



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:46 PM UTC

PDB ID : 6G2J / pdb_00006g2j
EMDB ID : EMD-4345
Title : Mouse mitochondrial complex I in the active state
Authors : Agip, A.N.A.; Blaza, J.N.; Bridges, H.R.; Viscomi, C.; Rawson, S.; Muench, S.P.; Hirst, J.
Deposited on : 2018-03-23
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

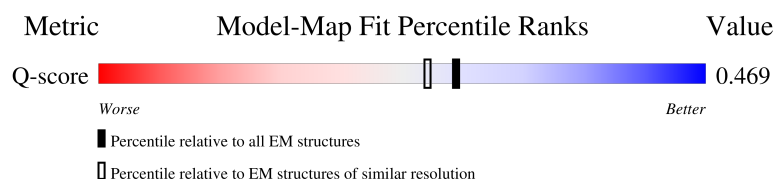
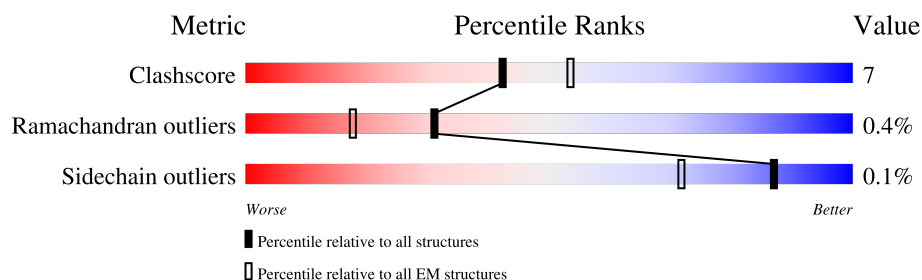
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	115	17% 82% 18%
2	B	224	7% 55% 13% 31%
3	C	263	13% 65% 13% 22%
4	D	463	11% 69% 24% 7%

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Mol	Chain	Length	Quality of chain
5	E	248	
6	F	428	
7	G	727	
8	H	318	
9	I	212	
10	J	172	
11	K	98	
12	L	607	
13	M	459	
14	N	345	
15	O	355	
16	P	377	
17	Q	175	
18	R	116	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	131	
23	X	172	
24	Y	143	
25	Z	144	
26	a	67	
27	b	84	
28	c	76	

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Mol	Chain	Length	Quality of chain
29	d	120	
30	e	106	
31	f	57	
32	g	151	
33	h	189	
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 66810 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	S	0	0
			933	633	133	160	7		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	155	Total	C	N	O	S	0	0
			1241	793	222	212	14		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1712	1105	294	310	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	430	Total	C	N	O	S	0	0
			3452	2207	593	628	24		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	212	Total	C	N	O	S	0	0
			1648	1048	277	312	11		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	428	Total	C	N	O	S	0	0
			3301	2080	590	609	22		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	688	Total	C	N	O	S	0	0
			5296	3321	919	1015	41		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2540	1706	384	428	22		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	178	Total	C	N	O	S	0	0
			1408	885	243	268	12		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	171	Total	C	N	O	S	0	0
			1300	874	185	226	15		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			737	477	112	137	11		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4800	3182	746	827	45		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3632	2408	567	617	40		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	344	Total	C	N	O	S	0	0
			2696	1791	416	452	37		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2607	1674	431	492	10		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	342	Total	C	N	O	S	0	0
			2748	1777	483	481	7		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	125	Total	C	N	O	S	0	0
			1015	642	179	190	4		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	95	Total	C	N	O	S	0	0
			748	464	138	143	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	83	Total	C	N	O	S	0	0
			667	419	126	119	3		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	75	Total	C	N	O	S	0	0
			604	388	89	122	5		
20	U	88	Total	C	N	O	S	0	0
			706	453	104	144	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	112	Total	C	N	O	S	0	0
			915	596	152	164	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1396	889	250	247	10		

- Molecule 24 is a protein called MCG5603.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	140	Total	C	N	O	S	0	0
			1037	662	175	192	8		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	139	Total	C	N	O	S	0	0
			1152	741	204	199	8		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	67	Total	C	N	O	S	0	0
			548	356	97	91	4		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			651	427	105	115	4		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	119	Total	C	N	O	S	0	0
			985	645	167	164	9		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	104	Total	C	N	O	S	0	0
			870	550	161	151	8		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	51	Total	C	N	O	S	0	0
			433	278	78	75	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	101	Total	C	N	O	S	0	0
			850	549	136	161	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	137	Total	C	N	O	S	0	0
			1154	758	192	201	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	101	Total	C	N	O	S	0	0
			820	534	141	142	3		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	60	Total	C	N	O	S	0	0
			525	345	88	91	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	72	Total	C	N	O	S	0	0
			582	384	100	97	1		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	152	Total	C	N	O	S	0	0
			1274	821	213	229	11		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	124	Total	C	N	O		0	0
			1035	667	186	182			

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	176	Total	C	N	O	S	0	0
			1527	976	274	266	11		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	105	Total	C	N	O	S	0	0
			898	565	167	158	8		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	170	Total	C	N	O	S	0	0
			1438	903	258	269	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	144	Total	C	N	O	S	0	0
			1203	773	213	212	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	1	AME	MET	conflict	UNP Q7TMF3

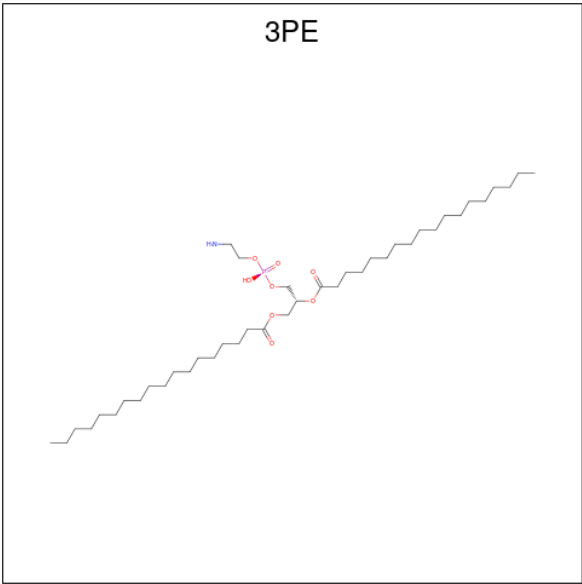
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	99	Total	C	N	O	S	0	0
			796	504	148	141	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

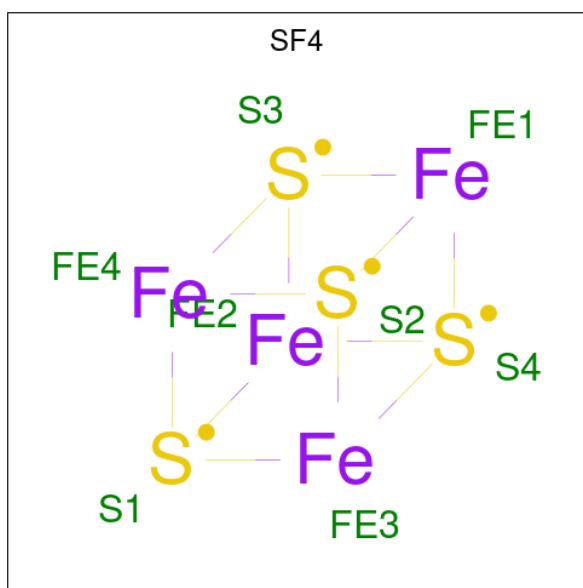
Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	40	Total	C	N	O	0	0
			336	211	60	65		

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



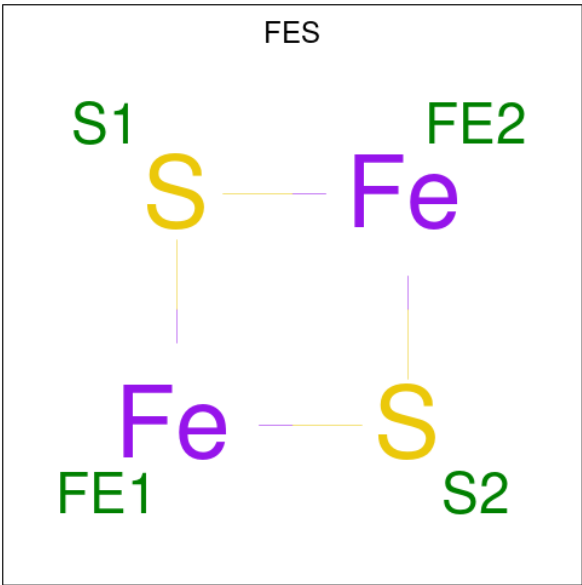
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
45	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	M	1	Total	C	O	P		0
			42	33	8	1		
45	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	M	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	N	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 46 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



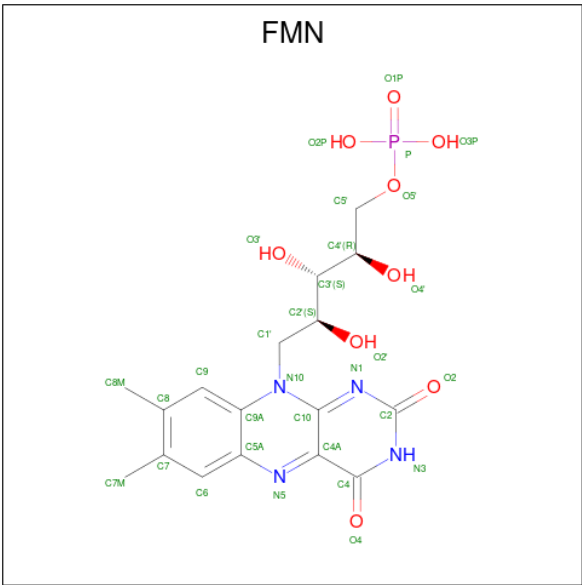
Mol	Chain	Residues	Atoms			AltConf
46	B	1	Total	Fe	S	0
			8	4	4	
46	F	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
47	E	1	Total	Fe	S	0
			4	2	2	
47	G	1	Total	Fe	S	0
			4	2	2	

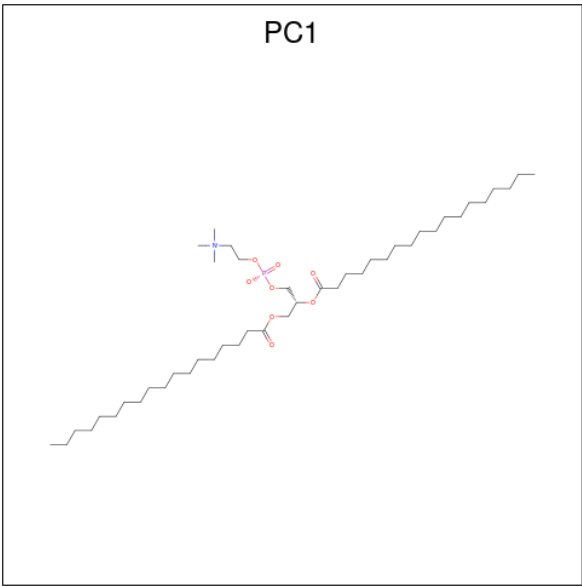
- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
48	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

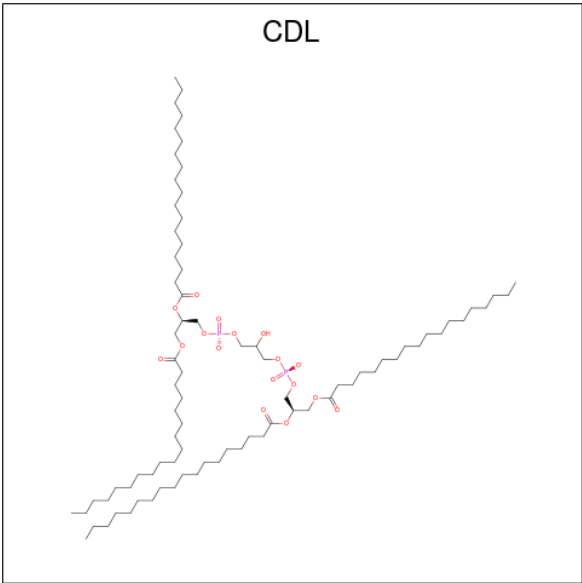
- Molecule 49 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1)

(formula: C₄₄H₈₈NO₈P).



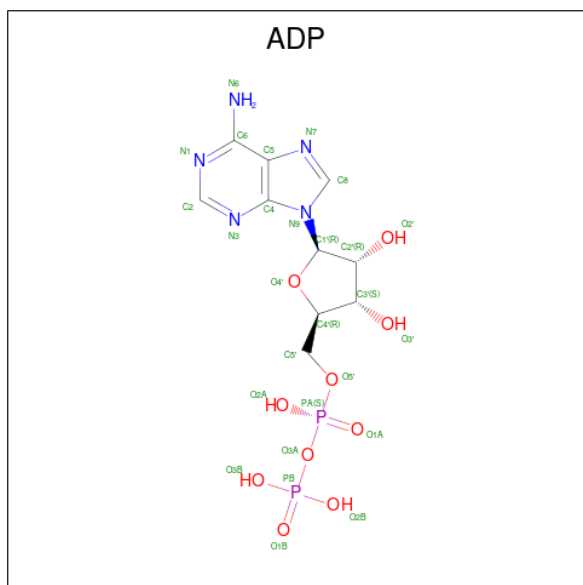
Mol	Chain	Residues	Atoms					AltConf
49	H	1	Total	C	N	O	P	0
			42	32	1	8	1	
49	H	1	Total	C	N	O	P	0
			47	37	1	8	1	
49	H	1	Total	C	N	O	P	0
			35	25	1	8	1	
49	P	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 50 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



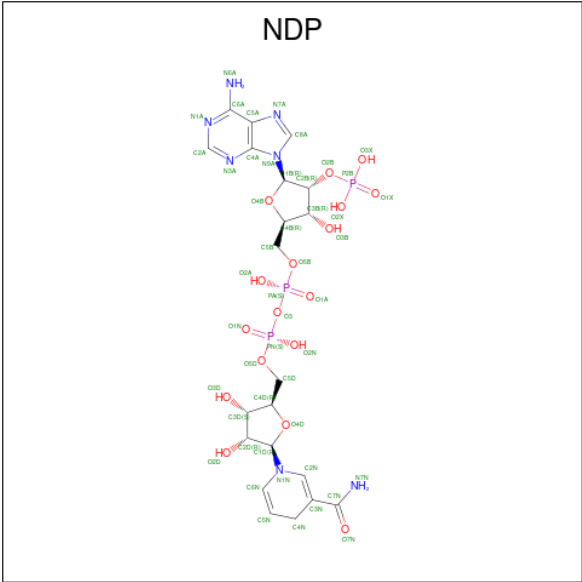
Mol	Chain	Residues	Atoms				AltConf
50	H	1	Total 57	C 38	O 17	P 2	0
50	L	1	Total 78	C 59	O 17	P 2	0
50	L	1	Total 70	C 51	O 17	P 2	0
50	M	1	Total 67	C 48	O 17	P 2	0

- Molecule 51 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
51	O	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).

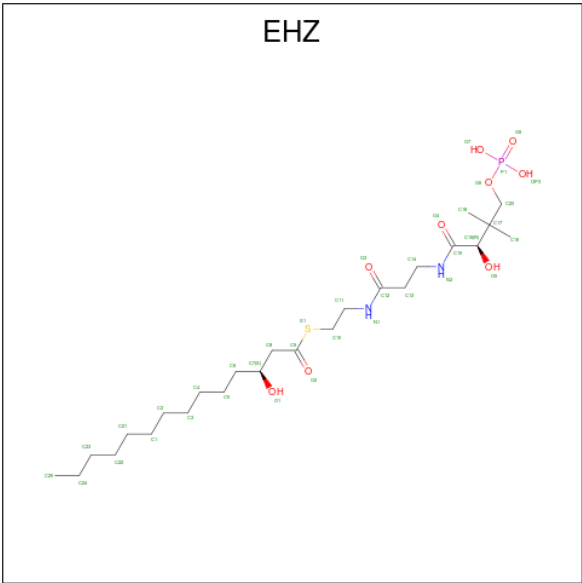


Mol	Chain	Residues	Atoms					AltConf
52	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

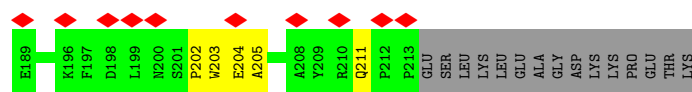
- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	R	1	Total	Zn	0
			1	1	

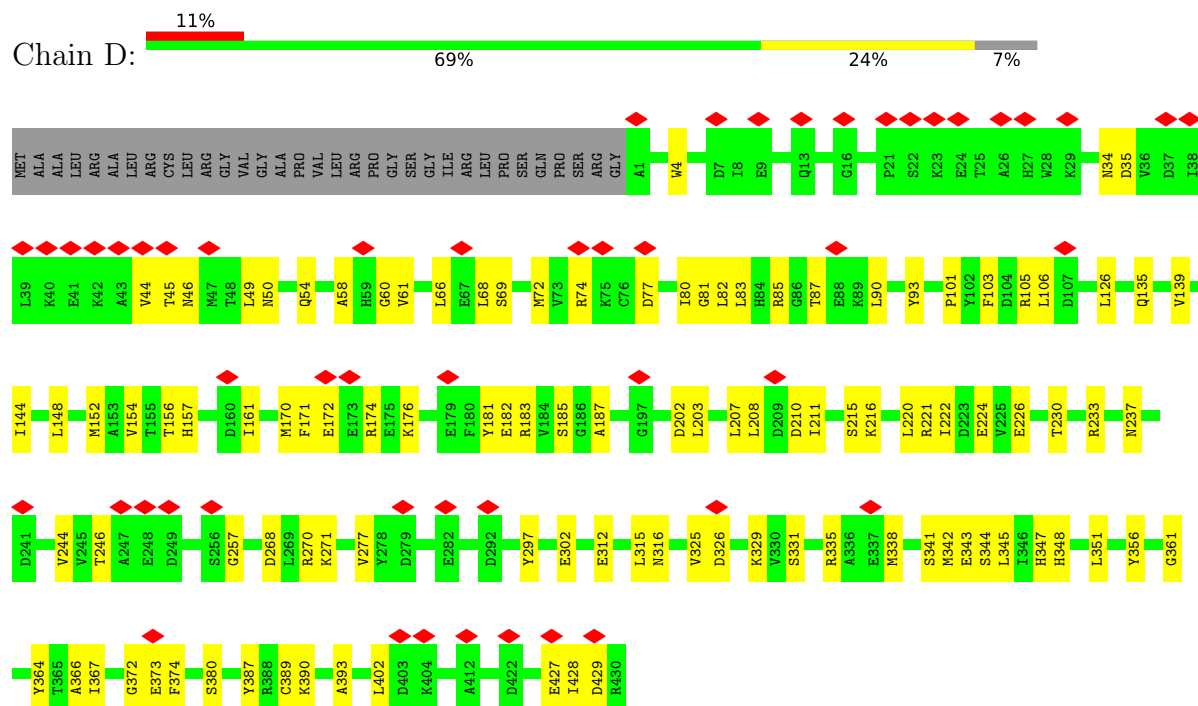
- Molecule 54 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



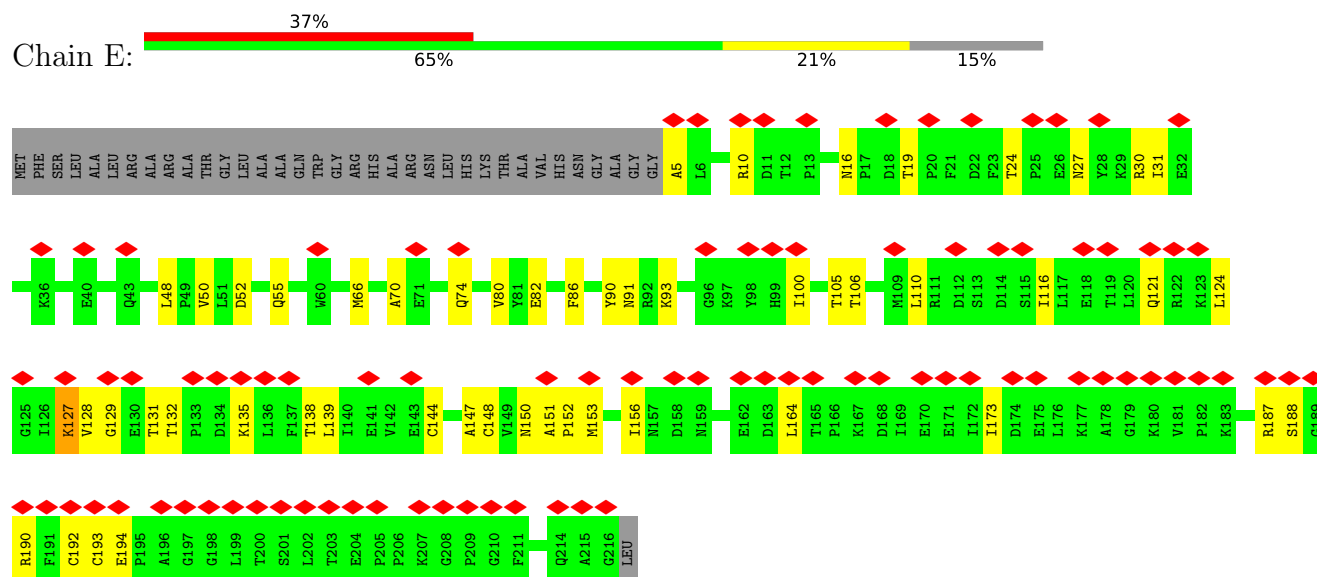
Mol	Chain	Residues	Atoms						AltConf
54	T	1	Total	C	N	O	P	S	0
			34	22	2	8	1	1	
54	U	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	



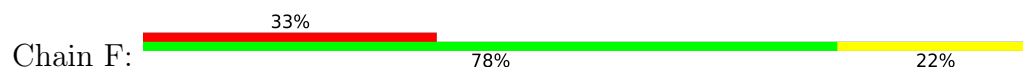
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

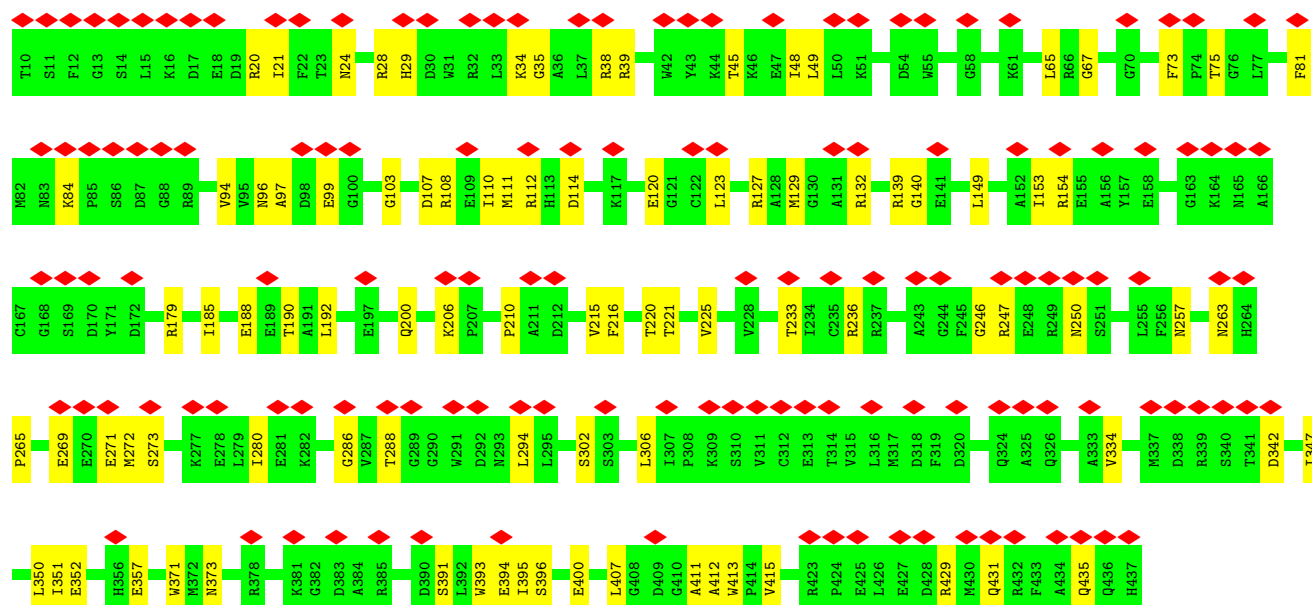


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

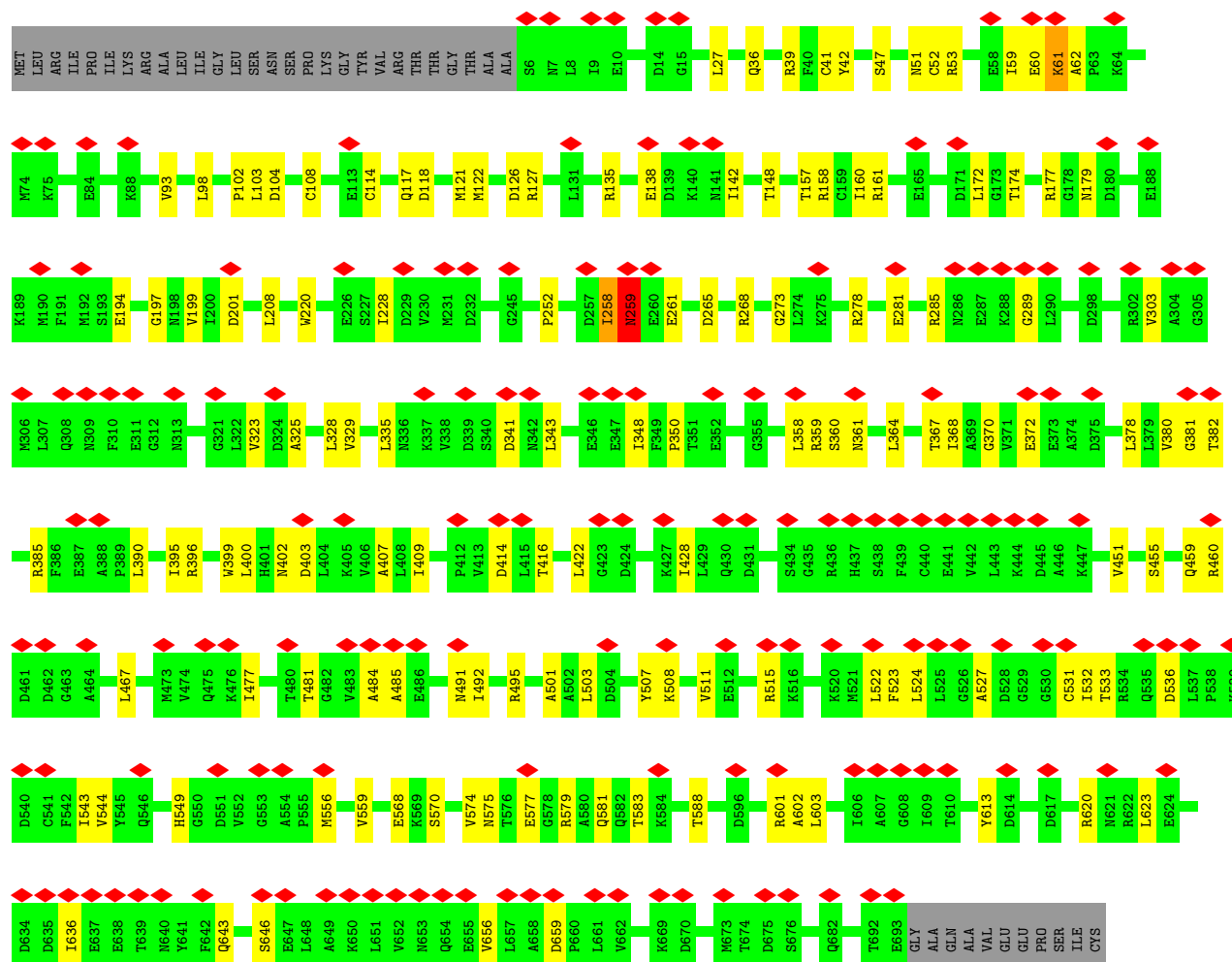
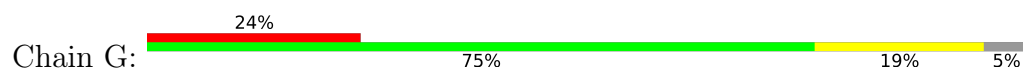


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

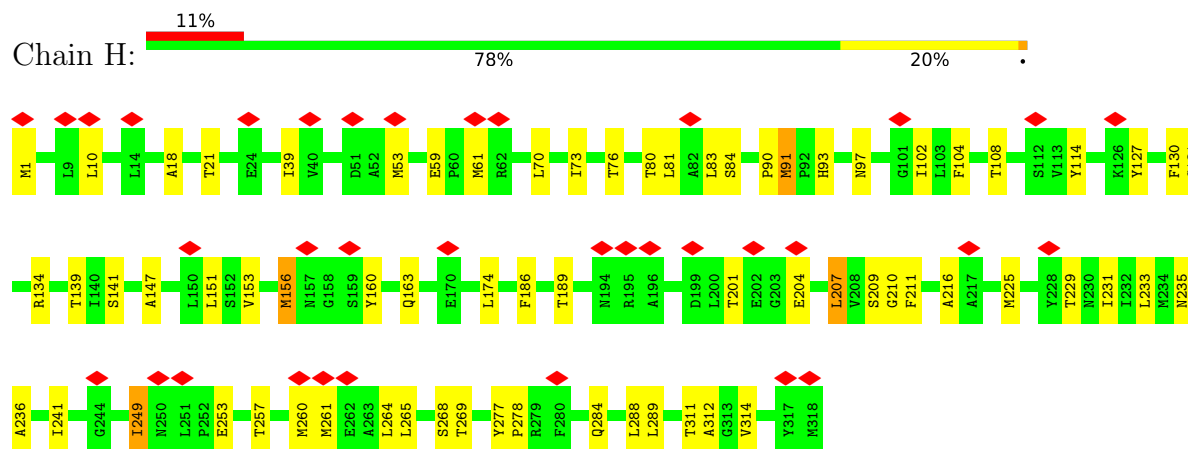




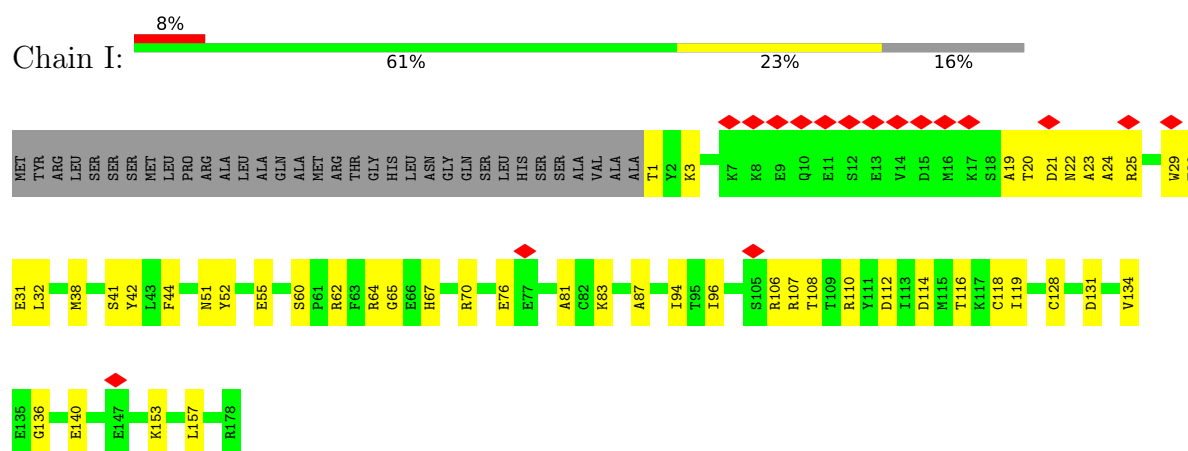
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



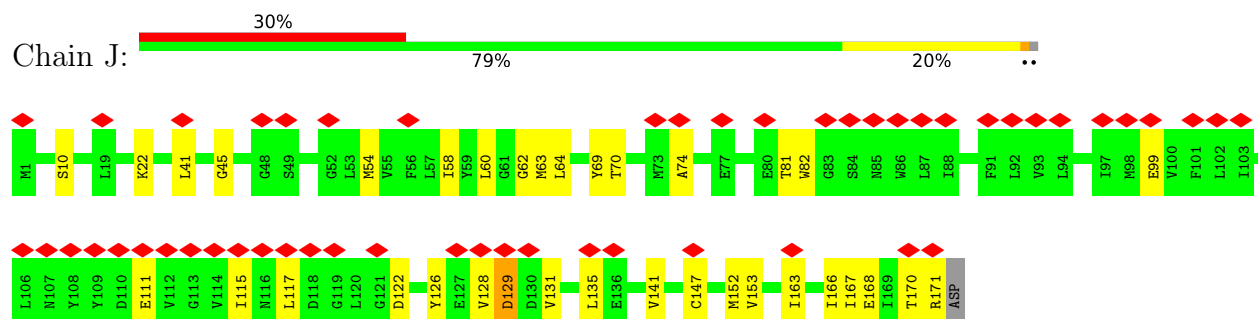
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



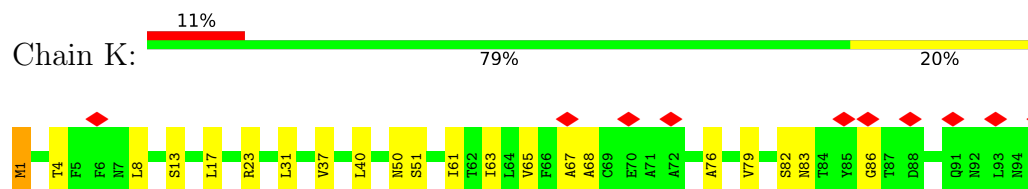
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



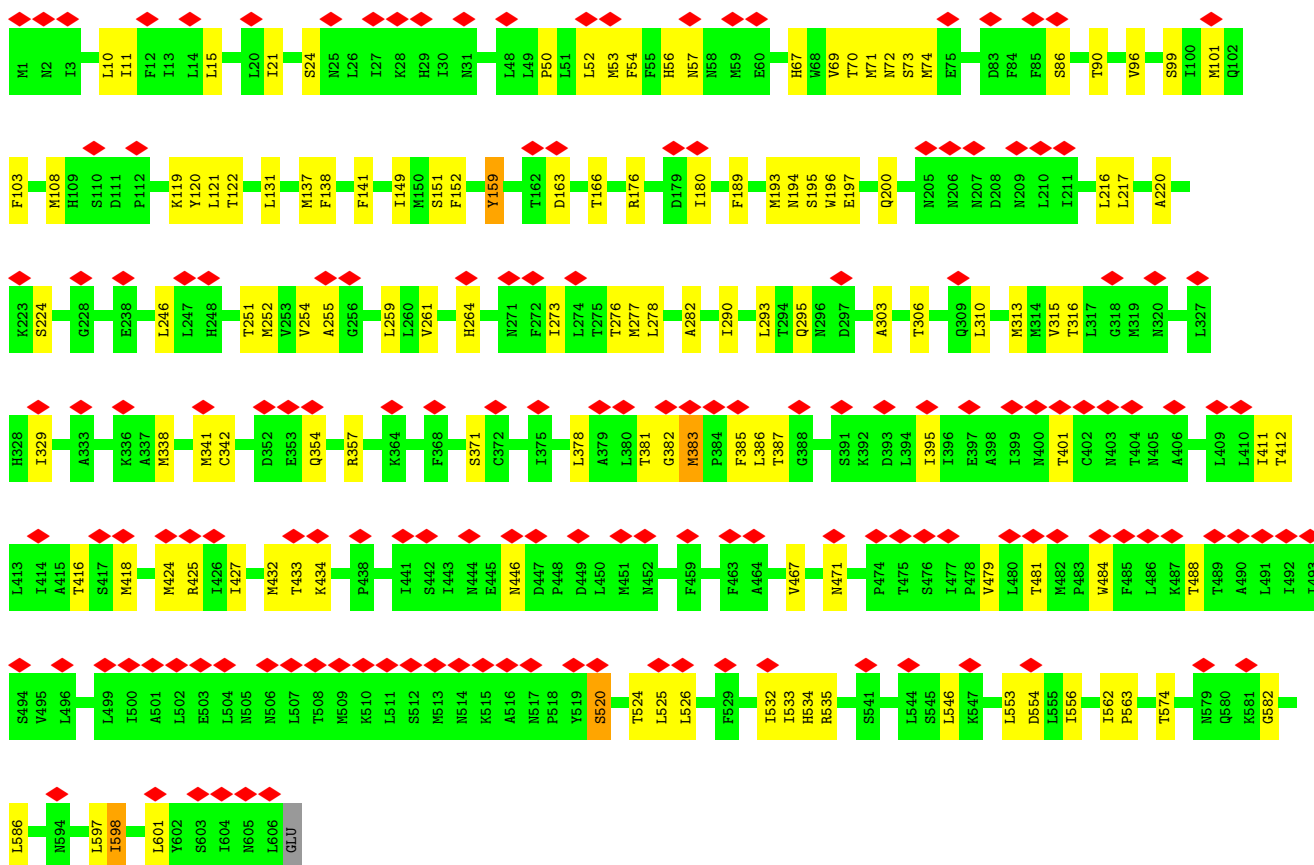
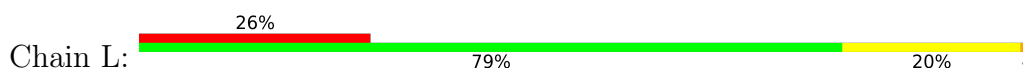
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



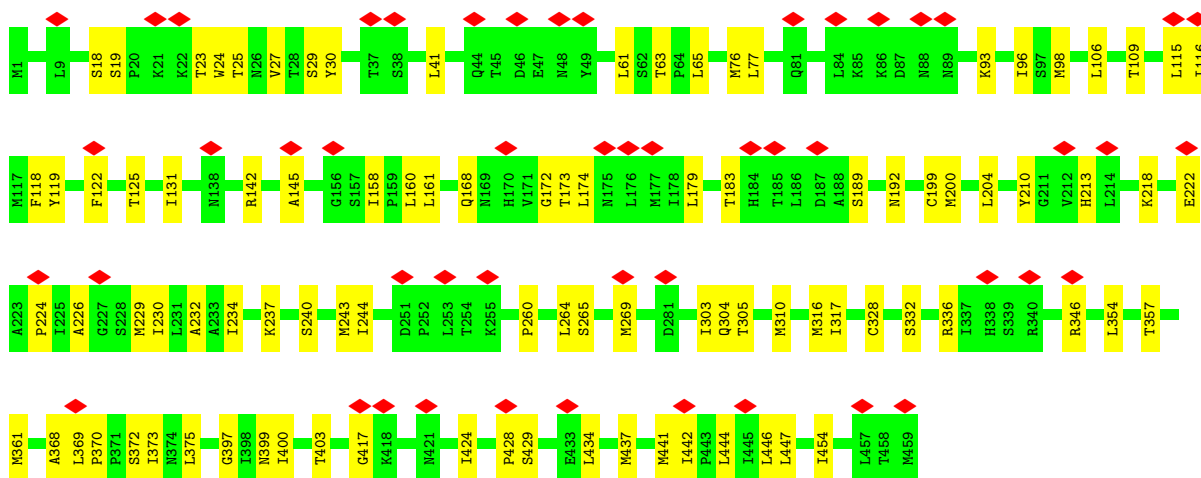
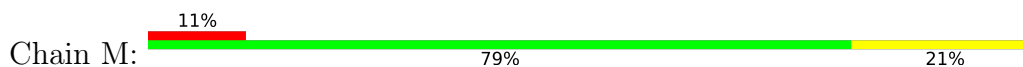
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



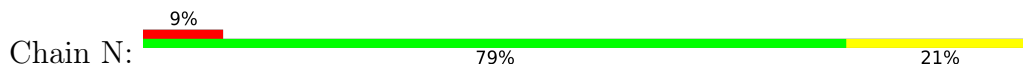
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

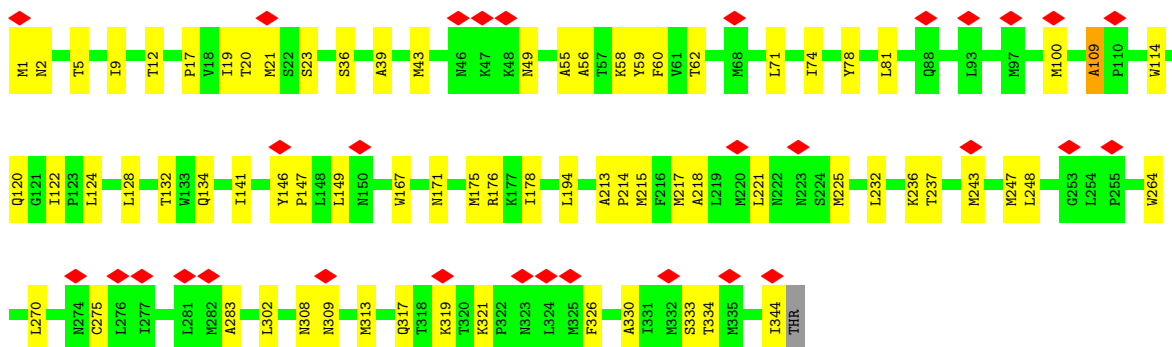


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

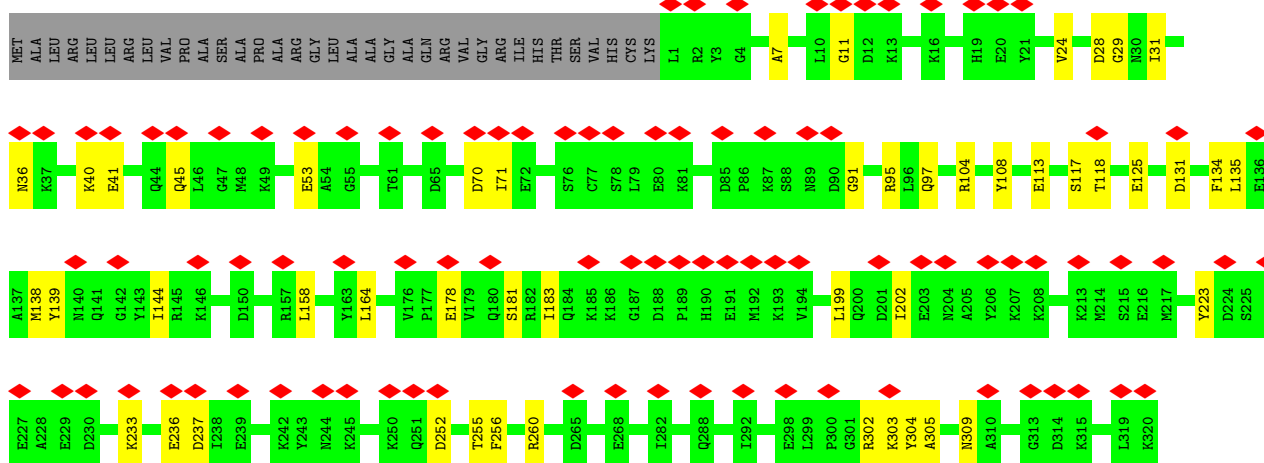
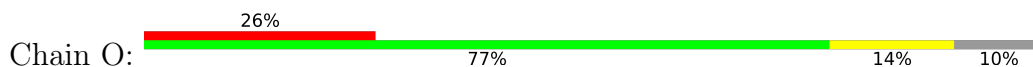


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

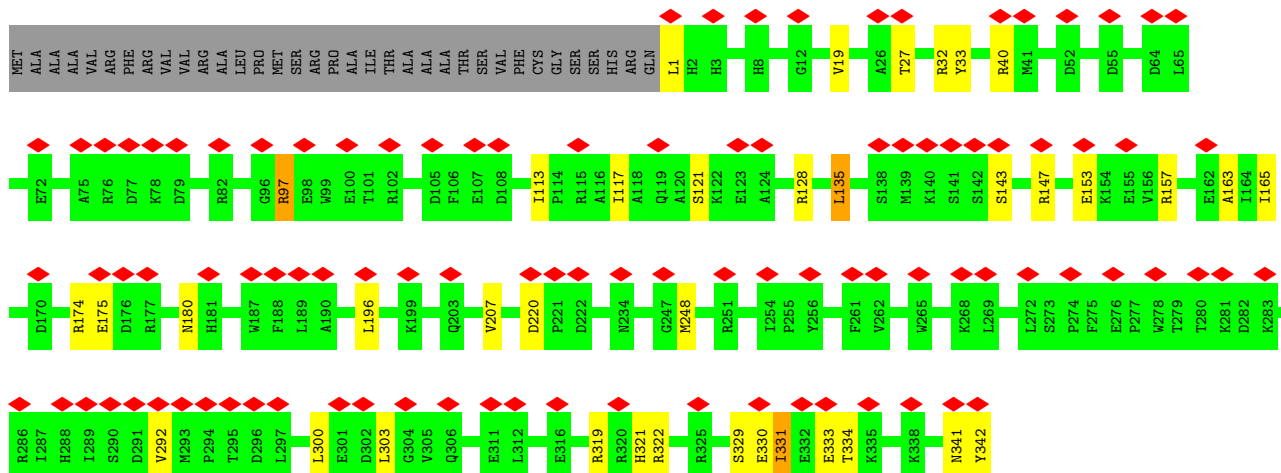
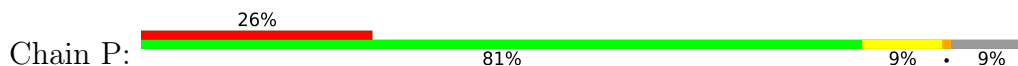




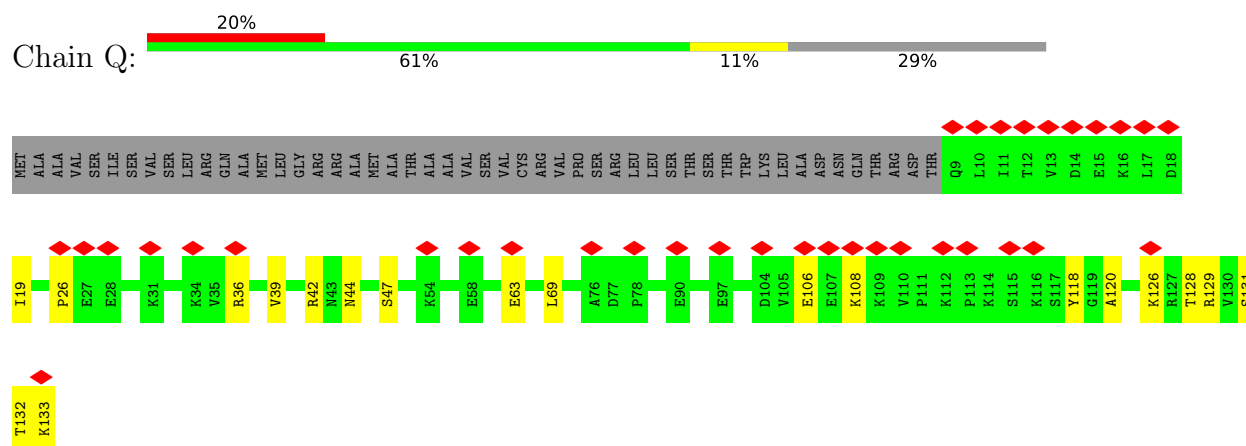
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



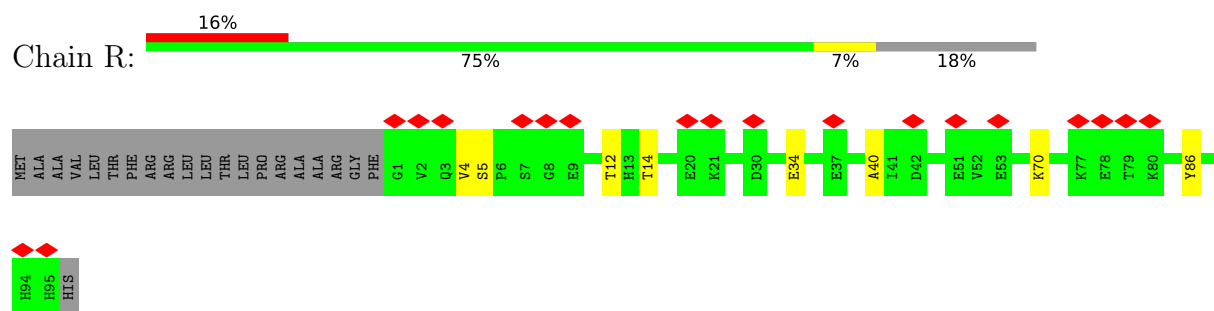
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



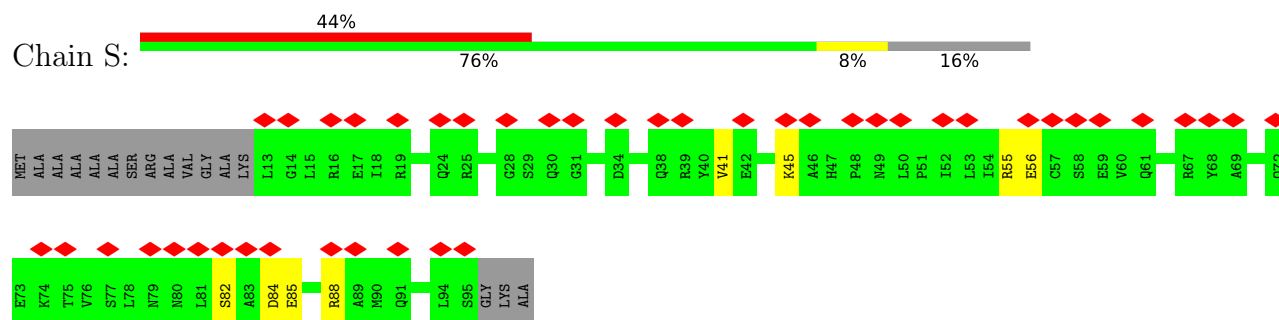
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



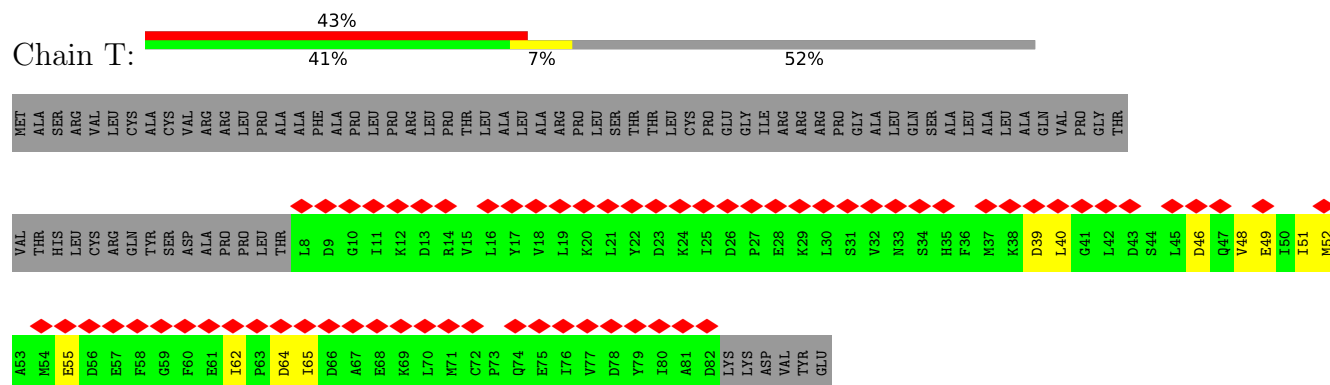
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



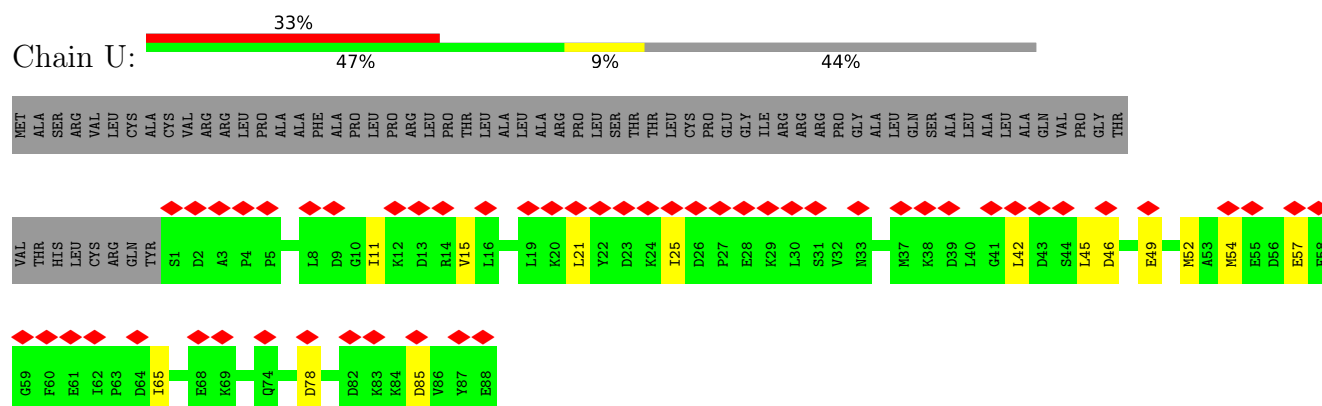
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



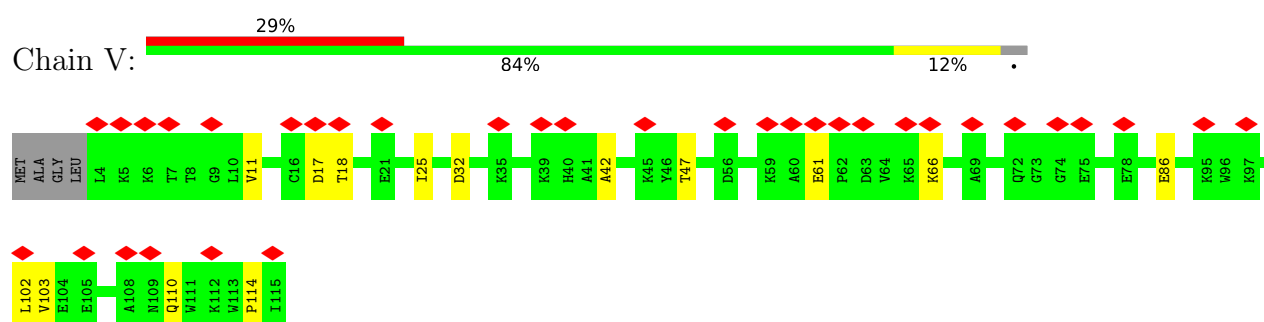
- Molecule 20: Acyl carrier protein, mitochondrial



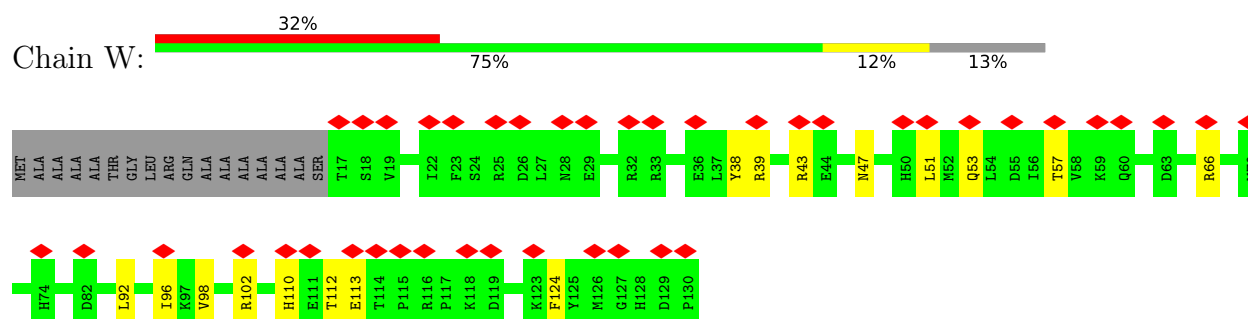
- Molecule 20: Acyl carrier protein, mitochondrial



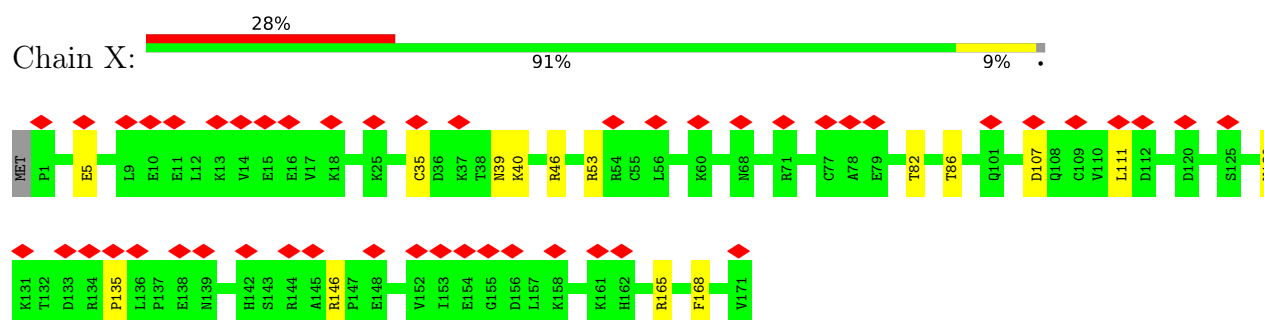
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



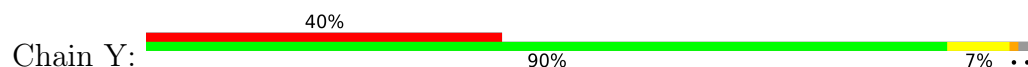
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

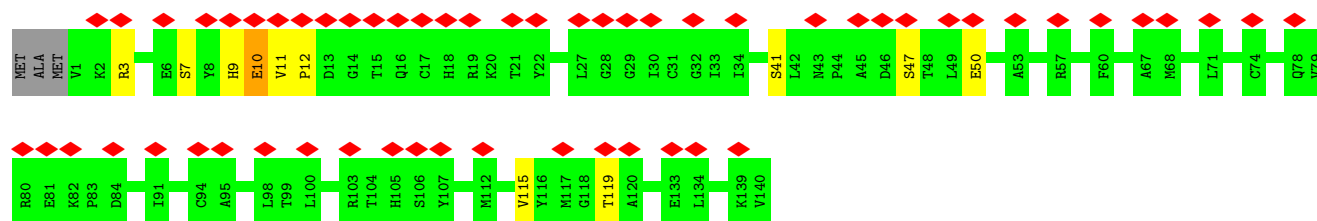


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

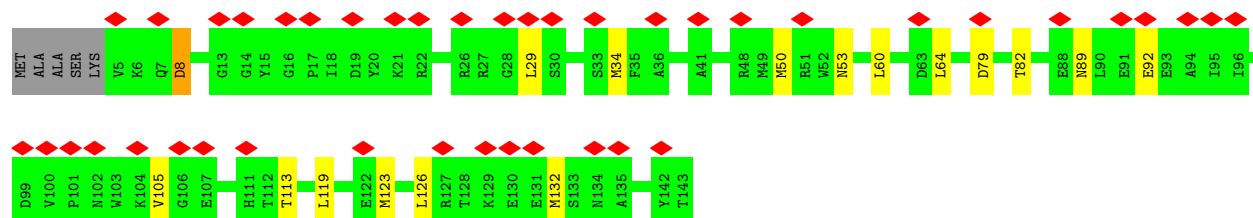
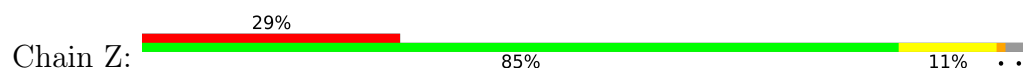


- Molecule 24: MCG5603

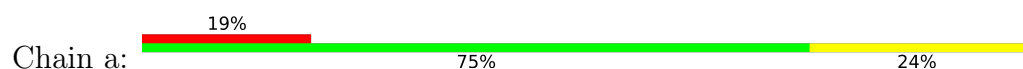




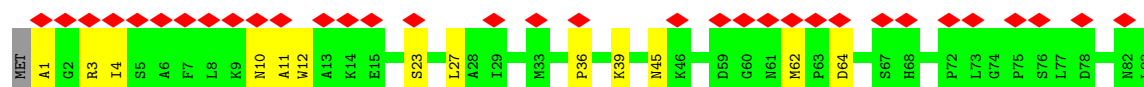
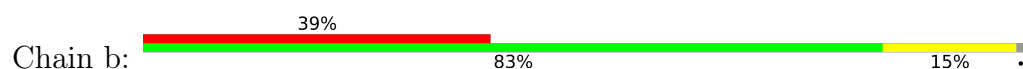
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



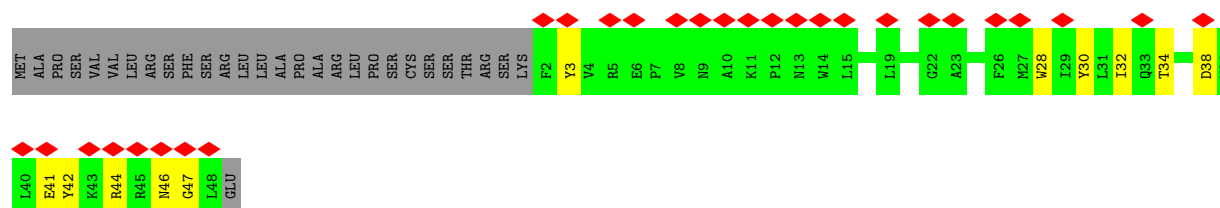
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



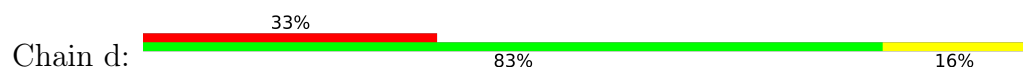
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

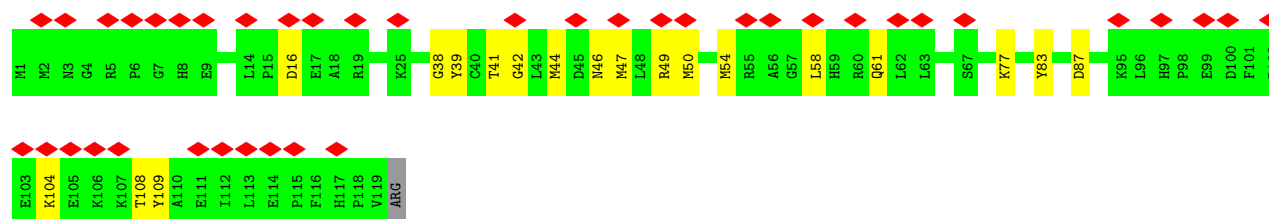


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

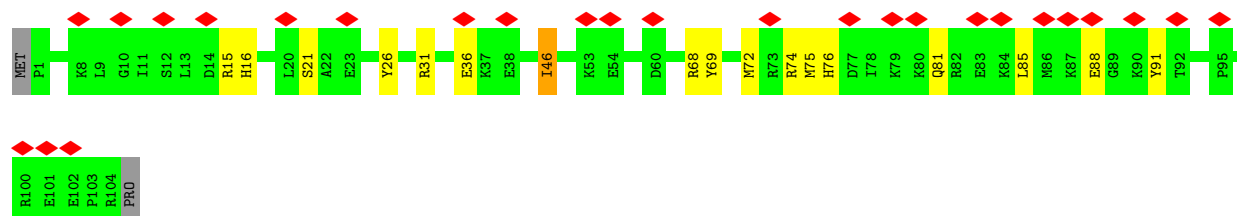
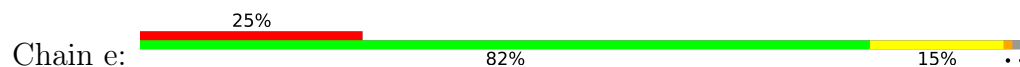


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

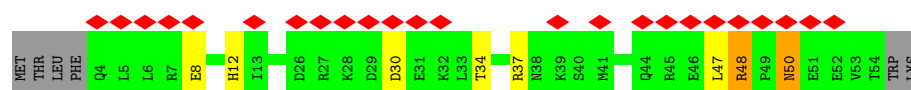
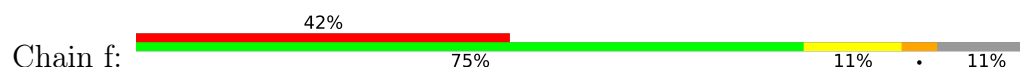




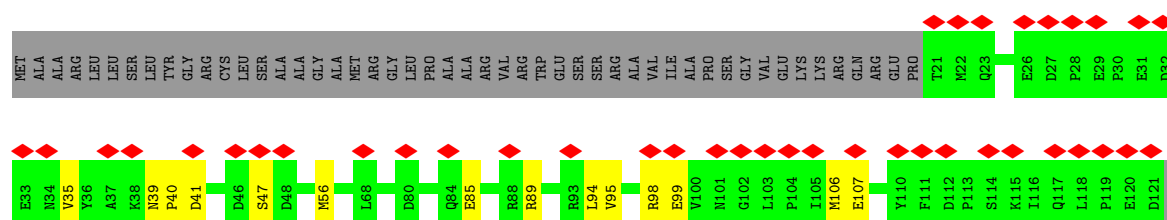
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



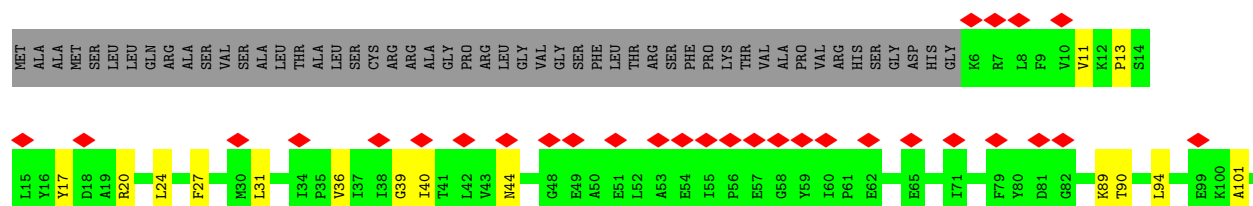
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

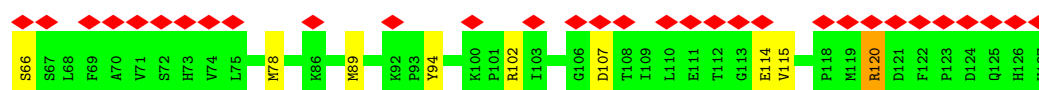
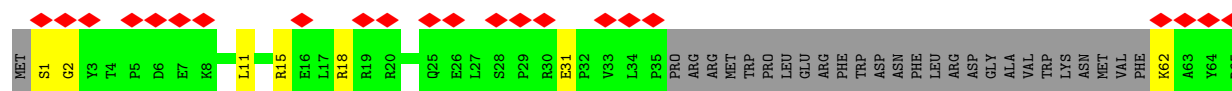
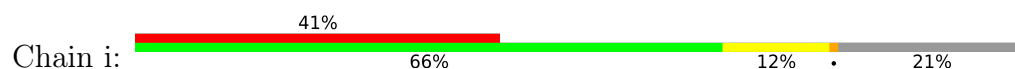


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

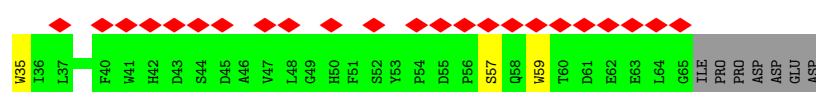
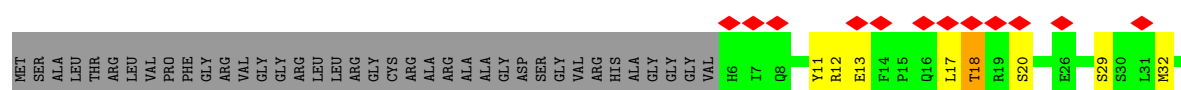




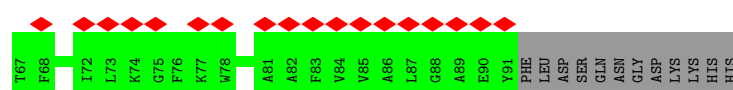
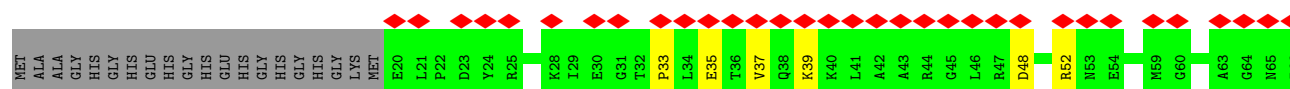
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



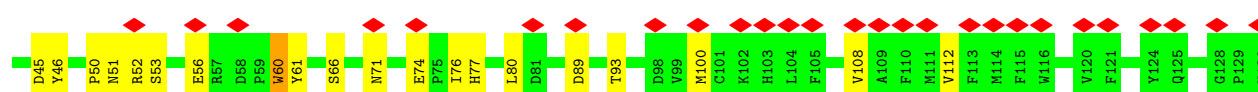
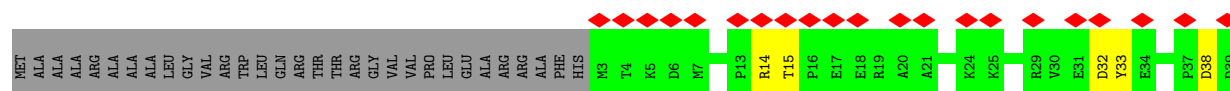
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

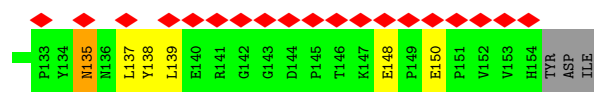


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

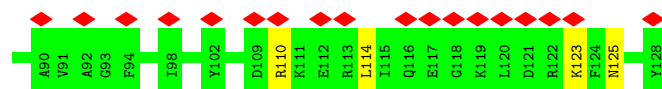
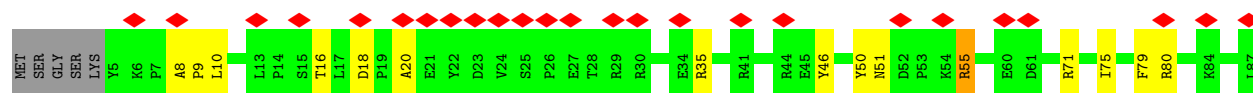
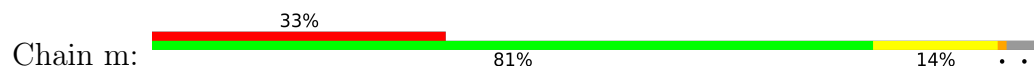


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

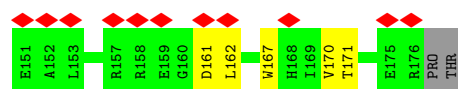
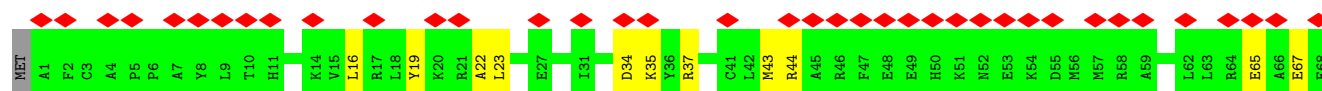
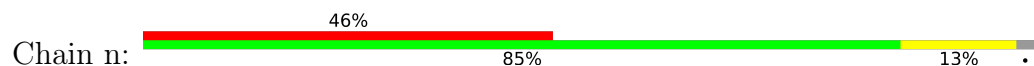




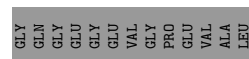
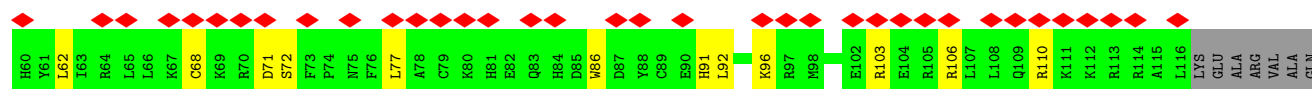
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



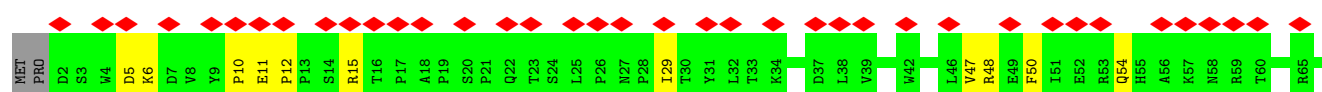
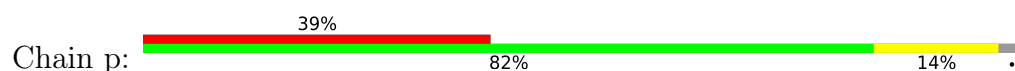
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

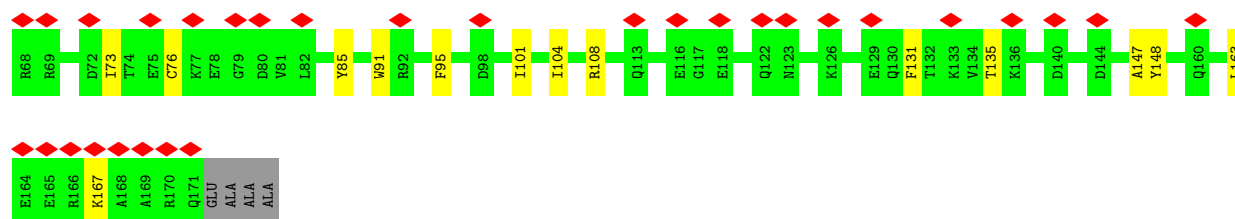


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

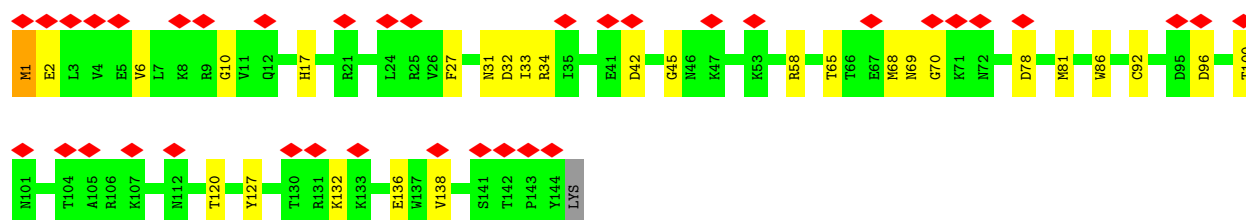
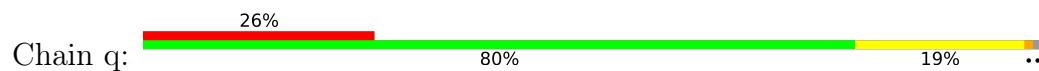


- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

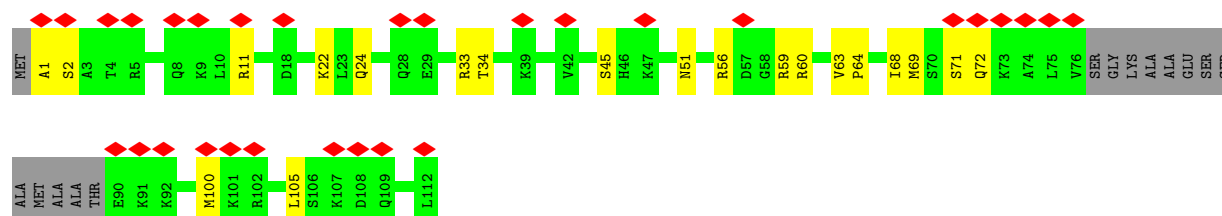




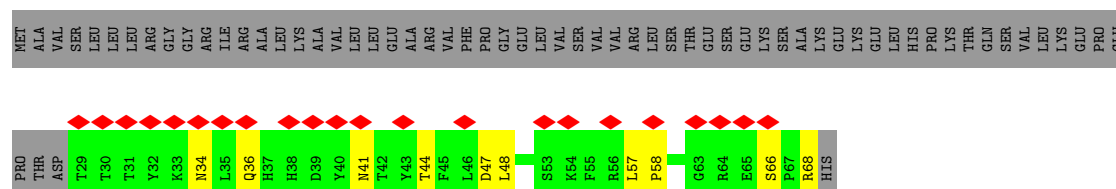
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	20370	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 ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	47600	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.450	Depositor
Minimum map value	-0.156	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	472.49997, 472.49997, 472.49997	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, NDP, 3PE, SAC, AYA, 2MR, ZN, FES, FMN, AME, PC1, ADP, FME, EHZ, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/949	0.67	0/1297
2	B	0.43	0/1272	0.61	0/1722
3	C	0.38	0/1762	0.58	0/2401
4	D	0.39	0/3528	0.57	0/4782
5	E	0.32	0/1688	0.64	0/2300
6	F	0.32	0/3376	0.57	0/4561
7	G	0.34	0/5383	0.58	0/7293
8	H	0.37	0/2607	0.60	0/3564
9	I	0.42	0/1438	0.68	0/1946
10	J	0.33	0/1322	0.57	0/1799
11	K	0.36	0/738	0.54	0/1002
12	L	0.35	0/4913	0.60	0/6686
13	M	0.37	0/3709	0.58	0/5052
14	N	0.37	0/2748	0.59	0/3741
15	O	0.31	0/2674	0.56	0/3626
16	P	0.31	0/2823	0.56	0/3828
17	Q	0.34	0/1038	0.53	0/1401
18	R	0.32	0/762	0.51	0/1026
19	S	0.30	0/678	0.58	0/915
20	T	0.21	0/613	0.42	0/826
20	U	0.30	0/718	0.56	0/970
21	V	0.29	0/937	0.65	0/1270
22	W	0.32	0/993	0.60	0/1335
23	X	0.30	0/1434	0.57	0/1937
24	Y	0.27	0/1061	0.50	0/1439
25	Z	0.32	0/1183	0.60	0/1597
26	a	0.33	0/561	0.68	1/755 (0.1%)
27	b	0.33	0/666	0.59	0/914
28	c	0.26	0/400	0.54	0/544
29	d	0.32	0/1017	0.55	0/1373
30	e	0.29	0/892	0.64	0/1187
31	f	0.32	0/443	0.60	0/596

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.28	0/878	0.59	0/1196
33	h	0.31	0/1189	0.53	0/1610
34	i	0.30	0/836	0.59	0/1138
35	j	0.31	0/548	0.70	0/748
36	k	0.27	0/601	0.54	0/814
37	l	0.31	0/1327	0.65	0/1811
38	m	0.32	0/1064	0.61	0/1444
39	n	0.31	0/1581	0.56	0/2140
40	o	0.29	0/919	0.60	0/1232
41	p	0.31	0/1471	0.59	0/1988
42	q	0.34	0/1234	0.59	1/1681 (0.1%)
43	r	0.34	0/806	0.64	0/1090
44	s	0.27	0/345	0.50	0/468
All	All	0.34	0/67125	0.59	2/91045 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	C	0	1
4	D	0	2
5	E	0	1
6	F	0	1
7	G	0	5
8	H	0	5
10	J	0	2
12	L	0	7
13	M	0	1
14	N	0	2
16	P	0	3
17	Q	0	1
20	U	0	1
22	W	0	1
23	X	0	1
25	Z	0	1
26	a	0	2
29	d	0	2
30	e	0	1
31	f	0	1

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	g	0	2
34	i	0	3
35	j	0	2
37	l	0	3
38	m	0	1
40	o	0	2
41	p	0	3
42	q	0	1
All	All	0	60

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	11	ILE	N-CA-C	-6.19	106.77	112.96
42	q	132	LYS	N-CA-CB	-5.78	107.58	114.17

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	119	GLU	Peptide
2	B	134	GLY	Peptide
3	C	8	ARG	Peptide
4	D	171	PHE	Peptide
4	D	87	THR	Peptide
5	E	150	ASN	Peptide
6	F	206	LYS	Peptide
7	G	258	ILE	Peptide
7	G	259	ASN	Peptide
7	G	484	ALA	Peptide
7	G	485	ALA	Peptide
7	G	61	LYS	Peptide
8	H	156	MET	Peptide
8	H	207	LEU	Peptide
8	H	249	ILE	Peptide
8	H	90	PRO	Peptide
8	H	91	MET	Peptide
10	J	129	ASP	Peptide
10	J	170	THR	Mainchain
12	L	108	MET	Peptide

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Mol	Chain	Res	Type	Group
12	L	159	TYR	Peptide
12	L	197	GLU	Peptide
12	L	383	MET	Peptide
12	L	434	LYS	Peptide
12	L	520	SER	Peptide
12	L	598	ILE	Mainchain
13	M	369	LEU	Peptide
14	N	109	ALA	Peptide
14	N	141	ILE	Peptide
16	P	331	ILE	Peptide
16	P	334	THR	Peptide
16	P	97	ARG	Peptide
17	Q	69	LEU	Peptide
20	U	65	ILE	Peptide
22	W	57	THR	Peptide
23	X	146	ARG	Peptide
25	Z	29	LEU	Peptide
26	a	55	SER	Peptide
26	a	61	TYR	Peptide
29	d	104	LYS	Peptide
29	d	16	ASP	Peptide
30	e	46	ILE	Peptide
31	f	48	ARG	Peptide
32	g	106	MET	Peptide
32	g	35	VAL	Peptide
34	i	114	GLU	Peptide
34	i	120	ARG	Peptide
34	i	31	GLU	Peptide
35	j	12	ARG	Peptide
35	j	18	THR	Peptide
37	l	135	ASN	Peptide
37	l	148	GLU	Peptide
37	l	60	TRP	Peptide
38	m	55	ARG	Peptide
40	o	13	SER	Peptide
40	o	20	LYS	Peptide
41	p	10	PRO	Peptide
41	p	11	GLU	Peptide
41	p	12	PRO	Peptide
42	q	120	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	933	0	969	22	0
2	B	1241	0	1250	23	0
3	C	1712	0	1667	27	0
4	D	3452	0	3390	86	0
5	E	1648	0	1639	37	0
6	F	3301	0	3252	64	0
7	G	5296	0	5322	105	0
8	H	2540	0	2626	49	0
9	I	1408	0	1344	40	0
10	J	1300	0	1315	27	0
11	K	737	0	768	16	0
12	L	4800	0	4985	91	0
13	M	3632	0	3853	77	0
14	N	2696	0	2895	48	0
15	O	2607	0	2566	30	0
16	P	2748	0	2768	26	0
17	Q	1015	0	1016	13	0
18	R	748	0	724	6	0
19	S	667	0	685	7	0
20	T	604	0	595	10	0
20	U	706	0	698	13	0
21	V	915	0	954	10	0
22	W	970	0	991	13	0
23	X	1396	0	1379	7	0
24	Y	1037	0	1027	6	0
25	Z	1152	0	1148	15	0
26	a	548	0	562	12	0
27	b	651	0	653	9	0
28	c	389	0	385	7	0
29	d	985	0	988	13	0
30	e	870	0	864	13	0
31	f	433	0	429	5	0
32	g	850	0	783	9	0
33	h	1154	0	1157	14	0
34	i	820	0	809	12	0
35	j	525	0	477	9	0
36	k	582	0	574	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	l	1274	0	1173	18	0
38	m	1035	0	1043	16	0
39	n	1527	0	1459	20	0
40	o	898	0	887	15	0
41	p	1438	0	1402	20	0
42	q	1203	0	1157	16	0
43	r	796	0	831	19	0
44	s	336	0	320	7	0
45	A	41	0	59	0	0
45	H	102	0	164	1	0
45	L	93	0	143	1	0
45	M	277	0	424	2	0
45	N	51	0	82	0	0
46	B	8	0	0	0	0
46	F	8	0	0	0	0
46	G	16	0	0	1	0
46	I	16	0	0	0	0
47	E	4	0	0	1	0
47	G	4	0	0	0	0
48	F	31	0	19	1	0
49	H	124	0	173	2	0
49	P	43	0	63	0	0
50	H	57	0	58	2	0
50	L	148	0	187	3	0
50	M	67	0	81	0	0
51	O	27	0	12	0	0
52	P	48	0	26	5	0
53	R	1	0	0	0	0
54	T	34	0	0	1	0
54	U	35	0	0	0	0
All	All	66810	0	67270	900	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 7.

All (900) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HD11	11:K:68:ALA:HB3	1.41	0.97
12:L:371:SER:HG	35:j:29:SER:HG	1.13	0.95
7:G:228:ILE:HG22	7:G:583:THR:HG22	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:M:505:3PE:H271	29:d:47:MET:HE3	1.57	0.86
50:H:405:CDL:H1O1	43:r:2:SER:HG	1.17	0.84
12:L:293:LEU:O	12:L:425:ARG:NH1	2.14	0.80
11:K:40:LEU:HD13	14:N:71:LEU:HD12	1.65	0.79
43:r:45:SER:O	43:r:51:ASN:ND2	2.16	0.79
6:F:99:GLU:OE2	6:F:108:ARG:N	2.16	0.78
12:L:151:SER:OG	12:L:252:MET:SD	2.42	0.78
23:X:165:ARG:NH2	29:d:87:ASP:OD1	2.15	0.78
20:U:46:ASP:OD1	39:n:44:ARG:NH2	2.17	0.77
4:D:183:ARG:NH1	4:D:210:ASP:OD2	2.17	0.77
7:G:396:ARG:NH1	7:G:416:THR:O	2.17	0.76
5:E:105:THR:OG1	47:E:301:FES:S2	2.44	0.76
9:I:55:GLU:OE2	42:q:34:ARG:NH2	2.18	0.76
23:X:35:CYS:O	23:X:39:ASN:ND2	2.19	0.76
4:D:335:ARG:NH2	9:I:128:CYS:O	2.17	0.76
1:A:81:THR:O	27:b:45:ASN:ND2	2.19	0.76
7:G:261:GLU:OE2	17:Q:42:ARG:NH2	2.19	0.76
15:O:97:GLN:NE2	15:O:131:ASP:OD1	2.19	0.76
37:l:46:TYR:OH	37:l:76:ILE:O	2.02	0.76
20:T:55:GLU:OE1	22:W:43:ARG:NH2	2.19	0.76
12:L:220:ALA:O	12:L:224:SER:OG	2.04	0.75
28:c:38:ASP:OD2	29:d:77:LYS:NZ	2.19	0.75
4:D:326:ASP:OD1	7:G:127:ARG:NH2	2.19	0.75
34:i:94:TYR:OH	41:p:6:LYS:O	2.05	0.75
11:K:1:FME:SD	11:K:50:ASN:ND2	2.59	0.75
2:B:159:CYS:SG	4:D:105:ARG:NH2	2.60	0.75
8:H:104:PHE:O	8:H:108:THR:OG1	2.04	0.75
6:F:24:ASN:ND2	6:F:28:ARG:O	2.20	0.74
4:D:246:THR:OG1	21:V:11:VAL:O	2.06	0.74
3:C:205:ALA:HB2	7:G:122:MET:HE1	1.67	0.74
6:F:263:ASN:ND2	6:F:286:GLY:O	2.21	0.74
20:U:15:VAL:HG22	20:U:54:MET:HE1	1.69	0.74
7:G:52:CYS:SG	7:G:53:ARG:N	2.61	0.74
13:M:240:SER:OG	13:M:316:MET:SD	2.43	0.73
6:F:49:LEU:O	6:F:127:ARG:NH1	2.21	0.73
2:B:127:GLY:O	2:B:131:ASN:ND2	2.21	0.73
5:E:194:GLU:OE2	6:F:28:ARG:NH2	2.20	0.73
24:Y:47:SER:OG	24:Y:50:GLU:OE1	2.06	0.73
2:B:92:GLN:NE2	8:H:209:SER:OG	2.21	0.73
12:L:86:SER:O	12:L:90:THR:OG1	2.05	0.73
4:D:224:GLU:OE1	9:I:42:TYR:OH	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:k:35:GLU:OE2	36:k:39:LYS:NZ	2.22	0.73
12:L:556:ILE:HD12	38:m:75:ILE:HG22	1.69	0.73
43:r:71:SER:OG	43:r:72:GLN:OE1	2.04	0.73
10:J:111:GLU:O	30:e:69:TYR:OH	2.07	0.72
42:q:42:ASP:OD1	42:q:86:TRP:NE1	2.22	0.72
8:H:18:ALA:O	8:H:21:THR:OG1	2.07	0.72
14:N:120:GLN:OE1	14:N:176:ARG:NH2	2.21	0.72
33:h:109:GLU:OE1	33:h:112:ARG:NH1	2.23	0.72
7:G:460:ARG:NH2	7:G:659:ASP:O	2.23	0.72
12:L:295:GLN:O	12:L:425:ARG:NH2	2.22	0.72
7:G:477:ILE:O	7:G:481:THR:OG1	2.07	0.72
6:F:34:LYS:O	6:F:38:ARG:NH1	2.23	0.72
16:P:97:ARG:NH1	52:P:501:NDP:O2X	2.22	0.72
34:i:102:ARG:O	41:p:15:ARG:NH2	2.23	0.72
4:D:237:ASN:O	8:H:284:GLN:NE2	2.23	0.71
16:P:27:THR:OG1	52:P:501:NDP:O3B	2.03	0.71
40:o:28:LEU:O	40:o:103:ARG:NH2	2.22	0.71
7:G:385:ARG:NH1	7:G:414:ASP:O	2.23	0.71
10:J:147:CYS:O	30:e:16:HIS:NE2	2.18	0.71
9:I:76:GLU:OE2	9:I:107:ARG:NH2	2.24	0.71
7:G:602:ALA:HB2	22:W:124:PHE:HZ	1.56	0.71
12:L:303:ALA:O	12:L:306:THR:OG1	2.09	0.71
13:M:179:LEU:O	13:M:183:THR:OG1	2.08	0.71
6:F:132:ARG:NH2	44:s:58:PRO:O	2.24	0.70
6:F:140:GLY:O	6:F:179:ARG:NH2	2.24	0.70
16:P:319:ARG:NH1	22:W:53:GLN:OE1	2.24	0.70
29:d:108:THR:OG1	41:p:76:CYS:O	2.05	0.70
3:C:211:GLN:NE2	21:V:114:PRO:O	2.24	0.70
13:M:116:ILE:HD12	13:M:174:LEU:HD12	1.73	0.70
3:C:43:SER:OG	3:C:45:LEU:O	2.10	0.70
29:d:39:TYR:OH	29:d:54:MET:SD	2.50	0.70
3:C:86:ARG:NH1	21:V:110:GLN:O	2.23	0.70
44:s:34:ASN:OD1	44:s:36:GLN:NE2	2.25	0.70
4:D:106:LEU:O	4:D:427:GLU:N	2.25	0.70
12:L:120:TYR:OH	50:L:702:CDL:OB3	2.09	0.70
32:g:41:ASP:OD1	33:h:20:ARG:NH2	2.25	0.70
8:H:265:LEU:O	8:H:269:THR:N	2.24	0.70
12:L:316:THR:HG22	12:L:395:ILE:HD12	1.75	0.69
4:D:182:GLU:OE2	9:I:60:SER:N	2.25	0.69
4:D:335:ARG:NH2	9:I:131:ASP:OD1	2.26	0.69
25:Z:82:THR:OG1	25:Z:123:MET:SD	2.46	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:ASP:O	2:B:48:ASN:ND2	2.25	0.69
6:F:246:GLY:N	6:F:271:GLU:OE2	2.25	0.69
12:L:246:LEU:O	12:L:251:THR:OG1	2.08	0.69
15:O:233:LYS:NZ	21:V:32:ASP:OD2	2.26	0.69
1:A:56:PHE:O	10:J:69:TYR:OH	2.10	0.69
15:O:252:ASP:O	15:O:255:THR:OG1	2.10	0.69
4:D:271:LYS:NZ	9:I:1:THR:OG1	2.25	0.68
4:D:329:LYS:NZ	7:G:126:ASP:OD1	2.25	0.68
12:L:73:SER:OG	12:L:194:ASN:ND2	2.26	0.68
4:D:341:SER:OG	4:D:344:SER:OG	2.06	0.68
6:F:29:HIS:O	6:F:39:ARG:NH1	2.26	0.68
12:L:520:SER:O	12:L:524:THR:OG1	2.11	0.68
7:G:199:VAL:HG12	7:G:208:LEU:HD11	1.76	0.68
15:O:31:ILE:HD11	15:O:183:ILE:HD11	1.76	0.68
7:G:303:VAL:HG11	7:G:603:LEU:HD11	1.76	0.67
21:V:47:THR:OG1	21:V:86:GLU:OE2	2.11	0.67
12:L:525:LEU:O	12:L:526:LEU:HD22	1.94	0.67
37:l:38:ASP:O	38:m:80:ARG:NH1	2.28	0.67
8:H:97:ASN:ND2	8:H:163:GLN:OE1	2.27	0.67
5:E:100:ILE:HG22	5:E:156:ILE:CD1	2.25	0.67
4:D:366:ALA:HB1	4:D:373:GLU:HG3	1.77	0.67
12:L:131:LEU:HD21	12:L:255:ALA:HB1	1.77	0.67
26:a:9:LEU:O	26:a:13:GLY:N	2.27	0.67
16:P:32:ARG:NH1	16:P:175:GLU:OE2	2.28	0.66
13:M:424:ILE:O	39:n:105:TYR:OH	2.13	0.66
15:O:108:TYR:OH	15:O:164:LEU:O	2.07	0.66
4:D:233:ARG:O	4:D:237:ASN:N	2.28	0.66
15:O:53:GLU:N	15:O:125:GLU:OE2	2.27	0.66
16:P:97:ARG:NH2	52:P:501:NDP:O1A	2.28	0.66
11:K:82:SER:O	11:K:86:GLY:N	2.27	0.66
34:i:120:ARG:NH2	40:o:38:MET:O	2.28	0.66
4:D:216:LYS:O	43:r:22:LYS:NZ	2.28	0.66
41:p:50:PHE:O	41:p:54:GLN:NE2	2.28	0.66
12:L:163:ASP:O	12:L:166:THR:OG1	2.13	0.66
2:B:144:ARG:NH2	3:C:169:THR:OG1	2.28	0.66
4:D:50:ASN:O	8:H:127:TYR:OH	2.14	0.66
12:L:224:SER:HB2	12:L:310:LEU:HD21	1.76	0.66
33:h:27:PHE:O	33:h:31:LEU:N	2.29	0.66
37:l:71:ASN:N	37:l:74:GLU:OE2	2.29	0.66
6:F:200:GLN:NE2	7:G:174:THR:O	2.28	0.65
7:G:117:GLN:NE2	46:G:801:SF4:S3	2.70	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:338:MET:HE3	4:D:348:HIS:HD1	1.61	0.65
7:G:455:SER:O	7:G:495:ARG:NH1	2.29	0.65
32:g:39:ASN:ND2	32:g:47:SER:O	2.29	0.65
44:s:41:ASN:OD1	44:s:44:THR:OG1	2.07	0.65
1:A:54:LYS:NZ	4:D:69:SER:O	2.19	0.65
23:X:5:GLU:O	23:X:53:ARG:NH1	2.28	0.65
17:Q:120:ALA:O	17:Q:128:THR:OG1	2.14	0.65
48:F:501:FMN:N1	48:F:501:FMN:O3'	2.24	0.65
8:H:284:GLN:O	8:H:288:LEU:N	2.28	0.65
8:H:201:THR:HG22	8:H:211:PHE:CD1	2.31	0.65
7:G:252:PRO:O	17:Q:44:ASN:ND2	2.30	0.64
12:L:176:ARG:NE	13:M:400:ILE:O	2.27	0.64
4:D:170:MET:O	4:D:174:ARG:N	2.29	0.64
29:d:38:GLY:O	29:d:41:THR:OG1	2.15	0.64
6:F:185:ILE:N	6:F:357:GLU:OE2	2.30	0.64
7:G:372:GLU:O	7:G:402:ASN:ND2	2.31	0.64
4:D:80:ILE:HD13	4:D:428:ILE:HG21	1.78	0.64
17:Q:36:ARG:NH2	17:Q:106:GLU:OE1	2.29	0.64
13:M:368:ALA:HB1	13:M:375:LEU:HD12	1.79	0.64
6:F:35:GLY:O	6:F:39:ARG:NH1	2.30	0.64
12:L:467:VAL:O	12:L:471:ASN:ND2	2.31	0.64
20:U:78:ASP:OD2	34:i:15:ARG:NH2	2.30	0.64
9:I:44:PHE:O	43:r:11:ARG:NH2	2.31	0.64
4:D:187:ALA:HB2	9:I:64:ARG:HE	1.63	0.64
18:R:12:THR:OG1	18:R:14:THR:O	2.15	0.63
40:o:50:LEU:O	40:o:55:ARG:NH2	2.30	0.63
4:D:347:HIS:ND1	7:G:121:MET:SD	2.66	0.63
11:K:4:THR:O	11:K:8:LEU:N	2.30	0.63
34:i:107:ASP:OD2	41:p:15:ARG:NH1	2.30	0.63
7:G:47:SER:O	7:G:161:ARG:NH1	2.32	0.63
6:F:407:LEU:O	6:F:411:ALA:N	2.32	0.63
12:L:195:SER:OG	12:L:200:GLN:OE1	2.16	0.63
13:M:269:MET:SD	13:M:399:ASN:ND2	2.72	0.63
34:i:1:SAC:OG	34:i:1:SAC:O	2.16	0.63
7:G:378:LEU:HD23	7:G:407:ALA:HB3	1.80	0.63
6:F:65:LEU:O	6:F:75:THR:OG1	2.14	0.62
35:j:57:SER:O	40:o:106:ARG:NH1	2.32	0.62
2:B:87:ARG:NH1	8:H:204:GLU:OE2	2.31	0.62
7:G:135:ARG:NH2	7:G:179:ASN:O	2.32	0.62
38:m:110:ARG:O	38:m:114:LEU:HD23	1.99	0.62
10:J:22:LYS:O	11:K:23:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:129:MET:SD	6:F:221:THR:OG1	2.56	0.62
12:L:217:LEU:HD11	12:L:277:MET:HE2	1.81	0.62
12:L:261:VAL:O	12:L:264:HIS:ND1	2.29	0.62
15:O:91:GLY:O	15:O:95:ARG:NE	2.33	0.62
18:R:34:GLU:O	42:q:127:TYR:OH	2.11	0.62
26:a:19:PRO:O	26:a:23:THR:OG1	2.17	0.62
20:U:25:ILE:HD13	20:U:42:LEU:HD11	1.82	0.62
7:G:348:ILE:N	7:G:459:GLN:OE1	2.33	0.61
14:N:122:ILE:O	14:N:176:ARG:NH1	2.33	0.61
37:l:14:ARG:O	37:l:15:THR:OG1	2.17	0.61
4:D:302:GLU:OE2	9:I:3:LYS:NZ	2.33	0.61
8:H:277:TYR:OH	9:I:32:LEU:O	2.18	0.61
8:H:10:LEU:HD22	8:H:83:LEU:HD21	1.82	0.61
1:A:2:ASN:O	1:A:5:THR:OG1	2.18	0.61
1:A:76:PRO:O	1:A:80:GLN:NE2	2.33	0.61
6:F:391:SER:O	6:F:394:GLU:N	2.34	0.61
50:H:405:CDL:OB4	26:a:2:TRP:NE1	2.33	0.61
13:M:260:PRO:O	13:M:264:LEU:N	2.33	0.61
2:B:78:ASP:OD2	2:B:81:ARG:N	2.33	0.61
20:U:49:GLU:OE2	39:n:19:TYR:OH	2.17	0.61
5:E:30:ARG:NH2	44:s:47:ASP:OD1	2.34	0.61
5:E:147:ALA:HB2	6:F:108:ARG:CD	2.30	0.61
6:F:81:PHE:O	6:F:84:LYS:NZ	2.33	0.61
15:O:309:ASN:OD1	28:c:3:TYR:OH	2.19	0.61
4:D:312:GLU:O	4:D:316:ASN:ND2	2.34	0.60
9:I:51:ASN:O	9:I:55:GLU:N	2.33	0.60
17:Q:118:TYR:OH	17:Q:133:LYS:NZ	2.27	0.60
12:L:338:MET:O	12:L:342:CYS:N	2.34	0.60
15:O:256:PHE:O	15:O:260:ARG:N	2.34	0.60
7:G:380:VAL:O	7:G:382:THR:N	2.34	0.60
1:A:63:LEU:HD13	11:K:68:ALA:HB1	1.82	0.60
3:C:82:ASP:O	4:D:387:TYR:OH	2.15	0.60
12:L:574:THR:HG23	14:N:167:TRP:O	2.02	0.60
14:N:74:ILE:O	14:N:78:TYR:N	2.34	0.60
42:q:96:ASP:OD2	42:q:100:THR:OG1	2.18	0.60
12:L:313:MET:O	12:L:316:THR:OG1	2.12	0.60
14:N:215:MET:HE2	14:N:248:LEU:HD21	1.81	0.60
6:F:96:ASN:OD1	6:F:192:LEU:HD22	2.02	0.60
14:N:128:LEU:O	14:N:132:THR:OG1	2.15	0.59
15:O:36:ASN:OD1	15:O:40:LYS:NZ	2.34	0.59
19:S:85:GLU:OE1	19:S:88:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:371:SER:OG	35:j:29:SER:OG	2.02	0.59
13:M:303:ILE:HG22	13:M:305:THR:HG23	1.83	0.59
4:D:208:LEU:HD22	4:D:315:LEU:HD23	1.85	0.59
14:N:308:ASN:OD1	14:N:309:ASN:N	2.35	0.59
15:O:305:ALA:N	29:d:50:MET:O	2.35	0.59
12:L:446:ASN:ND2	35:j:18:THR:OG1	2.35	0.59
42:q:32:ASP:OD2	42:q:58:ARG:NH2	2.36	0.59
5:E:147:ALA:HB3	5:E:153:MET:HE1	1.85	0.59
37:l:33:TYR:OH	37:l:45:ASP:O	2.16	0.58
3:C:119:SER:OG	3:C:144:ASN:O	2.21	0.58
5:E:121:GLN:NE2	5:E:127:LYS:O	2.37	0.58
13:M:304:GLN:O	41:p:147:ALA:N	2.37	0.58
41:p:131:PHE:O	41:p:135:THR:OG1	2.17	0.58
4:D:83:LEU:HD13	4:D:83:LEU:O	2.03	0.58
2:B:111:ARG:NH1	2:B:149:ILE:O	2.36	0.58
7:G:36:GLN:NE2	17:Q:47:SER:O	2.37	0.58
13:M:230:ILE:HD12	13:M:234:ILE:HD11	1.85	0.58
21:V:17:ASP:O	21:V:18:THR:OG1	2.17	0.58
38:m:18:ASP:O	38:m:20:ALA:N	2.36	0.58
40:o:54:GLN:NE2	40:o:62:LEU:HD13	2.18	0.58
7:G:378:LEU:HD12	7:G:451:VAL:HG12	1.86	0.58
7:G:273:GLY:O	7:G:549:HIS:NE2	2.18	0.58
8:H:147:ALA:O	8:H:151:LEU:N	2.34	0.58
40:o:106:ARG:O	40:o:110:ARG:N	2.36	0.58
8:H:225:MET:O	8:H:229:THR:OG1	2.16	0.57
12:L:484:TRP:O	12:L:488:THR:OG1	2.20	0.57
13:M:19:SER:OG	31:f:8:GLU:OE2	2.08	0.57
13:M:118:PHE:O	13:M:122:PHE:N	2.36	0.57
23:X:46:ARG:NH2	25:Z:79:ASP:OD1	2.37	0.57
30:e:21:SER:OG	30:e:36:GLU:OE1	2.21	0.57
3:C:86:ARG:NH1	3:C:91:GLU:OE2	2.37	0.57
7:G:194:GLU:OE2	7:G:385:ARG:NE	2.37	0.57
42:q:45:GLY:O	42:q:65:THR:OG1	2.17	0.57
5:E:148:CYS:SG	6:F:103:GLY:N	2.77	0.57
30:e:72:MET:O	30:e:76:HIS:N	2.37	0.57
12:L:189:PHE:O	12:L:193:MET:N	2.35	0.57
14:N:333:SER:O	14:N:334:THR:OG1	2.22	0.57
6:F:45:THR:HA	6:F:48:ILE:HD12	1.86	0.57
12:L:556:ILE:HD12	38:m:75:ILE:CG2	2.34	0.57
37:l:76:ILE:HG23	37:l:80:LEU:HD22	1.86	0.57
7:G:157:THR:O	7:G:161:ARG:NE	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:357:ARG:NH1	39:n:77:GLN:O	2.38	0.57
30:e:81:GLN:O	30:e:85:LEU:N	2.38	0.57
33:h:40:ILE:O	33:h:44:ASN:ND2	2.37	0.57
12:L:554:ASP:OD1	13:M:213:HIS:NE2	2.35	0.56
13:M:373:ILE:HD13	13:M:447:LEU:HD12	1.86	0.56
3:C:168:LEU:HD21	4:D:90:LEU:HD23	1.87	0.56
34:i:102:ARG:NE	40:o:48:ALA:O	2.37	0.56
6:F:20:ARG:NH1	6:F:269:GLU:O	2.37	0.56
7:G:194:GLU:N	7:G:194:GLU:OE1	2.37	0.56
7:G:259:ASN:CG	7:G:390:LEU:HD13	2.29	0.56
7:G:278:ARG:NH2	7:G:568:GLU:OE1	2.38	0.56
20:T:48:VAL:HG12	20:T:52:MET:HE3	1.86	0.56
43:r:105:LEU:HD13	43:r:105:LEU:O	2.06	0.56
16:P:143:SER:O	16:P:147:ARG:NE	2.37	0.56
21:V:102:LEU:HD23	21:V:103:VAL:H	1.71	0.56
34:i:89:MET:SD	34:i:89:MET:N	2.79	0.56
2:B:46:LEU:CD1	8:H:53:MET:HE1	2.35	0.56
6:F:351:ILE:HD11	6:F:415:VAL:CG2	2.35	0.56
42:q:1:AME:SD	42:q:2:GLU:N	2.79	0.56
14:N:19:ILE:O	14:N:23:SER:OG	2.18	0.56
15:O:134:PHE:O	15:O:138:MET:N	2.39	0.56
15:O:135:LEU:O	15:O:139:TYR:N	2.38	0.56
40:o:71:ASP:OD1	40:o:72:SER:N	2.39	0.56
13:M:373:ILE:HD11	13:M:444:LEU:CD2	2.36	0.56
4:D:226:GLU:O	4:D:230:THR:OG1	2.17	0.56
4:D:181:TYR:O	4:D:185:SER:N	2.39	0.56
28:c:38:ASP:O	28:c:42:TYR:N	2.39	0.55
41:p:5:ASP:O	41:p:108:ARG:NH2	2.36	0.55
1:A:70:ALA:HB1	10:J:54:MET:CE	2.37	0.55
4:D:183:ARG:O	9:I:62:ARG:NH1	2.39	0.55
9:I:38:MET:O	9:I:41:SER:OG	2.22	0.55
12:L:216:LEU:HD22	12:L:259:LEU:HD21	1.88	0.55
14:N:9:ILE:HG22	14:N:43:MET:HE2	1.87	0.55
3:C:149:ARG:NH2	4:D:77:ASP:OD1	2.40	0.55
15:O:41:GLU:OE2	15:O:45:GLN:NE2	2.39	0.55
43:r:51:ASN:OD1	43:r:56:ARG:NE	2.38	0.55
2:B:175:ARG:NH1	42:q:78:ASP:OD1	2.40	0.55
13:M:370:PRO:O	13:M:372:SER:N	2.40	0.55
7:G:118:ASP:O	7:G:121:MET:N	2.39	0.55
4:D:221:ARG:NH1	43:r:24:GLN:OE1	2.39	0.55
16:P:117:ILE:O	16:P:121:SER:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:10:ASN:OD1	27:b:11:ALA:N	2.39	0.55
32:g:56:MET:CE	33:h:24:LEU:HD13	2.36	0.55
6:F:306:LEU:HD21	6:F:347:ILE:HD11	1.88	0.55
28:c:41:GLU:OE2	28:c:44:ARG:NH2	2.40	0.55
8:H:39:ILE:HG23	49:H:406:PC1:H152	1.89	0.54
16:P:128:ARG:NH2	16:P:220:ASP:O	2.40	0.54
1:A:90:MET:HE2	10:J:152:MET:HG3	1.89	0.54
9:I:76:GLU:HA	18:R:40:ALA:HB1	1.90	0.54
28:c:30:TYR:O	28:c:34:THR:OG1	2.11	0.54
1:A:65:PHE:HE1	10:J:163:ILE:HD11	1.71	0.54
4:D:81:GLY:N	4:D:429:ASP:OD1	2.41	0.54
9:I:19:ALA:O	9:I:23:ALA:N	2.34	0.54
4:D:338:MET:HE3	4:D:348:HIS:ND1	2.21	0.54
12:L:273:ILE:HA	12:L:276:THR:HG22	1.89	0.54
7:G:602:ALA:HB2	22:W:124:PHE:CZ	2.42	0.54
12:L:290:ILE:HA	12:L:293:LEU:HD23	1.89	0.54
8:H:264:LEU:O	8:H:268:SER:N	2.37	0.54
13:M:200:MET:SD	13:M:243:MET:HE3	2.48	0.54
41:p:163:LEU:O	41:p:167:LYS:N	2.40	0.54
13:M:354:LEU:O	13:M:357:THR:OG1	2.20	0.53
23:X:107:ASP:O	23:X:111:LEU:N	2.41	0.53
6:F:247:ARG:N	6:F:250:ASN:O	2.41	0.53
7:G:358:LEU:O	7:G:360:SER:N	2.39	0.53
8:H:61:MET:H	8:H:216:ALA:HB3	1.73	0.53
20:T:49:GLU:OE2	22:W:38:TYR:OH	2.22	0.53
23:X:82:THR:O	23:X:86:THR:OG1	2.18	0.53
3:C:205:ALA:O	43:r:60:ARG:NH1	2.42	0.53
7:G:228:ILE:HD12	7:G:581:GLN:HB2	1.89	0.53
8:H:253:GLU:O	8:H:257:THR:OG1	2.20	0.53
12:L:354:GLN:OE1	12:L:354:GLN:N	2.42	0.53
15:O:138:MET:SD	15:O:144:ILE:HD11	2.49	0.53
32:g:94:LEU:HD11	32:g:98:ARG:CZ	2.39	0.53
37:l:135:ASN:ND2	37:l:150:GLU:OE2	2.41	0.53
15:O:223:TYR:OH	15:O:237:ASP:OD2	2.17	0.53
5:E:192:CYS:SG	5:E:193:CYS:N	2.81	0.53
12:L:586:LEU:HD22	24:Y:41:SER:O	2.09	0.53
1:A:67:LEU:HD13	11:K:65:VAL:HA	1.89	0.53
8:H:261:MET:O	8:H:265:LEU:HD23	2.09	0.53
12:L:137:MET:N	12:L:196:TRP:O	2.42	0.53
13:M:116:ILE:CD1	13:M:174:LEU:HD12	2.38	0.53
39:n:65:GLU:N	39:n:65:GLU:OE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:76:MET:HE3	13:M:226:ALA:HB1	1.91	0.53
23:X:40:LYS:HB2	23:X:130:VAL:HG11	1.91	0.53
34:i:11:LEU:HD23	34:i:15:ARG:HH22	1.73	0.53
2:B:58:MET:HE1	2:B:113:VAL:HG13	1.89	0.53
5:E:10:ARG:NH1	7:G:138:GLU:OE2	2.42	0.53
7:G:409:ILE:HG23	7:G:428:ILE:HD11	1.89	0.53
4:D:222:ILE:O	4:D:226:GLU:N	2.37	0.52
4:D:356:TYR:O	43:r:59:ARG:NH1	2.42	0.52
13:M:204:LEU:HD21	13:M:243:MET:HE1	1.91	0.52
14:N:124:LEU:CD2	14:N:225:MET:HE3	2.40	0.52
13:M:106:LEU:HD23	13:M:125:THR:HG21	1.92	0.52
13:M:115:LEU:O	13:M:119:TYR:N	2.41	0.52
13:M:168:GLN:O	13:M:172:GLY:N	2.43	0.52
16:P:27:THR:OG1	52:P:501:NDP:O1X	2.28	0.52
20:T:46:ASP:OD1	22:W:66:ARG:NH1	2.41	0.52
10:J:41:LEU:O	10:J:45:GLY:N	2.42	0.52
11:K:79:VAL:O	11:K:83:ASN:ND2	2.43	0.52
12:L:53:MET:HE1	41:p:29:ILE:HG23	1.90	0.52
15:O:178:GLU:O	15:O:181:SER:OG	2.17	0.52
7:G:368:ILE:N	7:G:577:GLU:OE2	2.43	0.52
9:I:22:ASN:OD1	9:I:25:ARG:NH1	2.43	0.52
17:Q:131:SER:O	17:Q:132:THR:OG1	2.18	0.52
1:A:79:ILE:O	27:b:45:ASN:ND2	2.42	0.52
2:B:125:SER:OG	2:B:131:ASN:OD1	2.24	0.52
7:G:335:LEU:HD12	7:G:343:LEU:HD21	1.92	0.52
10:J:166:ILE:HD11	11:K:76:ALA:HB2	1.92	0.52
19:S:41:VAL:HG12	19:S:45:LYS:HE3	1.92	0.52
5:E:128:VAL:HG12	5:E:139:LEU:HD12	1.91	0.52
1:A:80:GLN:O	30:e:26:TYR:OH	2.16	0.52
1:A:24:LEU:HD13	1:A:24:LEU:O	2.09	0.52
1:A:60:ILE:HG21	10:J:166:ILE:HG12	1.92	0.52
22:W:110:HIS:ND1	22:W:113:GLU:OE2	2.42	0.52
37:l:32:ASP:OD1	38:m:35:ARG:NH2	2.43	0.52
43:r:63:VAL:HG22	43:r:64:PRO:HD2	1.91	0.52
12:L:534:HIS:ND1	45:L:701:3PE:O32	2.42	0.52
37:l:150:GLU:N	37:l:150:GLU:OE1	2.43	0.52
38:m:46:TYR:O	38:m:50:TYR:N	2.40	0.52
5:E:48:LEU:O	5:E:90:TYR:OH	2.26	0.51
8:H:201:THR:HG22	8:H:211:PHE:HD1	1.75	0.51
12:L:533:ILE:HG22	12:L:533:ILE:O	2.10	0.51
14:N:17:PRO:O	14:N:21:MET:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:42:GLY:O	29:d:46:ASN:ND2	2.42	0.51
38:m:8:ALA:HB3	38:m:10:LEU:O	2.10	0.51
42:q:68:MET:O	42:q:70:GLY:N	2.43	0.51
9:I:114:ASP:OD1	9:I:116:THR:OG1	2.25	0.51
12:L:582:GLY:O	14:N:58:LYS:NZ	2.37	0.51
13:M:158:ILE:HG12	14:N:283:ALA:HB1	1.92	0.51
2:B:72:MET:HE1	2:B:166:LEU:HD12	1.91	0.51
6:F:210:PRO:O	6:F:220:THR:N	2.40	0.51
7:G:208:LEU:HD12	7:G:208:LEU:O	2.10	0.51
27:b:3:ARG:HD3	27:b:4:ILE:HG23	1.92	0.51
28:c:28:TRP:O	28:c:32:ILE:N	2.40	0.51
7:G:228:ILE:CG2	7:G:583:THR:HG22	2.36	0.51
12:L:193:MET:O	12:L:195:SER:N	2.43	0.51
12:L:10:LEU:HD13	34:i:78:MET:SD	2.50	0.51
13:M:317:ILE:HG13	13:M:454:ILE:HD11	1.93	0.51
12:L:401:THR:HG21	12:L:479:VAL:HG11	1.92	0.51
42:q:17:HIS:CE1	42:q:33:ILE:HG23	2.45	0.51
2:B:162:THR:O	2:B:165:ALA:N	2.41	0.51
5:E:116:ILE:HD11	5:E:164:LEU:HD11	1.92	0.51
8:H:314:VAL:O	25:Z:53:ASN:ND2	2.44	0.51
7:G:522:LEU:HB3	7:G:543:ILE:HG22	1.92	0.51
15:O:113:GLU:O	15:O:117:SER:OG	2.25	0.51
26:a:54:ILE:O	26:a:54:ILE:HG22	2.11	0.51
38:m:8:ALA:HB1	38:m:9:PRO:HD2	1.93	0.51
4:D:233:ARG:NH1	9:I:31:GLU:OE2	2.44	0.51
12:L:11:ILE:O	12:L:15:LEU:HD23	2.11	0.51
12:L:306:THR:O	12:L:310:LEU:N	2.41	0.51
16:P:33:TYR:CD2	16:P:207:VAL:HG11	2.46	0.51
20:U:15:VAL:HG22	20:U:54:MET:CE	2.39	0.51
32:g:85:GLU:OE2	32:g:89:ARG:NH1	2.44	0.51
2:B:128:SER:O	2:B:134:GLY:N	2.44	0.51
4:D:44:VAL:O	4:D:45:THR:OG1	2.25	0.51
7:G:278:ARG:N	42:q:136:GLU:O	2.44	0.51
22:W:47:ASN:O	22:W:51:LEU:HD23	2.11	0.51
3:C:205:ALA:HB2	7:G:122:MET:CE	2.40	0.50
19:S:82:SER:OG	19:S:84:ASP:OD1	2.24	0.50
5:E:132:THR:OG1	5:E:135:LYS:N	2.44	0.50
6:F:24:ASN:ND2	6:F:24:ASN:O	2.44	0.50
12:L:293:LEU:HD21	12:L:418:MET:HG3	1.94	0.50
12:L:381:THR:OG1	12:L:382:GLY:N	2.44	0.50
1:A:33:LYS:NZ	8:H:59:GLU:OE1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:579:ARG:NH2	7:G:636:ILE:HD12	2.26	0.50
8:H:76:THR:O	8:H:80:THR:OG1	2.19	0.50
8:H:130:PHE:O	8:H:134:ARG:N	2.42	0.50
12:L:597:LEU:O	12:L:601:LEU:N	2.42	0.50
6:F:257:ASN:O	6:F:334:VAL:N	2.44	0.50
7:G:577:GLU:OE1	7:G:636:ILE:HD11	2.11	0.50
8:H:102:ILE:HG22	8:H:160:TYR:HB3	1.94	0.50
12:L:103:PHE:HB2	12:L:341:MET:HE1	1.94	0.50
6:F:272:MET:O	6:F:273:SER:OG	2.26	0.50
16:P:341:ASN:OD1	16:P:342:TYR:N	2.45	0.50
6:F:108:ARG:O	6:F:112:ARG:NE	2.45	0.50
16:P:135:LEU:HD11	16:P:292:VAL:HG11	1.94	0.50
38:m:50:TYR:O	38:m:55:ARG:NH1	2.44	0.50
6:F:342:ASP:OD1	6:F:429:ARG:NH1	2.43	0.50
8:H:91:MET:O	8:H:93:HIS:N	2.45	0.50
14:N:149:LEU:HD22	14:N:194:LEU:HD12	1.93	0.50
26:a:49:GLU:O	26:a:53:ARG:NE	2.44	0.50
41:p:91:TRP:O	41:p:95:PHE:N	2.43	0.50
4:D:366:ALA:HB1	4:D:373:GLU:CG	2.42	0.50
6:F:400:GLU:OE1	6:F:413:TRP:NE1	2.45	0.50
13:M:361:MET:HB3	13:M:441:MET:HE2	1.93	0.50
31:f:47:LEU:HD13	31:f:50:ASN:O	2.11	0.50
40:o:68:CYS:O	40:o:72:SER:OG	2.13	0.50
12:L:21:ILE:O	12:L:24:SER:OG	2.20	0.50
16:P:157:ARG:NH1	16:P:163:ALA:O	2.45	0.50
27:b:27:LEU:HD13	27:b:27:LEU:O	2.12	0.50
30:e:15:ARG:NH1	33:h:129:GLU:OE1	2.45	0.50
3:C:32:ILE:HA	21:V:42:ALA:HB3	1.94	0.49
4:D:135:GLN:HB3	4:D:277:VAL:HG23	1.94	0.49
34:i:62:LYS:O	34:i:66:SER:OG	2.10	0.49
5:E:5:ALA:HB2	5:E:93:LYS:CE	2.42	0.49
8:H:312:ALA:O	8:H:314:VAL:N	2.44	0.49
10:J:58:ILE:O	10:J:62:GLY:N	2.45	0.49
13:M:24:TRP:CH2	13:M:96:ILE:HD11	2.47	0.49
37:l:53:SER:OG	37:l:56:GLU:OE1	2.30	0.49
13:M:23:THR:O	13:M:27:VAL:HG12	2.13	0.49
13:M:98:MET:HE1	45:M:505:3PE:H391	1.94	0.49
13:M:441:MET:O	13:M:444:LEU:N	2.45	0.49
6:F:294:LEU:O	6:F:294:LEU:HD23	2.13	0.49
7:G:142:ILE:HD12	7:G:148:THR:CG2	2.42	0.49
7:G:285:ARG:NH2	7:G:289:GLY:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:65:GLY:N	9:I:136:GLY:O	2.45	0.49
12:L:141:PHE:HE2	13:M:375:LEU:HD11	1.76	0.49
13:M:189:SER:O	13:M:192:ASN:N	2.46	0.49
7:G:364:LEU:HA	7:G:491:ASN:HB2	1.94	0.49
7:G:503:LEU:O	19:S:55:ARG:NH1	2.46	0.49
1:A:90:MET:HE1	10:J:153:VAL:HG12	1.94	0.49
6:F:107:ASP:HA	6:F:110:ILE:HG22	1.93	0.49
6:F:110:ILE:HG21	6:F:225:VAL:HG11	1.94	0.49
14:N:124:LEU:HD23	14:N:225:MET:HE3	1.95	0.49
39:n:116:ASP:OD1	39:n:117:TYR:N	2.44	0.49
39:n:170:VAL:HG12	39:n:171:THR:HG23	1.95	0.49
42:q:27:PHE:CD1	42:q:33:ILE:HD11	2.47	0.49
4:D:135:GLN:O	4:D:139:VAL:HG23	2.12	0.49
4:D:402:LEU:HD13	4:D:402:LEU:O	2.13	0.49
7:G:533:THR:OG1	7:G:556:MET:SD	2.57	0.49
10:J:168:GLU:OE1	10:J:171:ARG:NH1	2.45	0.49
24:Y:115:VAL:O	24:Y:119:THR:OG1	2.22	0.49
4:D:338:MET:HE2	4:D:345:LEU:HD23	1.95	0.49
4:D:389:CYS:SG	4:D:390:LYS:N	2.86	0.49
5:E:147:ALA:HB3	5:E:153:MET:CE	2.42	0.49
7:G:367:THR:HG22	7:G:636:ILE:HD13	1.94	0.49
19:S:84:ASP:OD1	19:S:85:GLU:N	2.46	0.49
25:Z:89:ASN:ND2	25:Z:126:LEU:HD21	2.28	0.49
6:F:351:ILE:HD11	6:F:415:VAL:HG22	1.94	0.49
6:F:393:TRP:O	6:F:396:SER:OG	2.24	0.49
7:G:41:CYS:O	7:G:161:ARG:NH2	2.43	0.49
9:I:110:ARG:NE	9:I:112:ASP:OD2	2.46	0.49
14:N:313:MET:O	14:N:317:GLN:NE2	2.46	0.49
1:A:57:LEU:HD11	10:J:167:ILE:HG22	1.93	0.48
7:G:460:ARG:NH2	7:G:659:ASP:OD1	2.46	0.48
9:I:83:LYS:HA	9:I:96:ILE:HD11	1.94	0.48
10:J:141:VAL:HG13	11:K:61:ILE:HD13	1.94	0.48
13:M:332:SER:O	13:M:336:ARG:NH1	2.46	0.48
14:N:236:LYS:HB3	14:N:319:LYS:HZ1	1.78	0.48
26:a:5:ILE:HG22	26:a:9:LEU:HD23	1.95	0.48
5:E:116:ILE:CD1	5:E:164:LEU:HD11	2.44	0.48
9:I:23:ALA:HB2	27:b:12:TRP:O	2.12	0.48
13:M:106:LEU:HD13	13:M:234:ILE:HD12	1.95	0.48
32:g:40:PRO:O	33:h:17:TYR:OH	2.24	0.48
6:F:188:GLU:OE1	6:F:190:THR:OG1	2.26	0.48
7:G:42:TYR:O	7:G:158:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:70:THR:OG1	10:J:74:ALA:O	2.28	0.48
11:K:50:ASN:OD1	11:K:51:SER:N	2.46	0.48
21:V:61:GLU:OE2	21:V:66:LYS:NZ	2.24	0.48
32:g:94:LEU:HD12	41:p:101:ILE:HD11	1.95	0.48
39:n:161:ASP:OD1	39:n:162:LEU:N	2.44	0.48
4:D:35:ASP:O	14:N:49:ASN:ND2	2.47	0.48
16:P:153:GLU:HG3	16:P:165:ILE:HD13	1.95	0.48
1:A:70:ALA:HB1	10:J:54:MET:HE3	1.94	0.48
4:D:347:HIS:O	4:D:351:LEU:HD23	2.13	0.48
6:F:149:LEU:O	6:F:153:ILE:N	2.43	0.48
12:L:119:LYS:O	12:L:122:THR:OG1	2.20	0.48
37:l:53:SER:N	37:l:56:GLU:OE2	2.47	0.48
5:E:82:GLU:OE2	17:Q:132:THR:HG22	2.14	0.48
31:f:34:THR:OG1	31:f:37:ARG:NH2	2.47	0.48
2:B:44:ASP:OD2	2:B:182:LYS:N	2.47	0.48
4:D:101:PRO:O	4:D:105:ARG:NH1	2.47	0.48
7:G:403:ASP:OD2	17:Q:126:LYS:NZ	2.37	0.48
12:L:50:PRO:O	12:L:54:PHE:N	2.47	0.48
13:M:145:ALA:HB2	13:M:218:LYS:HB3	1.95	0.48
20:U:85:ASP:OD1	34:i:18:ARG:NH2	2.47	0.48
39:n:22:ALA:HB3	39:n:43:MET:HE1	1.96	0.48
39:n:170:VAL:O	39:n:171:THR:OG1	2.20	0.48
40:o:45:MET:HE1	40:o:55:ARG:HD3	1.96	0.48
4:D:244:VAL:HG12	4:D:244:VAL:O	2.14	0.47
3:C:41:GLN:NE2	3:C:49:GLU:OE1	2.48	0.47
5:E:70:ALA:O	5:E:74:GLN:N	2.48	0.47
6:F:396:SER:HB2	6:F:412:ALA:HB1	1.95	0.47
12:L:574:THR:HG22	14:N:171:ASN:ND2	2.29	0.47
3:C:50:ILE:HD12	3:C:105:ILE:HD11	1.96	0.47
5:E:55:GLN:NE2	5:E:91:ASN:OD1	2.47	0.47
8:H:114:TYR:OH	10:J:60:LEU:O	2.31	0.47
20:U:11:ILE:O	20:U:15:VAL:HG23	2.15	0.47
24:Y:10:GLU:O	24:Y:11:VAL:HG13	2.14	0.47
5:E:100:ILE:HG22	5:E:156:ILE:HD13	1.93	0.47
5:E:106:THR:O	5:E:110:LEU:N	2.39	0.47
13:M:18:SER:O	13:M:93:LYS:NZ	2.43	0.47
4:D:202:ASP:OD1	4:D:203:LEU:N	2.45	0.47
5:E:86:PHE:O	7:G:177:ARG:NH2	2.45	0.47
7:G:511:VAL:HG12	7:G:511:VAL:O	2.15	0.47
8:H:141:SER:HB3	8:H:289:LEU:HD23	1.95	0.47
9:I:52:TYR:OH	9:I:140:GLU:OE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:67:HIS:NE2	9:I:118:CYS:SG	2.81	0.47
35:j:17:LEU:O	35:j:18:THR:OG1	2.30	0.47
4:D:364:TYR:CE2	4:D:366:ALA:HB2	2.50	0.47
13:M:41:LEU:HG	13:M:63:THR:HG23	1.96	0.47
14:N:321:LYS:O	29:d:49:ARG:NH2	2.44	0.47
16:P:300:LEU:O	16:P:303:LEU:N	2.47	0.47
22:W:53:GLN:O	22:W:102:ARG:NE	2.45	0.47
24:Y:3:ARG:O	24:Y:7:SER:N	2.48	0.47
12:L:432:MET:O	12:L:433:THR:OG1	2.23	0.47
15:O:302:ARG:O	15:O:304:TYR:N	2.47	0.47
16:P:322:ARG:NH2	16:P:329:SER:OG	2.48	0.47
36:k:33:PRO:O	36:k:37:VAL:HG23	2.15	0.47
2:B:82:PHE:CE2	2:B:167:LEU:HD21	2.49	0.47
8:H:249:ILE:HG23	8:H:249:ILE:O	2.15	0.47
31:f:30:ASP:OD1	33:h:89:LYS:NZ	2.37	0.47
37:l:108:VAL:O	37:l:112:VAL:N	2.44	0.47
8:H:233:LEU:O	8:H:236:ALA:N	2.48	0.47
24:Y:9:HIS:O	24:Y:11:VAL:N	2.48	0.47
7:G:142:ILE:HD12	7:G:148:THR:HG21	1.96	0.47
9:I:107:ARG:NH2	18:R:86:TYR:O	2.48	0.47
12:L:532:ILE:HG23	12:L:533:ILE:HG13	1.97	0.47
13:M:30:TYR:OH	31:f:12:HIS:ND1	2.36	0.47
40:o:77:LEU:HD12	40:o:77:LEU:O	2.14	0.47
42:q:6:VAL:O	42:q:10:GLY:N	2.47	0.47
3:C:203:TRP:O	7:G:122:MET:HE2	2.15	0.46
26:a:55:SER:OG	26:a:56:GLY:O	2.25	0.46
9:I:153:LYS:HE3	9:I:157:LEU:HD11	1.96	0.46
20:T:39:ASP:OD1	20:T:40:LEU:N	2.48	0.46
6:F:431:GLN:O	6:F:435:GLN:N	2.47	0.46
7:G:407:ALA:HB1	7:G:422:LEU:CD1	2.46	0.46
10:J:10:SER:OG	10:J:99:GLU:OE2	2.21	0.46
39:n:34:ASP:OD1	39:n:35:LYS:N	2.47	0.46
43:r:24:GLN:OE1	43:r:24:GLN:N	2.47	0.46
4:D:208:LEU:HD22	4:D:315:LEU:CD2	2.44	0.46
6:F:352:GLU:OE1	6:F:373:ASN:ND2	2.43	0.46
7:G:103:LEU:H	7:G:103:LEU:HD23	1.81	0.46
7:G:114:CYS:SG	7:G:117:GLN:N	2.83	0.46
30:e:46:ILE:HD12	30:e:46:ILE:O	2.15	0.46
9:I:81:ALA:O	9:I:106:ARG:NH2	2.49	0.46
13:M:244:ILE:O	41:p:148:TYR:OH	2.16	0.46
17:Q:19:ILE:HG22	17:Q:19:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:52:MET:HE1	22:W:39:ARG:HA	1.97	0.46
2:B:152:VAL:HG11	2:B:155:TYR:CE1	2.51	0.46
43:r:33:ARG:O	43:r:34:THR:OG1	2.28	0.46
5:E:144:CYS:O	6:F:139:ARG:NH1	2.45	0.46
13:M:428:PRO:O	13:M:429:SER:OG	2.27	0.46
22:W:92:LEU:O	22:W:96:ILE:HG22	2.16	0.46
2:B:189:ARG:NH1	52:P:501:NDP:O2X	2.49	0.46
4:D:4:TRP:O	13:M:142:ARG:NH2	2.49	0.46
13:M:161:LEU:HD21	14:N:264:TRP:CD1	2.51	0.46
20:U:11:ILE:O	20:U:15:VAL:N	2.42	0.46
35:j:32:MET:O	35:j:35:TRP:N	2.49	0.46
4:D:49:LEU:O	4:D:66:LEU:N	2.45	0.46
13:M:77:LEU:CD2	13:M:96:ILE:HD12	2.46	0.46
13:M:131:ILE:HD11	14:N:302:LEU:HD21	1.98	0.46
14:N:36:SER:O	14:N:134:GLN:NE2	2.44	0.46
1:A:78:ALA:O	1:A:81:THR:HG22	2.16	0.46
3:C:168:LEU:HD23	4:D:93:TYR:CE2	2.51	0.46
6:F:120:GLU:O	6:F:123:LEU:N	2.45	0.46
6:F:154:ARG:HH11	44:s:48:LEU:HD22	1.81	0.46
7:G:524:LEU:H	7:G:524:LEU:HD23	1.81	0.46
7:G:601:ARG:NE	7:G:613:TYR:O	2.49	0.46
9:I:108:THR:OG1	9:I:153:LYS:NZ	2.48	0.46
12:L:386:LEU:O	12:L:387:THR:OG1	2.22	0.46
13:M:346:ARG:NH2	37:l:66:SER:O	2.47	0.46
14:N:217:MET:HE3	14:N:326:PHE:HB2	1.98	0.46
7:G:361:ASN:O	7:G:492:ILE:HD13	2.16	0.45
12:L:71:MET:HG3	13:M:310:MET:HE1	1.97	0.45
13:M:232:ALA:O	13:M:237:LYS:NZ	2.45	0.45
13:M:437:MET:SD	13:M:437:MET:N	2.89	0.45
16:P:248:MET:SD	16:P:322:ARG:NH1	2.90	0.45
33:h:11:VAL:HG23	39:n:98:VAL:CG2	2.46	0.45
6:F:215:VAL:HG12	6:F:220:THR:CG2	2.46	0.45
7:G:643:GLN:O	7:G:646:SER:OG	2.25	0.45
10:J:115:ILE:HG22	10:J:117:LEU:HD12	1.97	0.45
13:M:61:LEU:HD22	13:M:244:ILE:HG21	1.97	0.45
13:M:442:ILE:O	13:M:446:LEU:HD23	2.16	0.45
15:O:31:ILE:CD1	15:O:183:ILE:HD11	2.45	0.45
54:T:201:EHZ:O2	54:T:201:EHZ:O1	2.31	0.45
27:b:23:SER:O	27:b:27:LEU:N	2.48	0.45
13:M:24:TRP:CZ3	13:M:96:ILE:HD11	2.51	0.45
14:N:270:LEU:HD12	14:N:275:CYS:SG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:105:VAL:O	30:e:74:ARG:NH2	2.49	0.45
33:h:36:VAL:O	33:h:39:GLY:N	2.49	0.45
40:o:62:LEU:HD12	40:o:86:TRP:CE2	2.51	0.45
6:F:21:ILE:HD11	6:F:233:THR:CG2	2.46	0.45
7:G:395:ILE:O	7:G:399:TRP:N	2.50	0.45
12:L:562:ILE:HB	12:L:563:PRO:HD3	1.98	0.45
13:M:145:ALA:HB3	13:M:222:GLU:OE1	2.16	0.45
14:N:55:ALA:O	14:N:59:TYR:N	2.49	0.45
14:N:175:MET:HE2	14:N:178:ILE:HD12	1.98	0.45
25:Z:8:ASP:OD1	25:Z:8:ASP:N	2.49	0.45
7:G:515:ARG:NH1	7:G:536:ASP:OD2	2.49	0.45
19:S:56:GLU:N	19:S:56:GLU:OE1	2.50	0.45
37:l:137:LEU:O	37:l:139:LEU:N	2.49	0.45
39:n:22:ALA:CB	39:n:43:MET:HE1	2.46	0.45
7:G:104:ASP:O	7:G:108:CYS:N	2.48	0.45
13:M:265:SER:O	13:M:269:MET:N	2.44	0.45
4:D:203:LEU:HD23	4:D:207:LEU:HD12	1.99	0.45
5:E:147:ALA:HB2	6:F:108:ARG:HD3	1.97	0.45
7:G:328:LEU:O	7:G:507:TYR:OH	2.28	0.45
13:M:77:LEU:HD21	13:M:96:ILE:HG23	1.98	0.45
33:h:107:GLU:OE2	33:h:111:ARG:NH2	2.49	0.45
1:A:111:LEU:HD12	1:A:111:LEU:O	2.16	0.45
15:O:7:ALA:O	15:O:11:GLY:N	2.49	0.45
16:P:19:VAL:HG12	16:P:19:VAL:O	2.17	0.45
25:Z:60:LEU:O	25:Z:64:LEU:N	2.47	0.45
6:F:21:ILE:HD11	6:F:233:THR:OG1	2.16	0.45
15:O:70:ASP:OD1	15:O:71:ILE:N	2.50	0.45
7:G:51:ASN:ND2	7:G:157:THR:OG1	2.50	0.45
13:M:77:LEU:HD22	13:M:96:ILE:HD12	1.98	0.45
38:m:123:LYS:O	38:m:125:ASN:N	2.50	0.45
1:A:79:ILE:HG22	8:H:314:VAL:HG23	2.00	0.44
2:B:167:LEU:HD13	2:B:167:LEU:O	2.16	0.44
4:D:325:VAL:O	4:D:331:SER:OG	2.33	0.44
13:M:119:TYR:CE2	13:M:161:LEU:HD23	2.52	0.44
28:c:46:ASN:OD1	28:c:47:GLY:N	2.50	0.44
36:k:48:ASP:OD1	39:n:37:ARG:NE	2.50	0.44
4:D:342:MET:HE1	7:G:102:PRO:C	2.42	0.44
12:L:96:VAL:O	12:L:99:SER:N	2.49	0.44
4:D:220:LEU:HD22	4:D:221:ARG:HH22	1.82	0.44
5:E:31:ILE:HD12	5:E:50:VAL:HG13	2.00	0.44
6:F:94:VAL:HG12	6:F:192:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:122:ASP:HA	25:Z:132:MET:HE2	1.99	0.44
14:N:56:ALA:O	14:N:60:PHE:N	2.50	0.44
14:N:62:THR:HG21	14:N:114:TRP:CG	2.51	0.44
14:N:81:LEU:HD12	14:N:81:LEU:O	2.17	0.44
16:P:330:GLU:O	16:P:333:GLU:N	2.43	0.44
7:G:59:ILE:CG2	7:G:62:ALA:HB3	2.48	0.44
12:L:378:LEU:HD11	12:L:383:MET:HE3	1.98	0.44
12:L:556:ILE:HD11	38:m:79:PHE:HB2	1.97	0.44
13:M:237:LYS:O	13:M:240:SER:OG	2.35	0.44
14:N:225:MET:SD	14:N:225:MET:N	2.90	0.44
4:D:361:GLY:N	4:D:380:SER:OG	2.51	0.44
14:N:5:THR:HG22	14:N:9:ILE:HD12	1.99	0.44
22:W:98:VAL:HG12	22:W:98:VAL:O	2.17	0.44
5:E:66:MET:O	5:E:80:VAL:HG11	2.17	0.44
13:M:160:LEU:HD23	13:M:199:CYS:HA	1.99	0.44
13:M:399:ASN:O	13:M:403:THR:N	2.46	0.44
14:N:214:PRO:O	14:N:218:ALA:N	2.51	0.44
16:P:196:LEU:HD13	16:P:196:LEU:O	2.17	0.44
39:n:100:GLU:OE2	39:n:121:ARG:NH1	2.50	0.44
3:C:39:GLN:N	43:r:69:MET:O	2.46	0.44
4:D:220:LEU:HD22	4:D:221:ARG:NH2	2.33	0.44
4:D:221:ARG:NH1	43:r:22:LYS:O	2.48	0.44
7:G:220:TRP:NE1	9:I:87:ALA:HB2	2.33	0.44
8:H:186:PHE:O	8:H:189:THR:OG1	2.30	0.44
10:J:135:LEU:HD13	10:J:135:LEU:O	2.18	0.44
25:Z:126:LEU:HD22	30:e:75:MET:HE1	1.99	0.44
35:j:18:THR:O	35:j:20:SER:N	2.42	0.44
39:n:167:TRP:O	39:n:171:THR:OG1	2.34	0.44
4:D:161:ILE:HG22	8:H:278:PRO:CB	2.48	0.44
4:D:161:ILE:HG22	8:H:278:PRO:HB2	1.99	0.44
7:G:27:LEU:HD23	7:G:39:ARG:HH21	1.82	0.44
7:G:258:ILE:HD12	7:G:259:ASN:N	2.32	0.44
12:L:316:THR:CG2	12:L:395:ILE:HD12	2.46	0.44
20:U:52:MET:SD	39:n:23:LEU:HD12	2.58	0.44
6:F:21:ILE:HD11	6:F:233:THR:HG23	1.99	0.44
7:G:118:ASP:O	7:G:122:MET:N	2.51	0.44
7:G:544:VAL:HG12	7:G:559:VAL:HG12	2.00	0.44
7:G:570:SER:O	7:G:620:ARG:NH2	2.51	0.44
8:H:311:THR:CG2	25:Z:50:MET:HE2	2.48	0.44
49:H:404:PC1:H141	9:I:21:ASP:OD1	2.18	0.44
12:L:412:THR:O	12:L:416:THR:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:113:ILE:HG22	16:P:117:ILE:HD12	1.99	0.44
20:U:45:LEU:HD23	39:n:16:LEU:HD13	1.99	0.44
37:l:93:THR:HG21	37:l:100:MET:HE1	2.00	0.44
4:D:144:ILE:HG22	4:D:148:LEU:CD2	2.48	0.43
4:D:152:MET:O	4:D:156:THR:OG1	2.23	0.43
4:D:367:ILE:O	4:D:374:PHE:N	2.50	0.43
6:F:67:GLY:N	6:F:73:PHE:O	2.51	0.43
7:G:201:ASP:OD2	7:G:268:ARG:NH2	2.50	0.43
7:G:523:PHE:HB3	7:G:544:VAL:HG22	1.99	0.43
15:O:302:ARG:O	15:O:309:ASN:ND2	2.47	0.43
41:p:104:ILE:O	41:p:108:ARG:N	2.47	0.43
4:D:46:ASN:O	4:D:68:LEU:N	2.51	0.43
12:L:598:ILE:HG13	14:N:100:MET:HE1	2.01	0.43
13:M:229:MET:HE2	13:M:328:CYS:SG	2.58	0.43
44:s:66:SER:OG	44:s:68:ARG:NH2	2.51	0.43
4:D:105:ARG:NH2	9:I:119:ILE:HG23	2.33	0.43
4:D:268:ASP:OD2	4:D:270:ARG:NH2	2.52	0.43
5:E:151:ALA:HB3	5:E:152:PRO:CD	2.48	0.43
6:F:114:ASP:OD1	6:F:114:ASP:N	2.51	0.43
7:G:281:GLU:OE2	16:P:1:LEU:N	2.48	0.43
14:N:221:LEU:HD11	14:N:237:THR:HG21	2.00	0.43
27:b:36:PRO:O	27:b:39:LYS:NZ	2.51	0.43
37:l:50:PRO:O	37:l:52:ARG:N	2.50	0.43
2:B:82:PHE:HE2	2:B:167:LEU:HD11	1.82	0.43
4:D:157:HIS:O	4:D:161:ILE:HD12	2.19	0.43
8:H:139:THR:HG21	10:J:64:LEU:HD13	2.00	0.43
9:I:24:ALA:HB1	25:Z:34:MET:SD	2.59	0.43
14:N:247:MET:HE1	14:N:330:ALA:HA	2.00	0.43
5:E:24:THR:OG1	5:E:27:ASN:ND2	2.51	0.43
6:F:302:SER:HB2	6:F:350:LEU:HD12	2.01	0.43
13:M:370:PRO:HA	13:M:375:LEU:HD13	2.01	0.43
25:Z:119:LEU:HD13	30:e:68:ARG:NH2	2.34	0.43
12:L:378:LEU:HD11	12:L:383:MET:CE	2.48	0.43
17:Q:39:VAL:HG21	17:Q:108:LYS:HD3	1.99	0.43
20:T:64:ASP:OD1	20:T:65:ILE:N	2.51	0.43
26:a:49:GLU:OE1	26:a:52:ARG:NE	2.44	0.43
6:F:216:PHE:HA	17:Q:129:ARG:HH22	1.83	0.43
7:G:588:THR:HG21	17:Q:63:GLU:HA	2.01	0.43
10:J:129:ASP:O	10:J:131:VAL:N	2.52	0.43
4:D:172:GLU:OE2	4:D:176:LYS:NZ	2.51	0.43
8:H:260:MET:HE2	26:a:17:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:106:LEU:O	13:M:109:THR:OG1	2.29	0.43
32:g:95:VAL:O	32:g:99:GLU:N	2.52	0.43
4:D:154:VAL:HG13	4:D:297:TYR:HE1	1.83	0.43
8:H:311:THR:HG23	25:Z:50:MET:HE2	2.00	0.43
9:I:20:THR:O	9:I:24:ALA:N	2.51	0.43
9:I:94:ILE:HG22	9:I:96:ILE:HG23	2.01	0.43
11:K:13:SER:O	11:K:17:LEU:N	2.42	0.43
32:g:94:LEU:HD13	32:g:94:LEU:O	2.18	0.43
2:B:58:MET:HE2	4:D:54:GLN:CD	2.44	0.43
3:C:171:TYR:C	3:C:188:VAL:HG23	2.43	0.43
6:F:48:ILE:HD11	6:F:236:ARG:HB3	2.00	0.43
12:L:53:MET:HE1	41:p:29:ILE:CG2	2.49	0.43
27:b:62:MET:O	27:b:64:ASP:N	2.49	0.43
35:j:59:TRP:O	40:o:106:ARG:NH2	2.43	0.43
44:s:57:LEU:H	44:s:57:LEU:HD23	1.83	0.43
7:G:583:THR:O	7:G:583:THR:OG1	2.34	0.42
8:H:207:LEU:O	8:H:210:GLY:N	2.52	0.42
10:J:81:THR:OG1	10:J:82:TRP:N	2.51	0.42
11:K:37:VAL:HG11	11:K:67:ALA:HB2	2.00	0.42
12:L:254:VAL:HG13	12:L:329:ILE:CG1	2.49	0.42
13:M:76:MET:HE1	13:M:230:ILE:HG13	2.01	0.42
13:M:106:LEU:CD2	13:M:125:THR:HG21	2.49	0.42
20:T:48:VAL:CG1	20:T:52:MET:HE3	2.49	0.42
42:q:92:CYS:O	43:r:33:ARG:NE	2.51	0.42
4:D:58:ALA:O	4:D:60:GLY:N	2.52	0.42
5:E:128:VAL:HG23	5:E:129:GLY:N	2.34	0.42
6:F:110:ILE:HG21	6:F:225:VAL:CG1	2.49	0.42
7:G:522:LEU:HD13	7:G:523:PHE:N	2.34	0.42
12:L:278:LEU:CD1	12:L:315:VAL:HG13	2.49	0.42
12:L:383:MET:O	12:L:385:PHE:N	2.52	0.42
13:M:41:LEU:H	13:M:41:LEU:HD23	1.84	0.42
15:O:199:LEU:O	15:O:202:ILE:HG22	2.19	0.42
4:D:126:LEU:HD11	4:D:356:TYR:CE2	2.54	0.42
7:G:399:TRP:HE3	7:G:400:LEU:HD12	1.84	0.42
14:N:17:PRO:O	14:N:20:THR:N	2.52	0.42
14:N:146:TYR:HB3	14:N:147:PRO:HD3	2.01	0.42
15:O:28:ASP:OD1	15:O:29:GLY:N	2.49	0.42
18:R:4:VAL:HG12	18:R:5:SER:O	2.19	0.42
4:D:72:MET:HE2	4:D:74:ARG:HE	1.84	0.42
4:D:257:GLY:HA3	4:D:372:GLY:HA3	2.00	0.42
5:E:131:THR:HG22	5:E:138:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:523:PHE:CB	7:G:544:VAL:HG22	2.49	0.42
12:L:481:THR:HG23	40:o:91:HIS:HE1	1.84	0.42
29:d:109:TYR:HB2	41:p:73:ILE:HG22	2.01	0.42
42:q:27:PHE:O	42:q:31:ASN:N	2.46	0.42
8:H:131:GLY:O	8:H:201:THR:HG23	2.20	0.42
12:L:138:PHE:HD2	50:L:703:CDL:H272	1.85	0.42
13:M:25:THR:O	13:M:29:SER:OG	2.22	0.42
20:U:21:LEU:HD12	36:k:52:ARG:O	2.20	0.42
42:q:138:VAL:HG23	42:q:138:VAL:O	2.20	0.42
3:C:178:ASP:O	3:C:181:LYS:NZ	2.49	0.42
6:F:97:ALA:CB	6:F:111:MET:HE3	2.48	0.42
6:F:371:TRP:CH2	6:F:395:ILE:HD13	2.55	0.42
7:G:574:VAL:HG12	7:G:575:ASN:O	2.20	0.42
8:H:153:VAL:HG11	8:H:241:ILE:CG2	2.49	0.42
13:M:173:THR:HB	33:h:101:ALA:HB2	2.01	0.42
13:M:303:ILE:CG2	13:M:305:THR:HG23	2.50	0.42
13:M:373:ILE:HD11	13:M:444:LEU:HD23	2.02	0.42
3:C:179:GLU:O	16:P:174:ARG:NH2	2.52	0.42
5:E:124:LEU:HD21	5:E:173:ILE:HD13	2.02	0.42
6:F:288:THR:HG23	6:F:288:THR:O	2.19	0.42
7:G:350:PRO:HG2	7:G:467:LEU:HD12	2.02	0.42
12:L:67:HIS:CE1	12:L:70:THR:HG23	2.55	0.42
45:H:403:3PE:H2A1	9:I:29:TRP:HH2	1.85	0.42
9:I:70:ARG:HD2	9:I:134:VAL:HG11	2.01	0.42
26:a:14:VAL:HG12	26:a:14:VAL:O	2.20	0.42
4:D:61:VAL:HG13	4:D:82:LEU:HB2	2.02	0.42
12:L:56:HIS:HD1	12:L:57:ASN:CG	2.27	0.42
25:Z:113:THR:HG22	25:Z:113:THR:O	2.20	0.42
7:G:367:THR:OG1	7:G:370:GLY:N	2.52	0.41
16:P:1:LEU:H1	16:P:1:LEU:HD22	1.85	0.41
7:G:524:LEU:HD12	7:G:527:ALA:HB3	2.01	0.41
12:L:282:ALA:HB1	12:L:411:ILE:HD11	2.01	0.41
16:P:180:ASN:OD1	16:P:321:HIS:NE2	2.34	0.41
2:B:167:LEU:HD12	9:I:52:TYR:CD2	2.55	0.41
4:D:211:ILE:O	4:D:215:SER:N	2.53	0.41
4:D:393:ALA:HB2	4:D:427:GLU:O	2.21	0.41
8:H:156:MET:HE1	8:H:174:LEU:HD22	2.02	0.41
9:I:153:LYS:CE	9:I:157:LEU:HD11	2.51	0.41
10:J:63:MET:HE1	11:K:31:LEU:HD22	2.02	0.41
12:L:69:VAL:HG13	12:L:71:MET:HE2	2.03	0.41
12:L:74:MET:HE3	12:L:194:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:520:SER:C	12:L:524:THR:HG1	2.26	0.41
12:L:535:ARG:NH1	37:l:89:ASP:OD2	2.53	0.41
12:L:546:LEU:HD22	38:m:71:ARG:NH2	2.35	0.41
15:O:236:GLU:CD	21:V:25:ILE:HD12	2.46	0.41
3:C:100:ARG:O	43:r:100:MET:N	2.47	0.41
5:E:187:ARG:O	5:E:188:SER:OG	2.28	0.41
11:K:63:ILE:CD1	14:N:71:LEU:HD11	2.50	0.41
37:l:51:ASN:OD1	37:l:77:HIS:NE2	2.52	0.41
12:L:149:ILE:O	12:L:152:PHE:N	2.53	0.41
12:L:424:MET:HA	12:L:427:ILE:HG22	2.03	0.41
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.55	0.41
14:N:213:ALA:HB3	14:N:214:PRO:HD3	2.01	0.41
8:H:231:ILE:O	8:H:235:ASN:ND2	2.53	0.41
50:L:703:CDL:OB3	41:p:48:ARG:NH2	2.54	0.41
14:N:344:ILE:O	29:d:83:TYR:OH	2.35	0.41
16:P:40:ARG:NH2	22:W:112:THR:O	2.54	0.41
20:U:57:GLU:OE2	35:j:11:TYR:OH	2.37	0.41
38:m:16:THR:HG21	39:n:67:GLU:HG2	2.02	0.41
7:G:197:GLY:N	7:G:265:ASP:OD1	2.50	0.41
7:G:341:ASP:O	7:G:508:LYS:NZ	2.48	0.41
15:O:24:VAL:HG13	15:O:24:VAL:O	2.20	0.41
4:D:34:ASN:HB2	15:O:158:LEU:HD22	2.02	0.41
12:L:72:ASN:C	12:L:73:SER:HG	2.22	0.41
12:L:180:ILE:HD12	13:M:397:GLY:HA2	2.03	0.41
12:L:553:LEU:HD22	13:M:210:TYR:CZ	2.56	0.41
13:M:65:LEU:HD22	13:M:317:ILE:HD11	2.02	0.41
38:m:51:ASN:O	39:n:128:ARG:NH2	2.54	0.41
3:C:40:VAL:O	43:r:68:ILE:N	2.45	0.41
6:F:400:GLU:OE2	6:F:412:ALA:HB3	2.21	0.41
7:G:103:LEU:HD21	18:R:70:LYS:O	2.21	0.41
7:G:325:ALA:HB2	7:G:501:ALA:HB1	2.02	0.41
8:H:81:LEU:O	8:H:84:SER:N	2.53	0.41
8:H:260:MET:HE3	26:a:13:GLY:O	2.21	0.41
9:I:25:ARG:HA	9:I:30:THR:HG22	2.03	0.41
12:L:67:HIS:HE1	12:L:70:THR:HG23	1.85	0.41
12:L:101:MET:HE1	12:L:121:LEU:HB2	2.02	0.41
13:M:131:ILE:CD1	14:N:302:LEU:HD21	2.50	0.41
14:N:232:LEU:HD12	14:N:232:LEU:O	2.21	0.41
25:Z:92:GLU:OE2	30:e:91:TYR:OH	2.27	0.41
33:h:90:THR:HG21	41:p:85:TYR:CZ	2.56	0.41
5:E:190:ARG:NH2	6:F:265:PRO:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:531:CYS:CB	7:G:532:ILE:HD12	2.51	0.41
10:J:126:TYR:HB3	30:e:31:ARG:HE	1.86	0.41
19:S:41:VAL:HG12	19:S:45:LYS:CE	2.50	0.41
40:o:92:LEU:O	40:o:96:LYS:N	2.49	0.41
29:d:58:LEU:N	29:d:61:GLN:OE1	2.44	0.40
3:C:150:ARG:NH2	3:C:157:PHE:O	2.54	0.40
5:E:16:ASN:OD1	5:E:19:THR:HG23	2.21	0.40
15:O:53:GLU:OE2	15:O:104:ARG:NH1	2.53	0.40
43:r:72:GLN:OE1	43:r:72:GLN:N	2.53	0.40
7:G:53:ARG:O	7:G:93:VAL:HG21	2.21	0.40
7:G:329:VAL:HG21	7:G:623:LEU:HD21	2.02	0.40
8:H:70:LEU:HA	8:H:73:ILE:HG22	2.03	0.40
8:H:260:MET:CE	26:a:17:VAL:HG23	2.52	0.40
12:L:159:TYR:O	13:M:417:GLY:N	2.53	0.40
20:T:65:ILE:HG23	20:T:65:ILE:O	2.21	0.40
41:p:47:VAL:O	41:p:50:PHE:N	2.54	0.40
3:C:32:ILE:HG23	3:C:33:LEU:HB2	2.03	0.40
4:D:103:PHE:HA	4:D:106:LEU:HD23	2.04	0.40
4:D:220:LEU:HD23	4:D:224:GLU:HG3	2.03	0.40
4:D:343:GLU:HG2	7:G:98:LEU:HD13	2.04	0.40
5:E:5:ALA:HB2	5:E:93:LYS:HE3	2.04	0.40
5:E:52:ASP:O	5:E:55:GLN:N	2.55	0.40
7:G:60:GLU:O	7:G:61:LYS:HG2	2.20	0.40
7:G:160:ILE:HG22	7:G:172:LEU:O	2.21	0.40
7:G:656:VAL:O	7:G:656:VAL:HG23	2.21	0.40
12:L:52:LEU:HD23	41:p:29:ILE:HD11	2.03	0.40
13:M:424:ILE:HD12	38:m:55:ARG:HE	1.85	0.40
14:N:243:MET:HG2	29:d:44:MET:HE2	2.03	0.40
15:O:117:SER:O	15:O:118:THR:OG1	2.30	0.40
3:C:81:VAL:N	3:C:91:GLU:O	2.49	0.40
3:C:114:LEU:O	3:C:115:THR:HG23	2.22	0.40
6:F:280:ILE:HG22	6:F:280:ILE:O	2.22	0.40
7:G:323:VAL:HG11	7:G:328:LEU:HD21	2.04	0.40
14:N:12:THR:OG1	14:N:39:ALA:HB2	2.21	0.40
20:T:51:ILE:HG21	20:T:62:ILE:HD11	2.02	0.40
33:h:90:THR:HG22	33:h:94:LEU:HD23	2.02	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	A	113/115 (98%)	90 (80%)	22 (20%)	1 (1%)	14	43
2	B	153/224 (68%)	134 (88%)	19 (12%)	0	100	100
3	C	204/263 (78%)	172 (84%)	30 (15%)	2 (1%)	12	40
4	D	427/463 (92%)	372 (87%)	55 (13%)	0	100	100
5	E	210/248 (85%)	169 (80%)	40 (19%)	1 (0%)	24	55
6	F	426/428 (100%)	360 (84%)	66 (16%)	0	100	100
7	G	686/727 (94%)	593 (86%)	90 (13%)	3 (0%)	30	60
8	H	316/318 (99%)	272 (86%)	44 (14%)	0	100	100
9	I	176/212 (83%)	145 (82%)	31 (18%)	0	100	100
10	J	169/172 (98%)	148 (88%)	20 (12%)	1 (1%)	21	52
11	K	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
12	L	604/607 (100%)	508 (84%)	96 (16%)	0	100	100
13	M	457/459 (100%)	413 (90%)	43 (9%)	1 (0%)	43	71
14	N	342/345 (99%)	309 (90%)	31 (9%)	2 (1%)	21	52
15	O	318/355 (90%)	273 (86%)	44 (14%)	1 (0%)	36	65
16	P	340/377 (90%)	280 (82%)	59 (17%)	1 (0%)	36	65
17	Q	123/175 (70%)	109 (89%)	13 (11%)	1 (1%)	16	45
18	R	93/116 (80%)	80 (86%)	13 (14%)	0	100	100
19	S	81/99 (82%)	69 (85%)	12 (15%)	0	100	100
20	T	73/156 (47%)	66 (90%)	7 (10%)	0	100	100
20	U	86/156 (55%)	69 (80%)	17 (20%)	0	100	100
21	V	110/116 (95%)	92 (84%)	18 (16%)	0	100	100
22	W	112/131 (86%)	101 (90%)	11 (10%)	0	100	100
23	X	169/172 (98%)	140 (83%)	27 (16%)	2 (1%)	10	37
24	Y	138/143 (96%)	120 (87%)	16 (12%)	2 (1%)	9	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Z	137/144 (95%)	114 (83%)	22 (16%)	1 (1%)	18	49
26	a	65/67 (97%)	55 (85%)	9 (14%)	1 (2%)	8	32
27	b	81/84 (96%)	63 (78%)	18 (22%)	0	100	100
28	c	45/76 (59%)	42 (93%)	3 (7%)	0	100	100
29	d	117/120 (98%)	98 (84%)	19 (16%)	0	100	100
30	e	102/106 (96%)	84 (82%)	17 (17%)	1 (1%)	12	40
31	f	49/57 (86%)	37 (76%)	11 (22%)	1 (2%)	6	27
32	g	99/151 (66%)	76 (77%)	22 (22%)	1 (1%)	12	40
33	h	135/189 (71%)	113 (84%)	21 (16%)	1 (1%)	18	49
34	i	97/128 (76%)	76 (78%)	19 (20%)	2 (2%)	5	26
35	j	58/105 (55%)	41 (71%)	16 (28%)	1 (2%)	7	30
36	k	70/104 (67%)	54 (77%)	16 (23%)	0	100	100
37	l	150/186 (81%)	112 (75%)	35 (23%)	3 (2%)	6	27
38	m	122/129 (95%)	102 (84%)	20 (16%)	0	100	100
39	n	174/179 (97%)	149 (86%)	25 (14%)	0	100	100
40	o	103/137 (75%)	85 (82%)	18 (18%)	0	100	100
41	p	168/176 (96%)	142 (84%)	26 (16%)	0	100	100
42	q	142/145 (98%)	108 (76%)	32 (22%)	2 (1%)	9	33
43	r	95/113 (84%)	77 (81%)	18 (19%)	0	100	100
44	s	38/104 (36%)	32 (84%)	6 (16%)	0	100	100
All	All	8069/9175 (88%)	6833 (85%)	1204 (15%)	32 (0%)	31	60

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	g	107	GLU
35	j	13	GLU
37	l	61	TYR
7	G	259	ASN
15	O	303	LYS
24	Y	10	GLU
26	a	62	VAL
37	l	60	TRP
34	i	2	GLY
37	l	138	TYR

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Mol	Chain	Res	Type
7	G	359	ARG
14	N	2	ASN
16	P	331	ILE
23	X	168	PHE
30	e	88	GLU
31	f	48	ARG
33	h	13	PRO
42	q	69	ASN
42	q	81	MET
3	C	204	GLU
13	M	224	PRO
24	Y	12	PRO
25	Z	8	ASP
1	A	25	PRO
5	E	127	LYS
14	N	109	ALA
34	i	115	VAL
7	G	381	GLY
3	C	202	PRO
17	Q	26	PRO
23	X	135	PRO
10	J	128	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	103/103 (100%)	103 (100%)	0	100	100
2	B	131/185 (71%)	130 (99%)	1 (1%)	73	79
3	C	188/227 (83%)	188 (100%)	0	100	100
4	D	367/394 (93%)	367 (100%)	0	100	100
5	E	183/206 (89%)	183 (100%)	0	100	100
6	F	343/343 (100%)	343 (100%)	0	100	100
7	G	580/610 (95%)	580 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	279/279 (100%)	279 (100%)	0	100	100
9	I	145/178 (82%)	145 (100%)	0	100	100
10	J	136/137 (99%)	136 (100%)	0	100	100
11	K	87/87 (100%)	87 (100%)	0	100	100
12	L	548/549 (100%)	548 (100%)	0	100	100
13	M	414/414 (100%)	413 (100%)	1 (0%)	87	88
14	N	306/307 (100%)	306 (100%)	0	100	100
15	O	284/309 (92%)	284 (100%)	0	100	100
16	P	299/325 (92%)	298 (100%)	1 (0%)	86	86
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	80/96 (83%)	80 (100%)	0	100	100
19	S	74/80 (92%)	74 (100%)	0	100	100
20	T	69/135 (51%)	69 (100%)	0	100	100
20	U	81/135 (60%)	81 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	153/154 (99%)	153 (100%)	0	100	100
24	Y	105/107 (98%)	105 (100%)	0	100	100
25	Z	120/123 (98%)	120 (100%)	0	100	100
26	a	57/57 (100%)	57 (100%)	0	100	100
27	b	72/73 (99%)	72 (100%)	0	100	100
28	c	41/67 (61%)	41 (100%)	0	100	100
29	d	106/107 (99%)	106 (100%)	0	100	100
30	e	92/94 (98%)	92 (100%)	0	100	100
31	f	47/53 (89%)	46 (98%)	1 (2%)	47	67
32	g	92/129 (71%)	92 (100%)	0	100	100
33	h	122/162 (75%)	122 (100%)	0	100	100
34	i	87/119 (73%)	87 (100%)	0	100	100
35	j	56/87 (64%)	56 (100%)	0	100	100
36	k	55/78 (70%)	55 (100%)	0	100	100
37	l	137/161 (85%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	m	110/114 (96%)	110 (100%)	0	100	100
39	n	161/164 (98%)	161 (100%)	0	100	100
40	o	98/121 (81%)	98 (100%)	0	100	100
41	p	155/158 (98%)	155 (100%)	0	100	100
42	q	129/130 (99%)	129 (100%)	0	100	100
43	r	88/96 (92%)	88 (100%)	0	100	100
44	s	39/95 (41%)	39 (100%)	0	100	100
All	All	7139/7917 (90%)	7135 (100%)	4 (0%)	87	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	64	CYS
13	M	434	LEU
16	P	135	LEU
31	f	50	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
2	B	92	GLN
3	C	160	HIS
4	D	54	GLN
4	D	79	HIS
4	D	232	ASN
4	D	237	ASN
4	D	409	HIS
5	E	27	ASN
6	F	263	ASN
7	G	255	HIS
7	G	259	ASN
7	G	546	GLN
8	H	235	ASN
8	H	304	HIS
9	I	172	GLN
11	K	25	HIS
11	K	92	ASN

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Mol	Chain	Res	Type
12	L	25	ASN
12	L	67	HIS
12	L	135	ASN
12	L	194	ASN
12	L	320	ASN
12	L	332	HIS
12	L	444	ASN
13	M	51	ASN
13	M	138	ASN
13	M	338	HIS
14	N	2	ASN
14	N	63	GLN
14	N	91	ASN
14	N	144	GLN
14	N	204	ASN
14	N	235	ASN
14	N	342	GLN
16	P	3	HIS
16	P	37	HIS
16	P	86	GLN
16	P	134	HIS
16	P	136	ASN
17	Q	29	HIS
17	Q	125	ASN
21	V	109	ASN
22	W	50	HIS
23	X	123	GLN
24	Y	18	HIS
24	Y	105	HIS
25	Z	53	ASN
25	Z	75	GLN
25	Z	111	HIS
27	b	45	ASN
29	d	117	HIS
30	e	97	HIS
31	f	50	ASN
32	g	34	ASN
33	h	95	GLN
33	h	124	GLN
34	i	12	GLN
36	k	38	GLN
37	l	103	HIS

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Mol	Chain	Res	Type
38	m	74	ASN
39	n	61	GLN
41	p	54	GLN
42	q	72	ASN
42	q	113	HIS
42	q	135	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
14	FME	N	1	14	8,9,10	0.98	0	8,9,11	1.28	1 (12%)
27	AYA	b	1	27	6,7,8	1.25	1 (16%)	6,8,10	1.05	1 (16%)
43	AYA	r	1	43	6,7,8	1.22	1 (16%)	6,8,10	1.13	1 (16%)
34	SAC	i	1	34	7,8,9	1.04	0	7,9,11	1.09	0
4	2MR	D	85	4	10,12,13	2.60	3 (30%)	5,13,15	1.69	1 (20%)
1	FME	A	1	1	8,9,10	1.01	1 (12%)	8,9,11	1.01	0
12	FME	L	1	12	8,9,10	0.98	0	8,9,11	0.73	0
42	AME	q	1	42	9,10,11	1.79	2 (22%)	9,11,13	1.83	4 (44%)
13	FME	M	1	13	8,9,10	1.01	0	8,9,11	0.79	0
11	FME	K	1	11	8,9,10	1.08	1 (12%)	8,9,11	1.20	1 (12%)
8	FME	H	1	8	8,9,10	0.97	0	8,9,11	1.21	1 (12%)
10	FME	J	1	10	8,9,10	0.95	0	8,9,11	0.86	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	N	1	14	-	3/7/9/11	-
27	AYA	b	1	27	-	1/5/6/8	-
43	AYA	r	1	43	-	1/5/6/8	-
34	SAC	i	1	34	-	2/7/8/10	-
4	2MR	D	85	4	-	4/10/13/15	-
1	FME	A	1	1	-	3/7/9/11	-
12	FME	L	1	12	-	3/7/9/11	-
42	AME	q	1	42	-	4/9/10/12	-
13	FME	M	1	13	-	1/7/9/11	-
11	FME	K	1	11	-	4/7/9/11	-
8	FME	H	1	8	-	4/7/9/11	-
10	FME	J	1	10	-	2/7/9/11	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NE	5.62	1.46	1.34
4	D	85	2MR	CZ-NH2	5.20	1.44	1.33
42	q	1	AME	CT1-N	4.15	1.47	1.34
43	r	1	AYA	CA-N	-2.36	1.44	1.46
27	b	1	AYA	CA-N	-2.23	1.44	1.46
11	K	1	FME	CA-N	-2.11	1.43	1.46
42	q	1	AME	OT-CT1	-2.06	1.18	1.23
1	A	1	FME	CA-N	-2.03	1.43	1.46
4	D	85	2MR	CQ1-NH1	-2.01	1.42	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	85	2MR	CD-NE-CZ	3.52	129.97	123.36
42	q	1	AME	CT2-CT1-N	3.13	121.31	116.12
8	H	1	FME	C-CA-N	2.96	115.21	109.50
14	N	1	FME	C-CA-N	2.64	114.60	109.50
43	r	1	AYA	CB-CA-N	2.41	112.40	109.68
42	q	1	AME	O-C-CA	-2.37	118.68	124.77
42	q	1	AME	CE-SD-CG	2.32	112.33	100.32
11	K	1	FME	CG-CB-CA	2.18	119.54	112.87
27	b	1	AYA	CB-CA-N	2.15	112.11	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	q	1	AME	C-CA-N	2.06	113.48	109.50

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	1	FME	N-CA-CB-CG
8	H	1	FME	O-C-CA-CB
11	K	1	FME	O1-CN-N-CA
13	M	1	FME	CB-CA-N-CN
14	N	1	FME	N-CA-CB-CG
14	N	1	FME	C-CA-CB-CG
34	i	1	SAC	C-CA-CB-OG
43	r	1	AYA	O-C-CA-CB
4	D	85	2MR	NE-CD-CG-CB
1	A	1	FME	CA-CB-CG-SD
42	q	1	AME	CT2-CT1-N-CA
42	q	1	AME	OT-CT1-N-CA
42	q	1	AME	CA-CB-CG-SD
4	D	85	2MR	CA-CB-CG-CD
34	i	1	SAC	N-CA-CB-OG
42	q	1	AME	CB-CG-SD-CE
1	A	1	FME	CB-CG-SD-CE
10	J	1	FME	CB-CG-SD-CE
27	b	1	AYA	C-CA-N-CT
14	N	1	FME	CB-CG-SD-CE
1	A	1	FME	N-CA-CB-CG
4	D	85	2MR	N-CA-CB-CG
8	H	1	FME	CB-CG-SD-CE
11	K	1	FME	CA-CB-CG-SD
12	L	1	FME	CB-CG-SD-CE
8	H	1	FME	CB-CA-N-CN
12	L	1	FME	CB-CA-N-CN
4	D	85	2MR	C-CA-CB-CG
12	L	1	FME	N-CA-CB-CG
10	J	1	FME	CA-CB-CG-SD
11	K	1	FME	N-CA-CB-CG
11	K	1	FME	CB-CG-SD-CE

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	i	1	SAC	1	0
42	q	1	AME	1	0
11	K	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 1 is monoatomic - leaving 33 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	3PE	H	403	-	50,50,50	0.88	3 (6%)	53,55,55	1.11	2 (3%)
49	PC1	H	406	-	34,34,53	1.19	4 (11%)	40,42,61	1.10	2 (5%)
50	CDL	M	507	-	66,66,99	1.06	8 (12%)	72,78,111	1.24	5 (6%)
46	SF4	I	202	9	0,12,12	-	-	-	-	-
46	SF4	G	801	7	0,12,12	-	-	-	-	-
45	3PE	L	701	-	50,50,50	0.86	4 (8%)	53,55,55	1.01	2 (3%)
49	PC1	H	402	-	41,41,53	1.08	3 (7%)	47,49,61	0.93	2 (4%)
46	SF4	B	201	2	0,12,12	-	-	-	-	-
54	EHZ	T	201	20	28,33,37	1.68	5 (17%)	33,41,47	1.40	4 (12%)
45	3PE	M	505	-	50,50,50	0.88	3 (6%)	53,55,55	1.03	3 (5%)
45	3PE	M	503	-	50,50,50	0.88	3 (6%)	53,55,55	1.07	2 (3%)
45	3PE	A	201	-	40,40,50	0.97	4 (10%)	43,45,55	1.07	2 (4%)
48	FMN	F	501	-	33,33,33	1.12	2 (6%)	48,50,50	1.42	7 (14%)
54	EHZ	U	201	20	29,34,37	1.66	5 (17%)	34,42,47	1.23	4 (11%)
51	ADP	O	401	-	28,29,29	1.39	4 (14%)	43,45,45	1.98	10 (23%)
45	3PE	L	704	-	41,41,50	0.96	4 (9%)	44,46,55	1.02	2 (4%)
46	SF4	F	502	6	0,12,12	-	-	-	-	-
52	NDP	P	501	-	51,52,52	2.36	8 (15%)	71,80,80	1.57	15 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	3PE	N	401	-	50,50,50	0.90	4 (8%)	53,55,55	1.10	3 (5%)
50	CDL	L	703	-	69,69,99	1.04	8 (11%)	75,81,111	1.09	4 (5%)
50	CDL	L	702	-	77,77,99	1.00	8 (10%)	83,89,111	1.14	4 (4%)
45	3PE	M	501	-	50,50,50	0.88	4 (8%)	53,55,55	0.98	2 (3%)
49	PC1	H	404	-	46,46,53	1.04	4 (8%)	52,54,61	1.03	2 (3%)
46	SF4	G	802	7	0,12,12	-	-	-	-	-
45	3PE	M	502	-	41,41,50	1.05	4 (9%)	44,46,55	1.24	3 (6%)
45	3PE	H	401	-	50,50,50	0.86	4 (8%)	53,55,55	0.99	2 (3%)
47	FES	E	301	5	0,4,4	-	-	-	-	-
49	PC1	P	401	-	42,42,53	1.08	4 (9%)	48,50,61	1.04	2 (4%)
45	3PE	M	506	-	30,30,50	1.11	4 (13%)	33,35,55	1.15	2 (6%)
45	3PE	M	504	-	50,50,50	0.87	4 (8%)	53,55,55	1.10	2 (3%)
46	SF4	I	201	9	0,12,12	-	-	-	-	-
47	FES	G	803	7	0,4,4	-	-	-	-	-
50	CDL	H	405	-	56,56,99	1.15	7 (12%)	62,68,111	1.12	4 (6%)

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
45	3PE	H	403	-	-	24/54/54/54	-
49	PC1	H	406	-	-	18/38/38/57	-
50	CDL	M	507	-	-	32/77/77/110	-
46	SF4	I	202	9	-	-	0/6/5/5
46	SF4	G	801	7	-	-	0/6/5/5
45	3PE	L	701	-	-	19/54/54/54	-
49	PC1	H	402	-	-	25/45/45/57	-
46	SF4	B	201	2	-	-	0/6/5/5
54	EHZ	T	201	20	-	8/39/41/45	-
45	3PE	M	505	-	-	25/54/54/54	-
45	3PE	M	503	-	-	21/54/54/54	-
45	3PE	A	201	-	-	18/44/44/54	-
48	FMN	F	501	-	-	7/18/18/18	0/3/3/3
54	EHZ	U	201	20	-	16/40/42/45	-
51	ADP	O	401	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	L	704	-	-	17/45/45/54	-
46	SF4	F	502	6	-	-	0/6/5/5
52	NDP	P	501	-	-	5/34/77/77	0/5/5/5
45	3PE	N	401	-	-	25/54/54/54	-
50	CDL	L	703	-	-	39/80/80/110	-
50	CDL	L	702	-	-	42/88/88/110	-
45	3PE	M	501	-	-	29/54/54/54	-
49	PC1	H	404	-	-	22/50/50/57	-
46	SF4	G	802	7	-	-	0/6/5/5
45	3PE	M	502	-	-	16/43/43/54	-
45	3PE	H	401	-	-	26/54/54/54	-
47	FES	E	301	5	-	-	0/1/1/1
49	PC1	P	401	-	-	26/46/46/57	-
45	3PE	M	506	-	-	14/34/34/54	-
45	3PE	M	504	-	-	23/54/54/54	-
46	SF4	I	201	9	-	-	0/6/5/5
47	FES	G	803	7	-	-	0/1/1/1
50	CDL	H	405	-	-	37/67/67/110	-

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	P2B-O2B	13.04	1.82	1.59
54	U	201	EHZ	C15-N2	5.15	1.45	1.33
54	T	201	EHZ	C15-N2	5.13	1.45	1.33
54	U	201	EHZ	C12-N1	5.10	1.45	1.33
54	T	201	EHZ	C12-N1	5.10	1.45	1.33
52	P	501	NDP	PA-O3	4.50	1.64	1.59
51	O	401	ADP	C5-C4	4.49	1.47	1.39
52	P	501	NDP	PN-O5D	3.65	1.73	1.59
52	P	501	NDP	O2B-C2B	-3.37	1.32	1.44
45	M	505	3PE	O21-C2	-2.95	1.39	1.46
48	F	501	FMN	C4A-N5	2.90	1.37	1.30
45	M	502	3PE	O31-C31	2.85	1.41	1.33
45	M	503	3PE	O21-C2	-2.84	1.39	1.46
45	M	502	3PE	P-O13	2.81	1.65	1.54
50	H	405	CDL	OB6-CB4	-2.77	1.40	1.46
45	H	403	3PE	O21-C2	-2.77	1.40	1.46
51	O	401	ADP	C5-C6	2.73	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	L	702	CDL	OA6-CA4	-2.71	1.40	1.46
45	N	401	3PE	O21-C2	-2.70	1.40	1.46
45	L	704	3PE	O21-C2	-2.67	1.40	1.46
45	M	502	3PE	O21-C2	-2.65	1.40	1.46
50	L	703	CDL	OA6-CA4	-2.64	1.40	1.46
50	H	405	CDL	OA6-CA4	-2.64	1.40	1.46
45	M	501	3PE	O21-C2	-2.62	1.40	1.46
45	M	505	3PE	O31-C3	-2.62	1.39	1.45
50	L	702	CDL	OB6-CB4	-2.61	1.40	1.46
49	H	404	PC1	O21-C2	-2.61	1.40	1.46
49	H	406	PC1	O21-C2	-2.60	1.40	1.46
49	H	402	PC1	O21-C2	-2.59	1.40	1.46
45	L	701	3PE	O21-C2	-2.56	1.40	1.46
48	F	501	FMN	C10-N1	2.55	1.38	1.33
49	H	404	PC1	O31-C31	2.55	1.40	1.33
50	M	507	CDL	OA8-CA7	2.52	1.40	1.33
54	U	201	EHZ	C9-S1	2.52	1.82	1.76
49	H	402	PC1	O31-C31	2.52	1.40	1.33
54	T	201	EHZ	C9-S1	2.52	1.82	1.76
45	M	504	3PE	O21-C2	-2.50	1.40	1.46
50	L	702	CDL	OA8-CA7	2.48	1.40	1.33
50	L	702	CDL	OB8-CB7	2.48	1.40	1.33
50	H	405	CDL	OA8-CA7	2.48	1.40	1.33
45	M	503	3PE	O31-C31	2.48	1.40	1.33
45	M	506	3PE	O21-C2	-2.47	1.40	1.46
52	P	501	NDP	O4B-C4B	-2.46	1.39	1.45
52	P	501	NDP	O5D-C5D	-2.44	1.35	1.44
50	H	405	CDL	OB8-CB7	2.44	1.40	1.33
45	A	201	3PE	O21-C2	-2.43	1.40	1.46
45	H	403	3PE	O31-C3	-2.43	1.39	1.45
52	P	501	NDP	O3B-C3B	-2.42	1.37	1.43
45	H	401	3PE	O21-C2	-2.41	1.40	1.46
45	N	401	3PE	O31-C3	-2.41	1.39	1.45
45	A	201	3PE	O21-C21	2.41	1.41	1.34
50	M	507	CDL	OB8-CB7	2.40	1.40	1.33
51	O	401	ADP	C5-N7	-2.39	1.34	1.39
51	O	401	ADP	C8-N7	2.39	1.36	1.31
45	M	502	3PE	O21-C21	2.38	1.41	1.34
45	L	704	3PE	O31-C31	2.38	1.40	1.33
45	A	201	3PE	O31-C3	-2.37	1.39	1.45
54	U	201	EHZ	O4-C15	-2.36	1.18	1.23
49	P	401	PC1	O21-C21	2.36	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	L	703	CDL	OB8-CB6	-2.35	1.39	1.45
50	M	507	CDL	OB6-CB5	2.35	1.40	1.34
49	H	406	PC1	O31-C3	-2.35	1.39	1.45
45	H	401	3PE	O31-C3	-2.35	1.39	1.45
45	A	201	3PE	O31-C31	2.34	1.40	1.33
49	H	406	PC1	O31-C31	2.34	1.40	1.33
45	M	506	3PE	O31-C31	2.34	1.40	1.33
45	M	504	3PE	O31-C31	2.34	1.40	1.33
54	T	201	EHZ	O4-C15	-2.33	1.18	1.23
50	M	507	CDL	OA6-CA4	-2.33	1.41	1.46
49	P	401	PC1	O31-C31	2.32	1.40	1.33
45	M	501	3PE	O31-C31	2.32	1.40	1.33
45	M	506	3PE	O31-C3	-2.32	1.40	1.45
50	L	703	CDL	OB8-CB7	2.32	1.40	1.33
54	U	201	EHZ	O3-C12	-2.30	1.18	1.23
50	M	507	CDL	OB6-CB4	-2.30	1.41	1.46
45	N	401	3PE	O31-C31	2.29	1.40	1.33
49	H	404	PC1	O21-C21	2.28	1.40	1.34
49	P	401	PC1	O31-C3	-2.28	1.40	1.45
50	L	703	CDL	OA8-CA7	2.28	1.40	1.33
45	M	506	3PE	O21-C21	2.28	1.40	1.34
45	M	501	3PE	O31-C3	-2.27	1.40	1.45
50	L	703	CDL	OB6-CB5	2.26	1.40	1.34
45	H	403	3PE	O31-C31	2.26	1.39	1.33
50	M	507	CDL	OB8-CB6	-2.25	1.40	1.45
45	M	501	3PE	O21-C21	2.24	1.40	1.34
45	M	504	3PE	O21-C21	2.24	1.40	1.34
54	T	201	EHZ	O3-C12	-2.22	1.18	1.23
49	H	406	PC1	O21-C21	2.22	1.40	1.34
50	L	703	CDL	OA8-CA6	-2.22	1.40	1.45
45	H	401	3PE	O31-C31	2.21	1.39	1.33
45	L	701	3PE	O31-C31	2.19	1.39	1.33
45	L	704	3PE	O31-C3	-2.19	1.40	1.45
49	H	402	PC1	O21-C21	2.18	1.40	1.34
50	L	703	CDL	OB6-CB4	-2.18	1.41	1.46
50	L	702	CDL	OB6-CB5	2.17	1.40	1.34
45	L	701	3PE	O31-C3	-2.15	1.40	1.45
50	M	507	CDL	OA6-CA5	2.15	1.40	1.34
45	M	503	3PE	O31-C3	-2.14	1.40	1.45
50	L	703	CDL	OA6-CA5	2.13	1.40	1.34
50	H	405	CDL	OB8-CB6	-2.13	1.40	1.45
49	P	401	PC1	O21-C2	-2.13	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	M	504	3PE	O31-C3	-2.13	1.40	1.45
50	H	405	CDL	OA6-CA5	2.12	1.40	1.34
45	N	401	3PE	O21-C21	2.12	1.40	1.34
45	L	701	3PE	O21-C21	2.09	1.40	1.34
49	H	404	PC1	O31-C3	-2.08	1.40	1.45
50	L	702	CDL	OA6-CA5	2.08	1.40	1.34
52	P	501	NDP	PA-O5B	2.07	1.67	1.59
45	M	505	3PE	O31-C31	2.07	1.39	1.33
50	M	507	CDL	OA8-CA6	-2.06	1.40	1.45
45	H	401	3PE	O21-C21	2.06	1.40	1.34
45	L	704	3PE	O21-C21	2.06	1.40	1.34
50	L	702	CDL	OB8-CB6	-2.04	1.40	1.45
50	H	405	CDL	OB6-CB5	2.02	1.40	1.34
50	L	702	CDL	OA8-CA6	-2.02	1.40	1.45

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	O	401	ADP	C5-C4-N3	-6.23	118.14	126.72
54	T	201	EHZ	C8-C9-S1	4.99	119.86	113.56
52	P	501	NDP	P2B-O2B-C2B	-4.92	110.30	123.43
51	O	401	ADP	N3-C4-N9	4.80	135.34	127.17
45	M	502	3PE	O31-C31-C32	4.77	126.36	111.83
50	M	507	CDL	OB6-CB5-C51	4.59	121.42	111.48
45	M	504	3PE	O21-C21-C22	4.52	121.26	111.48
49	H	404	PC1	O21-C21-C22	4.48	121.17	111.48
45	N	401	3PE	O21-C21-C22	4.42	121.05	111.48
45	H	403	3PE	O21-C21-C22	4.38	120.95	111.48
52	P	501	NDP	O3-PA-O1A	-4.36	97.60	110.70
50	L	702	CDL	OB6-CB5-C51	4.33	120.85	111.48
50	L	702	CDL	OA6-CA5-C11	4.32	120.82	111.48
49	H	406	PC1	O21-C21-C22	4.31	120.81	111.48
54	U	201	EHZ	C8-C9-S1	4.20	118.86	113.56
51	O	401	ADP	C2-N3-C4	4.17	122.02	111.83
45	M	503	3PE	O21-C21-C22	4.16	120.47	111.48
45	M	506	3PE	O21-C21-C22	3.96	120.05	111.48
45	M	501	3PE	O21-C21-C22	3.92	119.97	111.48
45	A	201	3PE	O21-C21-C22	3.91	119.93	111.48
49	P	401	PC1	O21-C21-C22	3.90	119.92	111.48
50	H	405	CDL	OB6-CB5-C51	3.85	119.81	111.48
50	H	405	CDL	OA6-CA5-C11	3.84	119.78	111.48
50	L	703	CDL	OB6-CB5-C51	3.82	119.75	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	H	402	PC1	O21-C21-C22	3.81	119.73	111.48
45	H	401	3PE	O21-C21-C22	3.79	119.68	111.48
51	O	401	ADP	N3-C2-N1	-3.75	122.90	128.58
48	F	501	FMN	C4-N3-C2	-3.74	119.00	125.64
50	L	703	CDL	OA6-CA5-C11	3.72	119.54	111.48
45	L	704	3PE	O21-C21-C22	3.67	119.42	111.48
52	P	501	NDP	O2B-P2B-O1X	-3.58	96.56	109.33
51	O	401	ADP	C4-C5-N7	-3.58	106.49	110.58
50	M	507	CDL	OA8-CA7-C31	3.53	122.59	111.83
45	L	701	3PE	O21-C21-C22	3.42	118.87	111.48
45	M	505	3PE	O21-C21-C22	3.39	118.82	111.48
51	O	401	ADP	O4'-C1'-N9	3.36	114.54	108.09
50	M	507	CDL	OA6-CA5-C11	3.34	118.70	111.48
45	M	505	3PE	C2-O21-C21	-3.21	110.11	117.80
49	H	404	PC1	O31-C31-C32	3.09	121.26	111.83
50	L	702	CDL	OA8-CA7-C31	3.07	121.21	111.83
45	M	502	3PE	O31-C31-O32	-3.01	116.09	123.63
48	F	501	FMN	O4-C4-C4A	-2.96	118.71	126.53
50	L	702	CDL	OB8-CB7-C71	2.91	120.72	111.83
49	H	406	PC1	O31-C31-C32	2.89	120.65	111.83
48	F	501	FMN	C4A-C10-N10	2.82	120.52	116.48
45	N	401	3PE	O31-C31-C32	2.81	120.40	111.83
48	F	501	FMN	C4A-C4-N3	2.81	120.39	113.25
45	M	504	3PE	O31-C31-C32	2.80	120.39	111.83
50	H	405	CDL	OA8-CA7-C31	2.79	120.34	111.83
50	M	507	CDL	OB8-CB7-C71	2.78	120.33	111.83
45	M	503	3PE	O31-C31-C32	2.76	120.24	111.83
51	O	401	ADP	C5-N7-C8	2.75	107.77	103.45
45	L	701	3PE	O31-C31-C32	2.73	120.17	111.83
50	L	703	CDL	OA8-CA7-C31	2.69	120.03	111.83
45	M	506	3PE	O31-C31-C32	2.69	120.03	111.83
50	H	405	CDL	OB8-CB7-C71	2.67	119.99	111.83
45	A	201	3PE	O31-C31-C32	2.66	119.95	111.83
48	F	501	FMN	C4A-C10-N1	-2.66	118.06	124.59
45	L	704	3PE	O31-C31-C32	2.65	119.92	111.83
45	M	502	3PE	O21-C21-C22	2.65	117.20	111.48
52	P	501	NDP	N3A-C4A-N9A	2.62	131.62	127.17
52	P	501	NDP	C2A-N1A-C6A	-2.62	114.43	118.73
50	L	703	CDL	OB8-CB7-C71	2.59	119.72	111.83
45	M	501	3PE	O31-C31-C32	2.58	119.71	111.83
52	P	501	NDP	O5D-PN-O1N	-2.57	98.75	108.94
54	U	201	EHZ	C19-C17-C16	2.55	113.11	108.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	H	403	3PE	O31-C31-C32	2.53	119.55	111.83
52	P	501	NDP	O3X-P2B-O2X	2.52	117.26	107.80
52	P	501	NDP	C4B-O4B-C1B	-2.50	103.94	109.47
49	P	401	PC1	O31-C31-C32	2.50	119.45	111.83
45	H	401	3PE	O31-C31-C32	2.49	119.44	111.83
45	M	505	3PE	O31-C31-C32	2.48	119.39	111.83
51	O	401	ADP	C4-N9-C8	2.48	108.34	105.74
54	T	201	EHZ	C10-S1-C9	2.46	109.12	101.84
51	O	401	ADP	C6-C5-N7	2.46	136.83	132.09
48	F	501	FMN	C4-C4A-C10	2.39	121.03	116.93
52	P	501	NDP	C5A-C4A-N3A	-2.36	123.46	126.72
52	P	501	NDP	O2N-PN-O1N	2.35	123.39	112.44
52	P	501	NDP	C5B-C4B-C3B	-2.35	106.75	115.21
54	T	201	EHZ	O2-C9-C8	-2.34	120.05	123.74
52	P	501	NDP	PN-O5D-C5D	-2.29	108.24	121.35
49	H	402	PC1	O31-C31-C32	2.27	118.74	111.83
52	P	501	NDP	O2N-PN-O3	2.26	113.39	107.27
48	F	501	FMN	C5A-C9A-N10	2.21	119.97	117.97
52	P	501	NDP	PA-O5B-C5B	-2.21	108.71	121.35
51	O	401	ADP	N9-C8-N7	-2.17	110.86	113.94
50	M	507	CDL	OA6-CA4-CA6	2.14	116.04	108.34
52	P	501	NDP	O3X-P2B-O2B	-2.13	97.55	105.85
54	U	201	EHZ	C10-S1-C9	2.12	108.11	101.84
54	T	201	EHZ	O2-C9-S1	-2.04	120.09	122.68
45	N	401	3PE	C2-O21-C21	-2.02	112.97	117.80
54	U	201	EHZ	O2-C9-C8	-2.01	120.57	123.74

There are no chirality outliers.

All (537) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C1-O11-P-O14
45	H	401	3PE	C11-O13-P-O11
45	H	401	3PE	C11-O13-P-O12
45	H	401	3PE	O13-C11-C12-N
45	H	401	3PE	C22-C21-O21-C2
45	H	403	3PE	C1-O11-P-O12
45	H	403	3PE	C1-O11-P-O13
45	H	403	3PE	C1-O11-P-O14
45	H	403	3PE	C11-O13-P-O11
45	H	403	3PE	C11-O13-P-O12
45	H	403	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
45	L	701	3PE	C1-O11-P-O13
45	L	701	3PE	C1-O11-P-O14
45	L	704	3PE	C1-O11-P-O12
45	L	704	3PE	C1-O11-P-O14
45	L	704	3PE	O13-C11-C12-N
45	M	501	3PE	C1-O11-P-O12
45	M	501	3PE	C1-O11-P-O13
45	M	501	3PE	O13-C11-C12-N
45	M	501	3PE	O22-C21-O21-C2
45	M	502	3PE	O32-C31-O31-C3
45	M	502	3PE	C32-C31-O31-C3
45	M	503	3PE	C11-O13-P-O11
45	M	503	3PE	C11-O13-P-O12
45	M	503	3PE	C11-O13-P-O14
45	M	503	3PE	O13-C11-C12-N
45	M	503	3PE	C22-C21-O21-C2
45	M	504	3PE	C11-O13-P-O11
45	M	504	3PE	C11-O13-P-O14
45	M	504	3PE	O13-C11-C12-N
45	M	504	3PE	C22-C21-O21-C2
45	M	505	3PE	O13-C11-C12-N
45	M	505	3PE	C22-C21-O21-C2
45	M	506	3PE	C1-O11-P-O13
45	M	506	3PE	O13-C11-C12-N
45	M	506	3PE	C22-C21-O21-C2
45	N	401	3PE	C1-O11-P-O12
45	N	401	3PE	C1-O11-P-O13
45	N	401	3PE	C1-O11-P-O14
45	N	401	3PE	C11-O13-P-O11
45	N	401	3PE	O13-C11-C12-N
45	N	401	3PE	O21-C2-C3-O31
45	N	401	3PE	C22-C21-O21-C2
48	F	501	FMN	N10-C1'-C2'-O2'
48	F	501	FMN	N10-C1'-C2'-C3'
48	F	501	FMN	C3'-C4'-C5'-O5'
48	F	501	FMN	O4'-C4'-C5'-O5'
48	F	501	FMN	C5'-O5'-P-O2P
49	H	402	PC1	C1-O11-P-O14
49	H	402	PC1	C1-O11-P-O13
49	H	402	PC1	O13-C11-C12-N
49	H	404	PC1	C11-O13-P-O14
49	H	404	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
49	H	406	PC1	C11-O13-P-O14
49	H	406	PC1	C1-O11-P-O12
49	H	406	PC1	C1-O11-P-O14
49	H	406	PC1	C1-O11-P-O13
49	H	406	PC1	O13-C11-C12-N
49	H	406	PC1	O22-C21-O21-C2
49	P	401	PC1	C11-O13-P-O12
49	P	401	PC1	C1-O11-P-O12
49	P	401	PC1	C1-O11-P-O13
49	P	401	PC1	O13-C11-C12-N
49	P	401	PC1	C3-C2-O21-C21
49	P	401	PC1	C22-C21-O21-C2
50	H	405	CDL	CA3-OA5-PA1-OA2
50	H	405	CDL	CA3-OA5-PA1-OA3
50	H	405	CDL	C11-CA5-OA6-CA4
50	H	405	CDL	C1-CB2-OB2-PB2
50	L	702	CDL	CA2-C1-CB2-OB2
50	L	702	CDL	CA2-OA2-PA1-OA5
50	L	702	CDL	CA3-OA5-PA1-OA2
50	L	702	CDL	CA3-OA5-PA1-OA3
50	L	702	CDL	OA7-CA5-OA6-CA4
50	L	702	CDL	CB2-OB2-PB2-OB5
50	L	702	CDL	OB7-CB5-OB6-CB4
50	L	703	CDL	CB2-C1-CA2-OA2
50	L	703	CDL	CA2-C1-CB2-OB2
50	L	703	CDL	CA2-OA2-PA1-OA3
50	L	703	CDL	CA2-OA2-PA1-OA4
50	L	703	CDL	CA2-OA2-PA1-OA5
50	L	703	CDL	CA3-OA5-PA1-OA3
50	L	703	CDL	CA3-OA5-PA1-OA4
50	L	703	CDL	CB3-OB5-PB2-OB2
50	L	703	CDL	CB3-OB5-PB2-OB4
50	M	507	CDL	CA3-OA5-PA1-OA2
50	M	507	CDL	CA3-OA5-PA1-OA3
50	M	507	CDL	CA3-OA5-PA1-OA4
50	M	507	CDL	OA5-CA3-CA4-OA6
50	M	507	CDL	OA7-CA5-OA6-CA4
50	M	507	CDL	C11-CA5-OA6-CA4
50	M	507	CDL	CB2-OB2-PB2-OB4
50	M	507	CDL	CB2-OB2-PB2-OB5
50	M	507	CDL	C51-CB5-OB6-CB4
52	P	501	NDP	C2N-C3N-C7N-N7N

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Mol	Chain	Res	Type	Atoms
54	T	201	EHZ	O1-C7-C8-C9
54	T	201	EHZ	C12-C13-C14-N2
54	T	201	EHZ	O2-C9-S1-C10
54	T	201	EHZ	C8-C9-S1-C10
54	U	201	EHZ	C15-C16-C17-C18
54	U	201	EHZ	C15-C16-C17-C19
54	U	201	EHZ	C15-C16-C17-C20
54	U	201	EHZ	O5-C16-C17-C18
54	U	201	EHZ	O5-C16-C17-C19
54	U	201	EHZ	O5-C16-C17-C20
54	U	201	EHZ	O2-C9-S1-C10
54	U	201	EHZ	C8-C9-S1-C10
45	H	401	3PE	C32-C31-O31-C3
45	H	401	3PE	O32-C31-O31-C3
45	M	505	3PE	O32-C31-O31-C3
49	H	406	PC1	O32-C31-O31-C3
50	H	405	CDL	OA9-CA7-OA8-CA6
50	H	405	CDL	OB9-CB7-OB8-CB6
50	L	702	CDL	OA9-CA7-OA8-CA6
50	L	703	CDL	OB9-CB7-OB8-CB6
45	H	401	3PE	O22-C21-O21-C2
45	M	505	3PE	O22-C21-O21-C2
45	M	506	3PE	O22-C21-O21-C2
45	N	401	3PE	O22-C21-O21-C2
50	H	405	CDL	OA7-CA5-OA6-CA4
50	M	507	CDL	OB7-CB5-OB6-CB4
49	H	406	PC1	C32-C31-O31-C3
50	H	405	CDL	C31-CA7-OA8-CA6
45	M	501	3PE	C22-C21-O21-C2
49	H	406	PC1	C22-C21-O21-C2
50	L	702	CDL	C11-CA5-OA6-CA4
50	L	702	CDL	C51-CB5-OB6-CB4
45	M	505	3PE	C32-C31-O31-C3
50	H	405	CDL	C71-CB7-OB8-CB6
50	L	702	CDL	C31-CA7-OA8-CA6
50	L	703	CDL	C71-CB7-OB8-CB6
45	M	503	3PE	O22-C21-O21-C2
45	M	504	3PE	O22-C21-O21-C2
49	P	401	PC1	O22-C21-O21-C2
50	L	702	CDL	O1-C1-CB2-OB2
50	L	703	CDL	O1-C1-CA2-OA2
50	L	703	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C32-C31-O31-C3
50	M	507	CDL	C71-CB7-OB8-CB6
45	N	401	3PE	O32-C31-O31-C3
50	H	405	CDL	C51-CB5-OB6-CB4
45	N	401	3PE	C32-C31-O31-C3
45	A	201	3PE	O32-C31-O31-C3
50	M	507	CDL	OB9-CB7-OB8-CB6
45	L	704	3PE	O32-C31-O31-C3
50	M	507	CDL	CB2-C1-CA2-OA2
45	L	704	3PE	C32-C31-O31-C3
45	M	501	3PE	C32-C31-O31-C3
45	M	506	3PE	C32-C31-O31-C3
50	M	507	CDL	O1-C1-CA2-OA2
45	M	501	3PE	O32-C31-O31-C3
50	H	405	CDL	OB7-CB5-OB6-CB4
49	H	402	PC1	C22-C21-O21-C2
52	P	501	NDP	C3D-C4D-C5D-O5D
45	H	401	3PE	C31-C32-C33-C34
45	M	506	3PE	C31-C32-C33-C34
45	M	506	3PE	O32-C31-O31-C3
45	A	201	3PE	C31-C32-C33-C34
50	H	405	CDL	CA4-CA6-OA8-CA7
45	L	701	3PE	C21-C22-C23-C24
49	H	402	PC1	C31-C32-C33-C34
50	L	702	CDL	CA7-C31-C32-C33
49	H	402	PC1	O22-C21-O21-C2
45	M	504	3PE	C32-C31-O31-C3
45	M	506	3PE	C21-C22-C23-C24
45	L	701	3PE	C22-C21-O21-C2
45	L	701	3PE	O22-C21-O21-C2
45	L	701	3PE	C32-C31-O31-C3
50	M	507	CDL	CA6-CA4-OA6-CA5
45	H	403	3PE	C22-C21-O21-C2
45	H	401	3PE	C38-C39-C3A-C3B
45	M	501	3PE	C3E-C3F-C3G-C3H
45	M	502	3PE	C28-C29-C2A-C2B
45	M	504	3PE	C37-C38-C39-C3A
50	L	702	CDL	CB5-C51-C52-C53
45	L	701	3PE	C35-C36-C37-C38
45	M	505	3PE	C2C-C2D-C2E-C2F
45	M	503	3PE	C35-C36-C37-C38
45	M	503	3PE	C3E-C3F-C3G-C3H

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Mol	Chain	Res	Type	Atoms
50	L	702	CDL	C74-C75-C76-C77
45	M	501	3PE	C38-C39-C3A-C3B
49	H	404	PC1	C24-C25-C26-C27
50	M	507	CDL	C54-C55-C56-C57
54	T	201	EHZ	S1-C10-C11-N1
45	M	506	3PE	C34-C35-C36-C37
45	A	201	3PE	C2B-C2C-C2D-C2E
50	L	702	CDL	C56-C57-C58-C59
49	P	401	PC1	C37-C38-C39-C3A
50	H	405	CDL	CA5-C11-C12-C13
45	H	403	3PE	C25-C26-C27-C28
45	M	504	3PE	C34-C35-C36-C37
50	H	405	CDL	CB7-C71-C72-C73
45	M	504	3PE	O32-C31-O31-C3
50	M	507	CDL	C31-CA7-OA8-CA6
45	H	401	3PE	C2B-C2C-C2D-C2E
45	M	503	3PE	C2B-C2C-C2D-C2E
50	L	703	CDL	C19-C20-C21-C22
50	M	507	CDL	C51-C52-C53-C54
49	H	402	PC1	C21-C22-C23-C24
49	P	401	PC1	C31-C32-C33-C34
45	H	401	3PE	C3E-C3F-C3G-C3H
49	H	402	PC1	C35-C36-C37-C38
49	H	404	PC1	C27-C28-C29-C2A
49	H	404	PC1	C33-C34-C35-C36
49	H	404	PC1	C35-C36-C37-C38
50	L	702	CDL	C51-C52-C53-C54
45	L	701	3PE	O32-C31-O31-C3
49	H	404	PC1	C29-C2A-C2B-C2C
45	N	401	3PE	C3C-C3D-C3E-C3F
45	N	401	3PE	C2C-C2D-C2E-C2F
45	M	501	3PE	C2-C1-O11-P
45	M	501	3PE	C24-C25-C26-C27
45	M	503	3PE	C24-C25-C26-C27
45	M	505	3PE	C29-C2A-C2B-C2C
50	M	507	CDL	C57-C58-C59-C60
50	H	405	CDL	CB5-C51-C52-C53
45	M	501	3PE	C22-C23-C24-C25
45	M	502	3PE	C22-C23-C24-C25
45	M	503	3PE	C32-C31-O31-C3
49	H	404	PC1	C22-C23-C24-C25
50	L	702	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
45	M	501	3PE	C28-C29-C2A-C2B
45	N	401	3PE	C28-C29-C2A-C2B
49	H	402	PC1	C26-C27-C28-C29
50	L	702	CDL	C77-C78-C79-C80
49	H	406	PC1	C23-C24-C25-C26
54	U	201	EHZ	C3-C4-C5-C6
45	H	403	3PE	O22-C21-O21-C2
45	L	704	3PE	C2D-C2E-C2F-C2G
45	M	505	3PE	C37-C38-C39-C3A
45	N	401	3PE	C2E-C2F-C2G-C2H
52	P	501	NDP	O4D-C4D-C5D-O5D
45	M	504	3PE	C27-C28-C29-C2A
45	M	505	3PE	C3A-C3B-C3C-C3D
50	L	703	CDL	C11-C12-C13-C14
50	M	507	CDL	OA9-CA7-OA8-CA6
50	L	702	CDL	CB7-C71-C72-C73
45	M	502	3PE	C38-C39-C3A-C3B
49	H	402	PC1	C24-C25-C26-C27
45	M	505	3PE	C24-C25-C26-C27
45	H	401	3PE	C36-C37-C38-C39
45	M	505	3PE	C25-C26-C27-C28
45	H	401	3PE	C2C-C2D-C2E-C2F
45	M	501	3PE	C2D-C2E-C2F-C2G
50	L	703	CDL	C22-C23-C24-C25
45	M	501	3PE	C39-C3A-C3B-C3C
45	H	401	3PE	C37-C38-C39-C3A
49	H	406	PC1	C2-C1-O11-P
50	L	702	CDL	C34-C35-C36-C37
45	A	201	3PE	C33-C34-C35-C36
45	M	504	3PE	C2-C3-O31-C31
50	L	703	CDL	C14-C15-C16-C17
45	M	504	3PE	C3C-C3D-C3E-C3F
49	H	404	PC1	O11-C1-C2-C3
50	M	507	CDL	OA5-CA3-CA4-CA6
45	M	505	3PE	C34-C35-C36-C37
45	M	503	3PE	O32-C31-O31-C3
50	L	702	CDL	C72-C73-C74-C75
49	H	402	PC1	C36-C37-C38-C39
45	M	504	3PE	C1-C2-C3-O31
50	H	405	CDL	CA3-CA4-CA6-OA8
50	L	702	CDL	CB3-CB4-CB6-OB8
49	P	401	PC1	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
45	L	701	3PE	C2C-C2D-C2E-C2F
45	H	403	3PE	C22-C23-C24-C25
50	H	405	CDL	C31-C32-C33-C34
50	M	507	CDL	C33-C34-C35-C36
45	H	403	3PE	C28-C29-C2A-C2B
48	F	501	FMN	C5'-O5'-P-O1P
45	M	503	3PE	C38-C39-C3A-C3B
50	H	405	CDL	C14-C15-C16-C17
49	H	404	PC1	C36-C37-C38-C39
45	H	401	3PE	C23-C24-C25-C26
45	A	201	3PE	C27-C28-C29-C2A
45	N	401	3PE	C34-C35-C36-C37
45	A	201	3PE	C35-C36-C37-C38
49	H	402	PC1	C3A-C3B-C3C-C3D
45	L	701	3PE	C2B-C2C-C2D-C2E
45	H	403	3PE	C32-C33-C34-C35
45	L	701	3PE	C32-C33-C34-C35
45	N	401	3PE	C36-C37-C38-C39
49	H	404	PC1	C32-C33-C34-C35
49	H	406	PC1	C31-C32-C33-C34
50	L	703	CDL	C31-CA7-OA8-CA6
50	H	405	CDL	C18-C19-C20-C21
45	M	501	3PE	C2F-C2G-C2H-C2I
50	L	703	CDL	C55-C56-C57-C58
45	N	401	3PE	C3F-C3G-C3H-C3I
45	N	401	3PE	C2F-C2G-C2H-C2I
49	H	402	PC1	C25-C26-C27-C28
54	U	201	EHZ	C1-C2-C3-C4
50	L	702	CDL	C11-C12-C13-C14
45	L	701	3PE	C2-C1-O11-P
50	L	703	CDL	C1-CA2-OA2-PA1
45	A	201	3PE	C2F-C2G-C2H-C2I
45	M	503	3PE	C2E-C2F-C2G-C2H
45	N	401	3PE	C37-C38-C39-C3A
50	M	507	CDL	C12-C13-C14-C15
45	H	401	3PE	C2F-C2G-C2H-C2I
45	L	704	3PE	O11-C1-C2-C3
45	M	505	3PE	C3F-C3G-C3H-C3I
50	L	702	CDL	C31-C32-C33-C34
49	H	402	PC1	C28-C29-C2A-C2B
45	L	701	3PE	C3A-C3B-C3C-C3D
49	H	402	PC1	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
45	M	505	3PE	C32-C33-C34-C35
50	M	507	CDL	C31-C32-C33-C34
45	H	401	3PE	C25-C26-C27-C28
50	M	507	CDL	C61-C62-C63-C64
45	H	403	3PE	C27-C28-C29-C2A
45	L	704	3PE	O11-C1-C2-O21
49	H	404	PC1	O11-C1-C2-O21
50	H	405	CDL	OA5-CA3-CA4-OA6
50	L	702	CDL	OB5-CB3-CB4-OB6
49	P	401	PC1	C3C-C3D-C3E-C3F
49	H	404	PC1	C38-C39-C3A-C3B
45	H	403	3PE	C2C-C2D-C2E-C2F
49	P	401	PC1	C3F-C3G-C3H-C3I
49	P	401	PC1	C34-C35-C36-C37
45	M	505	3PE	O21-C2-C3-O31
50	H	405	CDL	OB6-CB4-CB6-OB8
45	M	503	3PE	C39-C3A-C3B-C3C
45	N	401	3PE	C26-C27-C28-C29
45	M	505	3PE	C27-C28-C29-C2A
49	H	406	PC1	C33-C34-C35-C36
51	O	401	ADP	PB-O3A-PA-O5'
45	L	704	3PE	C34-C35-C36-C37
45	M	503	3PE	C28-C29-C2A-C2B
45	N	401	3PE	C2A-C2B-C2C-C2D
49	P	401	PC1	C39-C3A-C3B-C3C
54	T	201	EHZ	C6-C7-C8-C9
50	H	405	CDL	O1-C1-CB2-OB2
45	L	701	3PE	C3D-C3E-C3F-C3G
45	M	502	3PE	C26-C27-C28-C29
45	M	502	3PE	O11-C1-C2-C3
45	M	502	3PE	C2A-C2B-C2C-C2D
48	F	501	FMN	C5'-O5'-P-O3P
45	A	201	3PE	C21-C22-C23-C24
50	L	703	CDL	OA9-CA7-OA8-CA6
50	M	507	CDL	CB3-CB4-OB6-CB5
45	M	504	3PE	C24-C25-C26-C27
45	M	506	3PE	O11-C1-C2-O21
45	M	503	3PE	C26-C27-C28-C29
45	M	503	3PE	C12-C11-O13-P
45	N	401	3PE	C12-C11-O13-P
45	A	201	3PE	O21-C2-C3-O31
49	H	406	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
50	H	405	CDL	OA6-CA4-CA6-OA8
50	L	702	CDL	OB6-CB4-CB6-OB8
45	L	704	3PE	C36-C37-C38-C39
50	L	703	CDL	C11-CA5-OA6-CA4
45	M	501	3PE	C32-C33-C34-C35
45	M	503	3PE	C33-C34-C35-C36
45	A	201	3PE	C22-C23-C24-C25
45	M	502	3PE	C24-C25-C26-C27
50	M	507	CDL	C62-C63-C64-C65
50	L	703	CDL	C71-C72-C73-C74
45	M	503	3PE	C37-C38-C39-C3A
45	M	506	3PE	O11-C1-C2-C3
49	P	401	PC1	O11-C1-C2-C3
54	U	201	EHZ	C18-C17-C20-O6
45	M	504	3PE	C31-C32-C33-C34
45	M	503	3PE	C3C-C3D-C3E-C3F
49	H	406	PC1	C36-C37-C38-C39
54	T	201	EHZ	C11-C10-S1-C9
50	L	703	CDL	OA7-CA5-OA6-CA4
45	H	403	3PE	C2A-C2B-C2C-C2D
49	P	401	PC1	C21-C22-C23-C24
45	M	504	3PE	O21-C2-C3-O31
45	H	403	3PE	C3E-C3F-C3G-C3H
45	L	704	3PE	C25-C26-C27-C28
45	M	505	3PE	C1-C2-C3-O31
45	N	401	3PE	C1-C2-C3-O31
49	H	406	PC1	C1-C2-C3-O31
50	H	405	CDL	CB3-CB4-CB6-OB8
50	L	703	CDL	CA3-CA4-CA6-OA8
50	M	507	CDL	CB3-CB4-CB6-OB8
45	H	401	3PE	C24-C25-C26-C27
49	H	404	PC1	C2E-C2F-C2G-C2H
45	M	506	3PE	C23-C24-C25-C26
54	U	201	EHZ	C2-C1-C21-C22
45	A	201	3PE	C1-O11-P-O13
45	L	701	3PE	C1-O11-P-O12
45	L	701	3PE	C11-O13-P-O12
45	L	704	3PE	C1-O11-P-O13
45	M	501	3PE	C11-O13-P-O11
45	M	501	3PE	C11-O13-P-O12
45	M	504	3PE	C11-O13-P-O12
45	M	506	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
49	H	402	PC1	C11-O13-P-O11
49	H	404	PC1	C11-O13-P-O11
49	H	404	PC1	C1-O11-P-O12
49	H	404	PC1	C1-O11-P-O13
49	H	406	PC1	C11-O13-P-O11
49	P	401	PC1	C11-O13-P-O14
49	P	401	PC1	C11-O13-P-O11
49	P	401	PC1	C1-O11-P-O14
49	P	401	PC1	C11-C12-N-C14
50	H	405	CDL	CB2-OB2-PB2-OB3
50	H	405	CDL	CB2-OB2-PB2-OB4
50	H	405	CDL	CB2-OB2-PB2-OB5
50	L	702	CDL	CA2-OA2-PA1-OA3
50	L	702	CDL	CA3-OA5-PA1-OA4
50	L	702	CDL	CB2-OB2-PB2-OB3
50	L	703	CDL	CA3-OA5-PA1-OA2
50	L	703	CDL	CB2-OB2-PB2-OB3
50	M	507	CDL	CA2-OA2-PA1-OA3
50	M	507	CDL	CB2-OB2-PB2-OB3
50	L	703	CDL	CA7-C31-C32-C33
45	M	502	3PE	C2-C1-O11-P
50	L	702	CDL	CA4-CA3-OA5-PA1
50	L	703	CDL	CA4-CA3-OA5-PA1
45	H	403	3PE	C3C-C3D-C3E-C3F
45	H	403	3PE	C34-C35-C36-C37
45	M	505	3PE	C2F-C2G-C2H-C2I
45	H	401	3PE	C3-C2-O21-C21
45	L	701	3PE	C3-C2-O21-C21
45	M	502	3PE	C31-C32-C33-C34
45	M	505	3PE	C26-C27-C28-C29
45	M	501	3PE	O11-C1-C2-C3
51	O	401	ADP	C2'-C1'-N9-C8
50	L	702	CDL	C12-C13-C14-C15
45	M	502	3PE	O11-C1-C2-O21
50	L	703	CDL	C16-C17-C18-C19
52	P	501	NDP	O4D-C1D-N1N-C6N
45	M	502	3PE	C37-C38-C39-C3A
49	P	401	PC1	C3D-C3E-C3F-C3G
45	M	504	3PE	C29-C2A-C2B-C2C
50	L	702	CDL	C15-C16-C17-C18
50	L	702	CDL	C19-C20-C21-C22
51	O	401	ADP	C2'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
49	P	401	PC1	C11-C12-N-C15
54	U	201	EHZ	C4-C5-C6-C7
45	M	502	3PE	C35-C36-C37-C38
50	L	703	CDL	C72-C73-C74-C75
45	M	504	3PE	C25-C26-C27-C28
45	H	401	3PE	C28-C29-C2A-C2B
50	H	405	CDL	C11-C12-C13-C14
45	H	401	3PE	C2D-C2E-C2F-C2G
50	L	703	CDL	OA6-CA4-CA6-OA8
45	H	403	3PE	C29-C2A-C2B-C2C
45	H	401	3PE	C2E-C2F-C2G-C2H
45	M	502	3PE	C2B-C2C-C2D-C2E
50	L	703	CDL	C20-C21-C22-C23
49	P	401	PC1	C11-C12-N-C13
45	A	201	3PE	C1-C2-C3-O31
50	L	702	CDL	CA3-CA4-CA6-OA8
50	M	507	CDL	C60-C61-C62-C63
50	L	702	CDL	C52-C53-C54-C55
50	L	702	CDL	C16-C17-C18-C19
50	L	703	CDL	CA3-CA4-OA6-CA5
50	L	703	CDL	CB3-CB4-OB6-CB5
54	U	201	EHZ	C5-C6-C7-O1
49	P	401	PC1	C23-C24-C25-C26
45	M	501	3PE	O11-C1-C2-O21
45	M	504	3PE	C28-C29-C2A-C2B
45	H	401	3PE	C2-C1-O11-P
50	H	405	CDL	C12-C13-C14-C15
50	L	702	CDL	OB5-CB3-CB4-CB6
45	L	701	3PE	C39-C3A-C3B-C3C
45	L	701	3PE	O21-C2-C3-O31
45	M	502	3PE	C33-C34-C35-C36
45	M	504	3PE	C2F-C2G-C2H-C2I
49	H	404	PC1	O21-C21-C22-C23
45	M	505	3PE	C2E-C2F-C2G-C2H
49	H	402	PC1	C33-C34-C35-C36
45	A	201	3PE	C2-C1-O11-P
45	H	403	3PE	C2F-C2G-C2H-C2I
45	L	704	3PE	C1-C2-C3-O31
49	H	402	PC1	C1-C2-C3-O31
50	H	405	CDL	OB5-CB3-CB4-OB6
50	M	507	CDL	OB5-CB3-CB4-OB6
50	H	405	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
49	H	402	PC1	O32-C31-O31-C3
45	M	505	3PE	O11-C1-C2-C3
50	H	405	CDL	OA5-CA3-CA4-CA6
49	P	401	PC1	C24-C25-C26-C27
45	M	505	3PE	C39-C3A-C3B-C3C
50	H	405	CDL	O1-C1-CA2-OA2
45	N	401	3PE	O21-C21-C22-C23
49	H	404	PC1	C2F-C2G-C2H-C2I
49	H	402	PC1	C3-C2-O21-C21
45	H	403	3PE	C24-C25-C26-C27
45	H	403	3PE	C36-C37-C38-C39
45	L	704	3PE	C2C-C2D-C2E-C2F
45	L	704	3PE	C33-C34-C35-C36
45	M	505	3PE	C35-C36-C37-C38
45	M	501	3PE	C3C-C3D-C3E-C3F
49	P	401	PC1	C3E-C3F-C3G-C3H
49	H	402	PC1	C34-C35-C36-C37
45	M	501	3PE	O31-C31-C32-C33
45	N	401	3PE	C39-C3A-C3B-C3C
49	H	404	PC1	O31-C31-C32-C33
45	A	201	3PE	C28-C29-C2A-C2B
50	H	405	CDL	C32-C33-C34-C35
45	H	401	3PE	O31-C31-C32-C33
50	L	703	CDL	C72-C71-CB7-OB8
50	L	702	CDL	C53-C54-C55-C56
45	M	501	3PE	C3B-C3C-C3D-C3E
50	L	703	CDL	C51-C52-C53-C54
45	H	403	3PE	C3A-C3B-C3C-C3D
45	M	501	3PE	O21-C21-C22-C23
50	H	405	CDL	C52-C51-CB5-OB6
50	L	702	CDL	C12-C11-CA5-OA6
45	M	501	3PE	C3A-C3B-C3C-C3D
54	U	201	EHZ	C2-C3-C4-C5
45	A	201	3PE	O21-C21-C22-C23
49	H	402	PC1	O31-C31-C32-C33
45	M	504	3PE	C3B-C3C-C3D-C3E
49	H	402	PC1	C32-C31-O31-C3
49	H	402	PC1	C1-C2-O21-C21
50	H	405	CDL	CA3-CA4-OA6-CA5
50	L	703	CDL	CA6-CA4-OA6-CA5
45	M	505	3PE	C22-C23-C24-C25
50	L	703	CDL	C72-C71-CB7-OB9

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Mol	Chain	Res	Type	Atoms
50	L	702	CDL	C52-C51-CB5-OB6
50	L	702	CDL	C12-C11-CA5-OA7
45	H	403	3PE	C2B-C2C-C2D-C2E
45	M	501	3PE	C34-C35-C36-C37
50	H	405	CDL	C52-C51-CB5-OB7
45	M	501	3PE	O32-C31-C32-C33
49	H	404	PC1	O32-C31-C32-C33
45	L	704	3PE	O22-C21-O21-C2
49	H	406	PC1	O31-C31-C32-C33
54	T	201	EHZ	N2-C15-C16-O5
45	H	401	3PE	C32-C33-C34-C35
45	H	401	3PE	O32-C31-C32-C33
54	U	201	EHZ	C16-C17-C20-O6
45	M	504	3PE	O31-C31-C32-C33
52	P	501	NDP	PA-O3-PN-O2N
45	A	201	3PE	O22-C21-C22-C23
49	H	402	PC1	O32-C31-C32-C33
45	L	704	3PE	C31-C32-C33-C34
49	H	404	PC1	C34-C35-C36-C37
45	M	506	3PE	O31-C31-C32-C33
45	M	505	3PE	C2D-C2E-C2F-C2G
45	M	501	3PE	O22-C21-C22-C23

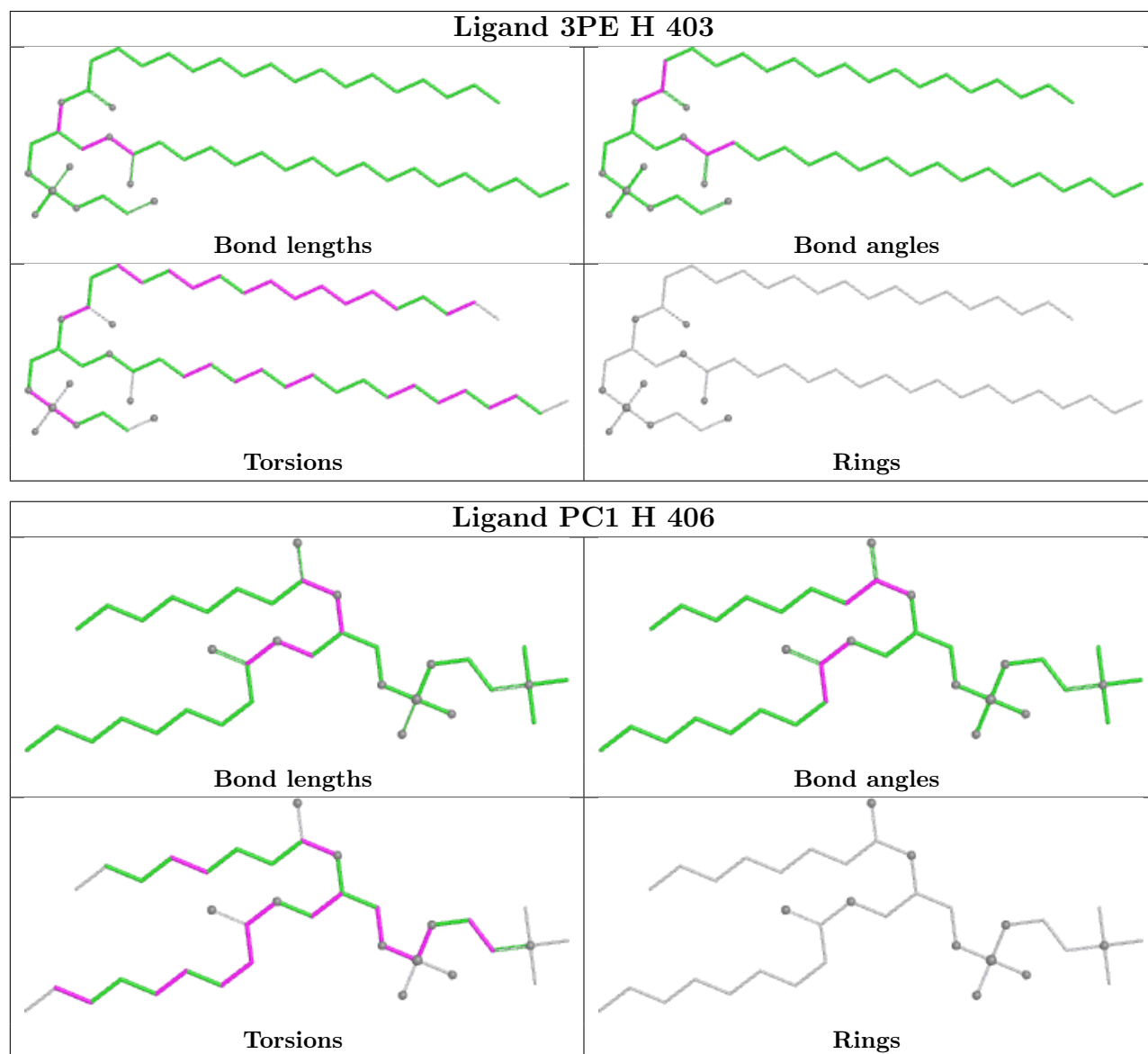
There are no ring outliers.

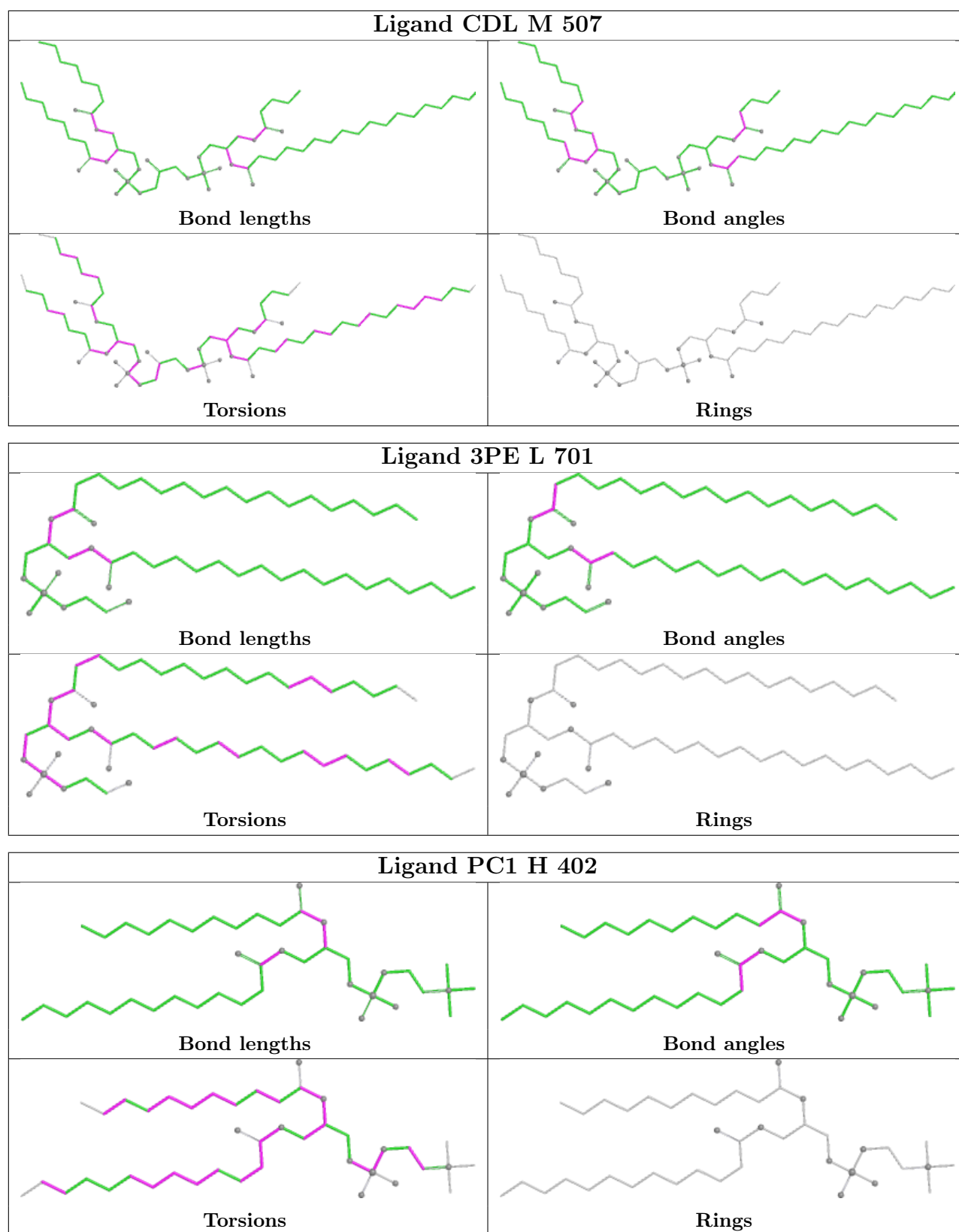
13 monomers are involved in 20 short contacts:

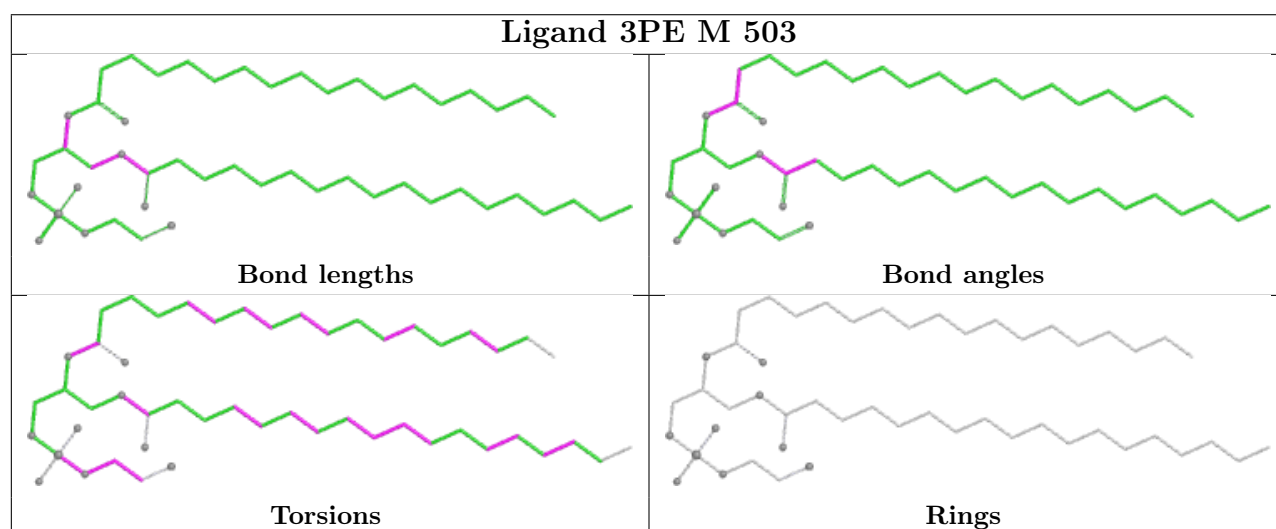
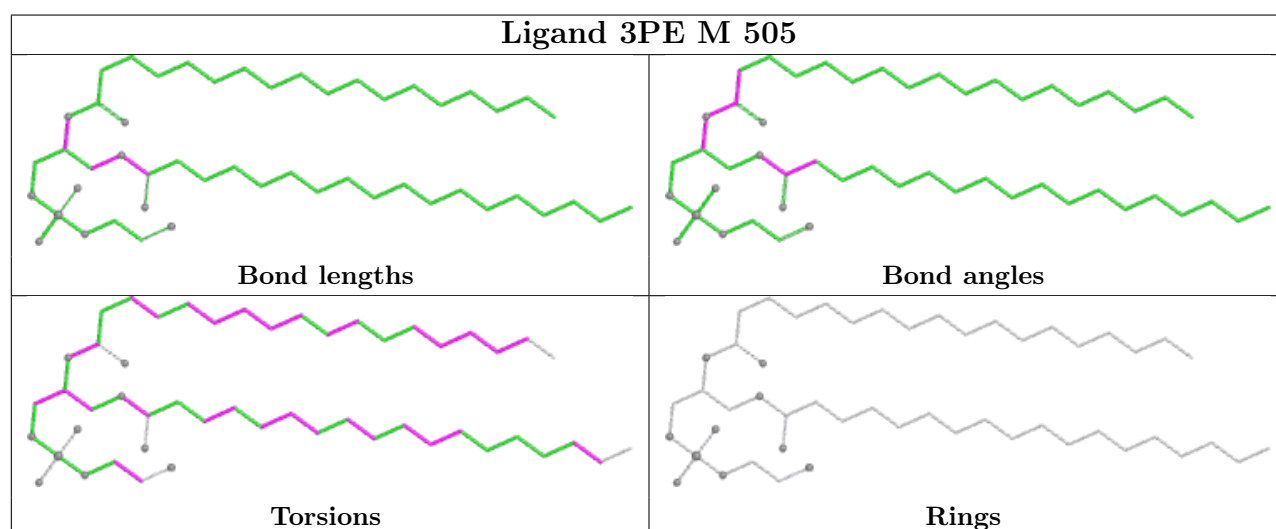
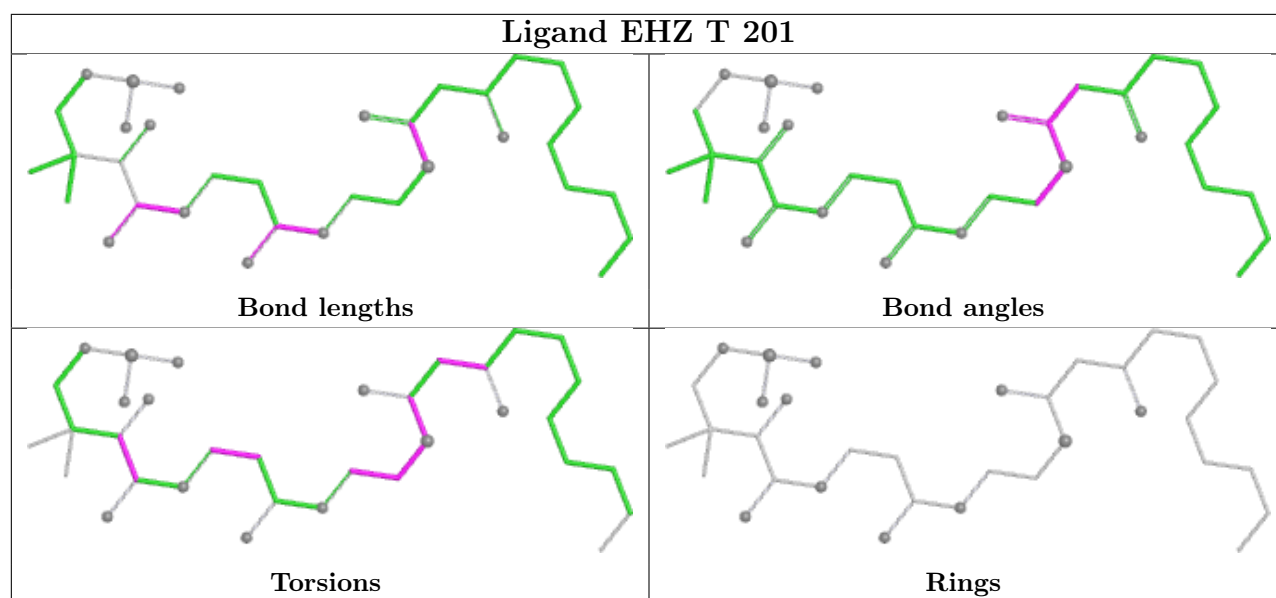
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	H	403	3PE	1	0
49	H	406	PC1	1	0
46	G	801	SF4	1	0
45	L	701	3PE	1	0
54	T	201	EHZ	1	0
45	M	505	3PE	2	0
48	F	501	FMN	1	0
52	P	501	NDP	5	0
50	L	703	CDL	2	0
50	L	702	CDL	1	0
49	H	404	PC1	1	0
47	E	301	FES	1	0
50	H	405	CDL	2	0

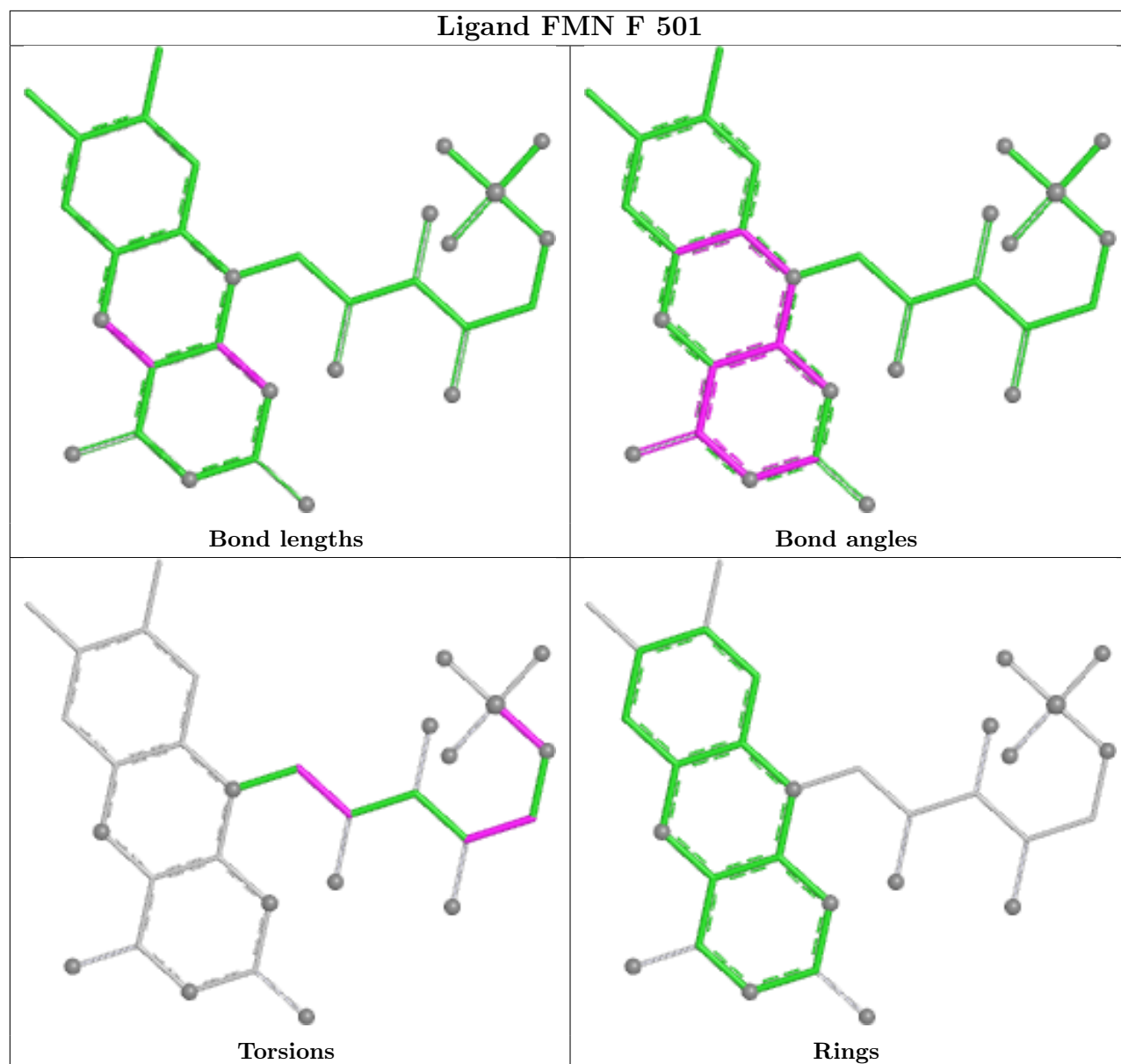
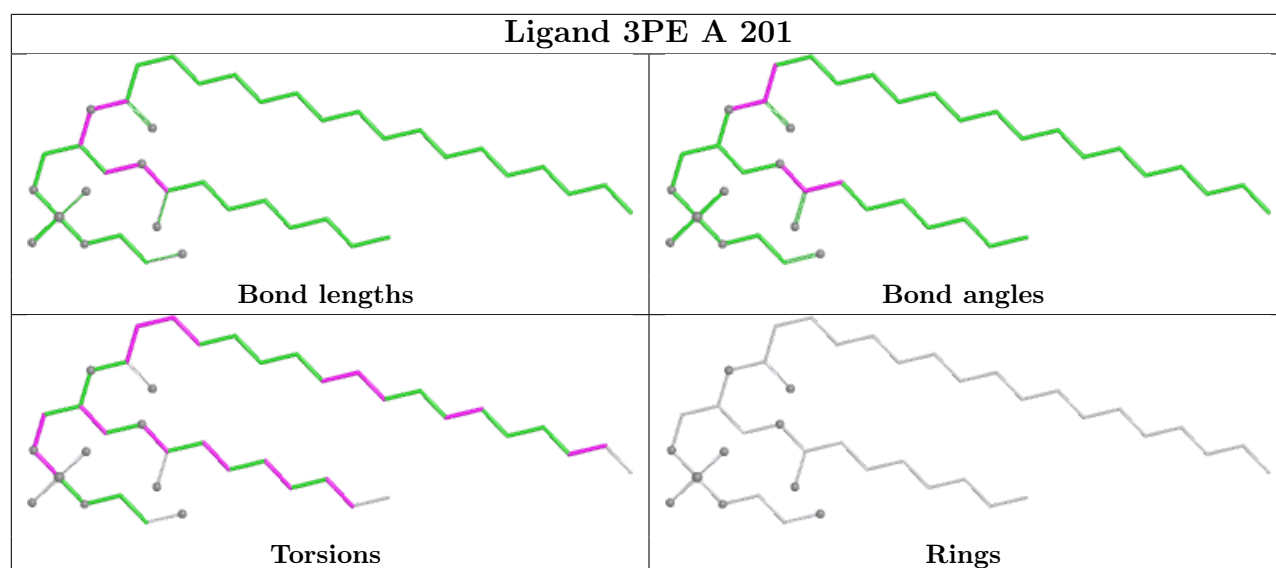
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

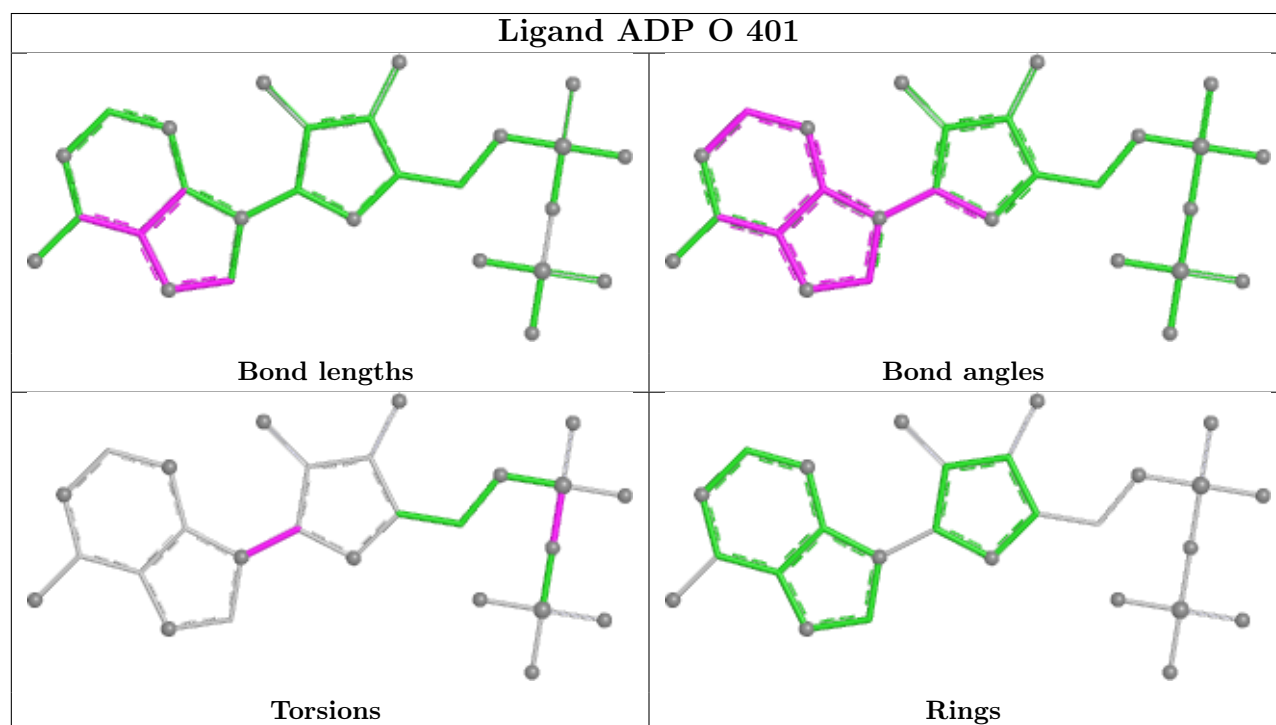
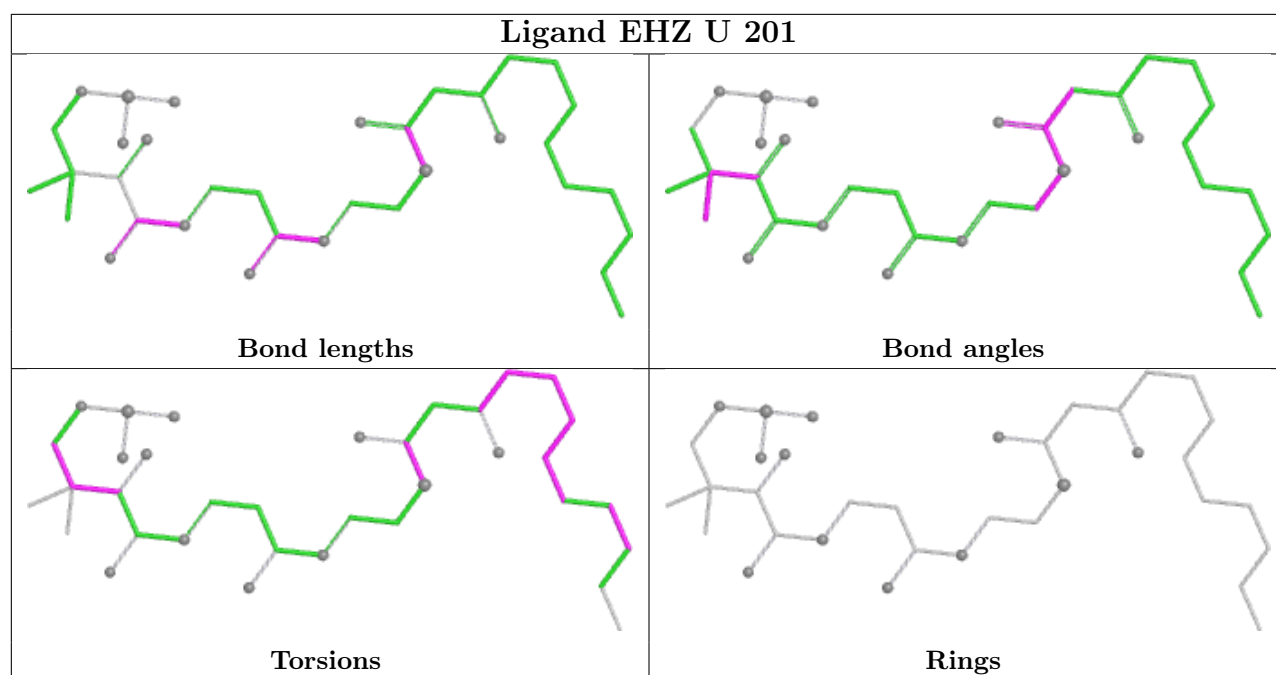
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

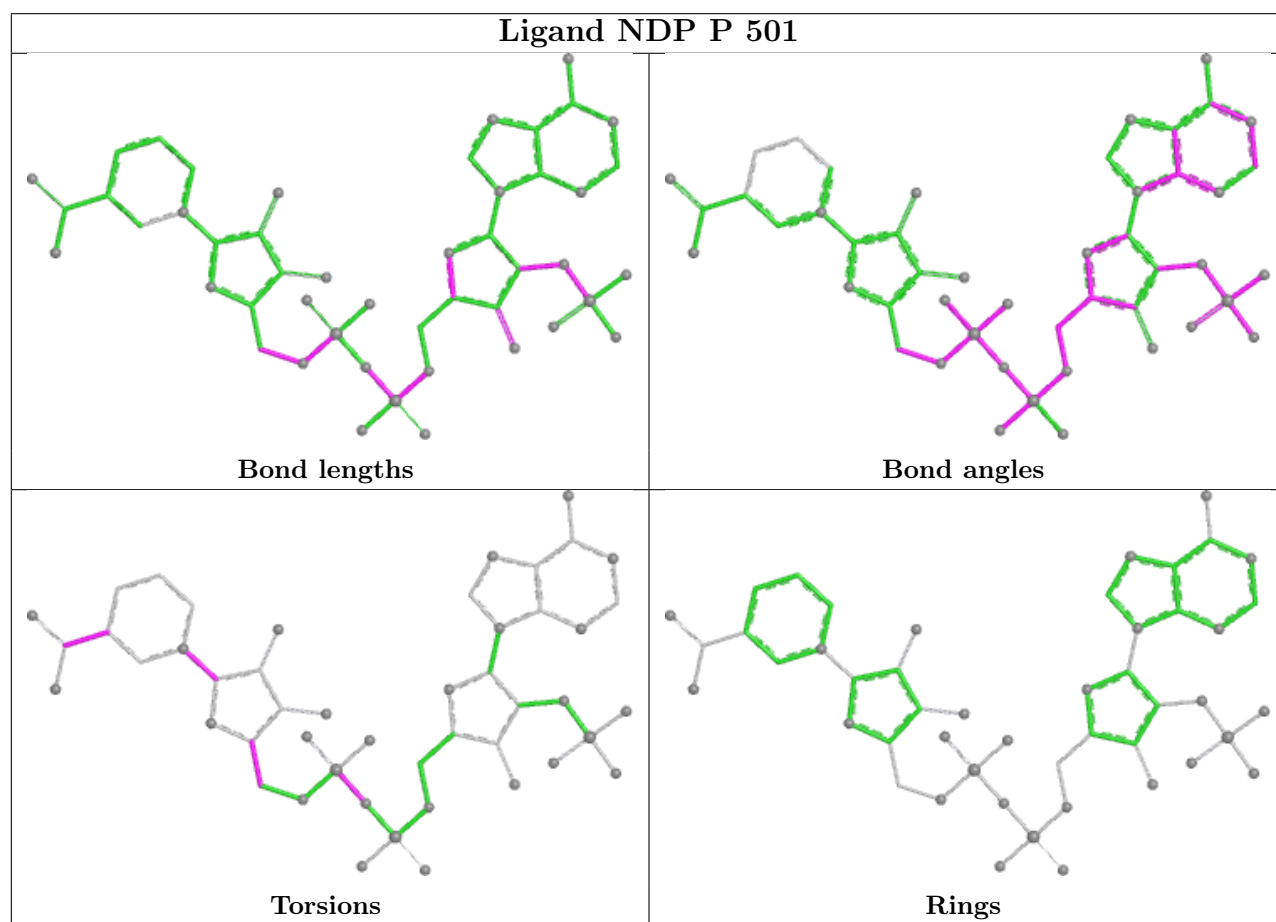
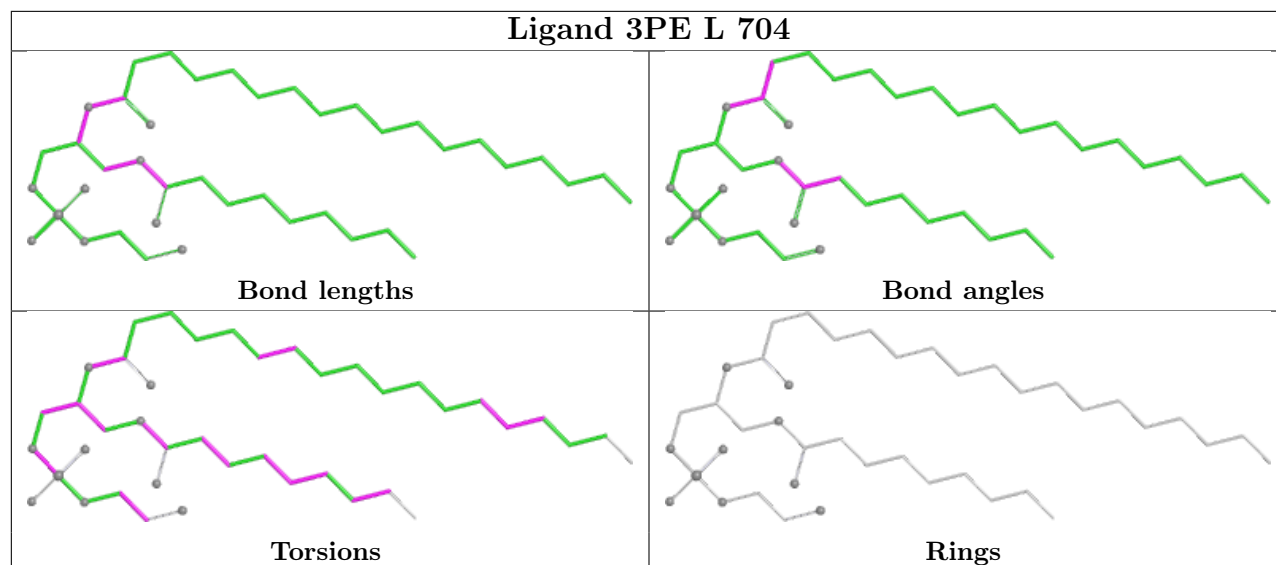


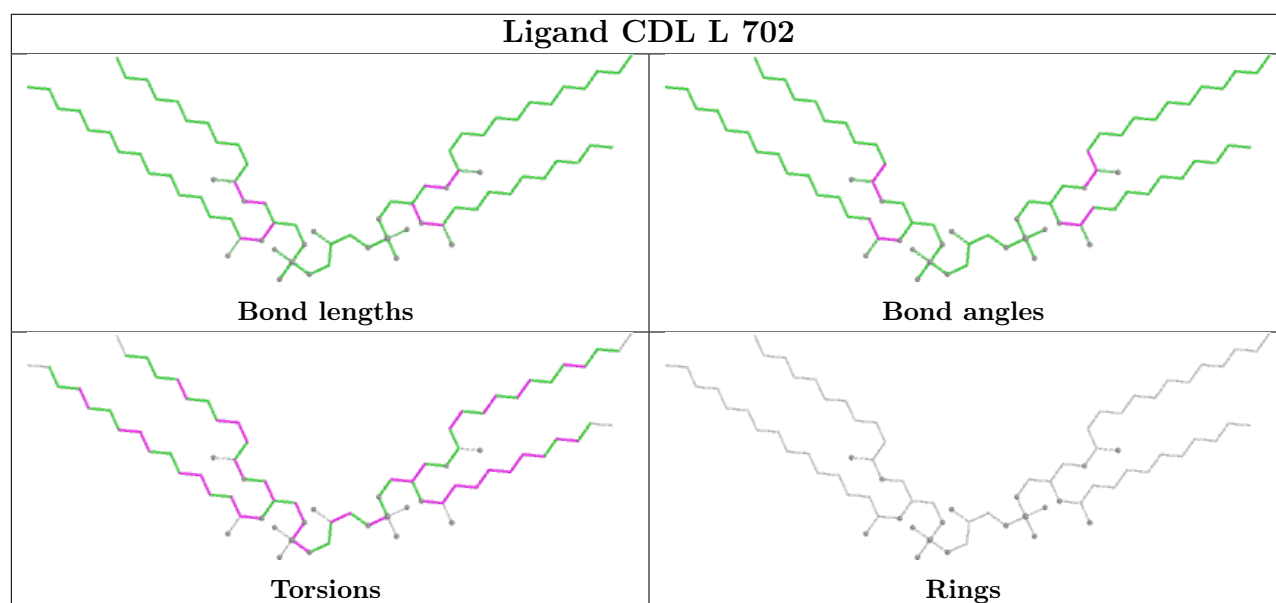
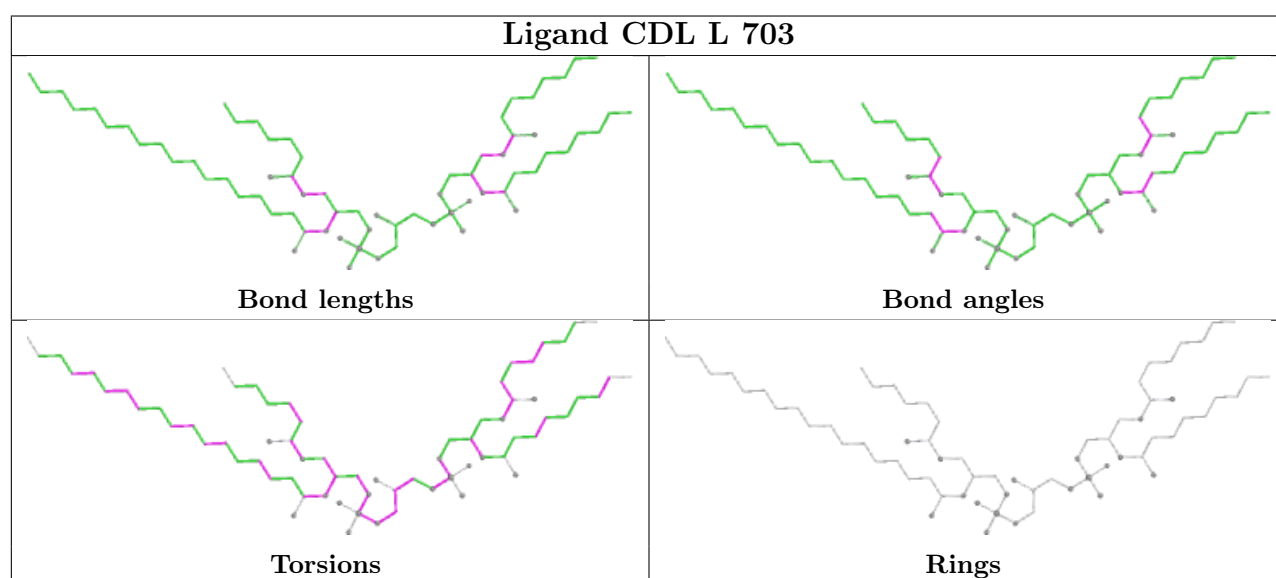
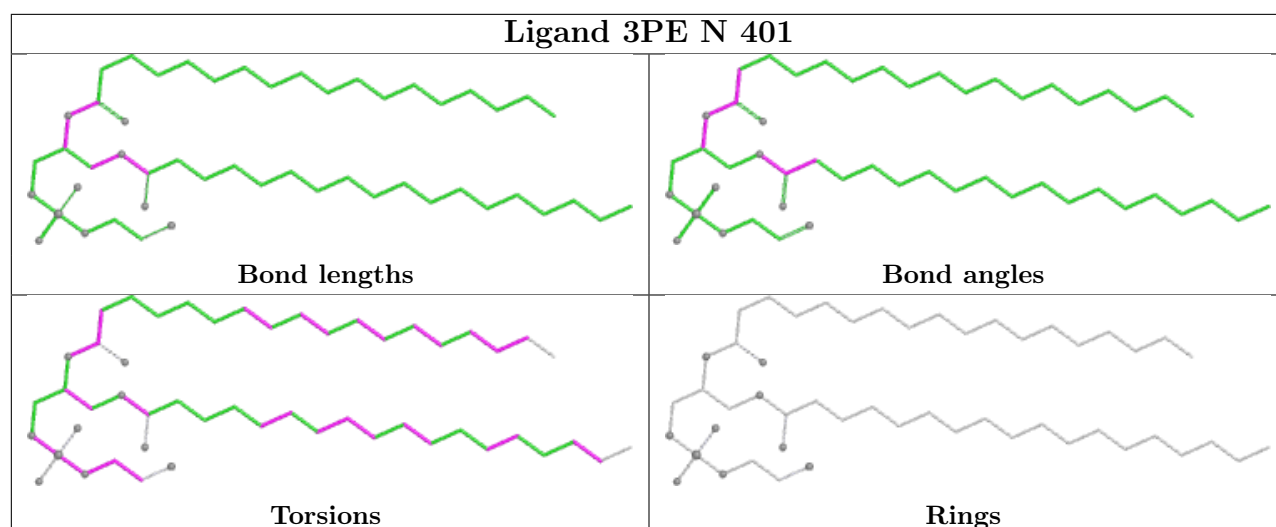


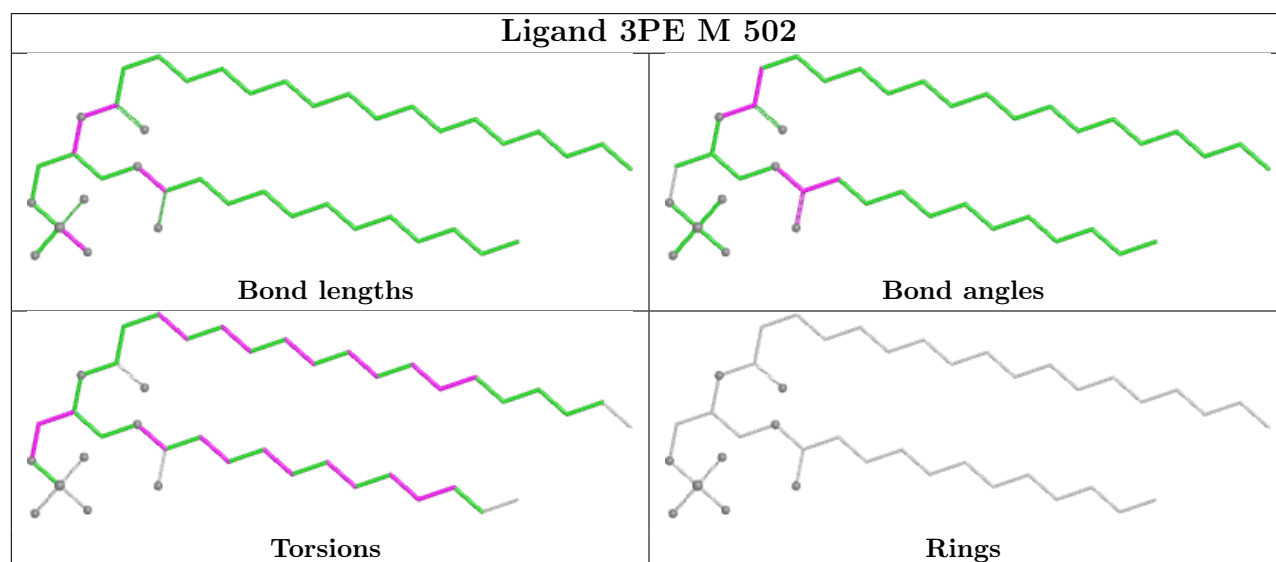
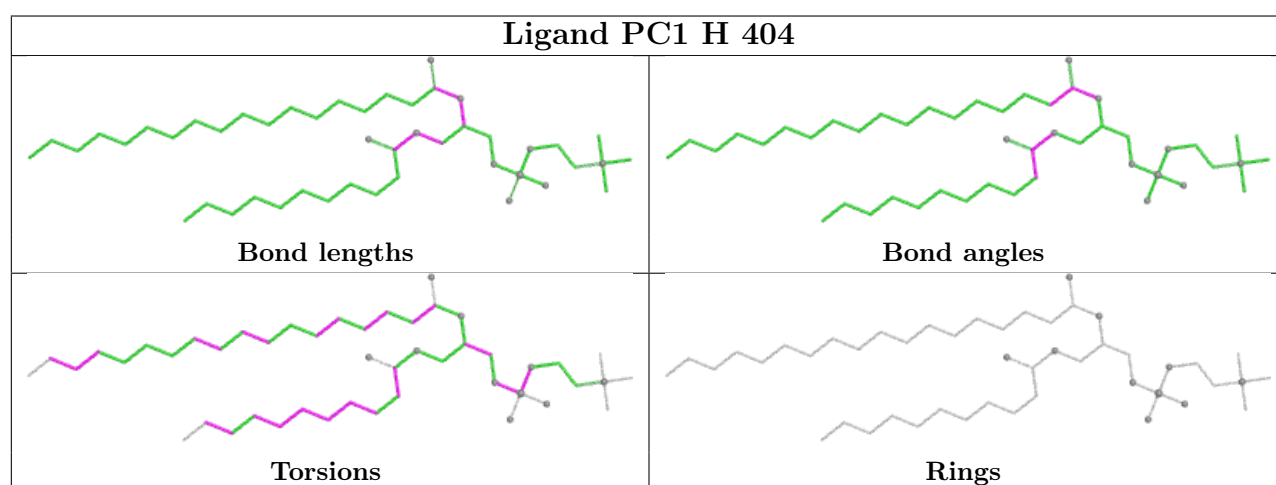
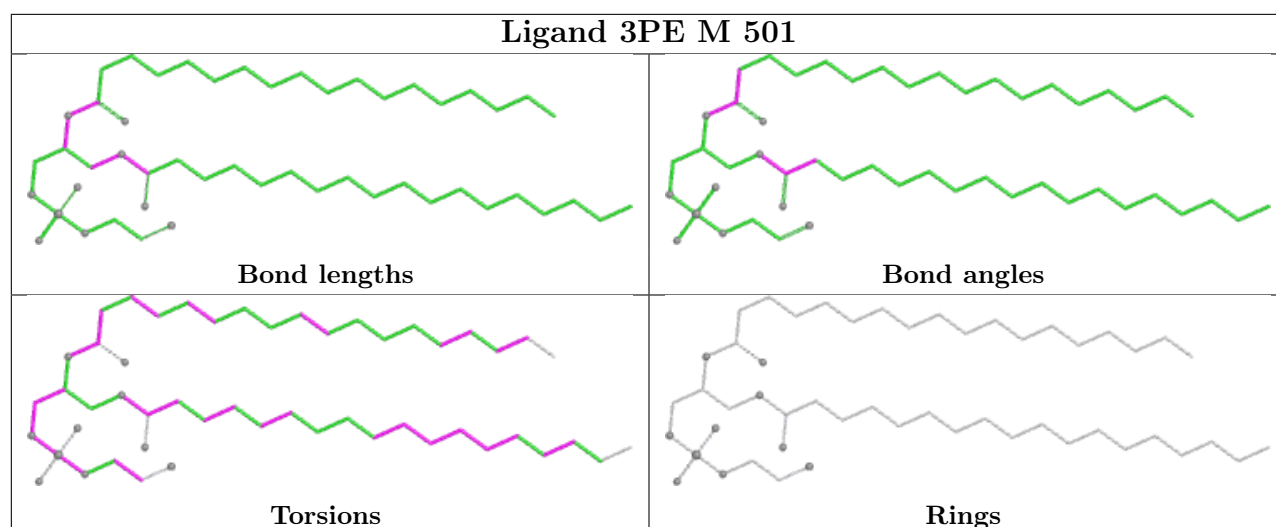


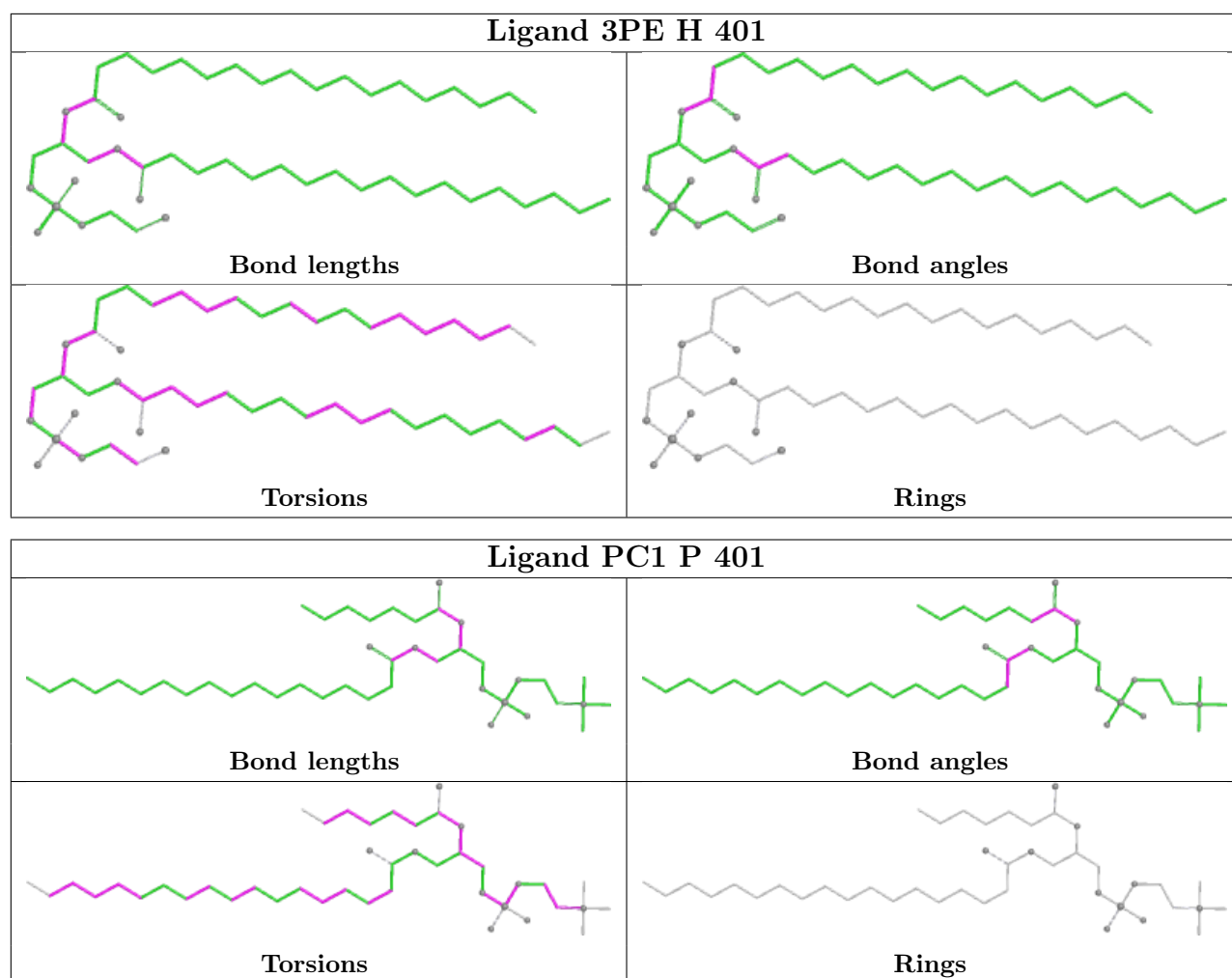


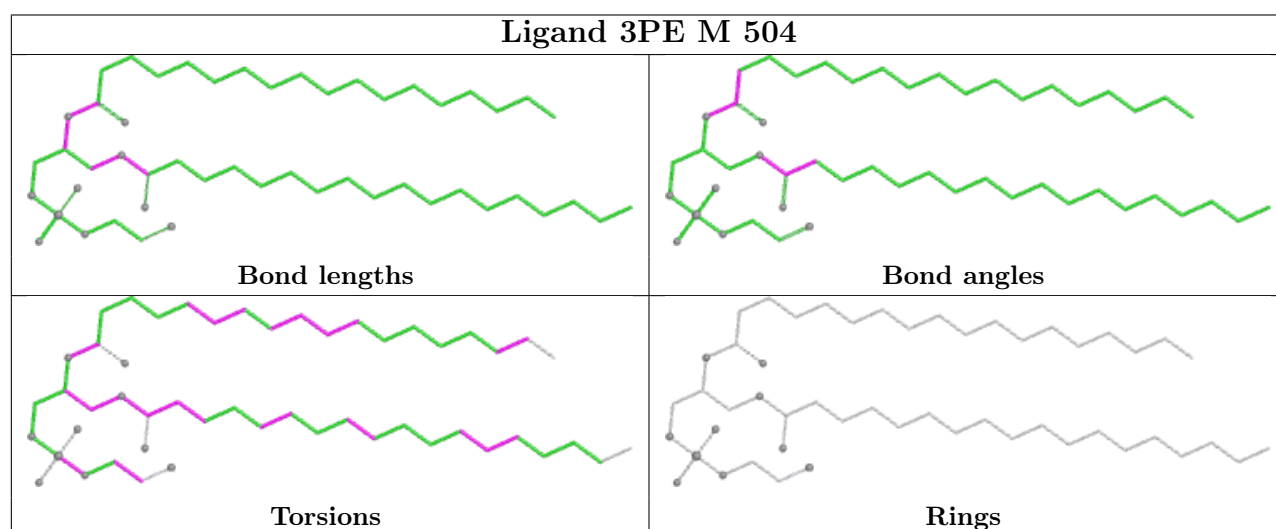
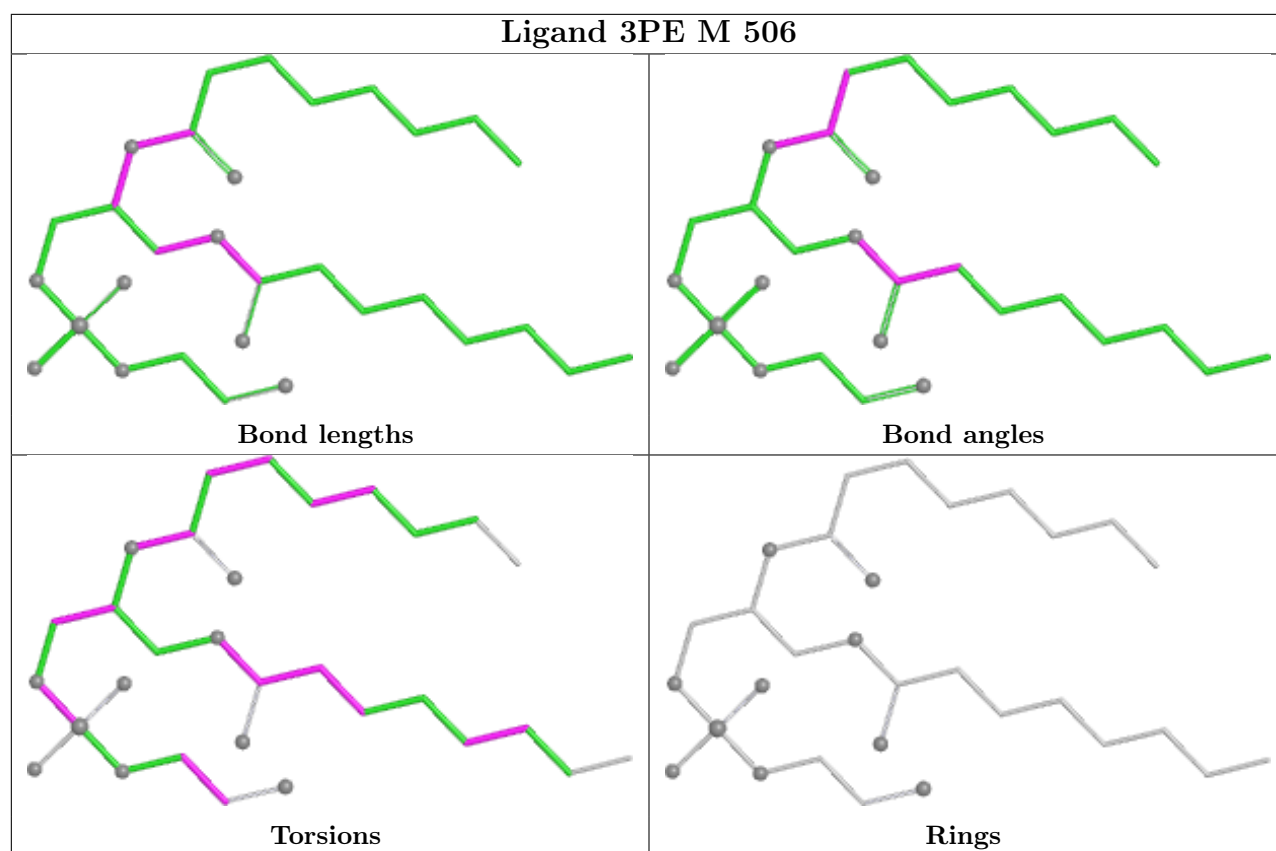


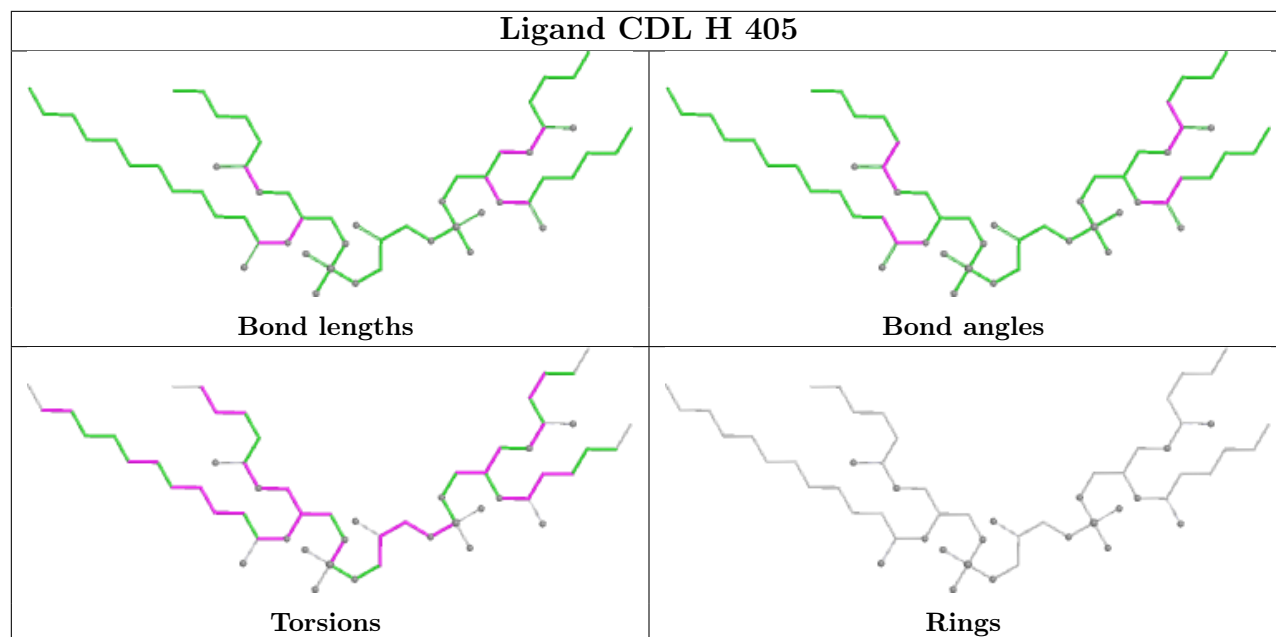












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

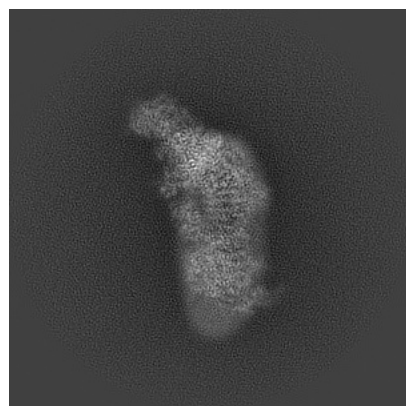
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4345. These allow visual inspection of the internal detail of the map and identification of artifacts.

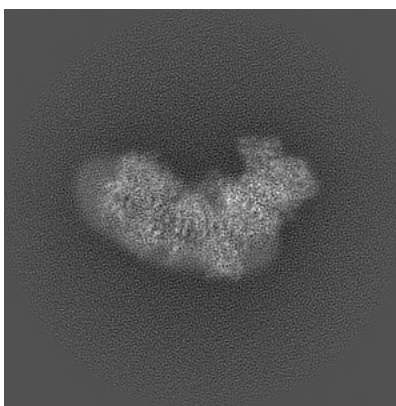
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

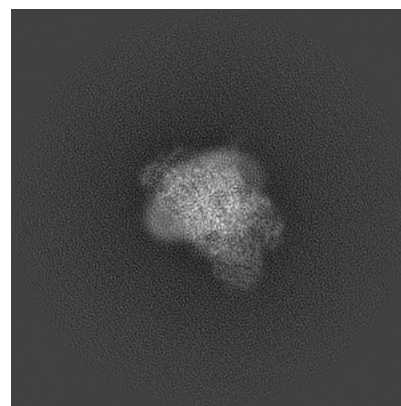
6.1.1 Primary map



X

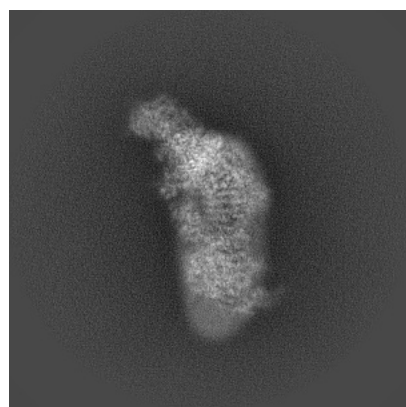


Y

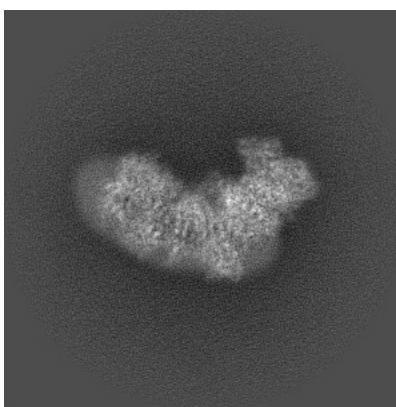


Z

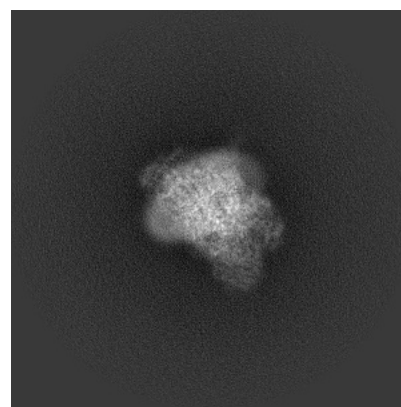
6.1.2 Raw map



X



Y

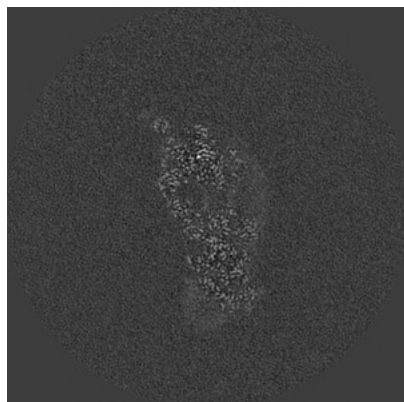


Z

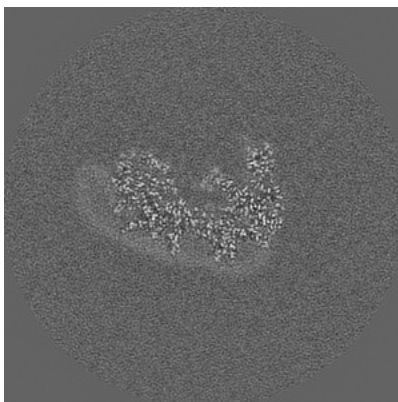
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

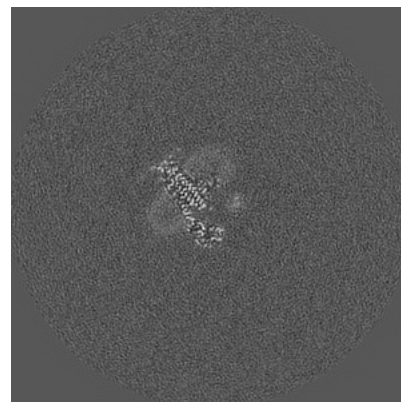
6.2.1 Primary map



X Index: 225

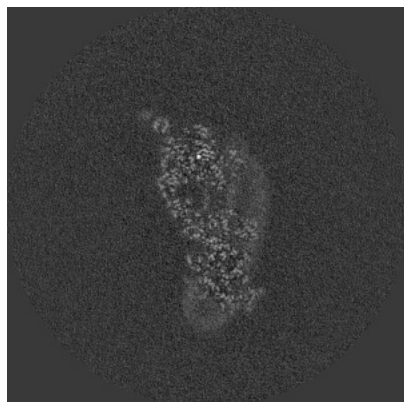


Y Index: 225

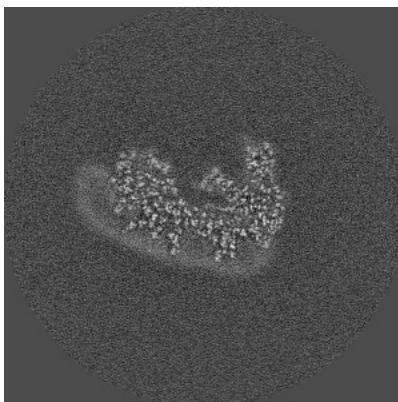


Z Index: 225

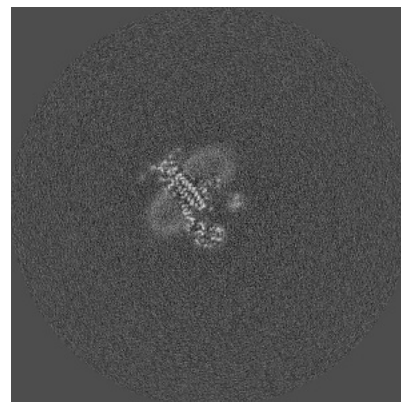
6.2.2 Raw map



X Index: 225



Y Index: 225

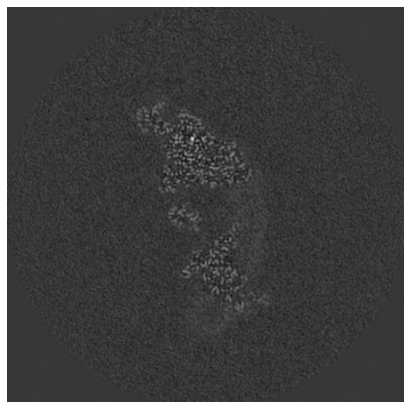


Z Index: 225

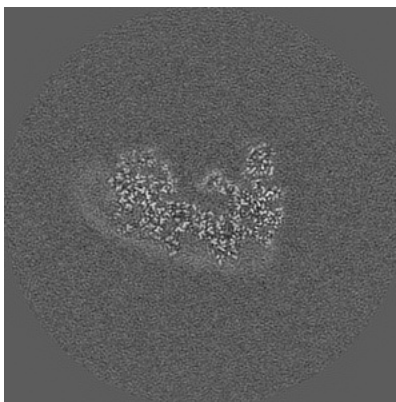
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

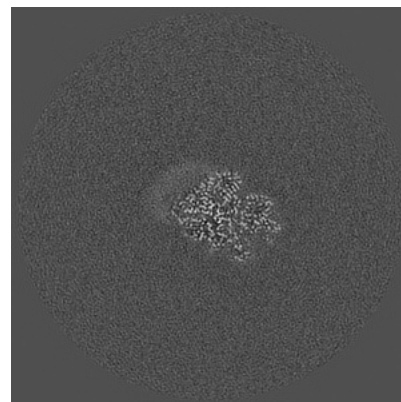
6.3.1 Primary map



X Index: 237

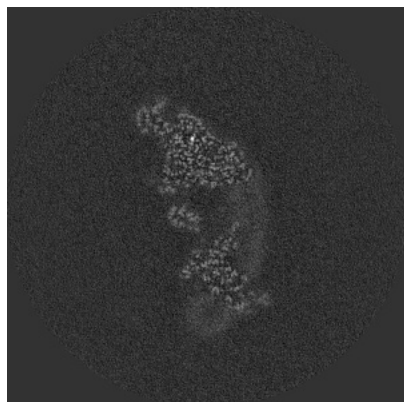


Y Index: 227

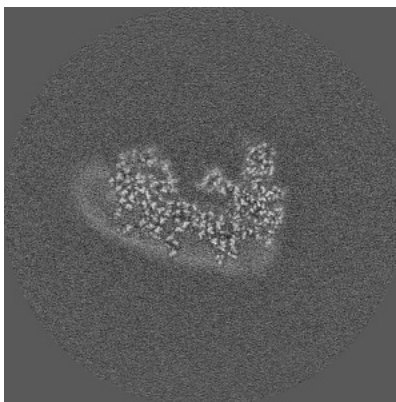


Z Index: 287

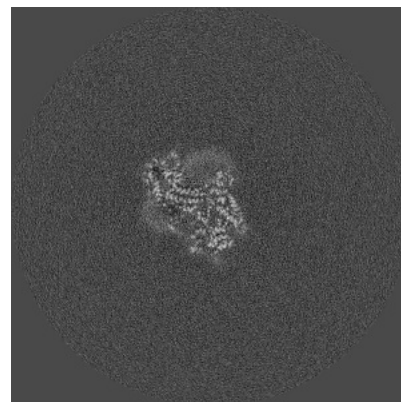
6.3.2 Raw map



X Index: 237



Y Index: 227

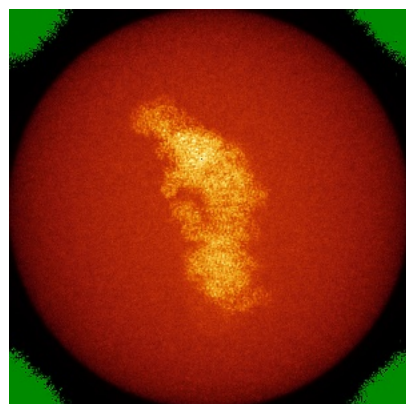


Z Index: 252

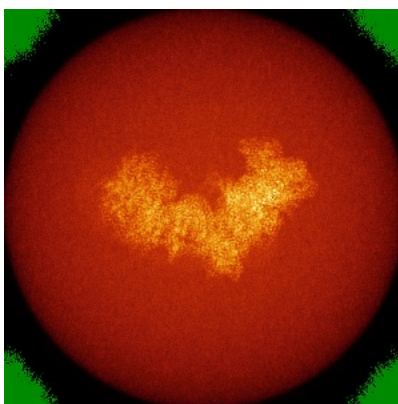
The images above show the largest variance slices of the map in three orthogonal directions.

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

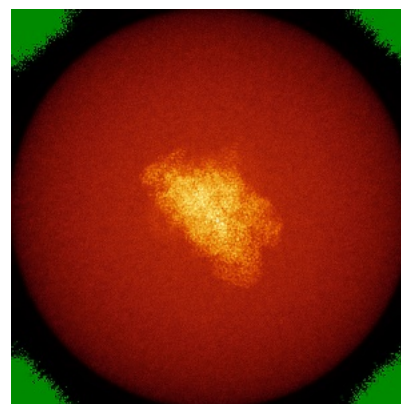
6.4.1 Primary map



X

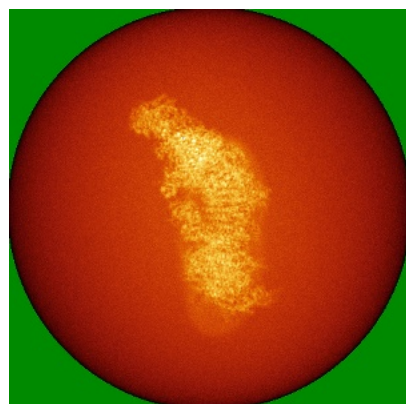


Y

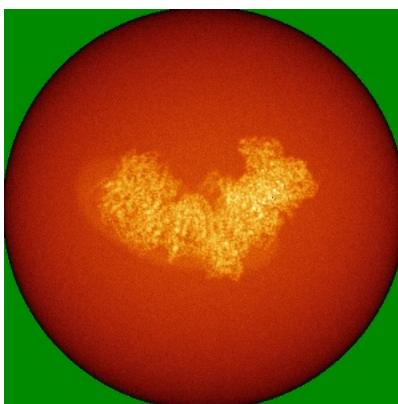


Z

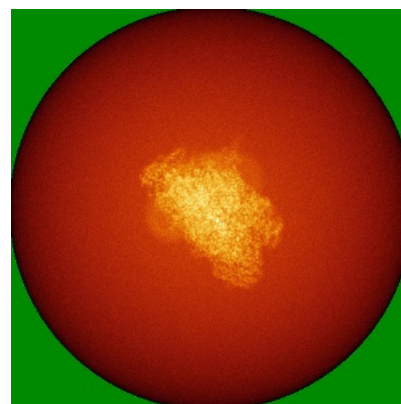
6.4.2 Raw map



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

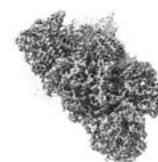
6.5.2 Raw map



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.

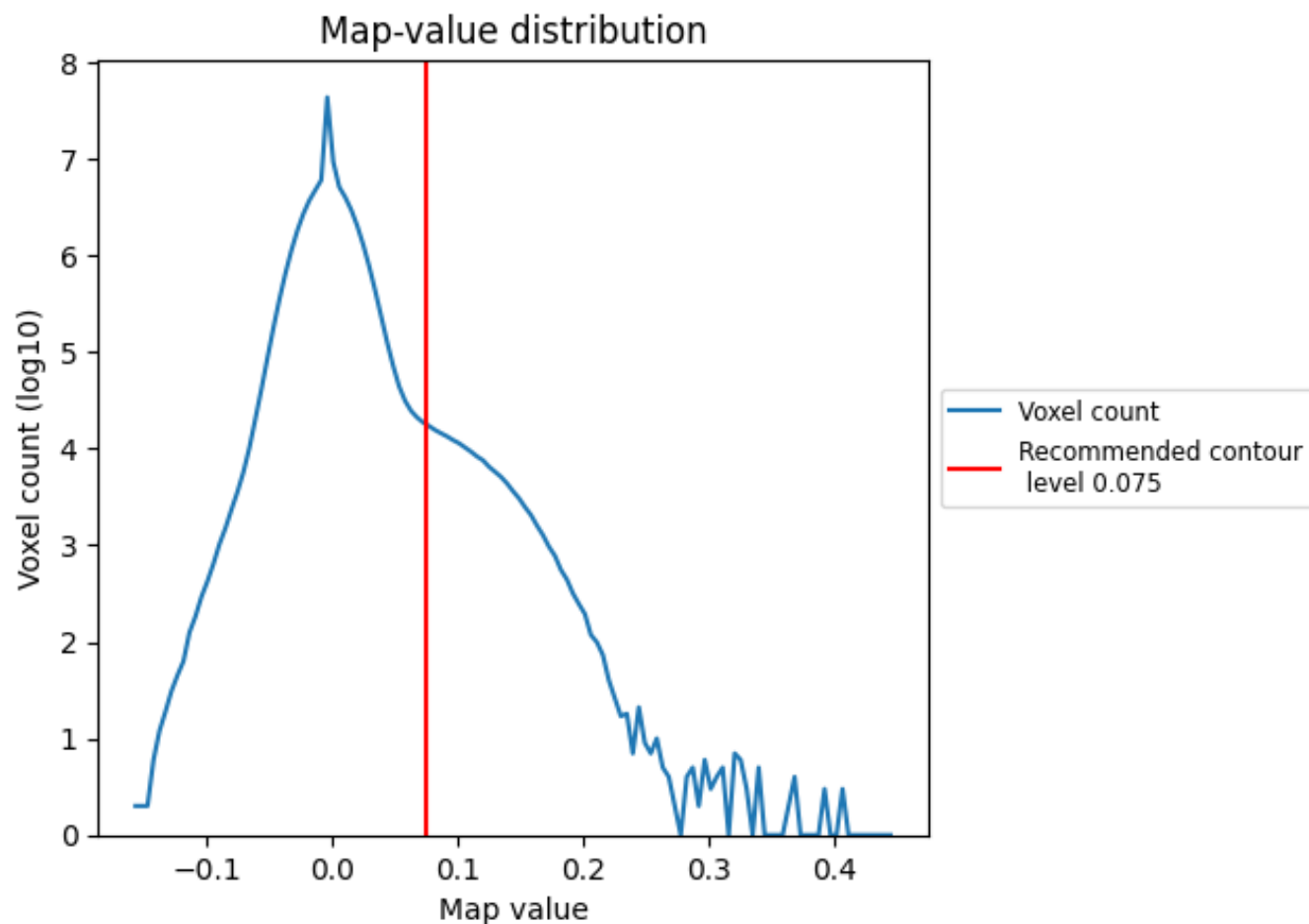
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

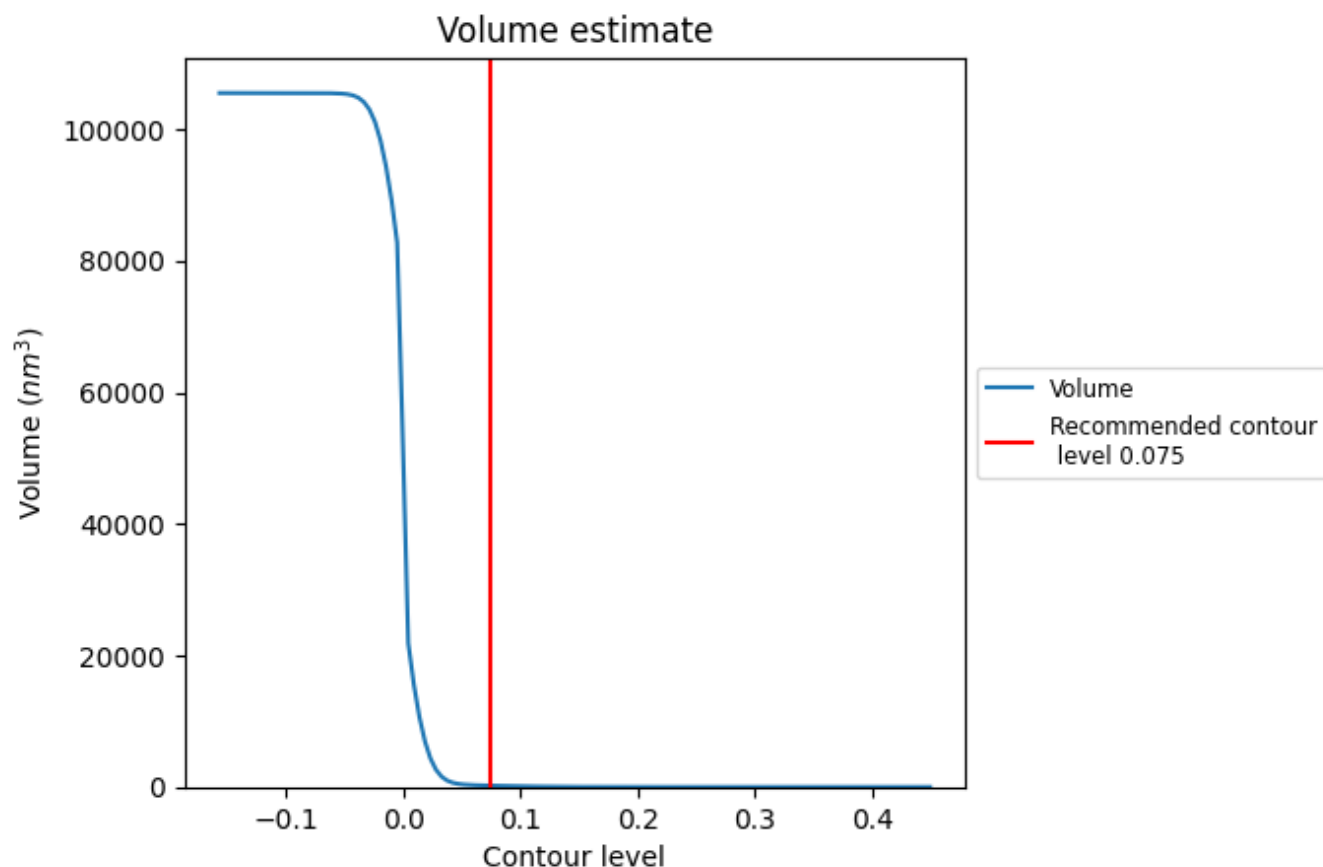
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

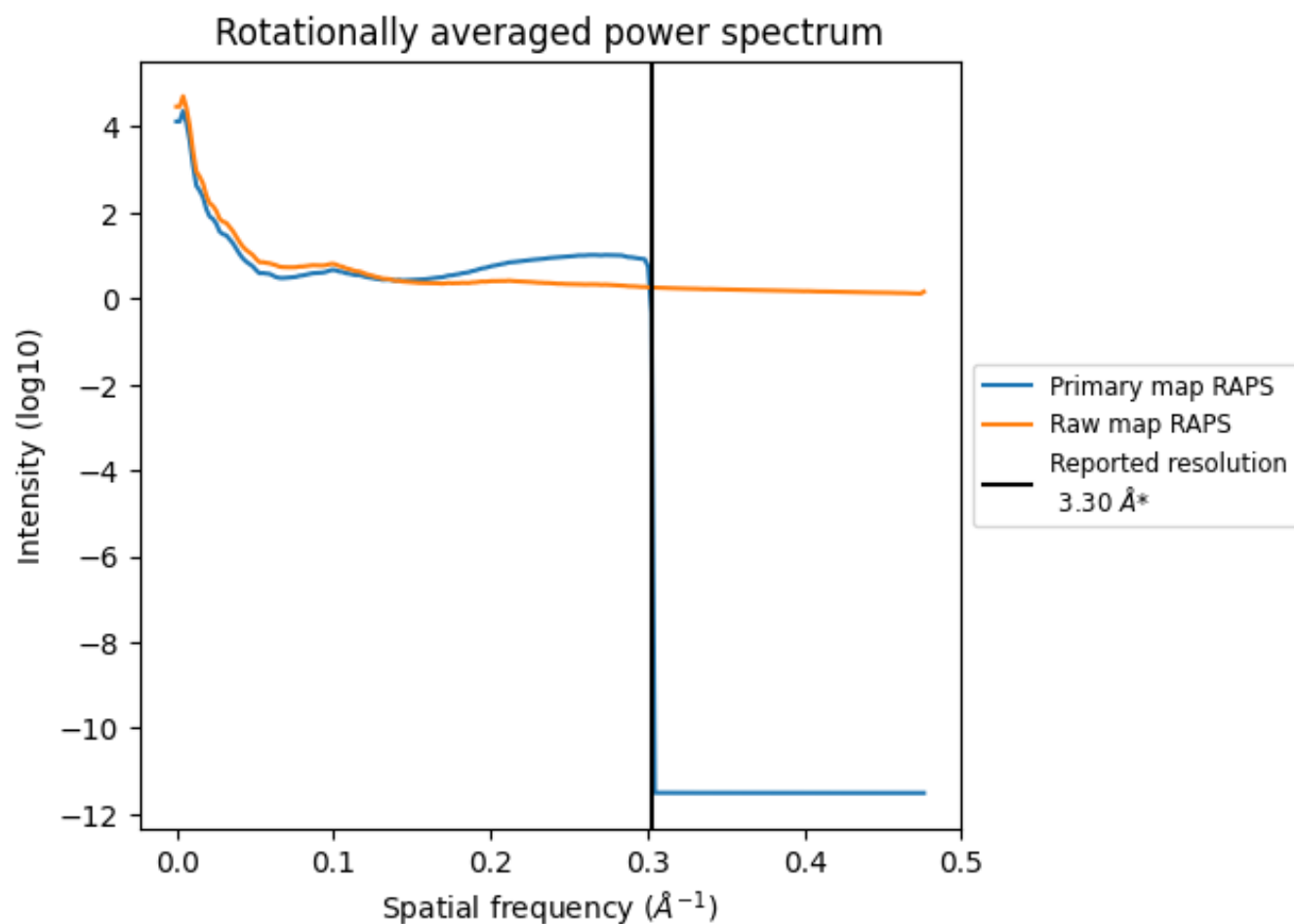
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 195 nm^3 ; this corresponds to an approximate mass of 176 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 ⓘ

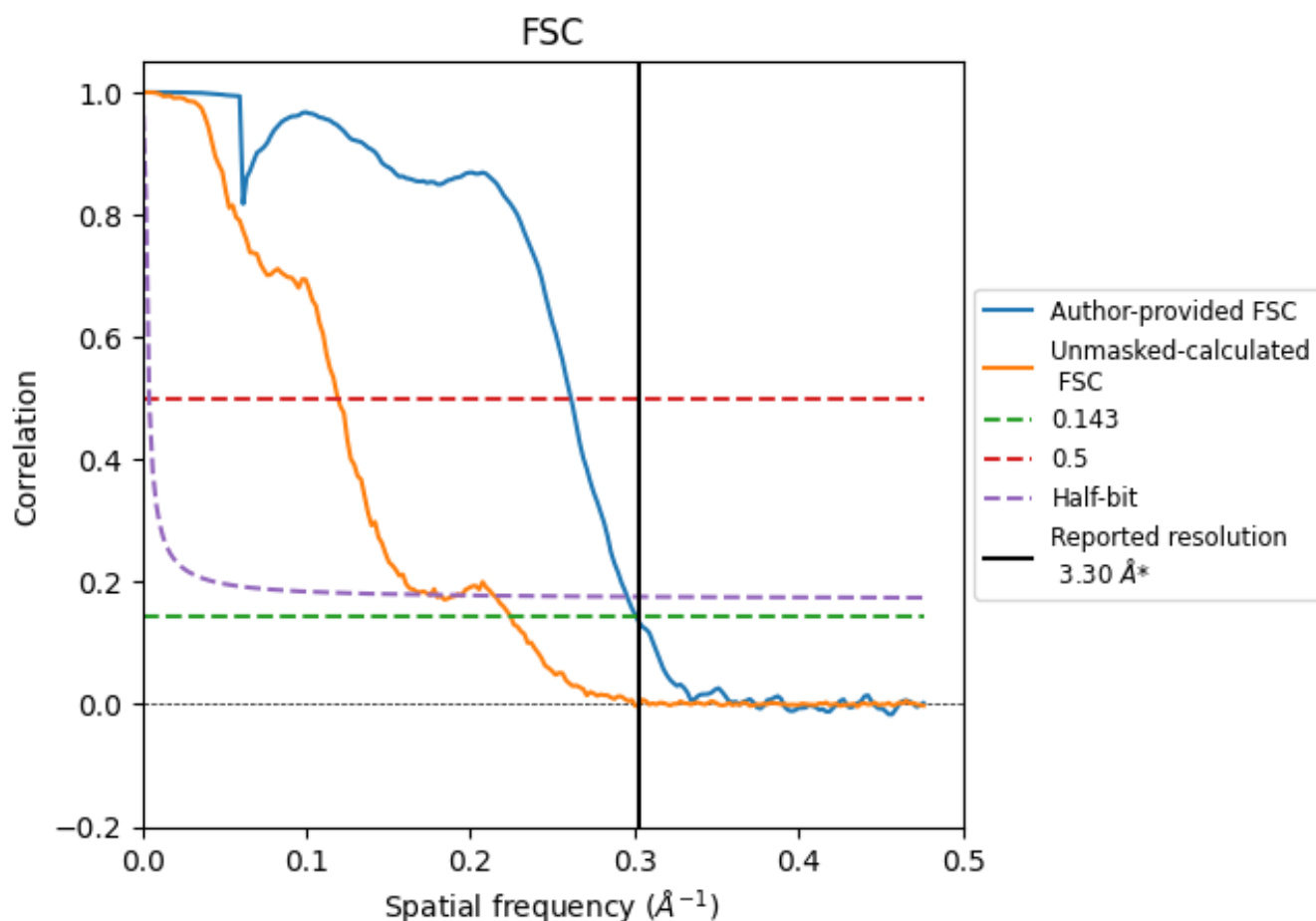


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

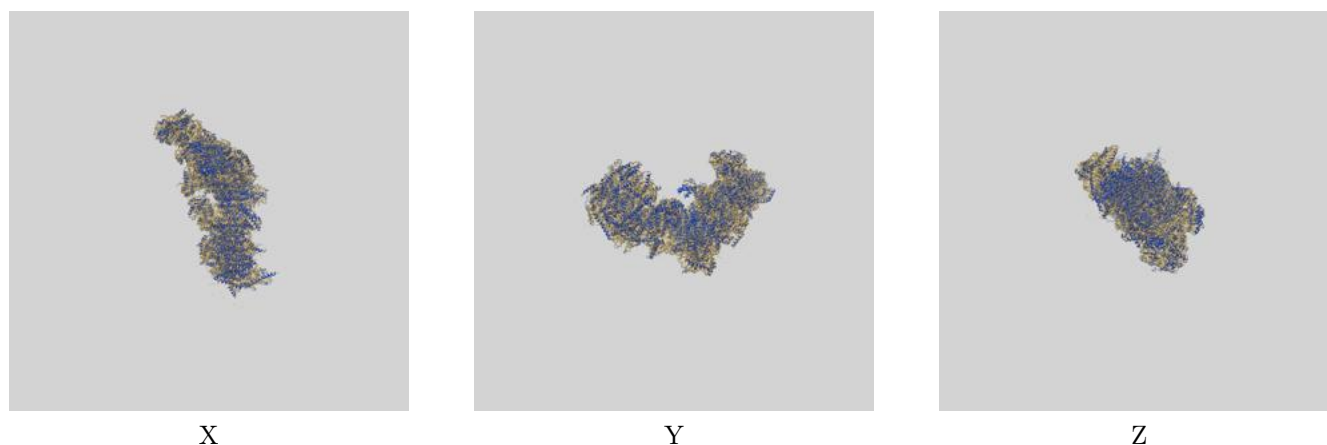
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.83	3.38
Unmasked-calculated*	4.45	8.39	5.70

*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 4.45 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

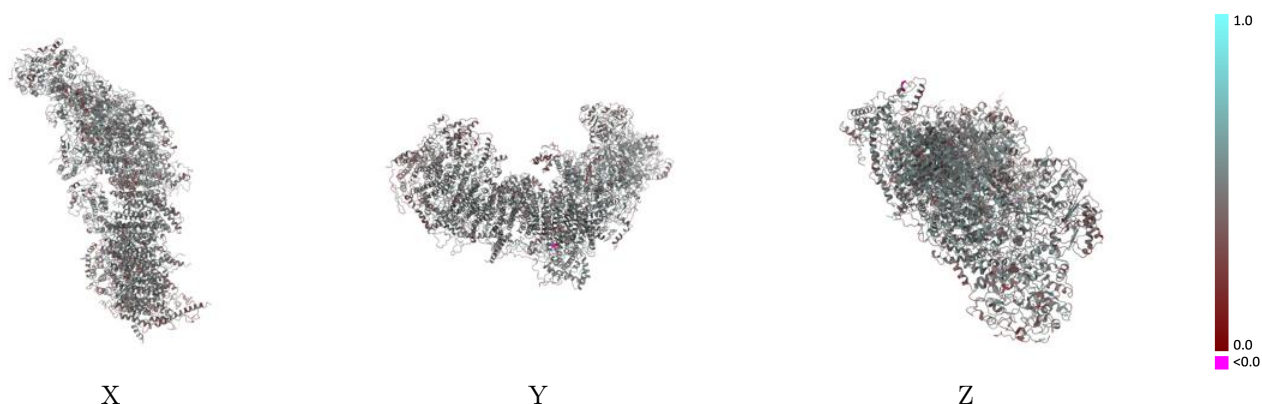
This section contains information regarding the fit between EMDB map EMD-4345 and PDB model 6G2J. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

9.1 Map-model overlay [i](#)



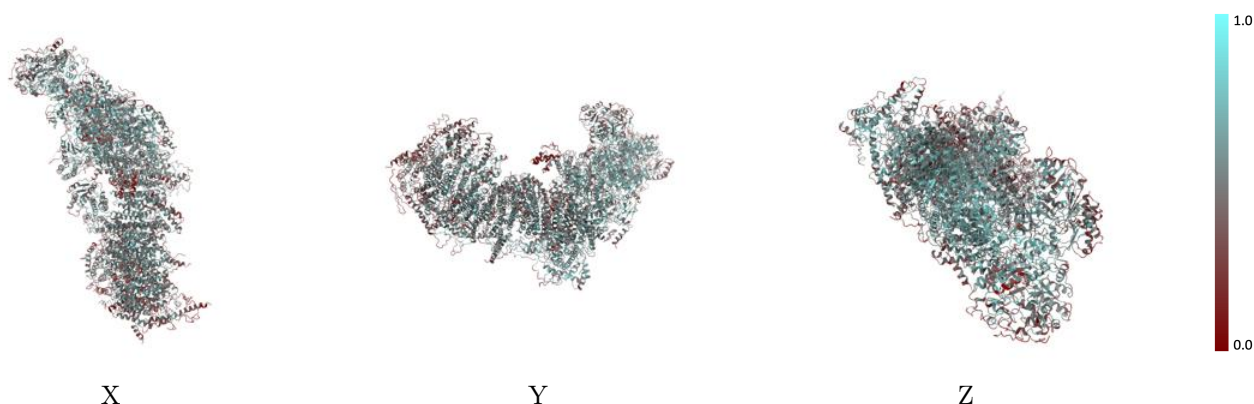
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



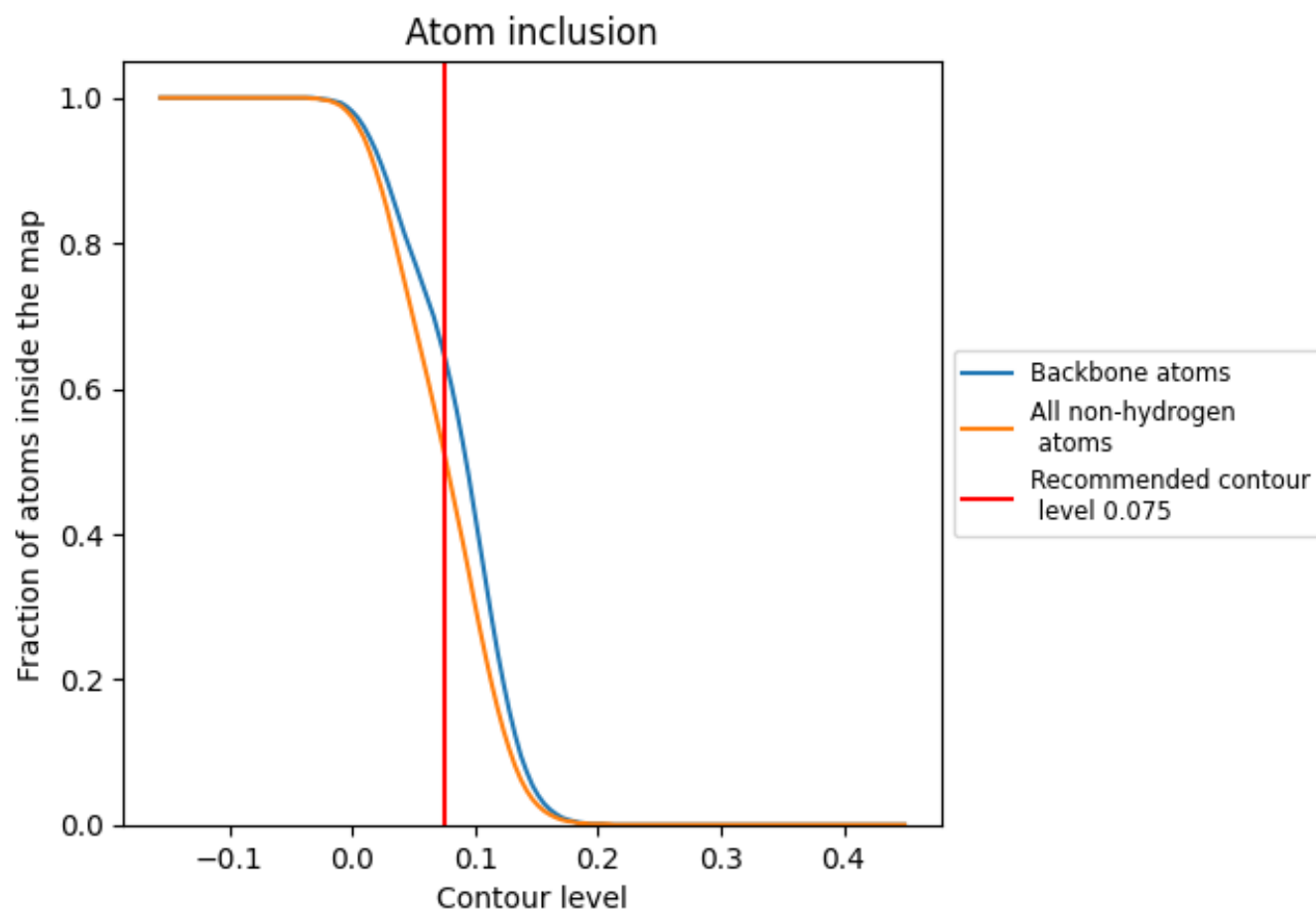
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 51% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5100	0.4690
A	0.5090	0.4820
B	0.6560	0.5030
C	0.6030	0.4980
D	0.6180	0.5020
E	0.4470	0.4570
F	0.4940	0.4600
G	0.5380	0.4760
H	0.5600	0.4960
I	0.6520	0.5070
J	0.4830	0.4650
K	0.5650	0.4900
L	0.4970	0.4760
M	0.5580	0.5020
N	0.5770	0.4920
O	0.5030	0.4640
P	0.5170	0.4680
Q	0.5330	0.4850
R	0.5400	0.4850
S	0.4140	0.4400
T	0.1780	0.3630
U	0.3540	0.4140
V	0.4730	0.4550
W	0.4950	0.4640
X	0.5180	0.4720
Y	0.4350	0.4490
Z	0.5160	0.4500
a	0.5670	0.4960
b	0.4630	0.4310
c	0.3810	0.4180
d	0.4960	0.4650
e	0.5200	0.4630
f	0.4180	0.4250
g	0.4330	0.4570
h	0.5140	0.4690



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Chain	Atom inclusion	Q-score
i	 0.3730	 0.4220
j	 0.3510	 0.3870
k	 0.3260	 0.4250
l	 0.4560	 0.4470
m	 0.4630	 0.4640
n	 0.4240	 0.4110
o	 0.3220	 0.3870
p	 0.4600	 0.4440
q	 0.5570	 0.4780
r	 0.4950	 0.4560
s	 0.3850	 0.4410