



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:54 AM UTC

PDB ID : 6RFQ / pdb_00006rfq
EMDB ID : EMD-4872
Title : Cryo-EM structure of a respiratory complex I assembly intermediate with ND-UFAF2
Authors : Parey, K.; Vonck, J.
Deposited on : 2019-04-16
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

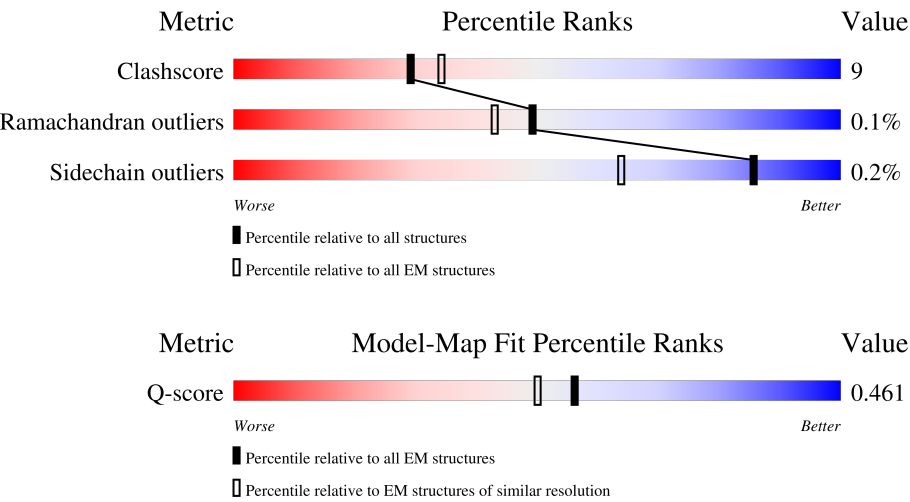
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	728	
2	B	488	
3	C	466	
4	D	87	

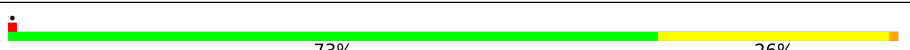
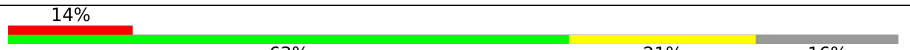
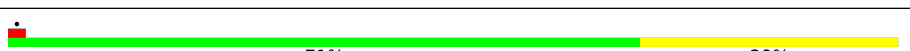
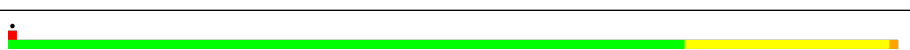
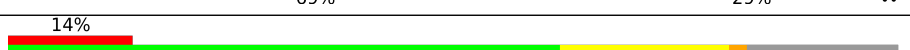
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Mol	Chain	Length	Quality of chain
5	E	375	
6	F	144	
7	G	281	
8	H	243	
9	I	229	
10	J	198	
11	K	210	
12	L	89	
13	O	109	
14	P	124	
15	Q	132	
16	R	109	
17	S	249	
18	U	172	
19	W	123	
20	X	169	
21	Y	161	
22	Z	182	
23	a	149	
24	b	74	
25	c	60	
26	d	92	
27	e	67	
28	f	87	
29	g	78	

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Mol	Chain	Length	Quality of chain
30	i	90	
31	j	93	
32	k	237	
33	n	120	
34	1	341	
35	2	469	
36	3	128	
37	4	486	
38	5	655	
39	6	185	
40	8	99	
41	9	89	

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
48	CDL	J	204	-	-	X	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 62052 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	694	Total	C	N	O	S	0	0
			5274	3275	928	1042	29		

- Molecule 2 is a protein called Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	441	Total	C	N	O	S	0	0
			3421	2161	601	635	24		

- Molecule 3 is a protein called Subunit NUCM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	430	Total	C	N	O	S	0	0
			3415	2170	583	640	22		

- Molecule 4 is a protein called Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	86	Total	C	N	O	S	0	0
			681	432	127	119	3		

- Molecule 5 is a protein called Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	263	Total	C	N	O	S	0	0
			2075	1315	362	390	8		

- Molecule 6 is a protein called Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I).

plex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	121	Total	C	N	O	S	0	0
			990	629	166	193	2		

- Molecule 7 is a protein called Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	210	Total	C	N	O	S	0	0
			1739	1119	297	319	4		

- Molecule 8 is a protein called Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	215	Total	C	N	O	S	0	0
			1680	1054	283	325	18		

- Molecule 9 is a protein called Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	190	Total	C	N	O	S	0	0
			1519	966	254	289	10		

- Molecule 10 is a protein called Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	179	Total	C	N	O	S	0	0
			1329	844	241	239	5		

- Molecule 11 is a protein called Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	153	Total	C	N	O	S	0	0
			1190	756	206	214	14		

- Molecule 12 is a protein called Subunit NULM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	89	Total	C	N	O	S	0	0
			691	464	109	115	3		

- Molecule 13 is a protein called Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	77	Total	C	N	O	S	0	0
			591	373	93	125			

- Molecule 14 is a protein called Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	123	Total	C	N	O	S	0	0
			1036	667	182	185	2		

- Molecule 15 is a protein called Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	85	Total	C	N	O	S	0	0
			648	405	103	138	2		

- Molecule 16 is a protein called Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	106	Total	C	N	O	S	0	0
			884	562	168	151	3		

- Molecule 17 is a protein called Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	174	Total	C	N	O	S	0	0
			1430	920	245	263	2		

- Molecule 18 is a protein called Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	171	Total	C	N	O	S	0	0
			1345	847	236	252	10		

- Molecule 19 is a protein called Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	119	Total	C	N	O	S	0	0
			961	615	176	165	5		

- Molecule 20 is a protein called Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	168	Total	C	N	O	S	0	0
			1305	845	223	233	4		

- Molecule 21 is a protein called Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	123	Total	C	N	O	S	0	0
			1021	651	187	181	2		

- Molecule 22 is a protein called Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	120	Total	C	N	O	S	0	0
			922	589	158	174	1		

- Molecule 23 is a protein called Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	124	Total	C	N	O	S	0	0
			1030	669	165	194	2		

- Molecule 24 is a protein called Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
24	b	64	Total	C	N	O	0	0
			490	326	83	81		

- Molecule 25 is a protein called Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
25	c	44	Total	C	N	O	0	0
			353	229	67	57		

- Molecule 26 is a protein called Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	90	Total	C	N	O	S	0	0
			760	472	137	148	3		

- Molecule 27 is a protein called Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	52	Total	C	N	O	S	0	0
			436	293	75	65	3		

- Molecule 28 is a protein called Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	79	Total	C	N	O	S	0	0
			620	389	118	112	1		

- Molecule 29 is a protein called Subunit NI9M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
29	g	76	Total	C	N	O	0	0
			617	405	112	100		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	71	GLY	GLN	conflict	UNP A0A1D8NJR0

- Molecule 30 is a protein called Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	i	83	Total	C	N	O	S	0	0
			646	413	117	115	1		

- Molecule 31 is a protein called Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	90	Total	C	N	O		0	0
			724	465	132	127			

- Molecule 32 is a protein called Subunit N7BML assembly factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	98	Total	C	N	O		0	0
			828	538	148	142			

- Molecule 33 is a protein called Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	n	114	Total	C	N	O	S	0	0
			914	588	156	169	1		

- Molecule 34 is a protein called Subunit NU1M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1	318	Total	C	N	O	S	0	0
			2540	1738	369	426	7		

- Molecule 35 is a protein called Subunit NU2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	2	469	Total	C	N	O	S	0	0
			3774	2557	550	655	12		

- Molecule 36 is a protein called Subunit NU3M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	3	108	Total	C	N	O	S	0	0
			869	600	127	140	2		

- Molecule 37 is a protein called Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4	486	Total	C	N	O	S	0	0
			3855	2600	586	654	15		

- Molecule 38 is a protein called Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	5	654	Total	C	N	O	S	0	0
			5197	3479	785	905	28		

- Molecule 39 is a protein called Subunit NU6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	6	183	Total	C	N	O	S	0	0
			1443	979	207	249	8		

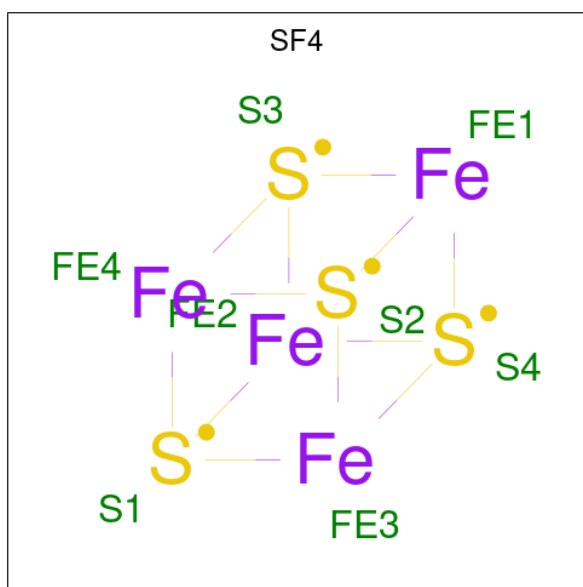
- Molecule 40 is a protein called Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	8	82	Total	C	N	O	S	0	0
			672	426	122	116	8		

- Molecule 41 is a protein called Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I).

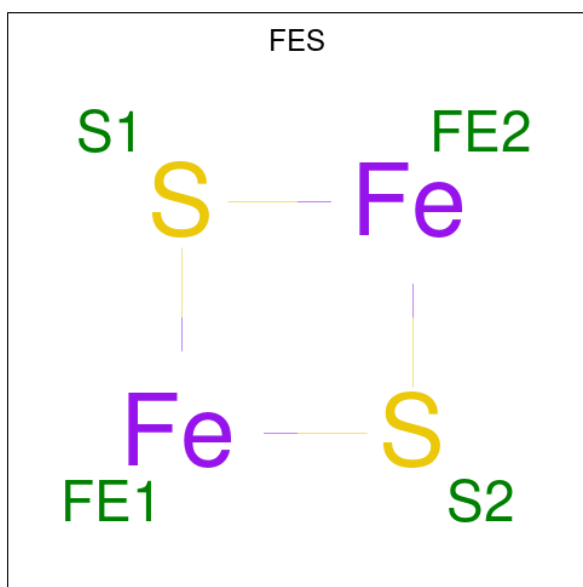
Mol	Chain	Residues	Atoms					AltConf	Trace
41	9	86	Total	C	N	O	S	0	0
			672	422	122	122	6		

- Molecule 42 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



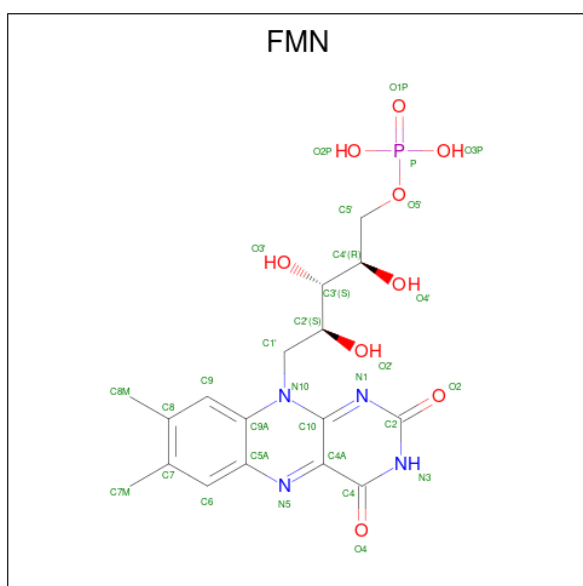
Mol	Chain	Residues	Atoms			AltConf
42	A	1	Total	Fe	S	0
			8	4	4	
42	A	1	Total	Fe	S	0
			8	4	4	
42	B	1	Total	Fe	S	0
			8	4	4	
42	I	1	Total	Fe	S	0
			8	4	4	
42	I	1	Total	Fe	S	0
			8	4	4	
42	K	1	Total	Fe	S	0
			8	4	4	

- Molecule 43 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total	Fe	S	0
			4	2	2	
43	H	1	Total	Fe	S	0
			4	2	2	

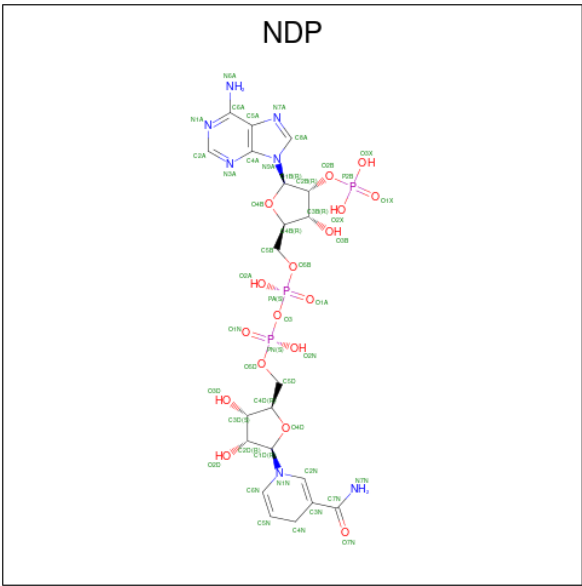
- Molecule 44 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

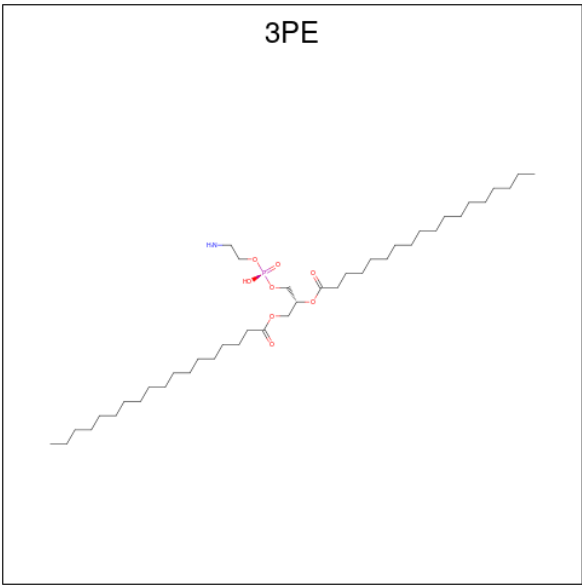
- Molecule 45 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



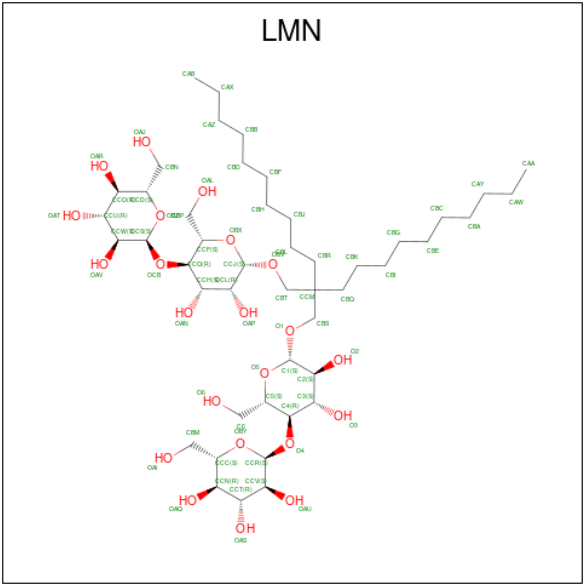
Mol	Chain	Residues	Atoms					AltConf
46	I	1	Total	C	N	O	P	0
			51	41	1	8	1	

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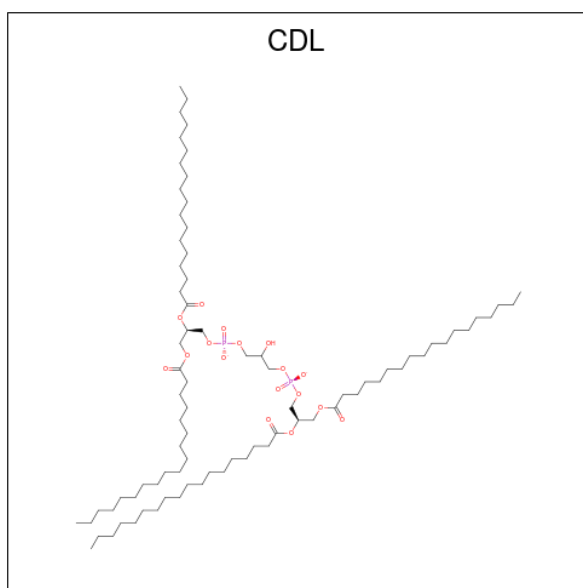
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Mol	Chain	Residues	Atoms					AltConf
46	J	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	J	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	g	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	4	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	4	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	4	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	5	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	6	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 47 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: C₄₇H₈₈O₂₂).

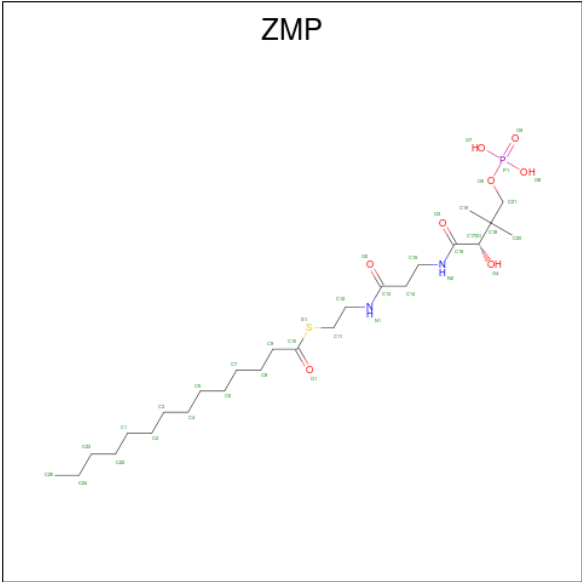


- Molecule 48 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



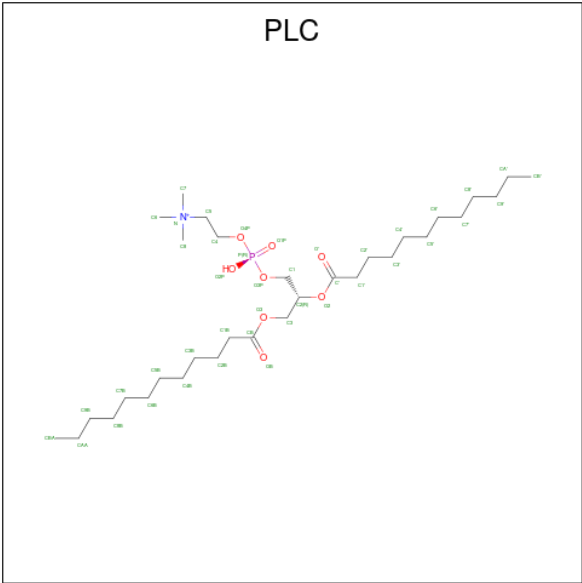
Mol	Chain	Residues	Atoms				AltConf
48	J	1	Total	C	O	P	0
			78	59	17	2	
48	X	1	Total	C	O	P	0
			82	63	17	2	
48	g	1	Total	C	O	P	0
			83	64	17	2	
48	4	1	Total	C	O	P	0
			92	73	17	2	

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



Mol	Chain	Residues	Atoms						AltConf
49	O	1	Total	C	N	O	P	S	0
			33	22	2	7	1	1	
49	Q	1	Total	C	N	O	P	S	0
			33	22	2	7	1	1	

- Molecule 50 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $C_{32}H_{65}NO_8P$).



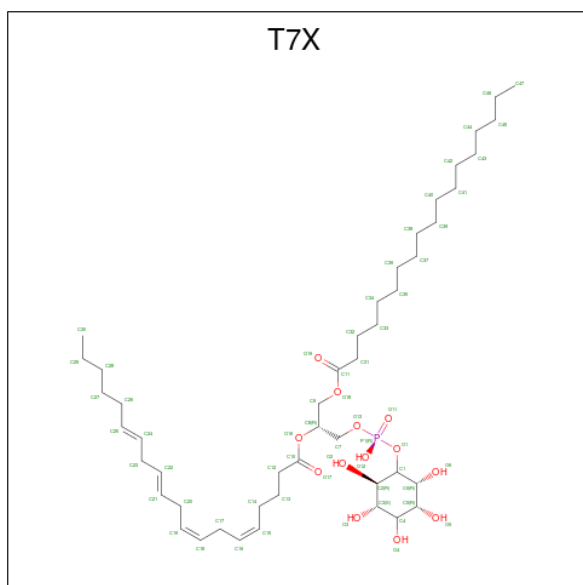
Mol	Chain	Residues	Atoms					AltConf
50	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
50	W	1	Total	C	N	O	P	0
			42	32	1	8	1	

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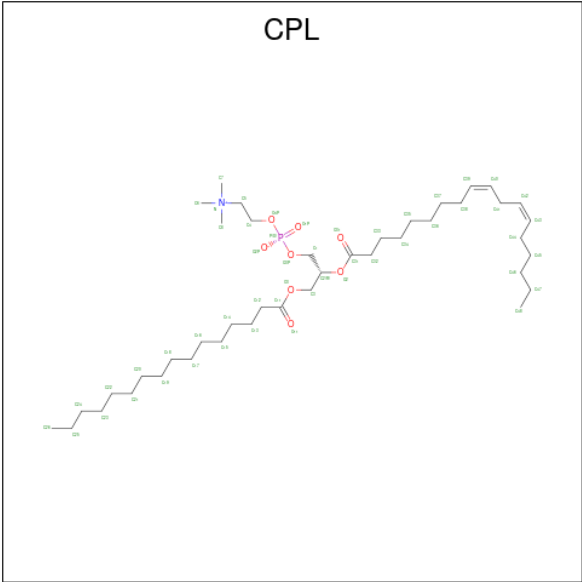
Mol	Chain	Residues	Atoms					AltConf
50	n	1	Total	C	N	O	P	0
			42	32	1	8	1	
50	5	1	Total	C	N	O	P	0
			31	21	1	8	1	

- Molecule 51 is Phosphatidylinositol (CCD ID: T7X) (formula: $C_{47}H_{83}O_{13}P$).



Mol	Chain	Residues	Atoms					AltConf
51	2	1	Total	C	O	P		0
			48	34	13	1		
51	2	1	Total	C	O	P		0
			52	38	13	1		
51	4	1	Total	C	O	P		0
			43	29	13	1		

- Molecule 52 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: CPL) (formula: $C_{42}H_{80}NO_8P$).

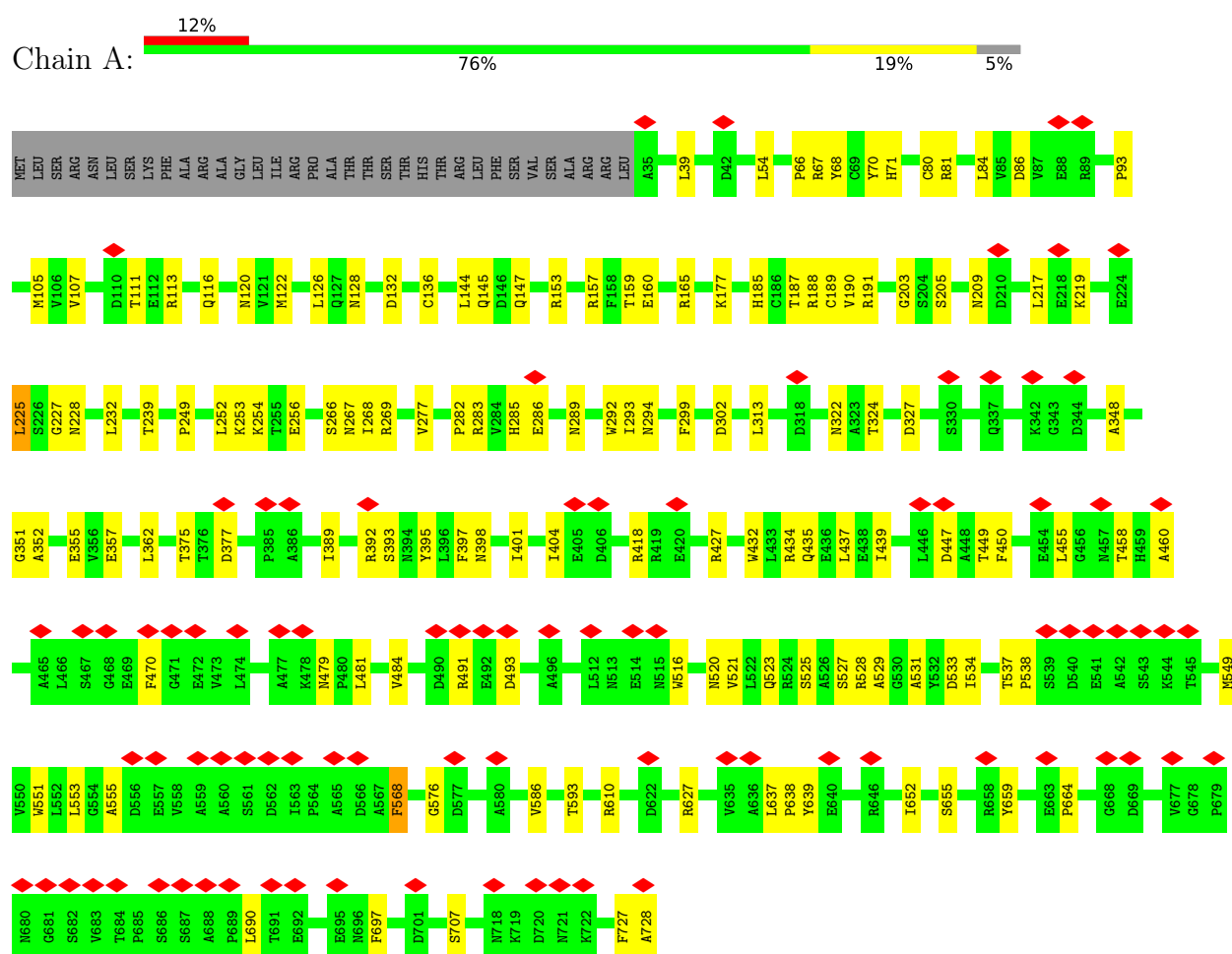


Mol	Chain	Residues	Atoms					AltConf
52	2	1	Total	C	N	O	P	0
			52	42	1	8	1	

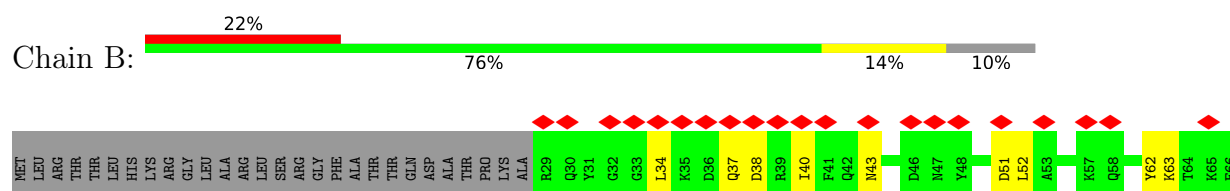
3 Residue-property plots

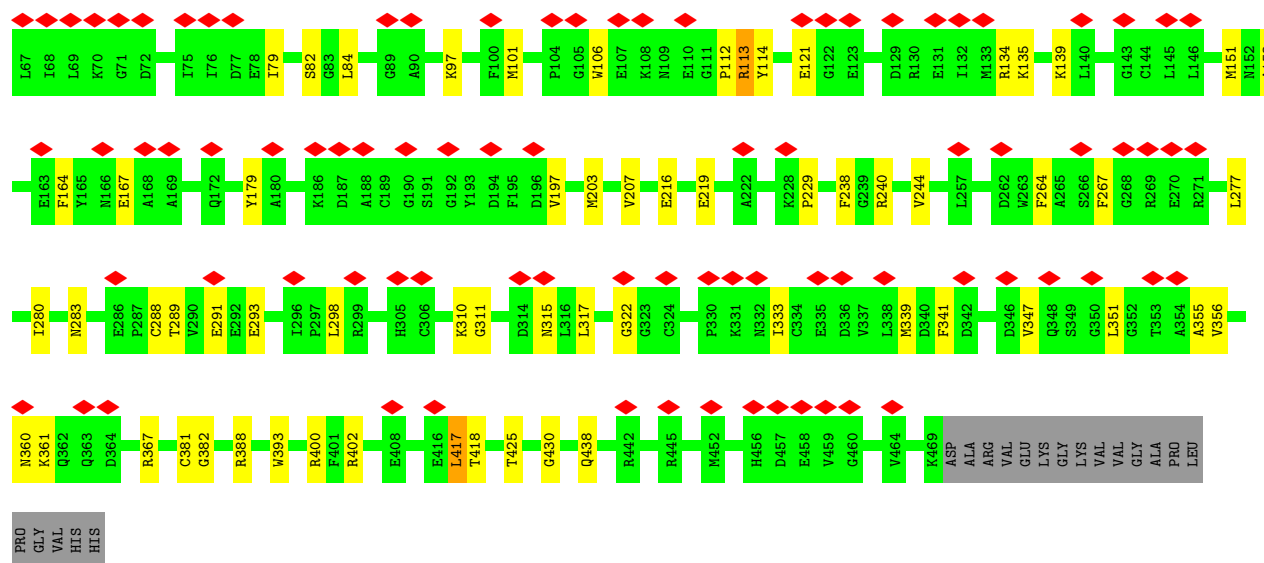
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I)

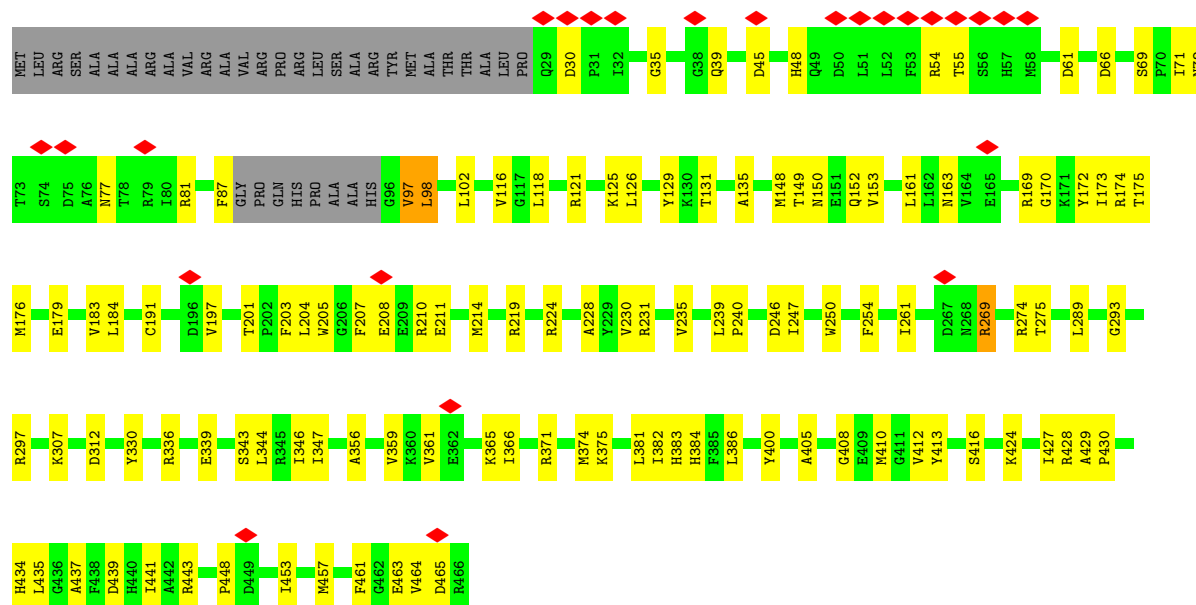


- Molecule 2: Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I)

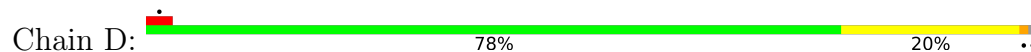




• Molecule 3: Subunit NUCM of NADH:Ubiquinone Oxidoreductase (Complex I)

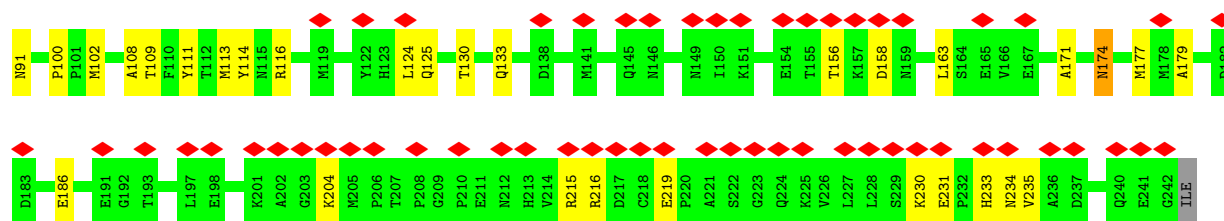


• Molecule 4: Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I)

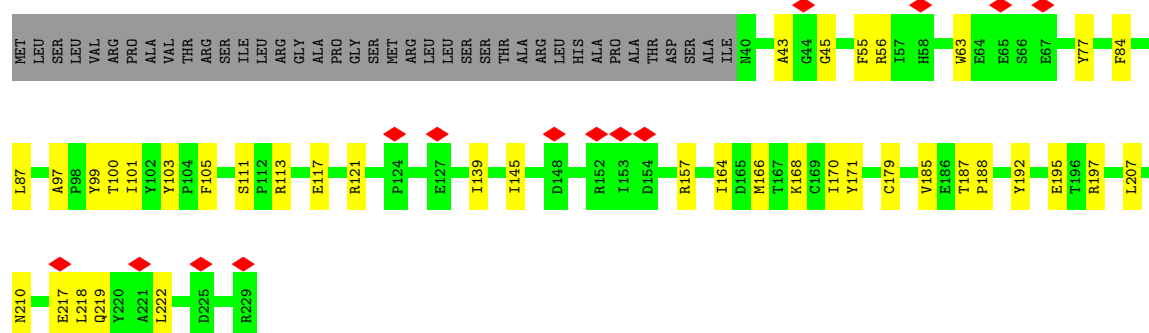


• Molecule 5: Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I)

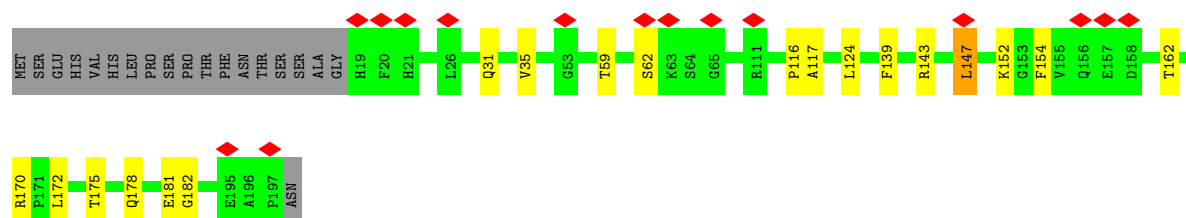
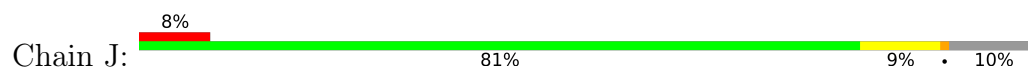




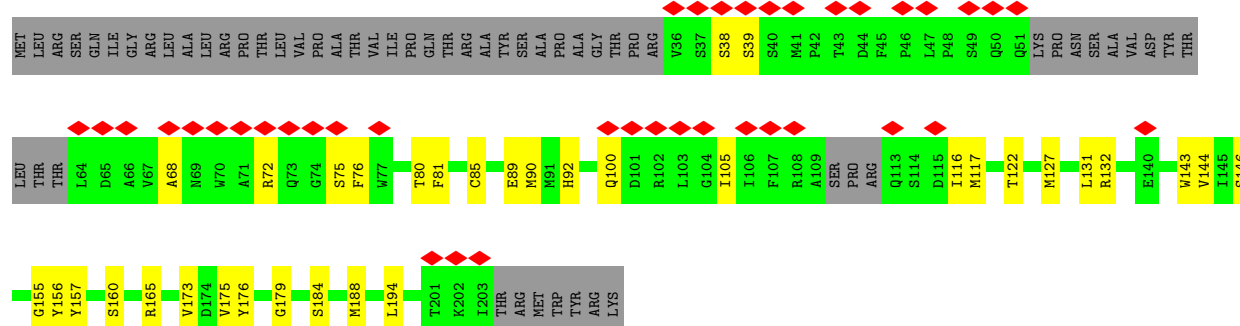
- Molecule 9: Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 10: Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I)



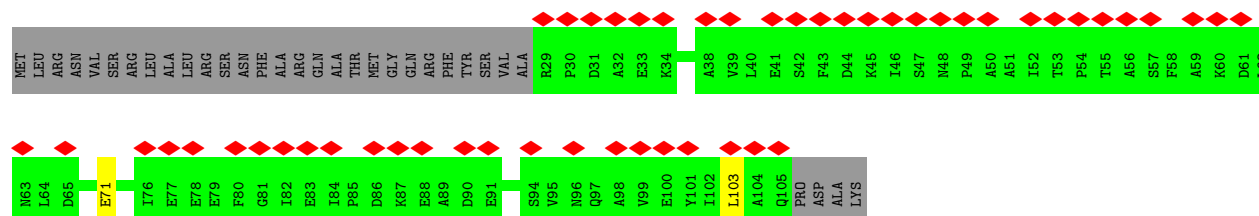
- Molecule 11: Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I)



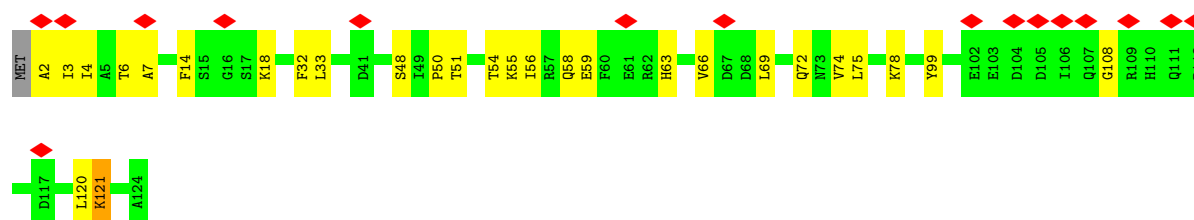
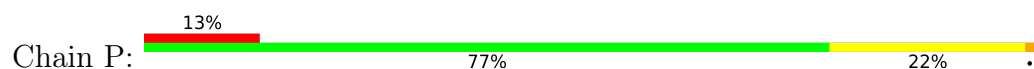
- Molecule 12: Subunit NULM of NADH:Ubiquinone Oxidoreductase (Complex I)



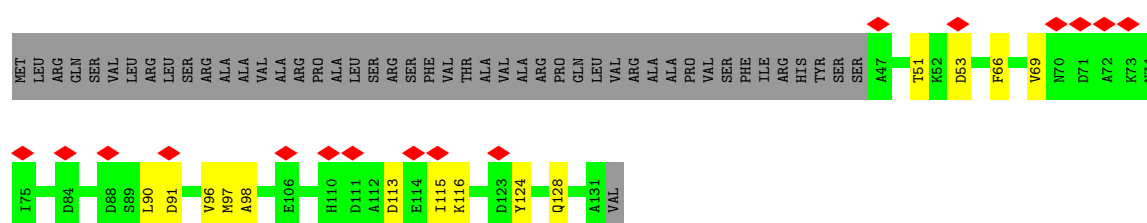
- Molecule 13: Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I)



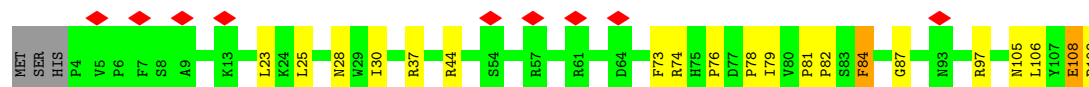
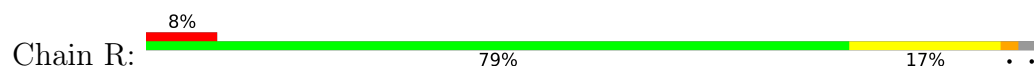
- Molecule 14: Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I)



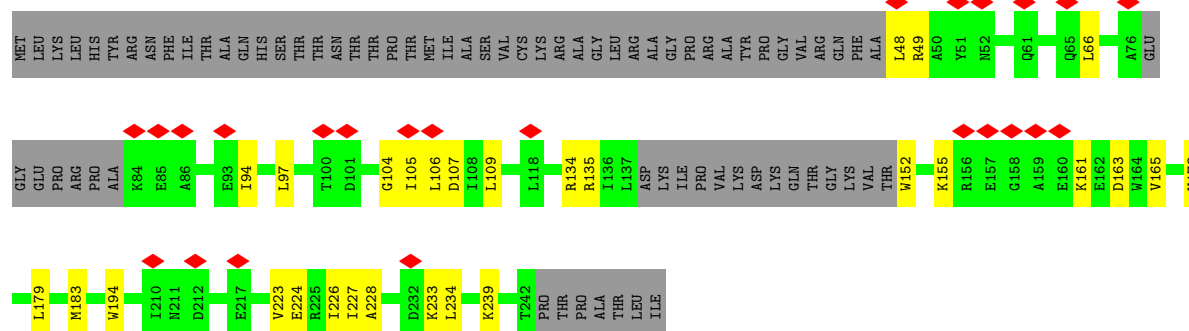
- Molecule 15: Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I)



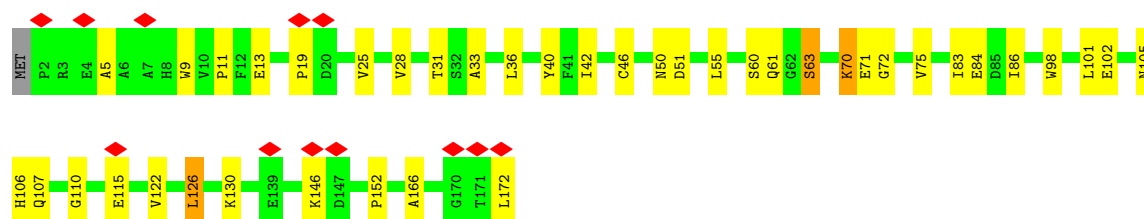
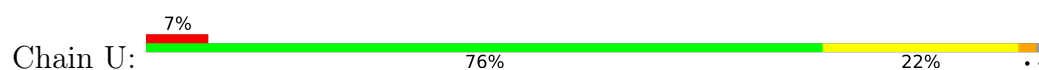
- Molecule 16: Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I)



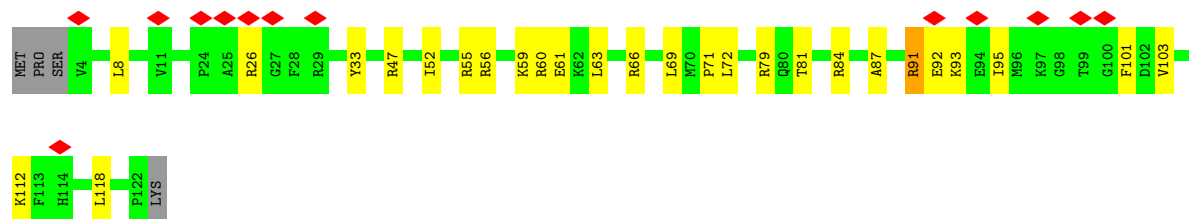
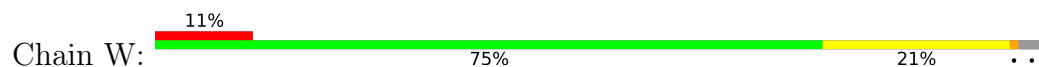
- Molecule 17: Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I)



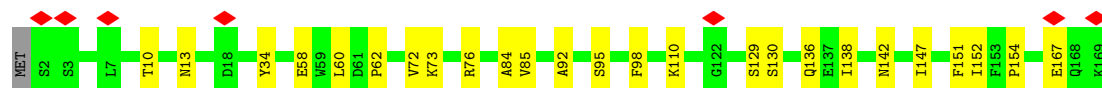
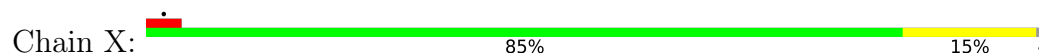
- Molecule 18: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)



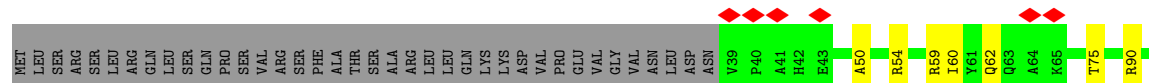
- Molecule 19: Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I)

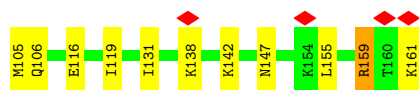


- Molecule 20: Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I)

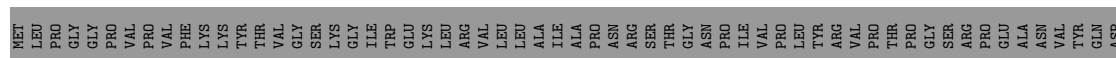


- Molecule 21: Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I)

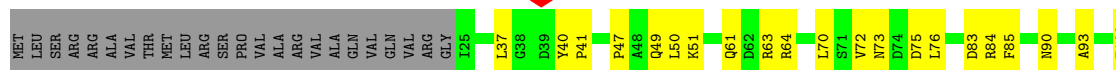




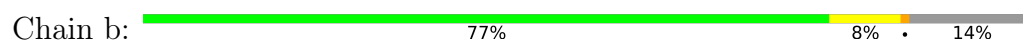
- Molecule 22: Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I)



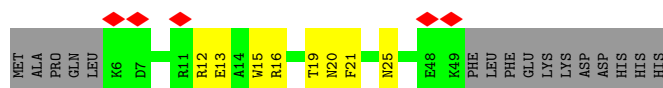
- Molecule 23: Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I)



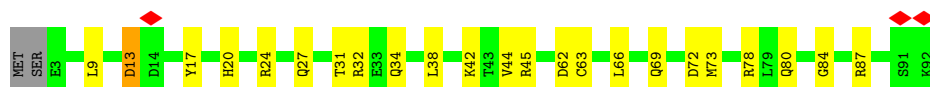
- Molecule 24: Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 25: Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I)

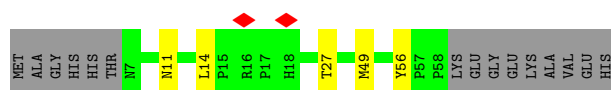


- Molecule 26: Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I)



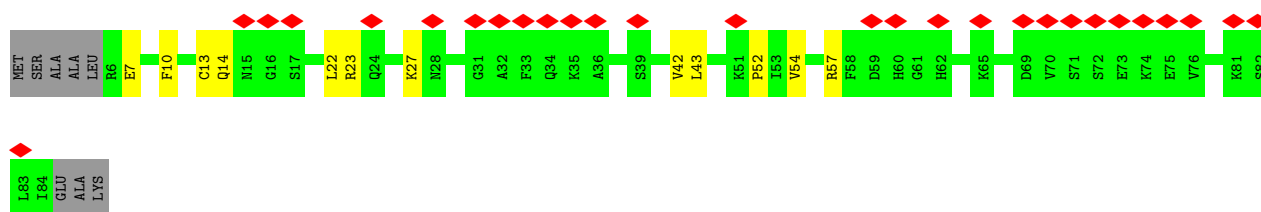
- Molecule 27: Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain e:  70% 7% 22%



- Molecule 28: Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain f:  32% 77% 14% 9%



- Molecule 29: Subunit NI9M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain g:  83% 14%



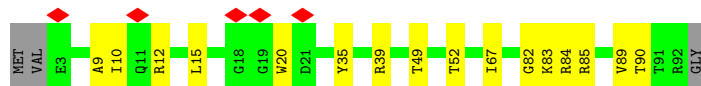
- Molecule 30: Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain i:  77% 16% 8%



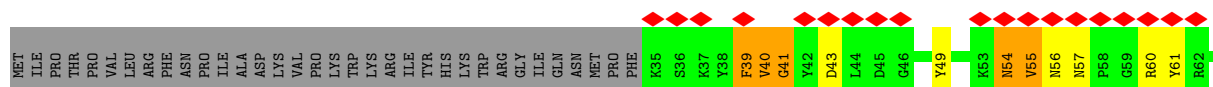
- Molecule 31: Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I)

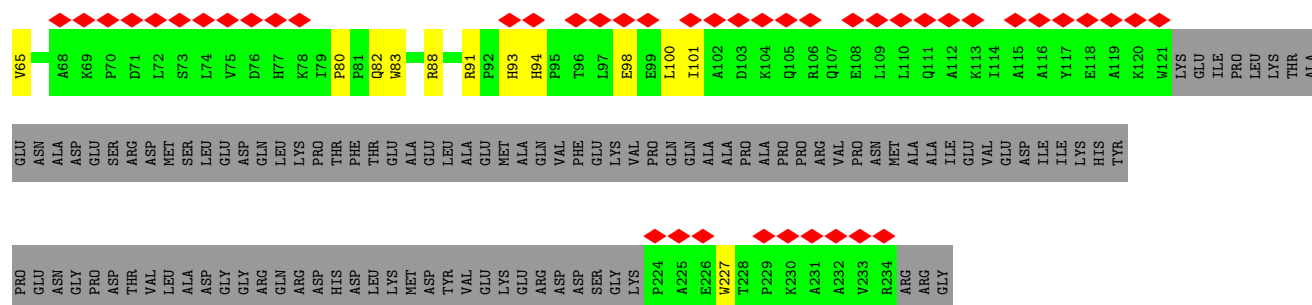
Chain j:  5% 80% 17%



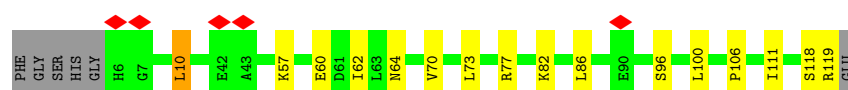
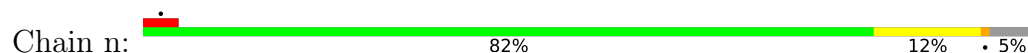
- Molecule 32: Subunit N7BML assembly factor

Chain k:  27% 32% 8% 59%

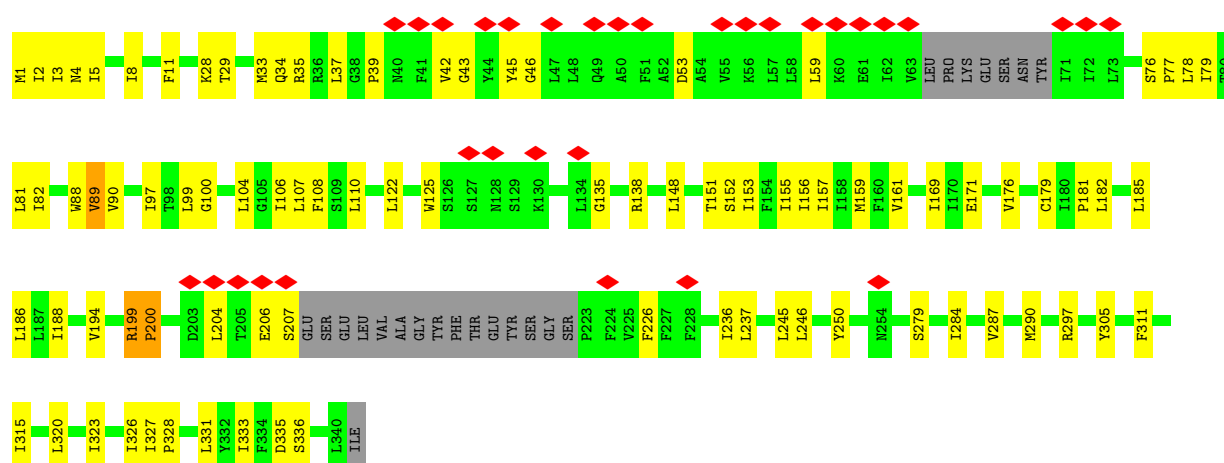




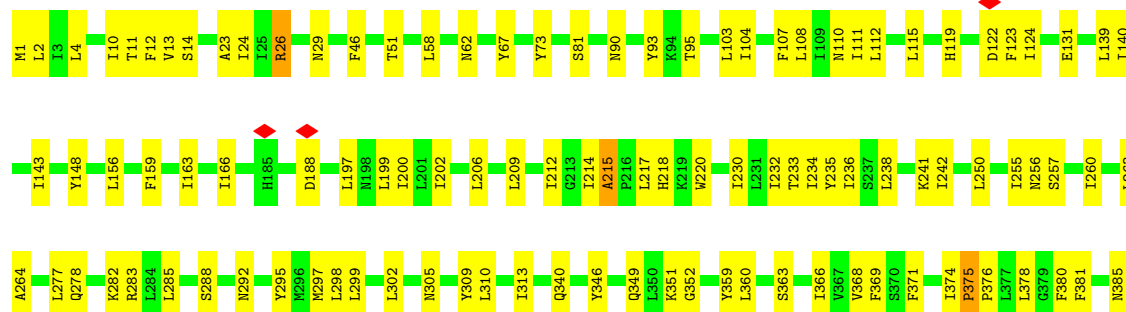
- Molecule 33: Subunit NUM of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 34: Subunit NU1M of NADH:Ubiquinone Oxidoreductase (Complex I)

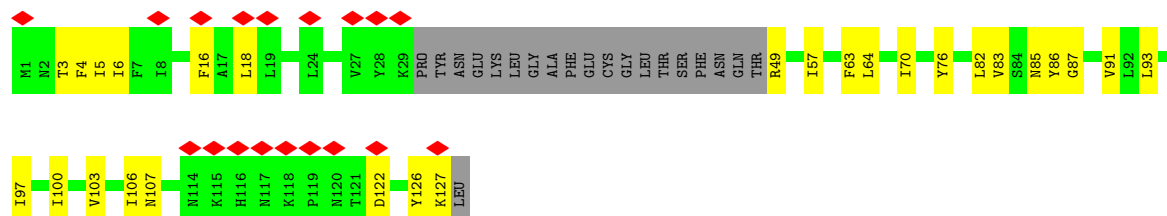


- Molecule 35: Subunit NU2M of NADH:Ubiquinone Oxidoreductase (Complex I)

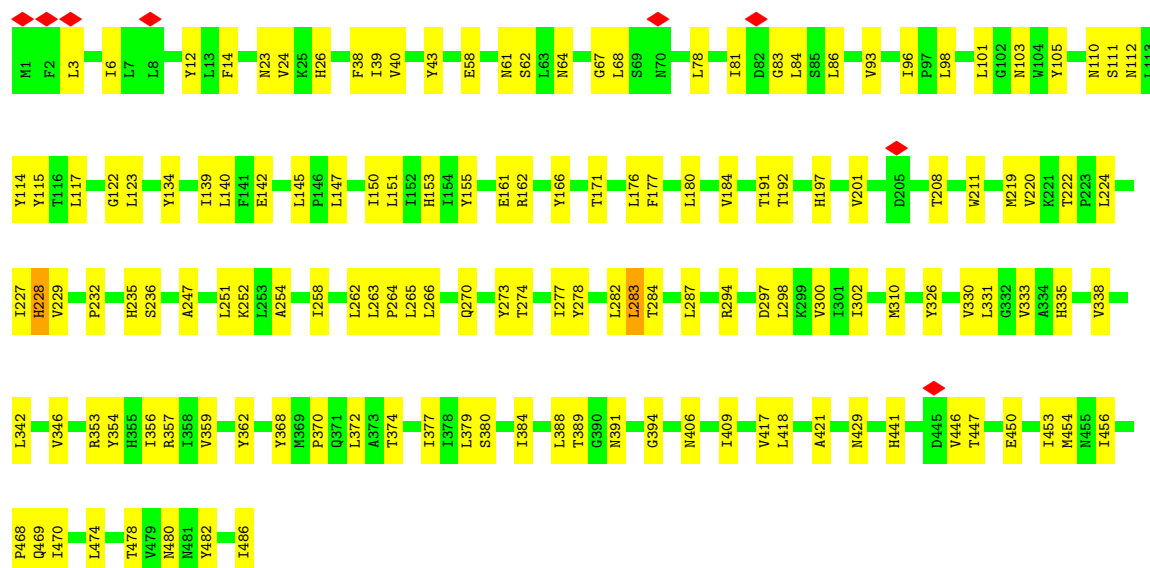




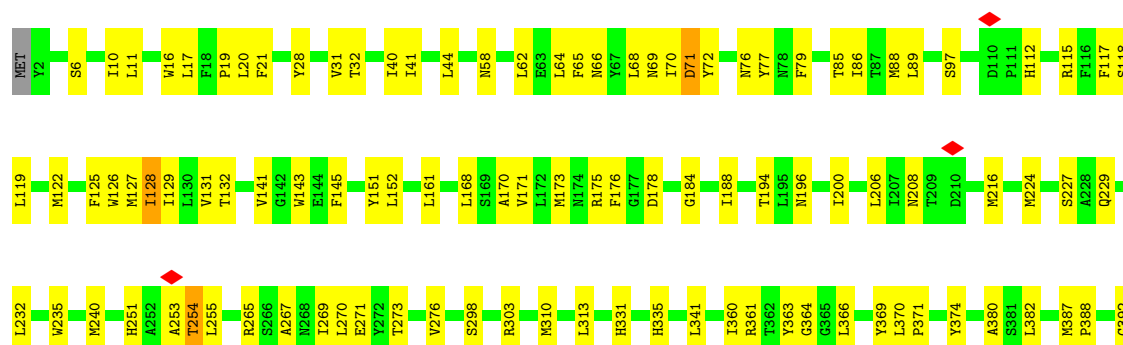
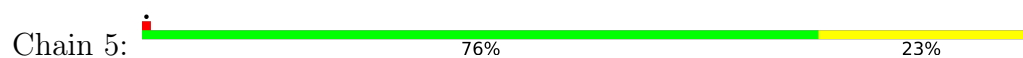
- Molecule 36: Subunit NU3M of NADH:Ubiquinone Oxidoreductase (Complex I)

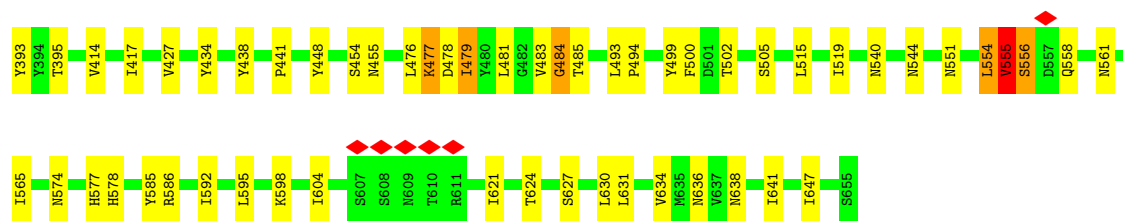


- Molecule 37: Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I)

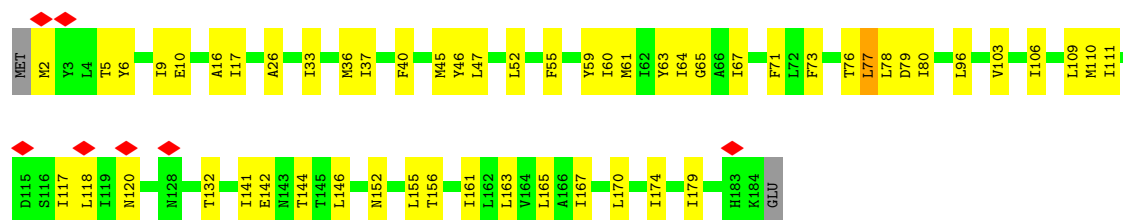


- Molecule 38: Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I)

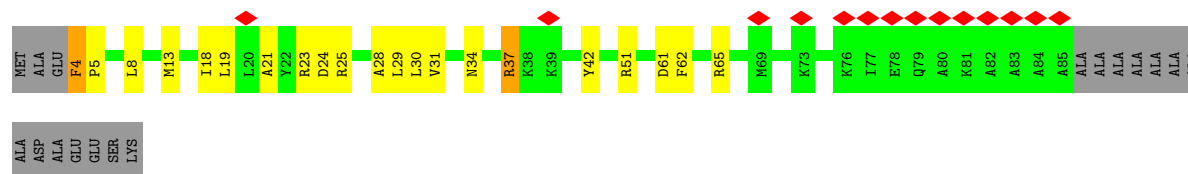




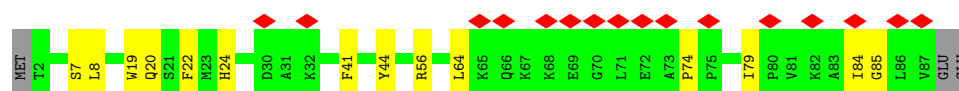
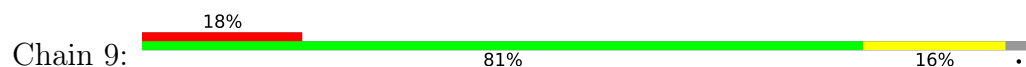
- Molecule 39: Subunit NU6M of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 40: Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 41: Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	112418	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	46425	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.202	Depositor
Minimum map value	-0.072	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	491.112, 491.112, 491.112	wwPDB
Map dimensions	456, 456, 456	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.077, 1.077, 1.077	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, CPL, FES, FMN, PLC, CDL, 3PE, LMN, T7X, ZMP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/5368	0.69	3/7285 (0.0%)
2	B	0.54	4/3496 (0.1%)	0.72	5/4717 (0.1%)
3	C	0.56	0/3492	0.81	2/4729 (0.0%)
4	D	0.50	0/697	0.70	1/940 (0.1%)
5	E	0.43	0/2113	0.71	2/2854 (0.1%)
6	F	0.38	0/1011	0.77	0/1371
7	G	0.55	0/1793	0.80	1/2441 (0.0%)
8	H	0.38	1/1717 (0.1%)	0.72	1/2332 (0.0%)
9	I	0.53	0/1557	0.77	1/2110 (0.0%)
10	J	0.45	0/1362	0.73	2/1855 (0.1%)
11	K	0.55	0/1220	0.80	0/1656
12	L	0.57	0/700	0.81	0/947
13	O	0.25	0/598	0.56	0/813
14	P	0.43	0/1061	0.73	2/1427 (0.1%)
15	Q	0.33	0/654	0.61	0/890
16	R	0.46	0/909	0.76	0/1229
17	S	0.41	0/1454	0.66	0/1960
18	U	0.46	0/1374	0.80	2/1856 (0.1%)
19	W	0.44	0/984	0.68	0/1327
20	X	0.48	0/1344	0.67	0/1822
21	Y	0.47	1/1051 (0.1%)	0.64	1/1420 (0.1%)
22	Z	0.40	0/947	0.65	0/1291
23	a	0.50	0/1064	0.76	0/1439
24	b	0.44	0/503	0.65	1/679 (0.1%)
25	c	0.39	0/364	0.55	0/491
26	d	0.57	0/776	0.75	0/1043
27	e	0.36	0/456	0.65	0/619
28	f	0.32	0/630	0.67	0/844
29	g	0.39	0/643	0.64	1/880 (0.1%)
30	i	0.48	0/666	0.65	0/907
31	j	0.43	0/745	0.66	0/1006
32	k	0.42	0/856	0.82	2/1163 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	n	0.48	0/943	0.71	2/1279 (0.2%)
34	1	0.60	0/2608	0.88	1/3558 (0.0%)
35	2	0.71	1/3854 (0.0%)	0.89	4/5252 (0.1%)
36	3	0.51	0/888	0.86	0/1210
37	4	0.66	0/3949	0.84	0/5392
38	5	0.62	2/5327 (0.0%)	0.86	8/7273 (0.1%)
39	6	0.55	0/1468	0.83	1/2003 (0.0%)
40	8	0.50	1/686 (0.1%)	0.77	2/918 (0.2%)
41	9	0.47	0/684	0.66	0/918
All	All	0.52	10/62012 (0.0%)	0.77	45/84146 (0.1%)

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
1	A	0	1
3	C	0	2
5	E	0	1
7	G	0	1
8	H	0	5
16	R	0	2
17	S	0	1
18	U	0	3
19	W	0	1
22	Z	0	1
26	d	0	1
31	j	0	1
32	k	0	2
34	1	0	2
37	4	0	3
38	5	0	5
40	8	0	1
All	All	0	33

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	113	ARG	NE-CZ	16.13	1.50	1.33
2	B	113	ARG	CZ-NH2	-9.30	1.21	1.33
2	B	113	ARG	CD-NE	-8.35	1.34	1.46

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	100	PRO	CA-C	-6.94	1.47	1.52
2	B	113	ARG	CZ-NH1	6.52	1.41	1.32
35	2	26	ARG	CZ-NH1	6.22	1.41	1.32
38	5	216	MET	SD-CE	6.00	1.94	1.79
38	5	71	ASP	CB-CG	-5.75	1.37	1.52
21	Y	105	MET	SD-CE	5.73	1.93	1.79
40	8	4	PHE	C-N	5.15	1.39	1.33

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	113	ARG	NE-CZ-NH1	9.93	131.43	121.50
38	5	254	THR	N-CA-C	7.11	118.72	110.97
3	C	381	LEU	CA-CB-CG	7.10	141.14	116.30
38	5	128	ILE	CG1-CB-CG2	-7.00	89.71	110.70
5	E	162	ARG	N-CA-C	6.76	120.73	111.54
10	J	147	LEU	CA-CB-CG	6.73	139.87	116.30
8	H	100	PRO	O-C-N	-6.58	118.06	121.15
3	C	71	ILE	N-CA-C	-6.51	106.45	112.96
40	8	4	PHE	CA-C-N	-6.32	113.88	120.38
40	8	4	PHE	C-N-CA	-6.32	113.88	120.38
21	Y	159	ARG	NE-CZ-NH2	6.28	124.85	119.20
5	E	150	ARG	NE-CZ-NH2	6.20	124.78	119.20
35	2	215	ALA	N-CA-C	6.10	123.29	109.81
38	5	479	ILE	N-CA-C	-5.85	106.78	111.81
32	k	41	GLY	N-CA-C	5.77	118.91	110.38
35	2	277	LEU	CA-CB-CG	5.69	136.22	116.30
10	J	182	GLY	O-C-N	5.68	125.03	121.85
1	A	225	LEU	CA-CB-CG	5.65	136.07	116.30
32	k	55	VAL	N-CA-C	5.56	120.91	109.34
14	P	121	LYS	CA-C-N	5.53	132.10	121.54
14	P	121	LYS	C-N-CA	5.53	132.10	121.54
39	6	77	LEU	CA-CB-CG	5.51	135.58	116.30
7	G	177	TRP	CA-CB-CG	5.43	123.92	113.60
2	B	417	LEU	CA-CB-CG	-5.38	97.47	116.30
1	A	659	TYR	CA-C-N	5.37	131.80	121.54
1	A	659	TYR	C-N-CA	5.37	131.80	121.54
35	2	375	PRO	N-CA-C	5.35	117.23	110.70
2	B	229	PRO	CA-C-N	-5.33	113.18	119.84
2	B	229	PRO	C-N-CA	-5.33	113.18	119.84
9	I	103	TYR	CA-CB-CG	-5.31	104.34	113.90
35	2	285	LEU	CA-CB-CG	5.28	134.76	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	5	555	VAL	N-CA-C	5.24	120.24	109.34
2	B	113	ARG	CG-CD-NE	-5.21	100.55	112.00
24	b	48	LEU	CA-CB-CG	5.20	134.48	116.30
29	g	69	ARG	CA-CB-CG	5.20	124.49	114.10
38	5	484	GLY	CA-C-N	-5.18	115.76	123.11
38	5	484	GLY	C-N-CA	-5.18	115.76	123.11
4	D	39	ARG	CB-CG-CD	5.15	123.15	111.30
18	U	126	LEU	CA-C-N	5.15	131.38	121.54
18	U	126	LEU	C-N-CA	5.15	131.38	121.54
33	n	10	LEU	CA-C-N	5.07	150.08	120.81
33	n	10	LEU	C-N-CA	5.07	150.08	120.81
34	1	45	TYR	CA-CB-CG	5.06	123.01	113.90
38	5	555	VAL	CA-C-N	5.01	131.10	121.54
38	5	555	VAL	C-N-CA	5.01	131.10	121.54

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	1	199	ARG	Sidechain
34	1	200	PRO	Peptide
37	4	228	HIS	Peptide
37	4	283	LEU	Peptide
37	4	81	ILE	Peptide
38	5	227	SER	Peptide
38	5	253	ALA	Peptide
38	5	454	SER	Peptide
38	5	554	LEU	Peptide
38	5	586	ARG	Sidechain
40	8	37	ARG	Sidechain
1	A	568	PHE	Peptide
3	C	269	ARG	Sidechain
3	C	336	ARG	Sidechain
5	E	51	ARG	Sidechain
7	G	148	ARG	Sidechain
8	H	174	ASN	Peptide
8	H	204	LYS	Peptide
8	H	216	ARG	Peptide
8	H	29	ILE	Peptide
8	H	54	ARG	Sidechain
16	R	108	GLU	Peptide
16	R	84	PHE	Peptide

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Mol	Chain	Res	Type	Group
17	S	134	ARG	Sidechain
18	U	5	ALA	Peptide
18	U	63	SER	Peptide
18	U	70	LYS	Peptide
19	W	91	ARG	Sidechain
22	Z	180	THR	Peptide
26	d	78	ARG	Sidechain
31	j	82	GLY	Peptide
32	k	39	PHE	Peptide
32	k	54	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5274	0	5173	99	0
2	B	3421	0	3372	44	0
3	C	3415	0	3353	111	0
4	D	681	0	671	20	0
5	E	2075	0	2064	46	0
6	F	990	0	977	15	0
7	G	1739	0	1678	38	0
8	H	1680	0	1649	28	0
9	I	1519	0	1460	40	0
10	J	1329	0	1311	27	0
11	K	1190	0	1163	33	0
12	L	691	0	754	26	0
13	O	591	0	585	4	0
14	P	1036	0	1018	21	0
15	Q	648	0	636	10	0
16	R	884	0	893	25	0
17	S	1430	0	1463	27	0
18	U	1345	0	1327	30	0
19	W	961	0	974	26	0
20	X	1305	0	1281	27	0
21	Y	1021	0	984	13	0
22	Z	922	0	908	17	0
23	a	1030	0	967	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	b	490	0	509	6	0
25	c	353	0	343	7	0
26	d	760	0	721	21	0
27	e	436	0	426	5	0
28	f	620	0	634	8	0
29	g	617	0	597	15	0
30	i	646	0	630	15	0
31	j	724	0	706	14	0
32	k	828	0	815	22	0
33	n	914	0	880	14	0
34	1	2540	0	2658	69	0
35	2	3774	0	4005	106	0
36	3	869	0	944	31	0
37	4	3855	0	4054	105	0
38	5	5197	0	5353	147	0
39	6	1443	0	1565	49	0
40	8	672	0	677	20	0
41	9	672	0	683	14	0
42	A	16	0	0	0	0
42	B	8	0	0	0	0
42	I	16	0	0	0	0
42	K	8	0	0	1	0
43	A	4	0	0	0	0
43	H	4	0	0	0	0
44	B	31	0	19	2	0
45	E	48	0	26	1	0
46	4	136	0	203	13	0
46	5	93	0	140	7	0
46	6	36	0	46	5	0
46	I	51	0	82	0	0
46	J	85	0	118	4	0
46	g	43	0	63	2	0
47	J	69	0	88	5	0
47	j	65	0	77	2	0
48	4	92	0	137	6	0
48	J	78	0	103	22	0
48	X	82	0	108	4	0
48	g	83	0	116	7	0
49	O	33	0	38	1	0
49	Q	33	0	38	0	0
50	5	31	0	36	1	0
50	W	83	0	123	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	n	42	0	64	1	0
51	2	100	0	0	0	0
51	4	43	0	0	1	0
52	2	52	0	80	4	0
All	All	62052	0	62566	1160	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 9.

All (1160) 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)
38:5:79:PHE:HE1	38:5:129:ILE:HG23	1.19	1.07
3:C:172:TYR:O	3:C:175:THR:HG22	1.56	1.05
1:A:375:THR:HG22	1:A:538:PRO:HG3	1.39	1.04
35:2:202:ILE:HG22	35:2:206:LEU:HD13	1.39	1.04
10:J:117:ALA:HA	48:J:204:CDL:HA4	1.45	0.99
17:S:49:ARG:HD3	17:S:105:ILE:HG12	1.45	0.98
38:5:478:ASP:OD1	40:8:51:ARG:NH2	2.01	0.93
3:C:269:ARG:HH12	9:I:77:TYR:HA	1.32	0.93
38:5:79:PHE:CE1	38:5:129:ILE:HG23	2.05	0.92
38:5:200:ILE:CG2	38:5:269:ILE:HD11	2.00	0.92
38:5:484:GLY:O	40:8:34:ASN:OD1	1.89	0.91
1:A:375:THR:HG22	1:A:538:PRO:CG	2.00	0.91
3:C:208:GLU:HG2	9:I:99:TYR:CE2	2.05	0.91
35:2:202:ILE:CG2	35:2:206:LEU:HD13	2.00	0.89
3:C:208:GLU:HG2	9:I:99:TYR:CD2	2.06	0.89
23:a:64:ARG:HE	23:a:70:LEU:HD21	1.37	0.88
38:5:200:ILE:HG22	38:5:269:ILE:HD11	1.54	0.87
39:6:45:MET:CG	46:6:301:3PE:H372	2.06	0.86
3:C:410:MET:HE3	3:C:427:ILE:HG23	1.58	0.86
38:5:16:TRP:CD1	38:5:16:TRP:O	2.29	0.86
20:X:73:LYS:HE3	48:g:201:CDL:OA3	1.76	0.85
39:6:45:MET:HG2	46:6:301:3PE:H372	1.60	0.83
38:5:298:SER:HB2	38:5:303:ARG:HD2	1.61	0.82
3:C:410:MET:HE3	3:C:427:ILE:CG2	2.10	0.81
38:5:16:TRP:CD1	38:5:16:TRP:C	2.52	0.80
33:n:77:ARG:HD2	37:4:191:THR:HG23	1.62	0.80
38:5:125:PHE:CE1	38:5:129:ILE:HD11	2.16	0.80
1:A:447:ASP:OD1	1:A:447:ASP:O	1.98	0.80
5:E:162:ARG:HA	5:E:162:ARG:HH21	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:184:LEU:HD21	3:C:210:ARG:NH2	1.98	0.79
20:X:72:VAL:HG13	20:X:76:ARG:HH22	1.49	0.78
13:O:103:LEU:HD12	13:O:103:LEU:O	1.83	0.77
3:C:428:ARG:HH12	3:C:430:PRO:HA	1.49	0.77
20:X:92:ALA:HA	20:X:147:ILE:HD11	1.66	0.76
32:k:49:TYR:HD1	32:k:65:VAL:HG23	1.51	0.75
5:E:367:GLU:HB3	12:L:82:GLY:HA3	1.67	0.75
15:Q:90:LEU:HB3	16:R:44:ARG:HH12	1.52	0.75
32:k:49:TYR:CD1	32:k:65:VAL:HG23	2.21	0.74
3:C:97:VAL:HG21	11:K:127:MET:HE1	1.70	0.74
5:E:162:ARG:HH21	5:E:162:ARG:CA	2.00	0.74
35:2:202:ILE:CG2	35:2:206:LEU:CD1	2.65	0.73
3:C:205:TRP:HE3	3:C:261:ILE:HG22	1.53	0.73
34:1:106:ILE:HD11	34:1:169:ILE:HD11	1.70	0.73
2:B:101:MET:O	2:B:113:ARG:NH1	2.21	0.73
18:U:166:ALA:HB1	18:U:172:LEU:HG	1.70	0.73
3:C:184:LEU:HD21	3:C:210:ARG:CZ	2.19	0.73
16:R:25:LEU:HD11	16:R:73:PHE:O	1.87	0.73
23:a:40:TYR:CE2	23:a:72:VAL:HG23	2.24	0.73
33:n:77:ARG:HD2	37:4:191:THR:CG2	2.17	0.73
3:C:204:LEU:HD22	34:1:34:GLN:CB	2.19	0.72
34:1:104:LEU:HD12	34:1:107:LEU:HD23	1.71	0.72
7:G:202:ASP:HB3	7:G:205:PHE:HB2	1.71	0.72
3:C:61:ASP:HB3	35:2:283:ARG:NH1	2.03	0.72
10:J:117:ALA:CA	48:J:204:CDL:HA4	2.18	0.71
17:S:228:ALA:O	30:i:77:ARG:NH2	2.23	0.71
20:X:84:ALA:HB1	35:2:4:LEU:HD21	1.73	0.71
3:C:428:ARG:NH1	3:C:430:PRO:HA	2.05	0.71
7:G:71:LEU:HD21	7:G:96:LEU:HB2	1.73	0.71
38:5:125:PHE:CZ	38:5:129:ILE:HD11	2.27	0.70
31:j:85:ARG:HA	38:5:208:ASN:HB3	1.73	0.70
7:G:124:ILE:HD11	7:G:145:LEU:HB2	1.74	0.70
20:X:34:TYR:CE1	20:X:110:LYS:HE2	2.26	0.70
3:C:150:ASN:ND2	3:C:410:MET:SD	2.65	0.70
2:B:43:ASN:OD1	2:B:43:ASN:O	2.10	0.69
32:k:83:TRP:HE1	32:k:100:LEU:HD11	1.55	0.69
3:C:121:ARG:HD3	11:K:122:THR:HG21	1.73	0.69
8:H:68:LYS:HE3	21:Y:155:LEU:CD2	2.23	0.69
16:R:105:ASN:HD21	37:4:105:TYR:HB3	1.59	0.68
48:4:502:CDL:H461	38:5:17:LEU:HD13	1.74	0.68
23:a:49:GLN:O	23:a:63:ARG:NH1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:49:ARG:HE	39:6:79:ASP:HB3	1.57	0.68
48:J:204:CDL:OA8	48:J:204:CDL:H111	1.94	0.68
11:K:100:GLN:HB2	11:K:188:MET:HE3	1.74	0.68
37:4:222:THR:HG23	37:4:254:ALA:HB3	1.76	0.68
38:5:151:TYR:HB2	38:5:171:VAL:HG21	1.76	0.68
36:3:122:ASP:OD1	36:3:122:ASP:O	2.12	0.67
5:E:126:VAL:HG12	5:E:164:ILE:HB	1.75	0.67
35:2:378:LEU:HD12	35:2:453:GLY:HA3	1.76	0.67
1:A:145:GLN:HG2	3:C:386:LEU:HD11	1.75	0.67
3:C:152:GLN:HG3	3:C:174:ARG:HD2	1.77	0.67
3:C:240:PRO:HG3	9:I:113:ARG:HH22	1.59	0.67
16:R:25:LEU:HD11	16:R:74:ARG:HA	1.77	0.67
38:5:71:ASP:OD1	38:5:71:ASP:N	2.23	0.67
10:J:147:LEU:CD2	10:J:152:LYS:HE2	2.23	0.67
37:4:197:HIS:HE1	37:4:264:PRO:HG2	1.59	0.67
48:4:502:CDL:H711	48:4:502:CDL:H531	1.77	0.67
3:C:175:THR:HG23	3:C:176:MET:N	2.09	0.67
35:2:403:ILE:HG13	37:4:180:LEU:HD11	1.77	0.66
39:6:45:MET:HG3	46:6:301:3PE:H372	1.76	0.66
3:C:97:VAL:HG11	11:K:127:MET:CE	2.26	0.66
38:5:85:THR:HG23	38:5:131:VAL:HG12	1.78	0.66
3:C:197:VAL:HG13	3:C:274:ARG:HD3	1.76	0.66
3:C:228:ALA:O	3:C:231:ARG:NH2	2.29	0.66
38:5:125:PHE:CZ	38:5:129:ILE:CD1	2.79	0.66
34:1:159:MET:HE1	34:1:328:PRO:HG3	1.77	0.65
40:8:5:PRO:HG2	40:8:29:LEU:HG	1.79	0.65
29:g:9:TRP:HE1	48:g:201:CDL:HA31	1.60	0.65
38:5:477:LYS:O	38:5:477:LYS:HG2	1.94	0.65
2:B:393:TRP:HE1	2:B:417:LEU:HD13	1.62	0.65
3:C:204:LEU:HD22	34:1:34:GLN:HB3	1.79	0.65
38:5:128:ILE:HG22	38:5:129:ILE:HD12	1.76	0.65
9:I:100:THR:HG21	34:1:37:LEU:HG	1.78	0.65
19:W:56:ARG:HH12	34:1:335:ASP:HB3	1.62	0.65
1:A:377:ASP:HB3	1:A:528:ARG:HH11	1.62	0.65
1:A:185:HIS:HB2	2:B:388:ARG:HH12	1.62	0.64
4:D:68:ALA:HB1	18:U:84:GLU:HG2	1.80	0.64
3:C:269:ARG:NH1	9:I:77:TYR:HA	2.07	0.64
36:3:126:TYR:C	36:3:127:LYS:HG2	2.21	0.64
36:3:126:TYR:O	36:3:127:LYS:HG2	1.97	0.64
9:I:170:ILE:HG21	11:K:156:TYR:HD1	1.63	0.64
29:g:60:GLN:HB3	33:n:111:ILE:HG13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:5:388:PRO:HG3	38:5:515:LEU:HD21	1.80	0.64
10:J:143:ARG:HH11	35:2:256:ASN:HB2	1.63	0.64
5:E:72:LYS:HE2	5:E:243:ALA:HA	1.80	0.64
1:A:67:ARG:HD2	1:A:70:TYR:HB3	1.80	0.63
14:P:18:LYS:HG2	14:P:69:LEU:HD13	1.79	0.63
34:1:148:LEU:HB2	36:3:63:PHE:HE1	1.63	0.63
38:5:479:ILE:HG23	40:8:42:TYR:HD2	1.64	0.63
5:E:110:ARG:HH12	5:E:137:ASN:HB3	1.64	0.63
6:F:99:LEU:HD23	9:I:56:ARG:HH11	1.62	0.63
3:C:204:LEU:CD2	34:1:34:GLN:HB3	2.28	0.63
5:E:162:ARG:HB3	5:E:162:ARG:NH2	2.14	0.63
35:2:299:LEU:O	35:2:305:ASN:ND2	2.31	0.63
7:G:68:VAL:O	7:G:72:HIS:ND1	2.30	0.63
17:S:49:ARG:HD3	17:S:105:ILE:CG1	2.26	0.63
48:J:204:CDL:HB32	38:5:598:LYS:HG3	1.80	0.62
26:d:87:ARG:HE	37:4:201:VAL:HG12	1.62	0.62
47:J:202:LMN:HBA	37:4:184:VAL:HG21	1.82	0.62
19:W:66:ARG:NH2	39:6:141:ILE:O	2.30	0.62
37:4:219:MET:HG3	37:4:224:LEU:HB2	1.80	0.62
1:A:491:ARG:HG2	1:A:493:ASP:H	1.64	0.62
37:4:370:PRO:HB3	46:5:901:3PE:H11	1.81	0.62
1:A:351:GLY:HA3	1:A:555:ALA:H	1.65	0.62
28:f:13:CYS:O	28:f:23:ARG:NH1	2.33	0.62
37:4:150:ILE:HG21	46:4:501:3PE:H272	1.82	0.62
16:R:108:GLU:HG2	16:R:109:PRO:CD	2.29	0.62
23:a:47:PRO:HB3	23:a:84:ARG:HH21	1.65	0.62
34:1:155:ILE:HD11	36:3:70:ILE:HG23	1.81	0.62
38:5:126:TRP:CZ3	38:5:141:VAL:HG12	2.35	0.62
38:5:224:MET:HG3	38:5:229:GLN:HB2	1.81	0.62
2:B:298:LEU:HB2	2:B:339:MET:HE3	1.80	0.61
10:J:116:PRO:HB2	48:J:204:CDL:HA32	1.82	0.61
48:J:204:CDL:H522	38:5:595:LEU:HD12	1.82	0.61
32:k:57:ASN:HB3	32:k:60:ARG:HB2	1.80	0.61
35:2:403:ILE:HD12	37:4:176:LEU:HD12	1.83	0.61
35:2:215:ALA:O	35:2:218:HIS:ND1	2.34	0.61
29:g:47:ARG:NE	34:1:333:ILE:O	2.34	0.61
34:1:181:PRO:HB2	34:1:182:LEU:HD12	1.83	0.61
38:5:16:TRP:O	38:5:16:TRP:HD1	1.79	0.61
3:C:97:VAL:HG11	11:K:127:MET:HE1	1.82	0.61
38:5:151:TYR:HD2	38:5:152:LEU:HD12	1.65	0.61
5:E:373:ILE:HG21	12:L:79:ARG:HH11	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:236:ILE:HG22	34:1:290:MET:HE2	1.82	0.61
1:A:267:ASN:HD22	1:A:285:HIS:HB2	1.66	0.60
5:E:112:LEU:HD21	5:E:150:ARG:HD2	1.82	0.60
40:8:61:ASP:OD2	40:8:65:ARG:NH2	2.34	0.60
10:J:181:GLU:HG3	10:J:181:GLU:O	2.01	0.60
48:J:204:CDL:H522	38:5:595:LEU:CD1	2.32	0.60
18:U:51:ASP:O	18:U:55:LEU:HG	2.01	0.60
37:4:112:ASN:OD1	46:4:501:3PE:H122	2.01	0.60
1:A:126:LEU:HD21	1:A:144:LEU:HD21	1.83	0.60
19:W:26:ARG:HG2	50:W:401:PLC:H8A1	1.84	0.60
23:a:40:TYR:CD1	23:a:41:PRO:HD2	2.37	0.60
32:k:39:PHE:O	32:k:41:GLY:N	2.32	0.60
38:5:271:GLU:HB3	38:5:493:LEU:HG	1.83	0.60
1:A:458:THR:HG22	1:A:460:ALA:H	1.67	0.60
12:L:81:ARG:NH2	35:2:148:TYR:O	2.35	0.60
35:2:202:ILE:HG23	35:2:206:LEU:CD1	2.31	0.60
9:I:97:ALA:O	34:1:35:ARG:NH2	2.35	0.60
10:J:147:LEU:HD23	10:J:152:LYS:HE2	1.83	0.60
20:X:13:ASN:HD21	20:X:167:GLU:HG2	1.66	0.60
1:A:439:ILE:HG21	1:A:450:PHE:HE2	1.66	0.60
3:C:126:LEU:HD23	7:G:216:LEU:HD11	1.83	0.60
10:J:124:LEU:HD13	48:J:204:CDL:H731	1.84	0.59
38:5:126:TRP:HZ3	38:5:141:VAL:HG12	1.67	0.59
38:5:298:SER:CB	38:5:303:ARG:HD2	2.32	0.59
2:B:367:ARG:HH21	2:B:402:ARG:HH12	1.49	0.59
2:B:288:CYS:SG	2:B:289:THR:N	2.75	0.59
12:L:69:ILE:HD12	35:2:139:LEU:HD11	1.83	0.59
17:S:227:ILE:HG12	26:d:44:VAL:HG22	1.84	0.59
8:H:125:GLN:HB2	8:H:179:ALA:HB3	1.83	0.59
48:J:204:CDL:H602	38:5:647:ILE:HG23	1.84	0.59
26:d:31:THR:HG23	37:4:480:ASN:HD22	1.68	0.59
1:A:375:THR:HG22	1:A:538:PRO:CB	2.32	0.59
19:W:52:ILE:HG12	19:W:55:ARG:HH22	1.66	0.59
5:E:247:ARG:NH1	5:E:334:ASP:O	2.36	0.59
15:Q:113:ASP:O	15:Q:116:LYS:HE3	2.03	0.59
34:1:284:ILE:HA	34:1:287:VAL:HG12	1.85	0.59
2:B:106:TRP:HB2	2:B:113:ARG:HH22	1.68	0.59
35:2:233:THR:HA	35:2:236:ILE:HG12	1.84	0.59
8:H:68:LYS:HE3	21:Y:155:LEU:HD23	1.85	0.59
3:C:175:THR:CG2	3:C:176:MET:N	2.66	0.58
35:2:13:VAL:HG22	35:2:24:ILE:HD13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:9:LEU:HD23	34:1:42:VAL:HG23	1.84	0.58
10:J:147:LEU:HD22	35:2:392:ASN:OD1	2.04	0.58
36:3:103:VAL:HA	36:3:106:ILE:HG22	1.85	0.58
3:C:54:ARG:HG2	3:C:55:THR:HG23	1.84	0.58
8:H:215:ARG:NH2	8:H:219:GLU:O	2.36	0.58
2:B:283:ASN:HD22	2:B:360:ASN:HB2	1.68	0.58
14:P:74:VAL:CG2	14:P:78:LYS:HE2	2.33	0.58
18:U:70:LYS:HB3	18:U:71:GLU:HG3	1.86	0.58
1:A:249:PRO:HA	1:A:252:LEU:HD23	1.86	0.58
3:C:172:TYR:C	3:C:175:THR:HG22	2.28	0.58
37:4:265:LEU:HD12	37:4:266:LEU:HD22	1.86	0.58
10:J:139:PHE:HZ	48:J:204:CDL:H673	1.67	0.58
11:K:80:THR:OG1	11:K:90:MET:SD	2.59	0.58
13:O:103:LEU:HD12	13:O:103:LEU:C	2.27	0.58
37:4:251:LEU:HD23	37:4:310:MET:HG3	1.85	0.58
20:X:130:SER:N	48:X:201:CDL:OA4	2.32	0.58
26:d:62:ASP:O	30:i:68:ASN:ND2	2.36	0.58
2:B:333:ILE:HG21	2:B:347:VAL:HG11	1.86	0.57
2:B:425:THR:HG21	2:B:430:GLY:HA3	1.86	0.57
3:C:176:MET:HE1	3:C:247:ILE:HD13	1.86	0.57
10:J:147:LEU:HG	10:J:152:LYS:HD3	1.84	0.57
37:4:96:ILE:HD12	37:4:122:GLY:HA3	1.85	0.57
38:5:485:THR:HG23	38:5:485:THR:O	2.04	0.57
41:9:20:GLN:O	41:9:24:HIS:ND1	2.37	0.57
34:1:226:PHE:CE1	36:3:18:LEU:HD23	2.39	0.57
37:4:220:VAL:HA	37:4:227:ILE:HG21	1.87	0.57
3:C:254:PHE:HD2	3:C:344:LEU:HD12	1.69	0.57
16:R:108:GLU:HG2	16:R:109:PRO:HD3	1.86	0.57
1:A:217:LEU:HD22	1:A:219:LYS:HB3	1.86	0.57
2:B:97:LYS:NZ	2:B:244:VAL:O	2.30	0.57
3:C:356:ALA:HB2	19:W:8:LEU:HD11	1.87	0.57
5:E:193:ILE:HD12	5:E:194:VAL:HG23	1.87	0.57
23:a:64:ARG:NE	23:a:70:LEU:HD21	2.13	0.57
23:a:140:SER:HB2	30:i:84:GLY:HA3	1.86	0.57
37:4:469:GLN:HE21	38:5:69:ASN:H	1.52	0.57
9:I:101:ILE:HG22	32:k:61:TYR:HB3	1.87	0.57
38:5:64:LEU:HB2	38:5:77:TYR:HB2	1.86	0.57
38:5:125:PHE:CE1	38:5:129:ILE:CD1	2.87	0.57
38:5:194:THR:HG22	38:5:196:ASN:H	1.70	0.57
20:X:58:GLU:HG3	20:X:62:PRO:HA	1.84	0.57
37:4:123:LEU:HD13	46:4:505:3PE:H2D2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:6:52:LEU:HB3	39:6:55:PHE:HD2	1.70	0.57
4:D:64:GLN:HA	18:U:31:THR:HG21	1.85	0.57
40:8:4:PHE:CE1	40:8:25:ARG:HB3	2.39	0.57
1:A:434:ARG:HG3	1:A:435:GLN:HG3	1.87	0.57
7:G:226:GLU:O	7:G:229:ARG:NH1	2.33	0.57
10:J:170:ARG:NH2	10:J:178:GLN:OE1	2.38	0.57
20:X:129:SER:OG	20:X:136:GLN:NE2	2.36	0.57
38:5:32:THR:HG22	38:5:117:PHE:HE2	1.70	0.57
38:5:341:LEU:HD12	38:5:380:ALA:HB2	1.87	0.57
34:1:153:ILE:HA	34:1:156:ILE:HG12	1.87	0.57
1:A:145:GLN:HG3	3:C:382:ILE:HG23	1.87	0.57
2:B:203:MET:HB3	8:H:113:MET:HB2	1.87	0.57
5:E:29:GLN:HG2	14:P:120:LEU:HB3	1.87	0.57
34:1:122:LEU:HA	34:1:125:TRP:HD1	1.68	0.57
38:5:11:LEU:HD21	38:5:41:ILE:HG13	1.85	0.57
18:U:33:ALA:HB1	18:U:98:TRP:HB2	1.87	0.56
1:A:86:ASP:OD1	1:A:113:ARG:NH2	2.39	0.56
11:K:68:ALA:HB1	34:1:59:LEU:HD21	1.87	0.56
33:n:82:LYS:HG2	33:n:86:LEU:HD13	1.87	0.56
40:8:8:LEU:HB2	40:8:13:MET:HE2	1.87	0.56
3:C:443:ARG:HH22	14:P:4:ILE:H	1.53	0.56
16:R:106:LEU:HD12	17:S:135:ARG:HG3	1.87	0.56
16:R:108:GLU:HG2	16:R:109:PRO:HG3	1.86	0.56
25:c:16:ARG:HD3	38:5:441:PRO:HG2	1.88	0.56
38:5:40:ILE:HD13	38:5:97:SER:HB2	1.85	0.56
2:B:134:ARG:O	2:B:134:ARG:HG2	2.04	0.56
37:4:103:ASN:O	37:4:115:TYR:OH	2.22	0.56
3:C:35:GLY:O	3:C:39:GLN:NE2	2.38	0.56
9:I:168:LYS:HA	11:K:155:GLY:HA2	1.87	0.56
20:X:73:LYS:HA	20:X:76:ARG:NH1	2.20	0.56
3:C:374:MET:HE3	3:C:384:HIS:CD2	2.40	0.56
7:G:105:VAL:HG22	7:G:157:THR:HG21	1.87	0.56
38:5:374:TYR:OH	38:5:438:TYR:OH	2.24	0.56
38:5:392:GLY:HA2	38:5:395:THR:HG22	1.86	0.56
4:D:39:ARG:HG3	4:D:62:ARG:HH22	1.71	0.56
20:X:151:PHE:O	35:2:73:TYR:OH	2.23	0.56
48:X:201:CDL:H752	48:X:201:CDL:H622	1.88	0.56
3:C:98:LEU:HD13	3:C:461:PHE:CZ	2.41	0.56
3:C:448:PRO:HG2	34:1:204:LEU:HD11	1.88	0.56
7:G:113:ARG:HE	7:G:171:LEU:HD22	1.70	0.56
7:G:120:TYR:HB3	7:G:144:PHE:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:188:PRO:O	32:k:88:ARG:NH2	2.39	0.56
37:4:326:TYR:OH	37:4:468:PRO:O	2.24	0.56
17:S:104:GLY:HA3	17:S:107:ASP:HB2	1.87	0.55
20:X:76:ARG:HD2	29:g:9:TRP:CE3	2.41	0.55
23:a:73:ASN:OD1	37:4:294:ARG:NH1	2.39	0.55
34:1:323:ILE:O	34:1:327:ILE:HG12	2.07	0.55
37:4:103:ASN:ND2	37:4:114:TYR:OH	2.39	0.55
37:4:389:THR:HG23	37:4:391:ASN:H	1.70	0.55
16:R:28:ASN:HD22	16:R:78:PRO:HA	1.70	0.55
38:5:574:ASN:HA	38:5:578:HIS:HD2	1.71	0.55
2:B:277:LEU:HA	2:B:291:GLU:HA	1.86	0.55
24:b:57:SER:HB2	35:2:466:VAL:HG21	1.89	0.55
25:c:20:ASN:ND2	38:5:369:TYR:OH	2.39	0.55
5:E:162:ARG:HH21	5:E:162:ARG:CB	2.19	0.55
10:J:139:PHE:CZ	48:J:204:CDL:H673	2.41	0.55
20:X:130:SER:O	36:3:85:ASN:ND2	2.39	0.55
26:d:69:GLN:HG3	30:i:74:TRP:CZ3	2.41	0.55
34:1:8:ILE:HG22	34:1:99:LEU:HD12	1.87	0.55
38:5:483:VAL:HG12	40:8:37:ARG:NH1	2.22	0.55
5:E:59:PHE:HB2	5:E:127:ASN:HA	1.89	0.55
7:G:176:ASN:HD21	14:P:2:ALA:HB3	1.72	0.55
38:5:540:ASN:O	38:5:544:ASN:ND2	2.40	0.55
4:D:10:PRO:HG3	34:1:42:VAL:HG11	1.89	0.55
4:D:84:ARG:HD2	39:6:6:TYR:CE1	2.42	0.55
5:E:22:ASN:HB2	5:E:46:GLY:O	2.07	0.55
5:E:30:ASP:HB2	14:P:121:LYS:HA	1.87	0.55
18:U:40:TYR:OH	19:W:61:GLU:O	2.24	0.55
18:U:122:VAL:HG13	18:U:126:LEU:HD12	1.88	0.55
38:5:28:TYR:HA	38:5:31:VAL:HG12	1.88	0.55
37:4:98:LEU:HD12	37:4:453:ILE:HG23	1.89	0.55
38:5:366:LEU:HD12	38:5:370:LEU:HD13	1.88	0.55
32:k:54:ASN:O	32:k:56:ASN:N	2.38	0.54
17:S:161:LYS:HG3	17:S:165:VAL:HG21	1.89	0.54
17:S:183:MET:HE2	37:4:470:ILE:HG22	1.89	0.54
20:X:142:ASN:ND2	36:3:86:TYR:OH	2.38	0.54
28:f:7:GLU:HG2	28:f:57:ARG:HB3	1.88	0.54
35:2:209:LEU:HB3	35:2:214:ILE:HG13	1.89	0.54
37:4:330:VAL:HA	37:4:333:VAL:HG12	1.88	0.54
47:J:202:LMN:HBFA	47:J:202:LMN:HAW	1.90	0.54
34:1:179:CYS:HB2	34:1:186:LEU:HD12	1.90	0.54
38:5:414:VAL:HA	38:5:417:ILE:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:6:73:PHE:O	39:6:76:THR:OG1	2.22	0.54
1:A:523:GLN:HG3	1:A:529:ALA:HB2	1.89	0.54
2:B:310:LYS:O	2:B:315:ASN:ND2	2.41	0.54
3:C:208:GLU:HA	3:C:208:GLU:OE1	2.07	0.54
48:J:204:CDL:CB7	48:J:204:CDL:H112	2.37	0.54
35:2:369:PHE:HD2	46:4:501:3PE:H2D1	1.71	0.54
37:4:235:HIS:HE1	37:4:247:ALA:HB2	1.72	0.54
1:A:111:THR:HG22	1:A:113:ARG:H	1.72	0.54
2:B:311:GLY:HA3	2:B:315:ASN:HD22	1.71	0.54
3:C:152:GLN:NE2	3:C:174:ARG:HG2	2.23	0.54
13:O:103:LEU:O	13:O:103:LEU:CD1	2.54	0.54
1:A:664:PRO:HD2	28:f:14:GLN:HE22	1.71	0.54
3:C:116:VAL:HG21	3:C:464:VAL:HG12	1.90	0.54
9:I:171:TYR:OH	9:I:192:TYR:OH	2.22	0.54
10:J:147:LEU:HG	10:J:152:LYS:CD	2.38	0.54
2:B:114:TYR:HA	2:B:153:ALA:HB1	1.88	0.54
19:W:93:LYS:HA	19:W:103:VAL:HG21	1.90	0.54
21:Y:90:ARG:NH1	21:Y:106:GLN:OE1	2.39	0.54
35:2:140:ILE:HG22	35:2:232:ILE:HG23	1.89	0.54
38:5:16:TRP:HH2	46:5:901:3PE:H3C2	1.72	0.54
7:G:115:ASN:HB3	7:G:118:THR:HB	1.90	0.53
9:I:84:PHE:HA	9:I:87:LEU:HD12	1.90	0.53
37:4:236:SER:O	37:4:357:ARG:NH2	2.41	0.53
26:d:38:LEU:HD11	38:5:72:TYR:H	1.72	0.53
34:1:171:GLU:OE2	34:1:250:TYR:OH	2.25	0.53
37:4:110:ASN:O	37:4:155:TYR:OH	2.27	0.53
7:G:180:ARG:HH12	7:G:197:ARG:HE	1.56	0.53
23:a:137:THR:N	23:a:140:SER:OG	2.39	0.53
35:2:456:TYR:HD1	35:2:459:LEU:HD12	1.73	0.53
36:3:126:TYR:O	36:3:127:LYS:CG	2.56	0.53
38:5:273:THR:HG22	38:5:276:VAL:H	1.72	0.53
38:5:479:ILE:HG23	40:8:42:TYR:CD2	2.42	0.53
1:A:534:ILE:HG23	1:A:652:ILE:HD13	1.90	0.53
7:G:112:LEU:HA	7:G:118:THR:HG22	1.89	0.53
28:f:42:VAL:HG12	28:f:43:LEU:N	2.23	0.53
35:2:378:LEU:HD11	52:2:502:CPL:H172	1.89	0.53
8:H:72:MET:O	8:H:114:TYR:OH	2.27	0.53
35:2:454:PHE:HZ	46:4:503:3PE:H3B2	1.72	0.53
36:3:64:LEU:HD11	39:6:67:ILE:HG22	1.89	0.53
14:P:55:LYS:HE2	14:P:99:TYR:HB3	1.90	0.53
18:U:51:ASP:OD2	29:g:67:ARG:NH2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ILE:HG13	1:A:537:THR:HG21	1.91	0.53
35:2:202:ILE:CD1	35:2:257:SER:OG	2.57	0.53
38:5:331:HIS:O	38:5:335:HIS:HB2	2.09	0.53
1:A:727:PHE:HD1	8:H:91:ASN:OD1	1.91	0.53
3:C:429:ALA:HB1	3:C:463:GLU:HB3	1.91	0.53
12:L:76:SER:HB2	39:6:179:ILE:HG21	1.91	0.53
17:S:109:LEU:HG	37:4:12:TYR:HE2	1.74	0.53
37:4:270:GLN:O	37:4:274:THR:N	2.41	0.53
2:B:418:THR:HG21	2:B:438:GLN:HG3	1.89	0.53
34:1:100:GLY:HA3	36:3:4:PHE:HD1	1.74	0.53
39:6:2:MET:O	39:6:5:THR:OG1	2.27	0.53
1:A:375:THR:HG22	1:A:538:PRO:HB3	1.91	0.52
3:C:81:ARG:NH2	36:3:49:ARG:O	2.42	0.52
3:C:163:ASN:HD22	22:Z:83:TYR:HA	1.74	0.52
4:D:84:ARG:CG	4:D:85:PRO:HD2	2.39	0.52
17:S:179:LEU:HD13	37:4:40:VAL:HG22	1.90	0.52
31:j:89:VAL:HG13	31:j:90:THR:HG23	1.91	0.52
39:6:76:THR:OG1	39:6:77:LEU:N	2.40	0.52
3:C:131:THR:O	3:C:135:ALA:N	2.43	0.52
21:Y:50:ALA:O	21:Y:54:ARG:HG2	2.09	0.52
35:2:108:LEU:HD23	35:2:111:ILE:HD12	1.90	0.52
3:C:169:ARG:HH11	3:C:239:LEU:HD12	1.74	0.52
26:d:72:ASP:OD1	31:j:84:ARG:NH2	2.43	0.52
37:4:379:LEU:HD22	37:4:454:MET:HE1	1.91	0.52
1:A:209:ASN:OD1	1:A:209:ASN:O	2.27	0.52
6:F:127:GLU:HG3	6:F:128:GLU:HG3	1.90	0.52
9:I:185:VAL:HG11	9:I:222:LEU:HD11	1.90	0.52
19:W:103:VAL:O	41:9:56:ARG:NH2	2.42	0.52
30:i:15:MET:HE2	38:5:21:PHE:HA	1.90	0.52
35:2:62:ASN:HD21	35:2:250:LEU:HD11	1.73	0.52
7:G:117:SER:HA	9:I:45:GLY:HA2	1.92	0.52
31:j:67:ILE:HD12	37:4:283:LEU:HD23	1.91	0.52
35:2:202:ILE:HG22	35:2:206:LEU:CD1	2.25	0.52
38:5:427:VAL:HG11	50:5:902:PLC:H5'1	1.92	0.52
2:B:101:MET:HE2	2:B:151:MET:HB3	1.92	0.52
22:Z:66:THR:O	22:Z:77:ARG:NH2	2.43	0.52
1:A:313:LEU:HB2	1:A:586:VAL:HG22	1.91	0.52
12:L:17:PHE:HZ	39:6:96:LEU:HD12	1.75	0.52
36:3:82:LEU:CD1	39:6:152:ASN:HD21	2.23	0.52
24:b:35:GLY:HA2	24:b:38:PHE:HD2	1.73	0.52
35:2:238:LEU:HD23	35:2:242:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ARG:NH2	22:Z:72:ASN:O	2.43	0.52
1:A:322:ASN:ND2	5:E:39:THR:OG1	2.42	0.52
2:B:112:PRO:O	2:B:240:ARG:NE	2.38	0.52
34:1:81:LEU:HD13	34:1:226:PHE:HD1	1.74	0.52
1:A:268:ILE:HG22	1:A:293:ILE:HD11	1.92	0.51
12:L:15:PHE:CE2	35:2:163:ILE:HD11	2.46	0.51
17:S:239:LYS:HG2	26:d:13:ASP:OD2	2.10	0.51
35:2:2:LEU:HD11	35:2:115:LEU:HD12	1.92	0.51
3:C:87:PHE:HB2	3:C:102:LEU:HD12	1.91	0.51
3:C:121:ARG:HD2	11:K:157:TYR:CE2	2.46	0.51
35:2:233:THR:HG21	35:2:282:LYS:HZ1	1.75	0.51
5:E:162:ARG:NH2	5:E:162:ARG:CB	2.73	0.51
8:H:124:LEU:HB2	8:H:163:LEU:HA	1.93	0.51
11:K:116:ILE:HD12	11:K:143:TRP:HB2	1.92	0.51
12:L:7:ILE:HD11	39:6:16:ALA:HB1	1.92	0.51
12:L:62:LEU:HD22	35:2:131:GLU:HG2	1.92	0.51
20:X:60:LEU:HD23	35:2:438:VAL:HB	1.92	0.51
20:X:72:VAL:HG13	20:X:76:ARG:NH2	2.21	0.51
8:H:52:MET:HE3	8:H:56:GLU:OE2	2.10	0.51
30:i:24:SER:HA	33:n:10:LEU:HD23	1.92	0.51
20:X:129:SER:HB2	48:X:201:CDL:OA4	2.10	0.51
34:1:4:ASN:HB2	36:3:3:THR:HB	1.93	0.51
1:A:418:ARG:NH1	1:A:449:THR:CG2	2.74	0.51
5:E:70:THR:HA	5:E:73:LEU:HB3	1.93	0.51
8:H:124:LEU:HG	8:H:163:LEU:HD23	1.91	0.51
34:1:78:LEU:HD21	36:3:16:PHE:HE1	1.75	0.51
35:2:46:PHE:HE2	35:2:467:TYR:HB3	1.75	0.51
35:2:302:LEU:HD12	35:2:393:ASN:HD22	1.75	0.51
1:A:348:ALA:HA	1:A:551:TRP:HB3	1.92	0.51
1:A:395:TYR:OH	1:A:533:ASP:OD1	2.28	0.51
1:A:728:ALA:HA	8:H:41:PRO:CB	2.41	0.51
11:K:144:VAL:HG13	11:K:173:VAL:HA	1.93	0.51
35:2:260:ILE:HG23	35:2:297:MET:HE2	1.93	0.51
37:4:23:ASN:ND2	37:4:111:SER:OG	2.44	0.51
37:4:356:ILE:O	37:4:362:TYR:OH	2.20	0.51
5:E:110:ARG:NH1	5:E:137:ASN:HB3	2.24	0.51
20:X:34:TYR:CD1	20:X:110:LYS:HE2	2.45	0.51
34:1:157:ILE:HG21	34:1:245:LEU:HB2	1.91	0.51
35:2:199:LEU:HG	39:6:111:ILE:HD11	1.92	0.51
37:4:418:LEU:HD12	38:5:176:PHE:HA	1.92	0.51
40:8:5:PRO:HB2	40:8:28:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2:197:LEU:HD23	35:2:200:ILE:HD13	1.92	0.51
3:C:203:PHE:CE2	3:C:207:PHE:CE2	2.99	0.50
4:D:84:ARG:HG2	4:D:85:PRO:HD2	1.91	0.50
14:P:48:SER:HB3	14:P:50:PRO:HD2	1.92	0.50
16:R:76:PRO:HB2	38:5:551:ASN:ND2	2.27	0.50
34:1:135:GLY:HA2	34:1:138:ARG:HE	1.75	0.50
35:2:288:SER:O	35:2:292:ASN:ND2	2.44	0.50
39:6:142:GLU:HG3	39:6:144:THR:HG23	1.93	0.50
20:X:95:SER:HA	20:X:98:PHE:HD2	1.75	0.50
37:4:43:TYR:HE1	37:4:474:LEU:HD21	1.76	0.50
1:A:375:THR:CG2	1:A:538:PRO:HB3	2.41	0.50
16:R:79:ILE:HD11	38:5:361:ARG:HE	1.75	0.50
18:U:25:VAL:HG11	19:W:79:ARG:HH12	1.76	0.50
35:2:366:ILE:HG22	46:4:501:3PE:H2D2	1.93	0.50
37:4:417:VAL:HG12	38:5:175:ARG:HD2	1.94	0.50
12:L:50:ILE:HG23	41:9:8:LEU:HA	1.94	0.50
16:R:108:GLU:HG2	16:R:109:PRO:CG	2.42	0.50
1:A:348:ALA:HB1	1:A:362:LEU:HD21	1.92	0.50
3:C:219:ARG:HA	9:I:111:SER:HB2	1.94	0.50
3:C:371:ARG:O	3:C:375:LYS:NZ	2.45	0.50
20:X:154:PRO:HB3	48:g:201:CDL:H271	1.92	0.50
32:k:80:PRO:HG2	32:k:83:TRP:HD1	1.75	0.50
1:A:484:VAL:HB	1:A:521:VAL:HG12	1.93	0.50
3:C:149:THR:HG21	3:C:405:ALA:HA	1.94	0.50
4:D:79:VAL:HG12	18:U:13:GLU:HB3	1.94	0.50
8:H:130:THR:HA	8:H:133:GLN:HB3	1.92	0.50
22:Z:110:ASP:O	22:Z:114:GLY:N	2.41	0.50
33:n:60:GLU:O	33:n:64:ASN:ND2	2.45	0.50
51:4:504:T7X:O5	51:4:504:T7X:O3	2.30	0.50
3:C:66:ASP:OD1	3:C:69:SER:OG	2.29	0.50
7:G:164:PRO:HB3	14:P:14:PHE:HE2	1.76	0.50
9:I:63:TRP:HZ3	29:g:17:ARG:HG2	1.76	0.50
12:L:6:ILE:HG21	39:6:17:ILE:HG12	1.93	0.50
4:D:84:ARG:HH22	39:6:10:GLU:HG3	1.75	0.50
5:E:115:ILE:HG12	5:E:151:ILE:HG22	1.93	0.50
7:G:268:LEU:HD22	22:Z:100:LEU:HD22	1.94	0.50
18:U:46:CYS:O	18:U:50:ASN:ND2	2.45	0.50
19:W:60:ARG:NH1	29:g:56:SER:O	2.44	0.50
23:a:37:LEU:HB2	23:a:40:TYR:HB3	1.94	0.50
35:2:23:ALA:HA	35:2:26:ARG:HD2	1.94	0.50
3:C:428:ARG:HE	7:G:124:ILE:HG23	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:203:ALA:HB3	5:E:236:VAL:HG23	1.94	0.50
10:J:154:PHE:CE2	33:n:77:ARG:NH2	2.80	0.50
34:1:157:ILE:HG13	34:1:245:LEU:HD13	1.92	0.50
1:A:256:GLU:HB3	1:A:283:ARG:NH2	2.28	0.49
1:A:352:ALA:O	1:A:525:SER:OG	2.29	0.49
3:C:30:ASP:OD2	35:2:351:LYS:NZ	2.42	0.49
8:H:230:LYS:HG3	8:H:231:GLU:HG2	1.94	0.49
18:U:33:ALA:HB2	18:U:106:HIS:HE1	1.77	0.49
18:U:50:ASN:HB3	19:W:71:PRO:HG2	1.93	0.49
23:a:118:LYS:HG2	23:a:120:ALA:H	1.77	0.49
37:4:258:ILE:HG13	37:4:262:LEU:HD22	1.94	0.49
37:4:468:PRO:HG2	38:5:68:LEU:HB3	1.94	0.49
39:6:117:ILE:HG13	39:6:120:ASN:HD22	1.77	0.49
1:A:355:GLU:HG2	1:A:357:GLU:H	1.77	0.49
2:B:341:PHE:HE1	2:B:351:LEU:HD12	1.77	0.49
36:3:82:LEU:HD12	39:6:152:ASN:HD21	1.77	0.49
38:5:364:GLY:HA3	38:5:441:PRO:HA	1.92	0.49
21:Y:62:GLN:NE2	21:Y:75:THR:O	2.43	0.49
26:d:24:ARG:NH2	26:d:27:GLN:OE1	2.45	0.49
37:4:227:ILE:HG22	37:4:228:HIS:H	1.77	0.49
1:A:54:LEU:HD11	1:A:107:VAL:HG21	1.94	0.49
1:A:68:TYR:HB2	1:A:80:CYS:HB2	1.95	0.49
1:A:227:GLY:HA3	1:A:299:PHE:HE2	1.76	0.49
9:I:195:GLU:HG2	11:K:175:VAL:HG22	1.93	0.49
16:R:106:LEU:HD22	31:j:20:TRP:HB2	1.94	0.49
29:g:25:HIS:CD2	34:1:315:ILE:HG22	2.48	0.49
3:C:214:MET:HE3	3:C:224:ARG:HB2	1.95	0.49
20:X:10:THR:HG23	33:n:100:LEU:HB2	1.95	0.49
2:B:216:GLU:OE1	21:Y:161:LYS:NZ	2.44	0.49
46:J:203:3PE:H3A1	38:5:630:LEU:HD23	1.94	0.49
1:A:266:SER:HB2	1:A:289:ASN:HD22	1.76	0.49
38:5:143:TRP:NE1	38:5:178:ASP:OD1	2.46	0.49
5:E:165:HIS:HB3	5:E:199:ILE:HG12	1.93	0.49
11:K:76:PHE:CD2	11:K:105:ILE:HD12	2.47	0.49
18:U:146:LYS:HD2	18:U:146:LYS:N	2.28	0.49
1:A:455:LEU:HD11	1:A:470:PHE:HE2	1.78	0.49
3:C:97:VAL:O	3:C:97:VAL:HG12	2.13	0.49
14:P:74:VAL:HG22	14:P:78:LYS:HE2	1.95	0.49
3:C:435:LEU:HD23	3:C:464:VAL:HG11	1.94	0.48
6:F:134:GLN:O	7:G:134:ARG:NH1	2.42	0.48
16:R:25:LEU:CD1	16:R:74:ARG:HA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:48:LEU:CD1	17:S:106:LEU:HB2	2.43	0.48
31:j:35:TYR:OH	31:j:39:ARG:NH2	2.46	0.48
34:1:29:THR:O	34:1:33:MET:HG2	2.12	0.48
35:2:263:LEU:HB2	35:2:297:MET:HE1	1.93	0.48
36:3:91:VAL:HG23	39:6:155:LEU:HD11	1.95	0.48
37:4:211:TRP:HZ2	37:4:277:ILE:HD11	1.77	0.48
1:A:254:LYS:HG2	1:A:269:ARG:HH21	1.79	0.48
3:C:184:LEU:HD21	3:C:210:ARG:NE	2.27	0.48
5:E:187:GLU:HG2	5:E:199:ILE:HG21	1.95	0.48
11:K:89:GLU:HA	11:K:92:HIS:HD2	1.78	0.48
17:S:163:ASP:HB3	37:4:26:HIS:HE1	1.78	0.48
25:c:19:THR:O	25:c:25:ASN:ND2	2.44	0.48
35:2:376:PRO:HG2	46:4:501:3PE:H2G1	1.95	0.48
4:D:54:LEU:HD22	41:9:84:ILE:HB	1.94	0.48
48:J:204:CDL:H791	48:J:204:CDL:H752	1.95	0.48
12:L:12:PHE:HA	12:L:32:MET:HE2	1.95	0.48
26:d:38:LEU:HD21	38:5:71:ASP:HA	1.95	0.48
29:g:26:LEU:HD22	46:g:202:3PE:H252	1.95	0.48
34:1:28:LYS:HD2	34:1:39:PRO:HD2	1.95	0.48
46:4:505:3PE:H242	46:4:505:3PE:H332	1.95	0.48
39:6:36:MET:HE3	39:6:40:PHE:HE2	1.77	0.48
40:8:37:ARG:HB3	40:8:42:TYR:CD1	2.48	0.48
3:C:152:GLN:NE2	3:C:312:ASP:OD2	2.44	0.48
3:C:161:LEU:HD21	3:C:416:SER:HB2	1.96	0.48
3:C:424:LYS:HD2	7:G:129:VAL:HG22	1.94	0.48
8:H:156:THR:HG22	8:H:158:ASP:H	1.77	0.48
20:X:138:ILE:HG21	39:6:156:THR:HB	1.95	0.48
33:n:96:SER:O	35:2:51:THR:HB	2.14	0.48
2:B:267:PHE:HB3	2:B:293:GLU:HG3	1.95	0.48
34:1:79:ILE:HA	34:1:82:ILE:HG12	1.94	0.48
35:2:112:LEU:HD23	39:6:167:ILE:HG21	1.96	0.48
11:K:72:ARG:HE	34:1:59:LEU:HD23	1.78	0.48
31:j:15:LEU:HD13	35:2:427:ILE:HG21	1.95	0.48
37:4:372:LEU:HD13	37:4:446:VAL:HG21	1.95	0.48
37:4:388:LEU:HD12	38:5:145:PHE:CZ	2.48	0.48
38:5:16:TRP:HE1	38:5:20:LEU:HD11	1.77	0.48
3:C:153:VAL:HG11	3:C:410:MET:HE2	1.96	0.48
3:C:184:LEU:CD2	3:C:210:ARG:NH2	2.75	0.48
38:5:627:SER:O	38:5:631:LEU:HB2	2.14	0.48
38:5:126:TRP:HZ3	38:5:141:VAL:CG1	2.25	0.48
9:I:105:PHE:HD1	32:k:65:VAL:HG13	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:51:LYS:O	23:a:63:ARG:NH1	2.47	0.48
24:b:23:LYS:HE2	35:2:359:TYR:CZ	2.49	0.48
35:2:212:ILE:HG23	35:2:241:LYS:HG2	1.95	0.48
37:4:208:THR:HG23	37:4:273:TYR:HE2	1.79	0.48
38:5:86:ILE:HD12	38:5:89:LEU:HD23	1.95	0.48
11:K:116:ILE:HD11	11:K:194:LEU:HD21	1.96	0.48
17:S:224:GLU:O	17:S:228:ALA:HB2	2.14	0.48
26:d:84:GLY:HA3	37:4:486:ILE:HA	1.96	0.48
38:5:478:ASP:OD2	40:8:37:ARG:NH2	2.46	0.48
3:C:125:LYS:HE3	7:G:216:LEU:HA	1.96	0.47
4:D:29:HIS:CE1	34:1:97:ILE:HG23	2.49	0.47
7:G:224:TRP:CZ3	11:K:132:ARG:HG2	2.48	0.47
9:I:117:GLU:O	9:I:187:THR:OG1	2.30	0.47
12:L:1:MET:HE3	39:6:109:LEU:HG	1.96	0.47
24:b:23:LYS:HE3	35:2:359:TYR:CE2	2.48	0.47
1:A:228:ASN:HB3	1:A:292:TRP:CZ3	2.49	0.47
1:A:375:THR:HA	1:A:538:PRO:HD3	1.96	0.47
5:E:247:ARG:HH21	14:P:108:GLY:HA2	1.79	0.47
8:H:78:GLY:HA3	8:H:89:VAL:HG21	1.95	0.47
37:4:98:LEU:HD12	37:4:453:ILE:HG12	1.96	0.47
37:4:258:ILE:HA	37:4:262:LEU:HD13	1.95	0.47
1:A:432:TRP:HD1	1:A:437:LEU:HB2	1.80	0.47
1:A:481:LEU:HD13	1:A:520:ASN:HD22	1.80	0.47
5:E:57:THR:OG1	5:E:122:SER:OG	2.28	0.47
14:P:51:THR:HA	14:P:54:THR:HG22	1.96	0.47
17:S:66:LEU:HD11	17:S:94:ILE:HD13	1.96	0.47
20:X:85:VAL:HA	35:2:1:MET:HE1	1.95	0.47
30:i:52:THR:HG22	38:5:62:LEU:HB3	1.95	0.47
30:i:63:ASP:HA	30:i:66:LYS:HE2	1.96	0.47
37:4:229:VAL:HG13	38:5:585:TYR:CE1	2.49	0.47
1:A:294:ASN:HD21	1:A:697:PHE:HZ	1.62	0.47
3:C:118:LEU:HB3	11:K:127:MET:HE3	1.96	0.47
7:G:256:GLY:O	22:Z:83:TYR:OH	2.32	0.47
17:S:152:TRP:HD1	17:S:155:LYS:HG3	1.79	0.47
34:1:90:VAL:HG21	34:1:108:PHE:CD2	2.48	0.47
38:5:200:ILE:HG21	38:5:269:ILE:HD11	1.91	0.47
6:F:77:HIS:HD2	9:I:43:ALA:HA	1.79	0.47
19:W:33:TYR:CD2	50:W:401:PLC:H1'1	2.50	0.47
21:Y:147:ASN:OD1	21:Y:159:ARG:NH2	2.48	0.47
4:D:25:MET:O	4:D:29:HIS:ND1	2.43	0.47
23:a:93:ALA:HB1	38:5:555:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:11:PHE:CG	34:1:99:LEU:HD21	2.49	0.47
35:2:215:ALA:HA	35:2:218:HIS:HB3	1.97	0.47
1:A:549:MET:HG3	1:A:568:PHE:HD2	1.80	0.47
2:B:79:ILE:HD11	2:B:84:LEU:HD22	1.95	0.47
3:C:45:ASP:H	3:C:48:HIS:CE1	2.32	0.47
5:E:27:LEU:HD11	5:E:52:THR:HG23	1.97	0.47
5:E:125:VAL:HG13	5:E:163:TYR:HD1	1.78	0.47
12:L:61:ILE:HD13	39:6:165:LEU:HD21	1.96	0.47
17:S:94:ILE:HA	17:S:97:LEU:HD23	1.95	0.47
23:a:47:PRO:HG2	23:a:50:LEU:HB2	1.96	0.47
26:d:20:HIS:HB2	33:n:70:VAL:HG11	1.97	0.47
35:2:264:ALA:HB1	35:2:298:LEU:HD12	1.96	0.47
37:4:38:PHE:HZ	46:4:505:3PE:H221	1.80	0.47
38:5:554:LEU:O	38:5:556:SER:N	2.37	0.47
1:A:128:ASN:HB3	1:A:165:ARG:HG2	1.96	0.47
9:I:187:THR:HG22	9:I:218:LEU:HD12	1.96	0.47
20:X:34:TYR:HE1	20:X:110:LYS:HE2	1.76	0.47
22:Z:80:ARG:HH11	22:Z:81:ARG:HH12	1.61	0.47
26:d:63:CYS:HB2	26:d:66:LEU:HB2	1.97	0.47
35:2:90:ASN:HB2	35:2:93:TYR:HD2	1.80	0.47
37:4:353:ARG:NH1	37:4:450:GLU:OE1	2.45	0.47
37:4:377:ILE:HD11	46:5:901:3PE:H261	1.97	0.47
39:6:61:MET:O	39:6:65:GLY:HA3	2.14	0.47
1:A:418:ARG:NH1	1:A:449:THR:HG23	2.30	0.47
1:A:627:ARG:HA	1:A:637:LEU:HD12	1.96	0.47
4:D:84:ARG:CG	4:D:85:PRO:CD	2.93	0.47
18:U:28:VAL:HG21	19:W:72:LEU:HD21	1.96	0.47
18:U:60:SER:HB2	18:U:63:SER:HB2	1.96	0.47
25:c:15:TRP:CZ3	27:e:11:ASN:HA	2.50	0.47
32:k:49:TYR:HE1	32:k:65:VAL:HG21	1.79	0.47
34:1:245:LEU:HD12	34:1:246:LEU:HG	1.96	0.47
35:2:29:ASN:ND2	35:2:81:SER:OG	2.44	0.47
37:4:302:ILE:HD13	37:4:342:LEU:HB3	1.96	0.47
38:5:119:LEU:O	38:5:122:MET:HG2	2.15	0.47
2:B:317:LEU:HB2	2:B:361:LYS:HA	1.96	0.47
8:H:174:ASN:HB3	8:H:186:GLU:HB3	1.97	0.47
12:L:75:VAL:HG21	36:3:57:ILE:HG12	1.97	0.47
48:X:201:CDL:H441	39:6:163:LEU:HG	1.96	0.47
30:i:75:ARG:HH11	30:i:82:SER:HA	1.80	0.47
32:k:49:TYR:CE1	32:k:65:VAL:CG2	2.98	0.47
50:n:1101:PLC:H31	38:5:65:PHE:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:4:58:GLU:HG2	37:4:78:LEU:HD23	1.96	0.47
37:4:232:PRO:HB3	37:4:300:VAL:HG23	1.97	0.47
40:8:4:PHE:CD1	40:8:25:ARG:HB3	2.50	0.47
2:B:37:GLN:HA	8:H:233:HIS:CE1	2.50	0.46
2:B:280:ILE:HG12	2:B:356:VAL:HB	1.95	0.46
15:Q:51:THR:OG1	15:Q:53:ASP:OD1	2.27	0.46
19:W:101:PHE:HZ	41:9:56:ARG:HG3	1.80	0.46
10:J:59:THR:HA	10:J:62:SER:HB3	1.96	0.46
46:J:203:3PE:H231	38:5:624:THR:HG22	1.98	0.46
15:Q:96:VAL:HG22	15:Q:115:ILE:HD11	1.97	0.46
15:Q:124:TYR:O	15:Q:128:GLN:NE2	2.47	0.46
16:R:82:PRO:HA	16:R:87:GLY:HA3	1.97	0.46
23:a:75:ASP:OD1	37:4:294:ARG:NH1	2.48	0.46
32:k:43:ASP:HB3	32:k:49:TYR:CE2	2.50	0.46
32:k:49:TYR:CD1	32:k:65:VAL:CG2	2.96	0.46
1:A:392:ARG:NH1	1:A:655:SER:OG	2.47	0.46
3:C:153:VAL:HG22	3:C:412:VAL:HG12	1.97	0.46
3:C:204:LEU:CD2	34:1:34:GLN:CB	2.90	0.46
3:C:240:PRO:HG3	9:I:113:ARG:NH2	2.29	0.46
9:I:185:VAL:HG21	9:I:218:LEU:HD11	1.97	0.46
9:I:197:ARG:HB2	11:K:176:TYR:HE2	1.79	0.46
33:n:57:LYS:HB2	33:n:62:ILE:HD11	1.97	0.46
34:1:200:PRO:HG2	34:1:297:ARG:HG3	1.96	0.46
37:4:162:ARG:HD2	37:4:166:TYR:OH	2.16	0.46
37:4:224:LEU:HA	37:4:284:THR:HG21	1.98	0.46
38:5:127:MET:HE3	38:5:254:THR:HB	1.97	0.46
39:6:37:ILE:HA	39:6:40:PHE:HD2	1.80	0.46
1:A:160:GLU:OE2	2:B:400:ARG:NH1	2.49	0.46
7:G:67:HIS:CE1	22:Z:155:PRO:HB2	2.50	0.46
29:g:25:HIS:CD2	29:g:26:LEU:HG	2.50	0.46
37:4:211:TRP:HD1	37:4:266:LEU:HG	1.80	0.46
37:4:380:SER:O	37:4:384:ILE:HD12	2.15	0.46
38:5:630:LEU:HD11	39:6:103:VAL:HG21	1.97	0.46
39:6:9:ILE:HG23	39:6:46:TYR:HE1	1.79	0.46
3:C:289:LEU:HD13	3:C:437:ALA:HB1	1.98	0.46
3:C:428:ARG:HG3	7:G:125:ASP:HB2	1.97	0.46
3:C:434:HIS:HB3	3:C:457:MET:HB2	1.97	0.46
12:L:61:ILE:HG21	39:6:165:LEU:HD11	1.97	0.46
8:H:174:ASN:ND2	8:H:215:ARG:HH11	2.13	0.46
46:J:203:3PE:H3A1	38:5:630:LEU:HB3	1.98	0.46
11:K:160:SER:O	11:K:165:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:98:ALA:HB1	25:c:12:ARG:HH12	1.81	0.46
19:W:112:LYS:HG3	33:n:119:ARG:HH12	1.80	0.46
27:e:27:THR:HG21	38:5:371:PRO:HB2	1.96	0.46
32:k:40:VAL:O	32:k:94:HIS:NE2	2.49	0.46
35:2:375:PRO:HA	35:2:380:PHE:CG	2.50	0.46
40:8:19:LEU:HD13	40:8:21:ALA:H	1.79	0.46
44:B:502:FMN:O4'	44:B:502:FMN:O2'	2.25	0.46
8:H:68:LYS:HE3	21:Y:155:LEU:HD21	1.98	0.46
10:J:143:ARG:NH1	35:2:256:ASN:HB2	2.27	0.46
14:P:6:THR:HG22	14:P:7:ALA:H	1.79	0.46
15:Q:91:ASP:OD1	16:R:44:ARG:NH2	2.48	0.46
23:a:61:GLN:HE22	38:5:161:LEU:HB2	1.81	0.46
35:2:110:ASN:HD22	35:2:235:TYR:HE2	1.63	0.46
46:4:501:3PE:H2B1	46:4:501:3PE:H2E2	1.68	0.46
46:4:505:3PE:H351	46:4:505:3PE:H322	1.72	0.46
38:5:592:ILE:HD12	38:5:595:LEU:HD23	1.96	0.46
1:A:232:LEU:HD22	1:A:292:TRP:HH2	1.81	0.46
3:C:172:TYR:O	3:C:175:THR:CG2	2.46	0.46
4:D:11:TYR:HE2	34:1:29:THR:HG21	1.81	0.46
20:X:152:ILE:HD11	35:2:119:HIS:CD2	2.50	0.46
27:e:49:MET:HG3	38:5:393:TYR:CZ	2.51	0.46
37:4:197:HIS:CE1	37:4:264:PRO:HG2	2.46	0.46
2:B:34:LEU:HD13	2:B:38:ASP:HB3	1.98	0.46
23:a:146:GLN:HE21	38:5:494:PRO:HB2	1.81	0.46
38:5:41:ILE:HA	38:5:44:LEU:HG	1.98	0.46
38:5:126:TRP:CZ3	38:5:141:VAL:CG1	2.99	0.46
1:A:393:SER:HA	1:A:398:ASN:HD21	1.81	0.46
3:C:184:LEU:CD2	3:C:210:ARG:HH21	2.29	0.46
11:K:146:SER:HB2	11:K:173:VAL:HG11	1.97	0.46
17:S:183:MET:HB3	37:4:470:ILE:HG22	1.98	0.46
34:1:206:GLU:OE1	34:1:207:SER:OG	2.32	0.46
34:1:290:MET:HE3	34:1:290:MET:HB2	1.71	0.46
1:A:66:PRO:HB2	1:A:147:GLN:HE21	1.80	0.45
3:C:204:LEU:HD22	34:1:34:GLN:OE1	2.16	0.45
7:G:167:SER:HB3	7:G:190:PHE:HB3	1.98	0.45
18:U:36:LEU:HD23	18:U:101:LEU:HD21	1.98	0.45
18:U:42:ILE:HD11	19:W:69:LEU:HD23	1.97	0.45
30:i:54:ARG:HD2	38:5:58:ASN:CG	2.41	0.45
2:B:40:ILE:O	2:B:139:LYS:NZ	2.49	0.45
2:B:322:GLY:N	2:B:355:ALA:O	2.48	0.45
5:E:259:PHE:CD1	5:E:328:LYS:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:83:ILE:HA	18:U:86:ILE:HG22	1.96	0.45
22:Z:135:SER:OG	22:Z:140:ILE:HD11	2.16	0.45
35:2:302:LEU:HD21	35:2:390:ILE:HD13	1.97	0.45
1:A:728:ALA:HA	8:H:41:PRO:HB2	1.99	0.45
4:D:80:TRP:HZ2	19:W:81:THR:HA	1.81	0.45
18:U:105:ASN:HD22	18:U:107:GLN:HE21	1.63	0.45
20:X:76:ARG:HD2	29:g:9:TRP:CZ3	2.51	0.45
34:1:161:VAL:HG21	34:1:169:ILE:HG12	1.98	0.45
52:2:502:CPL:H211	52:2:502:CPL:H182	1.43	0.45
37:4:67:GLY:HA2	46:4:503:3PE:H332	1.98	0.45
37:4:177:PHE:HA	37:4:180:LEU:HD13	1.98	0.45
39:6:161:ILE:O	39:6:165:LEU:HB2	2.16	0.45
2:B:393:TRP:HE1	2:B:417:LEU:HD22	1.80	0.45
3:C:443:ARG:HH22	14:P:3:ILE:HB	1.81	0.45
5:E:31:VAL:HG22	5:E:41:ILE:HG12	1.97	0.45
8:H:90:MET:HE3	8:H:108:ALA:HB3	1.99	0.45
17:S:194:TRP:HH2	26:d:32:ARG:HH21	1.64	0.45
35:2:95:THR:OG1	35:2:340:GLN:NE2	2.50	0.45
37:4:384:ILE:HG12	37:4:421:ALA:HA	1.98	0.45
38:5:173:MET:HB3	38:5:232:LEU:HD13	1.99	0.45
1:A:187:THR:HG22	1:A:191:ARG:HG3	1.97	0.45
2:B:164:PHE:HB3	2:B:167:GLU:HB3	1.98	0.45
5:E:339:GLU:HB3	5:E:341:PRO:HD2	1.97	0.45
18:U:110:GLY:HA2	18:U:152:PRO:HB3	1.97	0.45
22:Z:163:LYS:CG	22:Z:182:HIS:HD2	2.30	0.45
35:2:202:ILE:HD11	35:2:257:SER:OG	2.16	0.45
37:4:278:TYR:HB3	37:4:409:ILE:HG12	1.97	0.45
1:A:401:ILE:O	1:A:427:ARG:NH1	2.50	0.45
10:J:116:PRO:O	48:J:204:CDL:HA61	2.16	0.45
14:P:55:LYS:NZ	14:P:59:GLU:OE2	2.46	0.45
22:Z:92:LYS:O	22:Z:95:THR:OG1	2.29	0.45
22:Z:100:LEU:HD21	22:Z:118:LEU:HG	1.98	0.45
1:A:627:ARG:NE	1:A:639:TYR:O	2.34	0.45
4:D:59:GLY:N	41:9:85:GLY:O	2.50	0.45
12:L:20:ARG:NH1	39:6:26:ALA:O	2.49	0.45
48:g:201:CDL:H532	35:2:11:THR:HG21	1.99	0.45
37:4:117:LEU:HG	37:4:147:LEU:HD22	1.99	0.45
48:4:502:CDL:H222	48:4:502:CDL:H451	1.99	0.45
2:B:43:ASN:ND2	2:B:135:LYS:O	2.50	0.45
14:P:32:PHE:HB3	14:P:56:ILE:HD13	1.99	0.45
23:a:143:PHE:CD2	30:i:84:GLY:HA2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:4:139:ILE:HD12	37:4:140:LEU:HG	1.98	0.45
5:E:245:LEU:HA	5:E:248:ILE:HD12	1.98	0.45
31:j:85:ARG:HG3	38:5:206:LEU:O	2.16	0.45
36:3:5:ILE:HD13	46:6:301:3PE:H242	1.99	0.45
3:C:77:ASN:ND2	5:E:370:PHE:O	2.49	0.45
5:E:22:ASN:CB	5:E:46:GLY:O	2.65	0.45
48:J:204:CDL:CB3	38:5:598:LYS:HG3	2.46	0.45
34:1:194:VAL:HB	34:1:199:ARG:HB2	1.99	0.45
38:5:115:ARG:NH2	46:5:901:3PE:O11	2.50	0.45
39:6:59:TYR:HA	39:6:63:TYR:HD2	1.80	0.45
1:A:132:ASP:O	1:A:136:CYS:N	2.49	0.44
1:A:286:GLU:HG3	21:Y:138:LYS:HB2	1.99	0.44
5:E:234:ASN:HD21	5:E:262:TYR:HD2	1.64	0.44
6:F:67:TYR:CZ	6:F:117:MET:HG3	2.53	0.44
7:G:126:ILE:HG12	7:G:178:PHE:HB3	1.99	0.44
50:W:402:PLC:H1A1	50:W:402:PLC:H1'1	1.99	0.44
34:1:110:LEU:HD11	34:1:151:THR:HG23	1.99	0.44
34:1:311:PHE:CD1	34:1:315:ILE:HD11	2.52	0.44
35:2:51:THR:HG23	35:2:62:ASN:HB3	1.99	0.44
35:2:292:ASN:HA	35:2:295:TYR:HD2	1.82	0.44
38:5:360:ILE:HA	38:5:363:TYR:CD2	2.52	0.44
4:D:43:ASP:OD1	4:D:44:GLN:N	2.49	0.44
5:E:206:PHE:CD1	5:E:235:PRO:HB2	2.52	0.44
11:K:75:SER:CB	34:1:53:ASP:OD1	2.66	0.44
16:R:81:PRO:HB2	16:R:84:PHE:HD2	1.82	0.44
1:A:122:MET:HE2	1:A:122:MET:HB2	1.80	0.44
1:A:205:SER:HB2	8:H:109:THR:HG21	1.99	0.44
1:A:267:ASN:CG	1:A:283:ARG:HH11	2.25	0.44
1:A:610:ARG:HB2	21:Y:59:ARG:HH12	1.83	0.44
7:G:130:ASP:HB3	7:G:138:PHE:CE1	2.52	0.44
17:S:48:LEU:HB2	17:S:106:LEU:HD12	1.99	0.44
37:4:342:LEU:O	37:4:346:VAL:HG12	2.18	0.44
38:5:310:MET:HA	38:5:313:LEU:HG	1.99	0.44
1:A:377:ASP:HB3	1:A:528:ARG:NH1	2.31	0.44
3:C:201:THR:HG22	34:1:34:GLN:HE21	1.82	0.44
11:K:76:PHE:HZ	11:K:116:ILE:HD13	1.81	0.44
12:L:55:PHE:HD1	35:2:124:ILE:HG12	1.82	0.44
49:O:201:ZMP:H14A	14:P:72:GLN:HG2	1.99	0.44
14:P:66:VAL:O	14:P:72:GLN:NE2	2.45	0.44
24:b:45:GLY:HA2	24:b:48:LEU:HD23	1.98	0.44
48:g:201:CDL:HB61	46:g:202:3PE:H321	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:76:SER:HA	34:1:79:ILE:HG12	1.98	0.44
37:4:43:TYR:HD1	37:4:86:LEU:HD11	1.82	0.44
37:4:134:TYR:HD2	37:4:192:THR:HA	1.83	0.44
38:5:184:GLY:O	38:5:188:ILE:HG12	2.18	0.44
3:C:207:PHE:O	3:C:211:GLU:HG2	2.17	0.44
9:I:217:GLU:OE2	32:k:91:ARG:NH2	2.50	0.44
35:2:378:LEU:HD11	52:2:502:CPL:H191	1.99	0.44
14:P:63:HIS:HB3	14:P:75:LEU:HD21	2.00	0.44
15:Q:97:MET:HE3	16:R:23:LEU:HB2	2.00	0.44
17:S:48:LEU:HD12	17:S:106:LEU:HB2	1.99	0.44
28:f:22:LEU:HD13	28:f:52:PRO:HB2	1.99	0.44
30:i:15:MET:HE1	48:4:502:CDL:H132	2.00	0.44
35:2:156:LEU:HD21	35:2:220:TRP:HB2	1.99	0.44
38:5:125:PHE:CZ	38:5:129:ILE:HD13	2.52	0.44
38:5:173:MET:HG3	38:5:235:TRP:HB3	1.99	0.44
1:A:397:PHE:HZ	1:A:404:ILE:HD11	1.82	0.44
7:G:160:THR:HB	7:G:163:THR:HG22	1.99	0.44
7:G:180:ARG:NH1	7:G:197:ARG:HE	2.16	0.44
9:I:166:MET:HE3	9:I:166:MET:HB3	1.76	0.44
31:j:39:ARG:HH11	38:5:577:HIS:CE1	2.36	0.44
36:3:76:TYR:CG	36:3:91:VAL:HG21	2.53	0.44
38:5:561:ASN:HA	38:5:565:ILE:HD12	1.99	0.44
10:J:31:GLN:OE1	38:5:638:ASN:ND2	2.51	0.44
12:L:23:ILE:HA	12:L:26:PHE:HD2	1.83	0.44
35:2:368:VAL:HG11	35:2:417:LEU:HG	2.00	0.44
39:6:106:ILE:O	39:6:110:MET:HG2	2.17	0.44
3:C:219:ARG:NH1	3:C:246:ASP:OD2	2.47	0.44
10:J:143:ARG:HA	10:J:143:ARG:HD3	1.65	0.44
37:4:3:LEU:HD23	37:4:6:ILE:HD12	1.99	0.44
38:5:79:PHE:HD1	38:5:132:THR:HG23	1.83	0.44
1:A:203:GLY:HA3	8:H:102:MET:HE2	2.00	0.43
1:A:576:GLY:HA3	32:k:227:TRP:CG	2.52	0.43
2:B:382:GLY:HA2	2:B:388:ARG:HB2	1.98	0.43
3:C:179:GLU:HG3	3:C:346:ILE:HG21	2.00	0.43
7:G:144:PHE:HB2	7:G:153:ILE:HG22	2.00	0.43
48:J:204:CDL:C36	47:j:101:LMN:HAW	2.48	0.43
19:W:91:ARG:HD3	41:9:74:PRO:O	2.17	0.43
35:2:217:LEU:HD13	38:5:621:ILE:HG22	1.99	0.43
35:2:374:ILE:HA	35:2:375:PRO:HD3	1.85	0.43
36:3:126:TYR:C	36:3:127:LYS:CG	2.90	0.43
1:A:71:HIS:O	21:Y:142:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:THR:CG2	1:A:538:PRO:HG3	2.27	0.43
1:A:637:LEU:HA	1:A:638:PRO:HD3	1.89	0.43
3:C:374:MET:HE3	3:C:384:HIS:CG	2.52	0.43
14:P:55:LYS:HA	14:P:58:GLN:HG2	1.99	0.43
15:Q:66:PHE:HD2	15:Q:69:VAL:HG13	1.82	0.43
23:a:47:PRO:HB3	23:a:84:ARG:NH2	2.32	0.43
48:g:201:CDL:H192	48:g:201:CDL:H161	1.76	0.43
30:i:14:SER:OG	30:i:15:MET:N	2.52	0.43
37:4:298:LEU:HD13	37:4:359:VAL:HG22	2.00	0.43
38:5:129:ILE:HG22	38:5:129:ILE:O	2.17	0.43
1:A:157:ARG:O	1:A:159:THR:N	2.52	0.43
1:A:527:SER:O	1:A:531:ALA:N	2.40	0.43
3:C:72:ASN:O	3:C:72:ASN:OD1	2.36	0.43
3:C:129:TYR:HE2	7:G:216:LEU:HB2	1.83	0.43
3:C:293:GLY:HA3	3:C:408:GLY:HA2	2.00	0.43
16:R:97:ARG:O	37:4:368:TYR:OH	2.35	0.43
18:U:115:GLU:OE2	18:U:130:LYS:NZ	2.49	0.43
35:2:234:ILE:HD13	35:2:234:ILE:HG21	1.85	0.43
37:4:39:ILE:HD12	37:4:93:VAL:HG21	2.00	0.43
40:8:13:MET:HB3	40:8:23:ARG:HD3	2.00	0.43
3:C:441:ILE:HG22	3:C:453:ILE:HD11	2.01	0.43
26:d:87:ARG:NE	37:4:201:VAL:HG12	2.32	0.43
34:1:77:PRO:HB3	34:1:226:PHE:HB2	2.00	0.43
36:3:4:PHE:HE2	46:6:301:3PE:H241	1.84	0.43
38:5:66:ASN:HA	38:5:76:ASN:HD22	1.84	0.43
40:8:4:PHE:CE1	40:8:25:ARG:HD3	2.53	0.43
1:A:728:ALA:HA	8:H:41:PRO:HB3	2.00	0.43
12:L:4:GLY:HA3	12:L:39:ILE:HG13	2.00	0.43
18:U:72:GLY:HA2	18:U:75:VAL:HG22	2.00	0.43
23:a:90:ASN:ND2	38:5:558:GLN:HE21	2.17	0.43
23:a:130:LEU:HD22	23:a:133:GLU:HG3	1.99	0.43
48:g:201:CDL:H781	48:g:201:CDL:H752	1.78	0.43
35:2:278:GLN:HE21	38:5:604:ILE:HD11	1.82	0.43
39:6:146:LEU:HD12	41:9:8:LEU:HD12	2.00	0.43
3:C:371:ARG:NH2	9:I:179:CYS:O	2.41	0.43
9:I:170:ILE:HG21	11:K:156:TYR:CD1	2.49	0.43
28:f:23:ARG:HG2	28:f:27:LYS:HE3	2.00	0.43
32:k:82:GLN:HB3	32:k:91:ARG:HH22	1.84	0.43
35:2:10:ILE:HG21	36:3:100:ILE:HD13	1.99	0.43
35:2:58:LEU:HD11	39:6:161:ILE:HD11	2.01	0.43
35:2:103:LEU:HD13	35:2:143:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:100:ILE:HA	36:3:103:VAL:HG22	1.99	0.43
38:5:16:TRP:CH2	46:5:901:3PE:H3C2	2.53	0.43
38:5:119:LEU:HA	38:5:122:MET:HG2	2.00	0.43
1:A:228:ASN:HB3	1:A:292:TRP:HZ3	1.84	0.43
2:B:51:ASP:OD1	2:B:52:LEU:N	2.52	0.43
6:F:98:GLY:H	7:G:148:ARG:NH1	2.17	0.43
17:S:48:LEU:HD13	17:S:106:LEU:HD12	2.01	0.43
20:X:95:SER:HB2	20:X:147:ILE:HD12	2.01	0.43
37:4:283:LEU:HB2	37:4:287:LEU:HD23	2.01	0.43
48:4:502:CDL:H211	48:4:502:CDL:H242	1.66	0.43
38:5:476:LEU:HD22	38:5:479:ILE:HD12	2.00	0.43
2:B:207:VAL:HG21	2:B:381:CYS:HB3	2.00	0.43
12:L:27:ILE:HG21	39:6:33:ILE:HG22	2.01	0.43
17:S:224:GLU:O	17:S:228:ALA:CB	2.66	0.43
26:d:73:MET:HE3	26:d:73:MET:HB2	1.78	0.43
28:f:42:VAL:CG1	28:f:43:LEU:N	2.82	0.43
33:n:73:LEU:HD11	37:4:78:LEU:HD11	2.00	0.43
34:1:152:SER:HB3	34:1:320:LEU:HD21	2.00	0.43
37:4:101:LEU:HD22	37:4:453:ILE:HD11	2.00	0.43
37:4:247:ALA:O	37:4:252:LYS:NZ	2.52	0.43
38:5:636:ASN:HD21	39:6:118:LEU:HD11	1.84	0.43
2:B:121:GLU:HG2	44:B:502:FMN:HN3	1.83	0.43
46:J:203:3PE:H3A2	38:5:634:VAL:HG21	2.01	0.43
16:R:25:LEU:HG	16:R:25:LEU:O	2.19	0.43
29:g:47:ARG:HG3	29:g:51:LEU:HB2	2.01	0.43
34:1:1:MET:HG2	34:1:2:ILE:N	2.33	0.43
35:2:122:ASP:OD1	35:2:123:PHE:N	2.52	0.43
41:9:79:ILE:HD11	41:9:84:ILE:HD13	2.00	0.43
1:A:418:ARG:HH11	1:A:449:THR:N	2.17	0.43
5:E:112:LEU:CD2	5:E:150:ARG:HD2	2.47	0.43
5:E:124:ILE:HG22	5:E:162:ARG:HB2	2.01	0.43
18:U:166:ALA:HB3	18:U:172:LEU:CD1	2.49	0.43
21:Y:116:GLU:HA	21:Y:119:ILE:HG22	2.01	0.43
22:Z:163:LYS:HB2	22:Z:182:HIS:HB3	2.01	0.43
34:1:89:VAL:HG13	34:1:100:GLY:H	1.84	0.43
38:5:88:MET:HE3	38:5:88:MET:HB2	1.65	0.43
38:5:382:LEU:HD22	38:5:387:MET:HG3	2.00	0.43
1:A:277:VAL:HG21	1:A:593:THR:HG21	2.00	0.42
3:C:170:GLY:HA2	3:C:173:ILE:HG22	2.01	0.42
7:G:92:TRP:HB2	22:Z:86:THR:HG22	2.00	0.42
48:J:204:CDL:C60	38:5:647:ILE:HG23	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:d:34:GLN:NE2	26:d:80:GLN:H	2.16	0.42
32:k:91:ARG:HE	32:k:93:HIS:CE1	2.37	0.42
37:4:134:TYR:H	37:4:192:THR:HB	1.84	0.42
40:8:18:ILE:HD11	40:8:31:VAL:HG12	2.01	0.42
3:C:269:ARG:HH12	9:I:77:TYR:CA	2.18	0.42
9:I:121:ARG:NH2	9:I:219:GLN:OE1	2.52	0.42
11:K:76:PHE:CZ	11:K:116:ILE:HG21	2.54	0.42
28:f:10:PHE:HB3	28:f:54:VAL:HG22	2.00	0.42
29:g:47:ARG:HG3	29:g:51:LEU:HD12	2.01	0.42
35:2:200:ILE:HG13	39:6:111:ILE:HD13	2.01	0.42
35:2:309:TYR:CZ	35:2:313:ILE:HG13	2.55	0.42
38:5:434:TYR:HA	38:5:438:TYR:HD2	1.82	0.42
6:F:42:PRO:O	6:F:46:LEU:HB2	2.18	0.42
11:K:38:SER:OG	11:K:39:SER:N	2.51	0.42
11:K:85:CYS:HB3	42:K:301:SF4:S1	2.57	0.42
19:W:47:ARG:HE	34:1:176:VAL:HB	1.84	0.42
19:W:95:ILE:HG12	41:9:64:LEU:HD13	2.00	0.42
35:2:14:SER:HB2	36:3:107:ASN:HB2	2.01	0.42
37:4:153:HIS:CE1	37:4:161:GLU:HG2	2.53	0.42
1:A:362:LEU:HD22	1:A:553:LEU:HD13	2.02	0.42
3:C:77:ASN:H	5:E:369:THR:HA	1.83	0.42
3:C:207:PHE:HD1	3:C:207:PHE:HA	1.74	0.42
3:C:235:VAL:HB	3:C:359:VAL:HG22	2.00	0.42
3:C:361:VAL:HG11	3:C:366:ILE:HD11	2.02	0.42
5:E:205:MET:HB3	5:E:238:VAL:HG22	2.01	0.42
9:I:139:ILE:H	9:I:139:ILE:HG13	1.74	0.42
34:1:88:TRP:CE2	34:1:237:LEU:HD12	2.54	0.42
34:1:185:LEU:HD12	34:1:188:ILE:HD11	2.01	0.42
2:B:393:TRP:NE1	2:B:417:LEU:HD22	2.34	0.42
4:D:22:GLY:HA3	34:1:279:SER:HB3	2.01	0.42
10:J:35:VAL:HG21	38:5:641:ILE:HD12	2.01	0.42
19:W:63:LEU:HD21	29:g:58:LEU:HB3	2.02	0.42
21:Y:60:ILE:HB	21:Y:131:ILE:HA	2.02	0.42
31:j:52:THR:HG22	38:5:578:HIS:ND1	2.34	0.42
32:k:49:TYR:CE1	32:k:65:VAL:HG21	2.55	0.42
35:2:395:TYR:HB3	35:2:398:ILE:HB	2.01	0.42
37:4:64:ASN:ND2	37:4:68:LEU:O	2.52	0.42
37:4:406:ASN:HB3	37:4:409:ILE:HG22	2.01	0.42
1:A:302:ASP:HB3	1:A:707:SER:HB2	2.02	0.42
1:A:324:THR:HB	1:A:327:ASP:HB2	2.01	0.42
9:I:63:TRP:CZ3	29:g:17:ARG:HG2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:145:ILE:HD13	9:I:164:ILE:HG12	2.01	0.42
10:J:124:LEU:HD11	48:J:204:CDL:H732	2.01	0.42
10:J:162:THR:HB	47:J:202:LMN:HCU	2.01	0.42
26:d:42:LYS:HG2	26:d:45:ARG:HH12	1.85	0.42
26:d:69:GLN:HG2	26:d:73:MET:HE2	2.01	0.42
34:1:323:ILE:HA	34:1:326:ILE:HG22	2.01	0.42
35:2:230:ILE:HG13	35:2:282:LYS:HZ3	1.85	0.42
38:5:387:MET:HE1	38:5:519:ILE:HG12	2.01	0.42
41:9:7:SER:OG	41:9:8:LEU:N	2.53	0.42
1:A:479:ASN:HA	1:A:516:TRP:CZ2	2.55	0.42
3:C:439:ASP:O	3:C:443:ARG:NE	2.52	0.42
5:E:166:VAL:HG23	5:E:200:VAL:HG13	2.02	0.42
7:G:68:VAL:HG22	7:G:72:HIS:CE1	2.55	0.42
9:I:171:TYR:CE2	11:K:179:GLY:HA2	2.55	0.42
34:1:2:ILE:HA	34:1:5:ILE:HG22	2.02	0.42
37:4:61:ASN:OD1	37:4:62:SER:N	2.51	0.42
1:A:282:PRO:HB3	1:A:293:ILE:HB	2.02	0.42
3:C:54:ARG:HH22	5:E:365:ASN:HD21	1.68	0.42
23:a:85:PHE:HD2	38:5:558:GLN:HB2	1.85	0.42
24:b:18:LYS:HE3	24:b:35:GLY:HA3	2.02	0.42
37:4:117:LEU:HB3	37:4:151:LEU:HD12	2.02	0.42
37:4:374:THR:HG22	46:5:901:3PE:H242	2.02	0.42
38:5:265:ARG:HA	38:5:265:ARG:HD2	1.79	0.42
38:5:267:ALA:HA	38:5:270:LEU:HD12	2.02	0.42
6:F:99:LEU:HD11	9:I:55:PHE:CD2	2.54	0.42
10:J:124:LEU:HD13	48:J:204:CDL:C73	2.49	0.42
19:W:87:ALA:O	19:W:91:ARG:HG3	2.20	0.42
23:a:100:PHE:HA	23:a:103:ILE:HG22	2.01	0.42
41:9:19:TRP:HB2	41:9:44:TYR:CE1	2.54	0.42
1:A:189:CYS:SG	1:A:190:VAL:N	2.93	0.42
2:B:219:GLU:HA	2:B:238:PHE:HE1	1.85	0.42
34:1:89:VAL:HG22	34:1:99:LEU:HB2	2.02	0.42
35:2:352:GLY:HA3	35:2:424:LYS:HB2	2.01	0.42
39:6:60:ILE:HG23	39:6:64:ILE:HD11	2.01	0.42
1:A:39:LEU:HD22	1:A:105:MET:HB3	2.02	0.41
9:I:207:LEU:HD23	9:I:210:ASN:HD22	1.85	0.41
17:S:172:TYR:HE2	37:4:456:ILE:HD13	1.85	0.41
32:k:98:GLU:HA	32:k:101:ILE:HG22	2.02	0.41
35:2:360:LEU:O	35:2:363:SER:OG	2.33	0.41
35:2:381:PHE:O	35:2:385:ASN:ND2	2.53	0.41
36:3:93:LEU:O	36:3:97:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:4:335:HIS:HA	37:4:338:VAL:HG12	2.02	0.41
37:4:429:ASN:ND2	38:5:168:LEU:HB2	2.35	0.41
38:5:481:LEU:HD23	38:5:481:LEU:HA	1.79	0.41
38:5:484:GLY:HA3	40:8:30:LEU:HD11	2.02	0.41
2:B:62:TYR:CD2	2:B:63:LYS:HG2	2.55	0.41
3:C:410:MET:HE3	3:C:427:ILE:HG21	1.96	0.41
6:F:63:LYS:HA	6:F:68:ARG:HD3	2.01	0.41
7:G:67:HIS:HE1	22:Z:155:PRO:HB2	1.85	0.41
9:I:157:ARG:HA	9:I:157:ARG:HD2	1.83	0.41
17:S:233:LYS:HE3	26:d:9:LEU:HD11	2.02	0.41
18:U:13:GLU:HA	19:W:84:ARG:HH22	1.85	0.41
31:j:9:ALA:HB1	35:2:432:ASN:HB3	2.01	0.41
31:j:49:THR:N	31:j:52:THR:OG1	2.51	0.41
34:1:204:LEU:HD13	34:1:305:TYR:HB2	2.02	0.41
38:5:89:LEU:HA	38:5:89:LEU:HD12	1.81	0.41
38:5:254:THR:OG1	38:5:255:LEU:N	2.53	0.41
3:C:116:VAL:HG22	3:C:465:ASP:HB3	2.01	0.41
3:C:275:THR:O	3:C:330:TYR:HB2	2.20	0.41
5:E:372:HIS:CE1	12:L:82:GLY:HA2	2.55	0.41
19:W:118:LEU:H	39:6:132:THR:HA	1.84	0.41
36:3:57:ILE:HD12	39:6:73:PHE:HE2	1.86	0.41
3:C:191:CYS:O	3:C:203:PHE:HD1	2.04	0.41
3:C:307:LYS:HB3	22:Z:160:LYS:HE2	2.01	0.41
6:F:49:LEU:HD11	6:F:108:HIS:HA	2.01	0.41
11:K:89:GLU:OE2	11:K:184:SER:N	2.49	0.41
19:W:92:GLU:HA	19:W:95:ILE:HD12	2.02	0.41
35:2:12:PHE:HE2	35:2:24:ILE:HG12	1.84	0.41
37:4:297:ASP:OD1	37:4:298:LEU:N	2.53	0.41
1:A:116:GLN:HG3	1:A:120:ASN:HD21	1.85	0.41
7:G:176:ASN:OD1	7:G:177:TRP:N	2.53	0.41
11:K:117:MET:HE3	11:K:117:MET:HB2	1.73	0.41
16:R:25:LEU:HD11	16:R:74:ARG:CA	2.48	0.41
16:R:108:GLU:CG	16:R:109:PRO:HG3	2.50	0.41
17:S:223:VAL:HA	17:S:226:ILE:HD12	2.02	0.41
35:2:202:ILE:HD12	35:2:257:SER:OG	2.20	0.41
35:2:366:ILE:HD11	35:2:447:ILE:HG12	2.02	0.41
36:3:83:VAL:HB	36:3:87:GLY:HA3	2.03	0.41
41:9:22:PHE:CE1	41:9:41:PHE:HB2	2.56	0.41
6:F:89:GLU:HA	6:F:92:GLU:HG2	2.03	0.41
47:J:202:LMN:HBP	47:J:202:LMN:HCS	2.02	0.41
37:4:14:PHE:CE1	37:4:24:VAL:HG11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:5:240:MET:HE3	38:5:251:HIS:CE1	2.54	0.41
7:G:180:ARG:NH2	7:G:198:ARG:O	2.43	0.41
8:H:109:THR:HA	8:H:116:ARG:NH2	2.35	0.41
48:J:204:CDL:H361	47:j:101:LMN:HAW	2.02	0.41
31:j:10:ILE:HG22	31:j:12:ARG:HB3	2.02	0.41
35:2:313:ILE:HA	35:2:313:ILE:HD13	1.86	0.41
37:4:263:LEU:HD13	37:4:482:TYR:HB3	2.02	0.41
38:5:112:HIS:ND1	46:5:901:3PE:O14	2.54	0.41
38:5:477:LYS:HB3	38:5:477:LYS:HE3	1.66	0.41
1:A:227:GLY:HA3	1:A:299:PHE:CE2	2.55	0.41
3:C:365:LYS:HE2	3:C:383:HIS:HE1	1.86	0.41
6:F:99:LEU:HD11	9:I:55:PHE:HD2	1.86	0.41
10:J:172:LEU:HA	10:J:175:THR:HG22	2.02	0.41
18:U:61:GLN:HG2	33:n:118:SER:HB2	2.02	0.41
18:U:101:LEU:O	18:U:106:HIS:ND1	2.54	0.41
18:U:102:GLU:HA	18:U:106:HIS:CE1	2.55	0.41
34:1:331:LEU:O	34:1:336:SER:OG	2.38	0.41
40:8:62:PHE:HD1	40:8:65:ARG:HH11	1.68	0.41
3:C:230:VAL:HG12	3:C:235:VAL:HG22	2.02	0.41
7:G:126:ILE:HD13	7:G:126:ILE:HG21	1.85	0.41
8:H:72:MET:HG2	8:H:111:TYR:HE2	1.86	0.41
10:J:117:ALA:N	48:J:204:CDL:HA4	2.36	0.41
47:J:202:LMN:HAWA	35:2:396:TYR:HD1	1.84	0.41
12:L:15:PHE:HZ	35:2:159:PHE:HB3	1.85	0.41
15:Q:90:LEU:HB3	16:R:44:ARG:NH1	2.28	0.41
16:R:37:ARG:HG3	25:c:13:GLU:OE1	2.20	0.41
18:U:9:TRP:HZ3	18:U:11:PRO:HB3	1.86	0.41
19:W:59:LYS:O	19:W:63:LEU:HB2	2.20	0.41
22:Z:163:LYS:HG3	22:Z:182:HIS:HD2	1.85	0.41
23:a:76:LEU:O	23:a:84:ARG:NH1	2.53	0.41
23:a:123:ARG:HH22	38:5:500:PHE:HD2	1.69	0.41
23:a:123:ARG:NH1	40:8:24:ASP:OD2	2.54	0.41
30:i:44:VAL:HG11	38:5:10:ILE:HG13	2.02	0.41
30:i:75:ARG:NH1	30:i:82:SER:HA	2.36	0.41
32:k:40:VAL:H	32:k:40:VAL:HG23	1.62	0.41
35:2:46:PHE:CE2	35:2:467:TYR:HB3	2.55	0.41
35:2:255:ILE:H	35:2:255:ILE:HG13	1.66	0.41
35:2:368:VAL:HA	35:2:371:PHE:HD2	1.85	0.41
52:2:502:CPL:HC72	52:2:502:CPL:HC41	1.80	0.41
37:4:14:PHE:HE1	37:4:24:VAL:HG11	1.86	0.41
48:4:502:CDL:H512	48:4:502:CDL:HB4	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:5:16:TRP:HE1	38:5:20:LEU:CD1	2.34	0.41
38:5:68:LEU:HD12	38:5:68:LEU:O	2.21	0.41
38:5:170:ALA:HA	38:5:235:TRP:HB2	2.02	0.41
38:5:331:HIS:HA	38:5:395:THR:OG1	2.21	0.41
38:5:363:TYR:O	38:5:448:TYR:OH	2.25	0.41
1:A:81:ARG:HA	1:A:81:ARG:HD3	1.69	0.41
1:A:84:LEU:HB3	1:A:93:PRO:HB2	2.02	0.41
1:A:177:LYS:N	1:A:239:THR:O	2.53	0.41
3:C:400:TYR:HD1	3:C:413:TYR:HB2	1.86	0.41
5:E:107:MET:HE3	5:E:108:ASP:C	2.45	0.41
6:F:70:SER:O	6:F:74:LEU:HB2	2.20	0.41
8:H:234:ASN:OD1	8:H:235:VAL:N	2.54	0.41
10:J:124:LEU:CD1	48:J:204:CDL:C73	2.98	0.41
11:K:81:PHE:CE2	11:K:131:LEU:HD13	2.56	0.41
12:L:57:ILE:HD12	12:L:60:ILE:HD12	2.02	0.41
16:R:109:PRO:HD2	37:4:447:THR:HG21	2.03	0.41
37:4:145:LEU:HD21	37:4:171:THR:HG21	2.03	0.41
38:5:28:TYR:O	38:5:32:THR:HG23	2.21	0.41
39:6:78:LEU:HD23	39:6:80:ILE:HD11	2.02	0.41
41:9:20:GLN:HG2	41:9:24:HIS:CE1	2.56	0.41
8:H:171:ALA:HB3	8:H:177:MET:HE3	2.02	0.40
23:a:83:ASP:H	38:5:561:ASN:HD21	1.69	0.40
37:4:84:LEU:HB2	37:4:478:THR:HG21	2.03	0.40
37:4:354:TYR:OH	37:4:441:HIS:O	2.32	0.40
1:A:225:LEU:HB2	1:A:228:ASN:ND2	2.36	0.40
2:B:82:SER:HB3	2:B:264:PHE:HD2	1.86	0.40
2:B:179:TYR:OH	2:B:197:VAL:O	2.39	0.40
12:L:62:LEU:HD23	12:L:62:LEU:HA	1.86	0.40
27:e:56:TYR:OH	38:5:505:SER:O	2.38	0.40
35:2:95:THR:O	35:2:340:GLN:NE2	2.43	0.40
37:4:331:LEU:HG	37:4:394:GLY:HA3	2.03	0.40
46:4:501:3PE:H351	46:4:501:3PE:H321	1.83	0.40
38:5:19:PRO:HB2	38:5:118:SER:HB2	2.02	0.40
38:5:499:TYR:HA	38:5:502:THR:HG22	2.03	0.40
39:6:170:LEU:O	39:6:174:ILE:HG12	2.21	0.40
1:A:188:ARG:HA	1:A:191:ARG:HE	1.86	0.40
3:C:61:ASP:HB3	35:2:283:ARG:HH12	1.82	0.40
3:C:297:ARG:NH2	3:C:339:GLU:OE2	2.55	0.40
3:C:343:SER:O	3:C:347:ILE:HG12	2.21	0.40
4:D:84:ARG:HG2	4:D:85:PRO:CD	2.52	0.40
5:E:141:TYR:HE2	11:K:39:SER:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:227:ILE:HG23	26:d:69:GLN:HE22	1.85	0.40
35:2:12:PHE:CE2	35:2:24:ILE:HG12	2.57	0.40
35:2:346:TYR:HB2	35:2:349:GLN:HG3	2.04	0.40
38:5:70:ILE:HG22	38:5:71:ASP:H	1.86	0.40
3:C:148:MET:HE3	3:C:148:MET:HB3	1.97	0.40
3:C:183:VAL:HG11	3:C:250:TRP:HH2	1.86	0.40
5:E:143:VAL:HG12	45:E:401:NDP:H61A	1.87	0.40
6:F:56:GLU:HG3	6:F:115:LYS:HG2	2.03	0.40
12:L:13:LEU:HD22	12:L:17:PHE:HE2	1.86	0.40
25:c:21:PHE:HE2	27:e:14:LEU:HD12	1.87	0.40
31:j:67:ILE:HD13	37:4:282:LEU:HD23	2.04	0.40
35:2:104:ILE:HA	35:2:107:PHE:HD2	1.85	0.40
35:2:163:ILE:O	35:2:166:ILE:HG13	2.22	0.40
35:2:214:ILE:HD12	35:2:297:MET:SD	2.61	0.40
35:2:375:PRO:HG2	37:4:142:GLU:HB2	2.03	0.40
36:3:6:ILE:HG21	36:3:6:ILE:HD13	1.86	0.40
39:6:36:MET:HE1	39:6:71:PHE:HD2	1.86	0.40
39:6:47:LEU:HG	39:6:59:TYR:CE2	2.56	0.40
1:A:491:ARG:HH22	1:A:690:LEU:HA	1.87	0.40
6:F:121:LYS:HG3	6:F:123:TRP:CZ2	2.57	0.40
13:O:71:GLU:HA	14:P:33:LEU:HD21	2.04	0.40
34:1:43:GLY:C	34:1:46:GLY:H	2.29	0.40
35:2:67:TYR:HD2	35:2:310:LEU:HD22	1.87	0.40
38:5:6:SER:O	38:5:10:ILE:HB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	692/728 (95%)	642 (93%)	50 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	439/488 (90%)	409 (93%)	30 (7%)	0	100	100
3	C	426/466 (91%)	396 (93%)	30 (7%)	0	100	100
4	D	84/87 (97%)	79 (94%)	5 (6%)	0	100	100
5	E	255/375 (68%)	241 (94%)	14 (6%)	0	100	100
6	F	119/144 (83%)	109 (92%)	10 (8%)	0	100	100
7	G	208/281 (74%)	195 (94%)	13 (6%)	0	100	100
8	H	213/243 (88%)	191 (90%)	22 (10%)	0	100	100
9	I	188/229 (82%)	176 (94%)	12 (6%)	0	100	100
10	J	177/198 (89%)	164 (93%)	13 (7%)	0	100	100
11	K	147/210 (70%)	136 (92%)	11 (8%)	0	100	100
12	L	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
13	O	75/109 (69%)	71 (95%)	4 (5%)	0	100	100
14	P	121/124 (98%)	113 (93%)	8 (7%)	0	100	100
15	Q	83/132 (63%)	80 (96%)	3 (4%)	0	100	100
16	R	104/109 (95%)	93 (89%)	11 (11%)	0	100	100
17	S	168/249 (68%)	156 (93%)	12 (7%)	0	100	100
18	U	169/172 (98%)	153 (90%)	15 (9%)	1 (1%)	21	52
19	W	117/123 (95%)	112 (96%)	5 (4%)	0	100	100
20	X	166/169 (98%)	156 (94%)	10 (6%)	0	100	100
21	Y	121/161 (75%)	113 (93%)	8 (7%)	0	100	100
22	Z	118/182 (65%)	107 (91%)	11 (9%)	0	100	100
23	a	122/149 (82%)	109 (89%)	13 (11%)	0	100	100
24	b	62/74 (84%)	60 (97%)	2 (3%)	0	100	100
25	c	42/60 (70%)	38 (90%)	4 (10%)	0	100	100
26	d	88/92 (96%)	82 (93%)	5 (6%)	1 (1%)	11	39
27	e	50/67 (75%)	49 (98%)	1 (2%)	0	100	100
28	f	77/87 (88%)	67 (87%)	10 (13%)	0	100	100
29	g	74/78 (95%)	64 (86%)	10 (14%)	0	100	100
30	i	81/90 (90%)	77 (95%)	4 (5%)	0	100	100
31	j	88/93 (95%)	81 (92%)	6 (7%)	1 (1%)	11	39
32	k	94/237 (40%)	86 (92%)	6 (6%)	2 (2%)	5	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	n	112/120 (93%)	96 (86%)	15 (13%)	1 (1%)	14	43
34	1	312/341 (92%)	292 (94%)	20 (6%)	0	100	100
35	2	467/469 (100%)	436 (93%)	30 (6%)	1 (0%)	43	71
36	3	104/128 (81%)	98 (94%)	6 (6%)	0	100	100
37	4	484/486 (100%)	455 (94%)	28 (6%)	1 (0%)	43	71
38	5	652/655 (100%)	605 (93%)	44 (7%)	3 (0%)	24	55
39	6	181/185 (98%)	166 (92%)	15 (8%)	0	100	100
40	8	80/99 (81%)	75 (94%)	5 (6%)	0	100	100
41	9	84/89 (94%)	78 (93%)	6 (7%)	0	100	100
All	All	7531/8667 (87%)	6990 (93%)	530 (7%)	11 (0%)	49	75

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	k	40	VAL
32	k	55	VAL
38	5	555	VAL
38	5	556	SER
35	2	188	ASP
31	j	83	LYS
26	d	17	TYR
38	5	455	ASN
18	U	19	PRO
33	n	106	PRO
37	4	83	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	566/595 (95%)	565 (100%)	1 (0%)	87	88
2	B	353/389 (91%)	353 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	369/394 (94%)	367 (100%)	2 (0%)	81	83
4	D	68/69 (99%)	68 (100%)	0	100	100
5	E	225/329 (68%)	224 (100%)	1 (0%)	84	84
6	F	109/129 (84%)	108 (99%)	1 (1%)	70	78
7	G	188/245 (77%)	188 (100%)	0	100	100
8	H	190/212 (90%)	190 (100%)	0	100	100
9	I	156/187 (83%)	156 (100%)	0	100	100
10	J	130/147 (88%)	130 (100%)	0	100	100
11	K	131/180 (73%)	131 (100%)	0	100	100
12	L	77/77 (100%)	77 (100%)	0	100	100
13	O	65/91 (71%)	65 (100%)	0	100	100
14	P	109/110 (99%)	109 (100%)	0	100	100
15	Q	72/111 (65%)	72 (100%)	0	100	100
16	R	97/100 (97%)	96 (99%)	1 (1%)	68	76
17	S	149/211 (71%)	148 (99%)	1 (1%)	76	80
18	U	147/148 (99%)	147 (100%)	0	100	100
19	W	98/102 (96%)	98 (100%)	0	100	100
20	X	132/133 (99%)	132 (100%)	0	100	100
21	Y	105/140 (75%)	105 (100%)	0	100	100
22	Z	95/148 (64%)	95 (100%)	0	100	100
23	a	108/129 (84%)	108 (100%)	0	100	100
24	b	50/59 (85%)	50 (100%)	0	100	100
25	c	30/45 (67%)	30 (100%)	0	100	100
26	d	83/85 (98%)	82 (99%)	1 (1%)	63	75
27	e	44/55 (80%)	44 (100%)	0	100	100
28	f	68/73 (93%)	68 (100%)	0	100	100
29	g	62/64 (97%)	62 (100%)	0	100	100
30	i	64/68 (94%)	64 (100%)	0	100	100
31	j	71/73 (97%)	71 (100%)	0	100	100
32	k	86/207 (42%)	86 (100%)	0	100	100
33	n	98/102 (96%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	1	282/302 (93%)	280 (99%)	2 (1%)	76	80
35	2	433/433 (100%)	433 (100%)	0	100	100
36	3	97/114 (85%)	97 (100%)	0	100	100
37	4	434/434 (100%)	434 (100%)	0	100	100
38	5	579/580 (100%)	578 (100%)	1 (0%)	87	88
39	6	165/167 (99%)	165 (100%)	0	100	100
40	8	69/76 (91%)	69 (100%)	0	100	100
41	9	73/76 (96%)	73 (100%)	0	100	100
All	All	6527/7389 (88%)	6516 (100%)	11 (0%)	85	88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	LYS
3	C	97	VAL
3	C	98	LEU
5	E	162	ARG
6	F	111	LEU
16	R	30	ILE
17	S	234	LEU
26	d	13	ASP
34	1	3	ILE
34	1	89	VAL
38	5	477	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	147	GLN
1	A	209	ASN
1	A	212	GLN
1	A	220	ASN
1	A	240	ASN
1	A	322	ASN
1	A	398	ASN
2	B	47	ASN
3	C	163	ASN

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Mol	Chain	Res	Type
3	C	237	GLN
3	C	268	ASN
3	C	284	GLN
3	C	342	GLN
3	C	367	ASN
3	C	383	HIS
3	C	445	HIS
4	D	44	GLN
5	E	76	HIS
5	E	121	HIS
5	E	127	ASN
5	E	181	HIS
5	E	365	ASN
5	E	372	HIS
6	F	77	HIS
7	G	67	HIS
7	G	136	ASN
8	H	125	GLN
8	H	181	ASN
10	J	21	HIS
10	J	149	GLN
14	P	93	GLN
16	R	50	ASN
16	R	105	ASN
17	S	61	GLN
17	S	115	HIS
17	S	132	ASN
17	S	201	GLN
18	U	17	ASN
18	U	50	ASN
18	U	97	HIS
18	U	107	GLN
18	U	119	ASN
19	W	88	GLN
20	X	13	ASN
20	X	27	HIS
20	X	142	ASN
20	X	145	HIS
21	Y	99	GLN
21	Y	132	GLN
22	Z	182	HIS
23	a	61	GLN

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Mol	Chain	Res	Type
23	a	90	ASN
24	b	51	HIS
25	c	20	ASN
26	d	65	ASN
26	d	69	GLN
26	d	77	HIS
27	e	23	HIS
28	f	11	HIS
28	f	14	GLN
29	g	22	ASN
29	g	25	HIS
30	i	78	HIS
31	j	27	HIS
32	k	93	HIS
33	n	64	ASN
33	n	71	GLN
34	1	49	GLN
34	1	254	ASN
35	2	86	ASN
35	2	185	HIS
35	2	278	GLN
35	2	320	HIS
35	2	339	ASN
35	2	340	GLN
35	2	385	ASN
35	2	393	ASN
36	3	85	ASN
36	3	120	ASN
37	4	23	ASN
37	4	26	HIS
37	4	33	ASN
37	4	103	ASN
37	4	106	ASN
37	4	153	HIS
37	4	197	HIS
37	4	235	HIS
37	4	335	HIS
37	4	424	GLN
37	4	429	ASN
37	4	469	GLN
38	5	76	ASN
38	5	100	HIS

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Mol	Chain	Res	Type
38	5	251	HIS
38	5	450	ASN
38	5	491	HIS
38	5	529	ASN
38	5	578	HIS
38	5	636	ASN
38	5	638	ASN
39	6	90	ASN
39	6	120	ASN
39	6	152	ASN
39	6	157	ASN
40	8	10	GLN
40	8	34	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

36 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
46	3PE	J	203	-	43,43,50	0.92	3 (6%)	46,48,55	1.17	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	ZMP	Q	201	15	27,32,36	1.78	6 (22%)	31,39,45	2.00	8 (25%)
48	CDL	X	201	-	81,81,99	0.98	7 (8%)	87,93,111	1.20	5 (5%)
51	T7X	2	501	-	48,48,61	0.96	4 (8%)	57,60,73	1.30	6 (10%)
50	PLC	W	401	-	40,40,41	1.37	6 (15%)	46,48,49	1.22	3 (6%)
50	PLC	n	1101	-	41,41,41	1.34	6 (14%)	47,49,49	1.06	2 (4%)
42	SF4	A	801	1	0,12,12	-	-	-	-	-
48	CDL	J	204	-	77,77,99	1.04	4 (5%)	83,89,111	1.15	9 (10%)
43	FES	A	803	1	0,4,4	-	-	-	-	-
43	FES	H	301	8	0,4,4	-	-	-	-	-
46	3PE	I	303	-	50,50,50	0.89	4 (8%)	53,55,55	1.37	3 (5%)
46	3PE	g	202	-	42,42,50	0.92	3 (7%)	45,47,55	1.32	2 (4%)
48	CDL	g	201	-	82,82,99	0.96	6 (7%)	88,94,111	1.26	5 (5%)
45	NDP	E	401	-	51,52,52	3.57	21 (41%)	71,80,80	2.20	18 (25%)
46	3PE	J	201	-	40,40,50	1.00	3 (7%)	43,45,55	1.30	3 (6%)
46	3PE	6	301	-	35,35,50	1.03	4 (11%)	38,40,55	1.13	2 (5%)
51	T7X	2	503	-	52,52,61	0.94	4 (7%)	61,64,73	1.29	7 (11%)
42	SF4	A	802	1	0,12,12	-	-	-	-	-
46	3PE	4	505	-	50,50,50	0.83	3 (6%)	53,55,55	1.21	4 (7%)
47	LMN	j	101	-	68,68,72	1.61	12 (17%)	88,94,98	1.54	17 (19%)
46	3PE	5	901	-	41,41,50	1.00	3 (7%)	44,46,55	1.20	3 (6%)
51	T7X	4	504	-	43,43,61	0.97	4 (9%)	52,55,73	1.39	4 (7%)
48	CDL	4	502	-	91,91,99	0.96	8 (8%)	97,103,111	1.20	6 (6%)
49	ZMP	O	201	13	27,32,36	1.65	5 (18%)	31,39,45	1.87	8 (25%)
42	SF4	I	302	9	0,12,12	-	-	-	-	-
46	3PE	5	903	-	50,50,50	0.90	4 (8%)	53,55,55	1.18	2 (3%)
42	SF4	K	301	11	0,12,12	-	-	-	-	-
52	CPL	2	502	-	51,51,51	1.00	4 (7%)	57,59,59	1.11	3 (5%)
50	PLC	5	902	-	30,30,41	1.51	6 (20%)	36,38,49	1.05	3 (8%)
44	FMN	B	502	-	33,33,33	2.88	12 (36%)	48,50,50	1.64	9 (18%)
42	SF4	I	301	9	0,12,12	-	-	-	-	-
47	LMN	J	202	-	72,72,72	1.51	8 (11%)	92,98,98	1.62	18 (19%)
46	3PE	4	503	-	41,41,50	0.94	4 (9%)	44,46,55	1.14	3 (6%)
42	SF4	B	501	2	0,12,12	-	-	-	-	-
46	3PE	4	501	-	42,42,50	0.96	3 (7%)	45,47,55	1.24	3 (6%)
50	PLC	W	402	-	41,41,41	1.31	5 (12%)	47,49,49	1.22	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	J	203	-	-	23/47/47/54	-
49	ZMP	Q	201	15	-	7/37/39/43	-
48	CDL	X	201	-	-	27/92/92/110	-
51	T7X	2	501	-	-	14/43/67/80	0/1/1/1
50	PLC	W	401	-	-	20/44/44/45	-
50	PLC	n	1101	-	-	11/45/45/45	-
48	CDL	J	204	-	-	21/88/88/110	-
42	SF4	A	801	1	-	-	0/6/5/5
43	FES	A	803	1	-	-	0/1/1/1
43	FES	H	301	8	-	-	0/1/1/1
46	3PE	I	303	-	-	23/54/54/54	-
46	3PE	g	202	-	-	20/46/46/54	-
48	CDL	g	201	-	-	37/93/93/110	-
45	NDP	E	401	-	-	14/34/77/77	0/5/5/5
46	3PE	J	201	-	-	21/44/44/54	-
46	3PE	6	301	-	-	20/39/39/54	-
51	T7X	2	503	-	-	20/47/71/80	0/1/1/1
42	SF4	A	802	1	-	-	0/6/5/5
46	3PE	4	505	-	-	23/54/54/54	-
47	LMN	j	101	-	-	20/46/126/130	0/4/4/4
46	3PE	5	901	-	-	20/45/45/54	-
51	T7X	4	504	-	-	26/38/62/80	0/1/1/1
48	CDL	4	502	-	-	50/102/102/110	-
49	ZMP	O	201	13	-	13/37/39/43	-
42	SF4	I	302	9	-	-	0/6/5/5
46	3PE	5	903	-	-	18/54/54/54	-
42	SF4	K	301	11	-	-	0/6/5/5
52	CPL	2	502	-	-	26/55/55/55	-
50	PLC	5	902	-	-	17/34/34/45	-
44	FMN	B	502	-	-	10/18/18/18	0/3/3/3
42	SF4	I	301	9	-	-	0/6/5/5
47	LMN	J	202	-	-	26/50/130/130	0/4/4/4
46	3PE	4	503	-	-	20/45/45/54	-
42	SF4	B	501	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	4	501	-	-	22/46/46/54	-
50	PLC	W	402	-	-	22/45/45/45	-

All (162) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	E	401	NDP	C2B-C1B	-8.24	1.32	1.53
45	E	401	NDP	O4B-C1B	7.76	1.59	1.42
45	E	401	NDP	O4D-C1D	7.75	1.59	1.42
45	E	401	NDP	C2D-C1D	-7.40	1.30	1.53
45	E	401	NDP	C6N-C5N	7.17	1.55	1.33
44	B	502	FMN	C10-N1	7.14	1.47	1.33
45	E	401	NDP	O4D-C4D	-6.96	1.29	1.45
44	B	502	FMN	C4A-N5	6.62	1.45	1.30
45	E	401	NDP	O4B-C4B	-6.62	1.30	1.45
45	E	401	NDP	PN-O3	6.55	1.66	1.59
47	j	101	LMN	O1-C1	-5.87	1.30	1.40
47	J	202	LMN	O1-C1	-5.73	1.30	1.40
44	B	502	FMN	C5A-N5	5.36	1.49	1.39
44	B	502	FMN	C2-N1	5.32	1.48	1.36
45	E	401	NDP	C2N-C3N	5.28	1.49	1.35
47	j	101	LMN	O5-C1	5.10	1.55	1.41
49	Q	201	ZMP	C13-N1	5.10	1.45	1.33
49	O	201	ZMP	C13-N1	4.98	1.45	1.33
47	J	202	LMN	O5-C1	4.86	1.54	1.41
44	B	502	FMN	C9A-N10	4.86	1.49	1.41
45	E	401	NDP	PA-O3	4.74	1.64	1.59
49	O	201	ZMP	C16-N2	4.72	1.44	1.33
44	B	502	FMN	C2-N3	4.71	1.49	1.39
49	Q	201	ZMP	C16-N2	4.58	1.44	1.33
45	E	401	NDP	P2B-O2B	4.46	1.67	1.59
45	E	401	NDP	C6A-N6A	4.44	1.45	1.34
48	J	204	CDL	OB8-CB7	4.27	1.45	1.33
48	J	204	CDL	OA8-CA7	4.20	1.45	1.33
48	J	204	CDL	OA6-CA5	4.14	1.46	1.34
48	J	204	CDL	OB6-CB5	4.13	1.45	1.34
44	B	502	FMN	C4-N3	4.06	1.46	1.38
45	E	401	NDP	C4N-C3N	4.01	1.57	1.50
45	E	401	NDP	O2D-C2D	3.94	1.52	1.43
44	B	502	FMN	C10-N10	3.93	1.45	1.37
49	Q	201	ZMP	O3-C16	-3.65	1.16	1.23
50	n	1101	PLC	O2-C'	3.44	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	W	401	PLC	O2-C'	3.44	1.44	1.34
50	n	1101	PLC	O3-CB	3.37	1.43	1.33
45	E	401	NDP	C7N-N7N	3.30	1.42	1.33
50	W	402	PLC	O2-C'	3.21	1.43	1.34
48	X	201	CDL	OA6-CA4	-3.19	1.39	1.46
50	W	401	PLC	O3-CB	3.17	1.42	1.33
45	E	401	NDP	C6N-N1N	3.15	1.44	1.37
47	J	202	LMN	O4-C4	3.14	1.51	1.43
47	j	101	LMN	OBZ-CCS	3.12	1.49	1.41
45	E	401	NDP	C5A-C4A	-3.12	1.33	1.39
48	4	502	CDL	OA6-CA4	-3.08	1.39	1.46
47	j	101	LMN	CBT-CCM	3.08	1.60	1.53
50	5	902	PLC	O3-CB	3.05	1.42	1.33
48	g	201	CDL	OA6-CA4	-3.03	1.39	1.46
50	5	902	PLC	O2-C'	3.00	1.42	1.34
46	5	903	3PE	O21-C2	-2.99	1.39	1.46
46	J	203	3PE	O21-C2	-2.93	1.39	1.46
46	4	501	3PE	O21-C2	-2.93	1.39	1.46
50	W	402	PLC	O3-CB	2.89	1.41	1.33
47	J	202	LMN	OBY-CCR	2.88	1.49	1.41
45	E	401	NDP	C5D-C4D	2.86	1.60	1.51
46	4	505	3PE	O21-C2	-2.84	1.39	1.46
48	g	201	CDL	OB6-CB4	-2.84	1.39	1.46
48	4	502	CDL	OB6-CB4	-2.84	1.39	1.46
48	X	201	CDL	OA8-CA6	-2.84	1.38	1.45
51	2	503	T7X	O16-C8	-2.83	1.39	1.46
46	5	901	3PE	O21-C2	-2.82	1.40	1.46
47	J	202	LMN	CBT-CCM	2.81	1.59	1.53
46	J	201	3PE	O31-C3	-2.78	1.39	1.45
49	O	201	ZMP	O3-C16	-2.75	1.18	1.23
50	5	902	PLC	O2-C2	-2.74	1.40	1.46
46	g	202	3PE	O21-C21	2.74	1.42	1.34
47	j	101	LMN	OBY-CCR	2.73	1.48	1.41
48	X	201	CDL	OB6-CB4	-2.73	1.40	1.46
46	4	503	3PE	O21-C2	-2.72	1.40	1.46
45	E	401	NDP	C4N-C5N	2.71	1.56	1.49
47	j	101	LMN	CBS-CCM	2.68	1.59	1.53
51	4	504	T7X	O18-C9	-2.65	1.39	1.45
46	J	201	3PE	O21-C2	-2.65	1.40	1.46
46	5	903	3PE	O31-C3	-2.64	1.39	1.45
50	W	402	PLC	O2-C2	-2.64	1.40	1.46
46	6	301	3PE	O21-C2	-2.63	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	g	201	CDL	OA8-CA7	2.63	1.41	1.33
48	4	502	CDL	OA8-CA7	2.62	1.41	1.33
52	2	502	CPL	O2-C2	-2.60	1.40	1.46
46	5	901	3PE	O31-C31	2.59	1.40	1.33
47	j	101	LMN	O4-C4	2.58	1.50	1.43
49	Q	201	ZMP	O2-C13	-2.57	1.18	1.23
44	B	502	FMN	O4-C4	-2.54	1.18	1.23
46	I	303	3PE	O21-C2	-2.54	1.40	1.46
44	B	502	FMN	O2-C2	-2.52	1.19	1.24
46	I	303	3PE	O31-C3	-2.52	1.39	1.45
46	J	201	3PE	O21-C21	2.50	1.41	1.34
46	4	501	3PE	O31-C3	-2.50	1.39	1.45
47	J	202	LMN	OBZ-CCS	2.49	1.48	1.41
47	j	101	LMN	OBZ-CCD	2.49	1.50	1.44
44	B	502	FMN	C7M-C7	2.49	1.55	1.51
51	4	504	T7X	O16-C10	2.46	1.41	1.34
50	n	1101	PLC	O2-C2	-2.44	1.40	1.46
46	I	303	3PE	O21-C21	2.43	1.41	1.34
49	O	201	ZMP	O2-C13	-2.43	1.18	1.23
48	g	201	CDL	OB8-CB7	2.41	1.40	1.33
45	E	401	NDP	C5A-N7A	-2.41	1.34	1.39
48	4	502	CDL	PA1-OA5	2.40	1.68	1.59
46	I	303	3PE	O31-C31	2.39	1.40	1.33
46	5	903	3PE	O31-C31	2.37	1.40	1.33
51	2	503	T7X	O18-C11	2.37	1.40	1.33
50	W	401	PLC	P-O3P	2.37	1.68	1.59
51	2	501	T7X	O16-C10	2.37	1.41	1.34
46	4	503	3PE	O31-C31	2.35	1.40	1.33
46	g	202	3PE	O31-C3	-2.35	1.39	1.45
50	W	401	PLC	O2-C2	-2.34	1.41	1.46
51	2	501	T7X	O18-C9	-2.34	1.39	1.45
52	2	502	CPL	O3-C3	-2.33	1.40	1.45
49	O	201	ZMP	C10-S1	2.31	1.81	1.76
46	6	301	3PE	O31-C31	2.30	1.40	1.33
52	2	502	CPL	O2-C31	2.30	1.40	1.34
48	X	201	CDL	OB8-CB7	2.27	1.40	1.33
48	4	502	CDL	OA8-CA6	-2.27	1.40	1.45
47	J	202	LMN	OBY-CCC	2.26	1.49	1.44
46	5	901	3PE	O21-C21	2.26	1.40	1.34
47	J	202	LMN	CBS-CCM	2.26	1.58	1.53
46	J	203	3PE	O31-C31	2.25	1.39	1.33
51	2	501	T7X	O18-C11	2.25	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	W	401	PLC	P-O4P	2.24	1.68	1.59
51	2	503	T7X	O18-C9	-2.24	1.40	1.45
48	4	502	CDL	OB8-CB7	2.24	1.39	1.33
51	4	504	T7X	P1-O1	2.22	1.66	1.59
50	n	1101	PLC	P-O3P	2.22	1.68	1.59
50	5	902	PLC	P-O3P	2.22	1.68	1.59
48	X	201	CDL	OB8-CB6	-2.22	1.40	1.45
50	n	1101	PLC	P-O4P	2.20	1.68	1.59
49	Q	201	ZMP	C10-S1	2.19	1.81	1.76
46	4	505	3PE	O31-C31	2.19	1.39	1.33
46	6	301	3PE	O31-C3	-2.19	1.40	1.45
52	2	502	CPL	O3-C11	2.19	1.39	1.33
45	E	401	NDP	C8A-N9A	-2.18	1.33	1.37
46	6	301	3PE	O21-C21	2.17	1.40	1.34
47	j	101	LMN	OBX-CCC	2.16	1.49	1.44
50	W	402	PLC	P-O3P	2.16	1.67	1.59
48	g	201	CDL	OA8-CA6	-2.15	1.40	1.45
50	W	402	PLC	P-O4P	2.14	1.67	1.59
46	4	503	3PE	O21-C21	2.14	1.40	1.34
48	4	502	CDL	OB8-CB6	-2.13	1.40	1.45
47	j	101	LMN	OBX-CCJ	2.13	1.47	1.41
51	2	501	T7X	P1-O1	2.12	1.65	1.59
50	5	902	PLC	P-O4P	2.12	1.67	1.59
46	J	203	3PE	O31-C3	-2.11	1.40	1.45
44	B	502	FMN	P-O5'	2.11	1.67	1.60
51	2	503	T7X	O16-C10	2.11	1.40	1.34
48	4	502	CDL	OB6-CB5	2.09	1.40	1.34
46	4	501	3PE	O31-C31	2.09	1.39	1.33
47	j	101	LMN	CBQ-CCM	2.09	1.58	1.54
46	4	505	3PE	O31-C3	-2.08	1.40	1.45
51	4	504	T7X	O16-C8	-2.08	1.41	1.46
48	X	201	CDL	OA6-CA5	2.08	1.40	1.34
48	X	201	CDL	OB6-CB5	2.05	1.40	1.34
46	4	503	3PE	O31-C3	-2.05	1.40	1.45
50	W	401	PLC	C8-N	-2.05	1.44	1.50
47	j	101	LMN	OAN-CCH	2.02	1.48	1.43
46	g	202	3PE	O31-C31	2.02	1.39	1.33
48	g	201	CDL	OA6-CA5	2.02	1.40	1.34
50	5	902	PLC	C8-N	-2.01	1.44	1.50
49	Q	201	ZMP	C9-C10	2.01	1.52	1.50
46	5	903	3PE	O21-C21	2.01	1.39	1.34
50	n	1101	PLC	C1'-C'	2.01	1.56	1.50

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	E	401	NDP	N6A-C6A-N1A	-6.68	103.49	118.38
45	E	401	NDP	C4A-N9A-C1B	-6.48	111.49	126.63
49	Q	201	ZMP	C9-C10-S1	6.17	120.75	113.40
45	E	401	NDP	N3A-C2A-N1A	-6.16	119.25	128.58
45	E	401	NDP	C1B-N9A-C8A	6.06	140.54	127.09
47	J	202	LMN	CBR-CBL-CBJ	5.94	130.88	113.19
47	j	101	LMN	CBR-CBL-CBJ	5.93	130.84	113.19
50	W	401	PLC	O2-C'-C1'	5.48	123.33	111.48
45	E	401	NDP	C5A-C6A-N6A	5.14	136.02	123.29
50	W	402	PLC	O2-C'-C1'	5.13	122.58	111.48
44	B	502	FMN	C7M-C7-C6	-5.06	110.65	119.57
51	2	501	T7X	O16-C10-C12	4.97	122.23	111.48
45	E	401	NDP	C5A-C4A-N3A	-4.95	119.90	126.72
46	g	202	3PE	O21-C21-C22	4.87	122.02	111.48
49	O	201	ZMP	C9-C10-S1	4.78	119.10	113.40
51	2	503	T7X	O16-C10-C12	4.54	121.31	111.48
46	5	901	3PE	O21-C21-C22	4.49	121.20	111.48
46	I	303	3PE	O21-C21-C22	4.47	121.14	111.48
47	J	202	LMN	O3-C3-C2	-4.41	99.98	110.38
46	5	903	3PE	O21-C21-C22	4.37	120.94	111.48
47	J	202	LMN	CCL-CCH-CCQ	4.30	119.44	109.68
48	J	204	CDL	OA6-CA5-C11	4.28	120.73	111.48
46	J	203	3PE	O21-C21-C22	4.27	120.73	111.48
46	J	201	3PE	O21-C21-C22	4.25	120.67	111.48
45	E	401	NDP	N9A-C8A-N7A	-4.21	107.96	113.94
52	2	502	CPL	O2-C31-C32	4.19	120.54	111.48
48	g	201	CDL	OA6-CA5-C11	4.15	120.46	111.48
44	B	502	FMN	C7M-C7-C8	4.14	129.22	120.76
48	X	201	CDL	OB6-CB5-C51	4.05	120.25	111.48
46	I	303	3PE	O31-C31-C32	4.01	124.06	111.83
48	4	502	CDL	OA6-CA5-C11	3.98	120.10	111.48
48	g	201	CDL	OB6-CB5-C51	3.97	120.07	111.48
46	6	301	3PE	O21-C21-C22	3.96	120.04	111.48
49	Q	201	ZMP	C14-C15-N2	-3.84	103.82	112.00
46	4	501	3PE	O21-C21-C22	3.84	119.79	111.48
48	4	502	CDL	OB6-CB5-C51	3.84	119.78	111.48
49	O	201	ZMP	O1-C10-C9	-3.82	119.58	123.98
48	X	201	CDL	CA6-CA4-CA3	-3.81	102.91	111.78
47	j	101	LMN	OAN-CCH-CCL	-3.80	101.42	110.38
48	J	204	CDL	OB6-CB5-C51	3.77	119.65	111.48
51	4	504	T7X	O16-C10-C12	3.76	119.61	111.48
48	X	201	CDL	OA6-CA5-C11	3.68	119.45	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	4	505	3PE	O21-C21-C22	3.67	119.43	111.48
45	E	401	NDP	C2A-N3A-C4A	3.66	120.77	111.83
50	n	1101	PLC	O2-C'-C1'	3.66	119.40	111.48
49	Q	201	ZMP	O1-C10-C9	-3.59	119.84	123.98
47	J	202	LMN	CCJ-CCL-CCH	3.52	117.42	110.01
46	4	503	3PE	O21-C21-C22	3.50	119.05	111.48
44	B	502	FMN	C4-N3-C2	-3.48	119.45	125.64
48	g	201	CDL	OB8-CB7-C71	3.45	122.36	111.83
48	g	201	CDL	OB8-CB6-CB4	3.37	118.12	108.40
45	E	401	NDP	C2B-C1B-N9A	-3.36	108.22	113.75
50	5	902	PLC	O2-C'-C1'	3.35	118.73	111.48
46	4	501	3PE	C2-O21-C21	-3.32	109.86	117.80
45	E	401	NDP	C5B-C4B-C3B	-3.31	103.29	115.21
49	O	201	ZMP	C19-C18-C17	3.25	114.31	108.77
47	j	101	LMN	CCW-CCU-CCO	3.24	116.51	110.83
48	4	502	CDL	OB8-CB7-C71	3.22	121.67	111.83
47	J	202	LMN	O4-C4-C3	3.21	115.39	107.23
49	Q	201	ZMP	C15-C14-C13	3.21	117.73	112.39
50	n	1101	PLC	O3-CB-C1B	3.09	121.25	111.83
46	J	203	3PE	O31-C31-C32	3.08	121.21	111.83
52	2	502	CPL	O3-C11-C12	3.07	121.19	111.83
49	Q	201	ZMP	C20-C18-C17	3.05	113.97	108.77
47	J	202	LMN	C2-C3-C4	3.03	116.56	109.68
48	4	502	CDL	OA8-CA7-C31	3.00	120.98	111.83
51	2	503	T7X	O18-C11-C31	2.97	120.90	111.83
45	E	401	NDP	P2B-O2B-C2B	-2.97	115.51	123.43
51	4	504	T7X	C12-C13-C14	-2.94	106.93	113.35
46	J	201	3PE	O31-C31-C32	2.93	120.76	111.83
45	E	401	NDP	C5A-N7A-C8A	2.92	108.05	103.45
51	4	504	T7X	O1-C1-C2	2.92	114.92	108.73
46	5	901	3PE	O31-C31-C32	2.91	120.69	111.83
48	J	204	CDL	OA8-CA7-C31	2.90	120.68	111.83
46	4	505	3PE	O31-C31-C32	2.88	120.62	111.83
49	Q	201	ZMP	C11-S1-C10	2.86	110.30	101.84
45	E	401	NDP	N3A-C4A-N9A	2.86	132.03	127.17
44	B	502	FMN	O4-C4-C4A	-2.85	119.02	126.53
47	J	202	LMN	O5-C1-C2	-2.84	104.53	110.37
47	j	101	LMN	CBL-CBR-CCM	-2.84	108.58	117.19
46	5	903	3PE	O31-C31-C32	2.83	120.47	111.83
47	j	101	LMN	OAP-CCL-CCH	-2.83	103.71	110.38
51	4	504	T7X	C6-C1-C2	2.81	114.77	110.86
46	6	301	3PE	O31-C31-C32	2.80	120.38	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	2	503	T7X	C3-C2-C1	2.79	116.02	109.68
46	4	505	3PE	C2-O21-C21	-2.77	111.16	117.80
51	2	503	T7X	C5-C6-C1	2.77	115.97	109.68
47	j	101	LMN	CCR-O4-C4	-2.77	111.41	117.98
47	J	202	LMN	CBL-CBR-CCM	-2.77	108.79	117.19
49	O	201	ZMP	C15-N2-C16	-2.75	117.61	122.55
44	B	502	FMN	C5A-C9A-N10	2.75	120.45	117.97
51	2	501	T7X	C5-C4-C3	2.73	115.62	110.83
47	j	101	LMN	CCV-CCT-CCN	2.72	115.60	110.83
47	j	101	LMN	OCB-CCS-CCW	2.69	114.72	108.09
51	2	501	T7X	O18-C11-C31	2.69	120.05	111.83
49	O	201	ZMP	C11-C12-N1	-2.68	106.82	112.41
46	4	503	3PE	O31-C31-C32	2.67	119.97	111.83
47	J	202	LMN	O5-C5-C4	2.67	115.24	109.72
46	4	501	3PE	O31-C31-C32	2.66	119.94	111.83
47	J	202	LMN	OBX-CCC-CCN	2.65	114.48	109.70
44	B	502	FMN	C4A-C4-N3	2.64	119.97	113.25
51	2	501	T7X	C5-C6-C1	2.64	115.67	109.68
47	J	202	LMN	OCB-CCS-CCW	2.64	114.58	108.09
48	J	204	CDL	OB8-CB7-C71	2.61	119.80	111.83
48	g	201	CDL	OA8-CA7-C31	2.61	119.79	111.83
47	J	202	LMN	CBQ-CBK-CBI	-2.59	105.47	113.19
48	X	201	CDL	OA8-CA7-C31	2.58	119.71	111.83
49	Q	201	ZMP	O1-C10-S1	-2.58	119.40	122.68
47	j	101	LMN	CCS-OCB-CCQ	-2.56	111.91	117.98
47	J	202	LMN	O4-CCR-CCV	2.55	114.36	108.09
50	W	401	PLC	O3-CB-C1B	2.55	119.59	111.83
49	O	201	ZMP	C17-C16-N2	2.52	121.26	116.48
50	W	402	PLC	O3-CB-C1B	2.50	119.47	111.83
47	j	101	LMN	O3-C3-C2	-2.50	104.48	110.38
51	2	503	T7X	C6-C1-C2	2.49	114.32	110.86
47	j	101	LMN	OCB-CCQ-CCH	2.48	113.53	107.23
47	J	202	LMN	OBX-CCF-CBP	-2.41	100.46	106.44
48	J	204	CDL	CA4-OA6-CA5	-2.41	112.03	117.80
47	j	101	LMN	OBX-CCC-CCN	2.40	114.02	109.70
44	B	502	FMN	C9A-C5A-N5	-2.40	119.91	122.45
48	X	201	CDL	OB8-CB7-C71	2.36	119.03	111.83
46	I	303	3PE	O31-C31-O32	-2.36	117.73	123.63
46	4	505	3PE	C24-C23-C22	-2.34	104.54	113.13
47	j	101	LMN	CBQ-CBK-CBI	-2.33	106.25	113.19
47	J	202	LMN	CCV-CCT-CCN	2.32	114.91	110.83
46	J	201	3PE	C3-C2-C1	-2.32	106.37	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	O	201	ZMP	C11-S1-C10	2.32	108.69	101.84
49	O	201	ZMP	C14-C15-N2	-2.31	107.08	112.00
47	J	202	LMN	CCU-CCO-CCD	2.30	114.40	110.23
45	E	401	NDP	C4A-C5A-N7A	-2.29	107.96	110.58
48	4	502	CDL	CA6-CA4-CA3	-2.29	106.46	111.78
46	g	202	3PE	O31-C31-C32	2.28	118.80	111.83
48	J	204	CDL	OA6-CA5-OA7	-2.26	118.42	123.70
48	J	204	CDL	CA6-CA4-CA3	-2.26	106.51	111.78
50	5	902	PLC	O3-C3-C2	2.23	114.81	108.40
47	j	101	LMN	O4-CCR-CCV	2.22	113.54	108.09
47	J	202	LMN	CCW-CCU-CCO	2.21	114.72	110.83
50	5	902	PLC	C3-C2-C1	-2.21	106.62	111.78
49	Q	201	ZMP	C17-C16-N2	2.21	120.68	116.48
51	2	501	T7X	C6-C1-C2	2.20	113.91	110.86
45	E	401	NDP	O4B-C1B-N9A	2.16	112.24	108.09
50	W	401	PLC	C3-C2-C1	-2.14	106.78	111.78
46	5	901	3PE	C3-C2-C1	-2.14	106.79	111.78
46	4	503	3PE	C33-C32-C31	-2.12	105.92	113.69
44	B	502	FMN	C5'-C4'-C3'	-2.11	108.23	112.22
45	E	401	NDP	C4A-N9A-C8A	2.11	107.96	105.74
51	2	503	T7X	O16-C10-O17	-2.10	118.79	123.70
48	J	204	CDL	CB4-OB6-CB5	-2.08	112.82	117.80
52	2	502	CPL	C14-C13-C12	-2.07	105.50	113.13
47	j	101	LMN	OBZ-CCD-CCO	2.07	113.43	109.70
45	E	401	NDP	C5A-C4A-N9A	2.07	108.07	105.81
47	J	202	LMN	O4-C4-C5	-2.05	104.09	109.48
51	2	503	T7X	C6-C5-C4	2.04	114.41	110.83
45	E	401	NDP	C1D-N1N-C6N	-2.02	116.50	120.77
47	j	101	LMN	O4-C4-C3	2.02	112.37	107.23
47	j	101	LMN	CCJ-CCL-CCH	2.02	114.25	110.01
51	2	501	T7X	C32-C31-C11	-2.02	106.31	113.69
48	J	204	CDL	OA8-CA7-OA9	-2.01	118.59	123.63
48	4	502	CDL	OB8-CB7-OB9	-2.01	118.61	123.63
44	B	502	FMN	C4-C4A-C10	2.00	120.37	116.93

There are no chirality outliers.

All (591) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	B	502	FMN	N10-C1'-C2'-O2'
44	B	502	FMN	N10-C1'-C2'-C3'
44	B	502	FMN	C1'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
44	B	502	FMN	C1'-C2'-C3'-C4'
44	B	502	FMN	O2'-C2'-C3'-O3'
44	B	502	FMN	O2'-C2'-C3'-C4'
45	E	401	NDP	C5D-O5D-PN-O1N
46	I	303	3PE	C1-O11-P-O13
46	I	303	3PE	C1-O11-P-O14
46	I	303	3PE	C11-O13-P-O11
46	I	303	3PE	O13-C11-C12-N
46	I	303	3PE	O21-C2-C3-O31
46	J	201	3PE	C1-O11-P-O12
46	J	201	3PE	C1-O11-P-O13
46	J	201	3PE	C11-O13-P-O12
46	J	201	3PE	O21-C2-C3-O31
46	J	203	3PE	C1-O11-P-O12
46	J	203	3PE	C1-O11-P-O13
46	J	203	3PE	C22-C21-O21-C2
46	g	202	3PE	C1-O11-P-O12
46	g	202	3PE	C1-O11-P-O13
46	g	202	3PE	C1-O11-P-O14
46	g	202	3PE	C11-O13-P-O11
46	g	202	3PE	C11-O13-P-O14
46	g	202	3PE	C22-C21-O21-C2
46	4	501	3PE	C1-O11-P-O12
46	4	501	3PE	C1-O11-P-O13
46	4	501	3PE	C1-O11-P-O14
46	4	501	3PE	C22-C21-O21-C2
46	4	503	3PE	C1-O11-P-O12
46	4	503	3PE	C1-O11-P-O13
46	4	503	3PE	C1-O11-P-O14
46	4	503	3PE	C11-O13-P-O12
46	4	503	3PE	O13-C11-C12-N
46	4	503	3PE	O21-C2-C3-O31
46	4	505	3PE	C1-O11-P-O12
46	4	505	3PE	C1-O11-P-O13
46	4	505	3PE	C1-O11-P-O14
46	4	505	3PE	O22-C21-O21-C2
46	5	901	3PE	C1-O11-P-O12
46	5	901	3PE	C1-O11-P-O13
46	5	901	3PE	C1-O11-P-O14
46	5	901	3PE	C11-O13-P-O12
46	5	901	3PE	O13-C11-C12-N
46	5	903	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
46	5	903	3PE	C1-O11-P-O13
46	5	903	3PE	C1-O11-P-O14
46	5	903	3PE	O22-C21-O21-C2
46	6	301	3PE	C1-O11-P-O12
46	6	301	3PE	C1-O11-P-O14
46	6	301	3PE	O13-C11-C12-N
47	j	101	LMN	OBX-CCJ-OBV-CBT
48	J	204	CDL	C11-CA5-OA6-CA4
48	J	204	CDL	CB2-OB2-PB2-OB5
48	J	204	CDL	CB3-OB5-PB2-OB2
48	J	204	CDL	CB3-OB5-PB2-OB3
48	J	204	CDL	CB3-OB5-PB2-OB4
48	X	201	CDL	CB2-OB2-PB2-OB4
48	g	201	CDL	CB2-C1-CA2-OA2
48	g	201	CDL	CB3-OB5-PB2-OB2
48	g	201	CDL	CB3-OB5-PB2-OB3
48	g	201	CDL	CB3-OB5-PB2-OB4
48	4	502	CDL	OB7-CB5-OB6-CB4
48	4	502	CDL	C51-CB5-OB6-CB4
49	O	201	ZMP	O4-C17-C18-C21
49	O	201	ZMP	C16-C17-C18-C21
49	O	201	ZMP	O4-C17-C18-C19
49	O	201	ZMP	C16-C17-C18-C19
49	O	201	ZMP	O4-C17-C18-C20
49	O	201	ZMP	C16-C17-C18-C20
49	O	201	ZMP	C12-C11-S1-C10
49	O	201	ZMP	C7-C8-C9-C10
49	Q	201	ZMP	C19-C18-C21-O5
49	Q	201	ZMP	C20-C18-C21-O5
49	Q	201	ZMP	C17-C18-C21-O5
49	Q	201	ZMP	C13-C14-C15-N2
49	Q	201	ZMP	C12-C11-S1-C10
50	W	401	PLC	O4P-C4-C5-N
50	W	401	PLC	C1-O3P-P-O1P
50	W	401	PLC	C4-O4P-P-O2P
50	W	401	PLC	C4-O4P-P-O3P
50	W	402	PLC	O4P-C4-C5-N
50	W	402	PLC	C1'-C'-O2-C2
50	W	402	PLC	O'-C'-O2-C2
50	n	1101	PLC	C1-O3P-P-O1P
50	n	1101	PLC	C1-O3P-P-O2P
50	n	1101	PLC	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
50	5	902	PLC	C1-O3P-P-O2P
50	5	902	PLC	C4-O4P-P-O1P
51	2	501	T7X	C7-O13-P1-O1
51	2	501	T7X	C7-O13-P1-O12
51	2	501	T7X	C9-C8-O16-C10
51	2	501	T7X	C12-C10-O16-C8
51	2	501	T7X	C15-C16-C17-C18
51	2	501	T7X	C18-C19-C20-C21
51	2	501	T7X	C22-C23-C24-C25
51	2	503	T7X	C7-O13-P1-O1
51	2	503	T7X	C7-O13-P1-O11
51	2	503	T7X	C7-O13-P1-O12
51	2	503	T7X	O19-C11-O18-C9
51	2	503	T7X	C25-C26-C27-C28
51	4	504	T7X	C2-C1-O1-P1
51	4	504	T7X	C6-C1-O1-P1
51	4	504	T7X	C1-O1-P1-O11
51	4	504	T7X	C1-O1-P1-O13
51	4	504	T7X	C7-O13-P1-O1
51	4	504	T7X	C7-O13-P1-O11
51	4	504	T7X	C12-C10-O16-C8
52	2	502	CPL	O4P-C4-C5-N
52	2	502	CPL	C1-O3P-P-O1P
52	2	502	CPL	C1-O3P-P-O2P
52	2	502	CPL	C1-O3P-P-O4P
46	I	303	3PE	O32-C31-O31-C3
46	4	505	3PE	O32-C31-O31-C3
48	g	201	CDL	CB4-CB6-OB8-CB7
46	I	303	3PE	C32-C31-O31-C3
51	2	503	T7X	C31-C11-O18-C9
47	j	101	LMN	OBY-CCR-O4-C4
46	4	501	3PE	O32-C31-O31-C3
48	4	502	CDL	OA9-CA7-OA8-CA6
48	4	502	CDL	OB9-CB7-OB8-CB6
47	J	202	LMN	CCW-CCS-OCB-CCQ
46	J	203	3PE	O22-C21-O21-C2
48	J	204	CDL	OA7-CA5-OA6-CA4
48	g	201	CDL	OB7-CB5-OB6-CB4
51	2	501	T7X	O17-C10-O16-C8
51	4	504	T7X	O17-C10-O16-C8
46	4	501	3PE	C32-C31-O31-C3
46	4	505	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
48	4	502	CDL	C31-CA7-OA8-CA6
48	4	502	CDL	C71-CB7-OB8-CB6
47	J	202	LMN	C3-C4-O4-CCR
46	4	505	3PE	C22-C21-O21-C2
46	5	903	3PE	C22-C21-O21-C2
48	g	201	CDL	C51-CB5-OB6-CB4
48	g	201	CDL	OB9-CB7-OB8-CB6
47	j	101	LMN	OBZ-CCS-OCB-CCQ
47	J	202	LMN	O5-C5-C6-O6
50	W	402	PLC	C1B-CB-O3-C3
46	g	202	3PE	O22-C21-O21-C2
46	4	501	3PE	O22-C21-O21-C2
47	j	101	LMN	OAJ-CBN-CCD-OBZ
48	g	201	CDL	O1-C1-CA2-OA2
50	W	402	PLC	OB-CB-O3-C3
47	J	202	LMN	OAJ-CBN-CCD-OBZ
46	5	901	3PE	C22-C21-O21-C2
48	4	502	CDL	C11-CA5-OA6-CA4
50	W	401	PLC	C1'-C'-O2-C2
47	J	202	LMN	C4-C5-C6-O6
48	g	201	CDL	C71-CB7-OB8-CB6
47	J	202	LMN	OBZ-CCS-OCB-CCQ
47	J	202	LMN	OBX-CCJ-OBV-CBT
47	j	101	LMN	O5-C1-O1-CBS
47	j	101	LMN	OAJ-CBN-CCD-CCO
47	J	202	LMN	OAJ-CBN-CCD-CCO
45	E	401	NDP	C3B-C2B-O2B-P2B
46	5	901	3PE	O22-C21-O21-C2
48	4	502	CDL	OA7-CA5-OA6-CA4
50	W	401	PLC	O'-C'-O2-C2
48	J	204	CDL	C31-CA7-OA8-CA6
46	4	501	3PE	C2B-C2C-C2D-C2E
47	J	202	LMN	CAW-CAY-CBA-CBC
47	j	101	LMN	C2-C1-O1-CBS
46	6	301	3PE	C21-C22-C23-C24
48	4	502	CDL	O1-C1-CB2-OB2
47	J	202	LMN	CBC-CBE-CBG-CBI
50	5	902	PLC	C'-C1'-C2'-C3'
46	g	202	3PE	O21-C2-C3-O31
52	2	502	CPL	C18-C19-C20-C21
44	B	502	FMN	O3'-C3'-C4'-C5'
50	5	902	PLC	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
48	4	502	CDL	CA7-C31-C32-C33
51	2	501	T7X	C11-C31-C32-C33
51	2	503	T7X	C10-C12-C13-C14
51	2	503	T7X	C11-C31-C32-C33
51	4	504	T7X	C11-C31-C32-C33
48	J	204	CDL	OA9-CA7-OA8-CA6
47	J	202	LMN	O5-C1-O1-CBS
46	J	203	3PE	C31-C32-C33-C34
46	g	202	3PE	C31-C32-C33-C34
48	X	201	CDL	C11-CA5-OA6-CA4
46	4	505	3PE	C36-C37-C38-C39
46	g	202	3PE	C21-C22-C23-C24
48	4	502	CDL	C56-C57-C58-C59
48	X	201	CDL	OA7-CA5-OA6-CA4
46	5	901	3PE	C34-C35-C36-C37
47	J	202	LMN	CBJ-CBL-CBR-CCM
47	J	202	LMN	OAI-CBM-CCC-OBY
47	J	202	LMN	C2-C1-O1-CBS
44	B	502	FMN	C2'-C3'-C4'-C5'
50	5	902	PLC	C1B-CB-O3-C3
48	g	201	CDL	CA5-C11-C12-C13
48	g	201	CDL	CB5-C51-C52-C53
51	2	501	T7X	C31-C32-C33-C34
46	J	201	3PE	C3D-C3E-C3F-C3G
46	g	202	3PE	C26-C27-C28-C29
46	4	505	3PE	C23-C24-C25-C26
47	j	101	LMN	C4-C5-C6-O6
46	I	303	3PE	C37-C38-C39-C3A
46	g	202	3PE	C25-C26-C27-C28
48	g	201	CDL	CB7-C71-C72-C73
46	4	501	3PE	C29-C2A-C2B-C2C
46	6	301	3PE	C23-C24-C25-C26
50	W	402	PLC	C3B-C4B-C5B-C6B
46	J	203	3PE	C32-C33-C34-C35
46	J	203	3PE	C24-C25-C26-C27
48	X	201	CDL	C57-C58-C59-C60
50	W	402	PLC	C2B-C3B-C4B-C5B
46	J	203	3PE	C38-C39-C3A-C3B
48	J	204	CDL	C73-C74-C75-C76
48	4	502	CDL	O1-C1-CA2-OA2
46	5	901	3PE	C21-C22-C23-C24
46	J	203	3PE	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
48	J	204	CDL	C75-C76-C77-C78
48	X	201	CDL	C31-C32-C33-C34
52	2	502	CPL	C17-C18-C19-C20
52	2	502	CPL	C19-C20-C21-C22
46	I	303	3PE	C3C-C3D-C3E-C3F
46	4	505	3PE	C34-C35-C36-C37
46	J	203	3PE	C21-C22-C23-C24
50	W	401	PLC	C'-C1'-C2'-C3'
46	J	203	3PE	C23-C24-C25-C26
46	4	505	3PE	C38-C39-C3A-C3B
48	X	201	CDL	C58-C59-C60-C61
48	g	201	CDL	C22-C23-C24-C25
48	g	201	CDL	C71-C72-C73-C74
46	I	303	3PE	C39-C3A-C3B-C3C
48	X	201	CDL	C35-C36-C37-C38
46	J	201	3PE	C24-C25-C26-C27
46	I	303	3PE	C28-C29-C2A-C2B
51	2	503	T7X	C12-C13-C14-C15
51	2	501	T7X	C32-C33-C34-C35
48	4	502	CDL	CA5-C11-C12-C13
47	j	101	LMN	CAY-CBA-CBC-CBE
51	2	503	T7X	C33-C34-C35-C36
46	4	503	3PE	C33-C34-C35-C36
50	W	401	PLC	C1B-C2B-C3B-C4B
51	4	504	T7X	C31-C11-O18-C9
46	J	201	3PE	C35-C36-C37-C38
46	4	505	3PE	C26-C27-C28-C29
48	X	201	CDL	C52-C53-C54-C55
51	2	503	T7X	C35-C36-C37-C38
47	J	202	LMN	C5-C4-O4-CCR
46	4	501	3PE	C25-C26-C27-C28
48	4	502	CDL	C51-C52-C53-C54
50	W	402	PLC	C4'-C5'-C6'-C7'
51	2	501	T7X	C24-C25-C26-C27
48	g	201	CDL	C11-CA5-OA6-CA4
52	2	502	CPL	C32-C31-O2-C2
46	g	202	3PE	C2D-C2E-C2F-C2G
48	4	502	CDL	C42-C43-C44-C45
46	5	903	3PE	C34-C35-C36-C37
48	g	201	CDL	C23-C24-C25-C26
46	4	501	3PE	C36-C37-C38-C39
46	4	501	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
46	5	903	3PE	C3E-C3F-C3G-C3H
50	5	902	PLC	OB-CB-O3-C3
46	I	303	3PE	C31-C32-C33-C34
51	4	504	T7X	C34-C35-C36-C37
51	2	503	T7X	O13-C7-C8-O16
46	4	503	3PE	C32-C33-C34-C35
44	B	502	FMN	C2'-C3'-C4'-O4'
50	W	402	PLC	C'-C1'-C2'-C3'
48	4	502	CDL	C71-C72-C73-C74
46	I	303	3PE	C27-C28-C29-C2A
51	4	504	T7X	C31-C32-C33-C34
46	I	303	3PE	C33-C34-C35-C36
48	4	502	CDL	C34-C35-C36-C37
50	5	902	PLC	C2-C1-O3P-P
46	6	301	3PE	C29-C2A-C2B-C2C
48	X	201	CDL	C56-C57-C58-C59
48	4	502	CDL	C22-C23-C24-C25
48	g	201	CDL	OA7-CA5-OA6-CA4
52	2	502	CPL	O31-C31-O2-C2
49	Q	201	ZMP	C1-C2-C3-C4
48	X	201	CDL	C71-CB7-OB8-CB6
48	X	201	CDL	C51-CB5-OB6-CB4
48	4	502	CDL	C54-C55-C56-C57
46	4	501	3PE	C2A-C2B-C2C-C2D
46	6	301	3PE	C34-C35-C36-C37
50	W	402	PLC	C5B-C6B-C7B-C8B
48	4	502	CDL	C75-C76-C77-C78
48	4	502	CDL	C11-C12-C13-C14
46	g	202	3PE	C36-C37-C38-C39
48	4	502	CDL	C12-C13-C14-C15
48	4	502	CDL	C73-C74-C75-C76
46	I	303	3PE	C1-C2-C3-O31
46	J	203	3PE	C1-C2-C3-O31
46	g	202	3PE	C1-C2-C3-O31
46	4	503	3PE	C1-C2-C3-O31
46	6	301	3PE	C1-C2-C3-O31
50	W	401	PLC	C1-C2-C3-O3
51	4	504	T7X	C7-C8-C9-O18
46	4	501	3PE	C28-C29-C2A-C2B
47	j	101	LMN	O5-C5-C6-O6
51	4	504	T7X	O19-C11-O18-C9
46	6	301	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
48	4	502	CDL	C1-CA2-OA2-PA1
46	4	503	3PE	C36-C37-C38-C39
45	E	401	NDP	C1B-C2B-O2B-P2B
48	X	201	CDL	OB9-CB7-OB8-CB6
47	J	202	LMN	CAX-CAZ-CBB-CBD
46	g	202	3PE	C1-C2-O21-C21
51	4	504	T7X	C33-C34-C35-C36
46	5	903	3PE	C2A-C2B-C2C-C2D
48	4	502	CDL	C21-C22-C23-C24
47	J	202	LMN	CBI-CBK-CBQ-CCM
46	4	501	3PE	O11-C1-C2-O21
50	5	902	PLC	C1'-C'-O2-C2
48	g	201	CDL	C31-C32-C33-C34
46	J	203	3PE	O21-C2-C3-O31
46	6	301	3PE	O21-C2-C3-O31
52	2	502	CPL	O2-C2-C3-O3
51	2	503	T7X	C34-C35-C36-C37
50	W	402	PLC	C8'-C9'-CA'-CB'
51	4	504	T7X	O18-C11-C31-C32
47	J	202	LMN	OBY-CCR-O4-C4
46	4	505	3PE	C27-C28-C29-C2A
46	5	903	3PE	C37-C38-C39-C3A
46	I	303	3PE	C25-C26-C27-C28
48	J	204	CDL	C51-CB5-OB6-CB4
47	J	202	LMN	CAB-CAX-CAZ-CBB
50	W	401	PLC	C1B-CB-O3-C3
48	4	502	CDL	C15-C16-C17-C18
46	4	505	3PE	C3B-C3C-C3D-C3E
46	5	903	3PE	C33-C34-C35-C36
50	W	401	PLC	O3P-C1-C2-C3
51	2	503	T7X	O13-C7-C8-C9
47	J	202	LMN	CBB-CBD-CBF-CBH
47	j	101	LMN	CBC-CBE-CBG-CBI
48	X	201	CDL	C74-C75-C76-C77
46	5	903	3PE	C28-C29-C2A-C2B
51	2	503	T7X	C32-C33-C34-C35
48	J	204	CDL	C71-C72-C73-C74
46	4	505	3PE	C3F-C3G-C3H-C3I
46	4	501	3PE	C37-C38-C39-C3A
51	2	501	T7X	C12-C13-C14-C15
46	J	201	3PE	C3E-C3F-C3G-C3H
46	5	901	3PE	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
46	6	301	3PE	C25-C26-C27-C28
48	4	502	CDL	CA3-CA4-CA6-OA8
50	n	1101	PLC	C1-C2-C3-O3
52	2	502	CPL	C1-C2-C3-O3
46	J	201	3PE	C33-C34-C35-C36
48	g	201	CDL	C72-C73-C74-C75
48	g	201	CDL	C76-C77-C78-C79
48	g	201	CDL	OA5-CA3-CA4-OA6
48	4	502	CDL	C39-C40-C41-C42
45	E	401	NDP	C4B-C5B-O5B-PA
48	g	201	CDL	C40-C41-C42-C43
50	n	1101	PLC	C6'-C7'-C8'-C9'
50	W	401	PLC	O2-C2-C3-O3
50	n	1101	PLC	O2-C2-C3-O3
52	2	502	CPL	C39-C40-C41-C42
52	2	502	CPL	C40-C41-C42-C43
46	4	503	3PE	C21-C22-C23-C24
48	4	502	CDL	C35-C36-C37-C38
50	W	401	PLC	C4'-C5'-C6'-C7'
48	X	201	CDL	C71-C72-C73-C74
48	J	204	CDL	C63-C64-C65-C66
44	B	502	FMN	O3'-C3'-C4'-O4'
47	j	101	LMN	CBH-CBJ-CBL-CBR
52	2	502	CPL	C16-C17-C18-C19
46	4	501	3PE	C35-C36-C37-C38
50	W	401	PLC	C4B-C5B-C6B-C7B
48	4	502	CDL	C44-C45-C46-C47
48	4	502	CDL	CB7-C71-C72-C73
46	J	203	3PE	C36-C37-C38-C39
46	6	301	3PE	C22-C21-O21-C2
48	4	502	CDL	CB2-C1-CA2-OA2
48	g	201	CDL	OB5-CB3-CB4-CB6
47	j	101	LMN	CBG-CBI-CBK-CBQ
46	6	301	3PE	C35-C36-C37-C38
48	4	502	CDL	CB5-C51-C52-C53
48	X	201	CDL	OB7-CB5-OB6-CB4
50	5	902	PLC	O'-C'-O2-C2
46	J	203	3PE	C39-C3A-C3B-C3C
49	O	201	ZMP	C6-C7-C8-C9
48	g	201	CDL	C72-C71-CB7-OB8
50	W	401	PLC	C5'-C6'-C7'-C8'
50	W	401	PLC	OB-CB-O3-C3

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Mol	Chain	Res	Type	Atoms
47	j	101	LMN	CBA-CBC-CBE-CBG
50	W	401	PLC	C5B-C6B-C7B-C8B
46	4	505	3PE	O11-C1-C2-O21
48	g	201	CDL	OB5-CB3-CB4-OB6
50	W	401	PLC	O3P-C1-C2-O2
46	J	201	3PE	C1-C2-C3-O31
46	5	901	3PE	C1-C2-C3-O31
50	W	402	PLC	C1-C2-C3-O3
48	X	201	CDL	CB7-C71-C72-C73
46	I	303	3PE	O21-C21-C22-C23
46	4	505	3PE	C3C-C3D-C3E-C3F
46	J	201	3PE	C12-C11-O13-P
46	g	202	3PE	C12-C11-O13-P
46	g	202	3PE	C32-C33-C34-C35
46	5	901	3PE	O21-C2-C3-O31
48	4	502	CDL	OA6-CA4-CA6-OA8
48	J	204	CDL	OB7-CB5-OB6-CB4
46	4	505	3PE	C32-C33-C34-C35
46	4	505	3PE	C3A-C3B-C3C-C3D
45	E	401	NDP	C2D-C1D-N1N-C6N
48	4	502	CDL	C59-C60-C61-C62
50	n	1101	PLC	O4P-C4-C5-N
50	5	902	PLC	O4P-C4-C5-N
51	4	504	T7X	C1-O1-P1-O12
46	6	301	3PE	O22-C21-O21-C2
46	I	303	3PE	C23-C24-C25-C26
50	W	402	PLC	C4B-C5B-C6B-C7B
46	I	303	3PE	C3D-C3E-C3F-C3G
46	4	503	3PE	C3D-C3E-C3F-C3G
50	W	402	PLC	C1B-C2B-C3B-C4B
51	4	504	T7X	C35-C36-C37-C38
46	4	501	3PE	O11-C1-C2-C3
46	4	505	3PE	O11-C1-C2-C3
46	5	901	3PE	O11-C1-C2-C3
46	6	301	3PE	O11-C1-C2-C3
50	n	1101	PLC	O3P-C1-C2-C3
51	4	504	T7X	O13-C7-C8-C9
51	4	504	T7X	C10-C12-C13-C14
46	4	505	3PE	C2-C1-O11-P
48	4	502	CDL	CB4-CB3-OB5-PB2
46	5	901	3PE	O11-C1-C2-O21
46	5	903	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
48	4	502	CDL	OB5-CB3-CB4-OB6
50	n	1101	PLC	O3P-C1-C2-O2
50	5	902	PLC	O3P-C1-C2-O2
51	4	504	T7X	O13-C7-C8-O16
46	5	903	3PE	C36-C37-C38-C39
50	W	402	PLC	C1'-C2'-C3'-C4'
51	4	504	T7X	C32-C33-C34-C35
49	O	201	ZMP	C4-C5-C6-C7
46	5	903	3PE	C29-C2A-C2B-C2C
46	5	901	3PE	C39-C3A-C3B-C3C
48	g	201	CDL	C41-C42-C43-C44
45	E	401	NDP	O4D-C4D-C5D-O5D
45	E	401	NDP	C5B-O5B-PA-O1A
45	E	401	NDP	C5D-O5D-PN-O3
46	I	303	3PE	C1-O11-P-O12
46	I	303	3PE	C11-O13-P-O14
46	J	201	3PE	C1-O11-P-O14
46	J	201	3PE	C11-O13-P-O11
46	J	203	3PE	C1-O11-P-O14
46	4	503	3PE	C11-O13-P-O11
46	4	505	3PE	C11-O13-P-O14
46	5	901	3PE	C11-O13-P-O11
46	6	301	3PE	C1-O11-P-O13
46	6	301	3PE	C11-O13-P-O14
48	J	204	CDL	CB2-OB2-PB2-OB3
48	X	201	CDL	CB2-OB2-PB2-OB3
48	X	201	CDL	CB2-OB2-PB2-OB5
48	X	201	CDL	CB3-OB5-PB2-OB2
48	X	201	CDL	CB3-OB5-PB2-OB4
48	4	502	CDL	CA3-OA5-PA1-OA3
48	4	502	CDL	CB2-OB2-PB2-OB3
48	4	502	CDL	CB3-OB5-PB2-OB2
48	4	502	CDL	CB3-OB5-PB2-OB4
50	5	902	PLC	C1-O3P-P-O1P
50	5	902	PLC	C1-O3P-P-O4P
52	2	502	CPL	C4-O4P-P-O1P
48	X	201	CDL	C12-C13-C14-C15
51	4	504	T7X	C13-C14-C15-C16
48	X	201	CDL	C1-CA2-OA2-PA1
46	J	203	3PE	C26-C27-C28-C29
48	J	204	CDL	C62-C63-C64-C65
47	j	101	LMN	OAI-CBM-CCC-OBY

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Mol	Chain	Res	Type	Atoms
48	J	204	CDL	C11-C12-C13-C14
47	j	101	LMN	OAL-CBP-CCF-CCQ
48	4	502	CDL	OB5-CB3-CB4-CB6
50	5	902	PLC	O3P-C1-C2-C3
52	2	502	CPL	O11-C11-O3-C3
47	j	101	LMN	OAL-CBP-CCF-OBX
48	4	502	CDL	C14-C15-C16-C17
46	6	301	3PE	O21-C21-C22-C23
50	W	402	PLC	C2'-C3'-C4'-C5'
48	4	502	CDL	C76-C77-C78-C79
46	6	301	3PE	O11-C1-C2-O21
48	X	201	CDL	C13-C14-C15-C16
52	2	502	CPL	C12-C11-O3-C3
45	E	401	NDP	O4D-C1D-N1N-C6N
46	J	201	3PE	O31-C31-C32-C33
48	4	502	CDL	C74-C75-C76-C77
45	E	401	NDP	C2B-O2B-P2B-O3X
45	E	401	NDP	C2D-C1D-N1N-C2N
50	W	401	PLC	O2-C'-C1'-C2'
50	n	1101	PLC	C4'-C5'-C6'-C7'
48	g	201	CDL	C34-C35-C36-C37
48	g	201	CDL	C77-C78-C79-C80
51	2	503	T7X	C13-C14-C15-C16
47	J	202	LMN	CBE-CBG-CBI-CBK
50	W	401	PLC	C3B-C4B-C5B-C6B
48	4	502	CDL	C55-C56-C57-C58
49	O	201	ZMP	N2-C16-C17-O4
46	4	505	3PE	C22-C23-C24-C25
46	5	901	3PE	C27-C28-C29-C2A
48	J	204	CDL	C1-CA2-OA2-PA1
48	g	201	CDL	OA5-CA3-CA4-CA6
48	4	502	CDL	OB6-CB4-CB6-OB8
50	W	402	PLC	O2-C2-C3-O3
51	4	504	T7X	O16-C8-C9-O18
46	5	903	3PE	C2E-C2F-C2G-C2H
45	E	401	NDP	O4D-C1D-N1N-C2N
51	2	503	T7X	C16-C17-C18-C19
51	4	504	T7X	C15-C16-C17-C18
47	J	202	LMN	CCV-CCR-O4-C4
45	E	401	NDP	C2B-O2B-P2B-O1X
51	4	504	T7X	O19-C11-C31-C32
46	J	201	3PE	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
46	g	202	3PE	C27-C28-C29-C2A
46	J	203	3PE	C22-C23-C24-C25
47	j	101	LMN	CCF-CCQ-OCB-CCS
46	5	903	3PE	C1-C2-C3-O31
47	j	101	LMN	CCH-CCQ-OCB-CCS
46	I	303	3PE	C3A-C3B-C3C-C3D
50	W	402	PLC	C7B-C8B-C9B-CAA
47	J	202	LMN	CBD-CBF-CBH-CBJ
46	4	503	3PE	O11-C1-C2-C3
47	J	202	LMN	CBH-CBJ-CBL-CBR
46	4	501	3PE	C34-C35-C36-C37
48	g	201	CDL	C33-C34-C35-C36
52	2	502	CPL	C43-C44-C45-C46
46	J	201	3PE	C3B-C3C-C3D-C3E
51	2	503	T7X	C24-C25-C26-C27
52	2	502	CPL	C42-C43-C44-C45
46	4	501	3PE	C24-C25-C26-C27
48	g	201	CDL	C72-C71-CB7-OB9
50	W	402	PLC	C8B-C9B-CAA-CBA
48	X	201	CDL	C33-C34-C35-C36
52	2	502	CPL	C37-C38-C39-C40
48	g	201	CDL	C35-C36-C37-C38
52	2	502	CPL	C2-C1-O3P-P
48	X	201	CDL	C37-C38-C39-C40
51	2	501	T7X	O13-C7-C8-O16
48	X	201	CDL	C21-C22-C23-C24
49	Q	201	ZMP	C11-C12-N1-C13
46	4	501	3PE	C2F-C2G-C2H-C2I
46	J	203	3PE	C2A-C2B-C2C-C2D
46	5	901	3PE	C25-C26-C27-C28
50	5	902	PLC	C2B-C3B-C4B-C5B
46	4	503	3PE	C27-C28-C29-C2A
48	J	204	CDL	OA6-CA4-CA6-OA8
51	2	503	T7X	O16-C8-C9-O18
52	2	502	CPL	C13-C14-C15-C16
46	J	201	3PE	O21-C21-C22-C23
46	5	901	3PE	O21-C21-C22-C23
46	J	203	3PE	O11-C1-C2-C3
46	5	903	3PE	O11-C1-C2-C3
52	2	502	CPL	C35-C36-C37-C38
50	W	402	PLC	C6'-C7'-C8'-C9'
47	J	202	LMN	CBG-CBI-CBK-CBQ

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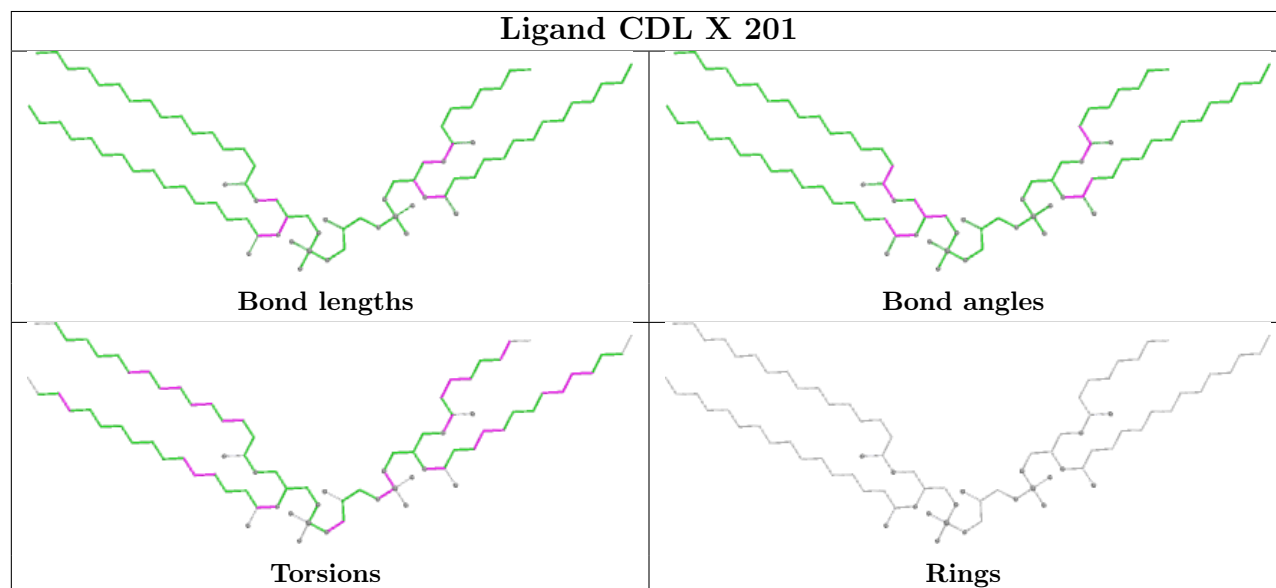
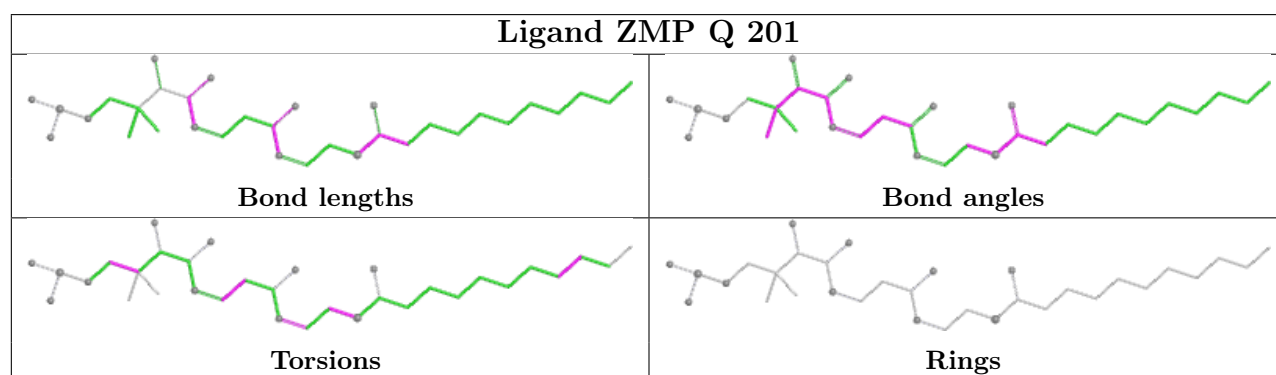
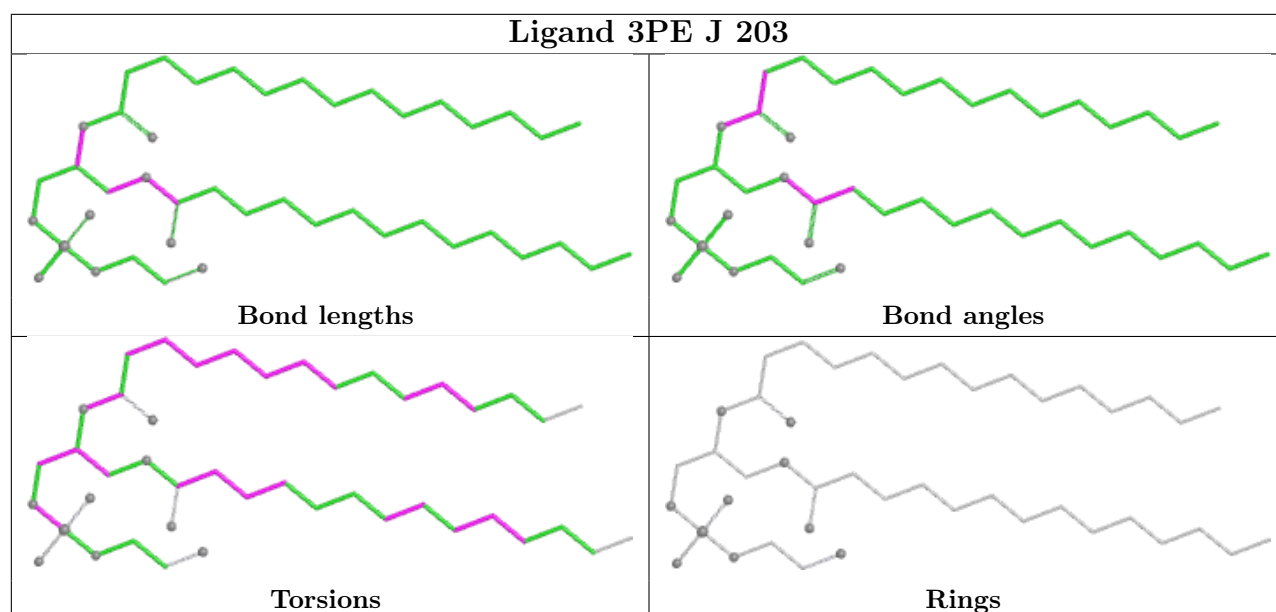
Mol	Chain	Res	Type	Atoms
47	j	101	LMN	CBF-CBH-CBJ-CBL
48	X	201	CDL	C51-C52-C53-C54
46	4	501	3PE	C22-C23-C24-C25
50	n	1101	PLC	C'-C1'-C2'-C3'
47	J	202	LMN	O1-CBS-CCM-CBR
49	O	201	ZMP	O3-C16-C17-C18
45	E	401	NDP	C2B-O2B-P2B-O2X
46	4	503	3PE	O31-C31-C32-C33
50	W	402	PLC	C2B-C1B-CB-O3
48	g	201	CDL	CB3-CB4-CB6-OB8
51	2	503	T7X	C7-C8-C9-O18
46	5	903	3PE	O21-C2-C3-O31
46	g	202	3PE	O21-C21-C22-C23
46	J	201	3PE	O11-C1-C2-C3
46	J	203	3PE	O31-C31-C32-C33
46	4	503	3PE	O21-C21-C22-C23
48	4	502	CDL	C12-C11-CA5-OA6
48	g	201	CDL	C32-C31-CA7-OA8
46	J	201	3PE	C32-C31-O31-C3
48	J	204	CDL	C76-C77-C78-C79
50	5	902	PLC	O2-C'-C1'-C2'
49	O	201	ZMP	N2-C16-C17-C18
46	J	201	3PE	O22-C21-C22-C23
46	I	303	3PE	O22-C21-C22-C23
48	J	204	CDL	C74-C75-C76-C77
46	J	201	3PE	O11-C1-C2-O21
46	4	503	3PE	O11-C1-C2-O21
46	6	301	3PE	O31-C31-C32-C33
48	4	502	CDL	C32-C33-C34-C35
46	J	203	3PE	O32-C31-C32-C33
48	4	502	CDL	C12-C11-CA5-OA7
50	W	402	PLC	C2B-C1B-CB-OB
48	g	201	CDL	C78-C79-C80-C81
52	2	502	CPL	C15-C16-C17-C18
46	4	503	3PE	C3B-C3C-C3D-C3E
46	4	503	3PE	O32-C31-C32-C33
46	J	203	3PE	C25-C26-C27-C28
46	5	901	3PE	O22-C21-C22-C23
50	5	902	PLC	O'-C'-C1'-C2'
52	2	502	CPL	O3-C11-C12-C13
48	g	201	CDL	C32-C31-CA7-OA9
52	2	502	CPL	C11-C12-C13-C14

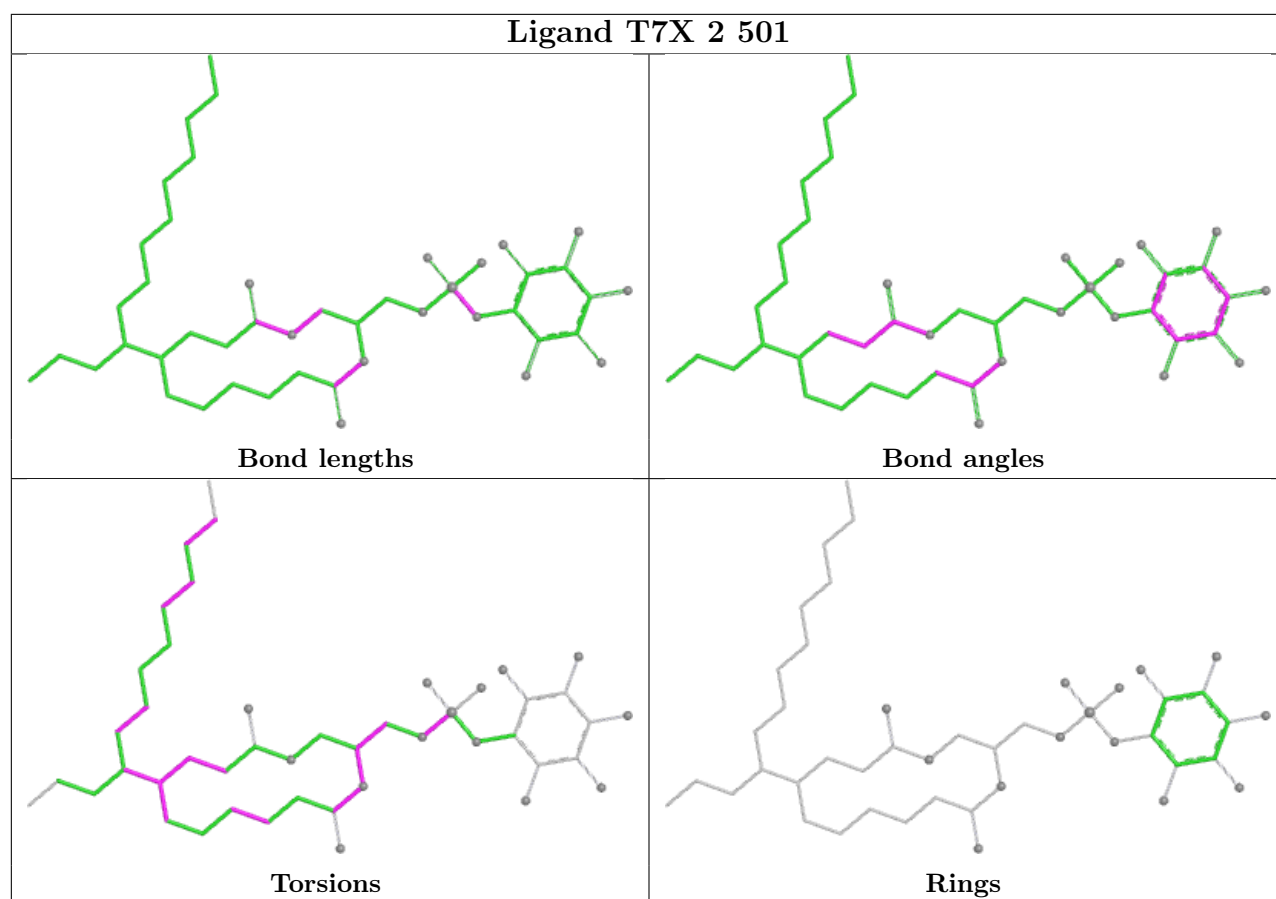
There are no ring outliers.

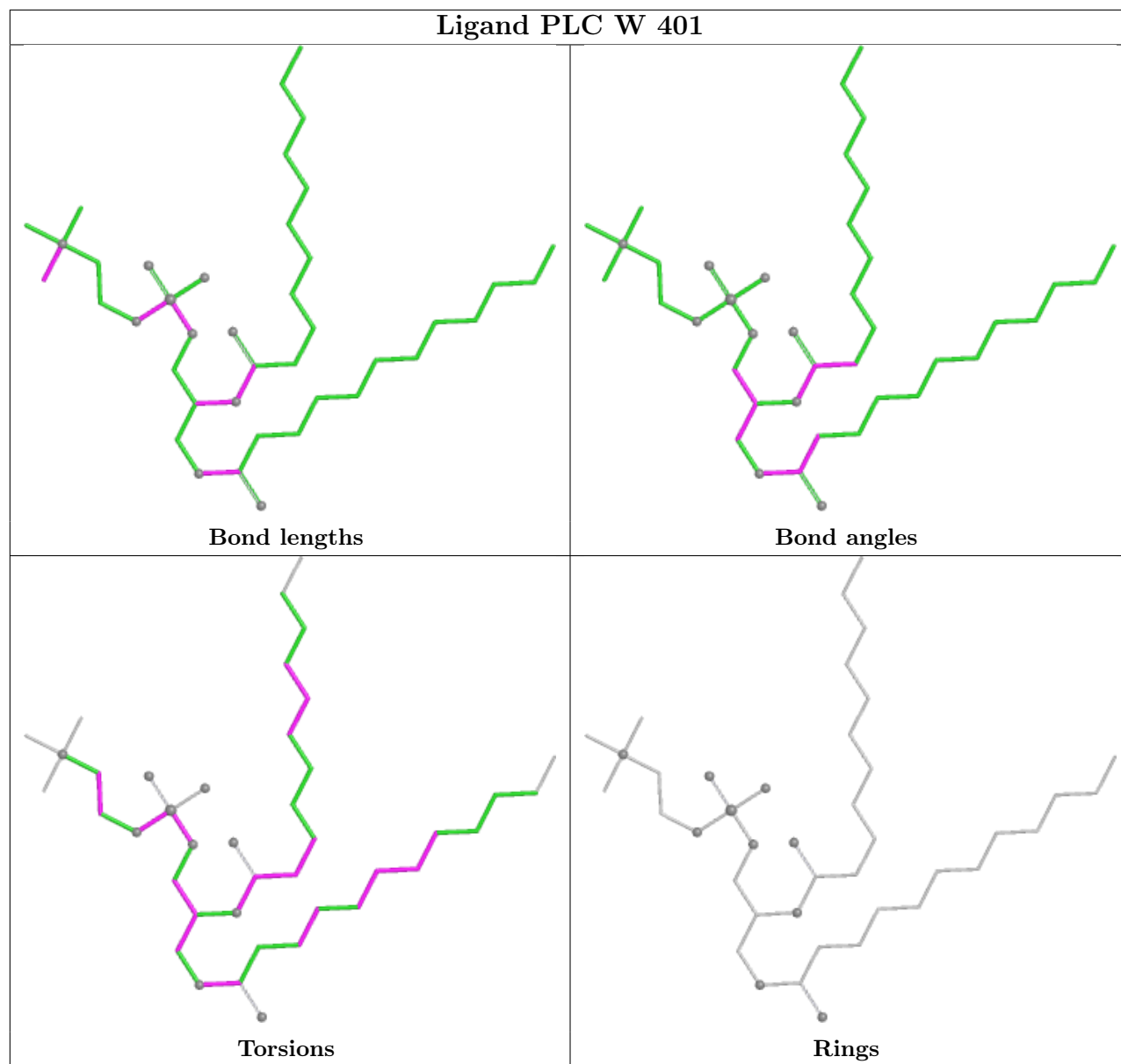
23 monomers are involved in 89 short contacts:

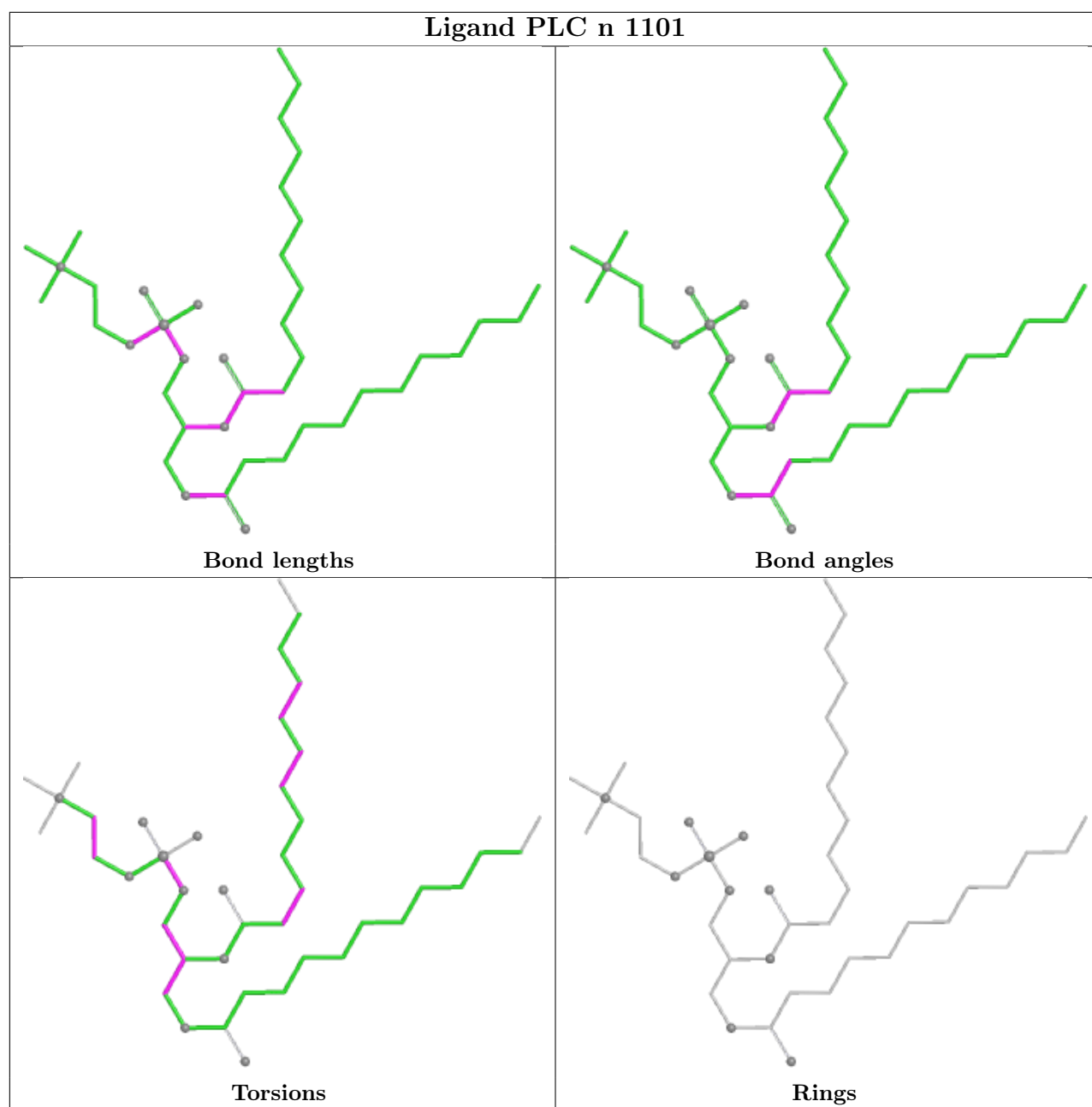
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	J	203	3PE	4	0
48	X	201	CDL	4	0
50	W	401	PLC	2	0
50	n	1101	PLC	1	0
48	J	204	CDL	22	0
46	g	202	3PE	2	0
48	g	201	CDL	7	0
45	E	401	NDP	1	0
46	6	301	3PE	5	0
46	4	505	3PE	4	0
47	j	101	LMN	2	0
46	5	901	3PE	7	0
51	4	504	T7X	1	0
48	4	502	CDL	6	0
49	O	201	ZMP	1	0
42	K	301	SF4	1	0
52	2	502	CPL	4	0
50	5	902	PLC	1	0
44	B	502	FMN	2	0
47	J	202	LMN	5	0
46	4	503	3PE	2	0
46	4	501	3PE	7	0
50	W	402	PLC	1	0

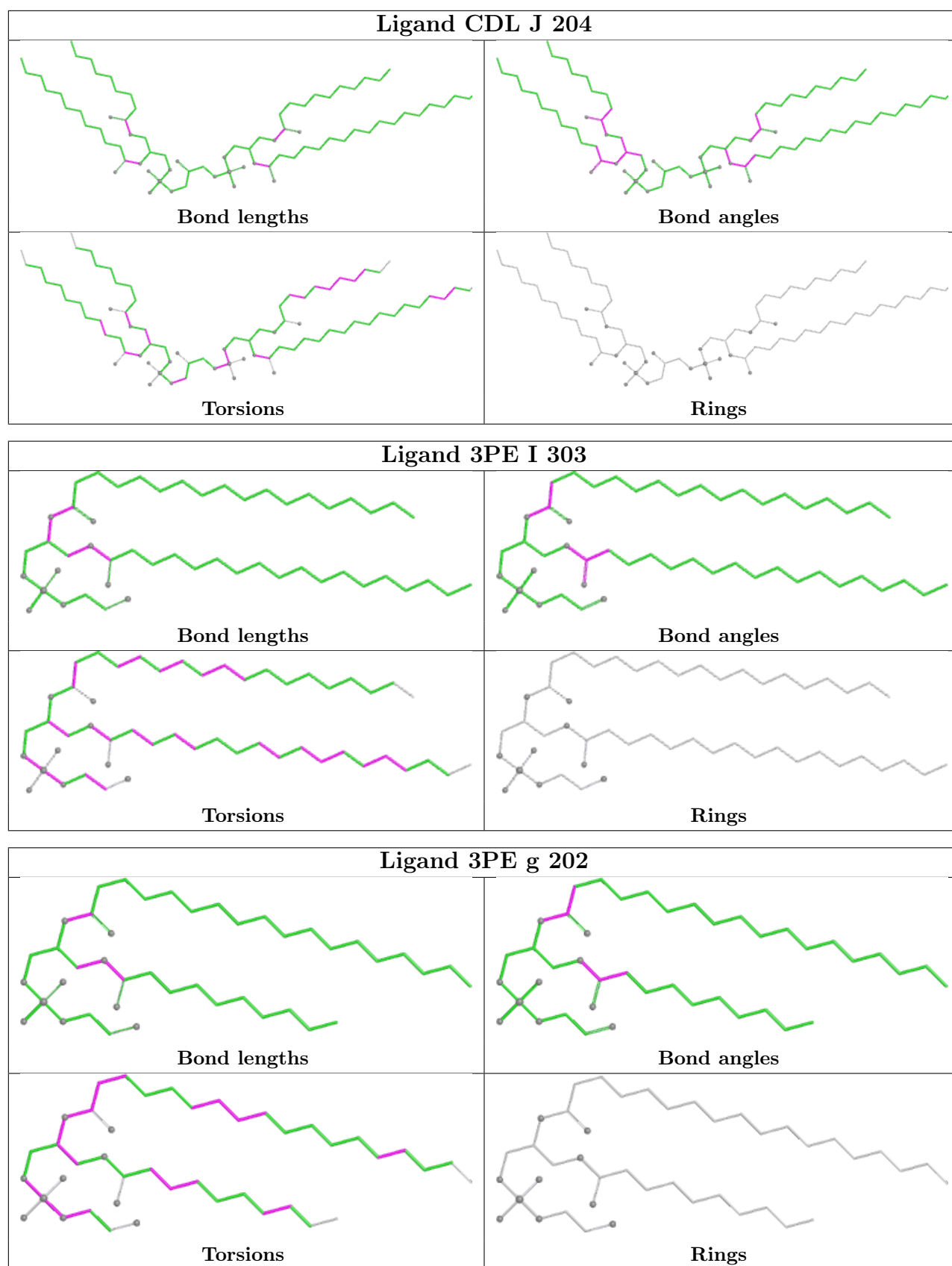
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

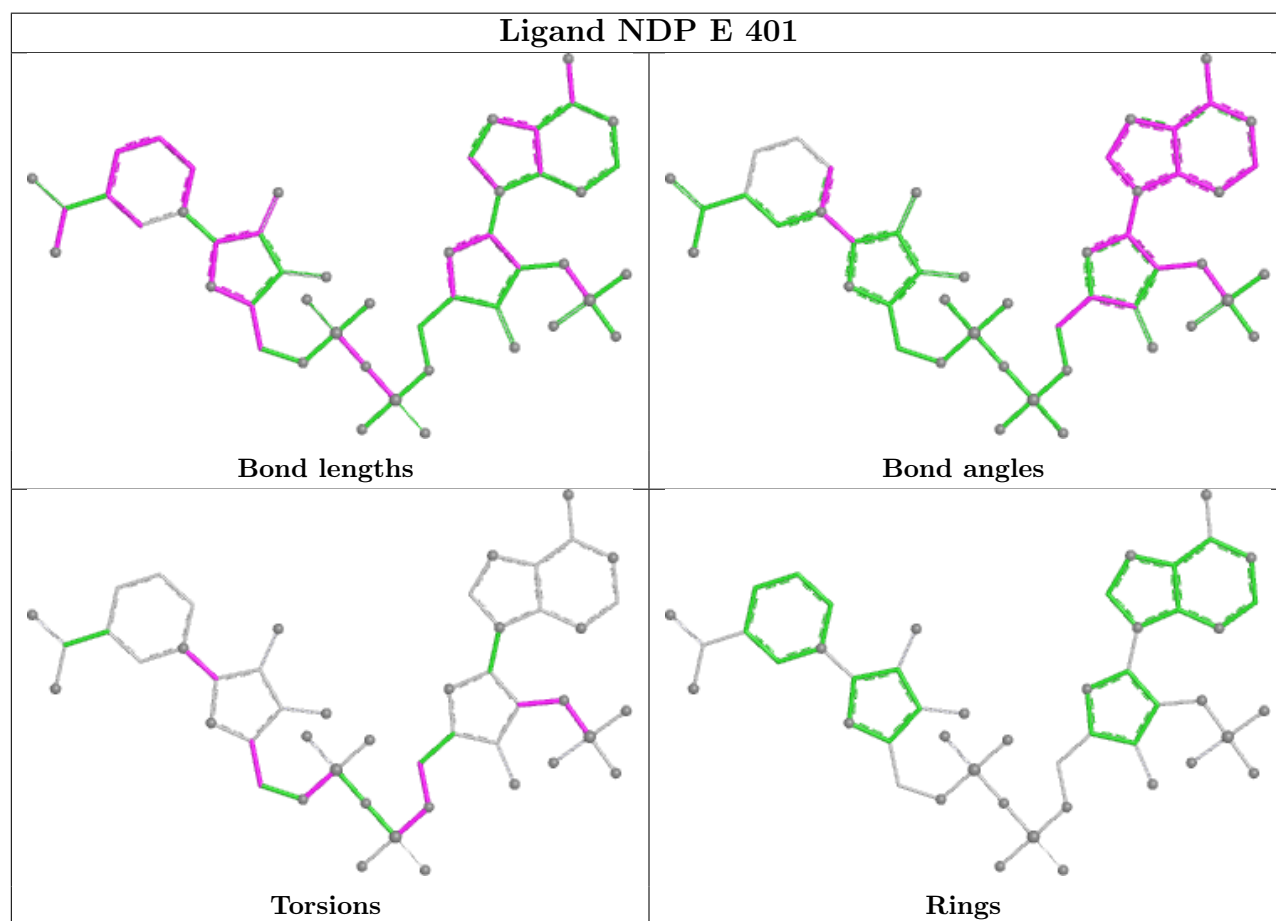
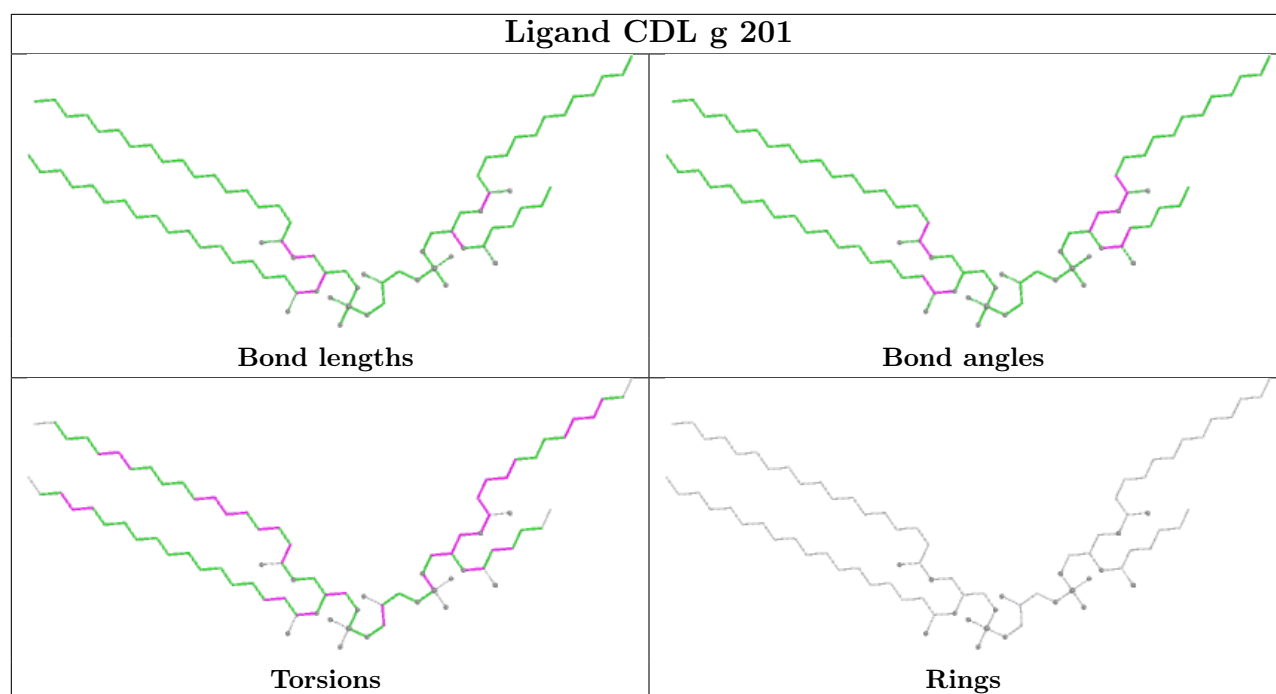


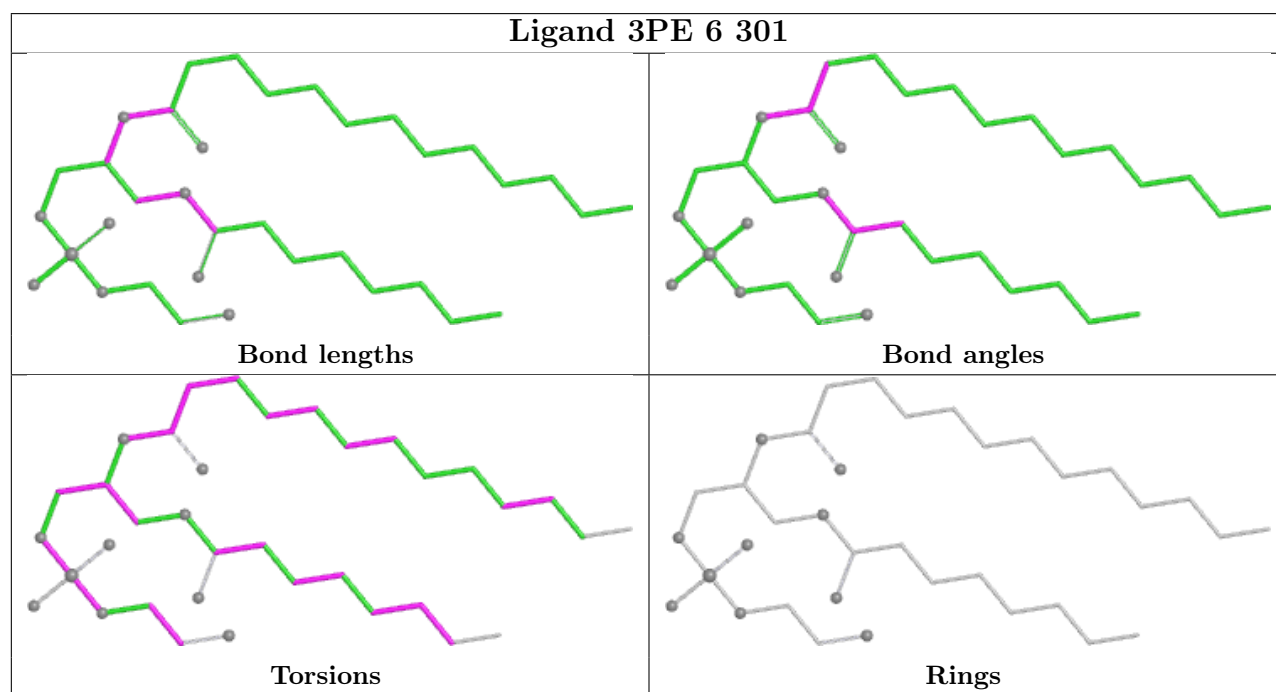
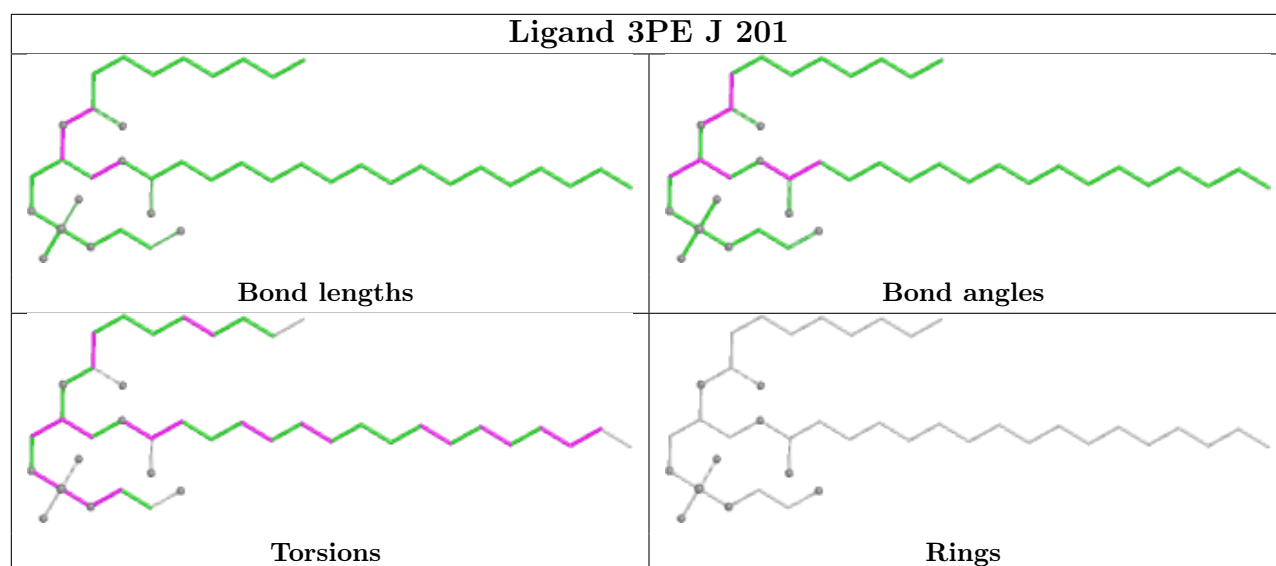


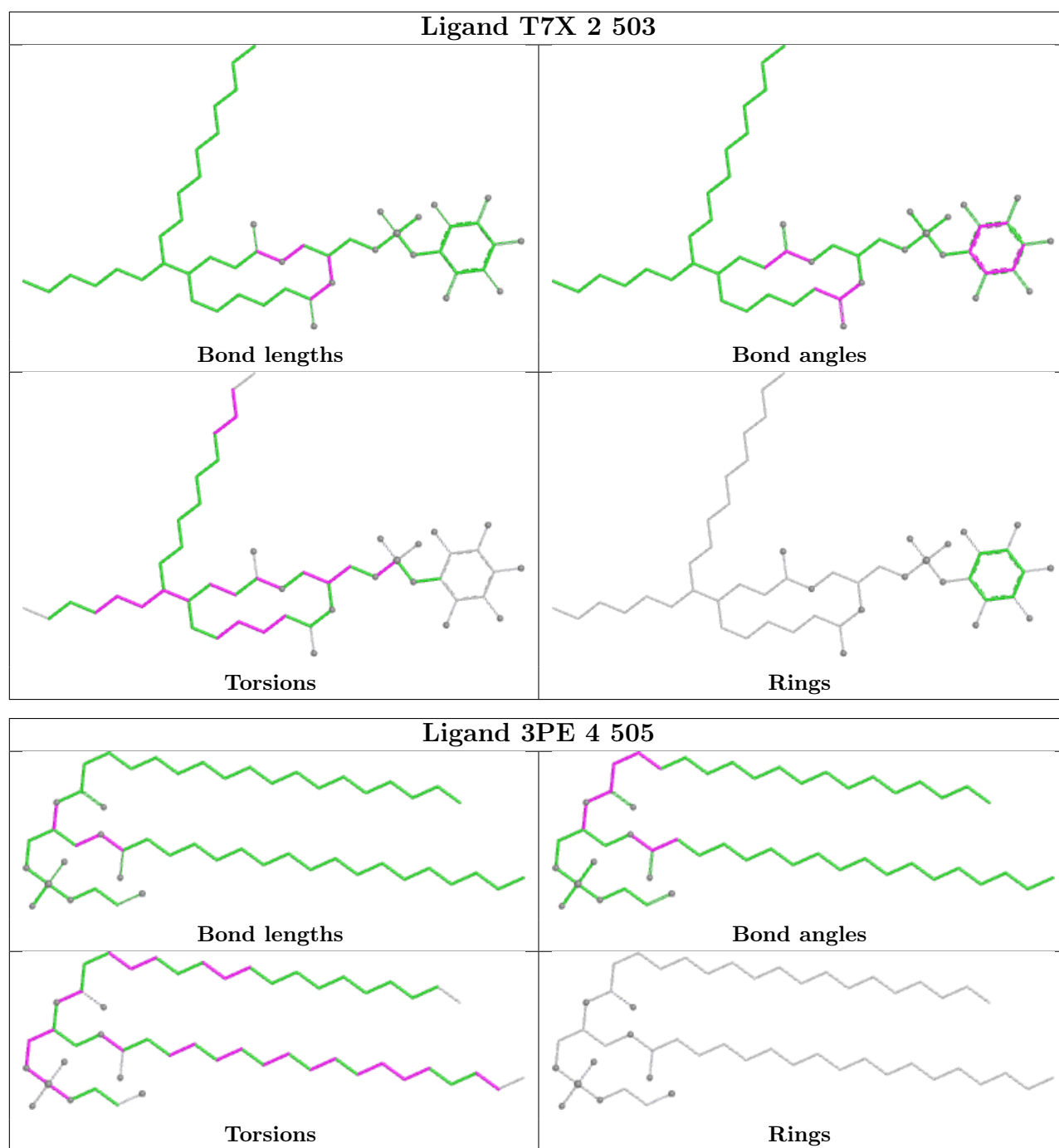


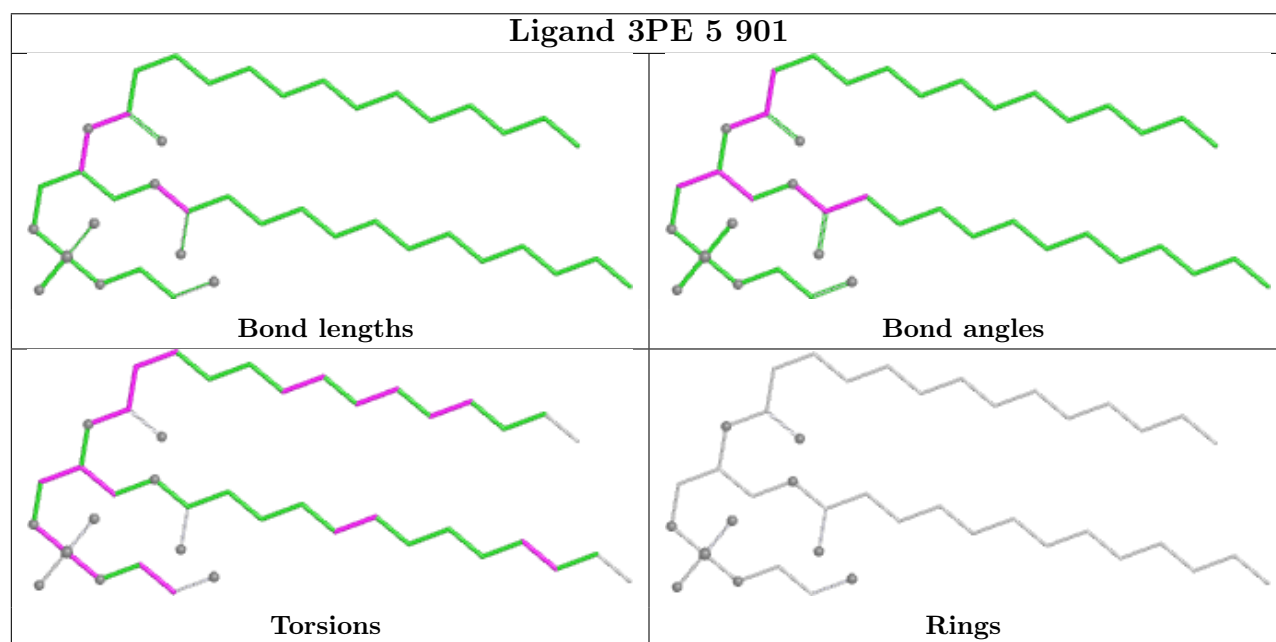
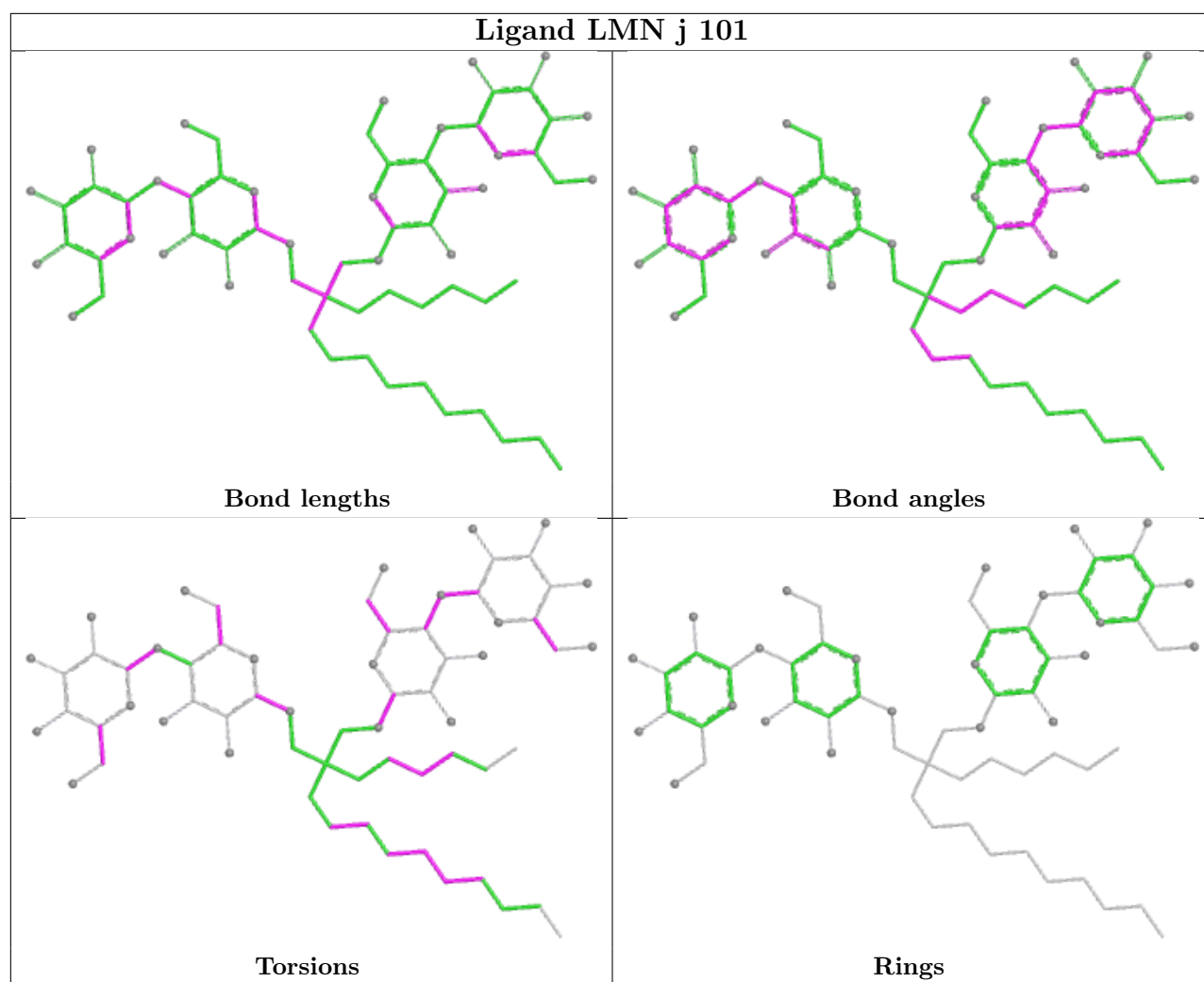


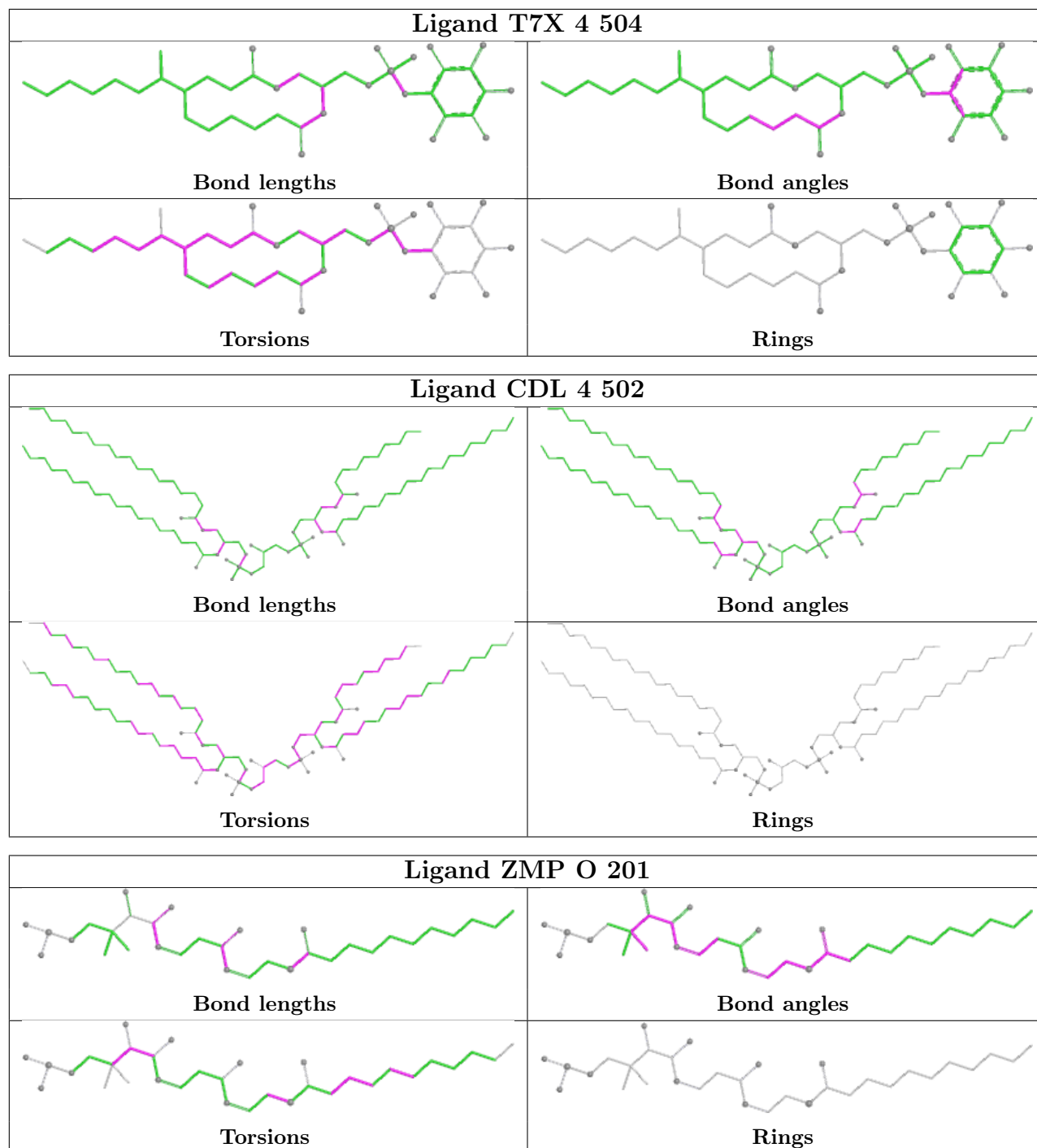


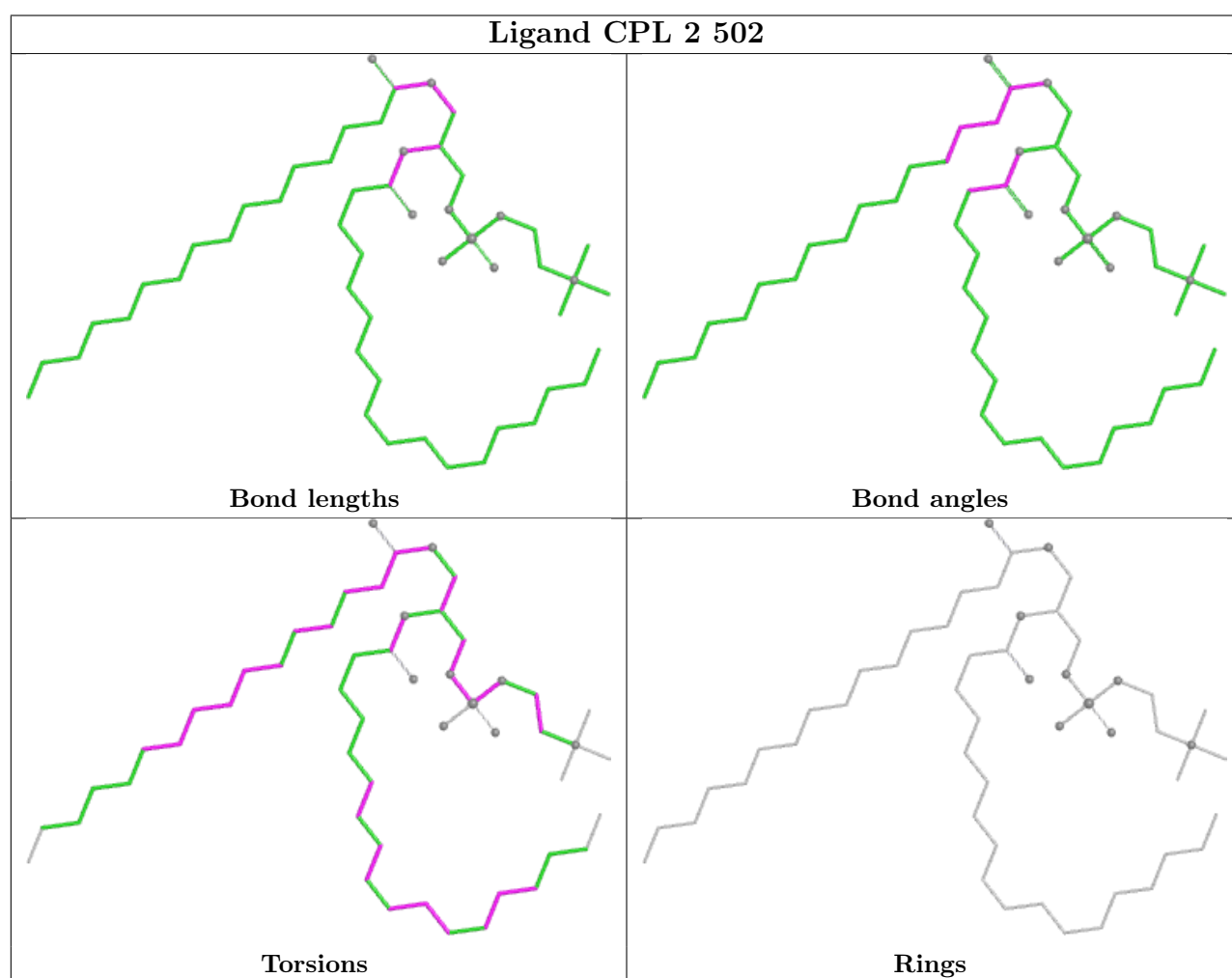
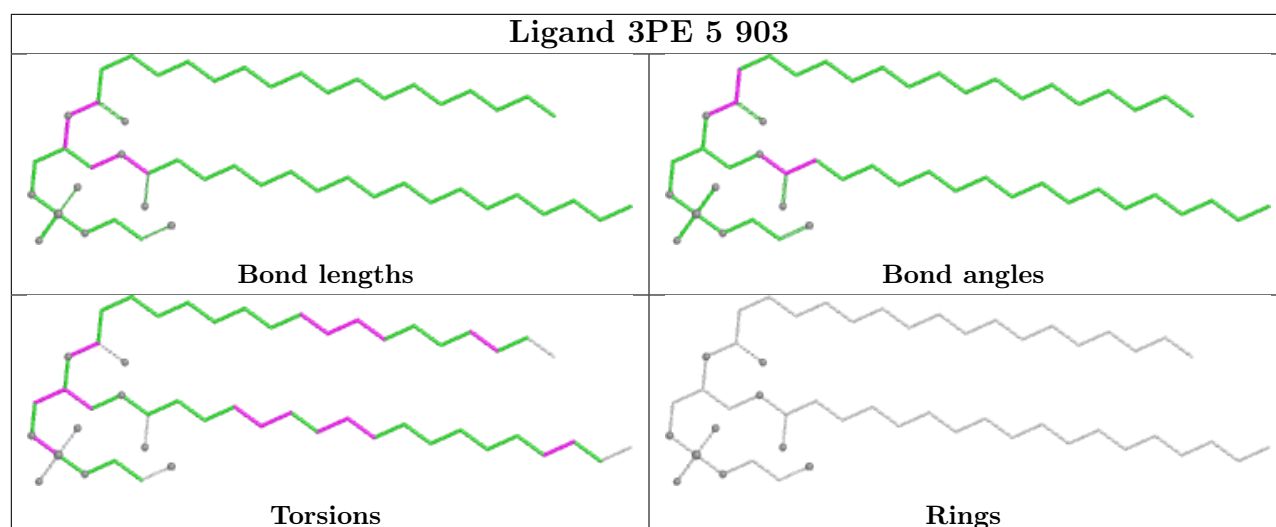


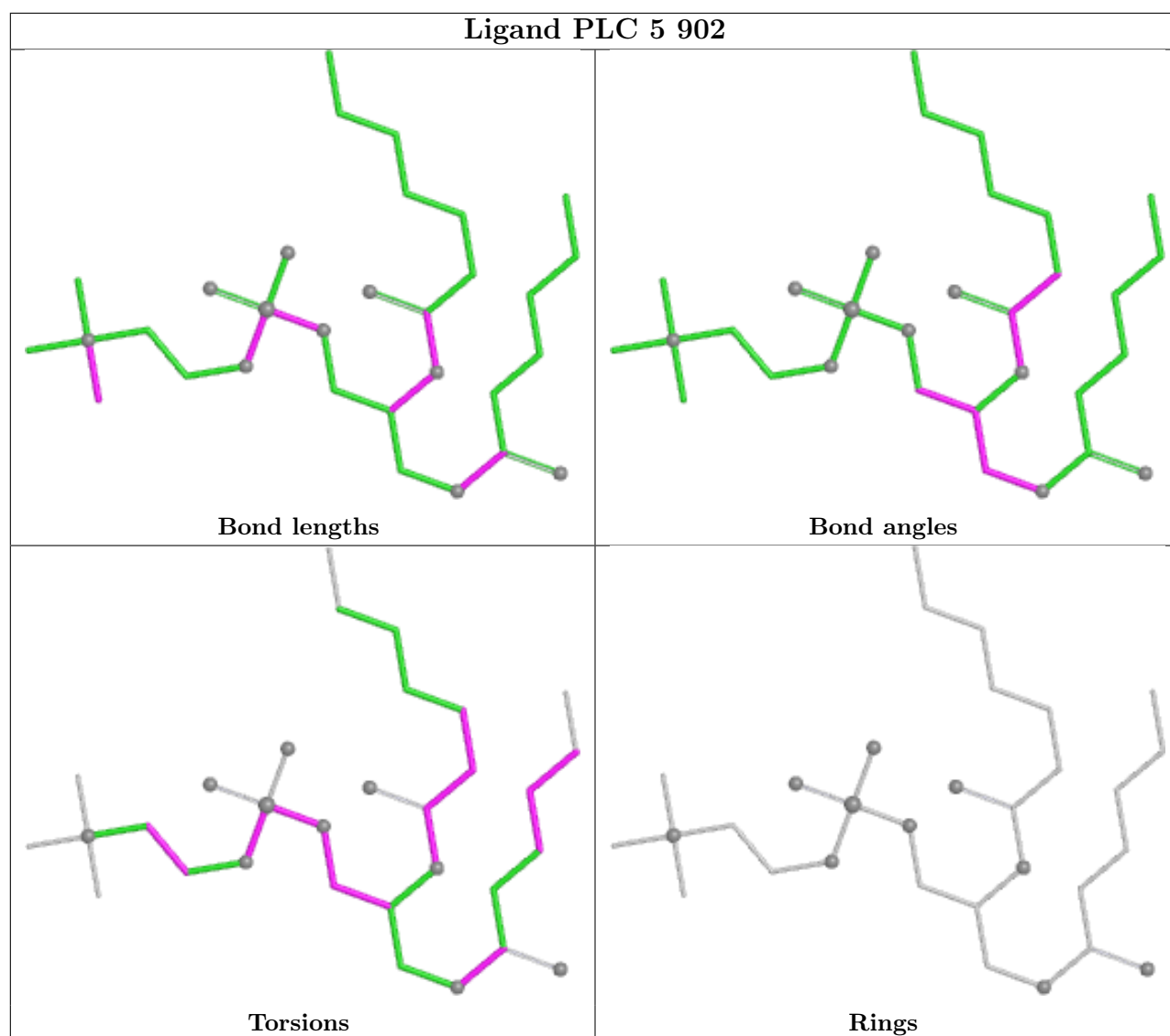


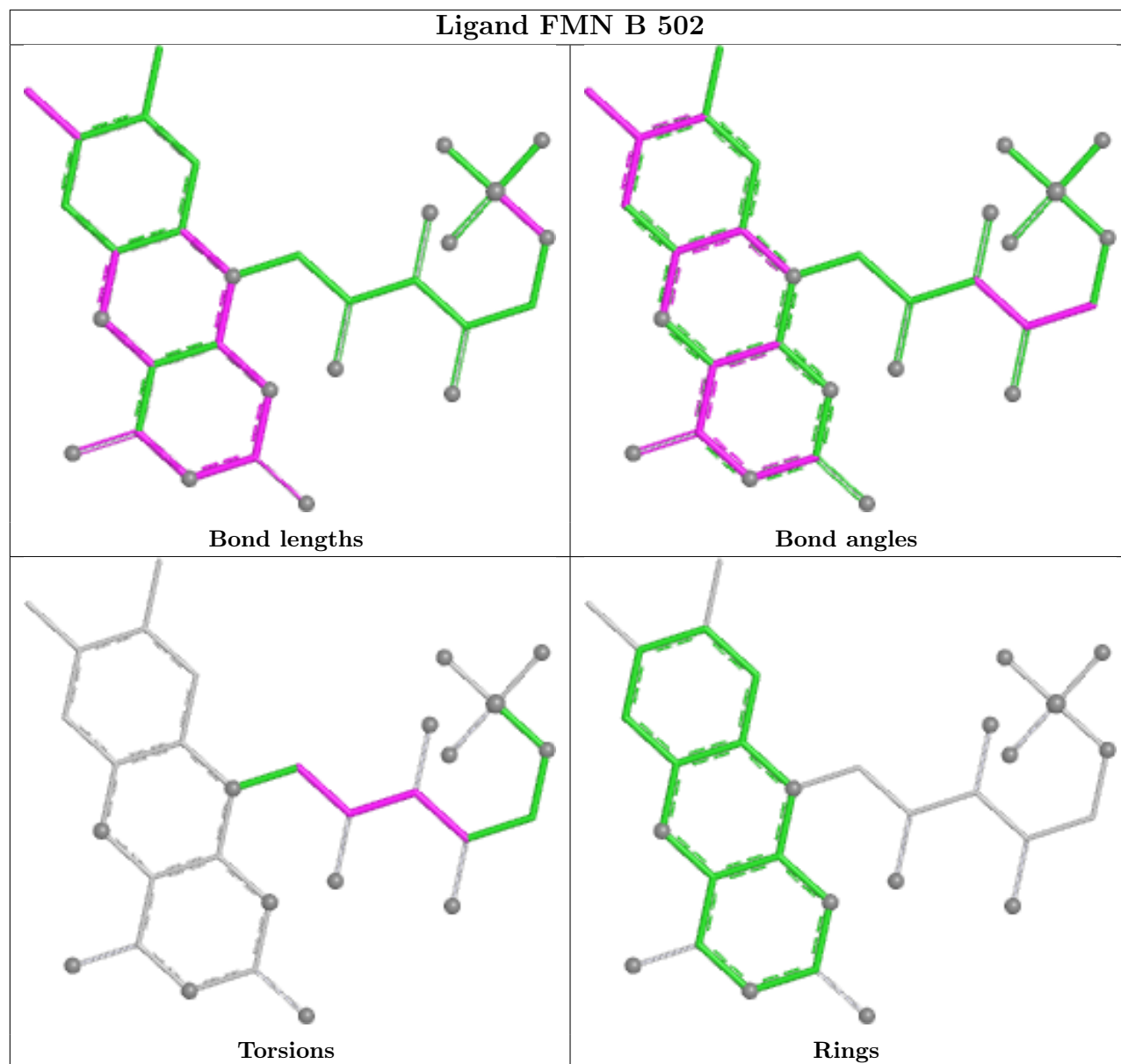


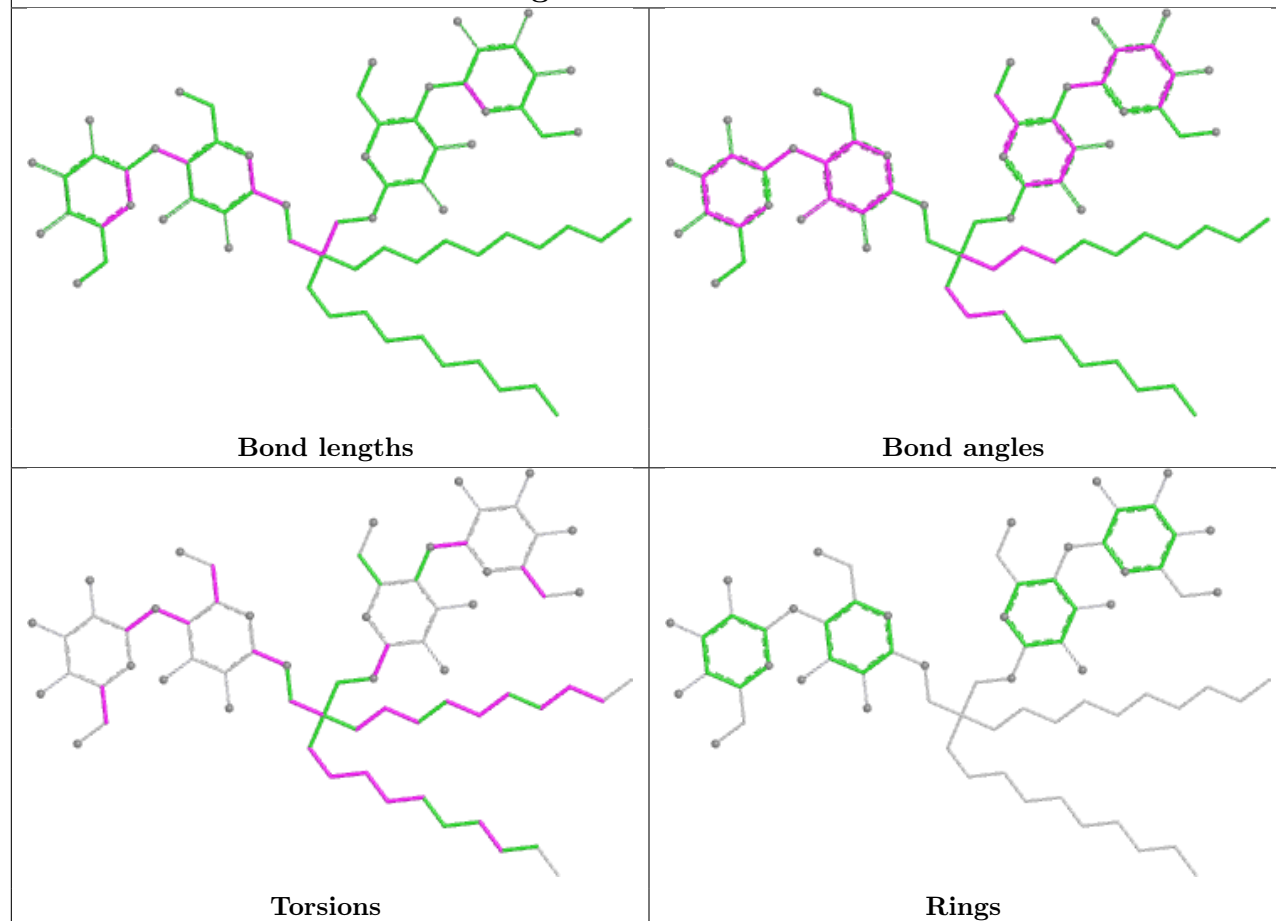
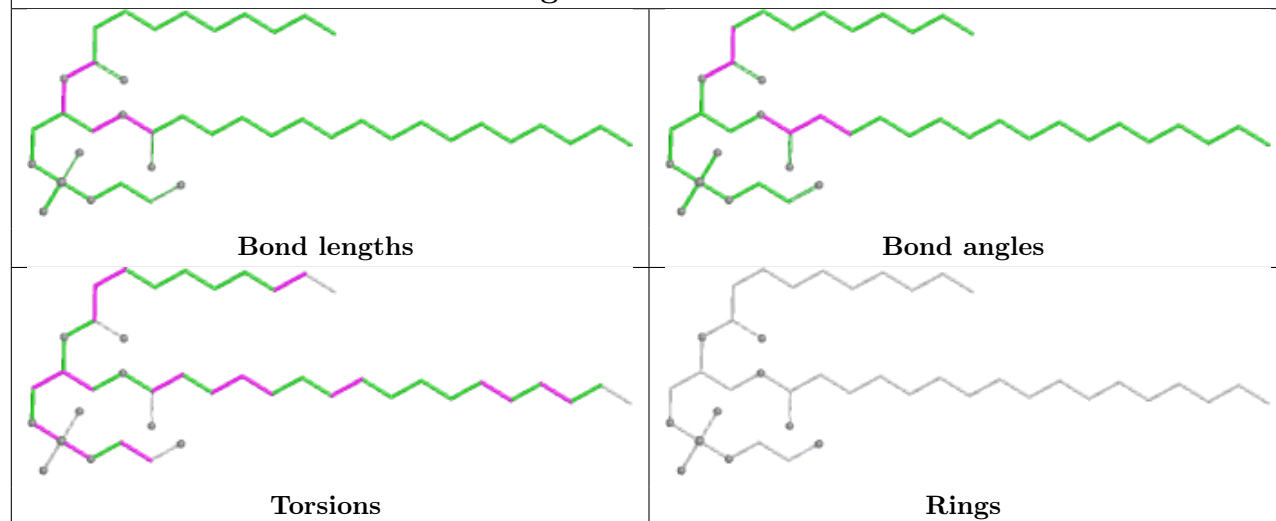


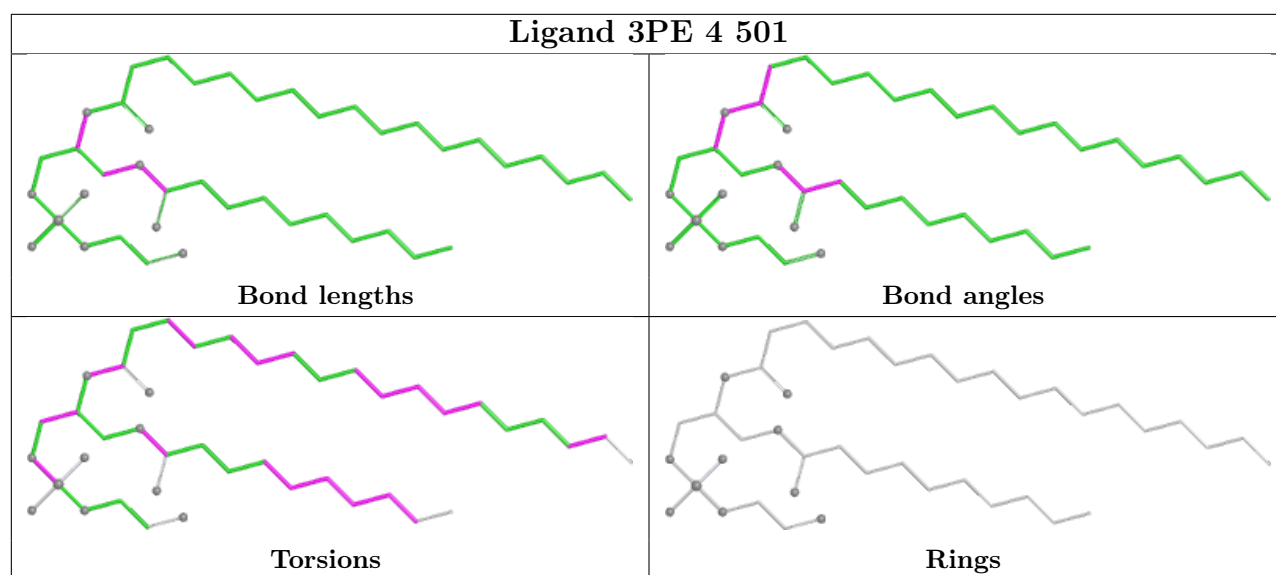


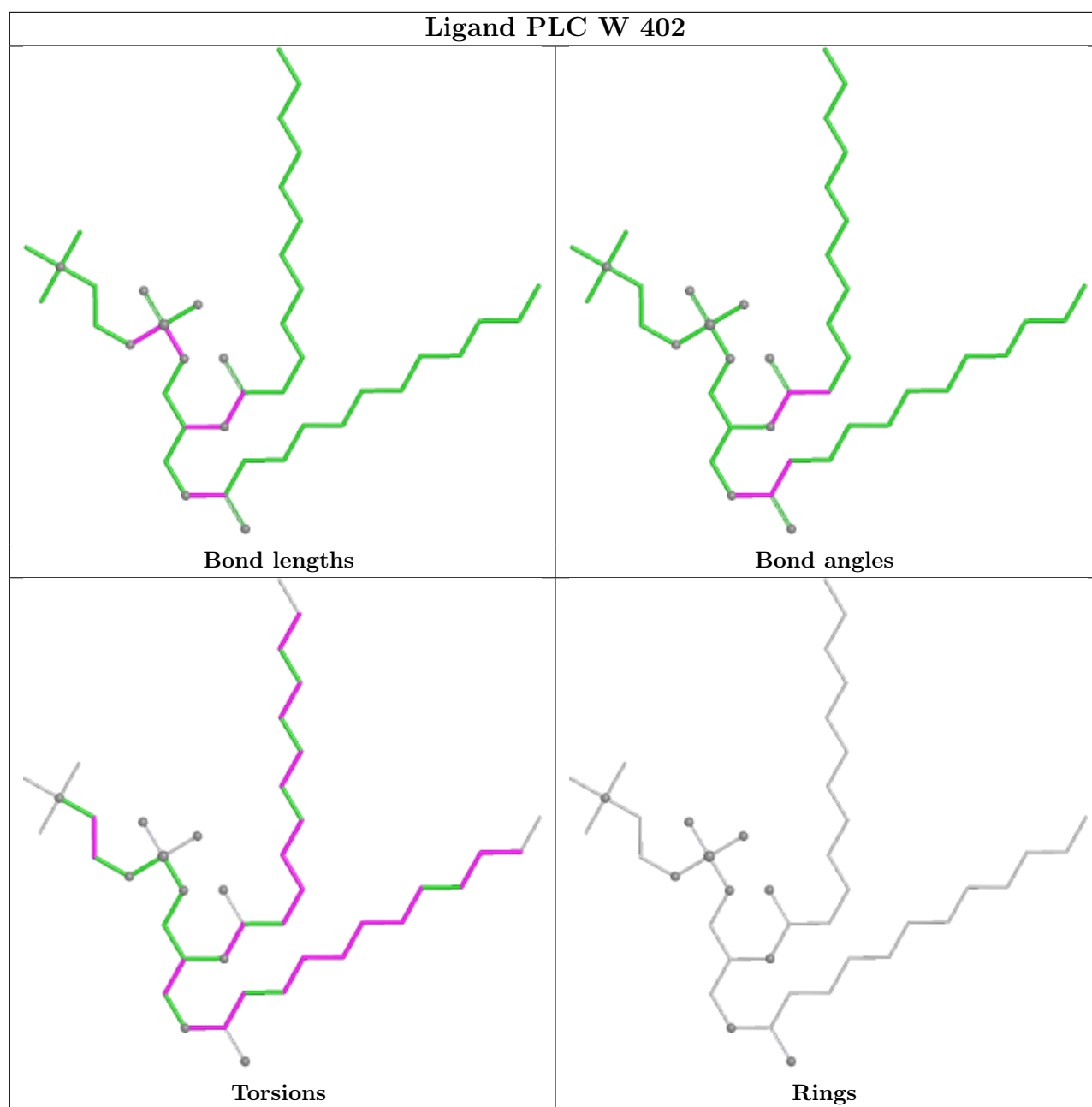






Ligand LMN J 202**Ligand 3PE 4 503**





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

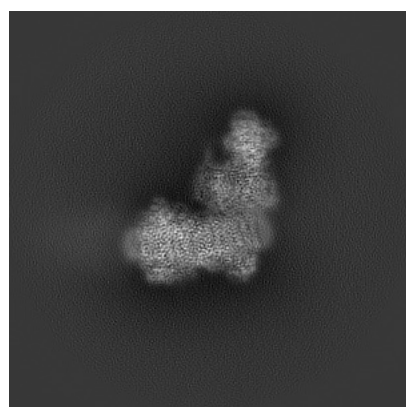
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4872. These allow visual inspection of the internal detail of the map and identification of artifacts.

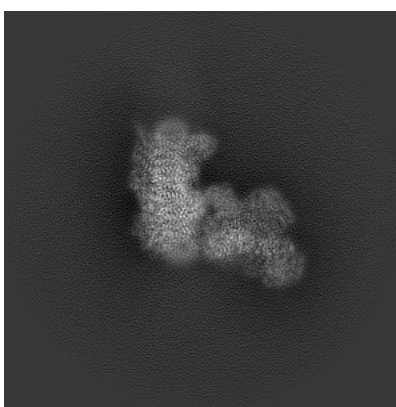
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

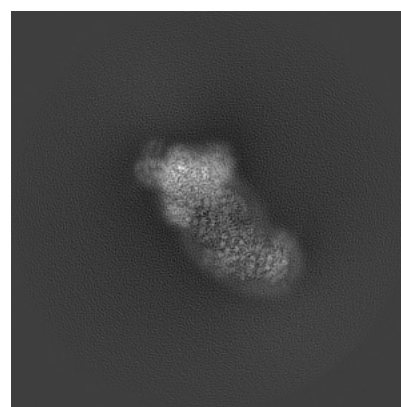
6.1.1 Primary map



X



Y

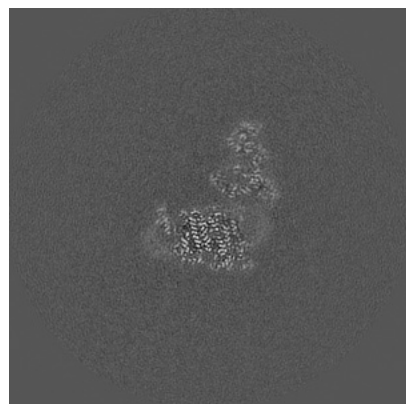


Z

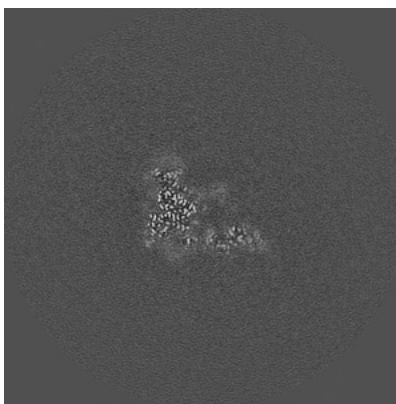
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

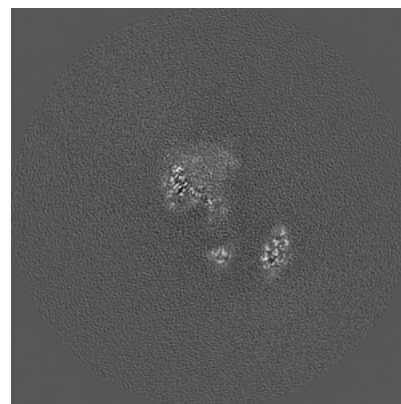
6.2.1 Primary map



X Index: 228



Y Index: 228

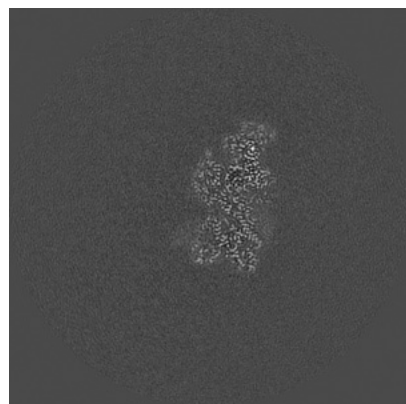


Z Index: 228

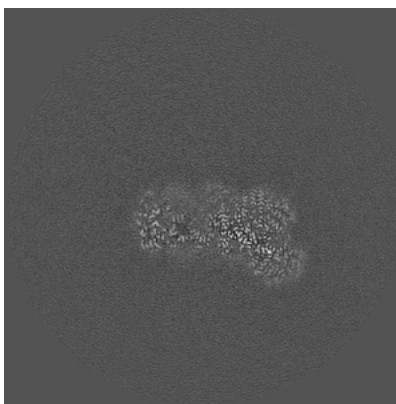
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

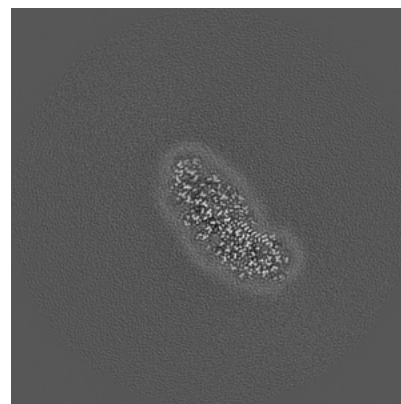
6.3.1 Primary map



X Index: 193



Y Index: 272

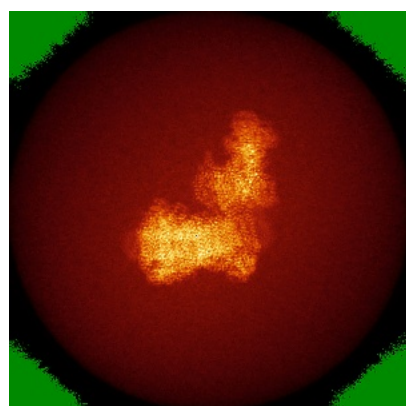


Z Index: 196

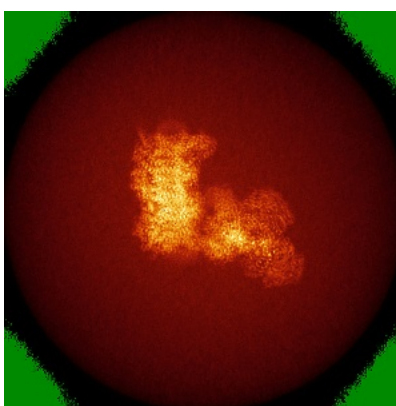
The images above show the largest variance slices of the map in three orthogonal directions.

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

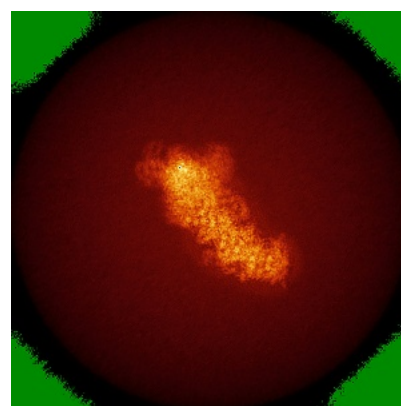
6.4.1 Primary map



X



Y

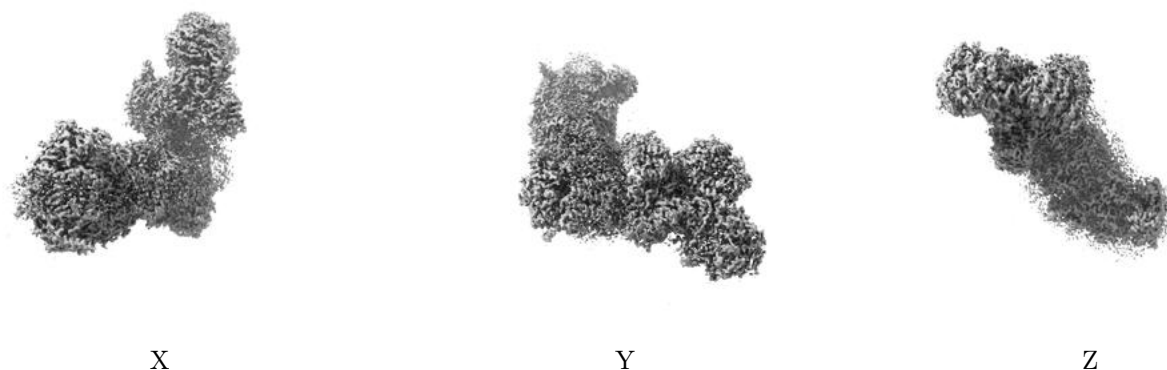


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

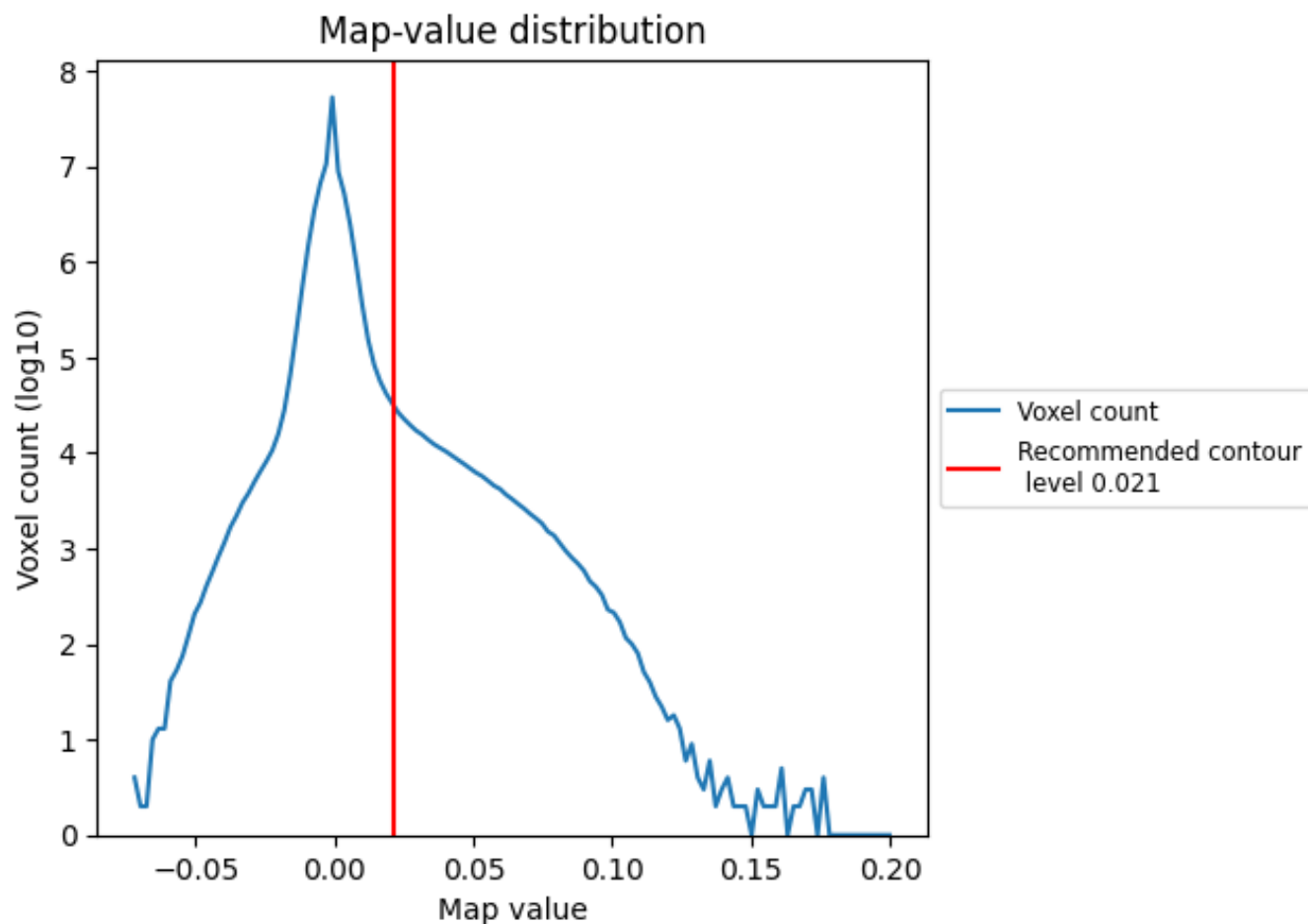
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

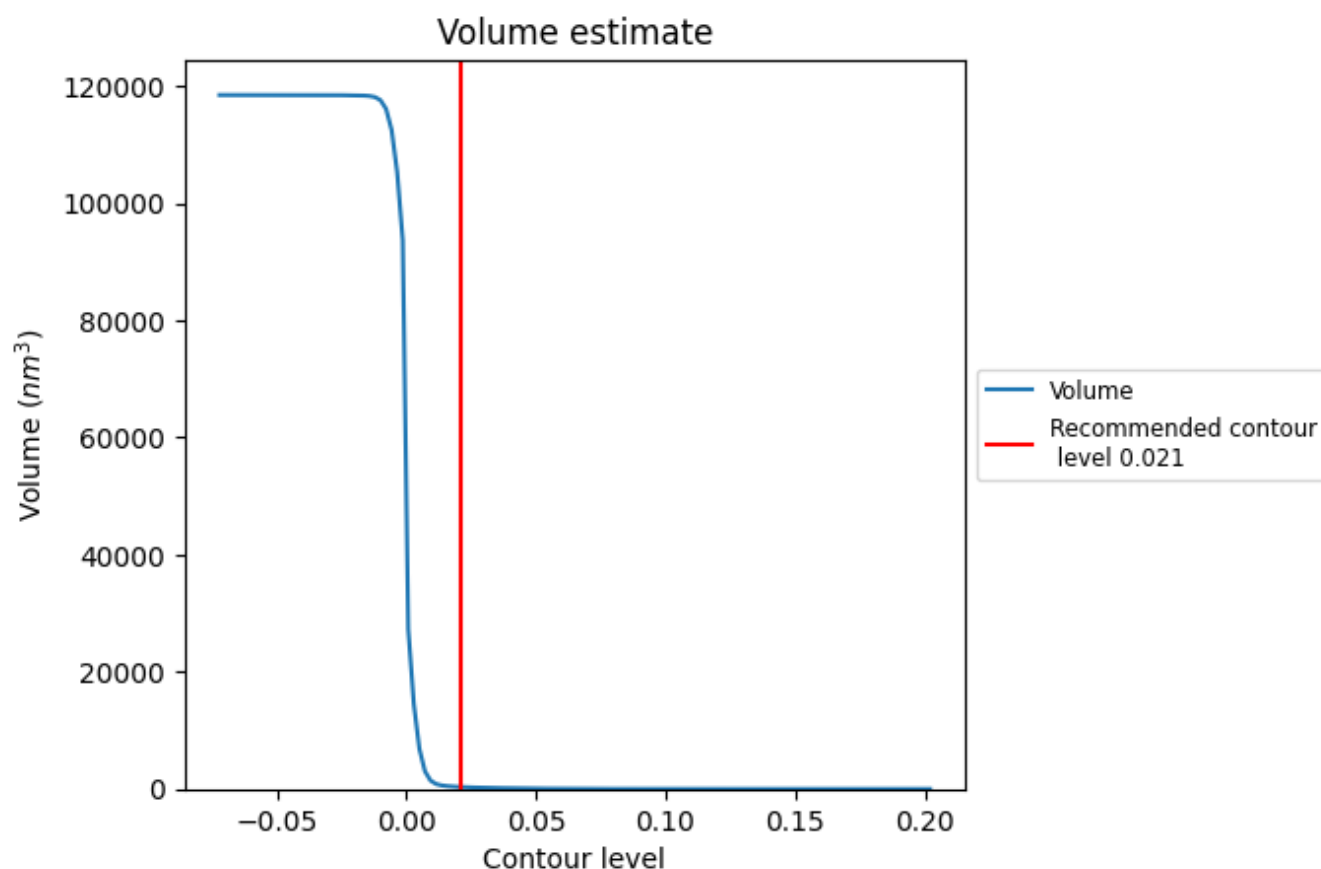
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

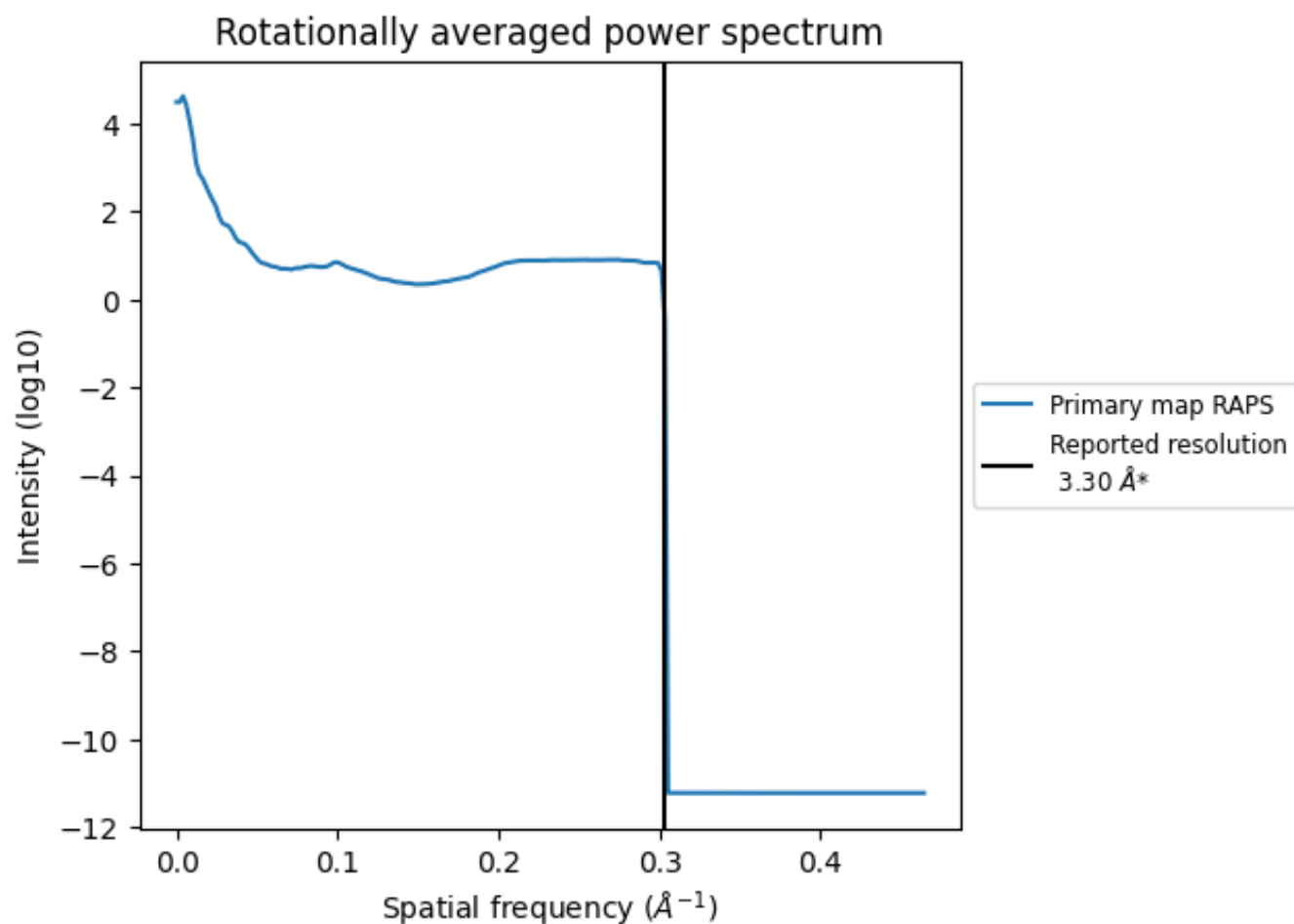
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 333 nm^3 ; this corresponds to an approximate mass of 300 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

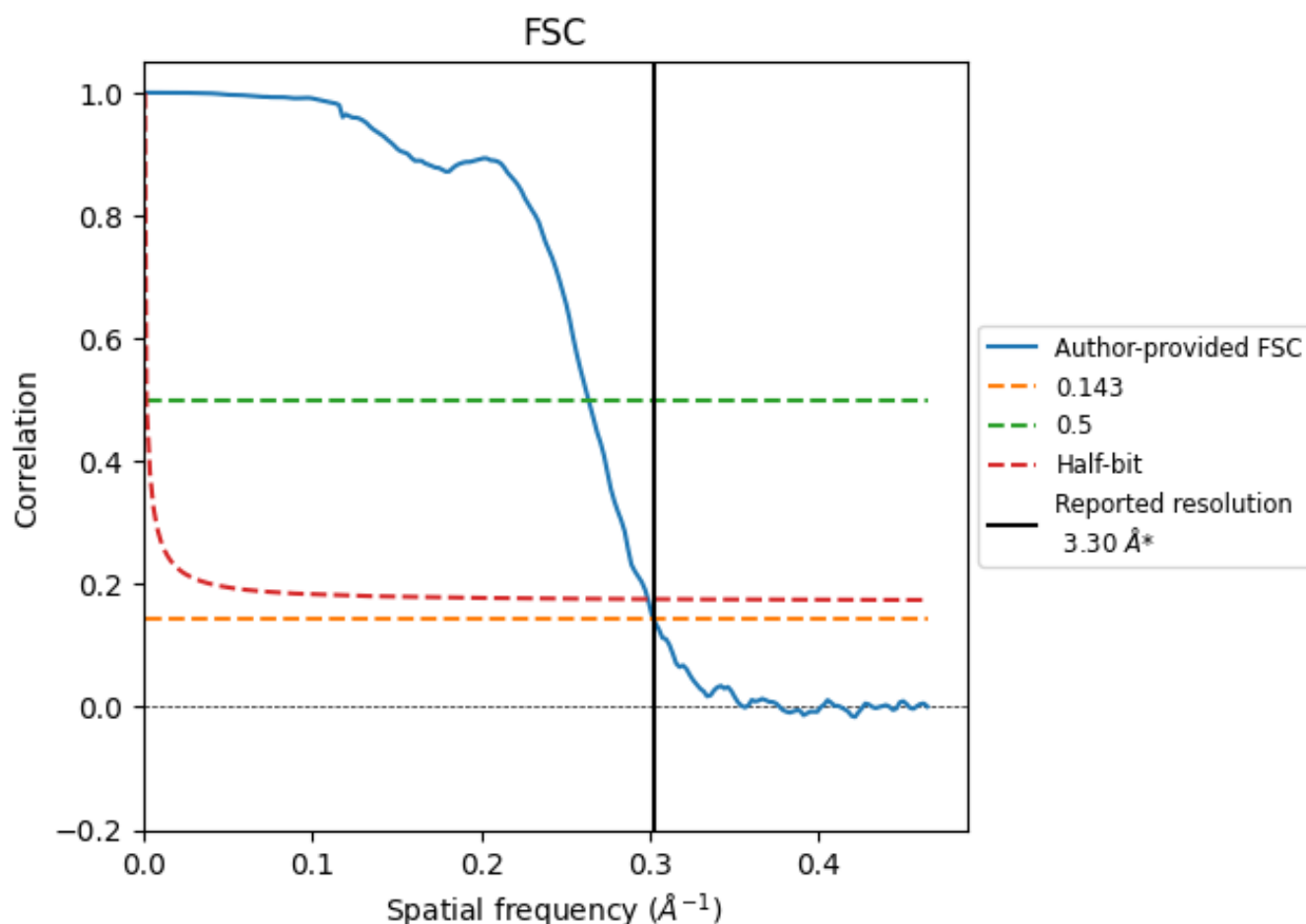


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

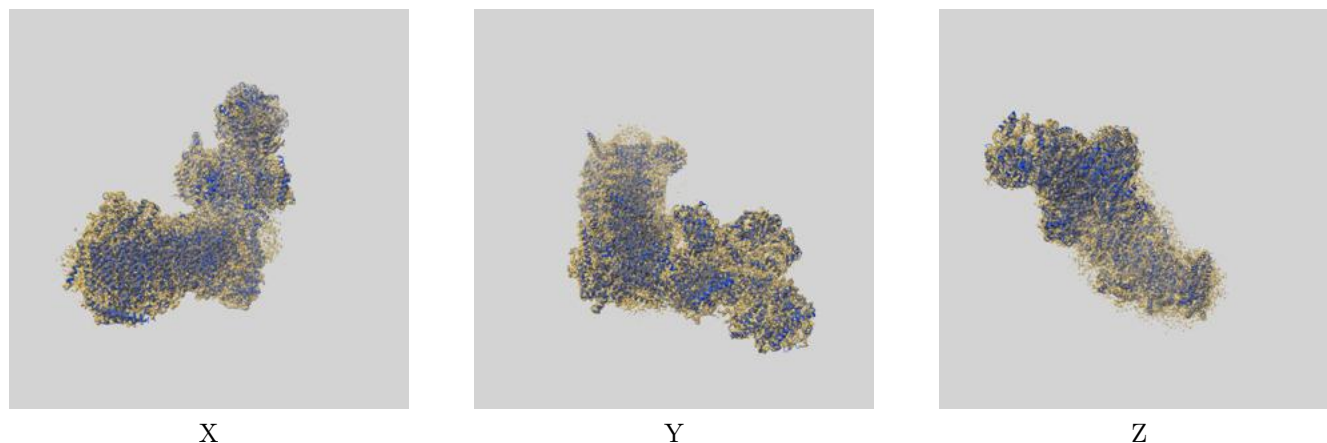
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.31	3.79	3.35
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

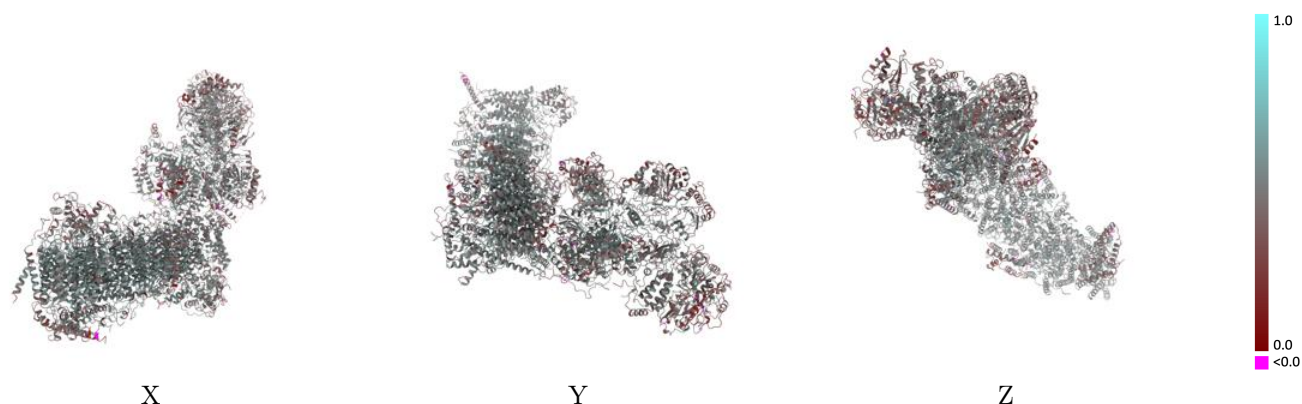
This section contains information regarding the fit between EMDB map EMD-4872 and PDB model 6RFQ. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.021 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](#)

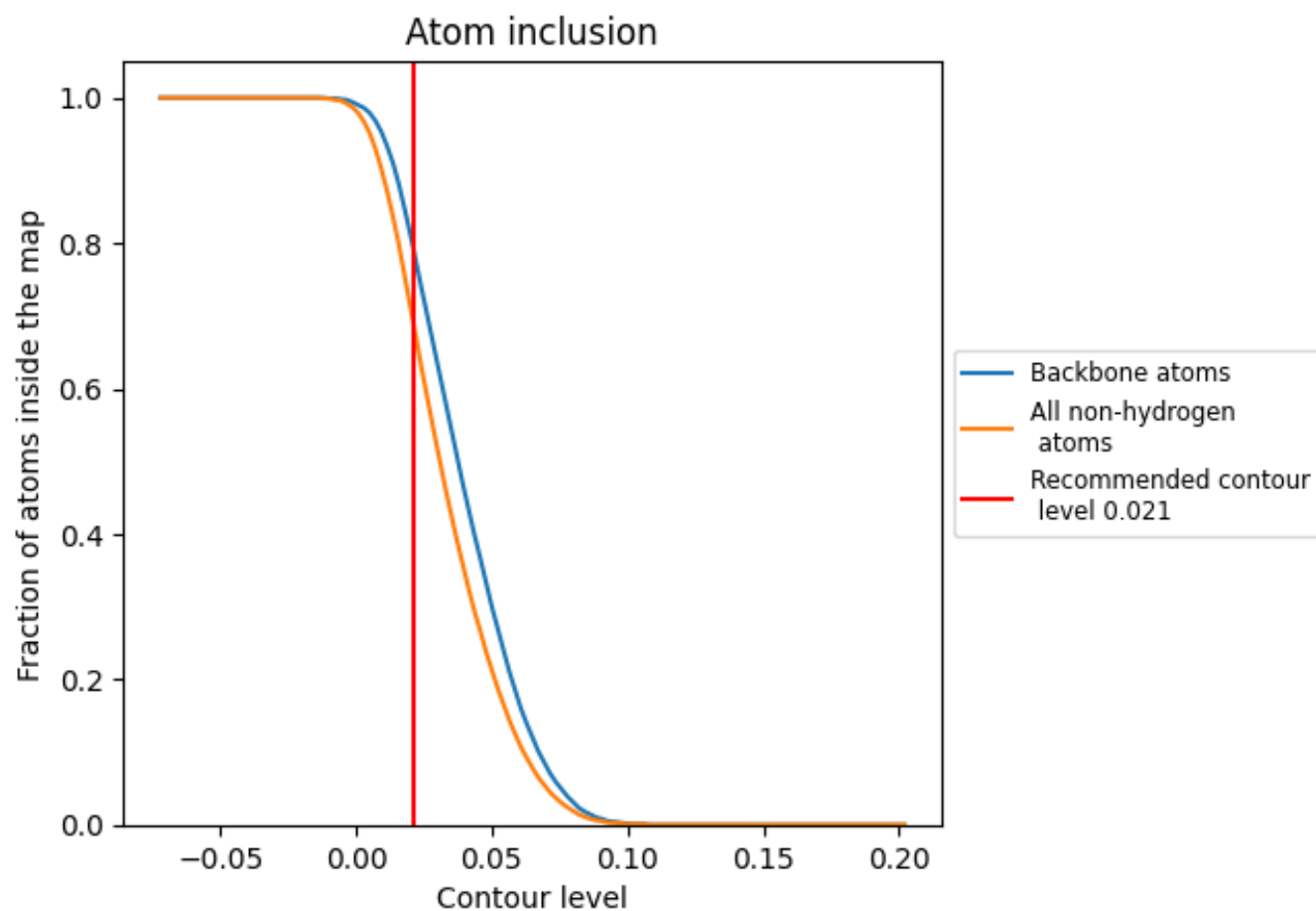


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 69% 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 (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6930	 0.4610
1	 0.6690	 0.4590
2	 0.8160	 0.5260
3	 0.6280	 0.4540
4	 0.7960	 0.5180
5	 0.7880	 0.5070
6	 0.6860	 0.4790
8	 0.6240	 0.3730
9	 0.6450	 0.4420
A	 0.6570	 0.4430
B	 0.5670	 0.4070
C	 0.7390	 0.4810
D	 0.7270	 0.4740
E	 0.5790	 0.4320
F	 0.6790	 0.4350
G	 0.7890	 0.5030
H	 0.5090	 0.3680
I	 0.7490	 0.4830
J	 0.7240	 0.4610
K	 0.6240	 0.4520
L	 0.7550	 0.4760
O	 0.3310	 0.3060
P	 0.6350	 0.4270
Q	 0.5900	 0.3990
R	 0.6970	 0.4260
S	 0.6480	 0.3910
U	 0.6920	 0.4590
W	 0.6840	 0.4630
X	 0.7590	 0.4860
Y	 0.7060	 0.4810
Z	 0.6550	 0.4430
a	 0.7480	 0.4430
b	 0.7930	 0.5000
c	 0.6870	 0.4150
d	 0.7840	 0.4840



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Chain	Atom inclusion	Q-score
e	 0.6990	 0.4640
f	 0.4840	 0.3600
g	 0.7760	 0.5230
i	 0.7540	 0.4620
j	 0.7250	 0.4790
k	 0.3270	 0.3570
n	 0.7130	 0.4680