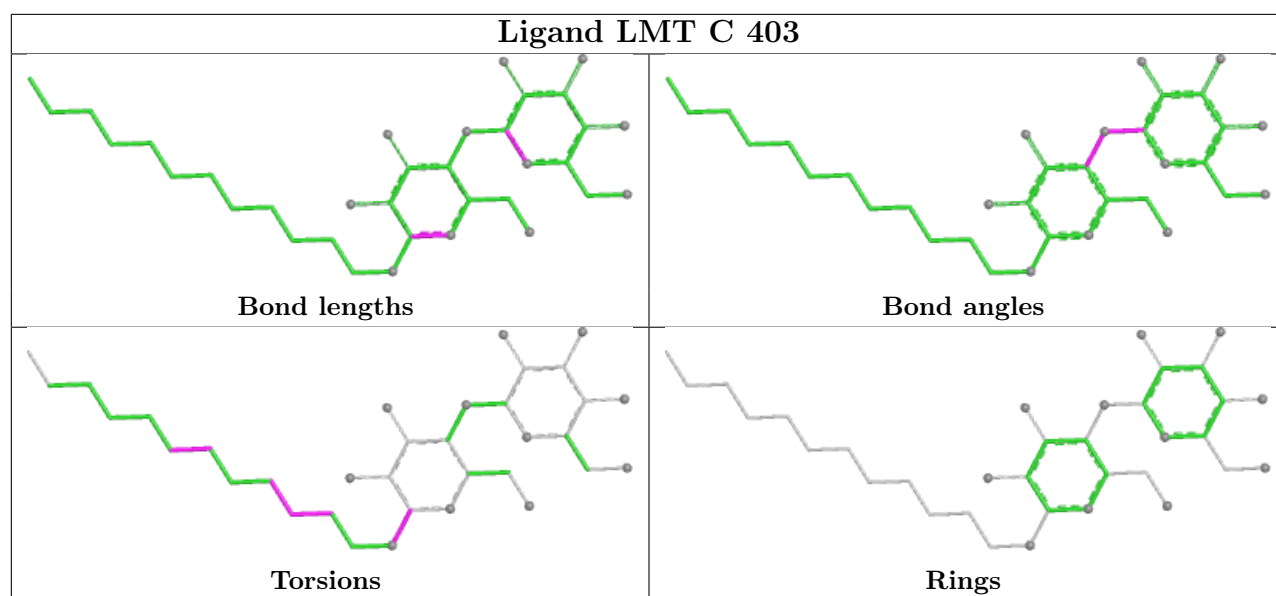


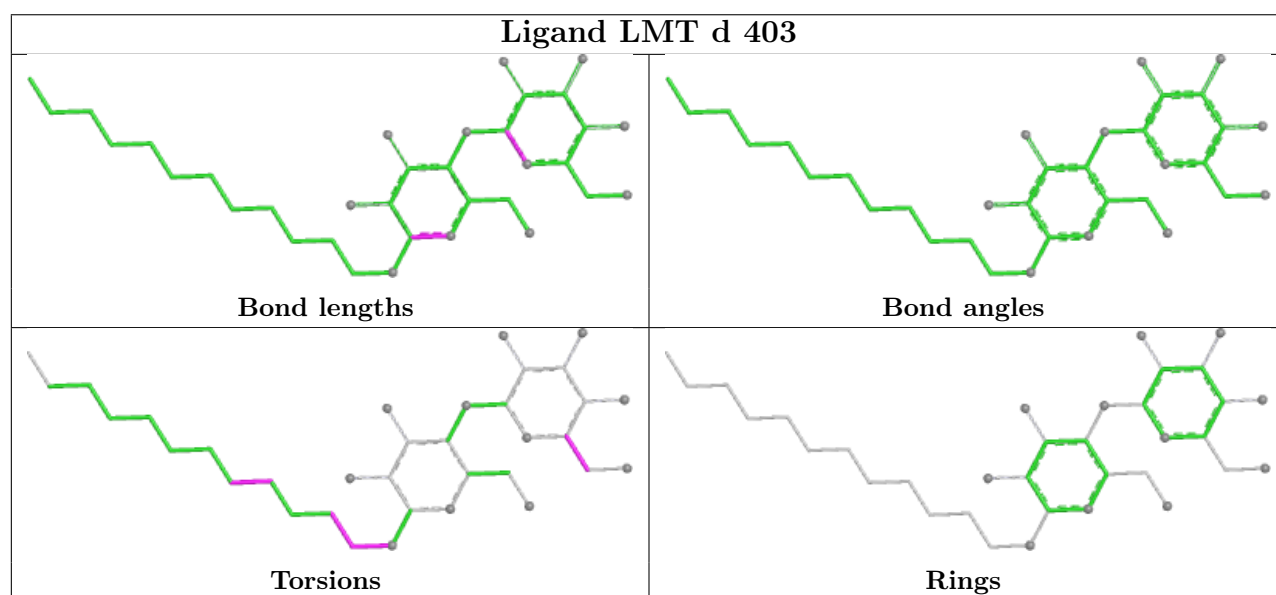
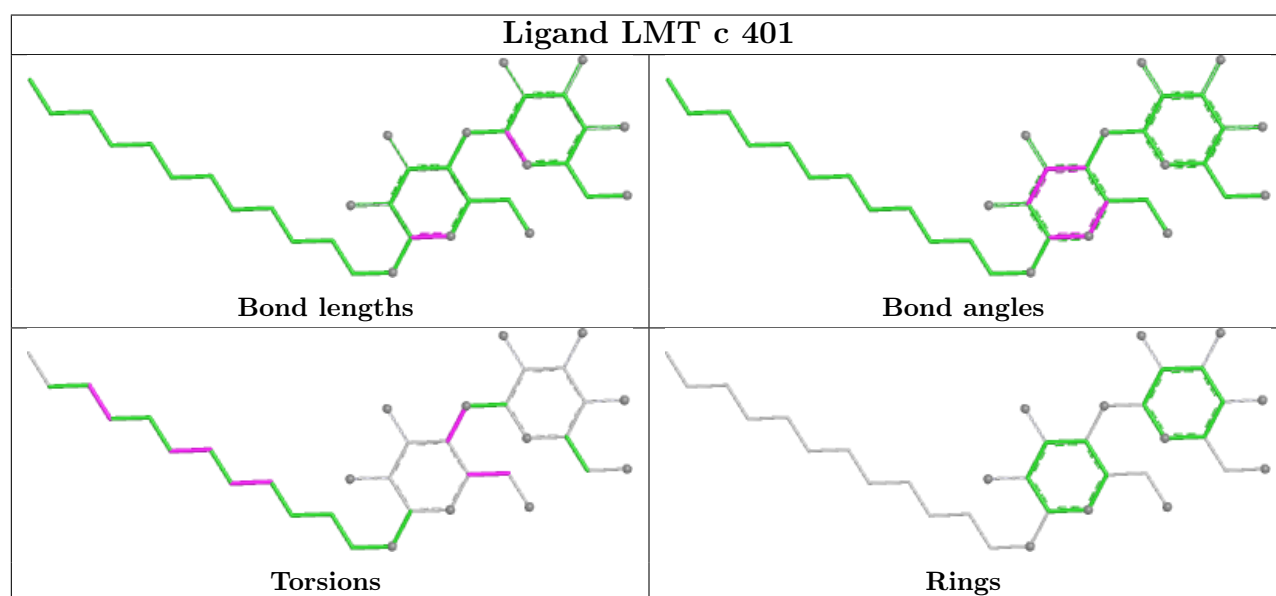
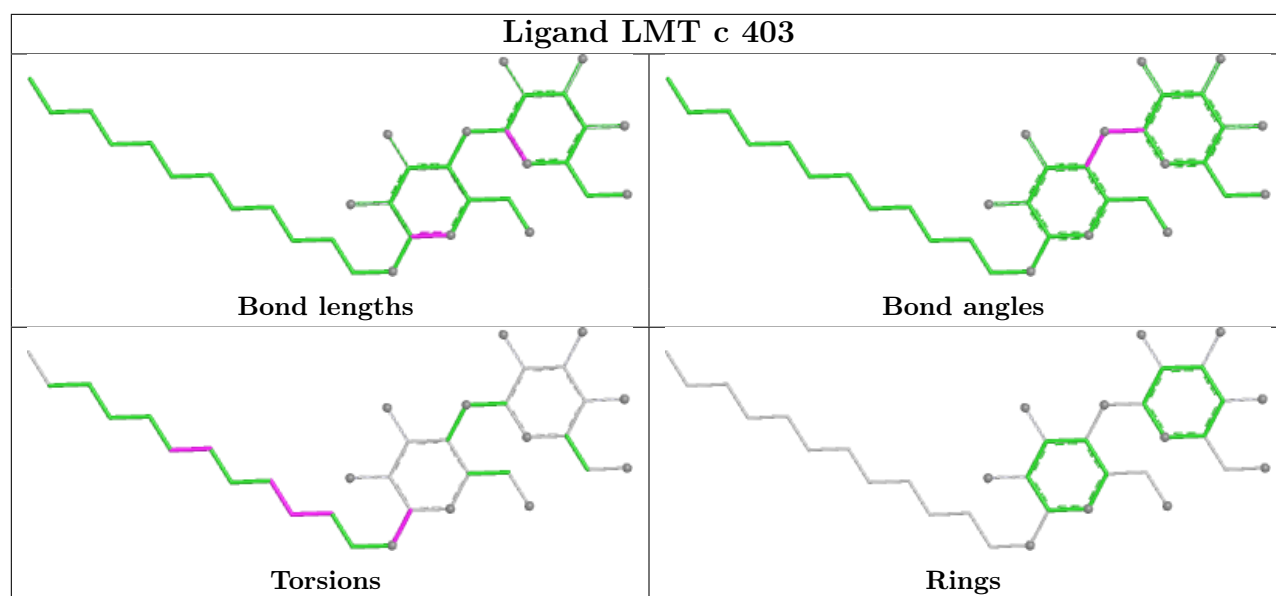


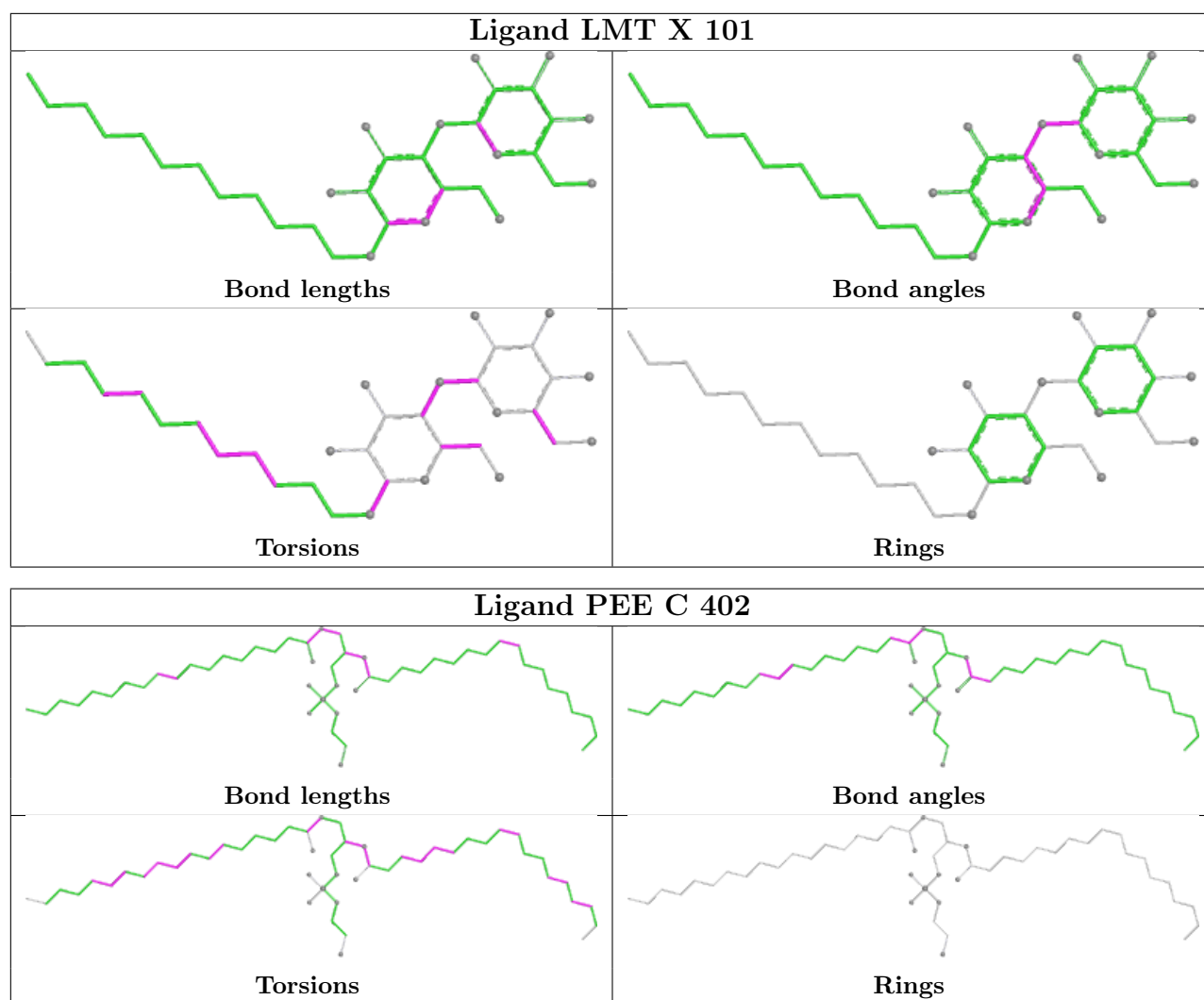












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

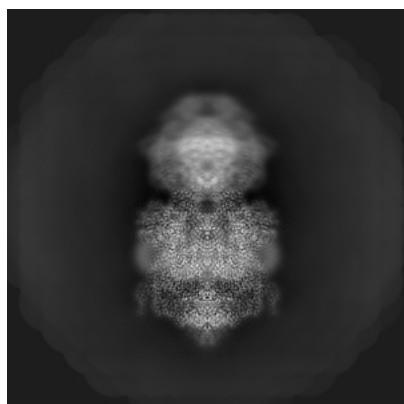
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10520. These allow visual inspection of the internal detail of the map and identification of artifacts.

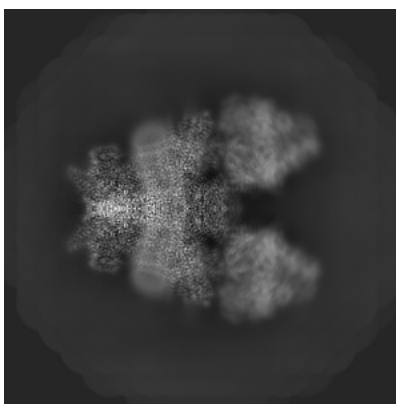
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

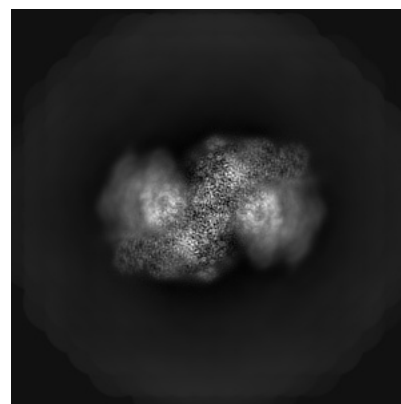
6.1.1 Primary map



X

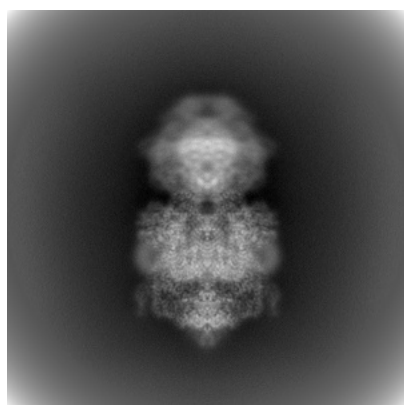


Y

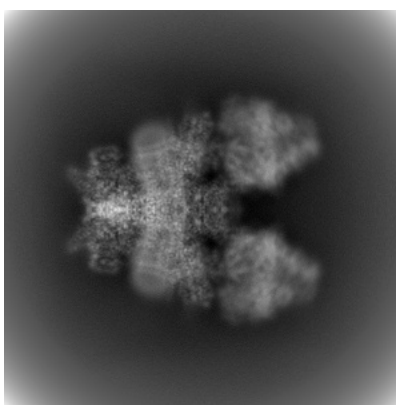


Z

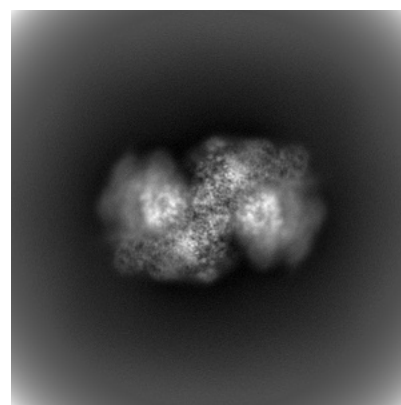
6.1.2 Raw map



X



Y

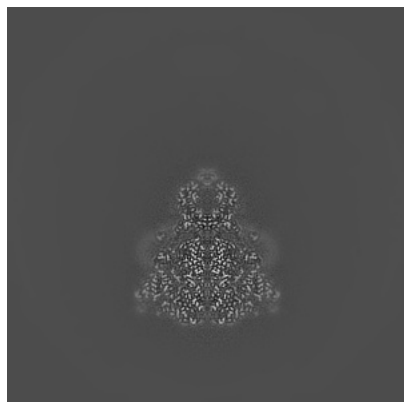


Z

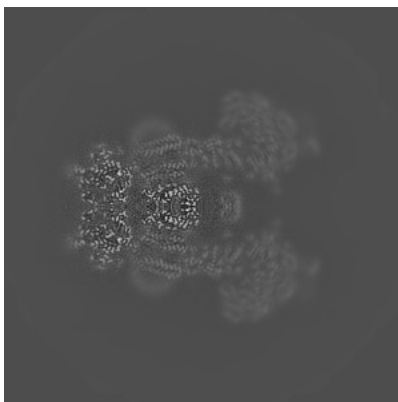
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

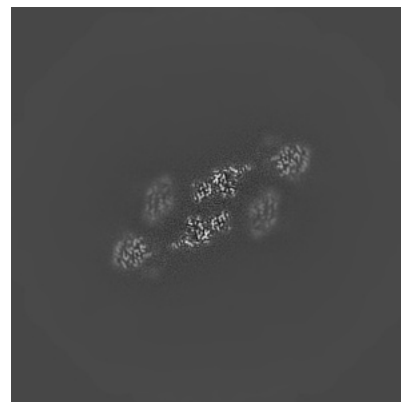
6.2.1 Primary map



X Index: 280

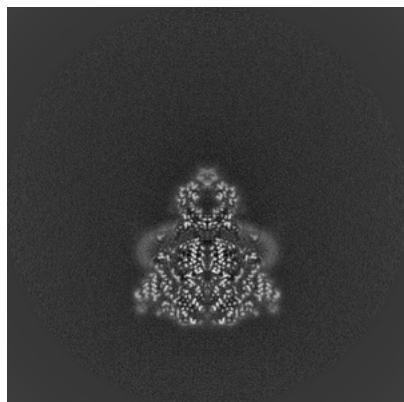


Y Index: 280

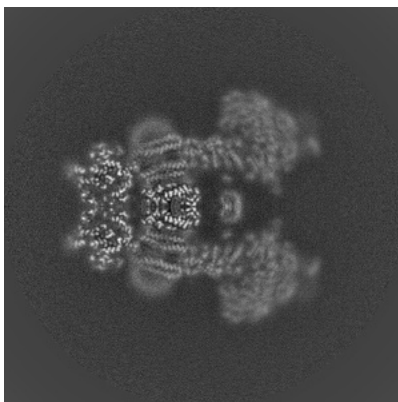


Z Index: 280

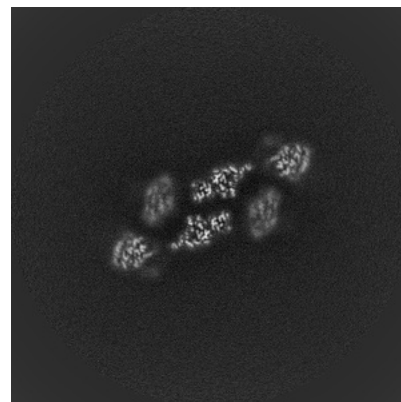
6.2.2 Raw map



X Index: 280



Y Index: 280

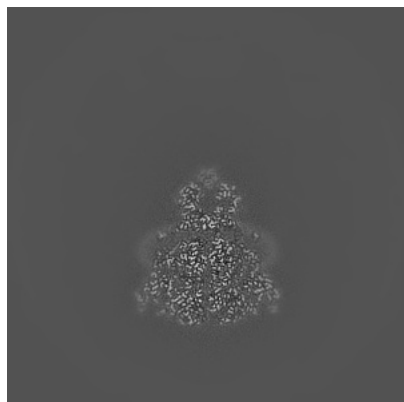


Z Index: 280

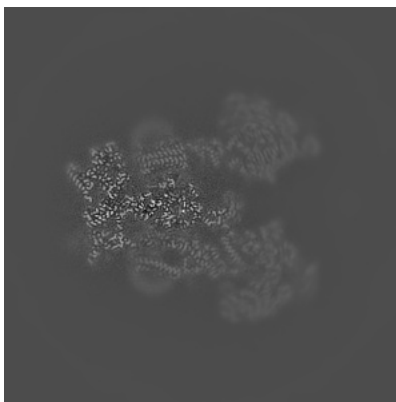
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

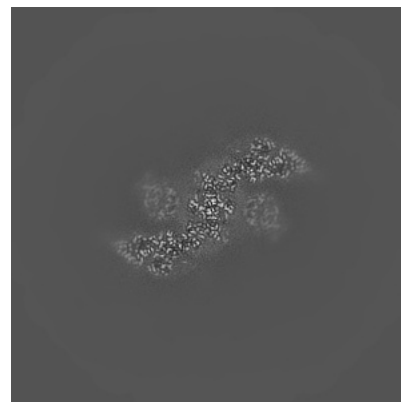
6.3.1 Primary map



X Index: 282

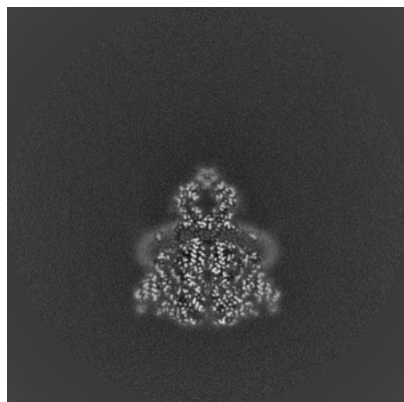


Y Index: 289

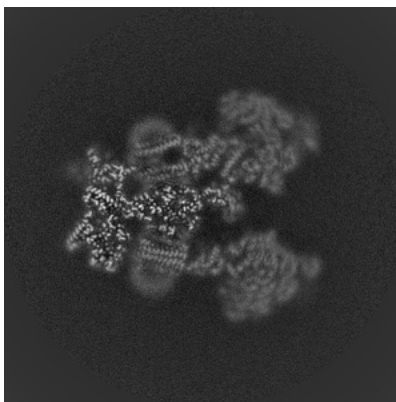


Z Index: 252

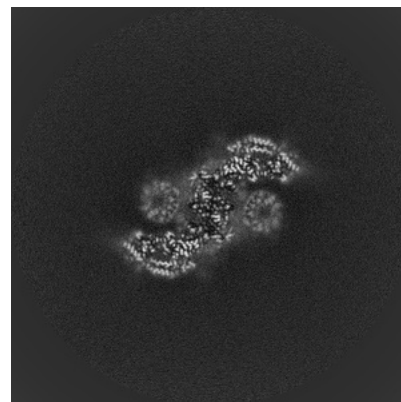
6.3.2 Raw map



X Index: 279



Y Index: 271

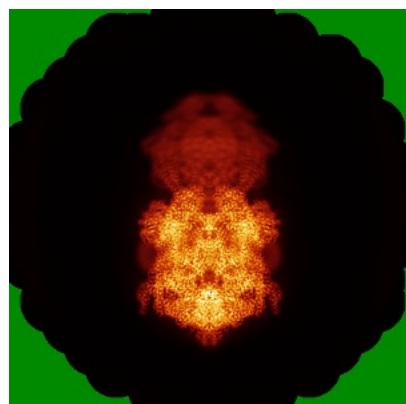


Z Index: 248

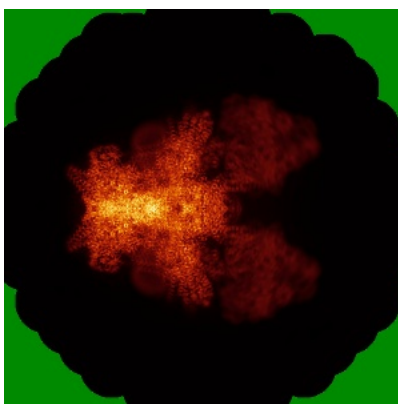
The images above show the largest variance slices of the map in three orthogonal directions.

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

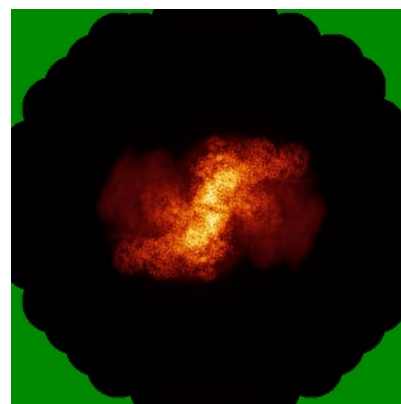
6.4.1 Primary map



X

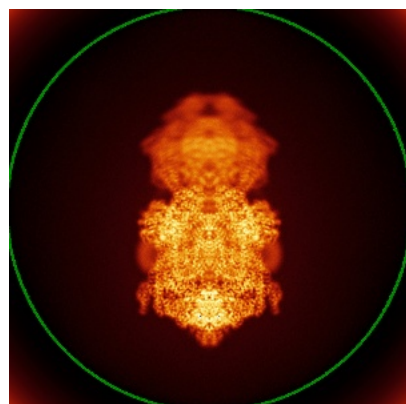


Y

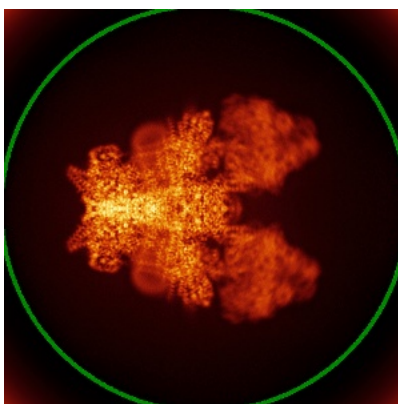


Z

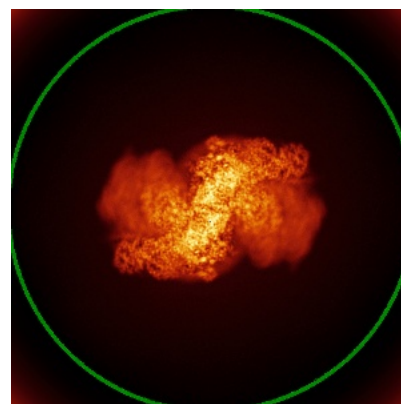
6.4.2 Raw map



X



Y

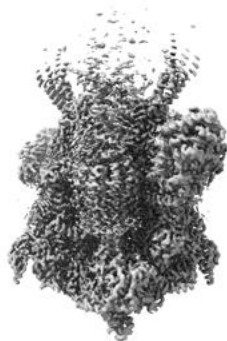


Z

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 0.04. 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.

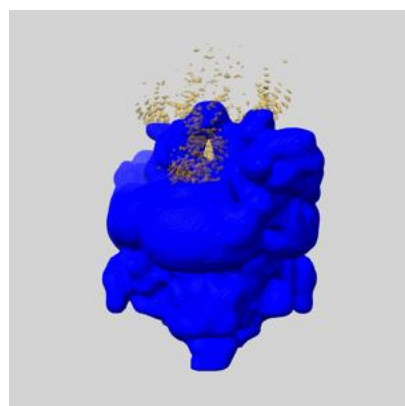
6.6 Mask visualisation [i](#)

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

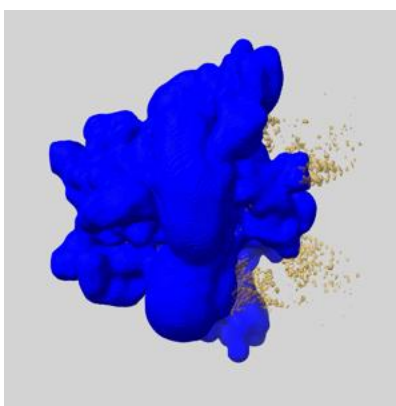
A mask typically either:

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

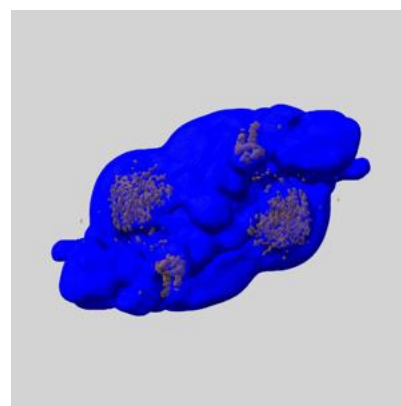
6.6.1 emd_10520_msk_1.map [i](#)



X



Y

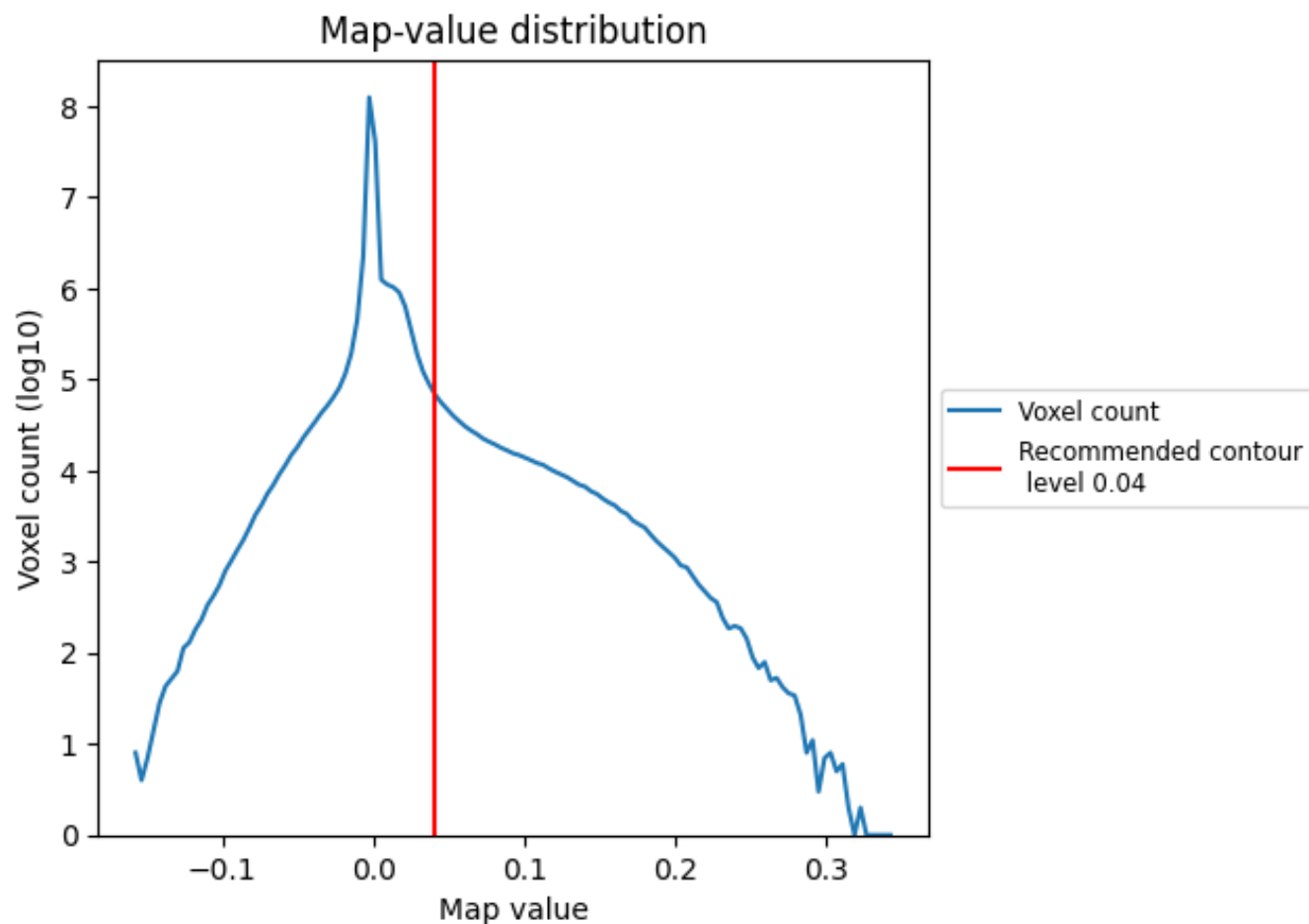


Z

7 Map analysis [i](#)

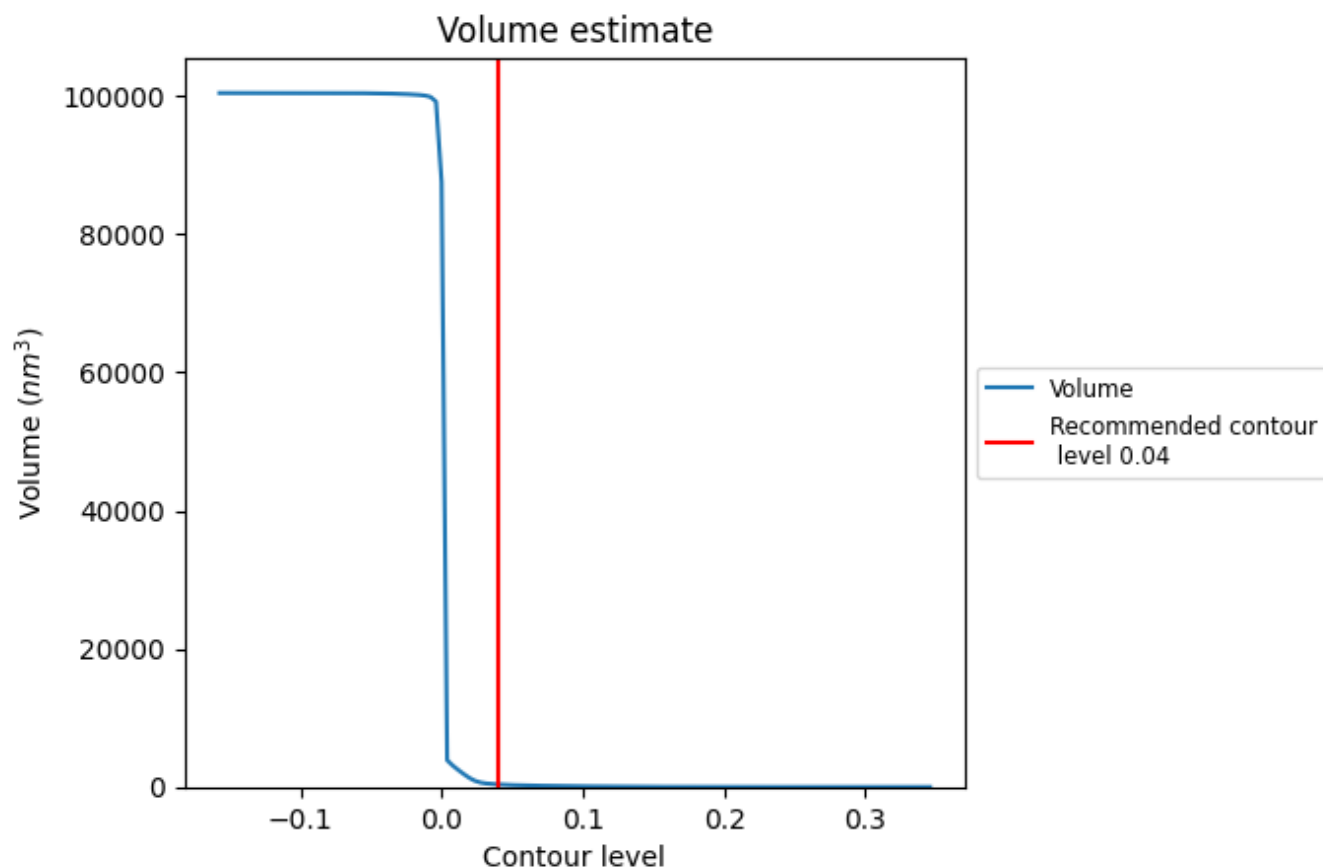
This section contains the results of statistical analysis of the map.

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.

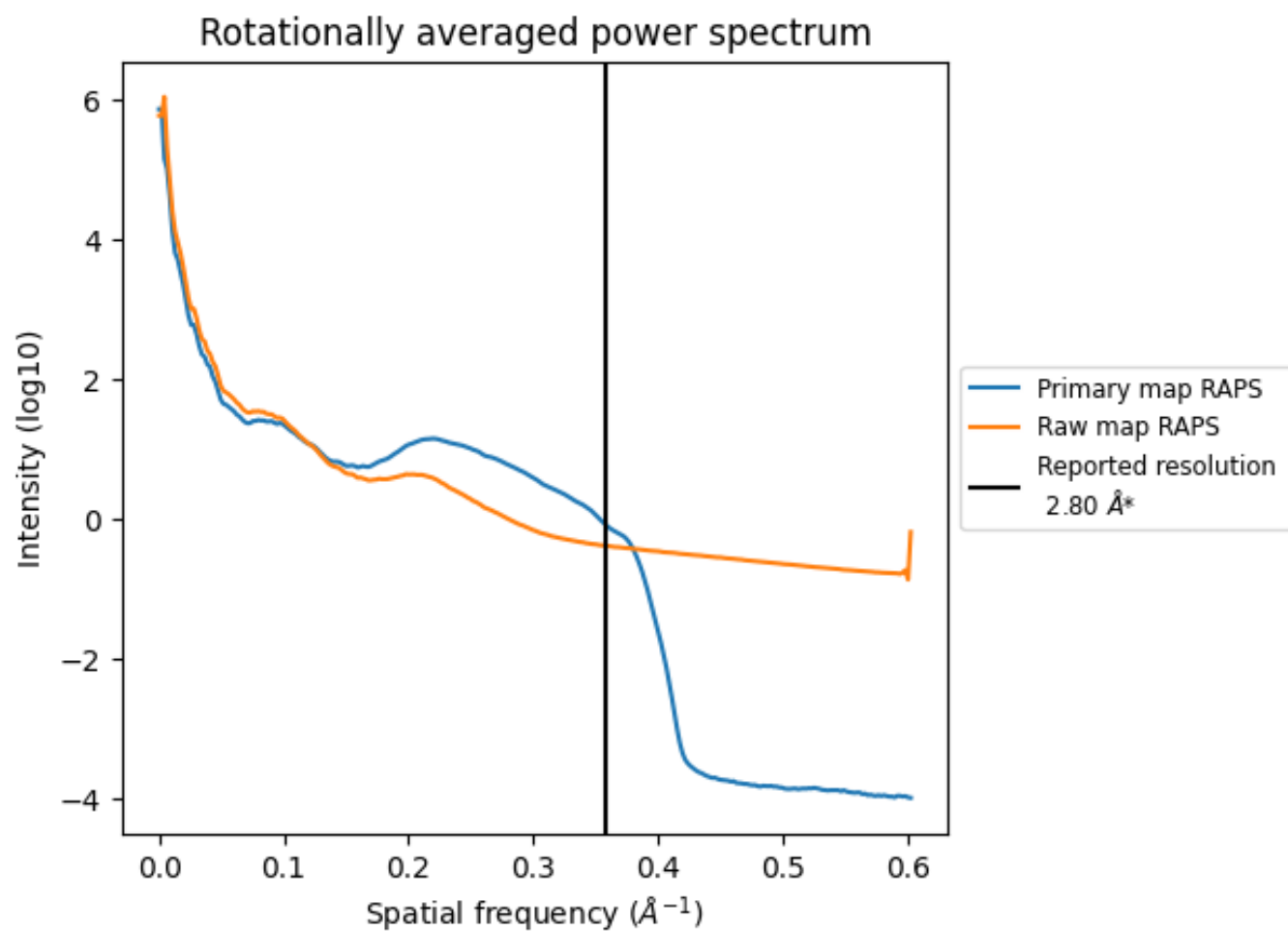
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 365 nm^3 ; this corresponds to an approximate mass of 329 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

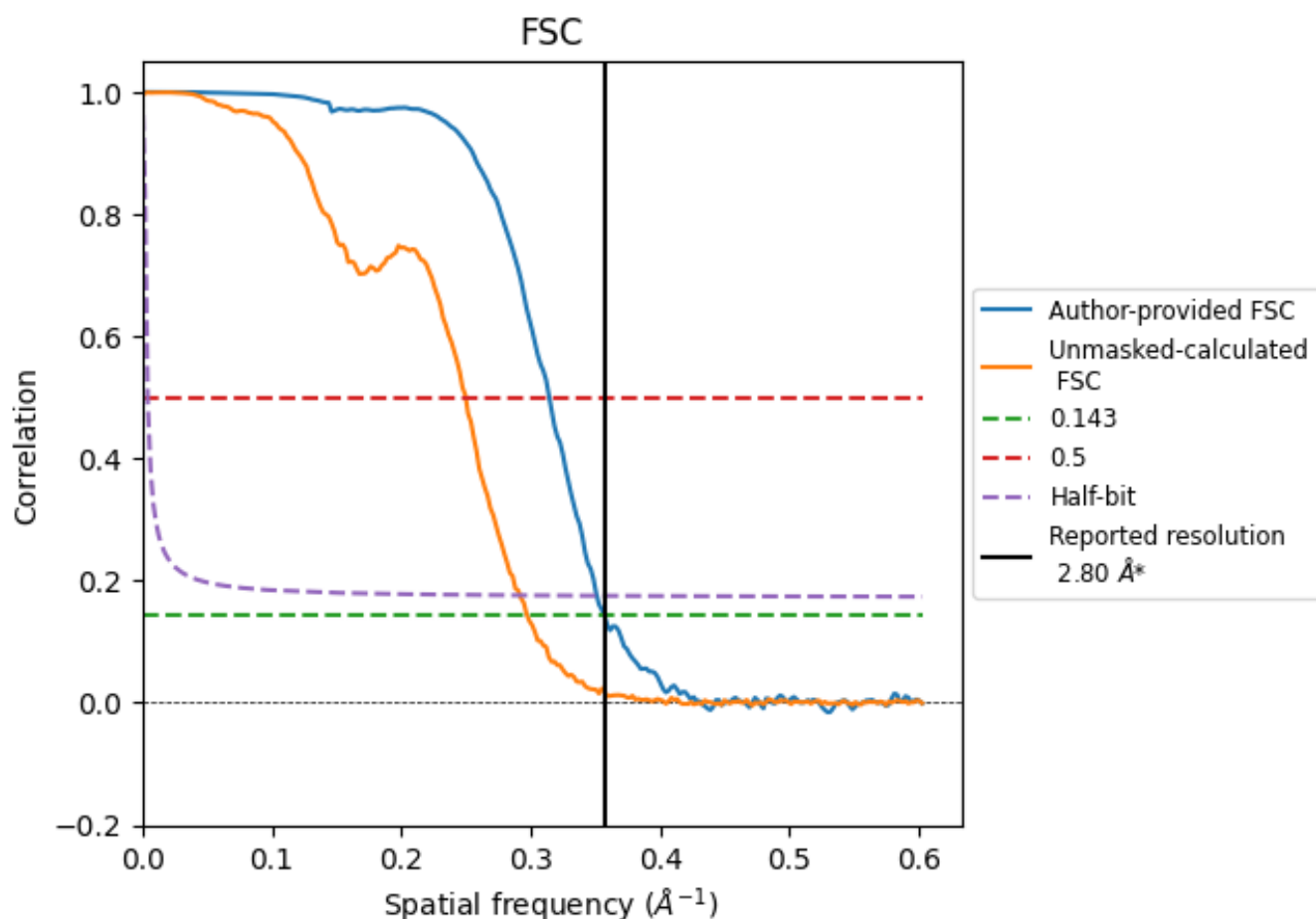


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.357 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

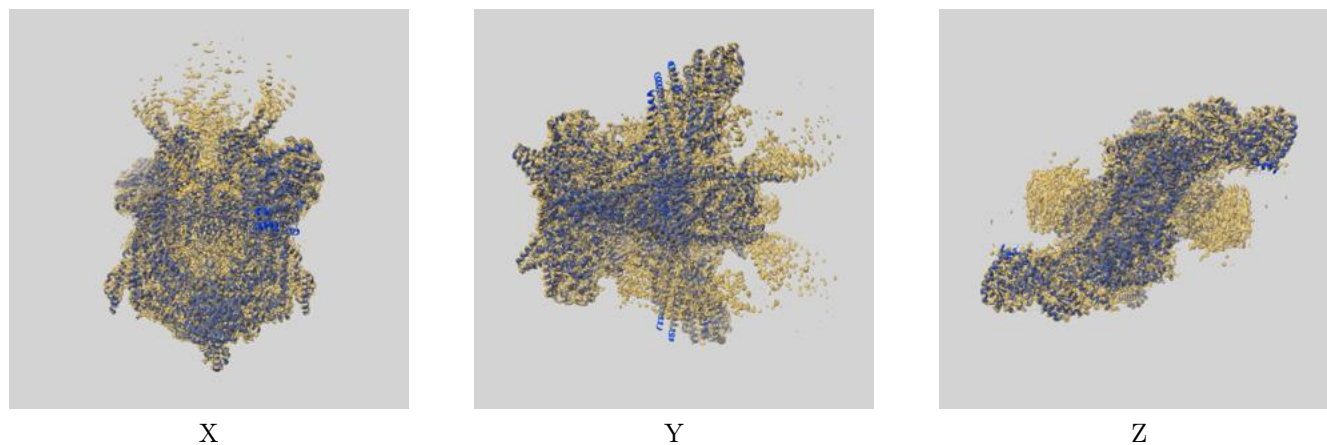
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.18	2.85
Unmasked-calculated*	3.36	4.00	3.43

*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 3.36 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

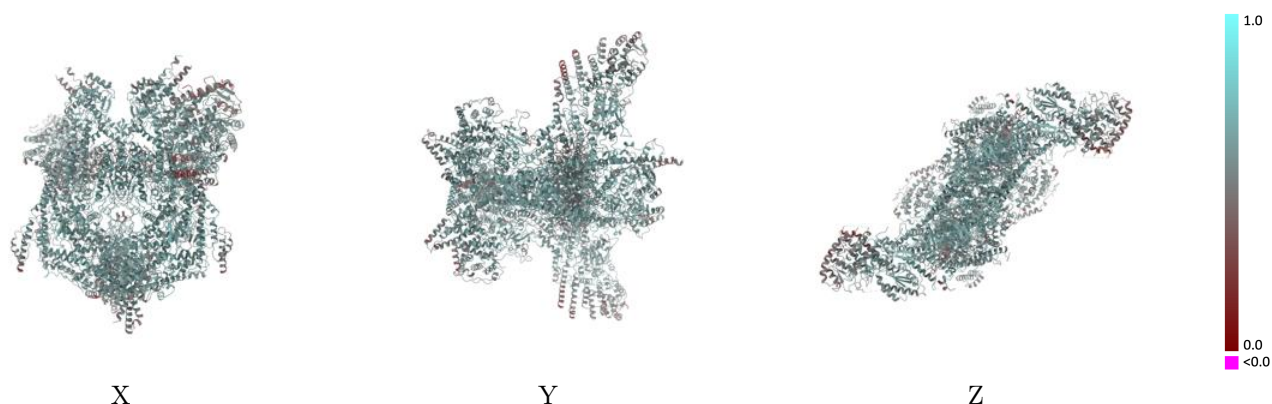
This section contains information regarding the fit between EMDB map EMD-10520 and PDB model 6TMG. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



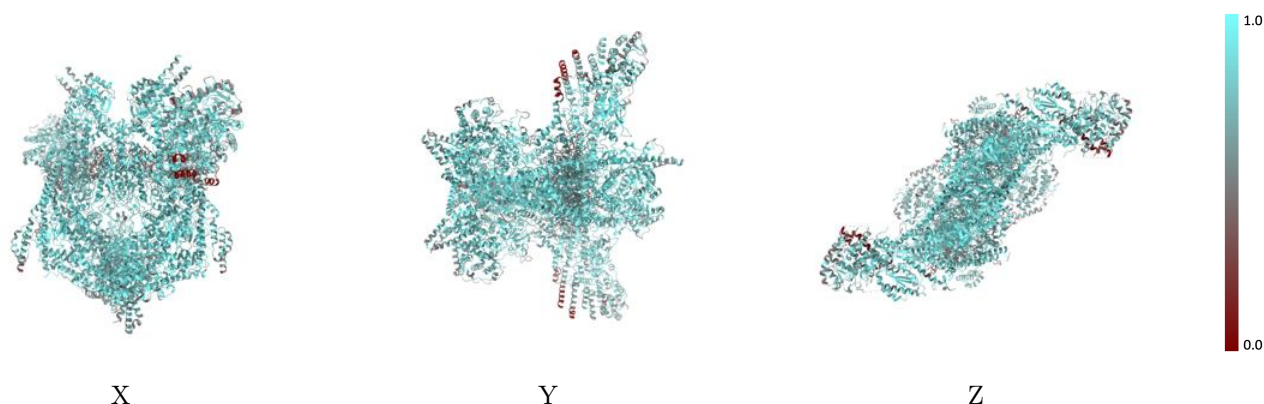
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



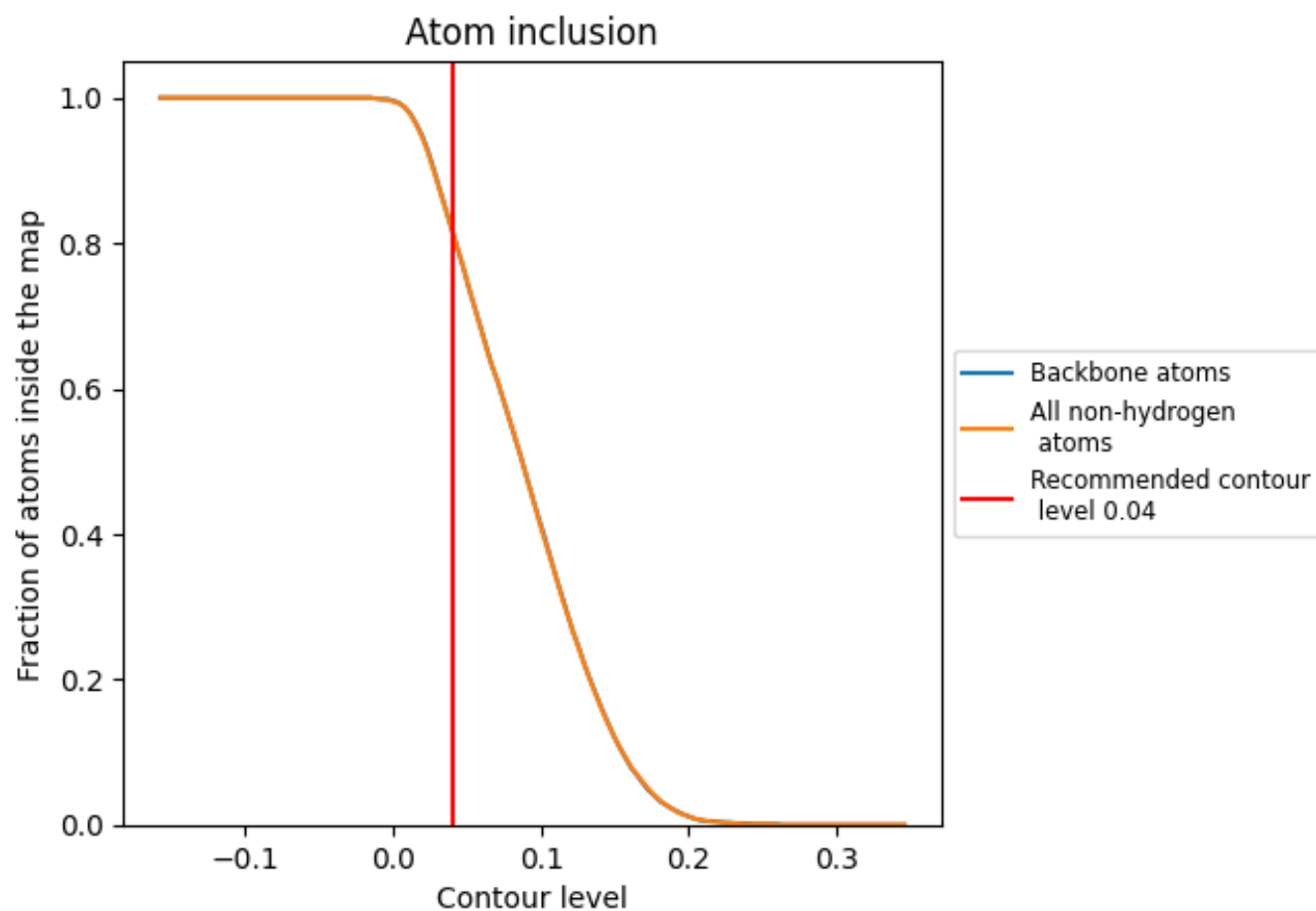
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 82% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8170	 0.5890
A	 0.7430	 0.5380
B	 0.8250	 0.5940
C	 0.7290	 0.5550
D	 0.8560	 0.6130
E	 0.8560	 0.6140
F	 0.8180	 0.5770
G	 0.8440	 0.5920
H	 0.8720	 0.6180
I	 0.7610	 0.5490
J	 0.9210	 0.6520
K	 0.7460	 0.5820
L	 0.8650	 0.6020
M	 0.8940	 0.6290
N	 0.7650	 0.5560
O	 0.7930	 0.5800
P	 0.8690	 0.6010
Q	 0.7190	 0.5150
R	 0.8430	 0.5950
S	 0.8360	 0.5860
T	 0.7700	 0.5560
U	 0.8200	 0.5840
V	 0.8290	 0.6100
W	 0.9230	 0.6320
X	 0.8610	 0.6130
a	 0.7410	 0.5390
b	 0.8330	 0.6010
c	 0.7300	 0.5560
d	 0.8570	 0.6120
e	 0.8550	 0.6160
f	 0.8170	 0.5760
g	 0.8500	 0.5940
h	 0.8710	 0.6190
i	 0.7660	 0.5510
j	 0.9230	 0.6510



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Chain	Atom inclusion	Q-score
k	 0.7410	 0.5810
l	 0.8630	 0.6010
m	 0.8910	 0.6270
n	 0.7640	 0.5560
o	 0.7940	 0.5830
p	 0.8700	 0.6030
q	 0.7110	 0.5160
r	 0.8380	 0.5930
s	 0.8330	 0.5840
t	 0.7540	 0.5540
u	 0.8230	 0.5860
v	 0.8510	 0.6170
w	 0.9190	 0.6320
x	 0.8580	 0.6110