



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 09:39 PM UTC

PDB ID : 7W0Y / pdb_00007w0y
EMDB ID : EMD-32249
Title : Active state CI from Q10-NADH dataset, Subclass 2
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-18
Resolution : 3.40 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:

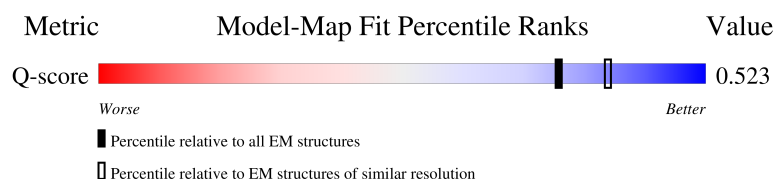
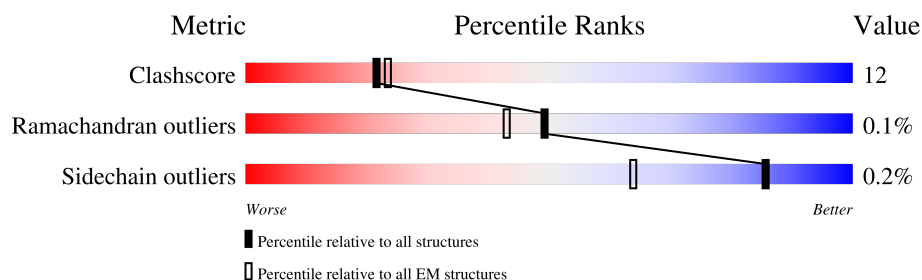
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.40 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	14717 (2.90 - 3.90)

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	 6% 77% 23%
2	B	176	 1% 85% 15%
3	C	156	 1% 86% 14%
4	E	115	 11% 78% 22%

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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	67	
23	Z	80	
24	a	138	
25	b	126	
26	c	156	
27	d	175	
28	e	104	

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Mol	Chain	Length	Quality of chain
29	f	49	
30	g	121	
31	h	105	
32	i	347	
33	j	115	
34	k	98	
35	l	606	
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	M	801	-	-	X	-

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 68093 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	433	Total	C	N	O	S	0	0
			3330	2103	593	614	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
			669	422	127	119	1		

- 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
			689	445	102	137	5		
6	X	88	Total	C	N	O	S	0	0
			704	454	104	141	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	43	Total	C	N	O	S	0	0
			366	228	68	69	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
			1016	642	181	190	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
			5289	3316	922	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
			1204	770	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
			1654	1054	278	312	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	430	Total	C	N	O	S	0	0
			3451	2208	594	625	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
			566	364	103	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
			1018	650	174	188	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
			1167	752	200	206	9		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	67	Total	C	N	O	S	0	0
			580	383	94	102	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	80	Total	C	N	O	S	0	0
			633	412	106	114	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	98	Total	C	N	O	S	0	0
			815	535	144	135	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	104	Total	C	N	O	S	0	0
			867	553	142	168	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	49	Total	C	N	O	0	0
			378	246	65	67		

- 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	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

- 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	606	Total	C	N	O	S	0	0
			4800	3182	744	823	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	175	Total	C	N	O	S	0	0
			1295	864	188	230	13		

- 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		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
			1530	980	279	263	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
			3629	2411	572	608	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	318	Total	C	N	O	S	0	0
			2501	1672	385	423	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
			1053	652	202	189	10		

- 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
			2575	1640	437	488	10		

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



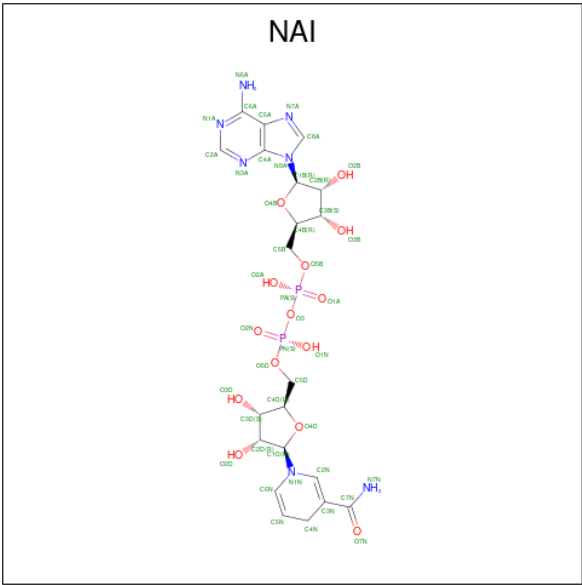
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- 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).



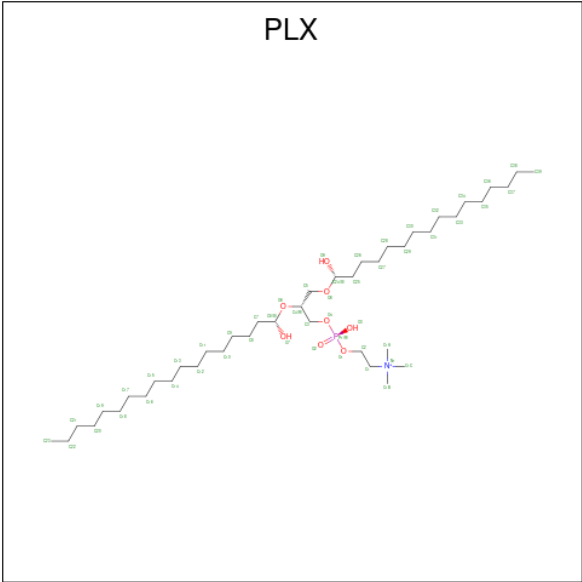
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- 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).



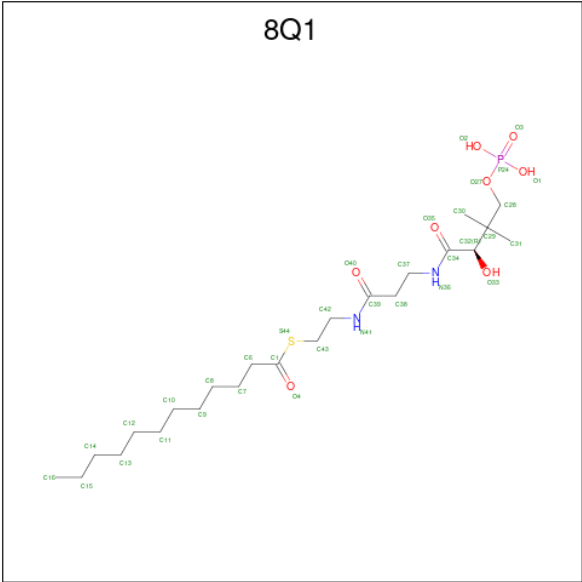
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	l	1	Total	C	N	O	P	0
			40	30	1	8	1	
48	l	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	s	1	Total	C	N	O	P	0
			41	31	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).



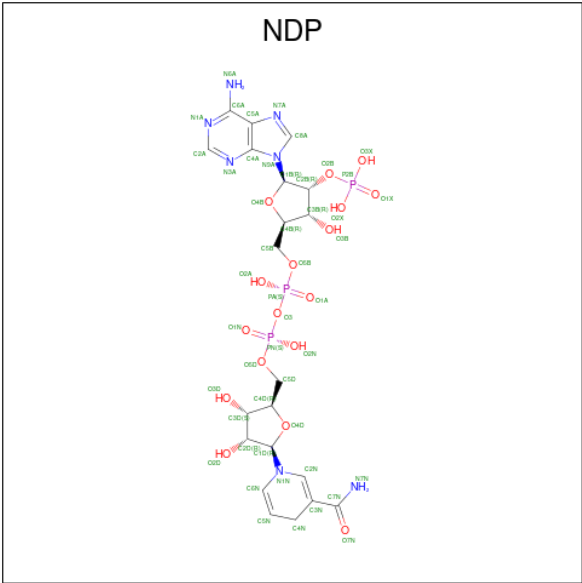
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

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



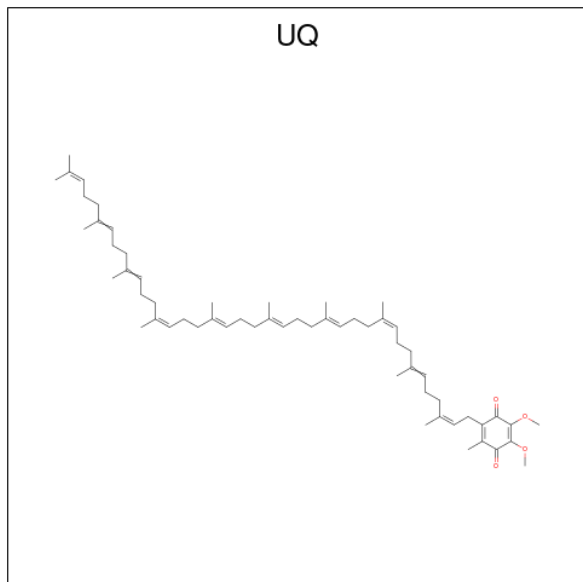
Mol	Chain	Residues	Atoms						AltConf
50	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
50	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 51 is 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).



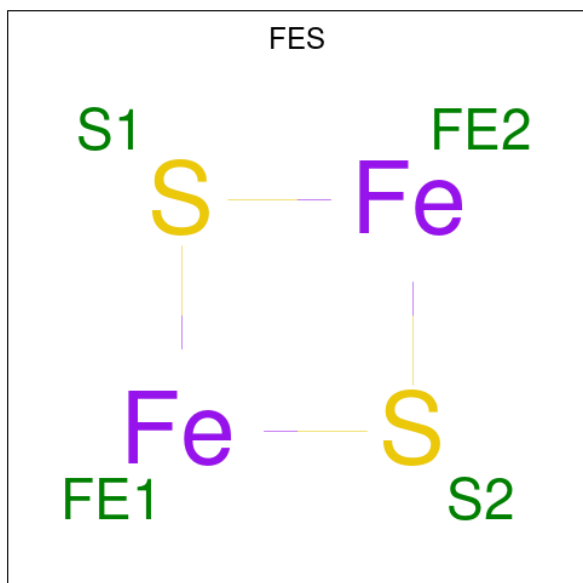
Mol	Chain	Residues	Atoms					AltConf
51	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 52 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
52	J	1	Total	C	O	0
			33	29	4	
52	s	1	Total	C	O	0
			38	34	4	

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

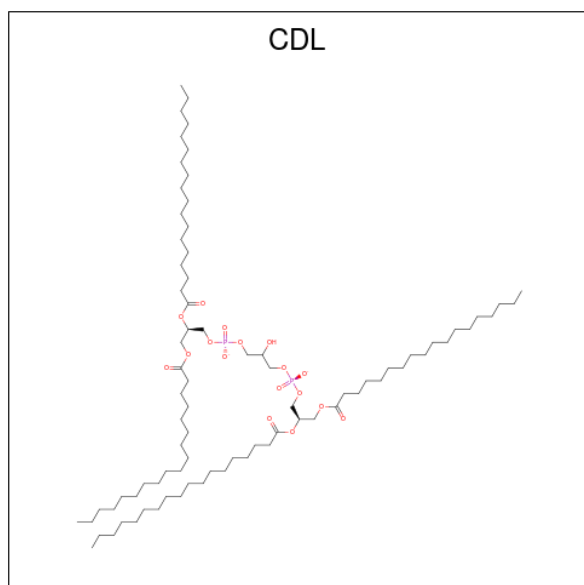


Mol	Chain	Residues	Atoms			AltConf
53	M	1	Total	Fe	S	0
			4	2	2	
53	O	1	Total	Fe	S	0
			4	2	2	

- 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 CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
55	N	1	Total	C	O	P	0
			51	32	17	2	
55	V	1	Total	C	O	P	0
			94	75	17	2	
55	V	1	Total	C	O	P	0
			100	81	17	2	
55	a	1	Total	C	O	P	0
			100	81	17	2	
55	l	1	Total	C	O	P	0
			99	80	17	2	
55	l	1	Total	C	O	P	0
			100	81	17	2	

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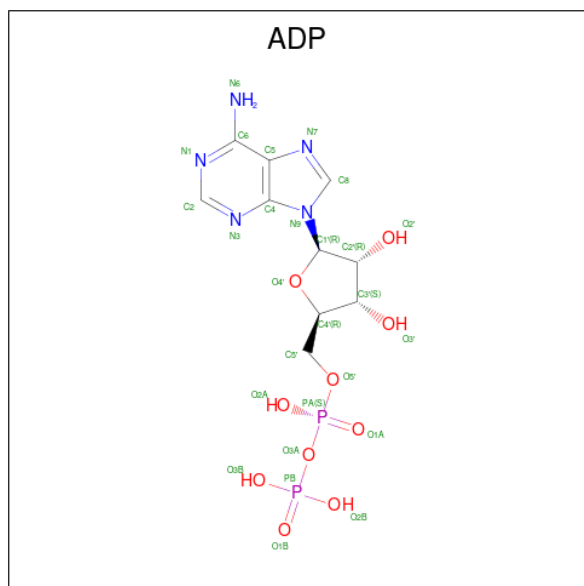
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Mol	Chain	Residues	Atoms				AltConf
55	m	1	Total	C	O	P	0
			100	81	17	2	
55	s	1	Total	C	O	P	0
			89	70	17	2	
55	u	1	Total	C	O	P	0
			55	36	17	2	
55	w	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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

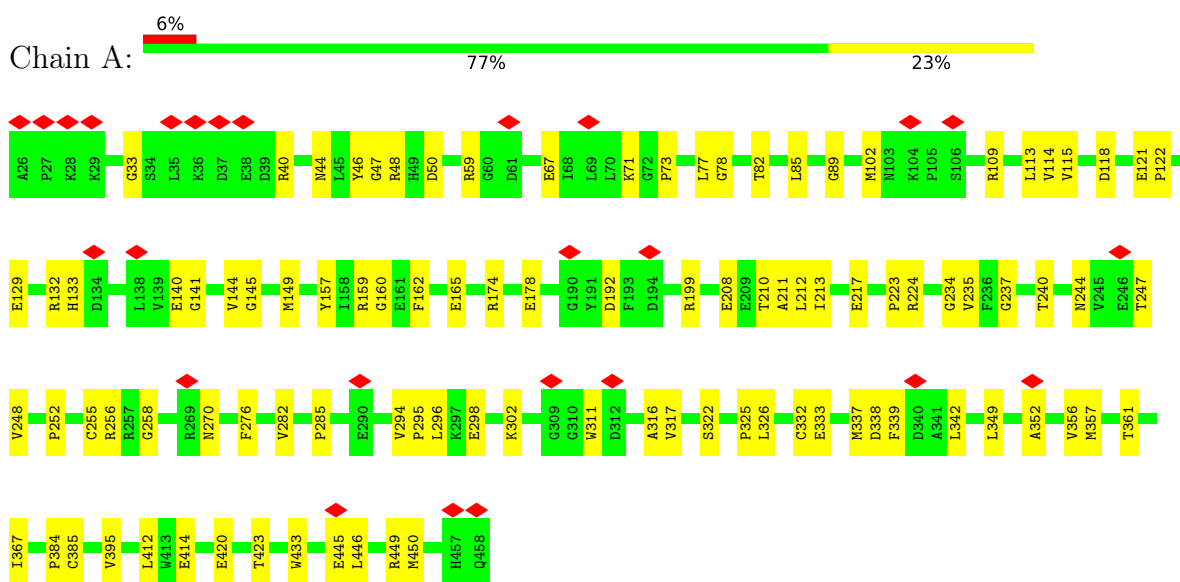


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

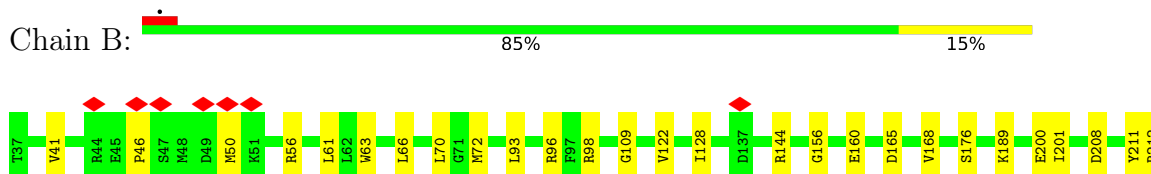
3 Residue-property plots

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.

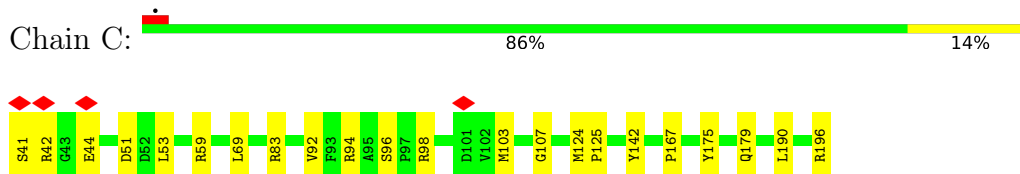
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



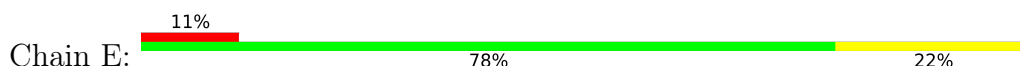
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

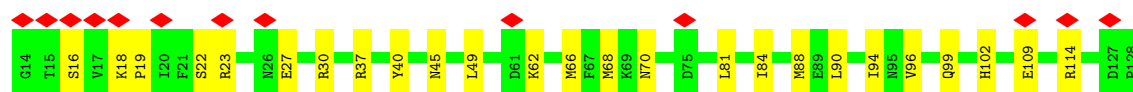


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

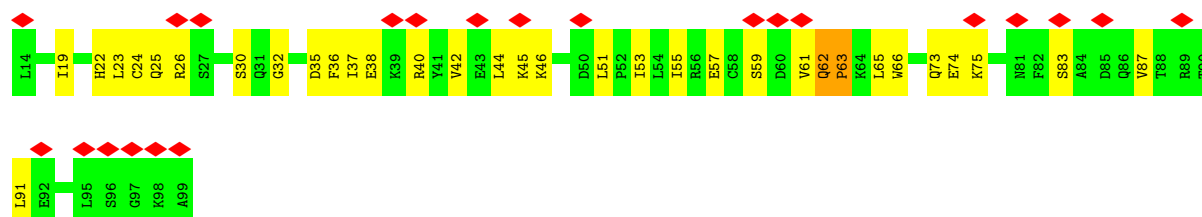


- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6





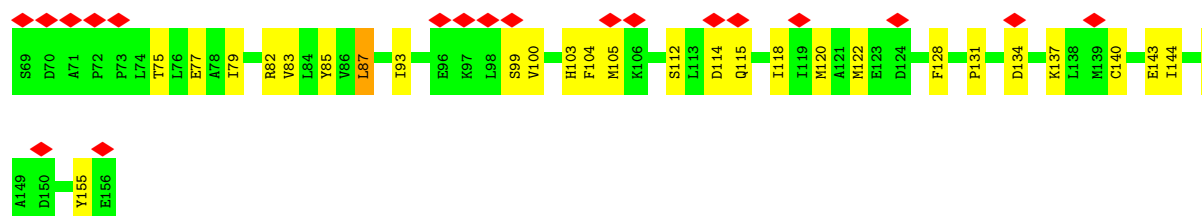
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



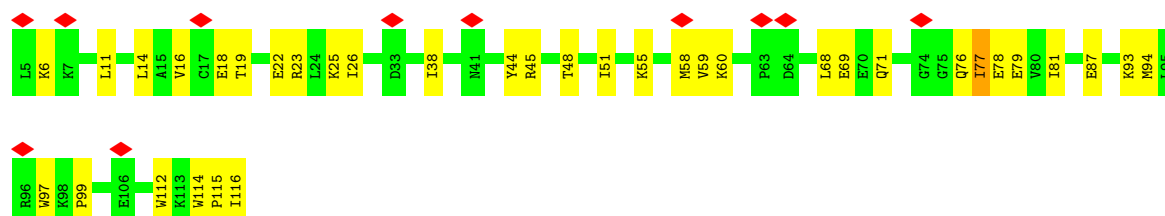
- Molecule 6: Acyl carrier protein



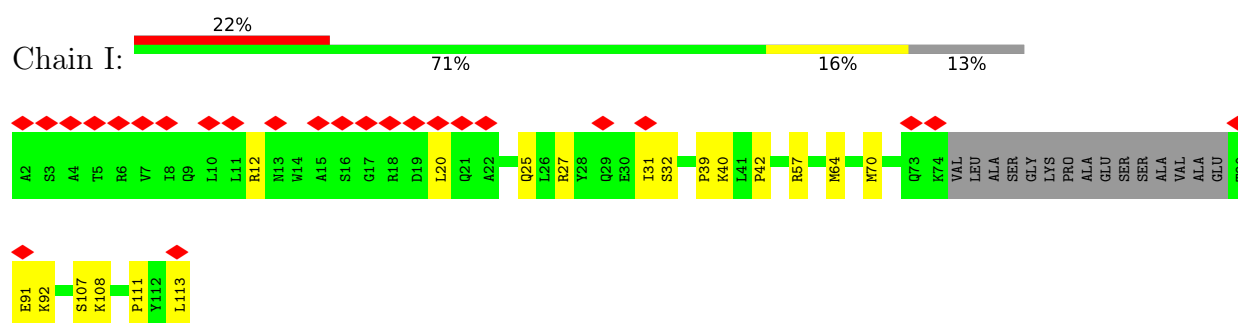
- Molecule 6: Acyl carrier protein



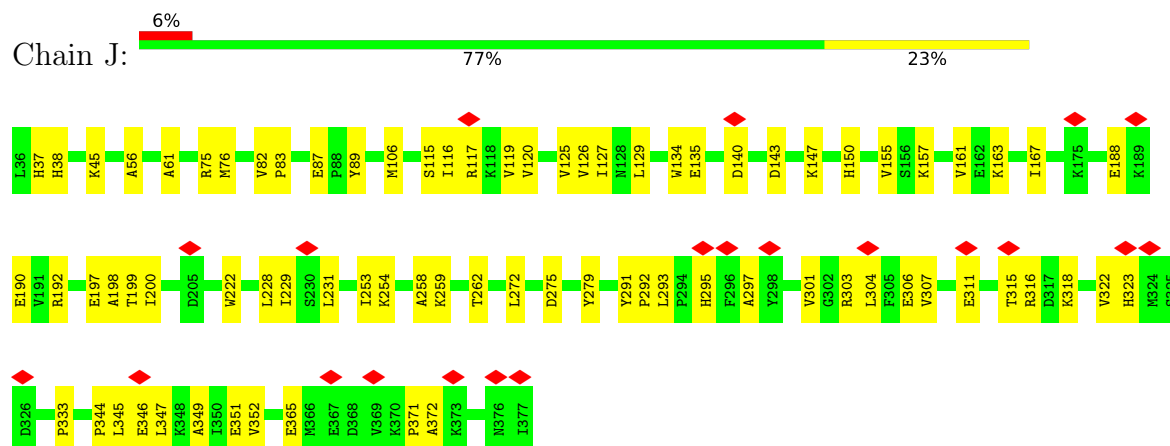
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



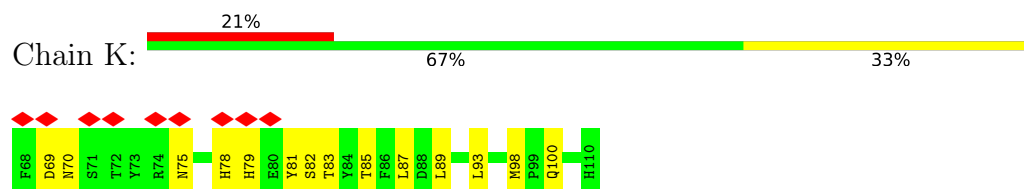
- Molecule 8: Complex I-B14.5a



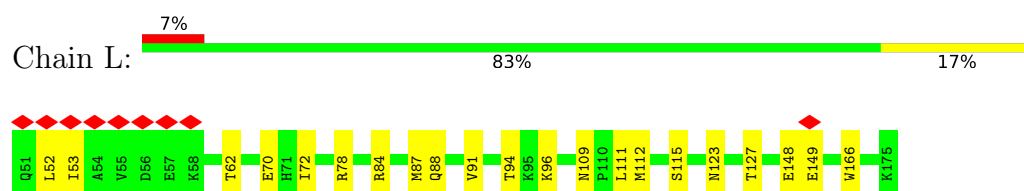
- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial



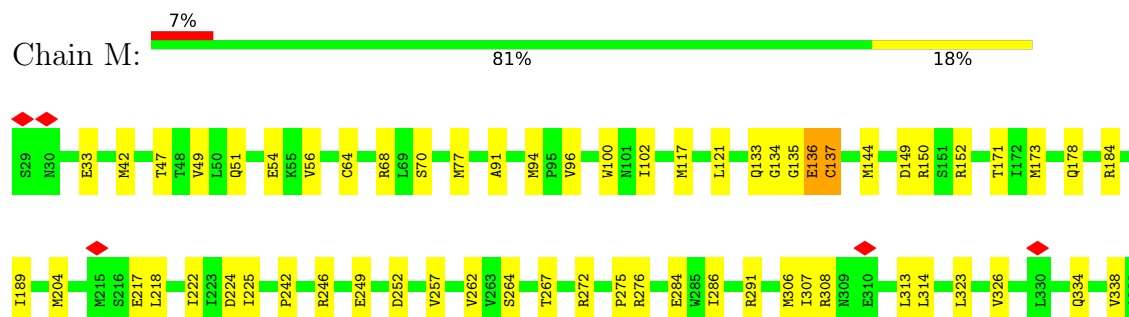
- Molecule 10: Complex I-9kD

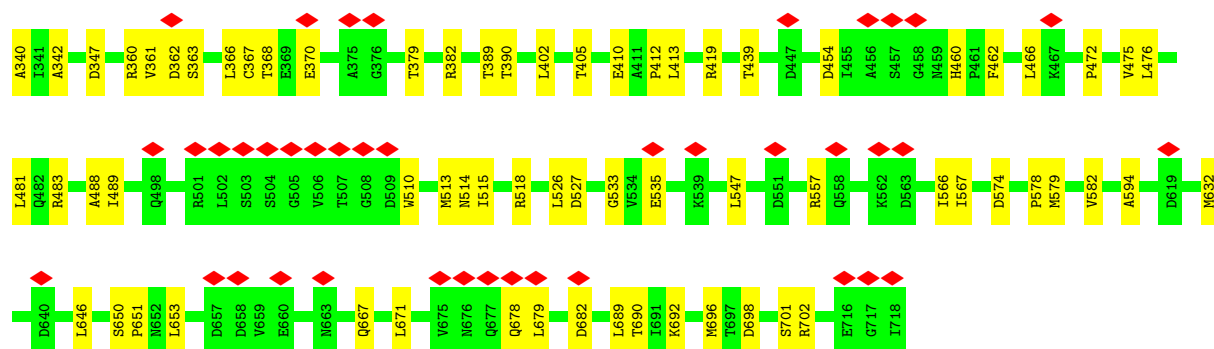


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

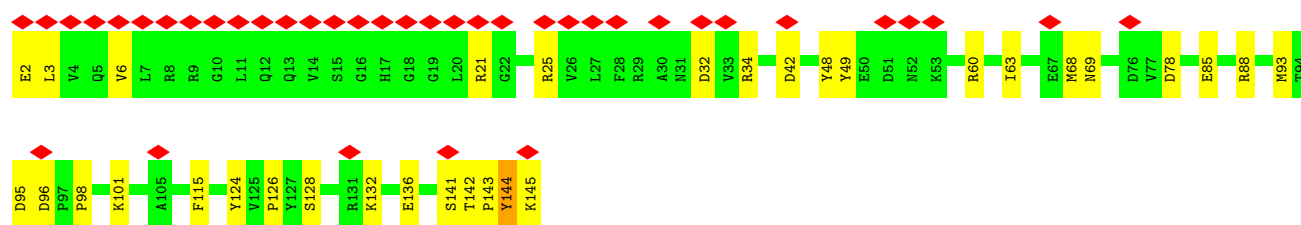
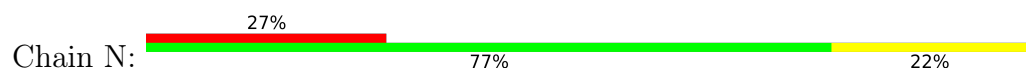


- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

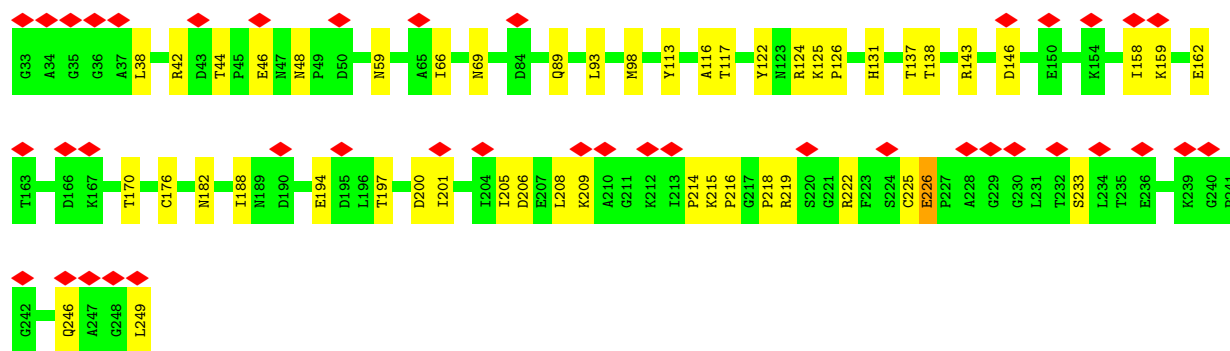
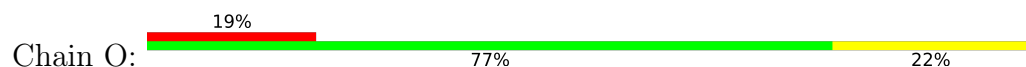




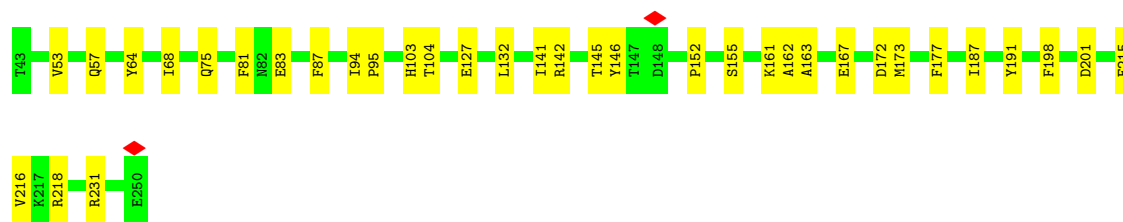
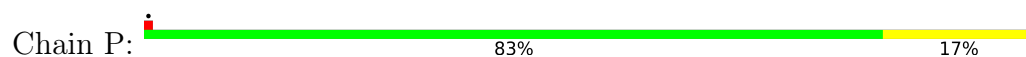
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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

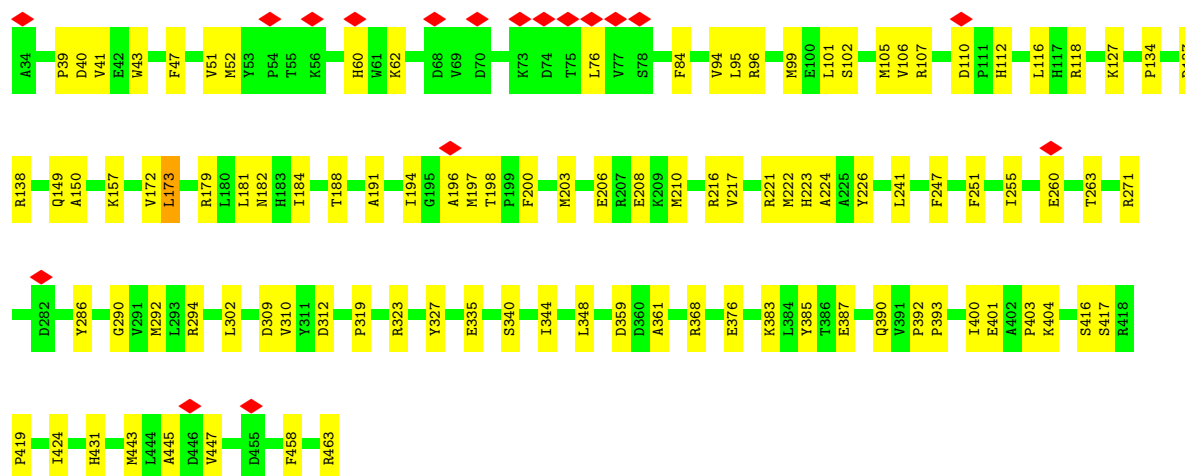


- Molecule 15: Complex I-30kD



- Molecule 16: Complex I-49kD

Chain Q:  77% 23%



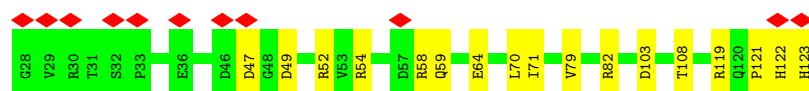
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S:  81% 19%



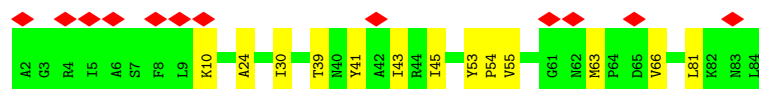
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T:  11% 82% 18%



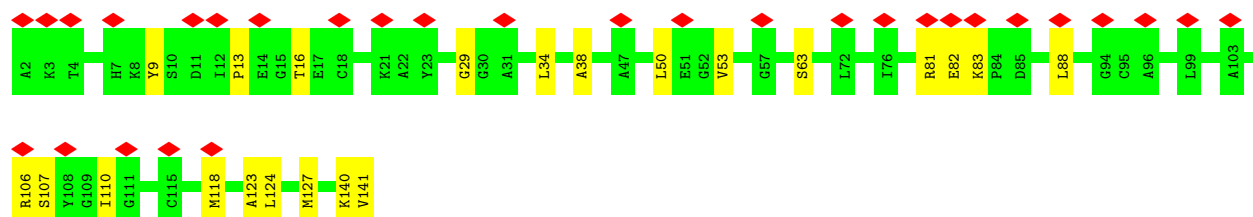
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:  14% 84% 16%

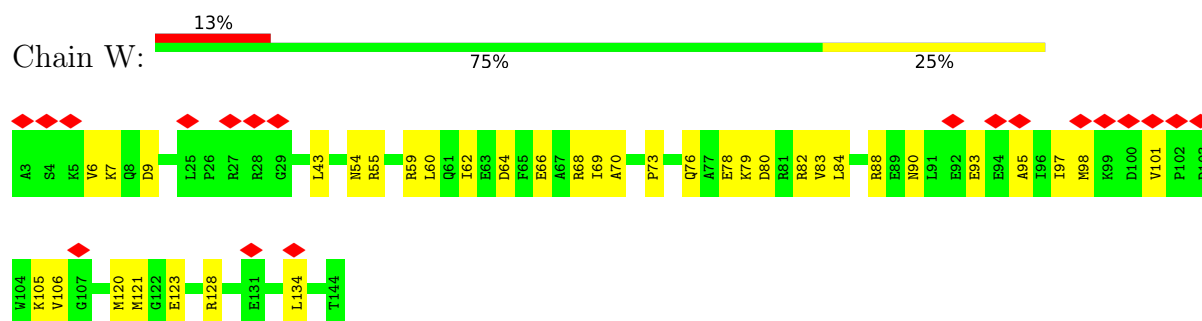


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

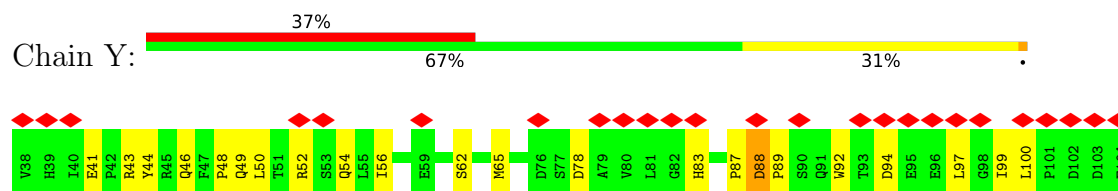
Chain V:  21% 84% 16%



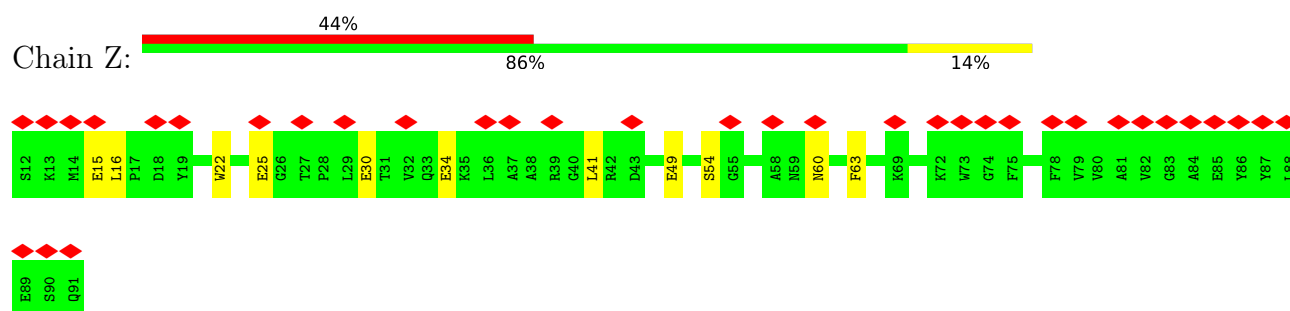
- Molecule 21: Complex I-B16.6



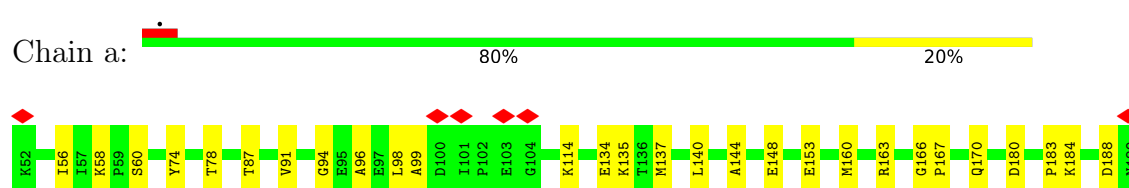
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



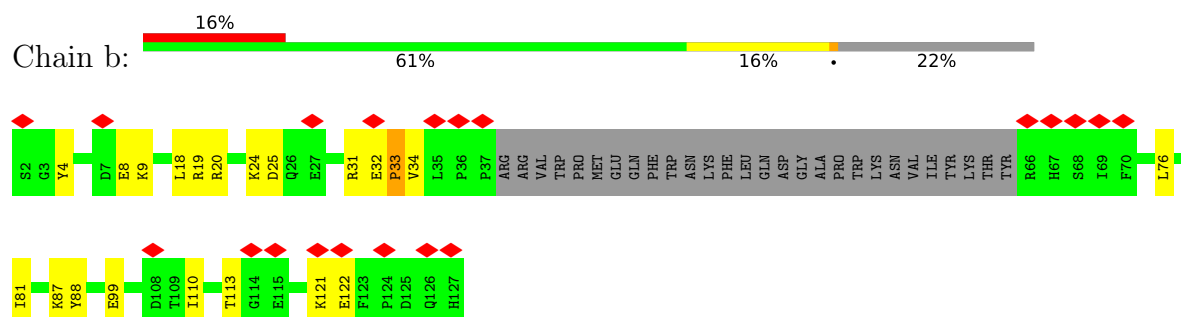
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



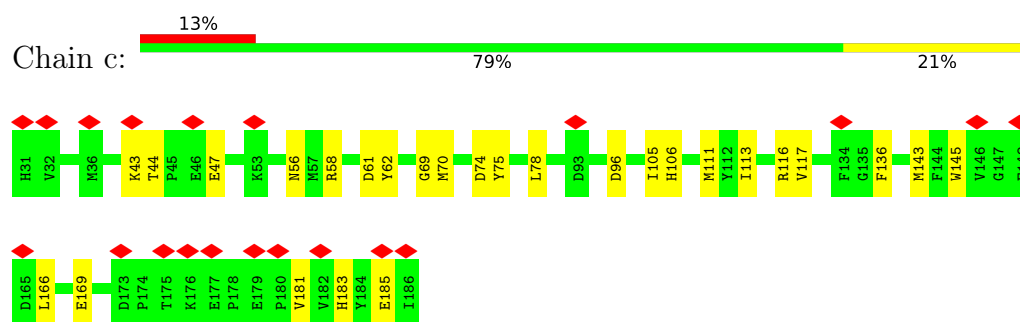
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



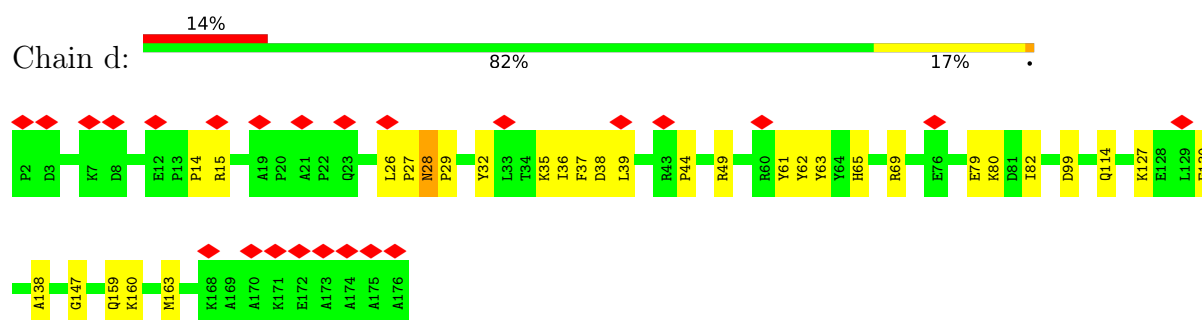
- Molecule 25: Complex I-B17



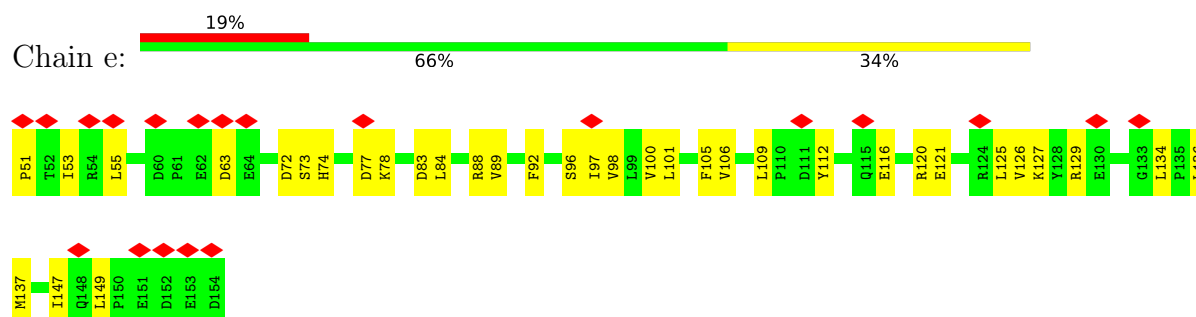
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



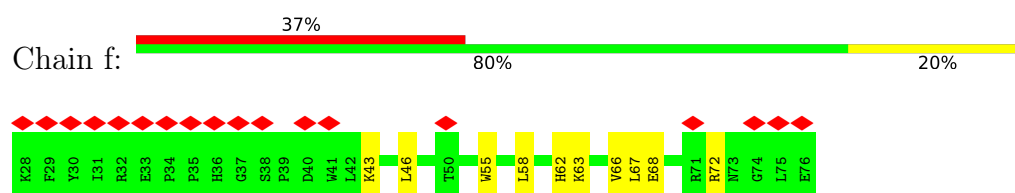
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



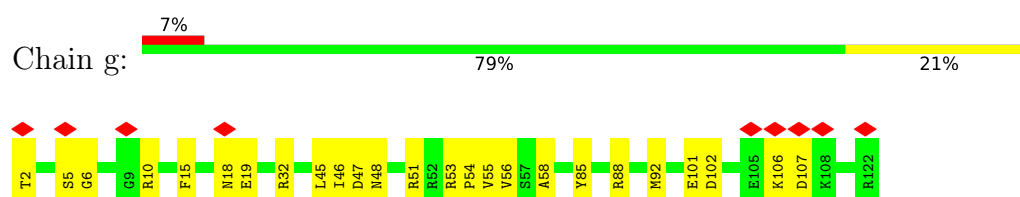
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



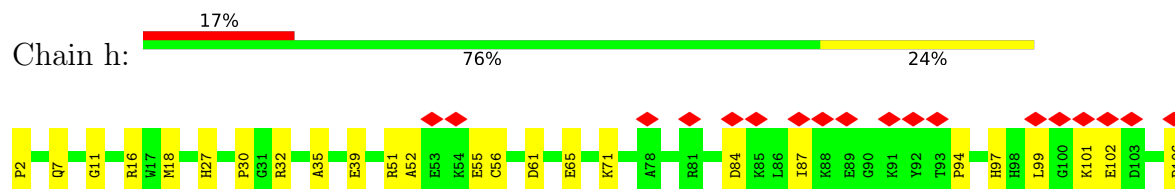
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



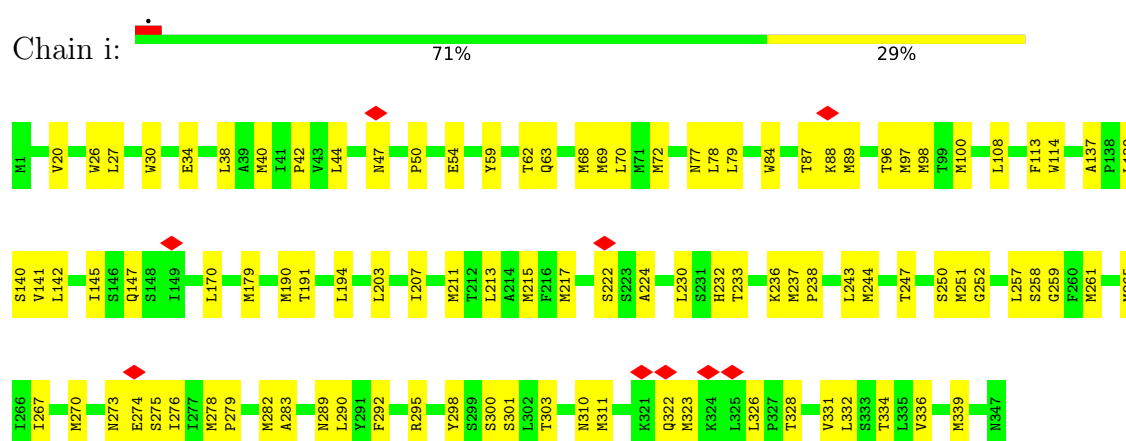
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



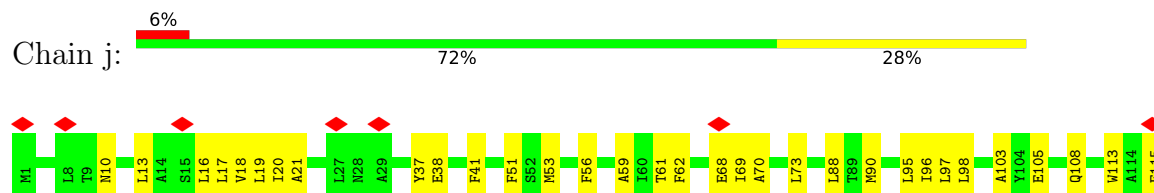
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



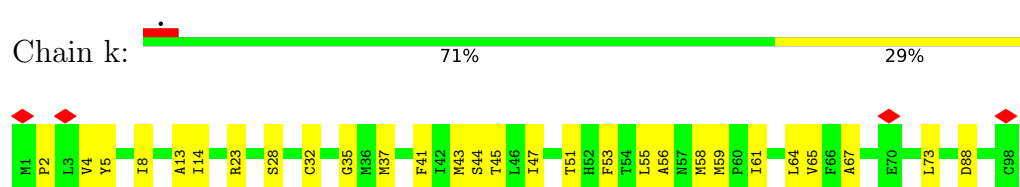
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



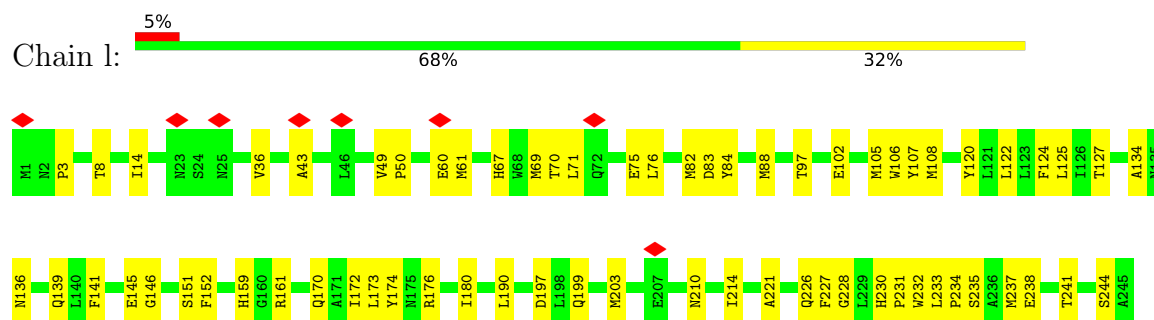
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

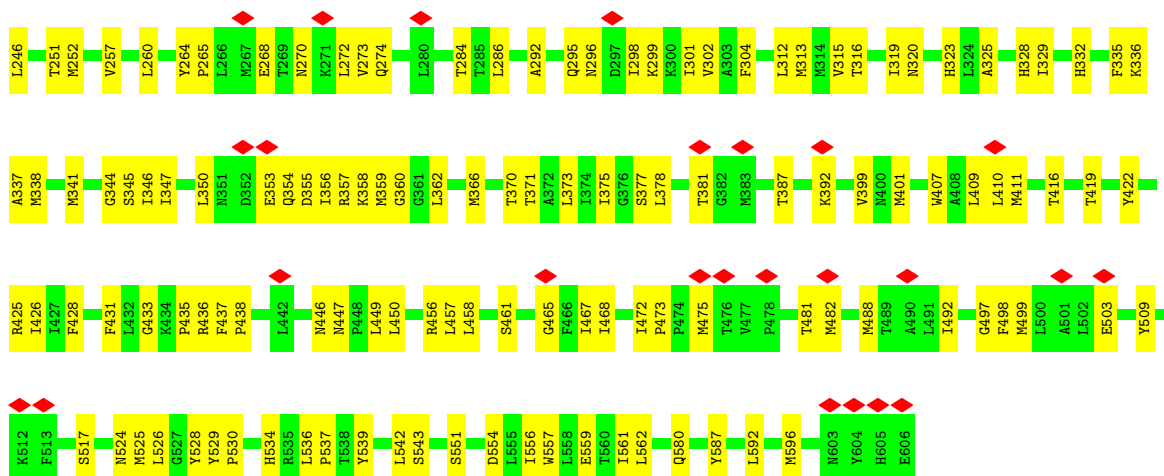


- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

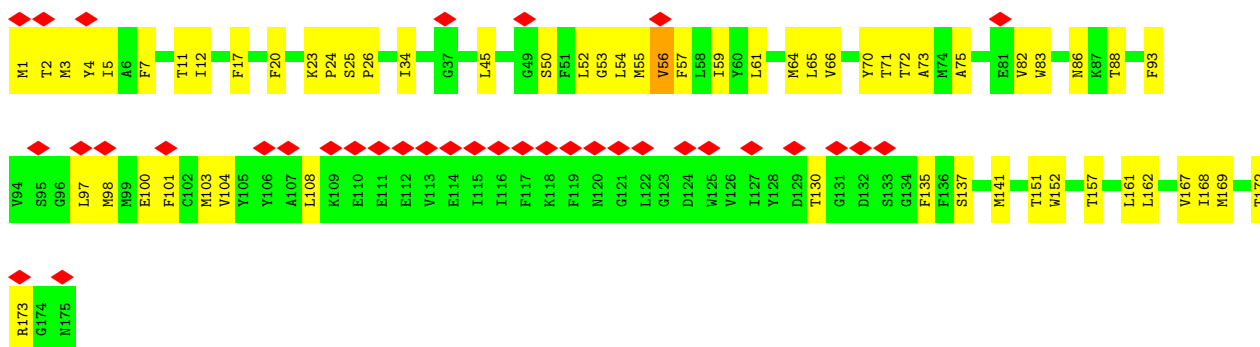


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

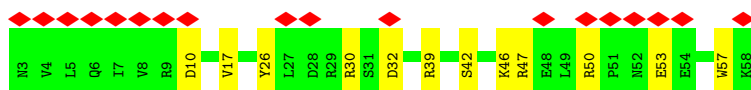
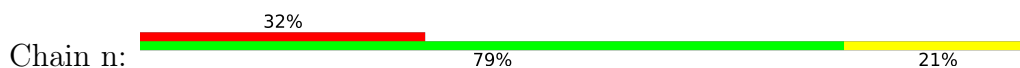




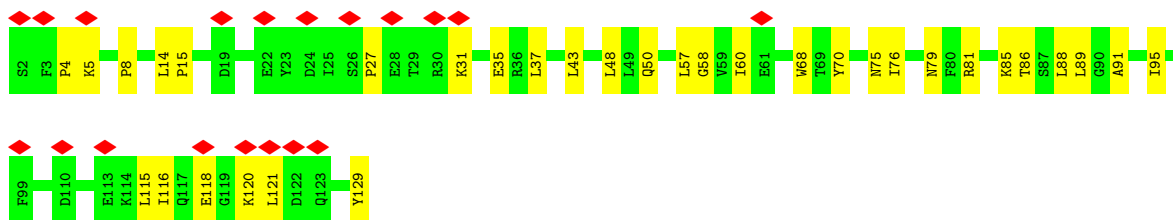
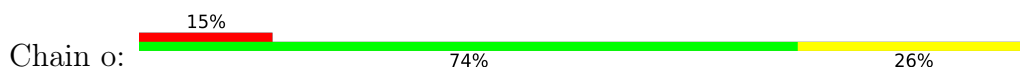
• Molecule 36: NADH-ubiquinone oxidoreductase chain 6



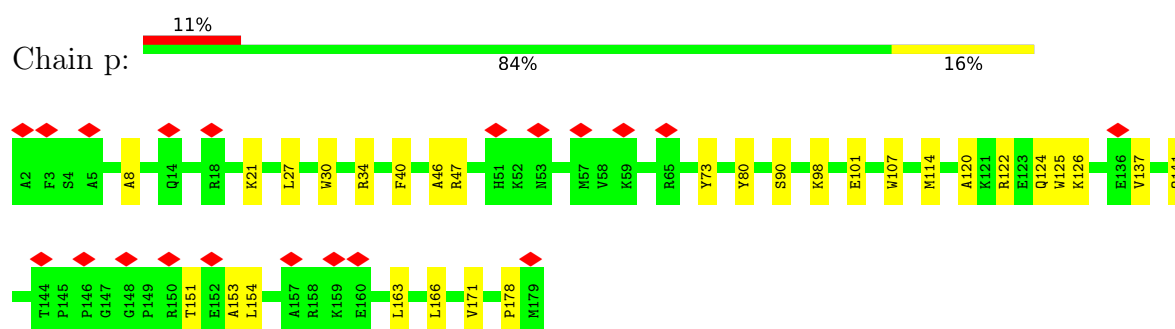
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



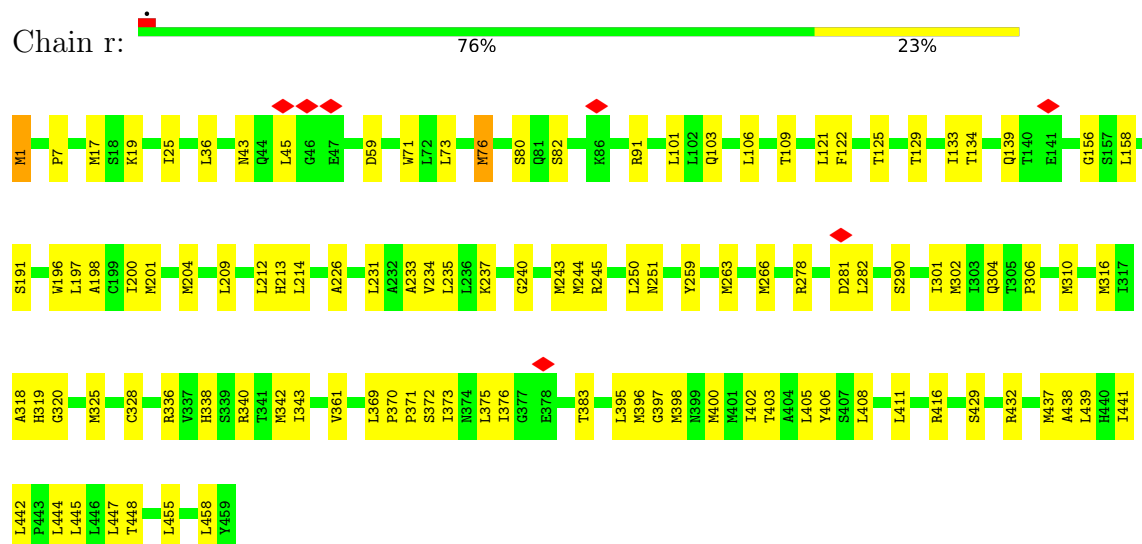
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



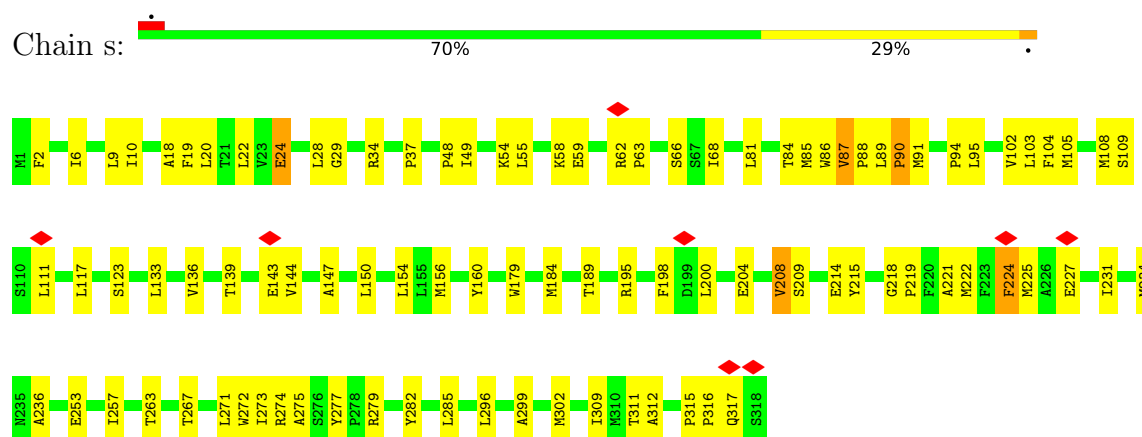
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



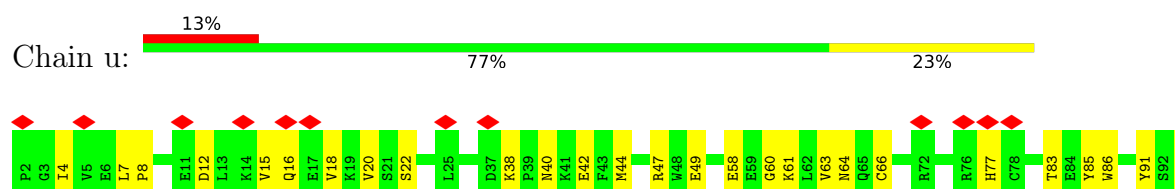
• Molecule 40: NADH-ubiquinone oxidoreductase chain 4

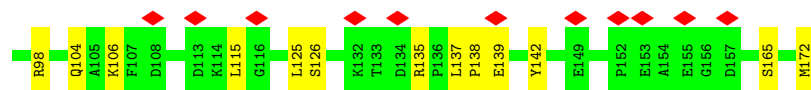


• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

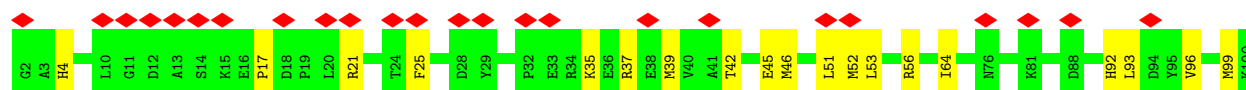
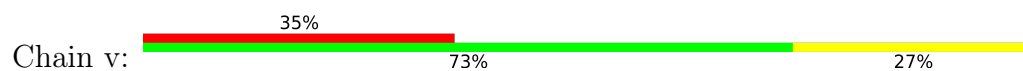


• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

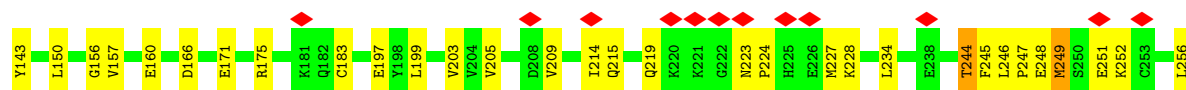
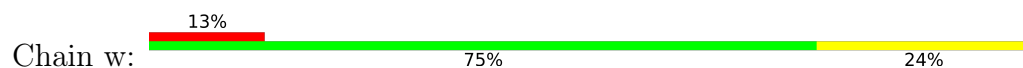




• Molecule 43: Complex I-B18



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27755	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	0.246	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0305	Depositor
Map size ($\text{\AA}$)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.14	0/3406	0.29	0/4603
2	B	0.16	0/1443	0.30	0/1952
3	C	0.15	0/1279	0.28	0/1730
4	E	0.16	0/995	0.29	0/1340
5	F	0.25	0/680	0.85	5/918 (0.5%)
6	G	0.17	0/701	0.39	0/951
6	X	0.20	0/716	0.38	0/968
7	H	0.16	0/929	0.34	0/1258
8	I	0.16	0/798	0.29	0/1079
9	J	0.13	0/2828	0.29	0/3834
10	K	0.14	0/377	0.24	0/509
11	L	0.15	0/1039	0.30	0/1403
12	M	0.15	0/5377	0.31	0/7287
13	N	0.15	0/1245	0.37	0/1694
14	O	0.16	0/1693	0.44	2/2306 (0.1%)
15	P	0.16	0/1789	0.31	0/2436
16	Q	0.19	0/3530	0.37	0/4785
17	S	0.16	0/581	0.37	0/781
18	T	0.15	0/755	0.29	0/1018
19	U	0.11	0/664	0.25	0/912
20	V	0.13	0/1039	0.26	0/1407
21	W	0.18	0/1198	0.40	0/1617
22	Y	0.22	0/606	0.58	2/831 (0.2%)
23	Z	0.14	0/652	0.30	0/884
24	a	0.14	0/1184	0.27	0/1603
25	b	0.18	0/840	0.41	0/1144
26	c	0.16	0/1371	0.33	0/1875
27	d	0.16	0/1494	0.38	2/2015 (0.1%)
28	e	0.13	0/891	0.29	0/1210
29	f	0.16	0/386	0.34	0/523
30	g	0.16	0/1031	0.33	0/1394
31	h	0.15	0/889	0.31	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.17	0/2773	0.35	0/3768
33	j	0.18	0/938	0.31	0/1281
34	k	0.18	0/759	0.35	0/1029
35	l	0.17	0/4929	0.35	1/6704 (0.0%)
36	m	0.20	0/1328	0.41	0/1804
37	n	0.11	0/491	0.30	0/663
38	o	0.13	0/1092	0.27	0/1481
39	p	0.13	0/1586	0.29	0/2150
40	r	0.17	0/3721	0.32	0/5075
41	s	0.23	0/2573	0.46	2/3518 (0.1%)
42	u	0.13	0/1436	0.32	0/1938
43	v	0.12	0/1076	0.35	0/1439
44	w	0.15	0/2635	0.39	2/3571 (0.1%)
All	All	0.16	0/67743	0.35	16/91878 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	62	GLN	N-CA-C	12.11	119.12	108.22
5	F	62	GLN	CA-C-N	9.53	131.75	119.84
5	F	62	GLN	C-N-CA	9.53	131.75	119.84
5	F	25	GLN	N-CA-C	7.58	119.54	111.28
5	F	61	VAL	N-CA-C	7.11	117.24	110.42
22	Y	88	ASP	CA-C-N	6.40	126.15	119.05
22	Y	88	ASP	C-N-CA	6.40	126.15	119.05
35	l	467	ILE	N-CA-C	5.99	116.16	110.53
41	s	86	TRP	N-CA-C	5.74	118.31	111.71
14	O	226	GLU	CA-C-N	5.69	125.70	119.90
14	O	226	GLU	C-N-CA	5.69	125.70	119.90
27	d	28	ASN	CA-C-N	5.48	125.13	119.05
27	d	28	ASN	C-N-CA	5.48	125.13	119.05
41	s	87	VAL	CB-CA-C	-5.34	108.69	114.35
44	w	244	THR	N-CA-C	5.12	119.27	112.72
44	w	245	PHE	N-CA-C	5.09	116.52	111.07

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	3330	0	3292	77	0
2	B	1412	0	1363	24	0
3	C	1248	0	1254	21	0
4	E	971	0	975	34	0
5	F	669	0	669	31	0
6	G	689	0	667	35	0
6	X	704	0	695	32	0
7	H	910	0	950	27	0
8	I	780	0	808	20	0
9	J	2751	0	2773	52	0
10	K	366	0	338	17	0
11	L	1016	0	1016	20	0
12	M	5289	0	5314	102	0
13	N	1204	0	1162	31	0
14	O	1654	0	1648	43	0
15	P	1738	0	1693	28	0
16	Q	3451	0	3383	91	0
17	S	566	0	561	18	0
18	T	741	0	702	15	0
19	U	643	0	642	10	0
20	V	1018	0	1023	17	0
21	W	1167	0	1155	37	0
22	Y	580	0	523	32	0
23	Z	633	0	598	13	0
24	a	1151	0	1164	29	0
25	b	815	0	831	20	0
26	c	1315	0	1208	35	0
27	d	1461	0	1429	29	0
28	e	867	0	817	33	0
29	f	378	0	356	8	0
30	g	1000	0	994	26	0
31	h	867	0	873	22	0
32	i	2710	0	2874	81	0
33	j	914	0	951	54	0
34	k	748	0	799	29	0
35	l	4800	0	4939	170	0
36	m	1295	0	1263	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	n	479	0	486	10	0
38	o	1062	0	1072	31	0
39	p	1530	0	1466	25	0
40	r	3629	0	3834	94	0
41	s	2501	0	2600	113	0
42	u	1398	0	1374	42	0
43	v	1053	0	1022	45	0
44	w	2575	0	2523	60	0
45	A	8	0	0	1	0
45	B	16	0	0	0	0
45	C	8	0	0	1	0
45	M	16	0	0	2	0
46	A	31	0	19	3	0
47	A	44	0	27	3	0
48	B	51	0	82	6	0
48	C	47	0	71	1	0
48	Q	47	0	71	1	0
48	W	41	0	59	0	0
48	b	46	0	69	4	0
48	j	51	0	82	4	0
48	l	91	0	136	3	0
48	r	51	0	82	9	0
48	s	41	0	59	3	0
49	C	52	0	88	5	0
49	a	52	0	88	1	0
49	g	52	0	88	7	0
49	j	52	0	88	2	0
49	r	104	0	176	7	0
50	G	35	0	0	6	0
50	X	35	0	0	3	0
51	J	48	0	25	3	0
52	J	33	0	39	2	0
52	s	38	0	47	10	0
53	M	4	0	0	0	0
53	O	4	0	0	0	0
54	M	1	0	0	0	0
55	N	51	0	46	1	0
55	V	194	0	294	8	0
55	a	100	0	156	2	0
55	l	199	0	307	16	0
55	m	100	0	156	13	0
55	s	89	0	125	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	u	55	0	54	4	0
55	w	100	0	156	13	0
56	T	1	0	0	0	0
57	w	27	0	11	2	0
All	All	68093	0	68780	1606	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 12.

All (1606) 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:G:112:SER:CB	50:G:201:8Q1:O1	1.72	1.36
6:X:112:SER:CB	50:X:201:8Q1:O1	1.75	1.33
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.20
51:J:401:NDP:O4D	51:J:401:NDP:C4D	1.68	1.18
35:l:8:THR:HB	35:l:82:MET:HE3	1.23	1.13
33:j:108:GLN:HB2	36:m:169:MET:HE1	1.25	1.10
41:s:81:LEU:HD11	41:s:111:LEU:HG	1.38	1.06
6:G:103:HIS:CG	6:G:139:MET:HE2	1.91	1.04
44:w:249:MET:CE	44:w:252:LYS:HE2	1.87	1.03
29:f:62:HIS:O	29:f:66:VAL:HG23	1.60	1.02
41:s:87:VAL:HG23	41:s:88:PRO:HD3	1.41	1.01
36:m:64:MET:HE2	36:m:64:MET:HA	1.41	1.01
6:G:103:HIS:ND1	6:G:139:MET:HE2	1.76	1.00
7:H:112:TRP:HZ3	15:P:127:GLU:OE1	1.45	1.00
40:r:375:LEU:HD23	40:r:375:LEU:O	1.61	0.98
30:g:2:THR:N	30:g:5:SER:HG	1.60	0.98
16:Q:210:MET:HE2	16:Q:247:PHE:HZ	1.28	0.97
22:Y:89:PRO:HB2	43:v:103:GLU:OE2	1.65	0.96
23:Z:63:PHE:HZ	35:l:498:PHE:HE1	1.14	0.94
30:g:48:ASN:OD1	30:g:53:ARG:HB2	1.69	0.93
23:Z:63:PHE:HZ	35:l:498:PHE:CE1	1.88	0.92
44:w:249:MET:HA	44:w:249:MET:HE2	1.51	0.91
43:v:111:ARG:HA	43:v:114:ARG:HH12	1.36	0.91
32:i:261:MET:HE1	32:i:336:VAL:HG12	1.51	0.90
16:Q:172:VAL:HG21	16:Q:310:VAL:HG22	1.55	0.89
5:F:24:CYS:SG	5:F:59:SER:O	2.30	0.88
4:E:68:MET:HA	4:E:68:MET:HE2	1.53	0.88
7:H:112:TRP:CZ3	15:P:127:GLU:OE1	2.27	0.88
1:A:192:ASP:HB3	10:K:98:MET:SD	2.13	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:65:LEU:CD1	41:s:139:THR:HG21	2.04	0.87
6:G:97:LYS:HZ3	6:G:108:LEU:HG	1.38	0.87
16:Q:181:LEU:HD21	16:Q:210:MET:HB2	1.55	0.87
8:I:70:MET:O	8:I:70:MET:SD	2.33	0.86
36:m:65:LEU:HD13	41:s:139:THR:HG21	1.58	0.86
8:I:40:LYS:HB2	21:W:7:LYS:H	1.38	0.85
35:l:8:THR:HB	35:l:82:MET:CE	2.07	0.85
41:s:24:GLU:HG2	41:s:271:LEU:HD22	1.58	0.85
16:Q:184:ILE:O	16:Q:188:THR:HG23	1.77	0.84
16:Q:173:LEU:O	16:Q:173:LEU:HD12	1.79	0.83
41:s:81:LEU:HD11	41:s:111:LEU:CG	2.07	0.83
43:v:111:ARG:HA	43:v:114:ARG:NH1	1.94	0.83
35:l:60:GLU:HG2	35:l:83:ASP:HA	1.58	0.83
44:w:249:MET:HE1	44:w:252:LYS:HE2	1.59	0.83
21:W:78:GLU:O	21:W:82:ARG:HG3	1.79	0.83
40:r:200:ILE:CG2	40:r:204:MET:HE2	2.10	0.82
41:s:24:GLU:CG	41:s:271:LEU:HD22	2.08	0.82
33:j:108:GLN:HB2	36:m:169:MET:CE	2.06	0.82
35:l:8:THR:CB	35:l:82:MET:HE3	2.09	0.82
43:v:104:ARG:O	43:v:108:LEU:HD23	1.80	0.81
6:G:112:SER:CB	50:G:201:8Q1:P24	2.67	0.81
1:A:337:MET:HA	1:A:337:MET:HE2	1.60	0.81
7:H:22:GLU:O	7:H:26:ILE:HG13	1.79	0.81
3:C:83:ARG:HE	16:Q:208:GLU:HG2	1.45	0.81
34:k:55:LEU:O	34:k:58:MET:HE3	1.80	0.81
16:Q:210:MET:HE2	16:Q:247:PHE:CZ	2.14	0.80
34:k:43:MET:O	34:k:47:ILE:HG13	1.80	0.80
9:J:365:GLU:OE1	9:J:365:GLU:N	2.15	0.80
33:j:53:MET:HE3	33:j:56:PHE:HA	1.64	0.79
1:A:282:VAL:HG13	1:A:356:VAL:HG21	1.65	0.79
12:M:33:GLU:HB2	12:M:42:MET:HE1	1.63	0.79
33:j:53:MET:HE3	33:j:56:PHE:HB3	1.64	0.79
35:l:170:GLN:NE2	35:l:235:SER:CB	2.45	0.79
41:s:117:LEU:CD2	41:s:136:VAL:HG23	2.13	0.79
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.63	0.78
12:M:134:GLY:HA2	45:M:801:SF4:S3	2.24	0.78
41:s:87:VAL:HG12	41:s:95:LEU:HD23	1.65	0.78
33:j:53:MET:HE3	33:j:56:PHE:CA	2.14	0.78
33:j:53:MET:HE1	36:m:70:TYR:CE1	2.19	0.77
12:M:178:GLN:HG2	12:M:204:MET:CE	2.12	0.77
41:s:87:VAL:HG23	41:s:88:PRO:CD	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:224:PHE:HE2	52:s:403:UQ:H112	1.50	0.77
4:E:96:VAL:HG12	4:E:96:VAL:O	1.85	0.77
44:w:266:ALA:O	44:w:270:VAL:HG23	1.84	0.77
27:d:99:ASP:OD2	28:e:137:MET:HE2	1.84	0.76
12:M:178:GLN:HG2	12:M:204:MET:HE3	1.68	0.76
38:o:70:TYR:HE1	38:o:75:ASN:HD22	1.33	0.76
41:s:208:VAL:HG12	41:s:209:SER:N	1.99	0.76
9:J:322:VAL:HG13	9:J:323:HIS:HD2	1.51	0.76
1:A:102:MET:O	1:A:102:MET:HG2	1.83	0.76
12:M:135:GLY:HA3	12:M:242:PRO:CG	2.16	0.76
33:j:53:MET:HE3	33:j:56:PHE:CB	2.14	0.76
22:Y:89:PRO:CB	43:v:103:GLU:OE2	2.33	0.76
15:P:216:VAL:HG23	15:P:218:ARG:HG2	1.66	0.76
43:v:46:MET:HE3	43:v:56:ARG:HD3	1.68	0.76
13:N:68:MET:HG3	13:N:69:ASN:H	1.48	0.76
16:Q:182:ASN:HD21	16:Q:404:LYS:NZ	1.85	0.76
35:l:286:LEU:HD13	35:l:411:MET:HE3	1.66	0.76
27:d:26:LEU:HD12	27:d:27:PRO:CD	2.16	0.75
10:K:79:HIS:ND1	14:O:215:LYS:NZ	2.34	0.75
23:Z:15:GLU:N	23:Z:15:GLU:OE1	2.19	0.75
22:Y:87:PRO:HG2	43:v:99:MET:HE1	1.68	0.75
44:w:57:SER:HB3	44:w:150:LEU:HD11	1.69	0.75
28:e:109:LEU:HD13	40:r:43:ASN:HB2	1.69	0.75
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.69	0.74
35:l:353:GLU:OE2	35:l:355:ASP:N	2.20	0.74
40:r:201:MET:HE3	40:r:201:MET:HA	1.69	0.74
22:Y:87:PRO:HG2	43:v:99:MET:CE	2.18	0.74
8:I:31:ILE:HD12	8:I:32:SER:O	1.88	0.74
7:H:94:MET:HE2	7:H:97:TRP:HE3	1.52	0.73
35:l:551:SER:O	35:l:556:ILE:HG12	1.88	0.73
12:M:313:LEU:CD2	13:N:141:SER:O	2.37	0.73
6:X:82:ARG:CD	22:Y:44:TYR:CE1	2.71	0.73
26:c:70:MET:CE	38:o:86:THR:HG22	2.18	0.73
32:i:278:MET:O	32:i:282:MET:HG3	1.88	0.73
30:g:106:LYS:HG2	30:g:107:ASP:N	2.02	0.73
16:Q:340:SER:O	16:Q:344:ILE:HG13	1.87	0.73
35:l:286:LEU:HD13	35:l:411:MET:CE	2.17	0.73
3:C:103:MET:HB2	3:C:124:MET:HE1	1.70	0.73
32:i:213:LEU:O	32:i:217:MET:HG3	1.89	0.73
41:s:117:LEU:HD21	41:s:136:VAL:HG23	1.69	0.73
36:m:64:MET:HA	36:m:64:MET:CE	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:HD13	1:A:149:MET:HE1	1.71	0.72
24:a:153:GLU:HB2	30:g:92:MET:CE	2.18	0.72
27:d:65:HIS:NE2	28:e:121:GLU:OE2	2.21	0.72
44:w:80:LYS:HD2	44:w:270:VAL:HG21	1.72	0.72
24:a:78:THR:HG21	28:e:96:SER:HA	1.71	0.72
32:i:222:SER:HB3	32:i:237:MET:HE1	1.72	0.72
40:r:375:LEU:HD23	40:r:375:LEU:C	2.15	0.72
6:G:112:SER:CA	50:G:201:8Q1:O1	2.38	0.72
10:K:79:HIS:CD2	14:O:216:PRO:HG2	2.24	0.72
12:M:313:LEU:HD21	13:N:141:SER:O	1.89	0.72
8:I:31:ILE:HD12	8:I:31:ILE:C	2.15	0.71
6:X:83:VAL:HG13	6:X:122:MET:HE1	1.72	0.71
35:l:237:MET:HA	35:l:237:MET:HE3	1.73	0.71
22:Y:65:MET:HE1	35:l:378:LEU:HD13	1.70	0.71
5:F:51:LEU:O	5:F:53:ILE:HD12	1.90	0.71
7:H:58:MET:HE3	7:H:71:GLN:CD	2.15	0.71
35:l:159:HIS:HB2	40:r:416:ARG:HG2	1.72	0.71
6:G:97:LYS:NZ	6:G:108:LEU:HG	2.05	0.71
36:m:65:LEU:HD23	36:m:65:LEU:O	1.90	0.71
37:n:10:ASP:OD1	40:r:19:LYS:NZ	2.22	0.71
22:Y:41:GLU:OE2	22:Y:41:GLU:N	2.23	0.71
28:e:55:LEU:HD23	44:w:320:GLY:HA2	1.72	0.71
34:k:41:PHE:O	34:k:45:THR:HG22	1.91	0.71
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.23	0.71
32:i:26:TRP:CH2	32:i:98:MET:HE2	2.26	0.71
33:j:108:GLN:CB	36:m:169:MET:HE1	2.12	0.71
32:i:77:ASN:ND2	32:i:89:MET:SD	2.64	0.71
32:i:232:HIS:HB3	32:i:311:MET:HE1	1.73	0.70
16:Q:172:VAL:HG21	16:Q:310:VAL:CG2	2.20	0.70
27:d:26:LEU:HD12	27:d:27:PRO:HD2	1.73	0.70
22:Y:78:ASP:HB2	22:Y:83:HIS:HB2	1.72	0.70
26:c:111:MET:HE2	35:l:542:LEU:HB2	1.73	0.70
7:H:44:TYR:HB2	15:P:68:ILE:HG23	1.73	0.70
33:j:18:VAL:HG23	41:s:222:MET:HE1	1.73	0.70
38:o:75:ASN:O	38:o:79:ASN:ND2	2.24	0.70
14:O:200:ASP:OD2	14:O:219:ARG:CB	2.40	0.69
23:Z:25:GLU:HA	23:Z:30:GLU:OE1	1.92	0.69
23:Z:60:ASN:ND2	35:l:433:GLY:O	2.25	0.69
12:M:133:GLN:HG3	12:M:133:GLN:O	1.92	0.69
36:m:52:LEU:O	36:m:56:VAL:HG12	1.91	0.69
16:Q:208:GLU:OE2	16:Q:221:ARG:NH2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:57:ARG:NH1	12:M:150:ARG:HH21	1.89	0.69
12:M:566:ILE:HD13	12:M:579:MET:HE3	1.74	0.69
24:a:137:MET:HE1	37:n:42:SER:HB3	1.72	0.69
5:F:51:LEU:O	5:F:53:ILE:CD1	2.40	0.69
6:G:141:PRO:O	6:G:145:VAL:HG23	1.93	0.69
9:J:318:LYS:O	9:J:322:VAL:HG12	1.92	0.69
16:Q:206:GLU:O	16:Q:210:MET:HG3	1.92	0.69
24:a:153:GLU:HB2	30:g:92:MET:HE1	1.74	0.69
35:l:422:TYR:O	35:l:426:ILE:HD12	1.91	0.69
36:m:65:LEU:HD23	36:m:65:LEU:C	2.17	0.69
21:W:128:ARG:NH1	31:h:102:GLU:OE2	2.25	0.69
38:o:118:GLU:OE1	38:o:120:LYS:NZ	2.25	0.69
41:s:89:LEU:HD21	41:s:105:MET:HE1	1.75	0.69
36:m:72:THR:HG21	41:s:133:LEU:HD21	1.75	0.69
1:A:317:VAL:HG22	1:A:356:VAL:HG12	1.73	0.68
8:I:31:ILE:CD1	8:I:32:SER:O	2.40	0.68
4:E:18:LYS:NZ	4:E:19:PRO:O	2.26	0.68
16:Q:182:ASN:ND2	16:Q:404:LYS:NZ	2.40	0.68
21:W:121:MET:HE3	36:m:130:THR:HG22	1.75	0.68
6:G:112:SER:N	50:G:201:8Q1:O1	2.25	0.68
32:i:328:THR:O	32:i:332:LEU:HD12	1.93	0.68
38:o:75:ASN:OD1	38:o:79:ASN:ND2	2.23	0.68
8:I:57:ARG:HH12	12:M:150:ARG:HH21	1.40	0.68
26:c:162:PRO:HG3	43:v:39:MET:HE2	1.75	0.68
1:A:48:ARG:NH1	10:K:70:ASN:O	2.27	0.68
26:c:58:ARG:HB2	26:c:61:ASP:HB2	1.75	0.68
41:s:87:VAL:CG2	41:s:88:PRO:HD3	2.21	0.68
44:w:139:ARG:NH1	44:w:166:ASP:OD2	2.27	0.68
1:A:285:PRO:HG3	14:O:143:ARG:NH1	2.09	0.68
41:s:208:VAL:HG12	41:s:209:SER:H	1.58	0.68
34:k:28:SER:HB3	36:m:23:LYS:HG2	1.75	0.67
4:E:84:ILE:HG22	4:E:88:MET:HE3	1.76	0.67
55:V:202:CDL:H712	55:V:202:CDL:H512	1.76	0.67
21:W:134:LEU:HD21	36:m:2:THR:HB	1.75	0.67
44:w:249:MET:CE	44:w:249:MET:HA	2.24	0.67
6:X:140:CYS:HB2	6:X:143:GLU:HG3	1.76	0.67
20:V:140:LYS:NZ	32:i:274:GLU:OE1	2.27	0.67
50:X:201:8Q1:C7	39:p:47:ARG:HG2	2.25	0.67
41:s:236:ALA:HA	41:s:263:THR:HG22	1.77	0.67
35:l:362:LEU:HB3	35:l:366:MET:HE2	1.77	0.67
36:m:82:VAL:HG11	55:s:402:CDL:HB31	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:93:PHE:CE2	36:m:97:LEU:HD11	2.31	0.66
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.36	0.66
7:H:25:LYS:HD2	7:H:60:LYS:HD3	1.76	0.66
23:Z:63:PHE:CZ	35:l:498:PHE:HE1	2.06	0.66
36:m:34:ILE:HG13	36:m:64:MET:HG3	1.77	0.66
20:V:81:ARG:HH12	20:V:83:LYS:HD2	1.60	0.66
35:l:375:ILE:HD12	35:l:458:LEU:HD11	1.77	0.66
48:B:303:PEE:H24	41:s:296:LEU:HD21	1.77	0.66
25:b:99:GLU:HG2	35:l:61:MET:HE2	1.77	0.66
34:k:37:MET:HE3	34:k:67:ALA:HB2	1.77	0.66
16:Q:182:ASN:HD21	16:Q:404:LYS:HZ1	1.43	0.66
6:G:132:ASP:C	6:G:133:ILE:HD12	2.21	0.66
9:J:83:PRO:HG3	9:J:119:VAL:HG11	1.78	0.66
32:i:334:THR:HG21	55:w:401:CDL:H391	1.77	0.66
24:a:153:GLU:OE1	30:g:88:ARG:HD2	1.96	0.65
35:l:190:LEU:HD12	40:r:383:THR:CG2	2.26	0.65
1:A:50:ASP:O	1:A:59:ARG:NH2	2.28	0.65
35:l:366:MET:O	35:l:370:THR:HG22	1.96	0.65
22:Y:83:HIS:O	22:Y:83:HIS:ND1	2.30	0.65
9:J:135:GLU:HG3	9:J:140:ASP:HA	1.78	0.65
19:U:30:ILE:HD11	33:j:96:ILE:HD11	1.78	0.65
26:c:70:MET:HE2	38:o:86:THR:HG22	1.78	0.65
27:d:79:GLU:OE2	27:d:80:LYS:HG2	1.96	0.65
41:s:85:MET:HE1	41:s:109:SER:HA	1.77	0.65
35:l:84:TYR:HE1	35:l:88:MET:HE3	1.61	0.65
23:Z:30:GLU:O	23:Z:34:GLU:HG2	1.96	0.65
35:l:274:GLN:NE2	35:l:320:ASN:OD1	2.30	0.65
1:A:102:MET:O	1:A:102:MET:CG	2.43	0.65
5:F:26:ARG:NH1	5:F:26:ARG:HB2	2.12	0.65
21:W:62:ILE:O	21:W:66:GLU:HG2	1.95	0.65
43:v:103:GLU:O	43:v:107:ARG:HG2	1.97	0.65
31:h:2:PRO:HA	32:i:140:SER:HB2	1.78	0.64
31:h:65:GLU:OE2	31:h:65:GLU:HA	1.96	0.64
32:i:77:ASN:HD21	32:i:89:MET:HA	1.62	0.64
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.77	0.64
12:M:535:GLU:OE1	12:M:535:GLU:N	2.19	0.64
35:l:190:LEU:HD12	40:r:383:THR:HG21	1.77	0.64
6:G:97:LYS:NZ	6:G:108:LEU:HA	2.13	0.64
12:M:308:ARG:NH2	12:M:578:PRO:O	2.30	0.64
16:Q:173:LEU:HD12	16:Q:173:LEU:C	2.20	0.64
6:X:112:SER:CB	50:X:201:8Q1:P24	2.86	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:69:MET:HE3	35:l:76:LEU:HD12	1.79	0.64
43:v:35:LYS:HA	43:v:35:LYS:HE2	1.78	0.64
1:A:234:GLY:HA3	1:A:240:THR:HG22	1.79	0.64
40:r:282:LEU:HD13	40:r:342:MET:HG3	1.79	0.64
55:w:401:CDL:H782	55:w:401:CDL:H241	1.79	0.64
43:v:51:LEU:O	43:v:52:MET:HG2	1.98	0.64
12:M:137:CYS:SG	45:M:801:SF4:FE4	1.89	0.64
21:W:88:ARG:NH2	42:u:7:LEU:O	2.31	0.64
26:c:185:GLU:OE2	43:v:37:ARG:HA	1.98	0.64
35:l:337:ALA:O	35:l:341:MET:HG3	1.97	0.64
40:r:447:LEU:HD11	49:r:503:PLX:H371	1.80	0.64
36:m:65:LEU:HD13	41:s:139:THR:CG2	2.28	0.63
25:b:4:TYR:HD2	25:b:9:LYS:HD3	1.63	0.63
28:e:125:LEU:HD23	28:e:129:ARG:HH12	1.62	0.63
33:j:19:LEU:HD11	48:s:401:PEE:H56	1.81	0.63
16:Q:181:LEU:HD21	16:Q:210:MET:CB	2.26	0.63
32:i:40:MET:HE3	32:i:44:LEU:HD21	1.79	0.63
17:S:12:MET:CE	41:s:20:LEU:HA	2.28	0.63
30:g:101:GLU:OE2	30:g:101:GLU:N	2.23	0.63
11:L:87:MET:HG3	12:M:136:GLU:OE2	1.98	0.63
49:g:201:PLX:H232	32:i:332:LEU:HB3	1.81	0.63
12:M:513:MET:C	12:M:514:ASN:HD22	2.05	0.63
21:W:98:MET:CE	21:W:101:VAL:HG21	2.29	0.63
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.81	0.63
40:r:91:ARG:NH2	44:w:325:ASP:OD2	2.31	0.63
40:r:240:GLY:O	40:r:244:MET:HG3	1.99	0.63
6:G:97:LYS:HE2	6:G:107:ASP:O	1.99	0.63
7:H:38:ILE:O	7:H:45:ARG:NH1	2.29	0.63
32:i:50:PRO:O	32:i:54:GLU:HG3	1.99	0.63
32:i:261:MET:HE1	32:i:336:VAL:CG1	2.27	0.63
26:c:111:MET:HE3	40:r:278:ARG:NH1	2.13	0.62
31:h:18:MET:HE3	34:k:56:ALA:HA	1.81	0.62
33:j:13:LEU:O	33:j:16:LEU:HG	1.99	0.62
44:w:41:LEU:O	44:w:45:LEU:HD23	1.98	0.62
12:M:33:GLU:CB	12:M:42:MET:HE1	2.29	0.62
31:h:18:MET:HE1	34:k:59:MET:HB2	1.81	0.62
1:A:145:GLY:O	1:A:149:MET:HE3	1.99	0.62
4:E:99:GLN:NE2	33:j:41:PHE:HB3	2.14	0.62
39:p:137:VAL:HG22	39:p:141:GLN:NE2	2.14	0.62
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.80	0.62
6:X:137:LYS:NZ	25:b:8:GLU:OE1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:170:GLN:NE2	35:l:235:SER:HB2	2.15	0.62
36:m:100:GLU:O	36:m:103:MET:HG3	2.00	0.62
9:J:229:ILE:H	9:J:323:HIS:CE1	2.18	0.62
40:r:396:MET:O	40:r:400:MET:HG3	1.99	0.62
9:J:87:GLU:HG3	9:J:89:TYR:H	1.63	0.62
36:m:71:THR:HA	36:m:75:ALA:HB3	1.82	0.62
44:w:70:LYS:NZ	44:w:160:GLU:OE1	2.32	0.62
9:J:222:TRP:HB3	52:J:402:UQ:H152	1.81	0.62
11:L:70:GLU:C	11:L:70:GLU:OE1	2.42	0.62
23:Z:41:LEU:HD21	39:p:46:ALA:HB2	1.80	0.62
35:l:488:MET:O	35:l:492:ILE:HG12	2.00	0.62
40:r:398:MET:O	40:r:402:ILE:HD12	2.00	0.62
41:s:24:GLU:HG3	41:s:271:LEU:HD22	1.81	0.62
4:E:16:SER:HA	11:L:52:LEU:HD13	1.82	0.61
9:J:229:ILE:H	9:J:323:HIS:HE1	1.47	0.61
35:l:387:THR:HG22	35:l:465:GLY:H	1.65	0.61
23:Z:63:PHE:CZ	35:l:498:PHE:CE1	2.81	0.61
20:V:38:ALA:HB2	55:m:201:CDL:H251	1.82	0.61
35:l:174:TYR:HD2	35:l:232:TRP:HB3	1.63	0.61
35:l:227:PHE:N	35:l:284:THR:OG1	2.33	0.61
10:K:79:HIS:CE1	14:O:215:LYS:HE3	2.35	0.61
27:d:26:LEU:CD1	27:d:27:PRO:HD2	2.31	0.61
36:m:93:PHE:O	36:m:97:LEU:HG	2.00	0.61
55:m:201:CDL:H402	55:m:201:CDL:H462	1.81	0.61
44:w:249:MET:HE2	44:w:252:LYS:HE2	1.80	0.61
35:l:71:LEU:HD12	40:r:310:MET:CE	2.31	0.61
2:B:50:MET:HE2	2:B:50:MET:HA	1.81	0.61
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.82	0.61
35:l:373:LEU:HD13	35:l:431:PHE:CE2	2.35	0.61
1:A:67:GLU:O	1:A:71:LYS:HG2	2.01	0.61
21:W:79:LYS:O	21:W:83:VAL:HG13	2.01	0.61
6:G:116:VAL:O	6:G:120:MET:HG3	2.01	0.60
9:J:192:ARG:NH1	9:J:198:ALA:O	2.34	0.60
44:w:88:GLU:OE1	44:w:139:ARG:NH2	2.35	0.60
14:O:208:LEU:HD13	14:O:214:PRO:CD	2.31	0.60
15:P:173:MET:HB3	15:P:198:PHE:HB2	1.82	0.60
41:s:222:MET:HA	41:s:225:MET:HE3	1.82	0.60
1:A:160:GLY:O	1:A:199:ARG:NH2	2.33	0.60
6:G:103:HIS:CE1	6:G:139:MET:HE2	2.36	0.60
32:i:328:THR:O	32:i:332:LEU:CD1	2.50	0.60
3:C:59:ARG:NH2	49:C:303:PLX:O3	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:243:LEU:HD23	55:w:401:CDL:H361	1.84	0.60
32:i:267:ILE:HG12	32:i:279:PRO:HB3	1.84	0.60
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.34	0.60
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.34	0.60
32:i:26:TRP:CZ3	32:i:98:MET:HE2	2.37	0.60
39:p:137:VAL:HG22	39:p:141:GLN:HE21	1.66	0.60
44:w:249:MET:HE1	44:w:252:LYS:CE	2.31	0.60
15:P:216:VAL:HG23	15:P:218:ARG:CG	2.31	0.60
16:Q:217:VAL:CG2	16:Q:226:TYR:CZ	2.84	0.60
28:e:136:LEU:HD12	28:e:136:LEU:O	2.01	0.60
35:l:84:TYR:CE1	35:l:88:MET:HE3	2.36	0.60
35:l:296:ASN:OD1	35:l:425:ARG:NH2	2.35	0.60
44:w:54:THR:HG23	44:w:56:THR:HG22	1.83	0.60
3:C:41:SER:N	3:C:44:GLU:OE2	2.35	0.60
15:P:81:PHE:HD1	15:P:83:GLU:HG3	1.67	0.60
27:d:69:ARG:NH2	37:n:46:LYS:O	2.35	0.60
12:M:472:PRO:O	12:M:510:TRP:NE1	2.35	0.60
24:a:140:LEU:HD23	27:d:82:ILE:HG13	1.84	0.60
35:l:71:LEU:HD12	40:r:310:MET:HE3	1.84	0.60
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.28	0.60
21:W:90:ASN:ND2	21:W:123:GLU:O	2.35	0.60
6:X:82:ARG:HD2	22:Y:44:TYR:CZ	2.36	0.60
35:l:227:PHE:O	35:l:230:HIS:ND1	2.34	0.60
40:r:438:ALA:O	40:r:442:LEU:HD12	2.01	0.60
2:B:50:MET:HE1	19:U:10:LYS:HD3	1.82	0.59
41:s:117:LEU:HD22	41:s:136:VAL:HG23	1.83	0.59
6:G:103:HIS:ND1	6:G:139:MET:HG2	2.17	0.59
30:g:106:LYS:HG2	30:g:107:ASP:H	1.66	0.59
21:W:54:ASN:ND2	41:s:156:MET:HE2	2.18	0.59
27:d:26:LEU:HD12	27:d:27:PRO:HD3	1.84	0.59
17:S:12:MET:HE2	41:s:20:LEU:HA	1.83	0.59
28:e:98:VAL:HG22	40:r:36:LEU:HB2	1.83	0.59
32:i:265:MET:HE3	32:i:265:MET:HA	1.83	0.59
1:A:40:ARG:NH1	14:O:233:SER:OG	2.35	0.59
11:L:78:ARG:NH2	11:L:148:GLU:OE2	2.33	0.59
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.83	0.59
17:S:47:LEU:HD22	42:u:22:SER:HB3	1.84	0.59
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.84	0.59
19:U:81:LEU:O	21:W:59:ARG:NH1	2.36	0.59
28:e:63:ASP:OD2	40:r:338:HIS:NE2	2.34	0.59
36:m:54:LEU:HD13	41:s:103:LEU:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:73:GLN:CD	5:F:75:LYS:HE3	2.28	0.59
16:Q:217:VAL:HG22	16:Q:226:TYR:CE1	2.38	0.59
22:Y:100:LEU:O	43:v:111:ARG:NH1	2.35	0.59
26:c:143:MET:HE3	35:l:407:TRP:CZ3	2.37	0.59
35:l:170:GLN:HE22	35:l:235:SER:HB2	1.66	0.59
40:r:444:LEU:O	40:r:448:THR:HG23	2.03	0.59
30:g:15:PHE:HB2	49:g:201:PLX:H6	1.84	0.59
3:C:94:ARG:NH1	52:s:403:UQ:H8	2.18	0.59
5:F:26:ARG:CB	5:F:26:ARG:HH11	2.15	0.59
22:Y:50:LEU:HD12	22:Y:50:LEU:N	2.17	0.59
32:i:38:LEU:HA	34:k:73:LEU:HD11	1.84	0.59
43:v:119:GLU:O	43:v:122:MET:HE3	2.03	0.59
12:M:135:GLY:HA3	12:M:242:PRO:HG3	1.82	0.59
26:c:162:PRO:HG3	43:v:39:MET:CE	2.32	0.59
28:e:126:VAL:HG22	28:e:136:LEU:HD11	1.84	0.59
35:l:346:ILE:HG12	35:l:366:MET:HE1	1.84	0.59
42:u:15:VAL:HG12	42:u:64:ASN:HD22	1.68	0.59
26:c:44:THR:HB	26:c:47:GLU:HG3	1.84	0.58
38:o:85:LYS:O	38:o:89:LEU:HG	2.03	0.58
22:Y:48:PRO:O	22:Y:50:LEU:HD12	2.03	0.58
36:m:45:LEU:HD23	36:m:50:SER:HA	1.85	0.58
35:l:106:TRP:CD1	35:l:447:ASN:HD22	2.22	0.58
41:s:89:LEU:HD21	41:s:105:MET:CE	2.33	0.58
6:X:83:VAL:HG13	6:X:122:MET:CE	2.33	0.58
29:f:63:LYS:O	29:f:67:LEU:HG	2.04	0.58
41:s:87:VAL:CG2	41:s:88:PRO:CD	2.80	0.58
22:Y:97:LEU:HD12	43:v:107:ARG:HD2	1.86	0.58
33:j:69:ILE:HD11	41:s:144:VAL:HA	1.83	0.58
42:u:139:GLU:OE2	42:u:139:GLU:N	2.35	0.58
5:F:45:LYS:HD3	5:F:53:ILE:HD13	1.86	0.58
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.86	0.58
35:l:190:LEU:HD13	35:l:190:LEU:C	2.27	0.58
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.36	0.58
16:Q:47:PHE:CD1	16:Q:52:MET:HE1	2.39	0.58
36:m:65:LEU:HD21	41:s:136:VAL:HG13	1.86	0.58
48:r:501:PEE:H79	48:r:501:PEE:H40	1.85	0.58
41:s:299:ALA:HA	41:s:302:MET:HE3	1.85	0.58
1:A:294:VAL:HG23	1:A:298:GLU:OE2	2.03	0.58
5:F:22:HIS:CD2	5:F:66:TRP:CD1	2.91	0.58
5:F:87:VAL:O	5:F:91:LEU:HD12	2.04	0.58
9:J:188:GLU:HG3	9:J:200:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:650:SER:HB3	12:M:653:LEU:HD12	1.86	0.58
35:l:377:SER:O	35:l:381:THR:HG23	2.04	0.58
40:r:200:ILE:HG22	40:r:204:MET:HE2	1.85	0.58
12:M:33:GLU:HG3	12:M:42:MET:CE	2.34	0.57
12:M:483:ARG:HH11	12:M:489:ILE:HD11	1.70	0.57
6:X:75:THR:O	6:X:79:ILE:HG13	2.04	0.57
40:r:263:MET:HE2	40:r:263:MET:N	2.19	0.57
16:Q:194:ILE:HG23	16:Q:271:ARG:HD3	1.85	0.57
38:o:31:LYS:O	38:o:35:GLU:HG2	2.04	0.57
11:L:88:GLN:HG2	12:M:136:GLU:O	2.04	0.57
20:V:123:ALA:O	20:V:127:MET:HG3	2.03	0.57
30:g:10:ARG:NH2	49:g:201:PLX:O3	2.37	0.57
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.86	0.57
35:l:127:THR:HG21	35:l:146:GLY:HA3	1.84	0.57
35:l:472:ILE:HG23	35:l:473:PRO:HD2	1.85	0.57
24:a:180:ASP:OD1	24:a:180:ASP:O	2.22	0.57
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.86	0.57
36:m:53:GLY:HA2	36:m:56:VAL:CG1	2.35	0.57
8:I:107:SER:HB3	8:I:111:PRO:HA	1.87	0.57
6:X:115:GLN:HA	6:X:118:ILE:HD12	1.86	0.57
33:j:53:MET:HE1	36:m:70:TYR:CD1	2.39	0.57
35:l:499:MET:O	35:l:503:GLU:HG2	2.04	0.57
39:p:154:LEU:HD21	39:p:166:LEU:HD12	1.85	0.57
44:w:300:ASN:OD1	44:w:300:ASN:O	2.23	0.57
1:A:357:MET:HB3	1:A:361:THR:HG21	1.86	0.57
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.85	0.57
7:H:55:LYS:HE3	15:P:104:THR:HG21	1.85	0.57
10:K:79:HIS:ND1	14:O:215:LYS:CE	2.67	0.57
32:i:298:TYR:CE1	40:r:134:THR:HG21	2.40	0.57
35:l:237:MET:HE1	35:l:244:SER:HB2	1.85	0.57
6:G:103:HIS:ND1	6:G:139:MET:CE	2.59	0.57
12:M:696:MET:HG2	12:M:702:ARG:HA	1.87	0.57
16:Q:182:ASN:ND2	16:Q:404:LYS:HZ2	2.02	0.57
40:r:204:MET:HG3	40:r:209:LEU:HB2	1.86	0.57
22:Y:94:ASP:OD1	22:Y:99:ILE:HB	2.04	0.57
28:e:77:ASP:OD1	28:e:78:LYS:N	2.38	0.57
30:g:19:GLU:H	30:g:19:GLU:CD	2.13	0.57
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.87	0.57
33:j:95:LEU:HD13	41:s:302:MET:HG3	1.87	0.57
11:L:111:LEU:HD11	13:N:126:PRO:HG2	1.87	0.57
32:i:247:THR:O	32:i:251:MET:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:103:ALA:HB2	48:j:201:PEE:H23	1.86	0.57
35:l:170:GLN:HE22	35:l:235:SER:CB	2.17	0.56
39:p:120:ALA:O	39:p:124:GLN:HG2	2.03	0.56
7:H:94:MET:HE2	7:H:97:TRP:CE3	2.38	0.56
33:j:61:THR:HG21	33:j:105:GLU:OE1	2.06	0.56
35:l:173:LEU:HD12	40:r:405:LEU:HD21	1.87	0.56
44:w:132:GLN:NE2	44:w:166:ASP:OD1	2.38	0.56
1:A:115:VAL:HG22	1:A:248:VAL:HG21	1.87	0.56
12:M:94:MET:HE2	12:M:100:TRP:HH2	1.71	0.56
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.40	0.56
34:k:13:ALA:HB1	55:m:201:CDL:H821	1.86	0.56
35:l:373:LEU:HD13	35:l:431:PHE:HE2	1.69	0.56
41:s:224:PHE:CD2	52:s:403:UQ:H152	2.40	0.56
43:v:46:MET:HE3	43:v:56:ARG:CD	2.35	0.56
7:H:44:TYR:O	7:H:48:THR:HG22	2.05	0.56
12:M:389:THR:O	12:M:390:THR:OG1	2.23	0.56
17:S:54:ILE:HD11	31:h:106:PRO:HB3	1.86	0.56
21:W:70:ALA:HB2	42:u:125:LEU:HD13	1.88	0.56
40:r:133:ILE:HD11	40:r:231:LEU:HD11	1.88	0.56
32:i:276:ILE:HG21	48:r:501:PEE:H7	1.86	0.56
39:p:101:GLU:OE1	39:p:122:ARG:NH2	2.39	0.56
39:p:151:THR:HG22	39:p:153:ALA:H	1.71	0.56
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.37	0.56
12:M:135:GLY:HA3	12:M:242:PRO:HG2	1.84	0.56
18:T:122:HIS:CD2	18:T:123:HIS:NE2	2.73	0.56
21:W:73:PRO:HA	42:u:44:MET:HE3	1.88	0.56
44:w:87:PRO:O	44:w:142:GLN:NE2	2.36	0.56
1:A:89:GLY:O	47:A:503:NAI:H2N	2.06	0.56
32:i:298:TYR:O	32:i:303:THR:OG1	2.23	0.56
35:l:170:GLN:HE21	35:l:235:SER:CB	2.16	0.56
12:M:405:THR:OG1	12:M:410:GLU:OE1	2.20	0.56
32:i:30:TRP:O	32:i:34:GLU:HG2	2.05	0.56
6:X:82:ARG:HD3	22:Y:44:TYR:CE1	2.39	0.56
10:K:100:GLN:NE2	14:O:69:ASN:O	2.39	0.55
40:r:403:THR:HA	40:r:406:TYR:CE2	2.40	0.55
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.88	0.55
16:Q:290:GLY:HA2	16:Q:294:ARG:HH21	1.71	0.55
25:b:31:ARG:HG3	25:b:31:ARG:O	2.06	0.55
44:w:248:GLU:O	44:w:251:GLU:OE1	2.24	0.55
3:C:175:TYR:HE1	13:N:78:ASP:HB2	1.72	0.55
6:G:97:LYS:HZ1	6:G:108:LEU:HA	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:212:LEU:HD21	49:r:502:PLX:H212	1.88	0.55
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.88	0.55
4:E:68:MET:HE1	50:G:201:8Q1:C30	2.37	0.55
12:M:313:LEU:HD22	13:N:141:SER:O	2.06	0.55
26:c:62:TYR:OH	26:c:74:ASP:O	2.22	0.55
32:i:72:MET:HE2	32:i:72:MET:HA	1.88	0.55
41:s:189:THR:HG22	41:s:234:MET:SD	2.47	0.55
55:s:402:CDL:H332	55:s:402:CDL:H182	1.87	0.55
12:M:690:THR:HG23	12:M:692:LYS:HG2	1.89	0.55
35:l:84:TYR:HE1	35:l:88:MET:CE	2.19	0.55
35:l:246:LEU:O	35:l:251:THR:OG1	2.22	0.55
40:r:373:ILE:HA	40:r:376:ILE:HD12	1.87	0.55
40:r:408:LEU:CD2	40:r:411:LEU:HD23	2.37	0.55
31:h:52:ALA:O	31:h:56:CYS:HB2	2.07	0.55
33:j:13:LEU:HA	33:j:16:LEU:CD2	2.37	0.55
40:r:375:LEU:C	40:r:375:LEU:CD2	2.80	0.55
44:w:246:LEU:HB2	44:w:247:PRO:HD3	1.87	0.55
4:E:19:PRO:HG3	4:E:23:ARG:HD3	1.87	0.55
41:s:84:THR:O	41:s:87:VAL:HG22	2.07	0.55
44:w:63:ASP:N	44:w:205:VAL:O	2.36	0.55
10:K:79:HIS:ND1	14:O:215:LYS:HE3	2.22	0.55
12:M:171:THR:HG23	12:M:173:MET:SD	2.47	0.55
4:E:96:VAL:O	4:E:96:VAL:CG1	2.53	0.55
11:L:109:ASN:ND2	11:L:111:LEU:O	2.40	0.55
6:X:77:GLU:OE1	6:X:77:GLU:N	2.38	0.55
25:b:121:LYS:O	25:b:121:LYS:HG3	2.07	0.55
35:l:180:ILE:HG23	40:r:397:GLY:HA3	1.88	0.55
40:r:259:TYR:O	40:r:263:MET:HG2	2.06	0.55
22:Y:89:PRO:HB3	43:v:103:GLU:CG	2.37	0.54
32:i:27:LEU:HD13	34:k:59:MET:HG2	1.87	0.54
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.88	0.54
38:o:8:PRO:HG3	38:o:14:LEU:HD12	1.89	0.54
44:w:171:GLU:O	44:w:175:ARG:HG2	2.07	0.54
1:A:102:MET:HE1	1:A:240:THR:HA	1.90	0.54
9:J:117:ARG:HA	9:J:120:VAL:HG12	1.88	0.54
9:J:345:LEU:HD23	9:J:349:ALA:HB2	1.89	0.54
6:X:104:PHE:CD2	6:X:115:GLN:NE2	2.75	0.54
22:Y:62:SER:OG	35:l:371:THR:OG1	2.25	0.54
55:l:702:CDL:H621	55:l:702:CDL:H432	1.89	0.54
44:w:108:LEU:HD12	44:w:331:PHE:HB2	1.89	0.54
2:B:144:ARG:NH2	13:N:128:SER:OG	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:16:LEU:O	33:j:20:ILE:HG22	2.08	0.54
35:l:170:GLN:HE21	35:l:235:SER:HB3	1.72	0.54
42:u:172:MET:HE3	55:u:201:CDL:OB4	2.07	0.54
1:A:73:PRO:O	1:A:77:LEU:HD22	2.06	0.54
36:m:53:GLY:O	36:m:56:VAL:HG13	2.07	0.54
1:A:337:MET:CE	1:A:342:LEU:HD11	2.37	0.54
2:B:72:MET:HE1	16:Q:260:GLU:OE1	2.08	0.54
9:J:322:VAL:HG13	9:J:323:HIS:CD2	2.38	0.54
22:Y:89:PRO:HA	22:Y:92:TRP:CE3	2.43	0.54
35:l:67:HIS:NE2	35:l:70:THR:OG1	2.35	0.54
1:A:145:GLY:C	1:A:149:MET:HE3	2.32	0.54
13:N:144:TYR:HD1	13:N:144:TYR:H	1.53	0.54
33:j:73:LEU:O	41:s:160:TYR:OH	2.23	0.54
55:l:702:CDL:H452	40:r:445:LEU:HB3	1.89	0.54
41:s:104:PHE:O	41:s:108:MET:HG2	2.07	0.54
35:l:401:MET:CE	35:l:482:MET:HB3	2.37	0.54
40:r:370:PRO:HG3	40:r:375:LEU:CD1	2.37	0.54
41:s:9:LEU:HD13	41:s:95:LEU:HD22	1.90	0.54
49:C:303:PLX:H381	49:C:303:PLX:H211	1.90	0.54
10:K:69:ASP:OD1	10:K:70:ASN:N	2.40	0.54
12:M:64:CYS:O	12:M:184:ARG:NH2	2.24	0.54
16:Q:107:ARG:NH2	33:j:115:GLU:O	2.37	0.54
12:M:121:LEU:HD13	16:Q:376:GLU:HG3	1.90	0.54
55:V:201:CDL:H512	35:l:580:GLN:HE22	1.73	0.54
33:j:88:LEU:HD13	41:s:309:ILE:HD12	1.88	0.54
40:r:191:SER:HB3	48:r:501:PEE:H3	1.89	0.54
17:S:11:VAL:HG11	41:s:19:PHE:CE1	2.43	0.54
18:T:122:HIS:NE2	18:T:123:HIS:CE1	2.77	0.54
6:X:122:MET:HE3	6:X:144:ILE:HG21	1.90	0.54
33:j:56:PHE:HB2	36:m:70:TYR:OH	2.07	0.54
42:u:83:THR:HA	42:u:86:TRP:CD1	2.42	0.54
25:b:34:VAL:O	39:p:114:MET:HG2	2.08	0.53
40:r:197:LEU:O	40:r:201:MET:HG2	2.06	0.53
40:r:237:LYS:HD2	40:r:316:MET:HG2	1.89	0.53
44:w:49:THR:HG21	44:w:291:PHE:HB3	1.90	0.53
2:B:200:GLU:HG3	13:N:88:ARG:HB2	1.88	0.53
3:C:142:TYR:CE2	16:Q:134:PRO:HB2	2.43	0.53
32:i:68:MET:HE1	34:k:37:MET:SD	2.47	0.53
33:j:59:ALA:HB1	36:m:66:VAL:HG13	1.90	0.53
3:C:41:SER:OG	3:C:42:ARG:N	2.42	0.53
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:76:LEU:H	16:Q:76:LEU:HD23	1.73	0.53
6:X:82:ARG:HD2	22:Y:44:TYR:CE1	2.42	0.53
35:l:199:GLN:OE1	35:l:199:GLN:N	2.39	0.53
1:A:159:ARG:NH2	14:O:176:CYS:O	2.39	0.53
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.26	0.53
14:O:38:LEU:O	14:O:124:ARG:NH2	2.41	0.53
16:Q:60:HIS:O	16:Q:62:LYS:NZ	2.42	0.53
17:S:57:VAL:HG12	17:S:57:VAL:O	2.08	0.53
26:c:145:TRP:O	26:c:149:ILE:HG22	2.08	0.53
32:i:261:MET:CE	32:i:336:VAL:HG12	2.30	0.53
39:p:122:ARG:O	39:p:126:LYS:HG3	2.08	0.53
1:A:414:GLU:OE1	12:M:152:ARG:NH1	2.33	0.53
35:l:88:MET:HE1	35:l:472:ILE:HG13	1.91	0.53
36:m:57:PHE:O	36:m:61:LEU:HG	2.08	0.53
40:r:251:ASN:ND2	40:r:304:GLN:OE1	2.35	0.53
12:M:338:VAL:O	12:M:363:SER:OG	2.23	0.53
4:E:19:PRO:HB3	11:L:53:ILE:HD13	1.89	0.53
40:r:129:THR:HG21	40:r:235:LEU:HD11	1.90	0.53
40:r:139:GLN:OE1	40:r:340:ARG:NH2	2.42	0.53
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.91	0.53
35:l:136:ASN:HA	35:l:197:ASP:HA	1.91	0.53
36:m:53:GLY:HA2	36:m:56:VAL:HG12	1.91	0.53
1:A:109:ARG:NH1	1:A:237:GLY:O	2.42	0.53
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.44	0.53
21:W:98:MET:HE3	21:W:101:VAL:HG21	1.90	0.53
30:g:51:ARG:HD3	32:i:322:GLN:HG2	1.90	0.53
35:l:264:TYR:O	35:l:268:GLU:HG3	2.09	0.53
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.91	0.53
40:r:302:MET:HE2	40:r:302:MET:HA	1.90	0.53
1:A:73:PRO:O	1:A:77:LEU:CD2	2.56	0.52
13:N:60:ARG:HH22	13:N:95:ASP:HA	1.75	0.52
35:l:152:PHE:CE1	40:r:408:LEU:HD13	2.44	0.52
42:u:15:VAL:CG1	42:u:64:ASN:HD22	2.23	0.52
27:d:32:TYR:HE1	27:d:36:ILE:HD11	1.74	0.52
32:i:70:LEU:HD11	32:i:98:MET:HE3	1.91	0.52
35:l:419:THR:HA	35:l:422:TYR:CE2	2.45	0.52
55:m:201:CDL:H632	55:m:201:CDL:H802	1.91	0.52
37:n:47:ARG:HG3	37:n:47:ARG:HH11	1.73	0.52
1:A:129:GLU:HA	1:A:132:ARG:HG2	1.90	0.52
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.91	0.52
4:E:99:GLN:HE22	33:j:41:PHE:HA	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:85:THR:O	10:K:89:LEU:HD12	2.10	0.52
6:X:77:GLU:H	6:X:77:GLU:CD	2.17	0.52
32:i:222:SER:CB	32:i:237:MET:HE1	2.39	0.52
33:j:97:LEU:HD22	36:m:162:LEU:HD13	1.91	0.52
4:E:99:GLN:HE22	33:j:41:PHE:CA	2.23	0.52
32:i:142:LEU:HB3	32:i:194:LEU:HD21	1.91	0.52
41:s:55:LEU:HD23	41:s:221:ALA:HB2	1.91	0.52
4:E:70:ASN:ND2	50:G:201:8Q1:O4	2.42	0.52
17:S:11:VAL:HG11	41:s:19:PHE:CZ	2.45	0.52
32:i:87:THR:HG22	32:i:88:LYS:H	1.74	0.52
40:r:201:MET:HE3	40:r:201:MET:CA	2.38	0.52
42:u:60:GLY:O	42:u:63:VAL:HG12	2.10	0.52
4:E:37:ARG:HG2	6:G:120:MET:SD	2.50	0.52
34:k:14:ILE:HG12	55:m:201:CDL:H771	1.91	0.52
48:C:302:PEE:H67	49:C:303:PLX:H212	1.91	0.52
16:Q:47:PHE:HD1	16:Q:52:MET:HE1	1.75	0.52
31:h:65:GLU:OE1	31:h:71:LYS:HB2	2.10	0.52
43:v:17:PRO:HB3	43:v:105:GLU:HG2	1.92	0.52
1:A:316:ALA:HB3	1:A:357:MET:HE3	1.92	0.52
6:G:126:PHE:CE2	6:G:148:ILE:HD13	2.45	0.52
9:J:344:PRO:HG2	9:J:347:LEU:HG	1.91	0.52
25:b:25:ASP:OD2	39:p:125:TRP:NE1	2.25	0.52
32:i:270:MET:O	32:i:275:SER:HB3	2.10	0.52
5:F:26:ARG:NH1	5:F:26:ARG:CB	2.73	0.52
5:F:83:SER:O	5:F:87:VAL:HG13	2.10	0.52
16:Q:41:VAL:HG23	28:e:55:LEU:HD11	1.91	0.52
32:i:84:TRP:HH2	34:k:59:MET:HE2	1.75	0.51
32:i:310:ASN:HB2	44:w:309:THR:HG22	1.91	0.51
33:j:10:ASN:ND2	41:s:10:ILE:HD11	2.25	0.51
4:E:68:MET:HA	4:E:68:MET:CE	2.34	0.51
16:Q:134:PRO:HA	16:Q:137:ASP:HB2	1.91	0.51
32:i:79:LEU:HB2	34:k:47:ILE:HD13	1.91	0.51
35:l:172:ILE:O	35:l:176:ARG:HG2	2.09	0.51
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.93	0.51
3:C:167:PRO:HD3	16:Q:223:HIS:CD2	2.45	0.51
13:N:144:TYR:CE2	13:N:145:LYS:HD3	2.46	0.51
6:X:114:ASP:O	6:X:118:ILE:HD12	2.10	0.51
26:c:143:MET:HE3	35:l:407:TRP:CE3	2.45	0.51
19:U:63:MET:HB3	19:U:66:VAL:HB	1.93	0.51
20:V:29:GLY:O	20:V:63:SER:HB3	2.11	0.51
21:W:93:GLU:O	21:W:97:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:70:ALA:HB2	36:m:59:ILE:HD11	1.92	0.51
43:v:46:MET:HE3	43:v:56:ARG:CG	2.41	0.51
9:J:126:VAL:HG23	9:J:161:VAL:HG11	1.92	0.51
31:h:16:ARG:HH11	31:h:16:ARG:HG2	1.75	0.51
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.76	0.51
14:O:182:ASN:ND2	14:O:222:ARG:NH1	2.58	0.51
14:O:194:GLU:O	14:O:218:PRO:HA	2.10	0.51
21:W:60:LEU:HD13	42:u:98:ARG:HD2	1.91	0.51
24:a:60:SER:HB2	39:p:107:TRP:HA	1.93	0.51
28:e:83:ASP:OD1	28:e:83:ASP:C	2.53	0.51
16:Q:184:ILE:HG23	16:Q:203:MET:HB3	1.92	0.51
55:V:202:CDL:H331	38:o:88:LEU:HD11	1.93	0.51
21:W:80:ASP:OD2	42:u:47:ARG:NE	2.28	0.51
29:f:55:TRP:CZ3	29:f:58:LEU:HD23	2.45	0.51
34:k:44:SER:HB2	34:k:59:MET:HE1	1.92	0.51
36:m:82:VAL:HG12	36:m:83:TRP:H	1.76	0.51
1:A:71:LYS:HE3	14:O:249:LEU:HD12	1.93	0.51
7:H:116:ILE:HG21	11:L:96:LYS:HE2	1.92	0.51
15:P:172:ASP:OD2	15:P:187:ILE:N	2.37	0.51
25:b:81:ILE:HG23	48:b:201:PEE:H58	1.93	0.51
29:f:68:GLU:OE2	29:f:72:ARG:HG3	2.11	0.51
33:j:68:GLU:HG2	36:m:161:LEU:HD13	1.93	0.51
12:M:646:LEU:HD22	12:M:653:LEU:HD13	1.92	0.51
17:S:51:ASP:OD2	42:u:22:SER:OG	2.21	0.51
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.39	0.51
9:J:304:LEU:O	9:J:307:VAL:HG12	2.10	0.51
15:P:155:SER:OG	15:P:167:GLU:OE2	2.27	0.51
16:Q:387:GLU:OE2	16:Q:390:GLN:NE2	2.44	0.51
40:r:200:ILE:CG2	40:r:204:MET:CE	2.86	0.51
11:L:88:GLN:CG	12:M:136:GLU:O	2.59	0.50
17:S:30:THR:OG1	17:S:31:ASN:OD1	2.28	0.50
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.93	0.50
1:A:140:GLU:O	1:A:144:VAL:HG22	2.10	0.50
9:J:150:HIS:HB2	9:J:190:GLU:HG2	1.94	0.50
14:O:208:LEU:HD13	14:O:214:PRO:HD3	1.93	0.50
16:Q:172:VAL:CG2	16:Q:310:VAL:HG22	2.35	0.50
18:T:122:HIS:CD2	18:T:123:HIS:CD2	2.99	0.50
26:c:117:VAL:HG21	35:l:539:TYR:HB2	1.91	0.50
26:c:70:MET:HE1	38:o:86:THR:HG22	1.93	0.50
31:h:39:GLU:OE2	42:u:142:TYR:HB3	2.11	0.50
32:i:222:SER:HB3	32:i:237:MET:CE	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:210:ASN:HD21	35:l:272:LEU:HD23	1.76	0.50
40:r:1:MET:O	40:r:1:MET:HG3	2.11	0.50
19:U:24:ALA:HB2	48:j:201:PEE:H76	1.93	0.50
28:e:97:ILE:O	28:e:101:LEU:HB2	2.12	0.50
33:j:16:LEU:C	33:j:16:LEU:HD12	2.37	0.50
35:l:106:TRP:HD1	35:l:447:ASN:HD22	1.59	0.50
35:l:296:ASN:HD22	35:l:357:ARG:CZ	2.24	0.50
40:r:17:MET:HE3	55:w:401:CDL:H562	1.93	0.50
9:J:303:ARG:HB2	9:J:316:ARG:HH11	1.76	0.50
11:L:149:GLU:OE1	11:L:149:GLU:HA	2.11	0.50
32:i:257:LEU:HD22	32:i:334:THR:HG23	1.92	0.50
36:m:65:LEU:CD1	41:s:139:THR:CG2	2.83	0.50
48:r:501:PEE:H20	48:r:501:PEE:H49	1.93	0.50
17:S:35:GLU:HG2	42:u:93:GLY:H	1.77	0.50
35:l:221:ALA:HA	35:l:226:GLN:HG2	1.93	0.50
1:A:85:LEU:HD21	1:A:247:THR:HG23	1.94	0.50
12:M:476:LEU:HD21	12:M:481:LEU:HD21	1.94	0.50
31:h:61:ASP:OD1	31:h:61:ASP:C	2.54	0.50
38:o:116:ILE:HG13	38:o:121:LEU:HD22	1.92	0.50
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.47	0.50
43:v:42:THR:N	43:v:45:GLU:OE1	2.42	0.50
5:F:22:HIS:HD2	5:F:66:TRP:NE1	2.09	0.50
44:w:80:LYS:CD	44:w:270:VAL:HG21	2.42	0.50
4:E:109:GLU:OE2	4:E:109:GLU:HA	2.11	0.50
6:G:103:HIS:CG	6:G:139:MET:CE	2.82	0.50
20:V:9:TYR:CD1	20:V:9:TYR:C	2.90	0.50
21:W:121:MET:HB2	36:m:130:THR:HG22	1.93	0.50
24:a:74:TYR:O	24:a:78:THR:HG22	2.12	0.50
35:l:298:ILE:O	35:l:302:VAL:HG23	2.12	0.50
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.47	0.50
36:m:65:LEU:C	36:m:65:LEU:CD2	2.85	0.50
41:s:102:VAL:CG1	41:s:150:LEU:HD21	2.41	0.50
8:I:42:PRO:HB3	21:W:6:VAL:HG21	1.94	0.49
9:J:76:MET:HE1	9:J:254:LYS:HD2	1.94	0.49
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.93	0.49
11:L:111:LEU:HG	11:L:112:MET:HG2	1.94	0.49
33:j:69:ILE:HD13	41:s:147:ALA:HB3	1.94	0.49
36:m:93:PHE:CD2	36:m:97:LEU:HD11	2.47	0.49
42:u:58:GLU:HA	42:u:61:LYS:HG3	1.94	0.49
16:Q:47:PHE:HD1	16:Q:52:MET:CE	2.25	0.49
16:Q:96:ARG:HB3	16:Q:112:HIS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:35:GLU:HG2	42:u:93:GLY:N	2.27	0.49
55:l:703:CDL:H592	55:l:703:CDL:H762	1.93	0.49
5:F:73:GLN:OE1	5:F:74:GLU:N	2.46	0.49
9:J:61:ALA:HB3	9:J:82:VAL:HG13	1.94	0.49
14:O:98:MET:HE2	14:O:116:ALA:CB	2.41	0.49
1:A:118:ASP:OD1	1:A:157:TYR:HE2	1.95	0.49
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.94	0.49
4:E:99:GLN:NE2	33:j:41:PHE:CB	2.75	0.49
9:J:199:THR:OG1	9:J:258:ALA:O	2.26	0.49
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.93	0.49
21:W:68:ARG:HD2	36:m:135:PHE:HD2	1.78	0.49
6:X:131:PRO:HG2	6:X:134:ASP:HB2	1.93	0.49
26:c:116:ARG:HG2	48:l:704:PEE:H49	1.94	0.49
34:k:51:THR:O	34:k:53:PHE:N	2.41	0.49
35:l:241:THR:HG21	35:l:344:GLY:HA3	1.93	0.49
35:l:359:MET:O	35:l:436:ARG:NH2	2.46	0.49
4:E:99:GLN:NE2	33:j:41:PHE:HD1	2.10	0.49
7:H:59:VAL:HG22	7:H:68:LEU:HD21	1.94	0.49
13:N:21:ARG:O	13:N:25:ARG:HG2	2.12	0.49
22:Y:65:MET:SD	35:l:375:ILE:HG12	2.52	0.49
26:c:111:MET:HE2	35:l:542:LEU:CB	2.42	0.49
27:d:147:GLY:N	38:o:129:TYR:OH	2.30	0.49
35:l:561:ILE:HG13	35:l:562:LEU:H	1.78	0.49
42:u:63:VAL:HA	42:u:66:CYS:SG	2.52	0.49
1:A:337:MET:HE1	1:A:342:LEU:HD11	1.94	0.49
12:M:678:GLN:OE1	12:M:679:LEU:O	2.30	0.49
14:O:131:HIS:HD2	14:O:170:THR:HB	1.78	0.49
16:Q:51:VAL:HG23	16:Q:52:MET:O	2.13	0.49
16:Q:94:VAL:HG21	16:Q:116:LEU:HB2	1.95	0.49
32:i:147:GLN:CD	32:i:147:GLN:H	2.20	0.49
35:l:345:SER:OG	35:l:450:LEU:HD21	2.13	0.49
35:l:401:MET:HE1	35:l:481:THR:O	2.13	0.49
9:J:197:GLU:OE2	9:J:197:GLU:N	2.42	0.49
13:N:3:LEU:HD12	13:N:3:LEU:H	1.78	0.49
25:b:18:LEU:HD11	39:p:163:LEU:HD22	1.95	0.49
27:d:37:PHE:CD2	35:l:3:PRO:HB3	2.48	0.49
32:i:258:SER:HB2	32:i:336:VAL:HB	1.94	0.49
55:w:401:CDL:H401	55:w:401:CDL:H221	1.94	0.49
2:B:109:GLY:HA3	18:T:70:LEU:HD23	1.95	0.49
14:O:158:ILE:HB	14:O:162:GLU:HG3	1.94	0.49
14:O:182:ASN:HD22	14:O:222:ARG:NH1	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:182:ASN:HD21	16:Q:404:LYS:HZ2	1.61	0.49
16:Q:241:LEU:HD22	16:Q:348:LEU:HD23	1.93	0.49
33:j:73:LEU:HD13	41:s:103:LEU:HD11	1.95	0.49
33:j:90:MET:SD	36:m:151:THR:HG23	2.53	0.49
35:l:437:PHE:HB2	35:l:438:PRO:HD2	1.95	0.49
35:l:517:SER:HB3	55:l:703:CDL:HA32	1.94	0.49
40:r:73:LEU:HA	40:r:76:MET:HE2	1.94	0.49
40:r:122:PHE:O	40:r:125:THR:OG1	2.31	0.49
41:s:22:LEU:HD12	41:s:22:LEU:O	2.12	0.49
44:w:65:ASN:OD1	44:w:66:ILE:N	2.41	0.49
7:H:58:MET:HE1	7:H:71:GLN:C	2.38	0.49
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.78	0.49
22:Y:54:GLN:OE1	35:l:446:ASN:ND2	2.43	0.49
35:l:401:MET:HE1	35:l:482:MET:HB3	1.95	0.49
36:m:24:PRO:HG3	36:m:83:TRP:NE1	2.27	0.49
41:s:2:PHE:O	41:s:6:ILE:HG13	2.13	0.49
44:w:83:LEU:HD22	44:w:156:GLY:HA3	1.93	0.49
1:A:102:MET:HE1	1:A:240:THR:CA	2.42	0.48
13:N:78:ASP:OD1	13:N:78:ASP:N	2.44	0.48
16:Q:271:ARG:HH22	16:Q:445:ALA:HB1	1.77	0.48
30:g:48:ASN:ND2	30:g:54:PRO:O	2.46	0.48
55:l:703:CDL:HB21	39:p:30:TRP:HZ3	1.78	0.48
37:n:17:VAL:HG13	40:r:7:PRO:HB3	1.95	0.48
41:s:85:MET:HE3	41:s:108:MET:C	2.38	0.48
6:G:84:LEU:O	6:G:88:LYS:HG3	2.12	0.48
6:G:97:LYS:HZ3	6:G:108:LEU:CG	2.18	0.48
35:l:102:GLU:HA	35:l:105:MET:HE3	1.95	0.48
55:w:401:CDL:H342	55:w:401:CDL:H181	1.95	0.48
1:A:270:ASN:HD22	1:A:338:ASP:HB2	1.78	0.48
9:J:134:TRP:CZ2	9:J:311:GLU:HG3	2.48	0.48
12:M:367:CYS:HB3	12:M:533:GLY:O	2.14	0.48
31:h:27:HIS:CD2	36:m:141:MET:HE2	2.48	0.48
32:i:233:THR:HG23	32:i:237:MET:HE2	1.95	0.48
42:u:172:MET:HE3	55:u:201:CDL:HB31	1.94	0.48
6:G:85:TYR:CE1	6:G:89:LEU:HD11	2.49	0.48
9:J:75:ARG:NH2	15:P:215:GLU:OE1	2.47	0.48
15:P:64:TYR:OH	15:P:103:HIS:NE2	2.40	0.48
18:T:54:ARG:O	18:T:58:ARG:NH2	2.43	0.48
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.44	0.48
24:a:144:ALA:O	24:a:148:GLU:HG3	2.13	0.48
29:f:72:ARG:NH2	30:g:18:ASN:OD1	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:170:LEU:O	32:i:295:ARG:NH2	2.42	0.48
35:l:14:ILE:HD11	35:l:43:ALA:HA	1.95	0.48
5:F:51:LEU:O	5:F:53:ILE:HD11	2.14	0.48
12:M:419:ARG:NH1	12:M:439:THR:O	2.46	0.48
22:Y:52:ARG:O	22:Y:56:ILE:HG23	2.14	0.48
24:a:160:MET:CE	24:a:167:PRO:HD2	2.43	0.48
25:b:19:ARG:HA	39:p:171:VAL:HG13	1.95	0.48
31:h:35:ALA:O	31:h:39:GLU:HG2	2.12	0.48
34:k:35:GLY:HA3	36:m:20:PHE:CZ	2.48	0.48
36:m:12:ILE:HG12	55:s:402:CDL:H862	1.96	0.48
44:w:246:LEU:N	44:w:247:PRO:CD	2.76	0.48
26:c:96:ASP:OD1	26:c:96:ASP:N	2.47	0.48
40:r:369:LEU:O	40:r:372:SER:OG	2.26	0.48
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.95	0.48
9:J:291:TYR:HE1	9:J:293:LEU:HD13	1.78	0.48
13:N:42:ASP:OD2	13:N:48:TYR:OH	2.29	0.48
35:l:36:VAL:HG13	35:l:122:LEU:HD22	1.95	0.48
35:l:392:LYS:HE2	35:l:416:THR:HG23	1.95	0.48
40:r:73:LEU:HD22	40:r:103:GLN:OE1	2.14	0.48
44:w:340:SER:HB2	44:w:343:TYR:HD1	1.79	0.48
48:B:303:PEE:H17	41:s:184:MET:HE3	1.94	0.48
14:O:98:MET:HE2	14:O:116:ALA:HB1	1.96	0.48
21:W:54:ASN:ND2	41:s:156:MET:CE	2.76	0.48
26:c:56:ASN:HD22	38:o:43:LEU:HD21	1.78	0.48
35:l:152:PHE:CE1	40:r:408:LEU:CD1	2.97	0.48
55:l:702:CDL:H391	40:r:371:PRO:HD2	1.96	0.48
36:m:86:ASN:OD1	36:m:88:THR:N	2.45	0.48
42:u:83:THR:HA	42:u:86:TRP:NE1	2.29	0.48
1:A:192:ASP:CB	10:K:98:MET:SD	2.95	0.48
16:Q:182:ASN:ND2	16:Q:404:LYS:HZ1	2.06	0.48
24:a:134:GLU:OE1	37:n:57:TRP:NE1	2.37	0.48
30:g:56:VAL:HG21	40:r:17:MET:HE1	1.96	0.48
41:s:59:GLU:O	41:s:59:GLU:HG3	2.14	0.48
1:A:46:TYR:CE1	14:O:226:GLU:HA	2.49	0.47
12:M:476:LEU:HB3	12:M:515:ILE:HD13	1.96	0.47
35:l:559:GLU:HG2	40:r:214:LEU:HD13	1.95	0.47
44:w:209:VAL:HB	44:w:214:ILE:HD11	1.96	0.47
1:A:295:PRO:HD2	1:A:298:GLU:OE2	2.13	0.47
4:E:102:HIS:CD2	15:P:191:TYR:HB2	2.49	0.47
12:M:370:GLU:OE2	12:M:518:ARG:NE	2.45	0.47
6:X:155:TYR:HA	25:b:20:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:323:HIS:ND1	35:l:475:MET:SD	2.87	0.47
1:A:114:VAL:HG11	1:A:212:LEU:HD21	1.96	0.47
6:X:83:VAL:HG22	6:X:122:MET:CE	2.44	0.47
28:e:73:SER:O	28:e:83:ASP:OD2	2.32	0.47
5:F:57:GLU:O	12:M:651:PRO:HG2	2.14	0.47
11:L:84:ARG:HD2	11:L:91:VAL:HG12	1.95	0.47
12:M:557:ARG:NE	13:N:144:TYR:HD2	2.13	0.47
27:d:38:ASP:OD1	27:d:39:LEU:N	2.47	0.47
32:i:69:MET:HE3	32:i:97:MET:HE3	1.96	0.47
35:l:525:MET:HE2	35:l:528:TYR:HE1	1.80	0.47
1:A:296:LEU:HD11	1:A:317:VAL:HG11	1.95	0.47
14:O:38:LEU:HD23	14:O:42:ARG:HH21	1.78	0.47
15:P:75:GLN:HB3	15:P:87:PHE:CD1	2.49	0.47
27:d:159:GLN:O	27:d:163:MET:HG3	2.15	0.47
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.95	0.47
1:A:122:PRO:HG2	1:A:322:SER:HB3	1.97	0.47
3:C:96:SER:HB2	41:s:209:SER:HB2	1.96	0.47
31:h:51:ARG:NE	31:h:55:GLU:OE1	2.35	0.47
3:C:51:ASP:OD1	3:C:190:LEU:HB2	2.14	0.47
3:C:196:ARG:NH1	51:J:401:NDP:O3X	2.48	0.47
21:W:98:MET:HE3	21:W:101:VAL:CG2	2.44	0.47
27:d:14:PRO:C	27:d:15:ARG:HG3	2.39	0.47
32:i:96:THR:HG22	32:i:100:MET:HE2	1.97	0.47
33:j:68:GLU:HG3	33:j:98:LEU:HD13	1.96	0.47
49:j:202:PLX:H121	36:m:152:TRP:HZ3	1.79	0.47
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.49	0.47
35:l:592:LEU:O	35:l:596:MET:HG3	2.14	0.47
44:w:353:TRP:CZ3	44:w:354:LEU:HD13	2.49	0.47
6:X:87:LEU:HD12	6:X:93:ILE:HD12	1.97	0.47
22:Y:43:ARG:HB3	22:Y:46:GLN:HB2	1.96	0.47
44:w:132:GLN:HE22	57:w:402:ADP:HN62	1.62	0.47
4:E:99:GLN:HE22	33:j:41:PHE:HB3	1.77	0.47
5:F:19:ILE:HD11	5:F:65:LEU:HD11	1.97	0.47
5:F:42:VAL:HG13	12:M:671:LEU:HD12	1.96	0.47
9:J:120:VAL:HG11	9:J:155:VAL:HG12	1.97	0.47
9:J:231:LEU:HD21	9:J:292:PRO:HD3	1.96	0.47
20:V:118:MET:HE2	20:V:118:MET:HB3	1.76	0.47
20:V:124:LEU:HD11	48:r:501:PEE:H64	1.96	0.47
25:b:32:GLU:N	25:b:33:PRO:CD	2.78	0.47
38:o:68:TRP:HZ3	40:r:343:ILE:HD11	1.80	0.47
41:s:81:LEU:CD1	41:s:111:LEU:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:15:VAL:CG2	42:u:61:LYS:HD3	2.45	0.47
35:l:60:GLU:HG2	35:l:83:ASP:CA	2.37	0.47
40:r:325:MET:HE1	40:r:441:ILE:HB	1.96	0.47
44:w:77:ILE:HD11	44:w:269:VAL:HG11	1.97	0.47
1:A:132:ARG:O	10:K:75:ASN:ND2	2.47	0.46
1:A:174:ARG:O	1:A:178:GLU:HG3	2.14	0.46
1:A:255:CYS:O	14:O:246:GLN:NE2	2.47	0.46
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.45	0.46
7:H:48:THR:HA	7:H:51:ILE:HG12	1.96	0.46
8:I:108:LYS:HD2	8:I:108:LYS:HA	1.76	0.46
16:Q:217:VAL:HG22	16:Q:226:TYR:CZ	2.49	0.46
19:U:41:TYR:O	19:U:45:ILE:HG13	2.15	0.46
22:Y:87:PRO:HG2	43:v:99:MET:HE2	1.97	0.46
22:Y:99:ILE:HD11	43:v:107:ARG:HG3	1.96	0.46
40:r:281:ASP:OD2	40:r:340:ARG:NH1	2.48	0.46
11:L:78:ARG:NH2	12:M:249:GLU:OE1	2.45	0.46
12:M:698:ASP:OD1	12:M:701:SER:OG	2.23	0.46
36:m:2:THR:C	36:m:3:MET:HG3	2.40	0.46
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.97	0.46
3:C:125:PRO:HG2	41:s:58:LYS:HE3	1.97	0.46
3:C:142:TYR:HE2	16:Q:134:PRO:HB2	1.80	0.46
9:J:262:THR:O	9:J:333:PRO:HD2	2.15	0.46
12:M:33:GLU:HG3	12:M:42:MET:HE2	1.96	0.46
17:S:31:ASN:ND2	17:S:36:LYS:HB2	2.30	0.46
20:V:140:LYS:HG3	20:V:141:VAL:HG23	1.98	0.46
55:a:201:CDL:H361	55:a:201:CDL:H392	1.51	0.46
28:e:106:VAL:HA	28:e:109:LEU:HG	1.96	0.46
40:r:263:MET:HE2	40:r:263:MET:CA	2.45	0.46
44:w:116:LYS:HB2	44:w:116:LYS:HE3	1.71	0.46
1:A:395:VAL:HG11	1:A:412:LEU:HD13	1.96	0.46
12:M:47:THR:HG23	12:M:51:GLN:HB2	1.96	0.46
14:O:201:ILE:O	14:O:205:ILE:HG12	2.16	0.46
16:Q:241:LEU:HG	21:W:9:ASP:OD2	2.15	0.46
17:S:50:ARG:O	17:S:54:ILE:HG12	2.16	0.46
23:Z:49:GLU:OE2	39:p:34:ARG:NH2	2.45	0.46
32:i:233:THR:HG23	32:i:237:MET:CE	2.45	0.46
55:l:702:CDL:H342	55:l:702:CDL:H372	1.57	0.46
36:m:168:ILE:O	36:m:172:THR:HG23	2.16	0.46
40:r:328:CYS:HB3	40:r:437:MET:HE1	1.97	0.46
6:G:132:ASP:O	6:G:133:ILE:HD12	2.16	0.46
13:N:49:TYR:CE2	13:N:63:ILE:HG12	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:145:THR:OG1	15:P:146:TYR:N	2.49	0.46
16:Q:127:LYS:O	16:Q:419:PRO:HD2	2.15	0.46
16:Q:292:MET:HG3	16:Q:431:HIS:CE1	2.51	0.46
55:V:202:CDL:H792	55:V:202:CDL:H761	1.63	0.46
22:Y:48:PRO:O	22:Y:50:LEU:CD1	2.63	0.46
48:b:201:PEE:H3	49:r:503:PLX:H1C3	1.97	0.46
41:s:22:LEU:CD1	41:s:37:PRO:HG2	2.45	0.46
43:v:51:LEU:HD21	43:v:64:ILE:HG12	1.96	0.46
2:B:189:LYS:HB2	13:N:124:TYR:CE2	2.50	0.46
14:O:59:ASN:ND2	14:O:89:GLN:HG3	2.30	0.46
15:P:81:PHE:CD1	15:P:83:GLU:HG3	2.49	0.46
16:Q:443:MET:HE1	33:j:113:TRP:CZ3	2.51	0.46
20:V:140:LYS:HE2	32:i:273:ASN:HA	1.97	0.46
6:X:122:MET:CE	6:X:144:ILE:HG21	2.45	0.46
28:e:51:PRO:HB2	28:e:53:ILE:HG12	1.98	0.46
48:j:201:PEE:H33	41:s:302:MET:HE1	1.96	0.46
34:k:2:PRO:HD2	34:k:5:TYR:CD2	2.51	0.46
41:s:102:VAL:HG12	41:s:150:LEU:HD21	1.96	0.46
43:v:46:MET:CE	43:v:56:ARG:HB3	2.46	0.46
44:w:256:LEU:HD11	44:w:276:LEU:HD11	1.96	0.46
13:N:49:TYR:HE2	13:N:63:ILE:HG12	1.80	0.46
14:O:188:ILE:HG21	14:O:208:LEU:HD21	1.98	0.46
16:Q:150:ALA:HB2	16:Q:400:ILE:HG12	1.98	0.46
16:Q:271:ARG:HD2	41:s:279:ARG:O	2.15	0.46
17:S:12:MET:HE1	41:s:20:LEU:HA	1.96	0.46
6:X:82:ARG:HD2	22:Y:44:TYR:OH	2.16	0.46
24:a:184:LYS:HB3	31:h:30:PRO:HB3	1.97	0.46
35:l:237:MET:HE2	35:l:299:LYS:HB3	1.98	0.46
41:s:63:PRO:HB2	41:s:66:SER:HB3	1.98	0.46
41:s:87:VAL:N	41:s:88:PRO:HD2	2.31	0.46
2:B:208:ASP:OD2	2:B:212:ARG:NE	2.48	0.46
4:E:45:ASN:O	4:E:49:LEU:HG	2.16	0.46
8:I:27:ARG:HG3	8:I:27:ARG:HH11	1.81	0.46
12:M:483:ARG:NH2	12:M:682:ASP:HB3	2.31	0.46
16:Q:40:ASP:OD1	16:Q:40:ASP:N	2.43	0.46
25:b:88:TYR:CE1	27:d:49:ARG:HG2	2.51	0.46
48:b:201:PEE:H33	48:b:201:PEE:H40	1.75	0.46
26:c:78:LEU:HB2	26:c:106:HIS:HD2	1.81	0.46
32:i:113:PHE:CD1	35:l:587:TYR:CE1	3.03	0.46
32:i:283:ALA:HB1	40:r:158:LEU:HD22	1.98	0.46
33:j:53:MET:CE	33:j:56:PHE:HA	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:557:TRP:O	35:l:561:ILE:HG12	2.16	0.46
38:o:37:LEU:HD13	39:p:8:ALA:HA	1.96	0.46
44:w:224:PRO:O	44:w:228:LYS:NZ	2.49	0.46
1:A:129:GLU:CD	14:O:225:CYS:HG	2.24	0.46
4:E:114:ARG:HH21	9:J:45:LYS:HB3	1.81	0.46
40:r:59:ASP:CG	40:r:245:ARG:HH22	2.24	0.46
41:s:267:THR:O	41:s:271:LEU:HG	2.16	0.46
42:u:18:VAL:HG12	42:u:20:VAL:HG22	1.97	0.46
44:w:300:ASN:OD1	44:w:300:ASN:C	2.59	0.46
1:A:33:GLY:O	1:A:302:LYS:NZ	2.48	0.46
2:B:168:VAL:HG21	2:B:201:ILE:HG21	1.98	0.46
5:F:73:GLN:OE1	5:F:75:LYS:HE3	2.16	0.46
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.48	0.46
55:V:202:CDL:H771	38:o:91:ALA:HB2	1.98	0.46
24:a:99:ALA:HB2	27:d:62:TYR:HD2	1.81	0.46
29:f:43:LYS:HA	29:f:46:LEU:CD2	2.45	0.46
49:g:201:PLX:H361	49:g:201:PLX:H311	1.97	0.46
35:l:237:MET:HE1	35:l:244:SER:CB	2.46	0.46
36:m:53:GLY:O	36:m:56:VAL:CG1	2.63	0.46
55:m:201:CDL:H632	55:m:201:CDL:H602	1.63	0.46
41:s:85:MET:HE1	41:s:109:SER:CA	2.46	0.46
16:Q:102:SER:HB3	16:Q:107:ARG:HE	1.81	0.45
48:Q:501:PEE:H37	48:Q:501:PEE:H60	1.97	0.45
36:m:1:MET:HA	36:m:4:TYR:CE1	2.52	0.45
41:s:91:MET:O	41:s:91:MET:HG3	2.16	0.45
44:w:129:TYR:CD1	44:w:183:CYS:HB3	2.51	0.45
55:w:401:CDL:H473	55:w:401:CDL:H191	1.99	0.45
1:A:258:GLY:HA2	14:O:246:GLN:CD	2.41	0.45
9:J:115:SER:O	9:J:119:VAL:HG23	2.16	0.45
11:L:62:THR:HG23	11:L:72:ILE:HG12	1.98	0.45
14:O:44:THR:HG22	14:O:46:GLU:H	1.81	0.45
25:b:87:LYS:HD3	25:b:88:TYR:CZ	2.51	0.45
48:b:201:PEE:H34	55:l:702:CDL:H242	1.97	0.45
49:g:201:PLX:H102	49:g:201:PLX:H71	1.68	0.45
35:l:88:MET:HE2	35:l:472:ILE:HD11	1.98	0.45
35:l:457:LEU:HD23	35:l:457:LEU:HA	1.83	0.45
38:o:4:PRO:HD2	39:p:73:TYR:CE1	2.51	0.45
40:r:306:PRO:HA	40:r:458:LEU:HG	1.99	0.45
44:w:197:GLU:HA	44:w:197:GLU:OE1	2.16	0.45
12:M:49:VAL:HB	12:M:91:ALA:HA	1.99	0.45
12:M:49:VAL:HG13	12:M:102:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:111:MET:CE	35:l:543:SER:N	2.79	0.45
55:s:402:CDL:H171	55:s:402:CDL:H141	1.55	0.45
2:B:96:ARG:HD2	16:Q:216:ARG:O	2.17	0.45
4:E:99:GLN:NE2	33:j:41:PHE:HA	2.31	0.45
5:F:32:GLY:HA2	5:F:35:ASP:OD2	2.15	0.45
6:G:78:ALA:O	6:G:81:ASP:OD1	2.34	0.45
9:J:143:ASP:OD1	9:J:147:LYS:HE3	2.16	0.45
9:J:365:GLU:H	9:J:365:GLU:CD	2.16	0.45
11:L:84:ARG:HB2	11:L:94:THR:HG21	1.99	0.45
12:M:150:ARG:NH1	16:Q:359:ASP:OD1	2.50	0.45
42:u:16:GLN:O	42:u:64:ASN:ND2	2.48	0.45
3:C:98:ARG:HH21	33:j:37:TYR:HB2	1.80	0.45
12:M:360:ARG:HG2	12:M:632:MET:HB2	1.97	0.45
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.97	0.45
15:P:163:ALA:O	15:P:167:GLU:HG3	2.16	0.45
17:S:1:MET:HE3	17:S:1:MET:HB3	1.77	0.45
24:a:78:THR:CG2	28:e:100:VAL:HG11	2.47	0.45
24:a:94:GLY:O	27:d:61:TYR:OH	2.29	0.45
24:a:135:LYS:HD2	37:n:32:ASP:HB2	1.98	0.45
33:j:18:VAL:HG12	48:s:401:PEE:H16	1.98	0.45
35:l:530:PRO:O	35:l:534:HIS:HB2	2.16	0.45
5:F:40:ARG:O	5:F:44:LEU:HD23	2.15	0.45
16:Q:271:ARG:NH2	16:Q:445:ALA:HB1	2.32	0.45
17:S:17:PHE:HE1	41:s:257:ILE:HA	1.82	0.45
6:X:85:TYR:CD2	23:Z:16:LEU:HD23	2.51	0.45
32:i:141:VAL:O	32:i:145:ILE:HG12	2.17	0.45
35:l:356:ILE:HA	35:l:359:MET:HG3	1.99	0.45
37:n:39:ARG:HG3	37:n:57:TRP:CE2	2.52	0.45
41:s:68:ILE:HG21	55:s:402:CDL:H111	1.97	0.45
41:s:227:GLU:OE2	41:s:227:GLU:HA	2.15	0.45
41:s:311:THR:HG22	41:s:311:THR:O	2.17	0.45
55:u:201:CDL:H742	55:u:201:CDL:H772	1.45	0.45
43:v:114:ARG:HH11	43:v:114:ARG:HB3	1.81	0.45
2:B:41:VAL:HA	8:I:113:LEU:HB3	1.99	0.45
14:O:206:ASP:HA	14:O:209:LYS:HG2	1.99	0.45
14:O:208:LEU:HD13	14:O:214:PRO:HD2	1.96	0.45
24:a:87:THR:O	24:a:91:VAL:HG13	2.16	0.45
35:l:286:LEU:HD13	35:l:411:MET:HE2	1.96	0.45
35:l:526:LEU:HD12	35:l:530:PRO:HG2	1.99	0.45
36:m:54:LEU:HB2	41:s:103:LEU:HD23	1.99	0.45
36:m:57:PHE:CE2	36:m:61:LEU:HD11	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:o:57:LEU:HD12	38:o:58:GLY:N	2.31	0.45
8:I:57:ARG:HH12	12:M:150:ARG:NH2	2.11	0.45
9:J:127:ILE:HD11	9:J:253:ILE:HD11	1.98	0.45
21:W:76:GLN:NE2	21:W:80:ASP:OD1	2.49	0.45
24:a:153:GLU:HB2	30:g:92:MET:HE2	1.95	0.45
31:h:101:LYS:HB3	31:h:101:LYS:HE2	1.78	0.45
32:i:238:PRO:HB2	55:w:401:CDL:HA31	1.99	0.45
35:l:210:ASN:O	35:l:214:ILE:HG12	2.17	0.45
43:v:25:PHE:CE1	43:v:112:LYS:HD2	2.52	0.45
9:J:56:ALA:HA	9:J:125:VAL:O	2.17	0.45
16:Q:263:THR:O	16:Q:327:TYR:OH	2.27	0.45
22:Y:43:ARG:NH2	22:Y:49:GLN:HB2	2.31	0.45
33:j:21:ALA:HB1	41:s:218:GLY:HA3	1.98	0.45
35:l:161:ARG:HH21	35:l:238:GLU:CD	2.25	0.45
35:l:325:ALA:O	35:l:329:ILE:HG13	2.17	0.45
55:m:201:CDL:H392	55:m:201:CDL:H362	1.82	0.45
2:B:176:SER:OG	3:C:179:GLN:OE1	2.34	0.45
48:B:303:PEE:H59	41:s:277:TYR:CE2	2.52	0.45
4:E:99:GLN:HE22	33:j:41:PHE:CB	2.30	0.45
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.99	0.45
16:Q:319:PRO:HG3	16:Q:335:GLU:HG3	1.99	0.45
26:c:143:MET:CE	35:l:407:TRP:CZ3	2.99	0.45
35:l:407:TRP:O	35:l:411:MET:HG2	2.17	0.45
41:s:123:SER:HB3	41:s:214:GLU:HG3	1.99	0.45
6:G:74:LEU:HD21	6:G:82:ARG:HH21	1.81	0.44
12:M:307:ILE:HG22	12:M:582:VAL:HG22	1.99	0.44
6:X:118:ILE:O	6:X:122:MET:HG2	2.17	0.44
6:X:128:PHE:HZ	6:X:148:ILE:HG12	1.81	0.44
25:b:4:TYR:HB2	25:b:9:LYS:HG2	1.99	0.44
12:M:222:ILE:HA	12:M:225:ILE:HG12	2.00	0.44
18:T:122:HIS:CD2	18:T:123:HIS:CE1	3.05	0.44
35:l:335:PHE:HB3	35:l:461:SER:OG	2.16	0.44
48:r:501:PEE:H74	48:r:501:PEE:H34	1.99	0.44
49:r:502:PLX:H51	49:r:502:PLX:H251	1.42	0.44
52:s:403:UQ:H262	52:s:403:UQ:H221	1.59	0.44
1:A:420:GLU:OE2	1:A:433:TRP:NE1	2.37	0.44
52:J:402:UQ:H221	52:J:402:UQ:H201	1.78	0.44
14:O:197:THR:OG1	14:O:200:ASP:HB2	2.18	0.44
15:P:53:VAL:O	15:P:57:GLN:HG3	2.17	0.44
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.52	0.44
30:g:85:TYR:CZ	42:u:165:SER:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:270:ASN:HB3	35:l:273:VAL:HG22	1.99	0.44
35:l:387:THR:HA	35:l:465:GLY:HA3	1.99	0.44
41:s:90:PRO:HB3	41:s:94:PRO:HD3	2.00	0.44
6:G:142:GLN:NE2	6:G:143:GLU:OE1	2.50	0.44
10:K:87:LEU:HD22	14:O:66:ILE:HD11	1.99	0.44
14:O:113:TYR:O	14:O:117:THR:HG23	2.18	0.44
15:P:201:ASP:OD1	15:P:201:ASP:C	2.60	0.44
6:X:103:HIS:CE1	6:X:105:MET:HB2	2.52	0.44
31:h:7:GLN:O	31:h:11:GLY:N	2.49	0.44
33:j:38:GLU:HB2	33:j:41:PHE:O	2.17	0.44
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.98	0.44
55:s:402:CDL:H362	55:s:402:CDL:H331	1.60	0.44
43:v:120:ALA:O	43:v:124:ARG:HG2	2.18	0.44
1:A:217:GLU:OE1	1:A:224:ARG:NH2	2.50	0.44
12:M:257:VAL:HG11	12:M:413:LEU:HB2	1.98	0.44
22:Y:88:ASP:HA	22:Y:89:PRO:HD3	1.80	0.44
24:a:98:LEU:HD11	28:e:120:ARG:HD3	1.99	0.44
49:g:201:PLX:H231	32:i:336:VAL:HG21	1.99	0.44
32:i:222:SER:O	32:i:224:ALA:N	2.51	0.44
35:l:399:VAL:HG12	35:l:409:LEU:HD13	1.99	0.44
35:l:428:PHE:HZ	35:l:509:TYR:HE2	1.66	0.44
40:r:233:ALA:HA	40:r:320:GLY:HA2	1.98	0.44
41:s:208:VAL:CG1	41:s:209:SER:N	2.70	0.44
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.99	0.44
3:C:92:VAL:HG21	52:s:403:UQ:H103	1.99	0.44
6:G:97:LYS:CE	6:G:107:ASP:O	2.65	0.44
12:M:454:ASP:OD1	12:M:460:HIS:N	2.50	0.44
24:a:160:MET:HE2	24:a:166:GLY:HA3	2.00	0.44
32:i:179:MET:SD	32:i:215:MET:HG2	2.58	0.44
36:m:173:ARG:HG3	36:m:173:ARG:HH11	1.82	0.44
38:o:81:ARG:HH11	38:o:81:ARG:HB3	1.83	0.44
41:s:28:LEU:CD1	41:s:275:ALA:HB2	2.48	0.44
41:s:62:ARG:NH2	48:s:401:PEE:O1P	2.31	0.44
41:s:317:GLN:OE1	41:s:317:GLN:HA	2.17	0.44
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.52	0.44
9:J:297:ALA:O	9:J:301:VAL:HG13	2.18	0.44
16:Q:84:PHE:HB2	16:Q:99:MET:HE2	2.00	0.44
16:Q:110:ASP:OD2	16:Q:112:HIS:NE2	2.51	0.44
20:V:50:LEU:O	20:V:53:VAL:HG12	2.18	0.44
21:W:105:LYS:HG2	42:u:4:ILE:HD11	1.98	0.44
26:c:56:ASN:ND2	38:o:43:LEU:HD21	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:139:LEU:HD11	32:i:190:MET:CE	2.48	0.44
34:k:88:ASP:OD1	34:k:88:ASP:C	2.61	0.44
38:o:115:LEU:HA	38:o:118:GLU:HG2	1.99	0.44
44:w:143:TYR:OH	44:w:199:LEU:O	2.28	0.44
44:w:354:LEU:HD12	44:w:354:LEU:HA	1.89	0.44
4:E:40:TYR:CB	6:G:120:MET:HE1	2.48	0.44
12:M:33:GLU:CG	12:M:42:MET:HE1	2.48	0.44
14:O:48:ASN:OD1	14:O:48:ASN:N	2.51	0.44
16:Q:251:PHE:O	16:Q:255:ILE:HG13	2.18	0.44
30:g:45:LEU:HD22	30:g:55:VAL:HG12	1.99	0.44
36:m:53:GLY:CA	36:m:56:VAL:HG12	2.48	0.44
41:s:225:MET:HG2	52:s:403:UQ:H212	2.00	0.44
44:w:91:ILE:HD12	44:w:91:ILE:H	1.83	0.44
1:A:133:HIS:HD2	10:K:75:ASN:HD22	1.66	0.44
1:A:141:GLY:HA2	1:A:252:PRO:HD3	1.99	0.44
11:L:115:SER:HB2	12:M:267:THR:HB	2.00	0.44
18:T:79:VAL:O	18:T:121:PRO:HD3	2.18	0.44
21:W:55:ARG:HH21	41:s:312:ALA:HB3	1.82	0.44
33:j:70:ALA:CB	36:m:55:MET:HE2	2.48	0.44
35:l:257:VAL:HG12	35:l:329:ILE:HD11	2.00	0.44
3:C:94:ARG:HH12	52:s:403:UQ:H8	1.81	0.43
7:H:94:MET:SD	7:H:99:PRO:HG3	2.58	0.43
12:M:51:GLN:HA	12:M:54:GLU:HG2	2.00	0.43
13:N:68:MET:HG2	13:N:115:PHE:CD2	2.53	0.43
15:P:161:LYS:HE3	15:P:161:LYS:HB3	1.81	0.43
35:l:228:GLY:HA3	48:l:704:PEE:H38	1.99	0.43
35:l:435:PRO:HB3	35:l:437:PHE:CZ	2.53	0.43
2:B:61:LEU:HD13	48:B:303:PEE:H27	1.99	0.43
48:B:303:PEE:H43	48:B:303:PEE:H37	1.74	0.43
5:F:24:CYS:O	5:F:30:SER:OG	2.26	0.43
8:I:91:GLU:C	8:I:92:LYS:HG3	2.43	0.43
9:J:116:ILE:O	9:J:120:VAL:HG12	2.18	0.43
16:Q:101:LEU:HD23	16:Q:106:VAL:HA	2.00	0.43
18:T:59:GLN:OE1	18:T:59:GLN:C	2.61	0.43
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.99	0.43
35:l:102:GLU:OE2	35:l:456:ARG:NH2	2.31	0.43
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.53	0.43
55:l:702:CDL:HA61	55:l:702:CDL:H312	1.53	0.43
36:m:45:LEU:CD2	36:m:50:SER:HA	2.48	0.43
7:H:11:LEU:HD12	7:H:14:LEU:HD22	1.99	0.43
12:M:547:LEU:HD11	12:M:579:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:163:ARG:NH1	30:g:102:ASP:OD2	2.39	0.43
34:k:35:GLY:HA3	36:m:20:PHE:HZ	1.83	0.43
55:m:201:CDL:H402	55:m:201:CDL:H432	1.82	0.43
5:F:23:LEU:HD21	5:F:55:ILE:CG2	2.48	0.43
5:F:62:GLN:HA	5:F:63:PRO:HD3	1.61	0.43
9:J:229:ILE:HD13	9:J:295:HIS:ND1	2.34	0.43
13:N:142:THR:HA	13:N:143:PRO:HD3	1.82	0.43
20:V:13:PRO:HB2	20:V:16:THR:HG23	2.01	0.43
28:e:127:LYS:HB2	28:e:127:LYS:HE3	1.76	0.43
36:m:2:THR:C	36:m:4:TYR:H	2.25	0.43
12:M:68:ARG:HE	12:M:284:GLU:HB2	1.84	0.43
13:N:63:ILE:HD13	13:N:63:ILE:N	2.34	0.43
27:d:138:ALA:HB1	28:e:137:MET:HG2	2.00	0.43
40:r:156:GLY:HA2	48:r:501:PEE:H38	2.00	0.43
41:s:18:ALA:HB1	41:s:48:PRO:HB3	2.00	0.43
52:s:403:UQ:H152	52:s:403:UQ:H121	1.74	0.43
42:u:12:ASP:O	42:u:61:LYS:NZ	2.38	0.43
55:w:401:CDL:H841	55:w:401:CDL:H872	1.78	0.43
4:E:90:LEU:O	4:E:94:ILE:HG13	2.18	0.43
5:F:45:LYS:HG2	12:M:671:LEU:HD21	2.00	0.43
5:F:46:LYS:HE3	5:F:46:LYS:HB3	1.74	0.43
28:e:74:HIS:HB2	28:e:83:ASP:OD1	2.18	0.43
32:i:47:ASN:OD1	32:i:47:ASN:O	2.36	0.43
35:l:596:MET:HB3	35:l:596:MET:HE3	1.86	0.43
36:m:104:VAL:O	36:m:108:LEU:HD12	2.18	0.43
1:A:325:PRO:HG3	1:A:433:TRP:HB3	2.00	0.43
5:F:53:ILE:HD12	5:F:53:ILE:N	2.34	0.43
7:H:93:LYS:HB3	7:H:97:TRP:CZ3	2.53	0.43
8:I:12:ARG:HB3	8:I:20:LEU:HD12	1.99	0.43
12:M:33:GLU:HG3	12:M:42:MET:HE1	2.00	0.43
12:M:334:GLN:HA	12:M:361:VAL:HG13	2.00	0.43
13:N:144:TYR:CD1	13:N:144:TYR:N	2.87	0.43
29:f:43:LYS:HE3	29:f:43:LYS:HB3	1.84	0.43
34:k:23:ARG:HG2	55:m:201:CDL:HB32	2.01	0.43
34:k:32:CYS:HA	36:m:20:PHE:HE1	1.83	0.43
35:l:316:THR:HA	35:l:319:ILE:HG12	2.00	0.43
55:m:201:CDL:H732	55:m:201:CDL:H762	1.85	0.43
40:r:243:MET:HB3	40:r:301:ILE:HG21	2.00	0.43
49:r:502:PLX:H112	49:r:502:PLX:H141	1.80	0.43
41:s:28:LEU:HD13	41:s:275:ALA:HB2	2.00	0.43
43:v:35:LYS:HA	43:v:35:LYS:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:140:CYS:HB2	6:G:143:GLU:OE2	2.18	0.43
9:J:163:LYS:NZ	9:J:253:ILE:O	2.40	0.43
12:M:574:ASP:OD2	12:M:702:ARG:NH2	2.33	0.43
18:T:47:ASP:O	18:T:52:ARG:NH1	2.52	0.43
20:V:88:LEU:HB2	49:r:502:PLX:H24	1.99	0.43
21:W:73:PRO:HG2	42:u:40:ASN:HB3	2.01	0.43
26:c:155:PRO:HG3	43:v:4:HIS:CE1	2.53	0.43
27:d:32:TYR:CE1	27:d:36:ILE:HD11	2.53	0.43
30:g:53:ARG:HD3	44:w:343:TYR:CZ	2.54	0.43
35:l:145:GLU:OE2	35:l:176:ARG:NH1	2.52	0.43
35:l:292:ALA:HB2	35:l:304:PHE:HB3	2.00	0.43
35:l:332:HIS:HA	35:l:335:PHE:CE2	2.54	0.43
35:l:410:LEU:HD12	35:l:410:LEU:HA	1.91	0.43
40:r:200:ILE:HG23	40:r:204:MET:HE2	1.98	0.43
42:u:106:LYS:HD2	42:u:106:LYS:HA	1.71	0.43
43:v:35:LYS:HE2	43:v:35:LYS:CA	2.43	0.43
9:J:157:LYS:NZ	9:J:197:GLU:OE1	2.51	0.43
9:J:272:LEU:HB2	9:J:275:ASP:OD2	2.17	0.43
26:c:111:MET:HE1	35:l:543:SER:CA	2.49	0.43
26:c:143:MET:HE3	35:l:407:TRP:CH2	2.54	0.43
27:d:163:MET:HE3	28:e:149:LEU:HD11	2.01	0.43
35:l:260:LEU:HD23	35:l:260:LEU:HA	1.78	0.43
35:l:338:MET:HB2	35:l:457:LEU:HB3	2.00	0.43
38:o:48:LEU:HB3	39:p:166:LEU:HD13	2.01	0.43
40:r:263:MET:HE2	40:r:263:MET:HA	2.01	0.43
42:u:15:VAL:HG22	42:u:61:LYS:HD3	2.00	0.43
44:w:52:LYS:HE2	44:w:52:LYS:HB3	1.78	0.43
55:w:401:CDL:H741	55:w:401:CDL:H772	1.57	0.43
1:A:256:ARG:O	14:O:246:GLN:HG2	2.19	0.43
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.76	0.43
3:C:53:LEU:HD22	49:C:303:PLX:H322	2.01	0.43
3:C:69:LEU:HB2	3:C:107:GLY:HA3	2.00	0.43
4:E:18:LYS:HG2	4:E:19:PRO:HD2	2.00	0.43
12:M:264:SER:OG	12:M:272:ARG:HG2	2.19	0.43
18:T:71:ILE:HD12	18:T:71:ILE:HA	1.84	0.43
23:Z:22:TRP:HZ3	23:Z:54:SER:HG	1.66	0.43
55:a:201:CDL:H401	27:d:44:PRO:HB3	2.00	0.43
26:c:43:LYS:HE3	26:c:43:LYS:HB2	1.60	0.43
31:h:32:ARG:HH21	34:k:51:THR:HG22	1.84	0.43
32:i:300:SER:OG	32:i:301:SER:N	2.52	0.43
55:l:703:CDL:H521	55:l:703:CDL:HB61	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:103:MET:HE2	36:m:103:MET:HB2	1.97	0.43
40:r:266:MET:HB3	40:r:395:LEU:HD13	2.00	0.43
41:s:88:PRO:HG3	41:s:104:PHE:CD2	2.54	0.43
41:s:184:MET:HE1	41:s:296:LEU:HB3	2.00	0.43
42:u:47:ARG:HD2	42:u:47:ARG:HA	1.77	0.43
44:w:244:THR:C	44:w:247:PRO:HD2	2.44	0.43
1:A:109:ARG:HG2	11:L:166:TRP:CD1	2.53	0.42
7:H:77:ILE:O	7:H:81:ILE:HG13	2.18	0.42
27:d:28:ASN:HA	27:d:29:PRO:HD3	1.80	0.42
27:d:35:LYS:HA	27:d:38:ASP:OD2	2.19	0.42
36:m:3:MET:HB2	36:m:5:ILE:HG13	2.00	0.42
36:m:173:ARG:HG3	36:m:173:ARG:NH1	2.34	0.42
41:s:198:PHE:CD1	41:s:285:LEU:HD13	2.54	0.42
52:s:403:UQ:H102	52:s:403:UQ:H122	1.81	0.42
12:M:342:ALA:HB3	12:M:368:THR:HG22	2.00	0.42
13:N:132:LYS:NZ	13:N:136:GLU:OE1	2.52	0.42
18:T:82:ARG:NH2	18:T:103:ASP:OD2	2.52	0.42
24:a:56:ILE:HG22	24:a:58:LYS:HG2	2.02	0.42
35:l:170:GLN:OE1	35:l:534:HIS:NE2	2.49	0.42
41:s:253:GLU:OE1	41:s:253:GLU:N	2.45	0.42
43:v:122:MET:SD	43:v:122:MET:C	3.02	0.42
1:A:446:LEU:O	1:A:450:MET:HG3	2.19	0.42
2:B:93:LEU:HB3	13:N:93:MET:HE2	2.01	0.42
3:C:167:PRO:HG3	16:Q:222:MET:SD	2.59	0.42
9:J:303:ARG:HB2	9:J:316:ARG:HD3	2.01	0.42
14:O:125:LYS:HB2	14:O:125:LYS:HE3	1.69	0.42
6:X:120:MET:HE2	39:p:21:LYS:HG3	2.02	0.42
32:i:236:LYS:HG3	32:i:237:MET:HG3	2.02	0.42
35:l:124:PHE:CE1	35:l:252:MET:HB2	2.55	0.42
35:l:472:ILE:HG23	35:l:475:MET:HE3	2.00	0.42
48:l:701:PEE:H14	48:l:701:PEE:H20	1.77	0.42
43:v:53:LEU:HA	43:v:53:LEU:HD12	1.87	0.42
43:v:115:ARG:O	43:v:119:GLU:HG2	2.20	0.42
44:w:340:SER:HB2	44:w:343:TYR:CD1	2.53	0.42
2:B:156:GLY:O	2:B:160:GLU:HG3	2.19	0.42
4:E:27:GLU:HB3	4:E:30:ARG:NH2	2.34	0.42
4:E:62:LYS:O	4:E:66:MET:HG2	2.20	0.42
9:J:351:GLU:HG3	9:J:352:VAL:HG23	2.00	0.42
12:M:306:MET:HE3	12:M:314:LEU:HB3	2.01	0.42
16:Q:179:ARG:HD2	16:Q:340:SER:OG	2.19	0.42
16:Q:182:ASN:OD1	16:Q:403:PRO:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:53:TYR:OH	42:u:44:MET:HG3	2.19	0.42
21:W:128:ARG:NH1	31:h:97:HIS:O	2.52	0.42
22:Y:50:LEU:N	22:Y:50:LEU:CD1	2.82	0.42
26:c:164:ASN:HA	26:c:181:VAL:HB	2.00	0.42
28:e:129:ARG:HA	28:e:134:LEU:HD12	2.02	0.42
33:j:16:LEU:HD12	33:j:17:LEU:N	2.34	0.42
35:l:105:MET:HB3	35:l:449:LEU:HD22	2.02	0.42
37:n:26:TYR:CZ	37:n:30:ARG:HD2	2.55	0.42
40:r:80:SER:OG	40:r:226:ALA:HB2	2.19	0.42
41:s:29:GLY:HA2	41:s:34:ARG:HG3	2.01	0.42
55:s:402:CDL:H382	55:s:402:CDL:H212	2.01	0.42
1:A:326:LEU:HD23	1:A:367:ILE:HD11	2.02	0.42
4:E:99:GLN:NE2	33:j:41:PHE:CD1	2.86	0.42
5:F:23:LEU:HD12	5:F:23:LEU:O	2.19	0.42
9:J:106:MET:HE2	9:J:106:MET:HB3	1.86	0.42
13:N:2:GLU:HG2	13:N:3:LEU:HD12	2.01	0.42
16:Q:416:SER:OG	16:Q:417:SER:N	2.53	0.42
55:V:201:CDL:H431	55:V:201:CDL:H461	1.74	0.42
26:c:113:ILE:HD11	26:c:116:ARG:HD2	2.02	0.42
32:i:62:THR:HG21	32:i:114:TRP:CD1	2.54	0.42
35:l:472:ILE:CG2	35:l:475:MET:HE3	2.50	0.42
35:l:524:ASN:C	35:l:524:ASN:HD22	2.28	0.42
36:m:17:PHE:HA	36:m:20:PHE:CD2	2.55	0.42
40:r:106:LEU:HD13	40:r:234:VAL:HG11	2.01	0.42
40:r:109:THR:OG1	40:r:121:LEU:HB3	2.18	0.42
41:s:85:MET:CE	41:s:109:SER:N	2.83	0.42
1:A:337:MET:HA	1:A:337:MET:CE	2.40	0.42
4:E:68:MET:HE2	4:E:68:MET:CA	2.38	0.42
4:E:84:ILE:CG2	4:E:88:MET:HE3	2.47	0.42
6:G:115:GLN:O	6:G:119:ILE:HG12	2.20	0.42
8:I:64:MET:HE3	8:I:64:MET:HB2	1.92	0.42
51:J:401:NDP:O5D	51:J:401:NDP:H2N	2.19	0.42
55:N:201:CDL:H542	55:N:201:CDL:H511	1.75	0.42
15:P:132:LEU:HB2	15:P:141:ILE:HG22	2.00	0.42
21:W:120:MET:O	21:W:120:MET:HG2	2.19	0.42
49:a:202:PLX:H22	49:a:202:PLX:H1C3	1.78	0.42
29:f:43:LYS:O	29:f:46:LEU:HD23	2.19	0.42
35:l:107:TYR:HD2	35:l:108:MET:HG2	1.85	0.42
40:r:101:LEU:HD13	55:w:401:CDL:H441	2.02	0.42
41:s:200:LEU:HD13	41:s:282:TYR:HB3	2.02	0.42
43:v:25:PHE:HE1	43:v:112:LYS:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:HD22	1:A:332:CYS:HB3	2.01	0.42
45:C:301:SF4:S2	16:Q:138:ARG:HG2	2.60	0.42
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.55	0.42
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	2.02	0.42
28:e:72:ASP:OD1	28:e:72:ASP:N	2.50	0.42
49:g:201:PLX:H122	49:g:201:PLX:H91	1.53	0.42
32:i:250:SER:O	32:i:259:GLY:HA3	2.20	0.42
32:i:278:MET:HB2	32:i:279:PRO:HD3	2.01	0.42
55:m:201:CDL:HA22	55:m:201:CDL:OA6	2.20	0.42
41:s:49:ILE:H	41:s:49:ILE:HG12	1.64	0.42
44:w:329:GLN:O	44:w:333:GLU:OE1	2.37	0.42
9:J:228:LEU:O	9:J:292:PRO:HA	2.19	0.42
9:J:318:LYS:HD2	9:J:318:LYS:HA	1.86	0.42
10:K:78:HIS:HA	10:K:81:TYR:CD2	2.54	0.42
12:M:252:ASP:OD1	12:M:252:ASP:C	2.62	0.42
21:W:95:ALA:HB2	21:W:106:VAL:HG11	2.02	0.42
32:i:139:LEU:HD23	32:i:139:LEU:HA	1.89	0.42
36:m:98:MET:HE2	36:m:98:MET:HB3	1.80	0.42
55:m:201:CDL:H581	55:m:201:CDL:H611	1.68	0.42
40:r:263:MET:N	40:r:263:MET:CE	2.83	0.42
40:r:372:SER:HA	40:r:448:THR:HG21	2.02	0.42
44:w:62:VAL:HG12	44:w:70:LYS:HB2	2.02	0.42
4:E:22:SER:HB3	4:E:27:GLU:HB2	2.01	0.42
5:F:26:ARG:HH11	5:F:26:ARG:HB3	1.85	0.42
12:M:488:ALA:HB1	12:M:679:LEU:HG	2.02	0.42
55:V:202:CDL:H802	38:o:95:ILE:HD11	2.02	0.42
21:W:84:LEU:HD22	42:u:8:PRO:HD2	2.01	0.42
30:g:32:ARG:HB3	32:i:339:MET:HE1	2.01	0.42
32:i:252:GLY:HA3	32:i:290:LEU:HD13	2.02	0.42
33:j:51:PHE:O	36:m:73:ALA:HA	2.20	0.42
34:k:23:ARG:HG3	36:m:23:LYS:HE2	2.00	0.42
34:k:64:LEU:O	34:k:67:ALA:HB3	2.20	0.42
35:l:134:ALA:HB1	35:l:139:GLN:HB3	2.02	0.42
38:o:5:LYS:HE3	38:o:5:LYS:HB3	1.64	0.42
40:r:455:LEU:HD23	40:r:455:LEU:HA	1.87	0.42
18:T:64:GLU:H	18:T:64:GLU:CD	2.27	0.42
6:X:99:SER:OG	6:X:100:VAL:N	2.53	0.42
27:d:127:LYS:O	27:d:130:GLU:HG3	2.20	0.42
31:h:94:PRO:HG2	31:h:99:LEU:HD11	2.00	0.42
35:l:312:LEU:O	35:l:315:VAL:HG22	2.20	0.42
35:l:336:LYS:HD3	35:l:336:LYS:HA	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:7:PHE:O	36:m:11:THR:OG1	2.35	0.42
43:v:107:ARG:HE	43:v:107:ARG:HB3	1.74	0.42
1:A:276:PHE:CD2	1:A:352:ALA:HB1	2.55	0.41
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.54	0.41
10:K:82:SER:OG	10:K:83:THR:N	2.53	0.41
12:M:189:ILE:HD13	12:M:189:ILE:N	2.35	0.41
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.50	0.41
15:P:64:TYR:CZ	15:P:68:ILE:HD11	2.55	0.41
15:P:162:ALA:HB2	16:Q:286:TYR:C	2.45	0.41
20:V:106:ARG:HD2	20:V:106:ARG:HA	1.68	0.41
25:b:4:TYR:CD2	25:b:9:LYS:HD3	2.49	0.41
27:d:160:LYS:HE2	28:e:147:ILE:HG23	2.01	0.41
33:j:62:PHE:HE1	41:s:143:GLU:HB3	1.85	0.41
35:l:295:GLN:HB2	35:l:301:ILE:HG12	2.01	0.41
55:l:702:CDL:H352	40:r:361:VAL:HG13	2.01	0.41
48:r:501:PEE:H26	48:r:501:PEE:H32	1.93	0.41
42:u:77:HIS:ND1	42:u:115:LEU:HD21	2.35	0.41
5:F:36:PHE:HD2	5:F:37:ILE:HD13	1.85	0.41
6:G:84:LEU:HD22	6:G:98:LEU:HD21	2.02	0.41
15:P:94:ILE:HB	15:P:95:PRO:HD3	2.02	0.41
28:e:92:PHE:O	28:e:96:SER:HB2	2.20	0.41
28:e:105:PHE:O	28:e:109:LEU:HD23	2.20	0.41
32:i:203:LEU:O	32:i:207:ILE:HG12	2.20	0.41
40:r:82:SER:HB2	40:r:432:ARG:CZ	2.49	0.41
2:B:70:LEU:HB3	41:s:272:TRP:CZ2	2.55	0.41
6:G:126:PHE:N	6:G:126:PHE:CD1	2.88	0.41
21:W:76:GLN:HG2	42:u:44:MET:HE1	2.02	0.41
24:a:188:ASP:OD1	24:a:188:ASP:N	2.52	0.41
25:b:76:LEU:HD12	25:b:76:LEU:HA	1.90	0.41
25:b:122:GLU:OE2	25:b:122:GLU:HA	2.21	0.41
26:c:169:GLU:HG2	43:v:56:ARG:HH11	1.85	0.41
32:i:217:MET:HB2	32:i:326:LEU:HD13	2.03	0.41
34:k:4:VAL:O	34:k:8:ILE:HG12	2.20	0.41
35:l:49:VAL:HB	35:l:50:PRO:HD3	2.02	0.41
39:p:90:SER:O	39:p:90:SER:OG	2.29	0.41
41:s:184:MET:HE1	41:s:296:LEU:HG	2.02	0.41
41:s:315:PRO:HA	41:s:316:PRO:HD3	1.93	0.41
44:w:223:ASN:O	44:w:227:MET:HE2	2.19	0.41
44:w:258:TYR:CE2	44:w:269:VAL:HG22	2.55	0.41
1:A:445:GLU:OE1	1:A:449:ARG:NH1	2.53	0.41
49:C:303:PLX:H272	49:C:303:PLX:H302	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:382:ARG:HE	12:M:527:ASP:CG	2.28	0.41
12:M:689:LEU:HD23	12:M:689:LEU:HA	1.88	0.41
16:Q:198:THR:OG1	41:s:275:ALA:O	2.25	0.41
16:Q:312:ASP:OD1	16:Q:312:ASP:N	2.50	0.41
19:U:39:THR:O	19:U:43:ILE:HG13	2.20	0.41
31:h:84:ASP:HA	31:h:87:ILE:HG12	2.02	0.41
32:i:207:ILE:HG22	32:i:211:MET:HE2	2.02	0.41
35:l:313:MET:HG3	35:l:328:HIS:HD2	1.86	0.41
35:l:347:ILE:HG12	35:l:354:GLN:HG2	2.03	0.41
40:r:71:TRP:CH2	40:r:439:LEU:HD22	2.55	0.41
43:v:21:ARG:O	43:v:21:ARG:HG2	2.19	0.41
43:v:93:LEU:HA	43:v:96:VAL:HG22	2.02	0.41
44:w:59:VAL:HG22	44:w:157:VAL:HG22	2.03	0.41
1:A:44:ASN:HD21	1:A:47:GLY:HA2	1.85	0.41
5:F:45:LYS:HA	5:F:45:LYS:HD2	1.87	0.41
7:H:6:LYS:NZ	7:H:78:GLU:OE1	2.53	0.41
7:H:6:LYS:O	7:H:16:VAL:HG11	2.21	0.41
14:O:125:LYS:HG3	14:O:126:PRO:HD2	2.02	0.41
16:Q:105:MET:HE3	16:Q:105:MET:HB3	1.96	0.41
26:c:69:GLY:HA3	38:o:86:THR:HG21	2.01	0.41
32:i:59:TYR:O	32:i:63:GLN:HG2	2.20	0.41
32:i:78:LEU:HD13	32:i:84:TRP:CE2	2.56	0.41
48:j:201:PEE:H27	48:j:201:PEE:H21	1.70	0.41
36:m:137:SER:O	36:m:141:MET:HG2	2.20	0.41
38:o:27:PRO:O	38:o:31:LYS:HG2	2.21	0.41
40:r:198:ALA:HB2	48:r:501:PEE:H22	2.03	0.41
43:v:103:GLU:OE1	43:v:106:ARG:HD3	2.20	0.41
1:A:311:TRP:NE1	1:A:333:GLU:OE2	2.46	0.41
1:A:339:PHE:CE1	1:A:349:LEU:HD23	2.55	0.41
5:F:38:GLU:HA	12:M:667:GLN:HE21	1.85	0.41
6:G:84:LEU:HD23	6:G:84:LEU:HA	1.87	0.41
12:M:323:LEU:HD23	12:M:323:LEU:HA	1.93	0.41
12:M:362:ASP:O	12:M:362:ASP:CG	2.64	0.41
12:M:557:ARG:NH2	13:N:144:TYR:HE2	2.19	0.41
18:T:108:THR:HG22	18:T:119:ARG:HB3	2.02	0.41
30:g:55:VAL:HG21	55:w:401:CDL:HB61	2.03	0.41
33:j:17:LEU:HD23	33:j:17:LEU:HA	1.93	0.41
35:l:554:ASP:OD1	40:r:213:HIS:NE2	2.54	0.41
38:o:50:GLN:HG3	38:o:60:ILE:HD13	2.03	0.41
40:r:318:ALA:HB2	40:r:373:ILE:HG13	2.01	0.41
40:r:336:ARG:HH22	40:r:429:SER:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:r:502:PLX:H121	49:r:502:PLX:H92	1.63	0.41
41:s:102:VAL:HG11	41:s:150:LEU:HD11	2.03	0.41
41:s:273:ILE:HG23	41:s:277:TYR:HD2	1.86	0.41
44:w:118:TYR:OH	57:w:402:ADP:O2'	2.38	0.41
55:w:401:CDL:H591	55:w:401:CDL:H561	1.77	0.41
6:G:97:LYS:CE	6:G:108:LEU:HA	2.50	0.41
12:M:262:VAL:HG23	12:M:276:ARG:HB2	2.03	0.41
12:M:326:VAL:HG13	12:M:567:ILE:HD13	2.02	0.41
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.56	0.41
20:V:34:LEU:HD23	20:V:34:LEU:HA	1.91	0.41
6:X:79:ILE:HD13	6:X:148:ILE:HG22	2.03	0.41
24:a:114:LYS:HB2	24:a:114:LYS:HE3	1.79	0.41
25:b:110:ILE:HG22	25:b:113:THR:H	1.86	0.41
35:l:358:LYS:HG3	39:p:80:TYR:CE1	2.55	0.41
35:l:472:ILE:HG22	35:l:473:PRO:O	2.21	0.41
36:m:24:PRO:HG3	36:m:83:TRP:CE2	2.56	0.41
40:r:281:ASP:OD1	40:r:340:ARG:HB3	2.20	0.41
41:s:68:ILE:HD13	41:s:68:ILE:HA	1.85	0.41
55:u:201:CDL:H581	55:u:201:CDL:H552	1.59	0.41
43:v:114:ARG:NH1	43:v:114:ARG:HB3	2.36	0.41
44:w:234:LEU:HD12	44:w:234:LEU:H	1.85	0.41
1:A:78:GLY:O	1:A:82:THR:HG23	2.20	0.41
8:I:25:GLN:H	8:I:25:GLN:HG3	1.71	0.41
9:J:259:LYS:HD3	9:J:259:LYS:HA	1.90	0.41
12:M:275:PRO:HG3	12:M:286:ILE:HG12	2.02	0.41
12:M:379:THR:HG21	12:M:526:LEU:HD22	2.02	0.41
12:M:413:LEU:HD13	12:M:413:LEU:HA	1.94	0.41
16:Q:157:LYS:HE3	16:Q:157:LYS:HB2	1.88	0.41
21:W:105:LYS:HE3	42:u:4:ILE:HD11	2.03	0.41
25:b:24:LYS:HD2	25:b:24:LYS:O	2.20	0.41
26:c:136:PHE:CE1	55:l:703:CDL:H831	2.56	0.41
49:j:202:PLX:H121	36:m:152:TRP:CZ3	2.55	0.41
35:l:350:LEU:O	35:l:353:GLU:HB3	2.20	0.41
38:o:37:LEU:HD13	39:p:8:ALA:CA	2.51	0.41
39:p:98:LYS:HG2	39:p:178:PRO:HG3	2.02	0.41
41:s:88:PRO:HG3	41:s:104:PHE:HD2	1.85	0.41
42:u:38:LYS:O	42:u:42:GLU:HG3	2.21	0.41
2:B:72:MET:CE	16:Q:260:GLU:OE1	2.69	0.41
2:B:128:ILE:O	15:P:231:ARG:NH2	2.54	0.41
48:B:303:PEE:H58	48:B:303:PEE:H64	1.80	0.41
8:I:40:LYS:HB3	8:I:40:LYS:HE3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:56:VAL:O	12:M:56:VAL:HG22	2.21	0.41
12:M:77:MET:HE1	12:M:117:MET:HG2	2.03	0.41
12:M:340:ALA:HB3	12:M:366:LEU:HD23	2.02	0.41
12:M:347:ASP:OD1	12:M:347:ASP:N	2.37	0.41
12:M:402:LEU:HD23	12:M:475:VAL:HB	2.03	0.41
16:Q:188:THR:HB	16:Q:200:PHE:HA	2.03	0.41
17:S:35:GLU:HB3	42:u:91:TYR:O	2.21	0.41
6:X:83:VAL:HG22	6:X:122:MET:HE1	2.02	0.41
26:c:161:TYR:O	26:c:183:HIS:HE1	2.04	0.41
30:g:46:ILE:HD12	32:i:331:VAL:HG23	2.03	0.41
30:g:48:ASN:HD21	30:g:58:ALA:HB3	1.85	0.41
35:l:230:HIS:N	35:l:231:PRO:HD3	2.36	0.41
35:l:468:ILE:N	35:l:468:ILE:HD12	2.36	0.41
36:m:65:LEU:CD2	41:s:136:VAL:HG13	2.50	0.41
55:m:201:CDL:H711	55:m:201:CDL:H562	2.01	0.41
38:o:14:LEU:HD23	38:o:15:PRO:O	2.20	0.41
2:B:46:PRO:HB2	2:B:56:ARG:NH1	2.36	0.41
7:H:23:ARG:NH1	44:w:275:TYR:CD2	2.89	0.41
11:L:70:GLU:OE1	11:L:70:GLU:O	2.39	0.41
16:Q:392:PRO:HA	16:Q:393:PRO:HD3	2.00	0.41
20:V:107:SER:HB3	20:V:110:ILE:HD12	2.02	0.41
24:a:78:THR:HG23	28:e:100:VAL:HG11	2.03	0.41
28:e:84:LEU:HD21	28:e:88:ARG:NH2	2.36	0.41
30:g:85:TYR:CE2	42:u:165:SER:HB2	2.56	0.41
35:l:170:GLN:NE2	35:l:235:SER:OG	2.54	0.41
39:p:27:LEU:HD21	39:p:40:PHE:HB3	2.03	0.41
40:r:444:LEU:HD23	40:r:444:LEU:HA	1.89	0.41
43:v:92:HIS:O	43:v:96:VAL:HG13	2.21	0.41
9:J:129:LEU:HD23	9:J:167:ILE:HG13	2.02	0.40
12:M:462:PHE:CE1	12:M:466:LEU:HG	2.56	0.40
15:P:152:PRO:HB3	15:P:177:PHE:HD2	1.85	0.40
16:Q:197:MET:HE1	52:s:403:UQ:HM33	2.03	0.40
18:T:122:HIS:HD2	18:T:123:HIS:CD2	2.39	0.40
20:V:82:GLU:OE1	20:V:82:GLU:HA	2.21	0.40
22:Y:89:PRO:HB3	43:v:103:GLU:HB2	2.02	0.40
24:a:96:ALA:HB3	27:d:63:TYR:HD2	1.86	0.40
32:i:179:MET:HA	32:i:179:MET:HE3	2.02	0.40
33:j:13:LEU:HA	33:j:16:LEU:HD21	2.04	0.40
34:k:61:ILE:HD13	34:k:61:ILE:HA	1.88	0.40
34:k:64:LEU:HD23	34:k:64:LEU:HA	1.95	0.40
35:l:141:PHE:CE2	40:r:375:LEU:HD11	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:26:PRO:HB2	36:m:71:THR:CG2	2.52	0.40
41:s:204:GLU:HA	41:s:208:VAL:O	2.21	0.40
44:w:215:GLN:O	44:w:219:GLN:OE1	2.39	0.40
44:w:296:MET:HA	44:w:296:MET:HE2	2.03	0.40
1:A:337:MET:HE2	1:A:342:LEU:HD11	2.04	0.40
8:I:31:ILE:C	8:I:31:ILE:CD1	2.85	0.40
19:U:54:PRO:HD3	21:W:69:ILE:HD13	2.03	0.40
55:V:201:CDL:H601	55:V:201:CDL:H732	2.03	0.40
26:c:75:TYR:OH	26:c:105:ILE:O	2.35	0.40
31:h:65:GLU:OE2	31:h:65:GLU:CA	2.67	0.40
35:l:472:ILE:HD13	35:l:472:ILE:HA	1.92	0.40
36:m:101:PHE:C	36:m:101:PHE:CD1	3.00	0.40
41:s:89:LEU:HA	41:s:90:PRO:HD3	1.92	0.40
41:s:215:TYR:HD2	41:s:219:PRO:HB2	1.86	0.40
44:w:314:LEU:HB2	44:w:317:ILE:HG12	2.03	0.40
7:H:76:GLN:O	7:H:79:GLU:N	2.43	0.40
13:N:32:ASP:OD1	13:N:34:ARG:HG3	2.21	0.40
13:N:96:ASP:OD2	13:N:101:LYS:NZ	2.45	0.40
14:O:93:LEU:HD12	14:O:122:TYR:HB3	2.03	0.40
14:O:215:LYS:HE3	14:O:215:LYS:HB3	1.96	0.40
17:S:51:ASP:CG	42:u:22:SER:HG	2.23	0.40
24:a:170:GLN:HB2	30:g:6:GLY:O	2.20	0.40
28:e:112:TYR:HB3	40:r:45:LEU:HD13	2.03	0.40
28:e:116:GLU:OE2	28:e:116:GLU:N	2.48	0.40
32:i:230:LEU:HD11	32:i:244:MET:SD	2.62	0.40
35:l:120:TYR:OH	55:l:702:CDL:OA4	2.37	0.40
40:r:290:SER:HB3	40:r:319:HIS:HE2	1.86	0.40
40:r:370:PRO:HG3	40:r:375:LEU:HD12	2.04	0.40
41:s:274:ARG:HG3	41:s:274:ARG:HH11	1.87	0.40
1:A:213:ILE:HG23	1:A:235:VAL:HA	2.04	0.40
7:H:69:GLU:OE1	7:H:77:ILE:HG22	2.22	0.40
12:M:47:THR:O	12:M:96:VAL:HG22	2.20	0.40
12:M:347:ASP:HB3	12:M:594:ALA:HB1	2.03	0.40
13:N:3:LEU:O	13:N:6:VAL:HG22	2.22	0.40
14:O:137:THR:HG22	14:O:138:THR:H	1.85	0.40
14:O:159:LYS:HB3	14:O:159:LYS:HE2	1.90	0.40
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	2.04	0.40
16:Q:222:MET:HE2	16:Q:223:HIS:CE1	2.56	0.40
16:Q:424:ILE:HB	16:Q:463:ARG:HD3	2.03	0.40
26:c:161:TYR:HB3	26:c:166:LEU:HG	2.02	0.40
27:d:26:LEU:HA	27:d:27:PRO:HD3	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:217:MET:CE	32:i:323:MET:HG3	2.51	0.40
35:l:375:ILE:CD1	35:l:458:LEU:HD11	2.48	0.40
35:l:497:GLY:HA2	55:l:703:CDL:H562	2.04	0.40
55:l:702:CDL:H581	55:l:702:CDL:H611	1.72	0.40
55:l:703:CDL:H382	55:l:703:CDL:H351	1.83	0.40
4:E:81:LEU:HD23	4:E:81:LEU:HA	1.90	0.40
7:H:18:GLU:O	7:H:19:THR:OG1	2.38	0.40
7:H:87:GLU:OE1	15:P:104:THR:OG1	2.34	0.40
12:M:70:SER:O	12:M:184:ARG:NH1	2.48	0.40
16:Q:323:ARG:HE	16:Q:323:ARG:HB3	1.68	0.40
19:U:55:VAL:HG21	24:a:183:PRO:HB3	2.03	0.40
21:W:60:LEU:O	21:W:64:ASP:OD1	2.40	0.40
35:l:67:HIS:CD2	35:l:75:GLU:HG3	2.57	0.40
35:l:151:SER:OG	35:l:252:MET:SD	2.72	0.40
35:l:556:ILE:HD11	38:o:76:ILE:CG2	2.52	0.40
37:n:50:ARG:HB2	37:n:53:GLU:HG2	2.03	0.40
41:s:54:LYS:HE3	41:s:54:LYS:HB3	1.82	0.40
42:u:85:TYR:CE1	42:u:104:GLN:HB2	2.56	0.40
43:v:116:GLU:C	43:v:116:GLU:OE2	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/433 (100%)	420 (97%)	11 (3%)	0	100	100
2	B	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
3	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
4	E	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
5	F	84/86 (98%)	81 (96%)	2 (2%)	1 (1%)	10	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	G	86/88 (98%)	78 (91%)	7 (8%)	1 (1%)	10	35
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	102 (93%)	7 (6%)	1 (1%)	14	42
8	I	93/112 (83%)	85 (91%)	8 (9%)	0	100	100
9	J	340/342 (99%)	325 (96%)	14 (4%)	1 (0%)	36	65
10	K	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
11	L	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
12	M	688/690 (100%)	670 (97%)	18 (3%)	0	100	100
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
15	P	206/208 (99%)	200 (97%)	6 (3%)	0	100	100
16	Q	427/430 (99%)	411 (96%)	16 (4%)	0	100	100
17	S	68/70 (97%)	63 (93%)	5 (7%)	0	100	100
18	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
19	U	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
20	V	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
21	W	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
22	Y	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
23	Z	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
24	a	136/138 (99%)	132 (97%)	4 (3%)	0	100	100
25	b	94/126 (75%)	90 (96%)	3 (3%)	1 (1%)	11	38
26	c	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
27	d	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
28	e	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
29	f	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
30	g	119/121 (98%)	113 (95%)	6 (5%)	0	100	100
31	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
32	i	345/347 (99%)	332 (96%)	13 (4%)	0	100	100
33	j	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
34	k	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
35	l	604/606 (100%)	575 (95%)	29 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	m	173/175 (99%)	166 (96%)	6 (4%)	1 (1%)	21	50
37	n	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
38	o	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
39	p	176/178 (99%)	170 (97%)	6 (3%)	0	100	100
40	r	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
41	s	316/318 (99%)	305 (96%)	9 (3%)	2 (1%)	21	50
42	u	169/171 (99%)	164 (97%)	5 (3%)	0	100	100
43	v	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
44	w	318/320 (99%)	311 (98%)	7 (2%)	0	100	100
All	All	8174/8312 (98%)	7886 (96%)	280 (3%)	8 (0%)	49	78

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	133	ILE
41	s	208	VAL
9	J	38	HIS
41	s	90	PRO
5	F	63	PRO
7	H	77	ILE
25	b	33	PRO
36	m	25	SER

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	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	107/107 (100%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	69/76 (91%)	69 (100%)	0	100	100
6	G	75/81 (93%)	75 (100%)	0	100	100
6	X	79/81 (98%)	78 (99%)	1 (1%)	61	71
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	87 (100%)	0	100	100
9	J	296/296 (100%)	296 (100%)	0	100	100
10	K	42/42 (100%)	42 (100%)	0	100	100
11	L	113/113 (100%)	112 (99%)	1 (1%)	70	76
12	M	578/580 (100%)	576 (100%)	2 (0%)	86	84
13	N	130/130 (100%)	129 (99%)	1 (1%)	73	77
14	O	179/183 (98%)	178 (99%)	1 (1%)	78	80
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	367/370 (99%)	366 (100%)	1 (0%)	86	84
17	S	57/58 (98%)	57 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	100/101 (99%)	100 (100%)	0	100	100
21	W	122/123 (99%)	122 (100%)	0	100	100
22	Y	61/62 (98%)	61 (100%)	0	100	100
23	Z	60/62 (97%)	60 (100%)	0	100	100
24	a	121/121 (100%)	121 (100%)	0	100	100
25	b	89/119 (75%)	89 (100%)	0	100	100
26	c	141/141 (100%)	141 (100%)	0	100	100
27	d	155/155 (100%)	155 (100%)	0	100	100
28	e	96/96 (100%)	96 (100%)	0	100	100
29	f	36/45 (80%)	36 (100%)	0	100	100
30	g	108/108 (100%)	107 (99%)	1 (1%)	70	76
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	311/311 (100%)	311 (100%)	0	100	100
33	j	100/100 (100%)	100 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	l	537/540 (99%)	537 (100%)	0	100	100
36	m	130/141 (92%)	129 (99%)	1 (1%)	73	77
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	158/159 (99%)	158 (100%)	0	100	100
40	r	409/410 (100%)	407 (100%)	2 (0%)	81	81
41	s	274/275 (100%)	272 (99%)	2 (1%)	76	78
42	u	153/153 (100%)	152 (99%)	1 (1%)	76	78
43	v	110/111 (99%)	110 (100%)	0	100	100
44	w	279/283 (99%)	278 (100%)	1 (0%)	84	83
All	All	7139/7240 (99%)	7124 (100%)	15 (0%)	85	85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	L	127	THR
12	M	136	GLU
12	M	137	CYS
13	N	144	TYR
14	O	146	ASP
16	Q	173	LEU
6	X	87	LEU
30	g	47	ASP
36	m	56	VAL
40	r	1	MET
40	r	76	MET
41	s	24	GLU
41	s	224	PHE
42	u	126	SER
44	w	249	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	393	ASN
1	A	441	HIS

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Mol	Chain	Res	Type
1	A	458	GLN
2	B	206	GLN
4	E	99	GLN
5	F	25	GLN
7	H	41	ASN
9	J	323	HIS
10	K	75	ASN
11	L	71	HIS
12	M	334	GLN
12	M	460	HIS
12	M	540	ASN
13	N	113	HIS
13	N	123	GLN
14	O	74	HIS
14	O	182	ASN
15	P	63	GLN
15	P	75	GLN
15	P	77	GLN
15	P	82	ASN
15	P	196	HIS
16	Q	60	HIS
16	Q	87	GLN
16	Q	182	ASN
16	Q	223	HIS
16	Q	454	GLN
17	S	44	GLN
18	T	123	HIS
19	U	52	ASN
20	V	134	GLN
21	W	76	GLN
6	X	115	GLN
6	X	142	GLN
22	Y	83	HIS
25	b	89	HIS
26	c	84	GLN
26	c	127	ASN
26	c	154	GLN
27	d	140	GLN
28	e	148	GLN
29	f	73	ASN
30	g	14	GLN
30	g	90	HIS

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Mol	Chain	Res	Type
31	h	98	HIS
32	i	77	ASN
32	i	174	GLN
32	i	221	HIS
33	j	10	ASN
34	k	7	ASN
35	l	30	ASN
35	l	34	ASN
35	l	135	ASN
35	l	175	ASN
35	l	210	ASN
35	l	226	GLN
35	l	270	ASN
35	l	309	GLN
35	l	348	HIS
35	l	524	ASN
35	l	580	GLN
39	p	51	HIS
39	p	78	GLN
39	p	141	GLN
39	p	169	HIS
40	r	144	ASN
40	r	175	ASN
40	r	366	ASN
40	r	422	HIS
40	r	434	ASN
41	s	47	GLN
41	s	235	ASN
41	s	287	HIS
42	u	64	ASN
43	v	84	GLN
44	w	85	HIS
44	w	132	GLN
44	w	149	HIS

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	1.99	1 (10%)	5,13,15	5.94	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	-	3/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.73	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.07	130.54	119.48
16	Q	118	2MR	CD-NE-CZ	4.27	131.39	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.37	130.89	123.65

There are no chirality outliers.

All (3) 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
16	Q	118	2MR	CG-CD-NE-CZ

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 44 ligands modelled in this entry, 2 are monoatomic - leaving 42 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
52	UQ	s	403	-	38,38,63	3.61	10 (26%)	48,49,79	2.80	16 (33%)
52	UQ	J	402	-	33,33,63	3.53	9 (27%)	42,43,79	2.69	14 (33%)
55	CDL	m	201	-	99,99,99	1.12	8 (8%)	105,111,111	0.85	4 (3%)
55	CDL	u	201	-	54,54,99	1.39	9 (16%)	60,66,111	1.09	4 (6%)
57	ADP	w	402	-	28,29,29	3.18	9 (32%)	43,45,45	1.92	9 (20%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
45	SF4	C	301	3	0,12,12	-	-	-	-	-
50	8Q1	X	201	-	32,34,34	1.66	6 (18%)	39,43,43	1.60	7 (17%)
47	NAI	A	503	-	47,48,48	4.03	22 (46%)	64,73,73	1.68	11 (17%)
49	PLX	C	303	-	51,51,51	1.21	4 (7%)	53,59,59	0.63	1 (1%)
49	PLX	g	201	-	51,51,51	1.20	4 (7%)	53,59,59	0.64	1 (1%)
48	PEE	l	701	-	39,39,50	1.32	6 (15%)	42,44,55	1.10	3 (7%)
55	CDL	s	402	-	88,88,99	1.17	9 (10%)	94,100,111	0.94	4 (4%)
55	CDL	N	201	-	50,50,99	1.43	8 (16%)	56,62,111	1.14	4 (7%)
55	CDL	l	702	-	98,98,99	1.12	8 (8%)	104,110,111	0.91	4 (3%)
48	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	1.00	2 (3%)
53	FES	M	803	12	0,4,4	-	-	-	-	-
48	PEE	s	401	-	40,40,50	1.17	5 (12%)	43,45,55	1.02	2 (4%)
48	PEE	Q	501	-	46,46,50	1.22	6 (13%)	49,51,55	1.02	2 (4%)
55	CDL	a	201	-	99,99,99	1.12	8 (8%)	105,111,111	0.85	4 (3%)
50	8Q1	G	201	-	32,34,34	1.61	6 (18%)	39,43,43	1.60	6 (15%)
48	PEE	b	201	-	45,45,50	1.24	6 (13%)	48,50,55	1.01	2 (4%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	PLX	a	202	-	51,51,51	1.21	5 (9%)	53,59,59	0.60	1 (1%)
51	NDP	J	401	-	51,52,52	4.28	25 (49%)	71,80,80	2.25	15 (21%)
49	PLX	j	202	-	51,51,51	1.21	5 (9%)	53,59,59	0.64	1 (1%)
55	CDL	w	401	-	99,99,99	1.11	8 (8%)	105,111,111	0.86	4 (3%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
49	PLX	r	503	-	51,51,51	1.20	4 (7%)	53,59,59	0.65	1 (1%)
48	PEE	C	302	-	46,46,50	1.23	6 (13%)	49,51,55	1.02	2 (4%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
48	PEE	W	201	-	40,40,50	1.17	5 (12%)	43,45,55	0.99	2 (4%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
49	PLX	r	502	-	51,51,51	1.21	5 (9%)	53,59,59	0.62	1 (1%)
53	FES	O	301	14	0,4,4	-	-	-	-	-
48	PEE	j	201	-	50,50,50	1.18	6 (12%)	53,55,55	0.98	2 (3%)
48	PEE	l	704	-	50,50,50	1.18	6 (12%)	53,55,55	0.94	2 (3%)
55	CDL	V	201	-	93,93,99	1.14	9 (9%)	99,105,111	0.89	4 (4%)
46	FMN	A	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.23	8 (16%)
55	CDL	l	703	-	99,99,99	1.11	8 (8%)	105,111,111	0.88	4 (3%)
48	PEE	B	303	-	50,50,50	1.18	6 (12%)	53,55,55	0.99	2 (3%)
55	CDL	V	202	-	99,99,99	1.11	8 (8%)	105,111,111	0.87	4 (3%)

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
52	UQ	s	403	-	-	15/33/57/87	0/1/1/1
52	UQ	J	402	-	-	9/27/51/87	0/1/1/1
55	CDL	m	201	-	-	59/110/110/110	-
55	CDL	u	201	-	-	38/65/65/110	-
57	ADP	w	402	-	-	4/16/32/32	0/3/3/3
45	SF4	B	302	2	-	-	0/6/5/5
50	8Q1	X	201	-	-	15/41/41/41	-
45	SF4	C	301	3	-	-	0/6/5/5
47	NAI	A	503	-	-	8/29/72/72	0/5/5/5
49	PLX	C	303	-	-	29/55/55/55	-
49	PLX	g	201	-	-	31/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PEE	l	701	-	-	26/43/43/54	-
55	CDL	s	402	-	-	52/99/99/110	-
55	CDL	N	201	-	-	31/61/61/110	-
55	CDL	l	702	-	-	64/109/109/110	-
48	PEE	r	501	-	-	26/54/54/54	-
53	FES	M	803	12	-	-	0/1/1/1
48	PEE	s	401	-	-	21/44/44/54	-
48	PEE	Q	501	-	-	20/50/50/54	-
55	CDL	a	201	-	-	57/110/110/110	-
50	8Q1	G	201	-	-	10/41/41/41	-
48	PEE	b	201	-	-	30/49/49/54	-
45	SF4	M	801	12	-	-	0/6/5/5
49	PLX	a	202	-	-	32/55/55/55	-
51	NDP	J	401	-	-	4/34/77/77	0/5/5/5
49	PLX	j	202	-	-	24/55/55/55	-
55	CDL	w	401	-	-	54/110/110/110	-
45	SF4	M	802	12	-	-	0/6/5/5
49	PLX	r	503	-	-	30/55/55/55	-
48	PEE	C	302	-	-	21/50/50/54	-
49	PLX	r	502	-	-	30/55/55/55	-
48	PEE	W	201	-	-	18/44/44/54	-
45	SF4	A	501	1	-	-	0/6/5/5
45	SF4	B	301	2	-	-	0/6/5/5
53	FES	O	301	14	-	-	0/1/1/1
48	PEE	j	201	-	-	30/54/54/54	-
48	PEE	l	704	-	-	29/54/54/54	-
55	CDL	V	201	-	-	53/104/104/110	-
46	FMN	A	502	-	-	5/18/18/18	0/3/3/3
55	CDL	l	703	-	-	55/110/110/110	-
48	PEE	B	303	-	-	23/54/54/54	-
55	CDL	V	202	-	-	65/110/110/110	-

All (257) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	C3B-C2B	-13.35	1.23	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	O4D-C4D	10.72	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.47	1.26	1.53
51	J	401	NDP	C3D-C4D	-10.05	1.27	1.53
52	J	402	UQ	C18-C19	9.99	1.56	1.33
52	s	403	UQ	C18-C19	9.92	1.55	1.33
52	J	402	UQ	C13-C14	9.64	1.55	1.33
52	s	403	UQ	C13-C14	9.49	1.54	1.33
47	A	503	NAI	O4B-C1B	9.43	1.63	1.42
52	s	403	UQ	C23-C24	9.41	1.54	1.33
52	J	402	UQ	C8-C9	9.38	1.54	1.33
52	s	403	UQ	C8-C9	9.13	1.54	1.33
57	w	402	ADP	C3'-C4'	-8.96	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.37	1.26	1.45
51	J	401	NDP	O4B-C4B	-7.90	1.27	1.45
57	w	402	ADP	O4'-C4'	7.84	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.70	1.29	1.53
52	J	402	UQ	C23-C24	7.46	1.54	1.32
52	s	403	UQ	C28-C29	7.41	1.54	1.32
47	A	503	NAI	C2B-C1B	-7.40	1.30	1.53
51	J	401	NDP	C2N-C3N	7.33	1.55	1.35
51	J	401	NDP	C6N-C5N	7.25	1.55	1.33
47	A	503	NAI	O4D-C4D	6.89	1.60	1.45
57	w	402	ADP	PA-O3A	6.46	1.66	1.59
51	J	401	NDP	PN-O3	6.40	1.66	1.59
47	A	503	NAI	PA-O3	6.36	1.66	1.59
47	A	503	NAI	C2D-C3D	6.03	1.69	1.53
51	J	401	NDP	P2B-O2B	5.94	1.69	1.59
51	J	401	NDP	C6A-N6A	5.77	1.48	1.34
47	A	503	NAI	O4D-C1D	5.62	1.55	1.42
47	A	503	NAI	PN-O3	5.58	1.65	1.59
57	w	402	ADP	C6-N6	5.45	1.48	1.34
51	J	401	NDP	PA-O3	5.43	1.65	1.59
47	A	503	NAI	C4N-C3N	-5.36	1.39	1.50
51	J	401	NDP	C3B-C4B	5.32	1.66	1.53
47	A	503	NAI	C7N-N7N	5.28	1.48	1.33
50	X	201	8Q1	C39-N41	5.15	1.45	1.33
50	X	201	8Q1	C34-N36	5.09	1.45	1.33
47	A	503	NAI	C6A-N6A	5.08	1.47	1.34
50	G	201	8Q1	C34-N36	5.04	1.45	1.33
50	G	201	8Q1	C39-N41	5.03	1.45	1.33
51	J	401	NDP	C6N-N1N	5.01	1.49	1.37
51	J	401	NDP	O4D-C1D	-4.98	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	O4B-C1B	4.66	1.52	1.42
51	J	401	NDP	C1B-N9A	-4.64	1.33	1.46
57	w	402	ADP	O4'-C1'	-4.52	1.31	1.42
47	A	503	NAI	O2B-C2B	4.30	1.53	1.43
51	J	401	NDP	O2D-C2D	-4.01	1.33	1.43
51	J	401	NDP	C7N-N7N	3.87	1.44	1.33
48	s	401	PEE	C18-C19	3.83	1.53	1.31
48	l	704	PEE	C18-C19	3.82	1.53	1.31
48	B	303	PEE	C18-C19	3.82	1.53	1.31
48	l	701	PEE	C18-C19	3.81	1.53	1.31
48	b	201	PEE	C18-C19	3.81	1.53	1.31
48	C	302	PEE	C18-C19	3.81	1.53	1.31
48	r	501	PEE	C18-C19	3.80	1.53	1.31
48	W	201	PEE	C18-C19	3.79	1.53	1.31
48	Q	501	PEE	C18-C19	3.79	1.53	1.31
48	j	201	PEE	C18-C19	3.78	1.53	1.31
48	j	201	PEE	C39-C38	3.73	1.52	1.31
48	r	501	PEE	C39-C38	3.73	1.52	1.31
48	l	701	PEE	C39-C38	3.72	1.52	1.31
48	l	704	PEE	C39-C38	3.71	1.52	1.31
48	Q	501	PEE	C39-C38	3.70	1.52	1.31
48	b	201	PEE	C39-C38	3.70	1.52	1.31
48	C	302	PEE	C39-C38	3.70	1.52	1.31
48	B	303	PEE	C39-C38	3.69	1.52	1.31
47	A	503	NAI	C7N-C3N	3.64	1.56	1.48
55	l	702	CDL	OA8-CA7	3.52	1.43	1.33
55	N	201	CDL	OA8-CA7	3.52	1.43	1.33
55	u	201	CDL	OA8-CA7	3.50	1.43	1.33
55	l	703	CDL	OA8-CA7	3.47	1.43	1.33
55	s	402	CDL	OA8-CA7	3.46	1.43	1.33
55	V	201	CDL	OA8-CA7	3.46	1.43	1.33
55	V	202	CDL	OA8-CA7	3.44	1.43	1.33
55	a	201	CDL	OA8-CA7	3.42	1.43	1.33
55	m	201	CDL	OA8-CA7	3.40	1.43	1.33
55	w	401	CDL	OA8-CA7	3.40	1.43	1.33
46	A	502	FMN	C4A-N5	3.36	1.38	1.30
57	w	402	ADP	C8-N9	-3.35	1.31	1.37
47	A	503	NAI	C4N-C5N	-3.34	1.40	1.49
51	J	401	NDP	C8A-N9A	-3.24	1.32	1.37
57	w	402	ADP	O2'-C2'	-3.19	1.35	1.43
55	m	201	CDL	OA6-CA5	3.12	1.43	1.34
55	V	201	CDL	OA6-CA5	3.11	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	201	CDL	OB8-CB7	3.07	1.42	1.33
55	V	202	CDL	OB6-CB5	3.06	1.42	1.34
55	l	702	CDL	OB8-CB7	3.04	1.42	1.33
55	w	401	CDL	OB6-CB5	3.04	1.42	1.34
55	a	201	CDL	OB6-CB5	3.04	1.42	1.34
55	s	402	CDL	OA6-CA5	3.04	1.42	1.34
55	m	201	CDL	OB6-CB5	3.04	1.42	1.34
55	u	201	CDL	OB8-CB7	3.03	1.42	1.33
55	N	201	CDL	OB6-CB5	3.02	1.42	1.34
55	l	702	CDL	OB6-CB5	3.00	1.42	1.34
55	V	202	CDL	OB8-CB7	3.00	1.42	1.33
55	l	703	CDL	OB6-CB5	3.00	1.42	1.34
55	m	201	CDL	OB8-CB7	2.99	1.42	1.33
55	N	201	CDL	OB8-CB7	2.99	1.42	1.33
55	V	201	CDL	OB6-CB5	2.98	1.42	1.34
55	s	402	CDL	OB6-CB5	2.98	1.42	1.34
51	J	401	NDP	C5A-N7A	-2.98	1.33	1.39
55	u	201	CDL	OA6-CA5	2.97	1.42	1.34
55	u	201	CDL	OB6-CB5	2.95	1.42	1.34
55	w	401	CDL	OB8-CB7	2.95	1.42	1.33
51	J	401	NDP	C7N-C3N	2.95	1.55	1.48
55	l	702	CDL	OA6-CA5	2.94	1.42	1.34
55	N	201	CDL	OA6-CA5	2.94	1.42	1.34
55	a	201	CDL	OA6-CA5	2.94	1.42	1.34
55	s	402	CDL	OB8-CB7	2.93	1.41	1.33
55	V	202	CDL	OA6-CA5	2.93	1.42	1.34
55	l	703	CDL	OA6-CA5	2.92	1.42	1.34
49	a	202	PLX	O6-C4	-2.92	1.40	1.44
57	w	402	ADP	O3'-C3'	2.92	1.50	1.43
55	l	703	CDL	OB8-CB7	2.91	1.41	1.33
55	V	201	CDL	OB8-CB7	2.90	1.41	1.33
55	w	401	CDL	OA6-CA5	2.89	1.42	1.34
49	r	503	PLX	O6-C4	-2.85	1.41	1.44
49	g	201	PLX	O6-C4	-2.83	1.41	1.44
51	J	401	NDP	O3D-C3D	2.82	1.49	1.43
49	C	303	PLX	O6-C4	-2.82	1.41	1.44
52	s	403	UQ	C6-C1	2.79	1.54	1.46
49	r	502	PLX	O6-C4	-2.79	1.41	1.44
49	j	202	PLX	O6-C4	-2.73	1.41	1.44
52	J	402	UQ	C6-C1	2.73	1.54	1.46
47	A	503	NAI	C8A-N9A	-2.70	1.32	1.37
48	Q	501	PEE	O2-C2	-2.65	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	401	CDL	OA6-CA4	-2.64	1.40	1.46
48	W	201	PEE	O2-C2	-2.63	1.40	1.46
48	B	303	PEE	O2-C2	-2.62	1.40	1.46
55	a	201	CDL	OA6-CA4	-2.61	1.40	1.46
55	u	201	CDL	OA6-CA4	-2.59	1.40	1.46
48	l	704	PEE	O2-C2	-2.59	1.40	1.46
50	X	201	8Q1	C6-C1	2.58	1.53	1.50
55	V	202	CDL	OA6-CA4	-2.56	1.40	1.46
48	C	302	PEE	O2-C2	-2.56	1.40	1.46
48	r	501	PEE	O2-C2	-2.56	1.40	1.46
55	s	402	CDL	OA6-CA4	-2.55	1.40	1.46
55	N	201	CDL	OA6-CA4	-2.55	1.40	1.46
55	l	702	CDL	OA6-CA4	-2.55	1.40	1.46
51	J	401	NDP	O2B-C2B	2.53	1.52	1.44
48	r	501	PEE	O3-C30	2.53	1.40	1.33
48	j	201	PEE	O2-C2	-2.52	1.40	1.46
47	A	503	NAI	PN-O5D	2.51	1.69	1.59
48	s	401	PEE	O2-C2	-2.50	1.40	1.46
50	X	201	8Q1	C1-S44	2.49	1.82	1.76
48	j	201	PEE	O3-C30	2.48	1.40	1.33
48	l	701	PEE	O2-C2	-2.48	1.40	1.46
48	b	201	PEE	O2-C2	-2.48	1.40	1.46
55	l	703	CDL	OA6-CA4	-2.48	1.40	1.46
48	s	401	PEE	O3-C30	2.47	1.40	1.33
48	B	303	PEE	O3-C30	2.47	1.40	1.33
48	l	704	PEE	O3-C30	2.45	1.40	1.33
48	W	201	PEE	O3-C30	2.45	1.40	1.33
48	C	302	PEE	O3-C30	2.45	1.40	1.33
49	j	202	PLX	C7-C6	2.45	1.55	1.50
47	A	503	NAI	C6N-C5N	2.44	1.40	1.33
48	b	201	PEE	O3-C30	2.44	1.40	1.33
46	A	502	FMN	C10-N1	2.44	1.38	1.33
48	l	701	PEE	O3-C30	2.44	1.40	1.33
49	g	201	PLX	C7-C6	2.43	1.55	1.50
48	Q	501	PEE	O3-C30	2.42	1.40	1.33
47	A	503	NAI	O3B-C3B	-2.40	1.37	1.43
55	V	201	CDL	OB6-CB4	-2.40	1.41	1.46
49	r	502	PLX	C7-C6	2.40	1.55	1.50
49	a	202	PLX	C7-C6	2.39	1.55	1.50
52	s	403	UQ	C7-C8	2.39	1.54	1.50
55	l	703	CDL	OB6-CB4	-2.39	1.41	1.46
55	m	201	CDL	OA6-CA4	-2.38	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	J	402	UQ	C7-C8	2.38	1.54	1.50
57	w	402	ADP	C5-N7	-2.38	1.34	1.39
50	X	201	8Q1	O35-C34	-2.36	1.18	1.23
55	m	201	CDL	OB6-CB4	-2.36	1.41	1.46
55	l	702	CDL	OB6-CB4	-2.36	1.41	1.46
49	r	503	PLX	C7-C6	2.36	1.55	1.50
50	G	201	8Q1	O40-C39	-2.35	1.18	1.23
50	G	201	8Q1	C1-S44	2.35	1.81	1.76
49	C	303	PLX	C7-C6	2.34	1.55	1.50
55	u	201	CDL	OB6-CB4	-2.34	1.41	1.46
55	N	201	CDL	OB6-CB4	-2.33	1.41	1.46
48	C	302	PEE	O2-C10	2.32	1.40	1.34
55	s	402	CDL	OB6-CB4	-2.32	1.41	1.46
50	G	201	8Q1	O35-C34	-2.32	1.18	1.23
51	J	401	NDP	C2D-C3D	2.31	1.59	1.53
48	B	303	PEE	O2-C10	2.30	1.40	1.34
50	X	201	8Q1	O40-C39	-2.30	1.18	1.23
48	b	201	PEE	O2-C10	2.30	1.40	1.34
55	V	202	CDL	PB2-OB2	2.30	1.68	1.59
47	A	503	NAI	C5B-C4B	2.29	1.58	1.51
55	V	201	CDL	PB2-OB2	2.29	1.68	1.59
48	s	401	PEE	O2-C10	2.29	1.40	1.34
55	a	201	CDL	PB2-OB2	2.28	1.68	1.59
48	l	701	PEE	O2-C10	2.28	1.40	1.34
48	j	201	PEE	O2-C10	2.27	1.40	1.34
55	l	703	CDL	PB2-OB2	2.27	1.68	1.59
48	W	201	PEE	O2-C10	2.27	1.40	1.34
55	l	702	CDL	PB2-OB2	2.26	1.68	1.59
55	m	201	CDL	PB2-OB5	2.26	1.68	1.59
48	l	704	PEE	O2-C10	2.25	1.40	1.34
55	N	201	CDL	PB2-OB2	2.25	1.68	1.59
55	a	201	CDL	OB6-CB4	-2.24	1.41	1.46
48	Q	501	PEE	O2-C10	2.24	1.40	1.34
55	m	201	CDL	PB2-OB2	2.24	1.68	1.59
55	a	201	CDL	PB2-OB5	2.24	1.68	1.59
55	u	201	CDL	PB2-OB2	2.24	1.68	1.59
52	s	403	UQ	O4-C4	-2.23	1.18	1.23
55	w	401	CDL	OB6-CB4	-2.23	1.41	1.46
55	l	702	CDL	PB2-OB5	2.23	1.68	1.59
55	w	401	CDL	PB2-OB2	2.23	1.68	1.59
55	V	202	CDL	OB6-CB4	-2.22	1.41	1.46
48	l	704	PEE	O3-C3	-2.21	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	401	CDL	PB2-OB5	2.21	1.68	1.59
55	s	402	CDL	PB2-OB5	2.21	1.68	1.59
52	s	403	UQ	O3-CM3	-2.21	1.40	1.45
55	V	202	CDL	PB2-OB5	2.20	1.68	1.59
55	V	201	CDL	OA6-CA4	-2.20	1.41	1.46
48	r	501	PEE	O2-C10	2.20	1.40	1.34
55	s	402	CDL	PB2-OB2	2.20	1.68	1.59
55	u	201	CDL	PB2-OB5	2.20	1.68	1.59
55	V	201	CDL	PB2-OB5	2.19	1.68	1.59
49	a	202	PLX	P1-O4	2.19	1.68	1.59
48	Q	501	PEE	O3-C3	-2.18	1.40	1.45
52	J	402	UQ	O4-C4	-2.17	1.18	1.23
49	g	201	PLX	P1-O4	2.17	1.67	1.59
55	N	201	CDL	PB2-OB5	2.17	1.67	1.59
49	r	503	PLX	P1-O4	2.16	1.67	1.59
48	W	201	PEE	O3-C3	-2.16	1.40	1.45
50	G	201	8Q1	C6-C1	2.16	1.53	1.50
55	l	703	CDL	PB2-OB5	2.16	1.67	1.59
48	r	501	PEE	O3-C3	-2.15	1.40	1.45
51	J	401	NDP	PA-O5B	2.15	1.67	1.59
47	A	503	NAI	C5A-N7A	-2.15	1.35	1.39
49	C	303	PLX	P1-O4	2.15	1.67	1.59
49	j	202	PLX	P1-O4	2.14	1.67	1.59
48	C	302	PEE	O3-C3	-2.14	1.40	1.45
51	J	401	NDP	O7N-C7N	-2.14	1.19	1.24
49	r	502	PLX	P1-O4	2.13	1.67	1.59
48	j	201	PEE	O3-C3	-2.13	1.40	1.45
48	b	201	PEE	O3-C3	-2.12	1.40	1.45
52	J	402	UQ	O3-CM3	-2.11	1.40	1.45
48	l	701	PEE	O3-C3	-2.10	1.40	1.45
49	C	303	PLX	P1-O1	2.09	1.67	1.59
48	B	303	PEE	O3-C3	-2.08	1.40	1.45
55	V	201	CDL	C11-CA5	2.08	1.56	1.50
49	r	502	PLX	P1-O1	2.08	1.67	1.59
48	s	401	PEE	O3-C3	-2.07	1.40	1.45
49	a	202	PLX	P1-O1	2.07	1.67	1.59
49	r	502	PLX	C25-C24	2.07	1.55	1.50
49	j	202	PLX	P1-O1	2.06	1.67	1.59
49	g	201	PLX	P1-O1	2.05	1.67	1.59
49	r	503	PLX	P1-O1	2.04	1.67	1.59
49	j	202	PLX	C25-C24	2.03	1.55	1.50
55	u	201	CDL	C11-CA5	2.03	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	s	403	UQ	O1-C1	-2.03	1.18	1.23
55	s	402	CDL	C11-CA5	2.02	1.56	1.50
49	a	202	PLX	C1-C2	2.02	1.57	1.51
52	J	402	UQ	C21-C19	2.01	1.55	1.51

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	J	402	UQ	C7-C8-C9	-8.15	112.79	126.83
52	s	403	UQ	C7-C8-C9	-7.47	113.96	126.83
51	J	401	NDP	C1D-N1N-C2N	-7.32	109.08	121.14
51	J	401	NDP	C3N-C2N-N1N	-7.30	112.48	123.20
51	J	401	NDP	C6N-N1N-C2N	-7.09	111.73	119.32
52	s	403	UQ	C12-C13-C14	-6.61	112.48	127.62
52	J	402	UQ	C17-C18-C19	-6.48	112.80	127.62
52	s	403	UQ	C22-C23-C24	-6.26	113.30	127.62
52	s	403	UQ	C17-C18-C19	-6.20	113.43	127.62
50	G	201	8Q1	C6-C1-S44	5.97	120.52	113.40
52	J	402	UQ	C12-C13-C14	-5.89	114.14	127.62
51	J	401	NDP	C5A-C4A-N3A	-5.59	119.02	126.72
47	A	503	NAI	C5A-C4A-N3A	-5.42	119.25	126.72
50	X	201	8Q1	C6-C1-S44	5.36	119.78	113.40
57	w	402	ADP	C5-C4-N3	-5.35	119.34	126.72
51	J	401	NDP	C1D-N1N-C6N	-5.16	109.87	120.77
57	w	402	ADP	N3-C2-N1	-4.57	121.66	128.58
52	s	403	UQ	C10-C9-C8	-4.44	112.23	123.63
52	s	403	UQ	C27-C28-C29	-4.41	112.95	127.64
52	J	402	UQ	C22-C23-C24	-4.40	112.96	127.64
47	A	503	NAI	N3A-C2A-N1A	-4.38	121.95	128.58
52	s	403	UQ	C25-C24-C23	-4.30	112.57	123.63
52	s	403	UQ	C11-C9-C8	-4.23	111.66	121.17
55	s	402	CDL	OA6-CA5-C11	4.21	120.58	111.48
57	w	402	ADP	N3-C4-N9	4.18	134.28	127.17
55	V	202	CDL	OB6-CB5-C51	4.15	120.46	111.48
55	l	702	CDL	OA6-CA5-C11	4.15	120.45	111.48
55	l	703	CDL	OB6-CB5-C51	4.13	120.41	111.48
51	J	401	NDP	N3A-C2A-N1A	-4.13	122.34	128.58
52	J	402	UQ	C20-C19-C18	-4.11	113.06	123.63
48	b	201	PEE	O2-C10-C11	4.10	120.36	111.48
55	V	201	CDL	OA6-CA5-C11	4.09	120.33	111.48
48	s	401	PEE	O2-C10-C11	4.08	120.31	111.48
52	J	402	UQ	C10-C9-C8	-4.08	113.15	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	r	501	PEE	O2-C10-C11	4.08	120.30	111.48
52	s	403	UQ	C15-C14-C13	-4.05	113.23	123.63
55	V	201	CDL	OB6-CB5-C51	4.02	120.18	111.48
48	l	701	PEE	O2-C10-C11	4.01	120.15	111.48
55	s	402	CDL	OB6-CB5-C51	3.99	120.11	111.48
52	s	403	UQ	C20-C19-C18	-3.96	113.44	123.63
48	C	302	PEE	O2-C10-C11	3.96	120.05	111.48
55	m	201	CDL	OB6-CB5-C51	3.95	120.03	111.48
55	a	201	CDL	OB6-CB5-C51	3.95	120.03	111.48
48	B	303	PEE	O2-C10-C11	3.95	120.02	111.48
55	l	702	CDL	OB6-CB5-C51	3.94	120.01	111.48
55	w	401	CDL	OB6-CB5-C51	3.94	120.01	111.48
55	u	201	CDL	OA6-CA5-C11	3.94	120.00	111.48
48	W	201	PEE	O2-C10-C11	3.94	120.00	111.48
48	j	201	PEE	O2-C10-C11	3.93	119.99	111.48
55	u	201	CDL	OB6-CB5-C51	3.91	119.95	111.48
48	Q	501	PEE	O2-C10-C11	3.90	119.93	111.48
51	J	401	NDP	N3A-C4A-N9A	3.90	133.81	127.17
55	l	703	CDL	OA6-CA5-C11	3.90	119.92	111.48
55	N	201	CDL	OA6-CA5-C11	3.89	119.91	111.48
55	N	201	CDL	OB6-CB5-C51	3.85	119.80	111.48
47	A	503	NAI	N3A-C4A-N9A	3.84	133.69	127.17
52	s	403	UQ	C21-C19-C18	-3.80	112.63	121.17
55	a	201	CDL	OA6-CA5-C11	3.79	119.68	111.48
48	l	704	PEE	O2-C10-C11	3.79	119.67	111.48
55	V	202	CDL	OA6-CA5-C11	3.73	119.56	111.48
55	w	401	CDL	OA6-CA5-C11	3.72	119.53	111.48
52	J	402	UQ	C15-C14-C13	-3.69	114.16	123.63
50	G	201	8Q1	O4-C1-C6	-3.69	119.73	123.98
47	A	503	NAI	C2A-N3A-C4A	3.66	120.76	111.83
52	J	402	UQ	C16-C14-C13	-3.64	112.99	121.17
55	m	201	CDL	OA6-CA5-C11	3.61	119.30	111.48
51	J	401	NDP	C2A-N3A-C4A	3.61	120.65	111.83
52	s	403	UQ	C16-C14-C13	-3.60	113.08	121.17
52	s	403	UQ	C26-C24-C23	-3.60	113.08	121.17
52	J	402	UQ	C21-C19-C18	-3.57	113.14	121.17
57	w	402	ADP	C2-N3-C4	3.55	120.49	111.83
57	w	402	ADP	N9-C8-N7	-3.52	108.94	113.94
47	A	503	NAI	C4A-C5A-N7A	-3.43	106.66	110.58
47	A	503	NAI	C5A-N7A-C8A	3.37	108.75	103.45
51	J	401	NDP	C4A-C5A-N7A	-3.36	106.74	110.58
52	J	402	UQ	C11-C9-C8	-3.35	113.64	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	502	FMN	C4-N3-C2	-3.34	119.71	125.64
47	A	503	NAI	C3D-C2D-C1D	3.34	107.78	101.46
52	J	402	UQ	C25-C24-C23	-3.28	112.80	122.66
47	A	503	NAI	N9A-C8A-N7A	-3.23	109.36	113.94
57	w	402	ADP	C5-N7-C8	3.21	108.50	103.45
57	w	402	ADP	C4-N9-C8	3.20	109.09	105.74
52	J	402	UQ	C26-C24-C23	-3.20	113.06	122.66
52	s	403	UQ	C30-C29-C28	-3.17	113.13	122.66
52	s	403	UQ	C31-C29-C28	-3.16	113.17	122.66
51	J	401	NDP	N9A-C8A-N7A	-3.14	109.48	113.94
51	J	401	NDP	C5A-N7A-C8A	3.10	108.32	103.45
57	w	402	ADP	C4-C5-N7	-3.05	107.09	110.58
50	X	201	8Q1	O4-C1-C6	-2.98	120.55	123.98
50	X	201	8Q1	C37-C38-C39	2.94	117.29	112.39
50	G	201	8Q1	C37-C38-C39	2.92	117.26	112.39
48	B	303	PEE	O3-C30-C31	2.92	120.72	111.83
47	A	503	NAI	C4D-O4D-C1D	-2.89	103.08	109.47
55	l	702	CDL	OA8-CA7-C31	2.88	120.62	111.83
55	u	201	CDL	OA8-CA7-C31	2.86	119.83	111.15
55	N	201	CDL	OB8-CB7-C71	2.84	120.50	111.83
48	r	501	PEE	O3-C30-C31	2.81	120.42	111.83
55	m	201	CDL	OB8-CB7-C71	2.80	120.39	111.83
48	Q	501	PEE	O3-C30-C31	2.80	120.38	111.83
48	C	302	PEE	O3-C30-C31	2.78	120.32	111.83
55	w	401	CDL	OB8-CB7-C71	2.77	120.28	111.83
55	N	201	CDL	OA8-CA7-C31	2.77	120.27	111.83
48	j	201	PEE	O3-C30-C31	2.77	120.27	111.83
55	m	201	CDL	OA8-CA7-C31	2.76	120.25	111.83
55	s	402	CDL	OA8-CA7-C31	2.75	120.22	111.83
55	a	201	CDL	OB8-CB7-C71	2.74	120.18	111.83
55	l	702	CDL	OB8-CB7-C71	2.73	120.17	111.83
55	l	703	CDL	OB8-CB7-C71	2.73	120.15	111.83
55	V	201	CDL	OB8-CB7-C71	2.72	120.13	111.83
50	X	201	8Q1	C43-S44-C1	2.71	109.85	101.84
55	s	402	CDL	OB8-CB7-C71	2.69	120.05	111.83
55	u	201	CDL	OB8-CB7-C71	2.69	120.02	111.83
55	a	201	CDL	OA8-CA7-C31	2.68	120.02	111.83
55	V	202	CDL	OB8-CB7-C71	2.68	120.01	111.83
49	r	503	PLX	C1A-N1-C1	2.67	120.51	109.91
55	V	202	CDL	OA8-CA7-C31	2.66	119.95	111.83
48	s	401	PEE	O3-C30-C31	2.65	119.92	111.83
48	l	704	PEE	O3-C30-C31	2.65	119.91	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	401	CDL	OA8-CA7-C31	2.65	119.91	111.83
51	J	401	NDP	C2B-C1B-N9A	-2.65	109.40	113.75
48	b	201	PEE	O3-C30-C31	2.64	119.88	111.83
46	A	502	FMN	C4A-C4-N3	2.63	119.95	113.25
48	W	201	PEE	O3-C30-C31	2.62	119.81	111.83
46	A	502	FMN	O4-C4-C4A	-2.60	119.68	126.53
48	l	701	PEE	O3-C30-C31	2.59	119.75	111.83
52	J	402	UQ	C7-C6-C5	-2.59	120.46	124.89
49	g	201	PLX	C1A-N1-C1	2.57	120.14	109.91
55	l	703	CDL	OA8-CA7-C31	2.56	119.64	111.83
49	j	202	PLX	C1A-N1-C1	2.53	119.98	109.91
46	A	502	FMN	C4A-C10-N10	2.53	120.10	116.48
46	A	502	FMN	C5A-C9A-N10	2.49	120.22	117.97
49	a	202	PLX	C1A-N1-C1	2.49	119.80	109.91
52	J	402	UQ	CM5-C5-C6	-2.48	120.38	124.45
55	V	201	CDL	OA8-CA7-C31	2.45	119.31	111.83
49	r	502	PLX	C1A-N1-C1	2.45	119.65	109.91
51	J	401	NDP	C4A-N9A-C8A	2.43	108.28	105.74
49	C	303	PLX	C1A-N1-C1	2.41	119.48	109.91
50	X	201	8Q1	C32-C34-N36	2.41	121.05	116.48
50	X	201	8Q1	O4-C1-S44	-2.37	119.67	122.68
48	l	701	PEE	C20-C19-C18	-2.35	112.31	126.42
47	A	503	NAI	C4A-N9A-C8A	2.32	108.17	105.74
47	A	503	NAI	C2D-C3D-C4D	2.31	107.08	102.61
50	G	201	8Q1	O4-C1-S44	-2.30	119.76	122.68
51	J	401	NDP	P2B-O2B-C2B	-2.26	117.41	123.43
52	s	403	UQ	C7-C6-C5	-2.23	121.06	124.89
50	G	201	8Q1	C43-S44-C1	2.22	108.41	101.84
46	A	502	FMN	C10-C4A-N5	-2.22	120.28	124.81
57	w	402	ADP	C4'-O4'-C1'	-2.21	104.59	109.47
51	J	401	NDP	C2D-C3D-C4D	2.19	106.84	102.61
50	G	201	8Q1	C38-C39-N41	2.18	120.31	116.34
46	A	502	FMN	C9A-C5A-N5	-2.16	120.17	122.45
46	A	502	FMN	C4A-C10-N1	-2.11	119.42	124.59
50	X	201	8Q1	C38-C39-N41	2.09	120.14	116.34

There are no chirality outliers.

All (1018) 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'

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Mol	Chain	Res	Type	Atoms
46	A	502	FMN	C5'-O5'-P-O1P
46	A	502	FMN	C5'-O5'-P-O2P
48	C	302	PEE	C11-C10-O2-C2
48	C	302	PEE	C1-O3P-P-O1P
48	C	302	PEE	C1-O3P-P-O4P
48	Q	501	PEE	C11-C10-O2-C2
48	Q	501	PEE	O4-C10-O2-C2
48	Q	501	PEE	C4-O4P-P-O1P
48	W	201	PEE	C1-O3P-P-O2P
48	W	201	PEE	C1-O3P-P-O1P
48	W	201	PEE	C1-O3P-P-O4P
48	j	201	PEE	C1-O3P-P-O1P
48	j	201	PEE	C1-O3P-P-O4P
48	j	201	PEE	C4-O4P-P-O3P
48	j	201	PEE	C4-O4P-P-O2P
48	j	201	PEE	C4-O4P-P-O1P
48	l	701	PEE	C11-C10-O2-C2
48	l	701	PEE	C1-O3P-P-O2P
48	l	701	PEE	C1-O3P-P-O1P
48	l	701	PEE	C1-O3P-P-O4P
48	l	701	PEE	C4-O4P-P-O3P
48	l	704	PEE	O3P-C1-C2-O2
48	l	704	PEE	C4-O4P-P-O3P
48	l	704	PEE	C4-O4P-P-O2P
48	l	704	PEE	C4-O4P-P-O1P
48	r	501	PEE	C1-O3P-P-O1P
48	r	501	PEE	C1-O3P-P-O4P
48	r	501	PEE	C4-O4P-P-O3P
48	r	501	PEE	C4-O4P-P-O2P
48	r	501	PEE	C4-O4P-P-O1P
48	s	401	PEE	C4-O4P-P-O3P
48	s	401	PEE	C4-O4P-P-O2P
49	C	303	PLX	N1-C1-C2-O1
49	C	303	PLX	O9-C24-O8-C5
49	a	202	PLX	O7-C6-O6-C4
49	a	202	PLX	C5-C4-O6-C6
49	a	202	PLX	C3-O4-P1-O1
49	a	202	PLX	C3-O4-P1-O2
49	a	202	PLX	C3-O4-P1-O3
49	a	202	PLX	C2-O1-P1-O4
49	a	202	PLX	C2-O1-P1-O2
49	a	202	PLX	C2-O1-P1-O3

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Mol	Chain	Res	Type	Atoms
49	a	202	PLX	O9-C24-C25-C26
49	g	201	PLX	O6-C4-C5-O8
49	g	201	PLX	C2-O1-P1-O4
49	g	201	PLX	C2-O1-P1-O3
49	g	201	PLX	O9-C24-C25-C26
49	j	202	PLX	O7-C6-C7-C8
49	j	202	PLX	O9-C24-O8-C5
49	j	202	PLX	O9-C24-C25-C26
49	r	502	PLX	O7-C6-C7-C8
49	r	502	PLX	O7-C6-O6-C4
49	r	502	PLX	C2-O1-P1-O4
49	r	502	PLX	C2-O1-P1-O2
49	r	502	PLX	C25-C24-O8-C5
49	r	502	PLX	O9-C24-C25-C26
49	r	503	PLX	O7-C6-O6-C4
49	r	503	PLX	C2-O1-P1-O4
49	r	503	PLX	C2-O1-P1-O2
49	r	503	PLX	O9-C24-O8-C5
50	G	201	8Q1	C42-C43-S44-C1
50	G	201	8Q1	C28-O27-P24-O3
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
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-O27-P24-O3
50	X	201	8Q1	C28-O27-P24-O2
50	X	201	8Q1	C28-O27-P24-O1
52	J	402	UQ	C7-C8-C9-C10
52	J	402	UQ	C7-C8-C9-C11
52	J	402	UQ	C12-C13-C14-C16
52	J	402	UQ	C17-C18-C19-C20
52	s	403	UQ	C7-C8-C9-C10
52	s	403	UQ	C7-C8-C9-C11
52	s	403	UQ	C22-C23-C24-C26
52	s	403	UQ	C23-C24-C26-C27
55	N	201	CDL	CA2-OA2-PA1-OA5
55	N	201	CDL	OA5-CA3-CA4-OA6
55	N	201	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
55	N	201	CDL	CB2-OB2-PB2-OB5
55	N	201	CDL	CB3-OB5-PB2-OB2
55	N	201	CDL	CB3-OB5-PB2-OB3
55	V	201	CDL	CB2-C1-CA2-OA2
55	V	201	CDL	CA2-OA2-PA1-OA3
55	V	201	CDL	CA2-OA2-PA1-OA4
55	V	201	CDL	CA2-OA2-PA1-OA5
55	V	201	CDL	C11-CA5-OA6-CA4
55	V	201	CDL	CB2-OB2-PB2-OB3
55	V	201	CDL	CB2-OB2-PB2-OB5
55	V	201	CDL	CB3-OB5-PB2-OB2
55	V	201	CDL	CB3-OB5-PB2-OB3
55	V	201	CDL	CB3-OB5-PB2-OB4
55	V	202	CDL	CB2-C1-CA2-OA2
55	V	202	CDL	CA2-C1-CB2-OB2
55	V	202	CDL	CA2-OA2-PA1-OA4
55	V	202	CDL	CA2-OA2-PA1-OA5
55	V	202	CDL	CB2-OB2-PB2-OB3
55	V	202	CDL	CB2-OB2-PB2-OB5
55	a	201	CDL	CB2-C1-CA2-OA2
55	a	201	CDL	CA2-C1-CB2-OB2
55	a	201	CDL	CB2-OB2-PB2-OB3
55	a	201	CDL	CB2-OB2-PB2-OB5
55	a	201	CDL	CB3-OB5-PB2-OB2
55	a	201	CDL	CB3-OB5-PB2-OB3
55	a	201	CDL	CB3-OB5-PB2-OB4
55	l	702	CDL	CA2-C1-CB2-OB2
55	l	702	CDL	CA2-OA2-PA1-OA5
55	l	702	CDL	OA5-CA3-CA4-OA6
55	l	702	CDL	OA9-CA7-OA8-CA6
55	l	702	CDL	C31-CA7-OA8-CA6
55	l	702	CDL	CB2-OB2-PB2-OB3
55	l	702	CDL	CB2-OB2-PB2-OB4
55	l	702	CDL	CB2-OB2-PB2-OB5
55	l	702	CDL	CB3-OB5-PB2-OB3
55	l	703	CDL	CB2-C1-CA2-OA2
55	l	703	CDL	CA3-OA5-PA1-OA2
55	l	703	CDL	CA3-OA5-PA1-OA3
55	l	703	CDL	CA3-OA5-PA1-OA4
55	m	201	CDL	CA2-OA2-PA1-OA3
55	m	201	CDL	CA3-OA5-PA1-OA2
55	m	201	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
55	m	201	CDL	OA5-CA3-CA4-OA6
55	m	201	CDL	CB2-OB2-PB2-OB3
55	m	201	CDL	CB2-OB2-PB2-OB5
55	m	201	CDL	CB3-OB5-PB2-OB2
55	m	201	CDL	CB3-OB5-PB2-OB3
55	m	201	CDL	CB3-OB5-PB2-OB4
55	s	402	CDL	CA2-OA2-PA1-OA3
55	s	402	CDL	CA2-OA2-PA1-OA4
55	s	402	CDL	CA2-OA2-PA1-OA5
55	s	402	CDL	OA5-CA3-CA4-OA6
55	s	402	CDL	C31-CA7-OA8-CA6
55	s	402	CDL	CB3-OB5-PB2-OB2
55	u	201	CDL	CB2-C1-CA2-OA2
55	u	201	CDL	CA2-C1-CB2-OB2
55	u	201	CDL	CA2-OA2-PA1-OA4
55	u	201	CDL	CA2-OA2-PA1-OA5
55	u	201	CDL	CA3-OA5-PA1-OA2
55	u	201	CDL	CA3-OA5-PA1-OA4
55	u	201	CDL	CB2-OB2-PB2-OB3
55	u	201	CDL	CB2-OB2-PB2-OB4
55	u	201	CDL	CB2-OB2-PB2-OB5
55	u	201	CDL	CB3-OB5-PB2-OB2
55	u	201	CDL	CB3-OB5-PB2-OB3
55	u	201	CDL	CB3-OB5-PB2-OB4
55	w	401	CDL	OA6-CA4-CA6-OA8
55	w	401	CDL	CB2-OB2-PB2-OB3
55	w	401	CDL	CB2-OB2-PB2-OB5
55	w	401	CDL	CB3-OB5-PB2-OB2
55	w	401	CDL	CB3-OB5-PB2-OB3
55	w	401	CDL	CB3-OB5-PB2-OB4
57	w	402	ADP	C5'-O5'-PA-O1A
57	w	402	ADP	C5'-O5'-PA-O2A
48	Q	501	PEE	O5-C30-O3-C3
55	s	402	CDL	OA9-CA7-OA8-CA6
48	Q	501	PEE	C31-C30-O3-C3
48	C	302	PEE	O4-C10-O2-C2
48	l	701	PEE	O4-C10-O2-C2
48	s	401	PEE	O4-C10-O2-C2
55	V	201	CDL	OA7-CA5-OA6-CA4
55	a	201	CDL	OB7-CB5-OB6-CB4
48	s	401	PEE	C11-C10-O2-C2
55	a	201	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
52	s	403	UQ	C18-C19-C21-C22
48	l	704	PEE	C31-C30-O3-C3
55	l	703	CDL	C71-CB7-OB8-CB6
52	s	403	UQ	C17-C18-C19-C21
48	l	704	PEE	O5-C30-O3-C3
55	N	201	CDL	O1-C1-CA2-OA2
55	V	201	CDL	O1-C1-CA2-OA2
55	V	201	CDL	O1-C1-CB2-OB2
55	V	202	CDL	O1-C1-CA2-OA2
55	a	201	CDL	O1-C1-CA2-OA2
55	l	702	CDL	O1-C1-CA2-OA2
55	l	703	CDL	O1-C1-CA2-OA2
55	s	402	CDL	O1-C1-CA2-OA2
55	s	402	CDL	O1-C1-CB2-OB2
55	u	201	CDL	O1-C1-CA2-OA2
48	B	303	PEE	C11-C10-O2-C2
48	l	704	PEE	C11-C10-O2-C2
55	V	202	CDL	C51-CB5-OB6-CB4
48	j	201	PEE	C30-C31-C32-C33
55	m	201	CDL	CB5-C51-C52-C53
47	A	503	NAI	C3D-C4D-C5D-O5D
48	l	701	PEE	C31-C30-O3-C3
55	V	201	CDL	C71-CB7-OB8-CB6
52	J	402	UQ	C13-C14-C16-C17
52	J	402	UQ	C18-C19-C21-C22
55	l	703	CDL	OB9-CB7-OB8-CB6
52	J	402	UQ	C19-C21-C22-C23
52	s	403	UQ	C14-C16-C17-C18
52	J	402	UQ	C22-C23-C24-C26
48	l	701	PEE	O5-C30-O3-C3
55	V	201	CDL	OB9-CB7-OB8-CB6
48	j	201	PEE	C31-C30-O3-C3
48	W	201	PEE	C17-C18-C19-C20
48	b	201	PEE	C37-C38-C39-C40
48	j	201	PEE	C17-C18-C19-C20
49	C	303	PLX	C27-C28-C29-C30
55	u	201	CDL	C55-C56-C57-C58
49	g	201	PLX	C7-C8-C9-C10
55	m	201	CDL	C73-C74-C75-C76
48	b	201	PEE	C11-C10-O2-C2
55	w	401	CDL	C51-CB5-OB6-CB4
49	g	201	PLX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
48	B	303	PEE	O4-C10-O2-C2
48	l	704	PEE	O4-C10-O2-C2
55	V	202	CDL	OB7-CB5-OB6-CB4
55	V	201	CDL	CA2-C1-CB2-OB2
55	s	402	CDL	CA2-C1-CB2-OB2
48	s	401	PEE	C31-C30-O3-C3
55	V	202	CDL	C71-CB7-OB8-CB6
55	l	702	CDL	C71-CB7-OB8-CB6
55	l	702	CDL	C55-C56-C57-C58
49	g	201	PLX	C17-C18-C19-C20
49	r	502	PLX	C11-C12-C13-C14
55	V	201	CDL	C59-C60-C61-C62
55	V	202	CDL	C32-C33-C34-C35
55	s	402	CDL	C37-C38-C39-C40
49	g	201	PLX	C2-C1-N1-C1A
55	w	401	CDL	C60-C61-C62-C63
55	w	401	CDL	C74-C75-C76-C77
49	r	502	PLX	C9-C10-C11-C12
55	u	201	CDL	C74-C75-C76-C77
55	u	201	CDL	CB5-C51-C52-C53
55	V	202	CDL	O1-C1-CB2-OB2
48	s	401	PEE	O5-C30-O3-C3
55	l	702	CDL	OB9-CB7-OB8-CB6
55	u	201	CDL	OA5-CA3-CA4-OA6
55	m	201	CDL	C11-CA5-OA6-CA4
55	V	202	CDL	OA6-CA4-CA6-OA8
55	l	703	CDL	OA6-CA4-CA6-OA8
51	J	401	NDP	C2D-C1D-N1N-C6N
55	l	703	CDL	CA7-C31-C32-C33
52	s	403	UQ	C12-C13-C14-C15
52	s	403	UQ	C27-C28-C29-C31
55	s	402	CDL	C71-CB7-OB8-CB6
55	V	201	CDL	C62-C63-C64-C65
55	m	201	CDL	C40-C41-C42-C43
52	s	403	UQ	C9-C11-C12-C13
55	l	702	CDL	C58-C59-C60-C61
55	l	703	CDL	C35-C36-C37-C38
49	g	201	PLX	C2-C1-N1-C1B
48	l	704	PEE	C33-C34-C35-C36
48	r	501	PEE	C10-C11-C12-C13
55	V	202	CDL	CB7-C71-C72-C73
55	w	401	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
48	W	201	PEE	C10-C11-C12-C13
55	a	201	CDL	CB5-C51-C52-C53
55	l	702	CDL	CB5-C51-C52-C53
55	l	702	CDL	CB7-C71-C72-C73
55	l	703	CDL	CB7-C71-C72-C73
55	m	201	CDL	CA7-C31-C32-C33
55	V	202	CDL	OB9-CB7-OB8-CB6
55	a	201	CDL	O1-C1-CB2-OB2
55	l	702	CDL	O1-C1-CB2-OB2
55	u	201	CDL	O1-C1-CB2-OB2
48	b	201	PEE	C31-C30-O3-C3
48	j	201	PEE	O5-C30-O3-C3
48	l	704	PEE	C30-C31-C32-C33
55	u	201	CDL	CB7-C71-C72-C73
48	b	201	PEE	O4-C10-O2-C2
55	m	201	CDL	OA7-CA5-OA6-CA4
55	w	401	CDL	OB7-CB5-OB6-CB4
48	l	701	PEE	C10-C11-C12-C13
55	N	201	CDL	CA7-C31-C32-C33
48	l	701	PEE	C11-C12-C13-C14
55	s	402	CDL	OB9-CB7-OB8-CB6
55	s	402	CDL	C14-C15-C16-C17
55	a	201	CDL	C36-C37-C38-C39
55	s	402	CDL	C33-C34-C35-C36
55	N	201	CDL	CB2-C1-CA2-OA2
55	l	702	CDL	CB2-C1-CA2-OA2
55	s	402	CDL	CB2-C1-CA2-OA2
55	w	401	CDL	C71-CB7-OB8-CB6
55	l	702	CDL	C34-C35-C36-C37
55	N	201	CDL	C71-CB7-OB8-CB6
55	m	201	CDL	C60-C61-C62-C63
49	C	303	PLX	O6-C6-C7-C8
49	r	502	PLX	O6-C6-C7-C8
48	j	201	PEE	C11-C10-O2-C2
48	r	501	PEE	C11-C10-O2-C2
48	j	201	PEE	O4-C10-O2-C2
48	r	501	PEE	O4-C10-O2-C2
48	r	501	PEE	C17-C18-C19-C20
55	V	201	CDL	C43-C44-C45-C46
49	C	303	PLX	C25-C26-C27-C28
55	V	202	CDL	C76-C77-C78-C79
48	b	201	PEE	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
49	j	202	PLX	C13-C14-C15-C16
55	V	201	CDL	C32-C33-C34-C35
55	m	201	CDL	C71-CB7-OB8-CB6
55	l	702	CDL	CA7-C31-C32-C33
49	r	503	PLX	C25-C26-C27-C28
55	V	201	CDL	C55-C56-C57-C58
55	l	702	CDL	C20-C21-C22-C23
55	a	201	CDL	C60-C61-C62-C63
55	a	201	CDL	C62-C63-C64-C65
55	l	702	CDL	C62-C63-C64-C65
55	l	703	CDL	C59-C60-C61-C62
55	s	402	CDL	C73-C74-C75-C76
48	l	701	PEE	C17-C18-C19-C20
48	l	704	PEE	C34-C35-C36-C37
49	a	202	PLX	C13-C14-C15-C16
49	C	303	PLX	O7-C6-C7-C8
49	g	201	PLX	O7-C6-C7-C8
48	B	303	PEE	C13-C14-C15-C16
48	s	401	PEE	C11-C12-C13-C14
49	j	202	PLX	C34-C35-C36-C37
49	r	502	PLX	C30-C31-C32-C33
49	r	503	PLX	C28-C29-C30-C31
50	X	201	8Q1	C11-C12-C13-C14
55	l	702	CDL	C74-C75-C76-C77
55	u	201	CDL	C52-C53-C54-C55
49	a	202	PLX	C10-C11-C12-C13
55	l	702	CDL	C19-C20-C21-C22
55	m	201	CDL	C59-C60-C61-C62
48	l	701	PEE	C32-C33-C34-C35
49	r	502	PLX	C34-C35-C36-C37
55	w	401	CDL	C23-C24-C25-C26
48	j	201	PEE	C19-C20-C21-C22
48	l	704	PEE	C19-C20-C21-C22
48	B	303	PEE	C23-C24-C25-C26
55	l	702	CDL	C56-C57-C58-C59
55	l	703	CDL	C75-C76-C77-C78
55	l	702	CDL	C11-CA5-OA6-CA4
55	V	202	CDL	C37-C38-C39-C40
48	j	201	PEE	C21-C22-C23-C24
49	a	202	PLX	C35-C36-C37-C38
55	m	201	CDL	O1-C1-CB2-OB2
55	s	402	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
48	W	201	PEE	C13-C14-C15-C16
48	b	201	PEE	C31-C32-C33-C34
49	a	202	PLX	C14-C15-C16-C17
49	r	503	PLX	C10-C11-C12-C13
55	V	201	CDL	C52-C53-C54-C55
55	l	703	CDL	C41-C42-C43-C44
55	w	401	CDL	OB9-CB7-OB8-CB6
48	r	501	PEE	C31-C32-C33-C34
49	g	201	PLX	C32-C33-C34-C35
55	l	702	CDL	C71-C72-C73-C74
55	l	702	CDL	C75-C76-C77-C78
55	w	401	CDL	C62-C63-C64-C65
48	r	501	PEE	C13-C14-C15-C16
49	g	201	PLX	C33-C34-C35-C36
49	j	202	PLX	C16-C17-C18-C19
55	u	201	CDL	C73-C74-C75-C76
49	r	503	PLX	C13-C14-C15-C16
55	V	202	CDL	C82-C83-C84-C85
48	W	201	PEE	C31-C30-O3-C3
55	a	201	CDL	C71-CB7-OB8-CB6
48	s	401	PEE	C14-C15-C16-C17
49	g	201	PLX	C27-C28-C29-C30
49	j	202	PLX	C14-C15-C16-C17
49	j	202	PLX	C7-C8-C9-C10
49	r	502	PLX	C33-C34-C35-C36
55	V	201	CDL	C12-C13-C14-C15
55	w	401	CDL	C43-C44-C45-C46
55	V	201	CDL	CA5-C11-C12-C13
55	l	703	CDL	CB5-C51-C52-C53
48	W	201	PEE	C21-C22-C23-C24
48	j	201	PEE	C13-C14-C15-C16
49	g	201	PLX	C30-C31-C32-C33
49	r	502	PLX	C12-C13-C14-C15
49	r	502	PLX	C31-C32-C33-C34
50	X	201	8Q1	C12-C13-C14-C15
55	V	202	CDL	C59-C60-C61-C62
55	a	201	CDL	C35-C36-C37-C38
55	l	702	CDL	C36-C37-C38-C39
55	l	703	CDL	C14-C15-C16-C17
55	N	201	CDL	OB9-CB7-OB8-CB6
55	V	201	CDL	C34-C35-C36-C37
55	V	201	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	C73-C74-C75-C76
55	w	401	CDL	C31-C32-C33-C34
55	V	202	CDL	C33-C34-C35-C36
55	l	702	CDL	C37-C38-C39-C40
55	m	201	CDL	C16-C17-C18-C19
55	u	201	CDL	C54-C55-C56-C57
49	C	303	PLX	C2-C1-N1-C1A
49	g	201	PLX	C2-C1-N1-C1C
48	l	701	PEE	C31-C32-C33-C34
55	V	201	CDL	C35-C36-C37-C38
55	a	201	CDL	C37-C38-C39-C40
55	a	201	CDL	C54-C55-C56-C57
55	s	402	CDL	C11-C12-C13-C14
55	s	402	CDL	C51-C52-C53-C54
55	V	202	CDL	CA7-C31-C32-C33
55	l	703	CDL	C51-CB5-OB6-CB4
48	r	501	PEE	C21-C22-C23-C24
55	l	703	CDL	C54-C55-C56-C57
55	m	201	CDL	C55-C56-C57-C58
55	m	201	CDL	C58-C59-C60-C61
55	s	402	CDL	C75-C76-C77-C78
55	w	401	CDL	C57-C58-C59-C60
49	r	503	PLX	C12-C13-C14-C15
49	r	502	PLX	C28-C29-C30-C31
55	V	202	CDL	C35-C36-C37-C38
55	m	201	CDL	OB9-CB7-OB8-CB6
49	g	201	PLX	C25-C26-C27-C28
49	j	202	PLX	C9-C10-C11-C12
49	j	202	PLX	C31-C32-C33-C34
48	b	201	PEE	C33-C34-C35-C36
49	C	303	PLX	C10-C11-C12-C13
55	w	401	CDL	C75-C76-C77-C78
52	s	403	UQ	C13-C14-C16-C17
48	b	201	PEE	C22-C23-C24-C25
48	b	201	PEE	C13-C14-C15-C16
49	a	202	PLX	C25-C26-C27-C28
55	l	702	CDL	C13-C14-C15-C16
55	m	201	CDL	C21-C22-C23-C24
55	a	201	CDL	OB9-CB7-OB8-CB6
49	C	303	PLX	C13-C14-C15-C16
55	l	703	CDL	C31-C32-C33-C34
55	m	201	CDL	C79-C80-C81-C82

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Mol	Chain	Res	Type	Atoms
55	V	201	CDL	C75-C76-C77-C78
55	V	202	CDL	C52-C53-C54-C55
48	B	303	PEE	C34-C35-C36-C37
48	W	201	PEE	C12-C13-C14-C15
55	l	703	CDL	C71-C72-C73-C74
49	g	201	PLX	C13-C14-C15-C16
49	r	503	PLX	C31-C32-C33-C34
55	l	703	CDL	C34-C35-C36-C37
55	s	402	CDL	C36-C37-C38-C39
55	s	402	CDL	C71-C72-C73-C74
55	w	401	CDL	C54-C55-C56-C57
49	C	303	PLX	C28-C29-C30-C31
49	C	303	PLX	C33-C34-C35-C36
55	m	201	CDL	C15-C16-C17-C18
55	m	201	CDL	C52-C53-C54-C55
55	N	201	CDL	C51-CB5-OB6-CB4
55	V	201	CDL	C51-CB5-OB6-CB4
55	V	201	CDL	CB7-C71-C72-C73
48	C	302	PEE	C32-C33-C34-C35
55	V	202	CDL	C60-C61-C62-C63
55	l	702	CDL	C52-C53-C54-C55
55	l	703	CDL	C58-C59-C60-C61
55	s	402	CDL	C59-C60-C61-C62
49	C	303	PLX	C11-C12-C13-C14
55	a	201	CDL	C22-C23-C24-C25
55	l	702	CDL	C59-C60-C61-C62
48	B	303	PEE	C19-C20-C21-C22
55	l	703	CDL	C11-C12-C13-C14
48	b	201	PEE	C10-C11-C12-C13
48	j	201	PEE	C42-C43-C44-C45
55	a	201	CDL	C31-C32-C33-C34
55	l	703	CDL	C43-C44-C45-C46
49	C	303	PLX	C14-C15-C16-C17
55	l	703	CDL	C74-C75-C76-C77
55	w	401	CDL	C63-C64-C65-C66
49	C	303	PLX	C2-C1-N1-C1C
48	r	501	PEE	C41-C42-C43-C44
49	j	202	PLX	C33-C34-C35-C36
55	V	202	CDL	C57-C58-C59-C60
55	a	201	CDL	C75-C76-C77-C78
55	u	201	CDL	C71-C72-C73-C74
48	l	701	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
49	r	502	PLX	C11-C10-C9-C8
55	m	201	CDL	C34-C35-C36-C37
55	w	401	CDL	C71-C72-C73-C74
55	l	702	CDL	OA7-CA5-OA6-CA4
55	l	703	CDL	OB7-CB5-OB6-CB4
55	m	201	CDL	OB5-CB3-CB4-OB6
55	m	201	CDL	C37-C38-C39-C40
55	s	402	CDL	C55-C56-C57-C58
55	l	702	CDL	C51-CB5-OB6-CB4
55	l	703	CDL	C51-C52-C53-C54
55	w	401	CDL	C32-C33-C34-C35
48	W	201	PEE	O5-C30-O3-C3
48	s	401	PEE	C30-C31-C32-C33
55	a	201	CDL	CA5-C11-C12-C13
48	C	302	PEE	C35-C36-C37-C38
48	Q	501	PEE	C19-C20-C21-C22
48	r	501	PEE	C15-C16-C17-C18
55	l	702	CDL	OA6-CA4-CA6-OA8
55	V	202	CDL	C11-C12-C13-C14
55	s	402	CDL	C16-C17-C18-C19
48	B	303	PEE	C22-C23-C24-C25
48	r	501	PEE	C11-C12-C13-C14
49	g	201	PLX	C28-C29-C30-C31
55	a	201	CDL	C32-C33-C34-C35
55	s	402	CDL	C52-C53-C54-C55
48	B	303	PEE	C36-C37-C38-C39
48	B	303	PEE	C38-C39-C40-C41
55	N	201	CDL	C11-C12-C13-C14
55	V	202	CDL	C73-C74-C75-C76
55	a	201	CDL	C71-C72-C73-C74
55	s	402	CDL	C32-C33-C34-C35
50	X	201	8Q1	C9-C10-C11-C12
55	N	201	CDL	OB7-CB5-OB6-CB4
55	V	201	CDL	OB7-CB5-OB6-CB4
49	a	202	PLX	C9-C10-C11-C12
55	w	401	CDL	C11-C12-C13-C14
48	j	201	PEE	C14-C15-C16-C17
49	a	202	PLX	C33-C34-C35-C36
55	m	201	CDL	C11-C12-C13-C14
55	u	201	CDL	C51-C52-C53-C54
49	j	202	PLX	C27-C28-C29-C30
55	N	201	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
49	g	201	PLX	C12-C13-C14-C15
55	s	402	CDL	C54-C55-C56-C57
55	V	202	CDL	C84-C85-C86-C87
55	V	202	CDL	C55-C56-C57-C58
49	g	201	PLX	C11-C12-C13-C14
49	g	201	PLX	C10-C11-C12-C13
55	V	202	CDL	C56-C57-C58-C59
48	C	302	PEE	C41-C42-C43-C44
49	r	502	PLX	C27-C28-C29-C30
49	r	503	PLX	C14-C15-C16-C17
55	l	702	CDL	C12-C13-C14-C15
48	B	303	PEE	C35-C36-C37-C38
48	s	401	PEE	C19-C20-C21-C22
48	l	704	PEE	C11-C12-C13-C14
55	l	703	CDL	C32-C33-C34-C35
48	l	704	PEE	O3P-C1-C2-C3
55	N	201	CDL	OA5-CA3-CA4-CA6
55	m	201	CDL	OA5-CA3-CA4-CA6
49	a	202	PLX	C27-C28-C29-C30
55	m	201	CDL	C41-C42-C43-C44
55	m	201	CDL	C20-C21-C22-C23
55	w	401	CDL	CA5-C11-C12-C13
49	j	202	PLX	O6-C6-C7-C8
49	r	503	PLX	C30-C31-C32-C33
55	l	702	CDL	C73-C74-C75-C76
55	w	401	CDL	C17-C18-C19-C20
55	a	201	CDL	C82-C83-C84-C85
55	l	702	CDL	C17-C18-C19-C20
48	s	401	PEE	C1-C2-C3-O3
49	C	303	PLX	C3-C4-C5-O8
49	g	201	PLX	C3-C4-C5-O8
49	r	503	PLX	C3-C4-C5-O8
55	l	703	CDL	CA3-CA4-CA6-OA8
48	C	302	PEE	C43-C44-C45-C46
48	Q	501	PEE	C35-C36-C37-C38
48	s	401	PEE	C15-C16-C17-C18
49	j	202	PLX	C26-C27-C28-C29
55	l	702	CDL	C51-C52-C53-C54
55	m	201	CDL	C62-C63-C64-C65
55	s	402	CDL	C17-C18-C19-C20
55	N	201	CDL	C51-C52-C53-C54
49	C	303	PLX	C2-C1-N1-C1B

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	C76-C77-C78-C79
55	w	401	CDL	C53-C54-C55-C56
48	r	501	PEE	C36-C37-C38-C39
55	w	401	CDL	C83-C84-C85-C86
55	m	201	CDL	C75-C76-C77-C78
55	V	201	CDL	CA6-CA4-OA6-CA5
48	l	704	PEE	C40-C41-C42-C43
55	V	202	CDL	C62-C63-C64-C65
55	l	702	CDL	C15-C16-C17-C18
55	m	201	CDL	C14-C15-C16-C17
55	m	201	CDL	C33-C34-C35-C36
52	s	403	UQ	C22-C23-C24-C25
48	l	704	PEE	C39-C40-C41-C42
49	r	503	PLX	C27-C28-C29-C30
55	s	402	CDL	C35-C36-C37-C38
55	w	401	CDL	C52-C53-C54-C55
55	w	401	CDL	C73-C74-C75-C76
49	C	303	PLX	C7-C8-C9-C10
55	m	201	CDL	C36-C37-C38-C39
55	a	201	CDL	C11-C12-C13-C14
55	s	402	CDL	C31-C32-C33-C34
48	W	201	PEE	C24-C25-C26-C27
49	C	303	PLX	O4-C3-C4-O6
55	V	202	CDL	OA5-CA3-CA4-OA6
55	l	702	CDL	OB5-CB3-CB4-OB6
48	Q	501	PEE	C11-C12-C13-C14
49	r	502	PLX	C14-C15-C16-C17
55	a	201	CDL	C55-C56-C57-C58
49	j	202	PLX	C29-C30-C31-C32
55	V	202	CDL	C17-C18-C19-C20
49	a	202	PLX	C18-C19-C20-C21
52	s	403	UQ	C12-C11-C9-C10
55	l	703	CDL	C64-C65-C66-C67
48	Q	501	PEE	C21-C22-C23-C24
55	V	202	CDL	C12-C13-C14-C15
55	V	202	CDL	C54-C55-C56-C57
55	w	401	CDL	C42-C43-C44-C45
55	w	401	CDL	C56-C57-C58-C59
55	V	201	CDL	C58-C59-C60-C61
55	a	201	CDL	C52-C53-C54-C55
55	a	201	CDL	C84-C85-C86-C87
49	a	202	PLX	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
48	b	201	PEE	O2-C2-C3-O3
49	C	303	PLX	O6-C4-C5-O8
55	s	402	CDL	OB6-CB4-CB6-OB8
49	j	202	PLX	C25-C26-C27-C28
55	u	201	CDL	C75-C76-C77-C78
55	w	401	CDL	C84-C85-C86-C87
48	B	303	PEE	C12-C13-C14-C15
55	V	202	CDL	C13-C14-C15-C16
55	w	401	CDL	C59-C60-C61-C62
49	j	202	PLX	C11-C12-C13-C14
49	C	303	PLX	C11-C10-C9-C8
49	g	201	PLX	C18-C19-C20-C21
55	l	702	CDL	C35-C36-C37-C38
48	B	303	PEE	C17-C18-C19-C20
49	r	503	PLX	C32-C33-C34-C35
48	l	701	PEE	C13-C14-C15-C16
55	m	201	CDL	C39-C40-C41-C42
50	X	201	8Q1	N41-C42-C43-S44
55	V	202	CDL	C75-C76-C77-C78
48	l	704	PEE	C13-C14-C15-C16
55	a	201	CDL	C20-C21-C22-C23
55	a	201	CDL	C74-C75-C76-C77
55	N	201	CDL	C52-C53-C54-C55
49	C	303	PLX	O4-C3-C4-C5
55	V	201	CDL	OA5-CA3-CA4-CA6
55	V	201	CDL	OB5-CB3-CB4-CB6
55	a	201	CDL	OB5-CB3-CB4-CB6
55	l	702	CDL	OA5-CA3-CA4-CA6
55	m	201	CDL	OB5-CB3-CB4-CB6
55	s	402	CDL	OA5-CA3-CA4-CA6
55	u	201	CDL	OA5-CA3-CA4-CA6
55	w	401	CDL	C64-C65-C66-C67
55	V	201	CDL	C73-C74-C75-C76
55	s	402	CDL	CB5-C51-C52-C53
47	A	503	NAI	O4D-C4D-C5D-O5D
48	j	201	PEE	C34-C35-C36-C37
48	r	501	PEE	C33-C34-C35-C36
48	Q	501	PEE	C18-C19-C20-C21
48	j	201	PEE	C38-C39-C40-C41
55	l	703	CDL	C84-C85-C86-C87
55	V	202	CDL	C34-C35-C36-C37
55	w	401	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
48	C	302	PEE	C13-C14-C15-C16
49	r	503	PLX	C7-C8-C9-C10
49	r	503	PLX	C36-C37-C38-C39
48	j	201	PEE	C22-C23-C24-C25
48	l	704	PEE	C32-C33-C34-C35
55	l	703	CDL	C52-C53-C54-C55
55	s	402	CDL	CA5-C11-C12-C13
55	m	201	CDL	C56-C57-C58-C59
48	b	201	PEE	C1-C2-C3-O3
48	r	501	PEE	C1-C2-C3-O3
49	a	202	PLX	C3-C4-C5-O8
49	r	502	PLX	C3-C4-C5-O8
55	V	202	CDL	CA3-CA4-CA6-OA8
55	l	702	CDL	CA3-CA4-CA6-OA8
55	m	201	CDL	CB3-CB4-CB6-OB8
55	s	402	CDL	CB3-CB4-CB6-OB8
48	Q	501	PEE	C24-C25-C26-C27
48	Q	501	PEE	C14-C15-C16-C17
55	s	402	CDL	C12-C13-C14-C15
55	l	703	CDL	C62-C63-C64-C65
48	Q	501	PEE	C23-C24-C25-C26
55	l	702	CDL	C76-C77-C78-C79
55	l	703	CDL	C38-C39-C40-C41
48	s	401	PEE	C13-C14-C15-C16
55	l	702	CDL	C31-C32-C33-C34
48	B	303	PEE	O3P-C1-C2-O2
55	V	201	CDL	OB5-CB3-CB4-OB6
55	a	201	CDL	OA5-CA3-CA4-OA6
49	r	503	PLX	C16-C17-C18-C19
55	s	402	CDL	C15-C16-C17-C18
55	a	201	CDL	C38-C39-C40-C41
48	b	201	PEE	C23-C24-C25-C26
55	V	202	CDL	C74-C75-C76-C77
49	C	303	PLX	C19-C20-C21-C22
55	l	702	CDL	C54-C55-C56-C57
52	s	403	UQ	C27-C28-C29-C30
48	s	401	PEE	C12-C13-C14-C15
48	l	701	PEE	O2-C2-C3-O3
48	s	401	PEE	O2-C2-C3-O3
55	V	202	CDL	OB6-CB4-CB6-OB8
55	m	201	CDL	OB6-CB4-CB6-OB8
55	l	702	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
55	l	703	CDL	C44-C45-C46-C47
55	V	201	CDL	C38-C39-C40-C41
48	j	201	PEE	C36-C37-C38-C39
49	g	201	PLX	O6-C6-C7-C8
49	a	202	PLX	C7-C8-C9-C10
55	m	201	CDL	C32-C33-C34-C35
55	V	201	CDL	C44-C45-C46-C47
55	s	402	CDL	C34-C35-C36-C37
49	a	202	PLX	C30-C31-C32-C33
55	V	201	CDL	C72-C73-C74-C75
55	a	201	CDL	C12-C13-C14-C15
48	l	704	PEE	C44-C45-C46-C47
55	V	201	CDL	C54-C55-C56-C57
55	V	201	CDL	C71-C72-C73-C74
55	V	201	CDL	C64-C65-C66-C67
48	W	201	PEE	O3P-C1-C2-C3
48	r	501	PEE	O3P-C1-C2-C3
55	N	201	CDL	OB5-CB3-CB4-CB6
55	V	202	CDL	OA5-CA3-CA4-CA6
55	a	201	CDL	OA5-CA3-CA4-CA6
48	B	303	PEE	C21-C22-C23-C24
48	b	201	PEE	C32-C33-C34-C35
49	a	202	PLX	C28-C29-C30-C31
55	w	401	CDL	C41-C42-C43-C44
49	r	502	PLX	C4-C5-O8-C24
55	l	702	CDL	OB7-CB5-OB6-CB4
48	l	704	PEE	C3-C2-O2-C10
55	m	201	CDL	CA6-CA4-OA6-CA5
49	C	303	PLX	C12-C13-C14-C15
55	s	402	CDL	C40-C41-C42-C43
55	V	201	CDL	C17-C18-C19-C20
55	w	401	CDL	C13-C14-C15-C16
48	l	704	PEE	C31-C32-C33-C34
48	s	401	PEE	C23-C24-C25-C26
48	W	201	PEE	O3P-C1-C2-O2
48	j	201	PEE	O3P-C1-C2-O2
49	r	502	PLX	O4-C3-C4-O6
49	r	503	PLX	O4-C3-C4-O6
55	N	201	CDL	OB5-CB3-CB4-OB6
55	a	201	CDL	OB5-CB3-CB4-OB6
55	l	703	CDL	OA5-CA3-CA4-OA6
55	u	201	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
48	l	701	PEE	C1-C2-C3-O3
55	w	401	CDL	CA3-CA4-CA6-OA8
48	j	201	PEE	C37-C38-C39-C40
55	a	201	CDL	C14-C15-C16-C17
48	j	201	PEE	C15-C16-C17-C18
48	r	501	PEE	O2-C2-C3-O3
49	j	202	PLX	C10-C11-C12-C13
55	l	703	CDL	C12-C13-C14-C15
55	s	402	CDL	C80-C81-C82-C83
55	w	401	CDL	C11-CA5-OA6-CA4
49	a	202	PLX	C11-C12-C13-C14
51	J	401	NDP	O4B-C4B-C5B-O5B
57	w	402	ADP	PB-O3A-PA-O1A
55	w	401	CDL	C15-C16-C17-C18
48	b	201	PEE	C34-C35-C36-C37
55	m	201	CDL	C71-C72-C73-C74
49	a	202	PLX	C25-C24-O8-C5
49	g	201	PLX	C25-C24-O8-C5
55	u	201	CDL	C71-CB7-OB8-CB6
48	j	201	PEE	O3P-C1-C2-C3
48	l	701	PEE	O3P-C1-C2-C3
49	r	502	PLX	O4-C3-C4-C5
49	r	503	PLX	O4-C3-C4-C5
55	l	703	CDL	OA5-CA3-CA4-CA6
50	G	201	8Q1	O27-C28-C29-C30
55	w	401	CDL	C77-C78-C79-C80
55	V	202	CDL	C64-C65-C66-C67
55	a	201	CDL	C18-C19-C20-C21
51	J	401	NDP	C3B-C4B-C5B-O5B
55	u	201	CDL	OB9-CB7-OB8-CB6
48	l	701	PEE	C2-C1-O3P-P
55	V	201	CDL	CB4-CB3-OB5-PB2
55	m	201	CDL	CA4-CA3-OA5-PA1
55	w	401	CDL	C1-CB2-OB2-PB2
55	V	201	CDL	C74-C75-C76-C77
55	s	402	CDL	C74-C75-C76-C77
49	j	202	PLX	O8-C24-C25-C26
49	r	502	PLX	O8-C24-C25-C26
48	b	201	PEE	O3P-C1-C2-O2
48	l	701	PEE	O3P-C1-C2-O2
48	r	501	PEE	O3P-C1-C2-O2
55	l	702	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
55	V	202	CDL	C15-C16-C17-C18
55	V	202	CDL	C58-C59-C60-C61
48	B	303	PEE	C16-C17-C18-C19
49	j	202	PLX	C15-C16-C17-C18
48	l	704	PEE	O2-C2-C3-O3
49	a	202	PLX	O6-C4-C5-O8
49	r	502	PLX	O6-C4-C5-O8
49	r	503	PLX	O6-C4-C5-O8
55	l	703	CDL	OB6-CB4-CB6-OB8
55	l	703	CDL	CB3-CB4-CB6-OB8
48	b	201	PEE	C14-C15-C16-C17
55	l	703	CDL	C55-C56-C57-C58
55	w	401	CDL	OA7-CA5-OA6-CA4
47	A	503	NAI	C5B-O5B-PA-O1A
47	A	503	NAI	C5B-O5B-PA-O2A
47	A	503	NAI	C5B-O5B-PA-O3
48	C	302	PEE	C1-O3P-P-O2P
48	Q	501	PEE	C1-O3P-P-O1P
48	Q	501	PEE	C4-O4P-P-O3P
48	Q	501	PEE	C4-O4P-P-O2P
48	b	201	PEE	C1-O3P-P-O2P
48	b	201	PEE	C1-O3P-P-O1P
48	b	201	PEE	C1-O3P-P-O4P
48	j	201	PEE	C1-O3P-P-O2P
48	l	701	PEE	C4-O4P-P-O1P
48	s	401	PEE	C4-O4P-P-O1P
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	C2-O1-P1-O3
49	r	503	PLX	C3-C4-O6-C6
49	r	503	PLX	C5-C4-O6-C6
49	r	503	PLX	C2-O1-P1-O3
55	N	201	CDL	CA2-OA2-PA1-OA4
55	N	201	CDL	CA3-OA5-PA1-OA3
55	N	201	CDL	CB2-OB2-PB2-OB4
55	N	201	CDL	CB3-OB5-PB2-OB4
55	V	201	CDL	CB2-OB2-PB2-OB4
55	V	202	CDL	CA3-OA5-PA1-OA2
55	V	202	CDL	CA3-OA5-PA1-OA3
55	V	202	CDL	CA3-OA5-PA1-OA4
55	V	202	CDL	CB2-OB2-PB2-OB4
55	V	202	CDL	CB3-OB5-PB2-OB2
55	V	202	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
55	V	202	CDL	CB3-OB5-PB2-OB4
55	a	201	CDL	CB2-OB2-PB2-OB4
55	l	702	CDL	CB3-OB5-PB2-OB2
55	l	702	CDL	CB3-OB5-PB2-OB4
55	l	703	CDL	CB3-OB5-PB2-OB3
55	m	201	CDL	CA2-OA2-PA1-OA5
55	m	201	CDL	CB2-OB2-PB2-OB4
55	w	401	CDL	CA3-OA5-PA1-OA3
55	w	401	CDL	CB2-OB2-PB2-OB4
57	w	402	ADP	C5'-O5'-PA-O3A
51	J	401	NDP	O4D-C1D-N1N-C6N
55	l	703	CDL	C12-C11-CA5-OA6
49	a	202	PLX	C34-C35-C36-C37
55	l	703	CDL	C39-C40-C41-C42
49	r	502	PLX	C16-C17-C18-C19
49	r	503	PLX	C11-C12-C13-C14
48	W	201	PEE	C23-C24-C25-C26
55	l	702	CDL	C80-C81-C82-C83
48	B	303	PEE	O3P-C1-C2-C3
48	b	201	PEE	O3P-C1-C2-C3
55	l	702	CDL	OB5-CB3-CB4-CB6
48	s	401	PEE	C18-C19-C20-C21
55	V	201	CDL	OA5-CA3-CA4-OA6
55	N	201	CDL	CB5-C51-C52-C53
55	u	201	CDL	C72-C73-C74-C75
55	w	401	CDL	C44-C45-C46-C47
55	s	402	CDL	C13-C14-C15-C16
52	s	403	UQ	C1-C2-O2-CM2
55	m	201	CDL	C54-C55-C56-C57
55	V	202	CDL	C83-C84-C85-C86
55	l	703	CDL	C60-C61-C62-C63
48	C	302	PEE	C11-C12-C13-C14
48	C	302	PEE	C34-C35-C36-C37
48	r	501	PEE	C20-C21-C22-C23
48	l	701	PEE	C18-C19-C20-C21
48	B	303	PEE	O5-C30-O3-C3
55	N	201	CDL	C31-CA7-OA8-CA6
55	V	202	CDL	CA5-C11-C12-C13
55	s	402	CDL	C83-C84-C85-C86
48	B	303	PEE	C31-C30-O3-C3
48	s	401	PEE	C16-C17-C18-C19
48	C	302	PEE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
55	l	703	CDL	C32-C31-CA7-OA8
49	r	502	PLX	C25-C26-C27-C28
55	a	201	CDL	C39-C40-C41-C42
52	J	402	UQ	C9-C11-C12-C13
55	V	202	CDL	C19-C20-C21-C22
48	C	302	PEE	C12-C13-C14-C15
55	s	402	CDL	C84-C85-C86-C87
48	B	303	PEE	C42-C43-C44-C45
49	g	201	PLX	C20-C21-C22-C23
55	w	401	CDL	C19-C20-C21-C22
48	l	704	PEE	C23-C24-C25-C26
55	a	201	CDL	C34-C35-C36-C37
49	C	303	PLX	O8-C24-C25-C26
49	a	202	PLX	O8-C24-C25-C26
55	m	201	CDL	C84-C85-C86-C87
55	V	201	CDL	CA4-CA3-OA5-PA1
49	j	202	PLX	C12-C13-C14-C15
55	l	703	CDL	C57-C58-C59-C60
55	N	201	CDL	OA9-CA7-OA8-CA6
48	C	302	PEE	C42-C43-C44-C45
48	r	501	PEE	C16-C17-C18-C19
55	N	201	CDL	O1-C1-CB2-OB2
55	s	402	CDL	C77-C78-C79-C80
50	G	201	8Q1	C29-C32-C34-N36
48	b	201	PEE	C15-C16-C17-C18
55	w	401	CDL	OB6-CB4-CB6-OB8
49	a	202	PLX	C24-C25-C26-C27
55	m	201	CDL	C13-C14-C15-C16
48	b	201	PEE	C16-C17-C18-C19
55	l	703	CDL	C1-CB2-OB2-PB2
55	u	201	CDL	C57-C58-C59-C60
48	r	501	PEE	C38-C39-C40-C41
55	V	202	CDL	CB3-CB4-CB6-OB8
48	W	201	PEE	C34-C35-C36-C37
55	u	201	CDL	C56-C57-C58-C59
50	X	201	8Q1	C10-C11-C12-C13
47	A	503	NAI	O4D-C1D-N1N-C2N
55	a	201	CDL	C40-C41-C42-C43
48	B	303	PEE	C44-C45-C46-C47
48	W	201	PEE	C33-C34-C35-C36
55	V	202	CDL	C77-C78-C79-C80
48	b	201	PEE	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
55	l	702	CDL	C24-C25-C26-C27
55	l	702	CDL	C33-C34-C35-C36
47	A	503	NAI	C2N-C3N-C7N-N7N
48	r	501	PEE	C31-C30-O3-C3
55	m	201	CDL	C31-CA7-OA8-CA6
55	V	202	CDL	C32-C31-CA7-OA8
48	C	302	PEE	C19-C20-C21-C22
48	l	704	PEE	C15-C16-C17-C18
48	j	201	PEE	C2-C3-O3-C30
55	s	402	CDL	C18-C19-C20-C21
55	V	202	CDL	C71-C72-C73-C74
49	g	201	PLX	O8-C24-C25-C26
49	C	303	PLX	C15-C16-C17-C18
55	u	201	CDL	CA5-C11-C12-C13
55	l	703	CDL	C15-C16-C17-C18
48	b	201	PEE	C11-C12-C13-C14
49	g	201	PLX	C16-C17-C18-C19
49	r	503	PLX	C33-C34-C35-C36
55	m	201	CDL	OA9-CA7-OA8-CA6
55	l	702	CDL	CB4-CB3-OB5-PB2
48	j	201	PEE	C32-C33-C34-C35
55	V	202	CDL	C42-C43-C44-C45
48	r	501	PEE	O5-C30-O3-C3
49	C	303	PLX	O9-C24-C25-C26
55	a	201	CDL	C79-C80-C81-C82
49	r	503	PLX	C35-C36-C37-C38
48	C	302	PEE	C38-C39-C40-C41
48	l	704	PEE	C16-C17-C18-C19
55	w	401	CDL	C72-C71-CB7-OB8
49	r	503	PLX	C15-C16-C17-C18
48	l	704	PEE	C10-C11-C12-C13
48	j	201	PEE	C40-C41-C42-C43
55	u	201	CDL	OB5-CB3-CB4-CB6
48	Q	501	PEE	C34-C35-C36-C37
55	l	702	CDL	OB6-CB4-CB6-OB8
55	u	201	CDL	OA6-CA4-CA6-OA8
55	s	402	CDL	C72-C71-CB7-OB8
55	s	402	CDL	C39-C40-C41-C42
48	b	201	PEE	C38-C39-C40-C41
48	b	201	PEE	C21-C22-C23-C24
48	B	303	PEE	C10-C11-C12-C13
48	B	303	PEE	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
46	A	502	FMN	C5'-O5'-P-O3P
49	C	303	PLX	C4-C5-O8-C24
48	W	201	PEE	C18-C19-C20-C21
48	l	701	PEE	C38-C39-C40-C41
55	V	201	CDL	C53-C54-C55-C56
49	C	303	PLX	C31-C32-C33-C34
48	Q	501	PEE	C16-C17-C18-C19
48	Q	501	PEE	C38-C39-C40-C41
48	l	701	PEE	C36-C37-C38-C39
55	a	201	CDL	C61-C62-C63-C64
49	j	202	PLX	C28-C29-C30-C31
48	C	302	PEE	C16-C17-C18-C19
47	A	503	NAI	C2D-C1D-N1N-C2N
48	s	401	PEE	C22-C23-C24-C25
48	l	704	PEE	C41-C42-C43-C44
48	l	704	PEE	C1-C2-C3-O3
48	W	201	PEE	C16-C17-C18-C19
55	l	702	CDL	C82-C83-C84-C85
55	a	201	CDL	C44-C45-C46-C47
49	r	502	PLX	C18-C19-C20-C21
49	C	303	PLX	C16-C17-C18-C19
55	l	703	CDL	C72-C71-CB7-OB8
55	s	402	CDL	C12-C11-CA5-OA6
48	s	401	PEE	C31-C32-C33-C34
55	a	201	CDL	C64-C65-C66-C67
49	j	202	PLX	C7-C6-O6-C4
55	V	201	CDL	C12-C11-CA5-OA6
55	V	202	CDL	C52-C51-CB5-OB6
49	r	503	PLX	C9-C10-C11-C12
55	N	201	CDL	C12-C11-CA5-OA6
55	l	702	CDL	C72-C71-CB7-OB8
48	l	704	PEE	C36-C37-C38-C39
48	j	201	PEE	C23-C24-C25-C26
48	b	201	PEE	C20-C21-C22-C23
48	C	302	PEE	O3-C30-C31-C32
55	u	201	CDL	C52-C51-CB5-OB6
55	a	201	CDL	C33-C34-C35-C36
55	l	703	CDL	C63-C64-C65-C66
50	G	201	8Q1	C11-C12-C13-C14
49	r	502	PLX	C35-C36-C37-C38
55	a	201	CDL	C58-C59-C60-C61
50	G	201	8Q1	C29-C32-C34-O35

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	C21-C22-C23-C24
48	b	201	PEE	O3-C30-C31-C32
55	N	201	CDL	C72-C71-CB7-OB8
55	w	401	CDL	C52-C51-CB5-OB6
50	G	201	8Q1	C12-C13-C14-C15
55	m	201	CDL	C52-C51-CB5-OB6
49	g	201	PLX	C11-C10-C9-C8
55	a	201	CDL	C32-C31-CA7-OA8
50	G	201	8Q1	O27-C28-C29-C31
55	m	201	CDL	CA2-C1-CB2-OB2
55	w	401	CDL	C12-C11-CA5-OA6
49	r	503	PLX	C18-C19-C20-C21
49	g	201	PLX	C6-C7-C8-C9
49	a	202	PLX	C12-C13-C14-C15
55	l	703	CDL	C40-C41-C42-C43
55	V	202	CDL	OA7-CA5-OA6-CA4
48	C	302	PEE	C44-C45-C46-C47
48	Q	501	PEE	C2-C1-O3P-P
55	l	702	CDL	C72-C71-CB7-OB9
48	l	701	PEE	O2-C10-C11-C12
55	V	201	CDL	C32-C31-CA7-OA8
55	V	202	CDL	C63-C64-C65-C66
49	a	202	PLX	C6-C7-C8-C9
55	l	703	CDL	C72-C71-CB7-OB9
55	w	401	CDL	C52-C51-CB5-OB7
55	l	703	CDL	C82-C83-C84-C85
49	a	202	PLX	O9-C24-O8-C5
48	C	302	PEE	O5-C30-C31-C32
48	b	201	PEE	O5-C30-C31-C32
55	V	201	CDL	C12-C11-CA5-OA7
48	l	701	PEE	C12-C13-C14-C15
50	X	201	8Q1	C6-C7-C8-C9
55	N	201	CDL	C12-C11-CA5-OA7
55	V	202	CDL	C52-C51-CB5-OB7
55	s	402	CDL	C12-C11-CA5-OA7
55	u	201	CDL	C52-C51-CB5-OB7
49	g	201	PLX	C4-C5-O8-C24
49	j	202	PLX	C4-C5-O8-C24
55	l	702	CDL	C63-C64-C65-C66
48	j	201	PEE	O3-C30-C31-C32
55	V	202	CDL	C11-CA5-OA6-CA4
55	l	703	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	C17-C18-C19-C20
55	l	702	CDL	C14-C15-C16-C17
55	m	201	CDL	C52-C51-CB5-OB7
55	u	201	CDL	C72-C71-CB7-OB8
55	m	201	CDL	C17-C18-C19-C20
55	w	401	CDL	C12-C11-CA5-OA7
48	B	303	PEE	C14-C15-C16-C17
55	a	201	CDL	C32-C31-CA7-OA9

There are no ring outliers.

36 monomers are involved in 150 short contacts:

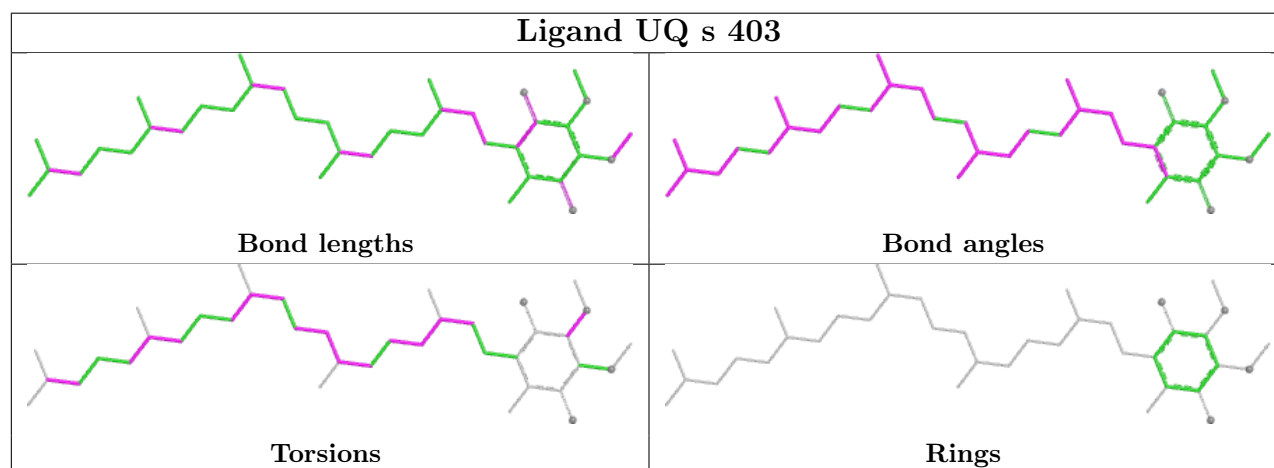
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	s	403	UQ	10	0
52	J	402	UQ	2	0
55	m	201	CDL	13	0
55	u	201	CDL	4	0
57	w	402	ADP	2	0
45	C	301	SF4	1	0
50	X	201	8Q1	3	0
47	A	503	NAI	3	0
49	C	303	PLX	5	0
49	g	201	PLX	7	0
48	l	701	PEE	1	0
55	s	402	CDL	7	0
55	N	201	CDL	1	0
55	l	702	CDL	9	0
48	r	501	PEE	9	0
48	s	401	PEE	3	0
48	Q	501	PEE	1	0
55	a	201	CDL	2	0
50	G	201	8Q1	6	0
48	b	201	PEE	4	0
45	M	801	SF4	2	0
49	a	202	PLX	1	0
51	J	401	NDP	3	0
49	j	202	PLX	2	0
55	w	401	CDL	13	0
49	r	503	PLX	2	0
48	C	302	PEE	1	0
45	A	501	SF4	1	0
49	r	502	PLX	5	0

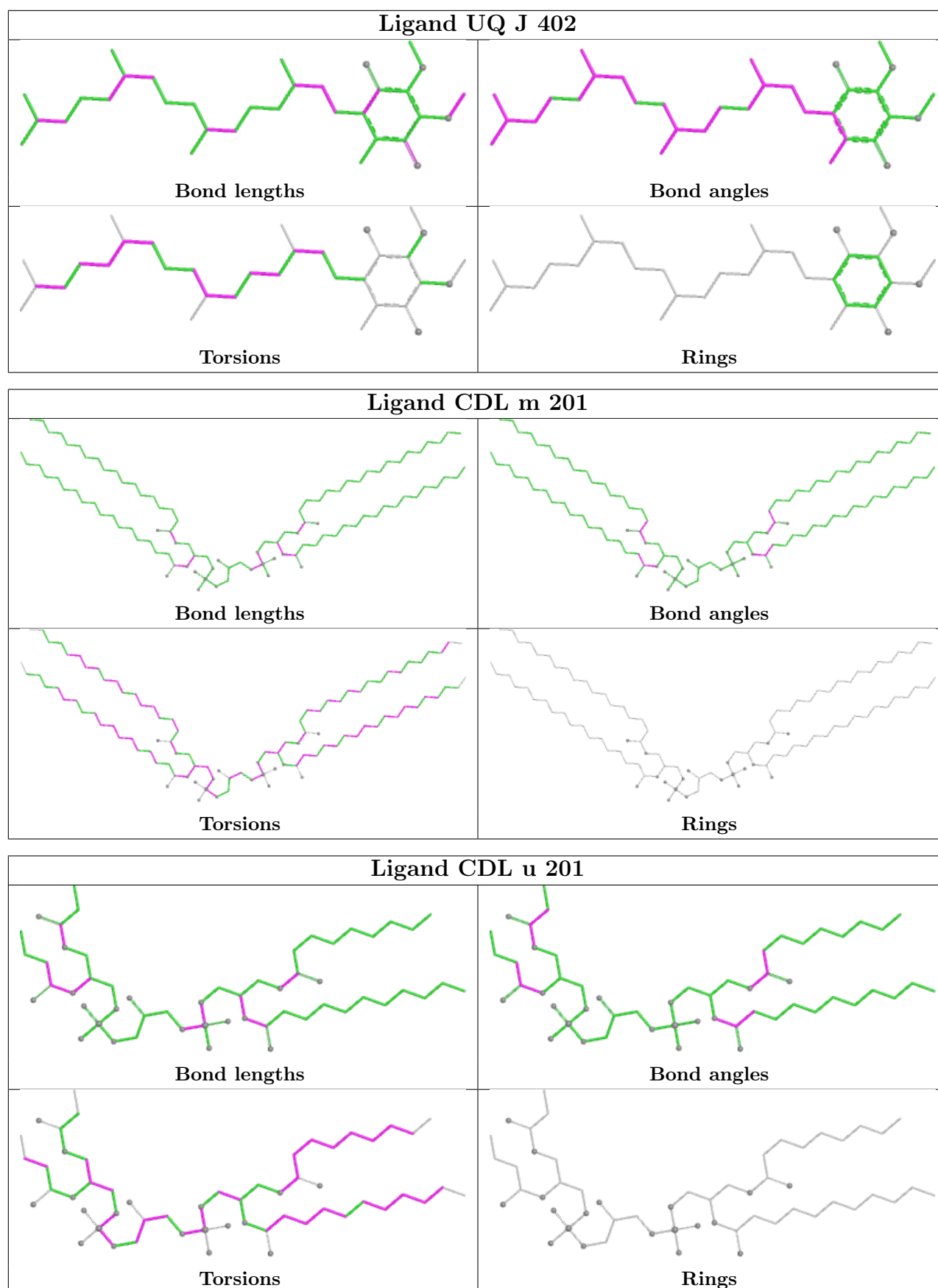
Continued on next page...

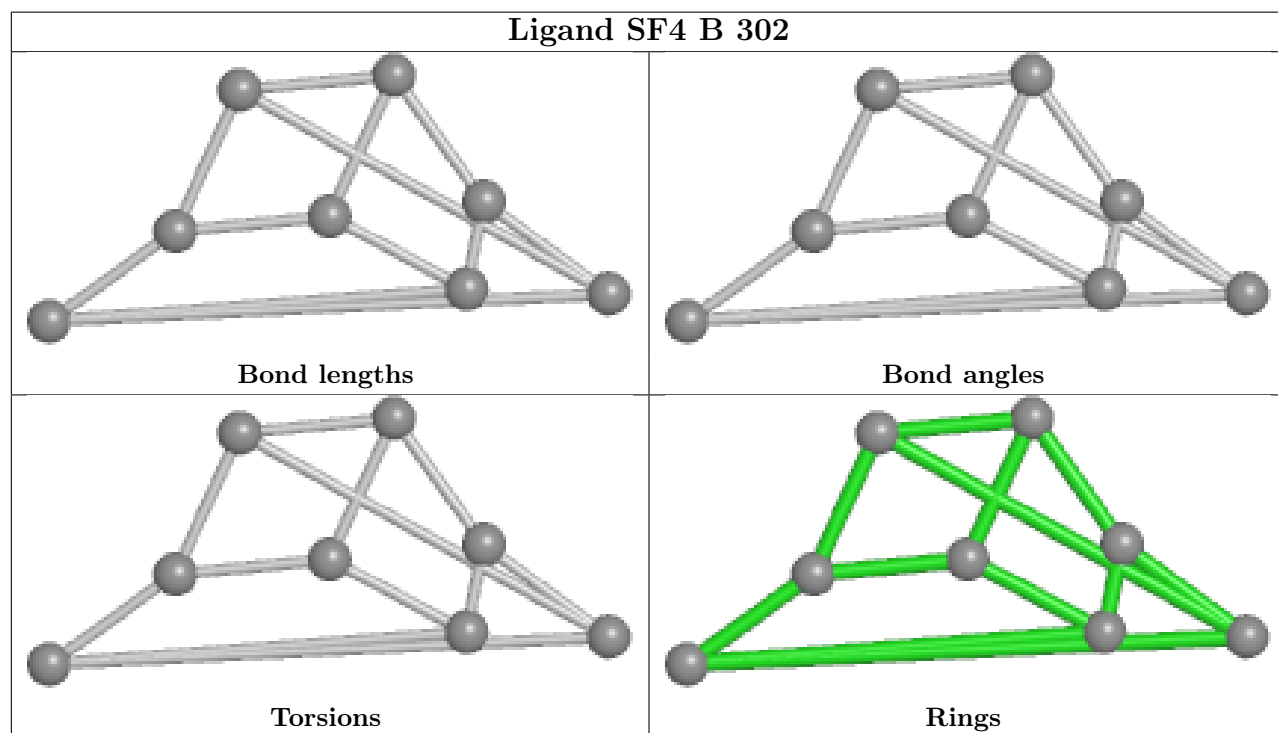
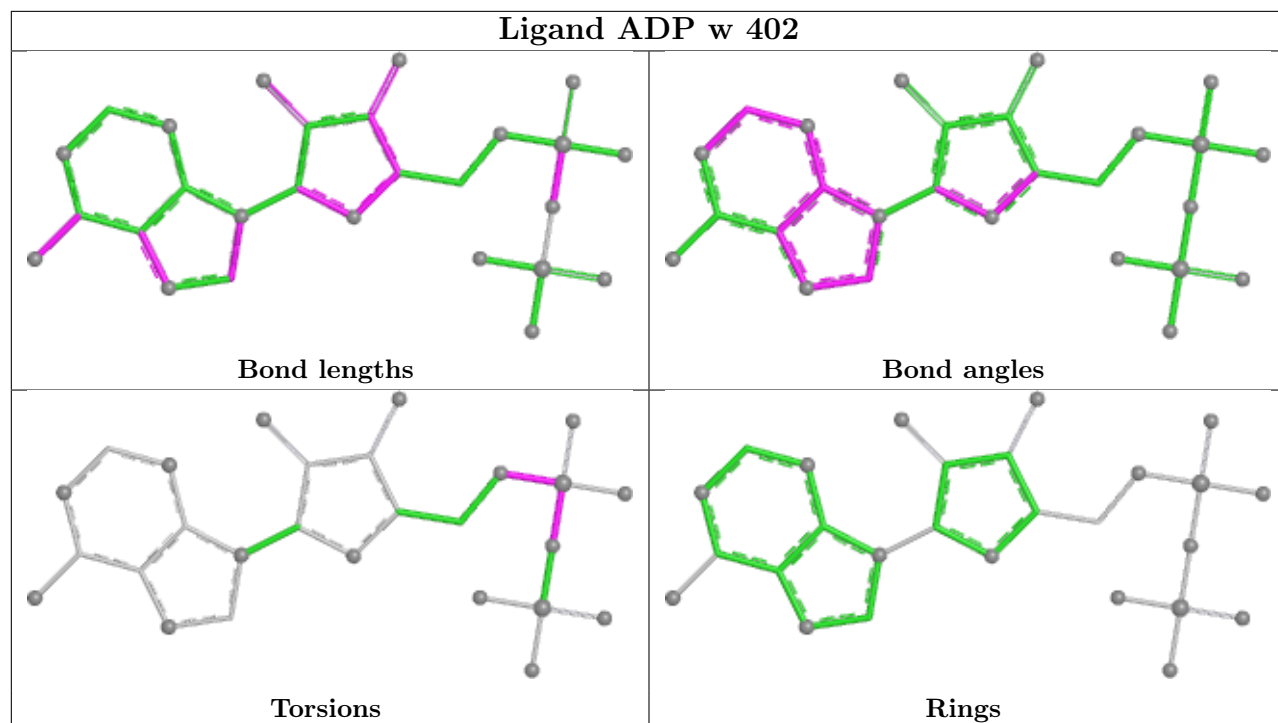
Continued from previous page...

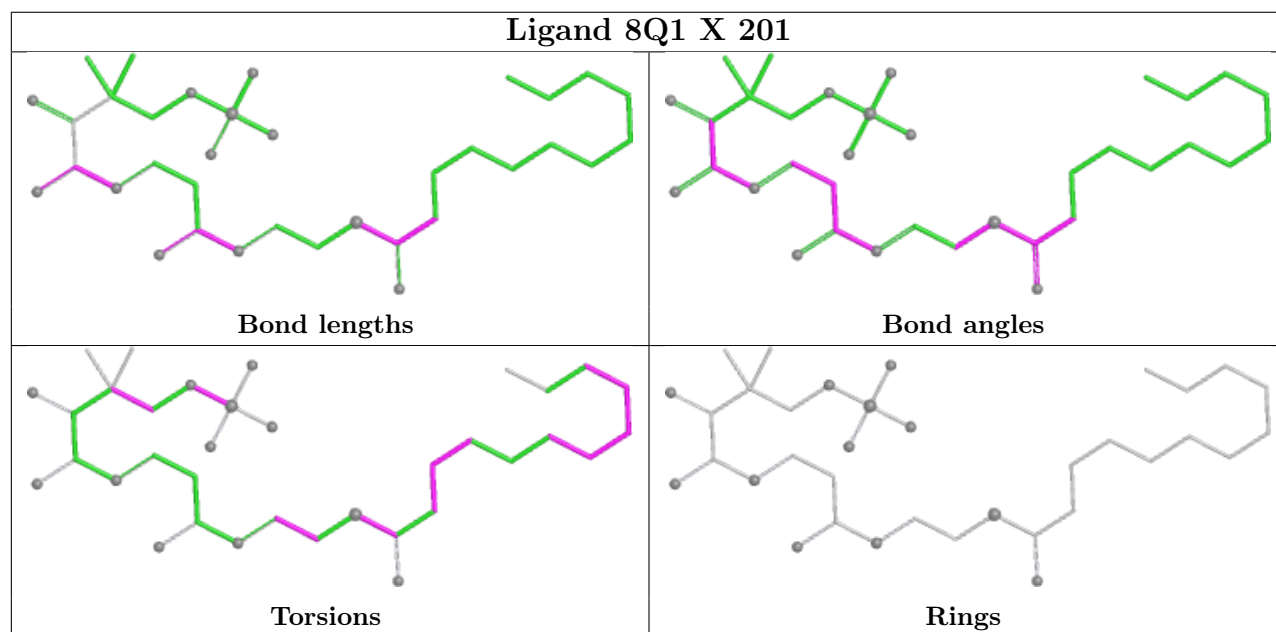
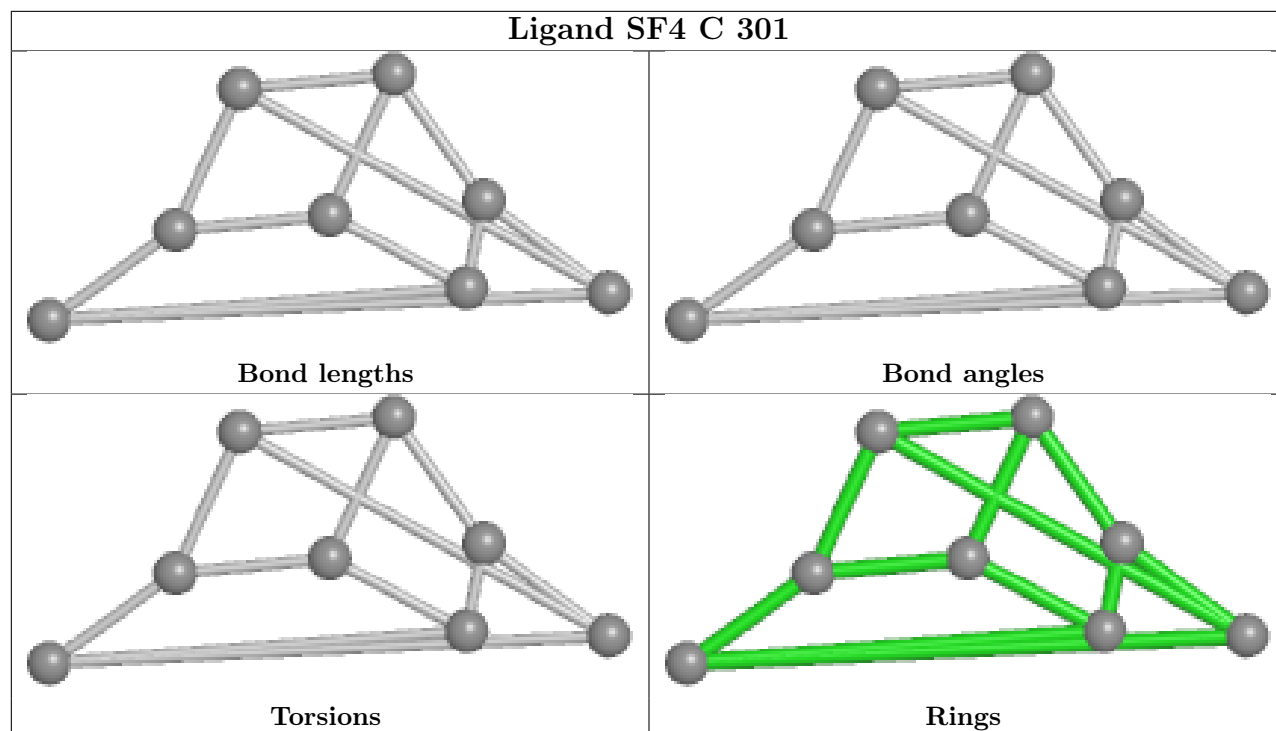
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	j	201	PEE	4	0
48	l	704	PEE	2	0
55	V	201	CDL	3	0
46	A	502	FMN	3	0
55	l	703	CDL	7	0
48	B	303	PEE	6	0
55	V	202	CDL	5	0

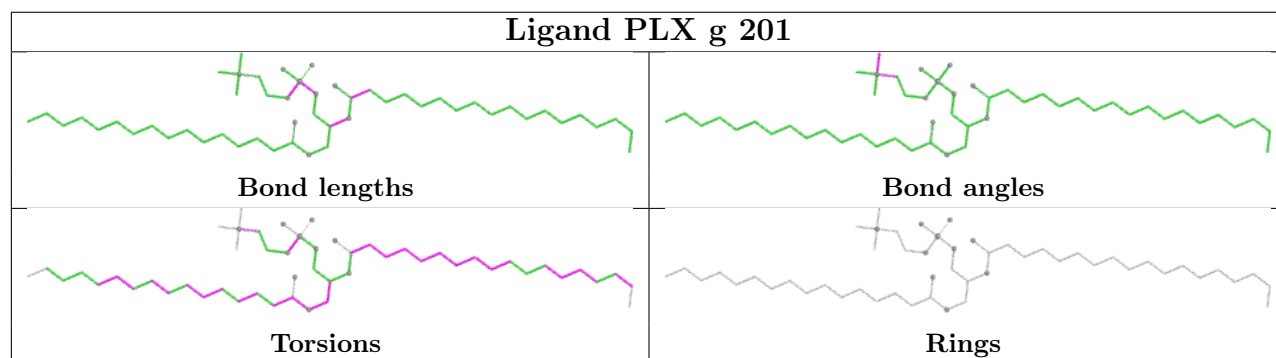
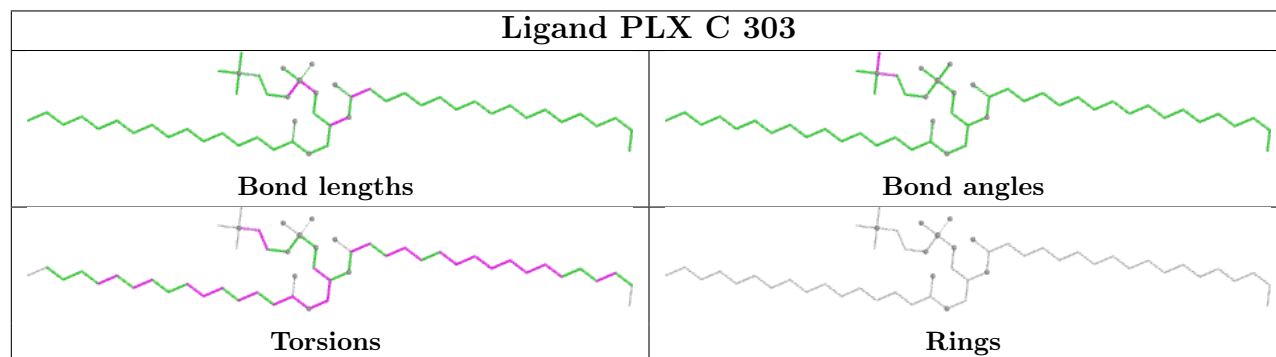
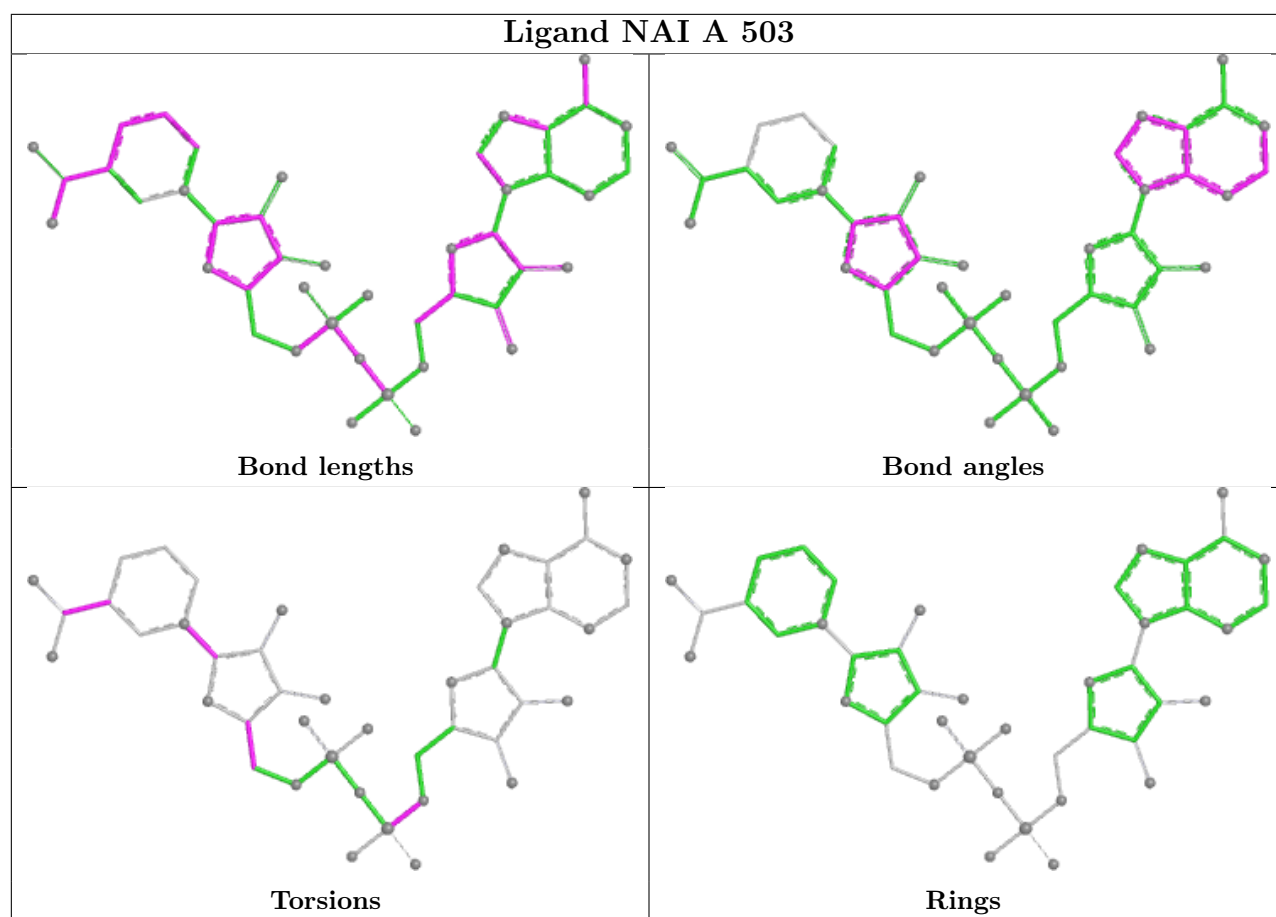
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

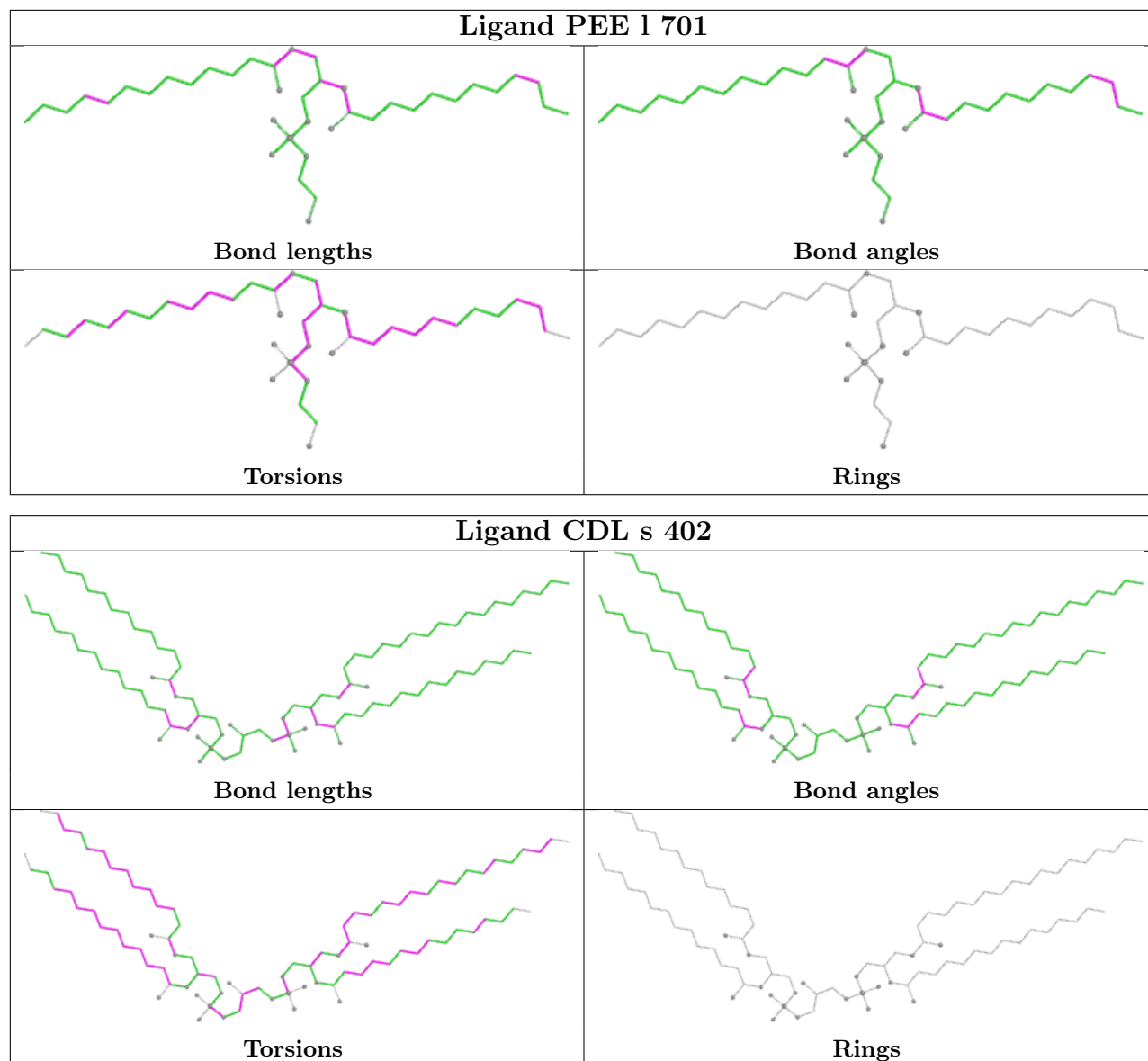


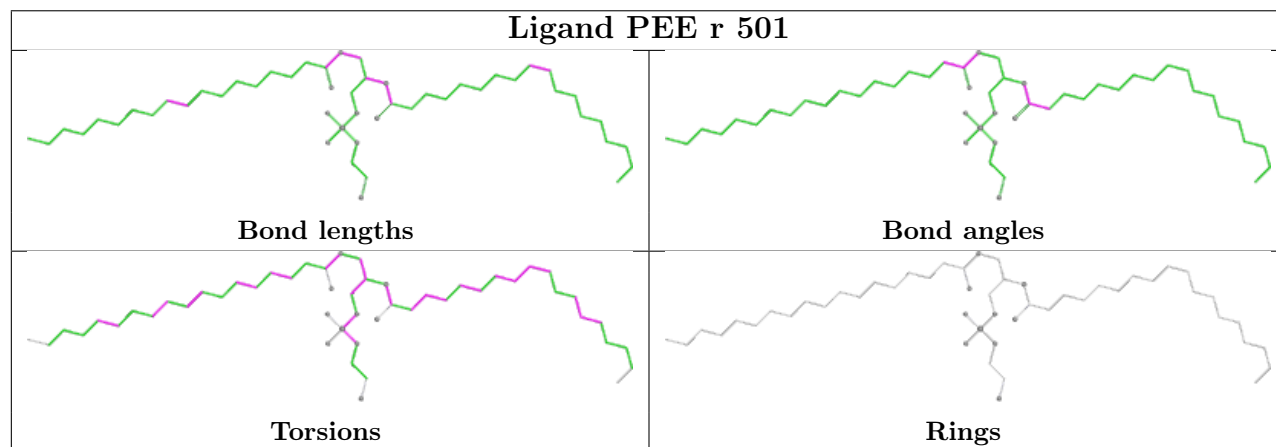
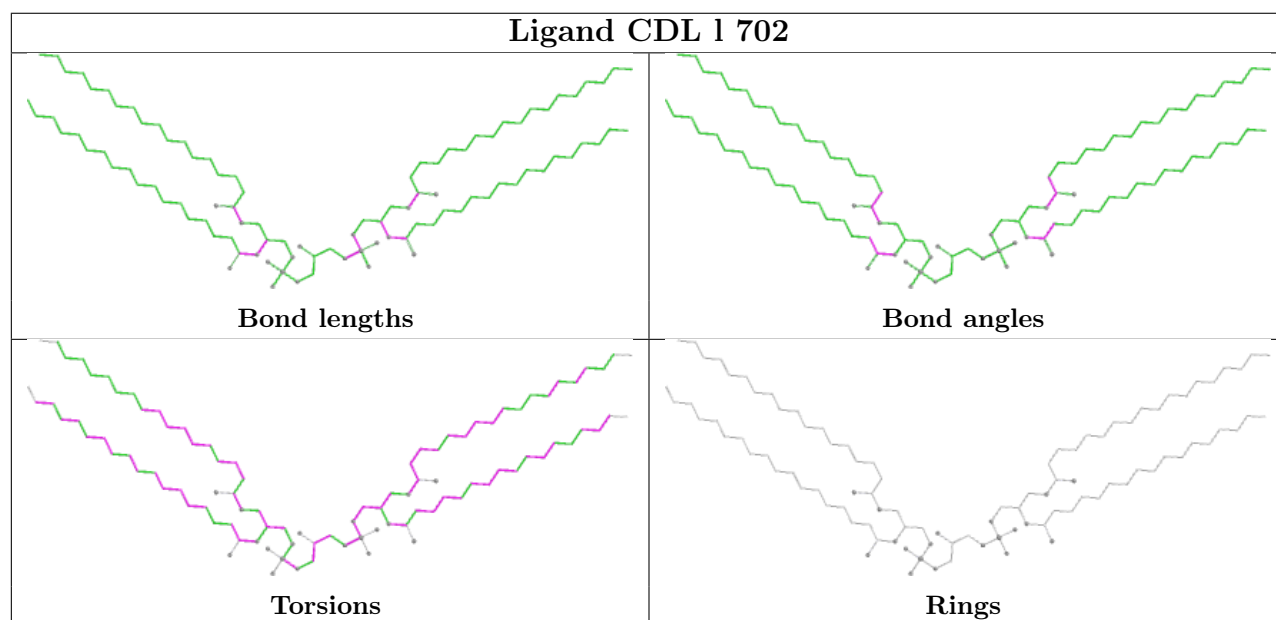
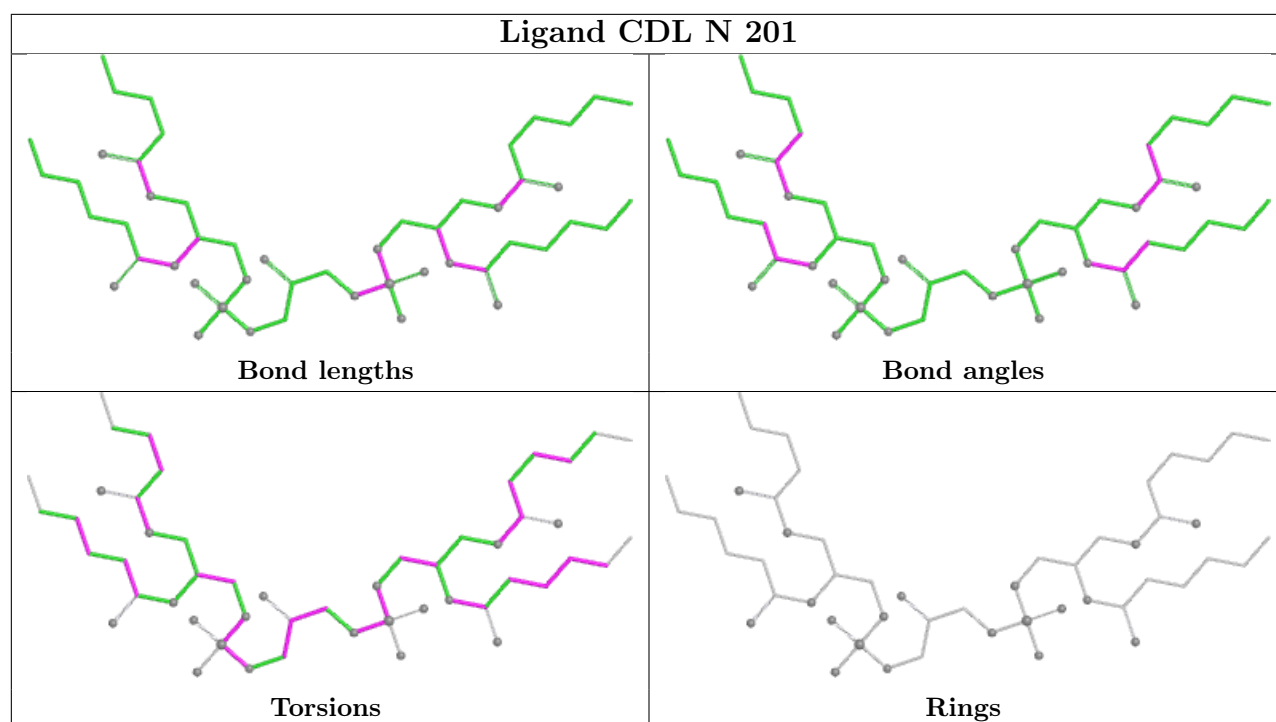


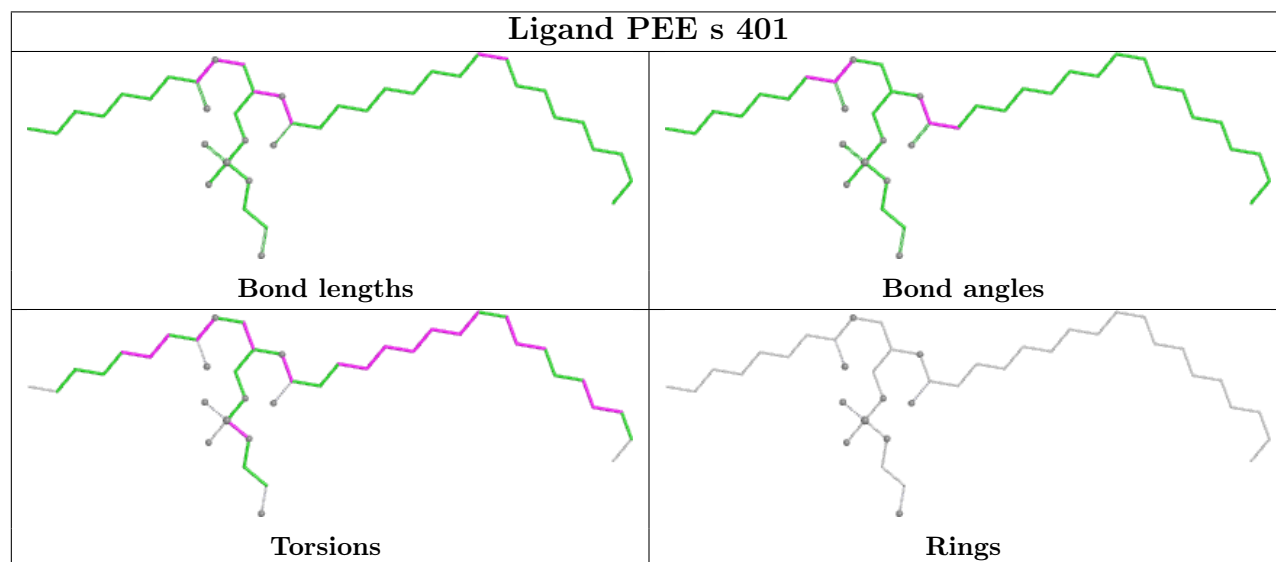
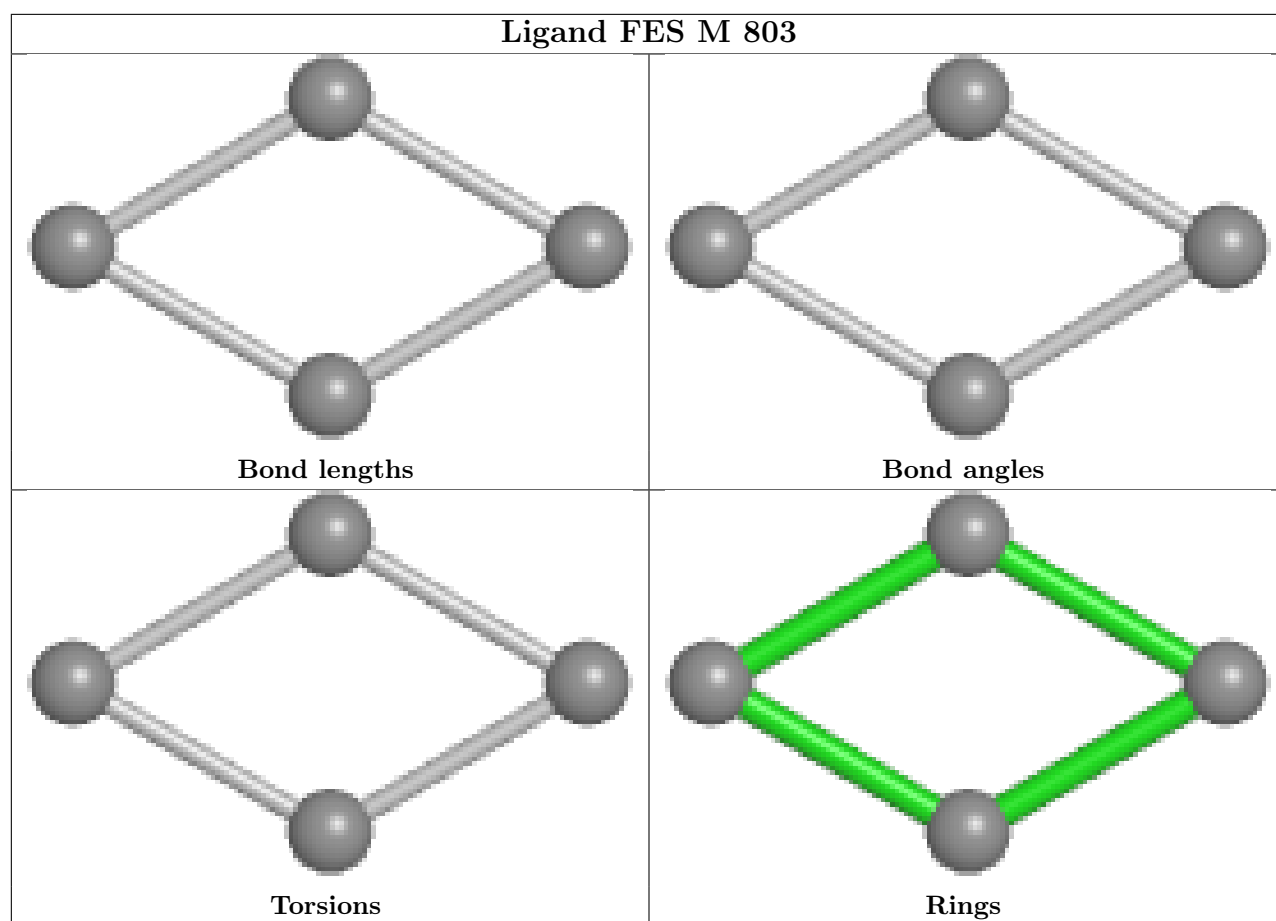


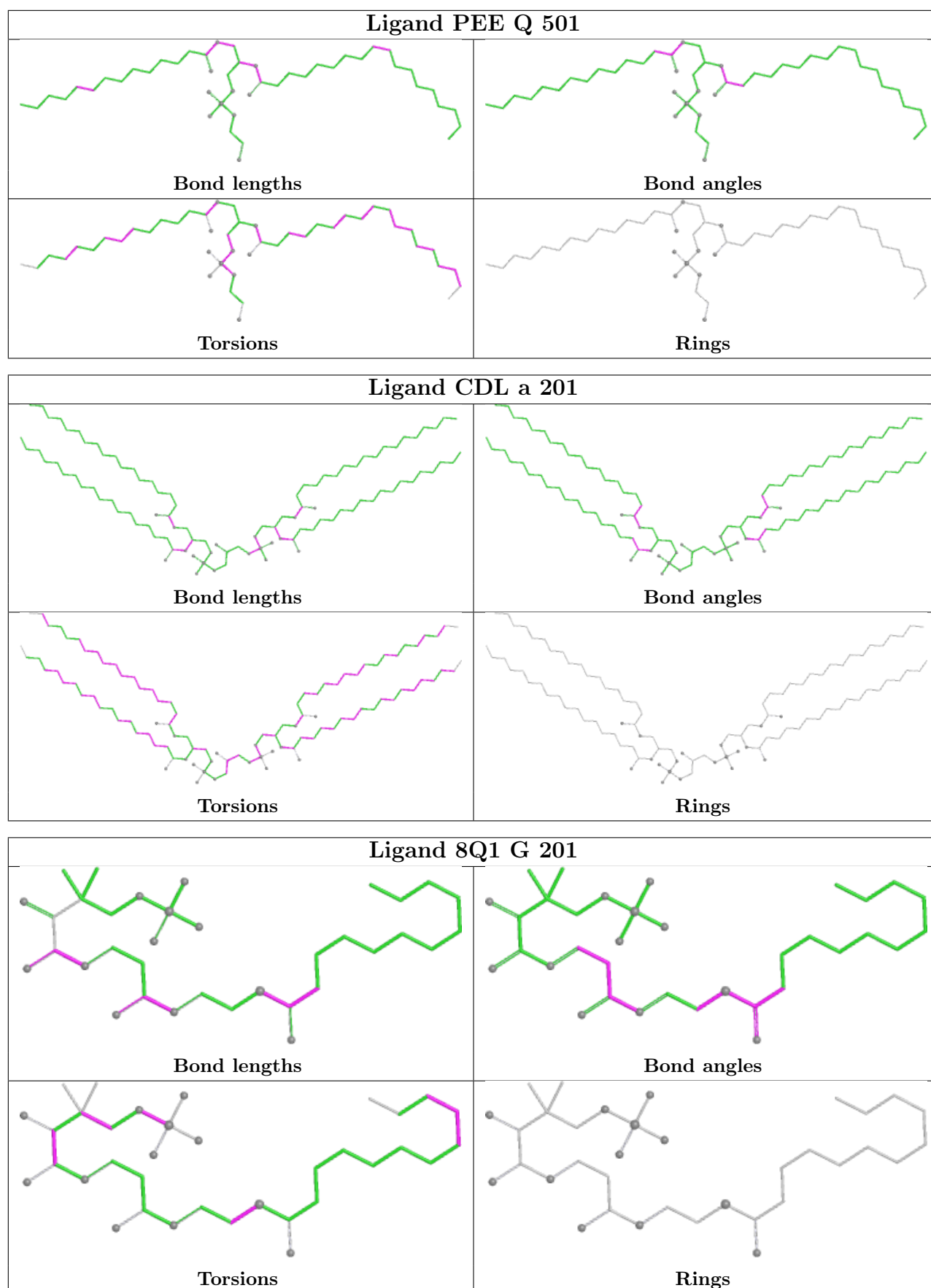


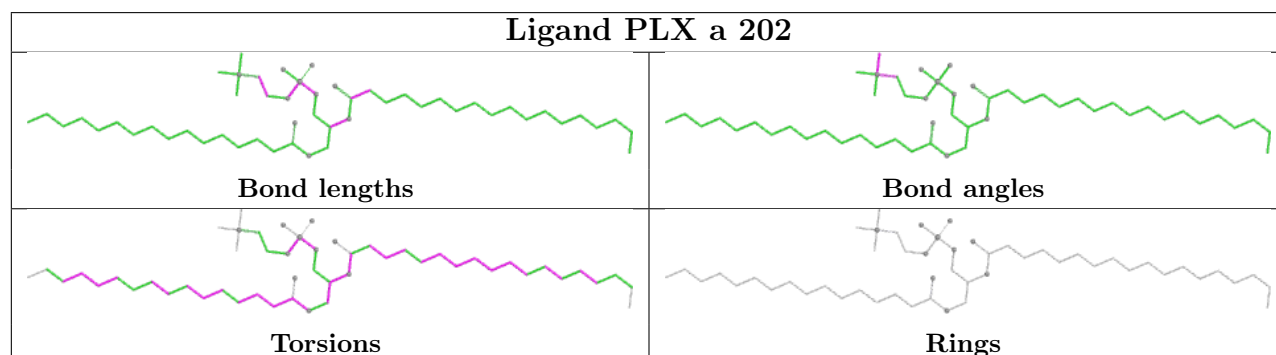
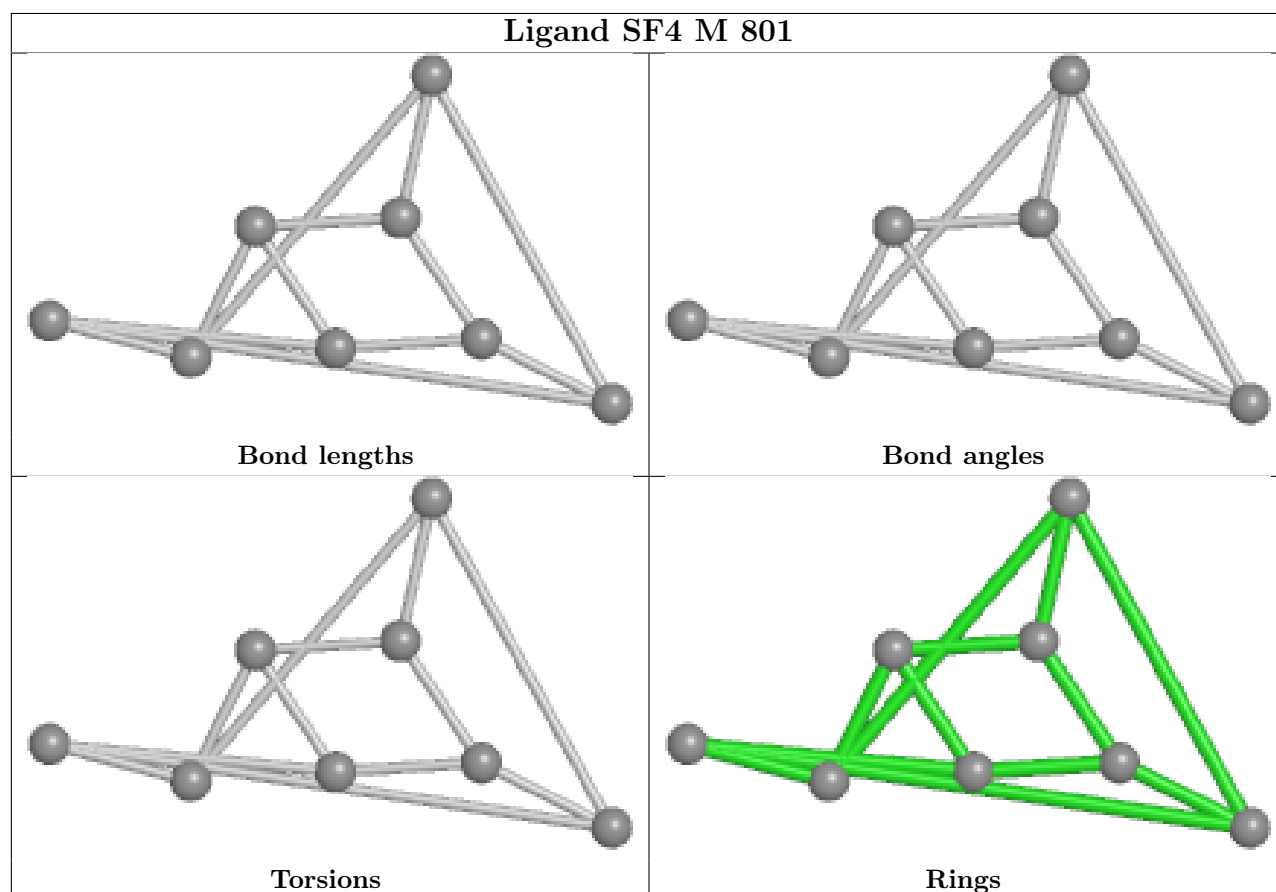
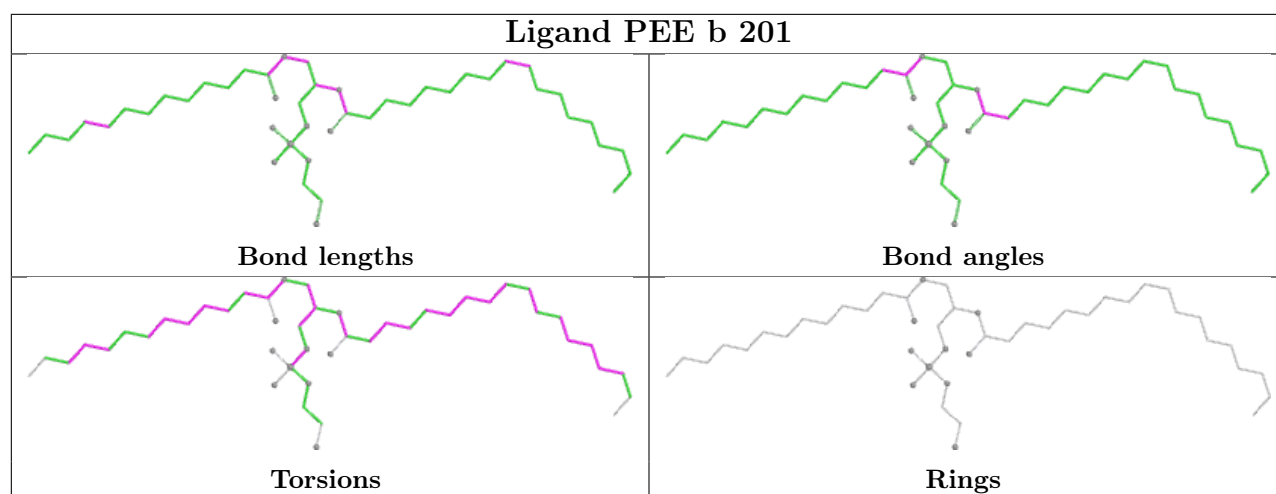


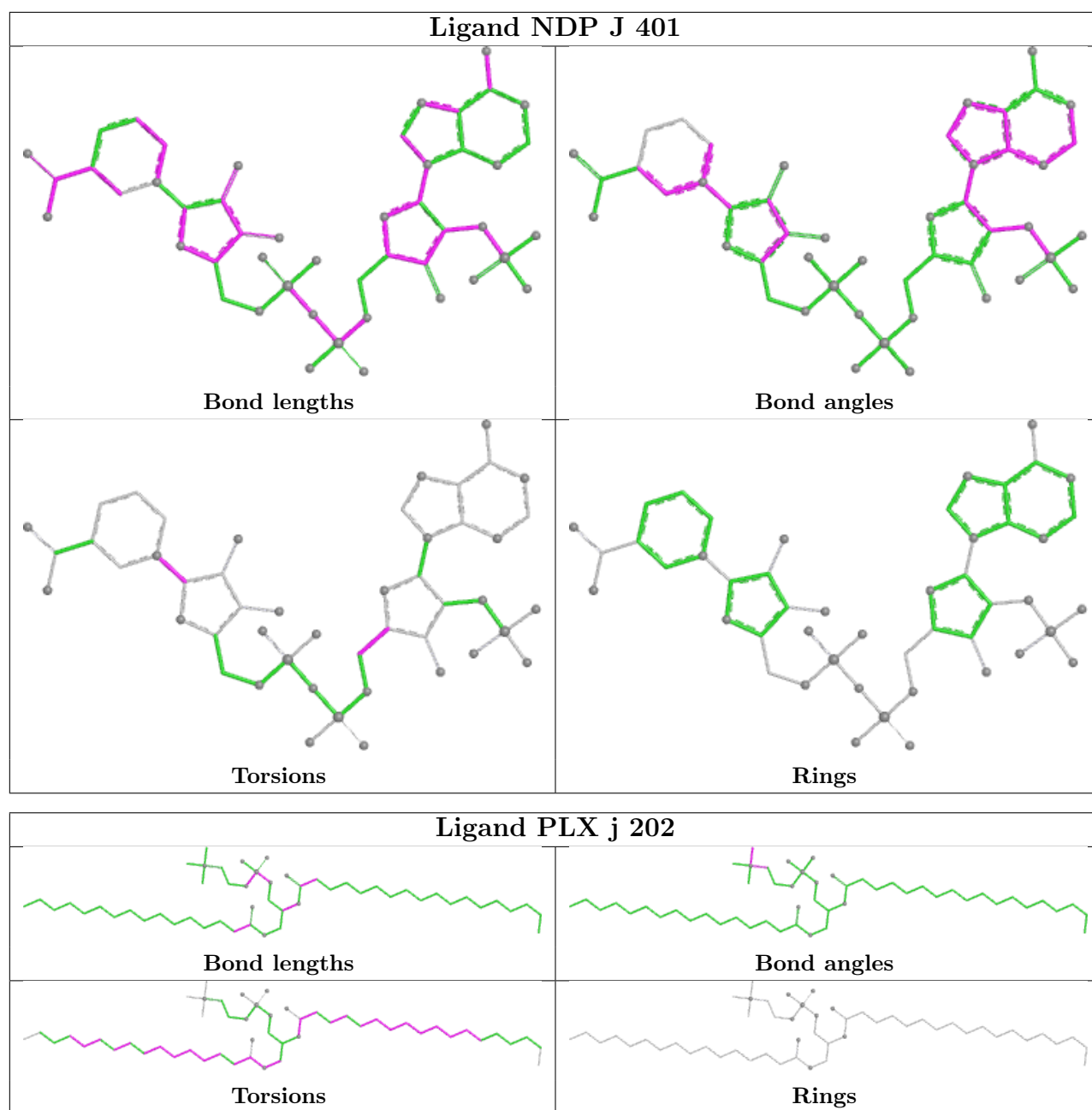


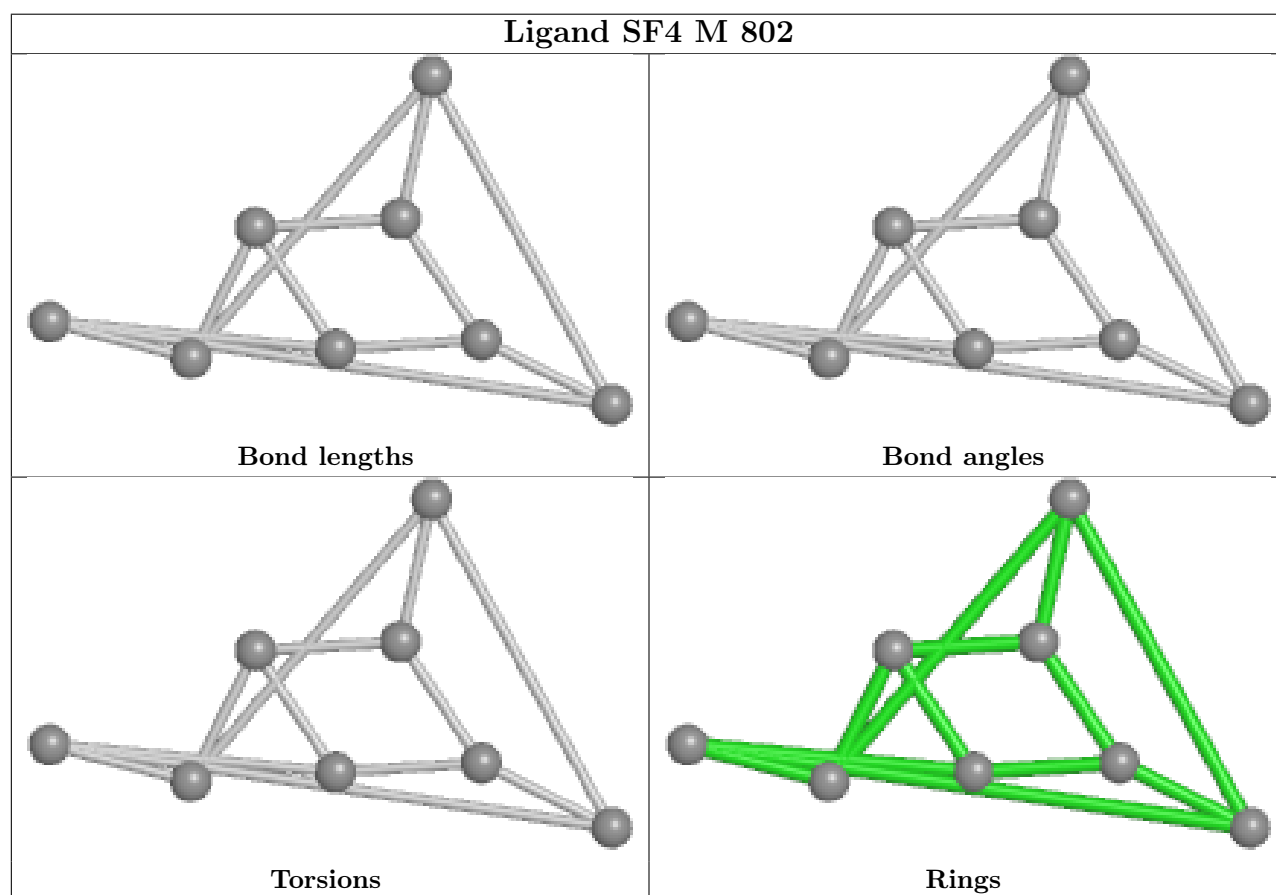
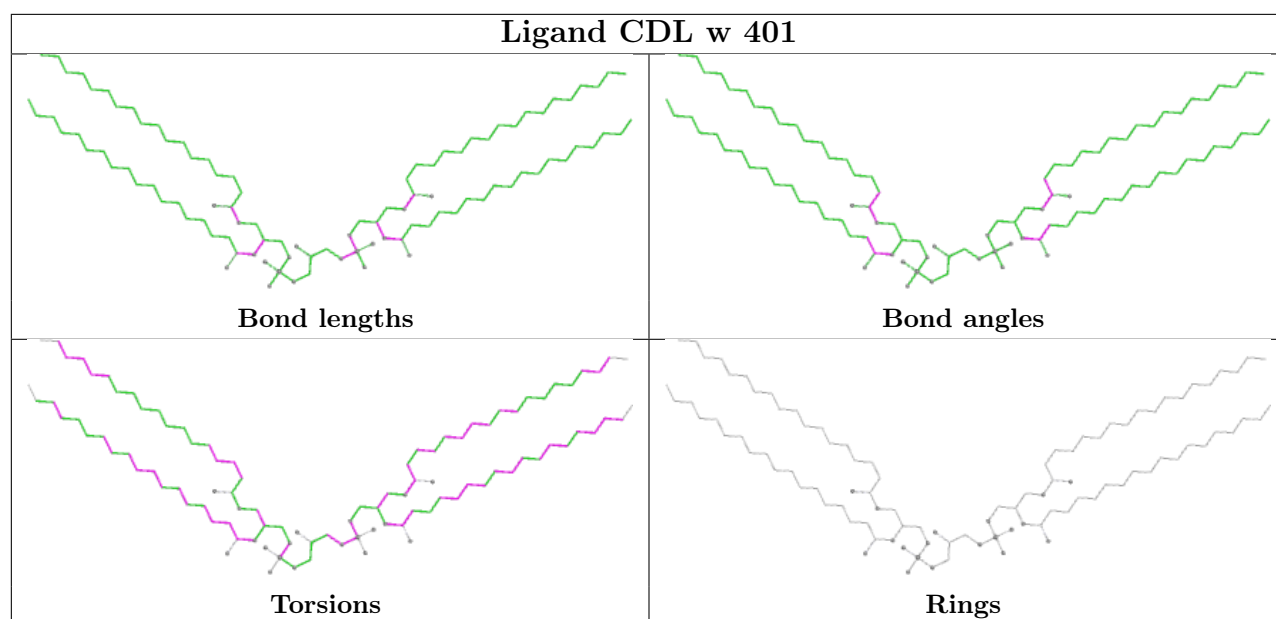


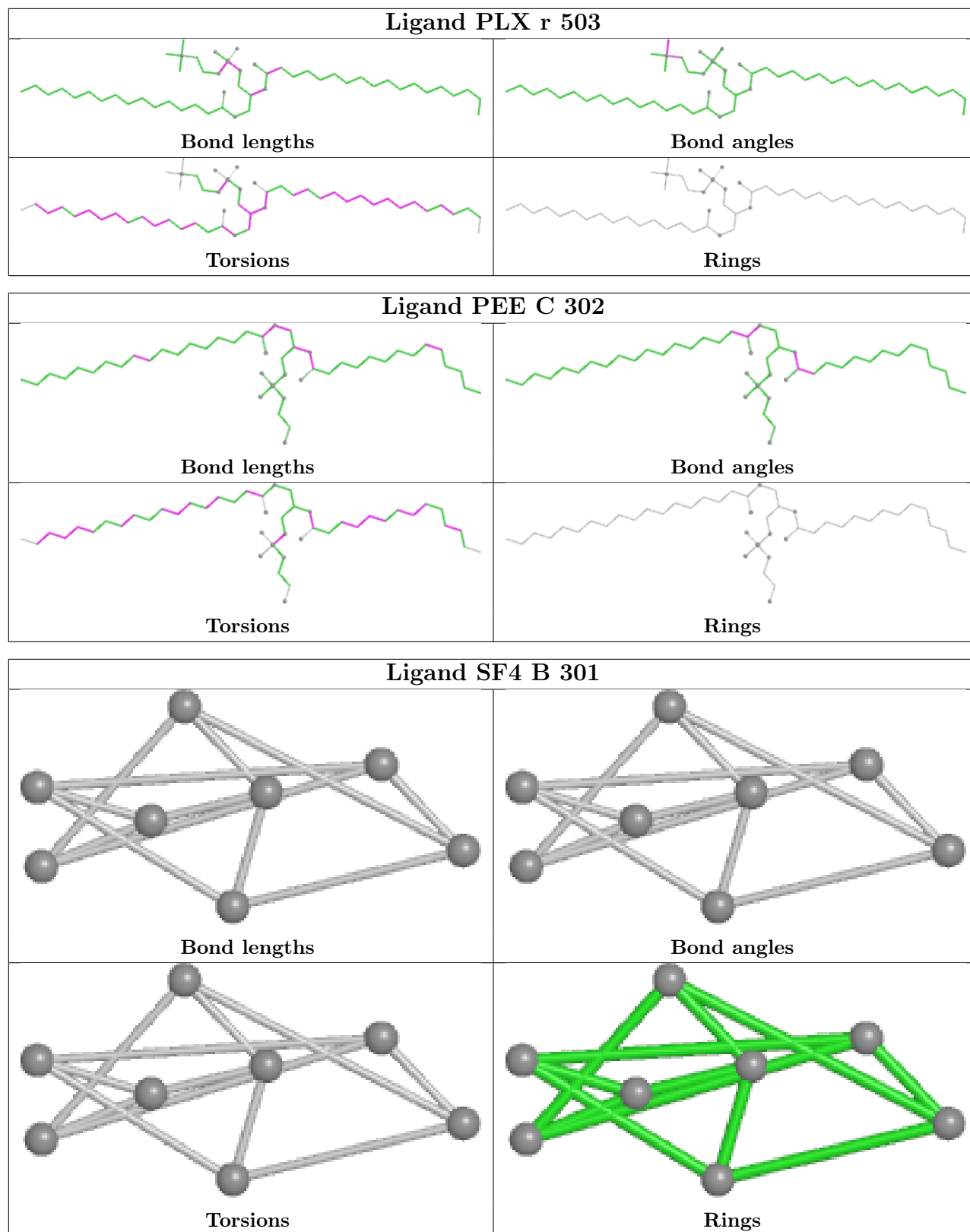


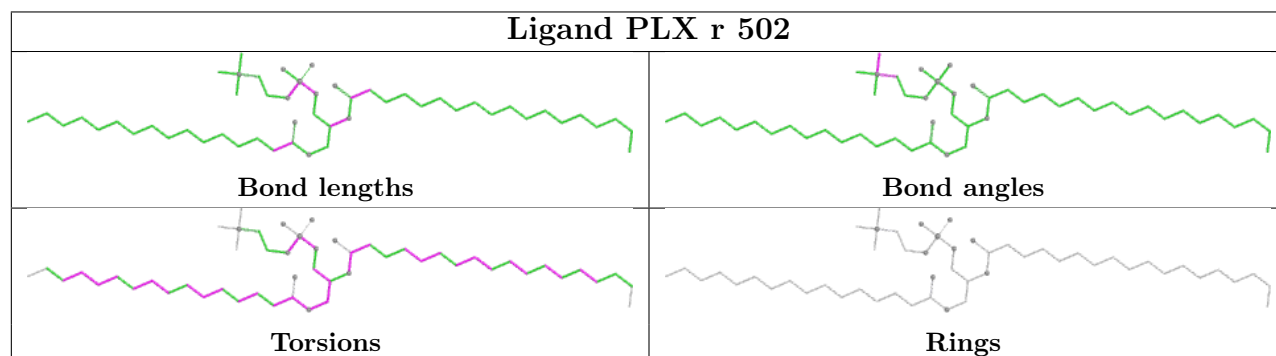
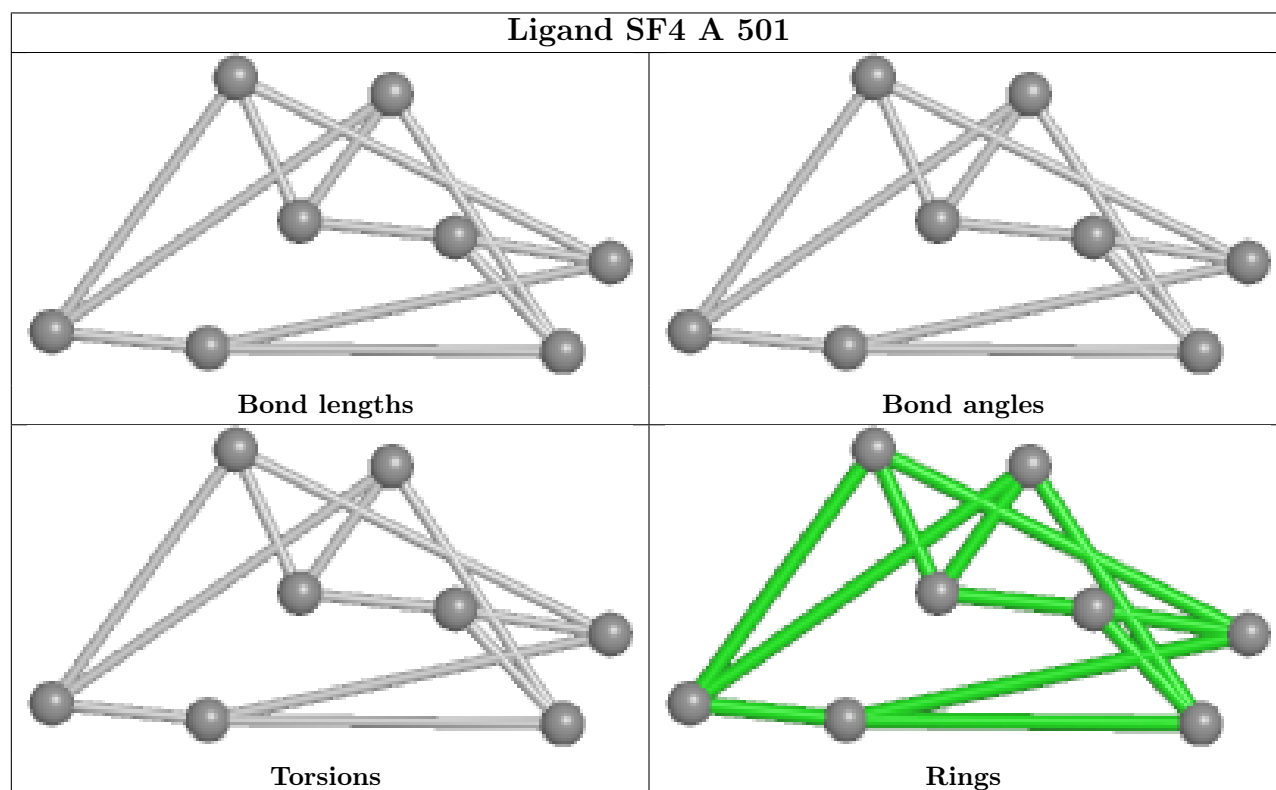
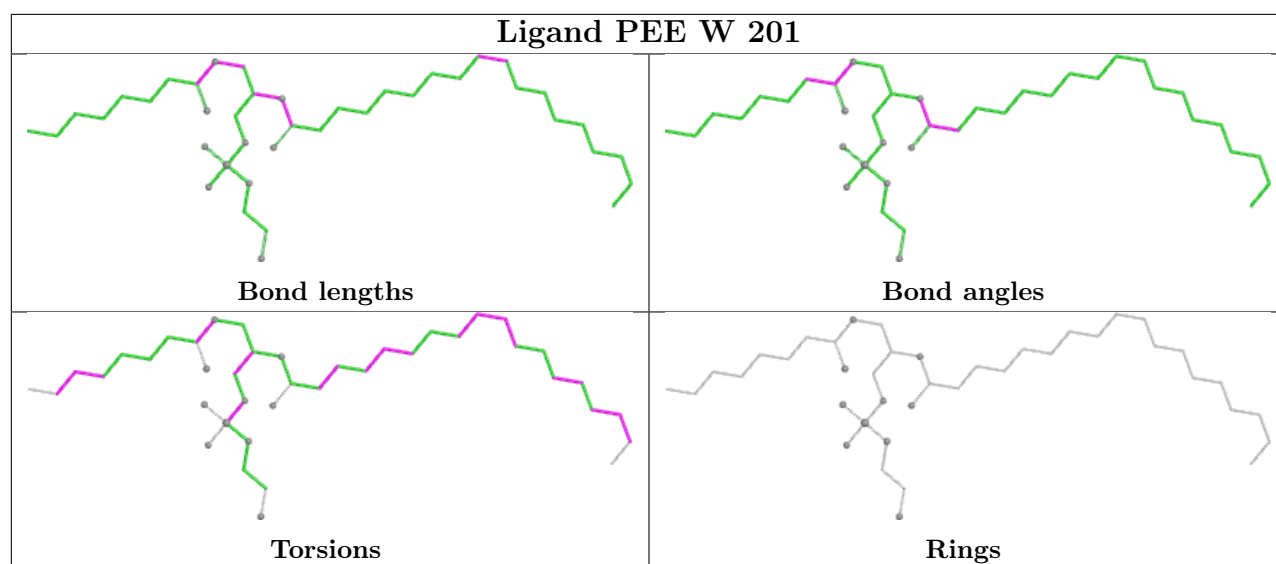


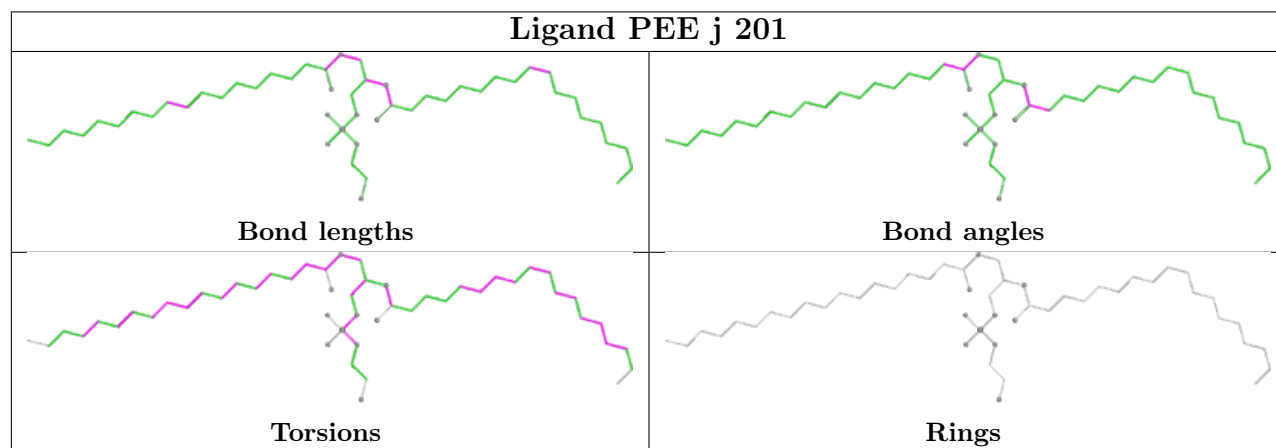
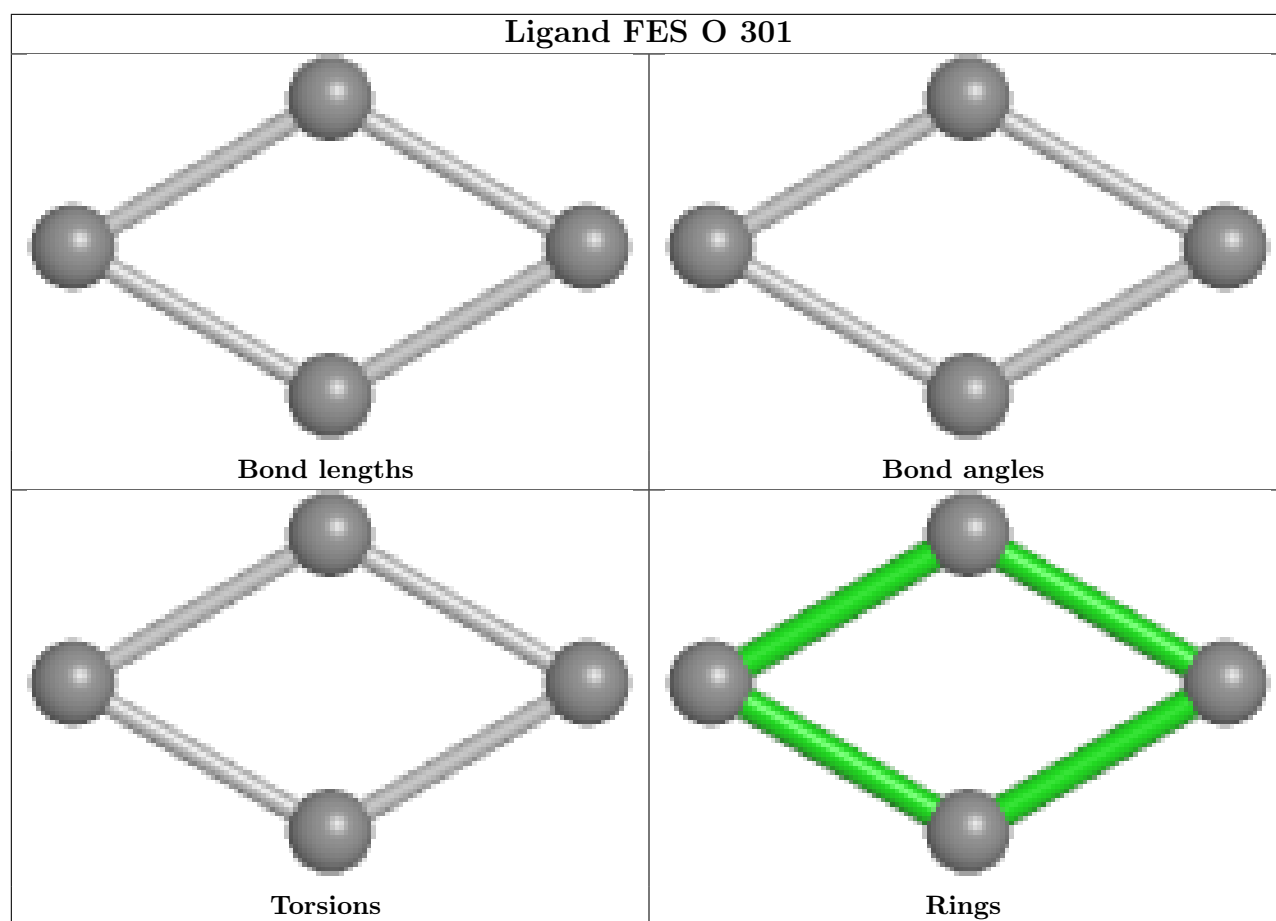


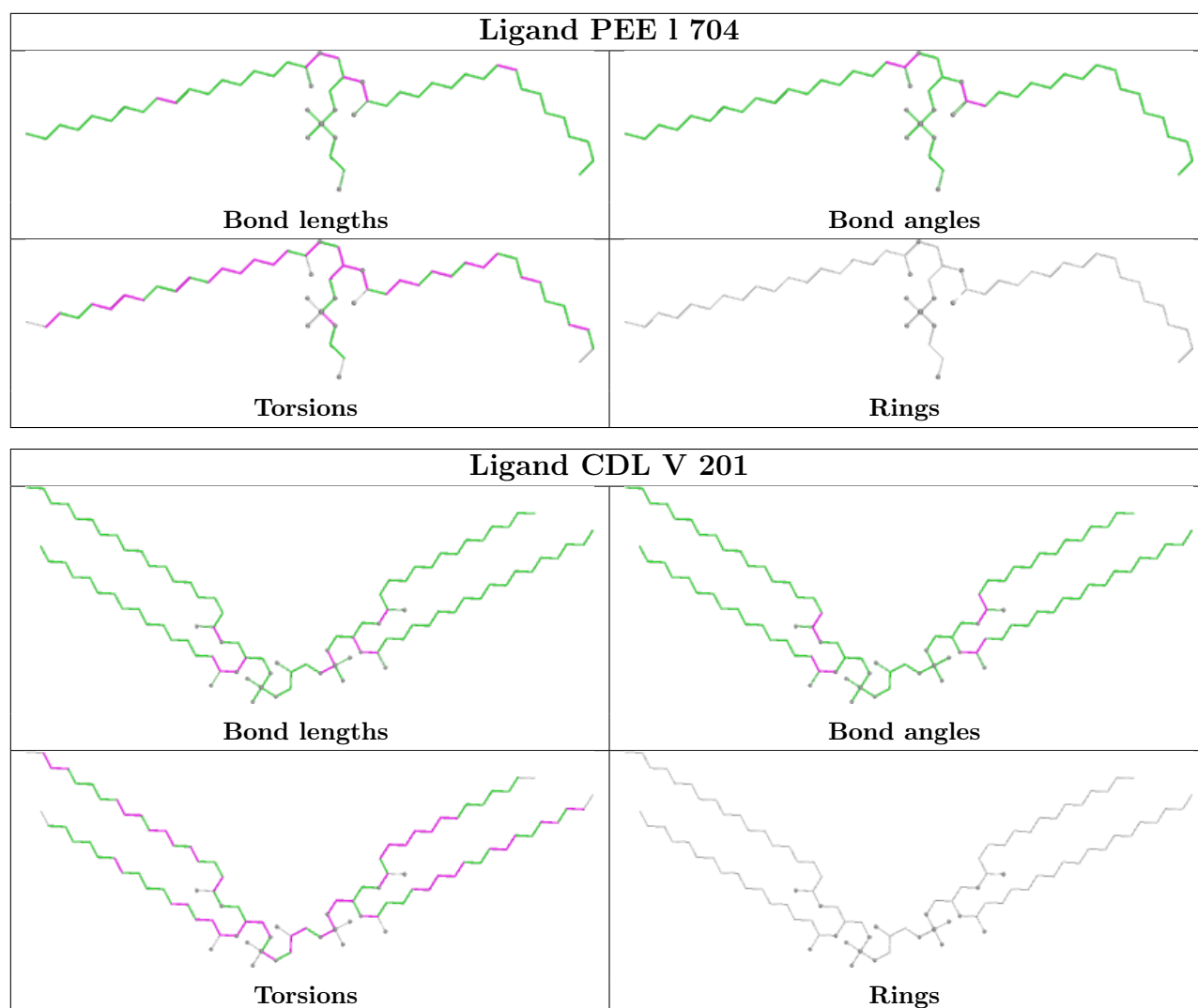


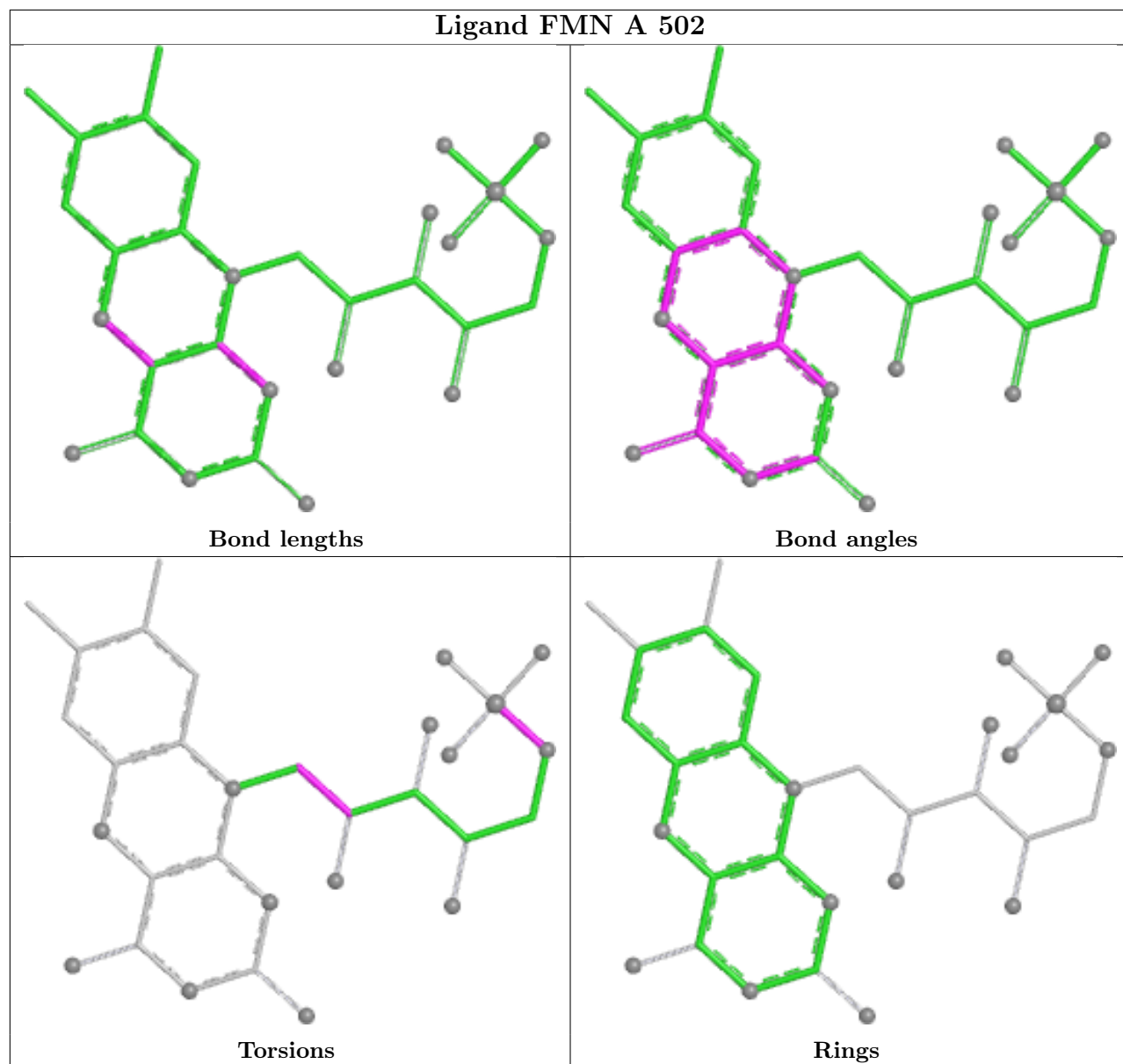


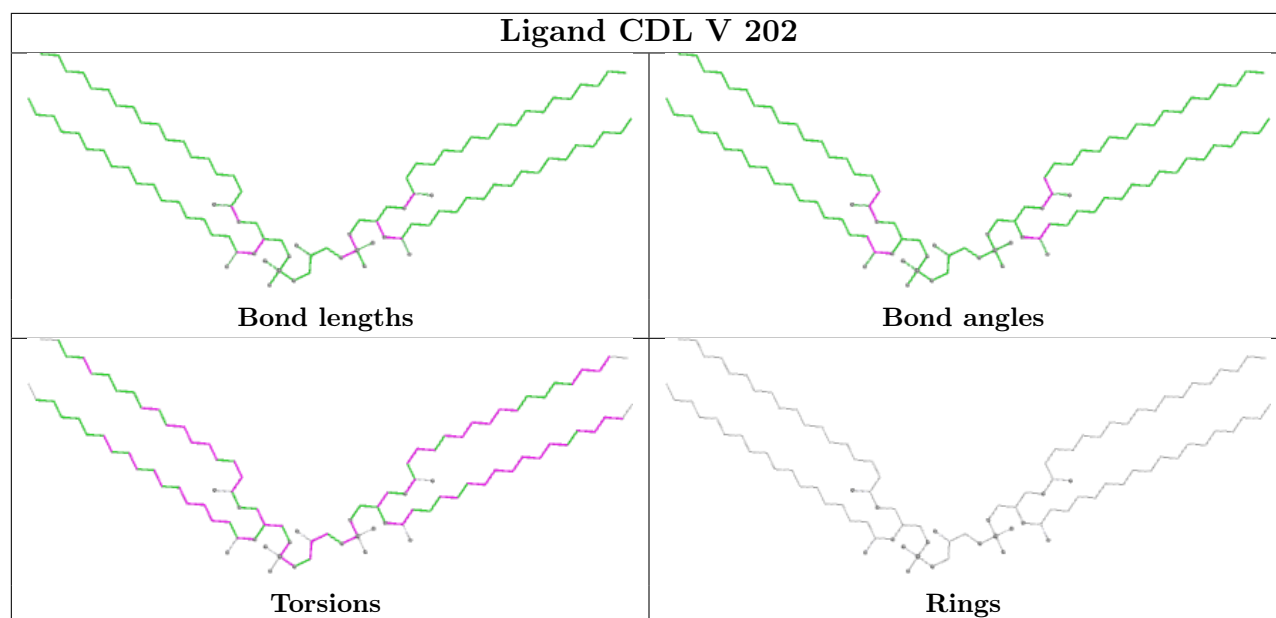
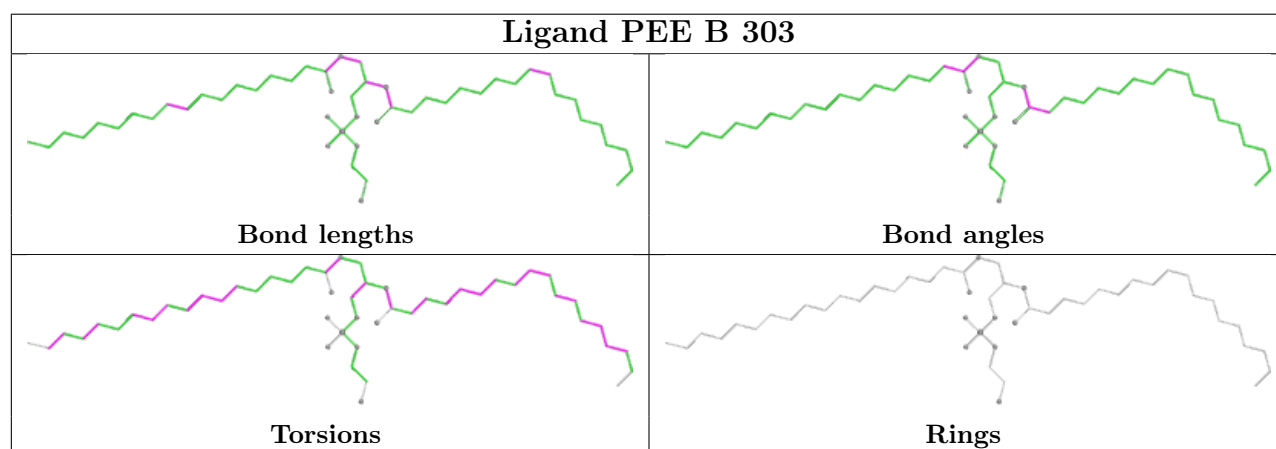
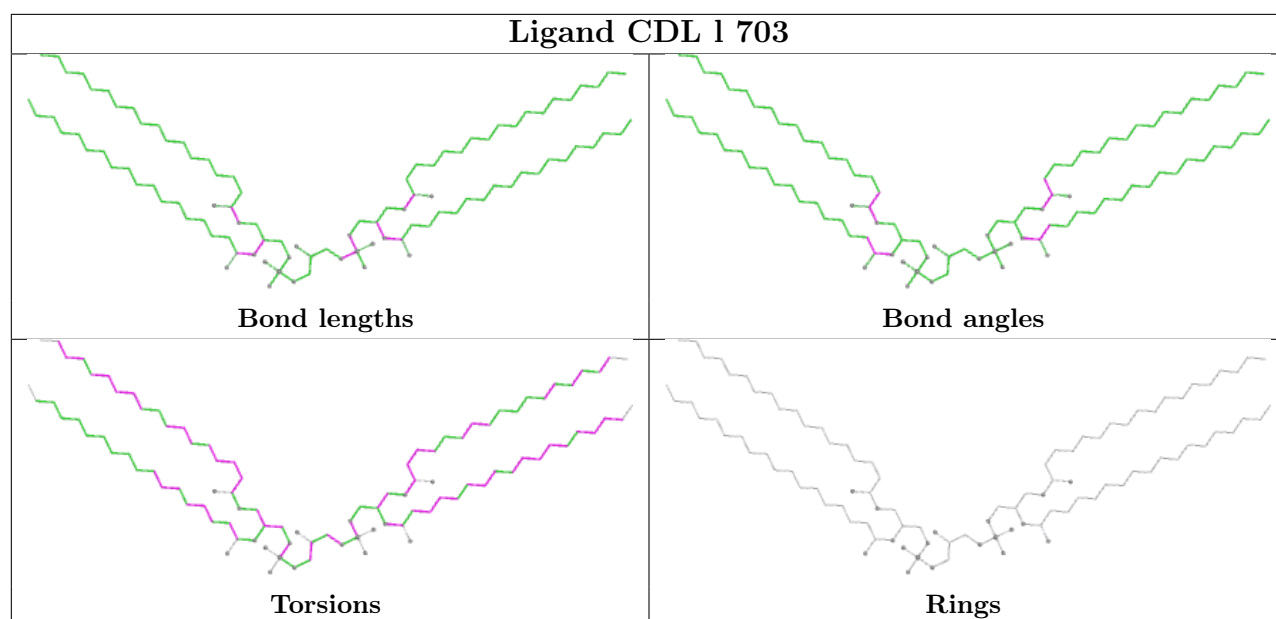












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

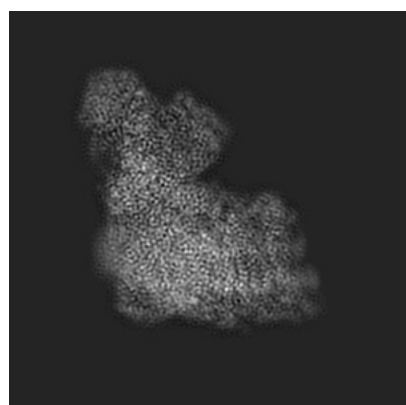
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32249. These allow visual inspection of the internal detail of the map and identification of artifacts.

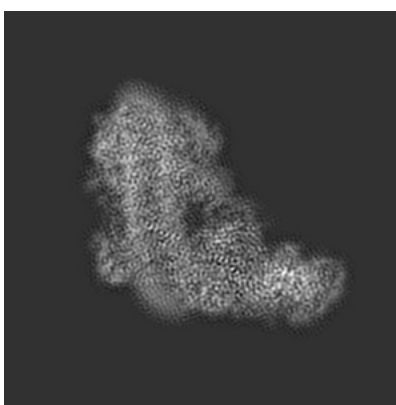
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

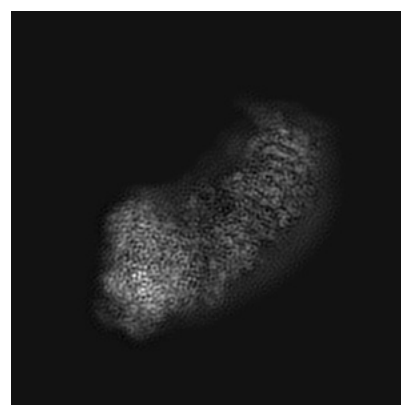
6.1.1 Primary map



X



Y

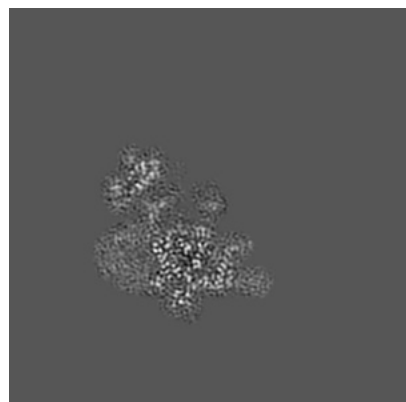


Z

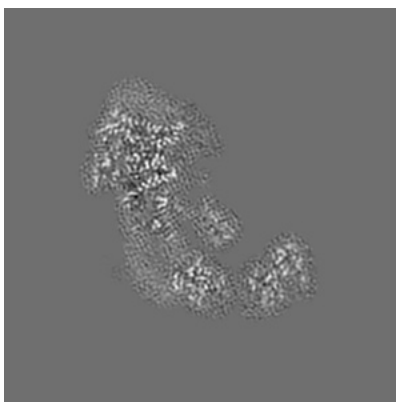
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

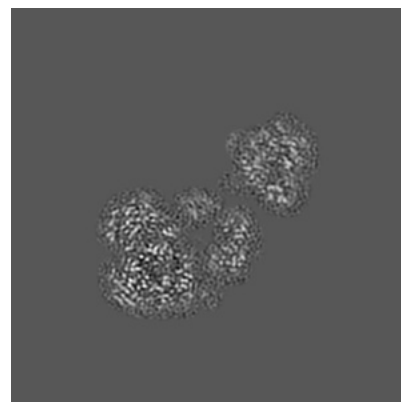
6.2.1 Primary map



X Index: 155



Y Index: 155

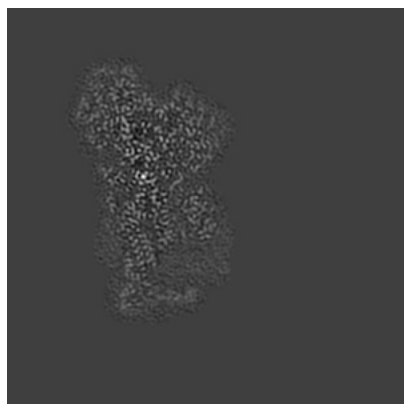


Z Index: 155

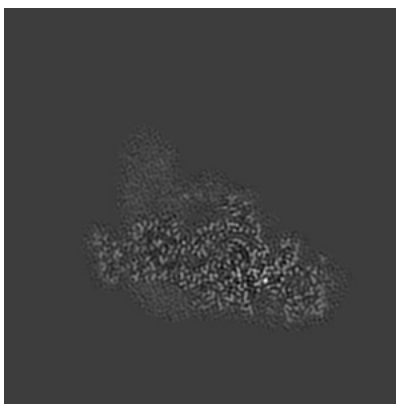
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

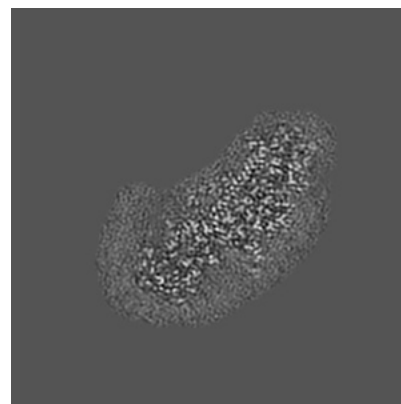
6.3.1 Primary map



X Index: 102



Y Index: 101

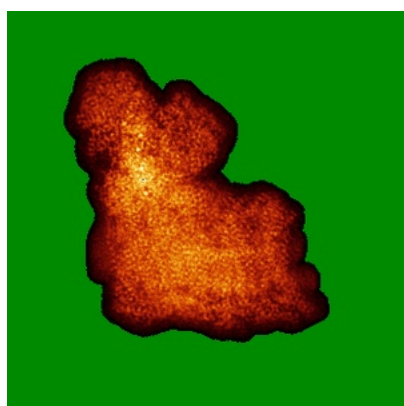


Z Index: 122

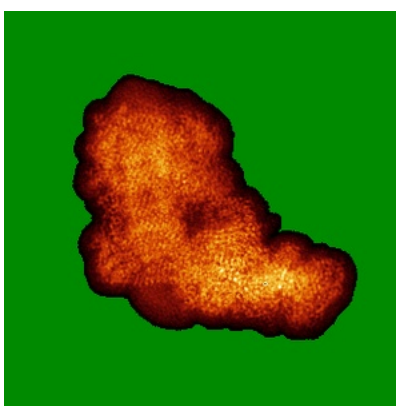
The images above show the largest variance slices of the map in three orthogonal directions.

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

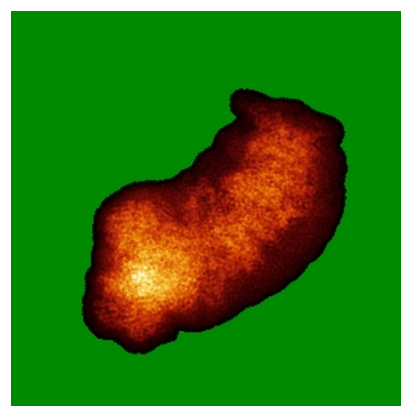
6.4.1 Primary map



X



Y

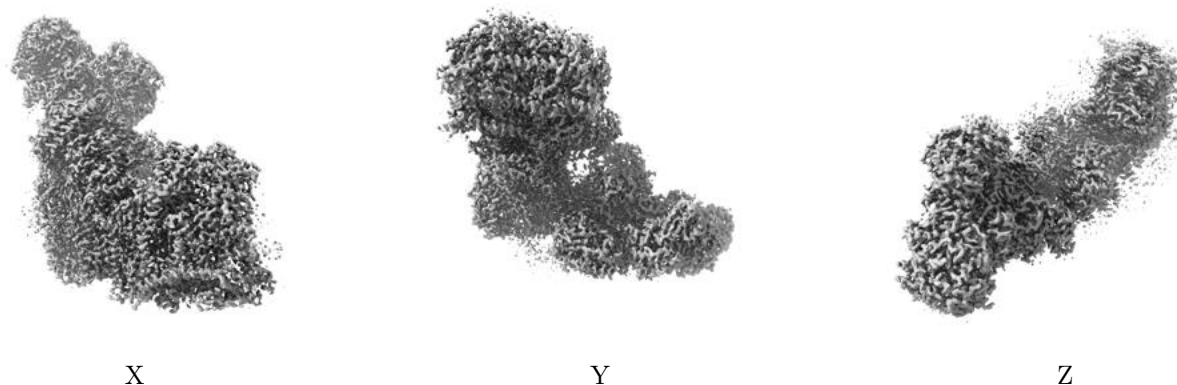


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0305. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

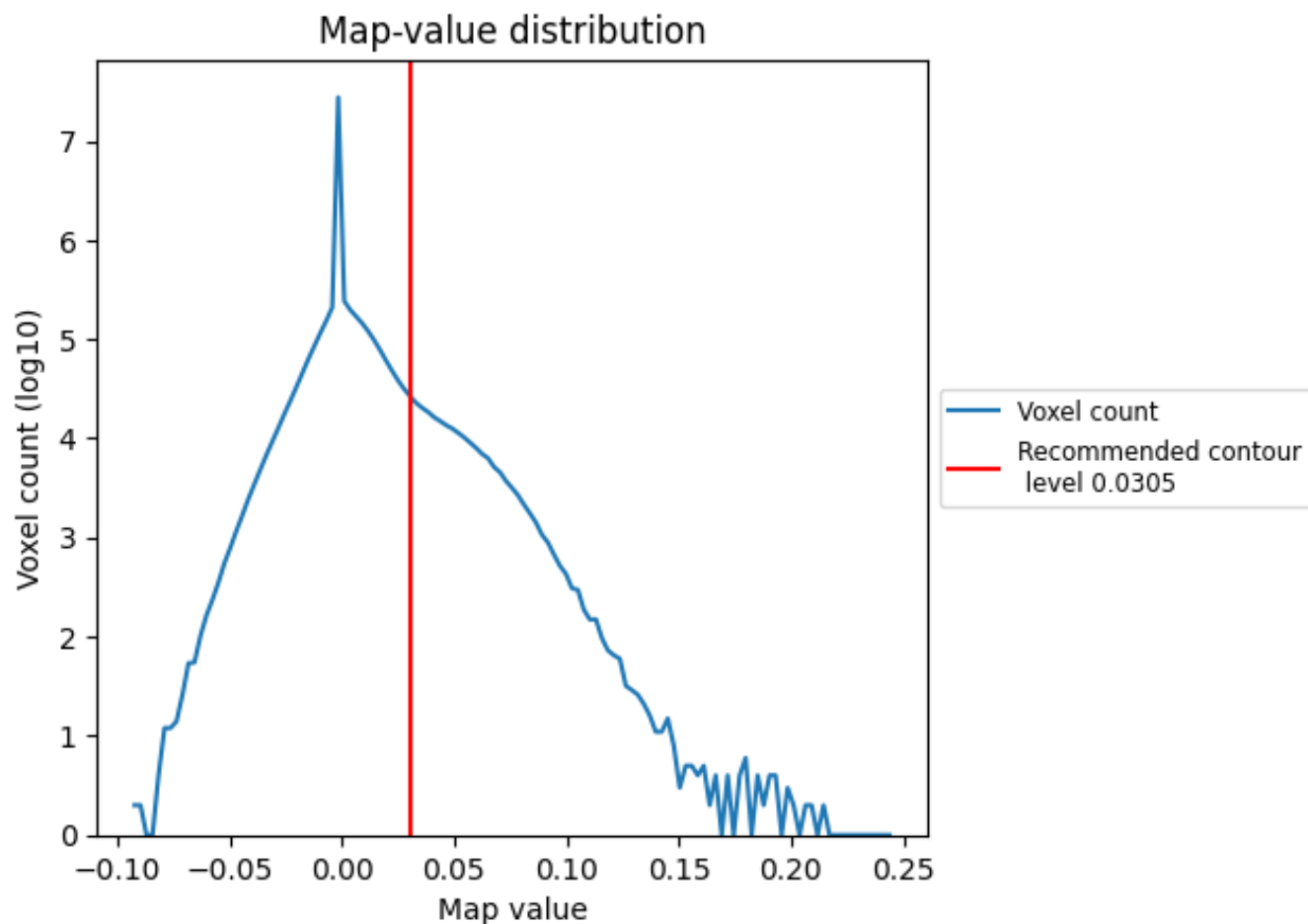
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

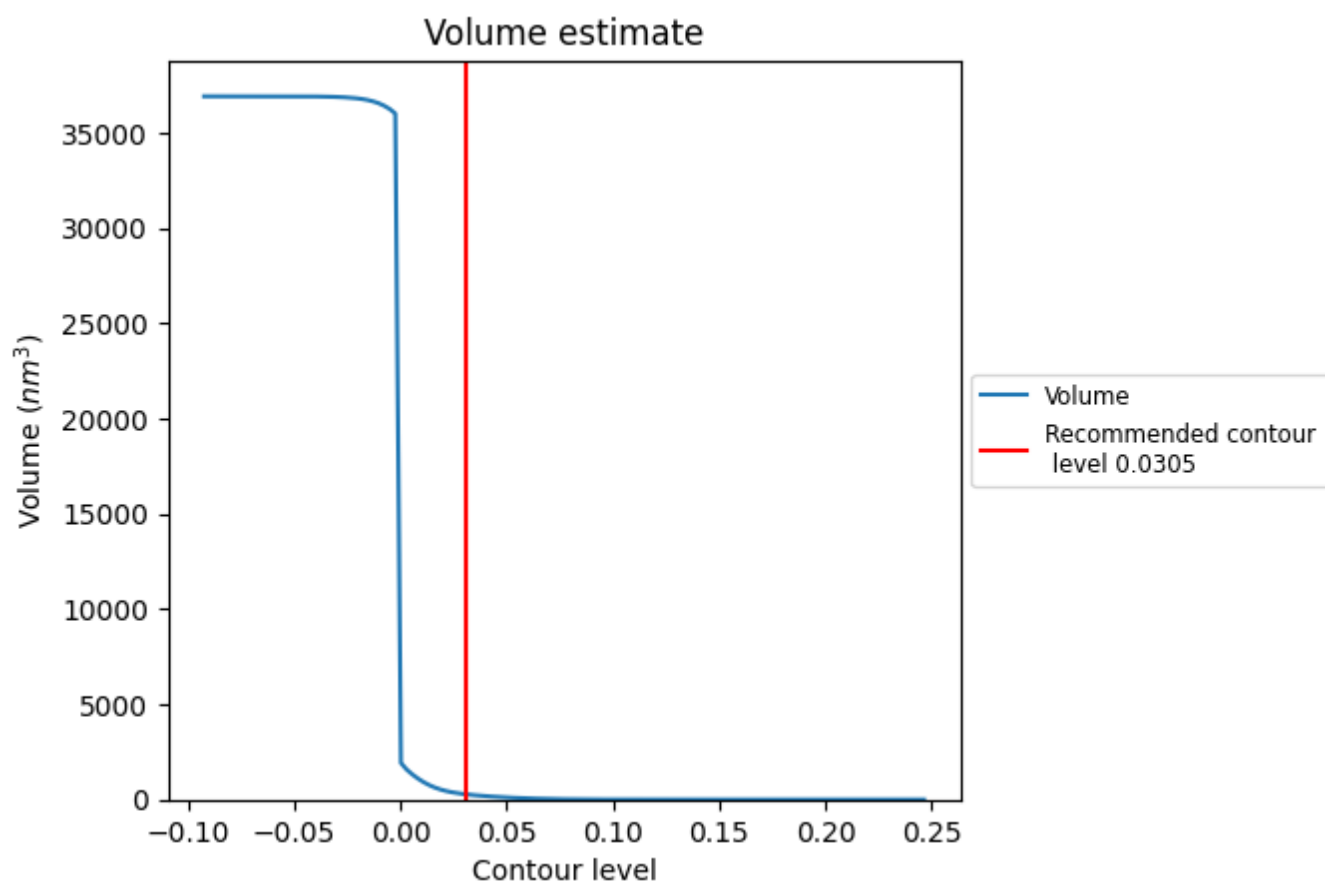
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

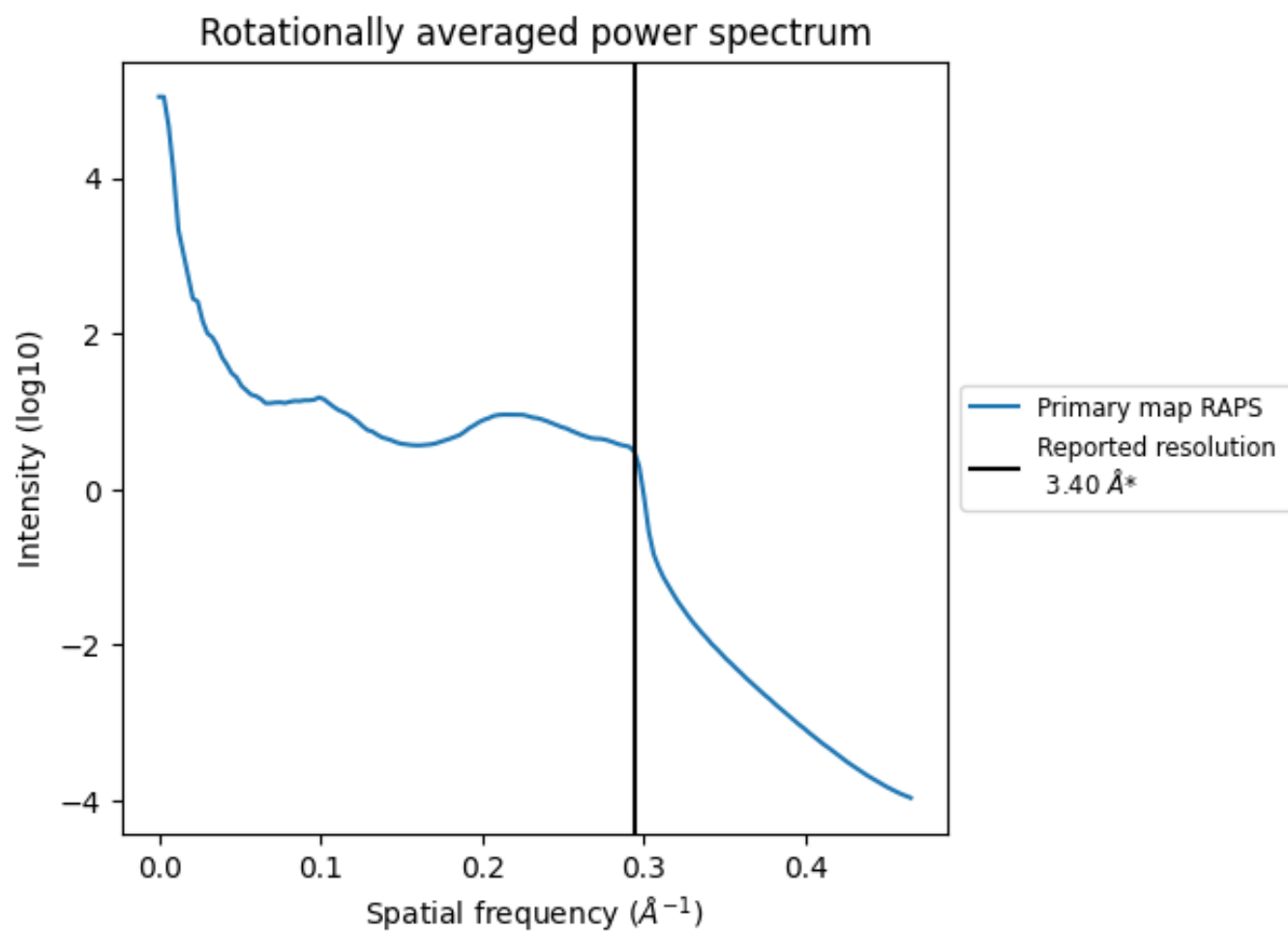
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 281 nm^3 ; this corresponds to an approximate mass of 254 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 0.294 Å⁻¹

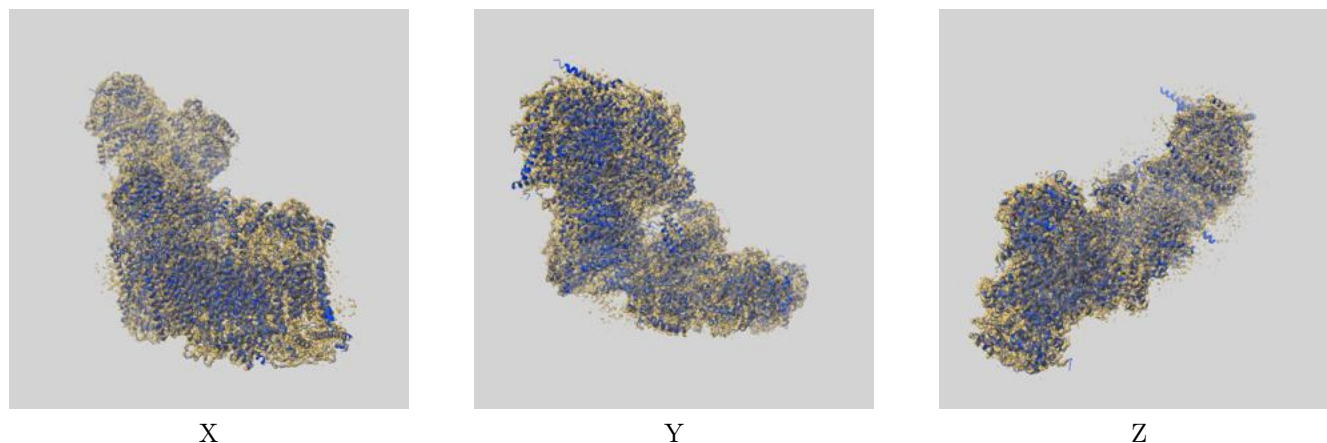
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

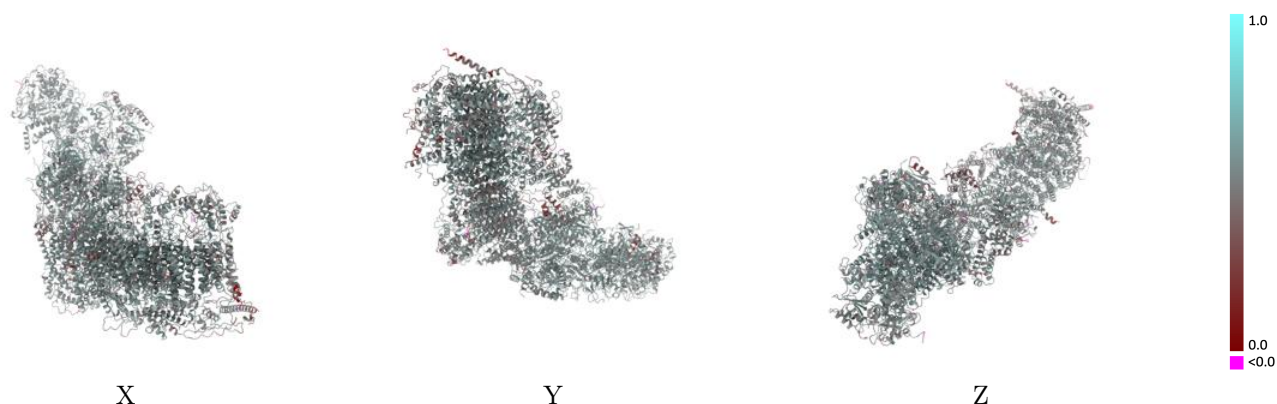
This section contains information regarding the fit between EMDB map EMD-32249 and PDB model 7W0Y. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



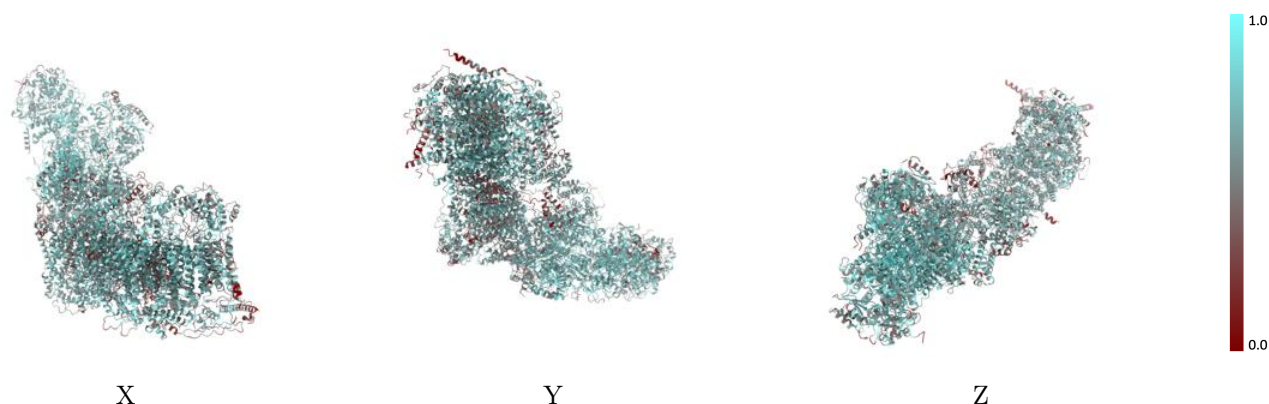
The images above show the 3D surface view of the map at the recommended contour level 0.0305 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



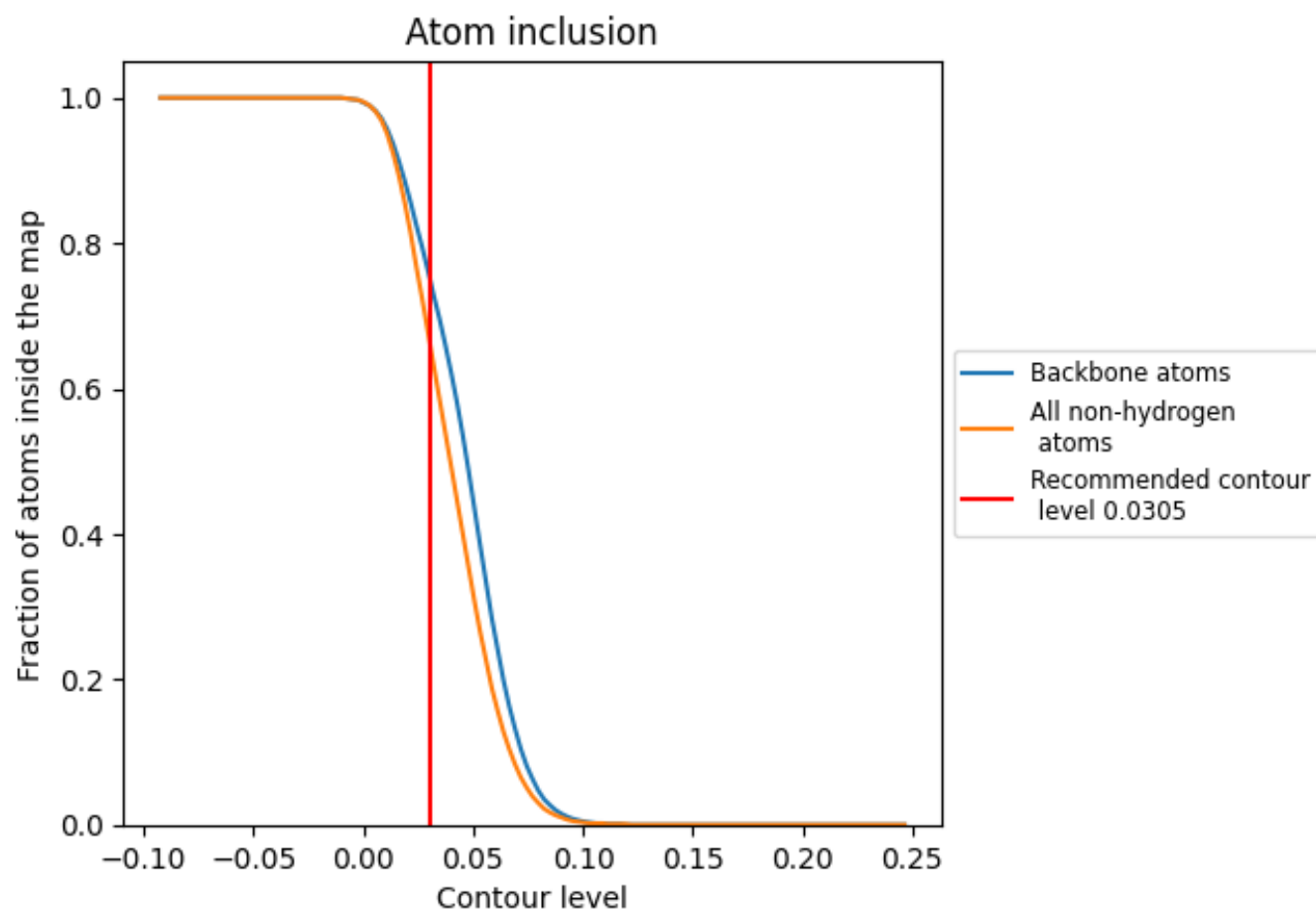
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0305).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 66% 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 (0.0305) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6590	 0.5230
A	 0.6700	 0.5240
B	 0.7860	 0.5630
C	 0.7610	 0.5660
E	 0.6800	 0.5350
F	 0.5750	 0.4700
G	 0.3260	 0.3600
H	 0.6370	 0.5180
I	 0.5990	 0.5140
J	 0.6880	 0.5340
K	 0.6310	 0.5220
L	 0.7170	 0.5480
M	 0.7170	 0.5420
N	 0.5780	 0.5090
O	 0.6430	 0.5110
P	 0.7950	 0.5700
Q	 0.7580	 0.5610
S	 0.6960	 0.5290
T	 0.6880	 0.5470
U	 0.6250	 0.4960
V	 0.4800	 0.4810
W	 0.6450	 0.5060
X	 0.5520	 0.4780
Y	 0.5190	 0.4490
Z	 0.4570	 0.4320
a	 0.6420	 0.5340
b	 0.5600	 0.4790
c	 0.6550	 0.5210
d	 0.6250	 0.5020
e	 0.6140	 0.5130
f	 0.4460	 0.4210
g	 0.6760	 0.5280
h	 0.6280	 0.5090
i	 0.7320	 0.5520
j	 0.6360	 0.5190



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Chain	Atom inclusion	Q-score
k	 0.6830	 0.5340
l	 0.6470	 0.5280
m	 0.5480	 0.4850
n	 0.5410	 0.4770
o	 0.6360	 0.5030
p	 0.6610	 0.5140
r	 0.7140	 0.5450
s	 0.6960	 0.5390
u	 0.6320	 0.5110
v	 0.5140	 0.4580
w	 0.6070	 0.5070