



Full wwPDB EM Validation Report ⓘ

Nov 3, 2025 – 04:11 pm GMT

PDB ID : 9I4I / pdb_00009i4i
EMDB ID : EMD-52619
Title : High resolution Cryo-EM structure of human complex I in mitochondria
Authors : Nguyen, M.D.; Singh, V.; Rorbach, J.
Deposited on : 2025-01-24
Resolution : 2.63 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

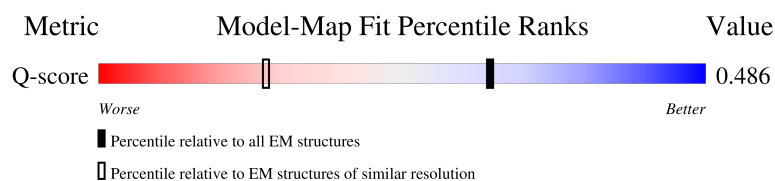
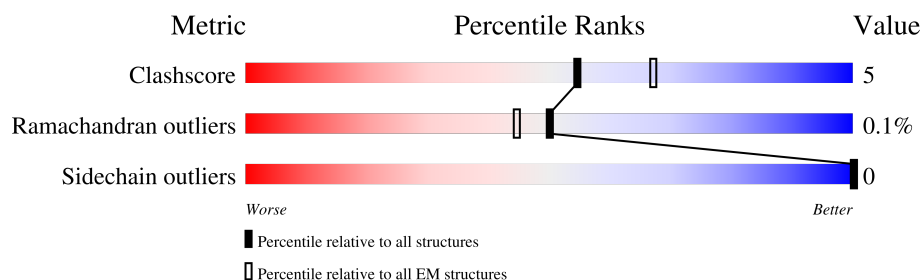
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up 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) : 2.46

1 Overall quality at a glance

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



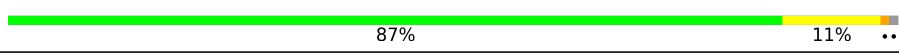
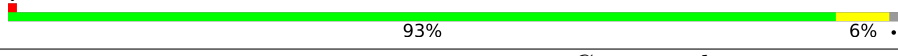
The reported resolution of this entry is 2.63 Å.

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.




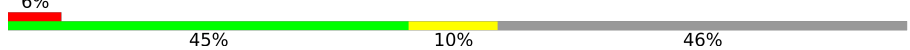


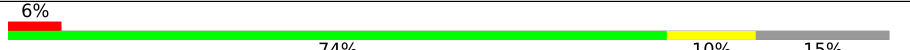


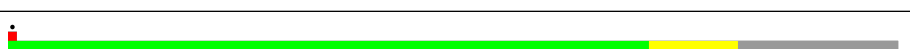
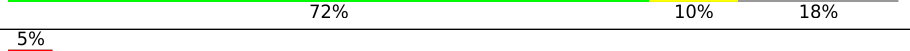


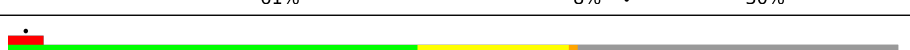
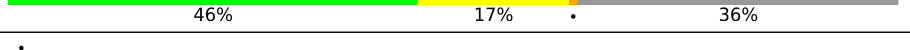

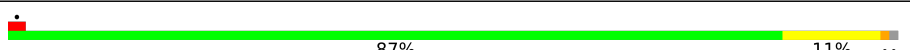

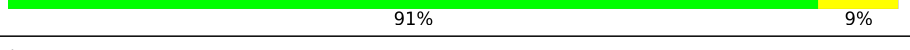
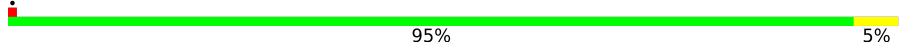
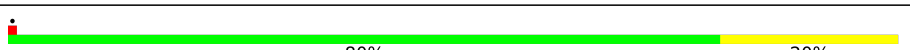




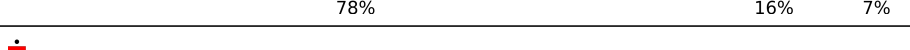
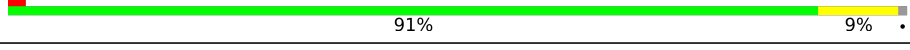
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	8888 (2.13 - 3.13)

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

Mol	Chain	Length	Quality of chain
1	Q	463	
2	S	70	
3	U	84	
4	V	141	

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Mol	Chain	Length	Quality of chain
5	W	144	
6	H	156	
6	X	156	
7	Y	105	
8	Z	98	
9	a	189	
10	b	128	
11	c	186	
12	d	172	
13	e	153	
14	f	76	
15	g	119	
16	h	106	
17	i	347	
18	j	115	
19	k	98	
20	l	603	
21	m	174	
22	n	58	
23	o	129	
24	p	179	
25	r	459	
26	s	318	
27	u	172	
28	v	137	

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Mol	Chain	Length	Quality of chain
29	w	355	
30	C	464	
31	D	210	
32	E	213	
33	F	128	
34	G	99	
35	I	116	
36	J	377	
37	K	108	
38	L	175	
39	M	727	
40	N	145	
41	O	249	
42	P	264	
43	T	124	
44	t	113	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
51	SF4	C	501	-	-	X	-
52	FMN	C	502	X	X	X	-

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 136393 atoms, of which 68697 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 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	Q	430	Total	C	H	N	O	S	0	0
			6894	2215	3433	599	624	23		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	S	70	Total	C	H	N	O	S	0	0
			1138	367	570	101	96	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	U	83	Total	C	H	N	O	S	0	0
			1302	427	655	105	113	2		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	V	140	Total	C	H	N	O	S	0	0
			2069	668	1031	178	187	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	W	140	Total	C	H	N	O	S	0	0
			2304	738	1153	205	202	6		

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	X	86	Total	C	H	N	O	S	0	0
			1386	448	690	102	140	6		
6	H	85	Total	C	H	N	O	S	0	0
			1369	443	681	101	139	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	Y	61	Total	C	H	N	O	S	0	0
			1035	361	491	89	93	1		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	Z	83	Total	C	H	N	O	S	0	0
			1339	447	660	115	115	2		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	a	138	Total	C	H	N	O	S	0	0
			2356	771	1182	199	202	2		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	b	120	Total	C	H	N	O	S	0	0
			2070	672	1049	176	169	4		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	c	152	Total	C	H	N	O	S	0	0
			2453	819	1180	215	227	12		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	d	169	Total	C	H	N	O	S	0	0
			2837	895	1404	262	264	12		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	e	107	Total	C	H	N	O	S	0	0
			1737	569	850	146	168	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	f	49	Total	C	H	N	O		0	0
			844	278	425	71	70			

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	g	119	Total	C	H	N	O	S	1	0
			2035	663	1023	176	169	4		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	h	105	Total	C	H	N	O	S	0	0
			1747	551	876	162	151	7		

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	i	347	Total	C	H	N	O	S	0	0
			5626	1818	2893	420	470	25		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
18	j	115	Total	C	H	N	O	S	0	0
			1890	631	964	132	154	9		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	k	98	Total	C	H	N	O	S	0	0
			1530	488	787	114	128	13		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	l	601	Total	C	H	N	O	S	0	0
			9583	3110	4880	739	823	31		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	m	173	Total	C	H	N	O	S	0	0
			2619	872	1317	192	227	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
22	n	54	Total	C	H	N	O	S	0	0
			923	295	466	82	77	3		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	o	128	Total	C	H	N	O	S	0	0
			2154	685	1088	192	187	2		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	p	173	Total	C	H	N	O	S	0	0
			2947	963	1448	266	262	8		

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	r	459	Total	C	H	N	O	S	0	0
			7444	2404	3821	569	620	30		

- Molecule 26 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	s	316	Total	C	H	N	O	S	0	0
			5091	1672	2593	376	435	15		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	u	171	Total	C	H	N	O	S	0	0
			2791	893	1386	249	254	9		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	v	121	Total	C	H	N	O	S	0	0
			2069	647	1032	200	180	10		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	w	320	Total	C	H	N	O	S	0	0
			5221	1680	2598	447	487	9		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	C	434	Total	C	H	N	O	S	0	0
			6668	2110	3321	601	616	20		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	D	176	Total	C	H	N	O	S	0	0
			2787	893	1367	243	271	13		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms							AltConf	Trace
32	E	161	Total	C	H	N	O	P	S	0	0
			2577	816	1290	233	223	1	14		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms							AltConf	Trace
33	F	118	Total	C	H	N	O	S		0	0
			2016	640	1017	183	171	5			

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms							AltConf	Trace
34	G	85	Total	C	H	N	O	S		0	0
			1380	430	697	127	124	2			

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms							AltConf	Trace
35	I	112	Total	C	H	N	O	S		0	0
			1875	593	953	157	169	3			

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms							AltConf	Trace
36	J	341	Total	C	H	N	O	S		0	0
			5547	1780	2802	490	467	8			

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms							AltConf	Trace
37	K	39	Total	C	H	N	O	S		0	0
			586	191	282	53	59	1			

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	L	121	Total	C	H	N	O	S	0	0
			1954	617	975	176	182	4		

- Molecule 39 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	M	687	Total	C	H	N	O	S	0	0
			10596	3310	5321	917	1009	39		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	N	144	Total	C	H	N	O	S	0	0
			2375	775	1172	211	213	4		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	O	212	Total	C	H	N	O	S	0	0
			3291	1047	1648	276	310	10		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	P	208	Total	C	H	N	O	S	0	0
			3421	1117	1691	297	313	3		

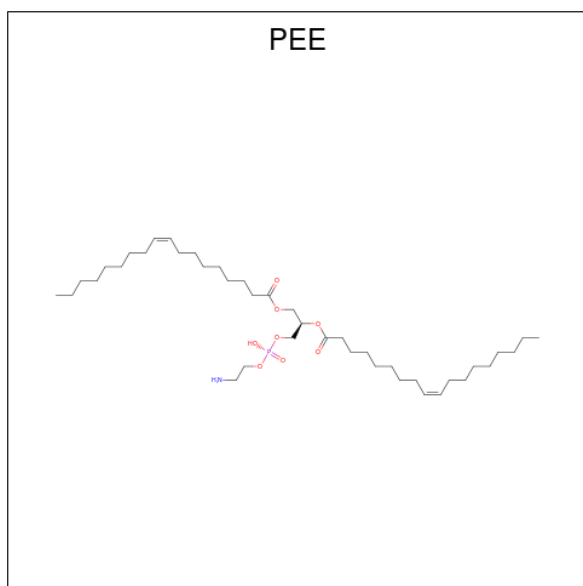
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	T	96	Total	C	H	N	O	S	0	0
			1484	465	732	141	143	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

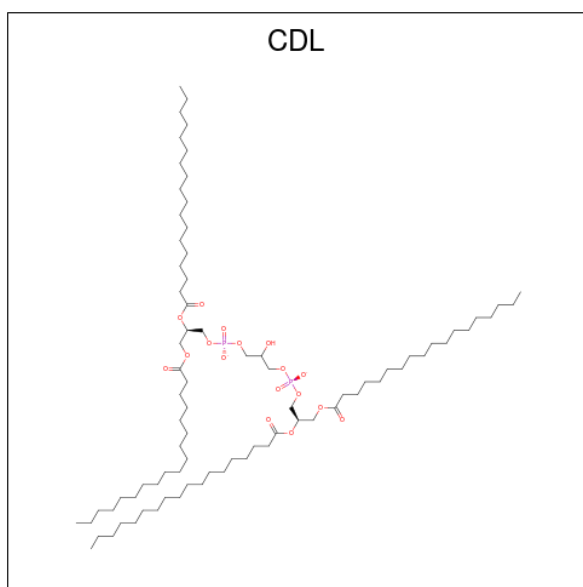
Mol	Chain	Residues	Atoms						AltConf	Trace
44	t	97	Total	C	H	N	O	S	0	0
			1582	489	802	148	141	2		

- Molecule 45 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



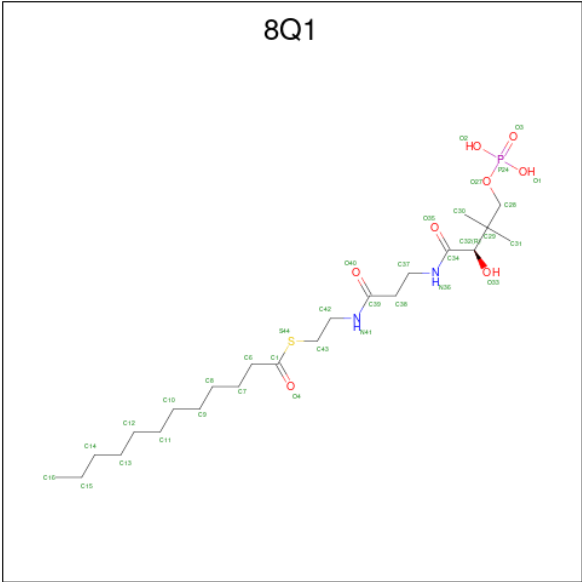
Mol	Chain	Residues	Atoms						AltConf
45	V	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	
45	W	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	
45	i	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	
45	i	1	Total	C	H	N	O	P	0
			121	39	72	1	8	1	
45	l	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	
45	E	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	
45	J	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	

- Molecule 46 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



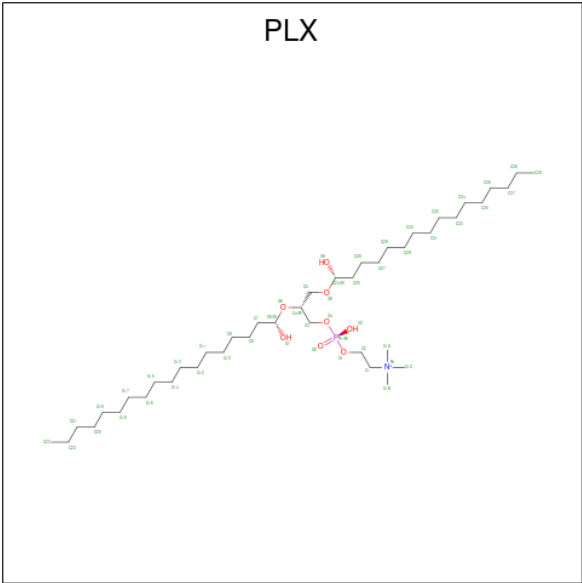
Mol	Chain	Residues	Atoms					AltConf
46	V	1	Total	C	H	O	P	0
			256	81	156	17	2	
46	V	1	Total	C	H	O	P	0
			256	81	156	17	2	
46	i	1	Total	C	H	O	P	0
			144	45	80	17	2	
46	l	1	Total	C	H	O	P	0
			144	45	80	17	2	
46	l	1	Total	C	H	O	P	0
			256	81	156	17	2	
46	u	1	Total	C	H	O	P	0
			144	45	80	17	2	

- Molecule 47 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
47	X	1	Total	C	H	N	O	P	S	0
			78	23	43	2	8	1	1	
47	F	1	Total	C	H	N	O	P	S	0
			78	23	43	2	8	1	1	

- Molecule 48 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P).



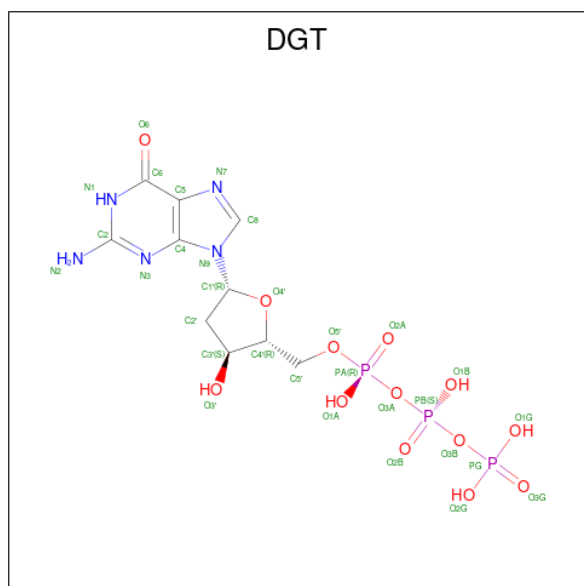
Mol	Chain	Residues	Atoms						AltConf
48	g	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	

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Mol	Chain	Residues	Atoms						AltConf
48	g	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	
48	j	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	
48	o	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	
48	r	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	
48	s	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	
48	N	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	

- Molecule 49 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

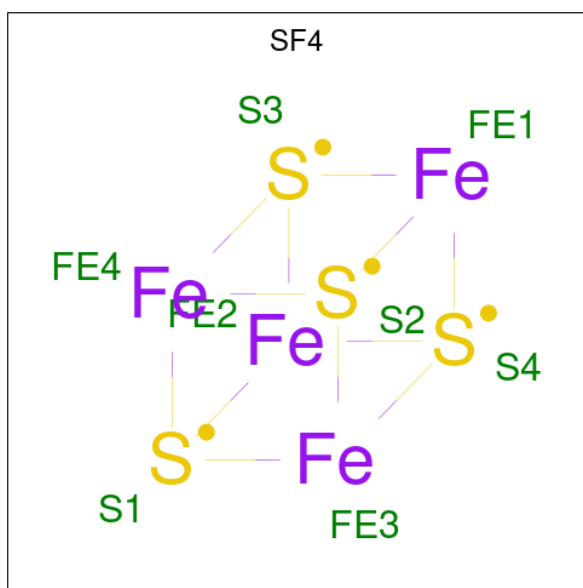


Mol	Chain	Residues	Atoms						AltConf
49	w	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 50 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

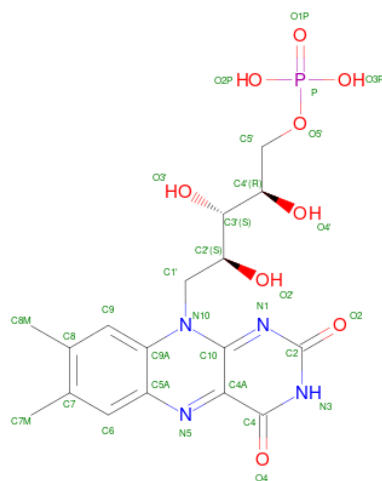
Mol	Chain	Residues	Atoms		AltConf
50	w	1	Total	Mg	0
			1	1	

- Molecule 51 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



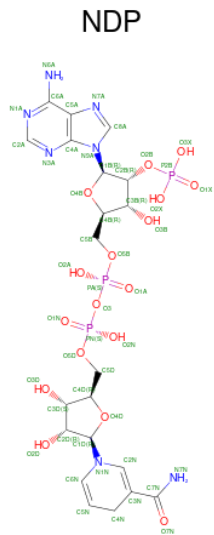
Mol	Chain	Residues	Atoms			AltConf
51	C	1	Total	Fe	S	0
			8	4	4	
51	D	1	Total	Fe	S	0
			8	4	4	
51	D	1	Total	Fe	S	0
			8	4	4	
51	E	1	Total	Fe	S	0
			8	4	4	
51	M	1	Total	Fe	S	0
			8	4	4	
51	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 52 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
52	C	1	Total	C	H	N	O	P	0
			50	17	19	4	9	1	

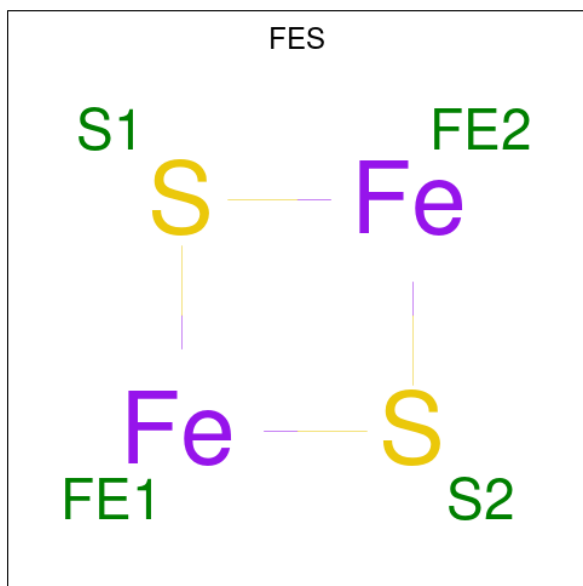
- Molecule 53 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
53	J	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled

as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
54	M	1	Total	Fe	S	0
			4	2	2	
54	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	T	1	Total	Zn	0
			1	1	

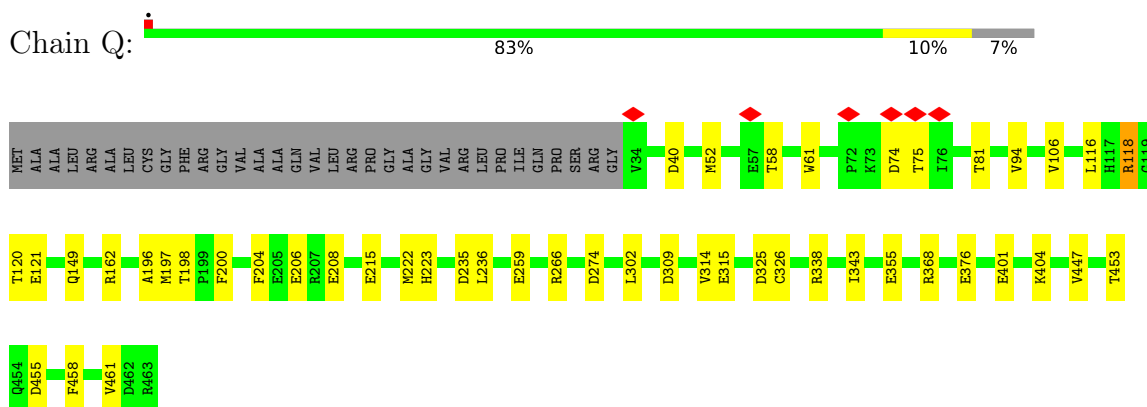
- Molecule 56 is water.

Mol	Chain	Residues	Atoms		AltConf
56	X	1	Total	O	0
			1	1	

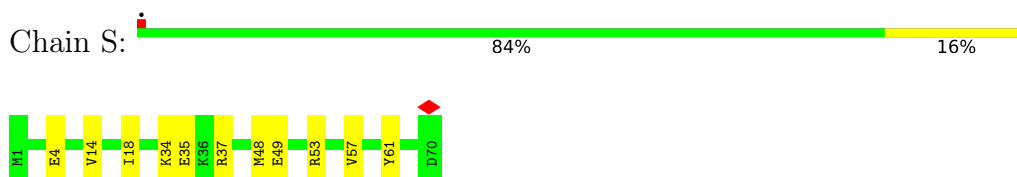
3 Residue-property plots

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

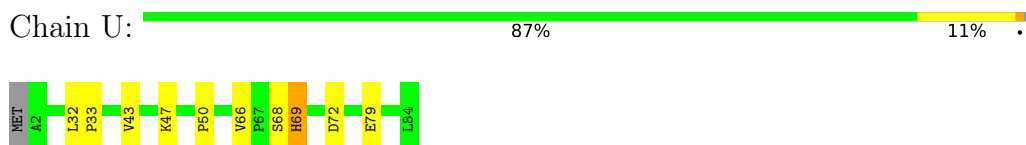
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



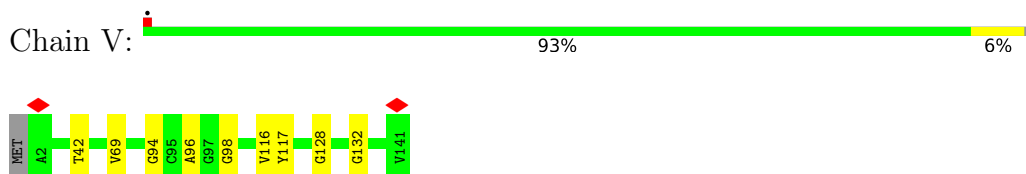
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1




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



- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



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

Chain W:  80% 15% . .

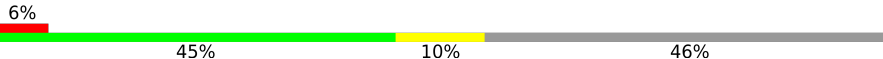


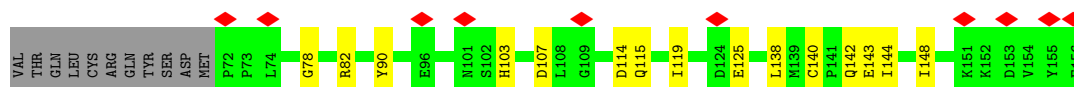
- Molecule 6: Acyl carrier protein, mitochondrial

Chain X:  51% . 45%



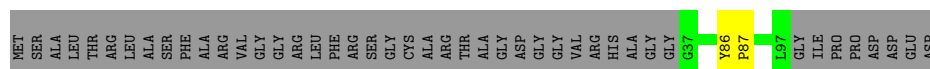
- Molecule 6: Acyl carrier protein, mitochondrial

Chain H:  6% 45% 10% 46%




- Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:  56% . 42%



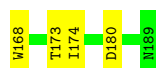
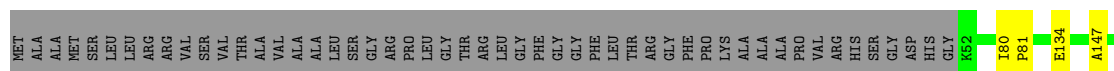
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:  6% 74% 10% 15%




- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  69% . 27%



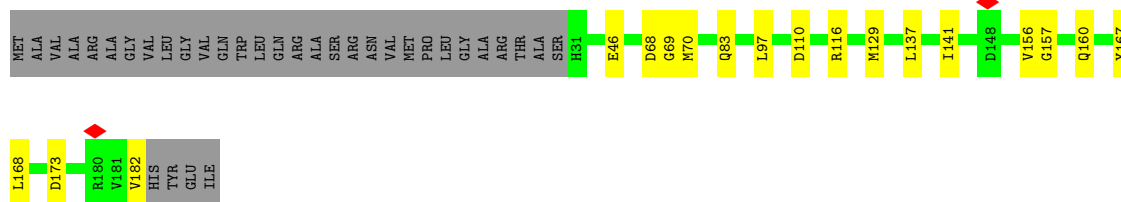
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b: 




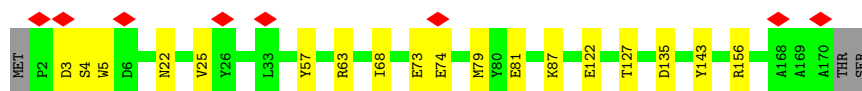
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c: 



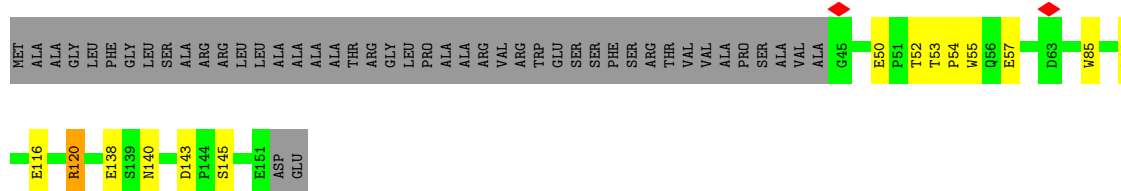
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d: 



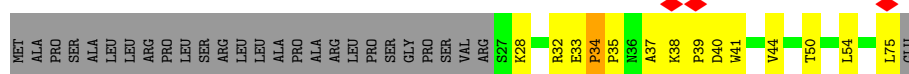
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e: 



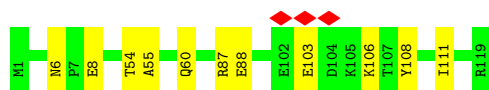
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f: 

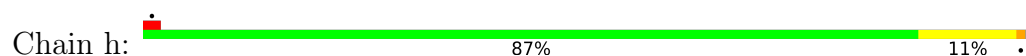


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g: 



- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



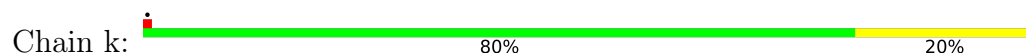
- Molecule 17: NADH-ubiquinone oxidoreductase chain 2



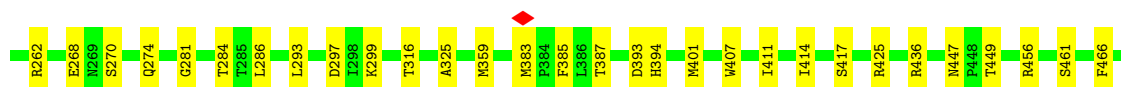
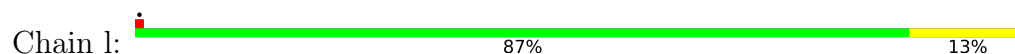
- Molecule 18: NADH-ubiquinone oxidoreductase chain 3




- Molecule 19: NADH-ubiquinone oxidoreductase chain 4L



- Molecule 20: NADH-ubiquinone oxidoreductase chain 5




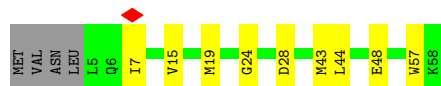
- Molecule 21: NADH-ubiquinone oxidoreductase chain 6

Chain m:  88% 11%




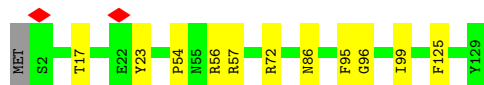
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n:  78% 16% 7%




- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o:  91% 9%




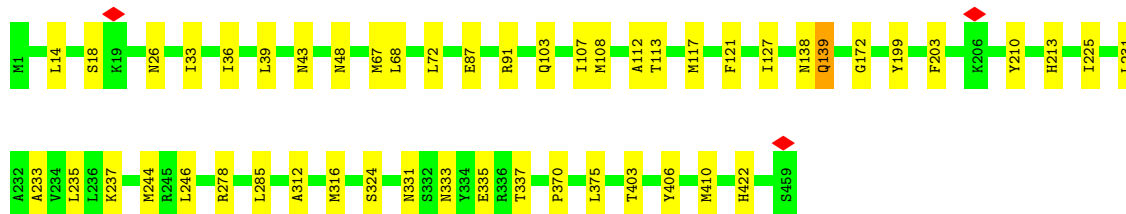
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p:  90% 7%




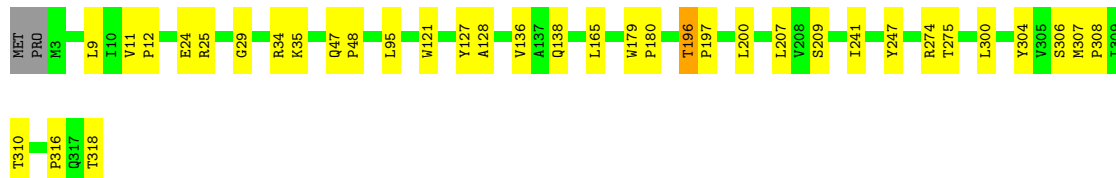
- Molecule 25: NADH-ubiquinone oxidoreductase chain 4

Chain r:  89% 11%




- Molecule 26: NADH-ubiquinone oxidoreductase chain 1

Chain s:  88% 11%




- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:  92% 8%




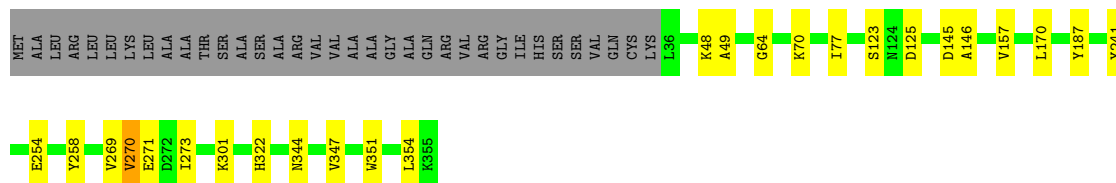
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:  78% 10% 12%




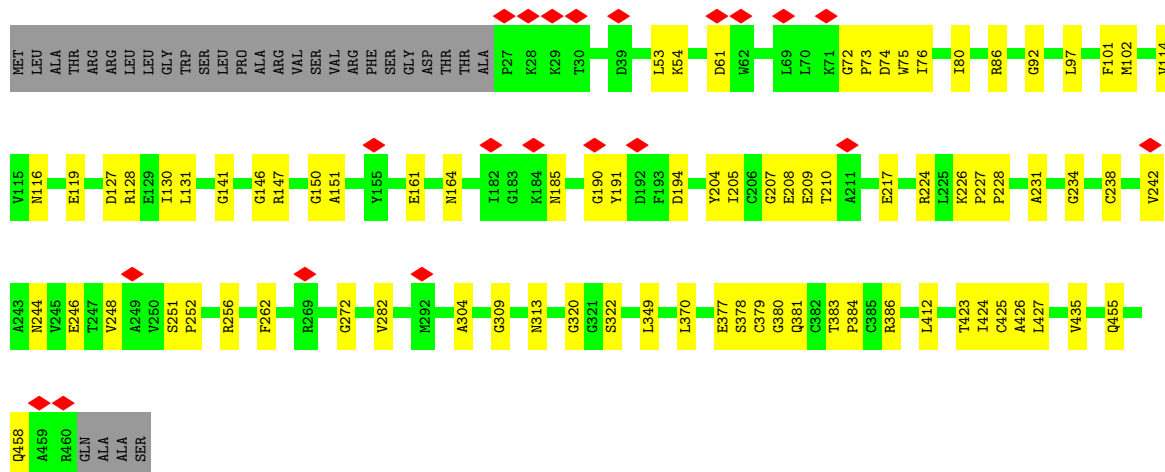
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w:  83% 7% 10%




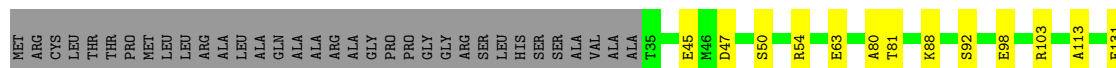
- Molecule 30: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

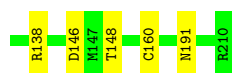
Chain C:  5% 76% 17% 6%



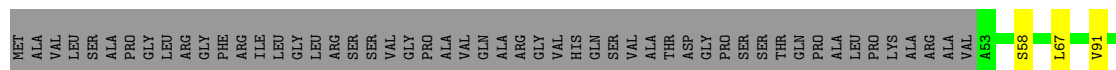
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain D:  75% 9% 16%

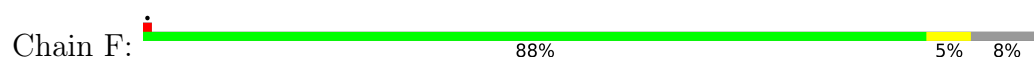




- Molecule 32: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



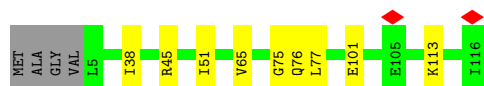
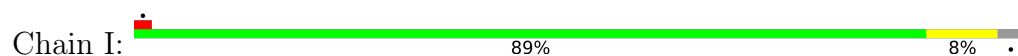
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



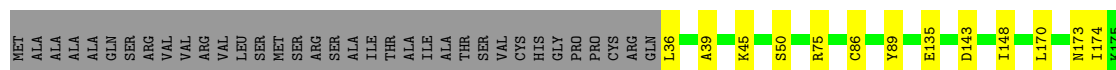
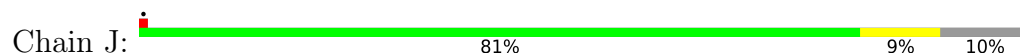
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

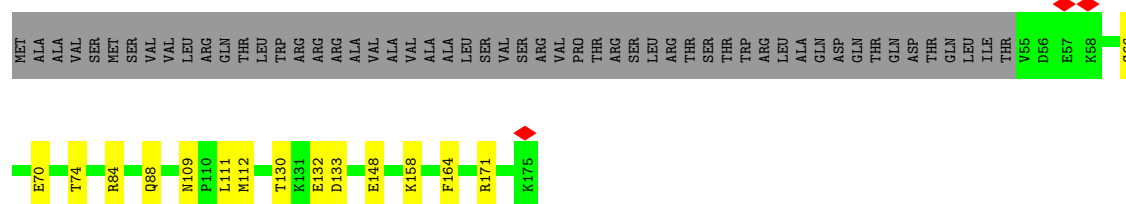


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

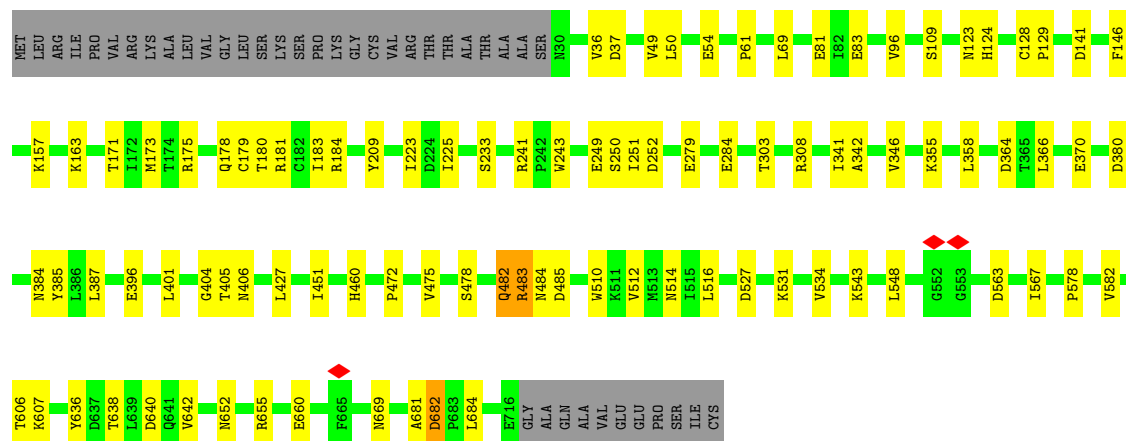


- Molecule 37: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

- Molecule 38: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



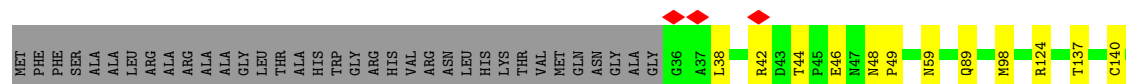
- Molecule 39: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

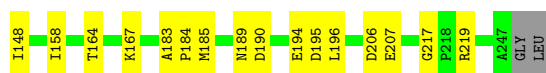


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



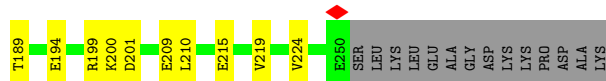
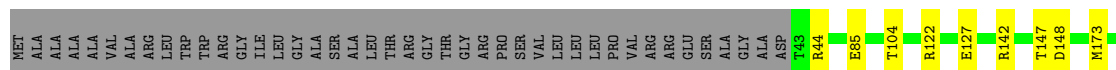
- Molecule 41: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial





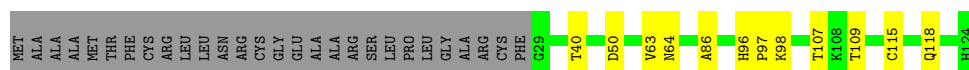
- Molecule 42: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain P: 72% 7% 21%



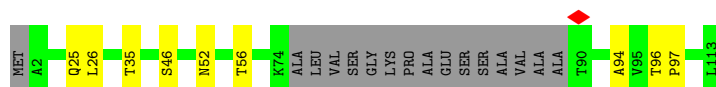
- Molecule 43: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T: 68% 10% 23%



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain t: 78% 8% 14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	168805	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.381	Depositor
Minimum map value	-1.294	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.109	Depositor
Recommended contour level	0.477	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.875, 0.875, 0.875	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, NDP, NMM, CDL, ZN, PEE, PLX, MG, DGT, 8Q1, SEP, FES, FMN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Q	0.22	0/3540	0.27	0/4798
2	S	0.18	0/583	0.25	0/785
3	U	0.18	0/670	0.34	0/920
4	V	0.17	0/1065	0.23	0/1450
5	W	0.18	0/1182	0.29	0/1600
6	H	0.13	0/700	0.27	0/945
6	X	0.15	0/708	0.23	0/956
7	Y	0.14	0/570	0.31	0/778
8	Z	0.15	0/702	0.33	0/945
9	a	0.16	0/1209	0.22	0/1639
10	b	0.15	0/1054	0.29	0/1423
11	c	0.16	0/1326	0.26	0/1809
12	d	0.15	0/1463	0.24	0/1968
13	e	0.21	0/915	0.37	0/1245
14	f	0.17	0/432	0.29	0/585
15	g	0.17	0/1046	0.23	0/1412
16	h	0.18	0/892	0.30	0/1193
17	i	0.20	0/2806	0.30	0/3840
18	j	0.21	0/952	0.30	0/1301
19	k	0.26	0/754	0.39	0/1024
20	l	0.16	0/4826	0.26	0/6594
21	m	0.20	0/1334	0.31	0/1816
22	n	0.14	0/468	0.26	0/630
23	o	0.16	0/1093	0.25	0/1479
24	p	0.16	0/1553	0.24	0/2104
25	r	0.18	0/3717	0.25	0/5082
26	s	0.22	0/2568	0.33	0/3523
27	u	0.15	0/1445	0.27	0/1953
28	v	0.13	0/1060	0.27	0/1417
29	w	0.19	0/2689	0.27	0/3637
30	C	0.15	0/3422	0.28	0/4620
31	D	0.22	0/1452	0.29	0/1964

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	E	0.25	0/1309	0.33	0/1771
33	F	0.19	0/1024	0.25	0/1378
34	G	0.14	0/695	0.26	0/938
35	I	0.19	0/941	0.26	0/1275
36	J	0.19	0/2820	0.26	0/3819
37	K	0.11	0/312	0.27	0/423
38	L	0.19	0/1002	0.25	0/1352
39	M	0.18	0/5363	0.29	0/7267
40	N	0.19	0/1244	0.29	0/1691
41	O	0.14	0/1682	0.28	0/2289
42	P	0.23	0/1780	0.29	0/2424
43	T	0.19	0/766	0.24	0/1032
44	t	0.20	0/799	0.29	0/1081
All	All	0.18	0/67933	0.28	0/92175

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	U	0	1
5	W	0	1
13	e	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	U	69	HIS	Peptide
5	W	27	ARG	Sidechain
13	e	120	ARG	Sidechain

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	Q	3461	3433	3418	36	0
2	S	568	570	567	9	0
3	U	647	655	653	13	0
4	V	1038	1031	1027	5	0
5	W	1151	1153	1151	18	0
6	H	688	681	680	10	0
6	X	696	690	688	5	0
7	Y	544	491	487	1	0
8	Z	679	660	657	8	0
9	a	1174	1182	1177	7	0
10	b	1021	1049	1043	14	0
11	c	1273	1180	1174	13	0
12	d	1433	1404	1402	18	0
13	e	887	850	848	15	0
14	f	419	425	423	11	0
15	g	1012	1023	1021	12	0
16	h	871	876	872	11	0
17	i	2733	2893	2892	20	0
18	j	926	964	978	4	0
19	k	743	787	794	17	0
20	l	4703	4880	4878	55	0
21	m	1302	1317	1326	15	0
22	n	457	466	463	7	0
23	o	1066	1088	1086	8	0
24	p	1499	1448	1442	9	0
25	r	3623	3821	3817	35	0
26	s	2498	2593	2602	33	0
27	u	1405	1386	1378	15	0
28	v	1037	1032	1026	10	0
29	w	2623	2598	2587	25	0
30	C	3347	3321	3310	57	0
31	D	1420	1367	1364	14	0
32	E	1287	1290	1286	16	0
33	F	999	1017	1011	4	0
34	G	683	697	695	10	0
35	I	922	953	950	7	0
36	J	2745	2802	2787	23	0
37	K	304	282	269	6	0
38	L	979	975	968	12	0
39	M	5275	5321	5311	69	0
40	N	1203	1172	1167	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	O	1643	1648	1644	22	0
42	P	1730	1691	1685	14	0
43	T	752	732	727	8	0
44	t	780	802	798	7	0
45	E	51	77	80	3	0
45	J	51	77	80	0	0
45	V	51	77	80	2	0
45	W	51	77	80	0	0
45	i	100	149	151	2	0
45	l	51	77	80	2	0
46	V	200	312	312	0	0
46	i	64	80	72	0	0
46	l	164	236	228	2	0
46	u	64	80	72	0	0
47	F	35	43	0	1	0
47	X	35	43	0	0	0
48	N	52	88	88	0	0
48	g	104	176	176	1	0
48	j	52	88	88	0	0
48	o	52	88	88	0	0
48	r	52	88	88	0	0
48	s	52	88	88	1	0
49	w	31	12	12	1	0
50	w	1	0	0	0	0
51	C	8	0	0	3	0
51	D	16	0	0	0	0
51	E	8	0	0	1	0
51	M	16	0	0	2	0
52	C	31	19	14	32	0
53	J	48	26	24	1	0
54	M	4	0	0	0	0
54	O	4	0	0	1	0
55	T	1	0	0	0	0
56	X	1	0	0	0	0
All	All	67696	68697	68430	672	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 5.

All (672) 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)
52:C:502:FMN:C4A	52:C:502:FMN:N5	1.70	1.54
52:C:502:FMN:C10	52:C:502:FMN:N1	1.71	1.50
52:C:502:FMN:C7	52:C:502:FMN:C7M	2.00	1.38
52:C:502:FMN:O5'	52:C:502:FMN:C5'	1.77	1.32
52:C:502:FMN:O2'	52:C:502:FMN:C3'	1.85	1.25
52:C:502:FMN:C4A	52:C:502:FMN:C10	2.22	1.17
52:C:502:FMN:C2'	52:C:502:FMN:C1'	2.23	1.17
52:C:502:FMN:C9A	52:C:502:FMN:C9	2.25	1.14
52:C:502:FMN:N5	52:C:502:FMN:C5A	2.10	1.13
52:C:502:FMN:O2'	52:C:502:FMN:C2'	0.78	1.08
52:C:502:FMN:O2'	52:C:502:FMN:H2'	1.43	1.07
26:s:196:THR:HG23	26:s:197:PRO:CD	1.89	1.03
39:M:124:HIS:CE1	51:M:801:SF4:S2	2.57	0.97
26:s:196:THR:HG23	26:s:197:PRO:HD3	1.49	0.93
20:l:529:TYR:O	20:l:533:THR:HG22	1.69	0.91
20:l:119:LYS:NZ	46:l:702:CDL:OB4	2.09	0.85
52:C:502:FMN:C8	52:C:502:FMN:C8M	2.56	0.83
25:r:87:GLU:OE2	25:r:91:ARG:NH1	2.15	0.79
29:w:70:LYS:N	49:w:401:DGT:O3G	2.15	0.79
39:M:638:THR:OG1	39:M:640:ASP:OD1	2.00	0.79
28:v:18:ASP:OD2	28:v:21:GLN:NE2	2.15	0.79
32:E:143:GLU:OE1	36:J:89:TYR:OH	1.99	0.79
29:w:269:VAL:HG12	29:w:270:VAL:HG23	1.65	0.78
19:k:58:ILE:HA	19:k:61:ILE:HD12	1.66	0.78
52:C:502:FMN:HM83	52:C:502:FMN:HM73	1.66	0.77
36:J:212:ARG:NH2	53:J:401:NDP:O1N	2.16	0.77
37:K:86:ASP:OD1	37:K:87:LEU:N	2.17	0.77
1:Q:198:THR:OG1	26:s:275:THR:O	2.02	0.77
39:M:370:GLU:OE2	39:M:478:SER:OG	2.03	0.76
1:Q:274:ASP:N	1:Q:325:ASP:OD2	2.19	0.76
6:X:91:ASP:OD1	8:Z:47:ARG:NH1	2.18	0.75
52:C:502:FMN:C8M	52:C:502:FMN:HM73	2.16	0.75
39:M:81:GLU:OE1	39:M:109:SER:OG	2.04	0.75
17:i:72:MET:HE1	19:k:43:MET:HE1	1.69	0.75
26:s:196:THR:HG23	26:s:197:PRO:HD2	1.68	0.75
39:M:387:LEU:HD12	39:M:514:ASN:HB2	1.68	0.74
21:m:76:GLU:N	21:m:76:GLU:OE1	2.20	0.74
52:C:502:FMN:C4A	52:C:502:FMN:N1	2.46	0.74
52:C:502:FMN:C7M	52:C:502:FMN:HM83	2.16	0.74
19:k:55:LEU:O	19:k:58:ILE:HG22	1.87	0.74
32:E:115:ARG:NH2	32:E:140:GLN:OE1	2.22	0.73
1:Q:206:GLU:OE2	44:t:25:GLN:NE2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:143:ASP:OD2	13:e:145:SER:OG	2.07	0.73
28:v:42:THR:OG1	28:v:45:GLU:OE1	2.05	0.73
5:W:28:ARG:HG3	5:W:29:GLY:H	1.52	0.72
20:l:534:HIS:O	20:l:538:PRO:HD2	1.89	0.71
26:s:304:TYR:O	26:s:308:PRO:HD2	1.90	0.71
43:T:86:ALA:HB1	43:T:98:LYS:HE2	1.73	0.70
19:k:56:ALA:O	19:k:60:PRO:HD2	1.92	0.70
25:r:103:GLN:O	25:r:107:ILE:HD12	1.92	0.70
39:M:475:VAL:HG11	39:M:516:LEU:HD23	1.74	0.70
30:C:427:LEU:HD12	52:C:502:FMN:O2	1.92	0.70
37:K:90:GLU:N	37:K:90:GLU:OE1	2.25	0.70
26:s:25:ARG:NH2	32:E:104:ASP:OD1	2.25	0.69
52:C:502:FMN:C7M	52:C:502:FMN:C8M	2.70	0.69
3:U:66:VAL:HG11	27:u:130:LYS:CD	2.21	0.69
30:C:151:ALA:O	30:C:191:TYR:OH	2.06	0.69
38:L:88:GLN:NE2	39:M:141:ASP:OD2	2.26	0.69
23:o:56:ARG:NH2	25:r:422:HIS:O	2.27	0.68
29:w:269:VAL:O	29:w:271:GLU:N	2.26	0.68
11:c:70:MET:SD	23:o:86:ASN:ND2	2.65	0.68
12:d:74:GLU:OE1	12:d:74:GLU:N	2.26	0.67
39:M:180:THR:OG1	39:M:184:ARG:NH1	2.27	0.67
39:M:483:ARG:NH2	39:M:682:ASP:O	2.27	0.67
26:s:196:THR:HG21	26:s:274:ARG:HA	1.75	0.67
36:J:173:ASN:OD1	36:J:174:ILE:N	2.26	0.67
13:e:50:GLU:OE1	13:e:50:GLU:N	2.28	0.67
20:l:281:GLY:O	20:l:284:THR:OG1	2.11	0.67
41:O:140:CYS:HA	41:O:183:ALA:HB1	1.77	0.67
30:C:458:GLN:N	30:C:458:GLN:OE1	2.28	0.66
36:J:211:ASP:OD1	36:J:212:ARG:N	2.29	0.66
21:m:112:VAL:HG23	21:m:113:VAL:H	1.60	0.65
34:G:30:SER:OG	34:G:34:ARG:NH1	2.29	0.65
39:M:482:GLN:O	39:M:484:ASN:N	2.29	0.65
16:h:32:ARG:NH1	19:k:50:ASN:OD1	2.28	0.65
9:a:173:THR:HG22	9:a:174:ILE:H	1.62	0.65
36:J:283:VAL:HG22	36:J:369:VAL:HG11	1.78	0.65
42:P:85:GLU:OE2	42:P:142:ARG:NE	2.29	0.65
5:W:23:ARG:HD3	5:W:25:LEU:HD13	1.77	0.64
20:l:561:LEU:O	20:l:565:THR:OG1	2.14	0.64
20:l:393:ASP:OD1	20:l:394:HIS:N	2.30	0.64
41:O:59:ASN:ND2	41:O:89:GLN:OE1	2.31	0.64
41:O:38:LEU:O	41:O:124:ARG:NH2	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:M:475:VAL:CG1	39:M:516:LEU:HD23	2.29	0.63
41:O:137:THR:OG1	54:O:301:FES:S2	2.56	0.63
2:S:34:LYS:NZ	2:S:61:TYR:O	2.28	0.63
1:Q:223:HIS:CE1	51:E:302:SF4:S4	2.92	0.63
1:Q:376:GLU:N	1:Q:376:GLU:OE1	2.32	0.62
2:S:4:GLU:OE1	2:S:4:GLU:N	2.32	0.62
11:c:110:ASP:OD2	25:r:278:ARG:NE	2.32	0.62
25:r:237:LYS:HG3	25:r:316:MET:HE2	1.81	0.62
36:J:135:GLU:OE2	36:J:179:ARG:NH1	2.32	0.62
5:W:63:GLU:OE2	27:u:119:ARG:NH2	2.32	0.62
6:X:114:ASP:OD1	24:p:45:ARG:NH1	2.31	0.62
16:h:59:GLU:OE1	27:u:145:ARG:NH2	2.32	0.62
25:r:331:ASN:ND2	25:r:335:GLU:OE2	2.32	0.62
41:O:194:GLU:N	41:O:217:GLY:O	2.31	0.61
20:l:102:GLU:OE1	20:l:456:ARG:NH2	2.33	0.61
17:i:268:GLU:OE1	27:u:168:TYR:OH	2.17	0.61
21:m:138:ASP:OD1	21:m:139:PRO:HD3	2.00	0.61
30:C:119:GLU:OE1	30:C:128:ARG:N	2.34	0.61
30:C:97:LEU:O	30:C:101:PHE:N	2.34	0.61
3:U:66:VAL:HG11	27:u:130:LYS:HD3	1.82	0.60
36:J:75:ARG:NH1	42:P:215:GLU:OE2	2.34	0.60
30:C:381:GLN:NE2	51:C:501:SF4:S4	2.74	0.60
3:U:66:VAL:HG11	27:u:130:LYS:HD2	1.84	0.60
30:C:217:GLU:OE2	38:L:171:ARG:NH1	2.35	0.60
30:C:116:ASN:ND2	30:C:207:GLY:O	2.34	0.60
38:L:130:THR:OG1	38:L:133:ASP:OD2	2.20	0.60
20:l:245:ALA:O	20:l:249:SER:OG	2.12	0.60
29:w:254:GLU:OE1	29:w:254:GLU:N	2.35	0.60
25:r:210:TYR:O	25:r:213:HIS:ND1	2.35	0.60
30:C:185:ASN:OD1	30:C:190:GLY:N	2.33	0.60
17:i:256:PRO:HG3	25:r:127:ILE:HD13	1.84	0.59
20:l:60:GLU:N	20:l:60:GLU:OE1	2.36	0.59
24:p:176:GLU:N	24:p:176:GLU:OE1	2.36	0.59
31:D:47:ASP:OD1	31:D:50:SER:OG	2.15	0.59
20:l:533:THR:HG23	20:l:534:HIS:N	2.17	0.59
11:c:68:ASP:OD1	11:c:69:GLY:N	2.35	0.59
26:s:304:TYR:O	26:s:308:PRO:CD	2.51	0.59
20:l:293:LEU:O	20:l:425:ARG:NE	2.36	0.59
20:l:546:GLN:OE1	23:o:72:ARG:NH2	2.36	0.59
5:W:27:ARG:O	5:W:28:ARG:C	2.45	0.59
26:s:24:GLU:OE2	26:s:274:ARG:NH1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:86:TYR:CG	7:Y:87:PRO:HD2	2.38	0.58
30:C:427:LEU:N	52:C:502:FMN:O2	2.36	0.58
11:c:46:GLU:OE1	11:c:46:GLU:N	2.36	0.58
20:l:161:ARG:NH2	24:p:88:GLY:O	2.36	0.58
15:g:103:GLU:OE1	15:g:103:GLU:N	2.36	0.58
19:k:59:VAL:HB	19:k:60:PRO:HD3	1.86	0.58
26:s:306:SER:O	26:s:310:THR:HG23	2.03	0.58
32:E:209:ILE:HD13	36:J:86:CYS:O	2.03	0.58
8:Z:51:TRP:O	8:Z:53:TYR:N	2.36	0.58
5:W:88:ARG:NH2	27:u:7:LEU:O	2.36	0.58
20:l:508:THR:O	24:p:36:LYS:NZ	2.29	0.58
42:P:210:LEU:HD12	42:P:219:VAL:HG12	1.86	0.58
1:Q:215:GLU:OE2	31:D:92:SER:OG	2.17	0.58
25:r:112:ALA:O	25:r:117:MET:HE3	2.03	0.57
30:C:119:GLU:OE2	30:C:127:ASP:N	2.35	0.57
8:Z:55:GLY:O	8:Z:57:PHE:N	2.37	0.57
12:d:4:SER:HG	12:d:5:TRP:CD1	2.22	0.57
39:M:83:GLU:OE1	39:M:83:GLU:N	2.36	0.57
30:C:226:LYS:N	30:C:227:PRO:HD2	2.19	0.57
32:E:103:MET:HE1	32:E:110:PHE:CD2	2.39	0.57
5:W:36:LEU:O	5:W:40:ILE:HD12	2.04	0.57
38:L:158:LYS:NZ	39:M:69:LEU:O	2.23	0.57
1:Q:40:ASP:HA	13:e:55:TRP:HH2	1.70	0.57
17:i:235:ASN:O	17:i:315:TRP:NE1	2.37	0.57
34:G:70:ALA:O	34:G:73:GLN:NE2	2.37	0.57
39:M:358:LEU:HD12	39:M:366:LEU:HD21	1.87	0.57
52:C:502:FMN:C5'	52:C:502:FMN:P	2.93	0.56
39:M:163:LYS:O	39:M:171:THR:OG1	2.22	0.56
41:O:46:GLU:OE1	41:O:46:GLU:N	2.38	0.56
10:b:78:PRO:O	10:b:82:ILE:HD12	2.05	0.56
16:h:80:ARG:NH1	21:m:121:VAL:HG21	2.20	0.56
26:s:165:LEU:HD21	26:s:241:ILE:HA	1.86	0.56
41:O:194:GLU:O	41:O:219:ARG:N	2.38	0.56
25:r:203:PHE:HE2	25:r:246:LEU:HD12	1.70	0.56
33:F:34:GLU:OE1	33:F:34:GLU:N	2.39	0.55
39:M:123:ASN:HA	39:M:157:LYS:HE2	1.88	0.55
6:H:125:GLU:OE1	6:H:125:GLU:N	2.33	0.55
39:M:346:VAL:HG22	39:M:548:LEU:HD13	1.89	0.55
17:i:200:MET:HE2	17:i:265:ALA:HB1	1.89	0.55
31:D:45:GLU:O	31:D:54:ARG:NH2	2.39	0.55
11:c:160:GLN:OE1	11:c:182:VAL:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:T:96:HIS:CD2	43:T:115:CYS:SG	3.00	0.55
11:c:137:LEU:O	11:c:141:ILE:HD12	2.07	0.55
26:s:207:LEU:O	26:s:209:SER:N	2.39	0.55
25:r:39:LEU:O	25:r:43:ASN:ND2	2.40	0.54
30:C:147:ARG:O	30:C:147:ARG:NE	2.40	0.54
20:l:274:GLN:OE1	20:l:274:GLN:N	2.39	0.54
41:O:42:ARG:NH2	43:T:107:THR:OG1	2.40	0.54
1:Q:404:LYS:NZ	1:Q:455:ASP:OD1	2.40	0.54
1:Q:94:VAL:HG21	1:Q:116:LEU:HB2	1.90	0.54
52:C:502:FMN:N5	52:C:502:FMN:C4	2.56	0.54
30:C:146:GLY:O	30:C:150:GLY:N	2.41	0.54
15:g:6:ASN:ND2	48:g:201:PLX:O3	2.40	0.53
39:M:209:TYR:HE2	41:O:98:MET:HE1	1.73	0.53
52:C:502:FMN:O2'	52:C:502:FMN:C1'	2.55	0.53
32:E:67:LEU:HD22	45:E:301:PEE:H66	1.89	0.53
18:j:54:LYS:HA	18:j:114:THR:HG22	1.90	0.53
20:l:401:MET:HE2	20:l:482:ILE:HG22	1.89	0.53
36:J:369:VAL:HG12	36:J:369:VAL:O	2.08	0.53
15:g:87:ARG:NH1	27:u:156:GLY:O	2.42	0.53
30:C:244:ASN:ND2	52:C:502:FMN:O3P	2.28	0.53
29:w:344:ASN:O	29:w:347:VAL:HG22	2.09	0.53
34:G:41:TYR:OH	39:M:380:ASP:OD2	2.26	0.53
39:M:534:VAL:HG13	39:M:534:VAL:O	2.08	0.53
1:Q:326:CYS:SG	1:Q:453:THR:HG21	2.49	0.53
2:S:57:VAL:HG12	2:S:57:VAL:O	2.07	0.53
3:U:68:SER:HA	27:u:129:THR:HG23	1.90	0.53
1:Q:315:GLU:N	1:Q:315:GLU:OE1	2.43	0.52
11:c:83:GLN:NE2	11:c:97:LEU:O	2.41	0.52
36:J:211:ASP:OD1	36:J:213:PHE:N	2.41	0.52
1:Q:266:ARG:NE	31:D:63:GLU:OE2	2.42	0.52
22:n:48:GLU:N	22:n:48:GLU:OE1	2.43	0.52
39:M:472:PRO:O	39:M:510:TRP:NE1	2.40	0.52
26:s:179:TRP:N	26:s:180:PRO:HD2	2.23	0.52
39:M:364:ASP:O	39:M:531:LYS:NZ	2.20	0.52
39:M:385:TYR:OH	39:M:527:ASP:OD1	2.25	0.52
36:J:36:LEU:HD22	43:T:50:ASP:HA	1.90	0.52
41:O:158:ILE:HD11	41:O:164:THR:HB	1.91	0.52
43:T:109:THR:OG1	43:T:118:GLN:OE1	2.25	0.52
21:m:2:MET:SD	21:m:121:VAL:HG23	2.50	0.52
39:M:681:ALA:O	39:M:682:ASP:CB	2.58	0.52
35:I:38:ILE:O	35:I:45:ARG:NH1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:79:GLU:OE1	3:U:79:GLU:N	2.38	0.52
20:l:316:THR:HG23	20:l:325:ALA:HB2	1.91	0.52
30:C:164:ASN:ND2	41:O:190:ASP:O	2.43	0.52
52:C:502:FMN:O2'	52:C:502:FMN:C4'	2.51	0.52
4:V:42:THR:HG21	20:l:593:PHE:HZ	1.74	0.52
31:D:103:ARG:NH2	43:T:64:ASN:OD1	2.43	0.52
21:m:105:TRP:CH2	21:m:114:VAL:HG22	2.45	0.52
1:Q:208:GLU:HG2	32:E:100:ARG:HE	1.75	0.51
5:W:31:SER:HB3	5:W:34:SER:HB2	1.92	0.51
6:X:136:GLU:OE1	10:b:2:THR:N	2.43	0.51
31:D:98:GLU:OE2	31:D:191:ASN:ND2	2.43	0.51
1:Q:162:ARG:NH2	42:P:44:ARG:O	2.43	0.51
25:r:127:ILE:HD12	25:r:127:ILE:H	1.75	0.51
6:H:140:CYS:N	6:H:143:GLU:OE1	2.41	0.51
29:w:351:TRP:CE2	29:w:354:LEU:HB2	2.44	0.51
30:C:226:LYS:O	30:C:227:PRO:C	2.53	0.51
15:g:54:THR:O	15:g:54:THR:HG23	2.10	0.51
28:v:41:ALA:O	28:v:42:THR:OG1	2.26	0.51
19:k:48:THR:HG22	19:k:56:ALA:HB1	1.92	0.51
25:r:14:LEU:O	25:r:18:SER:OG	2.27	0.51
30:C:246:GLU:OE1	30:C:246:GLU:N	2.32	0.51
30:C:378:SER:O	30:C:379:CYS:HB3	2.11	0.51
29:w:273:ILE:O	29:w:273:ILE:HG22	2.11	0.51
30:C:320:GLY:HA3	30:C:349:LEU:O	2.11	0.51
40:N:41:GLU:O	40:N:42:ASP:OD1	2.29	0.51
1:Q:149:GLN:NE2	1:Q:309:ASP:OD2	2.43	0.51
4:V:94:GLY:O	4:V:98:GLY:N	2.44	0.51
12:d:143:TYR:OH	25:r:244:MET:O	2.25	0.51
20:l:387:THR:OG1	20:l:461:SER:O	2.27	0.51
52:C:502:FMN:C9	52:C:502:FMN:C5A	2.86	0.51
14:f:50:THR:O	14:f:54:LEU:HD23	2.10	0.51
27:u:26:LYS:NZ	27:u:95:GLN:O	2.37	0.51
10:b:27:GLU:N	10:b:27:GLU:OE1	2.43	0.51
17:i:208:TYR:CE1	17:i:212:THR:HG21	2.46	0.50
25:r:33:ILE:O	25:r:36:ILE:HG22	2.11	0.50
21:m:112:VAL:HG23	21:m:113:VAL:N	2.24	0.50
29:w:77:ILE:HD11	29:w:270:VAL:HG21	1.93	0.50
1:Q:196:ALA:O	1:Q:197:MET:HG2	2.11	0.50
13:e:55:TRP:HE1	17:i:306:PRO:HB3	1.77	0.50
20:l:529:TYR:CE1	20:l:533:THR:HG21	2.46	0.50
39:M:179:CYS:O	51:M:802:SF4:S3	2.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:P:199:ARG:O	42:P:200:LYS:HB2	2.11	0.50
32:E:167:VAL:HG12	32:E:167:VAL:O	2.11	0.50
34:G:58:CYS:SG	39:M:655:ARG:NH1	2.85	0.50
35:I:113:LYS:O	42:P:122:ARG:NH2	2.42	0.50
36:J:298:TYR:CD2	36:J:319:VAL:HG13	2.47	0.50
11:c:168:LEU:HD23	11:c:168:LEU:H	1.76	0.50
30:C:208:GLU:OE1	30:C:210:THR:N	2.44	0.50
12:d:87:LYS:NZ	25:r:48:ASN:OD1	2.44	0.49
1:Q:222:MET:HE1	32:E:91:VAL:HG23	1.94	0.49
8:Z:30:GLU:OE1	8:Z:30:GLU:N	2.45	0.49
45:V:201:PEE:H3	17:i:276:LEU:HD13	1.93	0.49
12:d:22:ASN:O	12:d:25:VAL:HG22	2.12	0.49
13:e:52:THR:O	13:e:52:THR:HG22	2.12	0.49
20:l:246:LEU:O	20:l:251:THR:OG1	2.26	0.49
28:v:24:THR:OG1	28:v:105:GLU:OE2	2.26	0.49
38:L:84:ARG:NH2	39:M:284:GLU:OE2	2.41	0.49
20:l:481:THR:O	20:l:481:THR:HG23	2.12	0.49
25:r:138:ASN:OD1	25:r:139:GLN:N	2.41	0.49
28:v:12:ASP:OD1	28:v:13:ALA:N	2.45	0.49
13:e:138:GLU:OE1	13:e:140:ASN:N	2.42	0.49
26:s:9:LEU:HD22	26:s:95:LEU:HD22	1.95	0.49
6:H:140:CYS:HB2	6:H:142:GLN:OE1	2.13	0.49
1:Q:118:NMM:O	1:Q:120:THR:N	2.42	0.49
18:j:16:LEU:O	18:j:20:ILE:HD12	2.12	0.49
31:D:113:ALA:O	31:D:138:ARG:NH2	2.40	0.49
10:b:122:GLU:O	28:v:65:ARG:NH2	2.45	0.49
29:w:145:ASP:OD1	29:w:301:LYS:NZ	2.35	0.49
29:w:269:VAL:HG12	29:w:270:VAL:N	2.27	0.49
23:o:54:PRO:O	23:o:57:ARG:NH1	2.46	0.48
3:U:69:HIS:HB3	3:U:72:ASP:HB2	1.95	0.48
17:i:222:ASN:ND2	17:i:233:THR:HG22	2.29	0.48
20:l:7:MET:HB3	20:l:50:PRO:HG3	1.95	0.48
24:p:135:ARG:NH1	24:p:162:ASP:OD1	2.45	0.48
26:s:29:GLY:HA2	26:s:34:ARG:HE	1.77	0.48
28:v:8:ARG:O	28:v:13:ALA:HB2	2.14	0.48
41:O:190:ASP:C	41:O:190:ASP:OD1	2.56	0.48
20:l:54:PHE:O	20:l:58:ASP:N	2.32	0.48
20:l:414:ILE:O	20:l:417:SER:OG	2.31	0.48
24:p:26:HIS:ND1	24:p:75:GLN:O	2.47	0.48
30:C:379:CYS:SG	30:C:380:GLY:N	2.87	0.48
16:h:97:HIS:O	16:h:98:HIS:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:E:67:LEU:HD22	45:E:301:PEE:C40	2.43	0.48
33:F:24:ASP:N	33:F:27:GLU:OE2	2.37	0.48
39:M:81:GLU:OE1	39:M:81:GLU:N	2.38	0.48
20:l:537:ILE:HB	20:l:538:PRO:HD3	1.96	0.48
29:w:123:SER:OG	29:w:125:ASP:OD1	2.31	0.48
39:M:396:GLU:N	39:M:396:GLU:OE1	2.46	0.48
24:p:160:GLU:N	24:p:160:GLU:OE1	2.45	0.48
31:D:81:THR:HG22	32:E:99:PRO:O	2.14	0.48
37:K:87:LEU:O	37:K:87:LEU:HD23	2.12	0.48
20:l:466:PHE:O	20:l:470:ASN:ND2	2.46	0.48
9:a:168:TRP:NE1	15:g:88:GLU:OE1	2.45	0.48
16:h:65:GLU:O	16:h:69:ARG:N	2.38	0.48
19:k:56:ALA:O	19:k:60:PRO:CD	2.60	0.48
25:r:225:ILE:HD13	25:r:331:ASN:HB2	1.95	0.48
11:c:156:VAL:HG23	11:c:157:GLY:N	2.29	0.48
38:L:132:GLU:OE1	38:L:132:GLU:N	2.41	0.48
12:d:57:TYR:HE2	13:e:120:ARG:NH1	2.12	0.47
26:s:196:THR:CG2	26:s:197:PRO:CD	2.78	0.47
25:r:39:LEU:HA	25:r:67:MET:HE2	1.96	0.47
39:M:250:SER:OG	39:M:251:ILE:N	2.45	0.47
39:M:387:LEU:HA	39:M:514:ASN:HB2	1.95	0.47
2:S:37:ARG:HB3	2:S:48:MET:HE2	1.96	0.47
26:s:138:GLN:HE21	26:s:200:LEU:HD12	1.78	0.47
30:C:61:ASP:O	30:C:256:ARG:NH1	2.47	0.47
39:M:37:ASP:OD1	39:M:37:ASP:C	2.57	0.47
20:l:533:THR:CG2	20:l:534:HIS:N	2.77	0.47
39:M:178:GLN:OE1	39:M:178:GLN:N	2.48	0.47
20:l:132:VAL:O	20:l:262:ARG:NH2	2.43	0.47
20:l:359:MET:O	20:l:436:ARG:NH2	2.48	0.47
30:C:425:CYS:SG	30:C:427:LEU:HD13	2.54	0.47
52:C:502:FMN:C7	52:C:502:FMN:C8M	2.92	0.47
31:D:80:ALA:HB2	44:t:26:LEU:HD21	1.96	0.47
12:d:3:ASP:OD1	12:d:4:SER:N	2.47	0.47
15:g:55:ALA:O	15:g:60:GLN:NE2	2.46	0.47
45:i:402:PEE:H29	45:i:402:PEE:O5	2.15	0.47
35:I:51:ILE:HG21	42:P:104:THR:HG21	1.96	0.47
40:N:132:LYS:NZ	40:N:134:ILE:O	2.47	0.47
14:f:37:ALA:O	14:f:40:ASP:N	2.48	0.47
30:C:423:THR:HG22	30:C:424:ILE:N	2.30	0.47
31:D:63:GLU:N	31:D:63:GLU:OE1	2.44	0.47
35:I:51:ILE:HD11	44:t:94:ALA:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:94:VAL:O	1:Q:94:VAL:HG23	2.15	0.47
3:U:66:VAL:O	3:U:66:VAL:HG13	2.15	0.47
12:d:63:ARG:NH1	22:n:44:LEU:O	2.48	0.47
25:r:112:ALA:O	25:r:113:THR:OG1	2.25	0.47
30:C:205:ILE:HD11	30:C:377:GLU:O	2.14	0.47
32:E:190:LEU:O	32:E:194:ILE:HD12	2.14	0.47
45:E:301:PEE:O3P	45:E:301:PEE:O4	2.33	0.47
36:J:45:LYS:O	36:J:50:SER:OG	2.21	0.47
39:M:404:GLY:HA2	39:M:684:LEU:HD21	1.97	0.47
8:Z:51:TRP:C	8:Z:53:TYR:N	2.73	0.46
12:d:68:ILE:HG12	15:g:108:TYR:HD2	1.80	0.46
17:i:19:ILE:O	17:i:23:SER:OG	2.28	0.46
45:l:701:PEE:C44	45:l:701:PEE:H66	2.45	0.46
39:M:510:TRP:HD1	39:M:512:VAL:HG22	1.80	0.46
39:M:567:ILE:HG23	39:M:582:VAL:HG13	1.97	0.46
19:k:4:ILE:HD12	19:k:4:ILE:H	1.79	0.46
36:J:176:SER:O	36:J:177:SER:OG	2.28	0.46
42:P:127:GLU:OE1	42:P:127:GLU:N	2.48	0.46
2:S:18:ILE:HD12	2:S:18:ILE:H	1.81	0.46
13:e:116:GLU:OE1	13:e:116:GLU:N	2.48	0.46
21:m:126:ILE:O	21:m:127:TYR:HB2	2.15	0.46
41:O:48:ASN:N	41:O:49:PRO:CD	2.78	0.46
1:Q:259:GLU:OE2	1:Q:338:ARG:NH2	2.37	0.46
20:l:210:LEU:HD23	20:l:210:LEU:H	1.80	0.46
22:n:7:ILE:HD12	22:n:7:ILE:H	1.81	0.46
25:r:68:LEU:O	25:r:72:LEU:HD23	2.15	0.46
26:s:11:VAL:HB	26:s:12:PRO:HD3	1.98	0.46
26:s:127:TYR:O	26:s:128:ALA:HB3	2.15	0.46
12:d:73:GLU:OE2	15:g:106:LYS:O	2.34	0.46
20:l:447:ASN:OD1	20:l:449:THR:OG1	2.32	0.46
33:F:96:VAL:HG12	33:F:96:VAL:O	2.16	0.46
6:H:138:LEU:HD12	6:H:138:LEU:N	2.30	0.46
16:h:94:PRO:O	16:h:97:HIS:N	2.47	0.46
20:l:530:PRO:O	20:l:534:HIS:HB2	2.16	0.46
28:v:90:CYS:HA	28:v:93:ARG:HG2	1.98	0.46
20:l:230:HIS:N	20:l:231:PRO:CD	2.79	0.46
30:C:426:ALA:C	52:C:502:FMN:O2	2.59	0.46
13:e:85:TRP:O	13:e:89:LEU:HD23	2.16	0.46
19:k:59:VAL:HB	19:k:60:PRO:CD	2.46	0.46
30:C:119:GLU:H	52:C:502:FMN:C7M	2.29	0.46
24:p:54:GLU:N	24:p:54:GLU:OE1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:C:130:ILE:HG23	30:C:131:LEU:N	2.32	0.45
36:J:235:THR:HG23	36:J:273:LEU:HB2	1.97	0.45
19:k:95:LEU:O	19:k:96:LEU:HB2	2.15	0.45
10:b:105:PHE:O	10:b:107:GLY:N	2.49	0.45
22:n:15:VAL:O	22:n:19:MET:HG2	2.17	0.45
47:F:201:8Q1:N36	47:F:201:8Q1:O40	2.48	0.45
20:l:233:LEU:HB3	20:l:234:PRO:HD3	1.98	0.45
28:v:83:GLU:N	28:v:83:GLU:OE1	2.45	0.45
39:M:684:LEU:C	39:M:684:LEU:HD23	2.41	0.45
10:b:77:VAL:HB	10:b:78:PRO:HD3	1.98	0.45
39:M:50:LEU:O	39:M:54:GLU:HG2	2.16	0.45
14:f:38:LYS:HB3	14:f:39:PRO:CD	2.46	0.45
30:C:161:GLU:OE1	30:C:161:GLU:N	2.49	0.45
44:t:46:SER:O	44:t:52:ASN:ND2	2.39	0.45
26:s:307:MET:O	26:s:308:PRO:C	2.60	0.45
29:w:270:VAL:O	29:w:271:GLU:C	2.60	0.45
34:G:65:LEU:C	34:G:65:LEU:HD23	2.42	0.45
6:H:103:HIS:O	6:H:107:ASP:OD1	2.35	0.45
38:L:109:ASN:ND2	38:L:111:LEU:O	2.44	0.45
44:t:96:THR:HG23	44:t:97:PRO:HD2	1.97	0.45
3:U:43:VAL:HG12	3:U:47:LYS:NZ	2.32	0.45
12:d:127:THR:HG22	23:o:125:PHE:HZ	1.81	0.45
30:C:309:GLY:O	30:C:313:ASN:ND2	2.47	0.45
30:C:423:THR:CG2	51:C:501:SF4:S3	3.05	0.45
38:L:70:GLU:O	38:L:74:THR:OG1	2.29	0.45
39:M:543:LYS:HZ1	39:M:567:ILE:HD11	1.81	0.45
13:e:53:THR:N	13:e:54:PRO:HD2	2.32	0.45
36:J:36:LEU:HD21	36:J:39:ALA:HB3	1.99	0.45
39:M:482:GLN:C	39:M:484:ASN:H	2.25	0.45
3:U:33:PRO:HA	26:s:310:THR:HG22	1.99	0.44
29:w:64:GLY:O	29:w:241:TYR:OH	2.20	0.44
30:C:114:VAL:CG2	30:C:242:VAL:HG12	2.47	0.44
16:h:93:THR:HG22	16:h:95:PRO:HD2	1.99	0.44
20:l:286:LEU:HD22	20:l:411:ILE:HD12	1.99	0.44
25:r:108:MET:SD	25:r:121:PHE:CE1	3.10	0.44
29:w:271:GLU:N	29:w:271:GLU:OE1	2.42	0.44
39:M:223:ILE:HD13	39:M:233:SER:HB3	1.98	0.44
40:N:66:THR:O	40:N:66:THR:HG22	2.17	0.44
3:U:50:PRO:HB2	5:W:69:ILE:HD11	1.99	0.44
10:b:110:ILE:HD12	10:b:110:ILE:H	1.81	0.44
20:l:268:GLU:OE1	20:l:268:GLU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:F:22:SER:OG	33:F:31:ARG:NH1	2.49	0.44
6:X:111:ASP:OD1	6:X:112:SER:N	2.50	0.44
25:r:203:PHE:CE2	25:r:246:LEU:HD12	2.52	0.44
34:G:18:GLU:N	34:G:18:GLU:OE1	2.50	0.44
34:G:47:ALA:O	34:G:48:ASN:C	2.61	0.44
19:k:48:THR:HG22	19:k:56:ALA:CB	2.46	0.44
20:l:97:THR:HG21	20:l:125:LEU:HD12	1.99	0.44
29:w:170:LEU:HD22	29:w:187:TYR:CG	2.53	0.44
38:L:148:GLU:N	38:L:148:GLU:OE1	2.50	0.44
39:M:303:THR:O	39:M:303:THR:HG22	2.17	0.44
39:M:563:ASP:N	39:M:563:ASP:OD1	2.50	0.44
39:M:640:ASP:OD1	39:M:640:ASP:N	2.51	0.44
43:T:40:THR:HG22	43:T:63:VAL:HG12	1.99	0.44
20:l:238:GLU:OE1	20:l:238:GLU:N	2.48	0.44
41:O:148:ILE:O	41:O:148:ILE:HG22	2.18	0.44
42:P:199:ARG:C	42:P:201:ASP:H	2.26	0.44
43:T:96:HIS:ND1	43:T:97:PRO:O	2.51	0.44
20:l:407:TRP:CZ2	20:l:411:ILE:HD11	2.51	0.44
21:m:135:ILE:HG23	21:m:140:ILE:HG13	1.99	0.44
25:r:231:LEU:HD23	25:r:235:LEU:HD12	1.99	0.44
39:M:341:ILE:HG22	39:M:342:ALA:N	2.33	0.44
39:M:405:THR:HG22	39:M:406:ASN:N	2.33	0.44
1:Q:458:PHE:HA	1:Q:461:VAL:HG22	1.98	0.44
29:w:351:TRP:CD1	29:w:354:LEU:H	2.35	0.44
5:W:64:ASP:OD1	5:W:65:PHE:N	2.51	0.44
9:a:80:ILE:HB	9:a:81:PRO:HD3	2.00	0.44
30:C:76:ILE:O	30:C:80:ILE:HD12	2.18	0.44
39:M:171:THR:OG1	39:M:171:THR:O	2.36	0.44
17:i:115:VAL:HB	17:i:116:PRO:HD3	1.99	0.43
17:i:244:ILE:HB	17:i:245:PRO:HD3	1.99	0.43
30:C:74:ASP:OD1	30:C:75:TRP:N	2.47	0.43
39:M:308:ARG:NH2	39:M:578:PRO:O	2.51	0.43
4:V:116:VAL:HG23	4:V:117:TYR:N	2.34	0.43
45:V:201:PEE:H29	45:V:201:PEE:H35	1.80	0.43
13:e:53:THR:HG23	13:e:54:PRO:HD3	1.99	0.43
1:Q:355:GLU:OE1	1:Q:355:GLU:N	2.39	0.43
5:W:23:ARG:CD	5:W:25:LEU:HD13	2.46	0.43
10:b:44:GLU:OE1	10:b:44:GLU:N	2.45	0.43
12:d:81:GLU:OE1	22:n:43:MET:HB2	2.17	0.43
30:C:455:GLN:O	30:C:458:GLN:N	2.51	0.43
36:J:350:ILE:HD13	36:J:366:ILE:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:M:241:ARG:HG2	39:M:243:TRP:CH2	2.53	0.43
4:V:69:VAL:HG12	4:V:96:ALA:HB1	2.00	0.43
16:h:89:GLU:CD	16:h:89:GLU:O	2.61	0.43
20:l:383:MET:O	20:l:385:PHE:N	2.52	0.43
29:w:354:LEU:C	29:w:354:LEU:HD23	2.43	0.43
30:C:204:TYR:CD2	52:C:502:FMN:O4	2.70	0.43
39:M:451:ILE:HD12	39:M:460:HIS:CE1	2.53	0.43
1:Q:106:VAL:HG11	1:Q:447:VAL:HG21	2.00	0.43
5:W:58:ARG:O	5:W:62:ILE:HD12	2.19	0.43
12:d:122:GLU:OE1	12:d:122:GLU:N	2.52	0.43
17:i:211:LEU:HD23	17:i:333:THR:HG22	2.00	0.43
20:l:17:PRO:N	20:l:18:PRO:HD2	2.33	0.43
20:l:600:LEU:HG	20:l:601:LEU:HD22	2.00	0.43
25:r:14:LEU:HD21	25:r:26:ASN:HB3	1.99	0.43
25:r:285:LEU:HD22	25:r:410:MET:HE2	2.00	0.43
25:r:333:ASN:O	25:r:337:THR:HG22	2.17	0.43
6:H:90:TYR:OH	6:H:114:ASP:OD1	2.32	0.43
41:O:185:MET:HA	41:O:194:GLU:HA	1.98	0.43
1:Q:222:MET:HE1	32:E:91:VAL:CG2	2.49	0.43
10:b:34:VAL:O	10:b:35:LEU:C	2.62	0.43
10:b:99:GLU:OE1	10:b:99:GLU:N	2.50	0.43
12:d:73:GLU:OE2	15:g:111:ILE:HD11	2.19	0.43
30:C:227:PRO:HB2	30:C:228:PRO:HD3	2.00	0.43
31:D:131:GLU:N	31:D:131:GLU:OE1	2.52	0.43
32:E:167:VAL:O	32:E:167:VAL:CG1	2.66	0.43
42:P:44:ARG:NH1	44:t:56:THR:O	2.52	0.43
8:Z:22:TRP:CE3	8:Z:51:TRP:HA	2.54	0.43
12:d:135:ASP:OD1	12:d:156:ARG:NE	2.52	0.43
31:D:88:LYS:HD3	40:N:91:HIS:CE1	2.53	0.43
36:J:201:VAL:HG12	36:J:203:PRO:HD3	2.01	0.43
39:M:279:GLU:OE1	39:M:279:GLU:N	2.48	0.43
42:P:147:THR:HG22	42:P:148:ASP:O	2.19	0.43
17:i:255:PRO:O	17:i:337:LEU:HD22	2.19	0.43
23:o:17:THR:O	23:o:23:TYR:OH	2.32	0.43
27:u:18:VAL:O	27:u:18:VAL:HG23	2.19	0.43
39:M:36:VAL:O	39:M:37:ASP:OD1	2.37	0.43
39:M:180:THR:HB	39:M:183:ILE:HD11	2.01	0.43
41:O:148:ILE:HG23	41:O:196:LEU:HD11	1.99	0.43
41:O:164:THR:O	41:O:167:LYS:NZ	2.52	0.43
1:Q:302:LEU:HB2	1:Q:401:GLU:HG2	2.00	0.43
17:i:137:ALA:HB3	17:i:138:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:84:LEU:HD12	27:u:8:PRO:HD2	2.01	0.42
10:b:43:MET:HA	10:b:46:PHE:CE2	2.54	0.42
28:v:21:GLN:HG2	28:v:21:GLN:O	2.19	0.42
39:M:249:GLU:OE1	39:M:249:GLU:N	2.51	0.42
39:M:606:THR:HG22	39:M:607:LYS:N	2.33	0.42
1:Q:81:THR:HG21	18:j:44:MET:SD	2.59	0.42
1:Q:200:PHE:CE1	1:Q:204:PHE:CE2	3.07	0.42
9:a:134:GLU:OE1	22:n:57:TRP:NE1	2.48	0.42
20:l:32:TYR:N	20:l:33:PRO:HD2	2.34	0.42
21:m:122:GLY:O	21:m:123:SER:OG	2.32	0.42
26:s:300:LEU:O	26:s:304:TYR:HD2	2.02	0.42
30:C:322:SER:OG	30:C:370:LEU:HD22	2.20	0.42
35:I:75:GLY:O	35:I:76:GLN:HB2	2.19	0.42
40:N:117:VAL:HG23	40:N:117:VAL:O	2.18	0.42
1:Q:235:ASP:OD1	1:Q:236:LEU:N	2.50	0.42
3:U:69:HIS:HB3	3:U:72:ASP:CG	2.45	0.42
5:W:58:ARG:HE	26:s:316:PRO:HA	1.83	0.42
20:l:560:LYS:O	20:l:565:THR:HG23	2.20	0.42
30:C:209:GLU:OE1	30:C:209:GLU:N	2.48	0.42
39:M:251:ILE:HG22	39:M:252:ASP:N	2.33	0.42
1:Q:368:ARG:NH2	31:D:160:CYS:O	2.52	0.42
2:S:14:VAL:O	2:S:18:ILE:HD12	2.20	0.42
21:m:64:MET:HE2	26:s:136:VAL:HA	2.01	0.42
31:D:146:ASP:OD1	31:D:148:THR:OG1	2.38	0.42
6:H:115:GLN:O	6:H:119:ILE:HD12	2.20	0.42
37:K:101:SER:OG	37:K:102:GLY:N	2.51	0.42
5:W:29:GLY:O	5:W:30:LEU:HG	2.20	0.42
20:l:293:LEU:HD22	46:l:703:CDL:H122	2.01	0.42
36:J:210:GLU:OE1	36:J:210:GLU:N	2.52	0.42
39:M:173:MET:C	39:M:175:ARG:H	2.26	0.42
9:a:180:ASP:OD2	16:h:24:GLU:HA	2.20	0.42
10:b:32:GLU:O	10:b:34:VAL:HG23	2.20	0.42
10:b:52:GLU:O	10:b:52:GLU:CG	2.68	0.42
15:g:54:THR:O	29:w:354:LEU:HD12	2.19	0.42
20:l:270:SER:O	20:l:274:GLN:OE1	2.37	0.42
23:o:95:PHE:O	23:o:99:ILE:HD12	2.19	0.42
36:J:301:VAL:O	36:J:304:VAL:HG12	2.20	0.42
39:M:128:CYS:N	39:M:129:PRO:HD2	2.34	0.42
41:O:44:THR:HG23	41:O:44:THR:O	2.20	0.42
1:Q:325:ASP:OD1	1:Q:326:CYS:N	2.51	0.42
2:S:49:GLU:OE1	2:S:53:ARG:NE	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:68:SER:HB2	27:u:130:LYS:HG2	2.02	0.42
13:e:57:GLU:OE2	29:w:322:HIS:HB2	2.20	0.42
48:s:401:PLX:C3	48:s:401:PLX:O7	2.68	0.42
30:C:380:GLY:O	30:C:386:ARG:HD3	2.20	0.42
39:M:485:ASP:OD1	39:M:485:ASP:C	2.62	0.42
41:O:196:LEU:C	41:O:196:LEU:HD12	2.45	0.42
42:P:173:MET:HE1	42:P:189:THR:HG23	2.00	0.42
1:Q:121:GLU:OE1	1:Q:121:GLU:N	2.51	0.42
30:C:282:VAL:HG21	30:C:304:ALA:HB1	2.02	0.42
39:M:61:PRO:HG3	39:M:146:PHE:CE2	2.55	0.42
1:Q:314:VAL:HG11	1:Q:343:ILE:HG23	2.02	0.42
3:U:32:LEU:N	3:U:33:PRO:CD	2.82	0.42
14:f:38:LYS:HA	14:f:41:TRP:CD1	2.55	0.42
25:r:312:ALA:O	25:r:316:MET:HG3	2.19	0.42
29:w:270:VAL:O	29:w:273:ILE:N	2.51	0.42
34:G:86:GLN:OE1	34:G:86:GLN:N	2.53	0.42
2:S:57:VAL:O	2:S:57:VAL:CG1	2.67	0.42
17:i:255:PRO:N	17:i:256:PRO:HD2	2.35	0.42
17:i:300:THR:HG23	17:i:301:SER:N	2.35	0.42
29:w:146:ALA:HB1	29:w:157:VAL:HG11	2.01	0.42
29:w:258:TYR:CZ	29:w:269:VAL:HG13	2.54	0.42
41:O:184:PRO:O	41:O:195:ASP:N	2.53	0.42
41:O:206:ASP:OD1	41:O:207:GLU:N	2.52	0.42
5:W:43:LEU:O	5:W:47:HIS:ND1	2.53	0.41
19:k:41:PHE:CD1	19:k:64:LEU:HG	2.55	0.41
30:C:86:ARG:NE	30:C:92:GLY:O	2.44	0.41
34:G:65:LEU:HB2	34:G:79:LEU:HD11	2.02	0.41
6:H:78:GLY:O	6:H:82:ARG:HG2	2.20	0.41
35:I:101:GLU:OE1	35:I:101:GLU:N	2.47	0.41
36:J:143:ASP:O	36:J:148:ILE:HD12	2.19	0.41
4:V:128:GLY:O	4:V:132:GLY:N	2.52	0.41
14:f:33:GLU:HB2	14:f:34:PRO:HD3	2.02	0.41
25:r:285:LEU:C	25:r:285:LEU:HD23	2.46	0.41
30:C:102:MET:CG	30:C:231:ALA:HB1	2.50	0.41
38:L:66:GLY:HA3	42:P:194:GLU:HG3	2.01	0.41
39:M:401:LEU:C	39:M:401:LEU:HD23	2.45	0.41
9:a:147:ALA:HB1	25:r:172:GLY:HA3	2.01	0.41
14:f:40:ASP:HB3	14:f:44:VAL:HG23	2.03	0.41
14:f:75:LEU:HD12	14:f:75:LEU:C	2.46	0.41
21:m:26:ILE:HD13	26:s:121:TRP:CE2	2.54	0.41
23:o:95:PHE:O	23:o:96:GLY:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:J:197:GLU:N	36:J:197:GLU:OE1	2.53	0.41
8:Z:52:ARG:HA	8:Z:55:GLY:O	2.20	0.41
10:b:46:PHE:CD1	10:b:46:PHE:C	2.98	0.41
12:d:79:MET:SD	15:g:108:TYR:OH	2.71	0.41
30:C:194:ASP:OD2	37:K:96:MET:SD	2.79	0.41
30:C:224:ARG:HD2	38:L:164:PHE:CZ	2.55	0.41
38:L:111:LEU:O	38:L:112:MET:HB2	2.20	0.41
39:M:355:LYS:HA	39:M:366:LEU:CD1	2.51	0.41
39:M:636:TYR:CD1	39:M:642:VAL:HG22	2.55	0.41
20:l:16:ILE:N	20:l:17:PRO:CD	2.83	0.41
20:l:172:ILE:O	20:l:176:ARG:HG2	2.20	0.41
21:m:114:VAL:HG12	21:m:115:VAL:N	2.35	0.41
26:s:196:THR:HG21	26:s:274:ARG:CA	2.46	0.41
30:C:72:GLY:N	30:C:73:PRO:HD3	2.35	0.41
39:M:49:VAL:HG22	39:M:96:VAL:HG12	2.03	0.41
14:f:40:ASP:O	14:f:41:TRP:C	2.62	0.41
19:k:37:MET:HE3	19:k:67:ALA:HB2	2.03	0.41
25:r:199:TYR:HB3	25:r:246:LEU:HD13	2.03	0.41
25:r:233:ALA:HB2	25:r:324:SER:OG	2.20	0.41
37:K:91:LEU:HD12	37:K:91:LEU:C	2.46	0.41
39:M:181:ARG:HD3	39:M:225:ILE:HG13	2.02	0.41
39:M:358:LEU:CD1	39:M:366:LEU:HD21	2.50	0.41
1:Q:74:ASP:OD1	1:Q:75:THR:N	2.52	0.41
14:f:33:GLU:O	14:f:35:PRO:HD3	2.20	0.41
19:k:4:ILE:O	19:k:8:ILE:HG12	2.20	0.41
20:l:534:HIS:O	20:l:538:PRO:CD	2.64	0.41
25:r:331:ASN:O	25:r:335:GLU:OE1	2.39	0.41
29:w:170:LEU:HD22	29:w:187:TYR:CD1	2.56	0.41
30:C:262:PHE:CZ	30:C:272:GLY:HA3	2.56	0.41
8:Z:85:GLU:O	8:Z:89:GLU:OE1	2.38	0.41
13:e:50:GLU:O	13:e:50:GLU:HG2	2.21	0.41
14:f:28:LYS:CD	14:f:32:ARG:HD2	2.51	0.41
15:g:8:GLU:OE1	15:g:8:GLU:N	2.54	0.41
16:h:59:GLU:OE2	27:u:145:ARG:NE	2.48	0.41
16:h:77:GLY:HA3	21:m:118:PHE:CZ	2.56	0.41
45:i:402:PEE:H51	45:i:402:PEE:H58	2.02	0.41
19:k:26:LEU:HD23	19:k:26:LEU:H	1.85	0.41
20:l:297:ASP:OD1	20:l:299:LYS:N	2.54	0.41
20:l:578:SER:O	20:l:580:GLN:HG3	2.21	0.41
21:m:26:ILE:HG13	21:m:70:THR:HG21	2.01	0.41
22:n:24:GLY:O	22:n:28:ASP:OD1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:p:101:GLU:O	24:p:122:ARG:NH2	2.54	0.41
25:r:370:PRO:HB3	25:r:375:LEU:CD2	2.51	0.41
26:s:196:THR:O	26:s:197:PRO:C	2.63	0.41
29:w:48:LYS:O	29:w:49:ALA:HB3	2.21	0.41
29:w:77:ILE:CD1	29:w:270:VAL:HG21	2.51	0.41
30:C:119:GLU:H	52:C:502:FMN:HM71	1.85	0.41
30:C:427:LEU:HD12	52:C:502:FMN:C2	2.50	0.41
35:I:65:VAL:HG23	35:I:77:LEU:HD12	2.03	0.41
39:M:652:ASN:HB3	39:M:660:GLU:OE1	2.20	0.41
40:N:95:ASP:OD2	44:t:35:THR:N	2.54	0.41
42:P:209:GLU:OE1	42:P:224:VAL:HA	2.19	0.41
1:Q:58:THR:O	1:Q:58:THR:HG22	2.21	0.41
2:S:35:GLU:OE2	26:s:247:TYR:OH	2.39	0.41
17:i:146:SER:N	17:i:147:PRO:CD	2.84	0.41
32:E:205:ARG:NH1	32:E:208:GLN:OE1	2.54	0.41
6:H:107:ASP:OD1	6:H:107:ASP:N	2.52	0.41
36:J:170:LEU:HA	36:J:202:LYS:HB3	2.03	0.41
41:O:189:ASN:O	41:O:190:ASP:OD1	2.39	0.41
1:Q:61:TRP:CZ2	20:l:580:GLN:HB3	2.55	0.40
5:W:94:GLU:HA	5:W:97:ILE:HG22	2.03	0.40
13:e:54:PRO:O	13:e:55:TRP:HB2	2.21	0.40
17:i:290:LEU:HD23	17:i:290:LEU:O	2.21	0.40
26:s:179:TRP:N	26:s:180:PRO:CD	2.84	0.40
27:u:140:ASN:OD1	27:u:143:HIS:O	2.39	0.40
30:C:141:GLY:HA3	30:C:248:VAL:HG12	2.03	0.40
30:C:427:LEU:HD22	51:C:501:SF4:S2	2.61	0.40
6:H:144:ILE:O	6:H:148:ILE:HD12	2.21	0.40
5:W:61:GLN:O	5:W:64:ASP:OD1	2.40	0.40
11:c:116:ARG:HA	45:l:701:PEE:C30	2.51	0.40
18:j:80:GLN:HG3	26:s:318:THR:HG23	2.03	0.40
19:k:54:LEU:O	19:k:57:ASN:OD1	2.40	0.40
30:C:251:SER:N	30:C:252:PRO:HD2	2.36	0.40
11:c:167:TYR:OH	11:c:173:ASP:O	2.35	0.40
12:d:156:ARG:NH1	13:e:140:ASN:OD1	2.54	0.40
20:l:128:MET:HE2	20:l:251:THR:O	2.20	0.40
26:s:35:LYS:O	32:E:102:ASP:OD2	2.39	0.40
30:C:234:GLY:N	30:C:238:CYS:O	2.44	0.40
30:C:412:LEU:HD21	30:C:435:VAL:HG21	2.02	0.40
39:M:384:ASN:HB3	39:M:669:ASN:HD22	1.87	0.40
39:M:427:LEU:H	39:M:427:LEU:HD23	1.85	0.40
40:N:65:THR:HG22	40:N:66:THR:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:130:THR:O	5:W:130:THR:HG22	2.21	0.40
6:X:155:TYR:O	6:X:156:GLU:C	2.65	0.40
9:a:173:THR:HG22	9:a:174:ILE:N	2.33	0.40
12:d:3:ASP:O	12:d:4:SER:C	2.64	0.40
14:f:32:ARG:HD3	14:f:32:ARG:N	2.36	0.40
26:s:47:GLN:N	26:s:48:PRO:HD2	2.37	0.40
26:s:196:THR:CG2	26:s:197:PRO:HD2	2.46	0.40
30:C:383:THR:N	30:C:384:PRO:HD2	2.37	0.40
34:G:95:LEU:HD23	34:G:95:LEU:H	1.87	0.40
1:Q:52:MET:O	17:i:171:ASN:OD1	2.37	0.40
11:c:129:MET:HB3	20:l:532:ILE:HD11	2.04	0.40
11:c:141:ILE:HD12	11:c:141:ILE:H	1.86	0.40
25:r:403:THR:HA	25:r:406:TYR:CE2	2.56	0.40
30:C:53:LEU:O	30:C:54:LYS:HB3	2.21	0.40
52:C:502:FMN:C4A	52:C:502:FMN:C5A	3.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	427/463 (92%)	405 (95%)	22 (5%)	0	100	100
2	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
3	U	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
4	V	138/141 (98%)	129 (94%)	9 (6%)	0	100	100
5	W	138/144 (96%)	130 (94%)	5 (4%)	3 (2%)	5	7
6	H	83/156 (53%)	77 (93%)	6 (7%)	0	100	100
6	X	84/156 (54%)	79 (94%)	5 (6%)	0	100	100
7	Y	59/105 (56%)	54 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Z	81/98 (83%)	70 (86%)	11 (14%)	0	100	100
9	a	136/189 (72%)	133 (98%)	3 (2%)	0	100	100
10	b	116/128 (91%)	102 (88%)	14 (12%)	0	100	100
11	c	150/186 (81%)	137 (91%)	13 (9%)	0	100	100
12	d	167/172 (97%)	166 (99%)	1 (1%)	0	100	100
13	e	105/153 (69%)	94 (90%)	11 (10%)	0	100	100
14	f	47/76 (62%)	44 (94%)	2 (4%)	1 (2%)	5	7
15	g	118/119 (99%)	116 (98%)	2 (2%)	0	100	100
16	h	103/106 (97%)	91 (88%)	11 (11%)	1 (1%)	13	19
17	i	345/347 (99%)	329 (95%)	16 (5%)	0	100	100
18	j	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
19	k	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
20	l	599/603 (99%)	561 (94%)	37 (6%)	1 (0%)	44	59
21	m	171/174 (98%)	155 (91%)	16 (9%)	0	100	100
22	n	52/58 (90%)	47 (90%)	5 (10%)	0	100	100
23	o	126/129 (98%)	122 (97%)	4 (3%)	0	100	100
24	p	171/179 (96%)	161 (94%)	10 (6%)	0	100	100
25	r	457/459 (100%)	441 (96%)	15 (3%)	1 (0%)	44	59
26	s	314/318 (99%)	294 (94%)	19 (6%)	1 (0%)	37	51
27	u	169/172 (98%)	156 (92%)	13 (8%)	0	100	100
28	v	119/137 (87%)	110 (92%)	9 (8%)	0	100	100
29	w	318/355 (90%)	303 (95%)	14 (4%)	1 (0%)	37	51
30	C	430/464 (93%)	392 (91%)	38 (9%)	0	100	100
31	D	174/210 (83%)	169 (97%)	5 (3%)	0	100	100
32	E	158/213 (74%)	147 (93%)	11 (7%)	0	100	100
33	F	116/128 (91%)	110 (95%)	6 (5%)	0	100	100
34	G	83/99 (84%)	74 (89%)	9 (11%)	0	100	100
35	I	110/116 (95%)	102 (93%)	8 (7%)	0	100	100
36	J	339/377 (90%)	316 (93%)	23 (7%)	0	100	100
37	K	37/108 (34%)	31 (84%)	6 (16%)	0	100	100
38	L	119/175 (68%)	113 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	M	685/727 (94%)	620 (90%)	62 (9%)	3 (0%)	30	43
40	N	142/145 (98%)	131 (92%)	11 (8%)	0	100	100
41	O	210/249 (84%)	187 (89%)	23 (11%)	0	100	100
42	P	206/264 (78%)	189 (92%)	17 (8%)	0	100	100
43	T	94/124 (76%)	90 (96%)	4 (4%)	0	100	100
44	t	93/113 (82%)	83 (89%)	10 (11%)	0	100	100
All	All	8147/9202 (88%)	7597 (93%)	538 (7%)	12 (0%)	50	65

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	W	28	ARG
16	h	98	HIS
26	s	196	THR
29	w	270	VAL
39	M	483	ARG
39	M	682	ASP
5	W	30	LEU
20	l	532	ILE
39	M	482	GLN
5	W	32	GLY
14	f	34	PRO
25	r	139	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	370/392 (94%)	370 (100%)	0	100	100
2	S	59/59 (100%)	59 (100%)	0	100	100
3	U	72/73 (99%)	72 (100%)	0	100	100
4	V	102/103 (99%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	W	121/123 (98%)	121 (100%)	0	100	100
6	H	79/136 (58%)	79 (100%)	0	100	100
6	X	80/136 (59%)	80 (100%)	0	100	100
7	Y	58/87 (67%)	58 (100%)	0	100	100
8	Z	66/79 (84%)	66 (100%)	0	100	100
9	a	124/159 (78%)	124 (100%)	0	100	100
10	b	113/122 (93%)	113 (100%)	0	100	100
11	c	136/161 (84%)	136 (100%)	0	100	100
12	d	152/155 (98%)	152 (100%)	0	100	100
13	e	99/130 (76%)	99 (100%)	0	100	100
14	f	45/67 (67%)	45 (100%)	0	100	100
15	g	106/105 (101%)	106 (100%)	0	100	100
16	h	91/92 (99%)	91 (100%)	0	100	100
17	i	314/314 (100%)	314 (100%)	0	100	100
18	j	104/104 (100%)	104 (100%)	0	100	100
19	k	85/85 (100%)	85 (100%)	0	100	100
20	l	531/533 (100%)	531 (100%)	0	100	100
21	m	136/137 (99%)	136 (100%)	0	100	100
22	n	51/55 (93%)	51 (100%)	0	100	100
23	o	114/115 (99%)	114 (100%)	0	100	100
24	p	157/161 (98%)	157 (100%)	0	100	100
25	r	416/416 (100%)	416 (100%)	0	100	100
26	s	277/279 (99%)	277 (100%)	0	100	100
27	u	154/155 (99%)	154 (100%)	0	100	100
28	v	110/121 (91%)	110 (100%)	0	100	100
29	w	288/313 (92%)	288 (100%)	0	100	100
30	C	348/371 (94%)	348 (100%)	0	100	100
31	D	151/174 (87%)	151 (100%)	0	100	100
32	E	135/173 (78%)	135 (100%)	0	100	100
33	F	110/116 (95%)	110 (100%)	0	100	100
34	G	75/80 (94%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	I	100/102 (98%)	100 (100%)	0	100	100
36	J	295/323 (91%)	295 (100%)	0	100	100
37	K	32/93 (34%)	32 (100%)	0	100	100
38	L	107/157 (68%)	107 (100%)	0	100	100
39	M	577/608 (95%)	577 (100%)	0	100	100
40	N	130/131 (99%)	130 (100%)	0	100	100
41	O	181/206 (88%)	181 (100%)	0	100	100
42	P	190/229 (83%)	190 (100%)	0	100	100
43	T	80/100 (80%)	80 (100%)	0	100	100
44	t	88/98 (90%)	88 (100%)	0	100	100
All	All	7209/7928 (91%)	7209 (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 (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	442	HIS
6	X	142	GLN
8	Z	21	GLN
9	a	189	ASN
10	b	48	ASN
12	d	155	GLN
18	j	10	ASN
19	k	7	ASN
20	l	446	ASN
22	n	40	ASN
23	o	24	ASN
23	o	86	ASN
23	o	126	HIS
25	r	169	ASN
26	s	194	ASN
26	s	230	ASN
26	s	235	ASN
29	w	323	GLN
30	C	164	ASN
30	C	244	ASN
30	C	283	ASN

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Mol	Chain	Res	Type
30	C	284	HIS
31	D	124	GLN
31	D	204	GLN
33	F	70	ASN
36	J	72	HIS
36	J	102	GLN
36	J	122	HIS
36	J	323	HIS
36	J	356	HIS
37	K	77	HIS
38	L	86	ASN
39	M	148	ASN
39	M	688	GLN
40	N	72	ASN
40	N	116	ASN
40	N	135	GLN
41	O	59	ASN
42	P	103	HIS
43	T	124	HIS
44	t	21	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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
1	NMM	Q	118	1	9,11,12	1.74	1 (11%)	6,12,14	1.36	1 (16%)
32	SEP	E	58	32	8,9,10	1.55	1 (12%)	8,12,14	1.51	2 (25%)

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
1	NMM	Q	118	1	-	1/9/11/13	-
32	SEP	E	58	32	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	118	NMM	CZ-NH2	4.61	1.45	1.34
32	E	58	SEP	P-O1P	3.37	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	E	58	SEP	P-OG-CB	-2.89	110.34	118.30
1	Q	118	NMM	NE-CZ-NH2	2.75	122.00	119.48
32	E	58	SEP	OG-CB-CA	2.54	110.61	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	Q	118	NMM	O-C-CA-CB
32	E	58	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	Q	118	NMM	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 2 are monoatomic - leaving 33 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
53	NDP	J	401	-	45,52,52	4.27	20 (44%)	53,80,80	1.84	6 (11%)
48	PLX	s	401	-	51,51,51	0.97	3 (5%)	55,59,59	0.73	0
51	SF4	C	501	30	0,12,12	-	-	-		
46	CDL	i	401	-	63,63,99	1.37	7 (11%)	69,75,111	0.93	3 (4%)
46	CDL	V	203	-	99,99,99	1.21	7 (7%)	105,111,111	0.85	3 (2%)
47	8Q1	F	201	-	31,34,34	1.73	6 (19%)	40,43,43	1.41	5 (12%)
47	8Q1	X	201	-	31,34,34	1.73	6 (19%)	40,43,43	1.29	4 (10%)
45	PEE	E	301	-	50,50,50	1.12	3 (6%)	53,55,55	1.09	2 (3%)
45	PEE	i	402	-	50,50,50	1.14	3 (6%)	53,55,55	1.15	3 (5%)
48	PLX	r	501	-	51,51,51	1.00	4 (7%)	55,59,59	0.68	0
48	PLX	N	201	-	51,51,51	0.99	3 (5%)	55,59,59	0.71	0
51	SF4	M	801	39	0,12,12	-	-	-		
45	PEE	l	701	-	50,50,50	1.14	3 (6%)	53,55,55	1.28	3 (5%)
45	PEE	W	201	-	50,50,50	1.13	3 (6%)	53,55,55	1.02	2 (3%)
48	PLX	g	201	-	51,51,51	0.98	2 (3%)	55,59,59	0.69	0
52	FMN	C	502	-	33,33,33	22.73	32 (96%)	48,50,50	7.20	26 (54%)
46	CDL	l	702	-	63,63,99	1.37	7 (11%)	69,75,111	0.96	3 (4%)
51	SF4	D	301	31	0,12,12	-	-	-		
48	PLX	o	201	-	51,51,51	1.01	4 (7%)	55,59,59	0.68	1 (1%)
45	PEE	V	201	-	50,50,50	1.12	3 (6%)	53,55,55	1.05	2 (3%)
46	CDL	V	202	-	99,99,99	1.22	7 (7%)	105,111,111	1.25	5 (4%)
49	DGT	w	401	50	26,33,33	3.75	13 (50%)	32,52,52	1.49	7 (21%)
54	FES	O	301	41	0,4,4	-	-	-		
48	PLX	j	201	-	51,51,51	0.96	4 (7%)	55,59,59	0.76	2 (3%)
45	PEE	i	403	-	48,48,50	1.15	3 (6%)	51,53,55	1.04	3 (5%)
45	PEE	J	402	-	50,50,50	1.13	3 (6%)	53,55,55	1.29	4 (7%)
46	CDL	l	703	-	99,99,99	1.20	7 (7%)	105,111,111	0.92	2 (1%)
46	CDL	u	201	-	63,63,99	1.39	7 (11%)	69,75,111	0.82	2 (2%)
51	SF4	M	802	39	0,12,12	-	-	-		
51	SF4	E	302	32,1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	FES	M	803	39	0,4,4	-	-	-		
51	SF4	D	302	31	0,12,12	-	-	-		
48	PLX	g	202	-	51,51,51	1.01	3 (5%)	55,59,59	0.61	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
53	NDP	J	401	-	-	5/30/77/77	0/5/5/5
48	PLX	s	401	-	-	18/55/55/55	-
51	SF4	C	501	30	-	-	0/6/5/5
46	CDL	i	401	-	-	14/74/74/110	-
46	CDL	V	203	-	-	25/110/110/110	-
47	8Q1	F	201	-	-	8/41/41/41	-
47	8Q1	X	201	-	-	4/41/41/41	-
45	PEE	E	301	-	-	14/54/54/54	-
45	PEE	i	402	-	-	15/54/54/54	-
48	PLX	r	501	-	-	16/55/55/55	-
48	PLX	N	201	-	-	13/55/55/55	-
51	SF4	M	801	39	-	-	0/6/5/5
45	PEE	l	701	-	-	20/54/54/54	-
45	PEE	W	201	-	-	15/54/54/54	-
48	PLX	g	201	-	-	15/55/55/55	-
52	FMN	C	502	-	1/1/4/4	6/18/18/18	0/3/3/3
46	CDL	l	702	-	-	22/74/74/110	-
51	SF4	D	301	31	-	-	0/6/5/5
48	PLX	o	201	-	-	12/55/55/55	-
45	PEE	V	201	-	-	30/54/54/54	-
46	CDL	V	202	-	-	26/110/110/110	-
49	DGT	w	401	50	-	5/18/34/34	0/3/3/3
54	FES	O	301	41	-	-	0/1/1/1
48	PLX	j	201	-	-	18/55/55/55	-
45	PEE	i	403	-	-	14/52/52/54	-
45	PEE	J	402	-	-	13/54/54/54	-
46	CDL	l	703	-	-	14/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	CDL	u	201	-	-	12/74/74/110	-
51	SF4	M	802	39	-	-	0/6/5/5
51	SF4	E	302	32,1	-	-	0/6/5/5
54	FES	M	803	39	-	-	0/1/1/1
51	SF4	D	302	31	-	-	0/6/5/5
48	PLX	g	202	-	-	12/55/55/55	-

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	C	502	FMN	C8M-C8	52.75	2.56	1.51
52	C	502	FMN	C9-C9A	52.75	2.25	1.39
52	C	502	FMN	C1'-C2'	50.06	2.23	1.52
52	C	502	FMN	O4'-C4'	-49.06	0.39	1.43
52	C	502	FMN	C5A-N5	37.04	2.10	1.39
52	C	502	FMN	O2'-C2'	-30.49	0.78	1.43
52	C	502	FMN	C4A-C10	26.51	2.22	1.44
52	C	502	FMN	C7M-C7	24.61	2.00	1.51
52	C	502	FMN	C4-N3	-22.93	0.96	1.38
52	C	502	FMN	C4A-N5	20.70	1.71	1.30
52	C	502	FMN	C10-N1	18.32	1.70	1.33
52	C	502	FMN	C6-C5A	16.81	1.66	1.40
53	J	401	NDP	O4B-C1B	14.16	1.60	1.41
52	C	502	FMN	C5'-C4'	-12.53	1.34	1.51
53	J	401	NDP	C6N-C5N	12.29	1.55	1.33
52	C	502	FMN	C4'-C3'	-12.01	1.30	1.53
53	J	401	NDP	C2D-C3D	-11.04	1.23	1.53
52	C	502	FMN	P-O1P	10.80	1.85	1.50
52	C	502	FMN	O2-C2	10.07	1.42	1.24
52	C	502	FMN	C2-N3	-9.92	1.15	1.39
52	C	502	FMN	O4-C4	9.80	1.42	1.23
52	C	502	FMN	C10-N10	9.27	1.57	1.37
52	C	502	FMN	C9-C8	8.73	1.52	1.39
52	C	502	FMN	O5'-C5'	8.61	1.77	1.44
52	C	502	FMN	C9A-C5A	-8.58	1.26	1.41
52	C	502	FMN	C1'-N10	-8.49	1.26	1.48
52	C	502	FMN	C2'-C3'	-8.15	1.38	1.53
52	C	502	FMN	C2-N1	7.68	1.55	1.36
49	w	401	DGT	O4'-C4'	7.48	1.61	1.45
52	C	502	FMN	C9A-N10	7.20	1.53	1.41
53	J	401	NDP	C2N-C3N	7.00	1.54	1.34
52	C	502	FMN	P-O5'	6.86	1.82	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	w	401	DGT	C2'-C3'	-6.71	1.35	1.52
49	w	401	DGT	O4'-C1'	-6.31	1.28	1.42
49	w	401	DGT	C6-N1	6.27	1.47	1.37
53	J	401	NDP	O4D-C4D	-6.26	1.31	1.45
53	J	401	NDP	C3D-C4D	6.14	1.68	1.53
53	J	401	NDP	C7N-N7N	5.99	1.49	1.33
49	w	401	DGT	C2-N3	5.91	1.47	1.33
53	J	401	NDP	O4B-C4B	-5.85	1.31	1.45
47	X	201	8Q1	C34-N36	5.53	1.45	1.33
47	F	201	8Q1	C39-N41	5.51	1.45	1.33
47	F	201	8Q1	C34-N36	5.40	1.45	1.33
47	X	201	8Q1	C39-N41	5.32	1.45	1.33
49	w	401	DGT	C4-N3	5.15	1.49	1.37
53	J	401	NDP	C1D-N1N	-4.92	1.32	1.46
49	w	401	DGT	C2-N2	4.89	1.45	1.34
52	C	502	FMN	C6-C7	4.65	1.46	1.39
49	w	401	DGT	O3'-C3'	4.49	1.52	1.43
49	w	401	DGT	C2'-C1'	4.33	1.64	1.52
52	C	502	FMN	O3'-C3'	4.32	1.53	1.43
49	w	401	DGT	C5'-C4'	-3.91	1.39	1.51
45	l	701	PEE	O3-C30	3.75	1.44	1.33
53	J	401	NDP	C6A-N6A	3.75	1.47	1.34
52	C	502	FMN	P-O2P	-3.71	1.40	1.54
45	J	402	PEE	O3-C30	3.65	1.44	1.33
53	J	401	NDP	O4D-C1D	3.60	1.50	1.42
45	E	301	PEE	O3-C30	3.59	1.43	1.33
45	V	201	PEE	O3-C30	3.57	1.43	1.33
45	i	402	PEE	O3-C30	3.56	1.43	1.33
46	V	202	CDL	OA8-CA7	3.53	1.43	1.33
49	w	401	DGT	C5-C6	3.53	1.54	1.47
45	i	403	PEE	O3-C30	3.50	1.43	1.33
46	V	203	CDL	OB8-CB7	3.48	1.43	1.33
46	u	201	CDL	OB8-CB7	3.43	1.43	1.33
46	V	202	CDL	OB8-CB7	3.42	1.43	1.33
46	i	401	CDL	OB8-CB7	3.42	1.43	1.33
45	W	201	PEE	O3-C30	3.41	1.43	1.33
46	l	702	CDL	OA8-CA7	3.41	1.43	1.33
53	J	401	NDP	C6N-N1N	3.41	1.45	1.37
52	C	502	FMN	P-O3P	-3.36	1.41	1.54
46	l	703	CDL	OB8-CB7	3.32	1.43	1.33
46	i	401	CDL	OA8-CA7	3.31	1.43	1.33
46	V	203	CDL	OA6-CA5	3.30	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	u	201	CDL	OA6-CA5	3.29	1.43	1.34
46	V	202	CDL	OA6-CA5	3.27	1.43	1.34
46	l	703	CDL	OA6-CA5	3.27	1.43	1.34
46	V	203	CDL	OA8-CA7	3.26	1.42	1.33
46	l	703	CDL	OA8-CA7	3.26	1.42	1.33
46	u	201	CDL	OA8-CA7	3.23	1.42	1.33
46	l	702	CDL	OA6-CA5	3.22	1.43	1.34
46	l	702	CDL	OB8-CB7	3.20	1.42	1.33
45	W	201	PEE	O2-C2	-3.12	1.38	1.46
46	i	401	CDL	OA6-CA5	3.12	1.43	1.34
45	i	402	PEE	O2-C10	3.11	1.43	1.34
49	w	401	DGT	C2-N1	3.10	1.45	1.37
46	V	202	CDL	OB6-CB5	3.02	1.42	1.34
53	J	401	NDP	O3B-C3B	-2.99	1.35	1.43
46	V	203	CDL	OB6-CB4	-2.91	1.39	1.46
46	u	201	CDL	OB6-CB4	-2.88	1.39	1.46
46	l	703	CDL	OB6-CB5	2.88	1.42	1.34
45	i	403	PEE	O2-C2	-2.87	1.39	1.46
45	V	201	PEE	O2-C2	-2.84	1.39	1.46
45	l	701	PEE	O2-C2	-2.84	1.39	1.46
45	J	402	PEE	O2-C10	2.83	1.42	1.34
45	E	301	PEE	O2-C2	-2.83	1.39	1.46
45	V	201	PEE	O2-C10	2.82	1.42	1.34
46	i	401	CDL	OB6-CB4	-2.81	1.39	1.46
46	l	702	CDL	OA6-CA4	-2.77	1.39	1.46
45	l	701	PEE	O2-C10	2.77	1.42	1.34
46	V	203	CDL	OB6-CB5	2.76	1.42	1.34
46	V	202	CDL	OA6-CA4	-2.74	1.39	1.46
45	J	402	PEE	O2-C2	-2.74	1.39	1.46
52	C	502	FMN	C4A-C4	-2.73	1.34	1.44
46	u	201	CDL	OA6-CA4	-2.71	1.39	1.46
46	i	401	CDL	OB6-CB5	2.70	1.41	1.34
45	i	403	PEE	O2-C10	2.70	1.41	1.34
46	V	203	CDL	OA6-CA4	-2.70	1.39	1.46
53	J	401	NDP	C5A-C4A	-2.70	1.33	1.40
46	V	202	CDL	OB6-CB4	-2.68	1.39	1.46
46	i	401	CDL	OA6-CA4	-2.67	1.39	1.46
45	E	301	PEE	O2-C10	2.66	1.41	1.34
46	u	201	CDL	OB6-CB5	2.66	1.41	1.34
46	l	702	CDL	OB6-CB5	2.64	1.41	1.34
45	W	201	PEE	O2-C10	2.61	1.41	1.34
48	o	201	PLX	O6-C4	-2.61	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	l	703	CDL	OB6-CB4	-2.60	1.40	1.46
53	J	401	NDP	O2D-C2D	2.60	1.49	1.43
47	X	201	8Q1	C1-S44	2.60	1.82	1.76
48	g	202	PLX	C7-C6	2.60	1.56	1.50
53	J	401	NDP	C2D-C1D	2.59	1.61	1.53
46	l	703	CDL	OA6-CA4	-2.54	1.40	1.46
47	F	201	8Q1	C1-S44	2.53	1.82	1.76
53	J	401	NDP	O3D-C3D	2.52	1.48	1.43
46	l	702	CDL	OB6-CB4	-2.51	1.40	1.46
53	J	401	NDP	C2A-N3A	2.48	1.36	1.32
47	F	201	8Q1	O40-C39	-2.47	1.18	1.23
47	F	201	8Q1	O35-C34	-2.46	1.18	1.23
45	i	402	PEE	O2-C2	-2.42	1.40	1.46
47	X	201	8Q1	O40-C39	-2.40	1.18	1.23
53	J	401	NDP	PN-O5D	2.40	1.69	1.59
53	J	401	NDP	O7N-C7N	-2.40	1.18	1.24
48	g	202	PLX	O6-C4	-2.39	1.41	1.44
48	s	401	PLX	O6-C4	-2.39	1.41	1.44
48	N	201	PLX	O6-C4	-2.38	1.41	1.44
48	r	501	PLX	O6-C4	-2.35	1.41	1.44
47	X	201	8Q1	O35-C34	-2.34	1.18	1.23
48	s	401	PLX	C25-C24	2.34	1.55	1.50
48	j	201	PLX	C7-C6	2.31	1.55	1.50
49	w	401	DGT	PA-O1A	-2.31	1.44	1.55
48	g	201	PLX	C25-C24	2.30	1.55	1.50
48	N	201	PLX	C25-C24	2.29	1.55	1.50
48	r	501	PLX	C25-C24	2.29	1.55	1.50
48	o	201	PLX	C25-C24	2.28	1.55	1.50
46	V	203	CDL	PB2-OB2	2.27	1.68	1.59
48	g	201	PLX	C7-C6	2.24	1.55	1.50
48	o	201	PLX	C7-C6	2.23	1.55	1.50
48	r	501	PLX	C7-C6	2.22	1.55	1.50
47	X	201	8Q1	C6-C1	2.20	1.53	1.50
46	V	202	CDL	PB2-OB2	2.19	1.68	1.59
46	i	401	CDL	PB2-OB2	2.18	1.68	1.59
46	l	702	CDL	PB2-OB2	2.17	1.68	1.59
48	j	201	PLX	O6-C4	-2.16	1.41	1.44
48	r	501	PLX	P1-O4	2.13	1.67	1.59
48	g	202	PLX	P1-O4	2.10	1.67	1.59
48	j	201	PLX	C25-C24	2.10	1.55	1.50
48	s	401	PLX	C7-C6	2.09	1.55	1.50
48	N	201	PLX	C7-C6	2.09	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	o	201	PLX	P1-O4	2.08	1.67	1.59
46	l	703	CDL	PB2-OB2	2.08	1.67	1.59
46	u	201	CDL	PB2-OB2	2.08	1.67	1.59
48	j	201	PLX	P1-O4	2.05	1.67	1.59
47	F	201	8Q1	C6-C1	2.01	1.52	1.50

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	C	502	FMN	C5A-C9A-N10	22.74	141.43	117.95
52	C	502	FMN	C4A-C10-N1	-20.90	76.23	124.73
52	C	502	FMN	N10-C10-N1	17.30	168.11	118.35
52	C	502	FMN	C8M-C8-C7	-15.51	88.95	120.74
52	C	502	FMN	C8M-C8-C9	11.96	141.60	119.49
52	C	502	FMN	C6-C5A-C9A	11.05	134.58	118.94
52	C	502	FMN	C6-C5A-N5	-9.97	101.11	118.51
53	J	401	NDP	C5A-C6A-N6A	8.96	133.97	120.35
52	C	502	FMN	C5A-N5-C4A	-8.88	103.32	118.07
52	C	502	FMN	C10-N1-C2	8.65	134.20	116.90
52	C	502	FMN	C9-C9A-C5A	-7.86	105.26	120.11
52	C	502	FMN	O2-C2-N1	-7.38	109.60	121.83
52	C	502	FMN	C9-C8-C7	6.79	129.40	119.67
52	C	502	FMN	C4A-C4-N3	6.75	130.32	113.19
46	V	202	CDL	OB6-CB5-C51	6.32	125.12	111.50
52	C	502	FMN	C9-C9A-N10	-6.31	113.30	121.84
53	J	401	NDP	N6A-C6A-N1A	-6.09	105.94	118.57
52	C	502	FMN	C4-C4A-C10	5.95	126.79	116.79
52	C	502	FMN	O3'-C3'-C4'	5.66	122.48	108.81
53	J	401	NDP	N3A-C2A-N1A	-5.45	120.15	128.68
52	C	502	FMN	C9A-C9-C8	-5.44	108.36	119.30
46	V	202	CDL	OA6-CA5-C11	5.10	122.48	111.50
45	E	301	PEE	C40-C39-C38	5.06	163.53	124.73
45	W	201	PEE	C40-C39-C38	5.03	163.35	124.73
52	C	502	FMN	O4-C4-C4A	-5.02	113.28	126.60
45	V	201	PEE	C40-C39-C38	4.99	162.99	124.73
45	J	402	PEE	C40-C39-C38	4.93	162.56	124.73
45	i	402	PEE	C40-C39-C38	4.92	162.51	124.73
45	i	403	PEE	C40-C39-C38	4.77	161.33	124.73
45	l	701	PEE	C40-C39-C38	4.61	160.13	124.73
45	i	402	PEE	O2-C10-C11	4.51	121.22	111.50
52	C	502	FMN	N3-C2-N1	4.22	127.66	119.38
47	F	201	8Q1	C6-C1-S44	4.14	118.27	113.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	l	701	PEE	O2-C10-C11	3.83	119.75	111.50
47	X	201	8Q1	C6-C1-S44	3.68	117.74	113.46
46	l	702	CDL	OB6-CB5-C51	3.41	118.86	111.50
47	F	201	8Q1	C38-C39-N41	3.35	122.06	116.42
46	V	202	CDL	OA8-CA7-C31	3.35	122.41	111.91
49	w	401	DGT	C5-C6-N1	3.34	119.84	113.95
52	C	502	FMN	C7M-C7-C6	-3.33	113.33	119.49
45	J	402	PEE	O2-C10-C11	3.30	118.62	111.50
52	C	502	FMN	P-O5'-C5'	-3.27	109.28	118.30
47	X	201	8Q1	C43-S44-C1	3.27	112.04	101.87
47	F	201	8Q1	C43-S44-C1	3.19	111.80	101.87
46	i	401	CDL	OB6-CB5-C51	3.17	118.33	111.50
46	V	203	CDL	OA6-CA5-C11	3.16	118.30	111.50
45	J	402	PEE	O3-C30-C31	3.14	121.75	111.91
52	C	502	FMN	C9A-N10-C10	-2.97	116.13	120.77
45	l	701	PEE	O3-C30-C31	2.97	121.24	111.91
52	C	502	FMN	C4-C4A-N5	-2.94	114.05	118.23
49	w	401	DGT	C2-N1-C6	-2.91	119.75	125.10
49	w	401	DGT	PB-O3B-PG	-2.91	122.86	132.83
46	u	201	CDL	OA6-CA5-C11	2.90	117.75	111.50
47	F	201	8Q1	O4-C1-C6	-2.89	120.57	123.99
49	w	401	DGT	C8-N7-C5	2.83	108.39	102.99
46	l	703	CDL	OA6-CA5-C11	2.83	117.59	111.50
46	i	401	CDL	OA6-CA5-C11	2.81	117.56	111.50
46	l	703	CDL	OB6-CB5-C51	2.78	117.49	111.50
46	u	201	CDL	OB6-CB5-C51	2.76	117.45	111.50
45	E	301	PEE	O2-C10-C11	2.74	117.41	111.50
49	w	401	DGT	PA-O3A-PB	-2.74	123.42	132.83
47	X	201	8Q1	O4-C1-C6	-2.72	120.77	123.99
52	C	502	FMN	C10-C4A-N5	-2.68	119.16	124.86
45	J	402	PEE	C42-C41-C40	-2.65	102.25	113.79
46	V	202	CDL	OB6-CB5-OB7	-2.57	117.50	123.70
46	V	203	CDL	OB8-CB7-C71	2.56	119.95	111.91
52	C	502	FMN	O2'-C2'-C3'	2.51	115.21	109.10
46	l	702	CDL	OA6-CA5-C11	2.49	116.88	111.50
48	j	201	PLX	C26-C25-C24	-2.40	107.82	113.38
48	o	201	PLX	C5-O8-C24	2.36	118.36	113.80
49	w	401	DGT	N2-C2-N1	2.32	121.66	116.71
45	V	201	PEE	O2-C10-C11	2.28	116.41	111.50
45	i	403	PEE	O2-C10-C11	2.22	116.28	111.50
46	l	702	CDL	OA8-CA7-C31	2.21	118.84	111.91
48	j	201	PLX	C8-C7-C6	-2.20	108.29	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	w	401	DGT	O6-C6-C5	-2.20	120.08	124.37
53	J	401	NDP	PN-O3-PA	-2.20	125.29	132.83
45	i	403	PEE	O3-C30-C31	2.16	118.69	111.91
47	X	201	8Q1	C38-C39-N41	2.14	120.03	116.42
46	V	202	CDL	OA6-CA5-OA7	-2.14	118.54	123.70
52	C	502	FMN	O2-C2-N3	2.11	122.74	118.65
53	J	401	NDP	O4D-C1D-C2D	-2.11	102.05	106.64
47	F	201	8Q1	O40-C39-N41	-2.10	119.05	123.01
46	V	203	CDL	OB6-CB5-C51	2.09	116.00	111.50
53	J	401	NDP	C4D-O4D-C1D	-2.08	104.89	109.47
45	W	201	PEE	O3-C30-C31	2.03	118.29	111.91
45	i	402	PEE	O2-C10-O4	-2.03	118.79	123.70
46	i	401	CDL	OA8-CA7-C31	2.01	118.21	111.91

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
52	C	502	FMN	C4'

All (366) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	V	201	PEE	C2-C1-O3P-P
45	V	201	PEE	C1-O3P-P-O2P
45	V	201	PEE	O4P-C4-C5-N
45	W	201	PEE	C1-O3P-P-O1P
45	W	201	PEE	C4-O4P-P-O2P
45	W	201	PEE	C4-O4P-P-O1P
45	i	402	PEE	C11-C10-O2-C2
45	i	402	PEE	O4-C10-O2-C2
45	i	403	PEE	C1-O3P-P-O1P
45	i	403	PEE	C1-O3P-P-O4P
45	i	403	PEE	C4-O4P-P-O1P
45	i	403	PEE	C5-C4-O4P-P
45	l	701	PEE	C4-O4P-P-O3P
45	l	701	PEE	C4-O4P-P-O1P
45	l	701	PEE	O5-C30-O3-C3
45	l	701	PEE	C31-C30-O3-C3
45	E	301	PEE	C1-O3P-P-O2P
45	E	301	PEE	C1-O3P-P-O1P
45	E	301	PEE	O4P-C4-C5-N
45	J	402	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
46	V	202	CDL	CB2-C1-CA2-OA2
46	V	202	CDL	CA2-OA2-PA1-OA4
46	V	202	CDL	OA7-CA5-OA6-CA4
46	V	202	CDL	C11-CA5-OA6-CA4
46	V	202	CDL	OA9-CA7-OA8-CA6
46	V	202	CDL	C31-CA7-OA8-CA6
46	V	202	CDL	OB7-CB5-OB6-CB4
46	V	202	CDL	C51-CB5-OB6-CB4
46	V	203	CDL	OB9-CB7-OB8-CB6
46	V	203	CDL	C71-CB7-OB8-CB6
46	i	401	CDL	C1-CB2-OB2-PB2
46	l	702	CDL	CA2-OA2-PA1-OA3
46	l	702	CDL	CA2-OA2-PA1-OA4
46	l	703	CDL	CA3-OA5-PA1-OA3
46	u	201	CDL	C1-CA2-OA2-PA1
47	X	201	8Q1	C1-C6-C7-C8
47	F	201	8Q1	O33-C32-C34-N36
47	F	201	8Q1	C42-C43-S44-C1
48	g	201	PLX	N1-C1-C2-O1
48	g	201	PLX	O9-C24-O8-C5
48	j	201	PLX	C3-C4-O6-C6
48	j	201	PLX	C3-O4-P1-O2
48	j	201	PLX	O9-C24-O8-C5
48	r	501	PLX	C2-O1-P1-O3
48	s	401	PLX	O7-C6-C7-C8
48	s	401	PLX	N1-C1-C2-O1
48	N	201	PLX	C3-O4-P1-O3
48	N	201	PLX	C2-O1-P1-O2
48	N	201	PLX	C2-O1-P1-O3
48	N	201	PLX	O9-C24-O8-C5
49	w	401	DGT	C5'-O5'-PA-O3A
49	w	401	DGT	C5'-O5'-PA-O1A
49	w	401	DGT	C5'-O5'-PA-O2A
52	C	502	FMN	N10-C1'-C2'-O2'
52	C	502	FMN	N10-C1'-C2'-C3'
52	C	502	FMN	C1'-C2'-C3'-O3'
52	C	502	FMN	C3'-C4'-C5'-O5'
52	C	502	FMN	O4'-C4'-C5'-O5'
53	J	401	NDP	C5D-O5D-PN-O1N
53	J	401	NDP	C5D-O5D-PN-O2N
45	J	402	PEE	O5-C30-O3-C3
47	F	201	8Q1	C38-C39-N41-C42

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Mol	Chain	Res	Type	Atoms
46	V	202	CDL	O1-C1-CA2-OA2
46	u	201	CDL	O1-C1-CA2-OA2
46	u	201	CDL	CA4-CA3-OA5-PA1
48	g	201	PLX	C4-C3-O4-P1
47	F	201	8Q1	O40-C39-N41-C42
46	l	702	CDL	O1-C1-CA2-OA2
45	W	201	PEE	C11-C12-C13-C14
45	V	201	PEE	C30-C31-C32-C33
46	l	702	CDL	CB5-C51-C52-C53
46	l	702	CDL	CB7-C71-C72-C73
45	V	201	PEE	C1-O3P-P-O4P
45	W	201	PEE	C1-O3P-P-O4P
45	W	201	PEE	C4-O4P-P-O3P
45	E	301	PEE	C1-O3P-P-O4P
45	J	402	PEE	C1-O3P-P-O4P
46	V	203	CDL	CA3-OA5-PA1-OA2
46	l	702	CDL	CA2-OA2-PA1-OA5
46	l	702	CDL	CA3-OA5-PA1-OA2
46	u	201	CDL	CA2-OA2-PA1-OA5
46	u	201	CDL	CA3-OA5-PA1-OA2
48	g	201	PLX	C3-O4-P1-O1
48	r	501	PLX	C2-O1-P1-O4
48	N	201	PLX	C3-O4-P1-O1
48	N	201	PLX	C2-O1-P1-O4
46	u	201	CDL	CB2-C1-CA2-OA2
48	g	202	PLX	O6-C6-C7-C8
45	V	201	PEE	C12-C13-C14-C15
46	V	202	CDL	C12-C13-C14-C15
46	V	202	CDL	C53-C54-C55-C56
46	V	203	CDL	C14-C15-C16-C17
45	i	402	PEE	C10-C11-C12-C13
46	l	703	CDL	CB4-CB3-OB5-PB2
45	V	201	PEE	C22-C23-C24-C25
45	V	201	PEE	C20-C21-C22-C23
46	V	203	CDL	C16-C17-C18-C19
45	V	201	PEE	C33-C34-C35-C36
45	i	403	PEE	C35-C36-C37-C38
46	l	703	CDL	C71-C72-C73-C74
48	j	201	PLX	C12-C13-C14-C15
48	g	201	PLX	C7-C8-C9-C10
48	r	501	PLX	C18-C19-C20-C21
45	i	403	PEE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
45	l	701	PEE	C14-C15-C16-C17
46	l	702	CDL	C14-C15-C16-C17
48	g	201	PLX	C11-C10-C9-C8
46	V	203	CDL	C12-C13-C14-C15
48	g	201	PLX	O7-C6-C7-C8
48	g	202	PLX	O7-C6-C7-C8
45	V	201	PEE	C35-C36-C37-C38
45	V	201	PEE	C42-C43-C44-C45
48	s	401	PLX	C29-C30-C31-C32
46	V	203	CDL	C54-C55-C56-C57
48	o	201	PLX	C27-C28-C29-C30
45	J	402	PEE	C12-C13-C14-C15
45	i	402	PEE	C13-C14-C15-C16
45	i	402	PEE	O3P-C1-C2-O2
46	V	203	CDL	O1-C1-CB2-OB2
48	r	501	PLX	O6-C4-C5-O8
48	j	201	PLX	C18-C19-C20-C21
46	V	202	CDL	C55-C56-C57-C58
45	E	301	PEE	C11-C12-C13-C14
45	W	201	PEE	C43-C44-C45-C46
47	X	201	8Q1	C11-C12-C13-C14
45	i	403	PEE	C4-O4P-P-O3P
46	V	202	CDL	CA2-OA2-PA1-OA5
46	i	401	CDL	CA3-OA5-PA1-OA2
46	l	702	CDL	CB2-OB2-PB2-OB5
48	j	201	PLX	C3-O4-P1-O1
45	V	201	PEE	C14-C15-C16-C17
46	V	203	CDL	CA2-C1-CB2-OB2
45	i	402	PEE	C22-C23-C24-C25
47	F	201	8Q1	C6-C7-C8-C9
48	r	501	PLX	C3-C4-C5-O8
48	o	201	PLX	C4-C5-O8-C24
47	F	201	8Q1	O33-C32-C34-O35
45	i	402	PEE	C30-C31-C32-C33
46	V	203	CDL	C37-C38-C39-C40
48	r	501	PLX	C17-C18-C19-C20
46	V	203	CDL	CA7-C31-C32-C33
45	V	201	PEE	C11-C12-C13-C14
45	V	201	PEE	C43-C44-C45-C46
45	l	701	PEE	C40-C41-C42-C43
45	i	402	PEE	O3P-C1-C2-C3
48	o	201	PLX	O4-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
47	F	201	8Q1	C29-C32-C34-O35
48	j	201	PLX	C17-C18-C19-C20
46	V	202	CDL	C1-CA2-OA2-PA1
46	i	401	CDL	CA4-CA3-OA5-PA1
45	W	201	PEE	C33-C34-C35-C36
46	V	203	CDL	C33-C34-C35-C36
45	W	201	PEE	C30-C31-C32-C33
46	V	202	CDL	CA7-C31-C32-C33
45	E	301	PEE	C1-C2-C3-O3
46	V	202	CDL	CB3-CB4-CB6-OB8
48	j	201	PLX	C3-C4-C5-O8
48	s	401	PLX	C5-C4-O6-C6
46	V	202	CDL	CB5-C51-C52-C53
45	E	301	PEE	C34-C35-C36-C37
46	l	702	CDL	C31-C32-C33-C34
45	W	201	PEE	O2-C2-C3-O3
46	i	401	CDL	OA6-CA4-CA6-OA8
48	g	202	PLX	O6-C4-C5-O8
48	j	201	PLX	O6-C4-C5-O8
45	E	301	PEE	C32-C33-C34-C35
45	V	201	PEE	C31-C32-C33-C34
45	i	402	PEE	C2-C1-O3P-P
45	J	402	PEE	C2-C1-O3P-P
48	g	201	PLX	C27-C28-C29-C30
46	V	203	CDL	C17-C18-C19-C20
45	V	201	PEE	C13-C14-C15-C16
52	C	502	FMN	O2'-C2'-C3'-O3'
46	l	703	CDL	C72-C71-CB7-OB8
45	i	402	PEE	C18-C19-C20-C21
48	s	401	PLX	C13-C14-C15-C16
48	N	201	PLX	C35-C36-C37-C38
46	V	203	CDL	C15-C16-C17-C18
45	E	301	PEE	C39-C40-C41-C42
48	g	202	PLX	C3-C4-C5-O8
45	J	402	PEE	O3P-C1-C2-O2
48	o	201	PLX	O4-C3-C4-O6
45	i	403	PEE	C22-C23-C24-C25
48	j	201	PLX	C26-C27-C28-C29
46	l	702	CDL	CB2-C1-CA2-OA2
46	i	401	CDL	O1-C1-CA2-OA2
45	E	301	PEE	O2-C2-C3-O3
48	g	201	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
45	V	201	PEE	C39-C40-C41-C42
48	s	401	PLX	C28-C29-C30-C31
46	V	202	CDL	CB2-OB2-PB2-OB5
46	l	703	CDL	CA3-OA5-PA1-OA2
53	J	401	NDP	O4D-C1D-N1N-C6N
45	W	201	PEE	C2-C1-O3P-P
46	V	203	CDL	CB4-CB3-OB5-PB2
48	g	202	PLX	C4-C3-O4-P1
48	s	401	PLX	C7-C8-C9-C10
45	V	201	PEE	C1-O3P-P-O1P
45	J	402	PEE	C1-O3P-P-O1P
46	V	202	CDL	CA2-OA2-PA1-OA3
46	V	203	CDL	CA3-OA5-PA1-OA4
46	i	401	CDL	CB3-OB5-PB2-OB3
46	l	702	CDL	CA3-OA5-PA1-OA3
46	u	201	CDL	CA2-OA2-PA1-OA4
46	u	201	CDL	CA3-OA5-PA1-OA4
48	g	201	PLX	C3-O4-P1-O2
48	g	201	PLX	C3-O4-P1-O3
48	j	201	PLX	C3-O4-P1-O3
48	r	501	PLX	C2-O1-P1-O2
46	l	702	CDL	C31-CA7-OA8-CA6
46	i	401	CDL	OA5-CA3-CA4-CA6
45	W	201	PEE	C5-C4-O4P-P
45	l	701	PEE	C5-C4-O4P-P
45	J	402	PEE	C5-C4-O4P-P
48	j	201	PLX	C1-C2-O1-P1
48	N	201	PLX	C1-C2-O1-P1
48	o	201	PLX	C24-C25-C26-C27
46	i	401	CDL	OA5-CA3-CA4-OA6
45	i	403	PEE	C36-C37-C38-C39
45	l	701	PEE	C16-C17-C18-C19
45	E	301	PEE	C31-C32-C33-C34
45	i	402	PEE	C32-C33-C34-C35
46	u	201	CDL	C54-C55-C56-C57
48	g	201	PLX	C3-C4-C5-O8
48	g	202	PLX	N1-C1-C2-O1
48	o	201	PLX	N1-C1-C2-O1
48	N	201	PLX	N1-C1-C2-O1
46	V	202	CDL	OB6-CB4-CB6-OB8
48	g	202	PLX	C4-C5-O8-C24
48	r	501	PLX	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
45	i	402	PEE	C16-C17-C18-C19
45	i	403	PEE	C16-C17-C18-C19
48	s	401	PLX	C10-C11-C12-C13
48	g	201	PLX	C16-C17-C18-C19
45	l	701	PEE	C18-C19-C20-C21
48	s	401	PLX	C14-C15-C16-C17
46	l	702	CDL	CB6-CB4-OB6-CB5
46	l	703	CDL	CB6-CB4-OB6-CB5
48	g	202	PLX	C6-C7-C8-C9
45	i	403	PEE	C2-C1-O3P-P
48	r	501	PLX	C4-C3-O4-P1
48	r	501	PLX	C13-C14-C15-C16
45	W	201	PEE	C2-C3-O3-C30
48	j	201	PLX	C32-C33-C34-C35
45	i	403	PEE	C38-C39-C40-C41
45	J	402	PEE	C38-C39-C40-C41
47	X	201	8Q1	C6-C7-C8-C9
45	V	201	PEE	C4-O4P-P-O3P
45	l	701	PEE	C1-O3P-P-O4P
45	J	402	PEE	C4-O4P-P-O3P
46	V	202	CDL	CA3-OA5-PA1-OA2
46	V	203	CDL	CA2-OA2-PA1-OA5
46	i	401	CDL	CA2-OA2-PA1-OA5
46	l	702	CDL	CB3-OB5-PB2-OB2
46	u	201	CDL	CB2-OB2-PB2-OB5
48	g	202	PLX	C3-O4-P1-O1
48	j	201	PLX	C2-O1-P1-O4
48	r	501	PLX	C3-O4-P1-O1
48	s	401	PLX	C3-O4-P1-O1
48	s	401	PLX	C2-O1-P1-O4
46	l	703	CDL	C53-C54-C55-C56
45	W	201	PEE	C1-C2-C3-O3
45	E	301	PEE	C36-C37-C38-C39
49	w	401	DGT	PB-O3A-PA-O1A
46	i	401	CDL	C1-CA2-OA2-PA1
45	J	402	PEE	C18-C19-C20-C21
48	r	501	PLX	C10-C11-C12-C13
46	l	702	CDL	C33-C34-C35-C36
48	o	201	PLX	C13-C14-C15-C16
45	l	701	PEE	C37-C38-C39-C40
46	l	702	CDL	C73-C74-C75-C76
46	i	401	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
48	r	501	PLX	C33-C34-C35-C36
46	V	203	CDL	C71-C72-C73-C74
46	l	703	CDL	C18-C19-C20-C21
48	s	401	PLX	O6-C6-C7-C8
48	N	201	PLX	O8-C24-C25-C26
48	o	201	PLX	C17-C18-C19-C20
48	N	201	PLX	C4-C3-O4-P1
45	V	201	PEE	C19-C20-C21-C22
45	l	701	PEE	C19-C20-C21-C22
46	l	702	CDL	C32-C33-C34-C35
48	r	501	PLX	C29-C30-C31-C32
47	F	201	8Q1	C29-C32-C34-N36
45	V	201	PEE	C40-C41-C42-C43
46	l	703	CDL	CA6-CA4-OA6-CA5
45	V	201	PEE	C38-C39-C40-C41
45	J	402	PEE	C36-C37-C38-C39
46	V	203	CDL	C53-C54-C55-C56
48	g	201	PLX	C9-C10-C11-C12
48	s	401	PLX	C26-C27-C28-C29
48	N	201	PLX	O9-C24-C25-C26
48	s	401	PLX	C6-C7-C8-C9
45	i	402	PEE	C37-C38-C39-C40
45	V	201	PEE	O3P-C1-C2-C3
45	J	402	PEE	O3P-C1-C2-C3
45	V	201	PEE	C32-C33-C34-C35
45	i	402	PEE	C20-C21-C22-C23
45	l	701	PEE	C23-C24-C25-C26
45	l	701	PEE	C31-C32-C33-C34
45	l	701	PEE	C38-C39-C40-C41
45	V	201	PEE	O3P-C1-C2-O2
48	g	202	PLX	O8-C24-C25-C26
48	j	201	PLX	O6-C6-C7-C8
46	l	702	CDL	C11-CA5-OA6-CA4
47	X	201	8Q1	O33-C32-C34-O35
48	j	201	PLX	C11-C10-C9-C8
48	o	201	PLX	C6-C7-C8-C9
46	V	202	CDL	C52-C51-CB5-OB6
48	N	201	PLX	C31-C32-C33-C34
46	V	203	CDL	C12-C11-CA5-OA6
45	V	201	PEE	C16-C17-C18-C19
45	l	701	PEE	C36-C37-C38-C39
46	V	203	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
48	g	202	PLX	C7-C6-O6-C4
48	j	201	PLX	C7-C6-O6-C4
45	l	701	PEE	O3P-C1-C2-O2
46	V	202	CDL	C32-C31-CA7-OA8
45	i	402	PEE	C33-C34-C35-C36
48	g	202	PLX	C15-C16-C17-C18
46	V	202	CDL	OA6-CA4-CA6-OA8
46	l	702	CDL	OA9-CA7-OA8-CA6
45	V	201	PEE	O2-C10-C11-C12
48	o	201	PLX	O7-C6-C7-C8
48	s	401	PLX	O9-C24-C25-C26
53	J	401	NDP	C5D-O5D-PN-O3
46	l	702	CDL	C32-C31-CA7-OA8
46	l	703	CDL	C16-C17-C18-C19
53	J	401	NDP	O4B-C4B-C5B-O5B
45	l	701	PEE	O3-C30-C31-C32
49	w	401	DGT	PB-O3A-PA-O2A
45	i	403	PEE	C32-C33-C34-C35
45	E	301	PEE	C35-C36-C37-C38
45	E	301	PEE	C12-C13-C14-C15
48	r	501	PLX	C12-C13-C14-C15
48	r	501	PLX	C25-C26-C27-C28
46	V	203	CDL	C12-C11-CA5-OA7
46	V	202	CDL	C52-C51-CB5-OB7
46	i	401	CDL	CA3-CA4-CA6-OA8
46	V	203	CDL	CA4-CA3-OA5-PA1
45	V	201	PEE	O4-C10-C11-C12
45	V	201	PEE	C4-O4P-P-O1P
46	V	203	CDL	CB2-OB2-PB2-OB4
46	i	401	CDL	CA3-OA5-PA1-OA3
46	i	401	CDL	CA3-OA5-PA1-OA4
46	u	201	CDL	CB2-OB2-PB2-OB3
48	g	201	PLX	C2-O1-P1-O2
48	s	401	PLX	C3-O4-P1-O2
48	s	401	PLX	O4-C3-C4-C5
48	j	201	PLX	C27-C28-C29-C30
45	l	701	PEE	C15-C16-C17-C18
46	V	202	CDL	C32-C31-CA7-OA9
46	u	201	CDL	C31-C32-C33-C34
46	l	702	CDL	CB3-CB4-OB6-CB5
46	l	703	CDL	CA3-CA4-OA6-CA5
48	o	201	PLX	C25-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
48	s	401	PLX	C1-C2-O1-P1
48	o	201	PLX	C10-C11-C12-C13
45	V	201	PEE	C36-C37-C38-C39
46	l	703	CDL	C72-C71-CB7-OB9
45	i	403	PEE	O3-C30-C31-C32
46	l	703	CDL	C52-C51-CB5-OB6
46	l	703	CDL	C52-C51-CB5-OB7
45	W	201	PEE	O3-C30-C31-C32
45	l	701	PEE	O5-C30-C31-C32
46	V	203	CDL	C32-C31-CA7-OA8

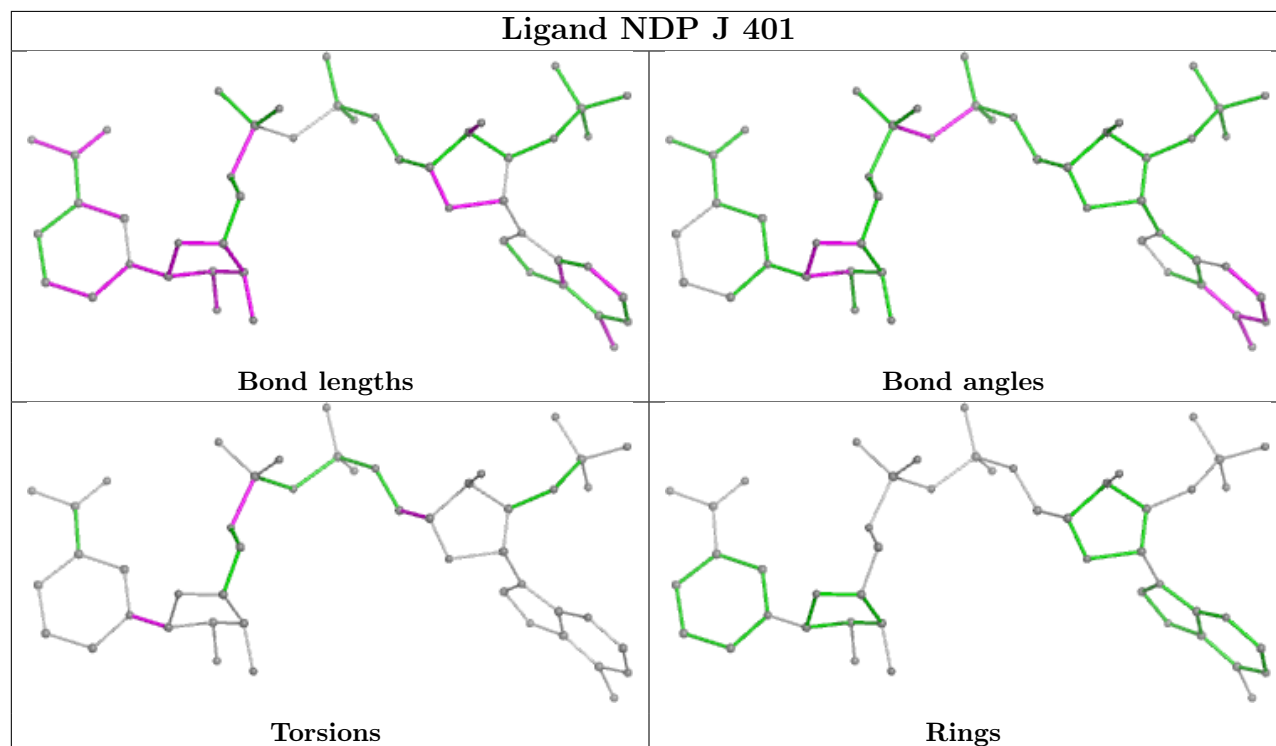
There are no ring outliers.

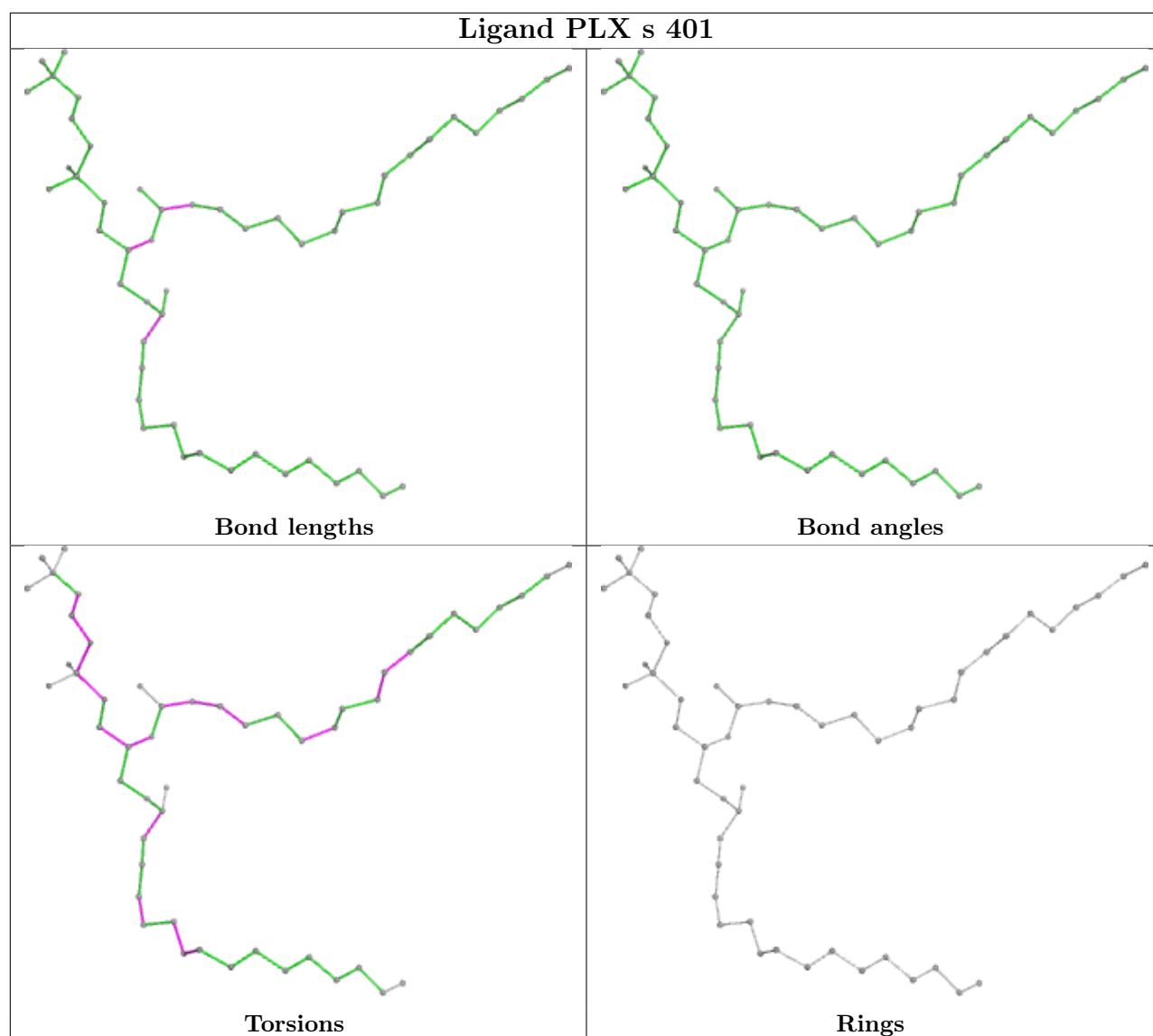
17 monomers are involved in 55 short contacts:

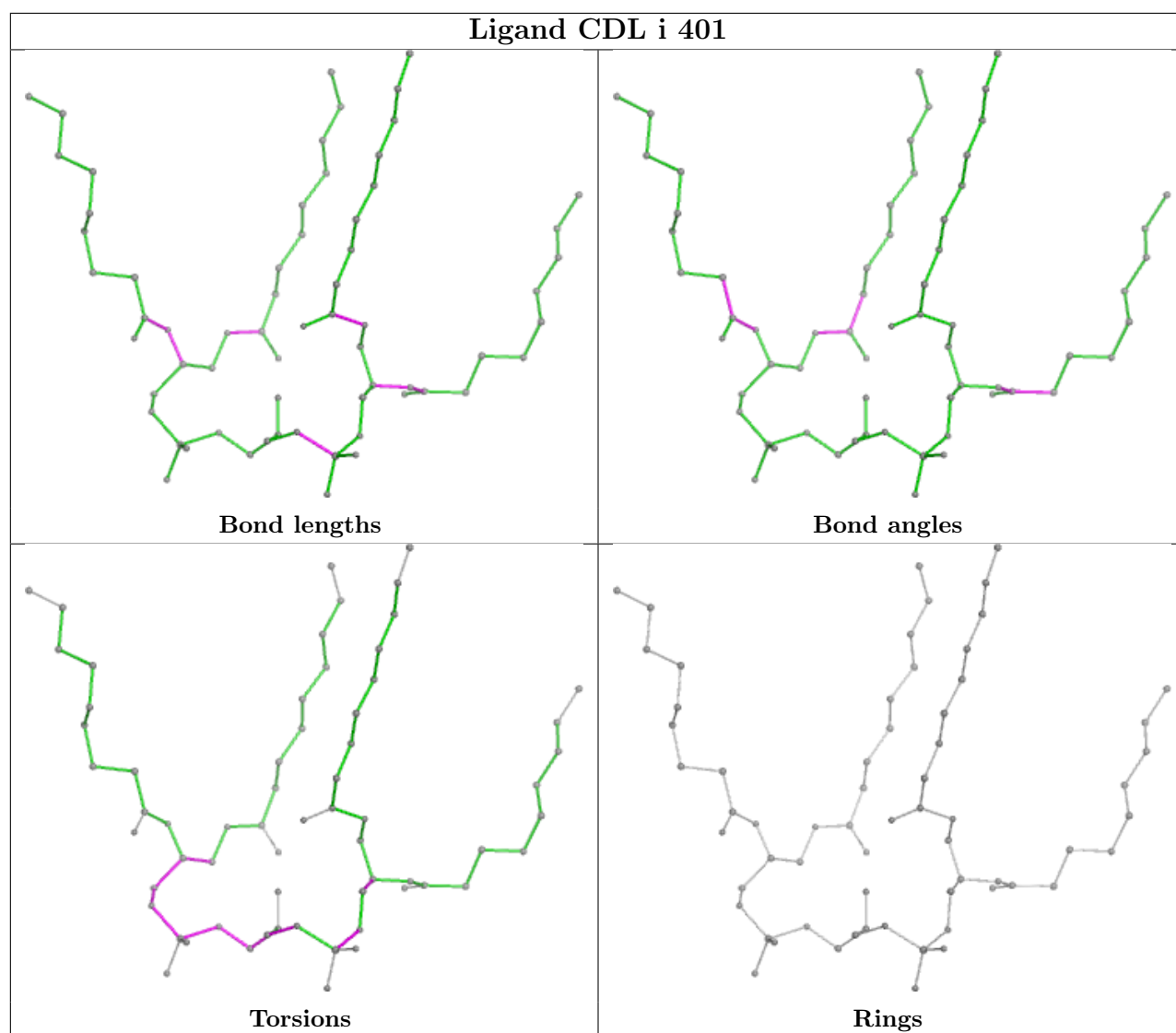
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	J	401	NDP	1	0
48	s	401	PLX	1	0
51	C	501	SF4	3	0
47	F	201	8Q1	1	0
45	E	301	PEE	3	0
45	i	402	PEE	2	0
51	M	801	SF4	1	0
45	l	701	PEE	2	0
48	g	201	PLX	1	0
52	C	502	FMN	32	0
46	l	702	CDL	1	0
45	V	201	PEE	2	0
49	w	401	DGT	1	0
54	O	301	FES	1	0
46	l	703	CDL	1	0
51	M	802	SF4	1	0
51	E	302	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

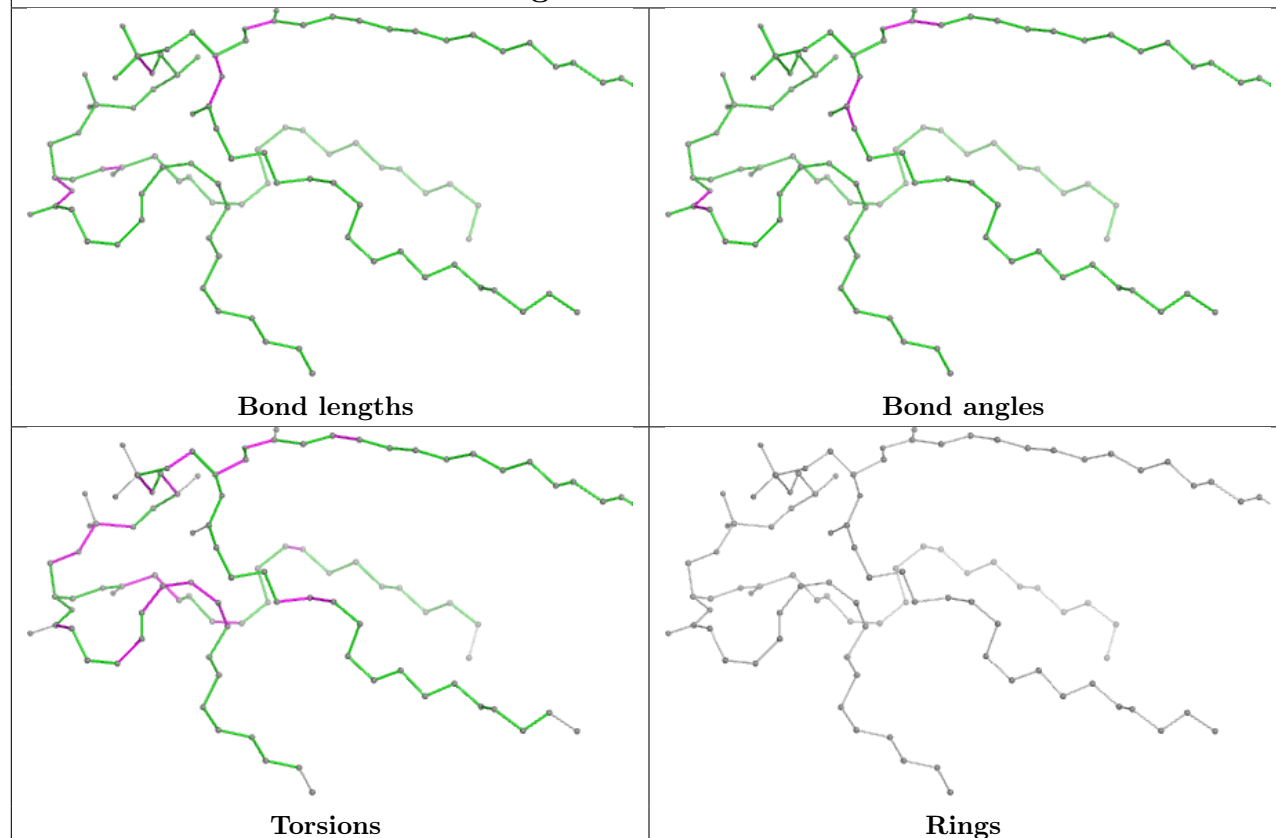
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



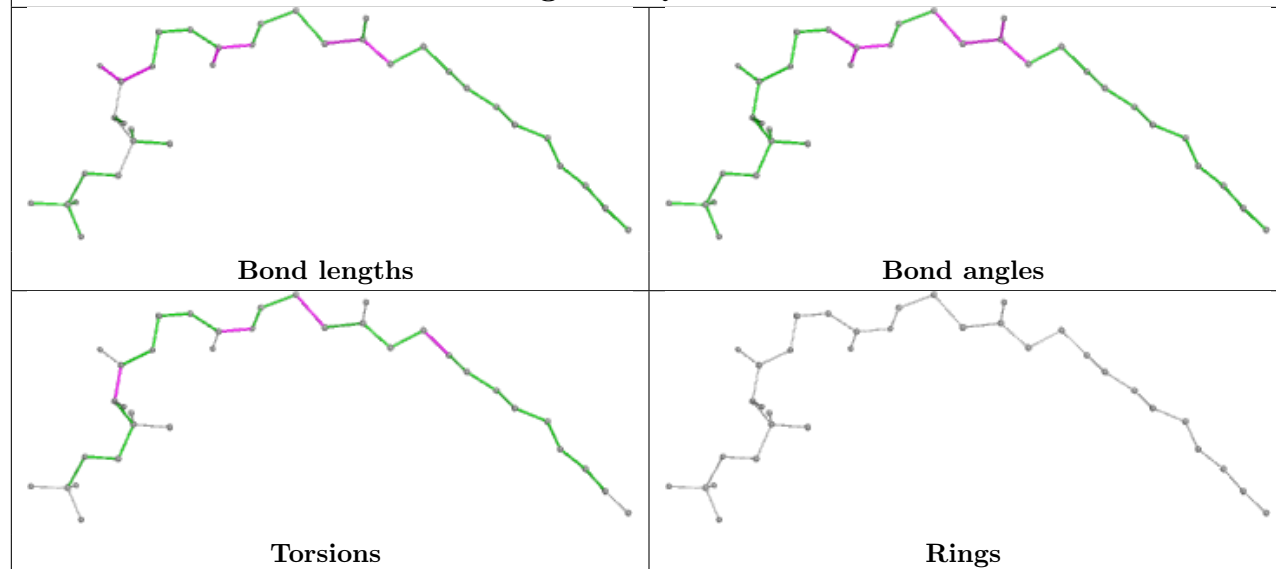


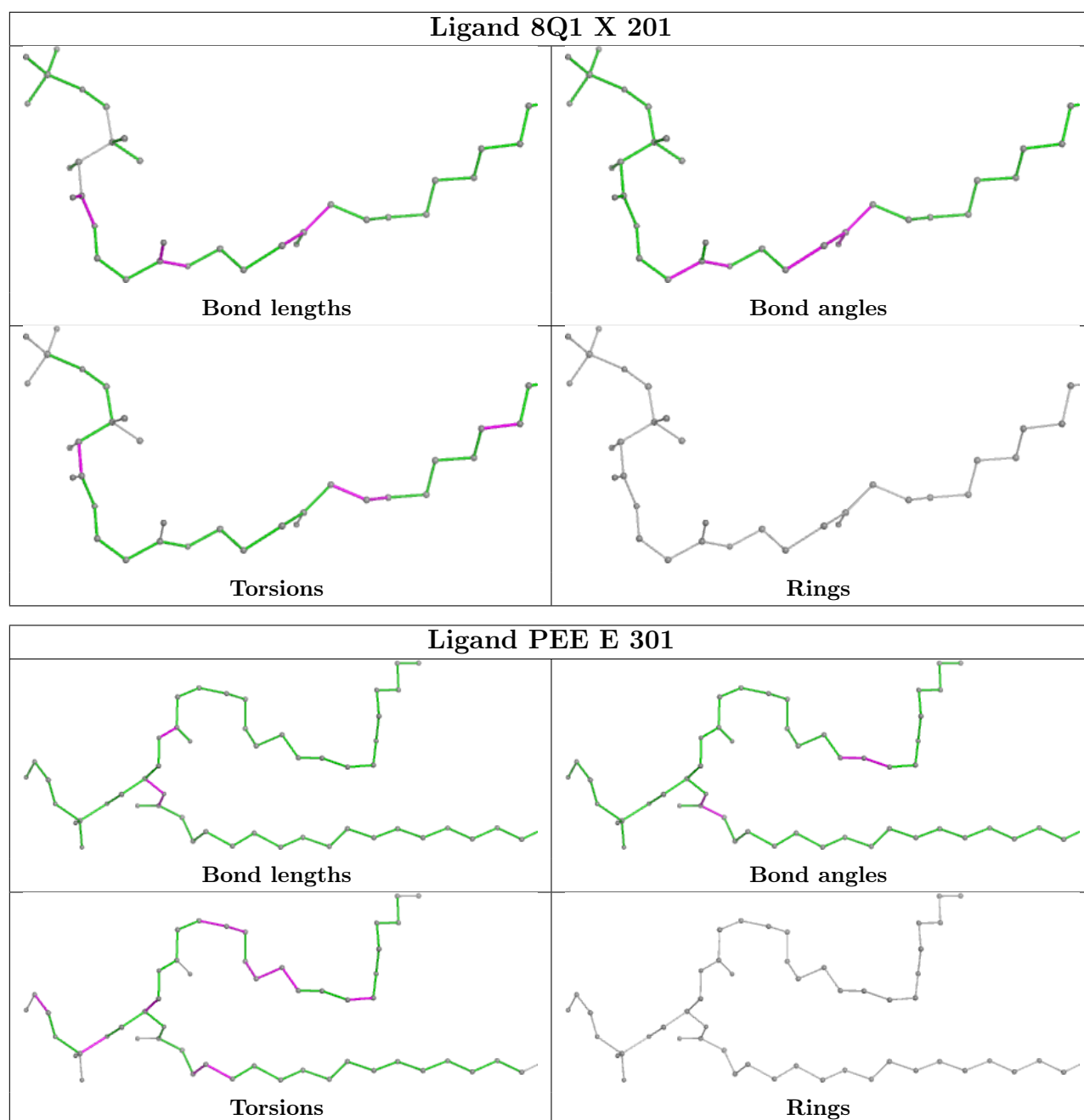


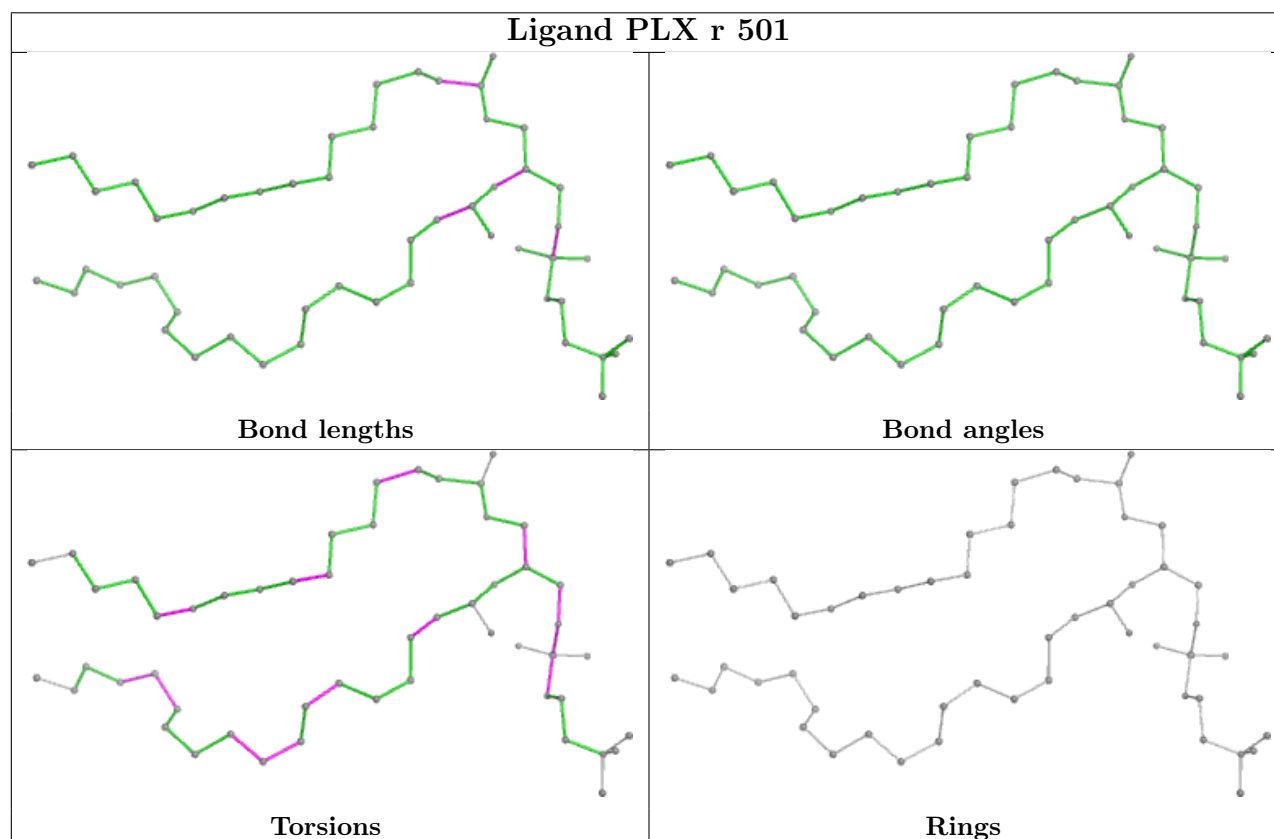
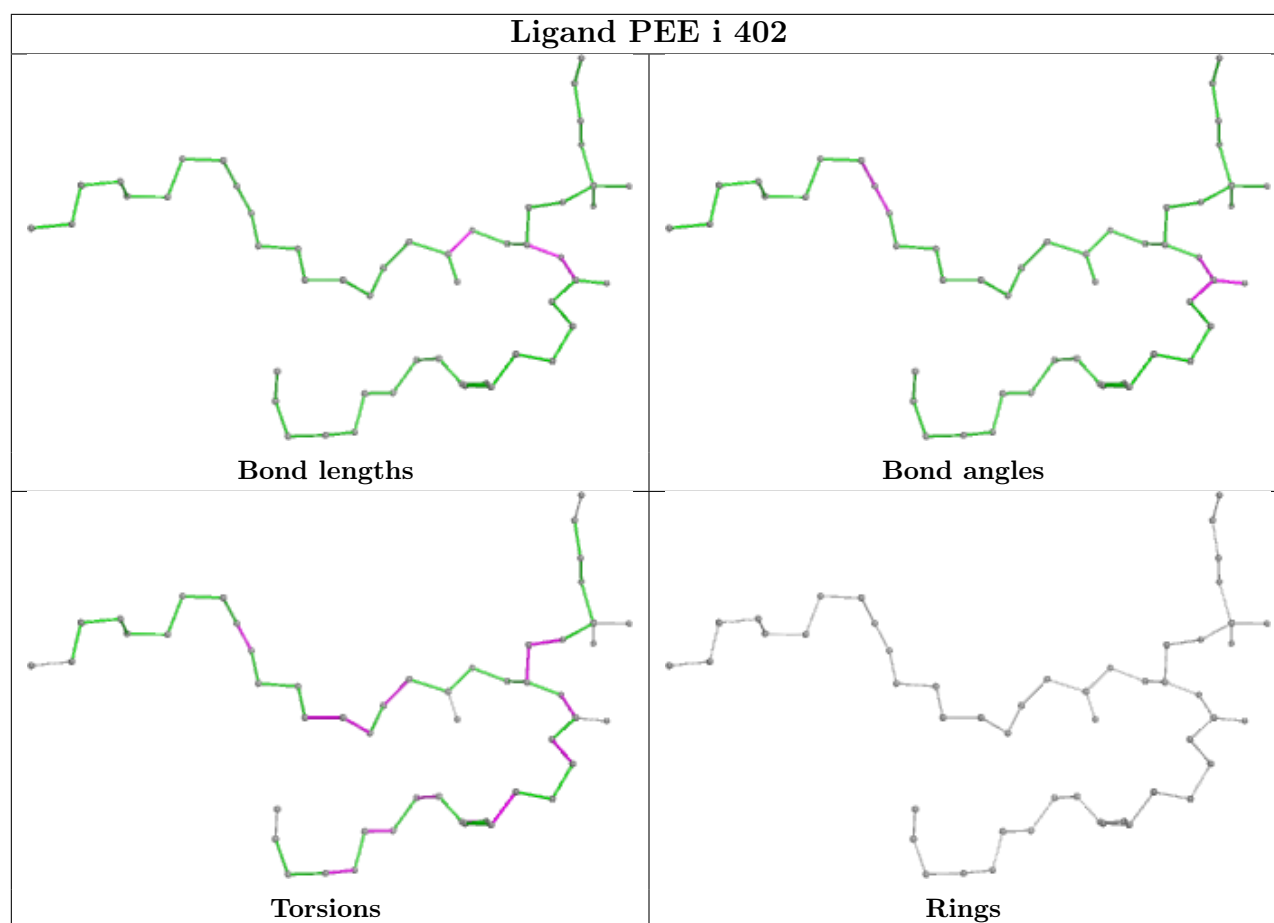
Ligand CDL V 203

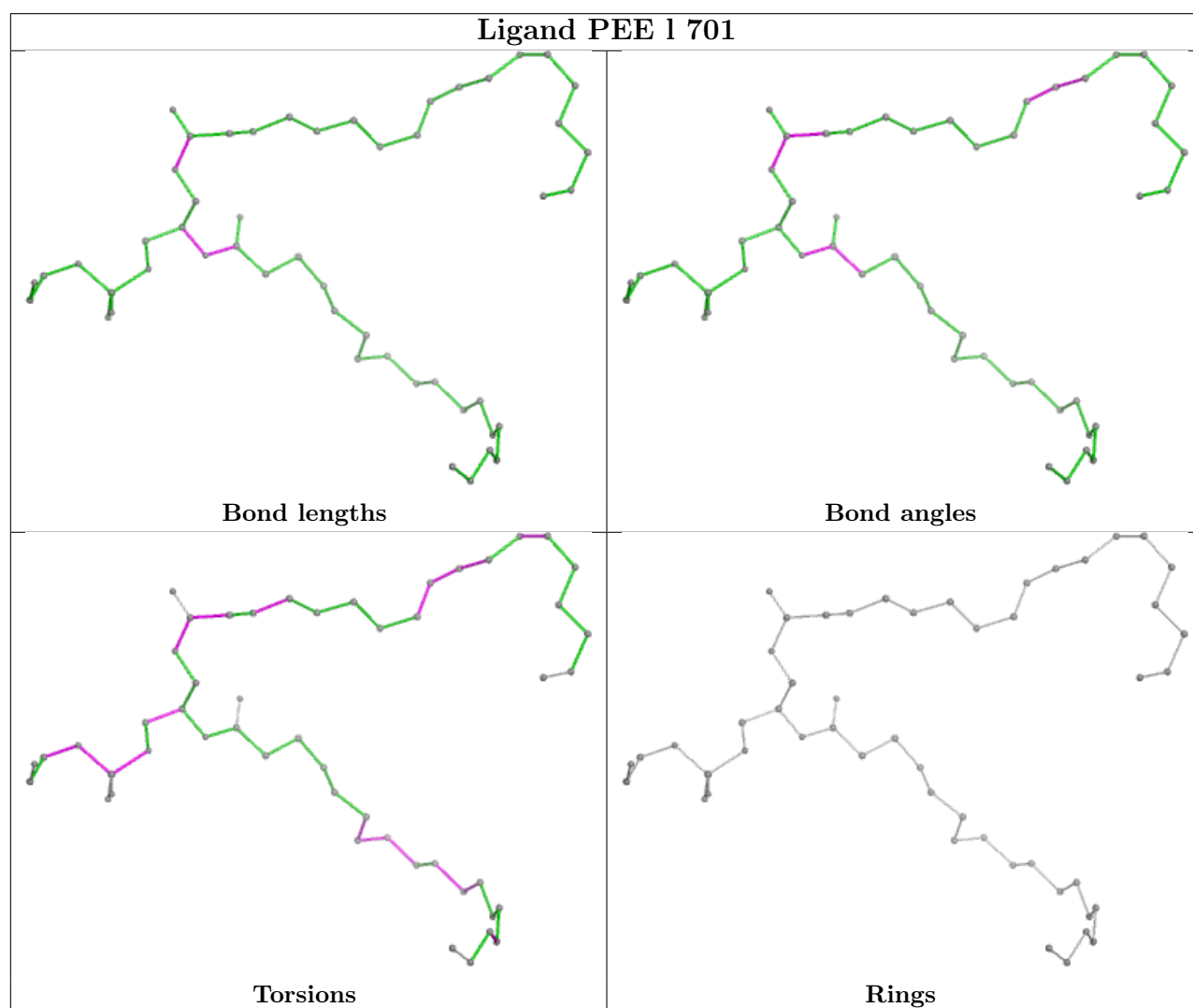
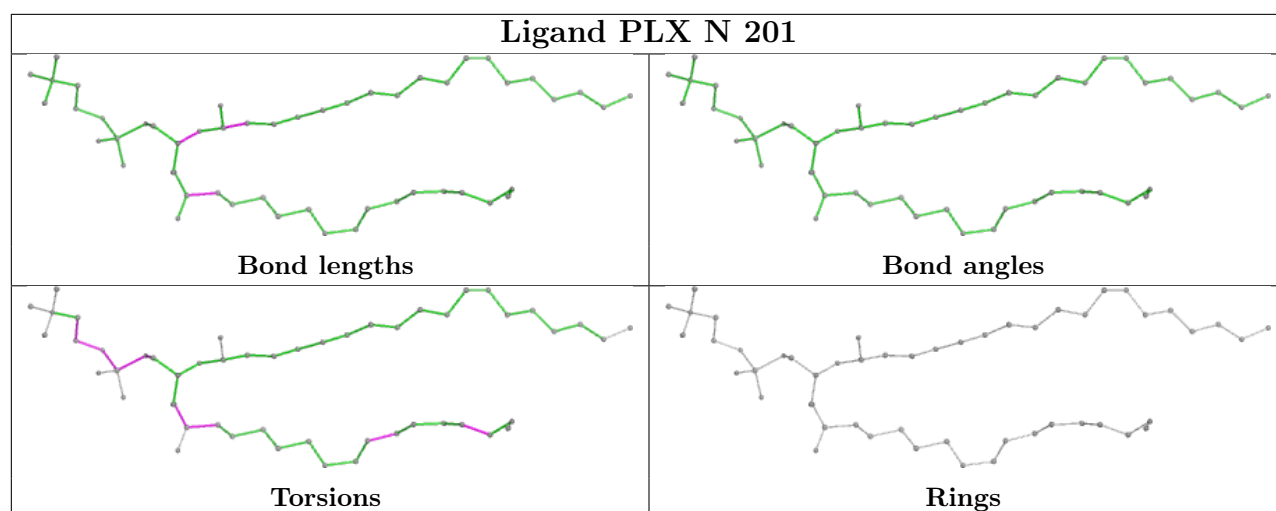


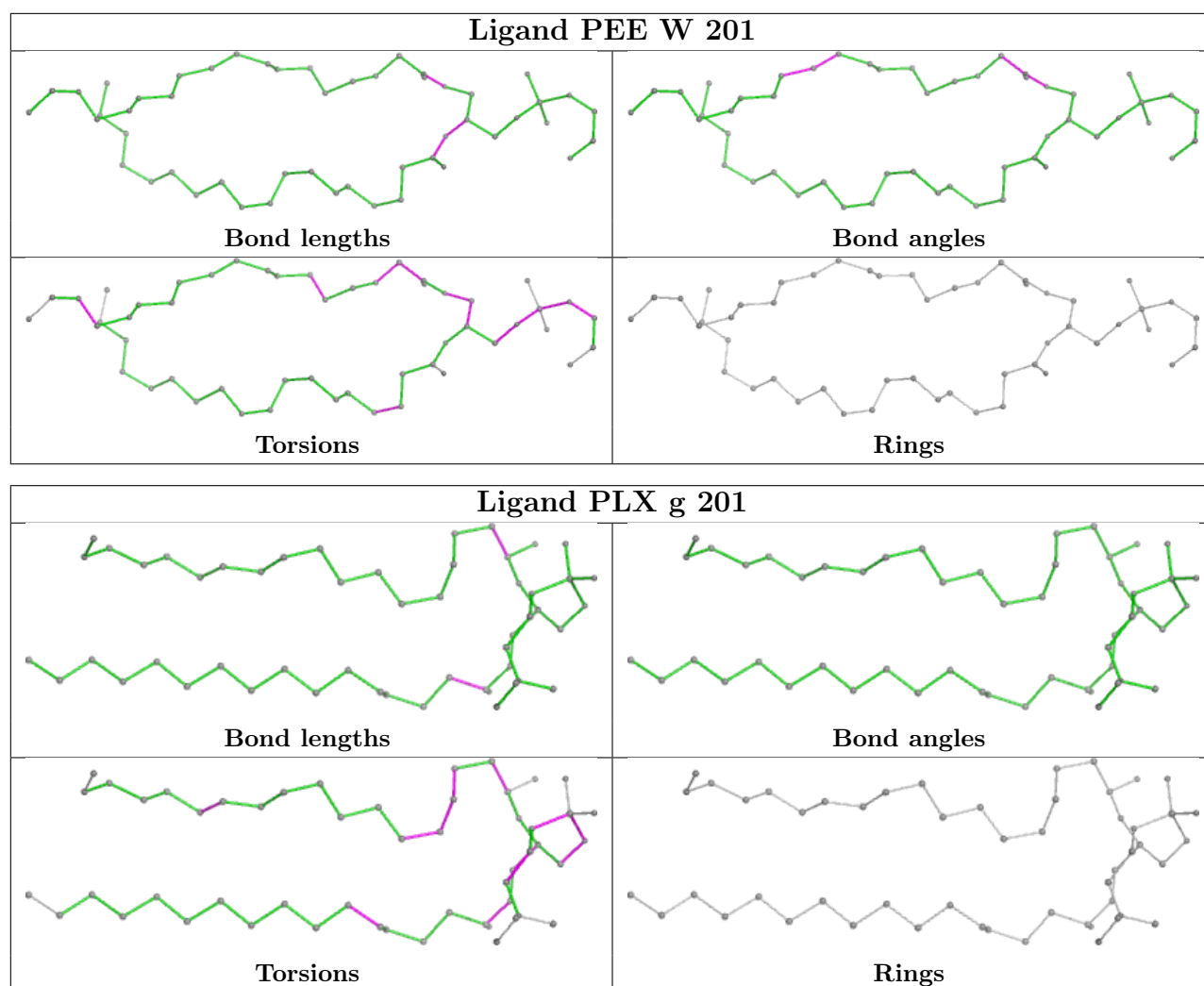
Ligand 8Q1 F 201

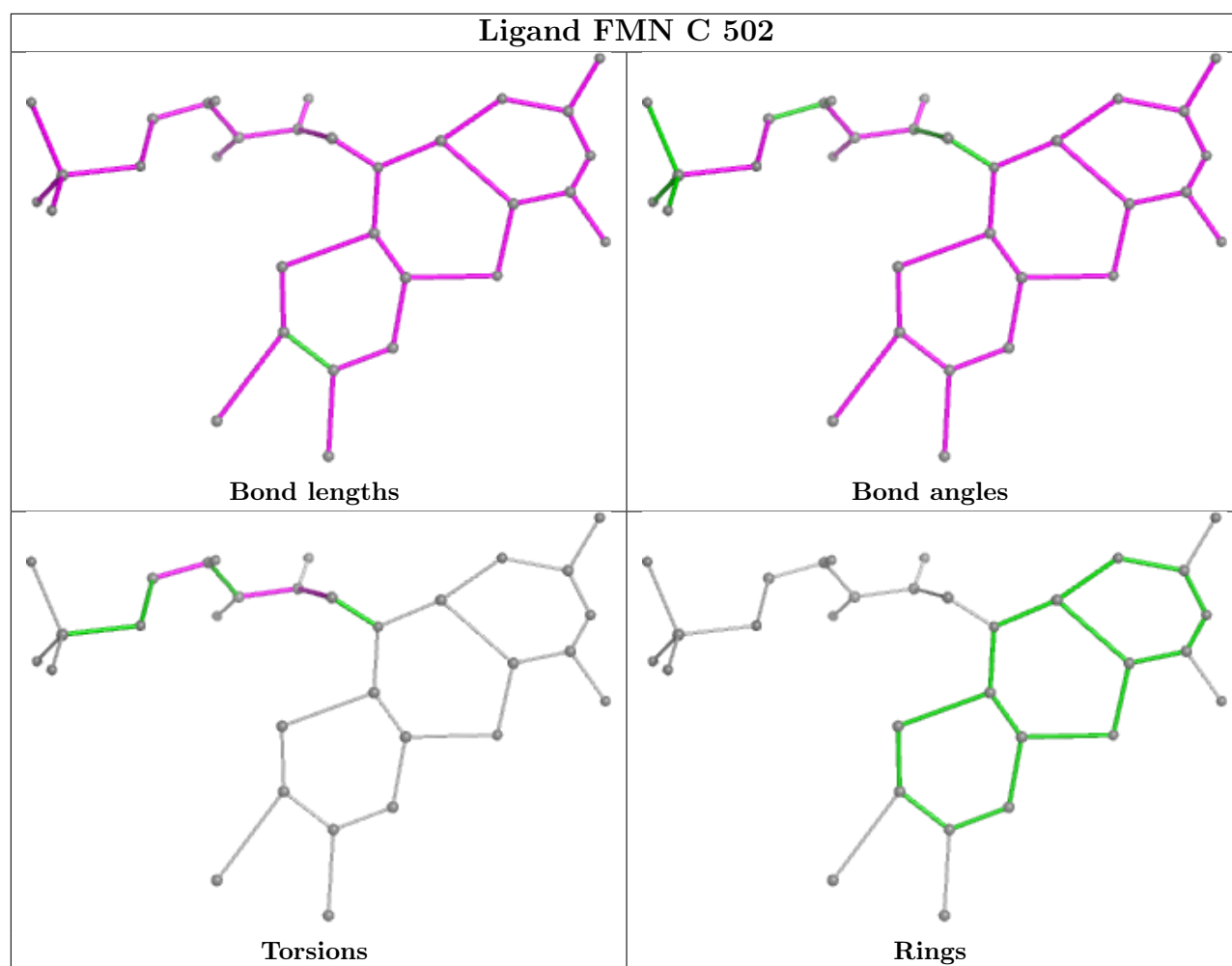


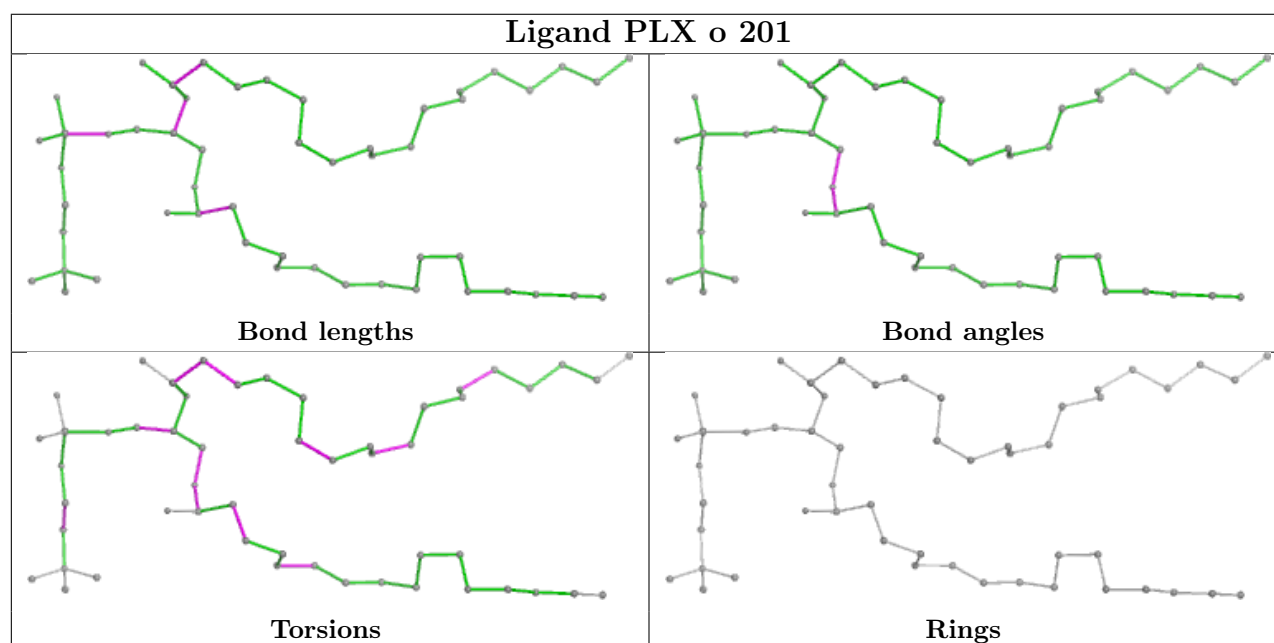
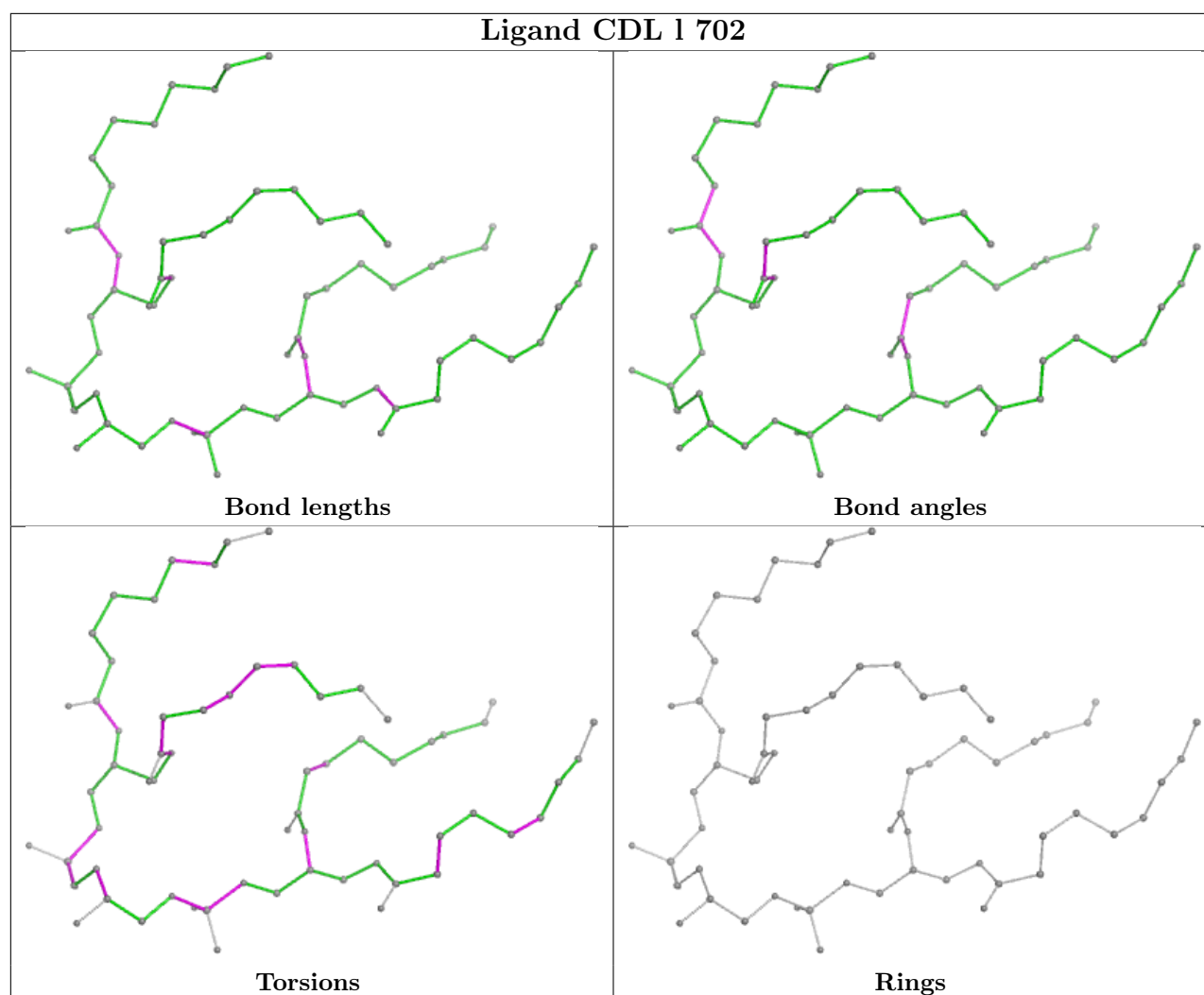


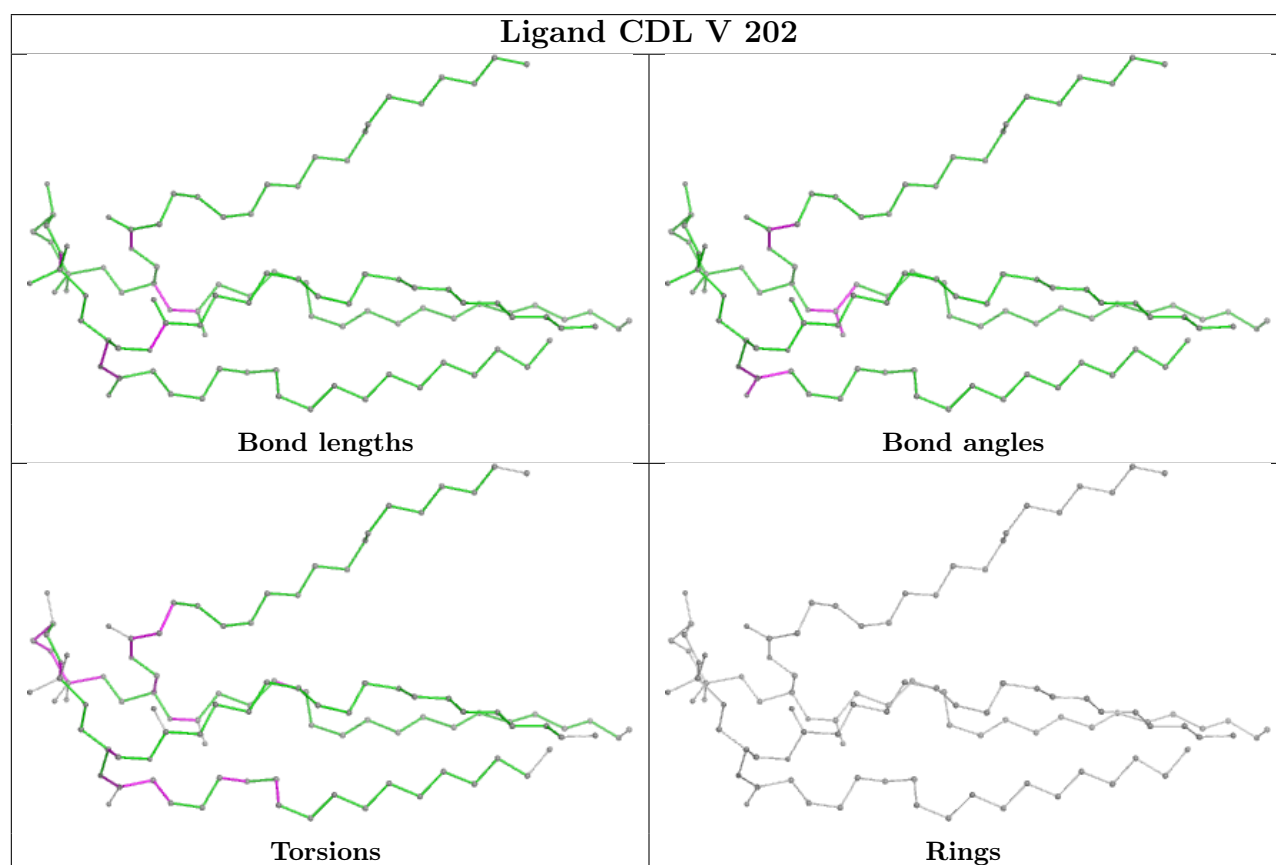
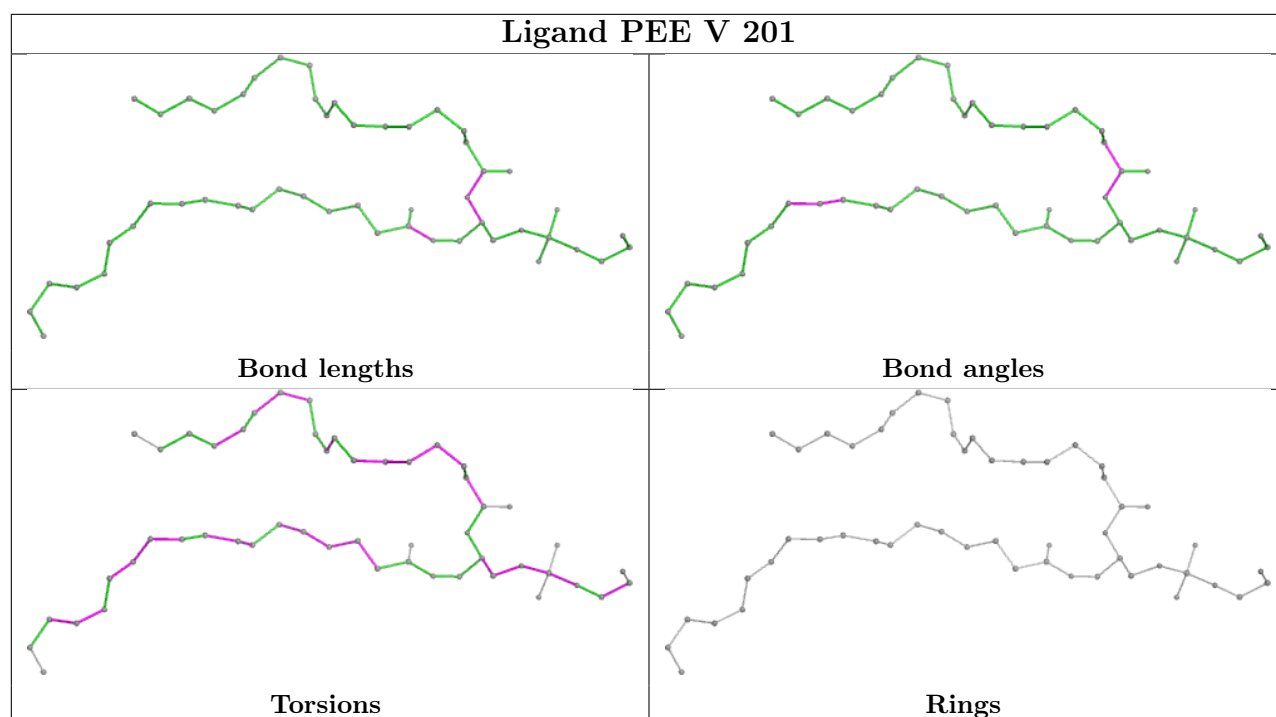


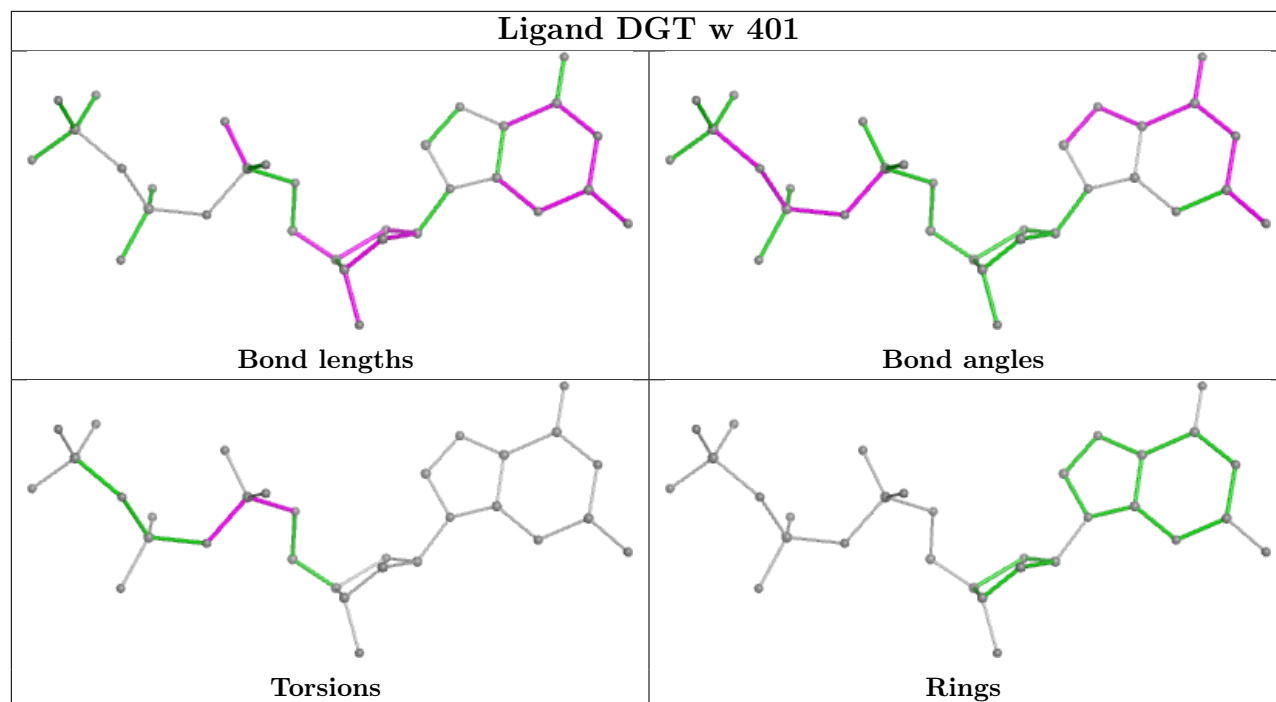


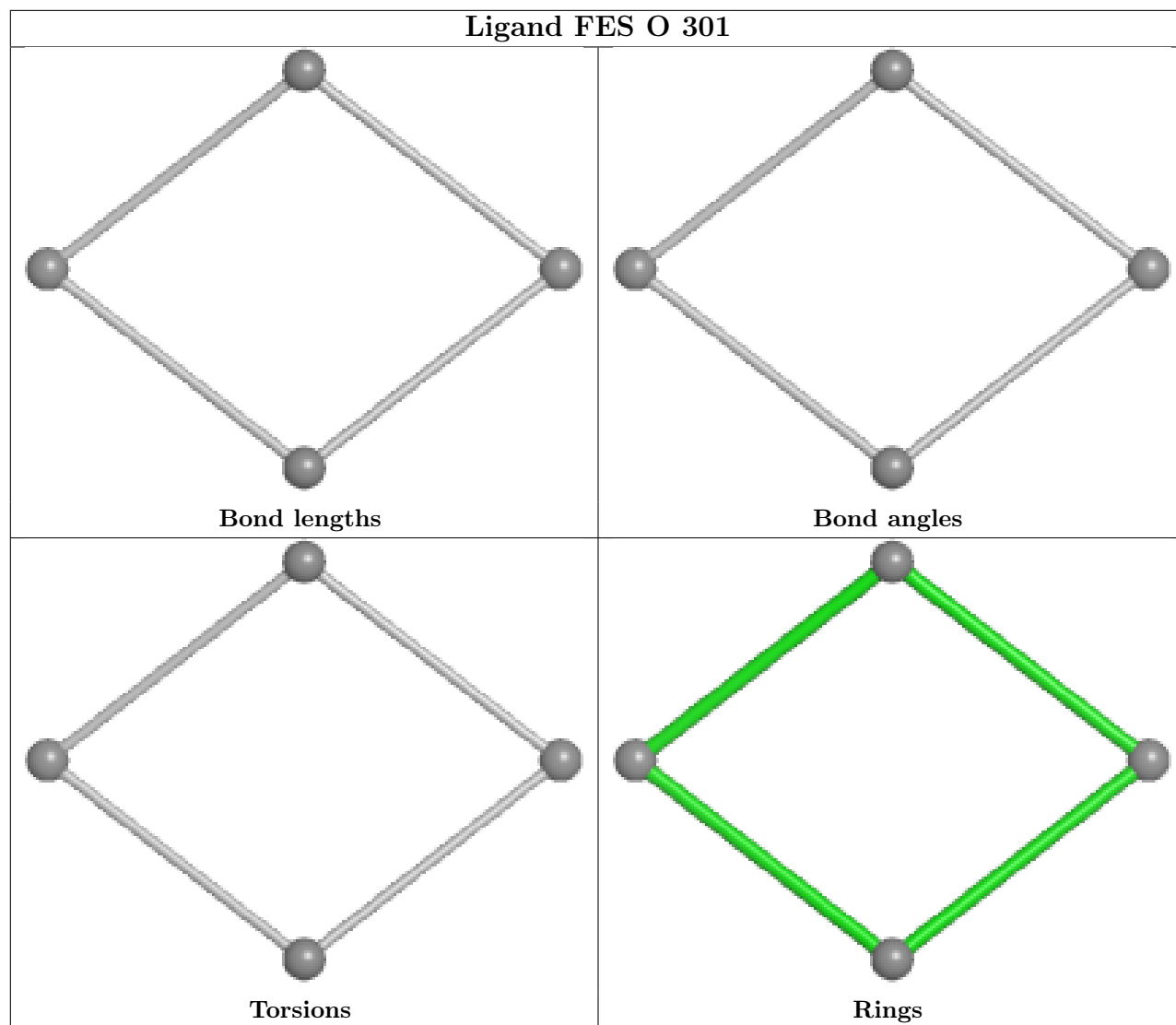




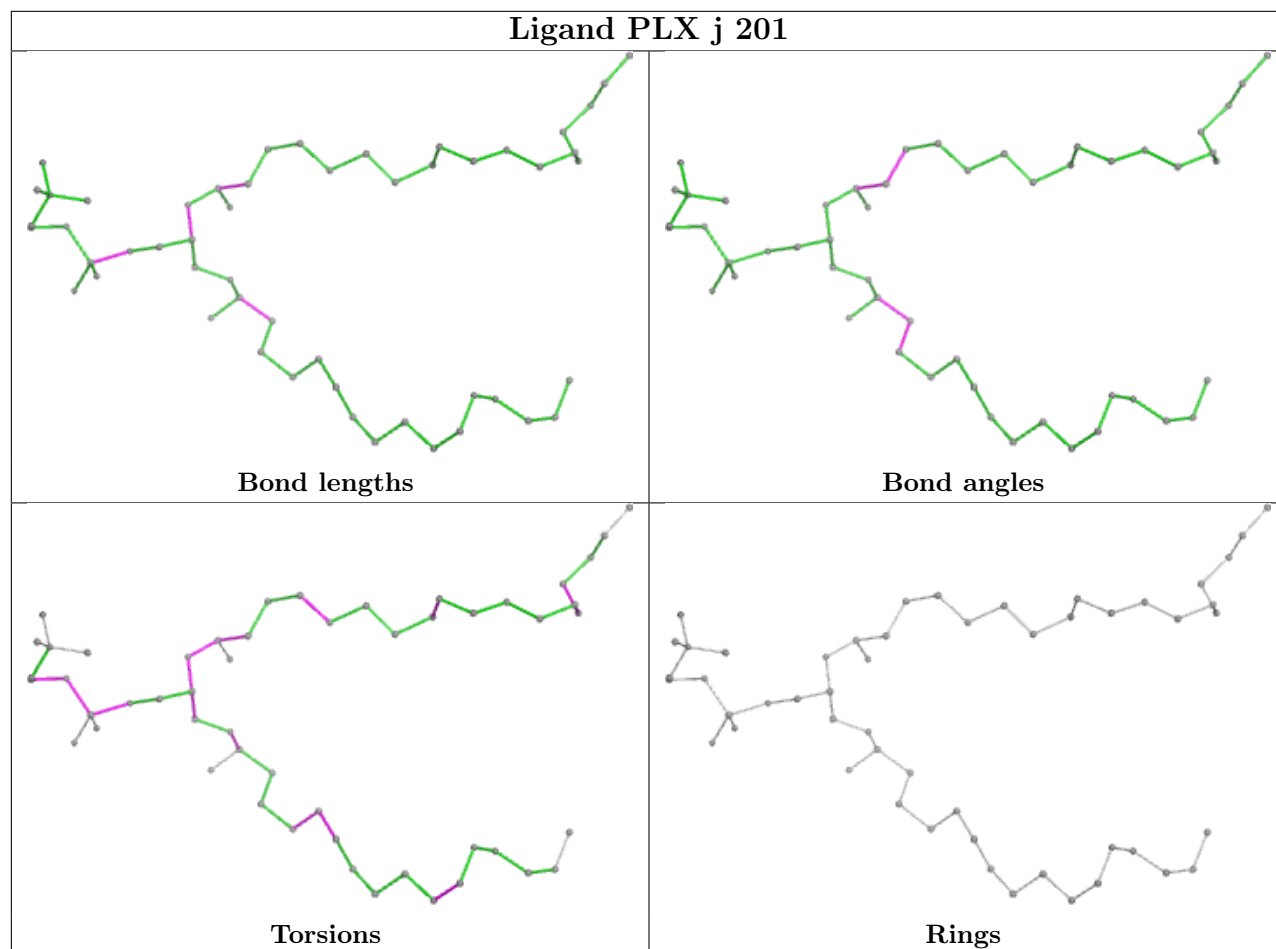




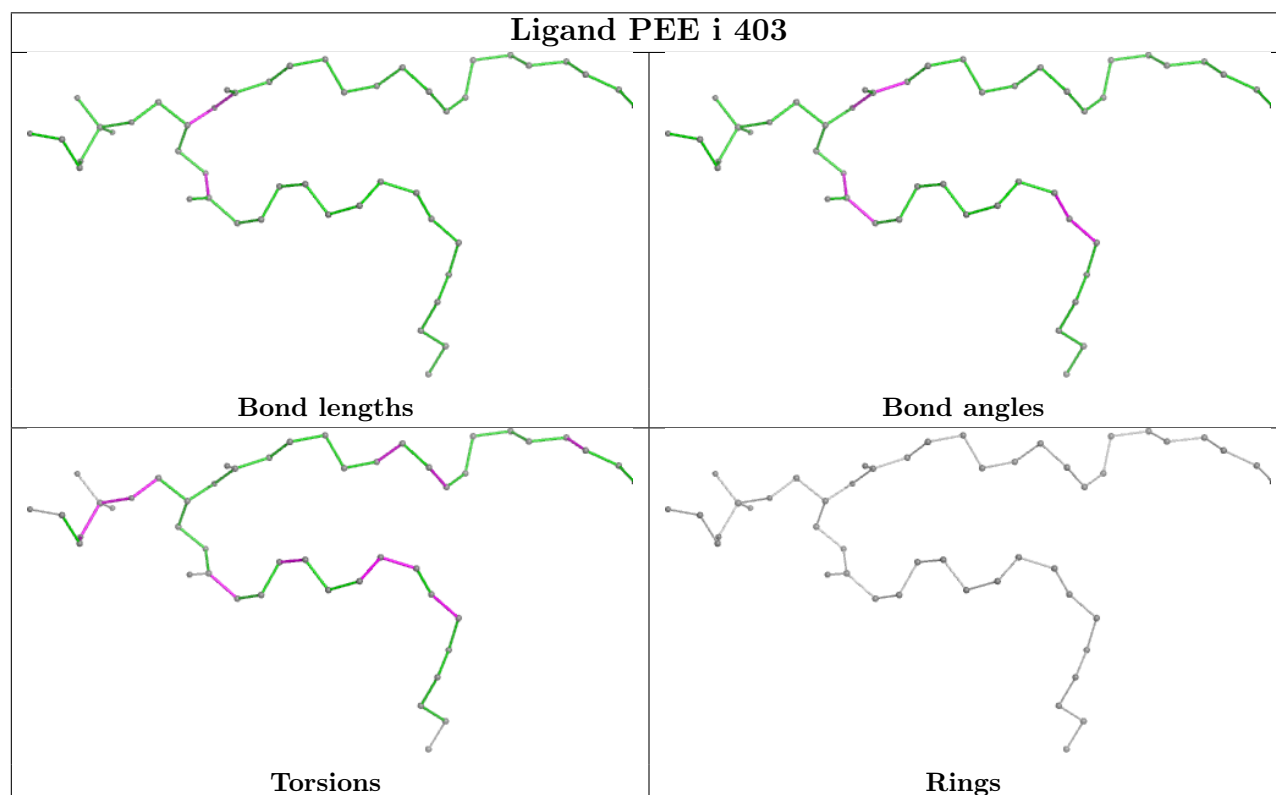


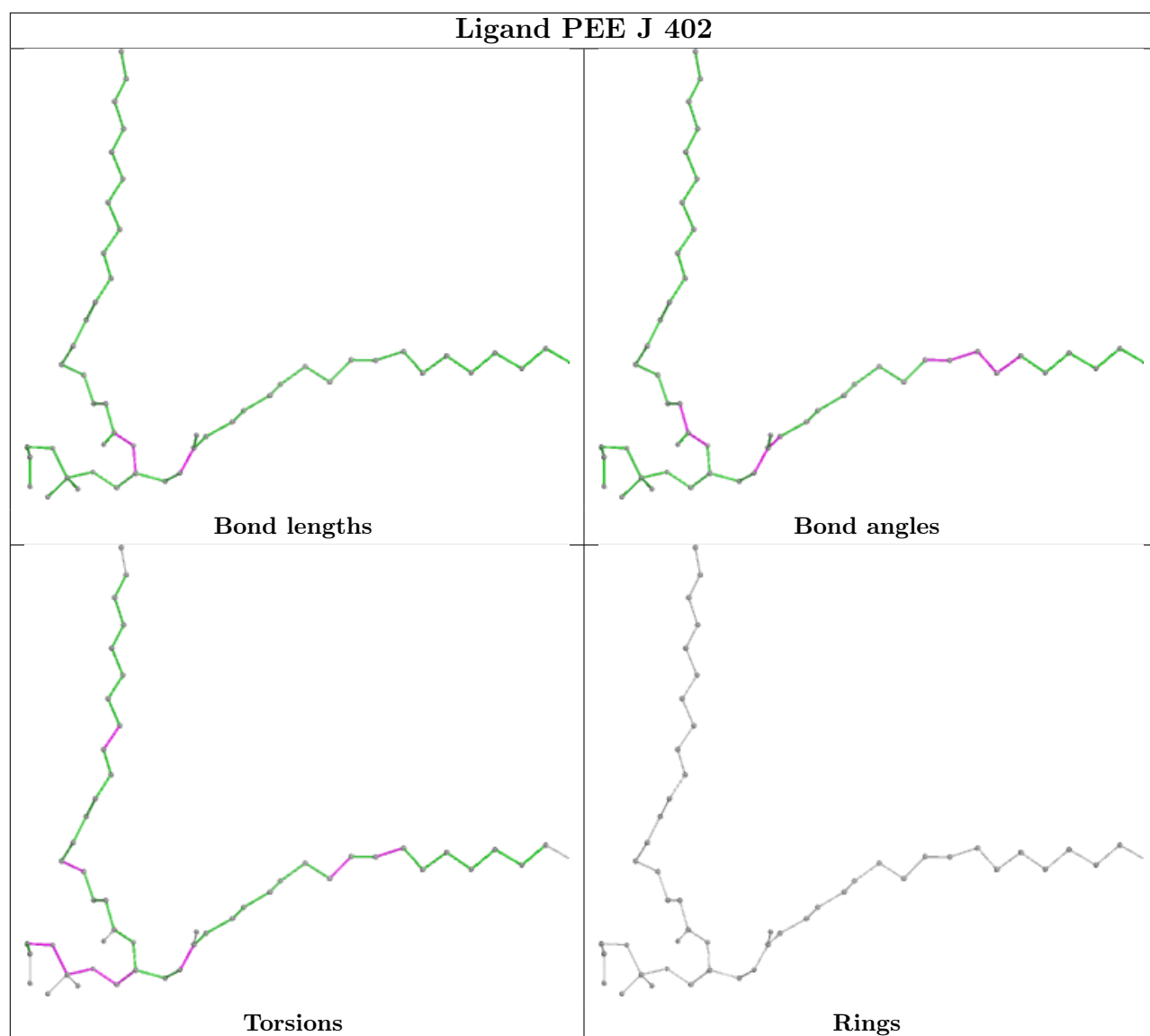


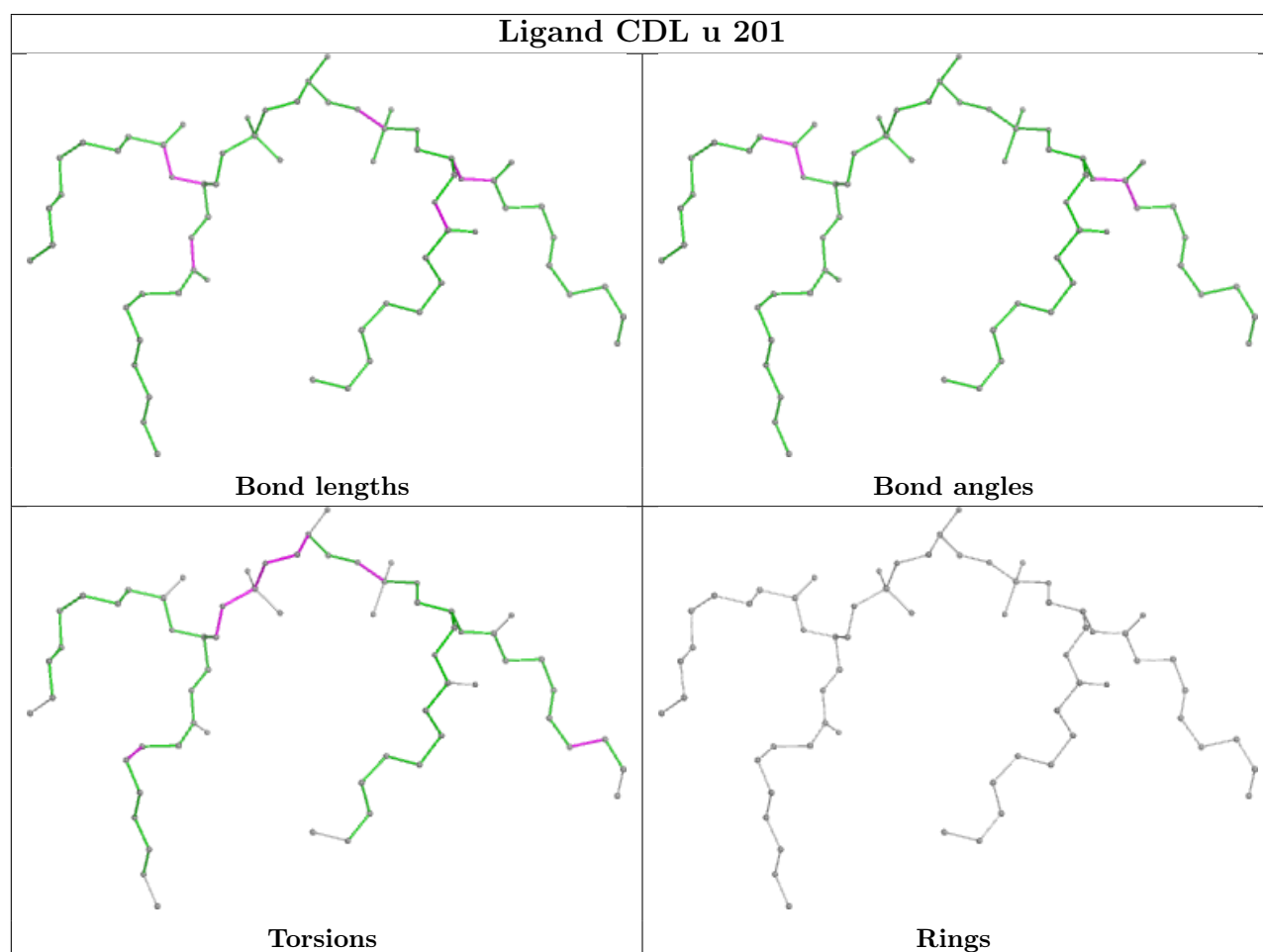
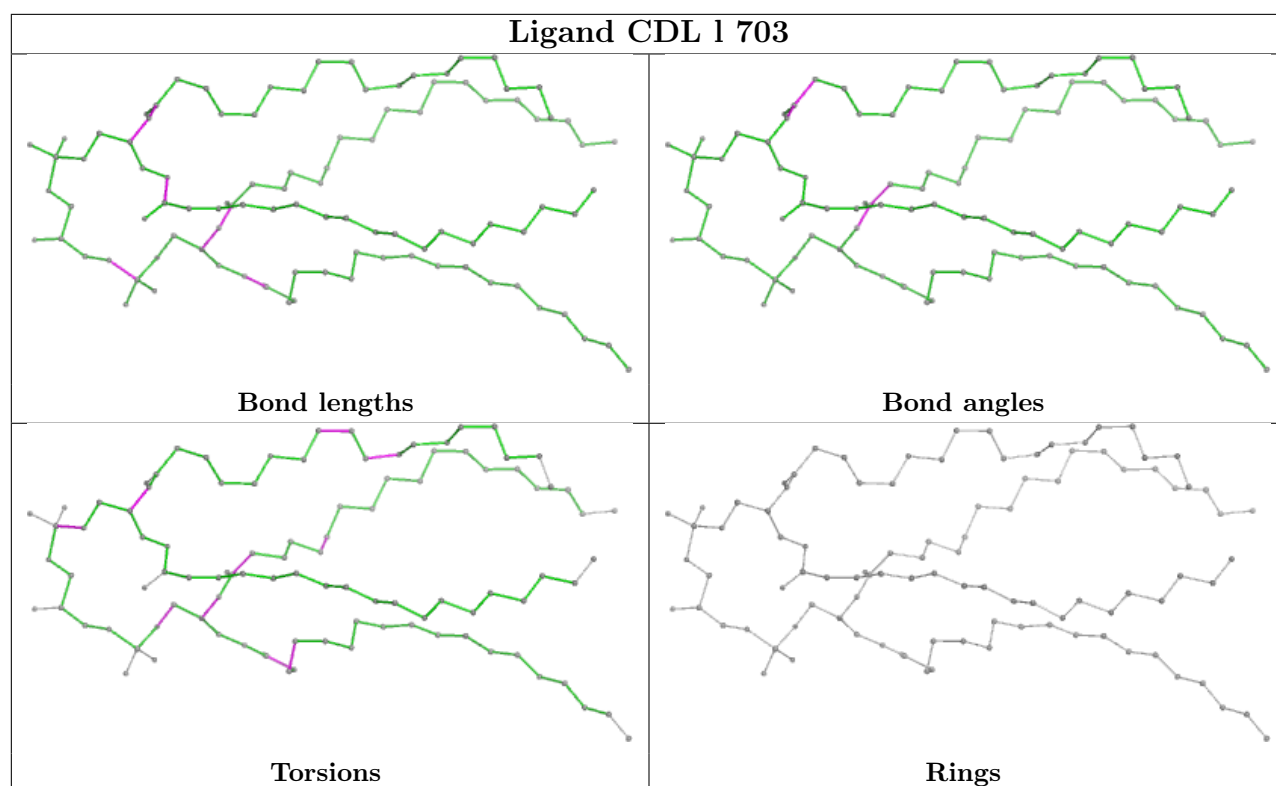
Ligand PLX j 201

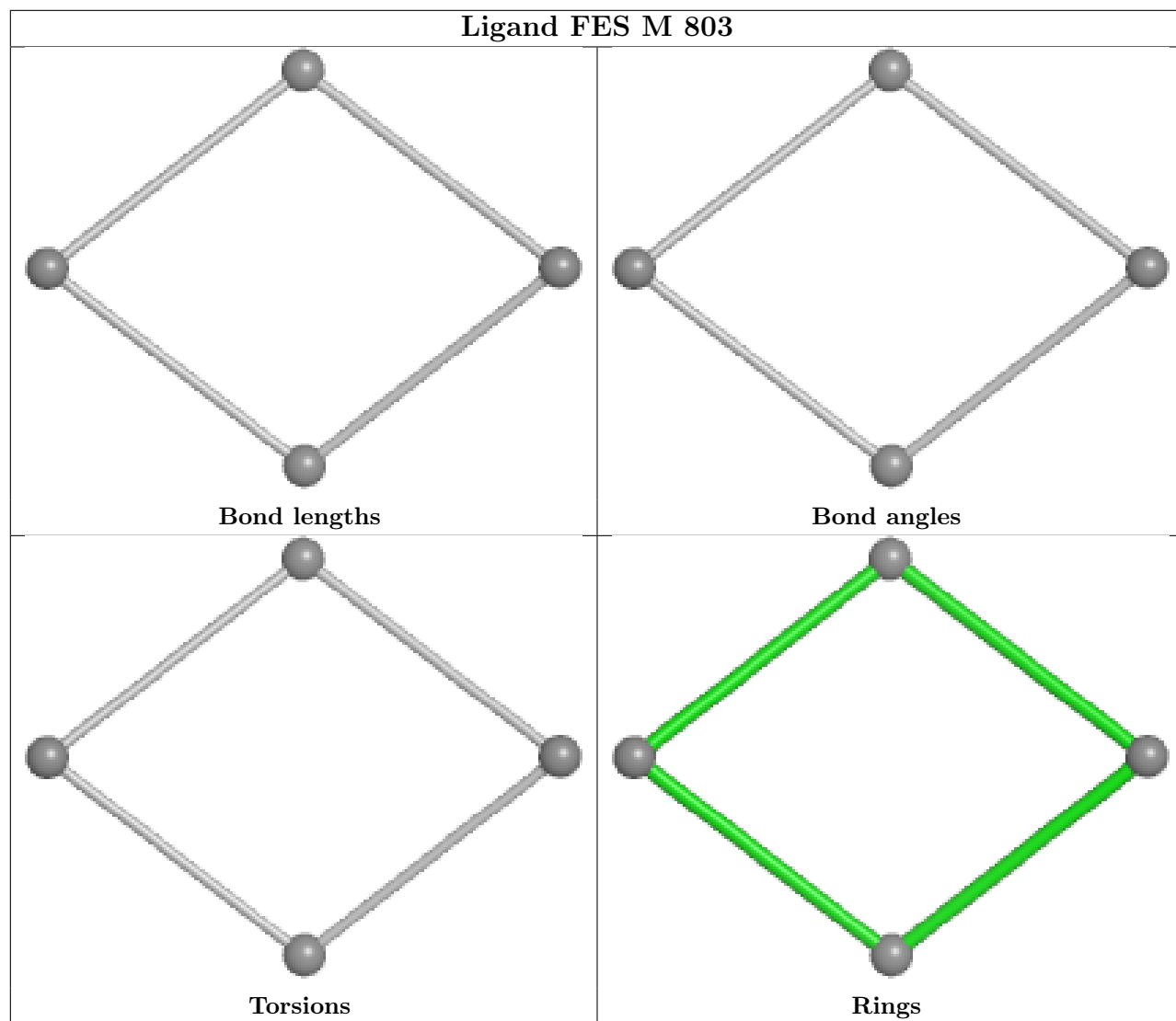


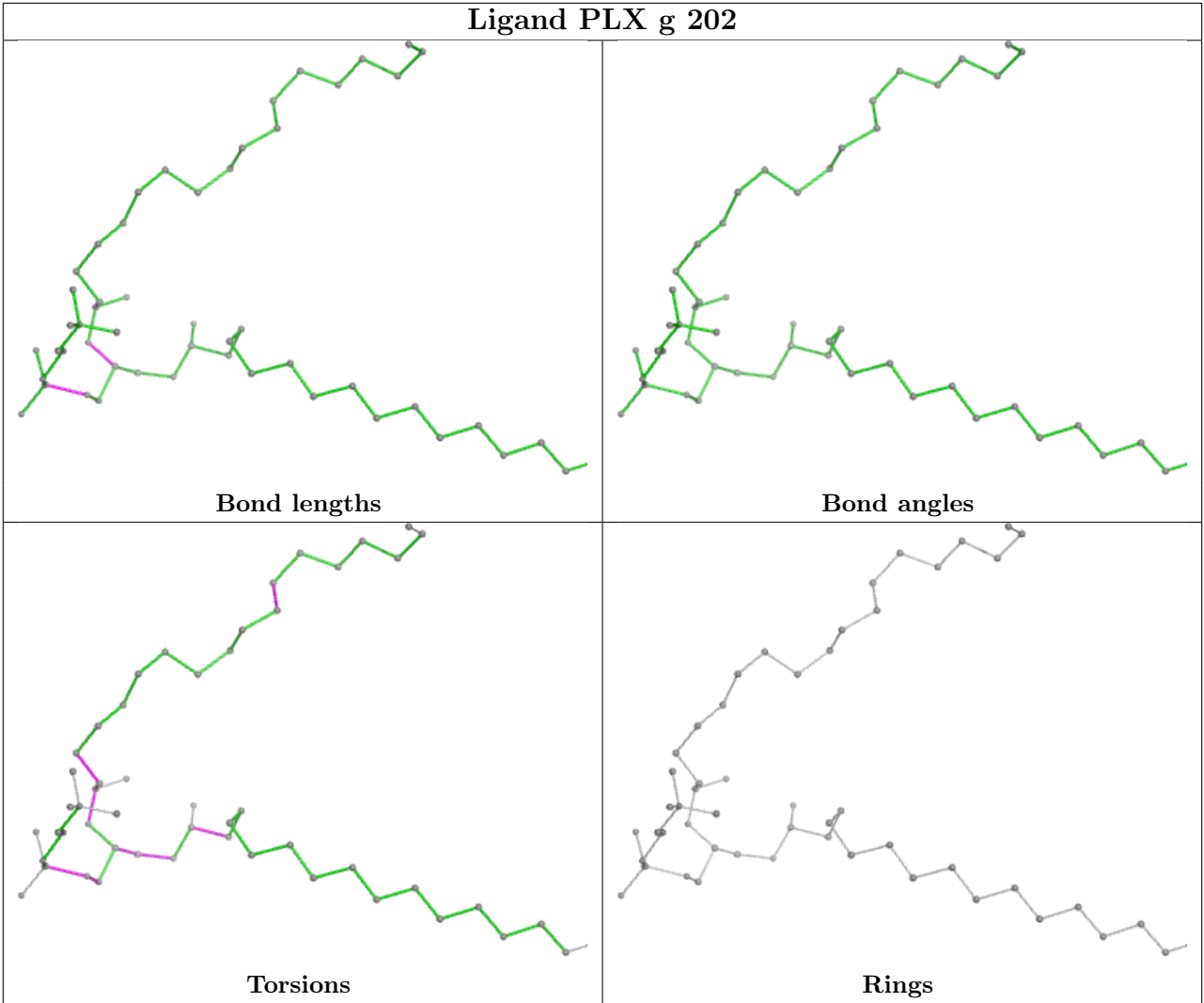
Ligand PEE i 403











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
30	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	457:HIS	C	458:GLN	N	3.27

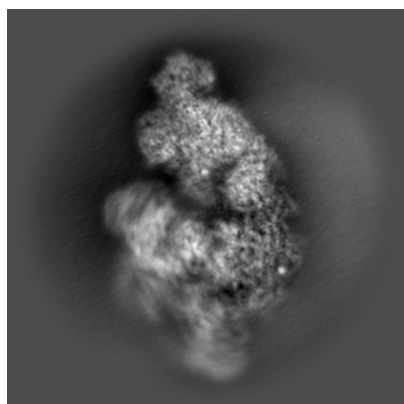
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52619. These allow visual inspection of the internal detail of the map and identification of artifacts.

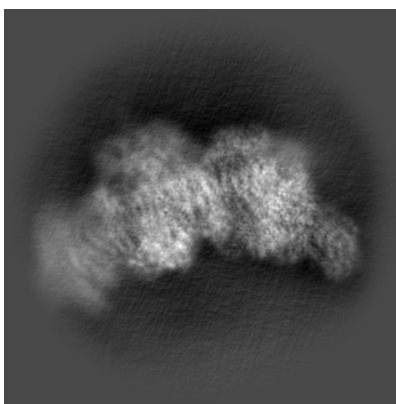
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

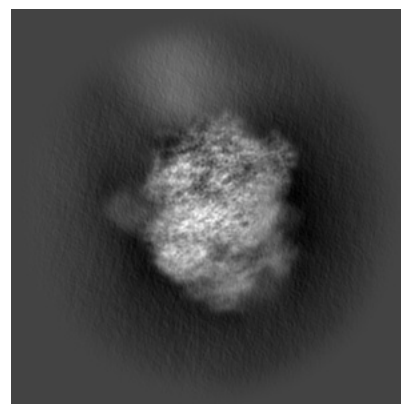
6.1.1 Primary map



X

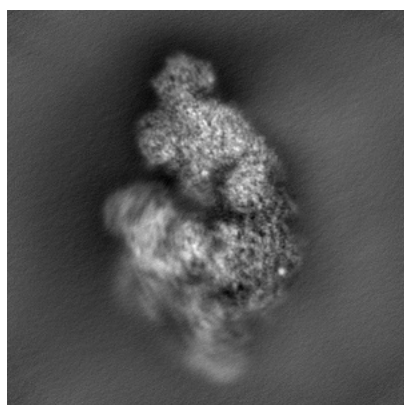


Y

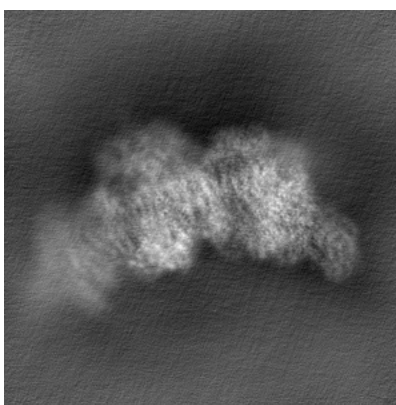


Z

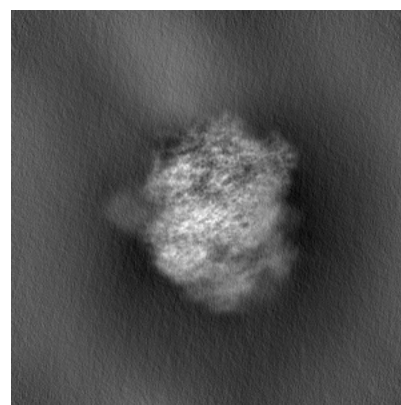
6.1.2 Raw map



X



Y

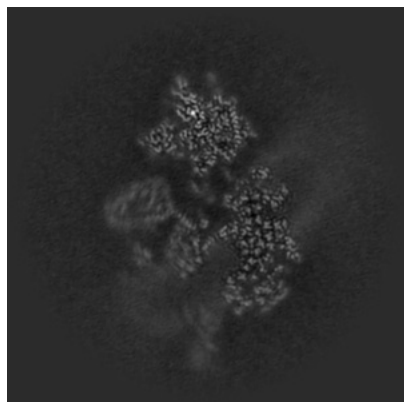


Z

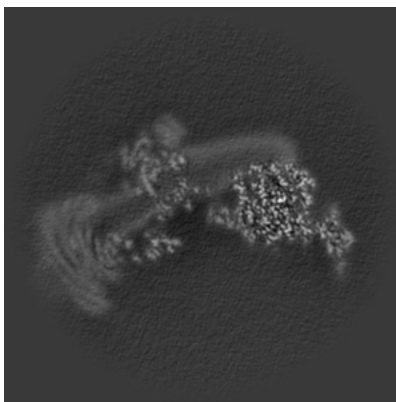
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

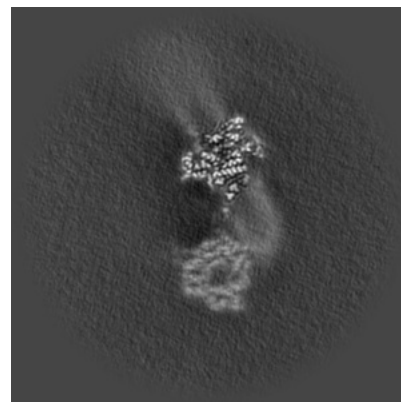
6.2.1 Primary map



X Index: 240

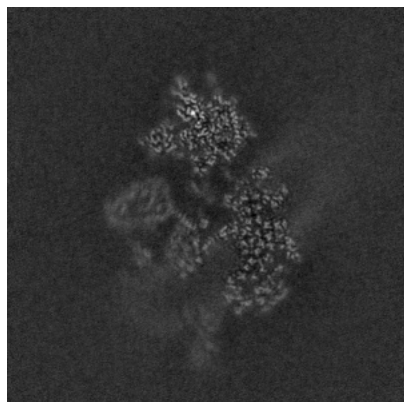


Y Index: 240

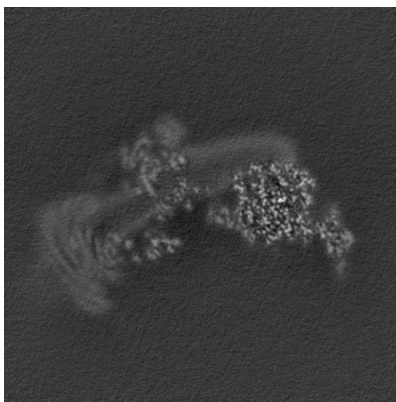


Z Index: 240

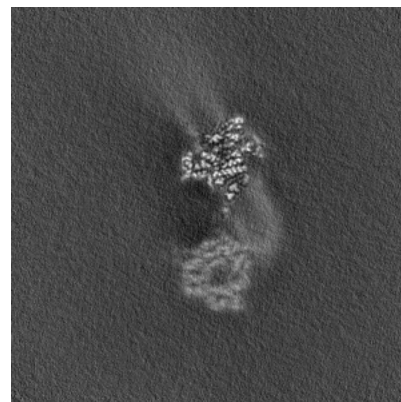
6.2.2 Raw map



X Index: 240



Y Index: 240

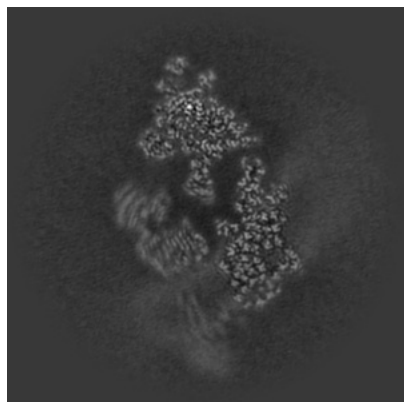


Z Index: 240

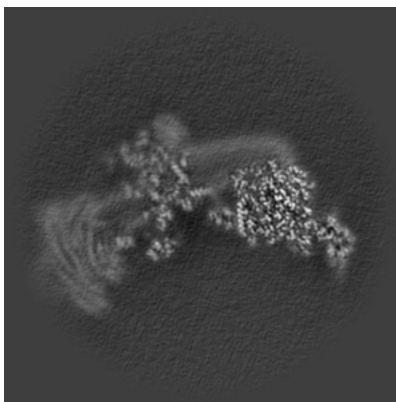
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

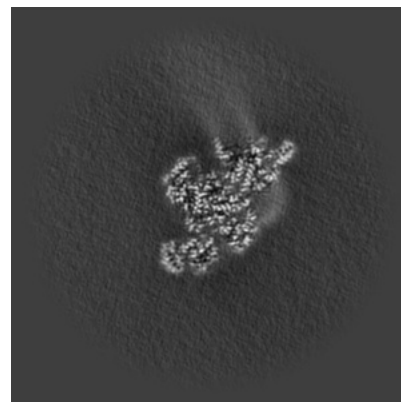
6.3.1 Primary map



X Index: 225

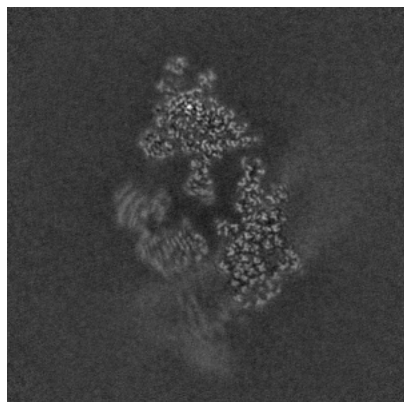


Y Index: 236

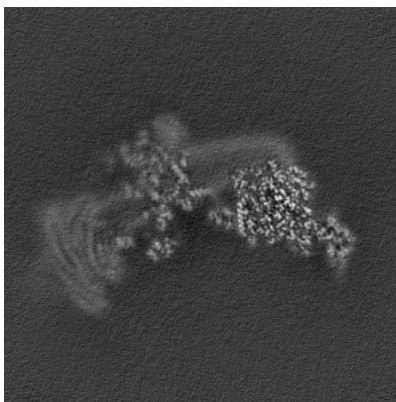


Z Index: 311

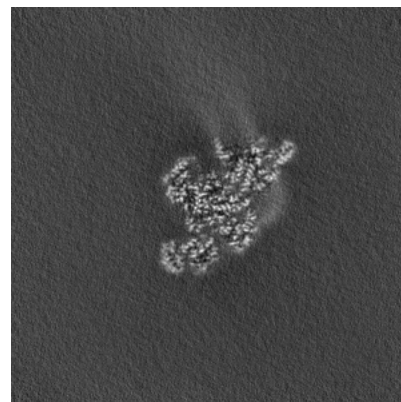
6.3.2 Raw map



X Index: 225



Y Index: 236

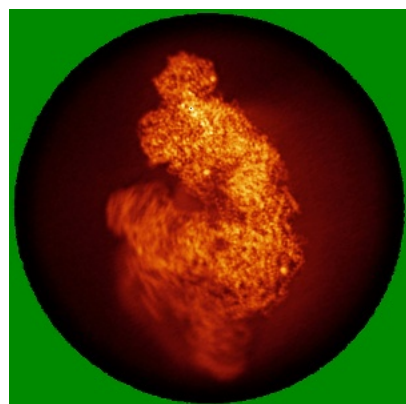


Z Index: 311

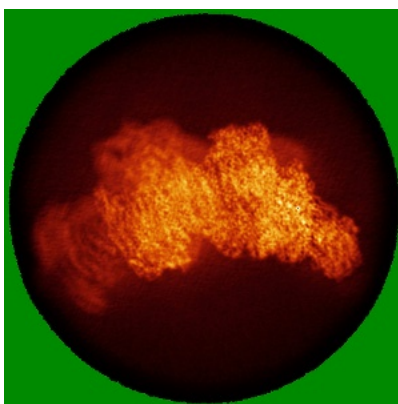
The images above show the largest variance slices of the map in three orthogonal directions.

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

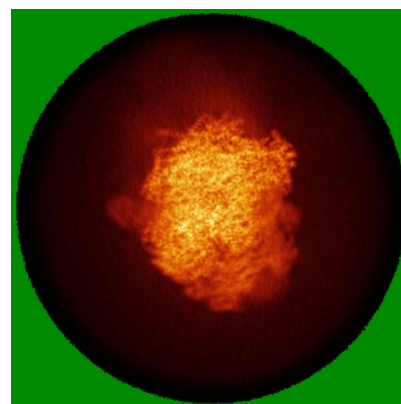
6.4.1 Primary map



X

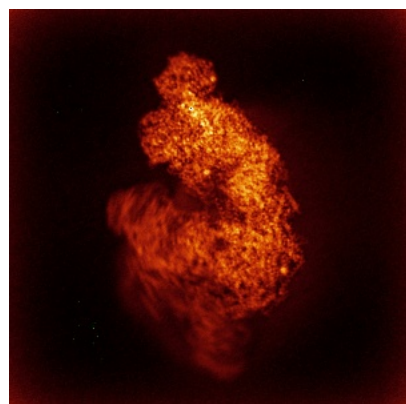


Y

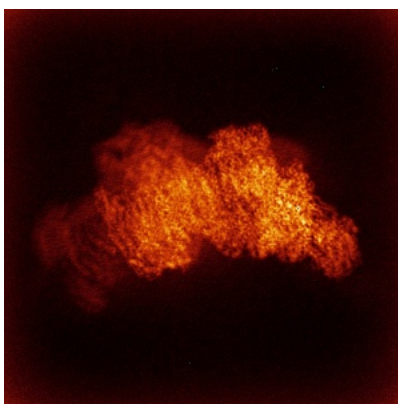


Z

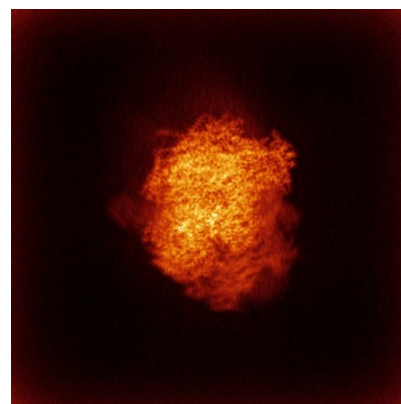
6.4.2 Raw map



X



Y

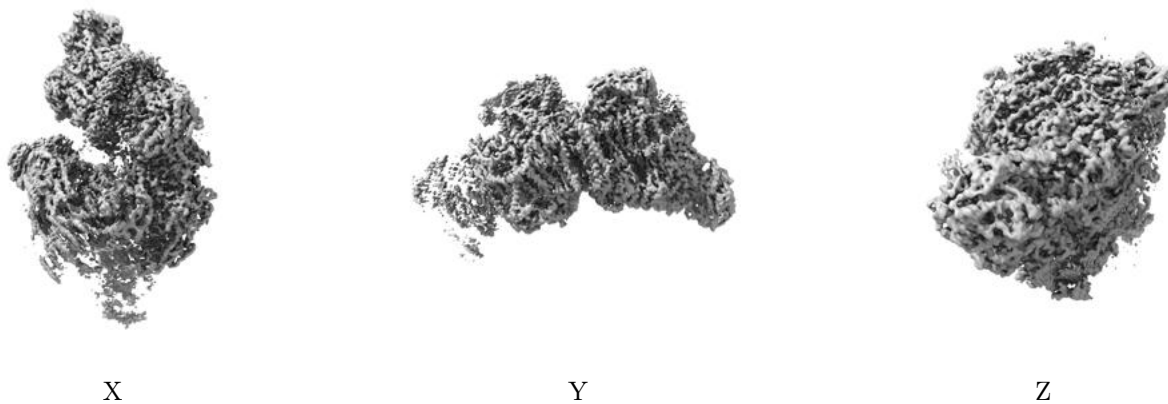


Z

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

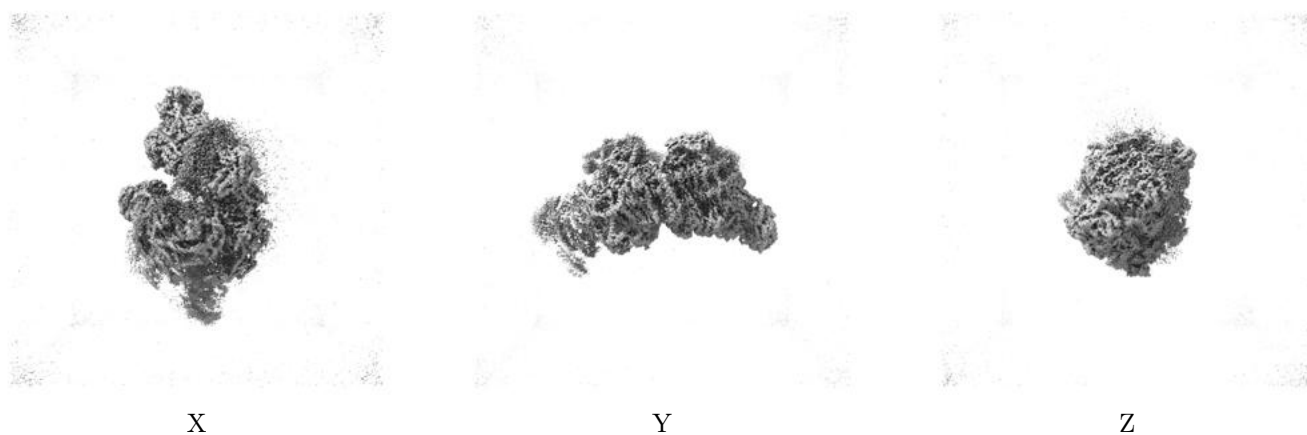
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.477. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

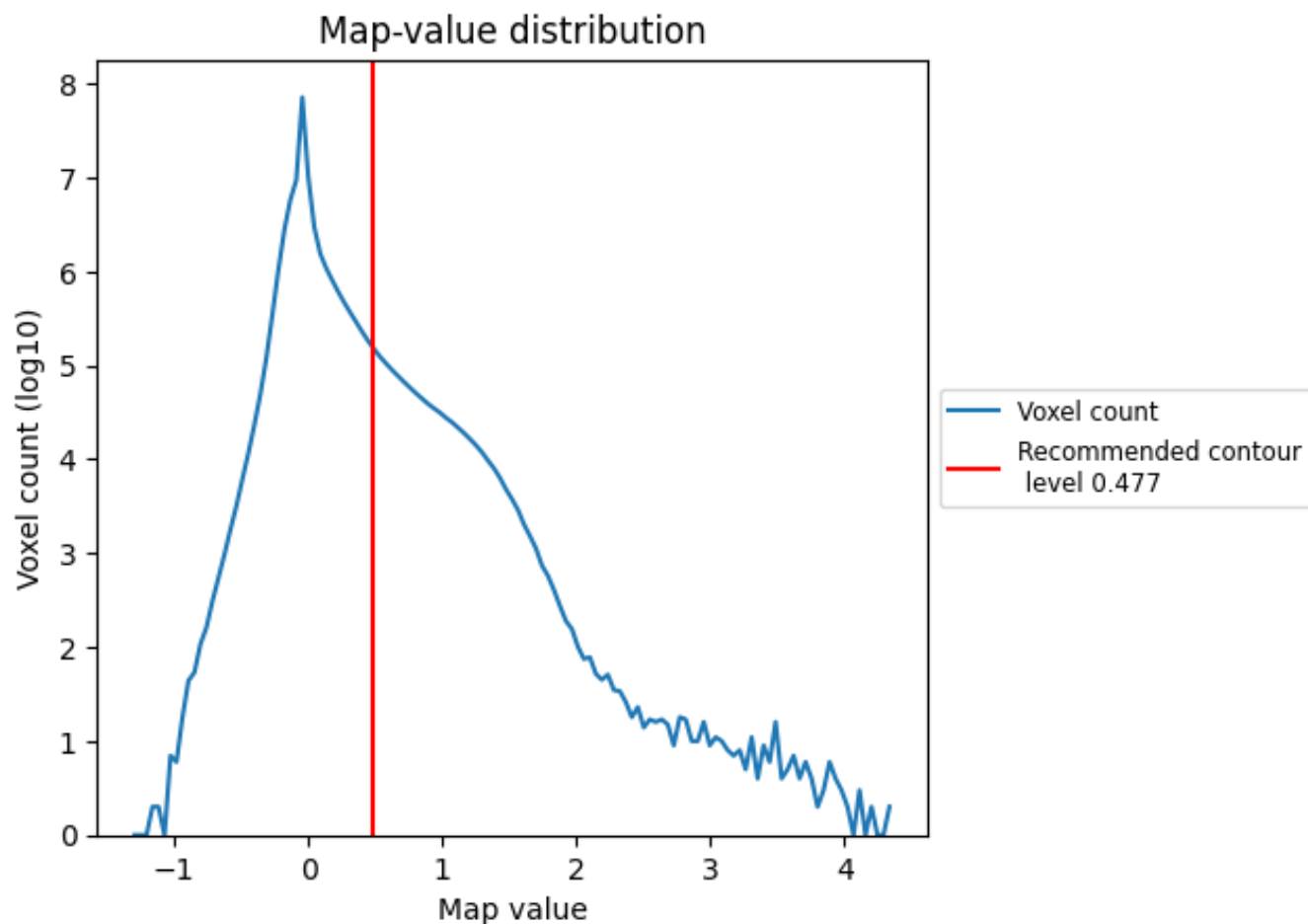
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

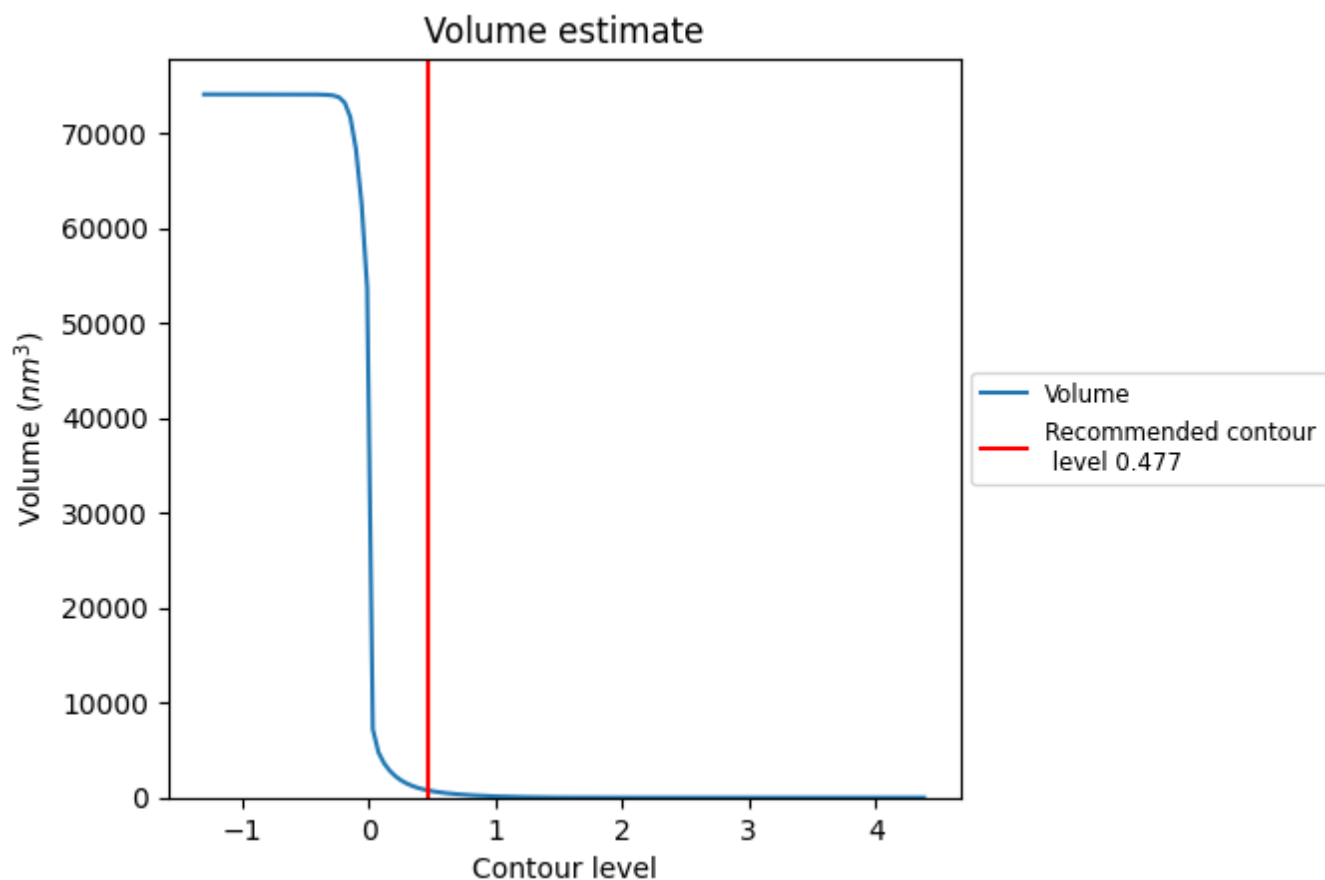
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

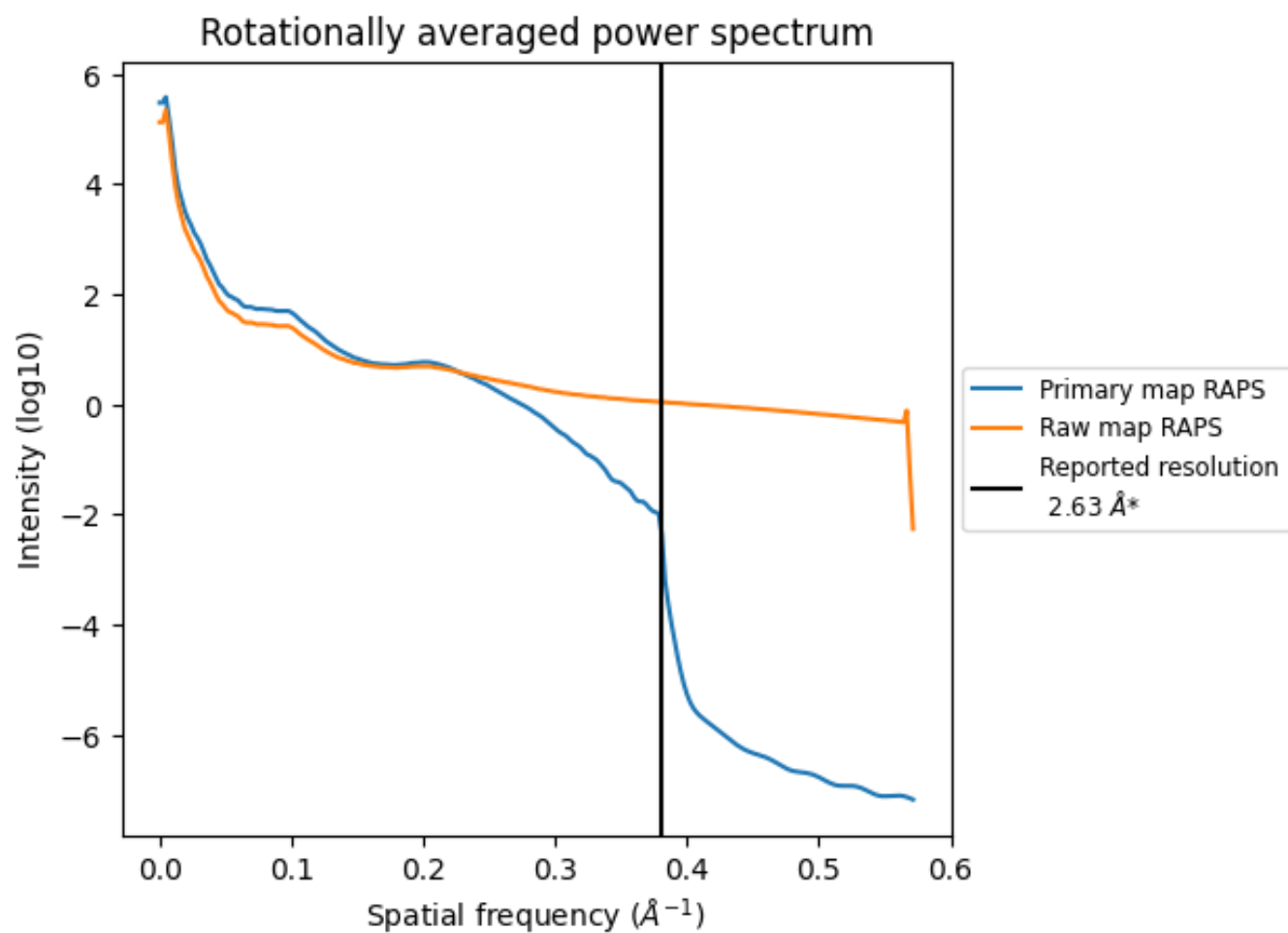
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 741 nm³; this corresponds to an approximate mass of 669 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

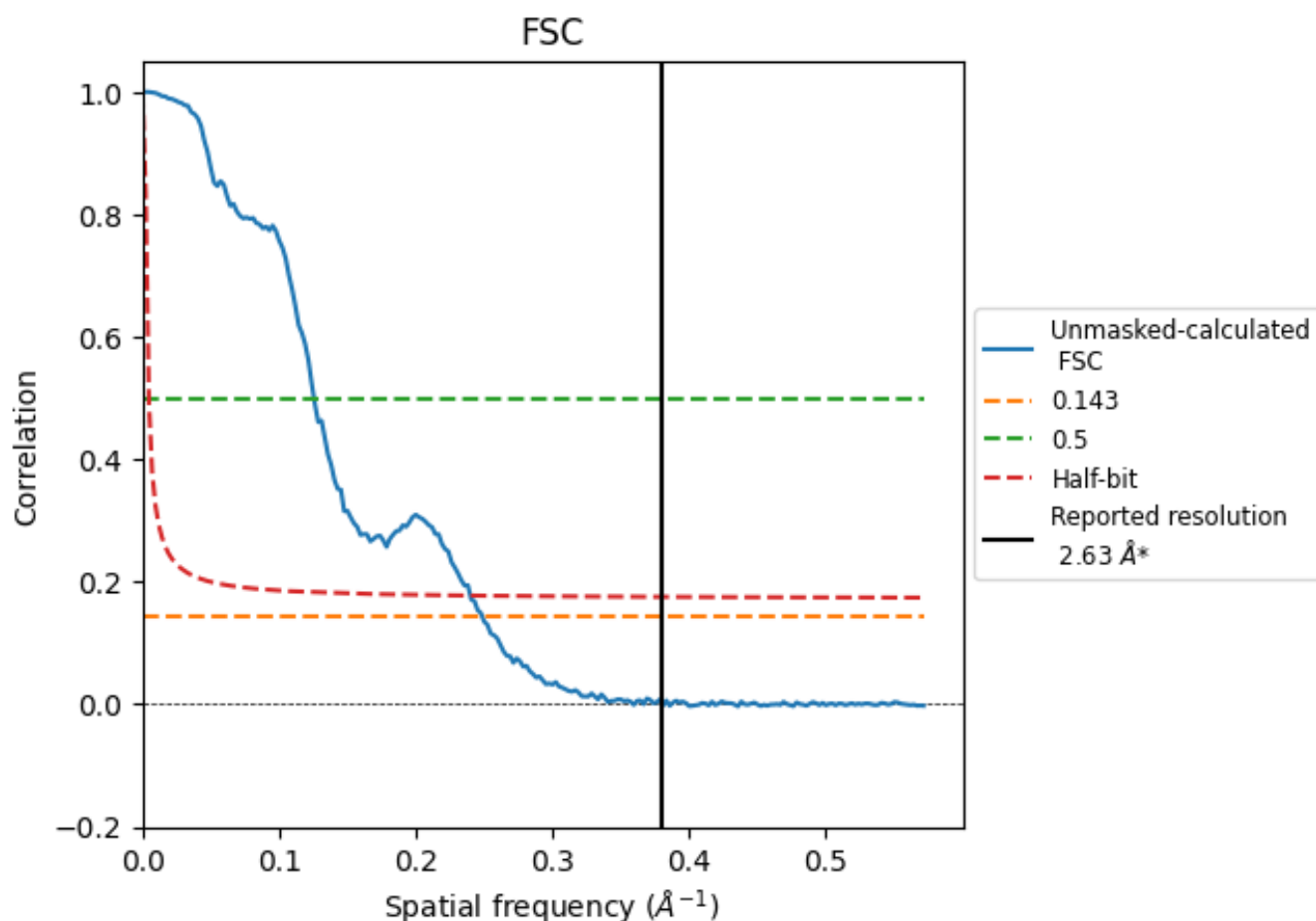


*Reported resolution corresponds to spatial frequency of 0.380 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.380 \AA^{-1}

8.2 Resolution estimates [i](#)

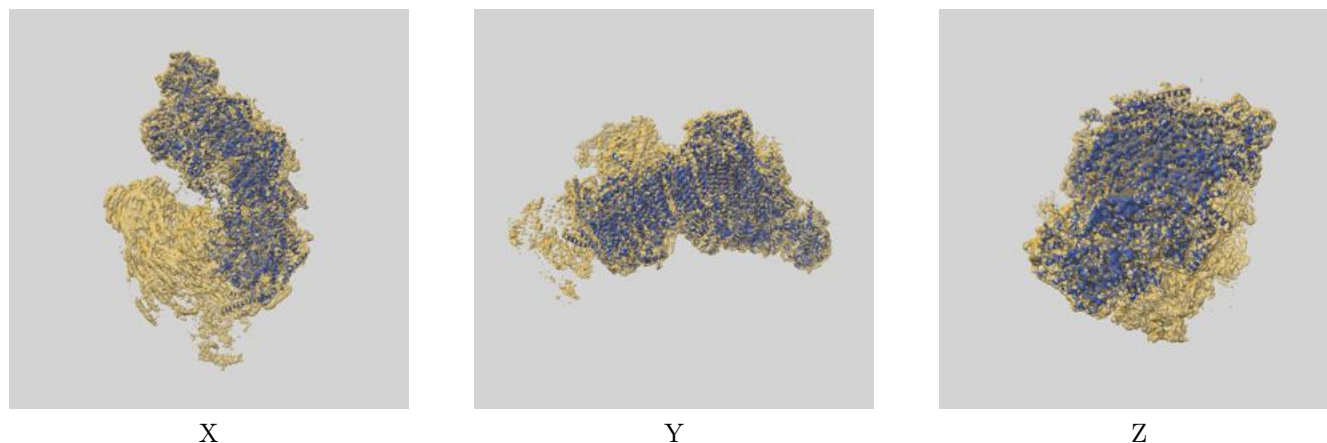
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.63	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.02	7.97	4.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 2.63 by more than 10 %

9 Map-model fit [i](#)

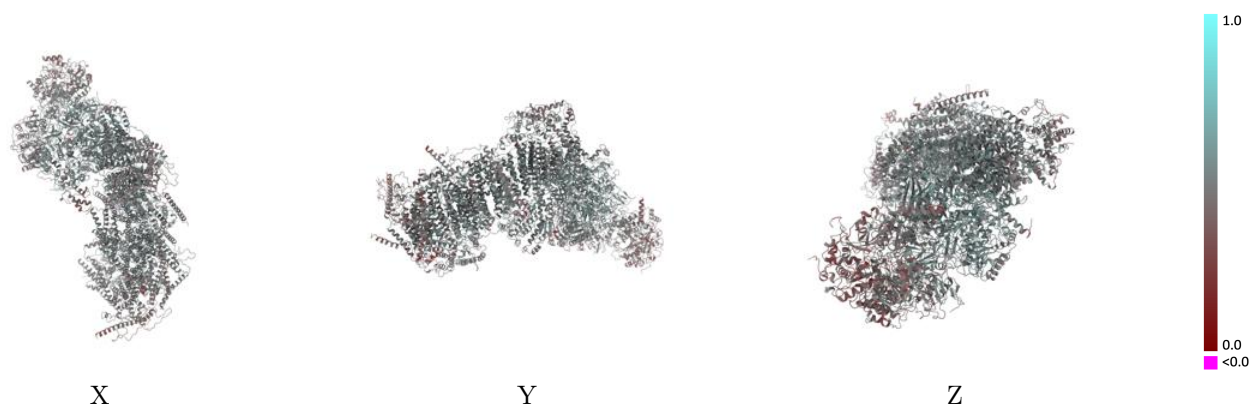
This section contains information regarding the fit between EMDB map EMD-52619 and PDB model 9I4I. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



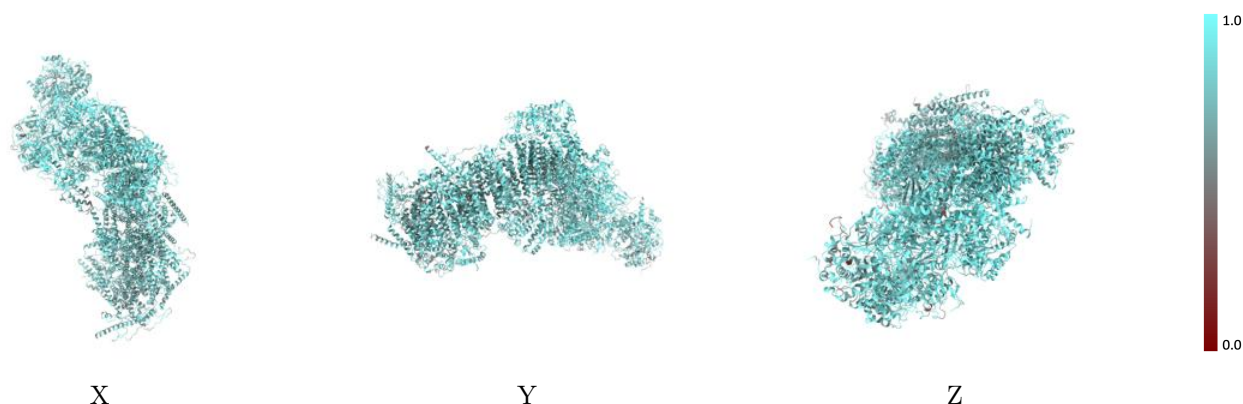
The images above show the 3D surface view of the map at the recommended contour level 0.477 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



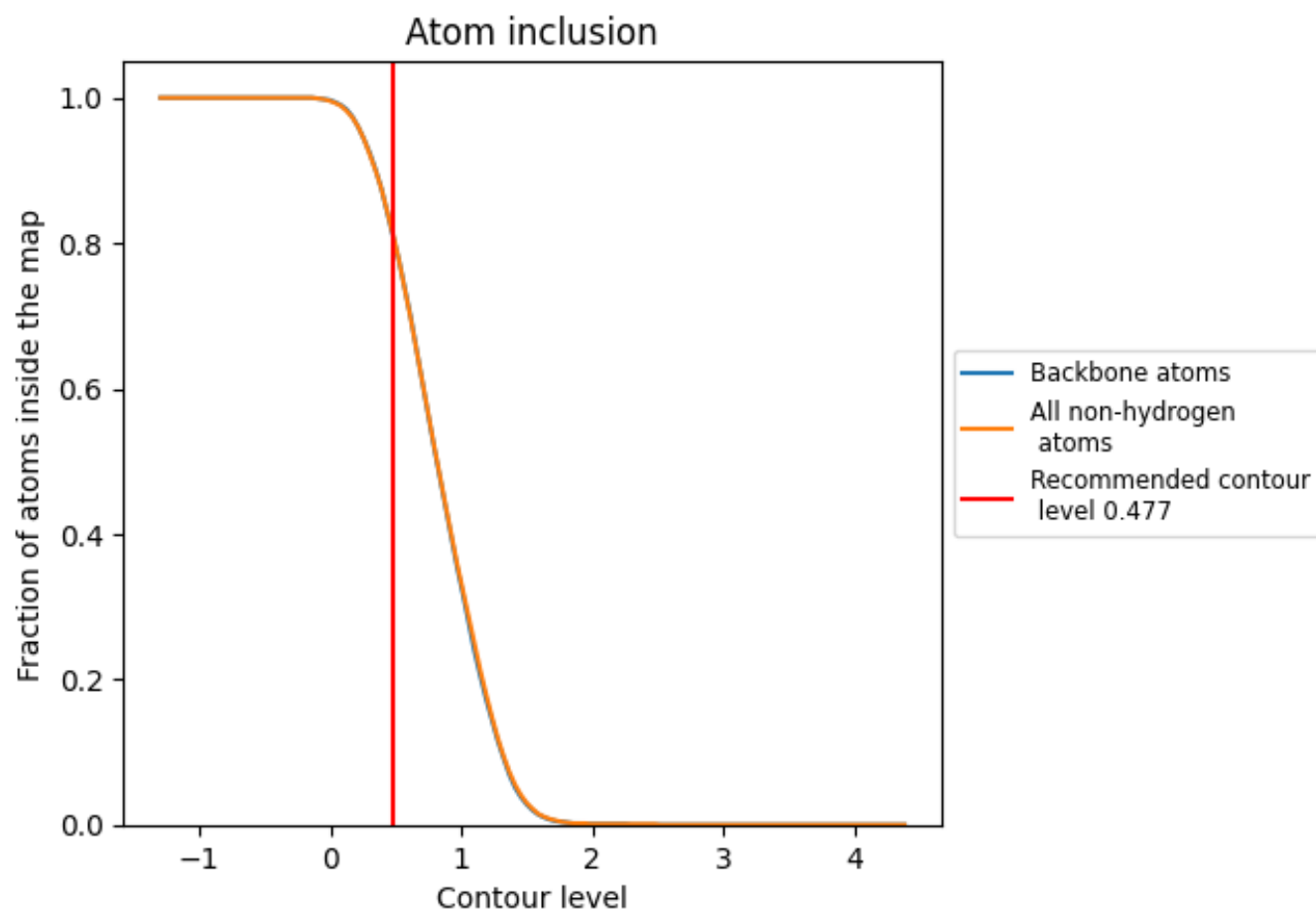
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.477).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.477) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8140	 0.4860
C	 0.7860	 0.3970
D	 0.9300	 0.5380
E	 0.9070	 0.5330
F	 0.8530	 0.5100
G	 0.8270	 0.4240
H	 0.6730	 0.3870
I	 0.8250	 0.4800
J	 0.8900	 0.5160
K	 0.8150	 0.3870
L	 0.8300	 0.5120
M	 0.8450	 0.4660
N	 0.9120	 0.5070
O	 0.8210	 0.4090
P	 0.8690	 0.5350
Q	 0.8750	 0.5390
S	 0.8840	 0.4830
T	 0.9240	 0.5140
U	 0.8450	 0.4820
V	 0.6960	 0.4890
W	 0.8540	 0.4900
X	 0.7850	 0.4540
Y	 0.7690	 0.4360
Z	 0.7070	 0.4190
a	 0.8450	 0.5020
b	 0.7270	 0.4070
c	 0.8140	 0.4960
d	 0.7780	 0.4610
e	 0.7930	 0.4670
f	 0.7030	 0.3960
g	 0.7770	 0.4980
h	 0.8570	 0.4820
i	 0.7940	 0.5220
j	 0.7950	 0.5150
k	 0.8260	 0.5100



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Chain	Atom inclusion	Q-score
l	 0.7500	 0.4860
m	 0.8290	 0.4900
n	 0.7720	 0.4650
o	 0.7870	 0.4880
p	 0.8490	 0.4890
r	 0.8100	 0.5200
s	 0.8830	 0.5250
t	 0.8760	 0.5070
u	 0.8360	 0.4680
v	 0.7520	 0.4030
w	 0.8490	 0.4990