



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:51 AM UTC

PDB ID : 7W4N / pdb_00007w4n
EMDB ID : EMD-32309
Title : Deactive state CI from Q1-NADH dataset, Subclass 5
Authors : Gu, J.; Yang, M.
Deposited on : 2021-11-28
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

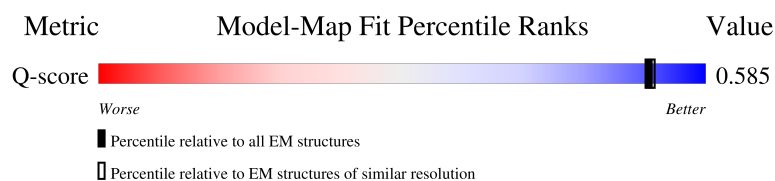
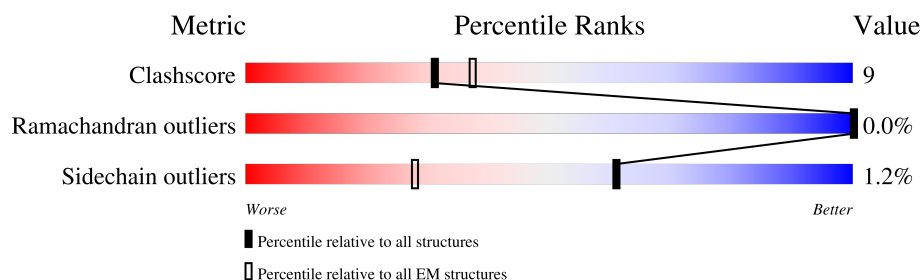
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

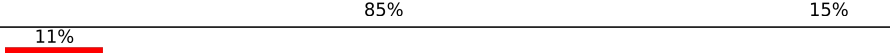
The reported resolution of this entry is 3.00 Å.

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	14081 (2.50 - 3.50)

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	433	
2	B	176	
3	C	156	
4	E	115	

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Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	70	
23	Z	84	
24	a	140	
25	b	126	
26	c	156	
27	d	175	
28	e	107	

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Mol	Chain	Length	Quality of chain
29	f	49	
30	g	122	
31	h	105	
32	i	347	
33	j	115	
34	k	98	
35	l	603	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	124	
44	w	320	

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
45	SF4	A	501	-	-	X	-
51	CDL	l	701	-	-	X	-

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 66477 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3313	2092	590	611	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1248	794	227	213	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	115	Total	C	N	O	S	0	0
			971	619	179	168	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			690	446	102	137	5		
6	X	88	Total	C	N	O	S	0	0
			696	449	103	139	5		

- Molecule 7 is a protein called Complex I subunit B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 8 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	297	Total	C	N	O	S	0	0
			2359	1514	421	416	8		

- Molecule 10 is a protein called Complex I-9kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	125	Total	C	N	O	S	0	0
			1013	641	181	188	3		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5292	3318	923	1012	39		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	144	Total	C	N	O	S	0	0
			1201	767	218	212	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	217	Total	C	N	O	S	0	0
			1671	1065	281	315	10		

- Molecule 15 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1738	1124	298	314	2		

- Molecule 16 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	419	Total	C	N	O	S	0	0
			3377	2162	578	613	24		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			567	364	104	94	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1009	646	171	186	6		

- Molecule 21 is a protein called Complex I-B16.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	142	Total	C	N	O	S	0	0
			1173	755	203	206	9		

- Molecule 22 is a protein called Complex I-AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	70	Total	C	N	O	S	0	0
			597	392	98	106	1		

- Molecule 23 is a protein called Complex I-B12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	84	Total	C	N	O	S	0	0
			674	437	116	120	1		

- Molecule 24 is a protein called Complex I-SGDH.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	140	Total	C	N	O	S	0	0
			1165	762	199	201	3		

- Molecule 25 is a protein called Complex I-B17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	103	Total	C	N	O	S	0	0
			879	573	158	147	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	156	Total	C	N	O	S	0	0
			1315	853	213	241	8		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	175	Total	C	N	O	S	0	0
			1461	916	265	272	8		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	107	Total	C	N	O	S	0	0
			890	568	145	173	4		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	42	Total	C	N	O	0	0
			342	225	58	59		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	99	Total	C	N	O	S	0	0
			800	545	118	132	5		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			4782	3172	740	819	51		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	129	Total	C	N	O	S	0	0
			946	635	138	165	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	128	Total	C	N	O	S	0	0
			1062	691	182	189			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	303	Total	C	N	O	S	0	0
			2394	1607	369	397	21		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

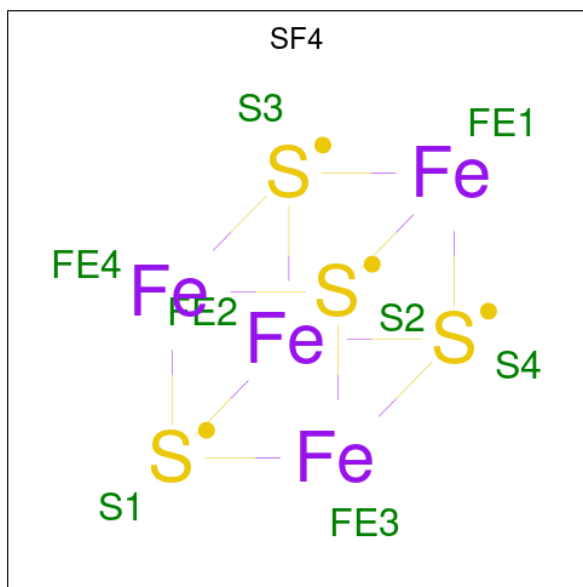
- Molecule 43 is a protein called Complex I-B18.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1028	642	195	182	9		

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

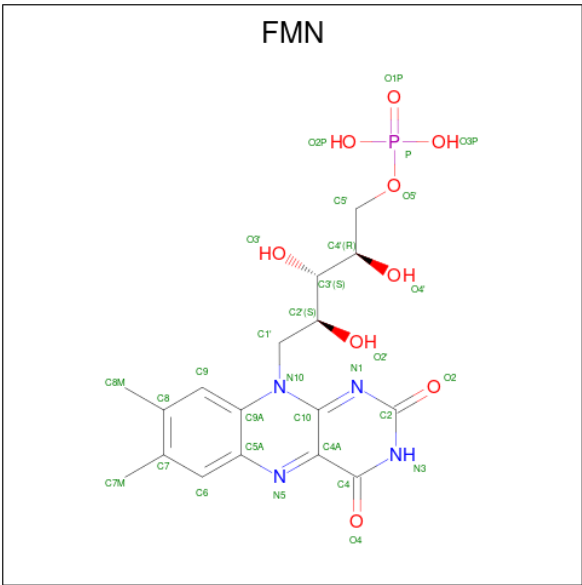
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2570	1636	436	488	10		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



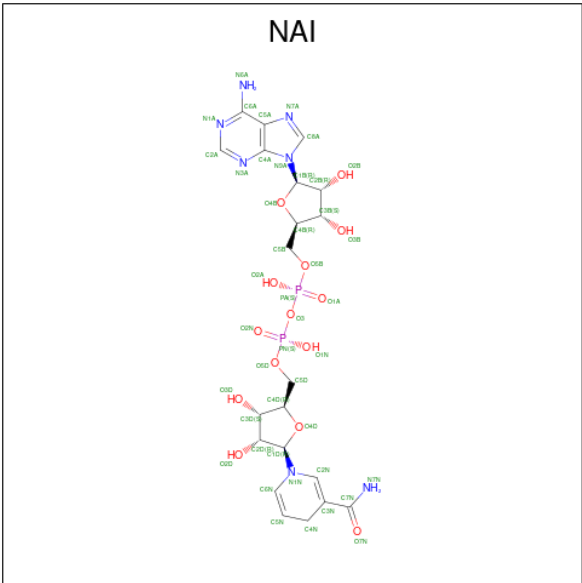
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



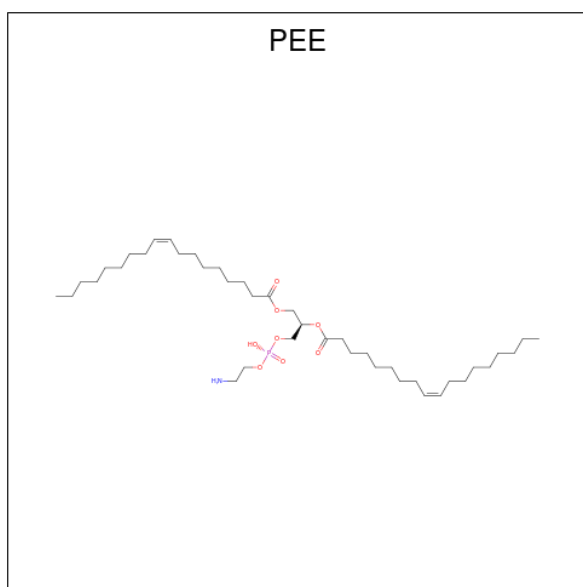
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



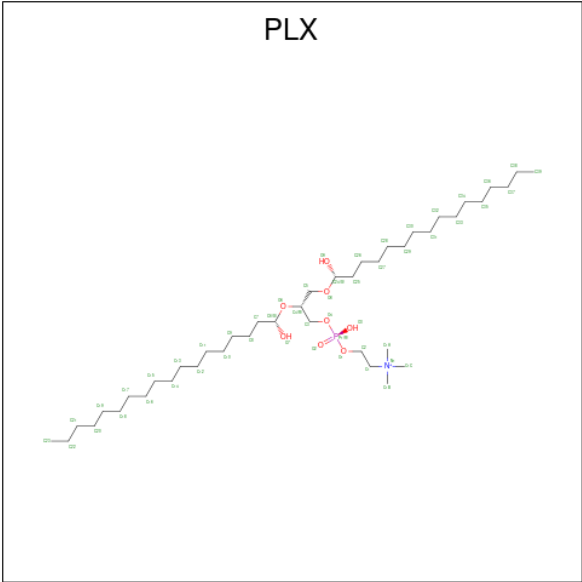
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



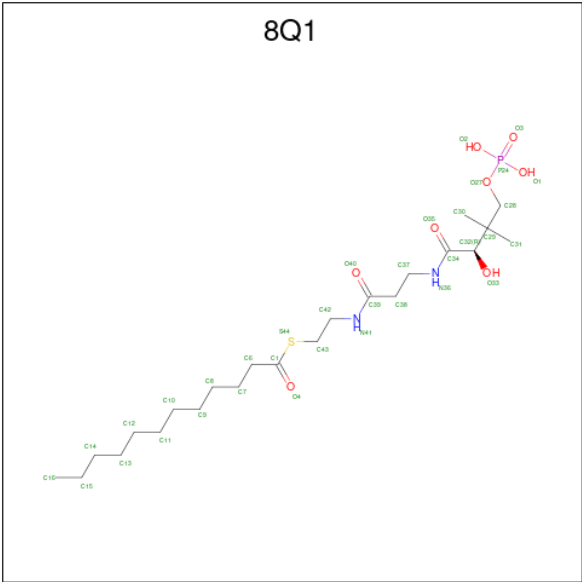
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 49 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



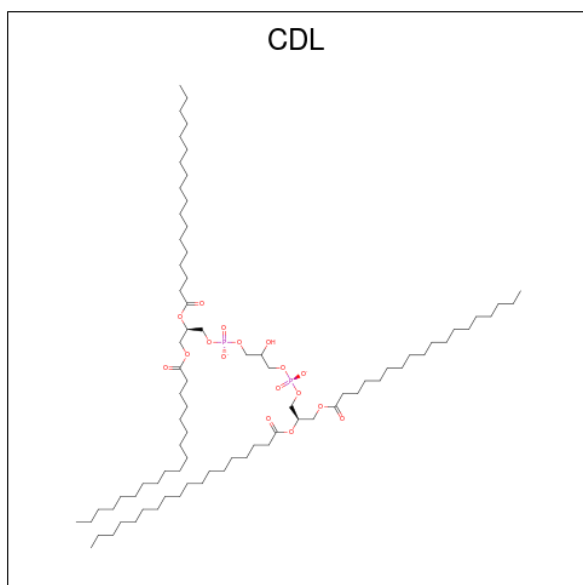
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 50 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-a
lanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as
"Ligand of Interest" by depositor).



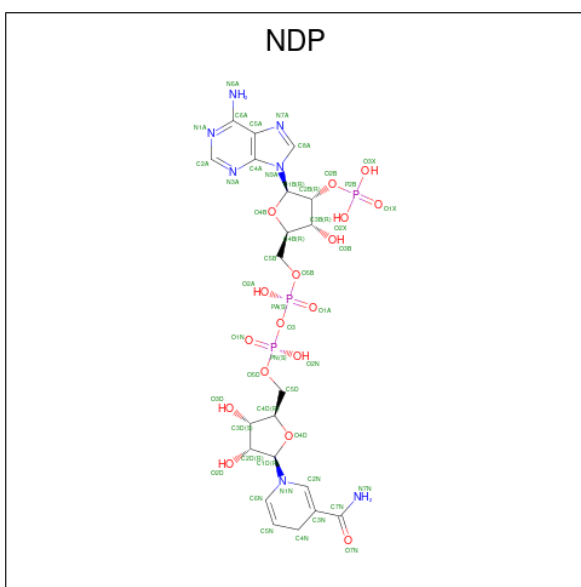
Mol	Chain	Residues	Atoms						AltConf
50	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
50	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 51 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



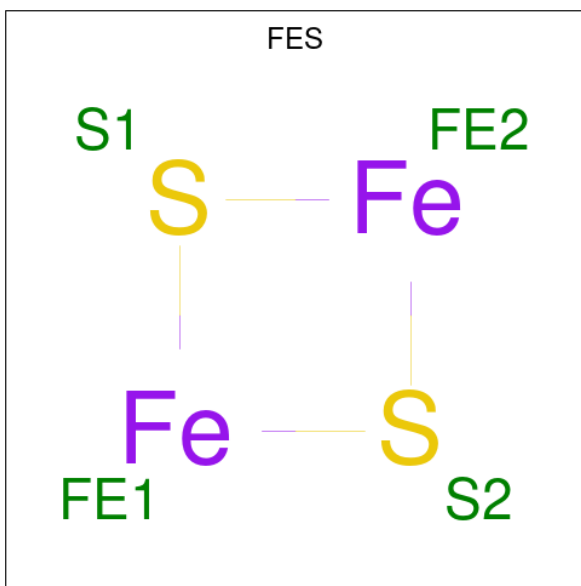
Mol	Chain	Residues	Atoms				AltConf
51	I	1	Total	C	O	P	0
			51	32	17	2	
51	a	1	Total	C	O	P	0
			91	72	17	2	
51	i	1	Total	C	O	P	0
			66	47	17	2	
51	l	1	Total	C	O	P	0
			99	80	17	2	
51	l	1	Total	C	O	P	0
			100	81	17	2	
51	r	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 53 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

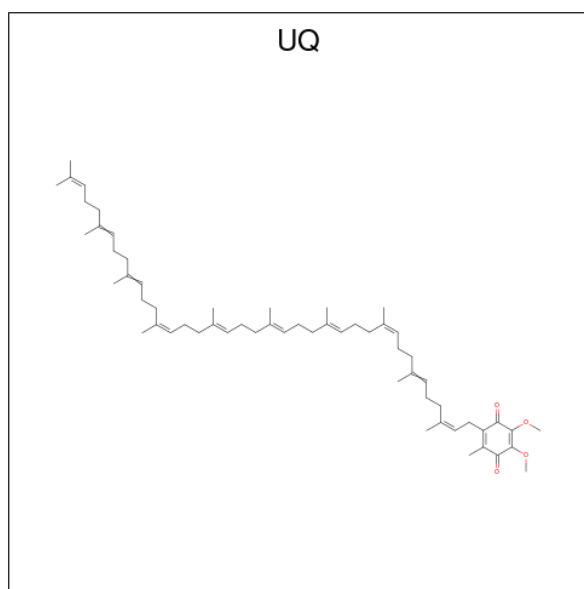
- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
54	M	1	Total	Mg	0
			1	1	

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

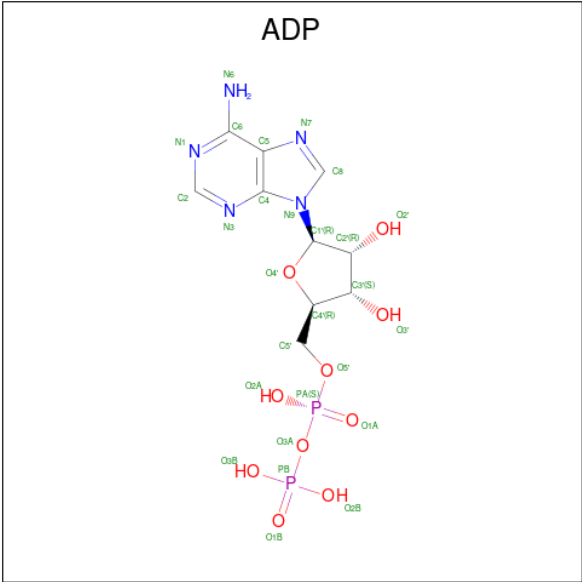
Mol	Chain	Residues	Atoms		AltConf
55	T	1	Total	Zn	0
			1	1	

- Molecule 56 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
56	s	1	Total	C	O	0
			28	24	4	

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

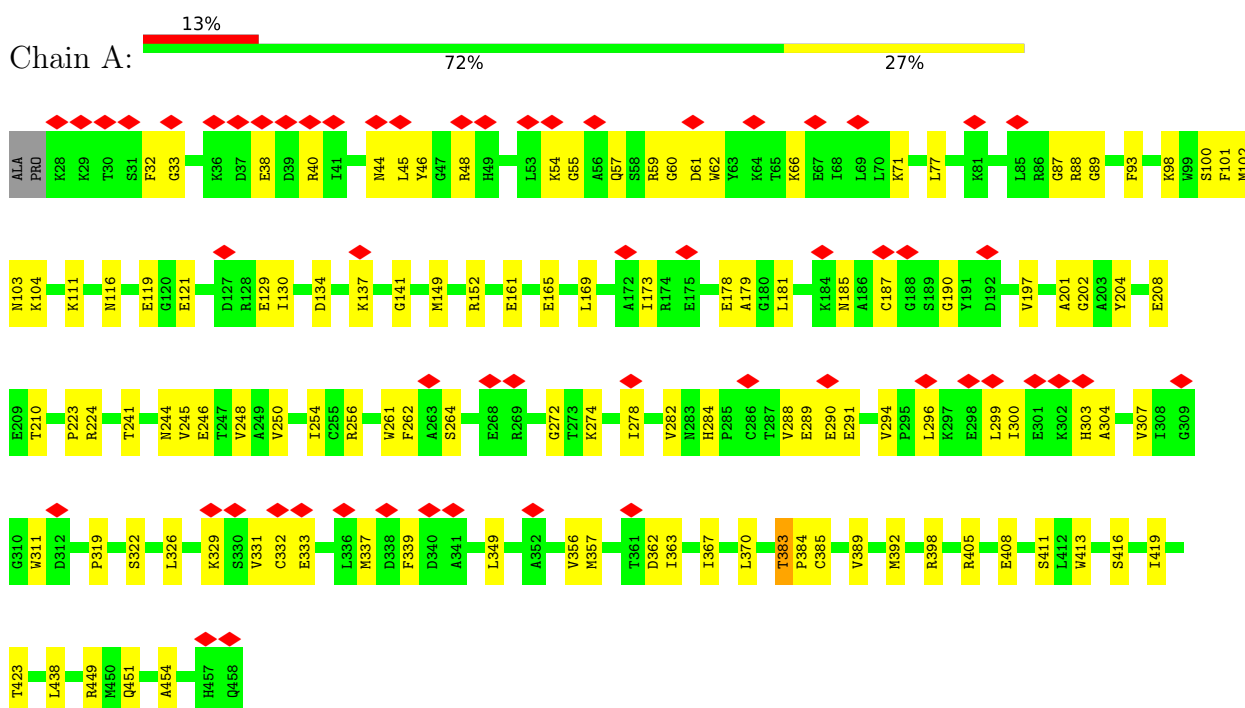


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

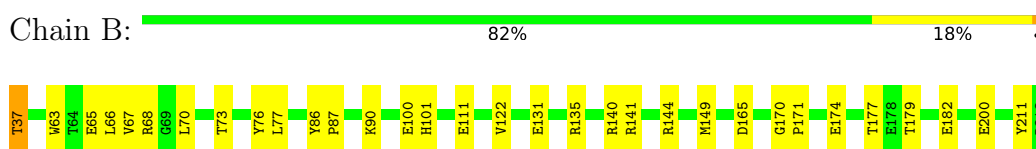
3 Residue-property plots

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

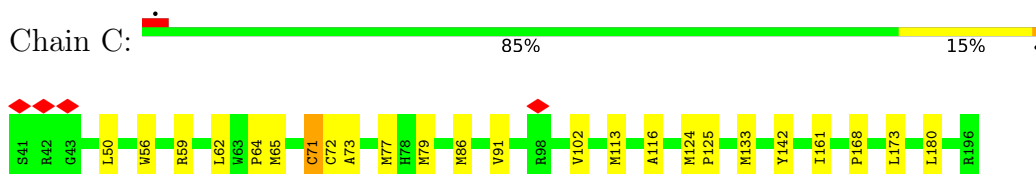
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



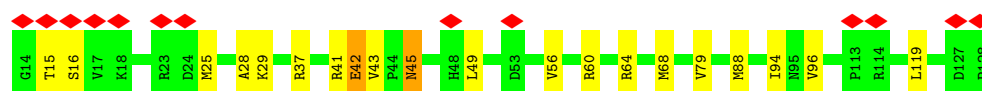
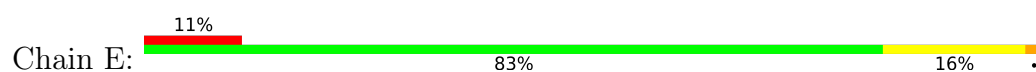
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



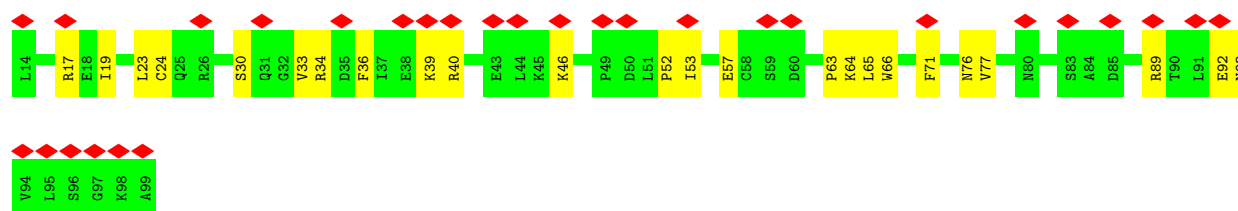
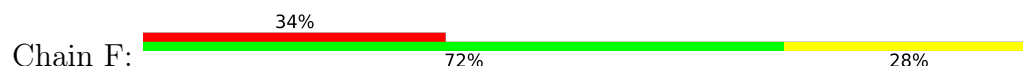
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



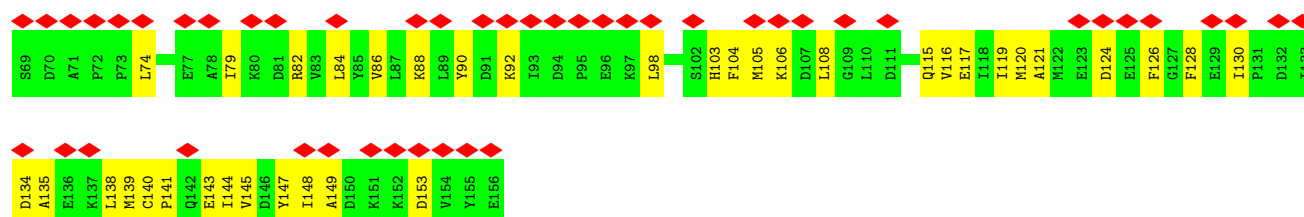
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



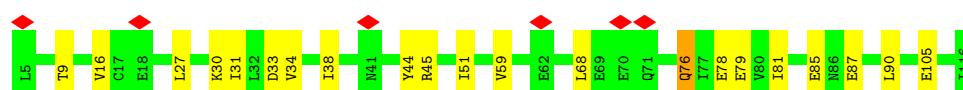
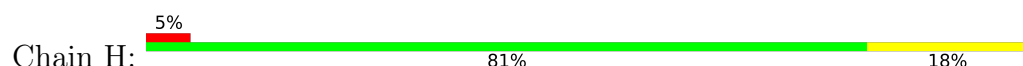
- Molecule 6: Acyl carrier protein



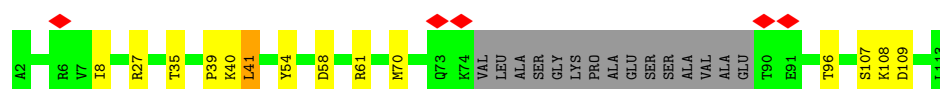
- Molecule 6: Acyl carrier protein



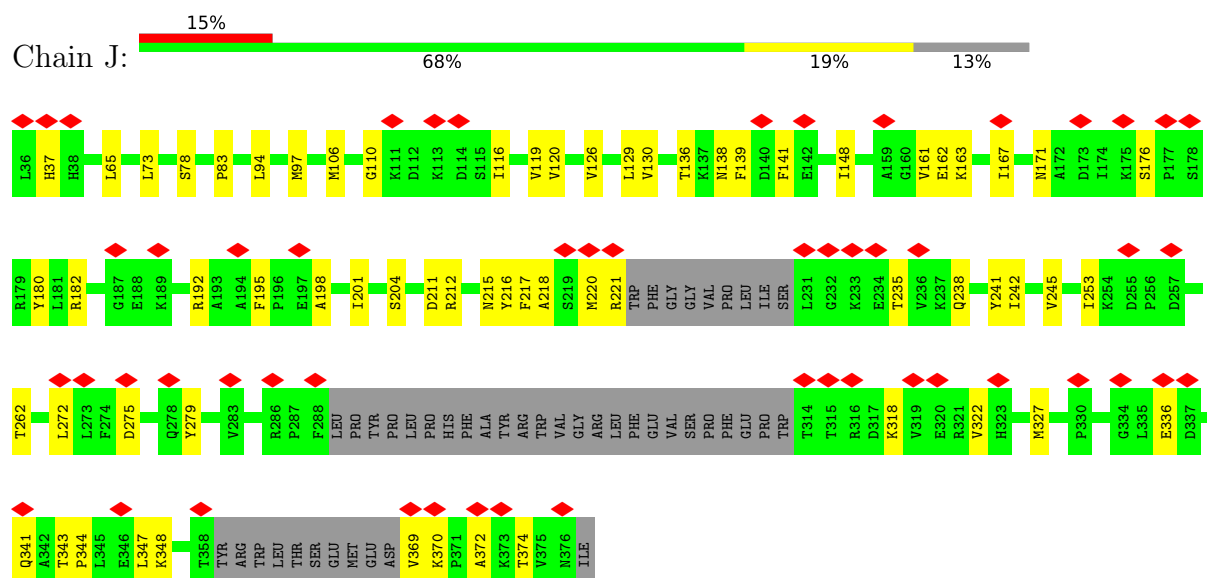
- Molecule 7: Complex I subunit B13



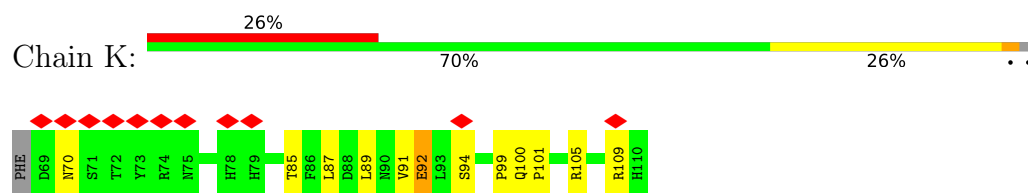
- Molecule 8: Complex I-B14.5a



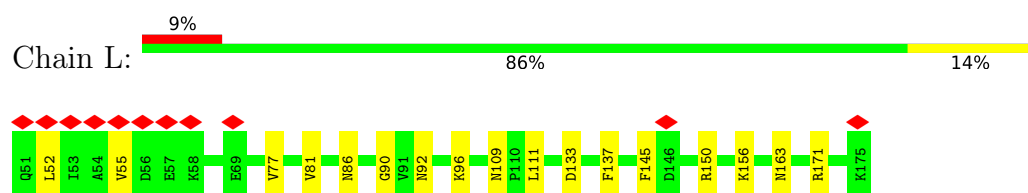
- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial



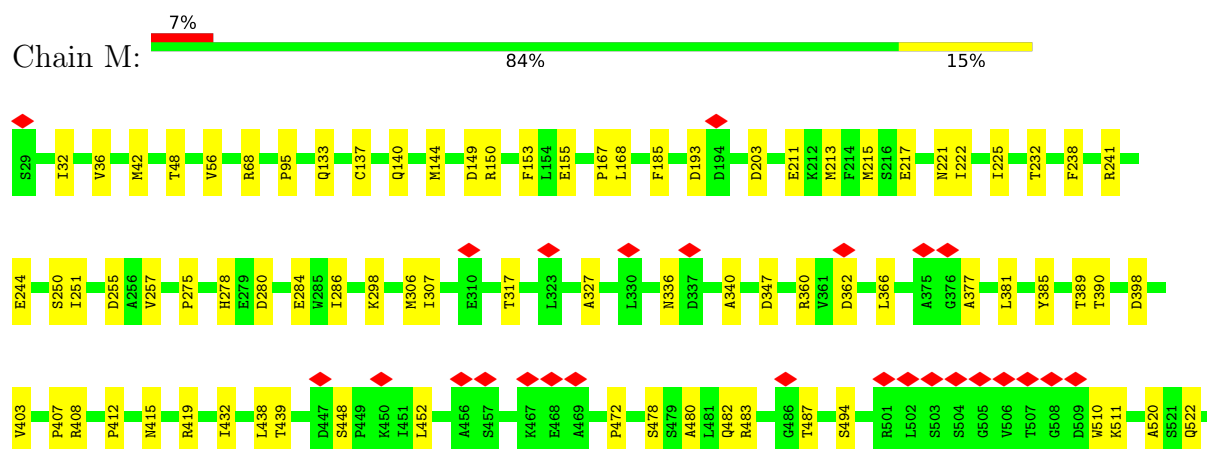
- Molecule 10: Complex I-9kD

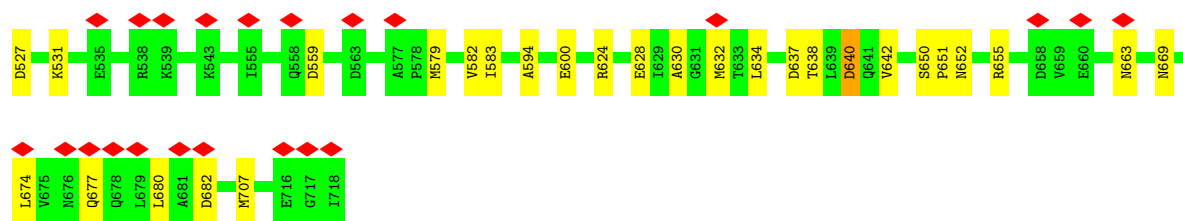


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

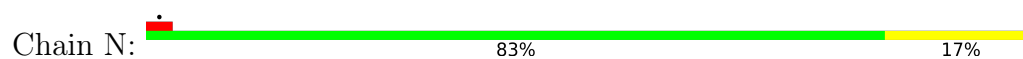


- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

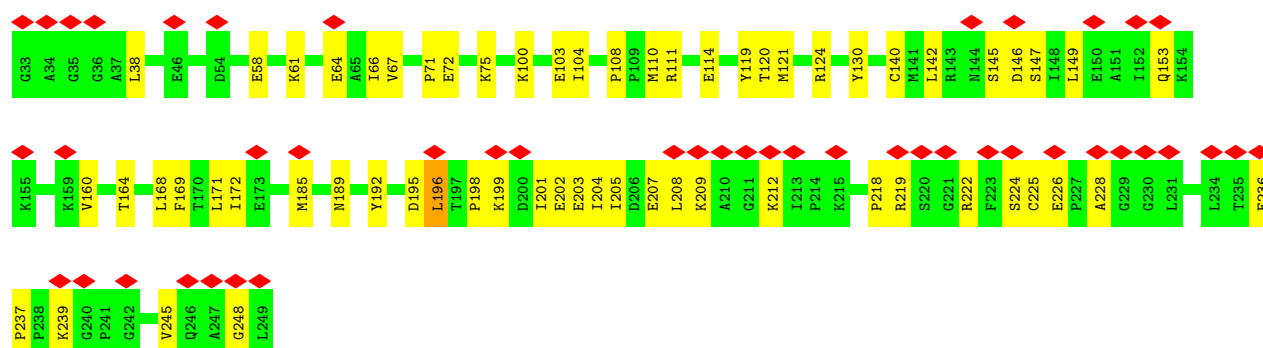




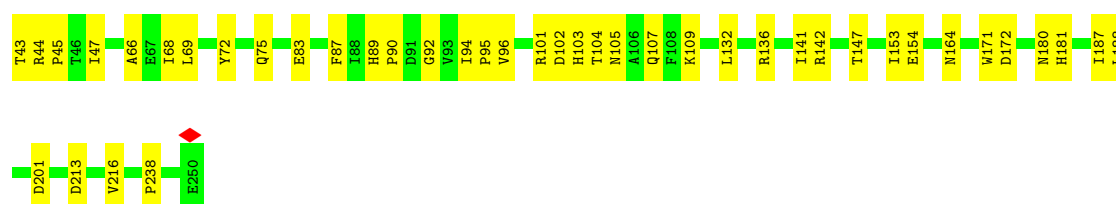
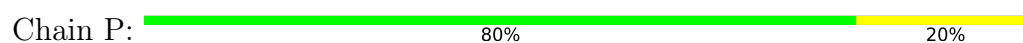
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



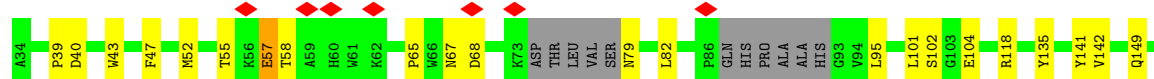
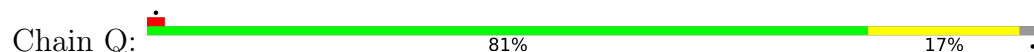
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

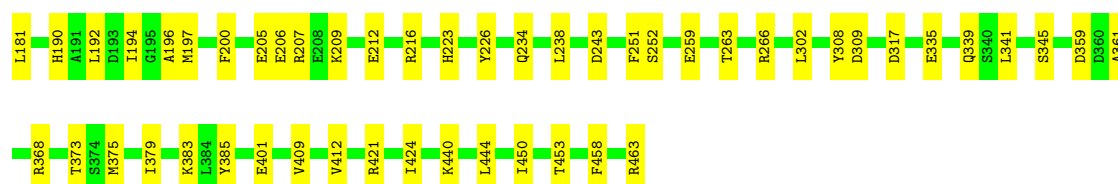


- Molecule 15: Complex I-30kD

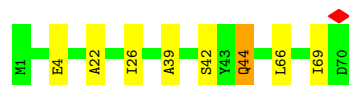


- Molecule 16: Complex I-49kD

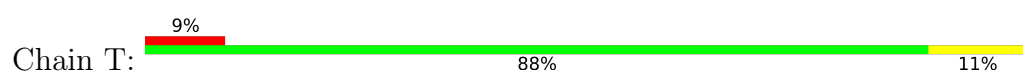




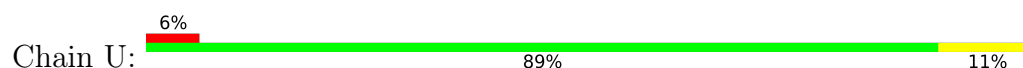
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



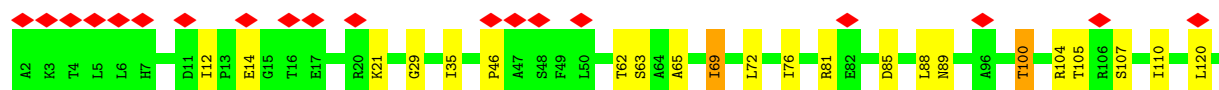
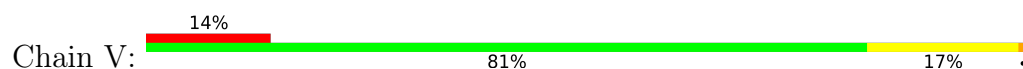
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



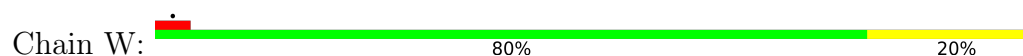
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



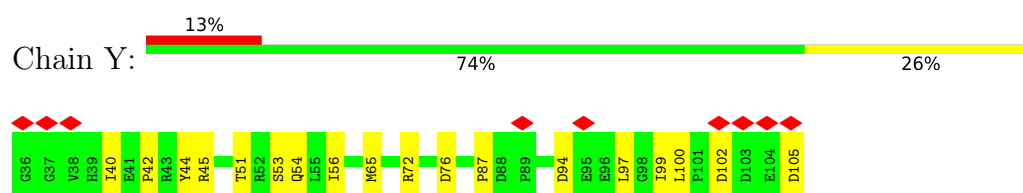
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



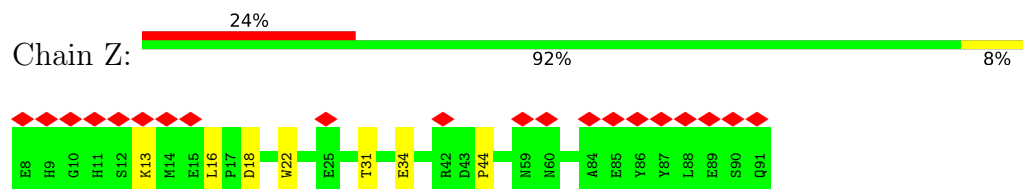
- Molecule 21: Complex I-B16.6



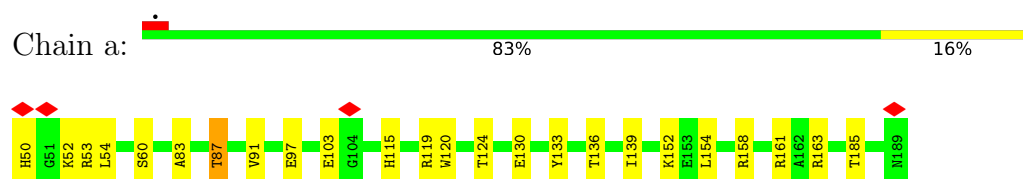
- Molecule 22: Complex I-AGGG



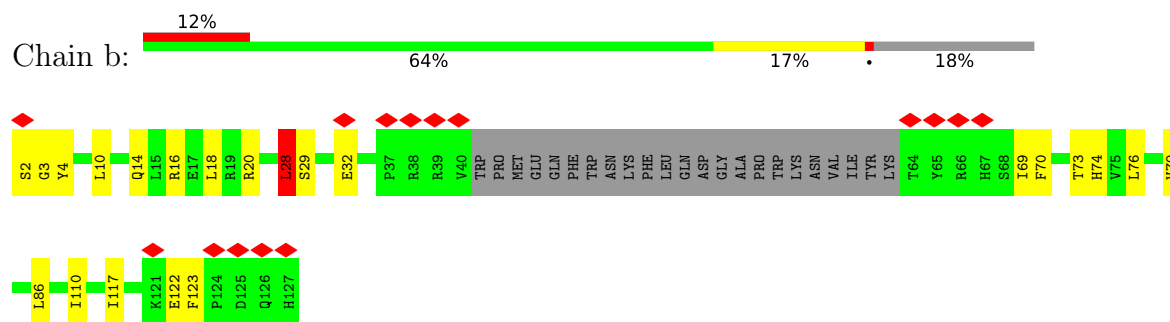
- Molecule 23: Complex I-B12



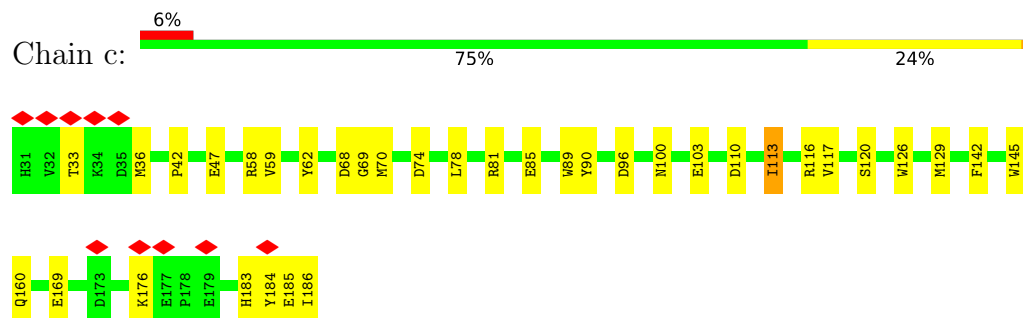
- Molecule 24: Complex I-SGDH



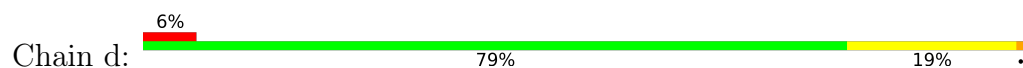
- Molecule 25: Complex I-B17

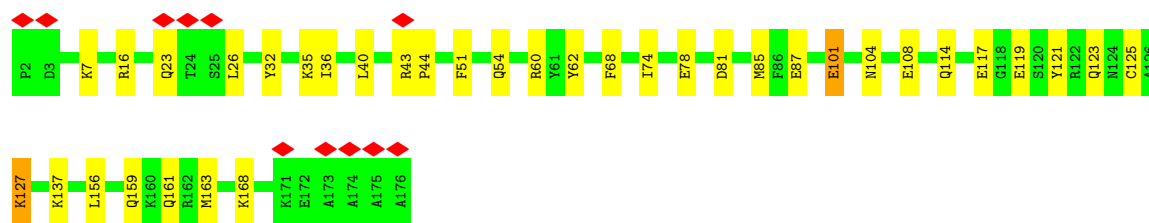


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

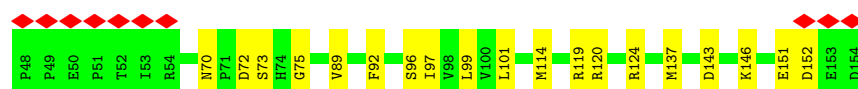
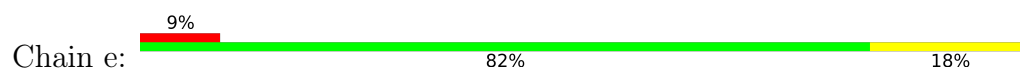


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

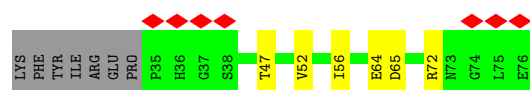




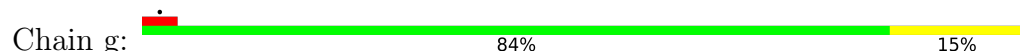
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



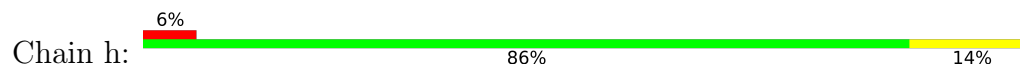
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



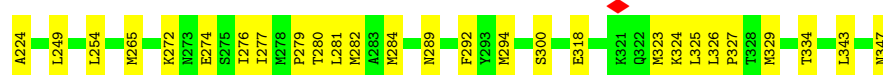
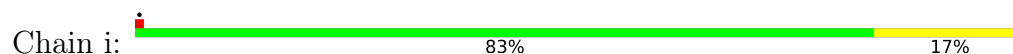
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



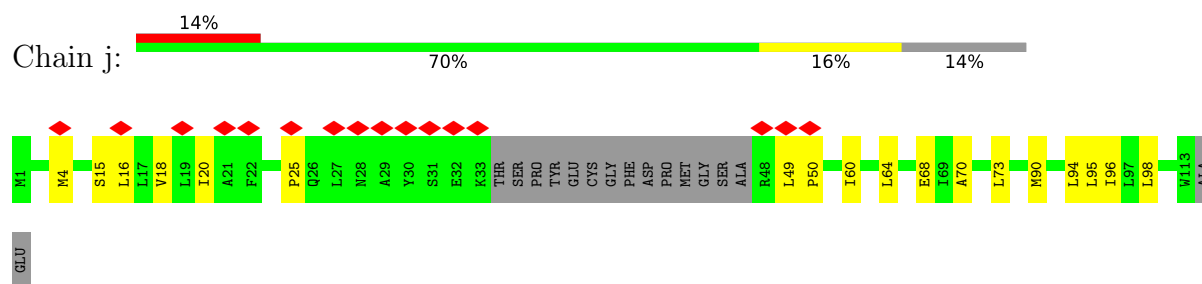
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



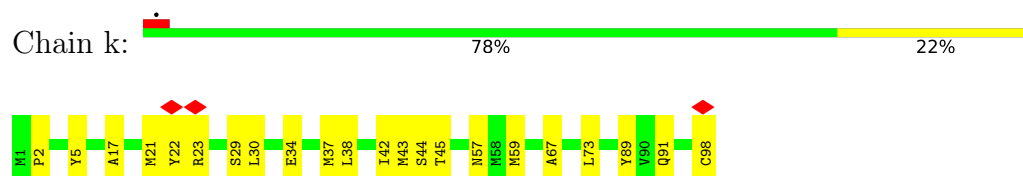
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



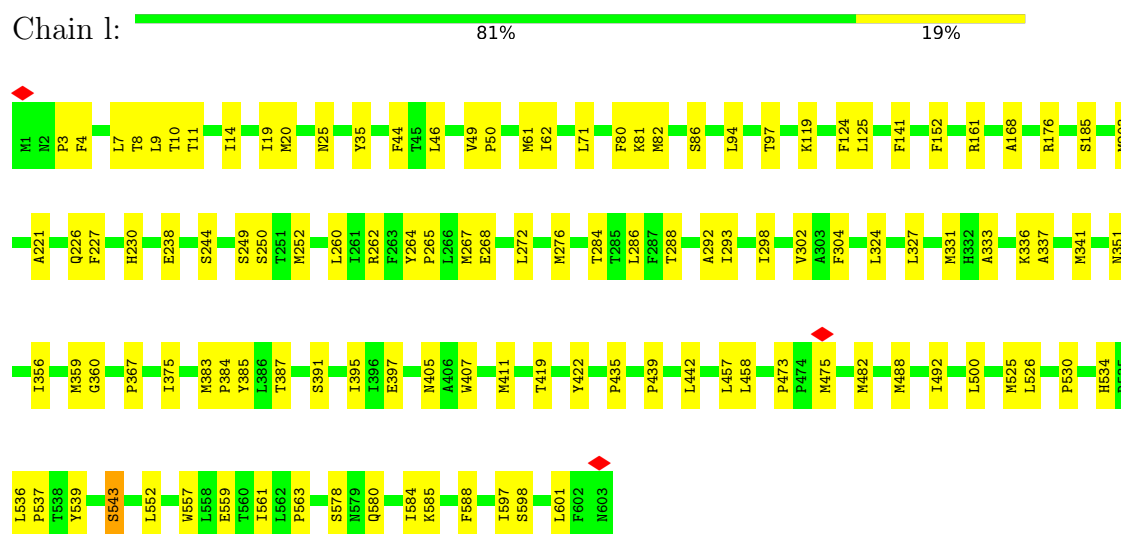
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



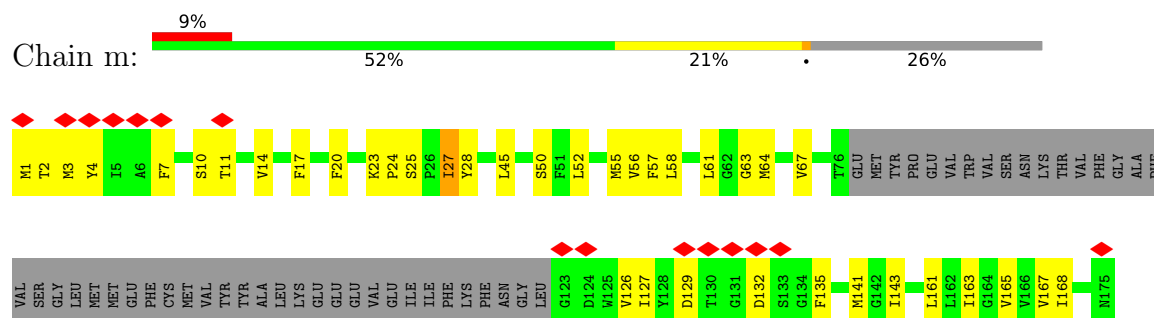
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



- Molecule 35: NADH-ubiquinone oxidoreductase chain 5



- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



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

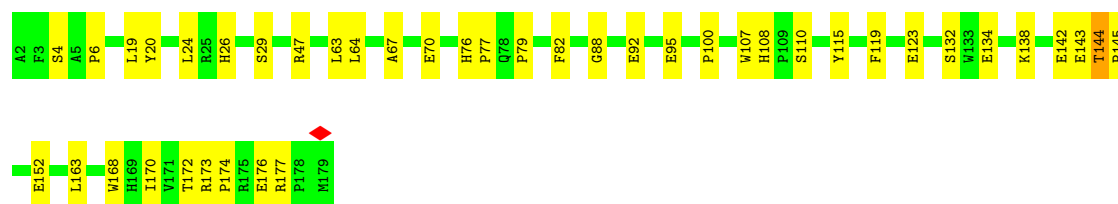
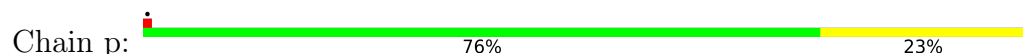




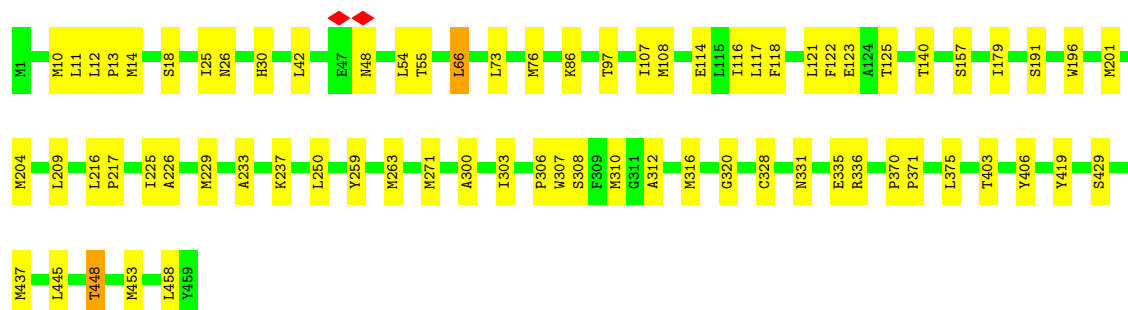
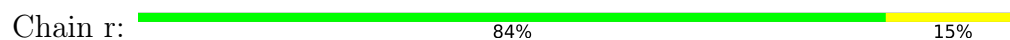
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



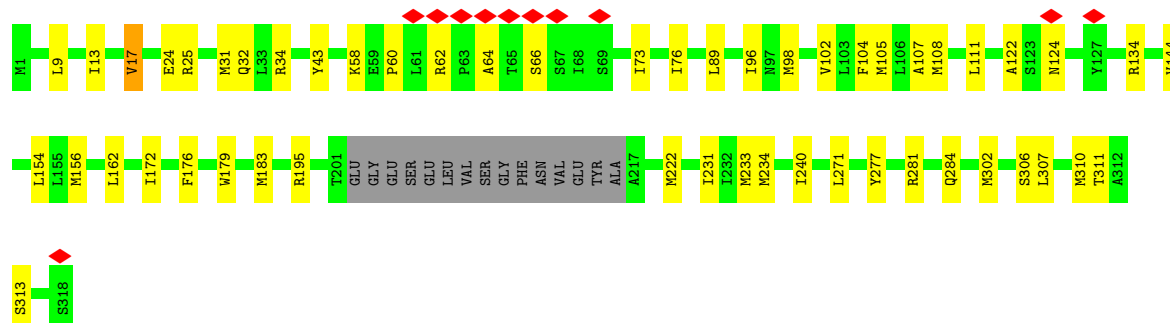
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

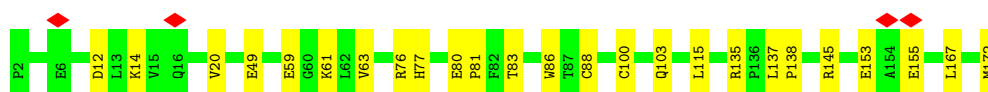


- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



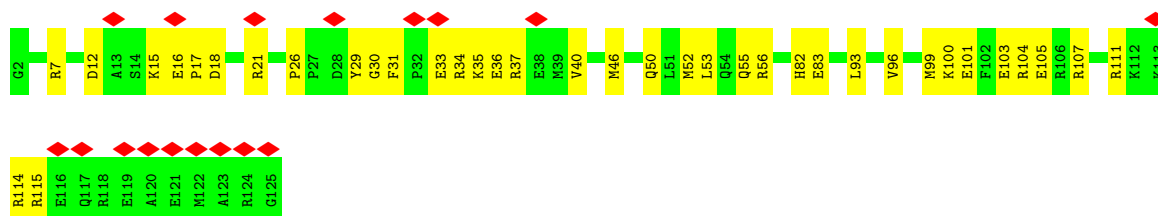
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:  85% 15%



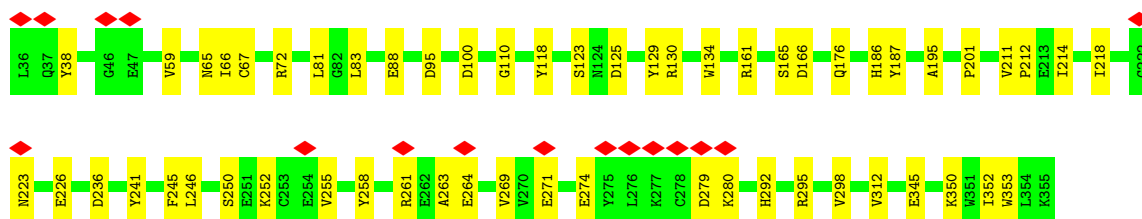
- Molecule 43: Complex I-B18

Chain v:  14% 70% 30%



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w:  5% 82% 18%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53905	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.205	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	333.7616, 333.7616, 333.7616	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PLX, ZN, FMN, ADP, PEE, 2MR, CDL, SF4, 8Q1, FES, MG, UQ, NDP, NAI

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	0.26	0/3388	0.42	2/4579 (0.0%)
2	B	0.40	0/1443	0.39	0/1952
3	C	0.37	0/1279	0.41	0/1730
4	E	0.28	0/995	0.51	2/1340 (0.1%)
5	F	0.26	0/702	0.51	1/945 (0.1%)
6	G	0.21	0/702	0.37	0/952
6	X	0.32	0/708	0.41	0/959
7	H	0.26	0/929	0.35	0/1258
8	I	0.28	0/798	0.37	0/1079
9	J	0.25	0/2411	0.32	0/3254
10	K	0.20	0/365	0.29	0/493
11	L	0.32	0/1036	0.31	0/1399
12	M	0.30	0/5380	0.37	1/7290 (0.0%)
13	N	0.29	0/1242	0.34	0/1690
14	O	0.25	0/1711	0.38	0/2328
15	P	0.36	0/1789	0.42	0/2436
16	Q	0.38	0/3451	0.41	1/4672 (0.0%)
17	S	0.33	0/582	0.37	0/783
18	T	0.28	0/755	0.35	0/1018
19	U	0.28	0/664	0.30	0/912
20	V	0.27	0/1030	0.48	0/1397
21	W	0.32	0/1204	0.44	2/1624 (0.1%)
22	Y	0.28	0/623	0.38	0/853
23	Z	0.24	0/695	0.26	0/939
24	a	0.35	0/1199	0.40	0/1623
25	b	0.31	0/906	0.48	1/1232 (0.1%)
26	c	0.34	0/1371	0.35	0/1875
27	d	0.33	0/1494	0.42	0/2015
28	e	0.31	0/916	0.35	0/1246
29	f	0.26	0/350	0.28	0/473
30	g	0.32	0/1031	0.33	0/1394
31	h	0.31	0/889	0.31	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.39	0/2773	0.39	0/3768
33	j	0.32	0/819	0.41	0/1117
34	k	0.35	0/759	0.38	0/1029
35	l	0.37	0/4911	0.39	0/6679
36	m	0.36	0/968	0.45	0/1313
37	n	0.27	0/491	0.35	0/663
38	o	0.33	0/1092	0.32	0/1481
39	p	0.34	0/1590	0.48	3/2155 (0.1%)
40	r	0.41	0/3723	0.41	0/5078
41	s	0.37	0/2464	0.41	0/3369
42	u	0.29	0/1436	0.36	0/1938
43	v	0.30	0/1052	0.42	0/1411
44	w	0.31	0/2630	0.40	2/3566 (0.1%)
All	All	0.33	0/66746	0.39	15/90497 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	522	GLN	N-CA-C	6.67	118.55	111.28
21	W	25	LEU	CA-C-N	6.22	126.19	120.03
21	W	25	LEU	C-N-CA	6.22	126.19	120.03
39	p	143	GLU	N-CA-C	6.09	118.00	111.36
39	p	144	THR	CA-C-N	6.02	126.58	120.38
39	p	144	THR	C-N-CA	6.02	126.58	120.38
4	E	43	VAL	CB-CA-C	-5.93	108.07	114.35
4	E	42	GLU	N-CA-C	5.71	117.50	111.28
5	F	52	PRO	CA-N-CD	-5.48	104.33	112.00
1	A	104	LYS	CA-C-N	5.45	125.38	119.76
1	A	104	LYS	C-N-CA	5.45	125.38	119.76
16	Q	142	VAL	N-CA-C	-5.27	107.69	112.96
25	b	28	LEU	N-CA-C	5.27	118.28	110.48
44	w	195	ALA	CA-C-N	-5.01	112.29	122.31
44	w	195	ALA	C-N-CA	-5.01	112.29	122.31

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3313	0	3266	115	0
2	B	1412	0	1363	25	0
3	C	1248	0	1254	25	0
4	E	971	0	975	21	0
5	F	691	0	704	23	0
6	G	690	0	669	32	0
6	X	696	0	680	26	0
7	H	910	0	950	13	0
8	I	780	0	808	12	0
9	J	2359	0	2402	47	0
10	K	355	0	329	11	0
11	L	1013	0	1014	13	0
12	M	5292	0	5322	77	0
13	N	1201	0	1153	20	0
14	O	1671	0	1673	55	0
15	P	1738	0	1693	32	0
16	Q	3377	0	3319	52	0
17	S	567	0	565	7	0
18	T	741	0	702	7	0
19	U	643	0	642	7	0
20	V	1009	0	1006	20	0
21	W	1173	0	1166	31	0
22	Y	597	0	537	17	0
23	Z	674	0	643	5	0
24	a	1165	0	1174	24	0
25	b	879	0	899	22	0
26	c	1315	0	1208	30	0
27	d	1461	0	1429	34	0
28	e	890	0	837	15	0
29	f	342	0	341	5	0
30	g	1000	0	994	14	0
31	h	867	0	871	10	0
32	i	2710	0	2874	45	0
33	j	800	0	855	16	0
34	k	748	0	799	21	0
35	l	4782	0	4929	90	0
36	m	946	0	955	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	n	479	0	486	3	0
38	o	1062	0	1072	11	0
39	p	1534	0	1470	31	0
40	r	3631	0	3839	59	0
41	s	2394	0	2508	56	0
42	u	1398	0	1378	21	0
43	v	1028	0	980	37	0
44	w	2570	0	2510	37	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	1	0
45	M	16	0	0	0	0
46	A	31	0	19	3	0
47	A	44	0	26	4	0
48	B	51	0	82	4	0
48	C	47	0	71	2	0
48	U	51	0	82	3	0
48	i	47	0	71	2	0
48	l	46	0	69	2	0
48	m	41	0	59	2	0
48	r	51	0	82	3	0
49	C	52	0	88	6	0
49	g	52	0	88	4	0
49	j	52	0	88	4	0
49	r	52	0	88	2	0
50	G	35	0	0	1	0
50	X	35	0	0	4	0
51	I	51	0	46	0	0
51	a	91	0	132	3	0
51	i	66	0	76	4	0
51	l	199	0	307	36	0
51	r	100	0	156	7	0
52	J	48	0	24	2	0
53	M	4	0	0	0	0
53	O	4	0	0	0	0
54	M	1	0	0	0	0
55	T	1	0	0	0	0
56	s	28	0	31	2	0
57	w	27	0	11	1	0
All	All	66477	0	66939	1176	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 (1176) 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)
6:X:112:SER:CB	50:X:201:8Q1:O1	1.65	1.44
52:J:401:NDP:O4D	52:J:401:NDP:C4D	1.68	1.16
51:l:701:CDL:H422	40:r:448:THR:HG21	1.44	1.00
51:l:701:CDL:C75	51:l:701:CDL:H312	1.93	0.99
51:l:701:CDL:H312	51:l:701:CDL:C74	1.95	0.97
43:v:33:GLU:OE2	43:v:33:GLU:N	1.98	0.97
1:A:102:MET:HG2	1:A:149:MET:HB3	1.43	0.96
26:c:33:THR:H	26:c:36:MET:HE3	1.33	0.94
6:X:76:LEU:HD12	6:X:156:GLU:C	1.92	0.94
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.48	0.93
1:A:54:LYS:O	1:A:54:LYS:HD3	1.67	0.93
1:A:296:LEU:HD23	1:A:337:MET:HE3	1.51	0.91
40:r:114:GLU:OE2	40:r:116:ILE:HG22	1.70	0.91
1:A:130:ILE:HD11	1:A:245:VAL:HG12	1.56	0.87
36:m:1:MET:HE3	36:m:4:TYR:H	1.39	0.87
51:l:701:CDL:H312	51:l:701:CDL:H742	1.58	0.85
21:W:120:MET:HE2	36:m:126:VAL:HG12	1.58	0.84
1:A:93:PHE:CD2	1:A:98:LYS:HG3	2.13	0.83
51:l:701:CDL:H581	51:l:701:CDL:H622	1.61	0.83
36:m:57:PHE:HE2	41:s:108:MET:HE1	1.42	0.82
4:E:37:ARG:HD2	6:G:120:MET:HE2	1.62	0.82
40:r:14:MET:HE2	40:r:30:HIS:ND1	1.95	0.82
35:l:383:MET:HE3	35:l:384:PRO:HD2	1.62	0.82
42:u:77:HIS:HD2	42:u:115:LEU:CD2	1.93	0.81
6:G:115:GLN:C	6:G:115:GLN:OE1	2.24	0.81
42:u:77:HIS:HD2	42:u:115:LEU:HD21	1.46	0.80
25:b:122:GLU:OE1	25:b:122:GLU:O	1.99	0.79
45:C:301:SF4:S4	16:Q:223:HIS:CD2	2.74	0.79
43:v:83:GLU:OE2	43:v:83:GLU:N	2.15	0.79
3:C:142:TYR:CE1	16:Q:135:TYR:CZ	2.71	0.79
51:l:701:CDL:H762	51:l:701:CDL:H722	1.64	0.77
1:A:44:ASN:HB2	1:A:59:ARG:HH12	1.46	0.77
42:u:77:HIS:CD2	42:u:115:LEU:HD21	2.20	0.77
1:A:54:LYS:HE2	1:A:54:LYS:HA	1.65	0.77
1:A:77:LEU:HD13	1:A:103:ASN:HD22	1.50	0.77
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.67	0.77
40:r:114:GLU:CD	40:r:116:ILE:HG22	2.09	0.76
24:a:97:GLU:OE1	27:d:62:TYR:CE2	2.38	0.76
35:l:351:ASN:O	35:l:351:ASN:ND2	2.19	0.76
9:J:141:PHE:HE2	9:J:180:TYR:HD1	1.32	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:18:VAL:HG22	41:s:222:MET:HG3	1.69	0.75
27:d:121:TYR:HD2	35:l:203:MET:HE3	1.52	0.74
1:A:102:MET:CB	1:A:149:MET:HG2	2.18	0.74
9:J:241:TYR:CE2	9:J:348:LYS:HG3	2.23	0.74
36:m:57:PHE:CE2	41:s:108:MET:HE1	2.23	0.74
1:A:77:LEU:CD1	1:A:103:ASN:HD22	2.01	0.74
6:X:112:SER:CB	50:X:201:8Q1:P24	2.75	0.74
12:M:211:GLU:OE1	12:M:211:GLU:N	2.20	0.73
1:A:93:PHE:CD2	1:A:98:LYS:CG	2.71	0.73
10:K:100:GLN:HG3	10:K:101:PRO:HD2	1.71	0.73
51:l:701:CDL:H762	51:l:701:CDL:C72	2.18	0.73
22:Y:87:PRO:HG2	43:v:99:MET:HE1	1.71	0.72
26:c:184:TYR:HD2	43:v:101:GLU:OE2	1.73	0.72
27:d:104:ASN:O	27:d:108:GLU:HG3	1.88	0.72
25:b:18:LEU:HD11	39:p:163:LEU:HD22	1.72	0.72
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.23	0.71
51:l:701:CDL:H312	51:l:701:CDL:H752	1.71	0.71
14:O:58:GLU:OE2	14:O:58:GLU:N	2.22	0.71
1:A:77:LEU:CD1	1:A:103:ASN:ND2	2.53	0.71
20:V:65:ALA:O	20:V:69:ILE:HG12	1.90	0.71
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.24	0.71
1:A:262:PHE:CE1	1:A:272:GLY:HA3	2.25	0.71
16:Q:52:MET:HE2	32:i:173:THR:HG22	1.73	0.71
16:Q:68:ASP:O	32:i:49:ASN:ND2	2.24	0.71
4:E:29:LYS:NZ	50:G:201:8Q1:O35	2.24	0.71
27:d:119:GLU:HB2	43:v:50:GLN:HB2	1.73	0.70
4:E:42:GLU:OE1	4:E:94:ILE:HG12	1.91	0.70
1:A:392:MET:HE3	1:A:419:ILE:HD12	1.73	0.70
28:e:143:ASP:OD1	28:e:146:LYS:HG3	1.91	0.70
1:A:102:MET:HB3	1:A:149:MET:HG2	1.72	0.70
20:V:69:ILE:HG13	20:V:100:THR:HG21	1.73	0.70
35:l:11:THR:HG22	35:l:46:LEU:HD12	1.74	0.70
44:w:67:CYS:HB2	44:w:218:ILE:HD11	1.73	0.70
21:W:134:LEU:HD13	36:m:1:MET:HA	1.74	0.70
1:A:93:PHE:CE2	1:A:98:LYS:HG3	2.25	0.69
6:G:88:LYS:HD3	6:G:98:LEU:HD21	1.73	0.69
35:l:161:ARG:NH1	35:l:238:GLU:OE1	2.25	0.69
1:A:54:LYS:HD3	1:A:54:LYS:C	2.17	0.69
51:l:701:CDL:H651	51:l:701:CDL:H862	1.75	0.69
13:N:68:MET:HG3	13:N:69:ASN:H	1.55	0.69
4:E:49:LEU:O	4:E:49:LEU:HD23	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:1:MET:CE	36:m:4:TYR:H	2.06	0.69
22:Y:94:ASP:OD1	43:v:107:ARG:NH1	2.25	0.68
5:F:89:ARG:O	5:F:93:ASN:ND2	2.26	0.68
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.75	0.68
36:m:57:PHE:HE2	41:s:108:MET:CE	2.06	0.68
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.26	0.68
35:l:341:MET:HE2	35:l:457:LEU:HD12	1.75	0.68
41:s:281:ARG:HB2	41:s:284:GLN:HG3	1.74	0.68
6:X:76:LEU:CD1	6:X:156:GLU:C	2.67	0.67
29:f:52:VAL:O	29:f:56:ILE:HG13	1.93	0.67
5:F:92:GLU:OE2	5:F:92:GLU:HA	1.93	0.67
43:v:31:PHE:HB2	43:v:33:GLU:OE2	1.93	0.67
28:e:120:ARG:O	28:e:124:ARG:HG3	1.94	0.67
14:O:171:LEU:O	14:O:172:ILE:HD13	1.95	0.67
1:A:102:MET:CG	1:A:149:MET:HB3	2.23	0.67
18:T:50:TYR:O	18:T:53:VAL:HG12	1.94	0.67
24:a:97:GLU:OE1	27:d:62:TYR:HE2	1.77	0.66
1:A:33:GLY:HA2	1:A:294:VAL:HG22	1.78	0.66
3:C:79:MET:HE2	3:C:86:MET:CE	2.25	0.66
1:A:48:ARG:NH2	14:O:226:GLU:OE1	2.29	0.66
41:s:62:ARG:HD3	41:s:64:ALA:H	1.59	0.66
1:A:88:ARG:HG2	1:A:246:GLU:HG2	1.76	0.66
3:C:59:ARG:NH1	49:C:303:PLX:O3	2.25	0.66
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.27	0.66
9:J:336:GLU:OE2	9:J:341:GLN:NE2	2.29	0.66
1:A:130:ILE:HD11	1:A:245:VAL:CG1	2.26	0.66
1:A:383:THR:HG23	1:A:384:PRO:HD3	1.75	0.66
3:C:125:PRO:HB2	41:s:58:LYS:HE3	1.78	0.66
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.28	0.66
37:n:26:TYR:OH	37:n:30:ARG:NH1	2.29	0.66
27:d:32:TYR:CE1	27:d:35:LYS:HE2	2.31	0.65
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.25	0.65
33:j:25:PRO:HB2	41:s:60:PRO:HD3	1.78	0.65
24:a:97:GLU:HG2	27:d:60:ARG:HD2	1.78	0.65
35:l:250:SER:HB2	35:l:333:ALA:HA	1.77	0.65
14:O:169:PHE:HZ	14:O:209:LYS:HG3	1.60	0.65
35:l:331:MET:HE2	35:l:331:MET:HA	1.79	0.65
1:A:98:LYS:HA	1:A:101:PHE:CD2	2.32	0.65
6:G:126:PHE:HB3	6:G:128:PHE:HE1	1.59	0.65
3:C:79:MET:HE2	3:C:86:MET:HE2	1.77	0.65
9:J:369:VAL:HG12	9:J:370:LYS:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:TRP:O	2:B:67:VAL:HG23	1.97	0.65
27:d:117:GLU:HA	27:d:117:GLU:OE1	1.97	0.64
34:k:23:ARG:HG2	36:m:23:LYS:HE2	1.78	0.64
21:W:28:ARG:HD2	21:W:28:ARG:N	2.11	0.64
1:A:201:ALA:HA	14:O:121:MET:HE2	1.77	0.64
12:M:42:MET:HE3	12:M:42:MET:HA	1.79	0.64
36:m:57:PHE:CE1	41:s:111:LEU:HG	2.32	0.64
10:K:100:GLN:HB3	14:O:72:GLU:OE1	1.96	0.64
35:l:227:PHE:O	35:l:230:HIS:ND1	2.30	0.64
35:l:391:SER:O	35:l:395:ILE:HG12	1.97	0.64
22:Y:51:THR:HG22	22:Y:53:SER:H	1.62	0.63
28:e:72:ASP:OD1	39:p:108:HIS:NE2	2.29	0.63
11:L:109:ASN:ND2	11:L:111:LEU:O	2.31	0.63
36:m:132:ASP:OD1	36:m:132:ASP:C	2.42	0.63
13:N:120:THR:HG22	13:N:122:GLN:H	1.63	0.63
6:G:126:PHE:HB3	6:G:128:PHE:CE1	2.33	0.63
8:I:40:LYS:HB3	21:W:7:LYS:H	1.64	0.63
36:m:55:MET:HA	36:m:55:MET:HE2	1.80	0.63
1:A:60:GLY:O	1:A:256:ARG:NH1	2.32	0.63
35:l:526:LEU:HD12	35:l:530:PRO:HG2	1.79	0.63
42:u:76:ARG:HE	42:u:77:HIS:CE1	2.17	0.63
44:w:125:ASP:O	44:w:130:ARG:NH2	2.32	0.63
2:B:111:GLU:O	2:B:141:ARG:NH1	2.32	0.63
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.81	0.63
4:E:37:ARG:HD3	6:G:116:VAL:HG13	1.80	0.62
35:l:11:THR:CG2	35:l:46:LEU:HD12	2.29	0.62
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.32	0.62
27:d:81:ASP:O	27:d:85:MET:HG3	1.99	0.62
22:Y:87:PRO:CG	43:v:99:MET:HE1	2.29	0.62
33:j:73:LEU:HD13	36:m:55:MET:HE1	1.80	0.62
35:l:557:TRP:O	35:l:561:ILE:HG12	2.00	0.62
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.40	0.62
1:A:282:VAL:HG13	1:A:356:VAL:HG21	1.82	0.62
14:O:168:LEU:HD23	14:O:169:PHE:HE1	1.65	0.62
24:a:120:TRP:O	24:a:124:THR:HG22	1.99	0.62
24:a:158:ARG:HH11	24:a:158:ARG:HG2	1.65	0.62
2:B:68:ARG:NH2	21:W:26:PRO:O	2.32	0.61
12:M:419:ARG:NH1	12:M:439:THR:O	2.32	0.61
2:B:177:THR:HG22	2:B:179:THR:H	1.65	0.61
26:c:186:ILE:HD13	43:v:100:LYS:HB3	1.81	0.61
12:M:677:GLN:OE1	12:M:677:GLN:N	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:h:97:HIS:HA	31:h:102:GLU:HB3	1.80	0.61
32:i:279:PRO:HA	32:i:282:MET:HG3	1.83	0.61
9:J:211:ASP:O	9:J:215:ASN:ND2	2.34	0.61
14:O:195:ASP:OD2	14:O:222:ARG:HD3	1.99	0.61
1:A:201:ALA:HA	14:O:121:MET:CE	2.29	0.61
4:E:64:ARG:NH2	6:G:117:GLU:OE1	2.34	0.61
7:H:76:GLN:O	7:H:79:GLU:HG2	2.00	0.61
22:Y:100:LEU:HB2	43:v:111:ARG:HH12	1.65	0.61
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.34	0.61
1:A:93:PHE:HD2	1:A:98:LYS:CD	2.13	0.61
9:J:110:GLY:HA3	9:J:148:ILE:HD11	1.83	0.60
22:Y:102:ASP:HA	43:v:115:ARG:HH12	1.66	0.60
3:C:142:TYR:HD1	3:C:142:TYR:O	1.85	0.60
14:O:239:LYS:HE2	14:O:239:LYS:HA	1.81	0.60
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.83	0.60
51:l:701:CDL:H742	51:l:701:CDL:C31	2.30	0.60
40:r:370:PRO:HB3	40:r:375:LEU:HD22	1.83	0.60
40:r:271:MET:HE2	40:r:271:MET:HA	1.84	0.60
12:M:377:ALA:HB1	12:M:381:LEU:HD23	1.84	0.60
1:A:185:ASN:ND2	1:A:187:CYS:O	2.35	0.59
7:H:33:ASP:OD1	7:H:33:ASP:C	2.45	0.59
26:c:113:ILE:HD11	26:c:116:ARG:HD2	1.84	0.59
5:F:36:PHE:O	5:F:40:ARG:HD2	2.01	0.59
33:j:70:ALA:HA	33:j:73:LEU:HD12	1.83	0.59
9:J:218:ALA:O	9:J:221:ARG:NH1	2.35	0.59
6:X:69:SER:OG	6:X:70:ASP:N	2.35	0.59
27:d:32:TYR:HE1	27:d:35:LYS:HE2	1.68	0.59
43:v:18:ASP:OD1	43:v:18:ASP:O	2.20	0.59
26:c:110:ASP:OD1	26:c:110:ASP:N	2.35	0.59
1:A:93:PHE:CD2	1:A:98:LYS:CD	2.86	0.59
35:l:203:MET:HE2	35:l:203:MET:HA	1.84	0.59
35:l:331:MET:HB3	35:l:387:THR:HG22	1.85	0.59
32:i:95:MET:HE2	32:i:149:ILE:HA	1.85	0.59
21:W:130:ASN:HB3	36:m:1:MET:N	2.18	0.58
40:r:114:GLU:OE1	40:r:117:LEU:N	2.28	0.58
39:p:170:ILE:O	39:p:173:ARG:NH1	2.36	0.58
3:C:72:CYS:HB3	3:C:133:MET:SD	2.44	0.58
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.85	0.58
1:A:296:LEU:O	1:A:300:ILE:HG22	2.03	0.58
22:Y:72:ARG:NH2	22:Y:76:ASP:OD2	2.35	0.58
27:d:68:PHE:HE2	28:e:114:MET:HE1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:85:THR:O	10:K:89:LEU:HD12	2.03	0.58
15:P:101:ARG:O	15:P:109:LYS:NZ	2.35	0.58
16:Q:104:GLU:OE2	41:s:134:ARG:NH1	2.35	0.58
41:s:234:MET:HE2	41:s:234:MET:HA	1.86	0.58
5:F:64:LYS:NZ	5:F:76:ASN:HB2	2.19	0.58
14:O:146:ASP:OD1	14:O:147:SER:N	2.37	0.58
16:Q:196:ALA:C	16:Q:197:MET:HG3	2.28	0.58
32:i:324:LYS:HD2	32:i:325:LEU:H	1.67	0.58
32:i:347:ASN:N	32:i:347:ASN:OD1	2.35	0.58
1:A:93:PHE:HD2	1:A:98:LYS:CG	2.16	0.58
11:L:137:PHE:HZ	15:P:201:ASP:OD2	1.87	0.58
15:P:72:TYR:CG	15:P:92:GLY:HA3	2.39	0.58
19:U:24:ALA:O	19:U:28:LEU:HD23	2.04	0.58
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.86	0.58
14:O:169:PHE:CZ	14:O:209:LYS:HG3	2.38	0.57
26:c:116:ARG:HG2	48:l:703:PEE:H49	1.86	0.57
35:l:272:LEU:HG	35:l:276:MET:HE2	1.85	0.57
30:g:31:PRO:HD2	42:u:172:MET:HE1	1.84	0.57
51:l:701:CDL:H331	51:l:701:CDL:OA9	2.03	0.57
40:r:204:MET:HE3	40:r:209:LEU:HD13	1.85	0.57
41:s:13:ILE:O	41:s:17:VAL:HG13	2.04	0.57
11:L:156:LYS:HE2	12:M:68:ARG:HE	1.68	0.57
21:W:85:GLN:OE1	31:h:105:ARG:NH1	2.36	0.57
31:h:73:MET:HE3	36:m:127:ILE:HG23	1.86	0.57
4:E:15:THR:OG1	11:L:55:VAL:O	2.22	0.57
6:G:104:PHE:HA	6:G:108:LEU:HD12	1.86	0.57
13:N:144:TYR:HD1	13:N:144:TYR:H	1.52	0.57
35:l:397:GLU:HG2	35:l:482:MET:HE1	1.86	0.57
5:F:33:VAL:O	5:F:36:PHE:HB3	2.04	0.57
40:r:48:ASN:N	40:r:48:ASN:OD1	2.37	0.57
1:A:93:PHE:HD2	1:A:98:LYS:HG3	1.63	0.57
1:A:185:ASN:OD1	1:A:190:GLY:N	2.20	0.57
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.85	0.57
42:u:80:GLU:HG2	42:u:81:PRO:HD3	1.87	0.57
1:A:204:TYR:OH	47:A:503:NAI:H5N	2.04	0.57
12:M:241:ARG:O	12:M:244:GLU:HG2	2.05	0.57
24:a:97:GLU:OE1	27:d:62:TYR:CD2	2.58	0.57
27:d:127:LYS:H	27:d:127:LYS:CE	2.17	0.57
27:d:161:GLN:OE1	30:g:118:PHE:HB3	2.04	0.57
51:l:701:CDL:H342	51:l:701:CDL:H392	1.86	0.57
1:A:55:GLY:O	1:A:59:ARG:NE	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:133:MET:HG3	3:C:173:LEU:HD13	1.86	0.57
33:j:95:LEU:HD13	41:s:302:MET:HG2	1.87	0.57
9:J:318:LYS:O	9:J:322:VAL:HG13	2.05	0.57
15:P:94:ILE:HB	15:P:95:PRO:HD3	1.87	0.57
24:a:87:THR:O	24:a:91:VAL:HG23	2.05	0.57
26:c:62:TYR:OH	26:c:74:ASP:OD1	2.22	0.57
34:k:44:SER:HB2	34:k:59:MET:HE1	1.87	0.57
51:l:701:CDL:H581	51:l:701:CDL:C62	2.33	0.56
38:o:35:GLU:O	38:o:39:ILE:HG23	2.04	0.56
14:O:218:PRO:HG3	14:O:224:SER:H	1.70	0.56
51:a:201:CDL:H772	51:a:201:CDL:H201	1.87	0.56
1:A:165:GLU:OE2	1:A:165:GLU:N	2.25	0.56
10:K:100:GLN:HG2	14:O:71:PRO:HA	1.87	0.56
12:M:680:LEU:HD21	12:M:682:ASP:OD2	2.05	0.56
14:O:38:LEU:O	14:O:124:ARG:NH2	2.39	0.56
48:i:402:PEE:H37	48:i:402:PEE:H60	1.86	0.56
51:l:701:CDL:H312	51:l:701:CDL:C76	2.34	0.56
40:r:114:GLU:CD	40:r:116:ILE:H	2.13	0.56
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.88	0.56
15:P:147:THR:HB	15:P:153:ILE:HD11	1.87	0.56
22:Y:94:ASP:HB3	22:Y:99:ILE:HB	1.87	0.56
33:j:90:MET:HE1	49:j:201:PLX:H281	1.88	0.56
8:I:39:PRO:HB2	8:I:41:LEU:HD23	1.86	0.56
19:U:30:ILE:HD11	33:j:96:ILE:HD11	1.88	0.56
26:c:33:THR:N	26:c:36:MET:HE3	2.14	0.56
41:s:105:MET:HE3	41:s:162:LEU:HD11	1.86	0.56
17:S:22:ALA:O	17:S:26:ILE:HD12	2.05	0.56
7:H:9:THR:HG23	7:H:16:VAL:HG22	1.87	0.56
12:M:398:ASP:N	12:M:398:ASP:OD1	2.38	0.56
6:G:141:PRO:O	6:G:145:VAL:HG23	2.06	0.56
14:O:61:LYS:O	14:O:64:GLU:HG3	2.06	0.56
6:X:111:ASP:OD1	6:X:112:SER:N	2.35	0.56
32:i:7:THR:HG22	32:i:11:MET:HE2	1.88	0.56
41:s:32:GLN:OE1	41:s:34:ARG:NH2	2.36	0.56
25:b:16:ARG:HD3	25:b:20:ARG:HH12	1.70	0.56
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.38	0.56
48:C:302:PEE:H32	48:C:302:PEE:H63	1.87	0.55
29:f:72:ARG:NH1	30:g:21:ARG:HB2	2.22	0.55
35:l:4:PHE:O	35:l:8:THR:HG23	2.06	0.55
42:u:76:ARG:HG3	42:u:77:HIS:ND1	2.21	0.55
34:k:2:PRO:HD2	34:k:5:TYR:CD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:225:ILE:HG13	40:r:229:MET:HE2	1.88	0.55
48:r:501:PEE:H71	48:r:501:PEE:H32	1.88	0.55
10:K:92:GLU:HA	10:K:92:GLU:OE1	2.06	0.55
12:M:140:GLN:HG2	16:Q:379:ILE:HG23	1.89	0.55
49:g:201:PLX:H301	32:i:347:ASN:HB3	1.88	0.55
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.87	0.55
13:N:78:ASP:OD2	13:N:80:SER:OG	2.24	0.55
3:C:113:MET:HE3	3:C:116:ALA:HB3	1.89	0.55
48:m:201:PEE:H52	41:s:104:PHE:HE1	1.72	0.55
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.87	0.55
43:v:96:VAL:HA	43:v:99:MET:HE2	1.88	0.55
3:C:73:ALA:O	3:C:77:MET:HG3	2.07	0.55
9:J:73:LEU:O	9:J:78:SER:OG	2.22	0.55
9:J:83:PRO:HG3	9:J:119:VAL:HG11	1.88	0.55
35:l:601:LEU:HD12	35:l:601:LEU:O	2.07	0.55
37:n:13:VAL:CG1	40:r:14:MET:HG2	2.37	0.55
21:W:85:GLN:O	21:W:89:GLU:HG3	2.07	0.55
26:c:145:TRP:CZ2	26:c:149:ILE:HD11	2.42	0.55
33:j:60:ILE:HG21	36:m:168:ILE:HG21	1.87	0.55
21:W:121:MET:HE2	21:W:121:MET:HA	1.89	0.54
24:a:158:ARG:HG2	24:a:158:ARG:NH1	2.22	0.54
32:i:265:MET:HE2	32:i:343:LEU:HD21	1.89	0.54
33:j:64:LEU:HD13	36:m:165:VAL:HG22	1.89	0.54
16:Q:206:GLU:OE2	16:Q:209:LYS:NZ	2.41	0.54
39:p:119:PHE:O	39:p:123:GLU:HG2	2.07	0.54
40:r:118:PHE:O	40:r:122:PHE:HB3	2.07	0.54
43:v:12:ASP:OD1	43:v:15:LYS:N	2.41	0.54
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.40	0.54
21:W:120:MET:HE3	36:m:127:ILE:HA	1.89	0.54
32:i:87:THR:HG22	32:i:88:LYS:N	2.22	0.54
39:p:138:LYS:NZ	39:p:142:GLU:OE1	2.37	0.54
20:V:62:THR:OG1	20:V:104:ARG:NH1	2.40	0.54
1:A:311:TRP:NE1	1:A:333:GLU:OE2	2.35	0.54
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.89	0.54
29:f:65:ASP:OD2	30:g:79:LYS:HE3	2.07	0.54
1:A:319:PRO:HB2	1:A:337:MET:HE1	1.89	0.54
17:S:4:GLU:HG2	41:s:43:TYR:CD2	2.43	0.54
30:g:36:MET:HE2	30:g:39:LEU:HD12	1.90	0.54
36:m:141:MET:HE2	36:m:141:MET:HA	1.89	0.54
1:A:48:ARG:HD2	10:K:70:ASN:O	2.08	0.54
7:H:59:VAL:HG23	7:H:68:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:241:TYR:HD1	9:J:242:ILE:H	1.56	0.54
25:b:110:ILE:HG12	27:d:16:ARG:HB2	1.90	0.54
1:A:152:ARG:NH2	10:K:99:PRO:O	2.41	0.54
14:O:110:MET:O	14:O:114:GLU:HG3	2.08	0.54
20:V:72:LEU:O	20:V:76:ILE:HG12	2.07	0.54
27:d:36:ILE:HG23	27:d:40:LEU:HD12	1.90	0.54
6:G:115:GLN:O	6:G:119:ILE:HG12	2.07	0.54
40:r:307:TRP:HA	40:r:310:MET:HE2	1.90	0.54
1:A:98:LYS:HA	1:A:101:PHE:HD2	1.73	0.53
6:G:144:ILE:O	6:G:148:ILE:HG12	2.09	0.53
18:T:79:VAL:O	18:T:121:PRO:HD3	2.07	0.53
23:Z:31:THR:HA	23:Z:34:GLU:HG3	1.89	0.53
36:m:1:MET:HE3	36:m:4:TYR:N	2.16	0.53
25:b:69:ILE:O	25:b:73:THR:HG23	2.08	0.53
44:w:271:GLU:HA	44:w:274:GLU:OE2	2.07	0.53
15:P:44:ARG:HB3	15:P:45:PRO:CD	2.38	0.53
20:V:72:LEU:C	20:V:72:LEU:HD13	2.34	0.53
51:l:701:CDL:H801	49:r:502:PLX:H212	1.90	0.53
43:v:18:ASP:OD1	43:v:21:ARG:N	2.39	0.53
12:M:306:MET:HE3	12:M:583:ILE:HD12	1.91	0.53
6:X:120:MET:HE1	39:p:24:LEU:HB3	1.89	0.53
2:B:37:THR:OG1	16:Q:317:ASP:OD1	2.24	0.53
8:I:27:ARG:NH1	16:Q:212:GLU:OE1	2.37	0.53
24:a:103:GLU:H	24:a:103:GLU:CD	2.17	0.53
51:r:503:CDL:H662	51:r:503:CDL:H612	1.90	0.53
20:V:85:ASP:HB3	20:V:130:LEU:HD21	1.91	0.53
21:W:120:MET:HE2	36:m:126:VAL:O	2.09	0.53
31:h:75:ARG:O	31:h:79:ILE:HD12	2.09	0.53
1:A:413:TRP:O	1:A:416:SER:OG	2.23	0.53
3:C:142:TYR:O	3:C:142:TYR:CD1	2.61	0.53
4:E:88:MET:HE1	15:P:171:TRP:HE1	1.74	0.53
6:G:74:LEU:HD12	6:G:79:ILE:HD11	1.91	0.53
14:O:130:TYR:HA	14:O:189:ASN:ND2	2.23	0.53
35:l:407:TRP:O	35:l:411:MET:HG2	2.09	0.53
35:l:473:PRO:HG2	35:l:475:MET:HE3	1.89	0.53
40:r:312:ALA:O	40:r:316:MET:HG3	2.09	0.53
40:r:403:THR:HA	40:r:406:TYR:CE2	2.44	0.53
44:w:123:SER:OG	44:w:125:ASP:OD1	2.25	0.53
1:A:40:ARG:NH1	1:A:289:GLU:O	2.42	0.52
14:O:168:LEU:HD23	14:O:169:PHE:CE1	2.44	0.52
26:c:96:ASP:N	26:c:96:ASP:OD1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:89:TYR:HB3	34:k:91:GLN:OE1	2.09	0.52
21:W:62:ILE:O	21:W:66:GLU:HG3	2.09	0.52
26:c:70:MET:SD	38:o:86:THR:HG22	2.50	0.52
27:d:68:PHE:CE2	28:e:114:MET:HE1	2.44	0.52
27:d:78:GLU:HB2	27:d:81:ASP:HB2	1.91	0.52
21:W:129:THR:O	21:W:133:ILE:HG13	2.10	0.52
12:M:213:MET:HB3	12:M:215:MET:HE2	1.92	0.52
5:F:46:LYS:HE2	12:M:674:LEU:HD21	1.92	0.52
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.90	0.52
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.44	0.52
35:l:286:LEU:HD22	35:l:411:MET:SD	2.48	0.52
42:u:59:GLU:O	42:u:63:VAL:HG13	2.10	0.52
44:w:258:TYR:HE2	44:w:269:VAL:HG13	1.74	0.52
32:i:334:THR:HG21	51:r:503:CDL:H391	1.91	0.52
34:k:57:ASN:HB3	36:m:143:ILE:HG13	1.92	0.52
36:m:45:LEU:HD23	36:m:50:SER:HA	1.92	0.52
1:A:290:GLU:HG3	1:A:291:GLU:N	2.24	0.52
9:J:141:PHE:HE2	9:J:180:TYR:CD1	2.22	0.52
21:W:130:ASN:HB3	36:m:1:MET:H3	1.74	0.52
31:h:24:GLU:HG3	31:h:24:GLU:O	2.09	0.52
40:r:191:SER:HB3	48:r:501:PEE:H3	1.92	0.52
2:B:70:LEU:HD11	48:B:303:PEE:H65	1.91	0.52
16:Q:192:LEU:HD12	16:Q:197:MET:HB3	1.91	0.52
25:b:28:LEU:HD12	25:b:28:LEU:N	2.25	0.52
48:i:402:PEE:H27	35:l:563:PRO:HA	1.91	0.52
34:k:22:TYR:CE2	35:l:588:PHE:CD2	2.98	0.52
35:l:375:ILE:HD12	35:l:458:LEU:HD11	1.92	0.52
44:w:67:CYS:HB2	44:w:218:ILE:CD1	2.39	0.52
26:c:58:ARG:NE	38:o:35:GLU:OE2	2.36	0.52
32:i:20:VAL:HG13	32:i:29:ILE:HG23	1.92	0.52
1:A:119:GLU:O	1:A:119:GLU:HG3	2.10	0.51
1:A:367:ILE:HG13	1:A:438:LEU:HD13	1.93	0.51
11:L:81:VAL:HG21	11:L:150:ARG:HG3	1.91	0.51
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.92	0.51
8:I:70:MET:HG3	15:P:66:ALA:HB1	1.92	0.51
32:i:294:MET:HA	32:i:294:MET:HE2	1.92	0.51
34:k:17:ALA:O	34:k:21:MET:HG2	2.10	0.51
35:l:559:GLU:O	35:l:563:PRO:HD2	2.10	0.51
1:A:54:LYS:C	1:A:54:LYS:CD	2.83	0.51
14:O:67:VAL:HG13	14:O:75:LYS:HG3	1.93	0.51
21:W:144:THR:HB	41:s:96:ILE:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:X:201:8Q1:O40	50:X:201:8Q1:N36	2.42	0.51
30:g:2:THR:HG22	30:g:4:MET:HG2	1.92	0.51
36:m:25:SER:O	36:m:27:ILE:N	2.43	0.51
38:o:9:SER:OG	38:o:10:ARG:N	2.43	0.51
43:v:18:ASP:OD1	43:v:18:ASP:C	2.52	0.51
33:j:49:LEU:N	33:j:50:PRO:HD2	2.26	0.51
36:m:57:PHE:CE2	41:s:108:MET:CE	2.91	0.51
14:O:140:CYS:O	14:O:145:SER:OG	2.25	0.51
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.91	0.51
51:l:701:CDL:C72	51:l:701:CDL:C76	2.86	0.51
9:J:217:PHE:HD1	9:J:220:MET:HE1	1.75	0.51
6:X:129:GLU:OE2	26:c:89:TRP:HZ2	1.93	0.51
35:l:324:LEU:HD13	35:l:395:ILE:HD13	1.91	0.51
36:m:57:PHE:O	36:m:57:PHE:CD1	2.64	0.51
40:r:42:LEU:HB3	40:r:453:MET:CE	2.41	0.51
42:u:83:THR:HA	42:u:86:TRP:CD1	2.46	0.51
40:r:12:LEU:HB2	40:r:13:PRO:HD3	1.93	0.51
12:M:650:SER:OG	12:M:652:ASN:OD1	2.28	0.51
15:P:44:ARG:HB3	15:P:45:PRO:HD3	1.92	0.51
17:S:39:ALA:HA	17:S:44:GLN:HG3	1.91	0.51
18:T:119:ARG:HD2	18:T:122:HIS:CD2	2.46	0.51
19:U:38:TYR:HB2	41:s:310:MET:O	2.11	0.51
21:W:51:MET:HA	41:s:313:SER:HB2	1.92	0.51
32:i:95:MET:HE3	32:i:99:THR:OG1	2.11	0.51
42:u:77:HIS:CD2	42:u:115:LEU:CD2	2.81	0.51
12:M:640:ASP:N	12:M:640:ASP:OD1	2.43	0.51
40:r:114:GLU:OE1	40:r:116:ILE:HG22	2.11	0.51
11:L:111:LEU:HD11	13:N:126:PRO:HG2	1.93	0.50
42:u:77:HIS:HD2	42:u:115:LEU:HD23	1.73	0.50
7:H:81:ILE:O	7:H:85:GLU:HG3	2.10	0.50
13:N:68:MET:CG	13:N:69:ASN:H	2.23	0.50
16:Q:196:ALA:O	16:Q:197:MET:HG3	2.10	0.50
22:Y:54:GLN:HE21	35:l:367:PRO:HD2	1.76	0.50
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.47	0.50
21:W:120:MET:CE	36:m:126:VAL:HG12	2.35	0.50
26:c:68:ASP:OD1	26:c:70:MET:HG2	2.10	0.50
1:A:451:GLN:O	1:A:451:GLN:OE1	2.29	0.50
5:F:24:CYS:O	5:F:34:ARG:NH1	2.44	0.50
6:G:115:GLN:OE1	6:G:115:GLN:O	2.28	0.50
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.92	0.50
41:s:306:SER:O	41:s:310:MET:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:241:TYR:CZ	9:J:348:LYS:HG3	2.47	0.50
26:c:185:GLU:OE2	43:v:37:ARG:HG2	2.12	0.50
9:J:343:THR:HG23	9:J:347:LEU:HD12	1.94	0.50
32:i:87:THR:CG2	32:i:88:LYS:H	2.24	0.50
15:P:43:THR:HA	15:P:47:ILE:HD12	1.93	0.50
35:l:161:ARG:NH2	39:p:88:GLY:O	2.45	0.50
16:Q:47:PHE:HD1	16:Q:52:MET:HE1	1.76	0.50
27:d:159:GLN:HG2	27:d:163:MET:HE2	1.93	0.50
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.47	0.50
39:p:29:SER:HB3	39:p:76:HIS:HD2	1.76	0.50
40:r:328:CYS:HB3	40:r:437:MET:HE1	1.93	0.50
5:F:64:LYS:HE3	5:F:66:TRP:NE1	2.26	0.50
44:w:38:TYR:OH	44:w:292:HIS:ND1	2.38	0.50
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.94	0.49
1:A:408:GLU:O	1:A:411:SER:HB3	2.11	0.49
1:A:451:GLN:OE1	1:A:451:GLN:CA	2.60	0.49
4:E:16:SER:HB3	11:L:52:LEU:HB3	1.93	0.49
35:l:525:MET:SD	39:p:77:PRO:HB2	2.52	0.49
51:l:701:CDL:H651	51:l:701:CDL:C86	2.42	0.49
38:o:113:GLU:OE1	38:o:113:GLU:HA	2.11	0.49
12:M:284:GLU:HG2	12:M:284:GLU:O	2.12	0.49
12:M:298:LYS:HA	13:N:134:ILE:HD13	1.94	0.49
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.94	0.49
51:l:701:CDL:C31	51:l:701:CDL:H761	2.41	0.49
15:P:172:ASP:OD2	15:P:187:ILE:N	2.44	0.49
24:a:154:LEU:HD21	32:i:272:LYS:HD2	1.93	0.49
12:M:390:THR:HA	12:M:600:GLU:HG2	1.95	0.49
35:l:331:MET:HE2	35:l:331:MET:CA	2.42	0.49
4:E:64:ARG:O	4:E:68:MET:HG2	2.13	0.49
6:G:84:LEU:O	6:G:88:LYS:HG2	2.13	0.49
15:P:164:ASN:OD1	15:P:181:HIS:NE2	2.45	0.49
15:P:213:ASP:HB3	15:P:216:VAL:HG22	1.94	0.49
28:e:92:PHE:O	28:e:96:SER:HB2	2.12	0.49
44:w:166:ASP:OD2	44:w:187:TYR:OH	2.24	0.49
6:G:74:LEU:H	6:G:74:LEU:HD23	1.77	0.49
9:J:192:ARG:NH2	9:J:262:THR:OG1	2.46	0.49
25:b:32:GLU:HG3	39:p:115:TYR:HA	1.95	0.49
35:l:4:PHE:CD2	35:l:61:MET:HG3	2.48	0.49
40:r:114:GLU:OE1	40:r:116:ILE:N	2.45	0.49
48:B:303:PEE:H20	41:s:183:MET:CE	2.42	0.49
14:O:130:TYR:HA	14:O:189:ASN:HD21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:149:ILE:HD11	32:i:195:PRO:HG3	1.93	0.49
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.93	0.49
36:m:57:PHE:CZ	41:s:111:LEU:HG	2.48	0.49
24:a:53:ARG:NH2	25:b:29:SER:O	2.44	0.49
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.47	0.49
34:k:34:GLU:OE1	36:m:64:MET:SD	2.71	0.49
1:A:88:ARG:HG3	1:A:274:LYS:NZ	2.27	0.49
9:J:136:THR:HG23	9:J:138:ASN:H	1.77	0.49
10:K:91:VAL:O	10:K:94:SER:OG	2.25	0.49
20:V:105:THR:HG21	20:V:110:ILE:HD13	1.95	0.49
44:w:261:ARG:NH1	44:w:264:GLU:HG3	2.27	0.49
1:A:250:VAL:O	1:A:254:ILE:HG12	2.11	0.49
6:G:138:LEU:HD23	6:G:144:ILE:HG12	1.95	0.49
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.47	0.49
14:O:153:GLN:HE22	14:O:160:VAL:HA	1.77	0.49
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.47	0.49
2:B:65:GLU:OE2	16:Q:266:ARG:NE	2.36	0.48
9:J:110:GLY:CA	9:J:148:ILE:HD11	2.43	0.48
13:N:11:LEU:HA	13:N:14:VAL:HG12	1.95	0.48
6:X:90:TYR:HE1	23:Z:44:PRO:HB2	1.77	0.48
22:Y:102:ASP:OD2	43:v:114:ARG:NH1	2.46	0.48
35:l:119:LYS:NZ	51:l:701:CDL:H512	2.28	0.48
40:r:331:ASN:O	40:r:335:GLU:HG3	2.13	0.48
1:A:102:MET:HG2	1:A:149:MET:CB	2.29	0.48
6:G:82:ARG:O	6:G:86:VAL:HG13	2.14	0.48
12:M:255:ASP:OD1	12:M:257:VAL:N	2.36	0.48
14:O:207:GLU:OE2	14:O:212:LYS:CE	2.61	0.48
3:C:71:CYS:HB3	16:Q:141:TYR:CB	2.42	0.48
21:W:50:MET:HE2	41:s:156:MET:HG3	1.94	0.48
33:j:68:GLU:OE1	33:j:98:LEU:HD13	2.13	0.48
36:m:1:MET:CE	36:m:4:TYR:HA	2.43	0.48
36:m:3:MET:N	36:m:3:MET:HE2	2.29	0.48
41:s:307:LEU:O	41:s:311:THR:OG1	2.30	0.48
1:A:98:LYS:HA	1:A:101:PHE:CE2	2.48	0.48
1:A:278:ILE:HD11	1:A:299:LEU:HD21	1.94	0.48
9:J:272:LEU:HB3	9:J:275:ASP:OD1	2.12	0.48
32:i:122:ILE:O	32:i:176:ARG:NH1	2.47	0.48
34:k:38:LEU:O	34:k:42:ILE:HG12	2.14	0.48
5:F:36:PHE:HD1	5:F:40:ARG:HD3	1.78	0.48
12:M:255:ASP:OD1	12:M:255:ASP:C	2.56	0.48
13:N:85:GLU:OE1	13:N:85:GLU:N	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:1:MET:CE	36:m:4:TYR:N	2.76	0.48
1:A:326:LEU:HD11	1:A:363:ILE:HD11	1.96	0.48
9:J:171:ASN:HA	9:J:327:MET:SD	2.54	0.48
13:N:68:MET:HG3	13:N:69:ASN:N	2.26	0.48
21:W:120:MET:HG3	36:m:126:VAL:O	2.13	0.48
22:Y:76:ASP:O	35:l:385:TYR:OH	2.26	0.48
34:k:5:TYR:CG	34:k:43:MET:HE1	2.48	0.48
13:N:68:MET:HG2	13:N:115:PHE:CE2	2.49	0.48
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.96	0.48
56:s:401:UQ:HM53	56:s:401:UQ:H72	1.69	0.48
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.30	0.48
6:G:147:TYR:HD1	6:G:148:ILE:HD13	1.78	0.48
12:M:203:ASP:OD1	12:M:203:ASP:N	2.35	0.48
12:M:250:SER:OG	12:M:251:ILE:N	2.47	0.48
19:U:8:PHE:CD1	19:U:8:PHE:C	2.91	0.48
49:j:201:PLX:H312	49:j:201:PLX:H282	1.63	0.48
4:E:45:ASN:N	4:E:45:ASN:OD1	2.47	0.48
36:m:57:PHE:HD1	36:m:61:LEU:HD12	1.78	0.48
2:B:101:HIS:ND1	2:B:149:MET:HE1	2.28	0.48
15:P:154:GLU:OE2	15:P:180:ASN:ND2	2.47	0.48
35:l:327:LEU:O	35:l:331:MET:HG2	2.14	0.48
36:m:23:LYS:N	36:m:24:PRO:HD3	2.29	0.48
44:w:67:CYS:SG	44:w:218:ILE:HD13	2.54	0.48
44:w:81:LEU:HB3	44:w:83:LEU:HG	1.95	0.48
26:c:126:TRP:HA	26:c:129:MET:HE2	1.96	0.47
30:g:36:MET:HE1	49:g:201:PLX:H382	1.96	0.47
32:i:87:THR:HG22	32:i:88:LYS:H	1.78	0.47
51:l:701:CDL:HA62	51:l:701:CDL:C54	2.43	0.47
36:m:52:LEU:O	36:m:56:VAL:HG23	2.14	0.47
1:A:89:GLY:O	47:A:503:NAI:H2N	2.13	0.47
9:J:195:PHE:HB3	9:J:198:ALA:HB2	1.96	0.47
36:m:10:SER:O	36:m:14:VAL:HG23	2.13	0.47
5:F:23:LEU:O	5:F:57:GLU:HA	2.14	0.47
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.29	0.47
35:l:119:LYS:NZ	51:l:701:CDL:C51	2.78	0.47
42:u:153:GLU:OE2	42:u:155:GLU:OE1	2.33	0.47
44:w:72:ARG:NH2	44:w:263:ALA:O	2.48	0.47
6:G:149:ALA:O	6:G:153:ASP:N	2.45	0.47
21:W:96:ILE:O	21:W:99:LYS:HD3	2.14	0.47
40:r:42:LEU:HB3	40:r:453:MET:HE1	1.95	0.47
1:A:385:CYS:O	1:A:389:VAL:HB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:C:303:PLX:H252	49:C:303:PLX:H82	1.96	0.47
9:J:204:SER:O	9:J:204:SER:OG	2.33	0.47
32:i:87:THR:CG2	32:i:88:LYS:N	2.78	0.47
49:j:201:PLX:H182	49:j:201:PLX:H152	1.78	0.47
34:k:30:LEU:O	34:k:34:GLU:HG2	2.14	0.47
41:s:124:ASN:C	41:s:124:ASN:HD22	2.22	0.47
1:A:46:TYR:CD2	14:O:226:GLU:HB3	2.49	0.47
5:F:65:LEU:HB3	5:F:77:VAL:HG23	1.97	0.47
9:J:192:ARG:NH1	9:J:198:ALA:O	2.48	0.47
40:r:108:MET:HE3	40:r:121:LEU:HD22	1.97	0.47
44:w:65:ASN:HB3	44:w:214:ILE:CD1	2.45	0.47
1:A:71:LYS:NZ	14:O:248:GLY:O	2.48	0.47
5:F:64:LYS:HZ1	5:F:76:ASN:HB2	1.77	0.47
12:M:408:ARG:HG3	12:M:415:ASN:ND2	2.30	0.47
13:N:65:THR:O	13:N:73:THR:OG1	2.32	0.47
15:P:72:TYR:CD1	15:P:92:GLY:HA3	2.50	0.47
19:U:14:ALA:O	19:U:15:LYS:HG2	2.14	0.47
21:W:120:MET:CE	36:m:127:ILE:HA	2.45	0.47
24:a:115:HIS:O	24:a:119:ARG:HG3	2.15	0.47
35:l:119:LYS:HZ1	51:l:701:CDL:H511	1.79	0.47
39:p:47:ARG:NH2	39:p:70:GLU:OE1	2.47	0.47
6:G:121:ALA:HA	6:G:124:ASP:OD1	2.15	0.47
50:X:201:8Q1:S44	39:p:63:LEU:HB3	2.55	0.47
24:a:136:THR:HG21	40:r:48:ASN:HD22	1.78	0.47
1:A:284:HIS:CE1	14:O:228:ALA:HB3	2.50	0.47
12:M:651:PRO:O	12:M:655:ARG:NH1	2.48	0.47
21:W:120:MET:HE2	36:m:126:VAL:C	2.40	0.47
6:X:129:GLU:OE2	26:c:89:TRP:CZ2	2.68	0.47
33:j:16:LEU:O	33:j:20:ILE:HG23	2.14	0.47
35:l:62:ILE:HD13	35:l:81:LYS:HA	1.95	0.47
40:r:14:MET:SD	40:r:26:ASN:HB3	2.54	0.47
3:C:64:PRO:HB3	3:C:102:VAL:HG13	1.97	0.47
14:O:185:MET:HE1	14:O:192:TYR:CD2	2.50	0.47
20:V:76:ILE:N	20:V:76:ILE:HD13	2.29	0.47
22:Y:45:ARG:HG2	35:l:439:PRO:HB3	1.97	0.47
25:b:86:LEU:HD11	35:l:9:LEU:HD12	1.96	0.47
27:d:119:GLU:OE2	43:v:52:MET:HG2	2.15	0.47
32:i:217:MET:HE1	32:i:329:MET:HG3	1.96	0.47
43:v:30:GLY:H	43:v:104:ARG:HH22	1.62	0.47
2:B:200:GLU:HG3	13:N:88:ARG:HB2	1.97	0.46
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:163:ASN:O	11:L:171:ARG:HA	2.15	0.46
21:W:68:ARG:HD2	36:m:135:PHE:HD2	1.80	0.46
24:a:50:HIS:HB3	24:a:52:LYS:HE3	1.97	0.46
35:l:284:THR:O	35:l:288:THR:OG1	2.28	0.46
49:r:502:PLX:H152	49:r:502:PLX:H121	1.53	0.46
4:E:42:GLU:OE1	4:E:94:ILE:CG1	2.60	0.46
4:E:49:LEU:HD23	4:E:49:LEU:C	2.39	0.46
14:O:201:ILE:O	14:O:205:ILE:HD13	2.15	0.46
20:V:140:LYS:HD2	32:i:274:GLU:OE1	2.15	0.46
32:i:249:LEU:HD22	32:i:254:LEU:HD12	1.97	0.46
33:j:15:SER:HA	41:s:76:ILE:HD12	1.96	0.46
35:l:534:HIS:CD2	48:l:703:PHE:H13	2.49	0.46
51:l:702:CDL:H382	51:l:702:CDL:H351	1.63	0.46
36:m:57:PHE:CE1	41:s:111:LEU:CG	2.97	0.46
43:v:115:ARG:HG3	43:v:115:ARG:HH11	1.79	0.46
3:C:124:MET:HA	3:C:125:PRO:HD3	1.79	0.46
28:e:152:ASP:OD1	28:e:152:ASP:N	2.43	0.46
35:l:488:MET:O	35:l:492:ILE:HG12	2.14	0.46
36:m:57:PHE:HE1	41:s:111:LEU:CG	2.27	0.46
44:w:165:SER:HB3	44:w:245:PHE:CE1	2.50	0.46
1:A:288:VAL:HG21	1:A:303:HIS:ND1	2.31	0.46
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.51	0.46
3:C:71:CYS:HB3	16:Q:141:TYR:HB2	1.97	0.46
12:M:336:ASN:O	12:M:336:ASN:ND2	2.48	0.46
16:Q:440:LYS:HA	16:Q:440:LYS:HD3	1.74	0.46
2:B:100:GLU:O	2:B:170:GLY:N	2.38	0.46
9:J:126:VAL:HG23	9:J:161:VAL:HG11	1.98	0.46
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.98	0.46
6:X:137:LYS:HD3	25:b:4:TYR:CE1	2.50	0.46
24:a:83:ALA:HA	51:a:201:CDL:H162	1.98	0.46
27:d:23:GLN:HA	27:d:23:GLN:OE1	2.14	0.46
31:h:69:ARG:HD2	31:h:72:THR:HG21	1.97	0.46
32:i:109:SER:O	32:i:157:MET:HG2	2.16	0.46
35:l:419:THR:HA	35:l:422:TYR:CE2	2.50	0.46
12:M:133:GLN:O	12:M:137:CYS:HB2	2.16	0.46
25:b:10:LEU:O	25:b:14:GLN:HG3	2.15	0.46
43:v:111:ARG:HH21	43:v:115:ARG:CZ	2.27	0.46
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.51	0.46
12:M:385:TYR:OH	12:M:527:ASP:OD1	2.29	0.46
18:T:84:ILE:HD12	18:T:84:ILE:HA	1.78	0.46
26:c:81:ARG:NH1	26:c:85:GLU:OE1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:121:TYR:CD2	35:l:203:MET:HE3	2.42	0.46
35:l:80:PHE:HB3	35:l:82:MET:HE2	1.97	0.46
35:l:260:LEU:HD22	35:l:267:MET:HE3	1.97	0.46
51:l:701:CDL:C54	51:l:701:CDL:CA6	2.94	0.46
39:p:144:THR:HA	39:p:145:PRO:HD3	1.73	0.46
1:A:32:PHE:HD2	1:A:291:GLU:OE2	1.98	0.46
16:Q:259:GLU:HG2	16:Q:263:THR:OG1	2.15	0.46
20:V:81:ARG:NH1	20:V:89:ASN:OD1	2.43	0.46
27:d:127:LYS:H	27:d:127:LYS:HE2	1.80	0.46
39:p:29:SER:HB3	39:p:76:HIS:CD2	2.51	0.46
39:p:100:PRO:HG3	40:r:419:TYR:CE1	2.51	0.46
9:J:204:SER:OG	9:J:238:GLN:O	2.32	0.46
11:L:133:ASP:OD1	11:L:133:ASP:N	2.48	0.46
12:M:193:ASP:OD1	14:O:111:ARG:NH2	2.47	0.46
22:Y:42:PRO:HB3	35:l:442:LEU:HD23	1.97	0.46
43:v:35:LYS:HD3	43:v:36:GLU:H	1.81	0.46
13:N:69:ASN:ND2	13:N:112:ASN:OD1	2.33	0.46
27:d:127:LYS:H	27:d:127:LYS:HE3	1.79	0.46
51:i:401:CDL:H151	51:i:401:CDL:H122	1.58	0.46
34:k:37:MET:HE2	34:k:67:ALA:HB3	1.98	0.46
44:w:95:ASP:OD1	44:w:95:ASP:N	2.49	0.46
1:A:392:MET:CE	1:A:419:ILE:HD12	2.45	0.45
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.96	0.45
38:o:105:PHE:CD2	40:r:263:MET:HE1	2.51	0.45
44:w:66:ILE:O	44:w:214:ILE:HD11	2.16	0.45
12:M:278:HIS:CE1	12:M:280:ASP:HB2	2.51	0.45
24:a:54:LEU:C	25:b:28:LEU:CD1	2.89	0.45
2:B:65:GLU:OE2	16:Q:266:ARG:HB3	2.16	0.45
5:F:64:LYS:NZ	5:F:64:LYS:HB3	2.31	0.45
6:X:129:GLU:HB3	39:p:82:PHE:CD2	2.51	0.45
22:Y:97:LEU:HD12	43:v:104:ARG:HB2	1.99	0.45
28:e:137:MET:HE3	28:e:137:MET:HB2	1.65	0.45
49:g:201:PLX:H72	49:g:201:PLX:H101	1.71	0.45
44:w:110:GLY:HA2	44:w:134:TRP:CD2	2.51	0.45
44:w:176:GLN:NE2	44:w:236:ASP:OD2	2.49	0.45
6:G:147:TYR:CD1	6:G:147:TYR:C	2.94	0.45
9:J:241:TYR:HD1	9:J:242:ILE:N	2.15	0.45
12:M:327:ALA:HB1	12:M:630:ALA:HB2	1.97	0.45
21:W:137:THR:HG22	21:W:138:TYR:CD1	2.52	0.45
51:i:401:CDL:H142	51:i:401:CDL:H171	1.53	0.45
39:p:26:HIS:CD2	39:p:79:PRO:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:63:LEU:O	39:p:64:LEU:HB3	2.16	0.45
40:r:10:MET:HE2	40:r:10:MET:HA	1.97	0.45
40:r:73:LEU:HA	40:r:76:MET:HE2	1.98	0.45
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.97	0.45
42:u:76:ARG:NE	42:u:77:HIS:CE1	2.84	0.45
1:A:451:GLN:OE1	1:A:451:GLN:HA	2.17	0.45
4:E:49:LEU:C	4:E:49:LEU:CD2	2.90	0.45
16:Q:40:ASP:OD1	16:Q:40:ASP:N	2.49	0.45
40:r:11:LEU:HD23	40:r:14:MET:HE3	1.99	0.45
41:s:66:SER:HB2	41:s:122:ALA:O	2.16	0.45
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.97	0.45
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.99	0.45
25:b:74:HIS:NE2	35:l:35:TYR:OH	2.39	0.45
41:s:107:ALA:O	41:s:111:LEU:HD23	2.16	0.45
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.98	0.45
1:A:102:MET:HE3	1:A:111:LYS:HB3	1.99	0.45
4:E:25:MET:O	4:E:29:LYS:HG3	2.17	0.45
4:E:88:MET:CE	15:P:171:TRP:HE1	2.29	0.45
5:F:36:PHE:CD1	5:F:40:ARG:HD3	2.52	0.45
15:P:44:ARG:HE	15:P:45:PRO:HD3	1.81	0.45
16:Q:335:GLU:CD	16:Q:339:GLN:HE21	2.24	0.45
10:K:85:THR:HG22	10:K:89:LEU:HD11	1.99	0.45
21:W:54:ASN:ND2	41:s:156:MET:HE2	2.32	0.45
30:g:73:PHE:HE2	49:g:201:PLX:H392	1.81	0.45
32:i:265:MET:HE1	42:u:167:LEU:HD11	1.99	0.45
32:i:329:MET:HE2	32:i:329:MET:HA	1.99	0.45
33:j:4:MET:HE2	48:m:201:PEE:H19	1.98	0.45
36:m:57:PHE:HE1	41:s:111:LEU:HG	1.76	0.45
43:v:103:GLU:OE2	43:v:107:ARG:NE	2.49	0.45
12:M:347:ASP:HB3	12:M:594:ALA:HB1	1.98	0.45
25:b:16:ARG:HD3	25:b:20:ARG:NH1	2.30	0.45
35:l:124:PHE:HE1	35:l:252:MET:HG3	1.82	0.45
40:r:226:ALA:HA	40:r:229:MET:HE3	1.99	0.45
1:A:185:ASN:C	1:A:187:CYS:H	2.25	0.45
2:B:131:GLU:HB2	2:B:144:ARG:HB3	2.00	0.45
9:J:116:ILE:O	9:J:120:VAL:HG22	2.17	0.45
27:d:168:LYS:HE3	27:d:168:LYS:HB2	1.83	0.45
32:i:280:THR:O	32:i:284:MET:HG2	2.16	0.45
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.52	0.45
1:A:129:GLU:OE1	1:A:129:GLU:HA	2.16	0.44
1:A:169:LEU:HD22	1:A:197:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:MET:HB3	16:Q:200:PHE:HZ	1.83	0.44
9:J:241:TYR:O	9:J:245:VAL:HG23	2.17	0.44
12:M:211:GLU:H	12:M:211:GLU:CD	2.13	0.44
12:M:531:LYS:HE3	12:M:531:LYS:HB2	1.72	0.44
14:O:168:LEU:HB3	14:O:169:PHE:CD1	2.52	0.44
16:Q:102:SER:O	16:Q:102:SER:OG	2.27	0.44
21:W:134:LEU:HD21	36:m:2:THR:OG1	2.17	0.44
24:a:133:TYR:OH	27:d:87:GLU:OE1	2.22	0.44
35:l:19:ILE:HG22	51:l:701:CDL:H831	1.99	0.44
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.98	0.44
43:v:17:PRO:HB3	43:v:105:GLU:HG2	1.97	0.44
4:E:119:LEU:HD21	12:M:628:GLU:HG2	1.99	0.44
6:G:134:ASP:O	6:G:138:LEU:HD13	2.18	0.44
8:I:108:LYS:HE2	8:I:108:LYS:HB2	1.74	0.44
13:N:68:MET:HG2	13:N:115:PHE:CD2	2.52	0.44
16:Q:79:ASN:HA	16:Q:101:LEU:O	2.17	0.44
26:c:42:PRO:HA	26:c:47:GLU:OE2	2.17	0.44
33:j:68:GLU:HG2	36:m:161:LEU:HD13	1.98	0.44
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.99	0.44
41:s:98:MET:HE1	41:s:104:PHE:HB2	1.99	0.44
14:O:204:ILE:HD11	14:O:219:ARG:HH21	1.82	0.44
6:X:80:LYS:HE3	6:X:80:LYS:HB3	1.57	0.44
6:X:154:VAL:O	6:X:154:VAL:HG12	2.16	0.44
25:b:28:LEU:N	25:b:28:LEU:CD1	2.81	0.44
35:l:337:ALA:O	35:l:341:MET:HG3	2.17	0.44
1:A:185:ASN:O	1:A:187:CYS:N	2.51	0.44
8:I:96:THR:HG22	15:P:105:ASN:HD22	1.82	0.44
35:l:249:SER:OG	35:l:336:LYS:HG3	2.16	0.44
40:r:259:TYR:O	40:r:263:MET:HG2	2.18	0.44
40:r:300:ALA:O	40:r:308:SER:HB3	2.17	0.44
51:r:503:CDL:H832	51:r:503:CDL:H862	1.31	0.44
1:A:202:GLY:H	14:O:121:MET:HE2	1.83	0.44
49:C:303:PLX:H311	49:C:303:PLX:H281	1.83	0.44
5:F:34:ARG:NH1	5:F:34:ARG:HB2	2.31	0.44
24:a:139:ILE:HG23	40:r:54:LEU:HD23	1.99	0.44
24:a:152:LYS:HE3	30:g:96:VAL:HG21	1.99	0.44
25:b:117:ILE:N	25:b:117:ILE:HD12	2.32	0.44
25:b:123:PHE:HD2	43:v:40:VAL:HG11	1.83	0.44
27:d:43:ARG:HB2	27:d:44:PRO:HD3	1.98	0.44
32:i:326:LEU:HB3	32:i:327:PRO:HD3	2.00	0.44
40:r:237:LYS:NZ	40:r:316:MET:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:LYS:NZ	2:B:174:GLU:OE2	2.49	0.44
48:B:303:PEE:H2O	41:s:183:MET:HE2	2.00	0.44
4:E:56:VAL:HG12	4:E:60:ARG:HD2	1.97	0.44
7:H:105:GLU:OE2	7:H:105:GLU:HA	2.18	0.44
9:J:148:ILE:HD13	9:J:148:ILE:HA	1.72	0.44
48:U:101:PEE:H67	48:U:101:PEE:H73	1.73	0.44
35:l:356:ILE:HA	35:l:359:MET:HG2	2.00	0.44
39:p:176:GLU:HG3	39:p:177:ARG:N	2.32	0.44
1:A:102:MET:HB3	1:A:149:MET:CG	2.43	0.44
11:L:77:VAL:HG23	11:L:145:PHE:HB3	1.99	0.44
12:M:638:THR:O	12:M:642:VAL:HG23	2.18	0.44
14:O:208:LEU:HD23	14:O:208:LEU:HA	1.81	0.44
20:V:29:GLY:O	20:V:63:SER:OG	2.32	0.44
44:w:211:VAL:N	44:w:212:PRO:CD	2.80	0.44
1:A:87:GLY:N	1:A:93:PHE:O	2.51	0.44
7:H:44:TYR:HB2	15:P:68:ILE:HG23	2.00	0.44
9:J:212:ARG:O	9:J:216:TYR:HB3	2.17	0.44
15:P:69:LEU:HD22	15:P:96:VAL:HG22	2.00	0.44
17:S:66:LEU:HD12	17:S:66:LEU:HA	1.84	0.44
26:c:169:GLU:HA	27:d:123:GLN:HB2	2.00	0.44
35:l:341:MET:CE	35:l:457:LEU:HD12	2.46	0.44
38:o:101:TRP:HB3	40:r:263:MET:CE	2.47	0.44
40:r:201:MET:HA	40:r:204:MET:HB2	2.00	0.44
42:u:76:ARG:HE	42:u:77:HIS:HE1	1.62	0.44
5:F:30:SER:OG	5:F:63:PRO:HG3	2.18	0.44
12:M:707:MET:HE2	12:M:707:MET:HA	1.99	0.44
14:O:196:LEU:HG	14:O:201:ILE:HD13	2.00	0.44
14:O:207:GLU:OE2	14:O:212:LYS:HE3	2.18	0.44
6:X:105:MET:SD	6:X:105:MET:N	2.91	0.44
22:Y:105:ASP:O	43:v:115:ARG:NE	2.48	0.44
32:i:323:MET:HG2	51:i:401:CDL:HA32	2.00	0.44
34:k:22:TYR:O	35:l:585:LYS:NZ	2.38	0.44
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.98	0.44
40:r:121:LEU:O	40:r:125:THR:HG23	2.18	0.44
44:w:250:SER:O	44:w:280:LYS:NZ	2.45	0.44
6:G:105:MET:HE2	6:G:105:MET:HA	2.00	0.43
20:V:107:SER:CB	20:V:110:ILE:HG22	2.48	0.43
24:a:163:ARG:HH22	30:g:102:ASP:CG	2.26	0.43
39:p:168:TRP:O	39:p:172:THR:OG1	2.26	0.43
9:J:129:LEU:HD23	9:J:167:ILE:HG13	2.00	0.43
9:J:141:PHE:CE2	9:J:180:TYR:HD1	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:100:LYS:O	14:O:104:ILE:HG13	2.17	0.43
20:V:140:LYS:NZ	32:i:274:GLU:OE1	2.32	0.43
6:X:119:ILE:HG21	6:X:135:ALA:HB1	2.00	0.43
26:c:69:GLY:HA3	38:o:86:THR:HG21	1.99	0.43
29:f:64:GLU:OE1	29:f:64:GLU:HA	2.18	0.43
36:m:25:SER:O	36:m:28:TYR:N	2.49	0.43
38:o:105:PHE:HD2	40:r:263:MET:HE1	1.82	0.43
40:r:306:PRO:HA	40:r:458:LEU:HD22	2.00	0.43
40:r:336:ARG:NH2	40:r:429:SER:HA	2.33	0.43
51:r:503:CDL:H362	51:r:503:CDL:H392	1.53	0.43
41:s:172:ILE:HG13	41:s:176:PHE:HD2	1.83	0.43
43:v:7:ARG:NE	43:v:16:GLU:OE2	2.45	0.43
1:A:201:ALA:O	14:O:119:TYR:HB3	2.18	0.43
1:A:261:TRP:O	1:A:264:SER:OG	2.31	0.43
12:M:478:SER:O	12:M:482:GLN:HG2	2.17	0.43
14:O:198:PRO:O	14:O:201:ILE:HG22	2.18	0.43
16:Q:57:GLU:HG2	16:Q:58:THR:N	2.33	0.43
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	2.00	0.43
26:c:149:ILE:O	26:c:151:PRO:HD3	2.18	0.43
27:d:74:ILE:HG23	27:d:156:LEU:HD22	2.00	0.43
51:l:701:CDL:CA6	51:l:701:CDL:H542	2.48	0.43
40:r:97:THR:HG21	51:r:503:CDL:H242	2.01	0.43
41:s:62:ARG:HH11	41:s:64:ALA:HA	1.82	0.43
1:A:54:LYS:HE2	1:A:54:LYS:CA	2.39	0.43
6:G:140:CYS:SG	6:G:143:GLU:HG3	2.58	0.43
9:J:106:MET:HE2	9:J:106:MET:HB3	1.82	0.43
12:M:389:THR:O	12:M:390:THR:OG1	2.30	0.43
14:O:222:ARG:NH2	14:O:225:CYS:HA	2.34	0.43
15:P:107:GLN:OE1	15:P:136:ARG:HG2	2.17	0.43
20:V:12:ILE:HB	20:V:21:LYS:HE3	2.00	0.43
20:V:126:LYS:HA	20:V:126:LYS:HD3	1.87	0.43
32:i:81:SER:O	32:i:83:GLN:N	2.48	0.43
32:i:222:SER:O	32:i:224:ALA:N	2.50	0.43
51:l:701:CDL:H742	51:l:701:CDL:CA7	2.49	0.43
40:r:14:MET:CE	40:r:30:HIS:ND1	2.76	0.43
1:A:208:GLU:OE1	1:A:223:PRO:HB3	2.19	0.43
1:A:319:PRO:CB	1:A:337:MET:HE1	2.48	0.43
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.83	0.43
8:I:109:ASP:OD1	8:I:109:ASP:C	2.62	0.43
12:M:255:ASP:O	12:M:520:ALA:HB2	2.19	0.43
14:O:100:LYS:O	14:O:103:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:4:GLU:HG2	41:s:43:TYR:CE2	2.53	0.43
28:e:70:ASN:O	28:e:73:SER:HB2	2.19	0.43
35:l:10:THR:O	35:l:14:ILE:HG23	2.19	0.43
3:C:133:MET:HE2	3:C:168:PRO:HD2	1.99	0.43
49:C:303:PLX:H21	49:C:303:PLX:H1C3	1.66	0.43
7:H:38:ILE:O	7:H:45:ARG:NH1	2.43	0.43
8:I:54:TYR:CE2	8:I:58:ASP:OD1	2.72	0.43
8:I:107:SER:C	8:I:109:ASP:H	2.27	0.43
12:M:36:VAL:HB	12:M:56:VAL:HG21	2.00	0.43
12:M:307:ILE:HG22	12:M:582:VAL:HG22	2.00	0.43
51:i:401:CDL:H312	51:i:401:CDL:H342	1.66	0.43
36:m:63:GLY:O	36:m:67:VAL:HG23	2.19	0.43
36:m:129:ASP:OD1	36:m:129:ASP:N	2.44	0.43
44:w:295:ARG:HA	44:w:298:VAL:HG22	2.00	0.43
1:A:100:SER:O	1:A:101:PHE:C	2.60	0.43
2:B:171:PRO:HB3	13:N:93:MET:HE1	2.00	0.43
4:E:28:ALA:HB1	4:E:79:VAL:HG11	2.01	0.43
9:J:275:ASP:OD1	9:J:275:ASP:N	2.40	0.43
12:M:632:MET:H	12:M:632:MET:HG2	1.73	0.43
26:c:148:GLU:OE2	35:l:405:ASN:ND2	2.38	0.43
51:r:503:CDL:H742	51:r:503:CDL:H271	2.01	0.43
44:w:246:LEU:HD12	44:w:255:VAL:HG11	2.00	0.43
9:J:136:THR:HG23	9:J:139:PHE:H	1.83	0.43
12:M:185:PHE:CZ	12:M:221:ASN:HB2	2.54	0.43
14:O:149:LEU:O	14:O:153:GLN:HG2	2.19	0.43
14:O:185:MET:HE1	14:O:192:TYR:CE2	2.54	0.43
14:O:236:GLU:HG2	14:O:237:PRO:HD2	2.00	0.43
28:e:151:GLU:N	28:e:151:GLU:OE1	2.52	0.43
32:i:276:ILE:HG21	48:r:501:PEE:H14	2.01	0.43
2:B:135:ARG:HD3	2:B:141:ARG:HG3	2.01	0.43
4:E:41:ARG:HD3	6:G:120:MET:SD	2.59	0.43
12:M:360:ARG:HE	12:M:634:LEU:HD23	1.83	0.43
14:O:164:THR:CG2	14:O:169:PHE:H	2.32	0.43
15:P:89:HIS:CG	15:P:90:PRO:HD2	2.54	0.43
16:Q:450:ILE:O	16:Q:453:THR:HG22	2.19	0.43
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.54	0.43
36:m:57:PHE:CE1	41:s:111:LEU:HD21	2.54	0.43
39:p:64:LEU:HA	39:p:67:ALA:HB3	2.01	0.43
51:r:503:CDL:H782	51:r:503:CDL:H381	2.01	0.43
44:w:59:VAL:HG13	44:w:201:PRO:HA	2.00	0.43
44:w:72:ARG:HH11	44:w:72:ARG:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:350:LYS:HA	44:w:350:LYS:HD3	1.84	0.43
2:B:77:LEU:HD12	41:s:31:MET:HG3	2.01	0.43
3:C:161:ILE:HG13	3:C:180:LEU:HB2	2.01	0.43
5:F:71:PHE:CD1	12:M:362:ASP:HB2	2.53	0.43
9:J:130:VAL:O	52:J:401:NDP:O3D	2.37	0.43
13:N:41:GLU:HG2	13:N:47:LYS:HD3	2.01	0.43
17:S:69:ILE:HD13	42:u:20:VAL:HG13	2.01	0.43
26:c:70:MET:HE1	35:l:552:LEU:HD13	2.00	0.43
26:c:184:TYR:HA	43:v:34:ARG:NH1	2.34	0.43
27:d:101:GLU:CG	28:e:119:ARG:HD2	2.48	0.43
34:k:37:MET:HE1	36:m:64:MET:HE1	2.00	0.43
35:l:20:MET:HG3	51:l:701:CDL:H832	2.01	0.43
35:l:49:VAL:HB	35:l:50:PRO:HD3	2.01	0.43
35:l:298:ILE:O	35:l:302:VAL:HG23	2.19	0.43
51:l:701:CDL:H542	51:l:701:CDL:HA61	2.00	0.43
38:o:3:PHE:CE2	39:p:70:GLU:HG3	2.54	0.43
1:A:62:TRP:CD2	1:A:181:LEU:HD13	2.53	0.42
1:A:134:ASP:OD2	1:A:137:LYS:HD2	2.19	0.42
6:G:119:ILE:HG21	6:G:135:ALA:HB1	2.01	0.42
7:H:90:LEU:HB2	15:P:102:ASP:HB3	2.01	0.42
16:Q:345:SER:HB2	21:W:19:ILE:HD12	2.01	0.42
30:g:52:ARG:HH21	32:i:318:GLU:CD	2.27	0.42
34:k:37:MET:HE2	34:k:67:ALA:CB	2.49	0.42
35:l:293:ILE:HD12	35:l:293:ILE:HA	1.82	0.42
35:l:536:LEU:HB3	35:l:537:PRO:HD3	2.00	0.42
51:l:701:CDL:H351	51:l:701:CDL:H322	1.84	0.42
41:s:233:MET:HE1	41:s:234:MET:HE3	2.00	0.42
43:v:93:LEU:O	43:v:96:VAL:HG12	2.20	0.42
5:F:17:ARG:NE	5:F:17:ARG:HA	2.34	0.42
11:L:96:LYS:HA	11:L:96:LYS:HD3	1.90	0.42
16:Q:205:GLU:OE2	16:Q:205:GLU:HA	2.19	0.42
18:T:69:ASP:O	18:T:73:GLU:HG3	2.19	0.42
6:X:151:LYS:HA	6:X:151:LYS:HD2	1.87	0.42
35:l:588:PHE:CD1	35:l:588:PHE:N	2.87	0.42
44:w:223:ASN:HB3	44:w:226:GLU:HB2	2.01	0.42
1:A:141:GLY:HA3	1:A:248:VAL:O	2.19	0.42
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.78	0.42
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.50	0.42
12:M:680:LEU:C	12:M:680:LEU:HD23	2.44	0.42
23:Z:13:LYS:HD2	23:Z:13:LYS:HA	1.81	0.42
26:c:176:LYS:HD2	26:c:176:LYS:HA	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:97:ILE:O	28:e:101:LEU:HB2	2.19	0.42
32:i:89:MET:HE1	32:i:98:MET:HE3	2.00	0.42
35:l:141:PHE:HE2	40:r:375:LEU:HD11	1.84	0.42
44:w:279:ASP:OD1	44:w:279:ASP:N	2.52	0.42
1:A:93:PHE:CD2	1:A:98:LYS:HD2	2.54	0.42
1:A:339:PHE:CE1	1:A:349:LEU:HD23	2.55	0.42
48:B:303:PEE:H16	48:B:303:PEE:H21	1.66	0.42
3:C:79:MET:HE2	3:C:86:MET:HE3	2.01	0.42
12:M:153:PHE:CZ	12:M:155:GLU:HB2	2.54	0.42
20:V:141:VAL:C	24:a:161:ARG:HD2	2.44	0.42
27:d:51:PHE:O	27:d:54:GLN:HG2	2.19	0.42
31:h:58:ILE:HD12	42:u:145:ARG:NH1	2.34	0.42
41:s:25:ARG:HD2	56:s:401:UQ:HM21	2.01	0.42
1:A:278:ILE:HG21	1:A:304:ALA:HB2	2.02	0.42
1:A:405:ARG:HH12	1:A:454:ALA:HB2	1.85	0.42
1:A:451:GLN:O	1:A:451:GLN:CD	2.62	0.42
5:F:64:LYS:HB3	5:F:64:LYS:HZ2	1.84	0.42
6:G:130:ILE:HG22	6:G:135:ALA:HB2	2.01	0.42
12:M:48:THR:HA	12:M:95:PRO:HA	2.01	0.42
14:O:185:MET:HE2	14:O:185:MET:HB2	1.55	0.42
16:Q:444:LEU:HD12	16:Q:444:LEU:O	2.19	0.42
18:T:104:LYS:HB2	18:T:104:LYS:HE3	1.70	0.42
29:f:47:THR:HG23	30:g:65:LEU:HD22	2.01	0.42
38:o:3:PHE:CZ	39:p:70:GLU:HG3	2.54	0.42
41:s:9:LEU:O	41:s:13:ILE:HG12	2.19	0.42
3:C:50:LEU:HD23	3:C:50:LEU:HA	1.88	0.42
5:F:19:ILE:HG23	5:F:53:ILE:HG23	2.02	0.42
9:J:176:SER:O	9:J:182:ARG:NH2	2.37	0.42
31:h:38:LYS:O	31:h:42:GLU:HG3	2.19	0.42
32:i:41:ILE:HG13	34:k:73:LEU:HD21	2.00	0.42
35:l:119:LYS:NZ	51:l:701:CDL:OA3	2.53	0.42
41:s:98:MET:HE1	41:s:104:PHE:CB	2.50	0.42
1:A:149:MET:HE3	1:A:241:THR:HB	2.02	0.42
5:F:64:LYS:HZ2	5:F:64:LYS:CB	2.32	0.42
48:U:101:PEE:H59	48:U:101:PEE:H64	1.72	0.42
35:l:152:PHE:CD1	35:l:168:ALA:HB1	2.54	0.42
35:l:264:TYR:O	35:l:268:GLU:HG2	2.20	0.42
35:l:539:TYR:O	35:l:543:SER:OG	2.33	0.42
51:l:701:CDL:C62	51:l:701:CDL:C58	2.94	0.42
1:A:161:GLU:OE1	1:A:161:GLU:N	2.53	0.42
1:A:178:GLU:OE1	1:A:179:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LYS:HA	1:A:332:CYS:SG	2.59	0.42
8:I:58:ASP:OD2	8:I:61:ARG:HD3	2.19	0.42
9:J:344:PRO:HG2	9:J:347:LEU:HG	2.00	0.42
12:M:167:PRO:HD2	12:M:215:MET:HE1	2.02	0.42
31:h:83:ARG:HE	31:h:83:ARG:HB3	1.60	0.42
32:i:325:LEU:O	32:i:329:MET:HG2	2.20	0.42
35:l:176:ARG:HA	35:l:176:ARG:HD2	1.68	0.42
36:m:163:ILE:HD13	36:m:163:ILE:HA	1.91	0.42
39:p:92:GLU:HB3	39:p:95:GLU:HG3	2.01	0.42
42:u:12:ASP:O	42:u:61:LYS:NZ	2.45	0.42
1:A:322:SER:OG	1:A:370:LEU:HD22	2.20	0.42
24:a:60:SER:HB3	39:p:107:TRP:HA	2.02	0.42
36:m:58:LEU:HD13	41:s:107:ALA:HA	2.02	0.42
44:w:353:TRP:CD1	44:w:353:TRP:H	2.38	0.42
1:A:66:LYS:H	1:A:66:LYS:HG2	1.71	0.42
1:A:93:PHE:CE2	1:A:98:LYS:CG	2.98	0.42
12:M:307:ILE:HG12	12:M:317:THR:HG21	2.01	0.42
26:c:100:ASN:O	26:c:103:GLU:HG2	2.20	0.42
33:j:94:LEU:HD23	33:j:94:LEU:HA	1.94	0.42
35:l:405:ASN:N	35:l:405:ASN:HD22	2.18	0.42
35:l:500:LEU:HD23	35:l:500:LEU:HA	1.80	0.42
39:p:132:SER:OG	39:p:163:LEU:HD12	2.20	0.42
40:r:233:ALA:HA	40:r:320:GLY:HA2	2.01	0.42
43:v:82:HIS:HB3	43:v:83:GLU:OE2	2.20	0.42
1:A:178:GLU:C	1:A:178:GLU:CD	2.88	0.41
2:B:131:GLU:HG3	2:B:144:ARG:HD2	2.02	0.41
9:J:94:LEU:HA	9:J:97:MET:HE3	2.02	0.41
14:O:199:LYS:O	14:O:203:GLU:HG3	2.20	0.41
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.44	0.41
19:U:52:ASN:HB3	24:a:185:THR:HG22	2.00	0.41
35:l:44:PHE:HB2	35:l:94:LEU:HB3	2.02	0.41
12:M:403:VAL:HG11	12:M:452:LEU:HD21	2.02	0.41
21:W:90:ASN:ND2	21:W:123:GLU:O	2.53	0.41
6:X:134:ASP:OD1	39:p:4:SER:OG	2.23	0.41
26:c:160:GLN:HB3	26:c:183:HIS:ND1	2.35	0.41
27:d:114:GLN:HG3	35:l:203:MET:HG2	2.02	0.41
40:r:66:LEU:HD21	40:r:107:ILE:HG23	2.01	0.41
40:r:114:GLU:OE2	40:r:116:ILE:CG2	2.55	0.41
10:K:109:ARG:NH1	14:O:108:PRO:HD3	2.35	0.41
12:M:32:ILE:C	12:M:42:MET:HE1	2.46	0.41
12:M:407:PRO:HD2	12:M:438:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:579:MET:O	12:M:579:MET:HG3	2.19	0.41
15:P:75:GLN:HB3	15:P:87:PHE:CD1	2.55	0.41
21:W:58:ARG:HD2	21:W:58:ARG:HA	1.86	0.41
6:X:99:SER:O	6:X:102:SER:OG	2.33	0.41
34:k:45:THR:HG23	36:m:52:LEU:HD13	2.03	0.41
35:l:3:PRO:O	35:l:7:LEU:HD23	2.19	0.41
35:l:221:ALA:HA	35:l:226:GLN:HG2	2.03	0.41
51:l:702:CDL:H112	51:l:702:CDL:H142	1.83	0.41
36:m:7:PHE:O	36:m:11:THR:HG23	2.20	0.41
40:r:14:MET:O	40:r:18:SER:OG	2.26	0.41
40:r:371:PRO:O	40:r:448:THR:OG1	2.39	0.41
44:w:129:TYR:OH	44:w:186:HIS:ND1	2.35	0.41
2:B:66:LEU:O	41:s:277:TYR:OH	2.32	0.41
5:F:34:ARG:HB2	5:F:34:ARG:CZ	2.50	0.41
9:J:163:LYS:NZ	9:J:253:ILE:O	2.45	0.41
16:Q:251:PHE:HB3	16:Q:341:LEU:HD11	2.02	0.41
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.85	0.41
6:X:113:LEU:O	6:X:116:VAL:HG12	2.20	0.41
25:b:123:PHE:HB3	43:v:40:VAL:HG21	2.02	0.41
37:n:13:VAL:HG12	40:r:14:MET:HG2	2.01	0.41
43:v:46:MET:CG	43:v:56:ARG:HG2	2.50	0.41
44:w:345:GLU:C	44:w:345:GLU:OE1	2.64	0.41
48:C:302:PEE:H75	49:C:303:PLX:H172	2.01	0.41
10:K:87:LEU:HD22	14:O:66:ILE:HD11	2.02	0.41
12:M:472:PRO:O	12:M:510:TRP:NE1	2.42	0.41
20:V:14:GLU:H	20:V:14:GLU:CD	2.29	0.41
3:C:142:TYR:CE1	16:Q:135:TYR:OH	2.74	0.41
6:G:103:HIS:ND1	6:G:106:LYS:HG2	2.36	0.41
12:M:275:PRO:HB3	12:M:286:ILE:HG23	2.02	0.41
14:O:58:GLU:HA	14:O:61:LYS:HG3	2.01	0.41
20:V:69:ILE:HG12	20:V:69:ILE:H	1.69	0.41
6:X:85:TYR:O	6:X:89:LEU:HD23	2.21	0.41
40:r:445:LEU:O	40:r:448:THR:HG22	2.21	0.41
1:A:45:LEU:HB3	1:A:46:TYR:CD1	2.54	0.41
6:G:79:ILE:HG22	6:G:145:VAL:HG13	2.02	0.41
6:G:103:HIS:CD2	6:G:139:MET:HG3	2.56	0.41
12:M:630:ALA:HB3	12:M:632:MET:HE2	2.03	0.41
48:U:101:PEE:H35	48:U:101:PEE:H30	1.93	0.41
51:a:201:CDL:H381	51:a:201:CDL:H412	1.84	0.41
28:e:99:LEU:HD12	28:e:99:LEU:HA	1.85	0.41
35:l:244:SER:O	35:l:249:SER:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:252:LYS:HE2	44:w:252:LYS:HB3	1.92	0.41
1:A:202:GLY:O	14:O:120:THR:HG22	2.21	0.41
4:E:42:GLU:HA	4:E:42:GLU:OE2	2.21	0.41
7:H:87:GLU:OE1	15:P:104:THR:OG1	2.32	0.41
9:J:65:LEU:HD23	9:J:129:LEU:HD22	2.02	0.41
14:O:207:GLU:HB3	14:O:212:LYS:HE3	2.02	0.41
15:P:92:GLY:C	15:P:95:PRO:HD2	2.46	0.41
16:Q:226:TYR:OH	16:Q:234:GLN:O	2.24	0.41
6:X:85:TYR:CD2	23:Z:16:LEU:HD23	2.56	0.41
30:g:47:ASP:OD1	30:g:53:ARG:NH2	2.54	0.41
35:l:588:PHE:N	35:l:588:PHE:HD1	2.18	0.41
36:m:57:PHE:CD1	36:m:57:PHE:C	2.96	0.41
43:v:7:ARG:NH2	43:v:16:GLU:OE2	2.50	0.41
43:v:26:PRO:HD2	43:v:29:TYR:HB2	2.03	0.41
44:w:38:TYR:HH	44:w:292:HIS:HD1	1.62	0.41
1:A:116:ASN:O	1:A:245:VAL:HG23	2.21	0.41
1:A:362:ASP:OD1	1:A:449:ARG:NH2	2.46	0.41
3:C:65:MET:HB2	3:C:65:MET:HE2	1.83	0.41
6:G:90:TYR:CE2	6:G:92:LYS:HB2	2.56	0.41
7:H:30:LYS:O	7:H:34:VAL:HG23	2.19	0.41
8:I:8:ILE:HD13	8:I:8:ILE:HA	1.93	0.41
9:J:162:GLU:HG2	9:J:163:LYS:HG3	2.01	0.41
9:J:167:ILE:HD13	9:J:201:ILE:HB	2.01	0.41
12:M:168:LEU:HD23	12:M:168:LEU:HA	1.91	0.41
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.56	0.41
16:Q:65:PRO:HB2	16:Q:67:ASN:O	2.20	0.41
16:Q:238:LEU:HD23	16:Q:238:LEU:HA	1.86	0.41
19:U:30:ILE:HG22	19:U:31:ILE:HD12	2.03	0.41
21:W:28:ARG:HD2	21:W:28:ARG:HA	1.89	0.41
6:X:82:ARG:HD3	22:Y:44:TYR:CE1	2.56	0.41
6:X:117:GLU:OE2	39:p:20:TYR:OH	2.37	0.41
6:X:137:LYS:HB3	6:X:137:LYS:HE3	1.88	0.41
25:b:2:SER:OG	25:b:3:GLY:N	2.54	0.41
25:b:70:PHE:O	25:b:74:HIS:HB2	2.21	0.41
25:b:76:LEU:O	25:b:79:VAL:HG12	2.21	0.41
25:b:122:GLU:O	25:b:122:GLU:CD	2.63	0.41
26:c:90:TYR:HE1	39:p:6:PRO:HG3	1.85	0.41
27:d:121:TYR:O	27:d:125:CYS:HB2	2.21	0.41
32:i:1:MET:HE1	32:i:9:LEU:HD12	2.02	0.41
49:j:201:PLX:H342	49:j:201:PLX:H372	1.42	0.41
51:l:702:CDL:H391	51:l:702:CDL:H421	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:152:GLU:O	39:p:152:GLU:HG3	2.20	0.41
43:v:52:MET:HB2	43:v:55:GLN:HG3	2.03	0.41
44:w:100:ASP:OD1	44:w:100:ASP:N	2.39	0.41
7:H:76:GLN:O	7:H:78:GLU:N	2.53	0.41
12:M:432:ILE:HD13	12:M:432:ILE:HA	1.93	0.41
12:M:494:SER:OG	12:M:669:ASN:OD1	2.39	0.41
13:N:85:GLU:H	13:N:85:GLU:CD	2.25	0.41
16:Q:375:MET:HE2	16:Q:379:ILE:HG13	2.03	0.41
22:Y:65:MET:SD	35:l:375:ILE:HG12	2.61	0.41
35:l:86:SER:OG	35:l:262:ARG:NH2	2.51	0.41
36:m:57:PHE:CD1	36:m:61:LEU:HD12	2.55	0.41
5:F:39:LYS:CB	5:F:40:ARG:HE	2.34	0.40
6:G:103:HIS:CE1	6:G:105:MET:HB2	2.57	0.40
9:J:235:THR:O	9:J:272:LEU:HD12	2.21	0.40
12:M:306:MET:CE	12:M:583:ILE:HD12	2.50	0.40
39:p:134:GLU:OE1	39:p:134:GLU:HA	2.20	0.40
40:r:123:GLU:OE2	40:r:157:SER:OG	2.32	0.40
1:A:45:LEU:HB3	1:A:46:TYR:HD1	1.87	0.40
1:A:244:ASN:N	46:A:502:FMN:O1P	2.48	0.40
1:A:357:MET:HE2	14:O:142:LEU:HD11	2.02	0.40
3:C:62:LEU:O	3:C:91:VAL:HA	2.22	0.40
9:J:241:TYR:HE2	9:J:348:LYS:HE3	1.86	0.40
12:M:32:ILE:C	12:M:42:MET:CE	2.94	0.40
13:N:85:GLU:HB2	13:N:98:PRO:HB3	2.03	0.40
14:O:204:ILE:HG22	14:O:205:ILE:HD12	2.03	0.40
16:Q:55:THR:OG1	16:Q:57:GLU:OE1	2.39	0.40
20:V:35:ILE:HD13	20:V:35:ILE:HA	1.82	0.40
32:i:96:THR:O	32:i:100:MET:HG3	2.22	0.40
34:k:22:TYR:O	35:l:585:LYS:HG2	2.21	0.40
41:s:24:GLU:HG3	41:s:271:LEU:HD22	2.02	0.40
41:s:172:ILE:HD12	41:s:172:ILE:HA	1.84	0.40
42:u:100:CYS:HB2	42:u:103:GLN:OE1	2.21	0.40
3:C:142:TYR:CZ	16:Q:135:TYR:CZ	3.09	0.40
12:M:32:ILE:O	12:M:42:MET:HE3	2.21	0.40
12:M:340:ALA:HB3	12:M:366:LEU:HD13	2.04	0.40
12:M:408:ARG:HD2	12:M:439:THR:HG23	2.02	0.40
12:M:480:ALA:O	12:M:483:ARG:HG2	2.21	0.40
12:M:511:LYS:HE3	12:M:663:ASN:HB2	2.04	0.40
14:O:207:GLU:OE2	14:O:212:LYS:HE2	2.21	0.40
17:S:4:GLU:HG2	41:s:43:TYR:HD2	1.86	0.40
28:e:73:SER:C	28:e:75:GLY:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:128:LEU:O	32:i:132:THR:OG1	2.26	0.40
32:i:277:ILE:O	32:i:281:LEU:HG	2.21	0.40
34:k:22:TYR:HE1	34:k:29:SER:HG	1.65	0.40
36:m:57:PHE:CE1	41:s:111:LEU:CD2	3.04	0.40
40:r:216:LEU:HB3	40:r:217:PRO:HD3	2.03	0.40
41:s:89:LEU:HD22	41:s:240:ILE:HD12	2.04	0.40
44:w:352:ILE:HD13	44:w:352:ILE:HA	1.81	0.40
1:A:210:THR:HB	1:A:224:ARG:HG2	2.03	0.40
1:A:423:THR:HB	45:A:501:SF4:S4	2.60	0.40
47:A:503:NAI:H6N	47:A:503:NAI:H2D	1.81	0.40
16:Q:190:HIS:O	16:Q:194:ILE:HG12	2.21	0.40
27:d:137:LYS:HA	27:d:137:LYS:HD3	1.91	0.40
30:g:48:ASN:HB3	30:g:55:VAL:HA	2.04	0.40
35:l:252:MET:HE2	35:l:252:MET:HB3	1.94	0.40
51:l:701:CDL:C42	40:r:448:THR:HG21	2.33	0.40
44:w:72:ARG:HB3	44:w:72:ARG:NH1	2.36	0.40
1:A:57:GLN:OE1	1:A:62:TRP:HB2	2.22	0.40
1:A:169:LEU:O	1:A:173:ILE:HG13	2.22	0.40
3:C:56:TRP:NE1	49:C:303:PLX:H71	2.36	0.40
7:H:27:LEU:O	7:H:31:ILE:HG13	2.21	0.40
16:Q:82:LEU:HD11	16:Q:101:LEU:HD11	2.03	0.40
20:V:35:ILE:HD12	35:l:597:ILE:HD11	2.04	0.40
24:a:130:GLU:H	24:a:130:GLU:CD	2.29	0.40
26:c:142:PHE:O	26:c:146:VAL:HG23	2.22	0.40
31:h:85:LYS:HD3	31:h:85:LYS:C	2.46	0.40
34:k:22:TYR:CD2	35:l:584:ILE:HG13	2.56	0.40
51:l:701:CDL:H312	51:l:701:CDL:H761	1.96	0.40
40:r:86:LYS:HZ3	40:r:86:LYS:HB2	1.87	0.40
44:w:118:TYR:OH	57:w:401:ADP:O2'	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/433 (99%)	414 (96%)	15 (4%)	0	100	100
2	B	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
3	C	154/156 (99%)	147 (96%)	7 (4%)	0	100	100
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
5	F	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
6	G	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
6	X	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
7	H	110/112 (98%)	103 (94%)	7 (6%)	0	100	100
8	I	93/112 (83%)	80 (86%)	13 (14%)	0	100	100
9	J	289/342 (84%)	273 (94%)	16 (6%)	0	100	100
10	K	40/43 (93%)	39 (98%)	1 (2%)	0	100	100
11	L	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
12	M	688/690 (100%)	668 (97%)	20 (3%)	0	100	100
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	201 (94%)	14 (6%)	0	100	100
15	P	206/208 (99%)	196 (95%)	10 (5%)	0	100	100
16	Q	412/430 (96%)	400 (97%)	12 (3%)	0	100	100
17	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
18	T	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
19	U	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
20	V	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	18	53
21	W	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
22	Y	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
23	Z	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
24	a	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
25	b	99/126 (79%)	93 (94%)	6 (6%)	0	100	100
26	c	154/156 (99%)	145 (94%)	9 (6%)	0	100	100
27	d	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
28	e	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
29	f	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
30	g	119/122 (98%)	115 (97%)	4 (3%)	0	100	100
31	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	i	345/347 (99%)	332 (96%)	13 (4%)	0	100	100
33	j	95/115 (83%)	90 (95%)	5 (5%)	0	100	100
34	k	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
35	l	601/603 (100%)	576 (96%)	25 (4%)	0	100	100
36	m	125/175 (71%)	112 (90%)	13 (10%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
39	p	176/178 (99%)	169 (96%)	6 (3%)	1 (1%)	21	56
40	r	457/459 (100%)	446 (98%)	11 (2%)	0	100	100
41	s	299/318 (94%)	286 (96%)	13 (4%)	0	100	100
42	u	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
43	v	122/124 (98%)	115 (94%)	7 (6%)	0	100	100
44	w	318/320 (99%)	304 (96%)	14 (4%)	0	100	100
All	All	8029/8322 (96%)	7717 (96%)	310 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	V	46	PRO
39	p	174	PRO

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	343/346 (99%)	338 (98%)	5 (2%)	57	80
2	B	151/151 (100%)	148 (98%)	3 (2%)	48	76
3	C	132/132 (100%)	131 (99%)	1 (1%)	73	86
4	E	107/107 (100%)	105 (98%)	2 (2%)	50	76
5	F	76/76 (100%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	75/81 (93%)	75 (100%)	0	100	100
6	X	77/81 (95%)	75 (97%)	2 (3%)	40	72
7	H	99/99 (100%)	97 (98%)	2 (2%)	48	76
8	I	87/97 (90%)	85 (98%)	2 (2%)	44	74
9	J	255/296 (86%)	254 (100%)	1 (0%)	84	90
10	K	41/42 (98%)	39 (95%)	2 (5%)	22	56
11	L	112/113 (99%)	111 (99%)	1 (1%)	70	85
12	M	579/580 (100%)	574 (99%)	5 (1%)	70	85
13	N	129/130 (99%)	128 (99%)	1 (1%)	73	86
14	O	183/183 (100%)	180 (98%)	3 (2%)	55	79
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	361/370 (98%)	356 (99%)	5 (1%)	59	80
17	S	58/58 (100%)	56 (97%)	2 (3%)	32	66
18	T	79/79 (100%)	77 (98%)	2 (2%)	42	72
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	97/101 (96%)	93 (96%)	4 (4%)	27	61
21	W	123/123 (100%)	122 (99%)	1 (1%)	73	86
22	Y	62/63 (98%)	60 (97%)	2 (3%)	34	67
23	Z	65/65 (100%)	64 (98%)	1 (2%)	57	80
24	a	122/122 (100%)	121 (99%)	1 (1%)	73	86
25	b	98/119 (82%)	97 (99%)	1 (1%)	68	84
26	c	141/141 (100%)	136 (96%)	5 (4%)	32	65
27	d	155/155 (100%)	151 (97%)	4 (3%)	40	72
28	e	99/99 (100%)	99 (100%)	0	100	100
29	f	35/45 (78%)	35 (100%)	0	100	100
30	g	108/109 (99%)	107 (99%)	1 (1%)	70	85
31	h	93/93 (100%)	92 (99%)	1 (1%)	65	83
32	i	311/311 (100%)	309 (99%)	2 (1%)	78	88
33	j	88/100 (88%)	88 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	536/537 (100%)	530 (99%)	6 (1%)	65	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	m	97/141 (69%)	96 (99%)	1 (1%)	68	84
37	n	53/53 (100%)	51 (96%)	2 (4%)	29	63
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	159/159 (100%)	157 (99%)	2 (1%)	61	81
40	r	410/410 (100%)	404 (98%)	6 (2%)	57	80
41	s	263/275 (96%)	260 (99%)	3 (1%)	65	83
42	u	153/153 (100%)	151 (99%)	2 (1%)	61	81
43	v	104/111 (94%)	103 (99%)	1 (1%)	68	84
44	w	278/283 (98%)	276 (99%)	2 (1%)	76	86
All	All	7051/7246 (97%)	6964 (99%)	87 (1%)	61	82

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	61	ASP
1	A	307	VAL
1	A	331	VAL
1	A	383	THR
2	B	37	THR
2	B	73	THR
2	B	76	TYR
3	C	71	CYS
4	E	45	ASN
4	E	96	VAL
7	H	51	ILE
7	H	76	GLN
8	I	35	THR
8	I	41	LEU
9	J	374	THR
10	K	92	GLU
10	K	105	ARG
11	L	86	ASN
12	M	232	THR
12	M	448	SER
12	M	487	THR
12	M	559	ASP
12	M	640	ASP
13	N	4	VAL

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Mol	Chain	Res	Type
14	O	196	LEU
14	O	202	GLU
14	O	245	VAL
16	Q	57	GLU
16	Q	252	SER
16	Q	308	TYR
16	Q	373	THR
16	Q	409	VAL
17	S	42	SER
17	S	44	GLN
18	T	78	GLU
18	T	84	ILE
20	V	69	ILE
20	V	88	LEU
20	V	100	THR
20	V	120	LEU
21	W	109	SER
6	X	100	VAL
6	X	108	LEU
22	Y	40	ILE
22	Y	56	ILE
23	Z	18	ASP
24	a	87	THR
25	b	28	LEU
26	c	59	VAL
26	c	78	LEU
26	c	113	ILE
26	c	117	VAL
26	c	120	SER
27	d	7	LYS
27	d	26	LEU
27	d	101	GLU
27	d	127	LYS
30	g	60	LEU
31	h	70	GLN
32	i	108	LEU
32	i	300	SER
35	l	25	ASN
35	l	71	LEU
35	l	185	SER
35	l	543	SER
35	l	578	SER

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Mol	Chain	Res	Type
35	l	598	SER
36	m	27	ILE
37	n	31	SER
37	n	48	GLU
39	p	19	LEU
39	p	110	SER
40	r	55	THR
40	r	66	LEU
40	r	140	THR
40	r	179	ILE
40	r	303	ILE
40	r	448	THR
41	s	17	VAL
41	s	73	ILE
41	s	144	VAL
42	u	14	LYS
42	u	88	CYS
43	v	53	LEU
44	w	241	TYR
44	w	312	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	270	ASN
1	A	283	ASN
1	A	436	GLN
4	E	51	GLN
5	F	25	GLN
5	F	81	ASN
8	I	21	GLN
9	J	122	HIS
9	J	376	ASN
12	M	278	HIS
12	M	388	ASN
12	M	464	GLN
12	M	688	GLN
14	O	123	ASN
15	P	77	GLN
15	P	105	ASN
15	P	107	GLN

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Mol	Chain	Res	Type
15	P	131	ASN
16	Q	60	HIS
16	Q	147	ASN
16	Q	160	ASN
16	Q	183	HIS
16	Q	190	HIS
16	Q	233	HIS
16	Q	285	ASN
16	Q	339	GLN
16	Q	431	HIS
18	T	63	ASN
18	T	117	GLN
19	U	71	GLN
21	W	8	GLN
22	Y	54	GLN
27	d	55	GLN
27	d	124	ASN
32	i	174	GLN
35	l	59	GLN
35	l	165	ASN
35	l	270	ASN
35	l	274	GLN
35	l	354	GLN
35	l	446	ASN
35	l	447	ASN
37	n	3	ASN
38	o	75	ASN
38	o	79	ASN
40	r	175	ASN
40	r	251	ASN
40	r	304	GLN
40	r	338	HIS
40	r	422	HIS
41	s	47	GLN
41	s	124	ASN
41	s	317	GLN
42	u	30	HIS
42	u	77	HIS
42	u	163	HIS
43	v	55	GLN
43	v	85	HIS
44	w	215	GLN

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Mol	Chain	Res	Type
44	w	344	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
16	2MR	Q	118	16	10,12,13	1.98	2 (20%)	5,13,15	6.41	3 (60%)

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
16	2MR	Q	118	16	-	2/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.18	1.45	1.34
16	Q	118	2MR	CQ2-NH2	-2.32	1.41	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	13.38	131.74	119.48
16	Q	118	2MR	CD-NE-CZ	3.88	130.65	123.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	CQ2-NH2-CZ	3.23	130.58	123.65

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	118	2MR	NE-CD-CG-CB
16	Q	118	2MR	CA-CB-CG-CD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PEE	m	201	-	40,40,50	1.15	5 (12%)	43,45,55	1.08	2 (4%)
49	PLX	C	303	-	51,51,51	1.20	5 (9%)	53,59,59	0.64	1 (1%)
51	CDL	I	201	-	50,50,99	1.42	9 (18%)	56,62,111	1.21	4 (7%)
51	CDL	l	701	-	98,98,99	0.93	4 (4%)	104,110,111	1.11	7 (6%)
56	UQ	s	401	-	28,28,63	3.30	9 (32%)	36,37,79	2.81	12 (33%)
50	8Q1	G	201	-	32,34,34	1.62	6 (18%)	39,43,43	1.68	8 (20%)
53	FES	M	803	12	0,4,4	-	-	-	-	-
49	PLX	j	201	-	51,51,51	1.18	5 (9%)	53,59,59	0.63	1 (1%)
49	PLX	r	502	-	51,51,51	1.19	4 (7%)	53,59,59	0.63	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	NAI	A	503	-	47,48,48	3.98	22 (46%)	64,73,73	1.68	11 (17%)
48	PEE	l	703	-	45,45,50	1.24	6 (13%)	48,50,55	1.05	2 (4%)
52	NDP	J	401	-	51,52,52	4.26	24 (47%)	71,80,80	2.20	13 (18%)
48	PEE	r	501	-	50,50,50	1.15	5 (10%)	53,55,55	1.08	2 (3%)
48	PEE	i	402	-	46,46,50	1.20	6 (13%)	49,51,55	1.07	2 (4%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
48	PEE	U	101	-	50,50,50	1.17	6 (12%)	53,55,55	0.95	2 (3%)
46	FMN	A	502	-	33,33,33	1.12	2 (6%)	48,50,50	1.27	8 (16%)
49	PLX	g	201	-	51,51,51	1.18	3 (5%)	53,59,59	0.65	1 (1%)
53	FES	O	301	14	0,4,4	-	-	-	-	-
45	SF4	B	301	2	0,12,12	-	-	-	-	-
51	CDL	a	201	-	90,90,99	1.15	7 (7%)	96,102,111	1.03	5 (5%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
51	CDL	l	702	-	99,99,99	1.10	8 (8%)	105,111,111	0.90	4 (3%)
48	PEE	C	302	-	46,46,50	1.24	6 (13%)	49,51,55	0.98	2 (4%)
51	CDL	r	503	-	99,99,99	1.10	8 (8%)	105,111,111	0.88	4 (3%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
45	SF4	C	301	3,16	0,12,12	-	-	-	-	-
50	8Q1	X	201	-	32,34,34	1.62	6 (18%)	39,43,43	1.64	7 (17%)
48	PEE	B	303	-	50,50,50	1.18	6 (12%)	53,55,55	1.09	3 (5%)
57	ADP	w	401	-	28,29,29	3.17	9 (32%)	43,45,45	1.94	9 (20%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
51	CDL	i	401	-	65,65,99	1.30	8 (12%)	71,77,111	1.05	4 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PEE	m	201	-	-	20/44/44/54	-
49	PLX	C	303	-	-	25/55/55/55	-
51	CDL	I	201	-	-	32/61/61/110	-
45	SF4	M	802	12	-	-	0/6/5/5
51	CDL	l	701	-	-	40/109/109/110	-
56	UQ	s	401	-	-	10/21/45/87	0/1/1/1
50	8Q1	G	201	-	-	17/41/41/41	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	FES	M	803	12	-	-	0/1/1/1
49	PLX	j	201	-	-	31/55/55/55	-
49	PLX	r	502	-	-	37/55/55/55	-
47	NAI	A	503	-	-	6/29/72/72	0/5/5/5
52	NDP	J	401	-	-	9/34/77/77	0/5/5/5
48	PEE	r	501	-	-	28/54/54/54	-
48	PEE	i	402	-	-	30/50/50/54	-
45	SF4	A	501	1	-	-	0/6/5/5
48	PEE	U	101	-	-	24/54/54/54	-
46	FMN	A	502	-	-	5/18/18/18	0/3/3/3
49	PLX	g	201	-	-	26/55/55/55	-
53	FES	O	301	14	-	-	0/1/1/1
45	SF4	B	301	2	-	-	0/6/5/5
51	CDL	a	201	-	-	35/101/101/110	-
45	SF4	B	302	2	-	-	0/6/5/5
51	CDL	l	702	-	-	59/110/110/110	-
48	PEE	C	302	-	-	22/50/50/54	-
51	CDL	r	503	-	-	66/110/110/110	-
45	SF4	M	801	12	-	-	0/6/5/5
45	SF4	C	301	3,16	-	-	0/6/5/5
50	8Q1	X	201	-	-	24/41/41/41	-
48	PEE	B	303	-	-	22/54/54/54	-
57	ADP	w	401	-	-	5/16/32/32	0/3/3/3
48	PEE	l	703	-	-	25/49/49/54	-
51	CDL	i	401	-	-	37/76/76/110	-

All (179) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	J	401	NDP	C3B-C2B	-13.20	1.24	1.53
52	J	401	NDP	O4D-C4D	10.67	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.43	1.26	1.53
52	J	401	NDP	C3D-C4D	-10.05	1.27	1.53
56	s	401	UQ	C13-C14	9.65	1.55	1.33
47	A	503	NAI	O4B-C1B	9.24	1.63	1.42
56	s	401	UQ	C8-C9	9.19	1.54	1.33
57	w	401	ADP	C3'-C4'	-8.98	1.30	1.53
52	J	401	NDP	O4B-C4B	-8.34	1.26	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O4B-C4B	-8.32	1.26	1.45
56	s	401	UQ	C18-C19	7.94	1.56	1.32
47	A	503	NAI	C2D-C1D	-7.68	1.29	1.53
57	w	401	ADP	O4'-C4'	7.60	1.61	1.45
47	A	503	NAI	C2B-C1B	-7.53	1.29	1.53
52	J	401	NDP	C2N-C3N	7.47	1.55	1.35
52	J	401	NDP	C6N-C5N	7.23	1.55	1.33
47	A	503	NAI	O4D-C4D	6.76	1.60	1.45
52	J	401	NDP	PN-O3	6.23	1.66	1.59
57	w	401	ADP	PA-O3A	6.04	1.66	1.59
47	A	503	NAI	C2D-C3D	5.87	1.69	1.53
47	A	503	NAI	PA-O3	5.83	1.65	1.59
52	J	401	NDP	P2B-O2B	5.68	1.69	1.59
47	A	503	NAI	O4D-C1D	5.54	1.54	1.42
47	A	503	NAI	C4N-C3N	-5.48	1.39	1.50
52	J	401	NDP	C6A-N6A	5.48	1.48	1.34
57	w	401	ADP	C6-N6	5.37	1.47	1.34
47	A	503	NAI	C7N-N7N	5.31	1.48	1.33
52	J	401	NDP	PA-O3	5.26	1.65	1.59
47	A	503	NAI	PN-O3	5.22	1.65	1.59
52	J	401	NDP	O4D-C1D	-5.18	1.30	1.42
52	J	401	NDP	C3B-C4B	5.13	1.66	1.53
50	G	201	8Q1	C34-N36	5.03	1.45	1.33
50	X	201	8Q1	C34-N36	5.00	1.45	1.33
47	A	503	NAI	C6A-N6A	4.97	1.46	1.34
52	J	401	NDP	C6N-N1N	4.94	1.49	1.37
50	G	201	8Q1	C39-N41	4.94	1.45	1.33
50	X	201	8Q1	C39-N41	4.77	1.44	1.33
57	w	401	ADP	O4'-C1'	-4.62	1.31	1.42
52	J	401	NDP	C1B-N9A	-4.53	1.33	1.46
52	J	401	NDP	O4B-C1B	4.30	1.51	1.42
51	l	701	CDL	OA8-CA7	4.28	1.45	1.33
47	A	503	NAI	O2B-C2B	4.22	1.53	1.43
52	J	401	NDP	O2D-C2D	-4.16	1.32	1.43
51	l	701	CDL	OB8-CB7	4.15	1.45	1.33
51	l	701	CDL	OB6-CB5	4.13	1.46	1.34
51	l	701	CDL	OA6-CA5	4.09	1.45	1.34
48	C	302	PEE	C18-C19	3.85	1.53	1.31
52	J	401	NDP	C7N-N7N	3.84	1.44	1.33
48	B	303	PEE	C18-C19	3.80	1.53	1.31
48	l	703	PEE	C18-C19	3.79	1.53	1.31
57	w	401	ADP	C8-N9	-3.77	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	C	302	PEE	C39-C38	3.76	1.53	1.31
48	m	201	PEE	C18-C19	3.74	1.52	1.31
48	U	101	PEE	C18-C19	3.74	1.52	1.31
48	U	101	PEE	C39-C38	3.70	1.52	1.31
48	r	501	PEE	C39-C38	3.70	1.52	1.31
48	r	501	PEE	C18-C19	3.70	1.52	1.31
48	i	402	PEE	C18-C19	3.69	1.52	1.31
48	B	303	PEE	C39-C38	3.68	1.52	1.31
48	l	703	PEE	C39-C38	3.66	1.52	1.31
48	i	402	PEE	C39-C38	3.65	1.52	1.31
51	i	401	CDL	OA8-CA7	3.55	1.43	1.33
47	A	503	NAI	C4N-C5N	-3.50	1.39	1.49
57	w	401	ADP	O2'-C2'	-3.48	1.34	1.43
52	J	401	NDP	C5A-N7A	-3.42	1.32	1.39
51	l	702	CDL	OA8-CA7	3.42	1.43	1.33
47	A	503	NAI	C7N-C3N	3.39	1.56	1.48
51	a	201	CDL	OA8-CA7	3.35	1.43	1.33
51	r	503	CDL	OA8-CA7	3.31	1.43	1.33
51	I	201	CDL	OA8-CA7	3.31	1.43	1.33
49	g	201	PLX	O6-C4	-3.27	1.40	1.44
52	J	401	NDP	C8A-N9A	-3.26	1.32	1.37
46	A	502	FMN	C4A-N5	3.25	1.37	1.30
49	C	303	PLX	O6-C4	-3.12	1.40	1.44
51	I	201	CDL	OB8-CB7	3.05	1.42	1.33
51	i	401	CDL	OB6-CB5	3.02	1.42	1.34
49	r	502	PLX	O6-C4	-3.02	1.40	1.44
51	I	201	CDL	OA6-CA5	3.01	1.42	1.34
51	a	201	CDL	OB8-CB7	3.01	1.42	1.33
51	r	503	CDL	OB8-CB7	2.98	1.42	1.33
51	l	702	CDL	OA6-CA5	2.95	1.42	1.34
52	J	401	NDP	C7N-C3N	2.95	1.55	1.48
51	i	401	CDL	OB8-CB7	2.95	1.41	1.33
52	J	401	NDP	O3D-C3D	2.94	1.50	1.43
51	a	201	CDL	OB6-CB5	2.94	1.42	1.34
51	i	401	CDL	OA6-CA5	2.94	1.42	1.34
51	l	702	CDL	OB8-CB7	2.94	1.41	1.33
57	w	401	ADP	O3'-C3'	2.93	1.50	1.43
51	l	702	CDL	OB6-CB5	2.93	1.42	1.34
51	I	201	CDL	OB6-CB5	2.92	1.42	1.34
51	r	503	CDL	OB6-CB5	2.91	1.42	1.34
51	a	201	CDL	OA6-CA5	2.90	1.42	1.34
51	r	503	CDL	OA6-CA5	2.90	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	C8A-N9A	-2.85	1.32	1.37
48	U	101	PEE	O2-C2	-2.84	1.39	1.46
51	r	503	CDL	OA6-CA4	-2.82	1.40	1.46
48	B	303	PEE	O2-C2	-2.77	1.40	1.46
48	C	302	PEE	O2-C2	-2.75	1.40	1.46
48	l	703	PEE	O2-C2	-2.73	1.40	1.46
51	i	401	CDL	OA6-CA4	-2.66	1.40	1.46
51	a	201	CDL	OA6-CA4	-2.65	1.40	1.46
49	j	201	PLX	O6-C4	-2.63	1.41	1.44
48	m	201	PEE	O2-C2	-2.61	1.40	1.46
48	r	501	PEE	O2-C2	-2.60	1.40	1.46
50	X	201	8Q1	O40-C39	-2.57	1.18	1.23
50	G	201	8Q1	O40-C39	-2.56	1.18	1.23
51	l	702	CDL	OA6-CA4	-2.54	1.40	1.46
52	J	401	NDP	O2B-C2B	2.53	1.52	1.44
51	I	201	CDL	OB6-CB4	-2.52	1.40	1.46
57	w	401	ADP	C5-N7	-2.52	1.34	1.39
48	i	402	PEE	O2-C2	-2.51	1.40	1.46
50	X	201	8Q1	O35-C34	-2.48	1.18	1.23
47	A	503	NAI	O3B-C3B	-2.48	1.36	1.43
51	I	201	CDL	OA6-CA4	-2.47	1.40	1.46
56	s	401	UQ	C6-C1	2.46	1.53	1.46
50	G	201	8Q1	O35-C34	-2.45	1.18	1.23
51	a	201	CDL	OB6-CB4	-2.44	1.40	1.46
51	l	702	CDL	OB6-CB4	-2.43	1.40	1.46
48	C	302	PEE	O3-C30	2.42	1.40	1.33
48	l	703	PEE	O3-C3	-2.41	1.39	1.45
51	r	503	CDL	OB6-CB4	-2.41	1.40	1.46
48	U	101	PEE	O3-C30	2.40	1.40	1.33
47	A	503	NAI	PN-O5D	2.40	1.68	1.59
48	B	303	PEE	O3-C30	2.40	1.40	1.33
48	i	402	PEE	O3-C30	2.34	1.40	1.33
52	J	401	NDP	O7N-C7N	-2.34	1.19	1.24
49	r	502	PLX	C7-C6	2.33	1.55	1.50
47	A	503	NAI	C5B-C4B	2.33	1.58	1.51
51	r	503	CDL	PB2-OB5	2.33	1.68	1.59
48	m	201	PEE	O2-C10	2.32	1.40	1.34
47	A	503	NAI	C5A-N7A	-2.30	1.34	1.39
51	i	401	CDL	OB6-CB4	-2.29	1.41	1.46
50	X	201	8Q1	C6-C1	2.29	1.53	1.50
47	A	503	NAI	C6N-C5N	2.28	1.40	1.33
48	m	201	PEE	O3-C3	-2.28	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	r	501	PEE	O3-C30	2.26	1.40	1.33
56	s	401	UQ	O1-C1	-2.26	1.18	1.23
48	r	501	PEE	O3-C3	-2.26	1.40	1.45
51	i	401	CDL	PB2-OB5	2.25	1.68	1.59
49	j	201	PLX	C7-C6	2.25	1.55	1.50
56	s	401	UQ	O4-C4	-2.25	1.18	1.23
48	l	703	PEE	O3-C30	2.25	1.39	1.33
48	m	201	PEE	O3-C30	2.25	1.39	1.33
48	i	402	PEE	O2-C10	2.25	1.40	1.34
49	g	201	PLX	C7-C6	2.24	1.55	1.50
48	U	101	PEE	O3-C3	-2.22	1.40	1.45
51	I	201	CDL	PB2-OB5	2.22	1.68	1.59
51	i	401	CDL	PB2-OB2	2.21	1.68	1.59
56	s	401	UQ	O3-CM3	-2.21	1.40	1.45
48	U	101	PEE	O2-C10	2.20	1.40	1.34
48	C	302	PEE	O2-C10	2.17	1.40	1.34
52	J	401	NDP	C2D-C3D	2.17	1.59	1.53
49	C	303	PLX	C7-C6	2.17	1.55	1.50
48	C	302	PEE	O3-C3	-2.17	1.40	1.45
48	l	703	PEE	O2-C10	2.16	1.40	1.34
51	r	503	CDL	PB2-OB2	2.16	1.67	1.59
49	r	502	PLX	P1-O4	2.15	1.67	1.59
48	B	303	PEE	O3-C3	-2.15	1.40	1.45
50	G	201	8Q1	C6-C1	2.15	1.53	1.50
50	G	201	8Q1	C1-S44	2.14	1.81	1.76
48	B	303	PEE	O2-C10	2.13	1.40	1.34
49	g	201	PLX	P1-O4	2.13	1.67	1.59
49	j	201	PLX	P1-O1	2.10	1.67	1.59
51	l	702	CDL	PB2-OB5	2.10	1.67	1.59
51	a	201	CDL	PB2-OB2	2.09	1.67	1.59
56	s	401	UQ	C6-C5	-2.09	1.31	1.35
48	i	402	PEE	O3-C3	-2.09	1.40	1.45
51	l	702	CDL	C11-CA5	2.08	1.56	1.50
46	A	502	FMN	C10-N1	2.07	1.37	1.33
49	j	201	PLX	P1-O4	2.07	1.67	1.59
49	C	303	PLX	P1-O4	2.06	1.67	1.59
56	s	401	UQ	O2-CM2	-2.05	1.40	1.45
49	C	303	PLX	P1-O1	2.04	1.67	1.59
51	I	201	CDL	PB2-OB2	2.04	1.67	1.59
49	j	201	PLX	C1-C2	2.03	1.57	1.51
51	I	201	CDL	C11-CA5	2.03	1.56	1.50
50	X	201	8Q1	C1-S44	2.03	1.81	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	C	303	PLX	C25-C24	2.01	1.54	1.50
49	r	502	PLX	P1-O1	2.00	1.67	1.59

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	401	UQ	C7-C8-C9	-9.91	109.76	126.83
52	J	401	NDP	C3N-C2N-N1N	-7.03	112.88	123.20
52	J	401	NDP	C1D-N1N-C2N	-7.03	109.57	121.14
50	X	201	8Q1	C6-C1-S44	6.53	121.19	113.40
50	G	201	8Q1	C6-C1-S44	6.15	120.73	113.40
56	s	401	UQ	C12-C13-C14	-6.09	113.68	127.62
52	J	401	NDP	C6N-N1N-C2N	-6.07	112.82	119.32
52	J	401	NDP	C1D-N1N-C6N	-5.92	108.26	120.77
52	J	401	NDP	C5A-C4A-N3A	-5.83	118.70	126.72
57	w	401	ADP	C5-C4-N3	-5.69	118.89	126.72
47	A	503	NAI	C5A-C4A-N3A	-5.52	119.11	126.72
48	B	303	PEE	O2-C10-C11	4.82	121.92	111.48
51	a	201	CDL	OA6-CA5-C11	4.75	121.75	111.48
51	a	201	CDL	OB6-CB5-C51	4.61	121.45	111.48
56	s	401	UQ	C10-C9-C8	-4.52	112.02	123.63
48	r	501	PEE	O2-C10-C11	4.47	121.16	111.48
57	w	401	ADP	N3-C2-N1	-4.44	121.86	128.58
51	l	701	CDL	OA6-CA5-C11	4.40	120.99	111.48
48	i	402	PEE	O2-C10-C11	4.37	120.94	111.48
51	l	701	CDL	OB6-CB5-C51	4.37	120.93	111.48
47	A	503	NAI	N3A-C2A-N1A	-4.37	121.97	128.58
56	s	401	UQ	C11-C9-C8	-4.27	111.58	121.17
51	l	702	CDL	OB6-CB5-C51	4.22	120.61	111.48
57	w	401	ADP	N3-C4-N9	4.22	134.34	127.17
51	I	201	CDL	OB6-CB5-C51	4.20	120.58	111.48
48	m	201	PEE	O2-C10-C11	4.15	120.45	111.48
48	l	703	PEE	O2-C10-C11	4.15	120.45	111.48
51	i	401	CDL	OA6-CA5-C11	4.12	120.39	111.48
51	I	201	CDL	OA6-CA5-C11	4.08	120.31	111.48
56	s	401	UQ	C16-C14-C13	-4.07	112.04	121.17
51	l	702	CDL	OA6-CA5-C11	4.05	120.24	111.48
56	s	401	UQ	C15-C14-C13	-4.00	113.34	123.63
51	r	503	CDL	OB6-CB5-C51	3.94	120.00	111.48
48	C	302	PEE	O2-C10-C11	3.89	119.90	111.48
51	i	401	CDL	OB6-CB5-C51	3.88	119.89	111.48
57	w	401	ADP	N9-C8-N7	-3.87	108.45	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	J	401	NDP	N3A-C4A-N9A	3.87	133.75	127.17
56	s	401	UQ	C17-C18-C19	-3.83	114.86	127.64
47	A	503	NAI	N3A-C4A-N9A	3.80	133.64	127.17
51	r	503	CDL	OA6-CA5-C11	3.80	119.71	111.48
52	J	401	NDP	N3A-C2A-N1A	-3.77	122.87	128.58
50	G	201	8Q1	O4-C1-C6	-3.77	119.63	123.98
47	A	503	NAI	C2A-N3A-C4A	3.72	120.92	111.83
57	w	401	ADP	C2-N3-C4	3.66	120.78	111.83
48	U	101	PEE	O2-C10-C11	3.64	119.35	111.48
46	A	502	FMN	C4-N3-C2	-3.63	119.19	125.64
52	J	401	NDP	C2A-N3A-C4A	3.57	120.55	111.83
57	w	401	ADP	C5-N7-C8	3.48	108.92	103.45
57	w	401	ADP	C4-C5-N7	-3.46	106.63	110.58
47	A	503	NAI	C4A-C5A-N7A	-3.43	106.66	110.58
56	s	401	UQ	C21-C19-C18	-3.39	112.47	122.66
57	w	401	ADP	C4-N9-C8	3.33	109.24	105.74
47	A	503	NAI	C5A-N7A-C8A	3.32	108.66	103.45
50	X	201	8Q1	O4-C1-S44	-3.30	118.48	122.68
52	J	401	NDP	C4A-C5A-N7A	-3.28	106.83	110.58
47	A	503	NAI	C3D-C2D-C1D	3.25	107.62	101.46
56	s	401	UQ	C7-C6-C5	-3.18	119.44	124.89
50	G	201	8Q1	C37-C38-C39	3.17	117.67	112.39
47	A	503	NAI	N9A-C8A-N7A	-3.16	109.45	113.94
50	X	201	8Q1	O4-C1-C6	-3.16	120.33	123.98
56	s	401	UQ	CM5-C5-C6	-3.13	119.30	124.45
51	a	201	CDL	OB8-CB7-C71	3.08	121.24	111.83
48	l	703	PEE	O3-C30-C31	3.07	121.20	111.83
47	A	503	NAI	C4D-O4D-C1D	-3.06	102.72	109.47
48	B	303	PEE	O3-C30-C31	3.02	121.05	111.83
52	J	401	NDP	C5A-N7A-C8A	3.02	108.20	103.45
51	r	503	CDL	OB8-CB7-C71	2.99	120.95	111.83
48	i	402	PEE	O3-C30-C31	2.98	120.93	111.83
52	J	401	NDP	N9A-C8A-N7A	-2.97	109.72	113.94
48	r	501	PEE	O3-C30-C31	2.97	120.88	111.83
51	I	201	CDL	OB8-CB7-C71	2.96	120.87	111.83
51	l	701	CDL	OA8-CA7-C31	2.89	120.64	111.83
52	J	401	NDP	O4B-C1B-C2B	-2.89	101.62	106.59
51	i	401	CDL	OA8-CA7-C31	2.87	120.58	111.83
51	I	201	CDL	OA8-CA7-C31	2.84	120.50	111.83
48	m	201	PEE	O3-C30-C31	2.80	120.39	111.83
56	s	401	UQ	C20-C19-C18	-2.80	114.24	122.66
46	A	502	FMN	C4A-C4-N3	2.79	120.34	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	l	701	CDL	CB4-OB6-CB5	-2.76	111.19	117.80
49	g	201	PLX	C1A-N1-C1	2.75	120.84	109.91
51	l	702	CDL	OB8-CB7-C71	2.74	120.20	111.83
48	U	101	PEE	O3-C30-C31	2.72	120.12	111.83
50	G	201	8Q1	C38-C39-N41	2.71	121.29	116.34
51	a	201	CDL	OA8-CA7-C31	2.71	120.11	111.83
49	r	502	PLX	C1A-N1-C1	2.71	120.69	109.91
51	l	701	CDL	OB8-CB7-C71	2.71	120.08	111.83
51	r	503	CDL	OA8-CA7-C31	2.67	119.98	111.83
51	l	702	CDL	OA8-CA7-C31	2.63	119.86	111.83
48	C	302	PEE	O3-C30-C31	2.63	119.84	111.83
51	l	701	CDL	CA4-OA6-CA5	-2.61	111.55	117.80
51	i	401	CDL	OB8-CB7-C71	2.58	119.69	111.83
49	j	201	PLX	C1A-N1-C1	2.56	120.07	109.91
46	A	502	FMN	C4A-C10-N10	2.53	120.10	116.48
52	J	401	NDP	C2B-C3B-C4B	2.52	107.41	101.99
46	A	502	FMN	O4-C4-C4A	-2.51	119.91	126.53
50	G	201	8Q1	O4-C1-S44	-2.40	119.63	122.68
46	A	502	FMN	C9A-C5A-N5	-2.37	119.94	122.45
49	C	303	PLX	C1A-N1-C1	2.35	119.24	109.91
47	A	503	NAI	C2D-C3D-C4D	2.34	107.14	102.61
46	A	502	FMN	C5A-C9A-N10	2.31	120.05	117.97
50	G	201	8Q1	C43-S44-C1	2.30	108.63	101.84
46	A	502	FMN	C10-C4A-N5	-2.27	120.17	124.81
50	X	201	8Q1	C38-C39-N41	2.26	120.47	116.34
50	X	201	8Q1	C38-C37-N36	-2.22	107.27	112.00
50	X	201	8Q1	C43-S44-C1	2.19	108.30	101.84
46	A	502	FMN	C4A-C10-N1	-2.13	119.37	124.59
47	A	503	NAI	C4A-N9A-C8A	2.13	107.97	105.74
48	B	303	PEE	O2-C10-O4	-2.10	118.80	123.70
50	X	201	8Q1	C37-C38-C39	2.09	115.88	112.39
50	G	201	8Q1	O40-C39-N41	-2.09	118.93	123.03
57	w	401	ADP	C2'-C3'-C4'	2.08	106.63	102.61
56	s	401	UQ	C7-C6-C1	2.08	120.93	118.52
50	G	201	8Q1	C42-N41-C39	-2.07	118.98	122.82
51	l	701	CDL	OB6-CB5-OB7	-2.04	118.94	123.70
51	a	201	CDL	OB6-CB5-OB7	-2.00	119.03	123.70

There are no chirality outliers.

All (635) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C1'-C2'-C3'-O3'
48	C	302	PEE	C1-O3P-P-O1P
48	C	302	PEE	C1-O3P-P-O4P
48	U	101	PEE	C1-O3P-P-O1P
48	U	101	PEE	C1-O3P-P-O4P
48	i	402	PEE	C11-C10-O2-C2
48	i	402	PEE	C1-O3P-P-O2P
48	i	402	PEE	C1-O3P-P-O1P
48	i	402	PEE	C1-O3P-P-O4P
48	l	703	PEE	C11-C10-O2-C2
48	l	703	PEE	C4-O4P-P-O3P
48	l	703	PEE	C4-O4P-P-O2P
48	l	703	PEE	C4-O4P-P-O1P
48	m	201	PEE	C11-C10-O2-C2
48	m	201	PEE	O4-C10-O2-C2
49	C	303	PLX	O7-C6-C7-C8
49	C	303	PLX	O4-C3-C4-O6
49	C	303	PLX	C3-O4-P1-O1
49	C	303	PLX	C3-O4-P1-O2
49	C	303	PLX	C3-O4-P1-O3
49	C	303	PLX	N1-C1-C2-O1
49	g	201	PLX	O7-C6-O6-C4
49	g	201	PLX	C25-C24-O8-C5
49	j	201	PLX	O7-C6-C7-C8
49	j	201	PLX	C3-O4-P1-O1
49	j	201	PLX	C3-O4-P1-O3
49	r	502	PLX	O7-C6-O6-C4
49	r	502	PLX	C3-O4-P1-O1
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	C2-O1-P1-O4
49	r	502	PLX	C2-O1-P1-O2
49	r	502	PLX	C2-O1-P1-O3
49	r	502	PLX	O9-C24-O8-C5
49	r	502	PLX	O9-C24-C25-C26
50	G	201	8Q1	C1-C6-C7-C8
50	G	201	8Q1	N41-C42-C43-S44
50	G	201	8Q1	C42-C43-S44-C1
50	G	201	8Q1	C28-O27-P24-O2
50	G	201	8Q1	C28-O27-P24-O1
50	X	201	8Q1	C1-C6-C7-C8
50	X	201	8Q1	O4-C1-S44-C43

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Mol	Chain	Res	Type	Atoms
50	X	201	8Q1	C6-C1-S44-C43
50	X	201	8Q1	O27-C28-C29-C30
50	X	201	8Q1	O27-C28-C29-C31
50	X	201	8Q1	O27-C28-C29-C32
50	X	201	8Q1	C28-C29-C32-C34
50	X	201	8Q1	C28-C29-C32-O33
50	X	201	8Q1	C30-C29-C32-C34
50	X	201	8Q1	C30-C29-C32-O33
50	X	201	8Q1	C31-C29-C32-C34
50	X	201	8Q1	C31-C29-C32-O33
50	X	201	8Q1	N36-C37-C38-C39
50	X	201	8Q1	C42-C43-S44-C1
50	X	201	8Q1	C28-O27-P24-O3
50	X	201	8Q1	C28-O27-P24-O2
50	X	201	8Q1	C28-O27-P24-O1
51	I	201	CDL	CA2-OA2-PA1-OA3
51	I	201	CDL	CA2-OA2-PA1-OA5
51	I	201	CDL	CA3-OA5-PA1-OA2
51	I	201	CDL	CA3-OA5-PA1-OA3
51	I	201	CDL	CA3-OA5-PA1-OA4
51	I	201	CDL	CB2-OB2-PB2-OB3
51	I	201	CDL	CB2-OB2-PB2-OB4
51	I	201	CDL	CB2-OB2-PB2-OB5
51	I	201	CDL	CB3-OB5-PB2-OB2
51	I	201	CDL	CB3-OB5-PB2-OB3
51	a	201	CDL	CA2-OA2-PA1-OA3
51	a	201	CDL	CA2-OA2-PA1-OA4
51	a	201	CDL	CA2-OA2-PA1-OA5
51	a	201	CDL	CA3-OA5-PA1-OA2
51	a	201	CDL	CA3-OA5-PA1-OA3
51	a	201	CDL	CA3-OA5-PA1-OA4
51	a	201	CDL	OA5-CA3-CA4-OA6
51	a	201	CDL	CB3-OB5-PB2-OB3
51	i	401	CDL	CA2-OA2-PA1-OA4
51	i	401	CDL	CA2-OA2-PA1-OA5
51	i	401	CDL	CA3-OA5-PA1-OA2
51	i	401	CDL	CA3-OA5-PA1-OA4
51	i	401	CDL	CB2-OB2-PB2-OB3
51	i	401	CDL	CB2-OB2-PB2-OB4
51	i	401	CDL	CB2-OB2-PB2-OB5
51	i	401	CDL	CB3-OB5-PB2-OB3
51	l	701	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
51	l	701	CDL	CA2-OA2-PA1-OA5
51	l	701	CDL	CB2-OB2-PB2-OB5
51	l	701	CDL	CB3-OB5-PB2-OB2
51	l	701	CDL	CB3-OB5-PB2-OB3
51	l	701	CDL	CB3-OB5-PB2-OB4
51	l	702	CDL	CA2-OA2-PA1-OA4
51	l	702	CDL	CA2-OA2-PA1-OA5
51	l	702	CDL	CA3-OA5-PA1-OA2
51	l	702	CDL	CA3-OA5-PA1-OA3
51	l	702	CDL	CA3-OA5-PA1-OA4
51	l	702	CDL	OA6-CA4-CA6-OA8
51	l	702	CDL	CB2-OB2-PB2-OB4
51	l	702	CDL	CB2-OB2-PB2-OB5
51	l	702	CDL	OB6-CB4-CB6-OB8
51	r	503	CDL	CA2-OA2-PA1-OA3
51	r	503	CDL	CA2-OA2-PA1-OA4
51	r	503	CDL	CA2-OA2-PA1-OA5
51	r	503	CDL	CA3-OA5-PA1-OA2
51	r	503	CDL	CA3-OA5-PA1-OA3
51	r	503	CDL	CA3-OA5-PA1-OA4
51	r	503	CDL	OA6-CA4-CA6-OA8
51	r	503	CDL	CB3-OB5-PB2-OB2
52	J	401	NDP	O4B-C4B-C5B-O5B
52	J	401	NDP	C2N-C3N-C7N-N7N
56	s	401	UQ	C7-C8-C9-C10
56	s	401	UQ	C7-C8-C9-C11
57	w	401	ADP	C5'-O5'-PA-O2A
56	s	401	UQ	C17-C18-C19-C21
48	i	402	PEE	O4-C10-O2-C2
48	l	703	PEE	O4-C10-O2-C2
51	r	503	CDL	C71-CB7-OB8-CB6
51	i	401	CDL	OA9-CA7-OA8-CA6
56	s	401	UQ	C12-C11-C9-C10
48	m	201	PEE	O5-C30-O3-C3
48	m	201	PEE	C31-C30-O3-C3
48	B	303	PEE	C37-C38-C39-C40
56	s	401	UQ	C12-C13-C14-C16
51	r	503	CDL	OB9-CB7-OB8-CB6
51	r	503	CDL	C83-C84-C85-C86
51	l	702	CDL	O1-C1-CB2-OB2
48	l	703	PEE	C31-C30-O3-C3
51	i	401	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
51	l	701	CDL	C31-CA7-OA8-CA6
51	l	702	CDL	C71-CB7-OB8-CB6
51	l	701	CDL	OA9-CA7-OA8-CA6
48	C	302	PEE	C11-C10-O2-C2
51	I	201	CDL	C11-CA5-OA6-CA4
51	r	503	CDL	C51-CB5-OB6-CB4
52	J	401	NDP	C2D-C1D-N1N-C6N
51	l	702	CDL	OB9-CB7-OB8-CB6
48	l	703	PEE	O5-C30-O3-C3
56	s	401	UQ	C14-C16-C17-C18
48	U	101	PEE	C17-C18-C19-C20
48	r	501	PEE	C17-C18-C19-C20
49	C	303	PLX	C28-C29-C30-C31
51	l	702	CDL	C11-C12-C13-C14
51	i	401	CDL	C14-C15-C16-C17
51	i	401	CDL	C31-C32-C33-C34
48	C	302	PEE	O4-C10-O2-C2
51	I	201	CDL	OA7-CA5-OA6-CA4
51	l	701	CDL	CB2-C1-CA2-OA2
51	r	503	CDL	CB2-C1-CA2-OA2
48	U	101	PEE	C31-C30-O3-C3
51	a	201	CDL	C71-CB7-OB8-CB6
49	j	201	PLX	C28-C29-C30-C31
51	r	503	CDL	C36-C37-C38-C39
49	j	201	PLX	C34-C35-C36-C37
49	r	502	PLX	C12-C13-C14-C15
49	g	201	PLX	C7-C8-C9-C10
51	l	702	CDL	C59-C60-C61-C62
56	s	401	UQ	C13-C14-C16-C17
51	l	702	CDL	O1-C1-CA2-OA2
51	a	201	CDL	OB9-CB7-OB8-CB6
51	r	503	CDL	OB7-CB5-OB6-CB4
51	I	201	CDL	C51-CB5-OB6-CB4
48	B	303	PEE	C12-C13-C14-C15
51	l	702	CDL	C35-C36-C37-C38
48	U	101	PEE	O5-C30-O3-C3
47	A	503	NAI	C3D-C4D-C5D-O5D
52	J	401	NDP	C3B-C4B-C5B-O5B
48	r	501	PEE	C10-C11-C12-C13
48	B	303	PEE	C30-C31-C32-C33
51	i	401	CDL	CA7-C31-C32-C33
51	r	503	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
51	l	702	CDL	C39-C40-C41-C42
51	l	702	CDL	C54-C55-C56-C57
51	i	401	CDL	O1-C1-CA2-OA2
51	r	503	CDL	O1-C1-CA2-OA2
48	i	402	PEE	C31-C30-O3-C3
49	j	201	PLX	C15-C16-C17-C18
51	I	201	CDL	OB7-CB5-OB6-CB4
48	i	402	PEE	C17-C18-C19-C20
48	U	101	PEE	C34-C35-C36-C37
51	a	201	CDL	CA7-C31-C32-C33
51	i	401	CDL	CB2-C1-CA2-OA2
51	r	503	CDL	CA7-C31-C32-C33
51	l	701	CDL	C16-C17-C18-C19
51	l	701	CDL	CB5-C51-C52-C53
56	s	401	UQ	C9-C11-C12-C13
48	i	402	PEE	O5-C30-O3-C3
48	i	402	PEE	C10-C11-C12-C13
48	i	402	PEE	C22-C23-C24-C25
48	l	703	PEE	C30-C31-C32-C33
51	l	701	CDL	C59-C60-C61-C62
49	C	303	PLX	C7-C8-C9-C10
49	r	502	PLX	C13-C14-C15-C16
51	a	201	CDL	C17-C18-C19-C20
48	U	101	PEE	C21-C22-C23-C24
48	l	703	PEE	C23-C24-C25-C26
51	l	702	CDL	C75-C76-C77-C78
49	r	502	PLX	C25-C26-C27-C28
51	l	702	CDL	C37-C38-C39-C40
49	g	201	PLX	C11-C10-C9-C8
49	g	201	PLX	C30-C31-C32-C33
49	j	201	PLX	C27-C28-C29-C30
49	r	502	PLX	C28-C29-C30-C31
49	g	201	PLX	C27-C28-C29-C30
51	r	503	CDL	C56-C57-C58-C59
51	I	201	CDL	CB7-C71-C72-C73
50	G	201	8Q1	C11-C12-C13-C14
48	B	303	PEE	O3P-C1-C2-C3
48	U	101	PEE	C11-C10-O2-C2
49	C	303	PLX	C17-C18-C19-C20
51	r	503	CDL	CB5-C51-C52-C53
49	r	502	PLX	C14-C15-C16-C17
51	a	201	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
48	C	302	PEE	C42-C43-C44-C45
49	g	201	PLX	C33-C34-C35-C36
51	a	201	CDL	C71-C72-C73-C74
51	r	503	CDL	C59-C60-C61-C62
49	j	201	PLX	C14-C15-C16-C17
49	r	502	PLX	C10-C11-C12-C13
51	i	401	CDL	C11-C12-C13-C14
51	l	701	CDL	C14-C15-C16-C17
48	U	101	PEE	C41-C42-C43-C44
51	I	201	CDL	C31-CA7-OA8-CA6
49	j	201	PLX	C12-C13-C14-C15
51	I	201	CDL	C11-C12-C13-C14
51	a	201	CDL	C76-C77-C78-C79
51	i	401	CDL	C52-C53-C54-C55
51	l	701	CDL	C51-C52-C53-C54
51	r	503	CDL	C41-C42-C43-C44
48	l	703	PEE	C31-C32-C33-C34
49	g	201	PLX	C32-C33-C34-C35
50	X	201	8Q1	C7-C8-C9-C10
49	C	303	PLX	C11-C12-C13-C14
51	r	503	CDL	C75-C76-C77-C78
51	i	401	CDL	CB5-C51-C52-C53
51	r	503	CDL	CA5-C11-C12-C13
48	i	402	PEE	C32-C33-C34-C35
48	r	501	PEE	C11-C10-O2-C2
48	B	303	PEE	C31-C30-O3-C3
48	U	101	PEE	C40-C41-C42-C43
49	g	201	PLX	C10-C11-C12-C13
48	B	303	PEE	C21-C22-C23-C24
48	B	303	PEE	C33-C34-C35-C36
50	G	201	8Q1	C10-C11-C12-C13
51	a	201	CDL	C73-C74-C75-C76
51	r	503	CDL	C73-C74-C75-C76
48	U	101	PEE	O4-C10-O2-C2
49	j	201	PLX	C13-C14-C15-C16
49	j	201	PLX	C35-C36-C37-C38
51	r	503	CDL	C82-C83-C84-C85
48	i	402	PEE	C14-C15-C16-C17
49	j	201	PLX	C25-C26-C27-C28
51	l	702	CDL	C14-C15-C16-C17
49	r	502	PLX	C29-C30-C31-C32
51	a	201	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
49	C	303	PLX	C35-C36-C37-C38
48	B	303	PEE	C14-C15-C16-C17
49	C	303	PLX	C25-C26-C27-C28
49	g	201	PLX	C9-C10-C11-C12
49	j	201	PLX	C10-C11-C12-C13
48	U	101	PEE	C36-C37-C38-C39
49	g	201	PLX	C14-C15-C16-C17
51	r	503	CDL	C17-C18-C19-C20
48	B	303	PEE	C11-C10-O2-C2
50	G	201	8Q1	N36-C37-C38-C39
51	I	201	CDL	CA7-C31-C32-C33
51	l	701	CDL	CA5-C11-C12-C13
51	l	701	CDL	C58-C59-C60-C61
48	r	501	PEE	O4-C10-O2-C2
51	r	503	CDL	C43-C44-C45-C46
48	U	101	PEE	C19-C20-C21-C22
51	i	401	CDL	C36-C37-C38-C39
51	i	401	CDL	C37-C38-C39-C40
48	m	201	PEE	C11-C12-C13-C14
51	l	702	CDL	C52-C53-C54-C55
49	C	303	PLX	C9-C10-C11-C12
51	i	401	CDL	C12-C13-C14-C15
49	r	502	PLX	C2-C1-N1-C1C
49	r	502	PLX	C2-C1-N1-C1A
49	j	201	PLX	C33-C34-C35-C36
51	a	201	CDL	C75-C76-C77-C78
48	C	302	PEE	C32-C33-C34-C35
48	l	703	PEE	O3P-C1-C2-O2
48	B	303	PEE	C20-C21-C22-C23
48	C	302	PEE	C13-C14-C15-C16
51	I	201	CDL	OA9-CA7-OA8-CA6
51	r	503	CDL	C35-C36-C37-C38
48	i	402	PEE	C19-C20-C21-C22
49	g	201	PLX	C28-C29-C30-C31
51	i	401	CDL	C71-CB7-OB8-CB6
48	B	303	PEE	O5-C30-O3-C3
51	i	401	CDL	C13-C14-C15-C16
48	r	501	PEE	C36-C37-C38-C39
50	G	201	8Q1	C12-C13-C14-C15
51	i	401	CDL	C32-C33-C34-C35
51	i	401	CDL	C35-C36-C37-C38
51	r	503	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
49	r	502	PLX	C11-C12-C13-C14
50	G	201	8Q1	C9-C10-C11-C12
51	l	702	CDL	CA2-C1-CB2-OB2
48	C	302	PEE	C11-C12-C13-C14
49	g	201	PLX	C25-C26-C27-C28
51	r	503	CDL	C37-C38-C39-C40
50	G	201	8Q1	C7-C8-C9-C10
51	i	401	CDL	C73-C74-C75-C76
49	r	502	PLX	C33-C34-C35-C36
49	r	502	PLX	C31-C32-C33-C34
48	l	703	PEE	C19-C20-C21-C22
51	a	201	CDL	C74-C75-C76-C77
48	B	303	PEE	O4-C10-O2-C2
49	C	303	PLX	O6-C6-C7-C8
49	g	201	PLX	O8-C24-C25-C26
51	l	701	CDL	C35-C36-C37-C38
48	l	703	PEE	C37-C38-C39-C40
48	C	302	PEE	C1-C2-C3-O3
49	j	201	PLX	C3-C4-C5-O8
51	I	201	CDL	CA3-CA4-CA6-OA8
51	r	503	CDL	CA3-CA4-CA6-OA8
49	j	201	PLX	C7-C8-C9-C10
51	i	401	CDL	OB9-CB7-OB8-CB6
48	B	303	PEE	C15-C16-C17-C18
48	C	302	PEE	C15-C16-C17-C18
48	C	302	PEE	C39-C40-C41-C42
48	i	402	PEE	C35-C36-C37-C38
48	l	703	PEE	C15-C16-C17-C18
51	a	201	CDL	C22-C23-C24-C25
48	l	703	PEE	C33-C34-C35-C36
49	g	201	PLX	C13-C14-C15-C16
49	r	502	PLX	C2-C1-N1-C1B
51	a	201	CDL	CB5-C51-C52-C53
48	m	201	PEE	C13-C14-C15-C16
51	r	503	CDL	C81-C82-C83-C84
50	G	201	8Q1	C28-O27-P24-O3
50	X	201	8Q1	C6-C7-C8-C9
51	l	702	CDL	C74-C75-C76-C77
51	I	201	CDL	CA6-CA4-OA6-CA5
49	C	303	PLX	C16-C17-C18-C19
49	C	303	PLX	C14-C15-C16-C17
51	r	503	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
51	l	702	CDL	CB7-C71-C72-C73
48	B	303	PEE	C17-C18-C19-C20
48	B	303	PEE	C34-C35-C36-C37
49	r	502	PLX	C27-C28-C29-C30
51	r	503	CDL	OB6-CB4-CB6-OB8
50	X	201	8Q1	C13-C14-C15-C16
51	r	503	CDL	C71-C72-C73-C74
51	l	702	CDL	C40-C41-C42-C43
51	l	702	CDL	C64-C65-C66-C67
49	j	201	PLX	C18-C19-C20-C21
51	r	503	CDL	C55-C56-C57-C58
49	g	201	PLX	C20-C21-C22-C23
49	r	502	PLX	C36-C37-C38-C39
48	r	501	PEE	C12-C13-C14-C15
49	j	201	PLX	C30-C31-C32-C33
48	C	302	PEE	C31-C30-O3-C3
49	g	201	PLX	O9-C24-C25-C26
51	r	503	CDL	C84-C85-C86-C87
50	G	201	8Q1	C6-C7-C8-C9
49	j	201	PLX	C9-C10-C11-C12
48	l	703	PEE	O3P-C1-C2-C3
49	C	303	PLX	O4-C3-C4-C5
51	I	201	CDL	OB5-CB3-CB4-CB6
51	a	201	CDL	OA5-CA3-CA4-CA6
47	A	503	NAI	O4D-C4D-C5D-O5D
51	r	503	CDL	C52-C53-C54-C55
49	r	502	PLX	C16-C17-C18-C19
51	a	201	CDL	C31-C32-C33-C34
49	r	502	PLX	C3-C4-C5-O8
51	l	702	CDL	CA3-CA4-CA6-OA8
51	l	702	CDL	CB3-CB4-CB6-OB8
51	r	503	CDL	CB3-CB4-CB6-OB8
51	r	503	CDL	C74-C75-C76-C77
48	r	501	PEE	C31-C32-C33-C34
51	l	702	CDL	C33-C34-C35-C36
48	i	402	PEE	C23-C24-C25-C26
49	j	201	PLX	C31-C32-C33-C34
51	r	503	CDL	C78-C79-C80-C81
48	r	501	PEE	C40-C41-C42-C43
48	B	303	PEE	O3P-C1-C2-O2
51	l	701	CDL	C51-CB5-OB6-CB4
48	i	402	PEE	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
51	l	702	CDL	CB5-C51-C52-C53
51	r	503	CDL	C14-C15-C16-C17
50	G	201	8Q1	O4-C1-S44-C43
51	l	701	CDL	C24-C25-C26-C27
56	s	401	UQ	C17-C18-C19-C20
48	r	501	PEE	O2-C2-C3-O3
49	j	201	PLX	O6-C4-C5-O8
49	r	502	PLX	O6-C4-C5-O8
51	i	401	CDL	OB6-CB4-CB6-OB8
48	B	303	PEE	C42-C43-C44-C45
51	l	701	CDL	C82-C83-C84-C85
51	r	503	CDL	C64-C65-C66-C67
49	r	502	PLX	C15-C16-C17-C18
49	r	502	PLX	C7-C8-C9-C10
49	r	502	PLX	O8-C24-C25-C26
48	B	303	PEE	C13-C14-C15-C16
51	l	702	CDL	C32-C33-C34-C35
49	C	303	PLX	C26-C27-C28-C29
49	C	303	PLX	C33-C34-C35-C36
48	l	703	PEE	C11-C12-C13-C14
46	A	502	FMN	O2'-C2'-C3'-C4'
50	G	201	8Q1	C6-C1-S44-C43
51	a	201	CDL	C16-C17-C18-C19
51	l	702	CDL	C43-C44-C45-C46
51	i	401	CDL	C15-C16-C17-C18
49	g	201	PLX	O4-C3-C4-C5
49	j	201	PLX	O4-C3-C4-C5
51	l	702	CDL	C55-C56-C57-C58
51	l	702	CDL	C62-C63-C64-C65
49	r	502	PLX	C35-C36-C37-C38
51	i	401	CDL	C71-C72-C73-C74
51	a	201	CDL	C52-C53-C54-C55
48	C	302	PEE	O5-C30-O3-C3
48	r	501	PEE	C41-C42-C43-C44
48	i	402	PEE	C24-C25-C26-C27
49	j	201	PLX	O4-C3-C4-O6
51	r	503	CDL	C33-C34-C35-C36
48	i	402	PEE	C1-C2-C3-O3
48	r	501	PEE	C1-C2-C3-O3
51	l	702	CDL	C73-C74-C75-C76
51	r	503	CDL	C20-C21-C22-C23
48	i	402	PEE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
48	i	402	PEE	O2-C2-C3-O3
51	i	401	CDL	OA6-CA4-CA6-OA8
48	r	501	PEE	C44-C45-C46-C47
48	U	101	PEE	C22-C23-C24-C25
49	r	502	PLX	C18-C19-C20-C21
51	a	201	CDL	C57-C58-C59-C60
51	l	702	CDL	C15-C16-C17-C18
48	m	201	PEE	O3-C30-C31-C32
51	r	503	CDL	C31-CA7-OA8-CA6
48	i	402	PEE	C2-C1-O3P-P
48	U	101	PEE	C12-C13-C14-C15
51	l	702	CDL	C57-C58-C59-C60
48	m	201	PEE	C33-C34-C35-C36
51	r	503	CDL	C42-C43-C44-C45
51	l	702	CDL	C77-C78-C79-C80
48	U	101	PEE	C38-C39-C40-C41
49	j	201	PLX	C25-C24-O8-C5
48	i	402	PEE	C31-C32-C33-C34
51	a	201	CDL	C35-C36-C37-C38
48	i	402	PEE	C18-C19-C20-C21
51	a	201	CDL	C21-C22-C23-C24
51	a	201	CDL	C43-C44-C45-C46
51	l	702	CDL	OA5-CA3-CA4-CA6
51	l	701	CDL	OB7-CB5-OB6-CB4
51	l	702	CDL	C51-C52-C53-C54
51	r	503	CDL	C31-C32-C33-C34
50	G	201	8Q1	O27-C28-C29-C30
50	G	201	8Q1	O27-C28-C29-C31
51	l	702	CDL	C12-C13-C14-C15
48	i	402	PEE	C21-C22-C23-C24
51	l	702	CDL	C34-C35-C36-C37
48	C	302	PEE	C38-C39-C40-C41
49	C	303	PLX	C13-C14-C15-C16
51	r	503	CDL	OA9-CA7-OA8-CA6
51	a	201	CDL	C33-C34-C35-C36
49	j	201	PLX	O6-C6-C7-C8
49	g	201	PLX	O4-C3-C4-O6
51	I	201	CDL	OB5-CB3-CB4-OB6
51	l	702	CDL	OA5-CA3-CA4-OA6
49	r	502	PLX	C9-C10-C11-C12
48	C	302	PEE	C33-C34-C35-C36
51	r	503	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
52	J	401	NDP	C2N-C3N-C7N-O7N
48	r	501	PEE	C38-C39-C40-C41
48	l	703	PEE	C13-C14-C15-C16
48	U	101	PEE	C30-C31-C32-C33
48	C	302	PEE	O2-C2-C3-O3
51	r	503	CDL	C44-C45-C46-C47
51	r	503	CDL	C57-C58-C59-C60
48	i	402	PEE	C38-C39-C40-C41
48	m	201	PEE	C16-C17-C18-C19
48	m	201	PEE	C24-C25-C26-C27
47	A	503	NAI	C5B-O5B-PA-O1A
48	B	303	PEE	C1-O3P-P-O1P
48	C	302	PEE	C1-O3P-P-O2P
48	U	101	PEE	C1-O3P-P-O2P
48	i	402	PEE	C4-O4P-P-O1P
48	m	201	PEE	C4-O4P-P-O3P
48	m	201	PEE	C4-O4P-P-O2P
48	m	201	PEE	C4-O4P-P-O1P
48	r	501	PEE	C1-O3P-P-O2P
48	r	501	PEE	C1-O3P-P-O1P
48	r	501	PEE	C1-O3P-P-O4P
48	r	501	PEE	C4-O4P-P-O1P
49	g	201	PLX	C3-O4-P1-O2
49	r	502	PLX	C5-C4-O6-C6
51	I	201	CDL	CA2-OA2-PA1-OA4
51	I	201	CDL	CB3-OB5-PB2-OB4
51	a	201	CDL	CB3-OB5-PB2-OB2
51	l	701	CDL	CA2-OA2-PA1-OA3
51	l	701	CDL	CB2-OB2-PB2-OB3
51	l	702	CDL	CA2-OA2-PA1-OA3
51	l	702	CDL	CB2-OB2-PB2-OB3
51	l	702	CDL	CB3-OB5-PB2-OB2
51	l	702	CDL	CB3-OB5-PB2-OB3
51	l	702	CDL	CB3-OB5-PB2-OB4
51	r	503	CDL	CB2-OB2-PB2-OB3
51	r	503	CDL	CB2-OB2-PB2-OB4
51	r	503	CDL	CB2-OB2-PB2-OB5
51	r	503	CDL	CB3-OB5-PB2-OB3
52	J	401	NDP	C5B-O5B-PA-O1A
52	J	401	NDP	C5B-O5B-PA-O2A
52	J	401	NDP	C5B-O5B-PA-O3
57	w	401	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
57	w	401	ADP	C5'-O5'-PA-O3A
50	X	201	8Q1	C9-C10-C11-C12
51	l	702	CDL	C56-C57-C58-C59
51	l	702	CDL	C60-C61-C62-C63
51	r	503	CDL	C40-C41-C42-C43
49	C	303	PLX	C15-C16-C17-C18
51	l	701	CDL	CA4-CA3-OA5-PA1
51	r	503	CDL	CB4-CB3-OB5-PB2
49	C	303	PLX	C27-C28-C29-C30
48	C	302	PEE	C43-C44-C45-C46
48	r	501	PEE	C24-C25-C26-C27
48	m	201	PEE	C3-C2-O2-C10
48	r	501	PEE	C11-C12-C13-C14
49	C	303	PLX	C31-C32-C33-C34
51	l	701	CDL	C37-C38-C39-C40
49	C	303	PLX	C30-C31-C32-C33
51	I	201	CDL	OA6-CA4-CA6-OA8
50	X	201	8Q1	C10-C11-C12-C13
51	i	401	CDL	C33-C34-C35-C36
51	l	702	CDL	C58-C59-C60-C61
52	J	401	NDP	PN-O3-PA-O1A
49	g	201	PLX	C18-C19-C20-C21
48	B	303	PEE	C19-C20-C21-C22
51	l	701	CDL	C33-C34-C35-C36
48	r	501	PEE	C30-C31-C32-C33
46	A	502	FMN	O2'-C2'-C3'-O3'
48	m	201	PEE	C19-C20-C21-C22
51	r	503	CDL	C80-C81-C82-C83
51	l	701	CDL	C61-C62-C63-C64
51	l	701	CDL	CB7-C71-C72-C73
48	m	201	PEE	C22-C23-C24-C25
48	l	703	PEE	C32-C33-C34-C35
48	r	501	PEE	C15-C16-C17-C18
50	X	201	8Q1	O33-C32-C34-N36
51	i	401	CDL	CB7-C71-C72-C73
48	l	703	PEE	C1-C2-O2-C10
48	l	703	PEE	C3-C2-O2-C10
47	A	503	NAI	O4D-C1D-N1N-C2N
47	A	503	NAI	C2D-C1D-N1N-C2N
49	j	201	PLX	C26-C27-C28-C29
51	a	201	CDL	C38-C39-C40-C41
51	l	701	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
49	r	502	PLX	C19-C20-C21-C22
48	i	402	PEE	O3P-C1-C2-C3
51	I	201	CDL	C51-C52-C53-C54
51	l	701	CDL	C11-C12-C13-C14
48	B	303	PEE	C22-C23-C24-C25
48	U	101	PEE	C43-C44-C45-C46
51	l	702	CDL	C71-C72-C73-C74
51	a	201	CDL	C32-C31-CA7-OA8
48	C	302	PEE	C18-C19-C20-C21
48	l	703	PEE	C24-C25-C26-C27
51	l	701	CDL	C76-C77-C78-C79
51	l	701	CDL	C52-C53-C54-C55
49	C	303	PLX	C18-C19-C20-C21
51	l	701	CDL	C72-C73-C74-C75
48	l	703	PEE	C20-C21-C22-C23
48	r	501	PEE	O3P-C1-C2-O2
49	g	201	PLX	C16-C17-C18-C19
49	g	201	PLX	C36-C37-C38-C39
51	i	401	CDL	CA4-CA3-OA5-PA1
51	l	701	CDL	C60-C61-C62-C63
51	l	701	CDL	OB9-CB7-OB8-CB6
48	i	402	PEE	C39-C40-C41-C42
49	j	201	PLX	C4-C5-O8-C24
51	r	503	CDL	C23-C24-C25-C26
48	B	303	PEE	C18-C19-C20-C21
48	C	302	PEE	C36-C37-C38-C39
48	i	402	PEE	C36-C37-C38-C39
48	U	101	PEE	C37-C38-C39-C40
48	r	501	PEE	O5-C30-O3-C3
51	i	401	CDL	C75-C76-C77-C78
51	r	503	CDL	C51-C52-C53-C54
48	l	703	PEE	C18-C19-C20-C21
48	l	703	PEE	C36-C37-C38-C39
49	r	502	PLX	C24-C25-C26-C27
48	r	501	PEE	C42-C43-C44-C45
48	r	501	PEE	C31-C30-O3-C3
48	r	501	PEE	C18-C19-C20-C21
49	g	201	PLX	C35-C36-C37-C38
51	l	702	CDL	C83-C84-C85-C86
51	i	401	CDL	CA3-CA4-CA6-OA8
51	i	401	CDL	CB3-CB4-CB6-OB8
48	C	302	PEE	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
51	a	201	CDL	C59-C60-C61-C62
49	j	201	PLX	C24-C25-C26-C27
51	I	201	CDL	C31-C32-C33-C34
49	r	502	PLX	C32-C33-C34-C35
48	m	201	PEE	C18-C19-C20-C21
51	r	503	CDL	C76-C77-C78-C79
49	j	201	PLX	C7-C6-O6-C4
48	U	101	PEE	C13-C14-C15-C16
49	j	201	PLX	C19-C20-C21-C22
51	I	201	CDL	C52-C51-CB5-OB6
51	l	701	CDL	C84-C85-C86-C87
49	g	201	PLX	C31-C32-C33-C34
51	I	201	CDL	C72-C71-CB7-OB8
51	l	702	CDL	C44-C45-C46-C47
56	s	401	UQ	C12-C11-C9-C8
48	r	501	PEE	C20-C21-C22-C23
49	r	502	PLX	C26-C27-C28-C29
48	C	302	PEE	O3-C30-C31-C32
48	U	101	PEE	O2-C10-C11-C12
48	U	101	PEE	O3-C30-C31-C32
51	l	702	CDL	C12-C11-CA5-OA6
51	a	201	CDL	C77-C78-C79-C80
57	w	401	ADP	C4'-C5'-O5'-PA
51	l	701	CDL	C73-C74-C75-C76
51	I	201	CDL	C52-C51-CB5-OB7
51	l	701	CDL	C12-C11-CA5-OA6
51	r	503	CDL	C72-C71-CB7-OB8
47	A	503	NAI	C2D-C1D-N1N-C6N
50	X	201	8Q1	C12-C13-C14-C15
49	g	201	PLX	O9-C24-O8-C5
49	j	201	PLX	O9-C24-O8-C5
48	U	101	PEE	O4-C10-C11-C12
48	m	201	PEE	O5-C30-C31-C32
51	l	701	CDL	C56-C57-C58-C59
48	m	201	PEE	C31-C32-C33-C34
51	l	702	CDL	C76-C77-C78-C79
51	I	201	CDL	C72-C71-CB7-OB9
51	l	702	CDL	C12-C11-CA5-OA7
48	i	402	PEE	C30-C31-C32-C33
51	l	702	CDL	C32-C31-CA7-OA8
51	r	503	CDL	C52-C51-CB5-OB6
48	r	501	PEE	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
48	m	201	PEE	C20-C21-C22-C23
51	l	701	CDL	C11-CA5-OA6-CA4
57	w	401	ADP	PB-O3A-PA-O2A
51	r	503	CDL	C72-C71-CB7-OB9

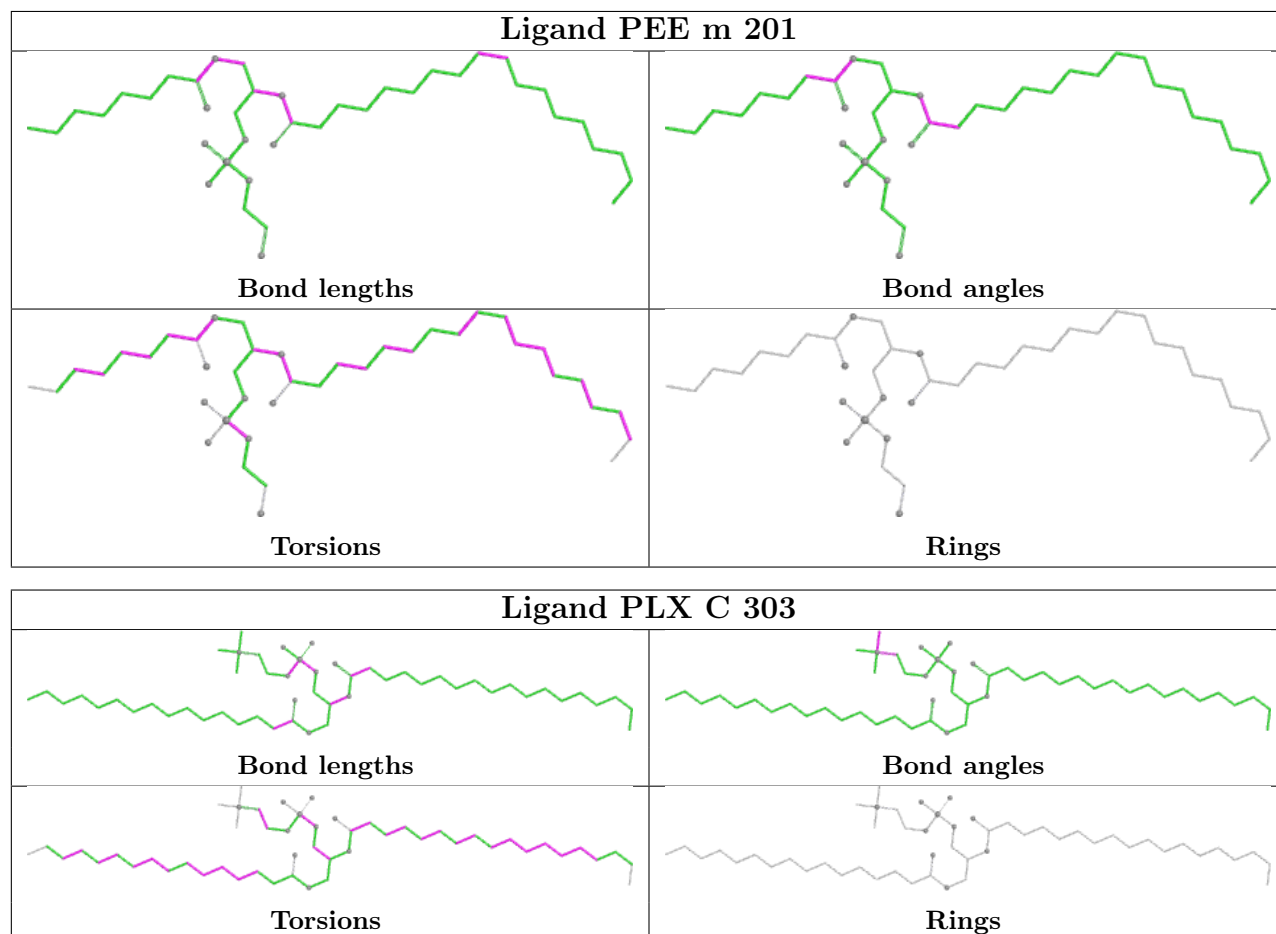
There are no ring outliers.

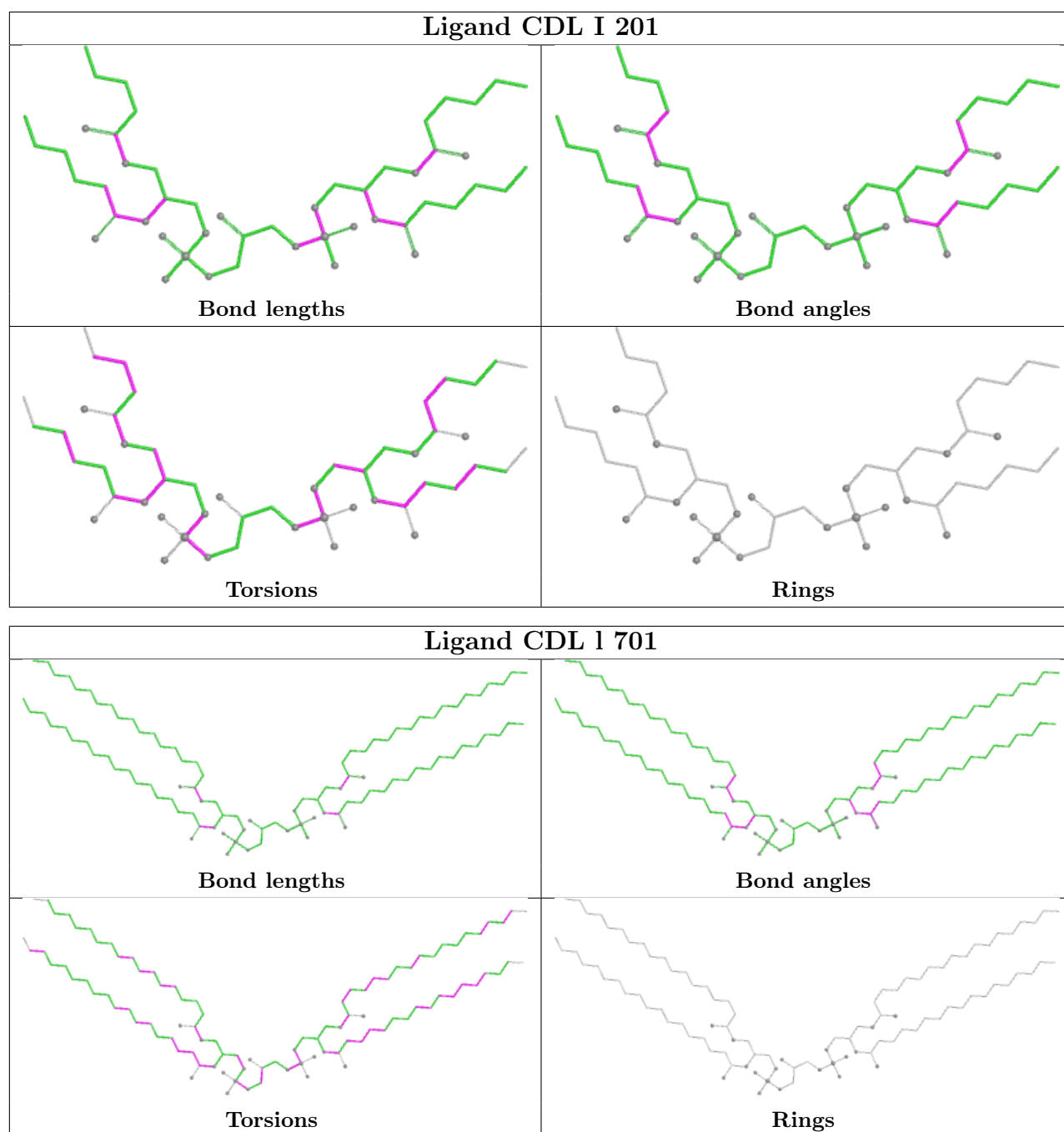
25 monomers are involved in 102 short contacts:

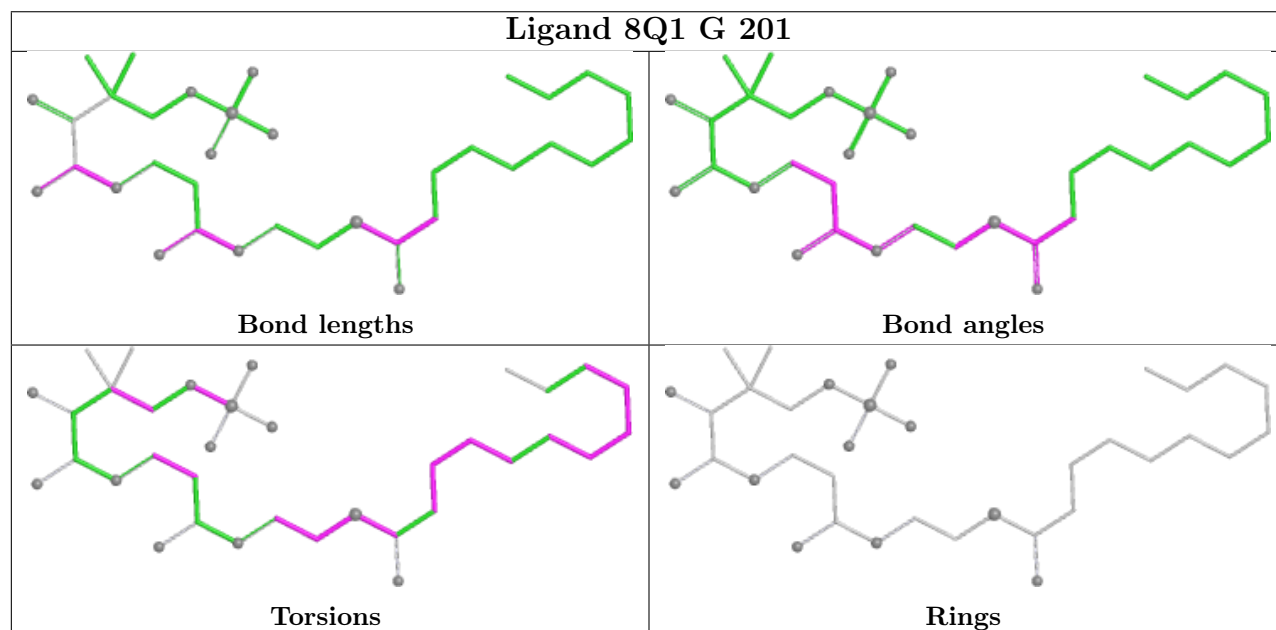
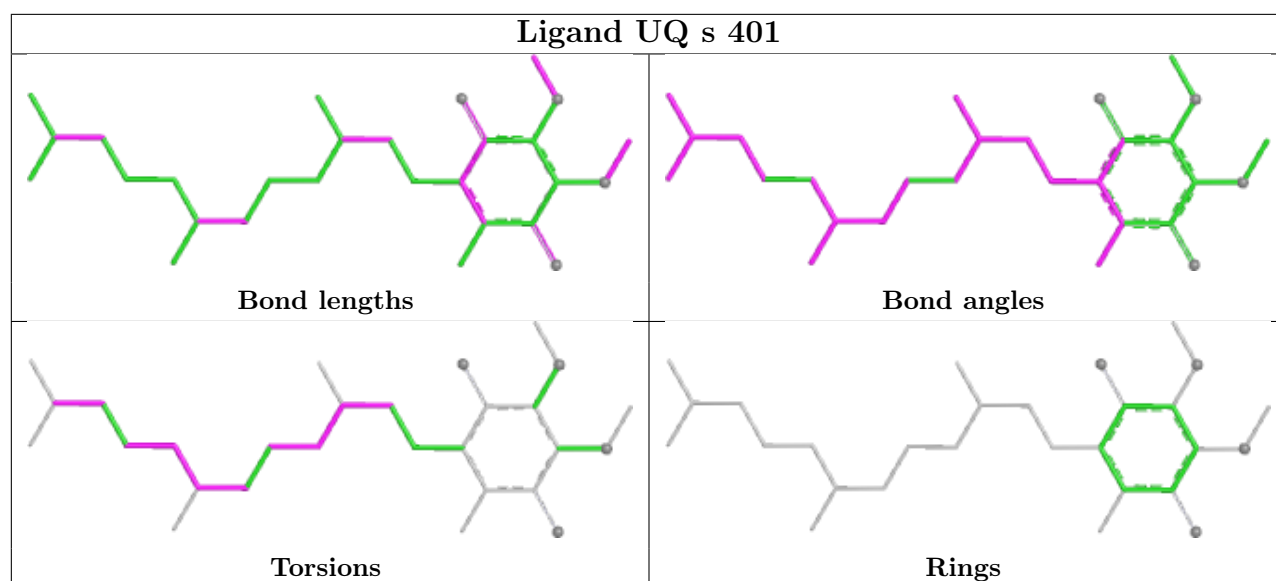
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	m	201	PEE	2	0
49	C	303	PLX	6	0
51	l	701	CDL	33	0
56	s	401	UQ	2	0
50	G	201	8Q1	1	0
49	j	201	PLX	4	0
49	r	502	PLX	2	0
47	A	503	NAI	4	0
48	l	703	PEE	2	0
52	J	401	NDP	2	0
48	r	501	PEE	3	0
48	i	402	PEE	2	0
45	A	501	SF4	2	0
48	U	101	PEE	3	0
46	A	502	FMN	3	0
49	g	201	PLX	4	0
51	a	201	CDL	3	0
51	l	702	CDL	3	0
48	C	302	PEE	2	0
51	r	503	CDL	7	0
45	C	301	SF4	1	0
50	X	201	8Q1	4	0
48	B	303	PEE	4	0
57	w	401	ADP	1	0
51	i	401	CDL	4	0

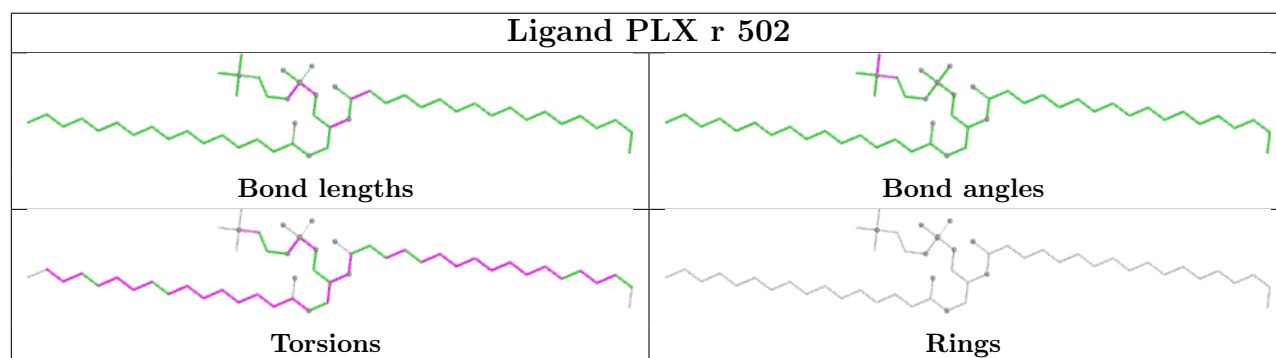
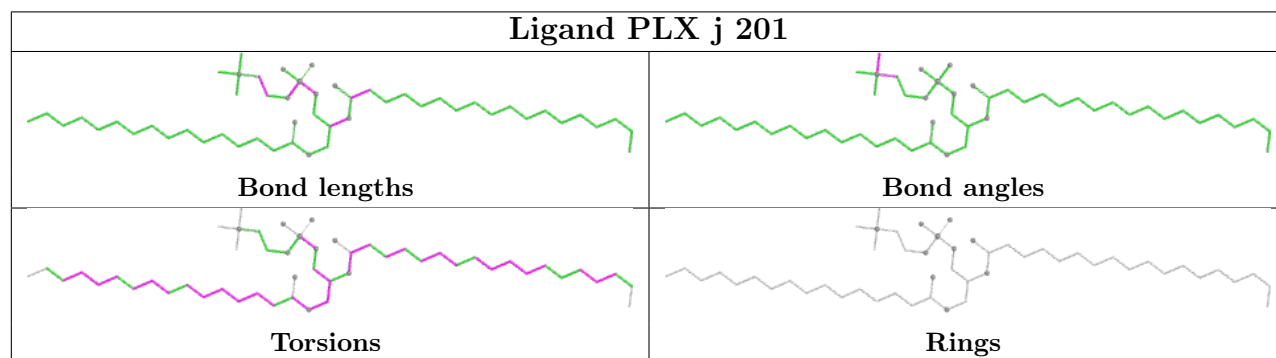
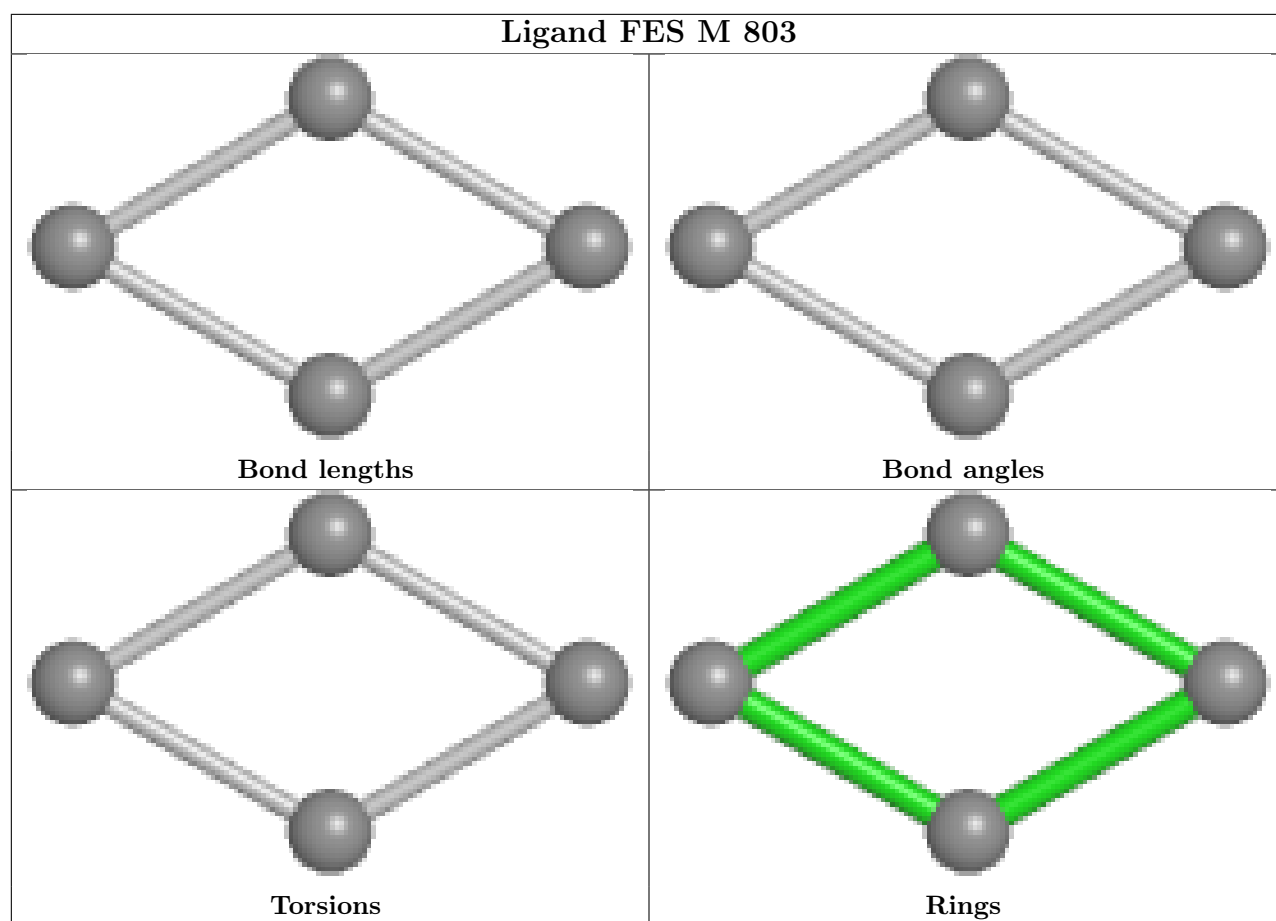
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

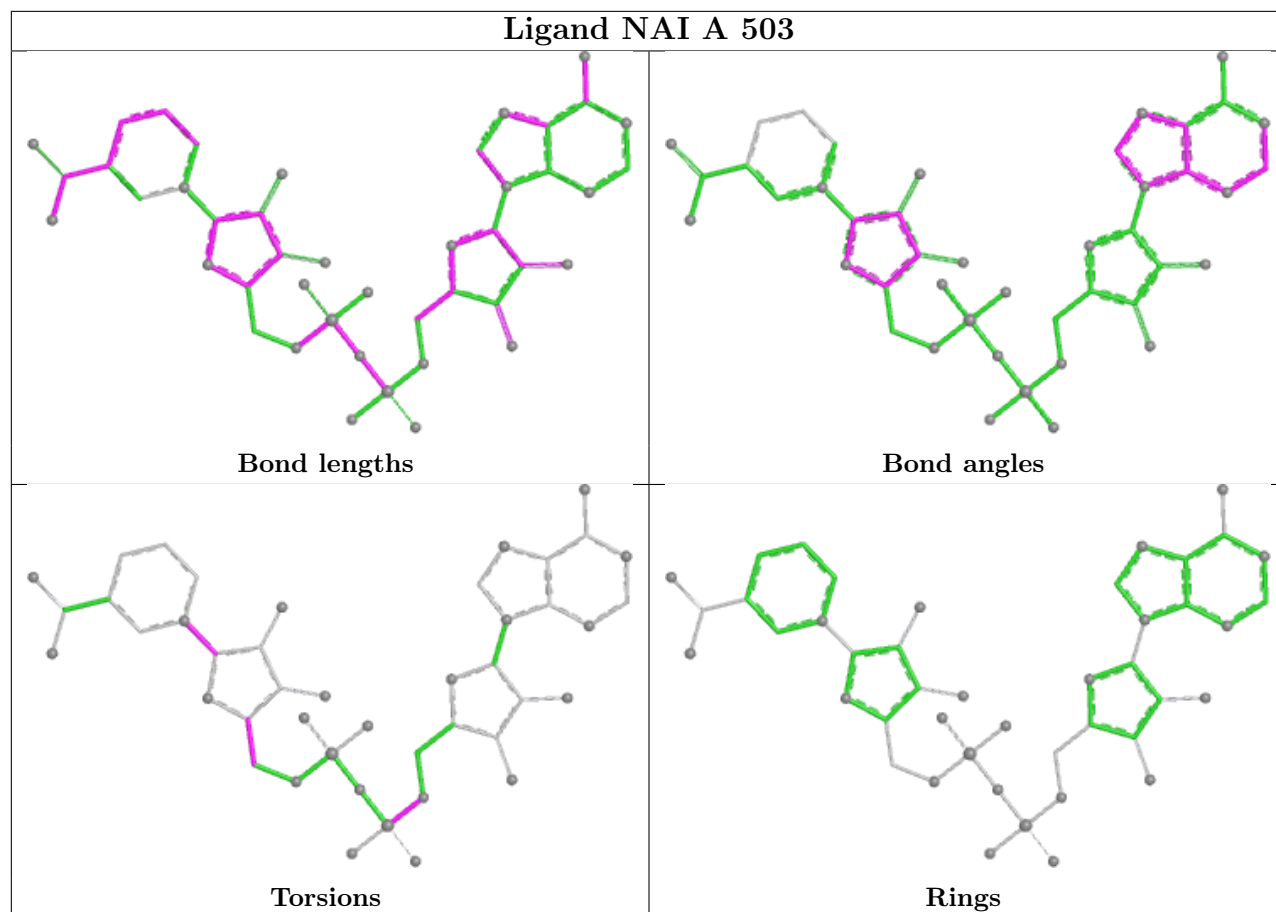




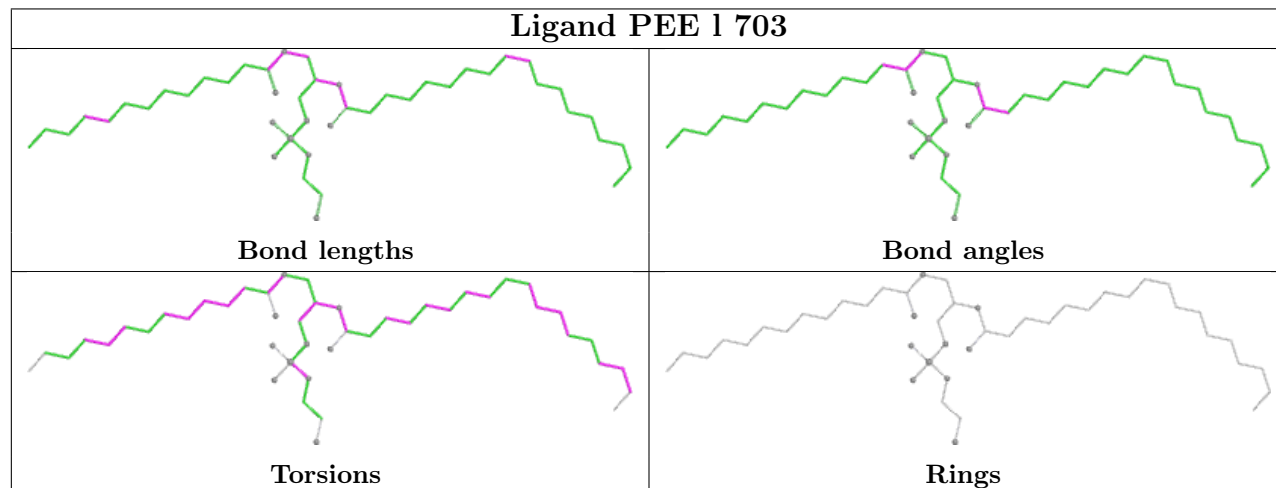




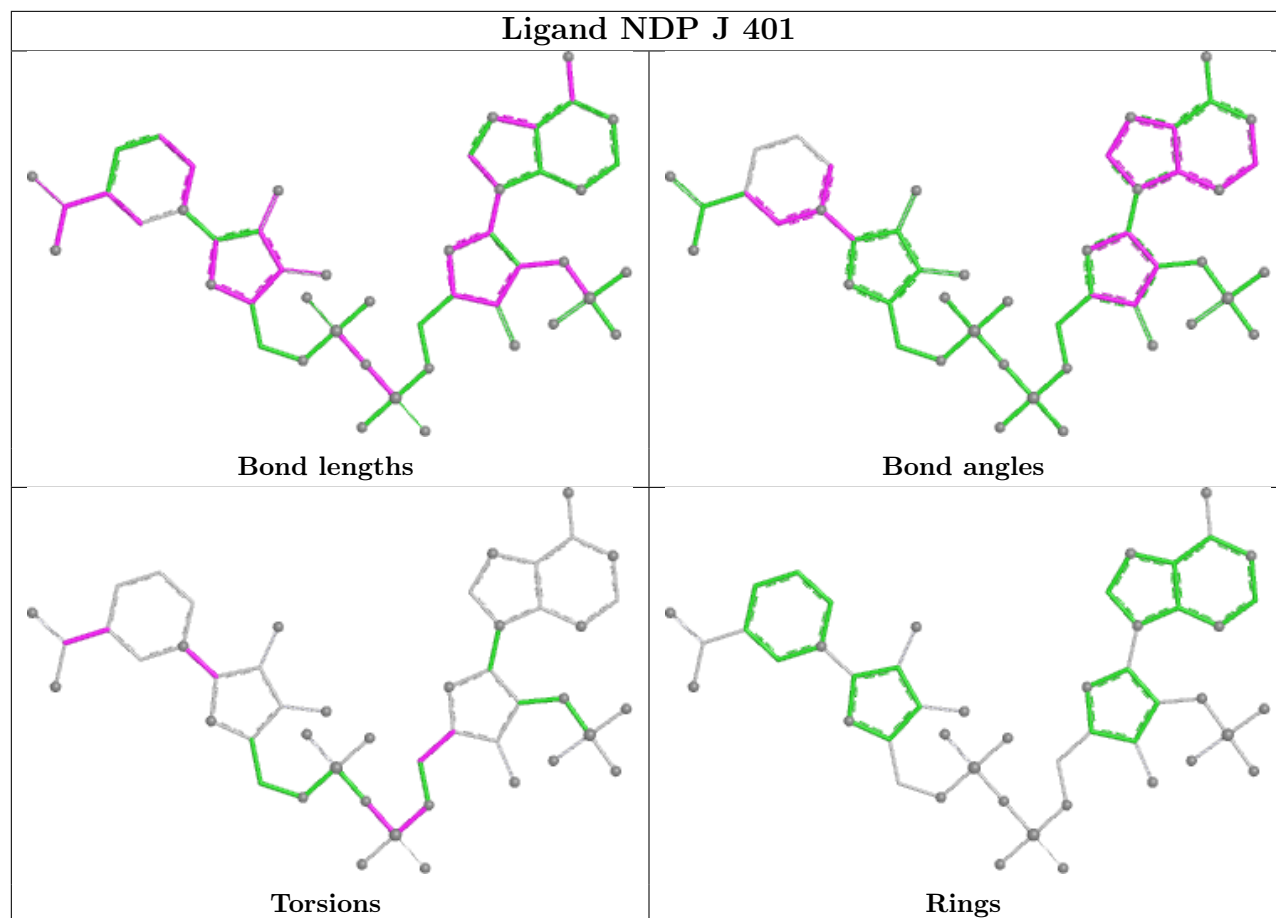
Ligand NAI A 503



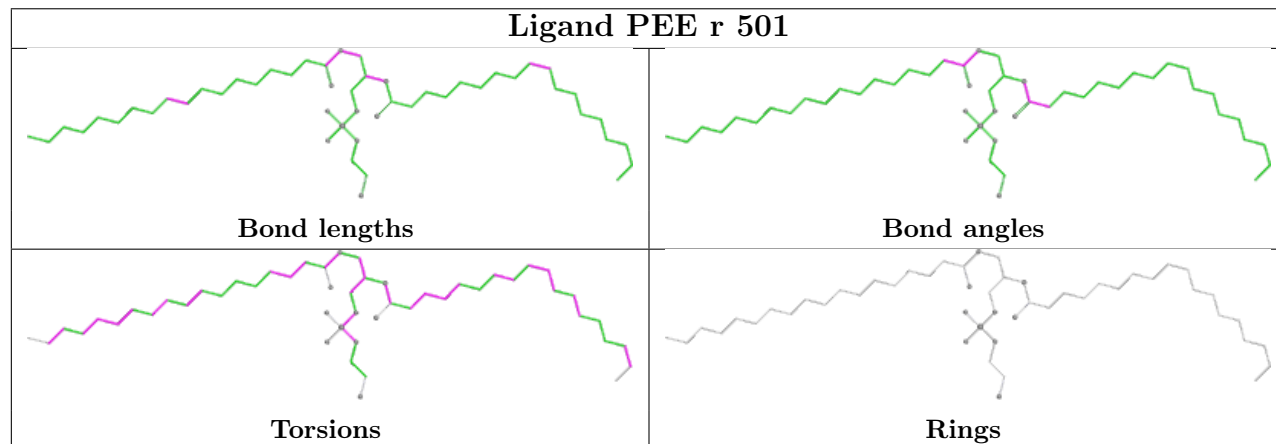
Ligand PEE 1 703

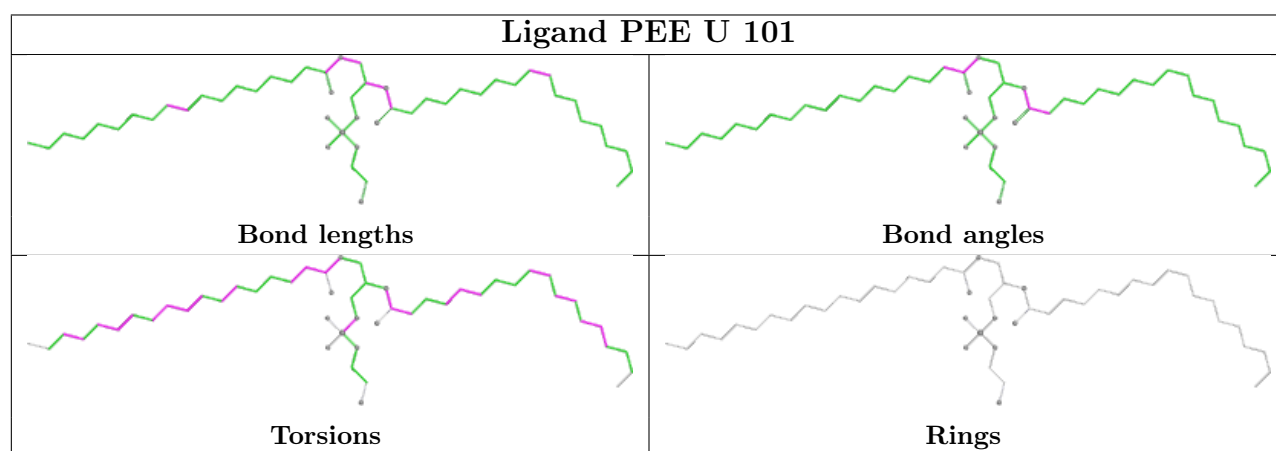
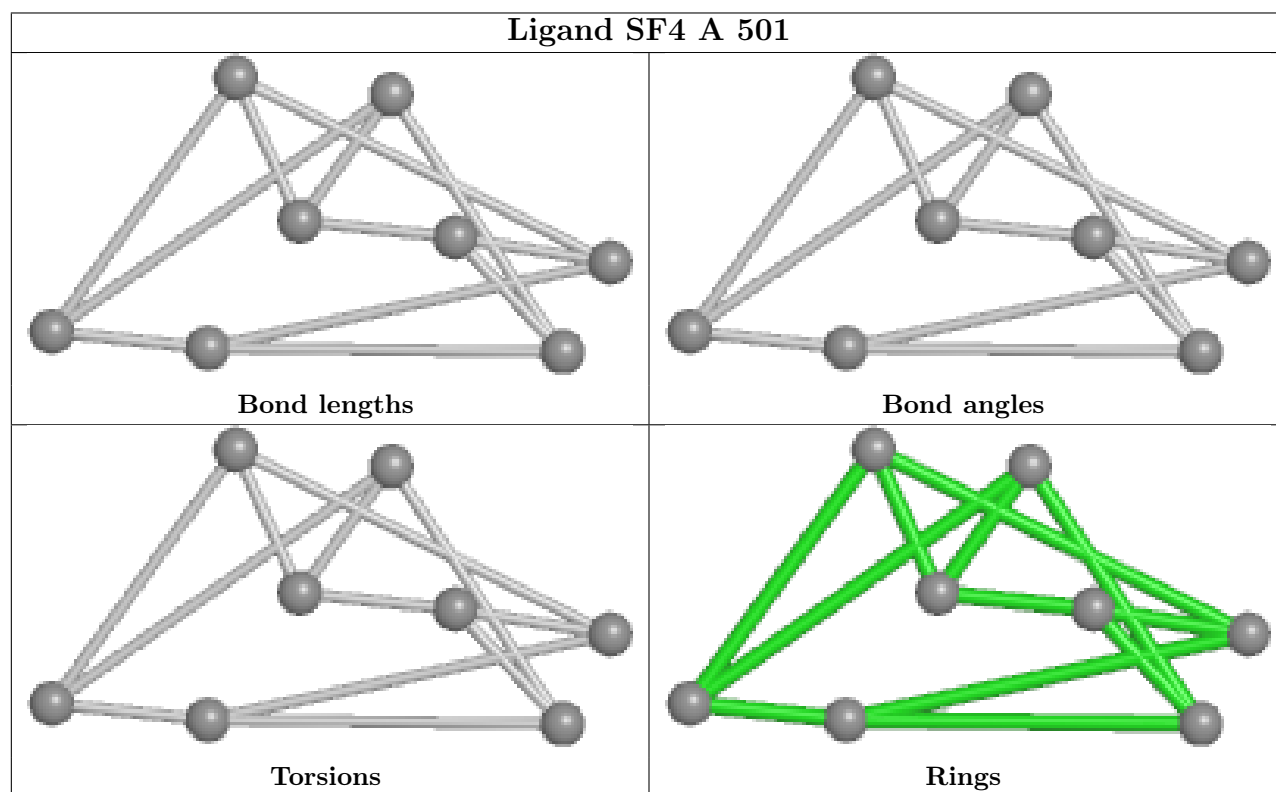
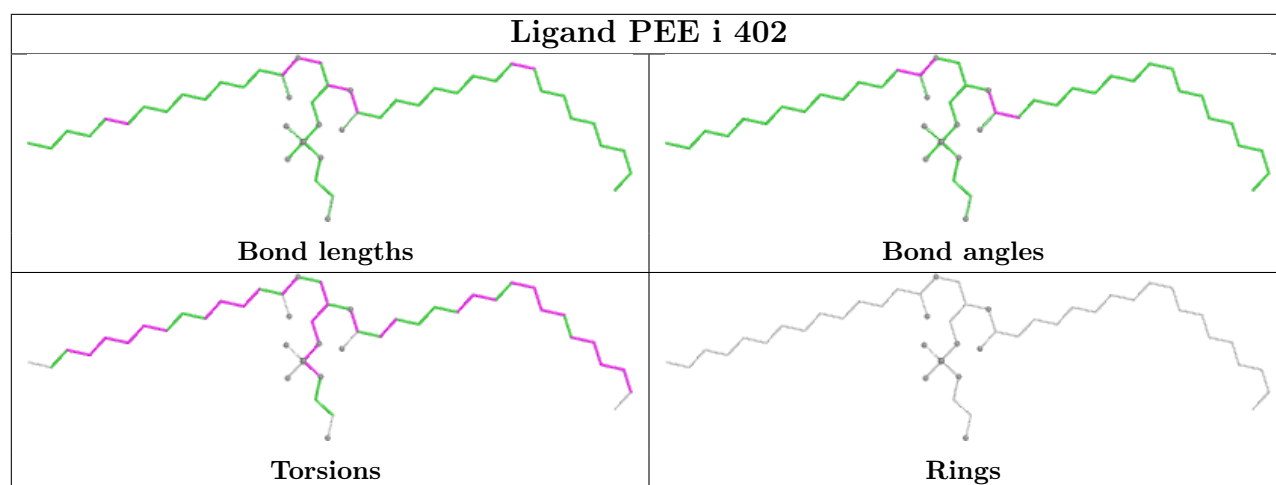


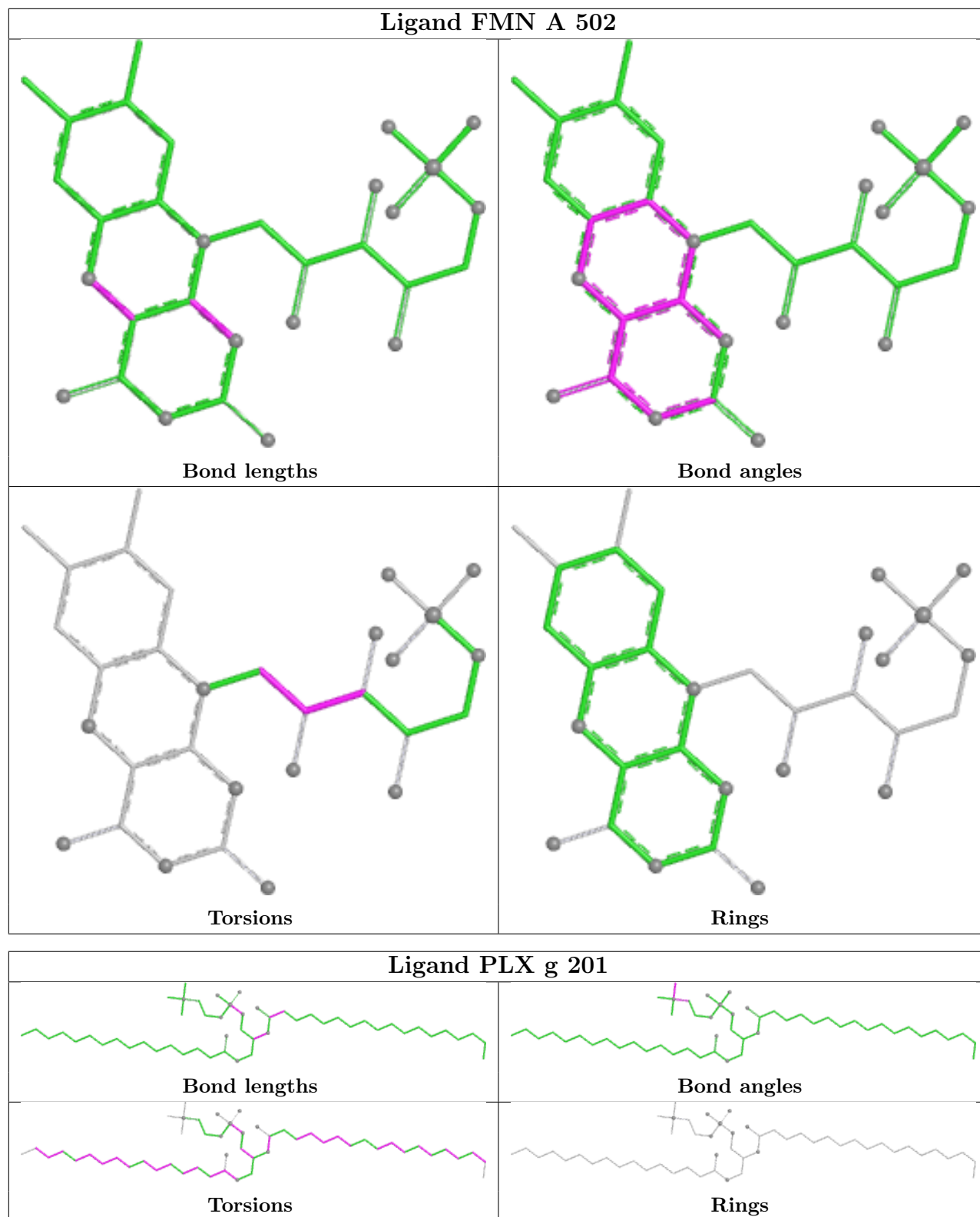
Ligand NDP J 401

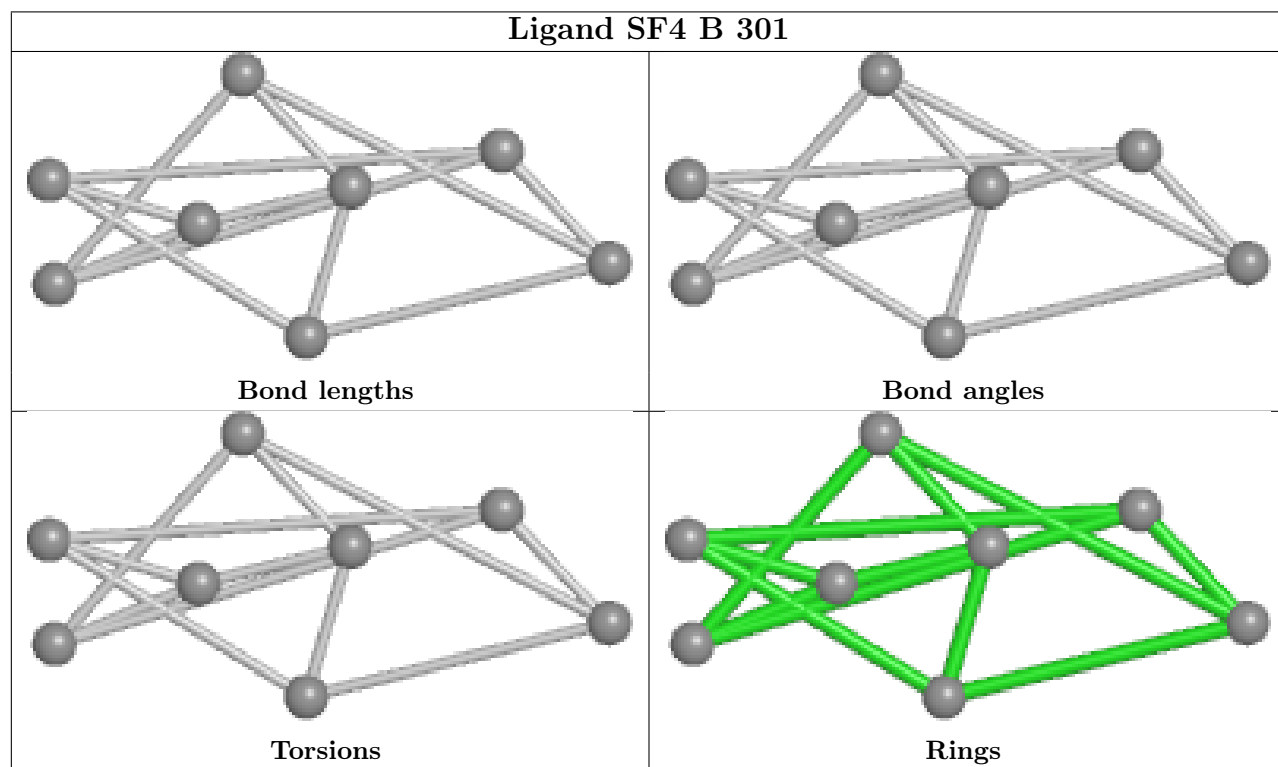
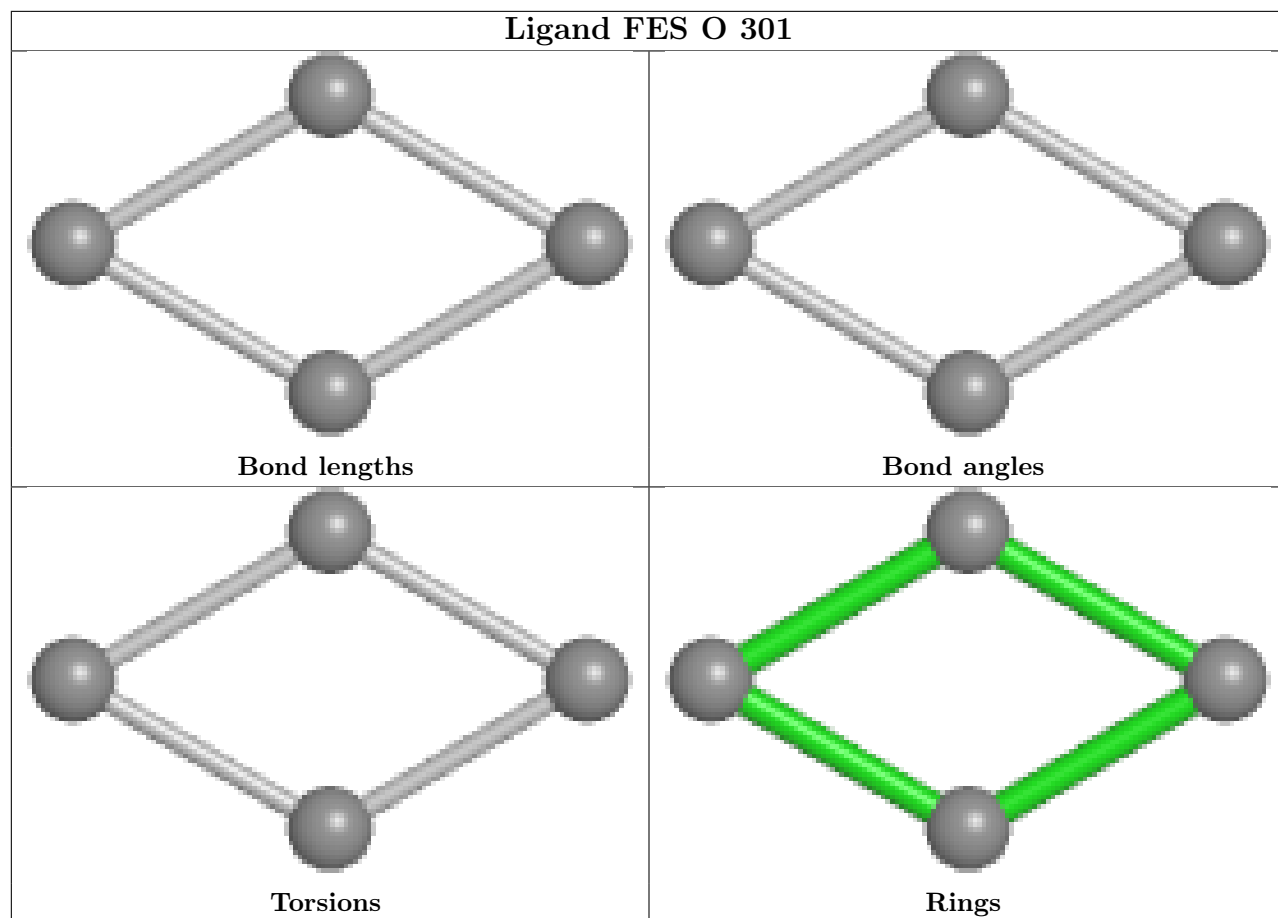


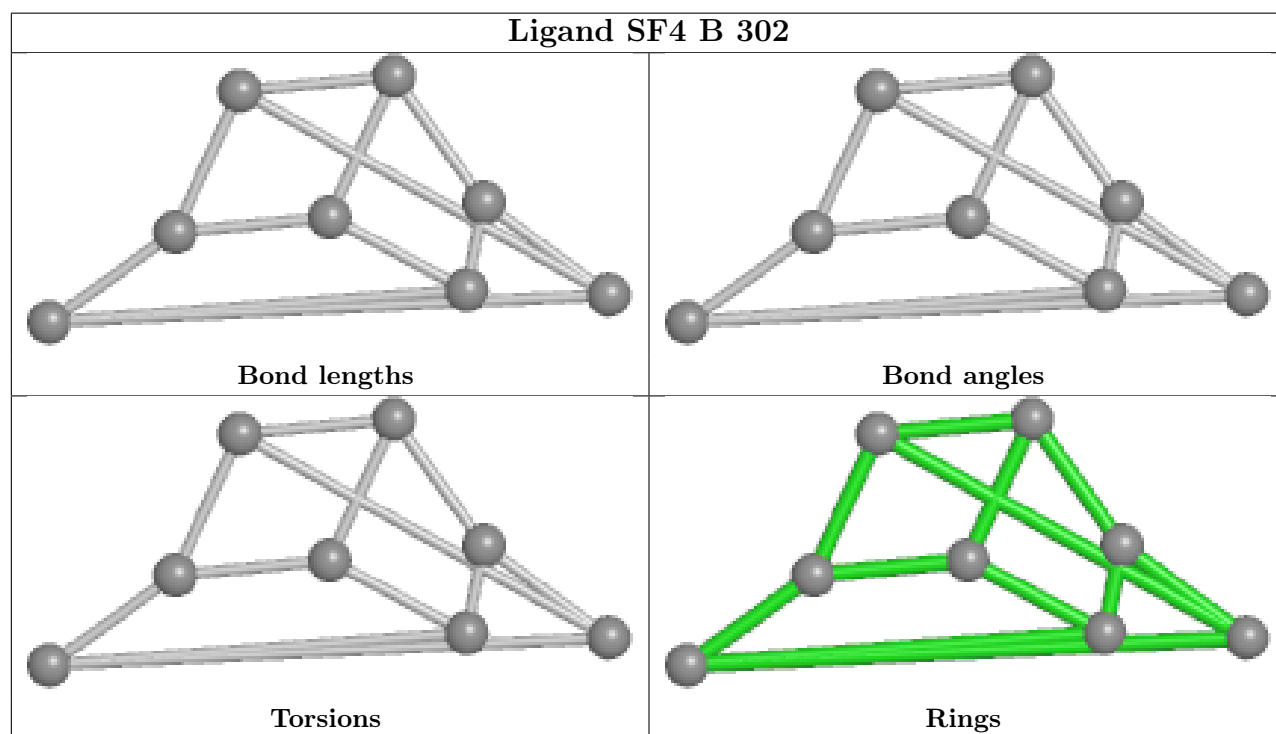
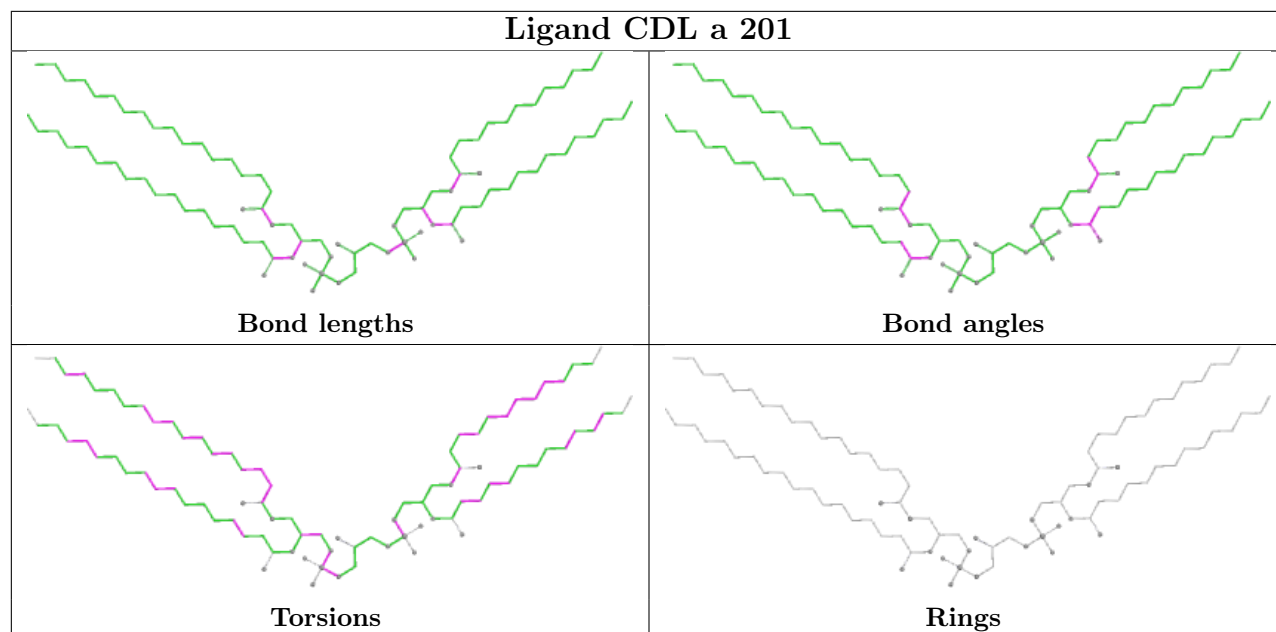
Ligand PEE r 501

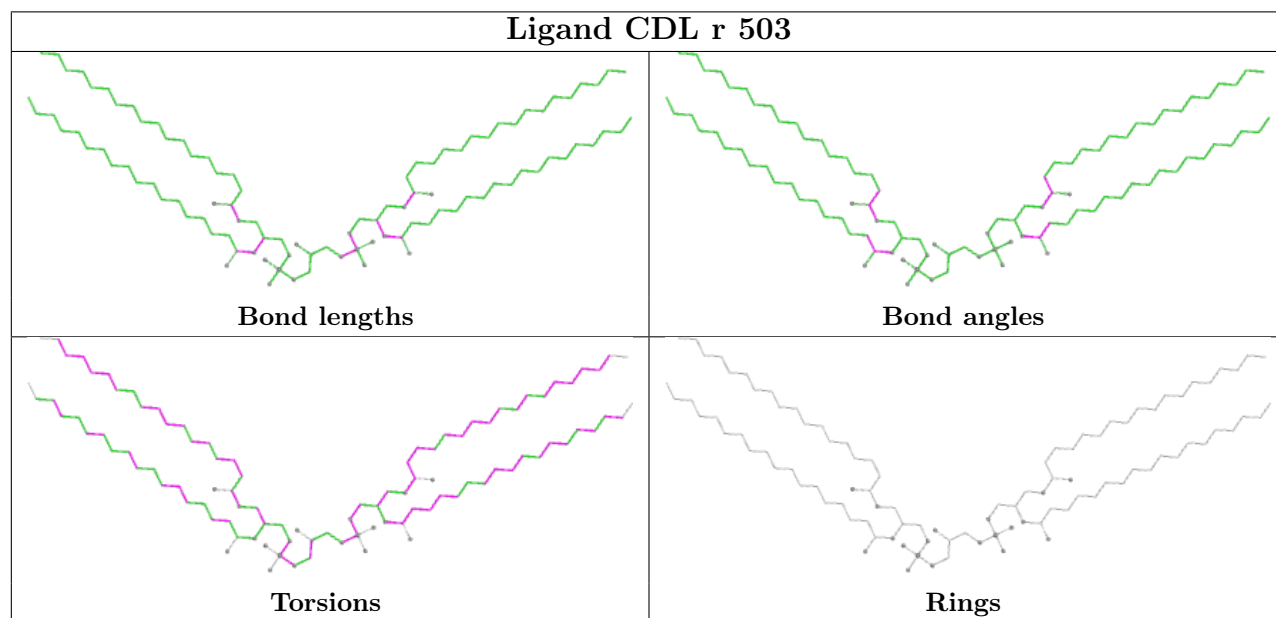
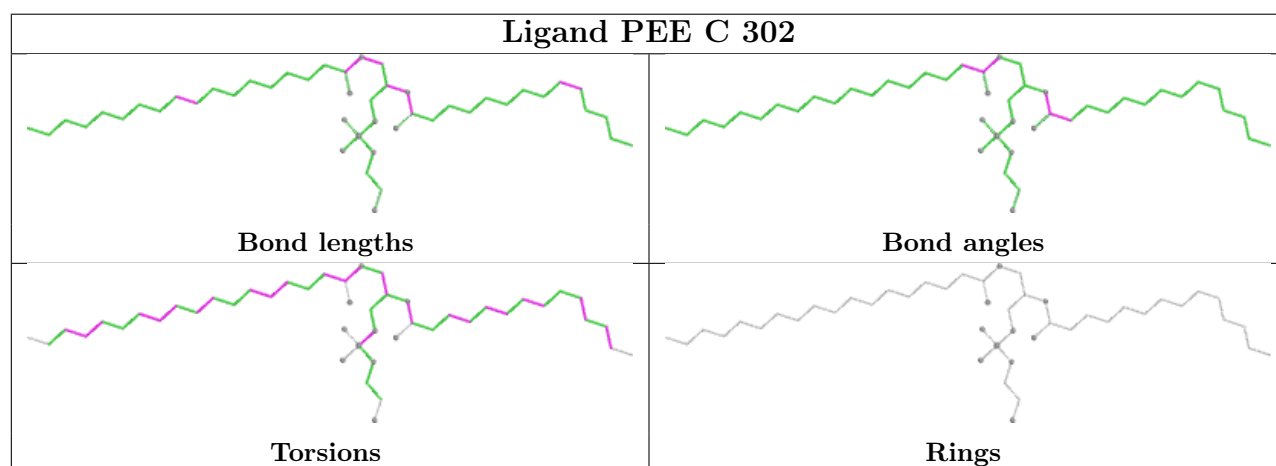
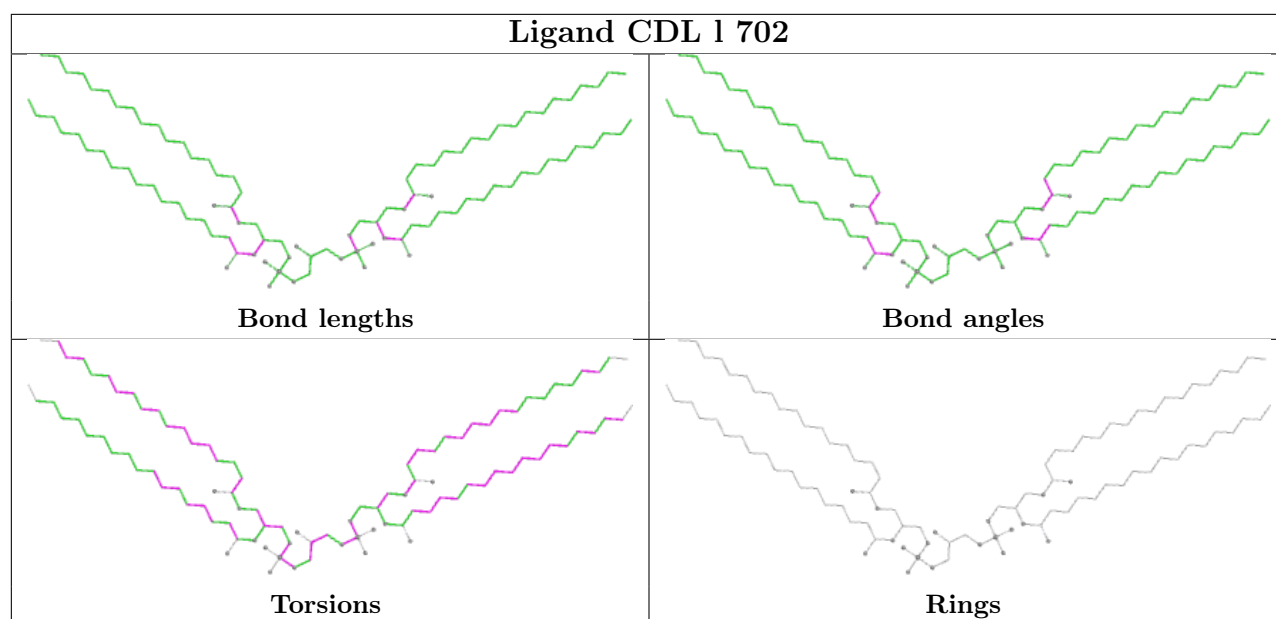




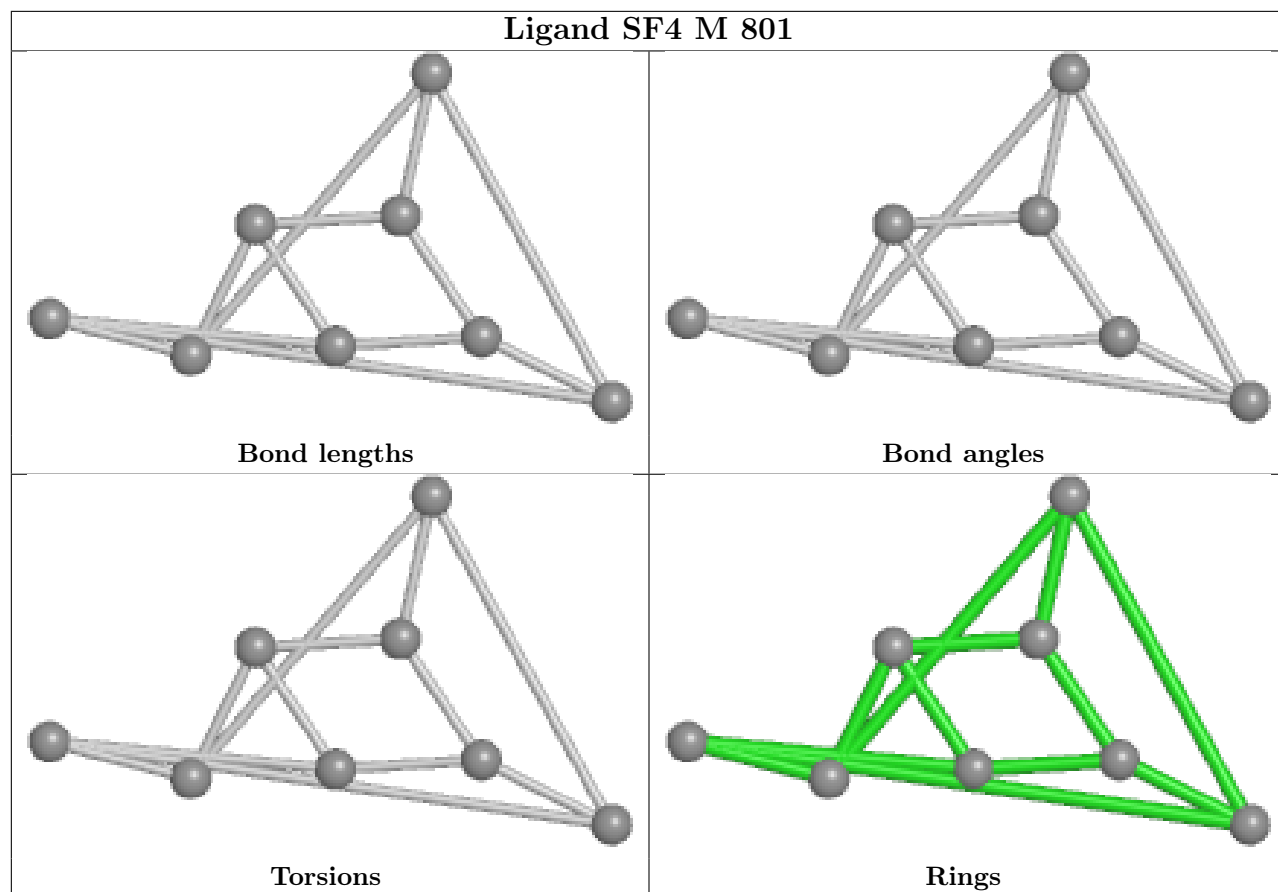




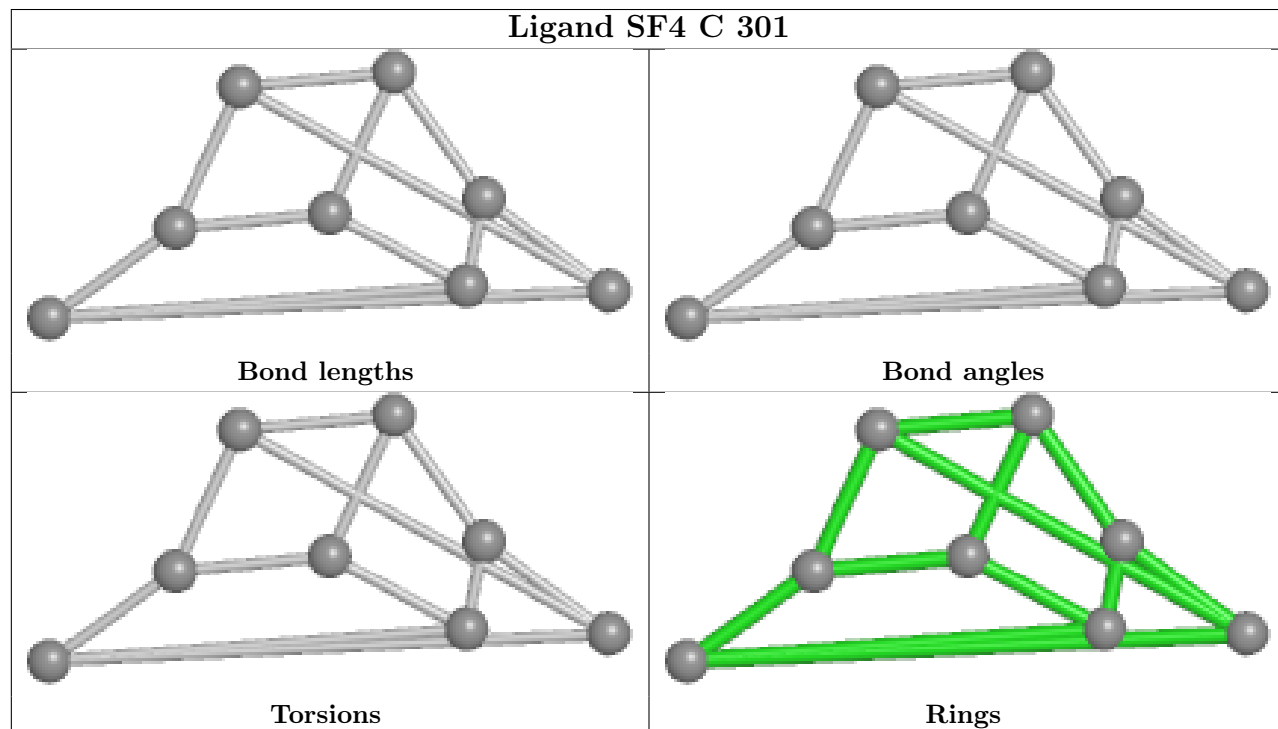


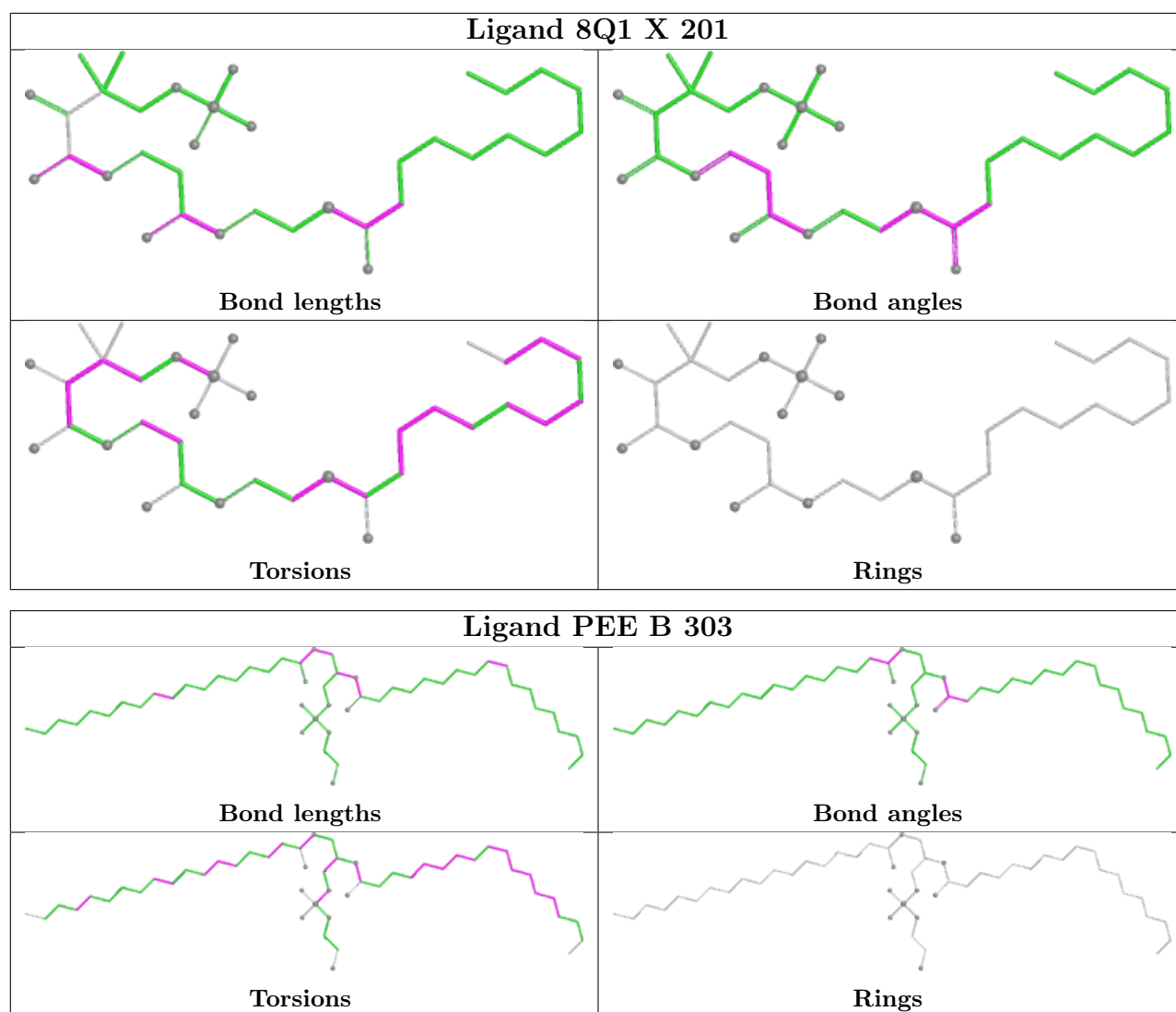


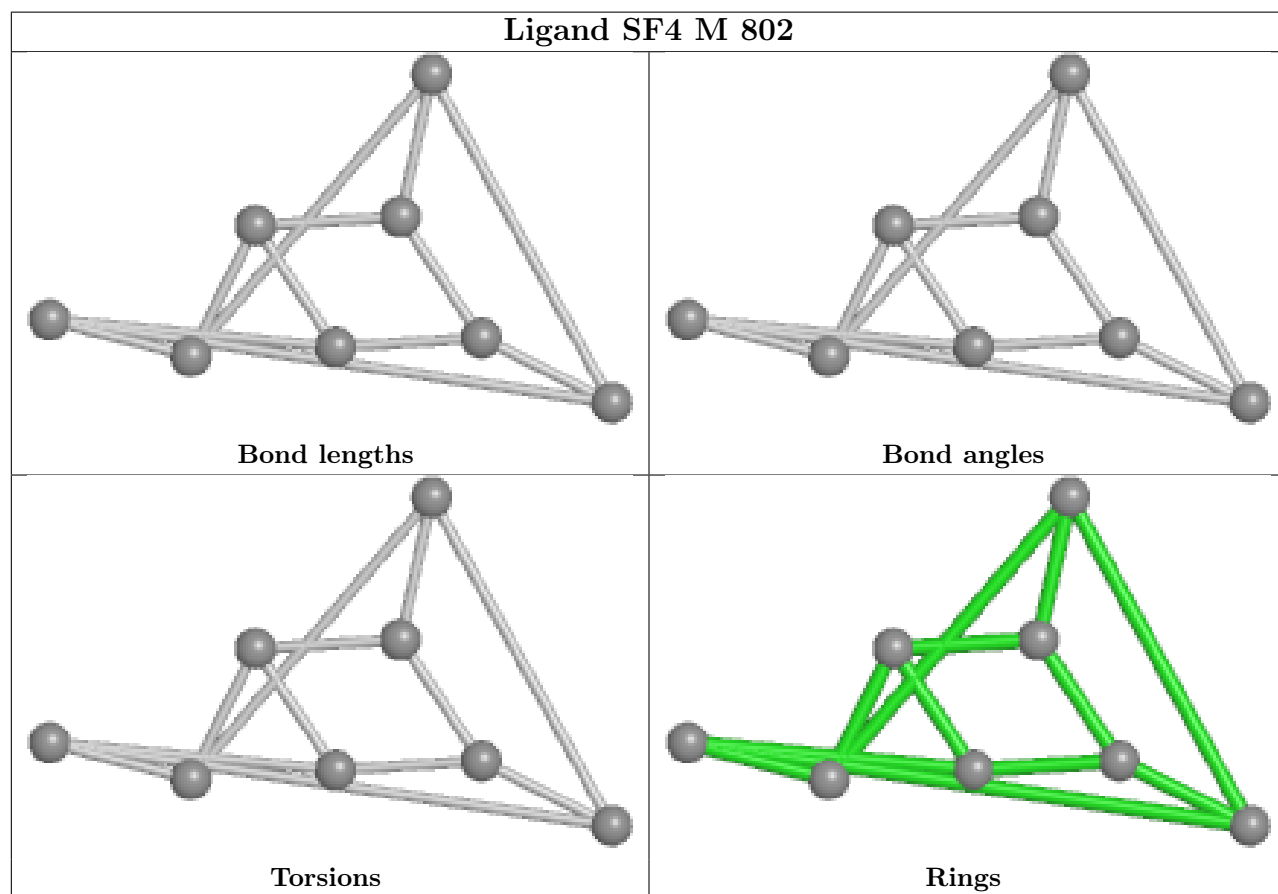
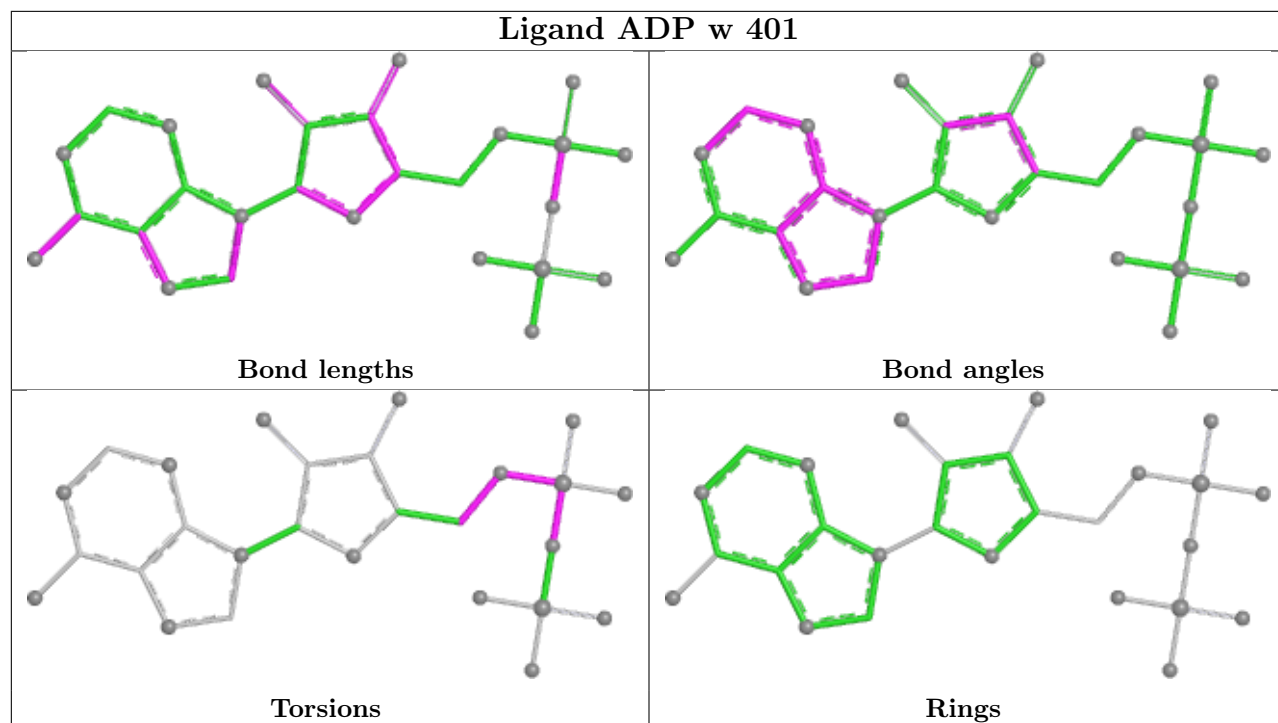
Ligand SF4 M 801

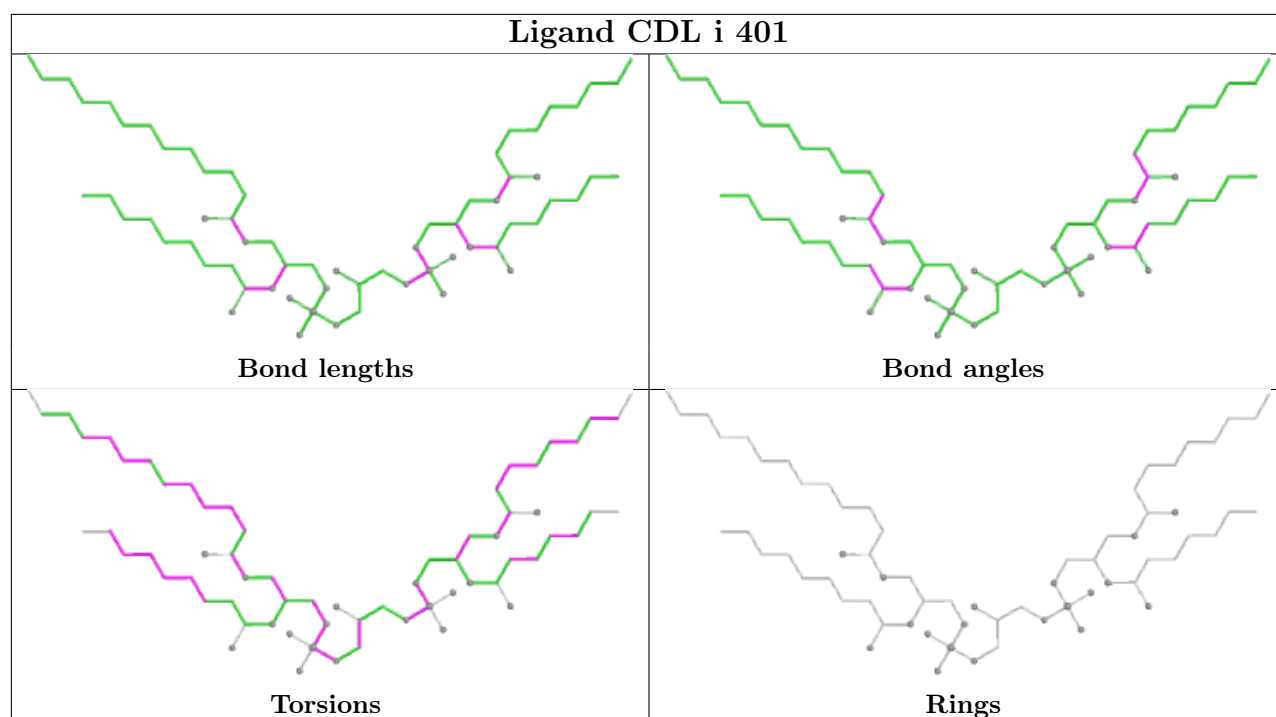


Ligand SF4 C 301









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.

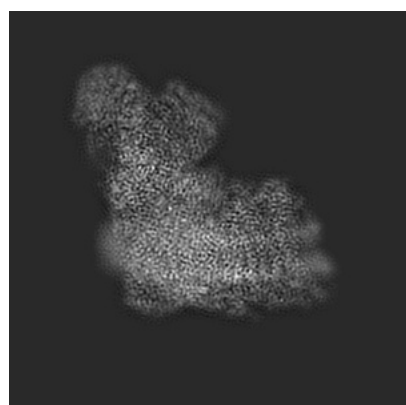
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32309. These allow visual inspection of the internal detail of the map and identification of artifacts.

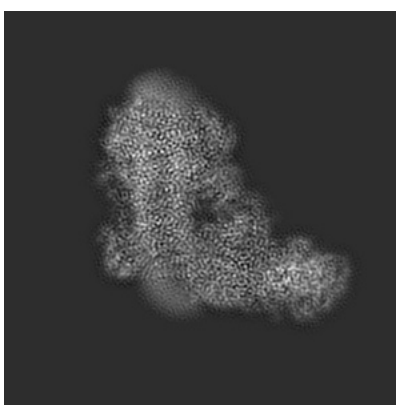
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

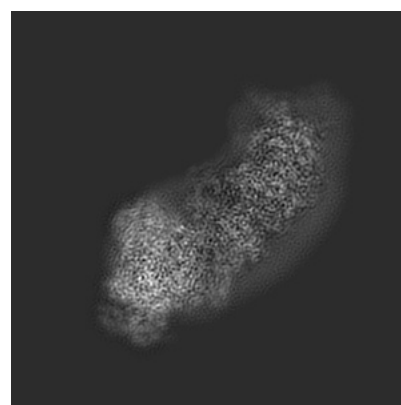
6.1.1 Primary map



X



Y

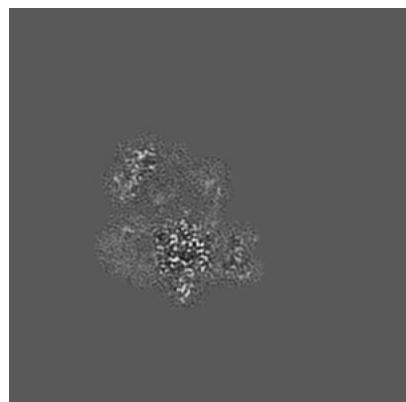


Z

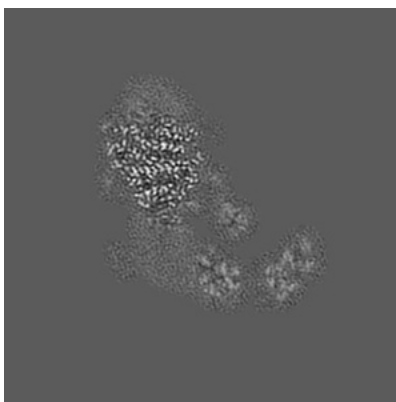
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

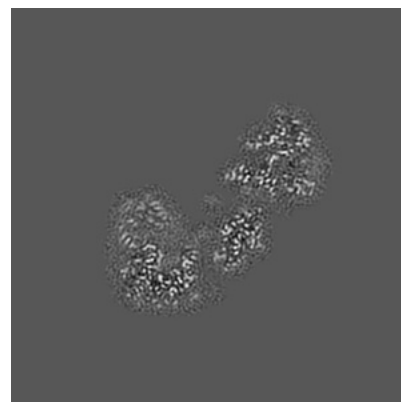
6.2.1 Primary map



X Index: 152



Y Index: 152

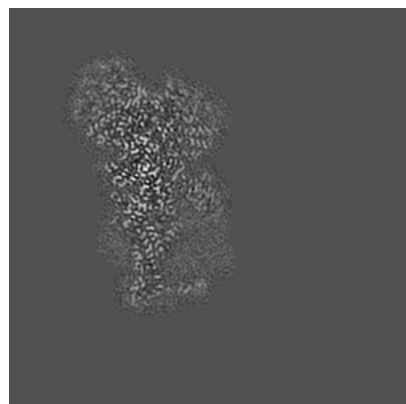


Z Index: 152

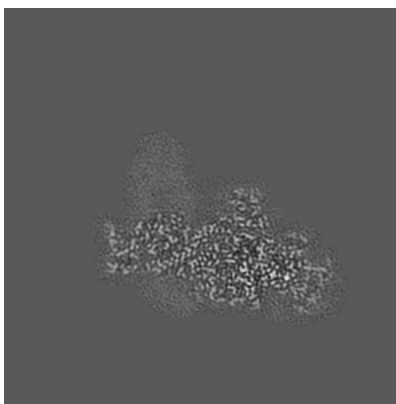
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

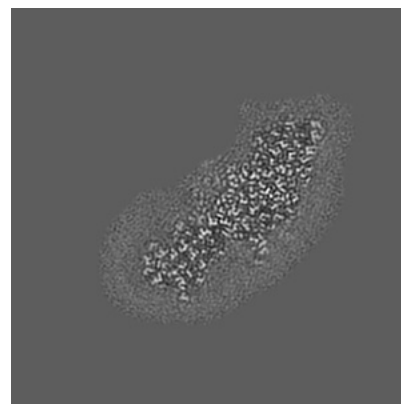
6.3.1 Primary map



X Index: 105



Y Index: 98

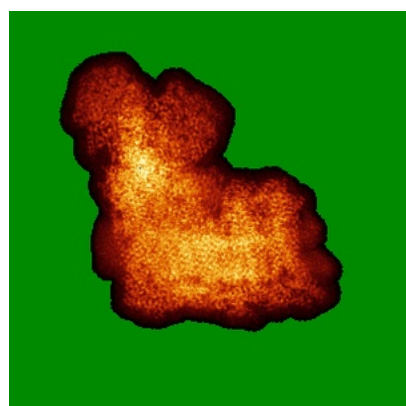


Z Index: 127

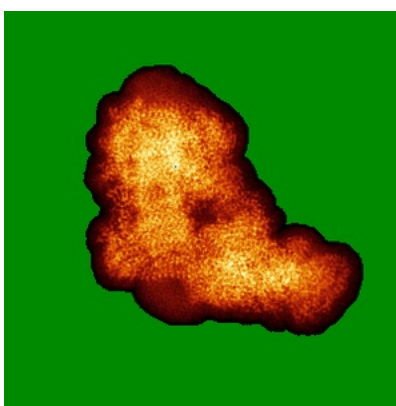
The images above show the largest variance slices of the map in three orthogonal directions.

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

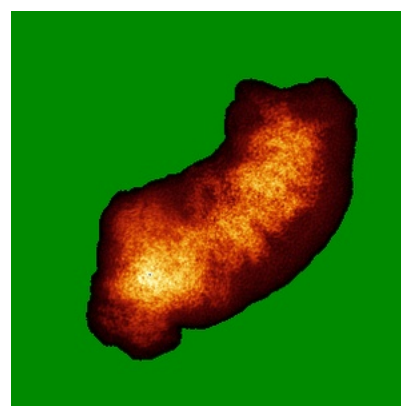
6.4.1 Primary map



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

This section was not generated.

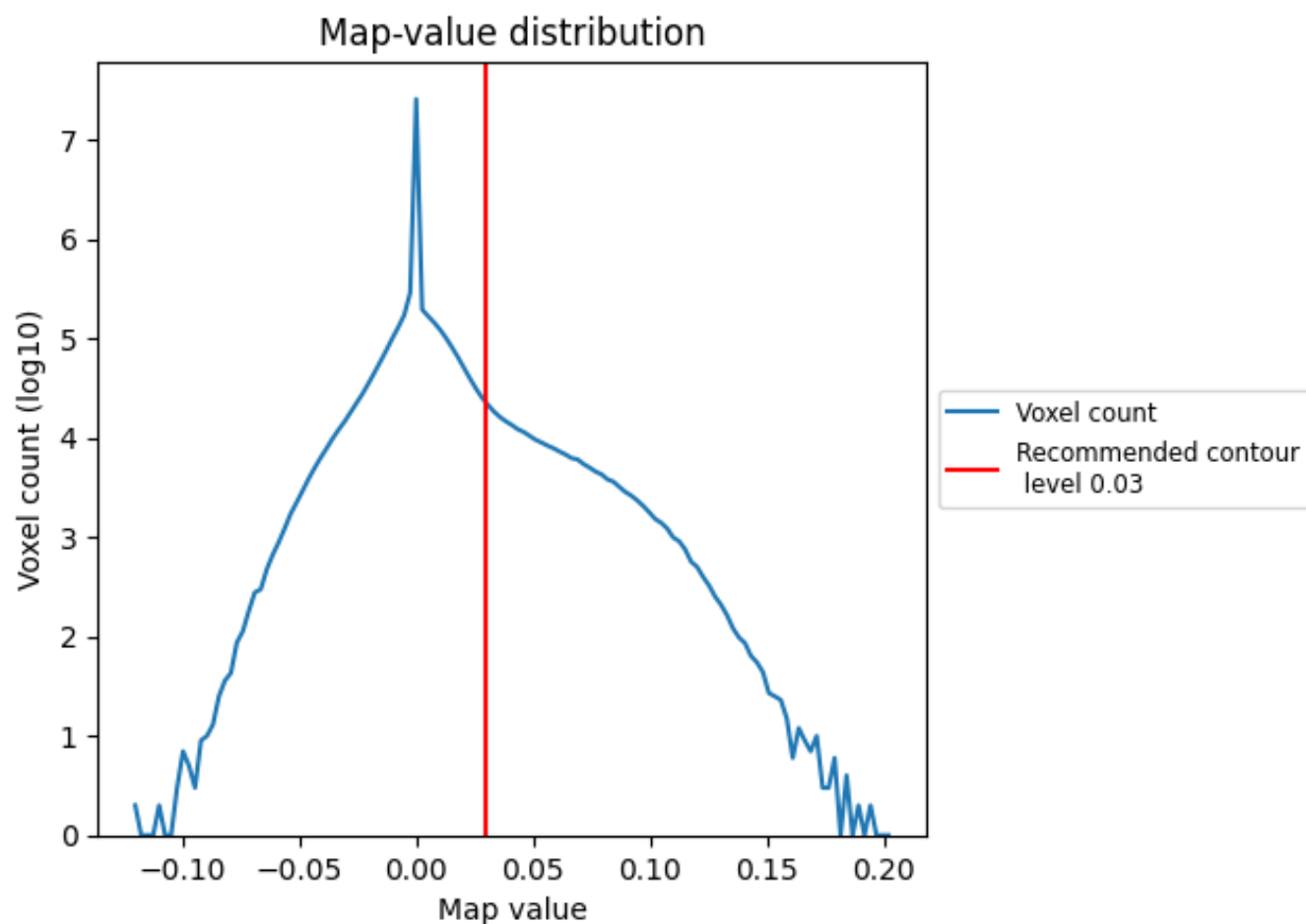
6.6 Mask visualisation

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

7 Map analysis [i](#)

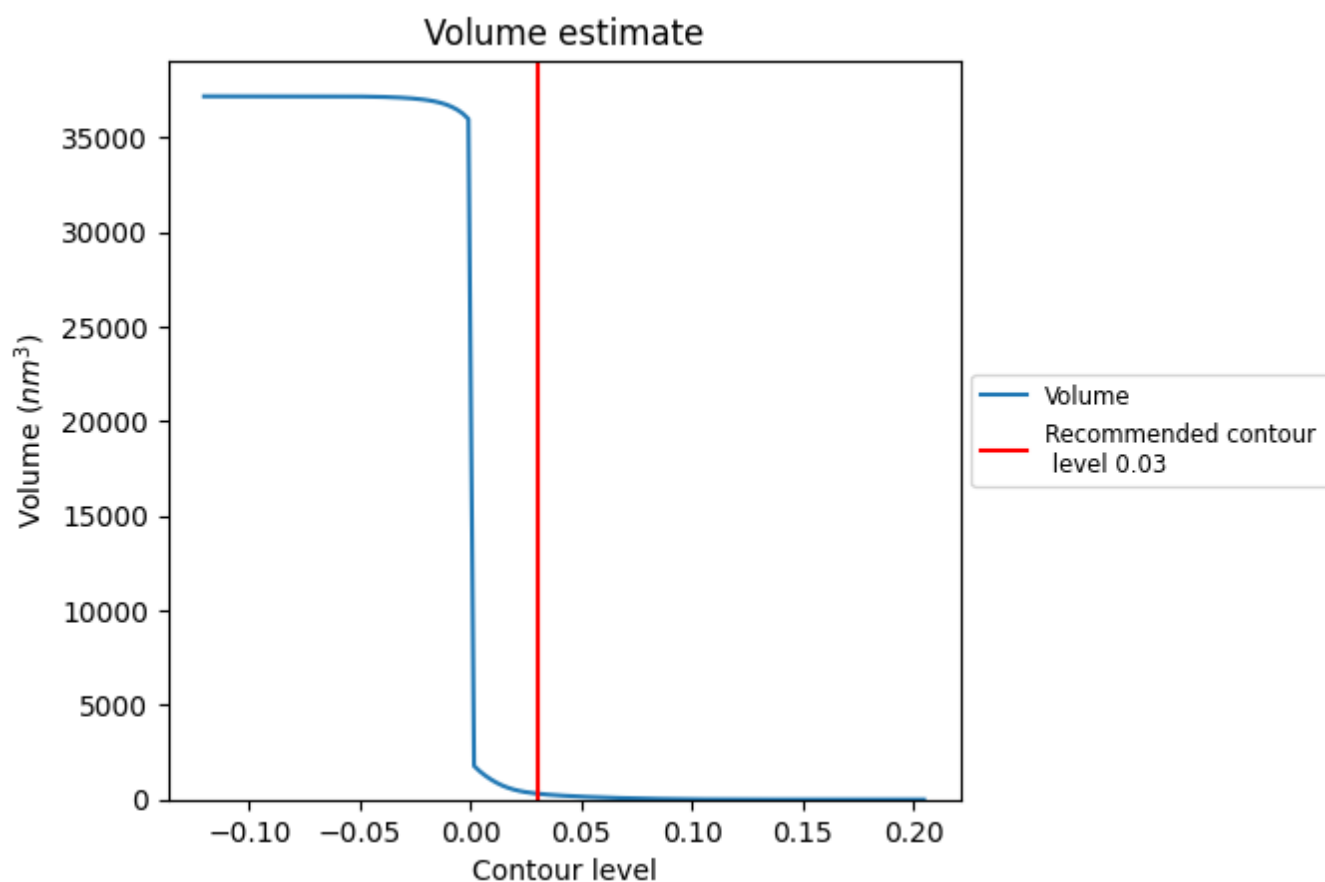
This section contains the results of statistical analysis of the map.

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.

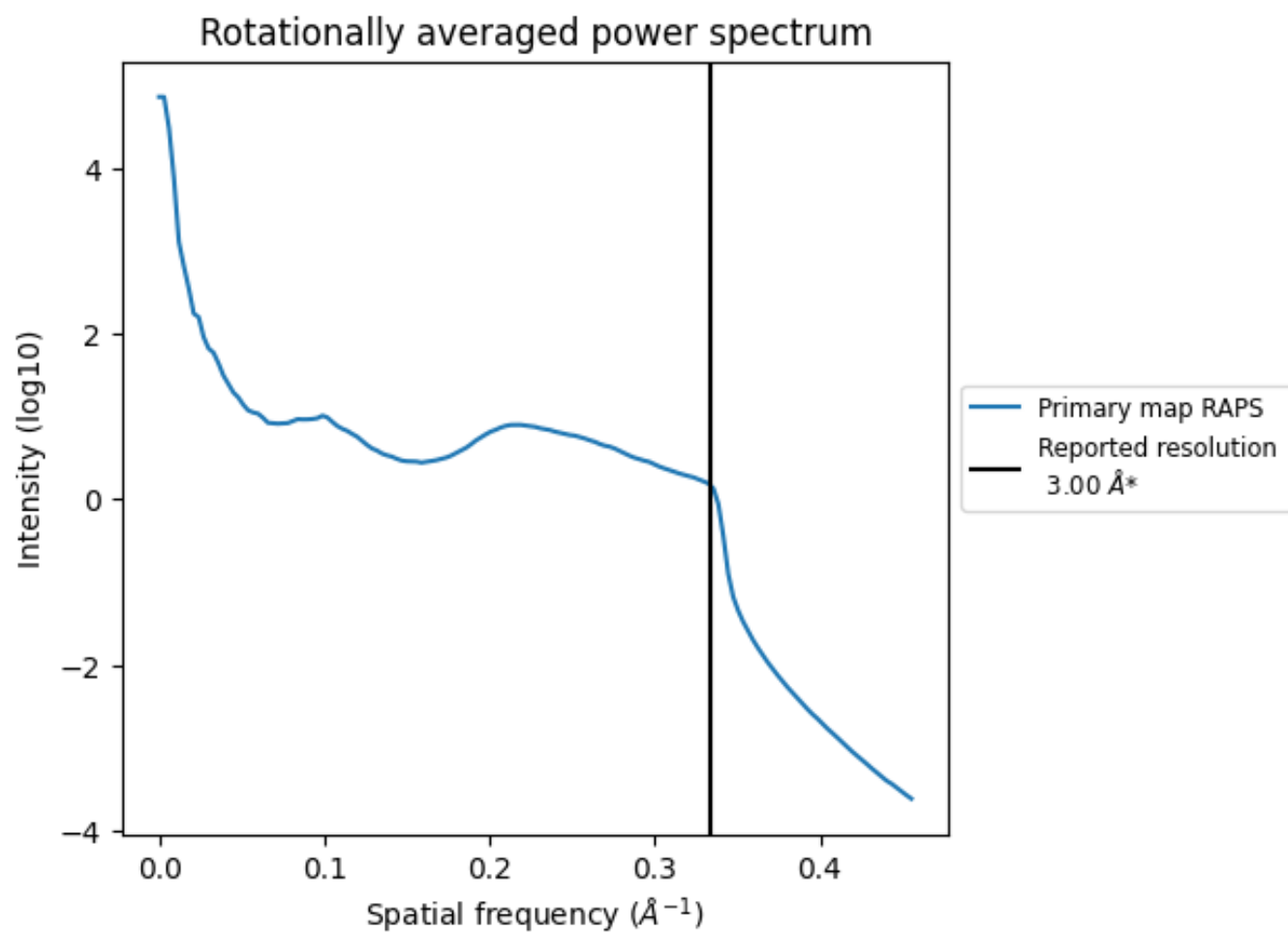
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 314 nm³; this corresponds to an approximate mass of 284 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 0.333 Å⁻¹

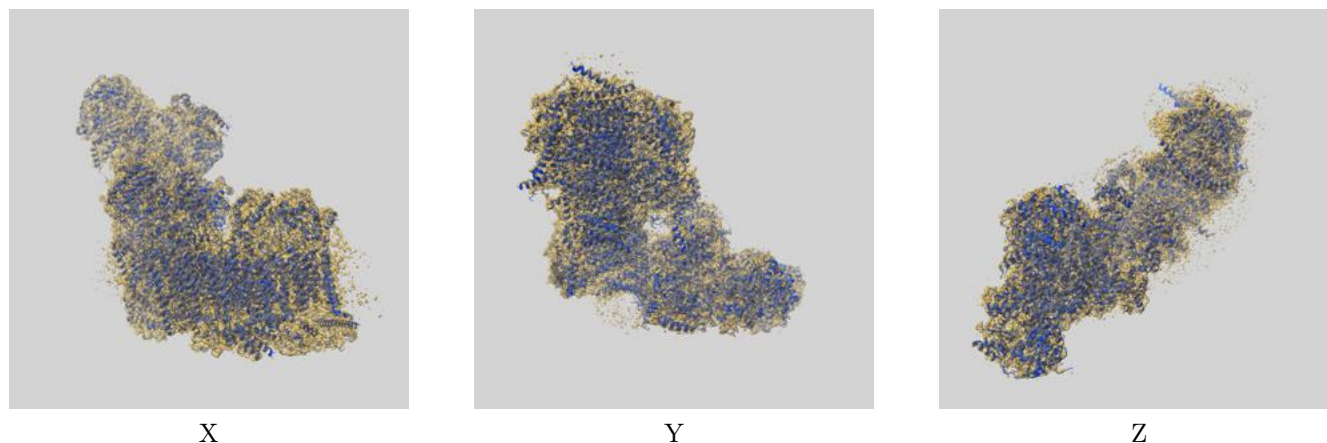
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

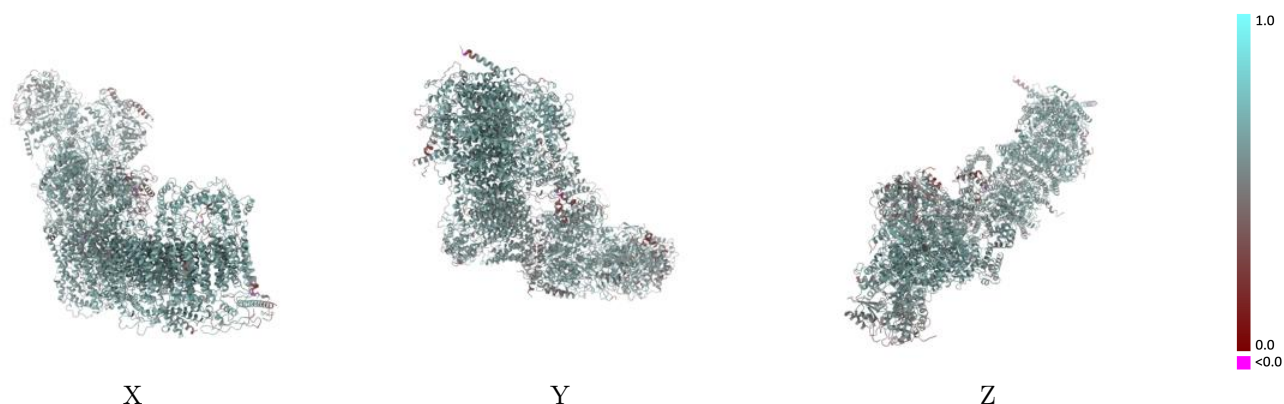
This section contains information regarding the fit between EMDB map EMD-32309 and PDB model 7W4N. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



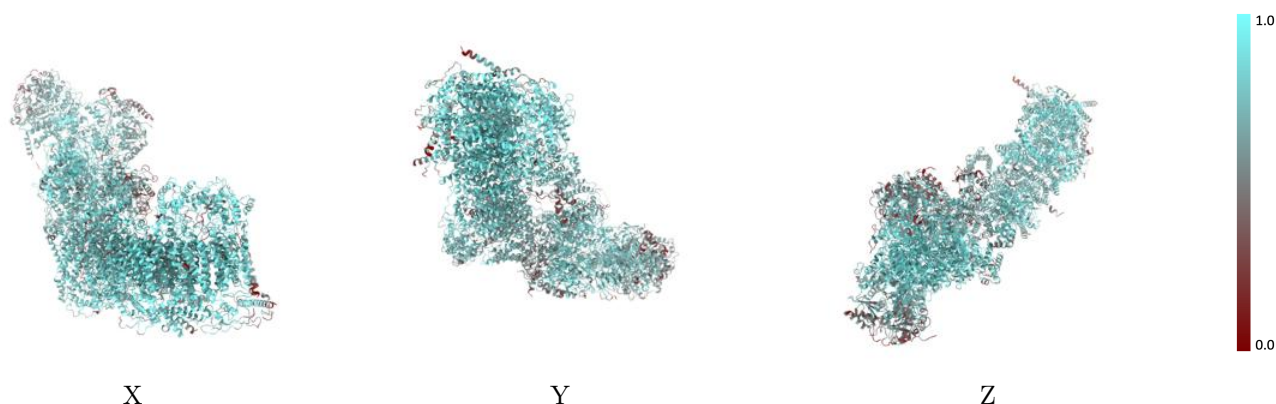
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



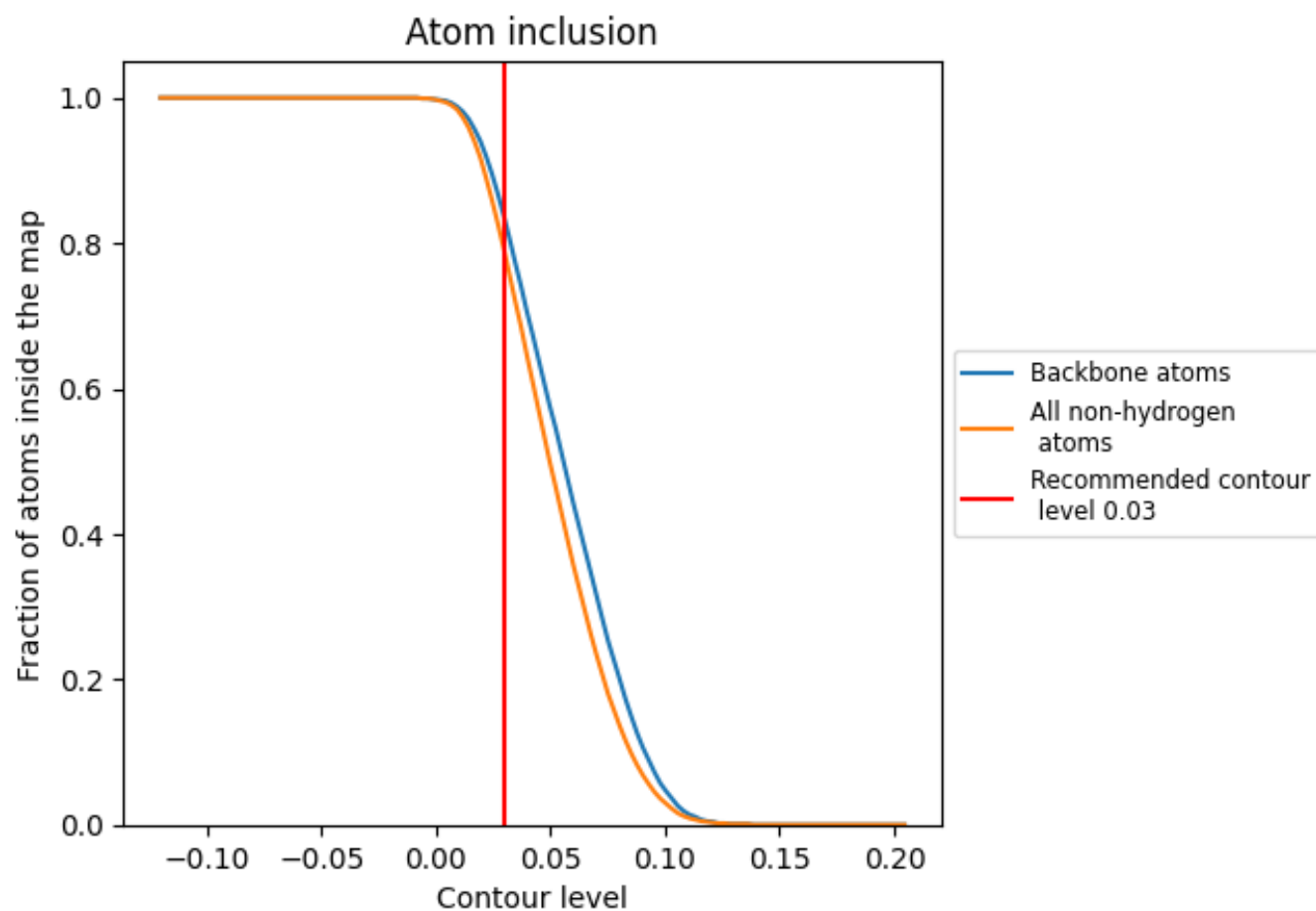
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 79% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7870	 0.5850
A	 0.6550	 0.5410
B	 0.9210	 0.6350
C	 0.8450	 0.6100
E	 0.7180	 0.5720
F	 0.5090	 0.4620
G	 0.4170	 0.4090
H	 0.7290	 0.5680
I	 0.7520	 0.5810
J	 0.6540	 0.5340
K	 0.5230	 0.5220
L	 0.8110	 0.6010
M	 0.7580	 0.5760
N	 0.8050	 0.6020
O	 0.6100	 0.5250
P	 0.8960	 0.6240
Q	 0.8870	 0.6270
S	 0.8370	 0.6050
T	 0.7730	 0.5900
U	 0.7760	 0.5760
V	 0.6650	 0.5530
W	 0.8030	 0.5920
X	 0.7990	 0.5890
Y	 0.7060	 0.5550
Z	 0.6350	 0.5190
a	 0.8450	 0.6130
b	 0.7330	 0.5570
c	 0.8230	 0.5970
d	 0.7960	 0.5860
e	 0.7700	 0.5720
f	 0.6950	 0.5470
g	 0.8360	 0.6100
h	 0.8040	 0.5880
i	 0.8920	 0.6230
j	 0.6810	 0.5530



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Chain	Atom inclusion	Q-score
k	 0.8190	 0.5960
l	 0.8660	 0.6150
m	 0.7500	 0.5720
n	 0.7050	 0.5700
o	 0.8200	 0.6010
p	 0.8380	 0.6000
r	 0.9000	 0.6230
s	 0.8420	 0.6000
u	 0.7960	 0.5860
v	 0.7180	 0.5460
w	 0.7910	 0.5830