



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 03:24 AM UTC

PDB ID : 8RGT / pdb_00008rgt
EMDB ID : EMD-19148
Title : Open Complex I from murine brain
Authors : Vercellino, I.; Sazanov, L.A.
Deposited on : 2023-12-14
Resolution : 3.10 Å(reported)
Based on initial model : 6g2j

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:

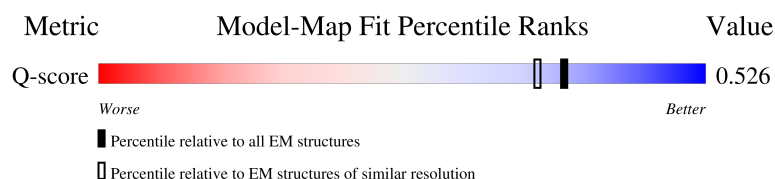
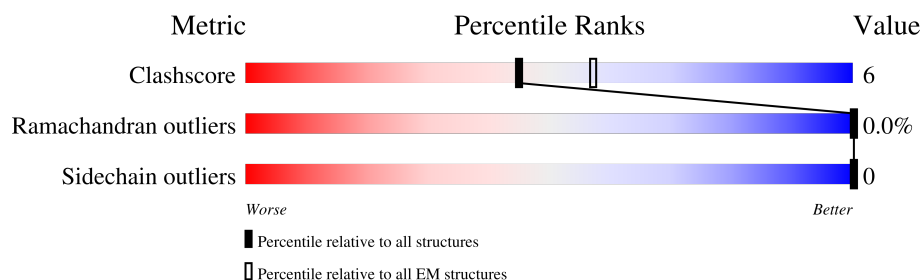
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.10 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	14724 (2.60 - 3.60)

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	6	224	 58% 12% 30%
2	C	263	 67% 12% 21%
3	D	463	 74% 17% 10%
4	2	248	 71% 15% 14%

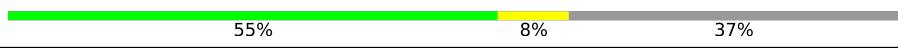
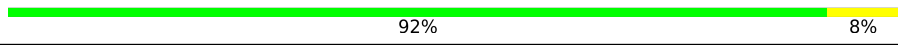
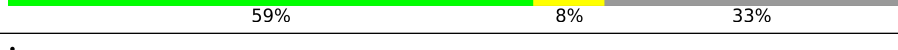
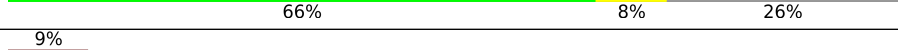
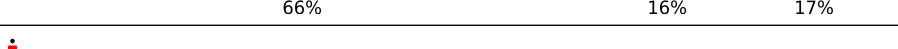
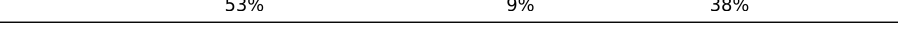
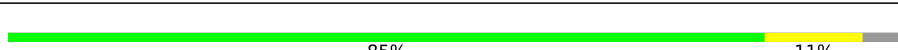
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Mol	Chain	Length	Quality of chain
5	1	464	
6	3	727	
7	9	212	
8	P	377	
9	Q	175	
10	7	116	
11	S	99	
12	T	156	
12	U	156	
13	V	116	
14	W	131	
15	q	145	
16	r	113	
17	s	104	
18	A	115	
19	H	318	
20	J	172	
21	K	98	
22	L	607	
23	M	459	
24	N	345	
25	O	355	
26	X	172	
27	Y	141	
28	Z	144	

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Mol	Chain	Length	Quality of chain
29	a	70	
30	b	84	
31	c	76	
32	d	120	
33	e	106	
34	f	57	
35	g	151	
36	h	189	
37	i	128	
38	j	105	
39	k	104	
40	l	186	
41	m	129	
42	n	179	
43	o	137	
44	p	176	

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 67123 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 dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	6	157	Total	C	N	O	S	0	0
			1258	802	227	215	14		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	208	Total	C	N	O	S	0	0
			1730	1116	297	314	3		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	418	Total	C	N	O	S	0	0
			3371	2156	577	614	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	214	Total	C	N	O	S	0	0
			1660	1056	279	314	11		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1	430	Total	C	N	O	S	0	0
			3321	2092	596	611	22		

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3	690	Total	C	N	O	S	0	0
			5305	3326	921	1017	41		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	314	Total	C	N	O	S	0	0
			2513	1611	453	442	7		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	126	Total	C	N	O	S	0	0
			1022	646	180	192	4		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	7	96	Total	C	N	O	S	0	0
			758	470	141	144	3		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	84	Total	C	N	O	S	0	0
			671	421	127	120	3		

- Molecule 12 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	79	Total	C	N	O	S	0	0
			637	410	95	127	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	88	Total	C	N	O	S	0	0
			706	453	104	144	5		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	113	Total	C	N	O	S	0	0
			923	602	153	165	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

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

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	q	145	Total	C	N	O	S	0	0
			1209	777	215	212	5		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	r	97	Total	C	N	O	S	0	0
			781	493	146	139	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	s	42	Total	C	N	O	0	0
			351	219	62	70		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A	94	Total	C	N	O	S	0	0
			771	533	108	125	5		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	H	306	Total	C	N	O	S	0	0
			2452	1652	371	407	22		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	164	Total	C	N	O	S	0	0
			1240	834	177	214	15		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	345	Total	C	N	O	S	0	0
			2703	1795	417	454	37		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	141	Total	C	N	O	S	0	0
			1167	750	207	202	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	70	Total	C	N	O	S	0	0
			572	370	101	97	4		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	82	Total	C	N	O	S	0	0
			643	422	104	113	4		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	48	Total	C	N	O	S	0	0
			398	261	69	67	1		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	53	Total	C	N	O	S	0	0
			456	295	82	77	2		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	139	Total	C	N	O	S	0	0
			1166	764	195	204	3		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	106	Total	C	N	O	S	0	0
			897	584	157	152	4		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	65	Total	C	N	O	S	0	0
			562	370	93	98	1		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	k	77	Total	C	N	O	S	0	0
			626	414	106	104	2		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	157	Total	C	N	O	S	0	0
			1323	855	220	237	11		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	m	126	Total	C	N	O	0	0
			1050	676	189	185		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		

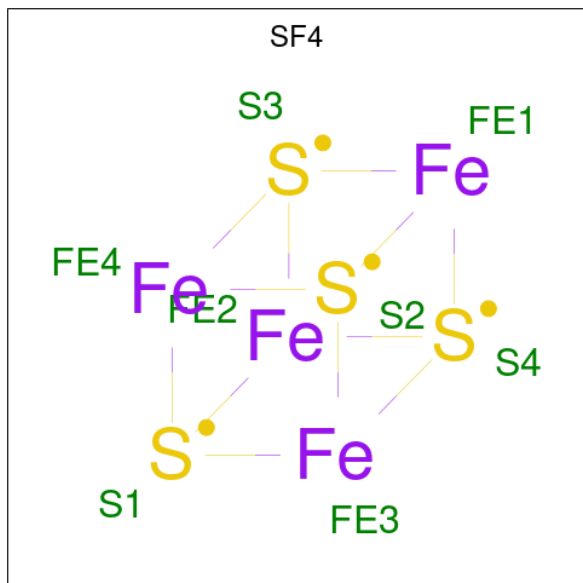
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	118	Total	C	N	O	S	0	0
			1014	639	190	177	8		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

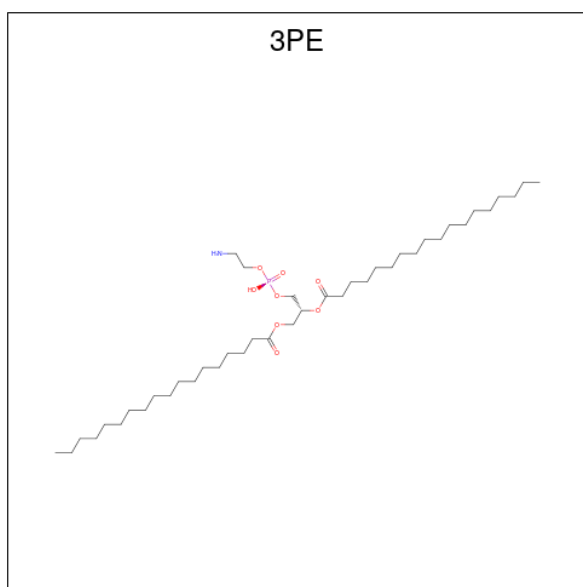
Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	169	Total	C	N	O	S	0	0
			1430	899	257	266	8		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
45	6	1	Total	Fe	S	0
			8	4	4	
45	1	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	9	1	Total	Fe	S	0
			8	4	4	
45	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $\text{C}_{41}\text{H}_{82}\text{NO}_8\text{P}$).



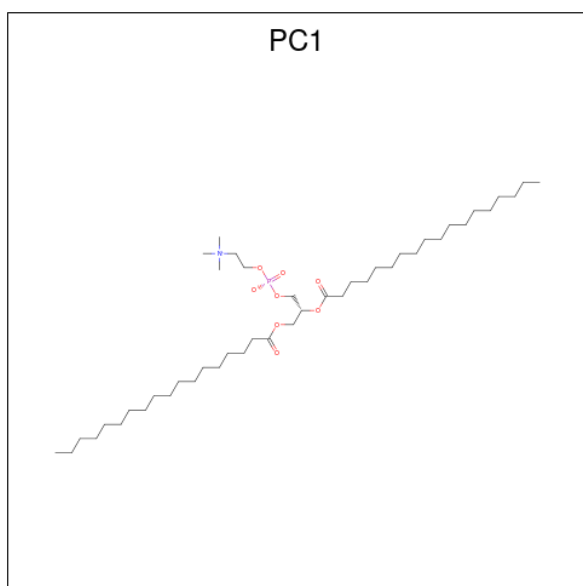
Mol	Chain	Residues	Atoms					AltConf
46	6	1	Total	C	N	O	P	0
			32	22	1	8	1	
46	r	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	K	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	M	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	N	1	Total	C	N	O	P	0
			38	28	1	8	1	
46	Y	1	Total	C	N	O	P	0
			28	18	1	8	1	
46	d	1	Total	C	N	O	P	0
			31	21	1	8	1	
46	d	1	Total	C	N	O	P	0
			32	22	1	8	1	

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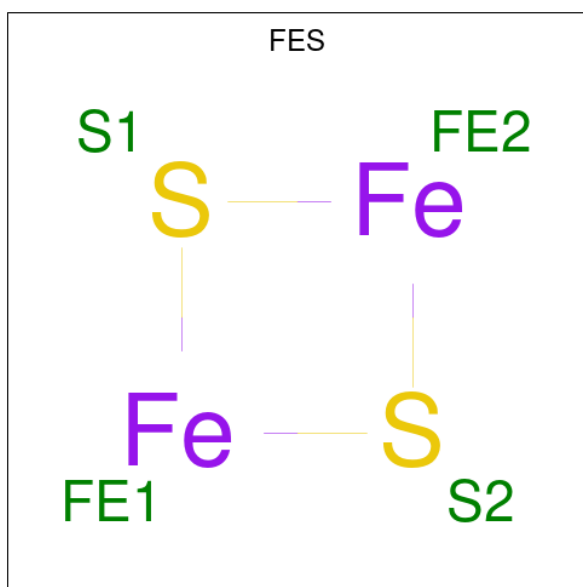
Mol	Chain	Residues	Atoms					AltConf
46	h	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	i	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	m	1	Total	C	N	O	P	0
			30	20	1	8	1	

- Molecule 47 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



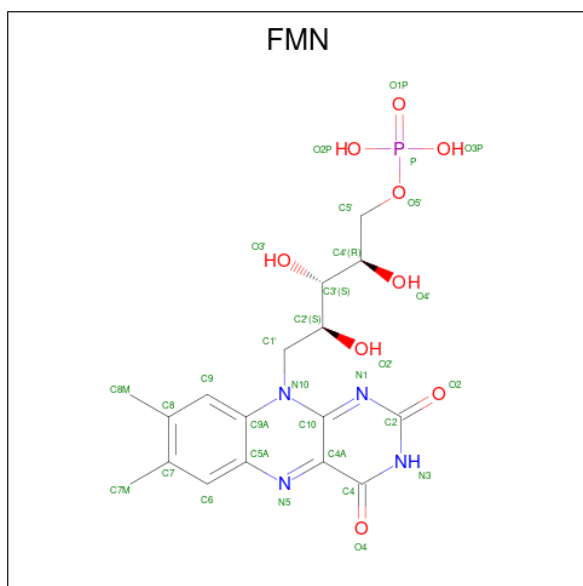
Mol	Chain	Residues	Atoms					AltConf
47	6	1	Total	C	N	O	P	0
			43	33	1	8	1	
47	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
47	9	1	Total	C	N	O	P	0
			47	37	1	8	1	
47	M	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
48	2	1	Total	Fe	S	0
			4	2	2	
48	3	1	Total	Fe	S	0
			4	2	2	

- Molecule 49 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

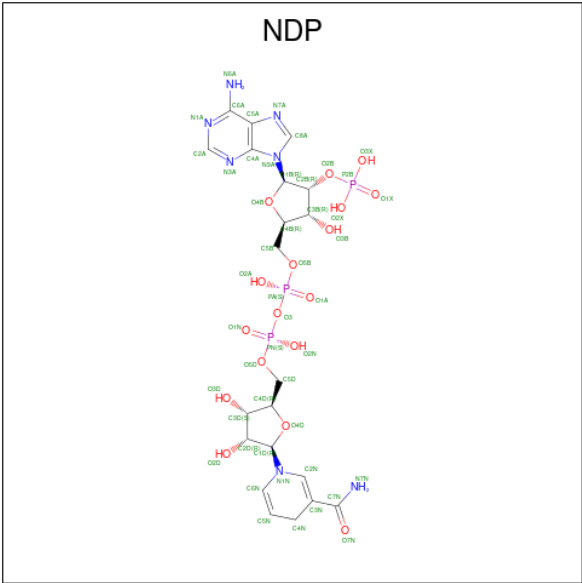


Mol	Chain	Residues	Atoms					AltConf
49	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
50	3	1	Total	K	0
			1	1	

- Molecule 51 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

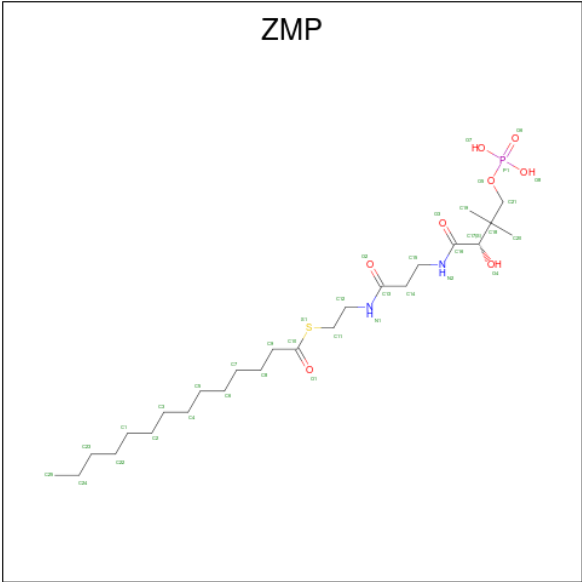


Mol	Chain	Residues	Atoms					AltConf
51	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

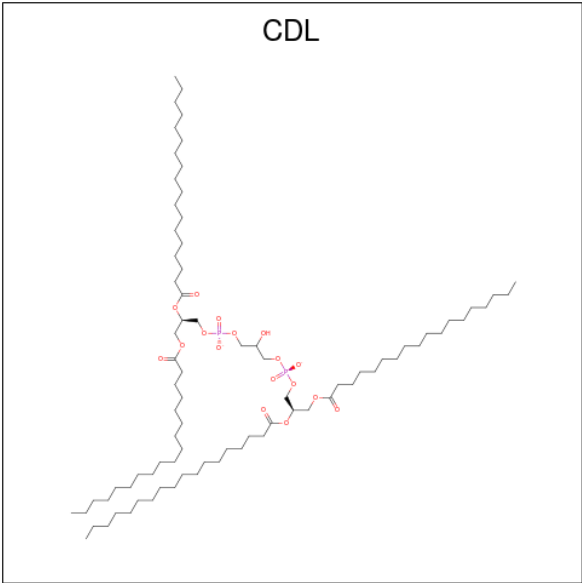
Mol	Chain	Residues	Atoms		AltConf
52	7	1	Total	Zn	0
			1	1	

- Molecule 53 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



Mol	Chain	Residues	Atoms						AltConf
53	T	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
53	U	1	Total	C	N	O	P	S	0
			32	21	2	7	1	1	

- Molecule 54 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



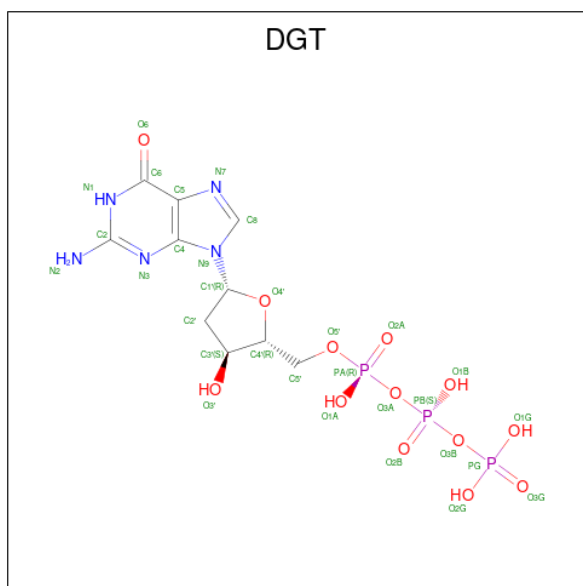
Mol	Chain	Residues	Atoms				AltConf
54	r	1	Total	C	O	P	0
			57	38	17	2	
54	L	1	Total	C	O	P	0
			78	59	17	2	

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Mol	Chain	Residues	Atoms				AltConf
54	N	1	Total	C	O	P	0
			90	71	17	2	
54	d	1	Total	C	O	P	0
			67	48	17	2	
54	h	1	Total	C	O	P	0
			70	51	17	2	
54	m	1	Total	C	O	P	0
			72	53	17	2	

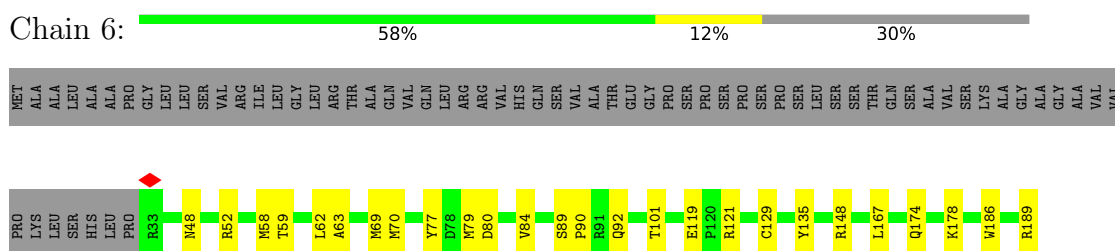
- Molecule 55 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



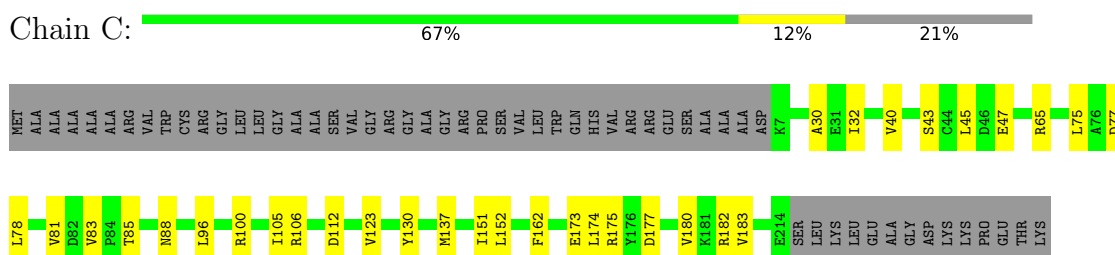
3 Residue-property plots

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

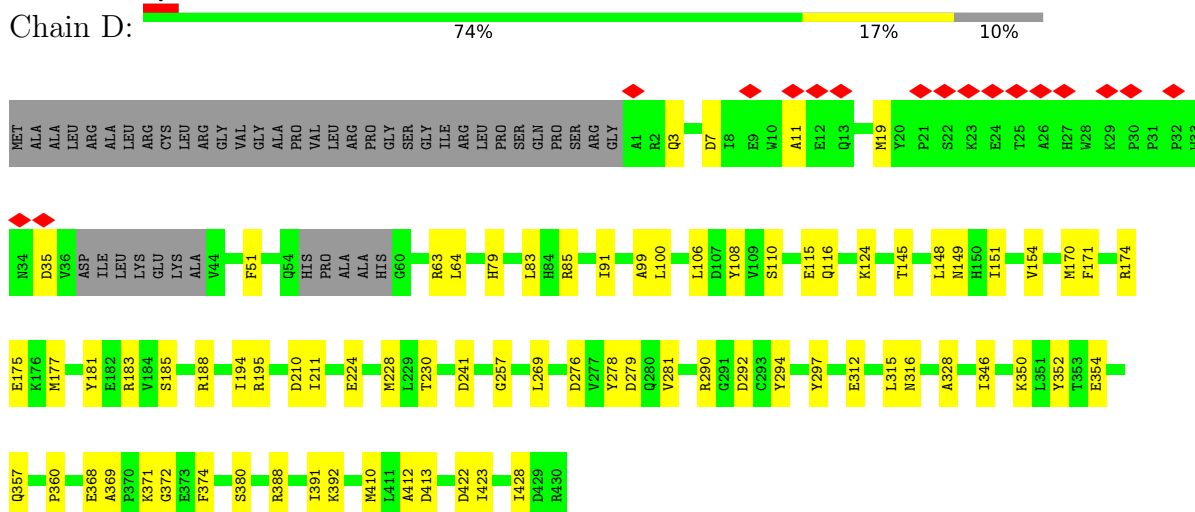
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

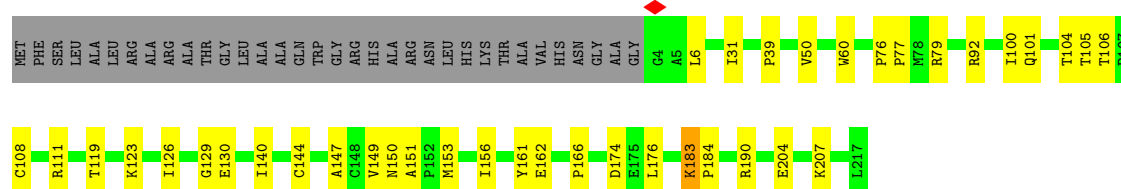


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



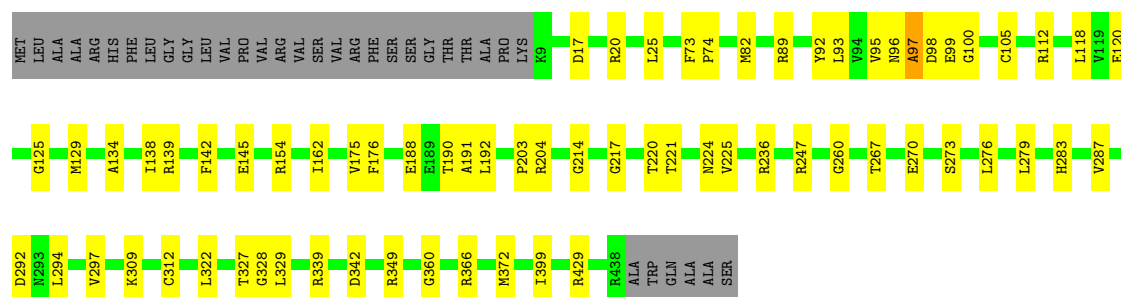
- Molecule 4: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 2: 



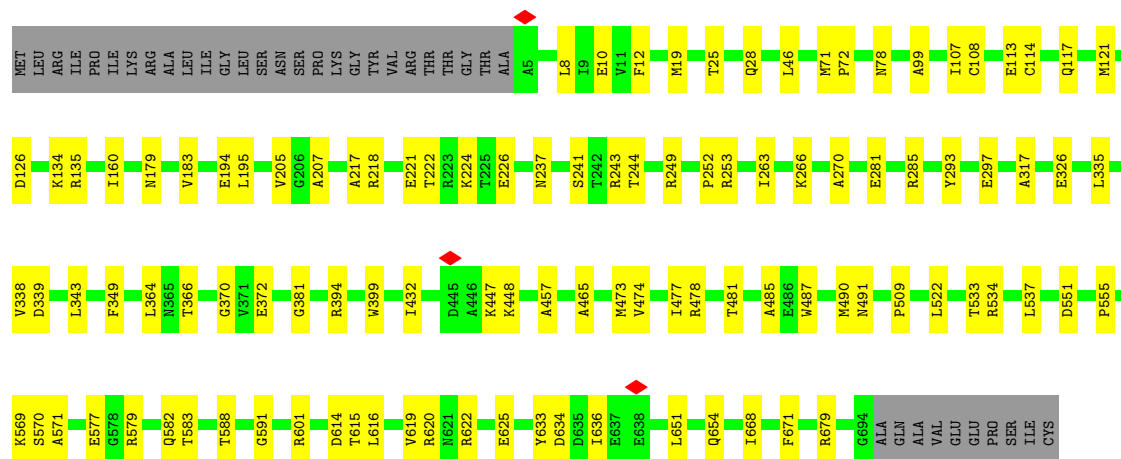
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1: 



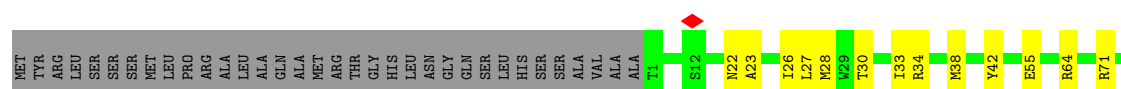
- Molecule 6: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 3: 



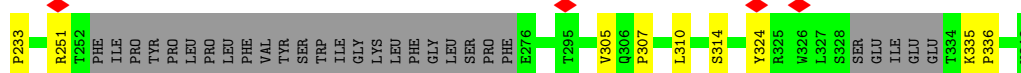
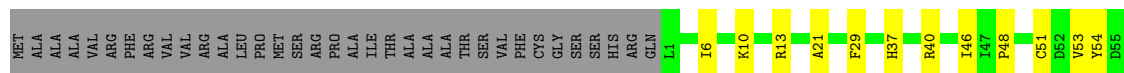
- Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 9: 

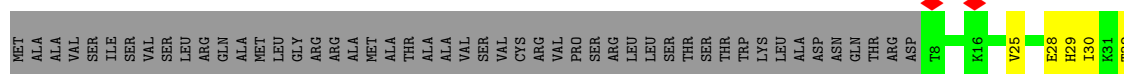




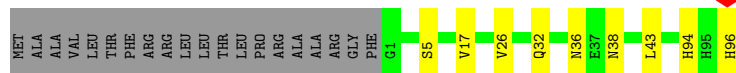
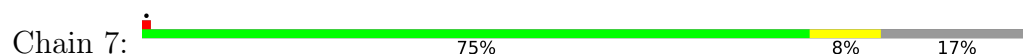
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



- Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

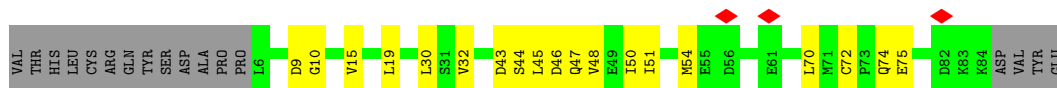


- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

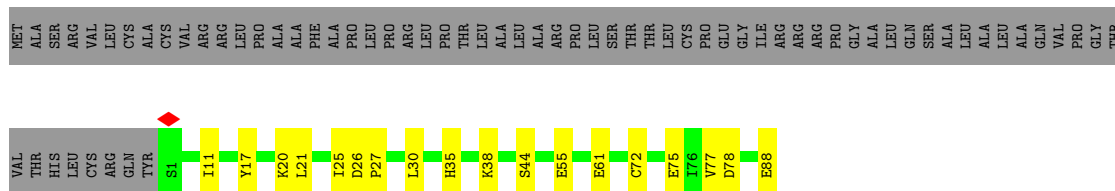


- Molecule 12: Acyl carrier protein, mitochondrial

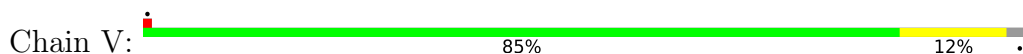




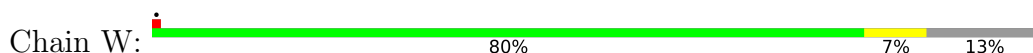
- Molecule 12: Acyl carrier protein, mitochondrial



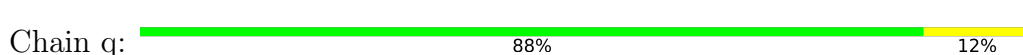
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



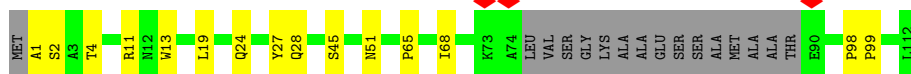
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



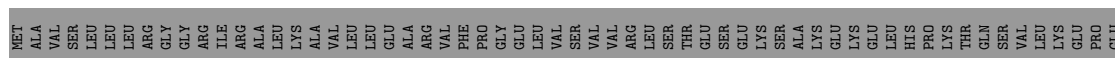
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 17: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial





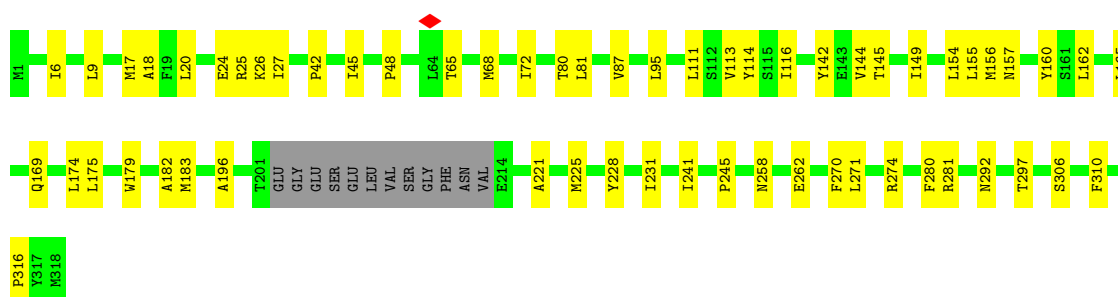
- Molecule 18: NADH-ubiquinone oxidoreductase chain 3

Chain A: 68% 14% 18%



- Molecule 19: NADH-ubiquinone oxidoreductase chain 1

Chain H: 78% 19% .



- Molecule 20: NADH-ubiquinone oxidoreductase chain 6

Chain J: 84% 12% 5%



- Molecule 21: NADH-ubiquinone oxidoreductase chain 4L

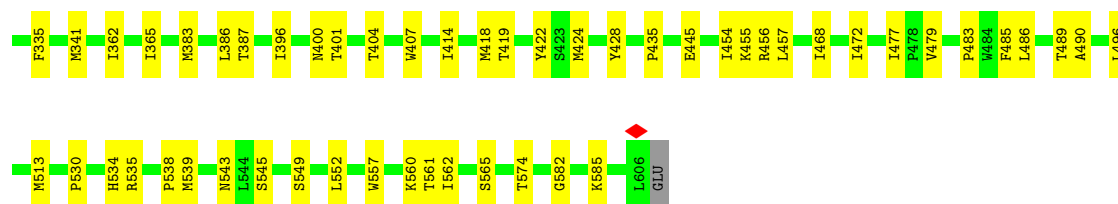
Chain K: 81% 18% .



- Molecule 22: NADH-ubiquinone oxidoreductase chain 5

Chain L: 80% 20%





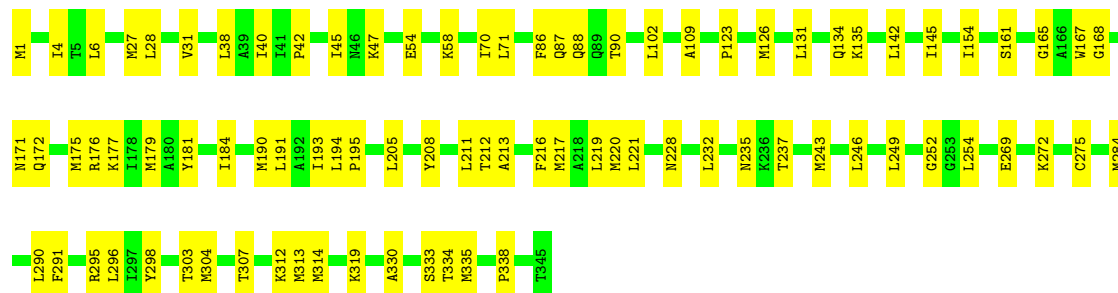
• Molecule 23: NADH-ubiquinone oxidoreductase chain 4

Chain M: 76% 24%



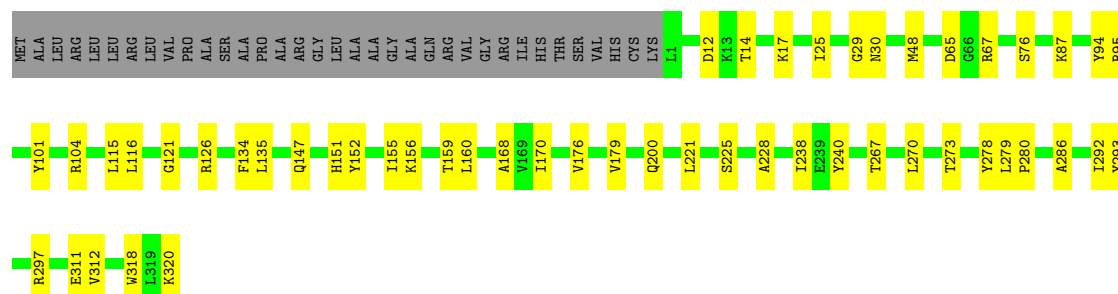
• Molecule 24: NADH-ubiquinone oxidoreductase chain 2

Chain N: 75% 25%



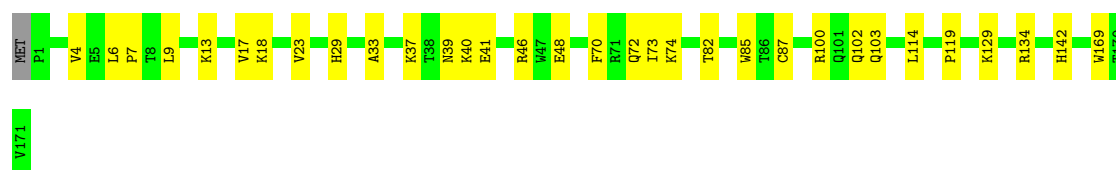
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 75% 15% 10%



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:  81% 19%



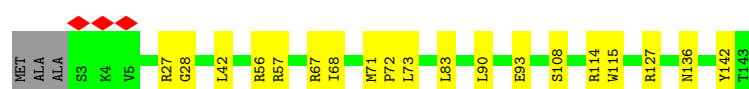
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:  84% 15%



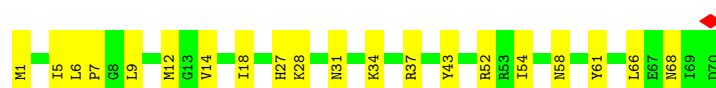
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:  85% 13%



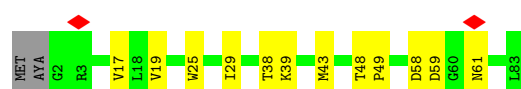
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:  71% 29%



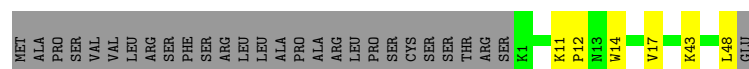
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:  83% 14%



- Molecule 31: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:  55% 8% 37%

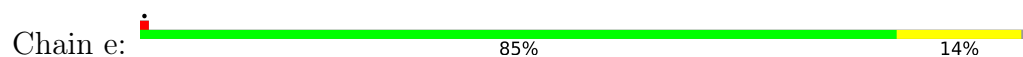


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:  92% 8%



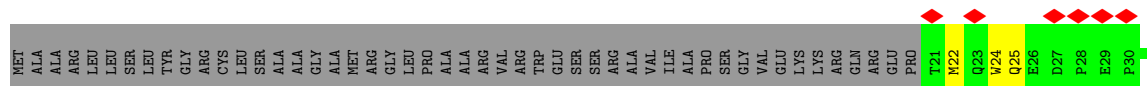
- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



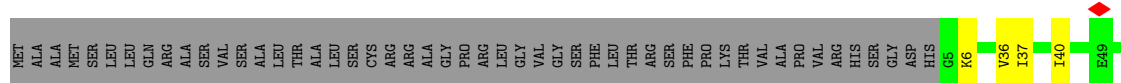
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



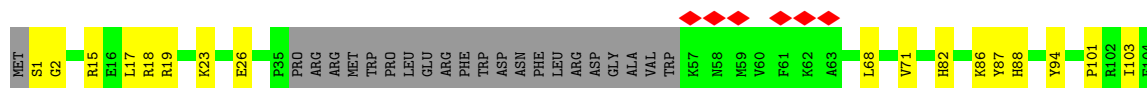
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

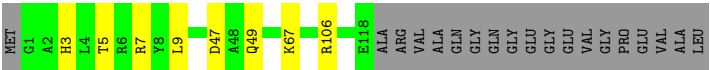


Chain o:

80%

6%

14%



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:

85%

11%

.



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54486	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.166	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	233.19998, 206.69998, 206.69998	wwPDB
Map dimensions	220, 195, 195	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MR, FME, FMN, PC1, 3PE, FES, ZN, DGT, AYA, K, CDL, SAC, ZMP, NDP, MG, 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	6	0.27	0/1289	0.55	0/1744
2	C	0.19	0/1780	0.38	0/2424
3	D	0.22	0/3442	0.42	0/4659
4	2	0.20	0/1700	0.44	0/2316
5	1	0.21	0/3396	0.47	1/4586 (0.0%)
6	3	0.21	0/5392	0.42	0/7305
7	9	0.24	0/1461	0.42	0/1974
8	P	0.19	0/2574	0.38	0/3483
9	Q	0.19	0/1045	0.34	0/1411
10	7	0.16	0/773	0.33	0/1041
11	S	0.22	0/682	0.56	0/920
12	T	0.25	0/646	0.67	0/869
12	U	0.20	0/718	0.41	0/970
13	V	0.20	0/945	0.38	0/1281
14	W	0.20	0/993	0.43	0/1335
15	q	0.20	0/1251	0.39	0/1702
16	r	0.18	0/791	0.30	0/1069
17	s	0.19	0/360	0.45	0/489
18	A	0.26	0/781	0.47	0/1066
19	H	0.27	0/2517	0.54	0/3441
20	J	0.23	0/1257	0.53	0/1707
21	K	0.25	0/738	0.49	0/1002
22	L	0.25	0/4913	0.52	0/6686
23	M	0.26	0/3709	0.52	2/5052 (0.0%)
24	N	0.26	0/2755	0.52	0/3751
25	O	0.18	0/2674	0.39	0/3626
26	X	0.17	0/1434	0.39	0/1937
27	Y	0.18	0/1061	0.43	0/1439
28	Z	0.17	0/1198	0.37	0/1616
29	a	0.21	0/585	0.47	0/788
30	b	0.17	0/666	0.40	0/914
31	c	0.18	0/409	0.40	0/555

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	d	0.18	0/1028	0.39	0/1387
33	e	0.16	0/900	0.36	0/1199
34	f	0.16	0/468	0.42	0/630
35	g	0.18	0/878	0.42	0/1196
36	h	0.18	0/1201	0.39	0/1626
37	i	0.19	0/917	0.40	0/1243
38	j	0.18	0/587	0.45	0/804
39	k	0.20	0/646	0.47	0/873
40	l	0.18	0/1379	0.40	0/1882
41	m	0.18	0/1079	0.41	0/1463
42	n	0.19	0/1596	0.48	2/2162 (0.1%)
43	o	0.19	0/1039	0.42	0/1394
44	p	0.18	0/1463	0.33	0/1977
All	All	0.21	0/67116	0.45	5/90994 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	n	55	ASP	CA-C-N	7.14	135.17	121.54
42	n	55	ASP	C-N-CA	7.14	135.17	121.54
5	1	97	ALA	N-CA-C	-6.89	104.18	112.59
23	M	243	MET	CG-SD-CE	6.01	114.13	100.90
23	M	243	MET	N-CA-CB	5.16	117.80	110.16

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6	1258	0	1268	19	0
2	C	1730	0	1686	21	0
3	D	3371	0	3320	56	0
4	2	1660	0	1653	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1	3321	0	3278	42	0
6	3	5305	0	5330	70	0
7	9	1431	0	1383	30	0
8	P	2513	0	2536	37	0
9	Q	1022	0	1023	18	0
10	7	758	0	731	7	0
11	S	671	0	688	12	0
12	T	637	0	640	10	0
12	U	706	0	699	13	0
13	V	923	0	965	9	0
14	W	970	0	991	7	0
15	q	1209	0	1170	13	0
16	r	781	0	811	10	0
17	s	351	0	331	5	0
18	A	771	0	824	15	0
19	H	2452	0	2547	54	0
20	J	1240	0	1265	18	0
21	K	737	0	768	18	0
22	L	4800	0	4985	86	0
23	M	3632	0	3853	80	0
24	N	2703	0	2902	68	0
25	O	2607	0	2566	34	0
26	X	1396	0	1385	24	0
27	Y	1037	0	1025	15	0
28	Z	1167	0	1166	19	0
29	a	572	0	583	15	0
30	b	643	0	644	9	0
31	c	398	0	401	5	0
32	d	996	0	1001	9	0
33	e	877	0	871	12	0
34	f	456	0	452	5	0
35	g	850	0	783	11	0
36	h	1166	0	1166	14	0
37	i	897	0	902	17	0
38	j	562	0	515	7	0
39	k	626	0	620	13	0
40	l	1323	0	1216	19	0
41	m	1050	0	1061	12	0
42	n	1541	0	1473	15	0
43	o	1014	0	1002	7	0
44	p	1430	0	1400	20	0
45	1	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	3	16	0	0	0	0
45	6	8	0	0	0	0
45	9	16	0	0	1	0
46	6	32	0	38	0	0
46	A	43	0	60	2	0
46	H	51	0	82	2	0
46	K	41	0	59	2	0
46	L	144	0	222	8	0
46	M	87	0	128	6	0
46	N	38	0	50	1	0
46	Y	28	0	30	1	0
46	d	63	0	74	0	0
46	h	51	0	82	2	0
46	i	42	0	61	5	0
46	m	30	0	34	1	0
46	r	46	0	66	0	0
47	6	43	0	63	0	0
47	9	101	0	159	11	0
47	M	54	0	88	5	0
48	2	4	0	0	0	0
48	3	4	0	0	0	0
49	1	31	0	19	3	0
50	3	1	0	0	0	0
51	P	48	0	26	1	0
52	7	1	0	0	0	0
53	T	34	0	40	2	0
53	U	32	0	36	3	0
54	L	78	0	100	1	0
54	N	90	0	133	3	0
54	d	67	0	81	1	0
54	h	70	0	87	6	0
54	m	72	0	91	1	0
54	r	57	0	58	4	0
55	O	31	0	12	1	0
56	O	1	0	0	0	0
All	All	67123	0	67858	845	0

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

All (845) 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)
8:P:310:LEU:O	8:P:314:SER:HB2	1.76	0.84
8:P:216:ASN:O	8:P:220:ASP:HB2	1.80	0.80
5:1:99:GLU:OE2	5:1:105:CYS:HA	1.85	0.75
31:c:11:LYS:HE3	31:c:12:PRO:HD2	1.69	0.75
4:2:119:THR:HG21	4:2:166:PRO:HB3	1.70	0.73
19:H:24:GLU:HG3	19:H:271:LEU:HD22	1.70	0.71
19:H:175:LEU:O	19:H:179:TRP:HB3	1.89	0.71
40:l:70:MET:HE1	40:l:76:ILE:HG12	1.71	0.71
5:1:93:LEU:O	5:1:134:ALA:HA	1.91	0.70
19:H:156:MET:HE3	19:H:174:LEU:HD22	1.73	0.70
22:L:545:SER:O	22:L:549:SER:HB2	1.90	0.70
5:1:99:GLU:OE2	5:1:105:CYS:CA	2.42	0.68
23:M:7:PRO:HB2	23:M:34:ILE:HD11	1.76	0.68
4:2:150:ASN:HB3	4:2:162:GLU:HB3	1.77	0.67
40:l:41:MET:HE1	41:m:85:ASN:HB3	1.77	0.67
6:3:364:LEU:HD12	6:3:491:ASN:HB3	1.76	0.66
23:M:138:ASN:ND2	23:M:334:TYR:OH	2.31	0.64
24:N:252:GLY:HA3	24:N:290:LEU:HD13	1.80	0.64
5:1:224:ASN:ND2	49:1:501:FMN:O2	2.30	0.64
22:L:243:VAL:O	22:L:247:LEU:HB2	1.98	0.64
47:9:204:PC1:H112	28:Z:28:GLY:HA3	1.80	0.64
1:6:79:MET:HB2	1:6:84:VAL:HB	1.79	0.64
3:D:151:ILE:HG12	3:D:170:MET:HE3	1.79	0.64
3:D:328:ALA:HB3	6:3:126:ASP:HB2	1.80	0.64
46:L:703:3PE:H3E1	47:M:501:PC1:H3H1	1.80	0.64
23:M:36:LEU:HB2	35:g:67:VAL:HG22	1.80	0.64
7:9:33:ILE:HG13	47:9:204:PC1:H242	1.80	0.63
39:k:32:THR:HG22	39:k:34:LEU:H	1.62	0.63
22:L:221:THR:HG23	22:L:226:GLN:HB2	1.81	0.63
19:H:26:LYS:HB3	29:a:5:ILE:HG12	1.81	0.63
2:C:77:ASP:HB3	3:D:392:LYS:HG3	1.81	0.63
7:9:171:ILE:O	7:9:175:TYR:HB3	1.99	0.63
3:D:110:SER:OG	3:D:149:ASN:ND2	2.31	0.62
23:M:48:ASN:ND2	44:p:89:MET:SD	2.71	0.62
24:N:172:GLN:HE21	24:N:177:LYS:HB3	1.65	0.62
23:M:232:ALA:O	23:M:237:LYS:NZ	2.32	0.61
5:1:112:ARG:HB3	5:1:145:GLU:HG3	1.82	0.61
20:J:67:PHE:HD1	21:K:27:MET:HE1	1.65	0.61
12:U:55:GLU:HG2	12:U:61:GLU:HA	1.81	0.61
4:2:144:CYS:O	5:1:139:ARG:NH2	2.33	0.61
13:V:32:ASP:HA	13:V:35:LYS:HE2	1.83	0.61
22:L:205:ASN:ND2	44:p:120:TYR:OH	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:231:LEU:HD23	23:M:235:LEU:HD12	1.82	0.61
6:3:570:SER:HA	6:3:583:THR:O	2.00	0.61
22:L:539:MET:HE3	22:L:543:ASN:HD21	1.66	0.60
40:l:15:THR:HG23	40:l:18:GLU:H	1.66	0.60
4:2:104:THR:HG23	5:1:349:ARG:HH21	1.67	0.60
7:9:77:GLU:O	7:9:107:ARG:NH1	2.35	0.60
24:N:109:ALA:HB3	24:N:161:SER:HA	1.84	0.60
24:N:165:GLY:HA2	24:N:181:TYR:HD1	1.67	0.60
16:r:45:SER:O	16:r:51:ASN:ND2	2.34	0.60
22:L:180:ILE:HD12	23:M:397:GLY:HA2	1.83	0.60
2:C:47:GLU:OE1	2:C:106:ARG:NH2	2.35	0.60
18:A:67:LEU:HD22	21:K:65:VAL:HA	1.84	0.59
6:3:114:CYS:HB3	6:3:117:GLN:HB2	1.84	0.59
6:3:474:VAL:HG21	6:3:490:MET:HG2	1.83	0.59
3:D:228:MET:HE3	7:9:38:MET:HE3	1.85	0.59
33:e:88:GLU:HG3	33:e:90:LYS:HG2	1.83	0.59
2:C:174:LEU:HD12	2:C:183:VAL:HG12	1.85	0.59
22:L:161:ARG:NH1	42:n:90:PHE:O	2.33	0.59
22:L:574:THR:OG1	24:N:167:TRP:O	2.19	0.59
26:X:100:ARG:NH1	26:X:103:GLN:OE1	2.36	0.59
6:3:194:GLU:HG2	6:3:195:LEU:HG	1.85	0.59
16:r:11:ARG:HB3	16:r:19:LEU:HD12	1.84	0.59
22:L:253:VAL:HB	22:L:310:LEU:HD11	1.84	0.59
22:L:341:MET:HG2	22:L:454:ILE:HG12	1.83	0.59
40:l:53:SER:HA	40:l:83:TYR:HB3	1.84	0.59
7:9:55:GLU:OE2	15:q:34:ARG:NH2	2.36	0.58
5:1:142:PHE:HB3	5:1:145:GLU:HB2	1.85	0.58
7:9:23:ALA:O	7:9:27:LEU:HB2	2.03	0.58
20:J:124:LEU:HD12	28:Z:136:ASN:HD21	1.68	0.58
7:9:71:ARG:NH2	10:7:36:ASN:OD1	2.37	0.58
22:L:197:GLU:HG3	44:p:110:LYS:HD3	1.84	0.58
44:p:139:GLN:HG2	44:p:143:LEU:HD22	1.86	0.58
42:n:26:LEU:HD22	42:n:43:MET:HE2	1.86	0.58
25:O:25:ILE:HG12	25:O:168:ALA:HB3	1.84	0.58
6:3:135:ARG:NH1	6:3:179:ASN:OD1	2.36	0.58
18:A:69:ILE:HD11	19:H:144:VAL:HG23	1.86	0.58
25:O:104:ARG:NH2	55:O:401:DGT:N7	2.52	0.58
26:X:46:ARG:NH2	36:h:142:ASP:OD1	2.37	0.58
8:P:177:ARG:NH2	51:P:501:NDP:O2N	2.36	0.58
41:m:114:LEU:HB3	41:m:120:LEU:HB2	1.85	0.58
8:P:90:VAL:HG21	8:P:218:THR:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:N:269:GLU:OE2	36:h:111:ARG:NH2	2.36	0.57
6:3:226:GLU:HG2	6:3:253:ARG:HD3	1.87	0.57
6:3:447:LYS:NZ	6:3:481:THR:O	2.37	0.57
6:3:601:ARG:NH2	6:3:614:ASP:OD1	2.36	0.57
3:D:35:ASP:OD2	24:N:176:ARG:NH1	2.36	0.57
46:i:201:3PE:H2I2	46:i:201:3PE:H381	1.86	0.57
4:2:111:ARG:NH1	5:1:260:GLY:O	2.37	0.57
6:3:620:ARG:NH1	6:3:633:TYR:OH	2.36	0.57
25:O:225:SER:O	25:O:228:ALA:C	2.47	0.57
19:H:154:LEU:HA	19:H:157:ASN:HB3	1.86	0.57
3:D:185:SER:O	7:9:64:ARG:NH1	2.38	0.57
22:L:424:MET:HE3	22:L:428:TYR:HB2	1.85	0.57
13:V:22:ARG:NH2	25:O:240:TYR:OH	2.37	0.57
19:H:24:GLU:OE1	19:H:274:ARG:NH1	2.37	0.57
34:f:38:ARG:NH1	34:f:56:TRP:O	2.38	0.57
7:9:30:THR:HB	47:9:204:PC1:H11	1.87	0.56
24:N:243:MET:HE2	24:N:330:ALA:HB1	1.87	0.56
23:M:173:THR:HB	36:h:101:ALA:HB2	1.87	0.56
5:1:270:GLU:OE1	5:1:283:HIS:NE2	2.36	0.56
23:M:50:LYS:HB2	23:M:58:SER:HB3	1.88	0.56
41:m:32:GLN:HG2	41:m:35:ARG:HH21	1.70	0.56
6:3:335:LEU:HA	6:3:338:VAL:HG12	1.87	0.56
42:n:103:LEU:O	42:n:111:LYS:NZ	2.39	0.56
23:M:207:MET:HE2	23:M:240:SER:HA	1.88	0.56
3:D:257:GLY:HA3	3:D:372:GLY:HA2	1.86	0.56
8:P:40:ARG:NH1	14:W:112:THR:O	2.39	0.56
23:M:36:LEU:HD21	46:h:202:3PE:H391	1.88	0.56
23:M:446:LEU:HB3	46:M:502:3PE:H342	1.88	0.56
22:L:135:ASN:ND2	22:L:197:GLU:OE2	2.38	0.56
23:M:98:MET:HE1	54:N:401:CDL:H801	1.88	0.56
3:D:149:ASN:HD21	3:D:371:LYS:HG3	1.68	0.56
8:P:109:VAL:HA	8:P:113:ILE:HD12	1.87	0.56
22:L:561:THR:HG23	46:L:704:3PE:H271	1.88	0.56
46:L:703:3PE:H2C2	24:N:284:MET:HB3	1.87	0.56
37:i:103:ILE:HB	43:o:47:ASP:HB3	1.86	0.56
22:L:139:GLN:HA	22:L:142:ILE:HD12	1.87	0.55
6:3:569:LYS:HG3	6:3:571:ALA:HB2	1.88	0.55
22:L:100:ILE:HG21	22:L:246:LEU:HB2	1.88	0.55
12:U:21:LEU:HD13	39:k:53:ASN:HA	1.87	0.55
6:3:399:TRP:O	9:Q:127:ARG:NH1	2.39	0.55
26:X:87:CYS:SG	26:X:102:GLN:NE2	2.79	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:3:LYS:NZ	34:f:27:ASP:OD2	2.40	0.55
23:M:275:ILE:O	23:M:279:GLN:HB2	2.07	0.55
30:b:59:ASP:OD2	30:b:61:ASN:ND2	2.38	0.55
22:L:483:PRO:HG2	22:L:486:LEU:HD13	1.89	0.55
23:M:197:LEU:HB3	47:M:501:PC1:H3A2	1.87	0.55
3:D:51:PHE:HB3	3:D:64:LEU:HB2	1.87	0.55
19:H:17:MET:HE2	19:H:225:MET:HB3	1.89	0.55
27:Y:94:CYS:HA	27:Y:114:CYS:HA	1.88	0.55
23:M:428:PRO:HD3	42:n:105:TYR:HD1	1.71	0.55
54:h:201:CDL:H152	46:i:201:3PE:H341	1.88	0.55
2:C:151:ILE:HG23	2:C:152:LEU:HG	1.88	0.55
5:1:99:GLU:HG2	5:1:99:GLU:O	2.07	0.55
18:A:11:ILE:HD13	19:H:80:THR:HG21	1.89	0.54
22:L:22:SER:HA	22:L:27:ILE:HD11	1.90	0.54
39:k:35:GLU:OE1	39:k:39:LYS:NZ	2.40	0.54
3:D:3:GLN:NE2	23:M:135:ARG:O	2.34	0.54
8:P:53:VAL:HA	8:P:56:ILE:HG12	1.88	0.54
40:l:57:ARG:NH2	40:l:74:GLU:OE1	2.40	0.54
1:6:58:MET:HE3	1:6:90:PRO:HG3	1.89	0.54
3:D:11:ALA:O	24:N:228:ASN:ND2	2.39	0.54
19:H:196:ALA:HB3	19:H:274:ARG:HA	1.88	0.54
22:L:97:THR:HG21	22:L:125:LEU:HD22	1.89	0.54
22:L:101:MET:HE1	22:L:118:ILE:HG23	1.90	0.54
24:N:131:LEU:HA	24:N:135:LYS:HE2	1.88	0.54
24:N:298:TYR:O	24:N:303:THR:OG1	2.24	0.54
5:1:100:GLY:HA2	5:1:139:ARG:NH1	2.22	0.54
22:L:161:ARG:NH2	22:L:238:GLU:OE2	2.33	0.54
3:D:410:MET:H	3:D:413:ASP:HB2	1.73	0.54
21:K:24:SER:HB3	21:K:89:TYR:HD1	1.73	0.54
23:M:278:ARG:HH12	40:l:82:MET:HE3	1.73	0.54
32:d:120:ARG:O	41:m:108:ARG:NH2	2.40	0.54
36:h:69:HIS:NE2	54:h:201:CDL:OA3	2.41	0.54
4:2:204:GLU:OE2	4:2:207:LYS:NZ	2.41	0.54
19:H:113:VAL:HA	19:H:116:ILE:HG12	1.89	0.54
6:3:366:THR:HG22	6:3:370:GLY:HA3	1.90	0.54
6:3:478:ARG:NH1	6:3:487:TRP:O	2.40	0.53
18:A:6:VAL:HG11	19:H:87:VAL:HG21	1.89	0.53
2:C:78:LEU:HB3	2:C:130:TYR:HB3	1.89	0.53
19:H:42:PRO:HD2	19:H:45:ILE:HG12	1.89	0.53
22:L:54:PHE:O	22:L:58:ASN:ND2	2.38	0.53
23:M:73:LEU:HB2	23:M:103:GLN:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:82:ASN:ND2	23:M:335:GLU:OE2	2.38	0.53
25:O:170:ILE:HD11	25:O:238:ILE:HD11	1.90	0.53
3:D:269:LEU:HB2	3:D:368:GLU:HB2	1.90	0.53
5:1:154:ARG:HB2	17:s:52:LEU:HD11	1.91	0.53
6:3:349:PHE:H	6:3:509:PRO:HB2	1.73	0.53
8:P:212:LYS:HB3	8:P:305:VAL:HG11	1.91	0.53
12:T:19:LEU:HB3	12:T:30:LEU:HD11	1.89	0.53
38:j:60:THR:HG23	38:j:63:GLU:H	1.72	0.53
24:N:232:LEU:HB2	24:N:307:THR:HG22	1.90	0.53
25:O:29:GLY:O	25:O:126:ARG:NH2	2.41	0.53
2:C:65:ARG:NH1	2:C:123:VAL:O	2.41	0.53
26:X:70:PHE:HA	26:X:73:ILE:HG22	1.91	0.53
32:d:108:THR:HA	44:p:77:LYS:HA	1.90	0.53
27:Y:47:SER:OG	27:Y:50:GLU:OE1	2.25	0.53
3:D:279:ASP:OD1	3:D:279:ASP:N	2.42	0.53
6:3:571:ALA:O	6:3:582:GLN:HA	2.09	0.53
39:k:59:MET:HA	39:k:63:ALA:HB2	1.91	0.53
8:P:194:VAL:O	8:P:199:LYS:NZ	2.42	0.53
18:A:73:LEU:O	19:H:160:TYR:OH	2.25	0.53
21:K:40:LEU:HD13	24:N:71:LEU:HD23	1.91	0.53
24:N:123:PRO:HG2	24:N:126:MET:HG2	1.91	0.53
32:d:112:ILE:O	44:p:159:LYS:NZ	2.42	0.53
8:P:66:GLY:HA3	9:Q:69:LEU:HD13	1.92	0.52
22:L:362:ILE:HD13	22:L:365:ILE:HD11	1.91	0.52
23:M:17:LEU:HD11	54:N:401:CDL:H141	1.91	0.52
19:H:228:TYR:HA	19:H:231:ILE:HD12	1.90	0.52
23:M:105:LEU:O	23:M:109:THR:OG1	2.23	0.52
25:O:147:GLN:HB3	25:O:279:LEU:HD11	1.90	0.52
32:d:109:TYR:OH	44:p:152:ARG:NH1	2.42	0.52
22:L:538:PRO:HB2	40:l:88:VAL:HG22	1.90	0.52
4:2:6:LEU:O	4:2:92:ARG:NH2	2.42	0.52
12:T:47:GLN:NE2	12:T:70:LEU:O	2.42	0.52
22:L:8:ILE:HA	22:L:11:ILE:HD12	1.92	0.52
23:M:260:PRO:HG3	46:M:503:3PE:H332	1.90	0.52
2:C:137:MET:HB3	2:C:162:PHE:HB2	1.91	0.52
6:3:28:GLN:NE2	9:Q:114:LYS:O	2.40	0.52
7:9:33:ILE:HD12	47:9:204:PC1:H3A2	1.92	0.52
6:3:281:GLU:HB2	6:3:293:TYR:HD2	1.75	0.52
8:P:108:ASP:OD1	8:P:112:ASN:ND2	2.38	0.52
25:O:65:ASP:OD2	25:O:67:ARG:NH2	2.43	0.52
2:C:32:ILE:HG23	13:V:43:TYR:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:241:ASP:OD1	3:D:290:ARG:NH2	2.43	0.52
5:1:327:THR:HG22	5:1:328:GLY:H	1.75	0.52
6:3:522:LEU:HD13	6:3:537:LEU:HD11	1.91	0.52
19:H:162:LEU:HD23	19:H:165:LEU:HD12	1.92	0.52
19:H:169:GLN:NE2	19:H:241:ILE:O	2.42	0.52
22:L:549:SER:OG	23:M:271:MET:SD	2.59	0.52
24:N:54:GLU:OE2	24:N:58:LYS:NZ	2.37	0.52
37:i:94:TYR:HD2	44:p:107:GLU:HG2	1.74	0.52
3:D:312:GLU:OE2	3:D:316:ASN:ND2	2.43	0.51
15:q:32:ASP:OD1	15:q:58:ARG:NH2	2.43	0.51
22:L:245:ALA:O	22:L:249:SER:HB2	2.10	0.51
26:X:9:LEU:O	26:X:13:LYS:HB2	2.10	0.51
53:T:201:ZMP:H19	14:W:70:MET:HE1	1.91	0.51
24:N:312:LYS:HZ2	25:O:292:ILE:HG21	1.74	0.51
3:D:413:ASP:OD1	19:H:281:ARG:NH1	2.44	0.51
6:3:551:ASP:OD2	6:3:679:ARG:NE	2.39	0.51
26:X:48:GLU:OE1	26:X:134:ARG:NH2	2.38	0.51
5:1:25:LEU:HD21	5:1:267:THR:HG22	1.92	0.51
22:L:485:PHE:O	22:L:489:THR:OG1	2.29	0.51
37:i:114:GLU:OE2	44:p:15:ARG:NH1	2.43	0.51
2:C:175:ARG:NH2	2:C:177:ASP:OD2	2.43	0.51
22:L:396:ILE:HG21	22:L:490:ALA:HB2	1.92	0.51
23:M:430:HIS:HB2	23:M:433:GLU:HG2	1.93	0.51
24:N:254:LEU:HG	24:N:290:LEU:HD21	1.92	0.51
2:C:100:ARG:NH2	13:V:78:GLU:OE1	2.44	0.51
16:r:13:TRP:O	28:Z:27:ARG:NH2	2.43	0.51
24:N:249:LEU:HD22	24:N:254:LEU:HD12	1.91	0.51
1:6:135:TYR:HE1	7:9:90:PRO:HB2	1.75	0.51
24:N:193:ILE:HD11	24:N:269:GLU:HB3	1.93	0.51
29:a:6:LEU:HA	29:a:9:LEU:HB2	1.93	0.51
13:V:17:ASP:OD1	13:V:17:ASP:N	2.43	0.51
54:L:702:CDL:H791	54:L:702:CDL:H582	1.91	0.51
4:2:76:PRO:HB2	4:2:79:ARG:HG2	1.91	0.51
6:3:372:GLU:OE2	6:3:394:ARG:NH1	2.43	0.51
22:L:246:LEU:O	22:L:251:THR:OG1	2.29	0.51
25:O:25:ILE:HD12	25:O:48:MET:HE1	1.93	0.51
53:U:201:ZMP:H7	42:n:66:ALA:HB1	1.93	0.51
26:X:129:LYS:HB2	30:b:58:ASP:HB3	1.93	0.51
40:l:124:TYR:OH	43:o:7:ARG:NH1	2.43	0.51
40:l:135:ASN:HA	40:l:152:VAL:HB	1.92	0.51
1:6:148:ARG:NH1	2:C:173:GLU:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:N:87:GLN:NE2	36:h:126:PRO:O	2.43	0.51
34:f:6:LEU:O	34:f:10:HIS:HB2	2.11	0.51
22:L:560:LYS:HE3	46:L:704:3PE:H221	1.93	0.50
23:M:370:PRO:HG3	23:M:375:LEU:HD13	1.94	0.50
12:U:35:HIS:HB3	12:U:38:LYS:HB2	1.93	0.50
6:3:465:ALA:HB2	6:3:654:GLN:HG2	1.92	0.50
6:3:622:ARG:NH1	6:3:625:GLU:OE2	2.40	0.50
21:K:59:ILE:HD12	24:N:27:MET:HG3	1.94	0.50
28:Z:115:TRP:NE1	36:h:142:ASP:OD2	2.43	0.50
44:p:107:GLU:HA	44:p:110:LYS:HE2	1.93	0.50
1:6:101:THR:HA	1:6:129:CYS:HB3	1.92	0.50
3:D:352:TYR:HD1	7:9:88:ILE:HG12	1.76	0.50
6:3:8:LEU:HD13	6:3:19:MET:HB3	1.94	0.50
18:A:4:TYR:HD1	46:H:401:3PE:H292	1.75	0.50
22:L:292:ALA:HB2	22:L:304:PHE:HB3	1.94	0.50
26:X:6:LEU:HD21	28:Z:90:LEU:HD22	1.94	0.50
2:C:96:LEU:HB2	2:C:105:ILE:HG22	1.93	0.50
3:D:354:GLU:OE2	3:D:357:GLN:NE2	2.42	0.50
6:3:217:ALA:HA	7:9:83:LYS:HE3	1.92	0.50
27:Y:105:HIS:HA	46:Y:201:3PE:H11	1.92	0.50
37:i:105:PRO:O	43:o:67:LYS:NZ	2.42	0.50
6:3:243:ARG:HG2	6:3:244:THR:HG23	1.94	0.50
15:q:106:ARG:HB2	15:q:109:ILE:HG13	1.93	0.50
12:U:17:TYR:OH	39:k:27:TRP:NE1	2.36	0.50
19:H:111:LEU:HA	19:H:114:TYR:HD2	1.77	0.50
24:N:172:GLN:NE2	24:N:177:LYS:HB3	2.27	0.50
25:O:76:SER:O	25:O:95:ARG:NH1	2.45	0.50
5:1:97:ALA:HB3	5:1:138:ILE:HA	1.92	0.50
11:S:17:GLU:HB3	11:S:67:ARG:HB3	1.94	0.50
23:M:429:SER:O	35:g:36:TYR:OH	2.29	0.50
35:g:24:TRP:H	35:g:24:TRP:CD1	2.29	0.50
1:6:89:SER:OG	1:6:92:GLN:OE1	2.30	0.50
12:T:72:CYS:N	12:T:75:GLU:OE2	2.41	0.50
23:M:11:LEU:HB3	23:M:100:ILE:HD13	1.94	0.50
34:f:43:LEU:HD11	44:p:67:TYR:HB3	1.93	0.50
54:h:201:CDL:OA7	46:i:201:3PE:N	2.45	0.50
20:J:47:GLY:HA3	21:K:49:LEU:HD22	1.93	0.49
24:N:304:MET:HE2	25:O:286:ALA:HB1	1.93	0.49
8:P:53:VAL:O	8:P:57:MET:HG2	2.12	0.49
24:N:175:MET:HE2	24:N:219:LEU:HD21	1.94	0.49
12:U:88:GLU:OE2	36:h:6:LYS:NZ	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:68:MET:SD	27:Y:99:THR:OG1	2.66	0.49
5:1:17:ASP:OD1	5:1:20:ARG:NH1	2.45	0.49
15:q:60:ARG:NH2	15:q:95:ASP:OD1	2.46	0.49
25:O:135:LEU:HD22	25:O:152:TYR:CD1	2.48	0.49
24:N:211:LEU:HG	24:N:333:SER:HB2	1.95	0.49
25:O:126:ARG:HD3	25:O:134:PHE:HE2	1.77	0.49
1:6:70:MET:HG3	3:D:171:PHE:HE2	1.77	0.49
4:2:147:ALA:HB3	4:2:153:MET:HE3	1.94	0.49
4:2:156:ILE:HD13	4:2:176:LEU:HD11	1.94	0.49
6:3:339:ASP:OD1	11:S:16:ARG:NH1	2.45	0.49
6:3:668:ILE:HA	6:3:671:PHE:HB3	1.95	0.49
11:S:23:CYS:O	11:S:33:ARG:NH1	2.42	0.49
25:O:14:THR:HG21	25:O:116:LEU:HD22	1.95	0.49
5:1:342:ASP:OD1	5:1:429:ARG:NH2	2.41	0.49
24:N:86:PHE:HB3	24:N:90:THR:HG21	1.95	0.49
24:N:154:ILE:HG23	24:N:191:LEU:HG	1.94	0.49
3:D:19:MET:HE1	24:N:295:ARG:CZ	2.43	0.49
7:9:119:ILE:HG12	45:9:201:SF4:S3	2.53	0.49
19:H:9:LEU:HD21	19:H:87:VAL:HA	1.93	0.49
22:L:154:LEU:HD13	22:L:247:LEU:HD21	1.94	0.49
23:M:115:LEU:HB2	23:M:174:LEU:HD21	1.95	0.49
5:1:188:GLU:O	5:1:192:LEU:HB2	2.12	0.49
47:9:203:PC1:H3F1	47:9:204:PC1:H2C2	1.95	0.49
5:1:120:GLU:OE2	5:1:236:ARG:NH1	2.38	0.49
6:3:205:VAL:HG23	6:3:207:ALA:H	1.76	0.49
11:S:21:HIS:HA	11:S:55:ARG:O	2.13	0.49
22:L:401:THR:HG21	22:L:479:VAL:HG21	1.95	0.49
3:D:149:ASN:OD1	3:D:371:LYS:NZ	2.37	0.48
3:D:346:ILE:HG23	6:3:117:GLN:HG2	1.95	0.48
5:1:214:GLY:HA3	5:1:220:THR:HG22	1.94	0.48
24:N:1:FME:HB3	24:N:6:LEU:HG	1.95	0.48
6:3:591:GLY:HA2	8:P:6:ILE:HG21	1.95	0.48
8:P:233:PRO:HG3	8:P:307:PRO:HB2	1.95	0.48
19:H:24:GLU:HA	19:H:271:LEU:HD13	1.95	0.48
33:e:86:MET:HE2	33:e:93:PRO:HG3	1.95	0.48
54:m:201:CDL:H771	46:m:202:3PE:H392	1.95	0.48
19:H:245:PRO:HB3	19:H:258:ASN:HB3	1.95	0.48
19:H:292:ASN:HA	30:b:17:VAL:HG11	1.95	0.48
23:M:154:LEU:HD11	24:N:254:LEU:HD21	1.95	0.48
4:2:129:GLY:HA2	4:2:140:ILE:HG22	1.95	0.48
22:L:15:LEU:HD11	22:L:129:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:233:LEU:HD23	22:L:307:SER:HB2	1.95	0.48
23:M:201:MET:O	23:M:205:ILE:HG12	2.13	0.48
10:7:32:GLN:HG2	15:q:122:GLU:HA	1.95	0.48
18:A:92:PHE:HZ	19:H:306:SER:HB2	1.79	0.48
21:K:41:PHE:HE2	21:K:64:LEU:HB2	1.78	0.48
24:N:42:PRO:HA	24:N:45:ILE:HG22	1.94	0.48
38:j:9:PRO:HB2	39:k:19:MET:HE1	1.95	0.48
47:9:204:PC1:H2C1	19:H:175:LEU:HD11	1.96	0.48
15:q:1:MET:HE3	15:q:3:LEU:HB3	1.95	0.48
15:q:9:ARG:HH21	54:r:202:CDL:HA22	1.79	0.48
22:L:83:ASP:N	22:L:86:SER:OG	2.43	0.48
40:l:81:ASP:OD1	40:l:81:ASP:N	2.43	0.48
13:V:8:THR:HG21	13:V:13:LEU:HB3	1.95	0.48
22:L:400:ASN:HB3	22:L:486:LEU:HD23	1.95	0.48
23:M:204:LEU:HD22	23:M:209:LEU:HD13	1.95	0.48
24:N:175:MET:O	24:N:179:MET:HG2	2.13	0.48
24:N:181:TYR:HA	24:N:184:ILE:HD12	1.95	0.48
24:N:213:ALA:O	24:N:217:MET:HG3	2.14	0.48
8:P:324:TYR:HB2	19:H:65:THR:HB	1.94	0.48
11:S:61:GLN:OE1	11:S:79:ASN:ND2	2.44	0.48
18:A:60:ILE:HG21	20:J:166:ILE:HG13	1.96	0.48
18:A:99:SER:HB3	46:A:201:3PE:H391	1.96	0.48
22:L:190:SER:HB2	22:L:196:TRP:NE1	2.29	0.48
25:O:115:LEU:HD12	25:O:121:GLY:HA2	1.94	0.48
27:Y:47:SER:N	27:Y:50:GLU:OE2	2.47	0.48
15:q:117:VAL:O	15:q:120:THR:OG1	2.27	0.48
24:N:208:TYR:O	24:N:212:THR:OG1	2.28	0.48
5:1:287:VAL:HG21	5:1:294:LEU:HB2	1.95	0.47
21:K:97:GLN:HB3	22:L:582:GLY:HA3	1.96	0.47
22:L:59:MET:HE1	37:i:101:PRO:HB3	1.96	0.47
25:O:176:VAL:HG21	25:O:200:GLN:HG2	1.95	0.47
3:D:63:ARG:HB3	3:D:79:HIS:HB2	1.96	0.47
6:3:107:ILE:HG23	7:9:80:ILE:HD12	1.96	0.47
6:3:432:ILE:HB	6:3:473:MET:HE2	1.97	0.47
15:q:2:GLU:HG3	16:r:4:THR:HB	1.95	0.47
41:m:28:THR:O	41:m:32:GLN:HG3	2.13	0.47
1:6:135:TYR:CD1	7:9:119:ILE:HG21	2.49	0.47
6:3:381:GLY:HA3	6:3:457:ALA:HB2	1.96	0.47
17:s:41:ASN:OD1	17:s:44:THR:OG1	2.27	0.47
19:H:68:MET:O	19:H:72:ILE:HG12	2.14	0.47
19:H:142:TYR:HA	19:H:145:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:J:20:ALA:HB1	46:K:201:3PE:H261	1.95	0.47
24:N:70:ILE:HD11	24:N:102:LEU:HG	1.96	0.47
29:a:14:VAL:O	29:a:18:ILE:HG12	2.15	0.47
3:D:211:ILE:HG22	3:D:315:LEU:HD11	1.97	0.47
6:3:113:GLU:HA	9:Q:46:GLN:HE21	1.79	0.47
6:3:221:GLU:OE2	7:9:83:LYS:HD3	2.13	0.47
8:P:153:GLU:OE1	8:P:167:ARG:NH1	2.46	0.47
9:Q:29:HIS:HA	9:Q:33:ARG:HG2	1.96	0.47
9:Q:33:ARG:HH12	9:Q:77:ASP:HB2	1.79	0.47
23:M:403:THR:HA	23:M:406:TYR:CE2	2.49	0.47
12:U:72:CYS:SG	12:U:75:GLU:HG2	2.53	0.47
28:Z:57:ARG:NH2	30:b:48:THR:OG1	2.44	0.47
25:O:293:TYR:OH	25:O:297:ARG:NH1	2.48	0.47
26:X:142:HIS:HB2	28:Z:114:ARG:HB3	1.96	0.47
2:C:75:LEU:HA	2:C:96:LEU:HD23	1.97	0.47
5:1:89:ARG:NH1	5:1:217:GLY:O	2.47	0.47
7:9:134:VAL:HG11	7:9:171:ILE:HD11	1.97	0.47
16:r:2:SER:O	54:r:202:CDL:O1	2.31	0.47
19:H:20:LEU:HA	29:a:12:MET:HE1	1.97	0.47
19:H:27:ILE:HD12	19:H:271:LEU:HD12	1.97	0.47
19:H:221:ALA:O	19:H:225:MET:HG3	2.14	0.47
22:L:62:MET:HB3	44:p:114:GLN:HG2	1.97	0.47
23:M:156:GLY:HA2	47:M:501:PC1:H3I2	1.96	0.47
24:N:86:PHE:HD2	24:N:145:ILE:HG21	1.80	0.47
24:N:190:MET:HE2	24:N:205:LEU:HA	1.96	0.47
12:U:20:LYS:O	39:k:52:ARG:NH2	2.47	0.47
6:3:99:ALA:O	6:3:134:LYS:NZ	2.45	0.47
26:X:82:THR:HA	26:X:85:TRP:CD1	2.50	0.47
28:Z:67:ARG:O	28:Z:71:MET:HG3	2.15	0.47
28:Z:127:ARG:HG3	33:e:97:HIS:HD2	1.80	0.47
2:C:40:VAL:HG12	16:r:68:ILE:HD12	1.97	0.47
3:D:148:LEU:HD23	3:D:174:ARG:HG2	1.97	0.47
6:3:588:THR:HG21	9:Q:63:GLU:HA	1.96	0.47
32:d:28:ASP:OD1	32:d:28:ASP:N	2.46	0.47
42:n:21:ARG:NH2	42:n:67:GLU:OE2	2.47	0.47
3:D:371:LYS:NZ	3:D:422:ASP:OD1	2.45	0.47
8:P:107:GLU:O	8:P:111:VAL:HB	2.15	0.47
8:P:134:HIS:ND1	8:P:135:LEU:O	2.32	0.47
25:O:94:TYR:OH	25:O:151:HIS:ND1	2.36	0.47
2:C:45:LEU:HD23	3:D:124:LYS:HG2	1.96	0.46
13:V:71:LEU:HD13	13:V:79:VAL:HG11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:K:41:PHE:HA	21:K:63:ILE:HD11	1.97	0.46
6:3:25:THR:HA	6:3:72:PRO:HA	1.95	0.46
23:M:458:THR:O	44:p:149:TYR:OH	2.32	0.46
28:Z:142:TYR:OH	29:a:37:ARG:O	2.30	0.46
3:D:224:GLU:OE1	7:9:42:TYR:OH	2.25	0.46
16:r:27:TYR:O	16:r:28:GLN:NE2	2.48	0.46
21:K:17:LEU:HG	46:K:201:3PE:H262	1.97	0.46
25:O:318:TRP:HE3	32:d:58:LEU:HD12	1.80	0.46
6:3:297:GLU:HG3	14:W:125:TYR:CZ	2.50	0.46
22:L:530:PRO:O	22:L:534:HIS:HB2	2.16	0.46
26:X:72:GLN:HG2	26:X:114:LEU:HD21	1.97	0.46
33:e:96:HIS:HA	33:e:101:GLU:HB3	1.97	0.46
39:k:67:THR:HG23	39:k:70:SER:H	1.81	0.46
3:D:115:GLU:HB3	3:D:194:ILE:HB	1.98	0.46
11:S:78:LEU:HB2	11:S:81:LEU:HD23	1.97	0.46
23:M:254:THR:O	23:M:258:ALA:HB2	2.16	0.46
8:P:29:PHE:HD1	8:P:175:GLU:HG2	1.81	0.46
22:L:112:PRO:HG3	42:n:178:THR:HG21	1.96	0.46
22:L:419:THR:HA	22:L:422:TYR:CE1	2.51	0.46
22:L:445:GLU:OE2	38:j:21:GLN:NE2	2.47	0.46
22:L:455:LYS:HD2	38:j:28:LEU:HD11	1.97	0.46
41:m:47:LEU:HB3	42:n:165:LEU:HD13	1.98	0.46
4:2:31:ILE:HG12	4:2:50:VAL:HG22	1.97	0.46
23:M:237:LYS:HE3	23:M:294:MET:HE3	1.98	0.46
38:j:61:ASP:OD2	43:o:106:ARG:NH1	2.48	0.46
9:Q:60:ASP:OD1	9:Q:60:ASP:N	2.47	0.46
53:T:201:ZMP:HN1	14:W:34:VAL:HG21	1.80	0.46
26:X:29:HIS:HB3	26:X:119:PRO:HD2	1.97	0.46
39:k:23:ASP:OD2	39:k:25:ARG:NE	2.44	0.46
6:3:634:ASP:OD2	9:Q:109:LYS:NZ	2.48	0.46
8:P:128:ARG:NH1	8:P:220:ASP:O	2.39	0.46
8:P:133:SER:OG	8:P:134:HIS:N	2.46	0.46
22:L:414:ILE:O	22:L:418:MET:HG2	2.16	0.46
12:U:20:LYS:HG2	12:U:27:PRO:HB3	1.97	0.46
26:X:33:ALA:HB2	26:X:119:PRO:HG3	1.97	0.46
40:l:6:ASP:N	40:l:6:ASP:OD1	2.49	0.46
40:l:96:SER:HB3	41:m:6:LYS:H	1.81	0.46
1:6:59:THR:HG21	1:6:69:MET:HG3	1.98	0.46
1:6:77:TYR:HB3	1:6:167:LEU:HD22	1.98	0.46
3:D:115:GLU:OE1	3:D:194:ILE:N	2.48	0.46
6:3:10:GLU:HB2	6:3:19:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:477:ILE:O	6:3:481:THR:OG1	2.29	0.46
15:q:60:ARG:HH22	15:q:95:ASP:HA	1.80	0.46
24:N:142:LEU:HB3	24:N:194:LEU:HD11	1.97	0.46
26:X:4:VAL:HG13	28:Z:108:SER:HB2	1.97	0.46
5:1:276:LEU:HD21	5:1:297:VAL:HG11	1.98	0.45
47:9:203:PC1:H3I2	19:H:182:ALA:HB1	1.98	0.45
24:N:221:LEU:HD21	24:N:237:THR:HG21	1.97	0.45
12:U:44:SER:HB2	42:n:16:LEU:HD11	1.97	0.45
26:X:17:VAL:HG21	28:Z:73:LEU:HD21	1.98	0.45
7:9:34:ARG:HB3	47:9:204:PC1:H31	1.99	0.45
19:H:149:ILE:HG13	19:H:297:THR:HG23	1.98	0.45
22:L:534:HIS:HB3	46:L:701:3PE:H2	1.98	0.45
6:3:577:GLU:OE1	6:3:579:ARG:NH1	2.49	0.45
23:M:307:TRP:CE2	23:M:459:MET:HE1	2.51	0.45
23:M:410:MET:O	23:M:414:THR:OG1	2.25	0.45
8:P:90:VAL:HG22	8:P:128:ARG:HB2	1.98	0.45
8:P:137:ALA:HB2	8:P:146:LEU:HD22	1.98	0.45
9:Q:36:ARG:O	9:Q:57:MET:HA	2.16	0.45
19:H:114:TYR:OH	20:J:60:LEU:O	2.29	0.45
37:i:86:LYS:HE3	37:i:87:TYR:CZ	2.51	0.45
1:6:62:LEU:HD12	3:D:83:LEU:HD13	1.98	0.45
4:2:108:CYS:HA	4:2:151:ALA:HB1	1.98	0.45
23:M:102:LEU:HD13	23:M:230:ILE:HG12	1.98	0.45
23:M:285:LEU:HD13	23:M:342:MET:HE2	1.98	0.45
26:X:13:LYS:HB2	26:X:13:LYS:HE3	1.78	0.45
15:q:5:GLU:OE2	15:q:9:ARG:NH1	2.50	0.45
20:J:44:LEU:HD23	20:J:49:SER:HA	1.97	0.45
21:K:22:PHE:CD2	22:L:585:LYS:HA	2.52	0.45
21:K:80:LYS:HA	21:K:80:LYS:HD2	1.81	0.45
53:U:201:ZMP:H15	53:U:201:ZMP:H17	1.66	0.45
27:Y:24:THR:HG21	27:Y:69:PHE:HD2	1.82	0.45
30:b:25:TRP:O	30:b:29:ILE:HG12	2.17	0.45
3:D:423:ILE:HD12	3:D:428:ILE:HD11	1.98	0.45
6:3:222:THR:O	6:3:224:LYS:NZ	2.48	0.45
6:3:252:PRO:HB3	6:3:263:ILE:HG23	1.99	0.45
8:P:13:ARG:NH2	8:P:63:GLY:O	2.50	0.45
8:P:46:ILE:HG12	10:7:26:VAL:HG21	1.99	0.45
21:K:70:GLU:HA	24:N:38:LEU:HD21	1.99	0.45
22:L:102:GLN:OE1	22:L:456:ARG:NH2	2.41	0.45
23:M:364:LEU:HD22	23:M:369:LEU:HD22	1.99	0.45
25:O:221:LEU:HD23	25:O:221:LEU:HA	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:h:201:CDL:OB4	44:p:48:ARG:NH1	2.44	0.45
9:Q:38:PHE:HE1	9:Q:58:GLU:HG2	1.82	0.45
20:J:165:ILE:HG12	24:N:42:PRO:HG2	1.98	0.45
22:L:67:HIS:NE2	22:L:70:THR:OG1	2.41	0.45
28:Z:93:GLU:OE2	33:e:74:ARG:NH1	2.50	0.45
4:2:101:GLN:HG2	4:2:140:ILE:HD11	1.99	0.45
20:J:136:GLU:HG3	20:J:138:GLY:H	1.82	0.45
25:O:320:LYS:HB3	31:c:12:PRO:HB3	1.99	0.45
53:U:201:ZMP:H3A	42:n:22:ALA:HB1	1.99	0.45
37:i:109:ILE:HG22	37:i:112:THR:H	1.82	0.45
41:m:124:PHE:HD1	44:p:135:THR:HG21	1.81	0.45
6:3:285:ARG:NH2	6:3:555:PRO:O	2.50	0.45
19:H:310:PHE:HA	30:b:38:THR:HG22	1.98	0.45
22:L:407:TRP:HE1	40:l:111:MET:HE3	1.82	0.45
46:L:703:3PE:H372	23:M:155:ILE:HD12	1.99	0.45
23:M:278:ARG:HD2	23:M:278:ARG:HA	1.72	0.45
23:M:447:LEU:HD21	46:M:502:3PE:H3G2	1.99	0.45
25:O:17:LYS:HB3	25:O:17:LYS:HE2	1.76	0.45
29:a:34:LYS:NZ	29:a:61:TYR:O	2.43	0.45
29:a:52:ARG:NH1	29:a:58:ASN:OD1	2.49	0.45
19:H:179:TRP:HE1	28:Z:42:LEU:HG	1.82	0.44
22:L:562:ILE:HG23	47:M:501:PC1:H2I1	1.98	0.44
23:M:203:PHE:O	23:M:207:MET:HG3	2.16	0.44
23:M:220:HIS:O	23:M:283:LYS:NZ	2.46	0.44
26:X:40:LYS:HA	26:X:40:LYS:HD3	1.80	0.44
32:d:100:ASP:OD1	36:h:117:ARG:NH2	2.50	0.44
35:g:96:LYS:NZ	44:p:5:ASP:OD2	2.40	0.44
54:r:202:CDL:H182	29:a:7:PRO:HD3	1.99	0.44
18:A:9:ILE:HD12	19:H:6:ILE:HD13	1.99	0.44
19:H:179:TRP:O	19:H:183:MET:HG3	2.17	0.44
22:L:74:MET:HE3	22:L:195:SER:HA	1.98	0.44
24:N:168:GLY:O	24:N:171:ASN:N	2.50	0.44
24:N:338:PRO:HA	26:X:169:TRP:HZ2	1.82	0.44
37:i:88:HIS:ND1	46:i:201:3PE:O22	2.50	0.44
4:2:149:VAL:O	4:2:190:ARG:NH2	2.46	0.44
6:3:577:GLU:HB3	6:3:636:ILE:HD11	1.99	0.44
9:Q:25:VAL:HB	9:Q:30:ILE:HD11	1.99	0.44
26:X:23:VAL:HG22	26:X:85:TRP:CD2	2.52	0.44
35:g:98:ARG:HG3	35:g:103:LEU:HB2	1.98	0.44
37:i:18:ARG:NH1	42:n:170:VAL:O	2.45	0.44
40:l:3:MET:HB3	40:l:8:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:30:ALA:HB2	2:C:40:VAL:HG21	1.99	0.44
3:D:100:LEU:HD11	3:D:195:ARG:HA	1.99	0.44
6:3:160:ILE:HD11	6:3:183:VAL:HG13	2.00	0.44
8:P:21:ALA:HA	8:P:90:VAL:O	2.17	0.44
15:q:144:TYR:OH	15:q:145:LYS:NZ	2.47	0.44
25:O:280:PRO:HB2	35:g:22:MET:HB3	1.99	0.44
1:6:52:ARG:O	1:6:174:GLN:NE2	2.50	0.44
4:2:123:LYS:NZ	4:2:174:ASP:OD1	2.39	0.44
10:7:5:SER:HB3	10:7:17:VAL:HG21	2.00	0.44
12:T:47:GLN:O	12:T:51:ILE:HG12	2.17	0.44
24:N:28:LEU:HA	24:N:31:VAL:HG22	1.98	0.44
38:j:10:ARG:HG3	38:j:15:PRO:HA	1.98	0.44
40:l:126:PRO:HD3	43:o:3:HIS:CE1	2.52	0.44
12:U:11:ILE:HG22	12:U:77:VAL:HG22	1.99	0.44
37:i:1:SAC:OG	37:i:2:GLY:N	2.44	0.44
3:D:145:THR:OG1	3:D:181:TYR:OH	2.36	0.44
3:D:350:LYS:HD2	3:D:350:LYS:HA	1.84	0.44
5:1:292:ASP:O	5:1:339:ARG:NH1	2.51	0.44
12:U:78:ASP:HB3	37:i:15:ARG:CZ	2.48	0.44
27:Y:8:TYR:HB2	27:Y:23:ILE:HG21	1.99	0.44
3:D:412:ALA:HB3	19:H:281:ARG:HG3	1.99	0.44
19:H:114:TYR:OH	20:J:64:LEU:HB2	2.17	0.44
46:L:704:3PE:O32	27:Y:109:THR:OG1	2.32	0.44
6:3:317:ALA:HB3	6:3:343:LEU:HD13	1.99	0.44
6:3:326:GLU:OE2	6:3:620:ARG:NE	2.51	0.44
12:T:9:ASP:OD1	12:T:10:GLY:N	2.50	0.44
19:H:316:PRO:HG3	28:Z:56:ARG:HB3	2.00	0.44
20:J:132:GLY:HA2	28:Z:67:ARG:HH21	1.83	0.44
22:L:78:MET:HA	54:h:201:CDL:H262	1.99	0.44
22:L:513:MET:HE3	22:L:513:MET:HB3	1.83	0.44
23:M:281:ASP:HB3	23:M:284:SER:HB2	1.98	0.44
12:U:26:ASP:OD1	12:U:26:ASP:N	2.46	0.44
47:9:204:PC1:H2E2	19:H:175:LEU:HD21	1.98	0.43
23:M:219:ALA:O	23:M:223:ALA:HB2	2.18	0.43
24:N:314:MET:HE3	24:N:314:MET:HB3	1.91	0.43
33:e:37:LYS:HG3	36:h:133:ILE:HG21	1.99	0.43
1:6:48:ASN:HB3	1:6:178:LYS:HA	1.99	0.43
2:C:180:VAL:HG23	2:C:182:ARG:HB2	2.01	0.43
6:3:478:ARG:HH22	6:3:485:ALA:HA	1.83	0.43
19:H:18:ALA:HB1	19:H:48:PRO:HB2	2.00	0.43
19:H:87:VAL:HG23	19:H:95:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:74:PRO:HA	23:M:77:LEU:HD12	2.00	0.43
26:X:18:LYS:HB2	29:a:68:ASN:HB3	2.01	0.43
35:g:79:PRO:HG3	36:h:72:SER:HB3	1.99	0.43
43:o:49:GLN:OE1	44:p:119:ASN:ND2	2.51	0.43
5:1:309:LYS:HA	5:1:312:CYS:HB2	2.00	0.43
26:X:39:ASN:HB3	28:Z:72:PRO:HG2	1.98	0.43
37:i:17:LEU:HD11	42:n:162:LEU:HD22	2.00	0.43
3:D:106:LEU:HD13	3:D:391:ILE:HG21	2.00	0.43
9:Q:42:ARG:HD3	9:Q:49:VAL:HG12	2.00	0.43
9:Q:64:ARG:HG2	9:Q:75:THR:HG22	2.00	0.43
22:L:341:MET:HE2	22:L:341:MET:HB2	1.87	0.43
22:L:468:ILE:O	22:L:472:ILE:HG12	2.19	0.43
23:M:106:LEU:HD13	23:M:234:ILE:HG21	2.00	0.43
23:M:367:LEU:HD23	23:M:407:SER:HB2	2.01	0.43
24:N:40:ILE:HD12	24:N:134:GLN:HE21	1.83	0.43
26:X:37:LYS:NZ	26:X:41:GLU:OE2	2.44	0.43
27:Y:36:SER:HB2	27:Y:55:VAL:HA	2.00	0.43
5:1:96:ASN:O	5:1:225:VAL:HG23	2.17	0.43
6:3:579:ARG:HB2	6:3:636:ILE:HD13	2.00	0.43
18:A:75:LEU:O	18:A:79:ILE:HG12	2.19	0.43
20:J:131:VAL:HG23	29:a:43:TYR:HD1	1.83	0.43
23:M:279:GLN:HG3	23:M:281:ASP:H	1.83	0.43
23:M:310:MET:HE1	23:M:380:PHE:CD2	2.54	0.43
4:2:39:PRO:HA	17:s:59:GLN:HB3	2.01	0.43
5:1:162:ILE:HG21	5:1:175:VAL:HG23	2.01	0.43
49:1:501:FMN:H9	49:1:501:FMN:H1'1	1.78	0.43
22:L:552:LEU:HG	22:L:557:TRP:HD1	1.84	0.43
24:N:216:PHE:O	24:N:220:MET:HG3	2.19	0.43
25:O:155:ILE:HD12	25:O:273:THR:HA	2.01	0.43
27:Y:13:ASP:HA	27:Y:20:LYS:HE2	2.01	0.43
36:h:36:VAL:O	36:h:40:ILE:HG12	2.18	0.43
2:C:88:ASN:HA	2:C:112:ASP:HB3	1.99	0.43
5:1:92:TYR:O	5:1:220:THR:HA	2.18	0.43
7:9:134:VAL:HG21	7:9:167:ILE:HG21	2.00	0.43
18:A:87:MET:HE3	18:A:87:MET:HB3	1.89	0.43
26:X:7:PRO:HD2	28:Z:83:LEU:HD12	2.01	0.43
3:D:91:ILE:HG12	3:D:99:ALA:HB1	2.00	0.43
5:1:190:THR:HB	5:1:204:ARG:HG2	2.00	0.43
22:L:129:LEU:HD23	22:L:129:LEU:HA	1.82	0.43
22:L:565:SER:HB2	27:Y:112:MET:HE1	2.00	0.43
35:g:112:ASP:HB3	35:g:115:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:l:42:GLY:HA2	41:m:78:ASN:HB2	2.01	0.43
13:V:54:LYS:O	13:V:58:VAL:HG23	2.18	0.43
25:O:12:ASP:OD1	25:O:17:LYS:NZ	2.46	0.43
4:2:60:TRP:CD1	4:2:60:TRP:H	2.37	0.43
5:1:191:ALA:HB2	5:1:203:PRO:HG3	2.01	0.43
5:1:322:LEU:HD12	5:1:329:LEU:HB2	2.01	0.43
6:3:448:LYS:HD2	6:3:487:TRP:CD2	2.54	0.43
16:r:98:PRO:HA	16:r:99:PRO:HD3	1.95	0.43
19:H:231:ILE:HG23	19:H:270:PHE:HD2	1.84	0.43
21:K:60:PRO:HA	21:K:63:ILE:HG12	2.01	0.43
22:L:36:THR:O	22:L:40:ILE:HG12	2.19	0.43
23:M:177:MET:HE3	36:h:94:LEU:HD21	2.01	0.43
29:a:54:ILE:HD11	33:e:105:PRO:HB3	2.00	0.43
1:6:119:GLU:O	8:P:54:TYR:OH	2.22	0.42
1:6:186:TRP:HA	1:6:189:ARG:HG2	2.01	0.42
3:D:145:THR:HA	3:D:148:LEU:HD12	2.01	0.42
22:L:293:LEU:HD23	22:L:293:LEU:HA	1.92	0.42
22:L:496:LEU:HD23	22:L:496:LEU:HA	1.88	0.42
30:b:39:LYS:O	30:b:43:MET:HG3	2.19	0.42
1:6:63:ALA:HA	3:D:108:TYR:CZ	2.55	0.42
1:6:80:ASP:OD1	19:H:25:ARG:NE	2.50	0.42
2:C:81:VAL:HG22	3:D:388:ARG:HG2	2.01	0.42
3:D:278:TYR:HA	3:D:281:VAL:HG22	2.00	0.42
4:2:76:PRO:HA	4:2:77:PRO:HD3	1.95	0.42
19:H:81:LEU:HD23	46:H:401:3PE:H3A1	2.00	0.42
22:L:9:LEU:HD13	46:i:201:3PE:H2D1	2.01	0.42
22:L:136:ASN:HB3	22:L:197:GLU:OE2	2.19	0.42
22:L:539:MET:HE3	22:L:543:ASN:ND2	2.32	0.42
23:M:347:GLY:HA3	23:M:419:LEU:HA	2.01	0.42
28:Z:68:ILE:HD11	30:b:49:PRO:HB2	2.01	0.42
3:D:116:GLN:NE2	3:D:276:ASP:OD2	2.45	0.42
24:N:319:LYS:HE2	25:O:267:THR:HG21	2.00	0.42
31:c:17:VAL:HG23	32:d:59:HIS:CG	2.54	0.42
3:D:7:ASP:OD1	3:D:7:ASP:N	2.45	0.42
3:D:360:PRO:HA	3:D:380:SER:O	2.19	0.42
6:3:636:ILE:HD12	6:3:636:ILE:HA	1.91	0.42
7:9:28:MET:HE2	19:H:179:TRP:HH2	1.83	0.42
19:H:169:GLN:OE1	19:H:174:LEU:N	2.52	0.42
23:M:76:MET:HE3	23:M:230:ILE:HB	2.01	0.42
23:M:319:HIS:HA	23:M:322:THR:HG22	2.02	0.42
23:M:368:ALA:HB1	23:M:375:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:49:ARG:HB2	34:f:52:GLU:HG2	2.01	0.42
39:k:30:GLU:HA	39:k:35:GLU:HG3	2.00	0.42
1:6:189:ARG:HH12	8:P:51:CYS:HB3	1.84	0.42
5:1:372:MET:HE2	5:1:399:ILE:HD13	2.00	0.42
6:3:108:CYS:O	6:3:218:ARG:NH1	2.35	0.42
11:S:32:VAL:HG21	11:S:62:PRO:HB3	2.01	0.42
46:L:704:3PE:H371	27:Y:113:GLY:HA2	2.00	0.42
23:M:11:LEU:HD23	23:M:14:LEU:HD23	2.00	0.42
23:M:139:GLN:HE22	23:M:340:ARG:HH12	1.67	0.42
37:i:68:LEU:HA	37:i:71:VAL:HG12	2.01	0.42
41:m:122:ARG:HB3	41:m:125:ASN:HB3	2.00	0.42
3:D:292:ASP:OD1	3:D:292:ASP:N	2.47	0.42
6:3:533:THR:OG1	6:3:534:ARG:N	2.53	0.42
8:P:48:PRO:HA	8:P:71:LEU:O	2.20	0.42
8:P:69:THR:HG21	10:7:26:VAL:HG22	2.02	0.42
11:S:41:VAL:O	11:S:45:LYS:HG2	2.19	0.42
13:V:42:ALA:HA	13:V:45:LYS:HE2	2.00	0.42
18:A:65:PHE:HB3	19:H:144:VAL:HG21	2.01	0.42
23:M:443:PRO:HB3	46:M:502:3PE:H3C1	2.01	0.42
47:M:501:PC1:H321	47:M:501:PC1:H352	1.90	0.42
37:i:82:HIS:ND1	44:p:36:TYR:OH	2.46	0.42
6:3:266:LYS:O	6:3:270:ALA:CB	2.68	0.42
6:3:616:LEU:O	6:3:620:ARG:HG2	2.20	0.42
17:s:34:ASN:O	17:s:37:HIS:ND1	2.40	0.42
26:X:74:LYS:HB2	29:a:66:LEU:HD12	2.01	0.42
33:e:53:LYS:HE2	33:e:53:LYS:HB2	1.79	0.42
3:D:350:LYS:HG3	6:3:121:MET:HG3	2.01	0.42
4:2:105:THR:HG22	4:2:106:THR:H	1.83	0.42
5:1:82:MET:SD	5:1:221:THR:OG1	2.70	0.42
6:3:651:LEU:HD22	11:S:45:LYS:HE2	2.02	0.42
7:9:34:ARG:NH1	47:9:204:PC1:O12	2.53	0.42
10:7:38:ASN:HB3	10:7:43:LEU:HD11	2.01	0.42
20:J:22:LYS:NZ	21:K:18:GLY:O	2.50	0.42
22:L:386:LEU:HD23	22:L:386:LEU:HA	1.93	0.42
22:L:435:PRO:HG2	39:k:57:ARG:HB3	2.02	0.42
23:M:67:ILE:HG22	46:M:502:3PE:H3D1	2.01	0.42
24:N:102:LEU:HD13	24:N:142:LEU:HG	2.01	0.42
25:O:101:TYR:HH	25:O:159:THR:HG1	1.66	0.42
31:c:43:LYS:HG2	31:c:48:LEU:HB2	2.02	0.42
32:d:29:PRO:HG3	54:d:201:CDL:H112	2.00	0.42
46:h:202:3PE:H3B2	46:h:202:3PE:H2B2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:i:15:ARG:O	37:i:19:ARG:HG2	2.19	0.42
37:i:94:TYR:OH	44:p:10:PRO:O	2.29	0.42
4:2:156:ILE:HB	4:2:161:TYR:HE2	1.84	0.42
46:M:502:3PE:H3A1	46:M:502:3PE:H372	1.79	0.42
24:N:172:GLN:HE22	24:N:181:TYR:HD2	1.68	0.42
27:Y:113:GLY:O	27:Y:117:MET:HB2	2.19	0.42
29:a:1:MET:HE3	29:a:1:MET:HB3	1.88	0.42
40:l:15:THR:OG1	40:l:17:GLU:OE1	2.36	0.42
22:L:101:MET:HE2	22:L:101:MET:HB3	1.92	0.42
22:L:176:ARG:O	22:L:180:ILE:HG12	2.20	0.42
22:L:223:LYS:HA	22:L:223:LYS:HD3	1.77	0.42
22:L:383:MET:HB3	22:L:386:LEU:HD12	2.02	0.42
23:M:78:MET:HE2	23:M:78:MET:HB3	1.79	0.42
24:N:154:ILE:HD13	24:N:195:PRO:HG3	2.02	0.42
24:N:235:ASN:HB2	24:N:307:THR:HG21	2.02	0.42
12:U:25:ILE:HG21	12:U:30:LEU:HD13	2.02	0.42
33:e:7:LYS:HB2	33:e:7:LYS:HE3	1.82	0.42
3:D:230:THR:O	3:D:294:TYR:OH	2.37	0.41
21:K:1:FME:HE3	21:K:1:FME:HB2	1.96	0.41
23:M:129:THR:HG21	23:M:235:LEU:HD11	2.01	0.41
23:M:237:LYS:H	23:M:237:LYS:HD2	1.85	0.41
24:N:47:LYS:HA	24:N:47:LYS:HD3	1.71	0.41
6:3:71:MET:HE2	6:3:71:MET:HB2	1.97	0.41
8:P:37:HIS:CD2	8:P:40:ARG:HH21	2.37	0.41
8:P:186:ARG:HD2	8:P:251:ARG:HB3	2.01	0.41
19:H:258:ASN:O	19:H:262:GLU:HG3	2.21	0.41
22:L:54:PHE:CZ	22:L:84:PHE:HB2	2.55	0.41
22:L:306:THR:HG23	22:L:332:HIS:CE1	2.55	0.41
23:M:34:ILE:HD13	23:M:34:ILE:HA	1.88	0.41
3:D:11:ALA:HB1	25:O:278:TYR:CZ	2.55	0.41
4:2:183:LYS:HA	4:2:184:PRO:HD3	1.87	0.41
7:9:150:LEU:HD23	9:Q:70:MET:HG3	2.01	0.41
20:J:164:PHE:HE2	24:N:4:ILE:HG22	1.84	0.41
22:L:75:GLU:OE1	22:L:77:LYS:NZ	2.51	0.41
22:L:313:MET:HE2	22:L:329:ILE:HA	2.03	0.41
23:M:46:ASP:OD2	23:M:47:GLU:N	2.53	0.41
23:M:166:LEU:HD23	23:M:195:LEU:HD12	2.02	0.41
23:M:383:MET:HE2	23:M:383:MET:HB3	1.86	0.41
25:O:311:GLU:HG2	25:O:312:VAL:HG13	2.02	0.41
31:c:14:TRP:HA	31:c:17:VAL:HG12	2.02	0.41
39:k:87:LEU:HD23	39:k:87:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:121:ARG:H	8:P:54:TYR:HH	1.62	0.41
4:2:207:LYS:HD3	4:2:207:LYS:HA	1.89	0.41
6:3:12:PHE:HB2	6:3:78:ASN:HA	2.03	0.41
22:L:75:GLU:HG3	44:p:103:ASN:ND2	2.35	0.41
22:L:535:ARG:NH1	40:l:91:SER:O	2.46	0.41
24:N:88:GLN:HG3	33:e:52:LYS:HE2	2.02	0.41
24:N:335:MET:HE3	24:N:335:MET:HB3	1.91	0.41
36:h:62:GLU:O	36:h:65:GLU:HB2	2.20	0.41
2:C:43:SER:HA	16:r:65:PRO:HB3	2.03	0.41
4:2:100:ILE:HG12	4:2:156:ILE:HG12	2.01	0.41
5:1:279:LEU:HD12	5:1:283:HIS:HD2	1.85	0.41
11:S:63:LYS:HE2	11:S:63:LYS:HB2	1.90	0.41
12:T:46:ASP:O	12:T:50:ILE:HD12	2.21	0.41
21:K:54:MET:HB2	33:e:25:PRO:HD2	2.02	0.41
23:M:331:ASN:O	23:M:335:GLU:HG3	2.21	0.41
24:N:275:CYS:HB3	27:Y:136:PRO:HG3	2.03	0.41
29:a:28:LYS:HE3	29:a:28:LYS:HB3	1.76	0.41
33:e:27:LYS:HA	33:e:27:LYS:HD3	1.92	0.41
38:j:11:TYR:HD2	39:k:22:PRO:HD2	1.85	0.41
4:2:126:ILE:HB	4:2:130:GLU:HG3	2.01	0.41
5:1:349:ARG:HA	5:1:349:ARG:HD2	1.84	0.41
6:3:237:ASN:HB3	6:3:253:ARG:CZ	2.51	0.41
11:S:18:ILE:O	11:S:52:ILE:HA	2.21	0.41
22:L:273:ILE:HG22	22:L:277:MET:HE2	2.03	0.41
22:L:477:ILE:H	22:L:477:ILE:HG13	1.67	0.41
24:N:334:THR:HG22	24:N:335:MET:HG2	2.03	0.41
25:O:30:ASN:HD22	25:O:179:VAL:HG21	1.86	0.41
42:n:94:GLU:OE2	42:n:97:LYS:NZ	2.40	0.41
43:o:5:THR:O	43:o:9:LEU:HB2	2.20	0.41
9:Q:33:ARG:HD2	9:Q:33:ARG:HA	1.82	0.41
14:W:37:LEU:HD13	14:W:89:LYS:HG2	2.02	0.41
18:A:63:LEU:HD11	20:J:66:VAL:HG11	2.03	0.41
23:M:305:THR:HG22	23:M:307:TRP:H	1.86	0.41
23:M:395:LEU:HD21	41:m:100:TRP:CE2	2.56	0.41
25:O:87:LYS:HE3	25:O:87:LYS:HB3	1.78	0.41
35:g:25:GLN:H	35:g:25:GLN:HG2	1.71	0.41
36:h:37:ILE:HG23	54:h:201:CDL:H552	2.02	0.41
2:C:83:VAL:HG12	2:C:85:THR:HG22	2.02	0.41
5:1:176:PHE:HE1	17:s:56:ARG:HD3	1.86	0.41
7:9:22:ASN:O	7:9:26:ILE:HG12	2.21	0.41
15:q:9:ARG:NE	54:r:202:CDL:OA4	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:J:93:VAL:HA	20:J:96:VAL:HG12	2.03	0.41
22:L:278:LEU:HD21	22:L:404:THR:HB	2.03	0.41
23:M:76:MET:HE2	23:M:99:LEU:HD22	2.03	0.41
23:M:139:GLN:NE2	23:M:340:ARG:HH12	2.18	0.41
3:D:369:ALA:HB2	3:D:374:PHE:HB2	2.02	0.41
5:1:360:GLY:O	5:1:366:ARG:NH1	2.46	0.41
6:3:218:ARG:HG2	7:9:83:LYS:HD2	2.01	0.41
6:3:241:SER:HB2	6:3:249:ARG:HB3	2.03	0.41
8:P:10:LYS:HE2	14:W:116:ARG:HD2	2.02	0.41
8:P:165:ILE:O	8:P:227:THR:HA	2.21	0.41
8:P:310:LEU:O	8:P:314:SER:CB	2.59	0.41
12:T:45:LEU:HA	12:T:48:VAL:HG22	2.02	0.41
46:A:201:3PE:H272	30:b:19:VAL:HG22	2.03	0.41
19:H:155:LEU:HD12	19:H:155:LEU:HA	1.80	0.41
20:J:136:GLU:OE2	20:J:137:GLY:N	2.53	0.41
22:L:335:PHE:HE1	22:L:387:THR:HB	1.86	0.41
22:L:457:LEU:HA	22:L:457:LEU:HD23	1.83	0.41
29:a:27:HIS:O	29:a:31:ASN:ND2	2.41	0.41
40:l:9:PRO:HD3	41:m:66:ARG:HG2	2.02	0.41
42:n:135:GLU:HB2	42:n:164:PRO:HA	2.02	0.41
9:Q:28:GLU:O	9:Q:32:THR:OG1	2.28	0.41
20:J:165:ILE:HG23	24:N:42:PRO:HG3	2.03	0.41
22:L:205:ASN:HA	22:L:266:LEU:HD23	2.03	0.41
37:i:23:LYS:NZ	37:i:26:GLU:OE2	2.54	0.41
3:D:175:GLU:OE2	3:D:188:ARG:NH1	2.37	0.40
19:H:111:LEU:O	19:H:114:TYR:HB2	2.21	0.40
21:K:24:SER:HB3	21:K:89:TYR:CD1	2.55	0.40
23:M:151:PHE:HZ	24:N:291:PHE:HA	1.86	0.40
24:N:71:LEU:HD12	24:N:71:LEU:HA	1.91	0.40
24:N:175:MET:HE1	24:N:296:LEU:HD21	2.02	0.40
5:1:247:ARG:HB2	5:1:273:SER:OG	2.21	0.40
7:9:89:CYS:HA	7:9:90:PRO:HD3	1.96	0.40
7:9:154:GLU:O	7:9:158:ASN:ND2	2.54	0.40
24:N:254:LEU:HD23	24:N:254:LEU:HA	1.94	0.40
24:N:313:MET:HB3	25:O:270:LEU:HD13	2.03	0.40
42:n:163:PRO:HA	42:n:164:PRO:HD3	1.97	0.40
3:D:174:ARG:HA	3:D:177:MET:HE3	2.03	0.40
4:2:153:MET:HE2	4:2:153:MET:HB2	1.99	0.40
5:1:95:VAL:HG11	5:1:118:LEU:HD11	2.02	0.40
6:3:46:LEU:O	9:Q:116:LYS:NZ	2.40	0.40
7:9:101:ARG:HD3	7:9:107:ARG:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:7:94:HIS:CE1	10:7:96:HIS:HB2	2.57	0.40
11:S:84:ASP:OD1	11:S:84:ASP:N	2.53	0.40
14:W:44:GLU:OE2	14:W:96:ILE:HD13	2.22	0.40
23:M:427:GLN:HB3	35:g:36:TYR:HE2	1.86	0.40
23:M:456:GLY:O	35:g:82:ARG:NH1	2.45	0.40
24:N:246:LEU:HD13	24:N:334:THR:HG21	2.04	0.40
3:D:154:VAL:HG13	3:D:297:TYR:HE1	1.86	0.40
3:D:183:ARG:NH1	3:D:210:ASP:OD2	2.32	0.40
49:1:501:FMN:N1	49:1:501:FMN:O3'	2.38	0.40
6:3:615:THR:O	6:3:619:VAL:HG23	2.22	0.40
47:9:203:PC1:H332	19:H:280:PHE:HE2	1.87	0.40
8:P:335:LYS:HA	8:P:336:PRO:HD3	1.94	0.40
12:T:15:VAL:HG13	12:T:54:MET:HE1	2.04	0.40
18:A:90:MET:HE3	18:A:90:MET:HB3	1.89	0.40
5:1:73:PHE:HA	5:1:74:PRO:HD3	1.95	0.40
5:1:125:GLY:O	5:1:129:MET:HG2	2.22	0.40
7:9:42:TYR:OH	16:r:24:GLN:NE2	2.54	0.40
12:T:32:VAL:HG12	12:T:74:GLN:OE1	2.21	0.40
12:T:43:ASP:OD2	12:T:44:SER:N	2.53	0.40
23:M:169:ASN:HD21	24:N:272:LYS:HA	1.86	0.40
54:N:401:CDL:H341	54:N:401:CDL:H312	1.92	0.40
46:N:402:3PE:H231	46:N:402:3PE:H332	2.03	0.40
25:O:156:LYS:HE2	25:O:160:LEU:HD22	2.04	0.40
27:Y:45:ALA:HB1	27:Y:50:GLU:HG2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	6	155/224 (69%)	148 (96%)	7 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	206/263 (78%)	199 (97%)	7 (3%)	0	100	100
3	D	411/463 (89%)	393 (96%)	18 (4%)	0	100	100
4	2	212/248 (86%)	200 (94%)	11 (5%)	1 (0%)	24	57
5	1	428/464 (92%)	406 (95%)	21 (5%)	1 (0%)	43	73
6	3	688/727 (95%)	660 (96%)	28 (4%)	0	100	100
7	9	176/212 (83%)	174 (99%)	2 (1%)	0	100	100
8	P	308/377 (82%)	294 (96%)	14 (4%)	0	100	100
9	Q	124/175 (71%)	119 (96%)	5 (4%)	0	100	100
10	7	94/116 (81%)	91 (97%)	3 (3%)	0	100	100
11	S	82/99 (83%)	79 (96%)	3 (4%)	0	100	100
12	T	77/156 (49%)	76 (99%)	1 (1%)	0	100	100
12	U	86/156 (55%)	84 (98%)	2 (2%)	0	100	100
13	V	111/116 (96%)	109 (98%)	2 (2%)	0	100	100
14	W	112/131 (86%)	106 (95%)	6 (5%)	0	100	100
15	q	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
16	r	93/113 (82%)	91 (98%)	2 (2%)	0	100	100
17	s	40/104 (38%)	39 (98%)	1 (2%)	0	100	100
18	A	90/115 (78%)	89 (99%)	1 (1%)	0	100	100
19	H	302/318 (95%)	289 (96%)	13 (4%)	0	100	100
20	J	160/172 (93%)	152 (95%)	8 (5%)	0	100	100
21	K	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
22	L	604/607 (100%)	571 (94%)	33 (6%)	0	100	100
23	M	457/459 (100%)	447 (98%)	10 (2%)	0	100	100
24	N	343/345 (99%)	329 (96%)	14 (4%)	0	100	100
25	O	318/355 (90%)	302 (95%)	16 (5%)	0	100	100
26	X	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
27	Y	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
28	Z	139/144 (96%)	137 (99%)	2 (1%)	0	100	100
29	a	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
30	b	80/84 (95%)	73 (91%)	7 (9%)	0	100	100
31	c	46/76 (60%)	45 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	d	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
33	e	103/106 (97%)	99 (96%)	4 (4%)	0	100	100
34	f	51/57 (90%)	51 (100%)	0	0	100	100
35	g	99/151 (66%)	96 (97%)	3 (3%)	0	100	100
36	h	137/189 (72%)	132 (96%)	5 (4%)	0	100	100
37	i	102/128 (80%)	96 (94%)	6 (6%)	0	100	100
38	j	63/105 (60%)	59 (94%)	4 (6%)	0	100	100
39	k	75/104 (72%)	72 (96%)	3 (4%)	0	100	100
40	l	155/186 (83%)	150 (97%)	5 (3%)	0	100	100
41	m	124/129 (96%)	123 (99%)	1 (1%)	0	100	100
42	n	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
43	o	116/137 (85%)	109 (94%)	7 (6%)	0	100	100
44	p	167/176 (95%)	163 (98%)	4 (2%)	0	100	100
All	All	8042/9212 (87%)	7734 (96%)	306 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	2	183	LYS
5	1	98	ASP

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	6	133/185 (72%)	133 (100%)	0	100	100
2	C	190/227 (84%)	190 (100%)	0	100	100
3	D	361/394 (92%)	361 (100%)	0	100	100
4	2	184/206 (89%)	184 (100%)	0	100	100
5	1	345/370 (93%)	345 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	3	580/610 (95%)	580 (100%)	0	100	100
7	9	152/178 (85%)	152 (100%)	0	100	100
8	P	273/325 (84%)	273 (100%)	0	100	100
9	Q	113/153 (74%)	113 (100%)	0	100	100
10	7	81/96 (84%)	81 (100%)	0	100	100
11	S	74/80 (92%)	74 (100%)	0	100	100
12	T	73/135 (54%)	73 (100%)	0	100	100
12	U	81/135 (60%)	81 (100%)	0	100	100
13	V	101/102 (99%)	101 (100%)	0	100	100
14	W	108/114 (95%)	108 (100%)	0	100	100
15	q	131/131 (100%)	131 (100%)	0	100	100
16	r	86/96 (90%)	86 (100%)	0	100	100
17	s	41/95 (43%)	41 (100%)	0	100	100
18	A	85/103 (82%)	85 (100%)	0	100	100
19	H	269/279 (96%)	269 (100%)	0	100	100
20	J	130/137 (95%)	130 (100%)	0	100	100
21	K	87/87 (100%)	87 (100%)	0	100	100
22	L	548/549 (100%)	548 (100%)	0	100	100
23	M	414/414 (100%)	414 (100%)	0	100	100
24	N	307/307 (100%)	307 (100%)	0	100	100
25	O	284/309 (92%)	284 (100%)	0	100	100
26	X	153/154 (99%)	153 (100%)	0	100	100
27	Y	105/106 (99%)	105 (100%)	0	100	100
28	Z	122/123 (99%)	122 (100%)	0	100	100
29	a	60/60 (100%)	60 (100%)	0	100	100
30	b	72/73 (99%)	72 (100%)	0	100	100
31	c	42/67 (63%)	42 (100%)	0	100	100
32	d	107/107 (100%)	107 (100%)	0	100	100
33	e	93/94 (99%)	93 (100%)	0	100	100
34	f	49/53 (92%)	49 (100%)	0	100	100
35	g	92/129 (71%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	h	123/162 (76%)	123 (100%)	0	100	100
37	i	99/119 (83%)	99 (100%)	0	100	100
38	j	61/87 (70%)	61 (100%)	0	100	100
39	k	60/78 (77%)	60 (100%)	0	100	100
40	l	142/161 (88%)	142 (100%)	0	100	100
41	m	112/114 (98%)	112 (100%)	0	100	100
42	n	163/164 (99%)	163 (100%)	0	100	100
43	o	109/121 (90%)	109 (100%)	0	100	100
44	p	154/158 (98%)	154 (100%)	0	100	100
All	All	7149/7947 (90%)	7149 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	6	104	ASN
2	C	211	GLN
3	D	13	GLN
3	D	217	ASN
4	2	42	HIS
4	2	58	ASN
4	2	155	GLN
5	1	96	ASN
5	1	356	HIS
5	1	373	ASN
6	3	110	GLN
6	3	430	GLN
6	3	535	GLN
6	3	581	GLN
8	P	87	HIS
8	P	93	ASN
8	P	288	HIS
13	V	40	HIS
15	q	113	HIS
16	r	24	GLN
16	r	46	HIS
19	H	258	ASN
22	L	56	HIS

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Mol	Chain	Res	Type
22	L	175	ASN
22	L	200	GLN
22	L	296	ASN
22	L	506	ASN
23	M	81	GLN
23	M	175	ASN
23	M	374	ASN
24	N	228	ASN
24	N	274	ASN
24	N	317	GLN
24	N	342	GLN
25	O	30	ASN
12	U	74	GLN
26	X	102	GLN
26	X	142	HIS
26	X	162	HIS
28	Z	75	GLN
32	d	61	GLN
34	f	13	HIS
35	g	55	ASN
35	g	101	ASN
36	h	86	ASN
38	j	6	HIS
39	k	26	GLN
42	n	13	GLN
42	n	74	GLN
43	o	84	HIS
44	p	54	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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	$\# Z > 2$
24	FME	N	1	24	8,9,10	0.98	0	8,9,11	1.02	0
21	FME	K	1	21	8,9,10	0.96	0	8,9,11	1.82	2 (25%)
3	2MR	D	85	3	10,12,13	2.64	2 (20%)	5,13,15	2.99	2 (40%)
18	FME	A	1	18	8,9,10	0.99	0	8,9,11	0.87	0
16	AYA	r	1	16	6,7,8	1.24	1 (16%)	6,8,10	1.08	1 (16%)
37	SAC	i	1	37	7,8,9	1.05	0	7,9,11	0.93	0
22	FME	L	1	22	8,9,10	0.98	0	8,9,11	0.94	0
19	FME	H	1	19	8,9,10	0.96	0	8,9,11	0.91	0
20	FME	J	1	20	8,9,10	0.96	0	8,9,11	0.90	0
23	FME	M	1	23	8,9,10	1.00	0	8,9,11	0.69	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
24	FME	N	1	24	-	3/7/9/11	-
21	FME	K	1	21	-	4/7/9/11	-
3	2MR	D	85	3	-	3/10/13/15	-
18	FME	A	1	18	-	1/7/9/11	-
16	AYA	r	1	16	-	0/5/6/8	-
37	SAC	i	1	37	-	1/7/8/10	-
22	FME	L	1	22	-	2/7/9/11	-
19	FME	H	1	19	-	2/7/9/11	-
20	FME	J	1	20	-	4/7/9/11	-
23	FME	M	1	23	-	1/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	85	2MR	CZ-NE	5.89	1.46	1.34
3	D	85	2MR	CZ-NH2	5.28	1.44	1.33
16	r	1	AYA	CA-N	-2.31	1.44	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	85	2MR	CD-NE-CZ	5.69	134.05	123.36
21	K	1	FME	C-CA-N	4.18	117.56	109.50
3	D	85	2MR	NE-CZ-NH2	-3.25	116.50	119.48
21	K	1	FME	O-C-CA	-2.29	118.89	124.77
16	r	1	AYA	CB-CA-N	2.21	112.18	109.68

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	85	2MR	C-CA-CB-CG
19	H	1	FME	N-CA-CB-CG
21	K	1	FME	O1-CN-N-CA
21	K	1	FME	N-CA-CB-CG
24	N	1	FME	N-CA-CB-CG
24	N	1	FME	C-CA-CB-CG
37	i	1	SAC	O-C-CA-CB
3	D	85	2MR	NE-CD-CG-CB
20	J	1	FME	CA-CB-CG-SD
21	K	1	FME	CA-CB-CG-SD
18	A	1	FME	N-CA-CB-CG
22	L	1	FME	N-CA-CB-CG
23	M	1	FME	N-CA-CB-CG
22	L	1	FME	CB-CG-SD-CE
3	D	85	2MR	CA-CB-CG-CD
20	J	1	FME	CB-CG-SD-CE
21	K	1	FME	C-CA-CB-CG
20	J	1	FME	CB-CA-N-CN
24	N	1	FME	CB-CG-SD-CE
19	H	1	FME	C-CA-CB-CG
20	J	1	FME	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	N	1	FME	1	0
21	K	1	FME	1	0
37	i	1	SAC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 3 are monoatomic - leaving 40 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	$\# Z > 2$
46	3PE	A	201	-	42,42,50	0.33	0	45,47,55	0.30	0
46	3PE	d	202	-	30,30,50	0.37	0	33,35,55	0.34	0
46	3PE	i	201	-	41,41,50	0.33	0	44,46,55	0.30	0
54	CDL	N	401	-	89,89,99	0.31	0	95,101,111	0.40	1 (1%)
46	3PE	M	502	-	50,50,50	0.30	0	53,55,55	0.29	0
54	CDL	m	201	-	71,71,99	0.35	0	77,83,111	0.43	1 (1%)
46	3PE	K	201	-	40,40,50	0.34	0	43,45,55	0.35	0
47	PC1	6	203	-	42,42,53	0.34	0	48,50,61	0.51	1 (2%)
46	3PE	N	402	-	37,37,50	0.34	0	40,42,55	0.32	0
51	NDP	P	501	-	51,52,52	0.35	0	71,80,80	0.42	0
53	ZMP	U	201	-	26,31,36	0.72	1 (3%)	30,38,45	0.94	1 (3%)
45	SF4	3	801	6	0,12,12	-	-	-	-	-
46	3PE	Y	201	-	27,27,50	0.40	0	30,32,55	0.39	0
45	SF4	6	201	1	0,12,12	-	-	-	-	-
46	3PE	d	203	-	31,31,50	0.37	0	34,36,55	0.36	0
46	3PE	M	503	-	35,35,50	0.36	0	38,40,55	0.31	0
46	3PE	L	701	-	50,50,50	0.31	0	53,55,55	0.48	0
46	3PE	h	202	-	50,50,50	0.30	0	53,55,55	0.27	0
48	FES	2	301	4	0,4,4	-	-	-	-	-
45	SF4	9	202	7	0,12,12	-	-	-	-	-
55	DGT	O	401	56	32,33,33	0.30	0	48,52,52	0.30	0
54	CDL	d	201	-	66,66,99	0.36	0	72,78,111	0.34	0
53	ZMP	T	201	-	28,33,36	0.61	0	32,40,45	1.16	4 (12%)
47	PC1	9	204	-	46,46,53	0.31	0	52,54,61	0.31	0
47	PC1	M	501	-	53,53,53	0.29	0	59,61,61	0.42	0
46	3PE	r	201	-	45,45,50	0.31	0	48,50,55	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	3PE	6	202	-	31,31,50	0.37	0	34,36,55	0.33	0
49	FMN	1	501	-	33,33,33	0.32	0	48,50,50	0.41	0
45	SF4	1	502	5	0,12,12	-	-	-		
45	SF4	3	802	6	0,12,12	-	-	-		
54	CDL	h	201	-	69,69,99	0.35	0	75,81,111	0.44	1 (1%)
47	PC1	9	203	-	53,53,53	0.30	0	59,61,61	0.46	1 (1%)
45	SF4	9	201	7	0,12,12	-	-	-		
46	3PE	H	401	-	50,50,50	0.31	0	53,55,55	0.48	1 (1%)
46	3PE	L	703	-	50,50,50	0.30	0	53,55,55	0.35	0
46	3PE	m	202	-	29,29,50	0.39	0	32,34,55	0.35	0
48	FES	3	803	6	0,4,4	-	-	-		
54	CDL	r	202	-	56,56,99	0.40	0	62,68,111	0.47	1 (1%)
54	CDL	L	702	-	77,77,99	0.34	0	83,89,111	0.29	0
46	3PE	L	704	-	41,41,50	0.33	0	44,46,55	0.35	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
46	3PE	A	201	-	-	9/46/46/54	-
46	3PE	d	202	-	-	7/34/34/54	-
46	3PE	i	201	-	-	9/45/45/54	-
54	CDL	N	401	-	-	16/100/100/110	-
46	3PE	M	502	-	-	10/54/54/54	-
54	CDL	m	201	-	-	21/82/82/110	-
46	3PE	K	201	-	-	10/44/44/54	-
47	PC1	6	203	-	-	10/46/46/57	-
46	3PE	N	402	-	-	9/41/41/54	-
51	NDP	P	501	-	-	7/34/77/77	0/5/5/5
53	ZMP	U	201	-	-	14/36/38/43	-
45	SF4	3	801	6	-	-	0/6/5/5
46	3PE	Y	201	-	-	6/31/31/54	-
45	SF4	6	201	1	-	-	0/6/5/5
46	3PE	d	203	-	-	4/35/35/54	-
46	3PE	M	503	-	-	11/39/39/54	-
46	3PE	L	701	-	-	10/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	h	202	-	-	11/54/54/54	-
48	FES	2	301	4	-	-	0/1/1/1
45	SF4	9	202	7	-	-	0/6/5/5
55	DGT	O	401	56	-	7/22/34/34	0/3/3/3
54	CDL	d	201	-	-	16/77/77/110	-
53	ZMP	T	201	-	-	10/38/40/43	-
47	PC1	9	204	-	-	17/50/50/57	-
47	PC1	M	501	-	-	10/57/57/57	-
46	3PE	r	201	-	-	7/49/49/54	-
46	3PE	6	202	-	-	4/35/35/54	-
49	FMN	1	501	-	-	5/18/18/18	0/3/3/3
45	SF4	1	502	5	-	-	0/6/5/5
54	CDL	h	201	-	-	20/80/80/110	-
45	SF4	3	802	6	-	-	0/6/5/5
47	PC1	9	203	-	-	10/57/57/57	-
45	SF4	9	201	7	-	-	0/6/5/5
46	3PE	H	401	-	-	9/54/54/54	-
46	3PE	L	703	-	-	7/54/54/54	-
46	3PE	m	202	-	-	10/33/33/54	-
48	FES	3	803	6	-	-	0/1/1/1
54	CDL	r	202	-	-	13/67/67/110	-
54	CDL	L	702	-	-	17/88/88/110	-
46	3PE	L	704	-	-	7/45/45/54	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	U	201	ZMP	C9-C10	2.34	1.53	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	T	201	ZMP	O1-C10-C9	-3.10	120.40	123.98
53	U	201	ZMP	O1-C10-C9	-2.52	121.07	123.98
53	T	201	ZMP	C15-C14-C13	-2.32	108.53	112.39
47	6	203	PC1	C2-O21-C21	2.14	122.93	117.80
46	H	401	3PE	C2-O21-C21	2.12	122.87	117.80
54	N	401	CDL	CB4-OB6-CB5	2.07	122.75	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	m	201	CDL	CA4-OA6-CA5	2.07	122.74	117.80
54	r	202	CDL	CA4-OA6-CA5	2.04	122.67	117.80
54	h	201	CDL	CB4-OB6-CB5	2.03	122.67	117.80
47	9	203	PC1	C2-O21-C21	2.03	122.66	117.80
53	T	201	ZMP	C9-C10-S1	2.03	115.82	113.40
53	T	201	ZMP	C8-C9-C10	-2.00	107.84	112.27

There are no chirality outliers.

All (333) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	6	202	3PE	C11-O13-P-O11
46	6	202	3PE	O13-C11-C12-N
46	r	201	3PE	C1-O11-P-O12
46	r	201	3PE	C1-O11-P-O14
46	r	201	3PE	C11-O13-P-O11
46	r	201	3PE	C11-O13-P-O12
46	A	201	3PE	C11-O13-P-O11
46	A	201	3PE	O13-C11-C12-N
46	K	201	3PE	C1-O11-P-O12
46	K	201	3PE	C11-O13-P-O11
46	K	201	3PE	C11-O13-P-O14
46	L	701	3PE	C1-O11-P-O13
46	L	701	3PE	C1-O11-P-O14
46	L	701	3PE	C11-O13-P-O11
46	L	701	3PE	C11-O13-P-O12
46	L	701	3PE	C11-O13-P-O14
46	L	703	3PE	C1-O11-P-O12
46	L	703	3PE	C1-O11-P-O13
46	L	703	3PE	O13-C11-C12-N
46	L	704	3PE	C1-O11-P-O12
46	L	704	3PE	C11-O13-P-O11
46	L	704	3PE	C11-O13-P-O12
46	L	704	3PE	C11-O13-P-O14
46	M	503	3PE	C1-O11-P-O14
46	M	503	3PE	C11-O13-P-O11
46	M	503	3PE	C11-O13-P-O12
46	M	503	3PE	C11-O13-P-O14
46	M	503	3PE	O13-C11-C12-N
46	N	402	3PE	C1-O11-P-O12
46	N	402	3PE	C1-O11-P-O13
46	N	402	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
46	N	402	3PE	C11-O13-P-O11
46	N	402	3PE	C11-O13-P-O14
46	Y	201	3PE	C1-O11-P-O12
46	Y	201	3PE	C1-O11-P-O13
46	Y	201	3PE	C1-O11-P-O14
46	Y	201	3PE	O13-C11-C12-N
46	d	202	3PE	C1-O11-P-O14
46	d	202	3PE	C11-O13-P-O12
46	d	202	3PE	O13-C11-C12-N
46	d	203	3PE	C1-O11-P-O12
46	d	203	3PE	C1-O11-P-O13
46	d	203	3PE	O13-C11-C12-N
46	h	202	3PE	C1-O11-P-O12
46	h	202	3PE	C1-O11-P-O13
46	h	202	3PE	C1-O11-P-O14
46	h	202	3PE	C11-O13-P-O11
46	h	202	3PE	C11-O13-P-O12
46	h	202	3PE	C11-O13-P-O14
46	i	201	3PE	C1-O11-P-O12
46	i	201	3PE	C1-O11-P-O13
46	i	201	3PE	C1-O11-P-O14
46	i	201	3PE	C11-O13-P-O12
46	m	202	3PE	C1-O11-P-O14
46	m	202	3PE	C11-O13-P-O11
46	m	202	3PE	C11-O13-P-O14
46	m	202	3PE	O13-C11-C12-N
47	6	203	PC1	C11-O13-P-O11
47	6	203	PC1	C1-O11-P-O12
47	6	203	PC1	C1-O11-P-O14
47	6	203	PC1	C1-O11-P-O13
47	9	203	PC1	C1-O11-P-O14
47	9	204	PC1	C11-O13-P-O12
47	9	204	PC1	C11-O13-P-O14
47	9	204	PC1	C11-O13-P-O11
47	9	204	PC1	C1-O11-P-O14
47	9	204	PC1	C1-O11-P-O13
47	M	501	PC1	C11-O13-P-O12
47	M	501	PC1	C11-O13-P-O14
47	M	501	PC1	C11-O13-P-O11
49	1	501	FMN	N10-C1'-C2'-O2'
49	1	501	FMN	N10-C1'-C2'-C3'
49	1	501	FMN	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
49	1	501	FMN	C5'-O5'-P-O3P
51	P	501	NDP	C5B-O5B-PA-O3
53	T	201	ZMP	C19-C18-C21-O5
53	T	201	ZMP	C20-C18-C21-O5
53	T	201	ZMP	C17-C18-C21-O5
53	T	201	ZMP	S1-C11-C12-N1
53	T	201	ZMP	O1-C10-S1-C11
53	T	201	ZMP	C9-C10-S1-C11
53	U	201	ZMP	C19-C18-C21-O5
53	U	201	ZMP	C20-C18-C21-O5
53	U	201	ZMP	C17-C18-C21-O5
53	U	201	ZMP	C17-C16-N2-C15
53	U	201	ZMP	C7-C8-C9-C10
54	r	202	CDL	CA2-OA2-PA1-OA3
54	r	202	CDL	CA2-OA2-PA1-OA4
54	r	202	CDL	CA2-OA2-PA1-OA5
54	r	202	CDL	CA3-OA5-PA1-OA4
54	L	702	CDL	CA2-OA2-PA1-OA3
54	L	702	CDL	CA2-OA2-PA1-OA4
54	L	702	CDL	CA2-OA2-PA1-OA5
54	L	702	CDL	CA3-OA5-PA1-OA2
54	L	702	CDL	CA3-OA5-PA1-OA3
54	L	702	CDL	CA3-OA5-PA1-OA4
54	L	702	CDL	CB2-OB2-PB2-OB3
54	L	702	CDL	CB2-OB2-PB2-OB4
54	L	702	CDL	CB2-OB2-PB2-OB5
54	L	702	CDL	CB3-OB5-PB2-OB2
54	L	702	CDL	CB3-OB5-PB2-OB3
54	L	702	CDL	CB3-OB5-PB2-OB4
54	N	401	CDL	CA2-OA2-PA1-OA3
54	N	401	CDL	CA3-OA5-PA1-OA2
54	N	401	CDL	CA3-OA5-PA1-OA3
54	N	401	CDL	OA6-CA4-CA6-OA8
54	N	401	CDL	CB2-OB2-PB2-OB3
54	N	401	CDL	CB2-OB2-PB2-OB5
54	d	201	CDL	CA2-OA2-PA1-OA3
54	d	201	CDL	CA2-OA2-PA1-OA4
54	d	201	CDL	CA3-OA5-PA1-OA2
54	d	201	CDL	CA3-OA5-PA1-OA3
54	d	201	CDL	CA3-OA5-PA1-OA4
54	h	201	CDL	CA2-OA2-PA1-OA3
54	h	201	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
54	h	201	CDL	CB2-OB2-PB2-OB4
54	h	201	CDL	CB2-OB2-PB2-OB5
54	h	201	CDL	CB3-OB5-PB2-OB2
54	h	201	CDL	CB3-OB5-PB2-OB3
54	h	201	CDL	CB3-OB5-PB2-OB4
54	m	201	CDL	CA2-OA2-PA1-OA3
54	m	201	CDL	CA3-OA5-PA1-OA2
54	m	201	CDL	CA3-OA5-PA1-OA3
54	m	201	CDL	CB2-OB2-PB2-OB3
54	m	201	CDL	CB2-OB2-PB2-OB4
54	m	201	CDL	CB2-OB2-PB2-OB5
54	m	201	CDL	CB3-OB5-PB2-OB2
54	m	201	CDL	CB3-OB5-PB2-OB3
54	m	201	CDL	CB3-OB5-PB2-OB4
55	O	401	DGT	PB-O3B-PG-O2G
55	O	401	DGT	C5'-O5'-PA-O3A
55	O	401	DGT	C5'-O5'-PA-O1A
55	O	401	DGT	C5'-O5'-PA-O2A
53	U	201	ZMP	O3-C16-N2-C15
54	m	201	CDL	OB5-CB3-CB4-OB6
46	L	701	3PE	C21-C22-C23-C24
46	H	401	3PE	C21-C22-C23-C24
46	M	503	3PE	C2-C1-O11-P
46	M	502	3PE	C21-C22-C23-C24
54	L	702	CDL	CA5-C11-C12-C13
47	6	203	PC1	C11-C12-N-C14
47	9	203	PC1	C11-C12-N-C13
46	H	401	3PE	C31-C32-C33-C34
46	h	202	3PE	C22-C23-C24-C25
47	9	204	PC1	C29-C2A-C2B-C2C
46	A	201	3PE	C39-C3A-C3B-C3C
53	U	201	ZMP	C6-C7-C8-C9
47	9	203	PC1	C11-C12-N-C14
47	9	203	PC1	C11-C12-N-C15
46	h	202	3PE	C26-C27-C28-C29
47	9	204	PC1	C34-C35-C36-C37
54	d	201	CDL	C54-C55-C56-C57
54	d	201	CDL	C55-C56-C57-C58
47	6	203	PC1	C11-C12-N-C13
47	6	203	PC1	C11-C12-N-C15
46	L	703	3PE	C38-C39-C3A-C3B
47	M	501	PC1	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
53	U	201	ZMP	O3-C16-C17-O4
54	d	201	CDL	C62-C63-C64-C65
46	M	502	3PE	O11-C1-C2-C3
54	N	401	CDL	CA3-CA4-CA6-OA8
49	l	501	FMN	C5'-O5'-P-O1P
46	M	502	3PE	C36-C37-C38-C39
46	M	502	3PE	C22-C23-C24-C25
46	L	703	3PE	C31-C32-C33-C34
47	M	501	PC1	C3B-C3C-C3D-C3E
47	9	204	PC1	C11-C12-N-C15
46	L	703	3PE	C32-C33-C34-C35
47	9	203	PC1	C28-C29-C2A-C2B
54	d	201	CDL	OB5-CB3-CB4-CB6
54	m	201	CDL	OB5-CB3-CB4-CB6
53	U	201	ZMP	N2-C16-C17-O4
54	m	201	CDL	CB3-CB4-CB6-OB8
54	d	201	CDL	OB5-CB3-CB4-OB6
53	U	201	ZMP	C3-C4-C5-C6
46	H	401	3PE	O31-C31-C32-C33
47	9	204	PC1	C11-C12-N-C14
46	M	502	3PE	O11-C1-C2-O21
46	m	202	3PE	O11-C1-C2-O21
54	d	201	CDL	CA3-CA4-CA6-OA8
54	d	201	CDL	OA6-CA4-CA6-OA8
54	h	201	CDL	OB6-CB4-CB6-OB8
54	m	201	CDL	OB6-CB4-CB6-OB8
54	r	202	CDL	C52-C51-CB5-OB6
47	M	501	PC1	O13-C11-C12-N
51	P	501	NDP	PN-O3-PA-O2A
55	O	401	DGT	PB-O3A-PA-O2A
46	A	201	3PE	C38-C39-C3A-C3B
54	N	401	CDL	C81-C82-C83-C84
46	m	202	3PE	O11-C1-C2-C3
53	U	201	ZMP	C16-C17-C18-C21
46	A	201	3PE	C34-C35-C36-C37
46	M	502	3PE	C3D-C3E-C3F-C3G
54	N	401	CDL	C82-C83-C84-C85
46	A	201	3PE	C2-C1-O11-P
53	U	201	ZMP	C12-C11-S1-C10
54	h	201	CDL	OB5-CB3-CB4-OB6
46	6	202	3PE	C1-O11-P-O14
46	6	202	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
46	r	201	3PE	C1-O11-P-O13
46	A	201	3PE	C11-O13-P-O14
46	K	201	3PE	C1-O11-P-O13
46	K	201	3PE	C1-O11-P-O14
46	L	701	3PE	C1-O11-P-O12
46	L	701	3PE	O13-C11-C12-N
46	M	503	3PE	C1-O11-P-O12
46	M	503	3PE	C1-O11-P-O13
46	N	402	3PE	C11-O13-P-O12
46	d	202	3PE	C1-O11-P-O12
46	d	202	3PE	C1-O11-P-O13
46	d	202	3PE	C11-O13-P-O11
46	d	202	3PE	C11-O13-P-O14
46	i	201	3PE	C11-O13-P-O11
46	i	201	3PE	C11-O13-P-O14
46	i	201	3PE	O13-C11-C12-N
47	9	203	PC1	C1-O11-P-O13
47	9	204	PC1	C1-O11-P-O12
47	9	204	PC1	C11-C12-N-C13
51	P	501	NDP	C5B-O5B-PA-O2A
54	r	202	CDL	CA3-OA5-PA1-OA2
54	r	202	CDL	CA3-OA5-PA1-OA3
54	r	202	CDL	CB2-OB2-PB2-OB3
54	N	401	CDL	CB2-OB2-PB2-OB4
54	d	201	CDL	CA2-OA2-PA1-OA5
54	h	201	CDL	CA2-OA2-PA1-OA4
46	K	201	3PE	C2-C1-O11-P
46	M	502	3PE	C2-C1-O11-P
54	N	401	CDL	C1-CA2-OA2-PA1
54	h	201	CDL	CA4-CA3-OA5-PA1
54	m	201	CDL	C1-CB2-OB2-PB2
46	H	401	3PE	C33-C34-C35-C36
46	L	704	3PE	C23-C24-C25-C26
51	P	501	NDP	C2D-C1D-N1N-C6N
47	9	203	PC1	C3-C2-O21-C21
46	H	401	3PE	O11-C1-C2-C3
54	r	202	CDL	OB5-CB3-CB4-CB6
54	h	201	CDL	OB5-CB3-CB4-CB6
53	U	201	ZMP	C13-C14-C15-N2
55	O	401	DGT	PB-O3A-PA-O1A
47	M	501	PC1	C21-C22-C23-C24
54	m	201	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
47	6	203	PC1	C35-C36-C37-C38
51	P	501	NDP	O4D-C1D-N1N-C6N
46	L	703	3PE	O21-C21-C22-C23
46	N	402	3PE	O21-C2-C3-O31
47	M	501	PC1	O21-C2-C3-O31
46	M	502	3PE	C37-C38-C39-C3A
54	r	202	CDL	C1-CB2-OB2-PB2
53	T	201	ZMP	C5-C6-C7-C8
47	9	203	PC1	O11-C1-C2-C3
47	9	204	PC1	O11-C1-C2-C3
54	L	702	CDL	OB5-CB3-CB4-CB6
54	N	401	CDL	C56-C57-C58-C59
46	i	201	3PE	C2D-C2E-C2F-C2G
54	L	702	CDL	C1-CB2-OB2-PB2
54	h	201	CDL	C1-CA2-OA2-PA1
46	N	402	3PE	C1-C2-C3-O31
46	h	202	3PE	C1-C2-C3-O31
54	r	202	CDL	OB5-CB3-CB4-OB6
54	L	702	CDL	OA5-CA3-CA4-OA6
46	r	201	3PE	O31-C31-C32-C33
46	H	401	3PE	C2-C1-O11-P
55	O	401	DGT	C4'-C5'-O5'-PA
46	i	201	3PE	C27-C28-C29-C2A
54	d	201	CDL	C60-C61-C62-C63
47	9	203	PC1	C3D-C3E-C3F-C3G
53	T	201	ZMP	C6-C7-C8-C9
46	H	401	3PE	C3-C2-O21-C21
46	L	701	3PE	C3-C2-O21-C21
54	h	201	CDL	CB6-CB4-OB6-CB5
54	m	201	CDL	C81-C82-C83-C84
51	P	501	NDP	C2D-C1D-N1N-C2N
47	9	204	PC1	O11-C1-C2-O21
54	h	201	CDL	CB3-CB4-CB6-OB8
46	h	202	3PE	C12-C11-O13-P
54	m	201	CDL	C75-C76-C77-C78
47	9	203	PC1	C2D-C2E-C2F-C2G
46	A	201	3PE	C23-C24-C25-C26
51	P	501	NDP	O4D-C1D-N1N-C2N
46	K	201	3PE	O21-C21-C22-C23
54	L	702	CDL	C11-C12-C13-C14
46	m	202	3PE	O31-C31-C32-C33
46	m	202	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
54	N	401	CDL	CA7-C31-C32-C33
54	h	201	CDL	C32-C31-CA7-OA8
46	A	201	3PE	C33-C34-C35-C36
46	M	503	3PE	C26-C27-C28-C29
54	d	201	CDL	C53-C54-C55-C56
54	m	201	CDL	C12-C11-CA5-OA6
47	9	204	PC1	C26-C27-C28-C29
47	9	204	PC1	C24-C25-C26-C27
46	K	201	3PE	O31-C31-C32-C33
54	N	401	CDL	OB6-CB4-CB6-OB8
46	L	704	3PE	O31-C31-C32-C33
46	M	502	3PE	O31-C31-C32-C33
46	Y	201	3PE	O31-C31-C32-C33
53	T	201	ZMP	C16-C17-C18-C21
54	r	202	CDL	C52-C51-CB5-OB7
47	6	203	PC1	C1-C2-O21-C21
47	6	203	PC1	C3-C2-O21-C21
54	r	202	CDL	CA3-CA4-OA6-CA5
54	N	401	CDL	CB3-CB4-OB6-CB5
54	N	401	CDL	CB6-CB4-OB6-CB5
54	m	201	CDL	CA6-CA4-OA6-CA5
47	9	204	PC1	C35-C36-C37-C38
54	d	201	CDL	C57-C58-C59-C60
47	M	501	PC1	C24-C25-C26-C27
54	m	201	CDL	C76-C77-C78-C79
46	K	201	3PE	O32-C31-C32-C33
46	H	401	3PE	O32-C31-C32-C33
46	M	503	3PE	C34-C35-C36-C37
46	M	503	3PE	C36-C37-C38-C39
53	U	201	ZMP	C2-C3-C4-C5
46	K	201	3PE	O22-C21-C22-C23
46	m	202	3PE	O32-C31-C32-C33
47	M	501	PC1	C3A-C3B-C3C-C3D
54	h	201	CDL	C72-C71-CB7-OB8
54	m	201	CDL	C12-C11-CA5-OA7
46	Y	201	3PE	O32-C31-C32-C33
47	9	204	PC1	O21-C21-C22-C23
46	H	401	3PE	C2A-C2B-C2C-C2D
53	T	201	ZMP	N2-C16-C17-O4
46	L	701	3PE	C35-C36-C37-C38
54	h	201	CDL	C32-C31-CA7-OA9
46	h	202	3PE	O21-C21-C22-C23

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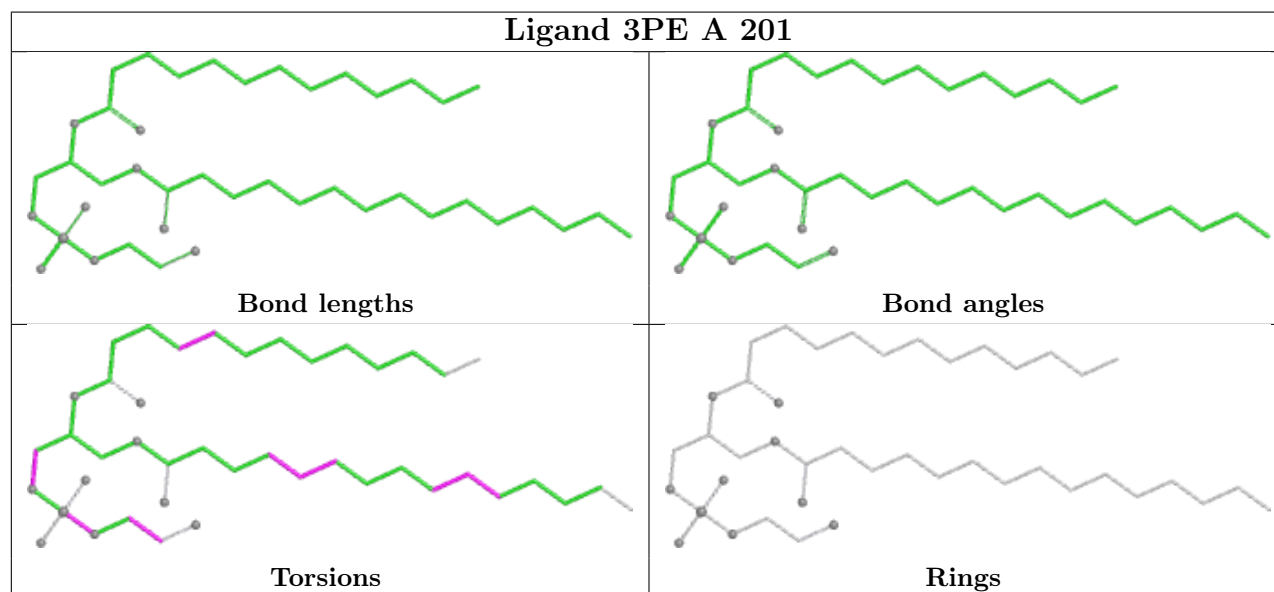
Mol	Chain	Res	Type	Atoms
54	h	201	CDL	C12-C11-CA5-OA6
46	r	201	3PE	C22-C23-C24-C25
46	N	402	3PE	O31-C31-C32-C33
46	m	202	3PE	O22-C21-C22-C23
46	L	704	3PE	O32-C31-C32-C33
46	d	203	3PE	C33-C34-C35-C36
46	M	502	3PE	O32-C31-C32-C33
54	h	201	CDL	C72-C71-CB7-OB9

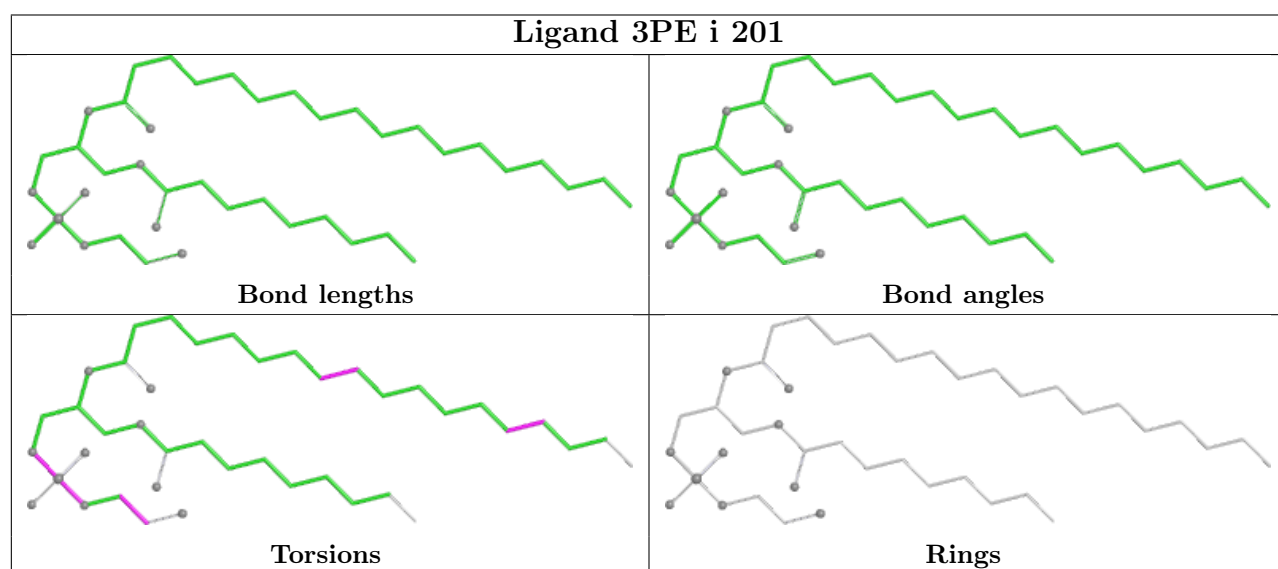
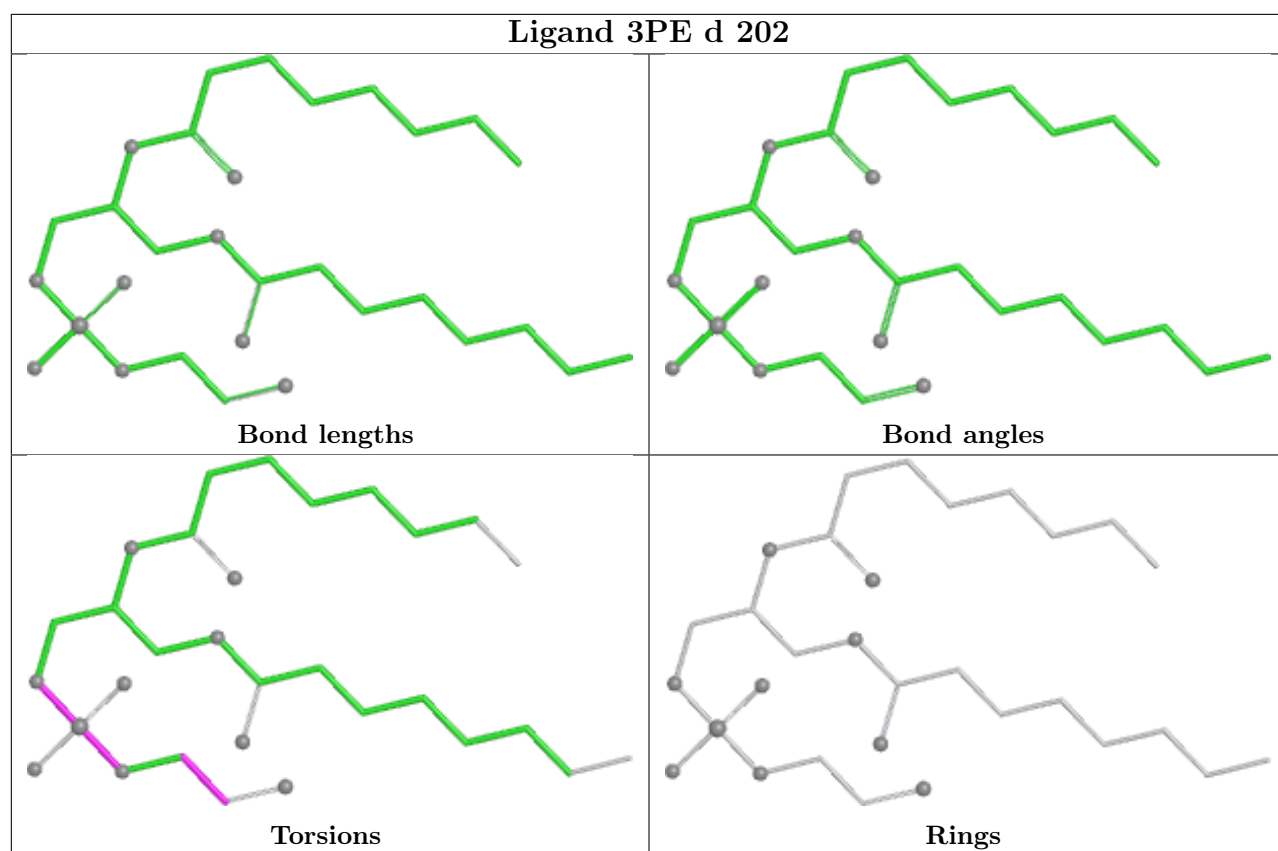
There are no ring outliers.

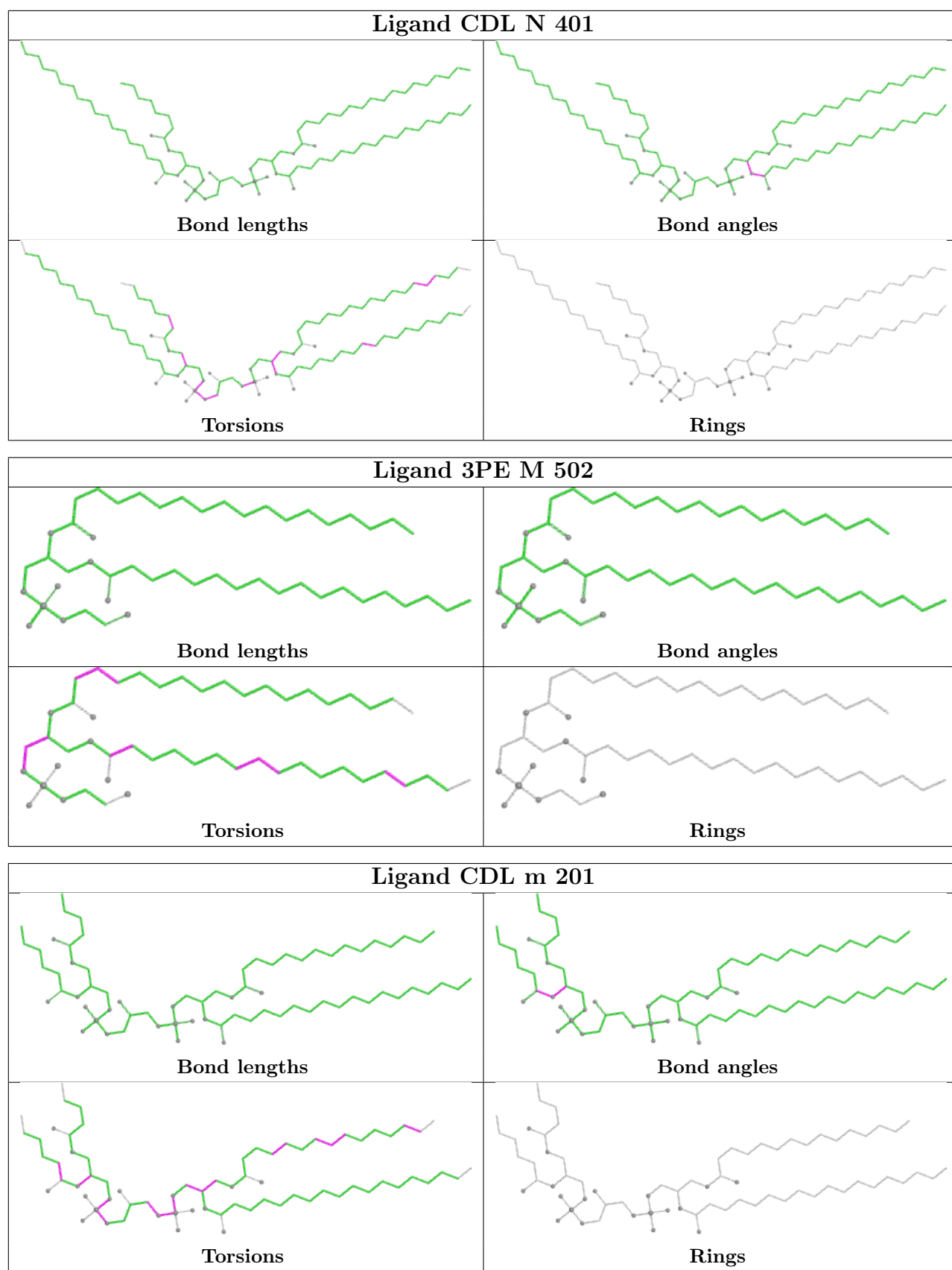
28 monomers are involved in 69 short contacts:

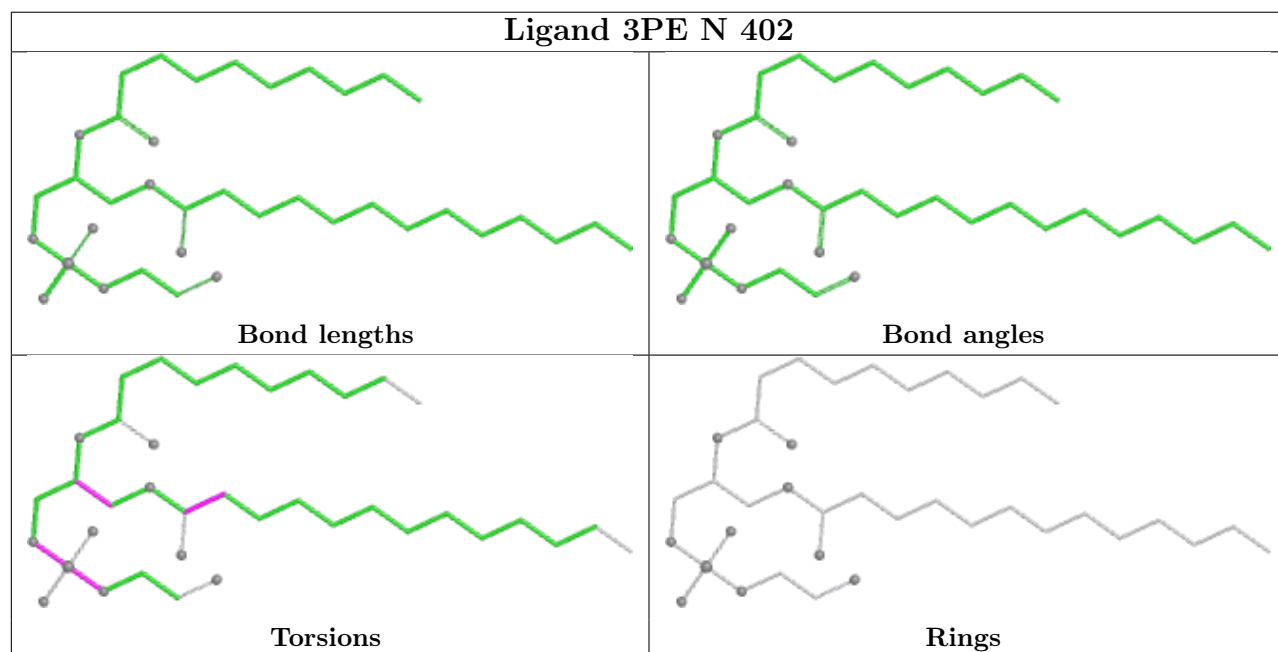
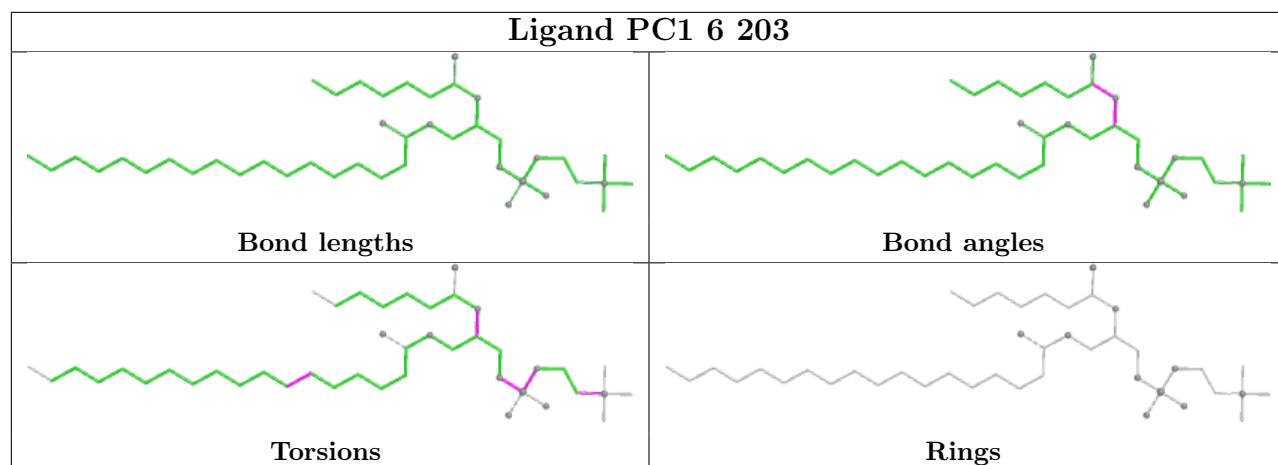
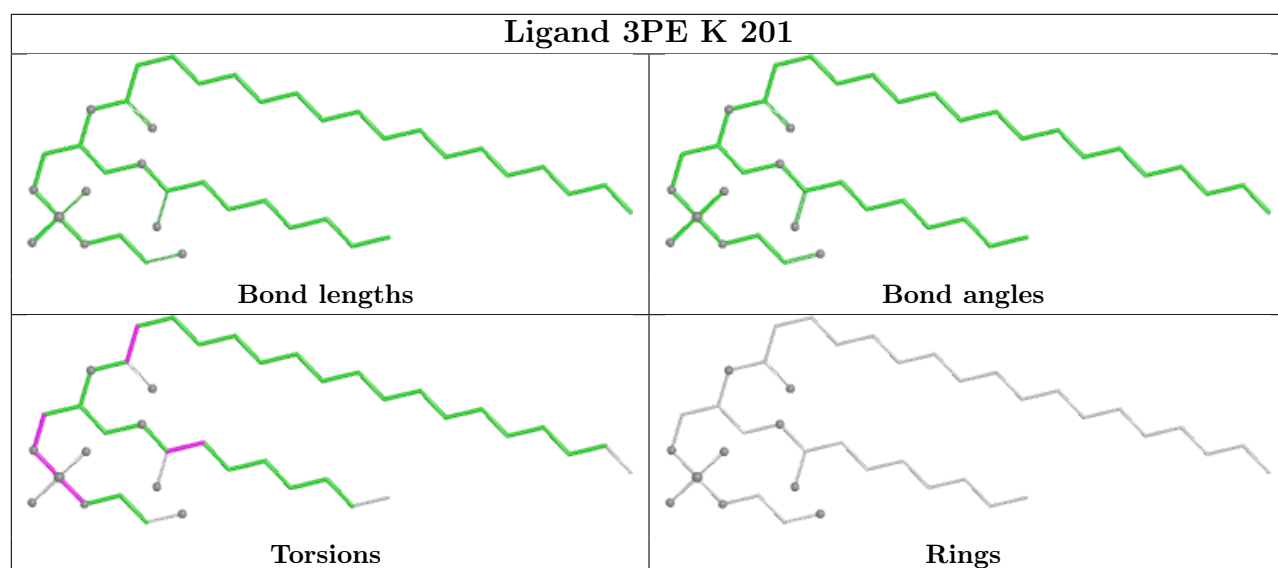
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	A	201	3PE	2	0
46	i	201	3PE	5	0
54	N	401	CDL	3	0
46	M	502	3PE	5	0
54	m	201	CDL	1	0
46	K	201	3PE	2	0
46	N	402	3PE	1	0
51	P	501	NDP	1	0
53	U	201	ZMP	3	0
46	Y	201	3PE	1	0
46	M	503	3PE	1	0
46	L	701	3PE	1	0
46	h	202	3PE	2	0
55	O	401	DGT	1	0
54	d	201	CDL	1	0
53	T	201	ZMP	2	0
47	9	204	PC1	9	0
47	M	501	PC1	5	0
49	1	501	FMN	3	0
54	h	201	CDL	6	0
47	9	203	PC1	3	0
45	9	201	SF4	1	0
46	H	401	3PE	2	0
46	L	703	3PE	3	0
46	m	202	3PE	1	0
54	r	202	CDL	4	0
54	L	702	CDL	1	0
46	L	704	3PE	4	0

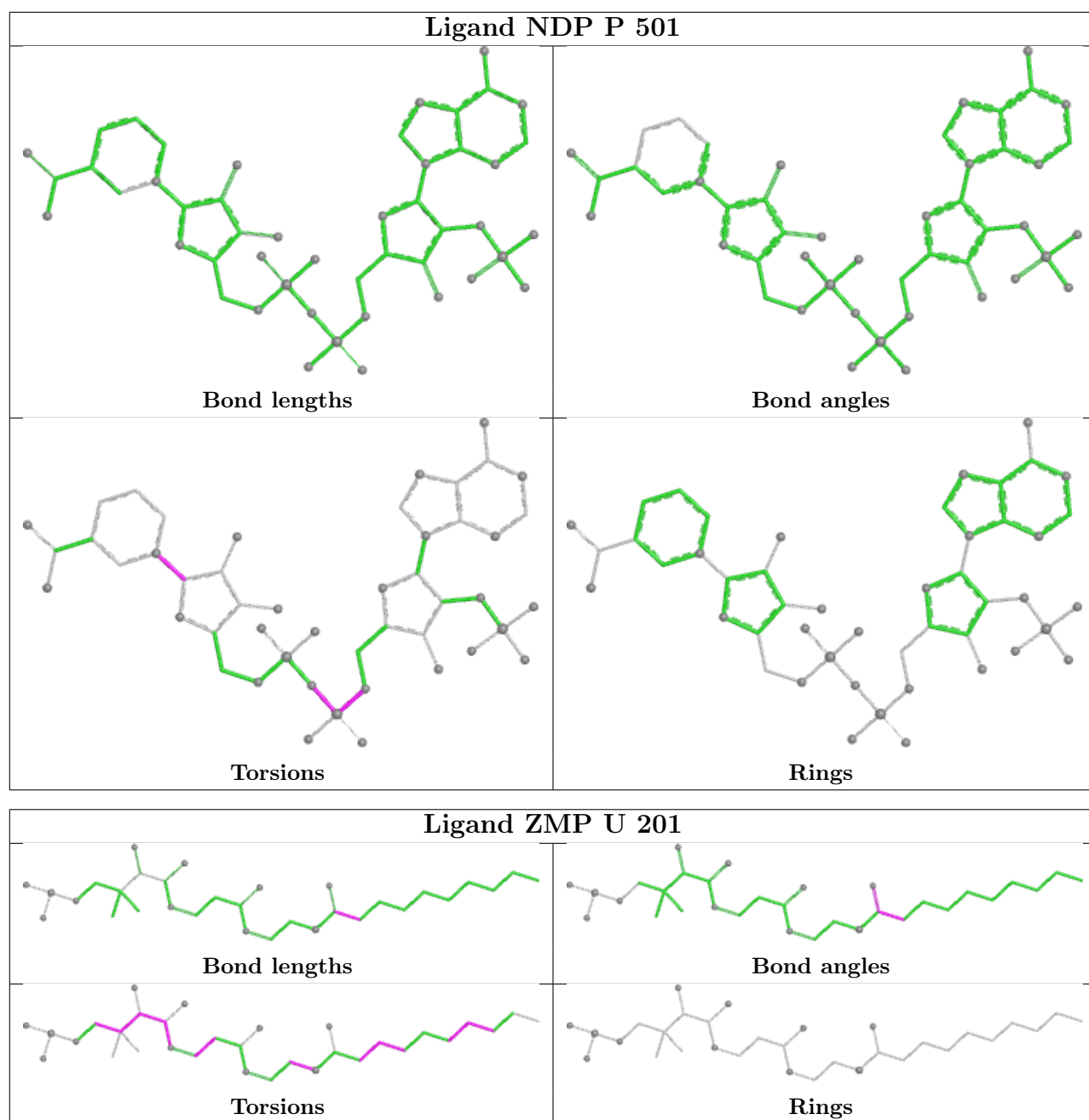
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

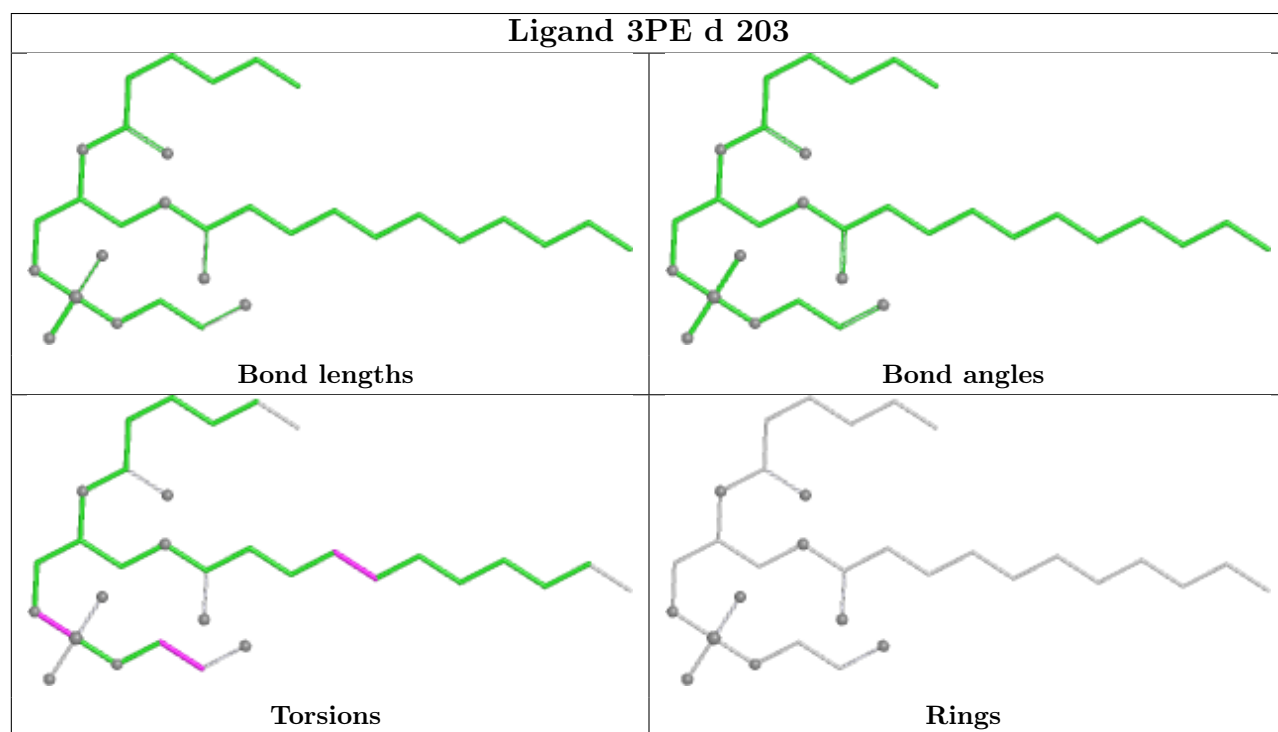
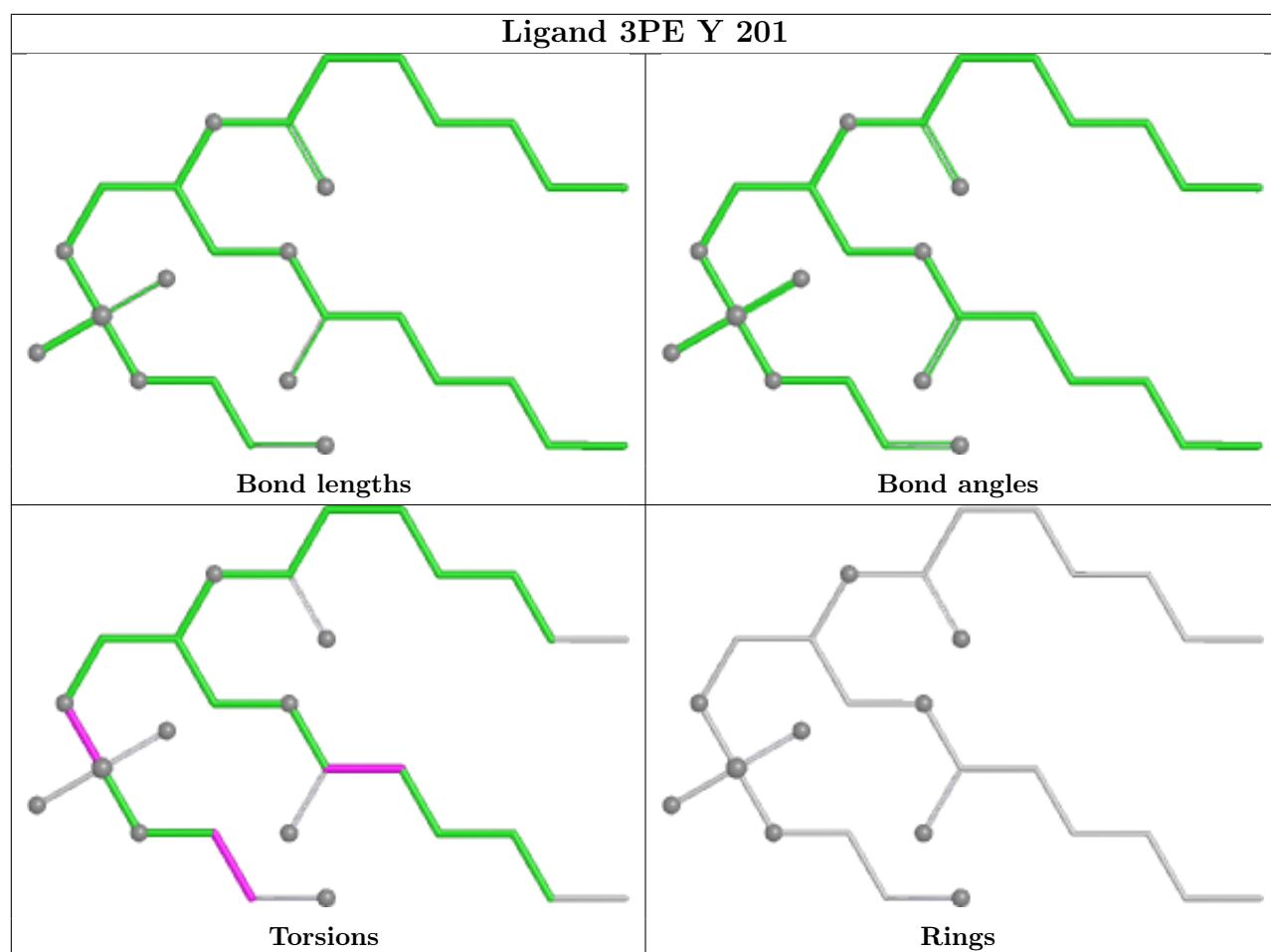


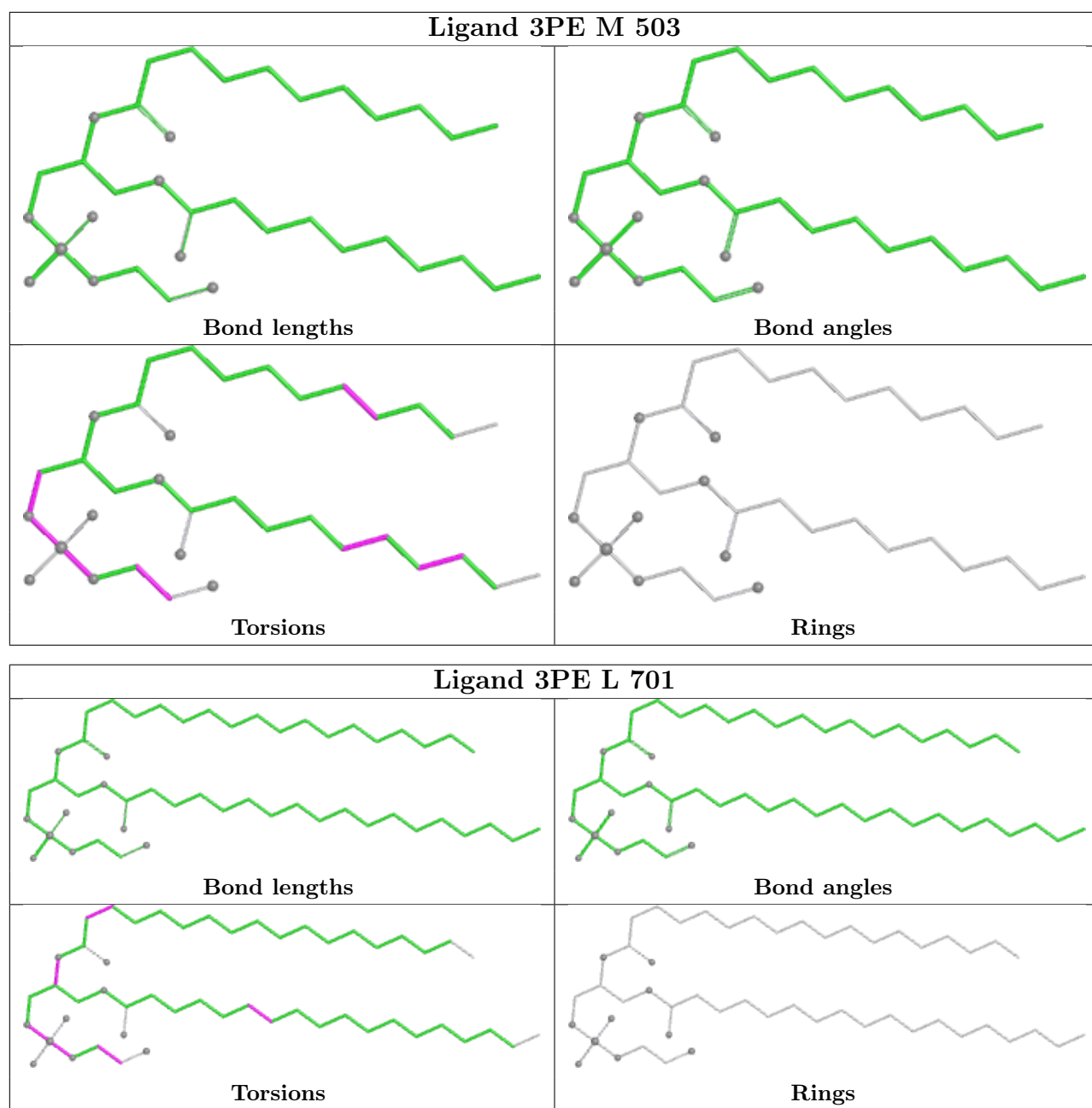


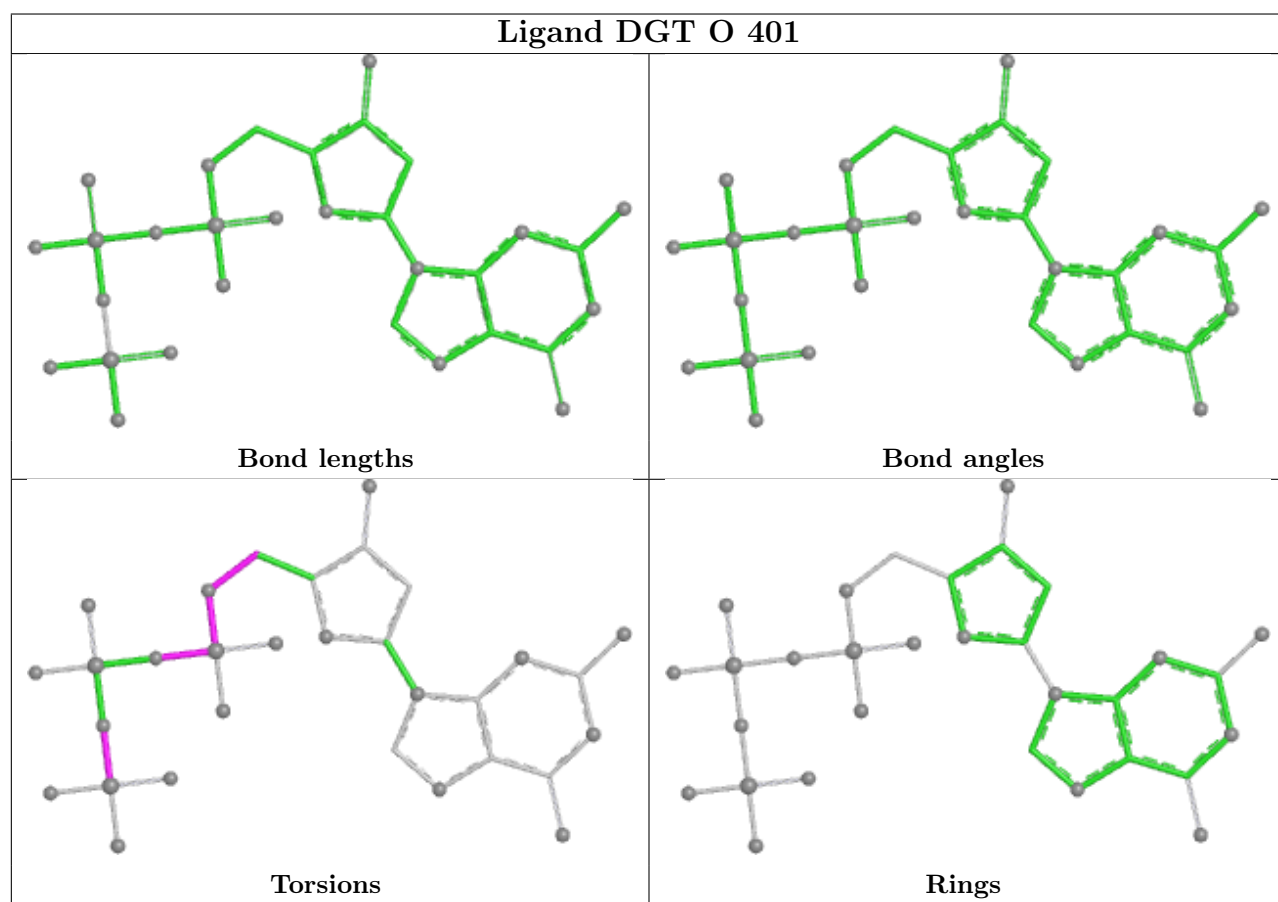
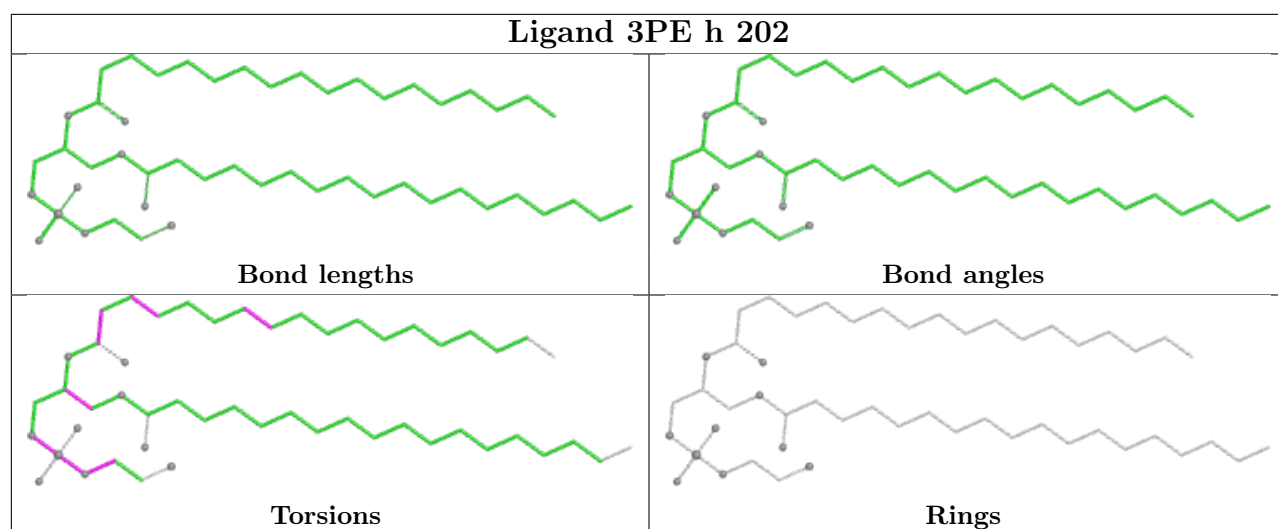


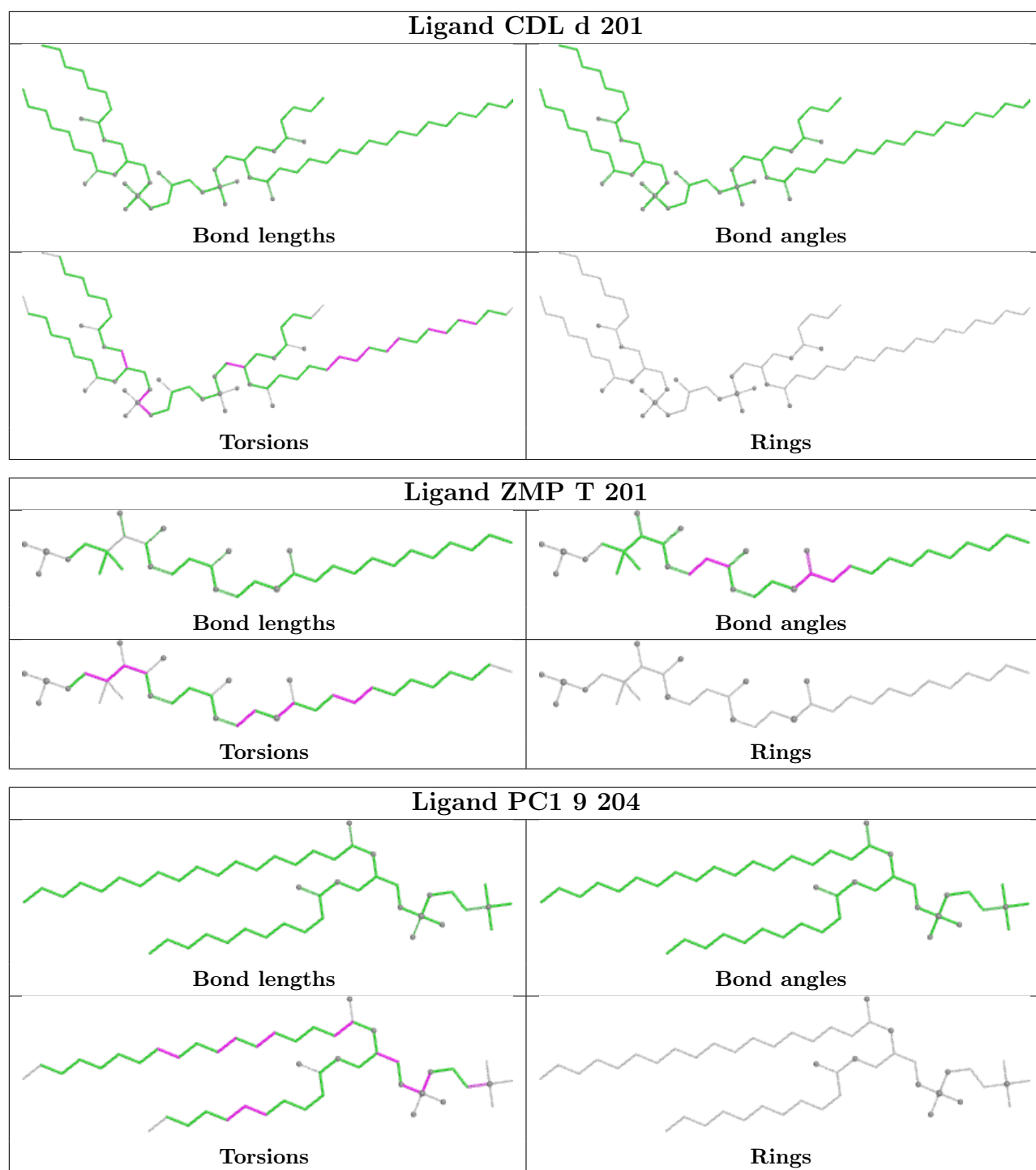


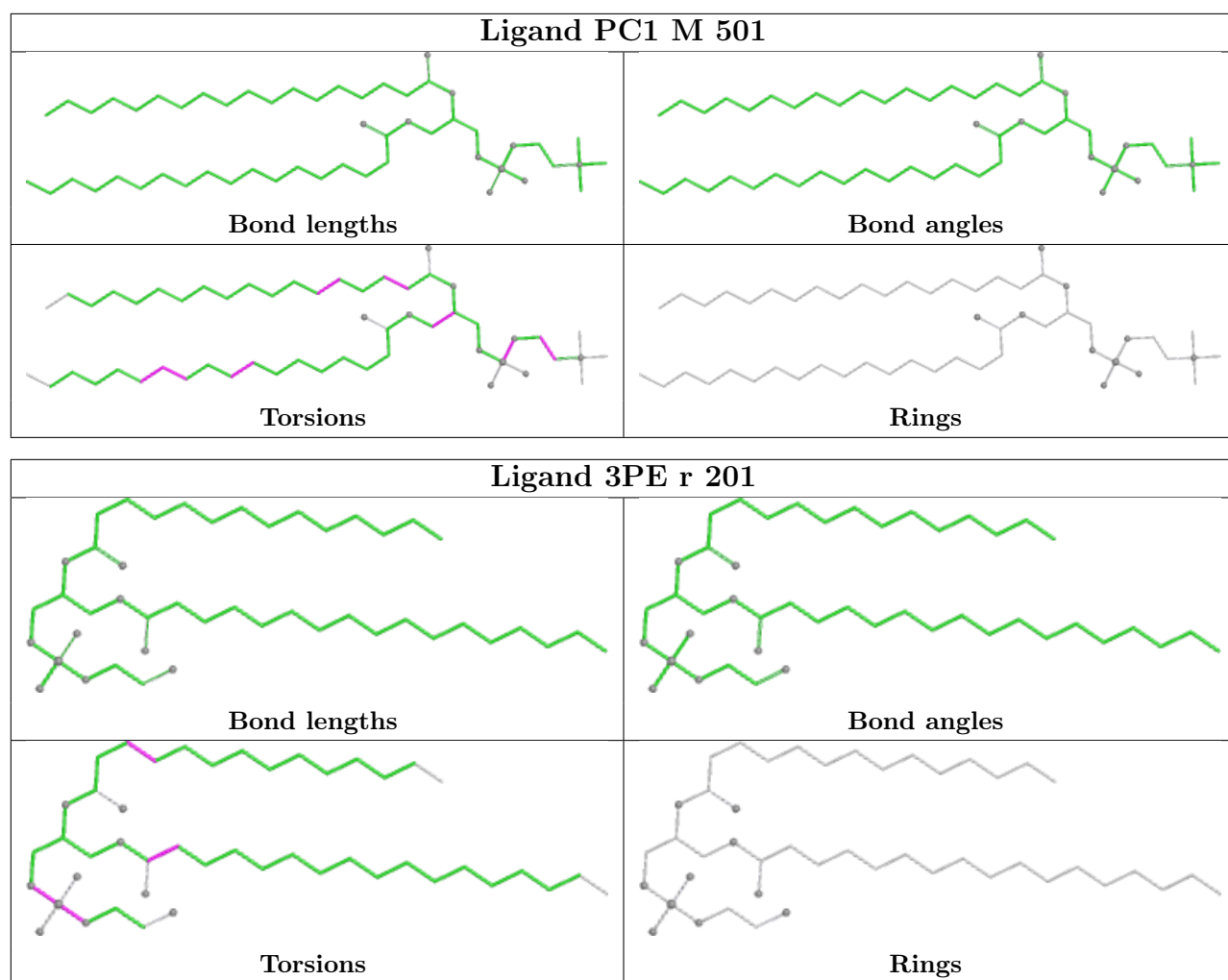


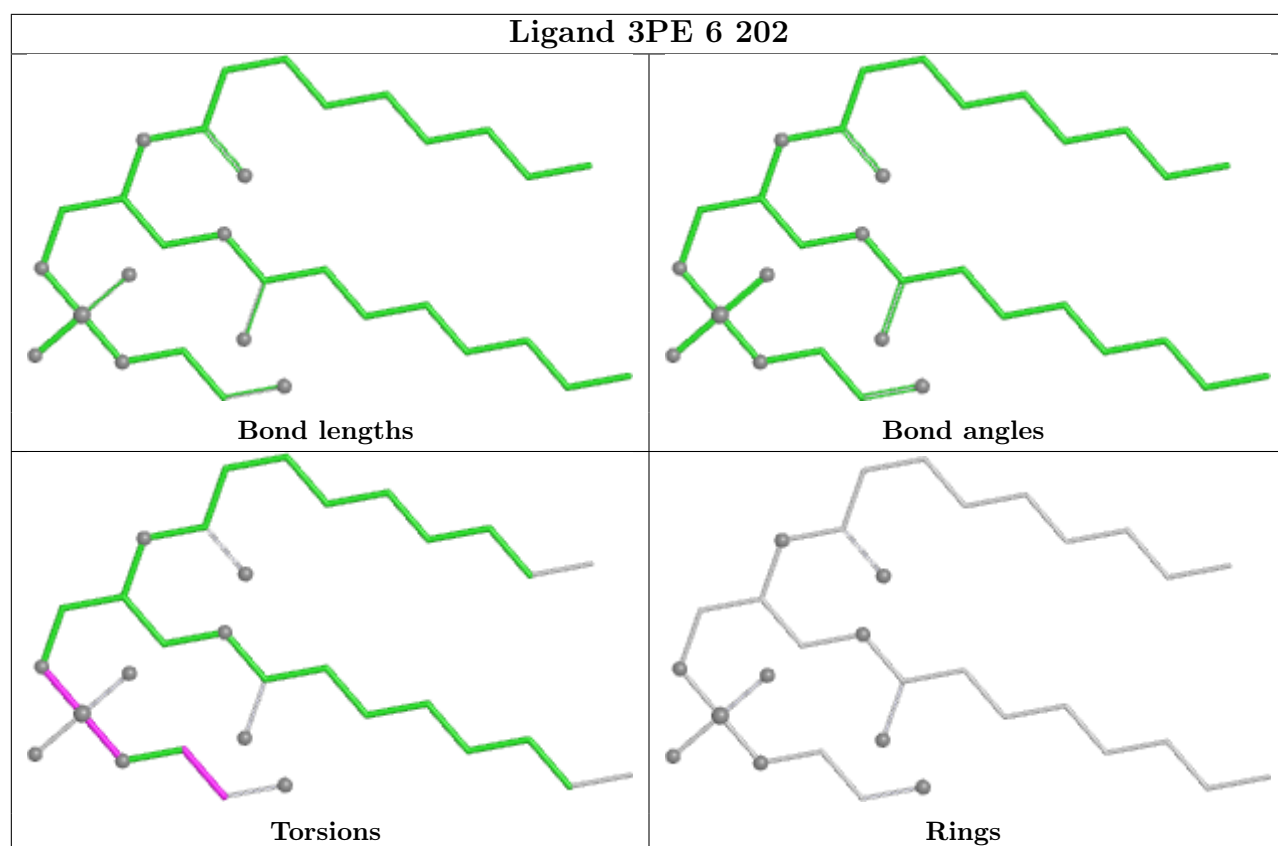


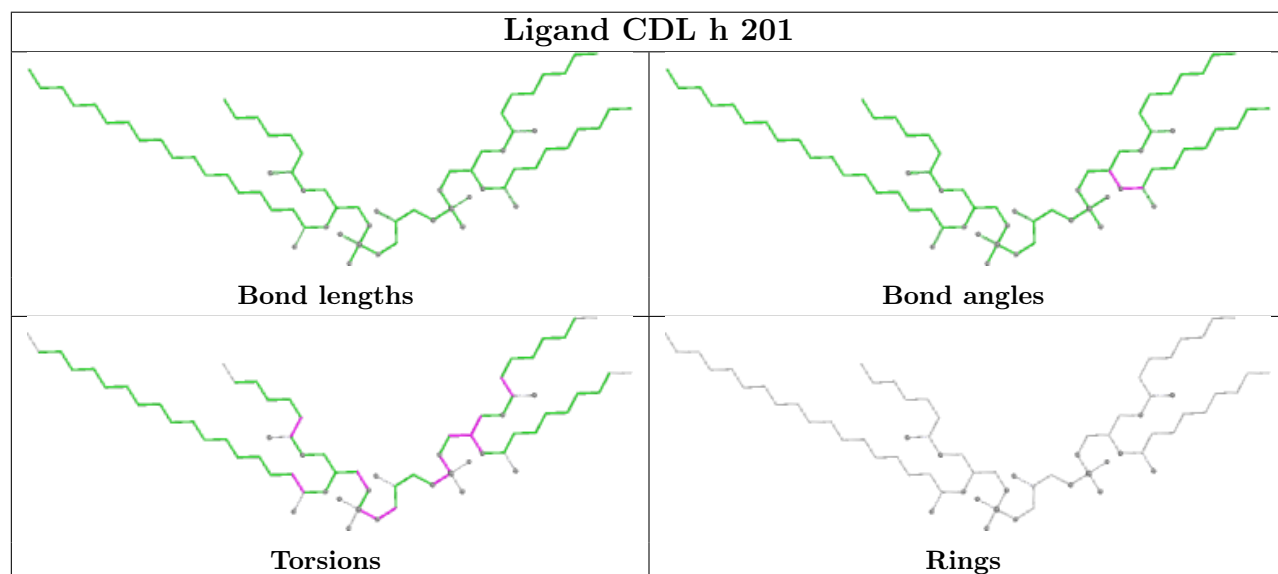
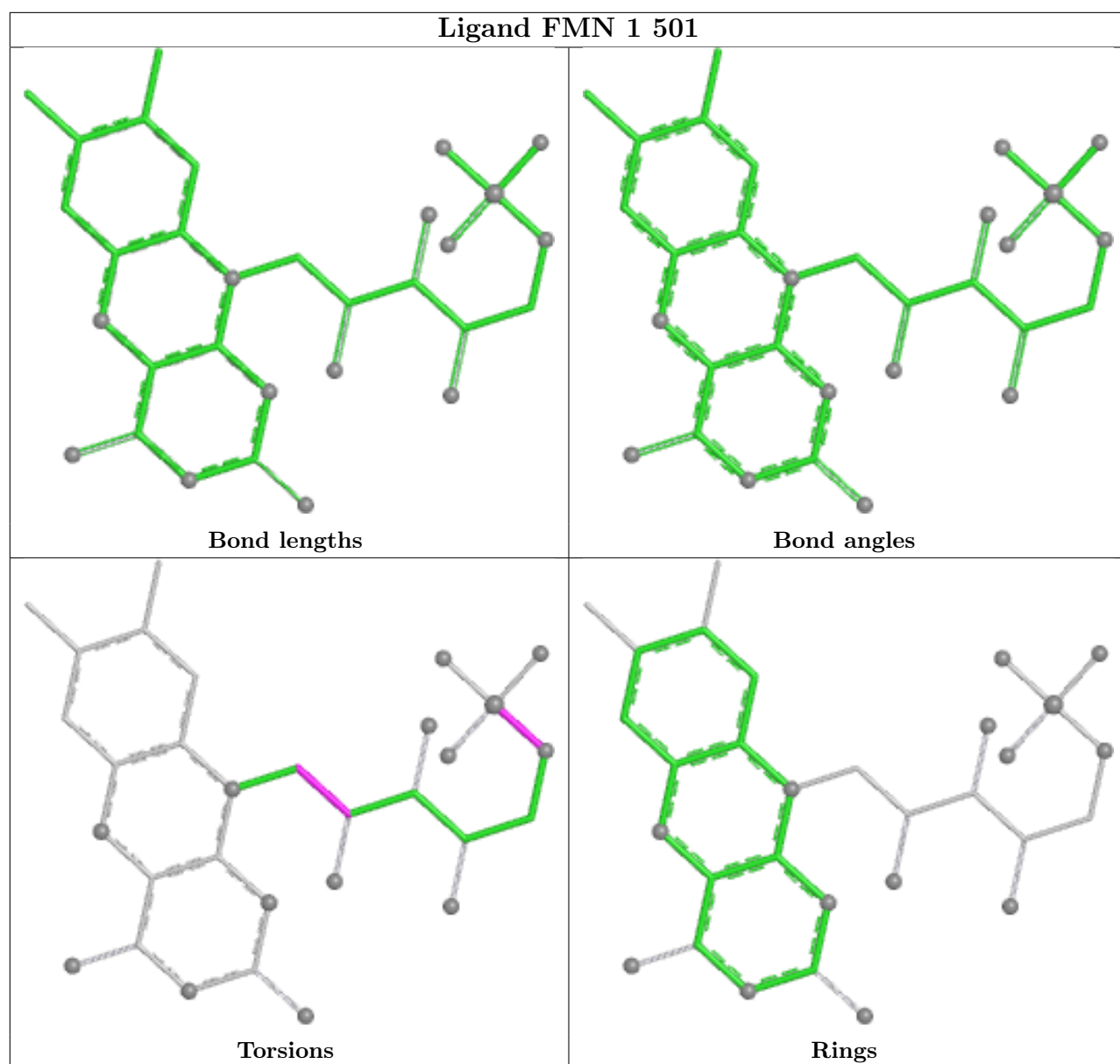


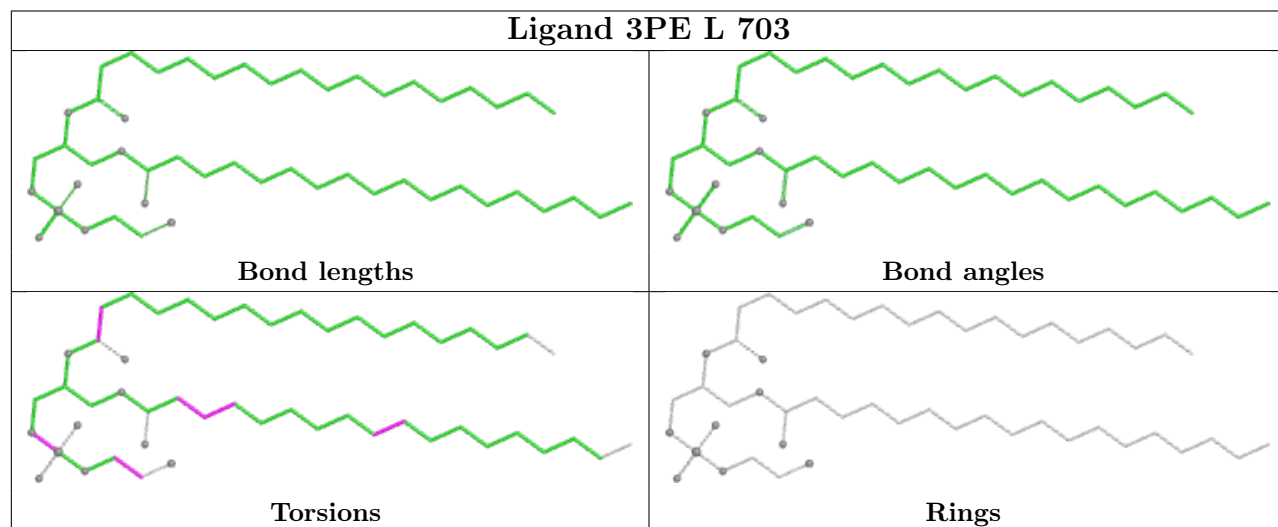
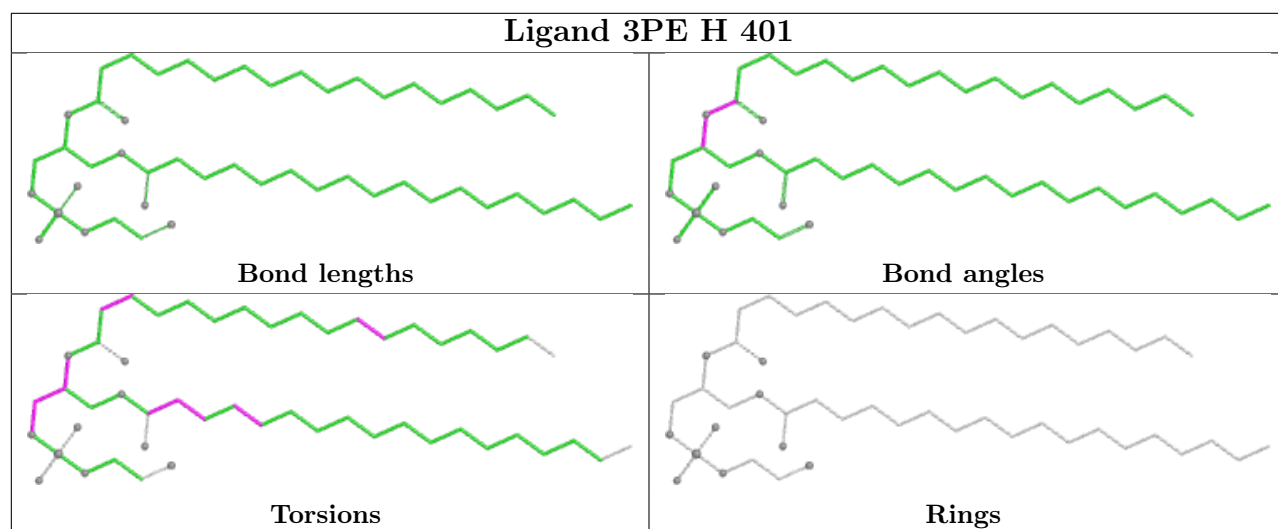
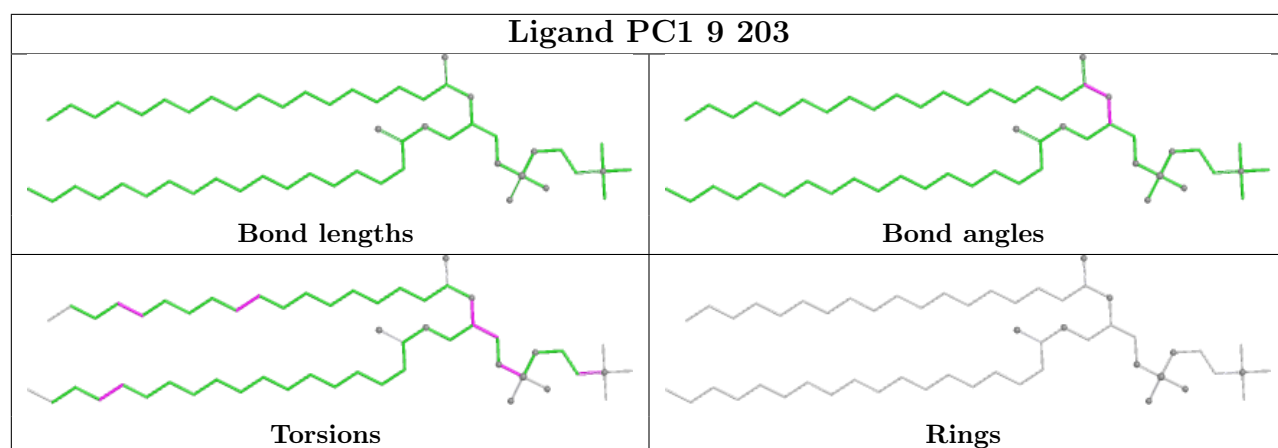


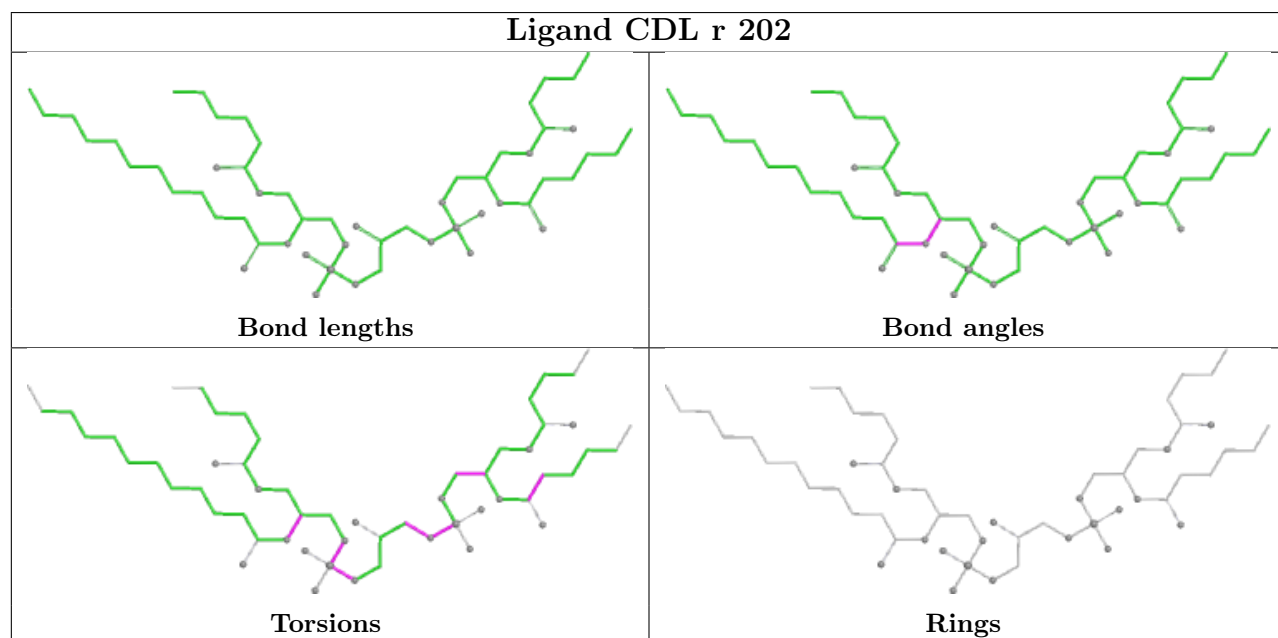
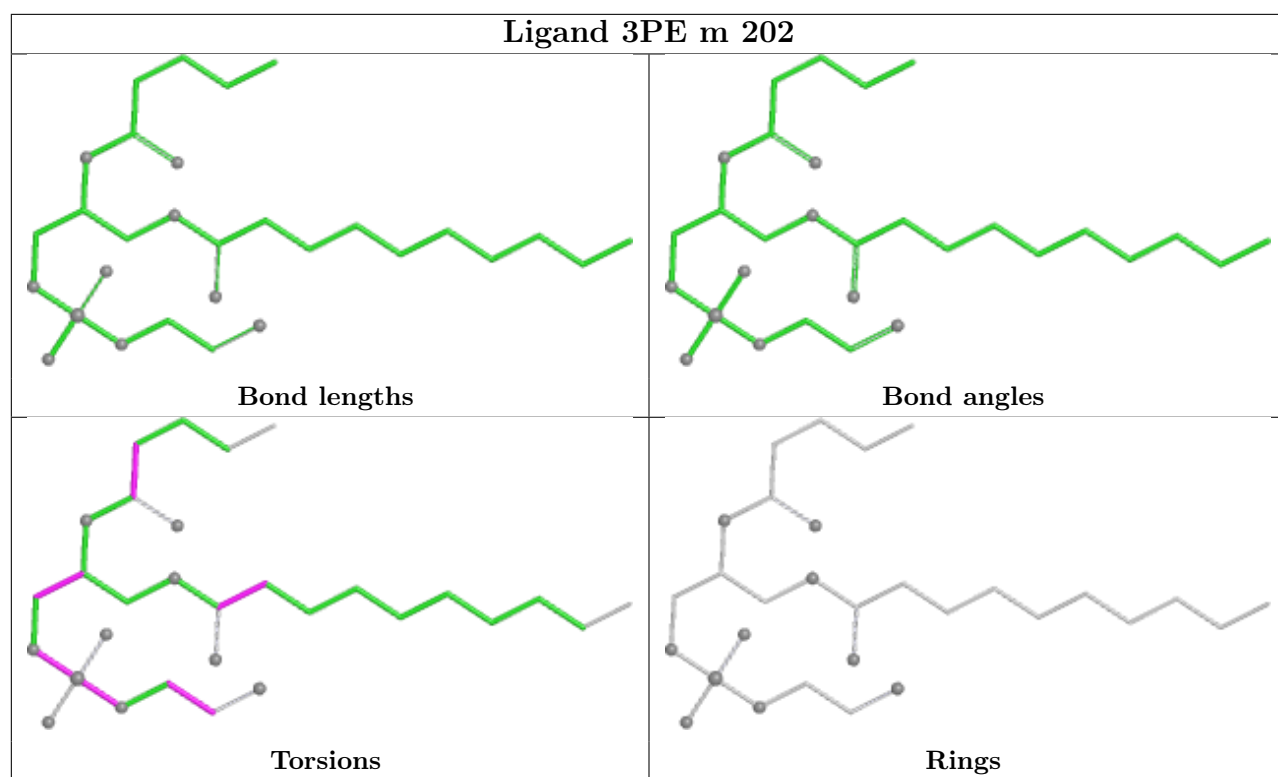


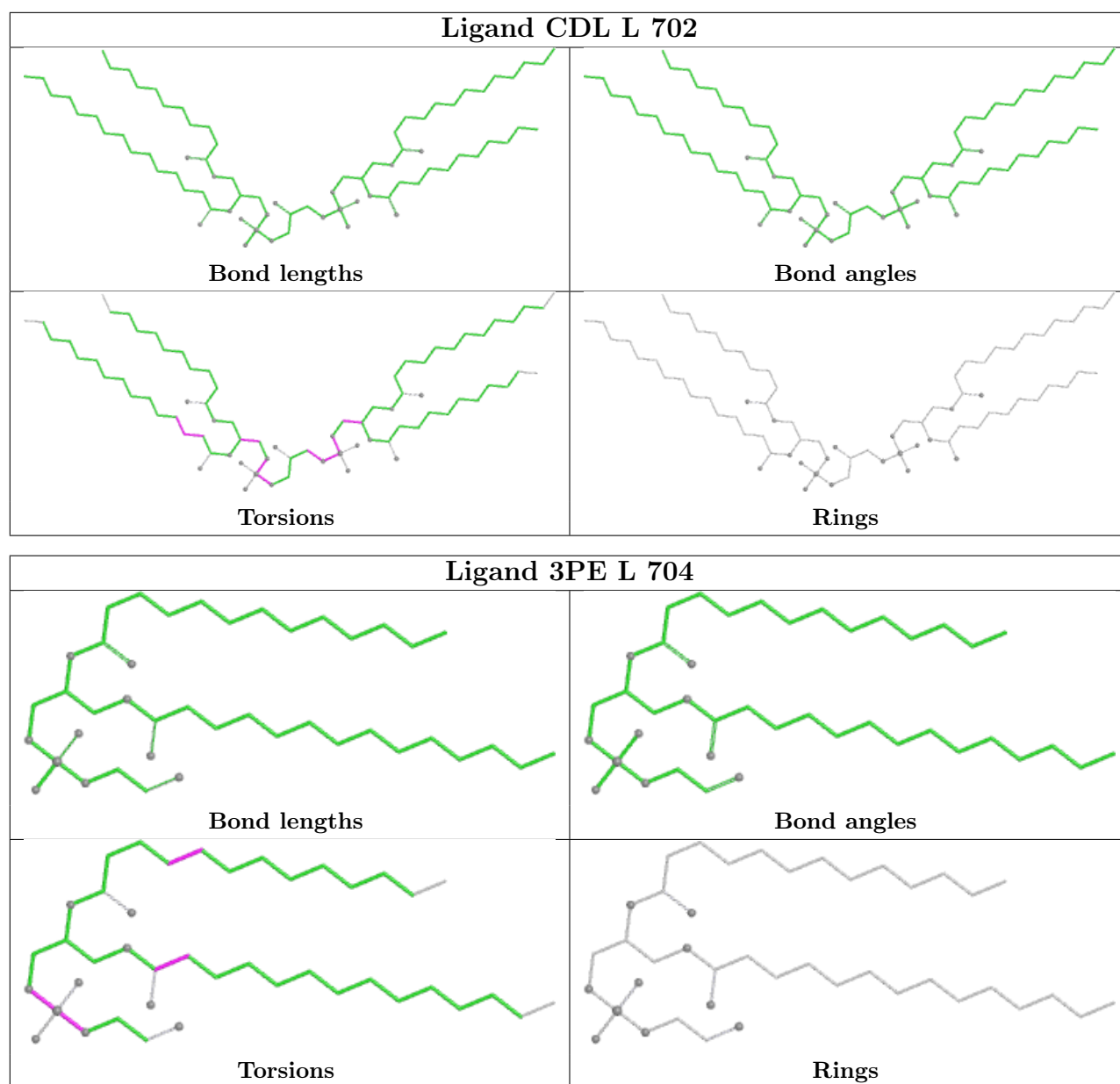












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

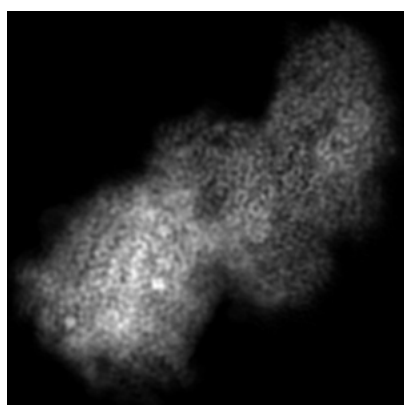
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19148. These allow visual inspection of the internal detail of the map and identification of artifacts.

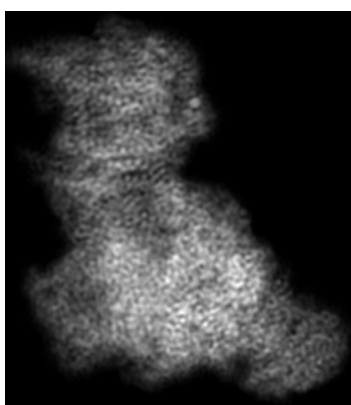
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

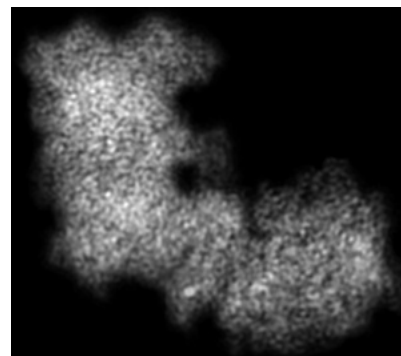
6.1.1 Primary map



X



Y

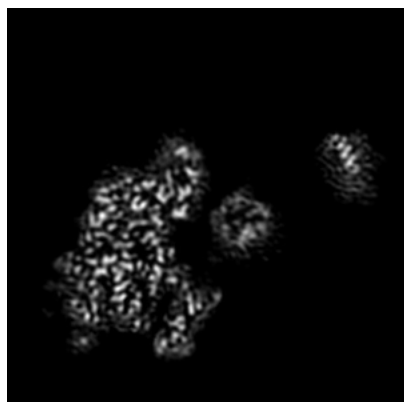


Z

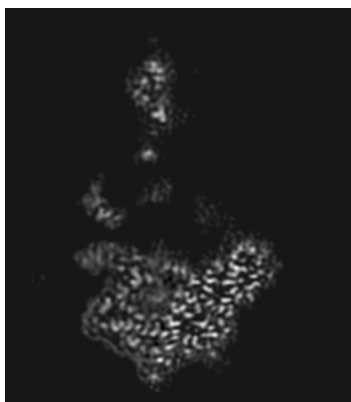
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

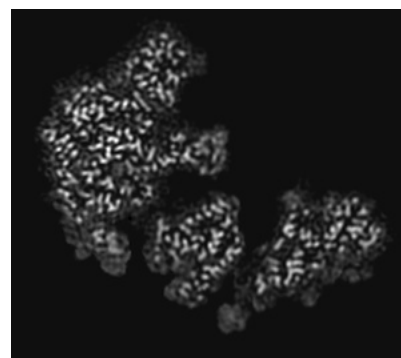
6.2.1 Primary map



X Index: 110



Y Index: 97

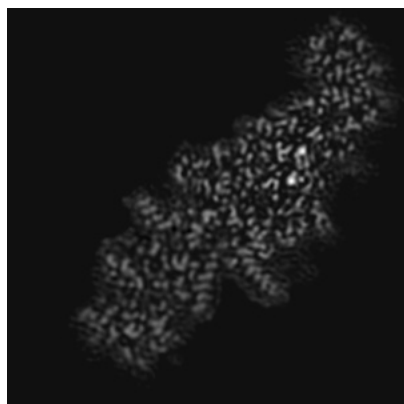


Z Index: 97

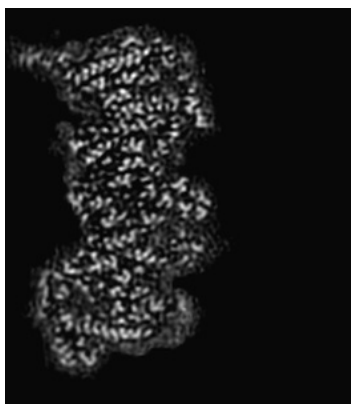
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 46



Y Index: 62



Z Index: 62

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

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

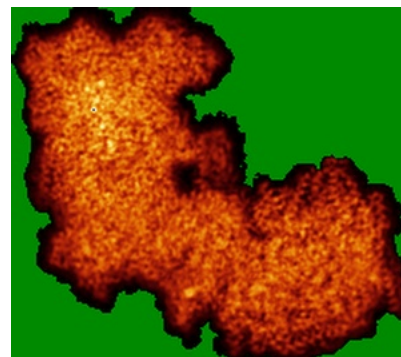
6.4.1 Primary map



X



Y

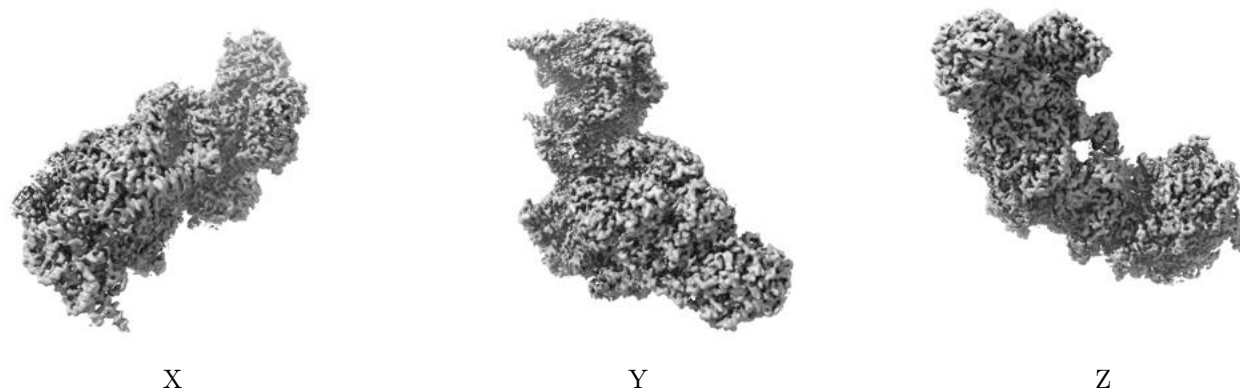


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

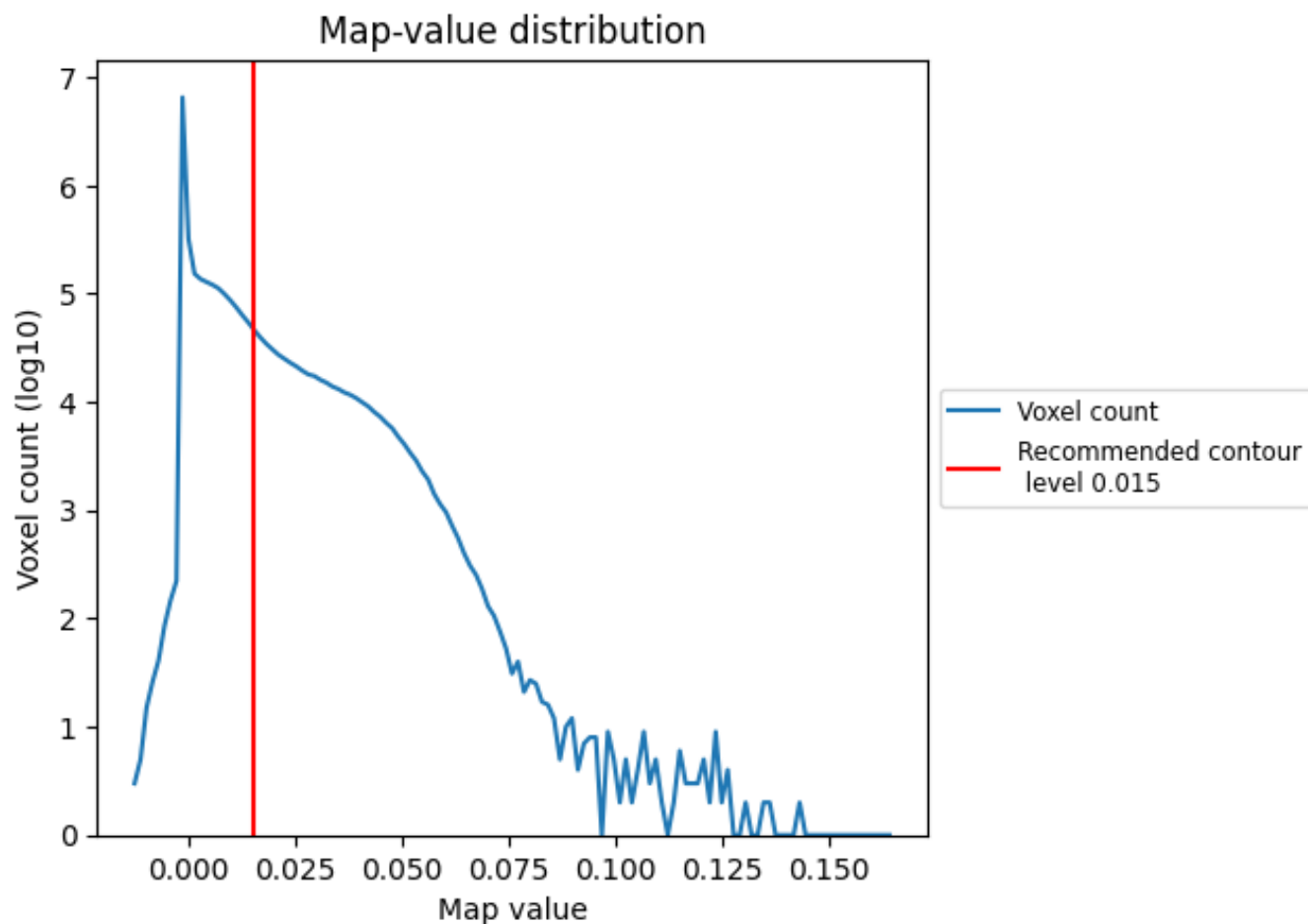
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

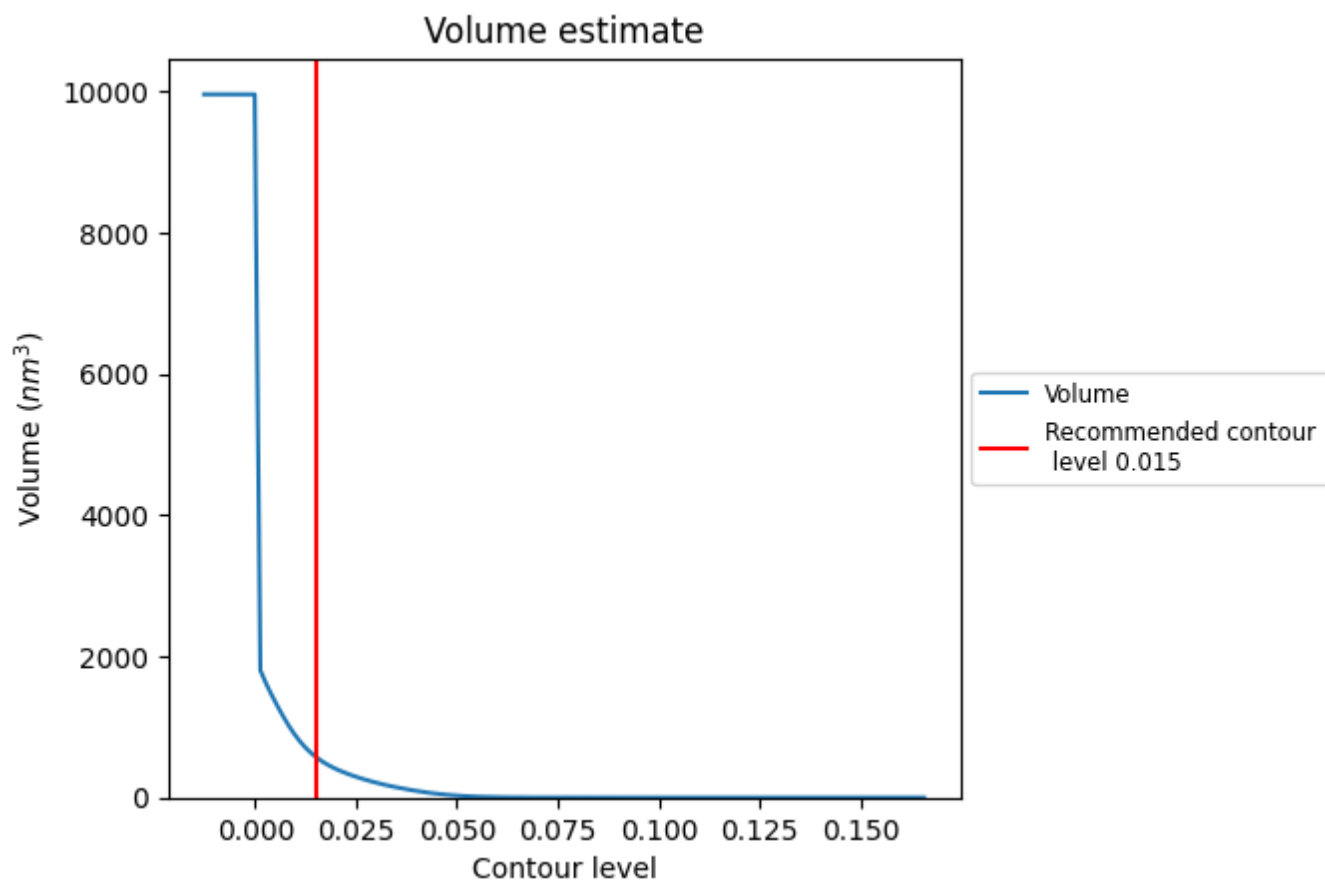
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 579 nm³; this corresponds to an approximate mass of 523 kDa.

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

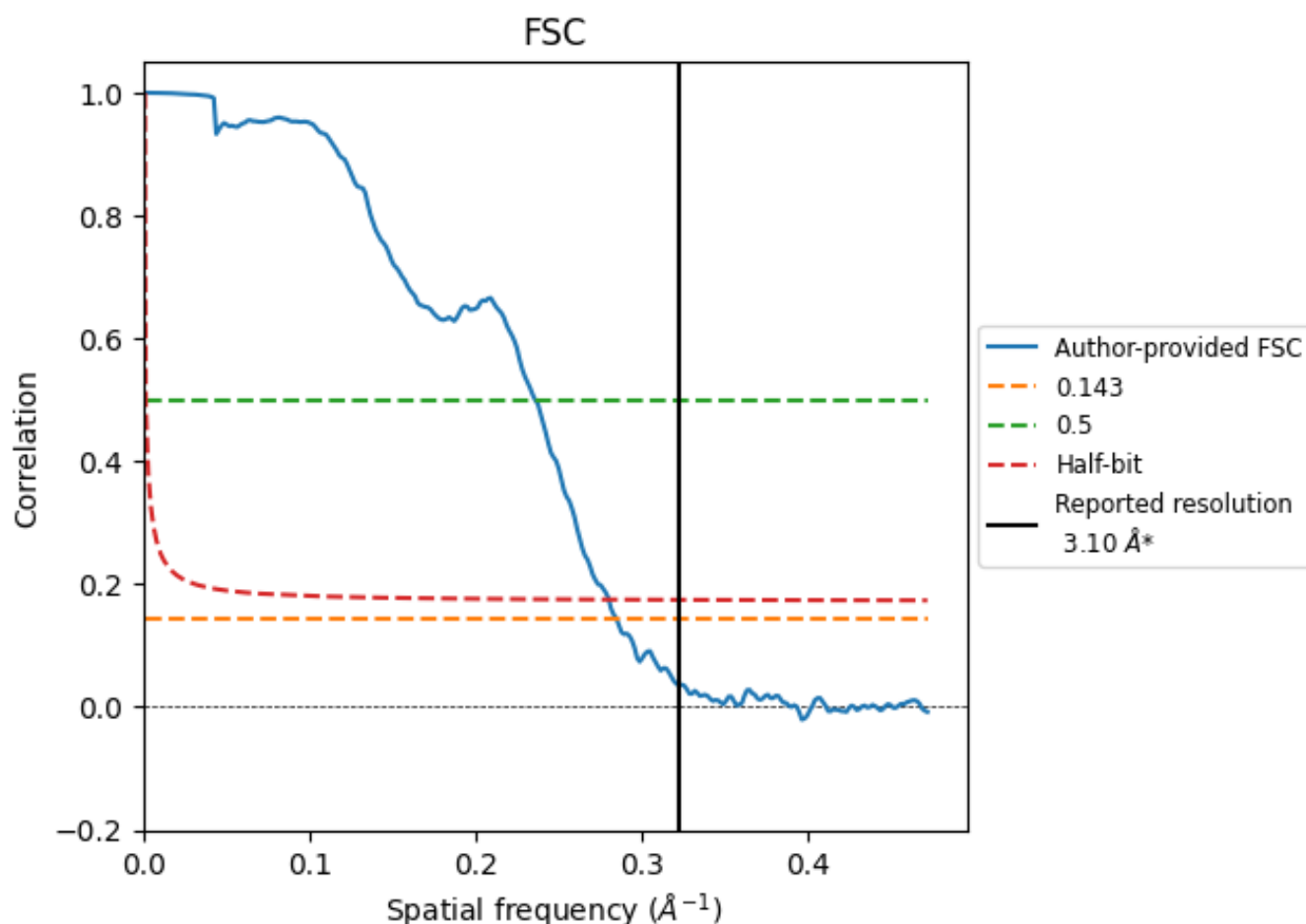
7.3 Rotationally averaged power spectrum [i](#)

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

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

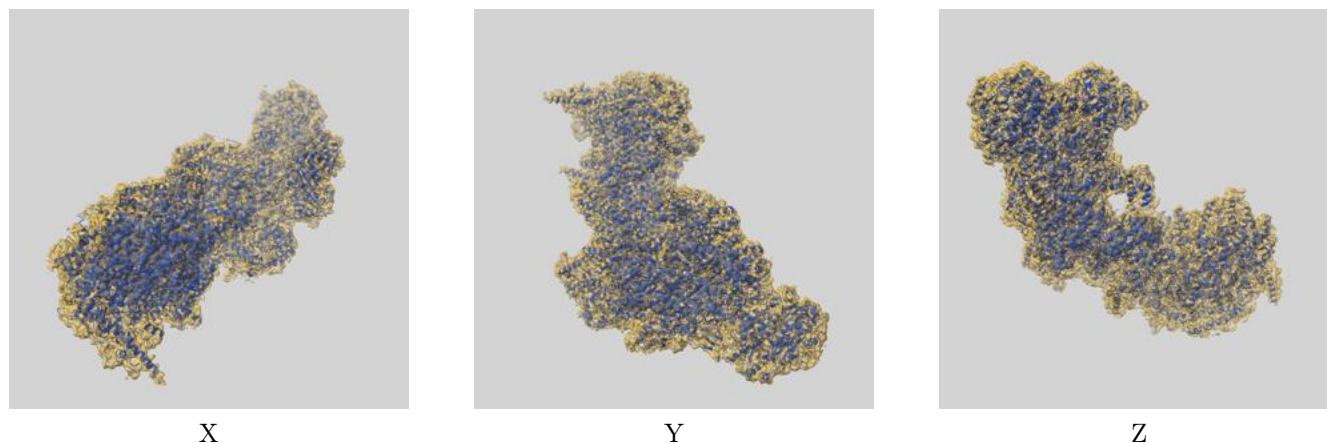
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.51	4.24	3.57
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.51 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

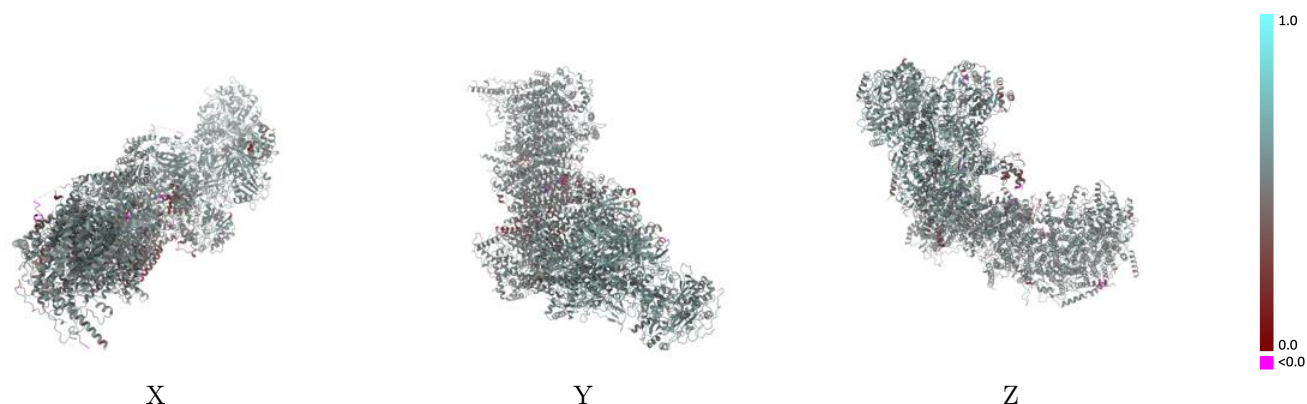
This section contains information regarding the fit between EMDB map EMD-19148 and PDB model 8RGT. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



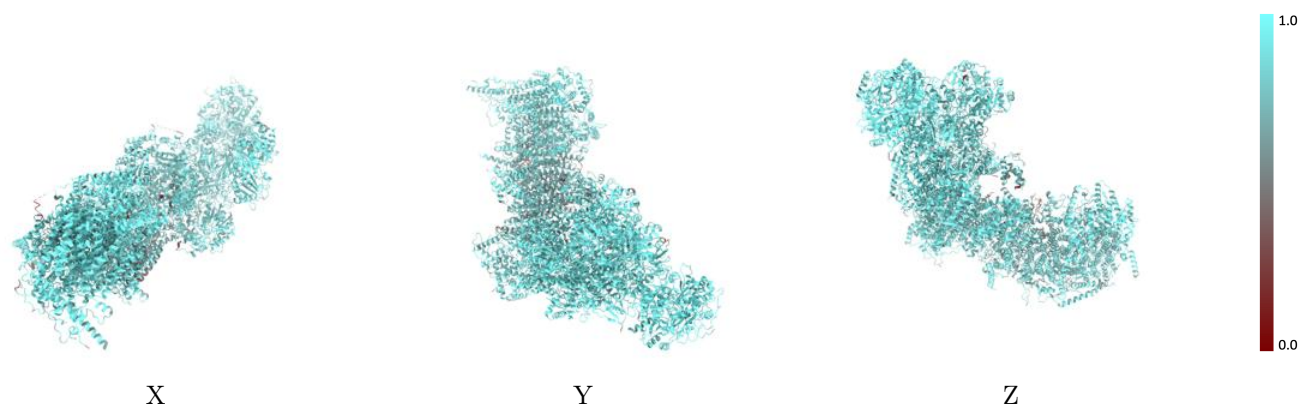
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



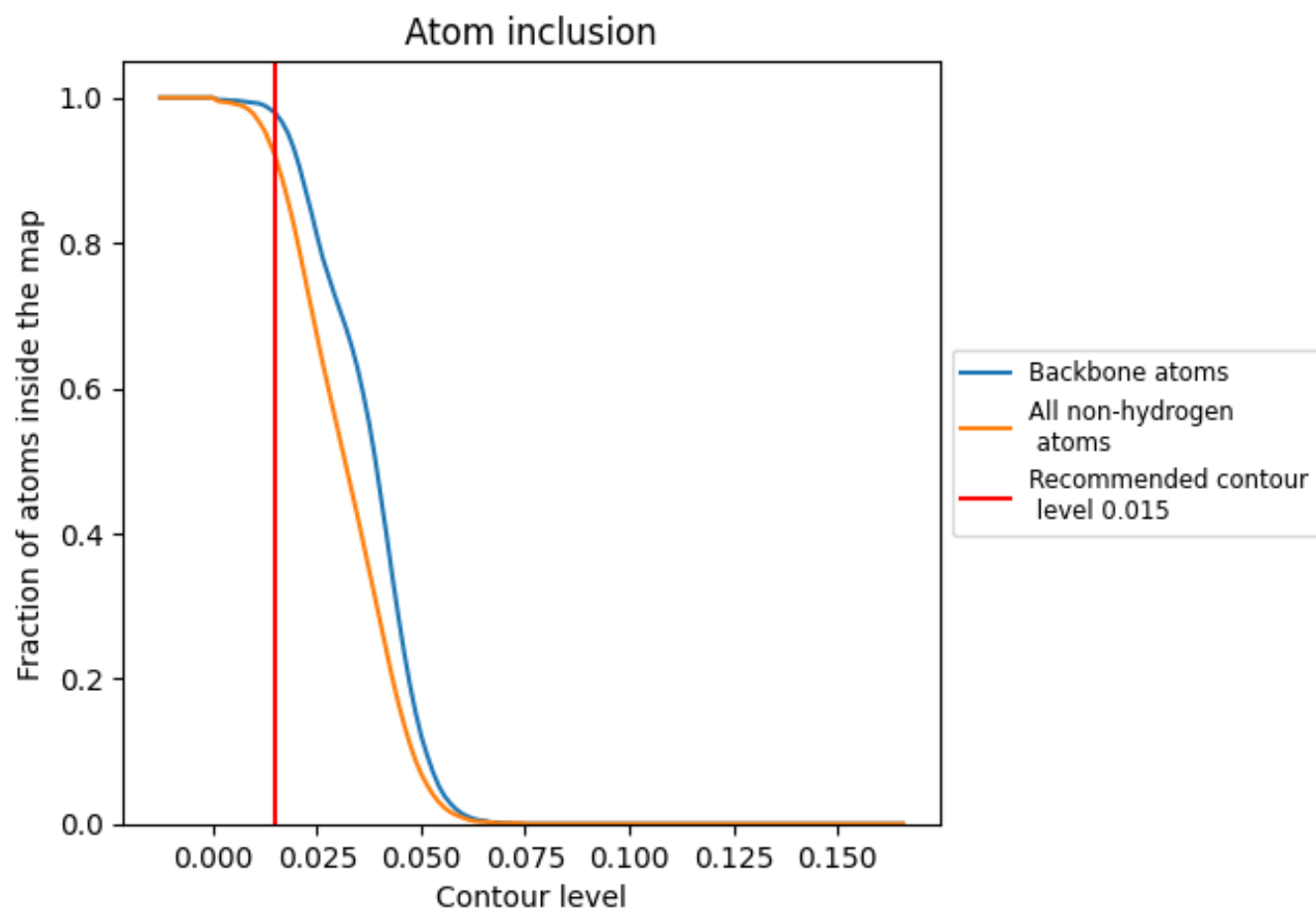
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 92% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9190	 0.5260
1	 0.9520	 0.5510
2	 0.9350	 0.5390
3	 0.9340	 0.5530
6	 0.9480	 0.5350
7	 0.9500	 0.5640
9	 0.9550	 0.5600
A	 0.8920	 0.4960
C	 0.9510	 0.5820
D	 0.9300	 0.5450
H	 0.9240	 0.5020
J	 0.8530	 0.4490
K	 0.8590	 0.4930
L	 0.9210	 0.5250
M	 0.9270	 0.5350
N	 0.9140	 0.5290
O	 0.9230	 0.5150
P	 0.8980	 0.5060
Q	 0.9290	 0.5690
S	 0.8900	 0.4910
T	 0.7760	 0.3940
U	 0.9130	 0.5210
V	 0.9120	 0.5460
W	 0.9320	 0.5470
X	 0.9210	 0.5100
Y	 0.8770	 0.5000
Z	 0.9280	 0.5040
a	 0.9400	 0.5130
b	 0.9110	 0.4790
c	 0.9100	 0.5050
d	 0.8940	 0.5200
e	 0.9230	 0.5200
f	 0.8830	 0.5060
g	 0.8690	 0.5000
h	 0.9140	 0.5220



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Chain	Atom inclusion	Q-score
i	 0.8360	 0.4720
j	 0.9090	 0.4910
k	 0.9230	 0.5100
l	 0.9200	 0.5330
m	 0.8300	 0.4870
n	 0.9390	 0.5350
o	 0.8980	 0.4980
p	 0.9280	 0.5200
q	 0.9710	 0.5600
r	 0.9150	 0.5440
s	 0.9620	 0.5390