



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:35 AM UTC

PDB ID : 7ZMB / pdb_00007zmb
EMDB ID : EMD-14794
Title : CryoEM structure of mitochondrial complex I from *Chaetomium thermophilum* (state 2)
Authors : Laube, E.; Kuehlbrandt, W.
Deposited on : 2022-04-19
Resolution : 2.75 Å (reported)
Based on initial models : 6RFR, 6RFQ

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:

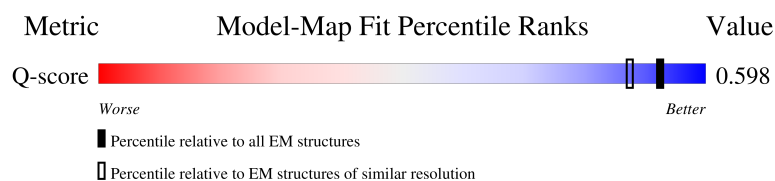
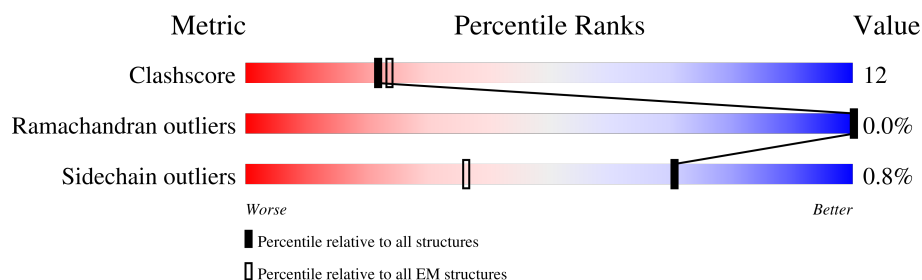
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.75 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.



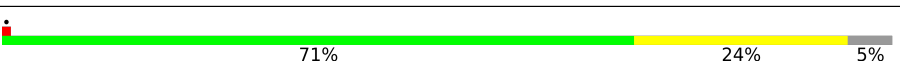
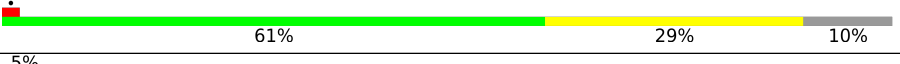
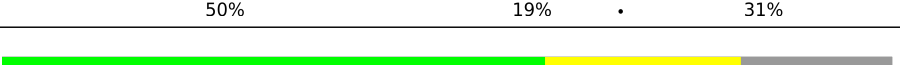
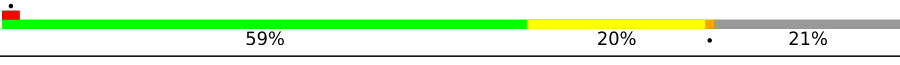
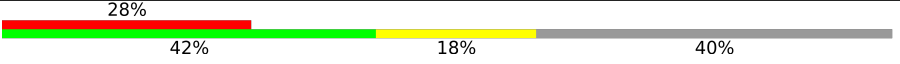
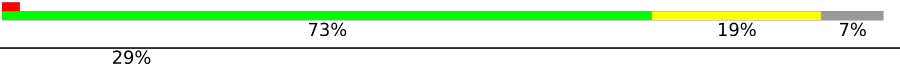
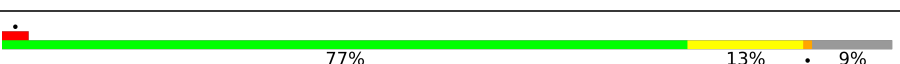
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10570 (2.25 - 3.25)

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	1	378	
2	2	571	
3	3	146	
4	4	542	

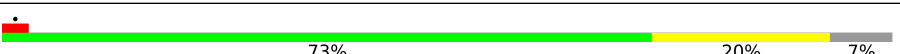
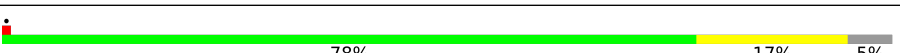
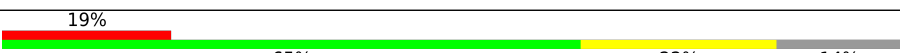
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Mol	Chain	Length	Quality of chain
5	5	679	
6	6	224	
7	8	86	
8	9	785	
9	A	749	
10	B	507	
11	C	499	
12	D	86	
13	E	378	
14	F	261	
15	G	293	
16	H	318	
17	I	223	
18	J	199	
19	K	230	
20	L	89	
21	M	168	
22	O	141	
22	Q	141	
23	P	124	
24	R	99	
25	S	143	
26	U	186	
27	W	121	
28	X	191	

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Mol	Chain	Length	Quality of chain
29	Y	210	
30	Z	196	
31	a	203	
32	b	94	
33	c	93	
34	d	105	
35	e	46	
36	f	95	
37	g	82	
38	h	134	
39	i	93	
40	j	75	
41	n	184	
42	o	380	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 69495 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-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	334	Total	C	N	O	S	0	0
			2573	1728	388	446	11		

- Molecule 2 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	558	Total	C	N	O	S	0	0
			4456	2993	672	780	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	130	Total	C	N	O	S	0	0
			1026	695	153	175	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	494	Total	C	N	O	S	0	0
			3904	2650	572	670	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	670	Total	C	N	O	S	0	0
			5272	3551	792	904	25		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	445	ARG	-	insertion	UNP G1DJA3
5	446	LEU	-	insertion	UNP G1DJA3
5	447	ALA	-	insertion	UNP G1DJA3

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Chain	Residue	Modelled	Actual	Comment	Reference
5	448	ILE	-	insertion	UNP G1DJA3
5	449	ASP	-	insertion	UNP G1DJA3
5	450	ASN	-	insertion	UNP G1DJA3
5	451	PHE	-	insertion	UNP G1DJA3
5	452	PHE	-	insertion	UNP G1DJA3
5	453	SER	-	insertion	UNP G1DJA3
5	454	ALA	-	insertion	UNP G1DJA3
5	455	GLN	-	insertion	UNP G1DJA3
5	456	ALA	-	insertion	UNP G1DJA3
5	457	ILE	-	insertion	UNP G1DJA3
5	458	LYS	-	insertion	UNP G1DJA3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	190	Total	C	N	O	S	0	0
			1452	982	217	247	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	77	Total	C	N	O	S	0	0
			658	408	126	118	6		

- Molecule 8 is a protein called Subunit NDUF5 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	103	Total	C	N	O	S	0	0
			807	500	147	154	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	100	VAL	-	insertion	UNP G0SG48

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	711	Total	C	N	O	S	0	0
			5476	3444	966	1035	31		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP G0RYA1
A	72	TYR	VAL	conflict	UNP G0RYA1
A	73	CYS	SER	conflict	UNP G0RYA1
A	74	TYR	MET	conflict	UNP G0RYA1
A	75	HIS	ARG	conflict	UNP G0RYA1
A	76	GLU	ARG	conflict	UNP G0RYA1

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	456	Total	C	N	O	S	0	0
			3538	2225	638	648	27		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase 49 kDa subunit-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	441	Total	C	N	O	S	0	0
			3468	2205	604	640	19		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LYS	deletion	UNP G0SCG0
C	?	-	LEU	deletion	UNP G0SCG0
C	?	-	THR	deletion	UNP G0SCG0
C	?	-	ILE	deletion	UNP G0SCG0
C	?	-	ALA	deletion	UNP G0SCG0
C	?	-	PRO	deletion	UNP G0SCG0
C	?	-	LYS	deletion	UNP G0SCG0

- Molecule 12 is a protein called Subunit NDUFA1 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	85	Total	C	N	O	S	0	0
			678	432	127	115	4		

- Molecule 13 is a protein called NADH dehydrogenase (Ubiquinone)-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	337	Total	C	N	O	S	0	0
			2741	1743	484	505	9		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	103	GLU	-	insertion	UNP G0SB35
E	104	PHE	-	insertion	UNP G0SB35
E	105	ASP	-	insertion	UNP G0SB35
E	106	LEU	-	insertion	UNP G0SB35
E	107	ARG	-	insertion	UNP G0SB35
E	108	ASN	-	insertion	UNP G0SB35
E	109	THR	-	insertion	UNP G0SB35
E	110	GLN	-	insertion	UNP G0SB35
E	233	HIS	-	insertion	UNP G0SB35
E	234	VAL	-	insertion	UNP G0SB35

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	238	Total	C	N	O	S	0	0
			1884	1189	328	366	1		

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase 30.4 kDa subunit-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	242	Total	C	N	O	S	0	0
			1968	1271	329	361	7		

- Molecule 16 is a protein called Subunit NDUFV2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	221	Total	C	N	O	S	0	0
			1698	1069	288	327	14		

- Molecule 17 is a protein called Oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	185	Total	C	N	O	S	0	0
			1487	941	252	282	12		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	186	Total	C	N	O	S	0	0
			1375	872	259	242	2		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	182	Total	C	N	O	S	0	0
			1454	927	255	257	15		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	88	Total	C	N	O	S	0	0
			671	450	103	115	3		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	117	Total	C	N	O	S	0	0
			930	581	177	167	5		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	149	ALA	SER	conflict	UNP G0S6J1
M	150	ASN	-	insertion	UNP G0S6J1
M	151	GLU	-	insertion	UNP G0S6J1
M	152	HIS	-	insertion	UNP G0S6J1
M	153	HIS	-	insertion	UNP G0S6J1
M	154	ARG	-	insertion	UNP G0S6J1
M	155	LYS	-	insertion	UNP G0S6J1
M	156	TYR	-	insertion	UNP G0S6J1
M	157	LEU	-	insertion	UNP G0S6J1
M	158	GLU	-	insertion	UNP G0S6J1
M	159	SER	-	insertion	UNP G0S6J1
M	160	LEU	-	insertion	UNP G0S6J1
M	161	PRO	-	insertion	UNP G0S6J1
M	162	GLN	-	insertion	UNP G0S6J1
M	163	THR	-	insertion	UNP G0S6J1
M	164	SER	-	insertion	UNP G0S6J1
M	165	TYR	-	insertion	UNP G0S6J1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	166	PRO	-	insertion	UNP G0S6J1
M	167	LEU	-	insertion	UNP G0S6J1
M	168	ASN	-	insertion	UNP G0S6J1

- Molecule 22 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	82	Total	C	N	O	S	0	0
			631	397	102	131	1		
22	Q	85	Total	C	N	O	S	0	0
			666	419	109	137	1		

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase B14 subunit-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	115	Total	C	N	O	S	0	0
			962	613	180	166	3		

- Molecule 24 is a protein called Complex I-B22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	98	Total	C	N	O	S	0	0
			807	520	149	137	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
25	S	74	Total	C	N	O	0	0
			610	401	98	111		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	169	Total	C	N	O	S	0	0
			1365	860	254	242	9		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	120	Total	C	N	O	S	0	0
			976	623	182	168	3		

- Molecule 28 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	187	Total	C	N	O	S	0	0
			1472	937	267	260	8		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	154	Total	C	N	O	S	0	0
			1240	788	219	229	4		

- Molecule 30 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	186	Total	C	N	O	S	0	0
			1432	898	254	278	2		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	189	SER	-	insertion	UNP G0SEF0
Z	190	TYR	-	insertion	UNP G0SEF0
Z	191	PRO	-	insertion	UNP G0SEF0
Z	192	CYS	-	insertion	UNP G0SEF0
Z	193	ARG	-	insertion	UNP G0SEF0
Z	194	SER	-	insertion	UNP G0SEF0
Z	195	PHE	-	insertion	UNP G0SEF0
Z	196	VAL	-	insertion	UNP G0SEF0

- Molecule 31 is a protein called NADH dehydrogenase (Ubiquinone)-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	143	Total	C	N	O	S	0	0
			1167	750	195	217	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	166	VAL	ALA	conflict	UNP G0RXU4
a	168	ALA	MET	conflict	UNP G0RXU4
a	?	-	GLU	deletion	UNP G0RXU4
a	?	-	GLY	deletion	UNP G0RXU4
a	?	-	ASP	deletion	UNP G0RXU4
a	?	-	PRO	deletion	UNP G0RXU4
a	?	-	ASP	deletion	UNP G0RXU4
a	?	-	PRO	deletion	UNP G0RXU4

- Molecule 32 is a protein called Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	81	Total	C	N	O	S	0	0
			683	445	125	110	3		

- Molecule 33 is a protein called Subunit NDUF3 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	60	Total	C	N	O	S	0	0
			490	320	86	82	2		

- Molecule 34 is a protein called Subunit NDUF10 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	99	Total	C	N	O	S	0	0
			822	523	145	150	4		

- Molecule 35 is a protein called Subunit NDUF2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	37	Total	C	N	O	S	0	0
			309	211	54	43	1		

- Molecule 36 is a protein called NADH dehydrogenase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	88	Total	C	N	O	S	0	0
			717	459	127	128	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	?	-	ALA	deletion	UNP G0S1P3

- Molecule 37 is a protein called Subunit NDUFA3 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	78	Total	C	N	O	S	0	0
			610	399	105	105	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	133	Total	C	N	O	S	0	0
			1118	723	194	200	1		

- Molecule 39 is a protein called Subunit NDUF6 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	80	Total	C	N	O	S	0	0
			677	447	117	111	2		

- Molecule 40 is a protein called Subunit NDUF4 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	73	Total	C	N	O	S	0	0
			603	391	108	101	3		

- Molecule 41 is a protein called Subunit NDUF5 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
41	n	135	Total	C	N	O	S	0	0
			1061	680	186	194	1		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	1	MET	-	initiating methionine	UNP G0S086

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Chain	Residue	Modelled	Actual	Comment	Reference
n	2	LEU	-	insertion	UNP G0S086
n	3	ALA	-	insertion	UNP G0S086
n	4	LEU	-	insertion	UNP G0S086
n	5	ARG	-	insertion	UNP G0S086
n	6	GLN	-	insertion	UNP G0S086
n	7	ARG	-	insertion	UNP G0S086
n	8	ALA	-	insertion	UNP G0S086
n	9	ALA	-	insertion	UNP G0S086
n	10	LEU	-	insertion	UNP G0S086
n	11	LEU	-	insertion	UNP G0S086
n	12	ALA	-	insertion	UNP G0S086
n	13	ARG	-	insertion	UNP G0S086
n	14	ARG	-	insertion	UNP G0S086
n	15	VAL	-	insertion	UNP G0S086
n	16	ARG	-	insertion	UNP G0S086
n	17	PRO	-	insertion	UNP G0S086
n	18	THR	-	insertion	UNP G0S086
n	19	VAL	-	insertion	UNP G0S086
n	20	VAL	-	insertion	UNP G0S086
n	21	VAL	-	insertion	UNP G0S086
n	22	PRO	-	insertion	UNP G0S086
n	23	ARG	-	insertion	UNP G0S086
n	24	ASN	-	insertion	UNP G0S086
n	25	ALA	-	insertion	UNP G0S086
n	26	ARG	-	insertion	UNP G0S086
n	27	THR	-	insertion	UNP G0S086
n	28	TYR	-	insertion	UNP G0S086
n	29	ALA	-	insertion	UNP G0S086
n	30	SER	-	insertion	UNP G0S086
n	31	SER	-	insertion	UNP G0S086
n	32	HIS	-	insertion	UNP G0S086
n	33	ASP	-	insertion	UNP G0S086
n	34	HIS	-	insertion	UNP G0S086
n	35	ASP	-	insertion	UNP G0S086
n	36	HIS	-	insertion	UNP G0S086
n	37	HIS	-	insertion	UNP G0S086
n	38	ASP	-	insertion	UNP G0S086
n	39	HIS	-	insertion	UNP G0S086
n	40	HIS	-	insertion	UNP G0S086
n	41	HIS	-	insertion	UNP G0S086
n	42	ASP	-	insertion	UNP G0S086
n	43	HIS	-	insertion	UNP G0S086

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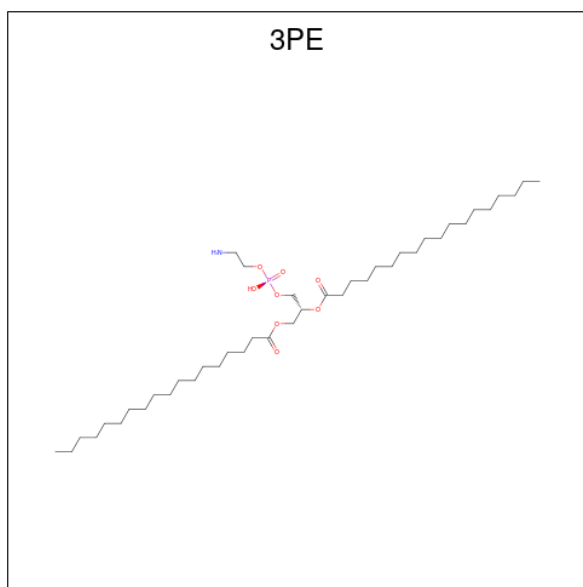
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Chain	Residue	Modelled	Actual	Comment	Reference
n	44	GLY	-	insertion	UNP G0S086
n	45	HIS	-	insertion	UNP G0S086
n	46	ASN	-	insertion	UNP G0S086
n	47	VAL	-	insertion	UNP G0S086
n	48	GLU	-	insertion	UNP G0S086
n	49	GLU	-	insertion	UNP G0S086
n	50	PRO	-	insertion	UNP G0S086
n	51	LEU	-	insertion	UNP G0S086
n	52	GLY	-	insertion	UNP G0S086

- Molecule 42 is a protein called Oxidoreductase-like domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	o	32	Total	C	N	O	0	0
			252	165	43	44		

- Molecule 43 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



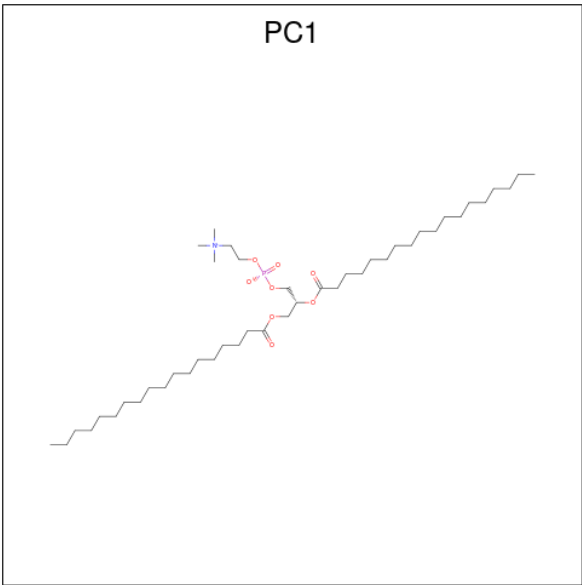
Mol	Chain	Residues	Atoms					AltConf
43	1	1	Total	C	N	O	P	0
			50	40	1	8	1	
43	1	1	Total	C	N	O	P	0
			27	18	1	7	1	
43	4	1	Total	C	N	O	P	0
			33	23	1	8	1	

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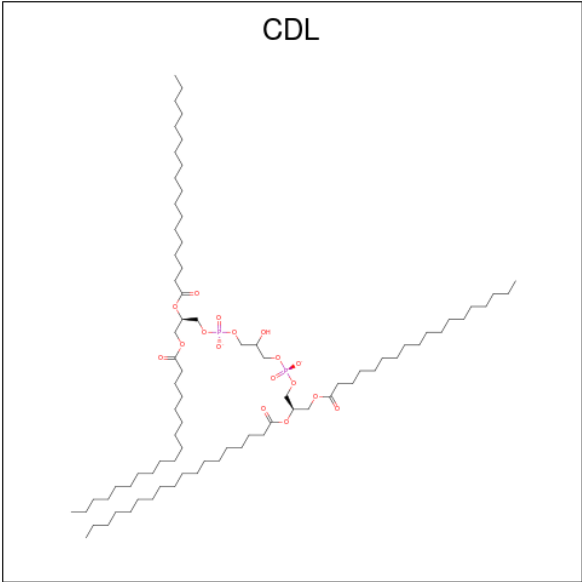
Mol	Chain	Residues	Atoms					AltConf
43	4	1	Total	C	N	O	P	0
			31	21	1	8	1	
43	5	1	Total	C	N	O	P	0
			40	30	1	8	1	
43	5	1	Total	C	N	O	P	0
			32	22	1	8	1	
43	5	1	Total	C	N	O	P	0
			32	22	1	8	1	
43	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
43	5	1	Total	C	N	O	P	0
			41	31	1	8	1	
43	8	1	Total	C	N	O	P	0
			36	26	1	8	1	
43	E	1	Total	C	N	O	P	0
			27	17	1	8	1	
43	J	1	Total	C	N	O	P	0
			32	22	1	8	1	
43	W	1	Total	C	N	O	P	0
			34	24	1	8	1	
43	W	1	Total	C	N	O	P	0
			40	30	1	8	1	
43	g	1	Total	C	N	O	P	0
			35	25	1	8	1	
43	i	1	Total	C	N	O	P	0
			39	29	1	8	1	
43	n	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 44 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



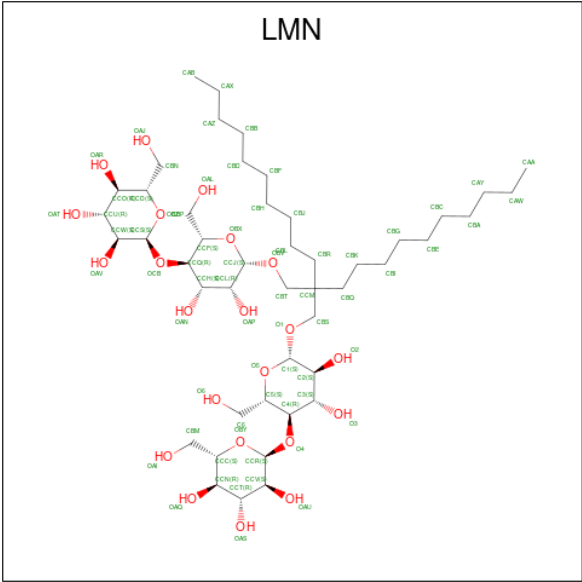
Mol	Chain	Residues	Atoms					AltConf
44	1	1	Total	C	N	O	P	0
			43	33	1	8	1	
44	2	1	Total	C	N	O	P	0
			30	20	1	8	1	
44	3	1	Total	C	N	O	P	0
			49	39	1	8	1	
44	4	1	Total	C	N	O	P	0
			50	40	1	8	1	
44	5	1	Total	C	N	O	P	0
			46	36	1	8	1	
44	5	1	Total	C	N	O	P	0
			43	33	1	8	1	
44	K	1	Total	C	N	O	P	0
			34	24	1	8	1	
44	S	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 45 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



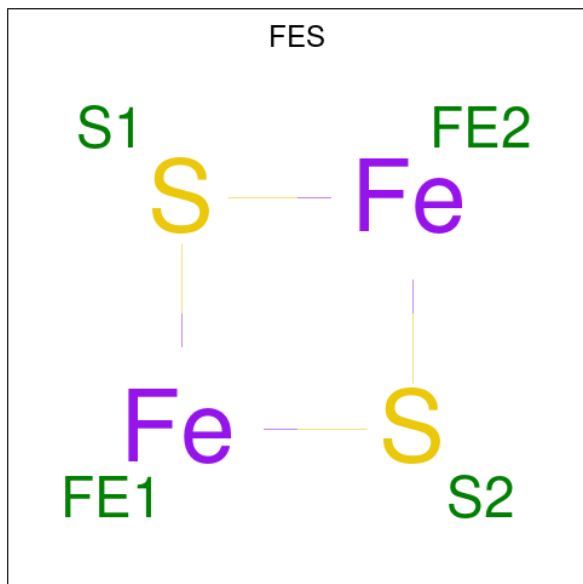
Mol	Chain	Residues	Atoms				AltConf
45	2	1	Total	C	O	P	0
			85	66	17	2	
45	4	1	Total	C	O	P	0
			83	64	17	2	
45	X	1	Total	C	O	P	0
			78	59	17	2	
45	g	1	Total	C	O	P	0
			57	38	17	2	
45	h	1	Total	C	O	P	0
			65	46	17	2	

- Molecule 46 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: C₄₇H₈₈O₂₂).



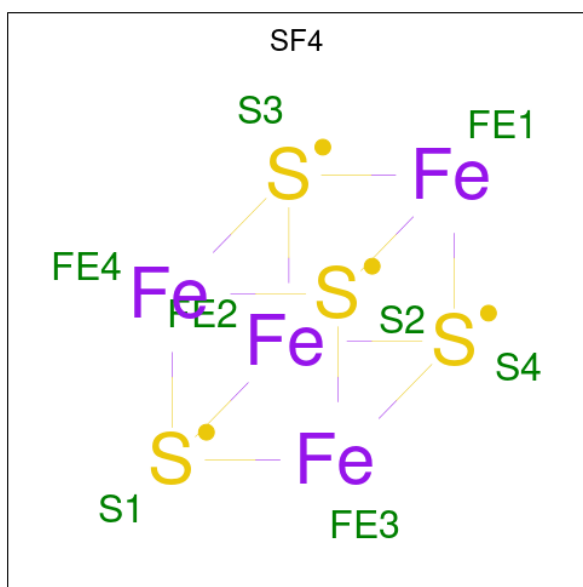
Mol	Chain	Residues	Atoms			AltConf
46	2	1	Total	C	O	0
			58	41	17	
46	J	1	Total	C	O	0
			58	41	17	
46	j	1	Total	C	O	0
			68	46	22	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



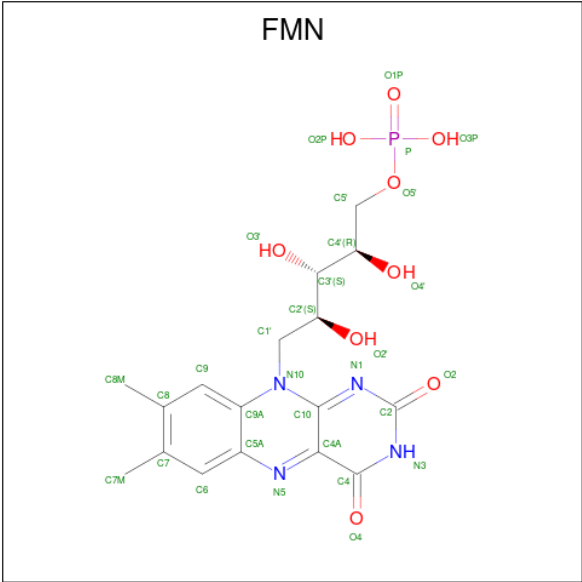
Mol	Chain	Residues	Atoms			AltConf
47	A	1	Total	Fe	S	0
			4	2	2	
47	H	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



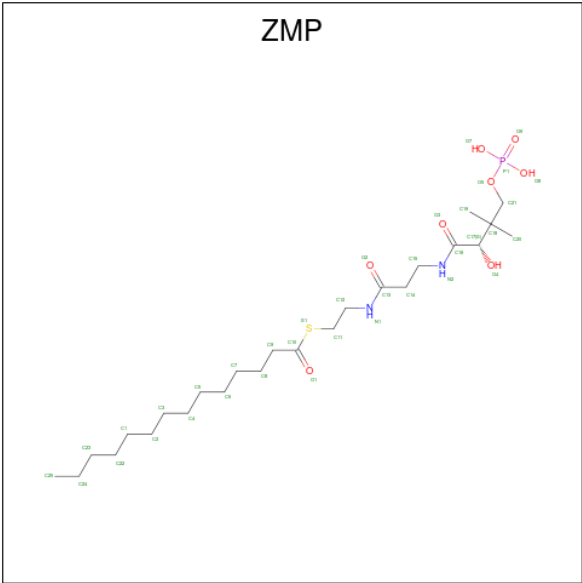
Mol	Chain	Residues	Atoms			AltConf
48	A	1	Total	Fe	S	0
			8	4	4	
48	A	1	Total	Fe	S	0
			8	4	4	
48	B	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	
48	K	1	Total	Fe	S	0
			8	4	4	

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



Mol	Chain	Residues	Atoms		AltConf
51	M	1	Total	Zn	0
			1	1	

- Molecule 52 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



Mol	Chain	Residues	Atoms						AltConf
52	O	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	
52	Q	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- Molecule 53 is water.

Mol	Chain	Residues	Atoms		AltConf
53	1	90	Total	O	0
			90	90	
53	2	137	Total	O	0
			137	137	
53	3	39	Total	O	0
			39	39	
53	4	56	Total	O	0
			56	56	
53	5	16	Total	O	0
			16	16	
53	6	43	Total	O	0
			43	43	

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Mol	Chain	Residues	Atoms		AltConf
53	9	14	Total 14	O 14	0
53	A	197	Total 197	O 197	0
53	B	30	Total 30	O 30	0
53	C	166	Total 166	O 166	0
53	D	22	Total 22	O 22	0
53	E	62	Total 62	O 62	0
53	F	29	Total 29	O 29	0
53	G	99	Total 99	O 99	0
53	H	5	Total 5	O 5	0
53	I	84	Total 84	O 84	0
53	K	83	Total 83	O 83	0
53	L	11	Total 11	O 11	0
53	M	34	Total 34	O 34	0
53	P	24	Total 24	O 24	0
53	S	1	Total 1	O 1	0
53	U	38	Total 38	O 38	0
53	W	39	Total 39	O 39	0
53	X	50	Total 50	O 50	0
53	Y	91	Total 91	O 91	0
53	Z	40	Total 40	O 40	0
53	a	4	Total 4	O 4	0

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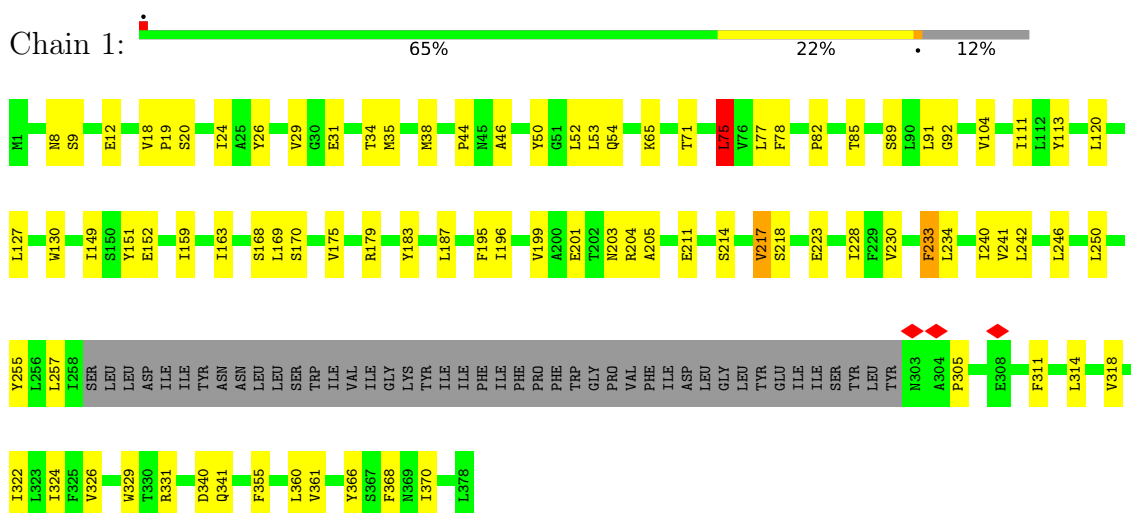
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Mol	Chain	Residues	Atoms		AltConf
53	b	2	Total 2	O 2	0
53	d	4	Total 4	O 4	0
53	f	1	Total 1	O 1	0
53	g	9	Total 9	O 9	0
53	h	46	Total 46	O 46	0
53	j	3	Total 3	O 3	0
53	n	24	Total 24	O 24	0

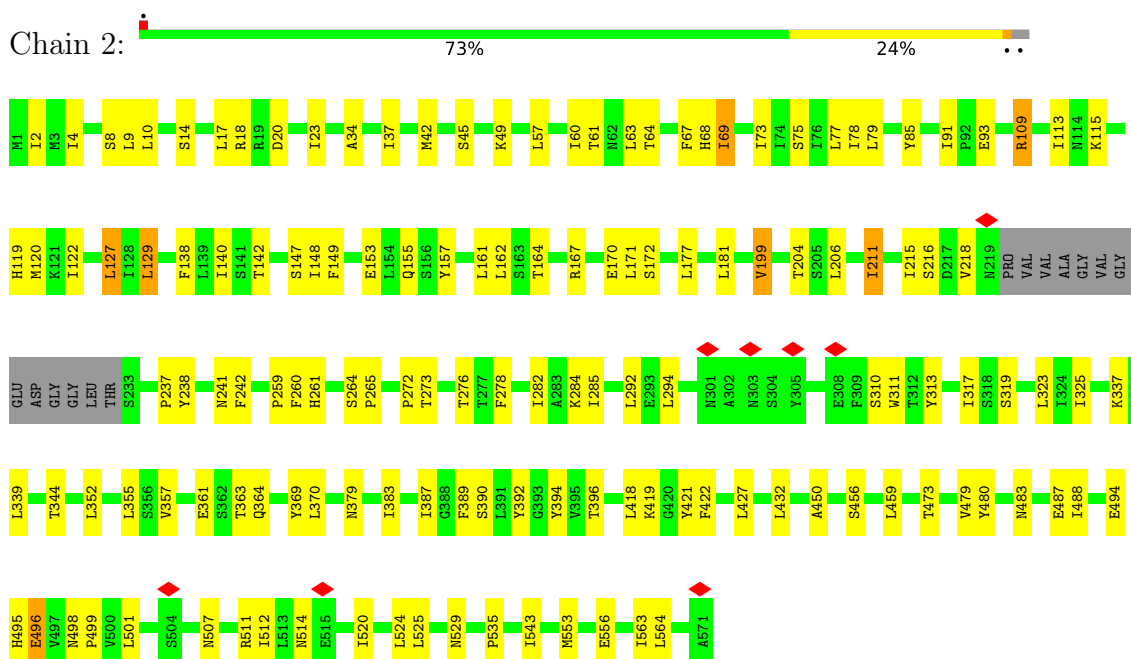
3 Residue-property plots

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.

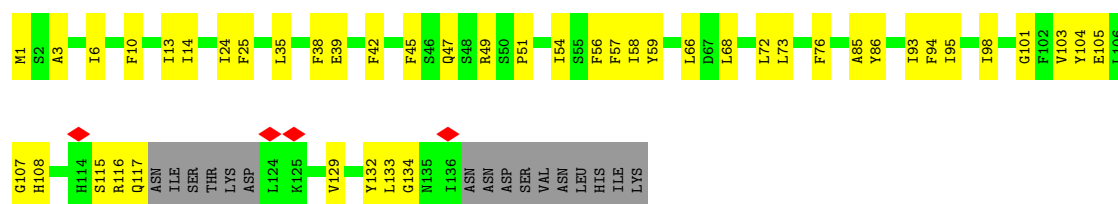
- Molecule 1: NADH-ubiquinone oxidoreductase chain 1



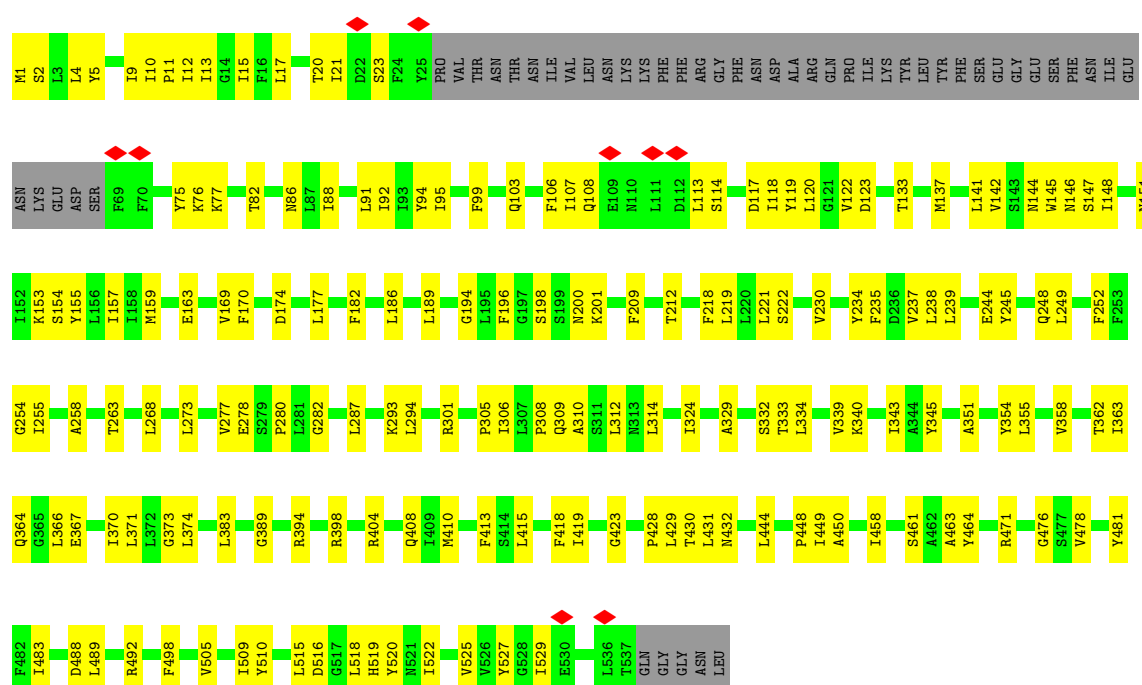
- Molecule 2: NADH dehydrogenase subunit 2



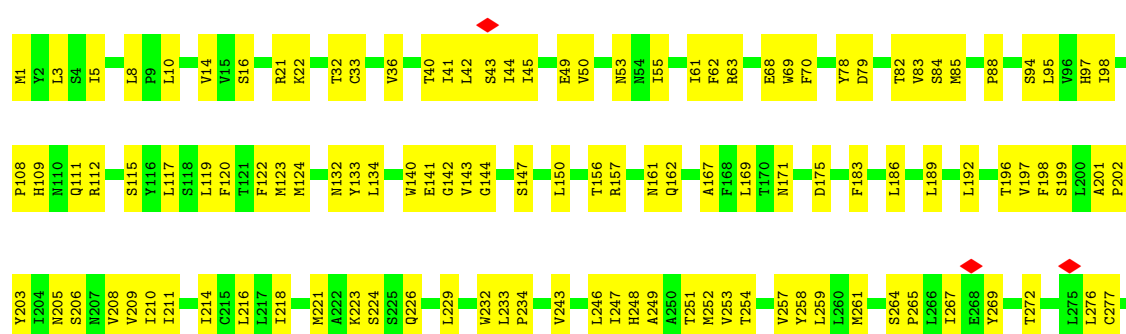
Chain 3: 58% 31% 11%

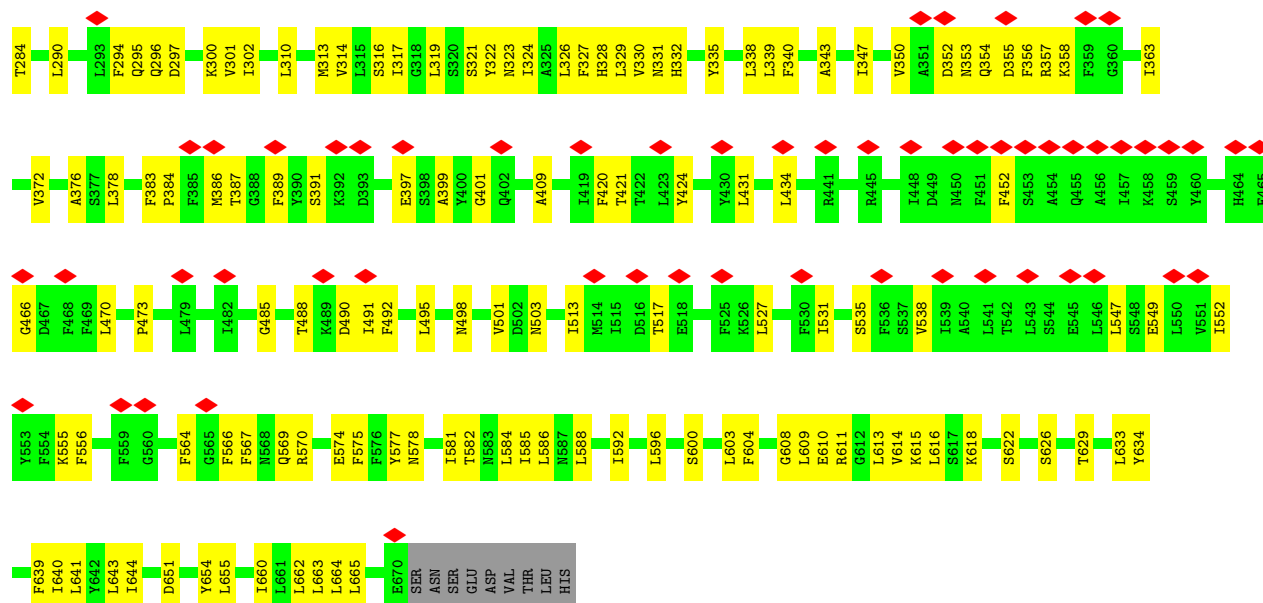


Chain 4:

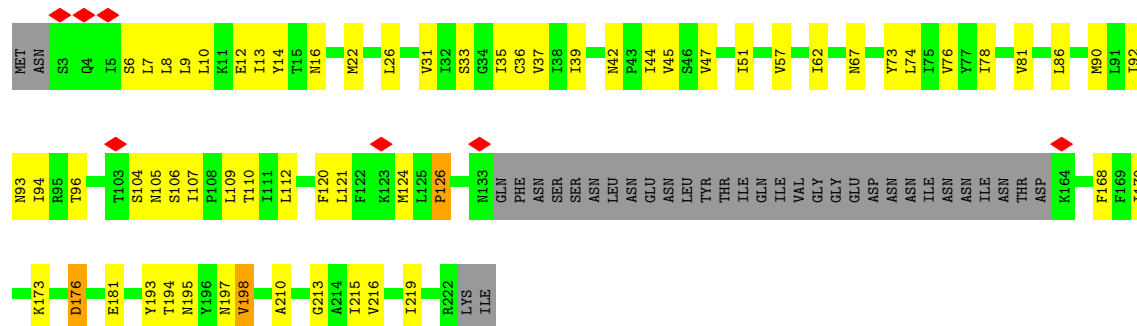


Chain 5: 9% 62% 36%

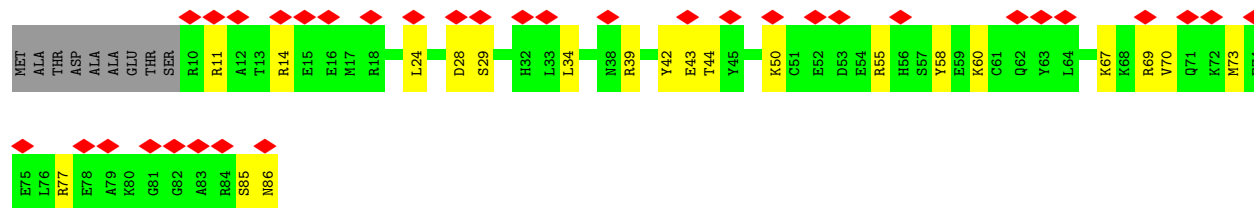
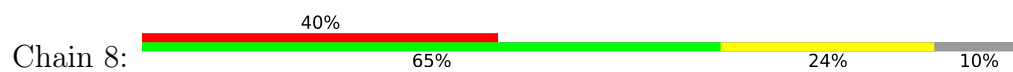




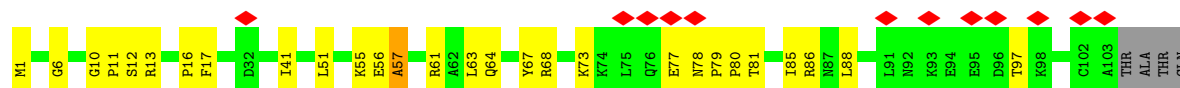
• Molecule 6: NADH-ubiquinone oxidoreductase chain 6



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

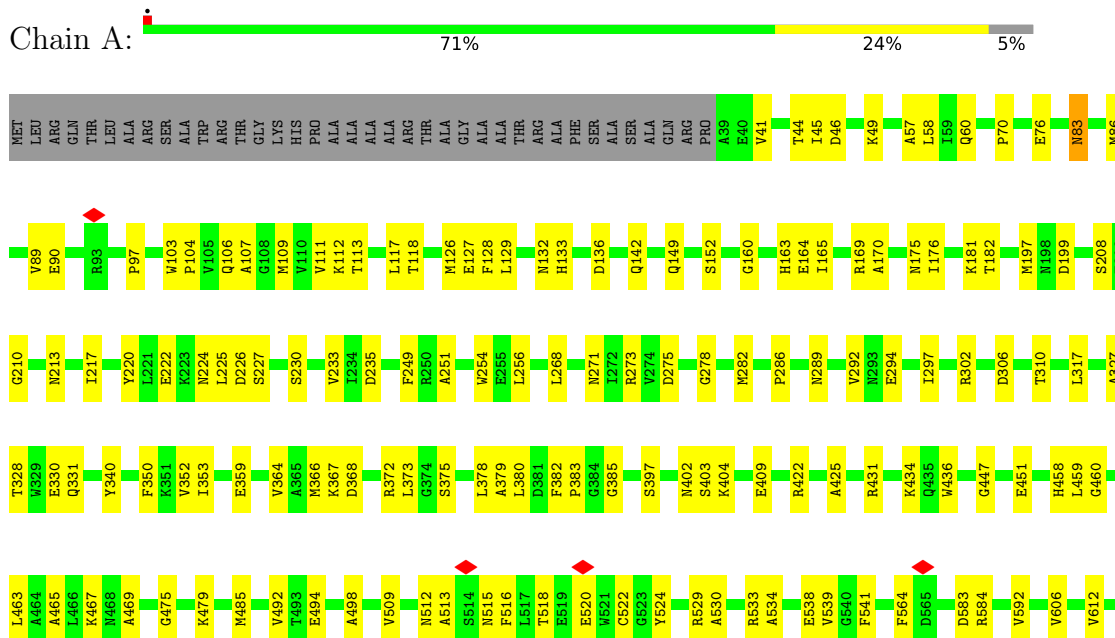


• Molecule 8: Subunit NDUF55 of NADH-ubiquinone oxidoreductase (Complex I)



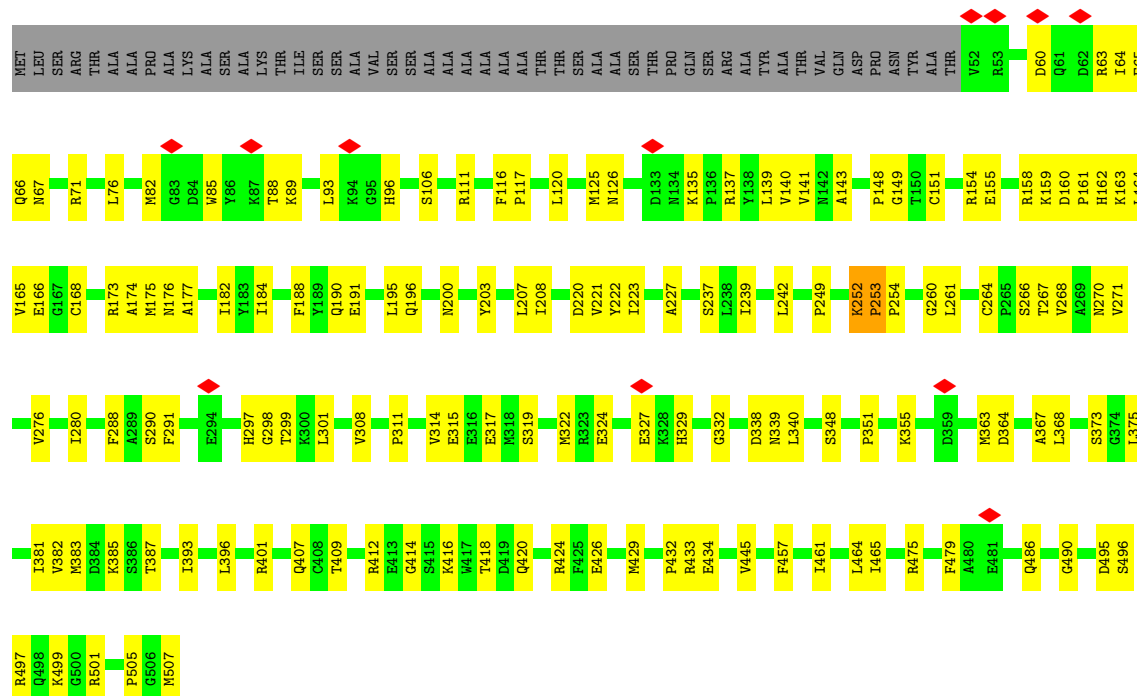
[illegible]

- Molecule 9: NADH-ubiquinone oxidoreductase-like protein

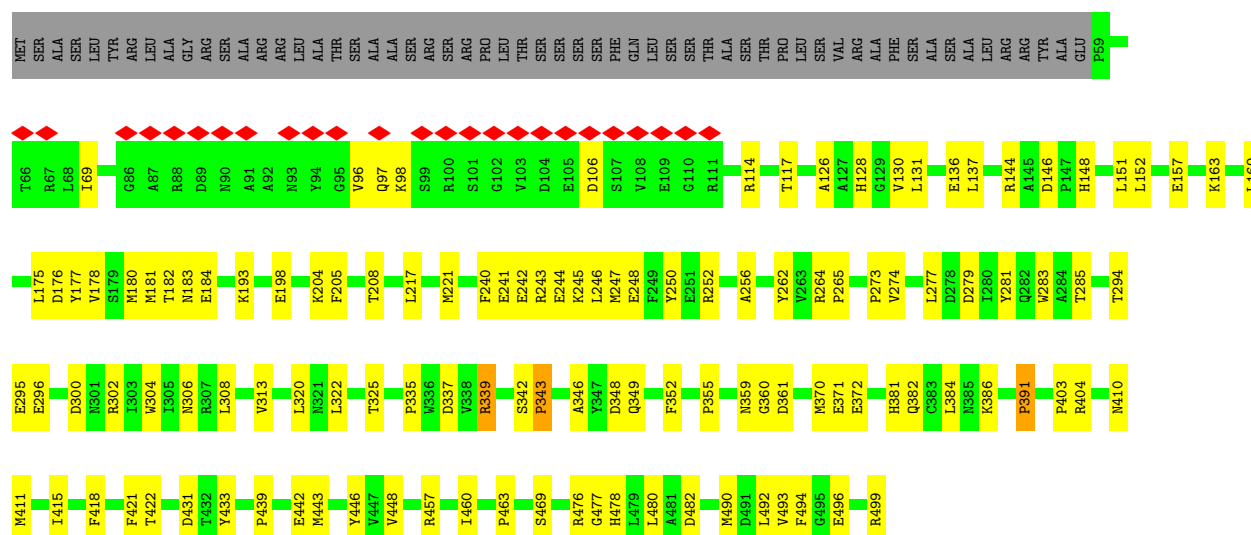




- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



- Molecule 11: NADH-ubiquinone oxidoreductase 49 kDa subunit-like protein



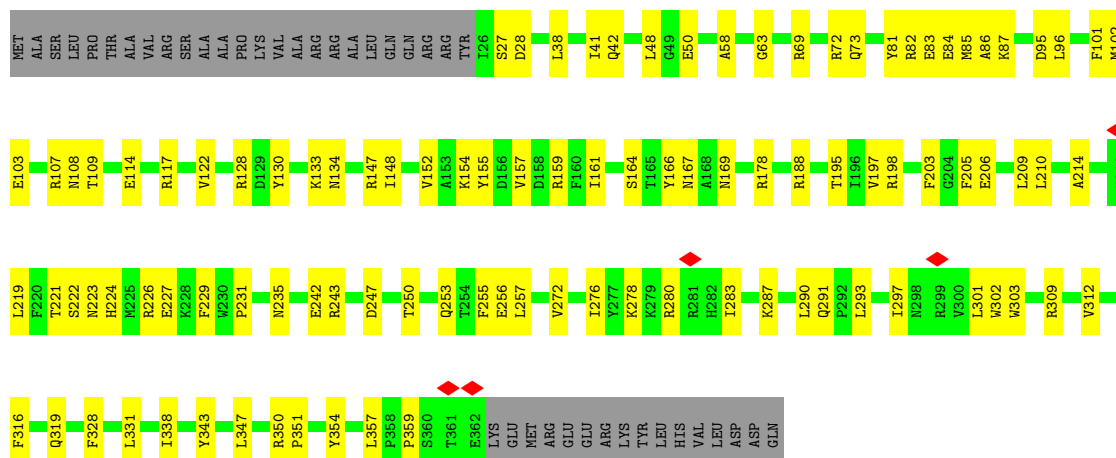
- Molecule 12: Subunit NDUFA1 of NADH-ubiquinone oxidoreductase (Complex I)

Chain D:  83% 15% ..



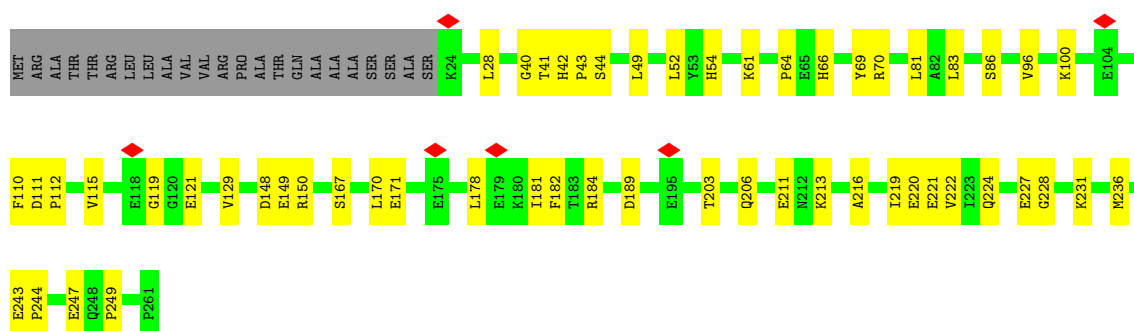
• Molecule 13: NADH dehydrogenase (Ubiquinone)-like protein

Chain E:  62% 27% 11%



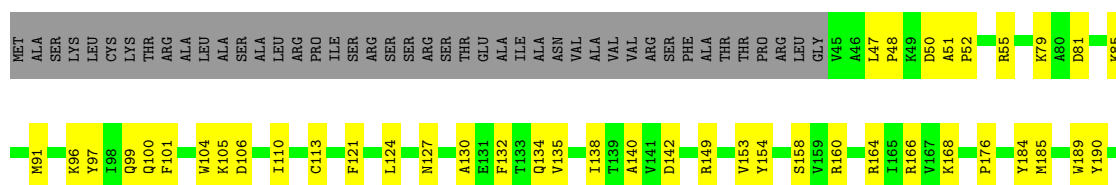
• Molecule 14: NADH-ubiquinone oxidoreductase-like protein

Chain F:  70% 21% 9%

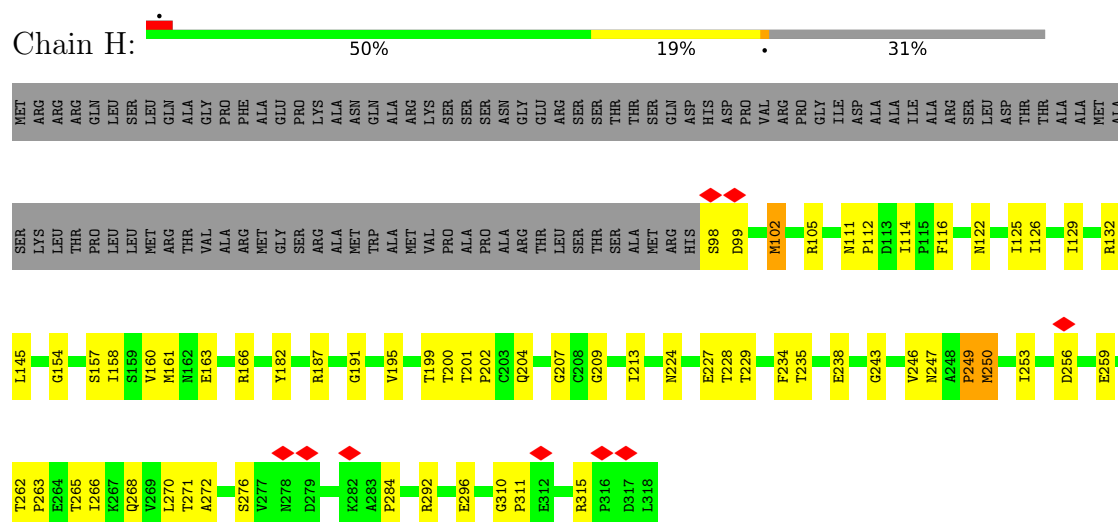


• Molecule 15: NADH-ubiquinone oxidoreductase 30.4 kDa subunit-like protein

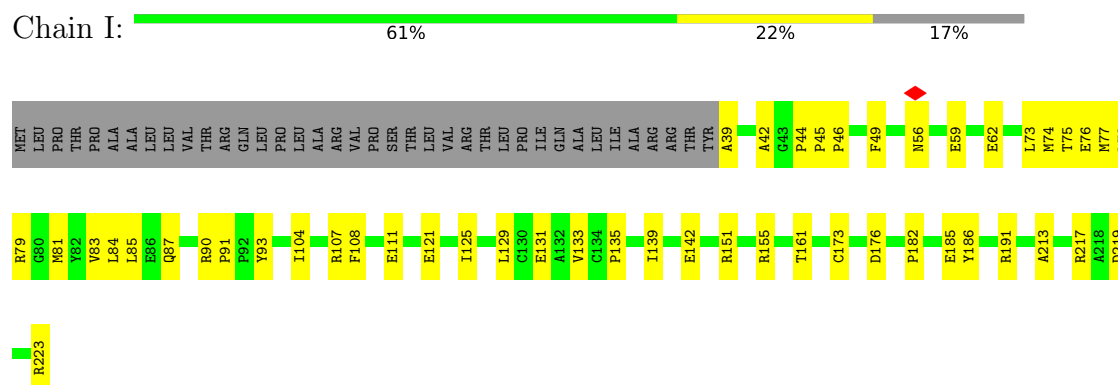
Chain G:  59% 24% 17%



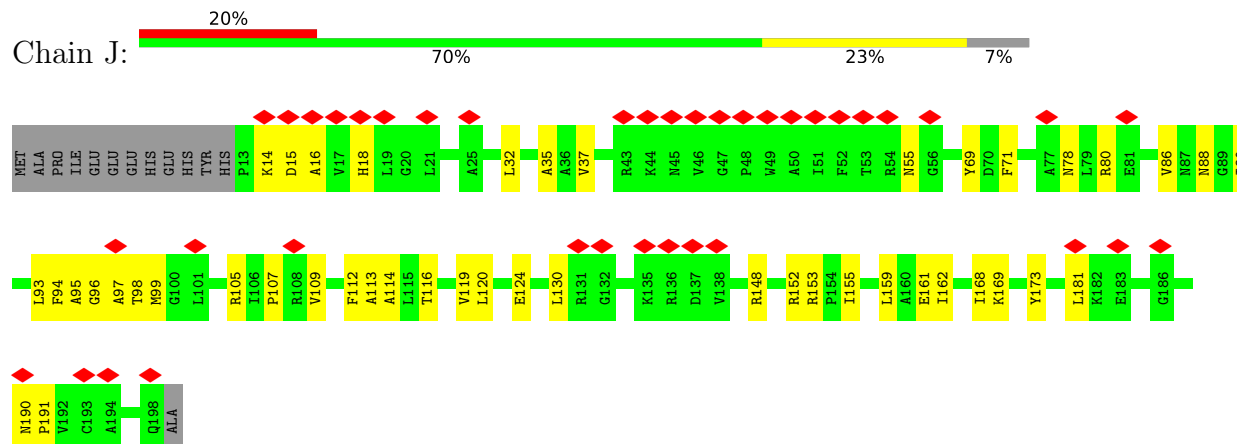
- Molecule 16: Subunit NDUFV2 of NADH-ubiquinone oxidoreductase (Complex I)



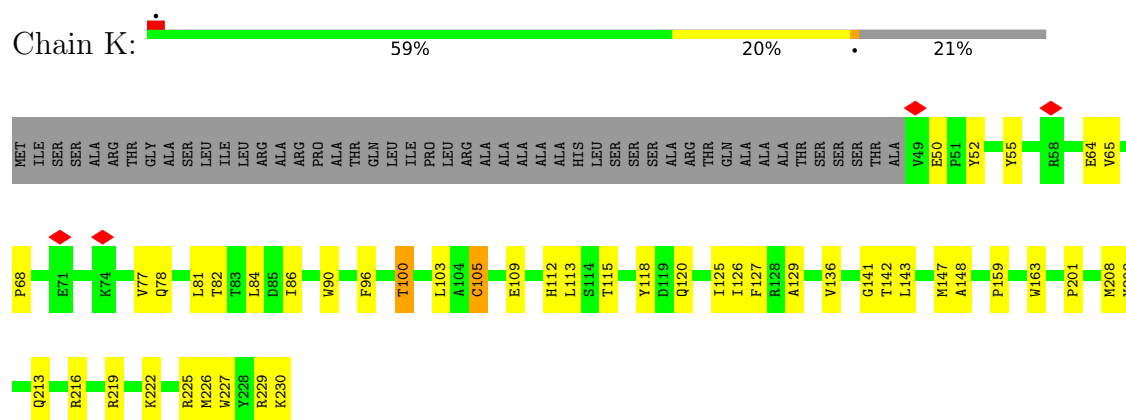
- Molecule 17: Oxidoreductase-like protein



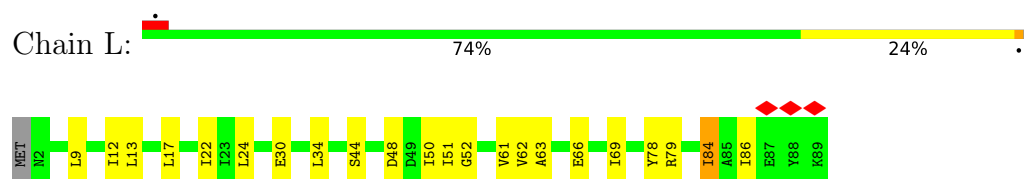
- Molecule 18: NADH-ubiquinone oxidoreductase-like protein.



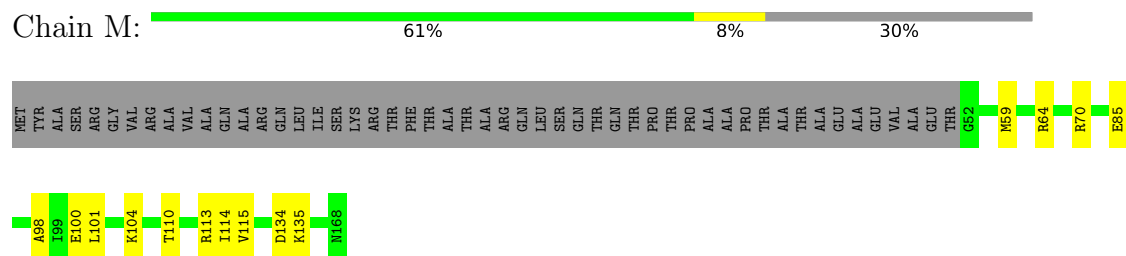
- Molecule 19: NADH-ubiquinone oxidoreductase-like protein



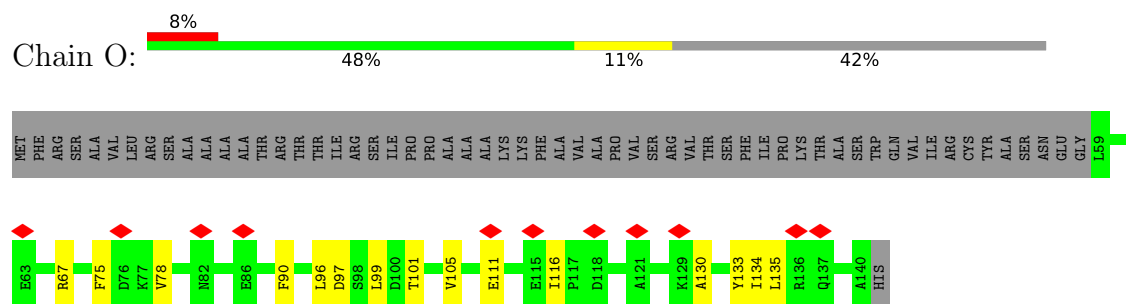
- Molecule 20: NADH-ubiquinone oxidoreductase chain 4L



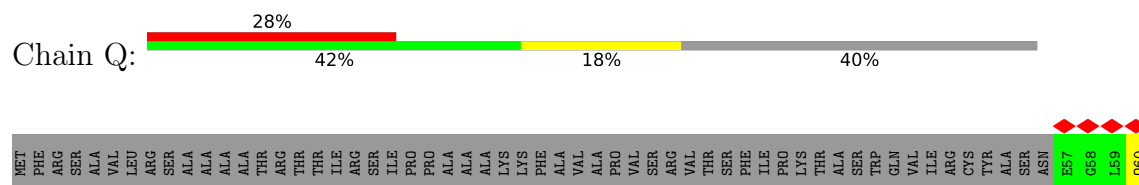
- Molecule 21: NADH-ubiquinone oxidoreductase-like protein

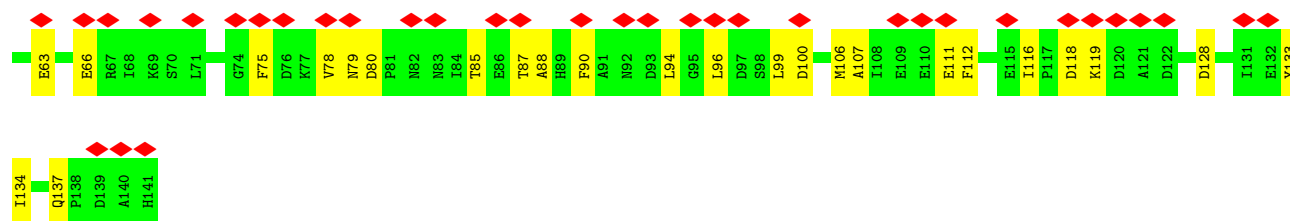


- Molecule 22: Acyl carrier protein



- Molecule 22: Acyl carrier protein

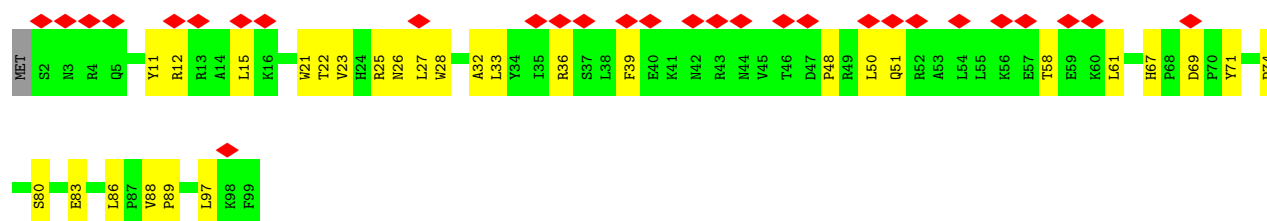




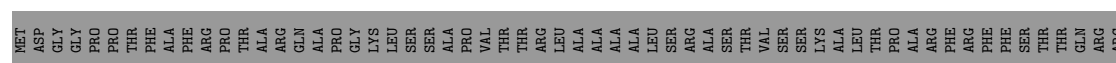
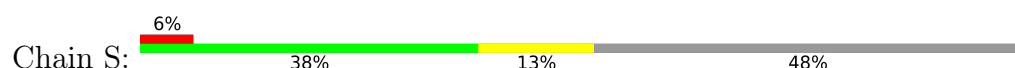
- Molecule 23: NADH-ubiquinone oxidoreductase B14 subunit-like protein



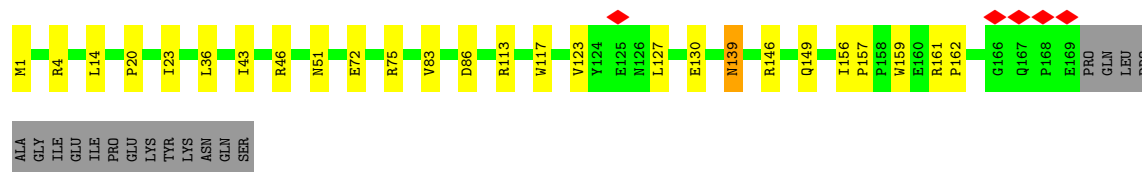
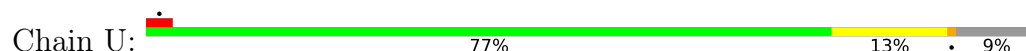
- Molecule 24: Complex I-B22



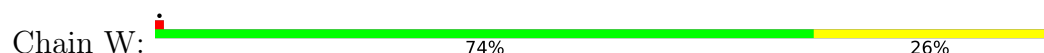
- Molecule 25: Complex I-ESSS



- Molecule 26: NADH-ubiquinone oxidoreductase

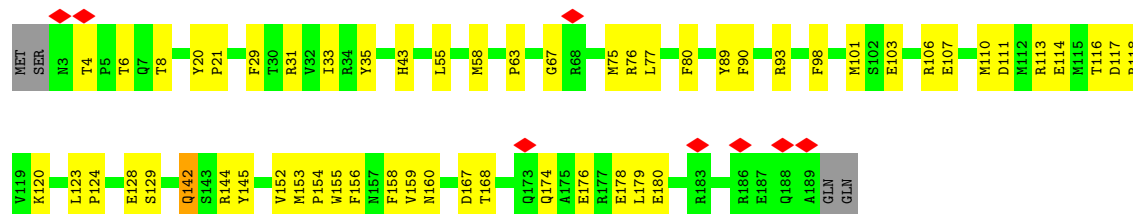


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

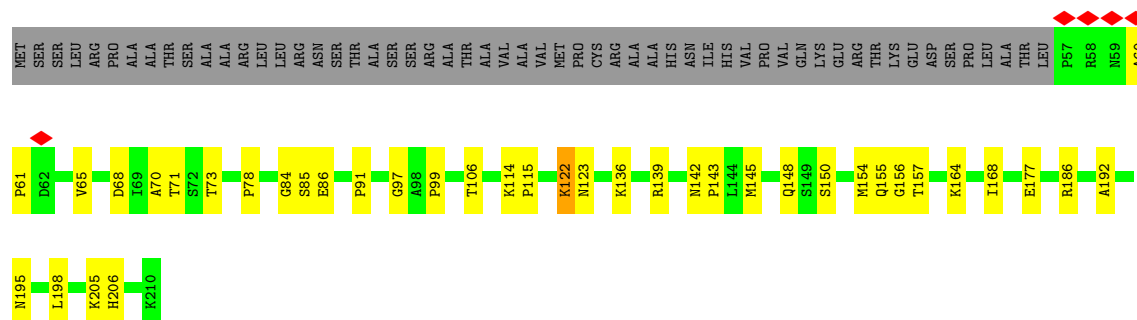




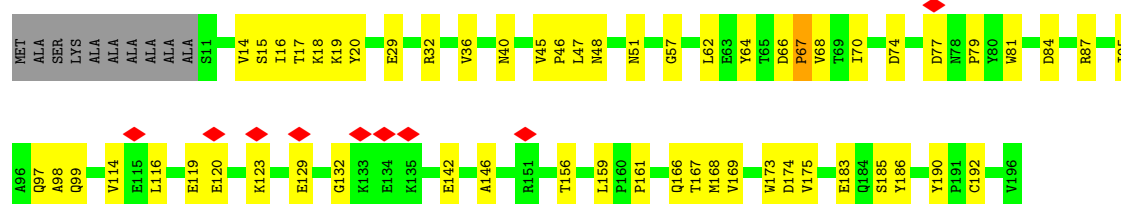
- Molecule 28: NADH-ubiquinone oxidoreductase-like protein



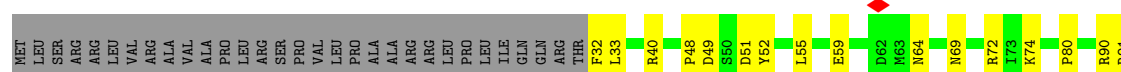
- Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

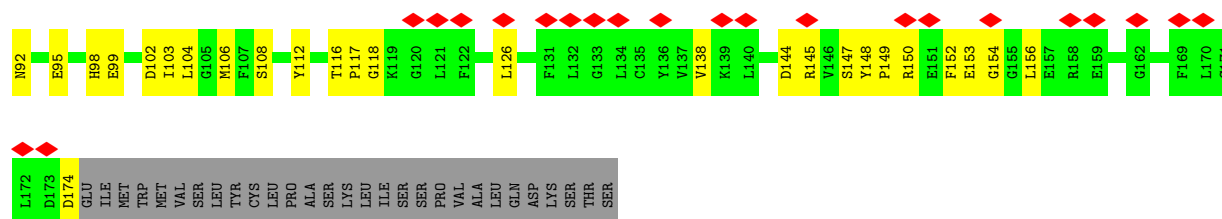


- Molecule 30: NADH-ubiquinone oxidoreductase-like protein



- Molecule 31: NADH dehydrogenase (Ubiquinone)-like protein

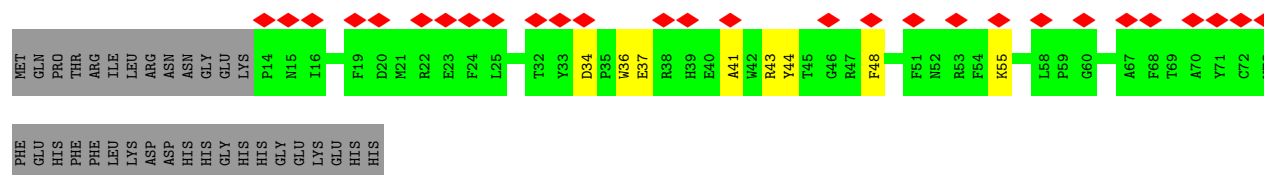




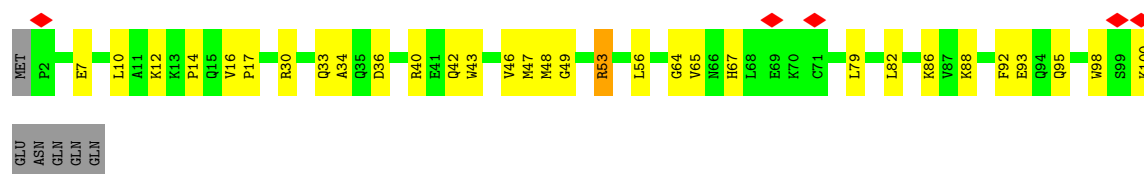
- Molecule 32: Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I)



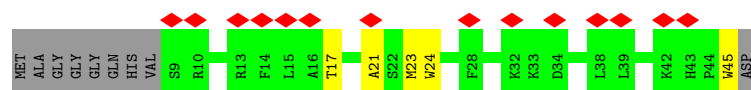
- Molecule 33: Subunit NDUFB3 of NADH-ubiquinone oxidoreductase (Complex I)



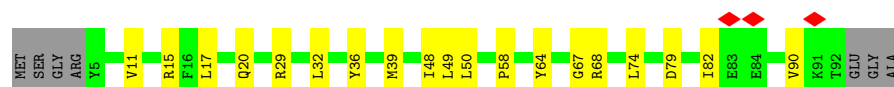
- Molecule 34: Subunit NDUFB10 of NADH-ubiquinone oxidoreductase (Complex I)



- Molecule 35: Subunit NDUFB2 of NADH-ubiquinone oxidoreductase (Complex I)

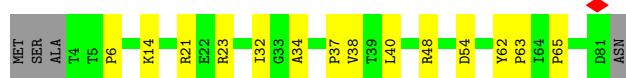


- Molecule 36: NADH dehydrogenase-like protein



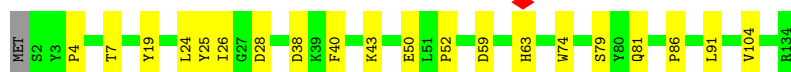
- Molecule 37: Subunit NDUFA3 of NADH-ubiquinone oxidoreductase (Complex I)

Chain g: 



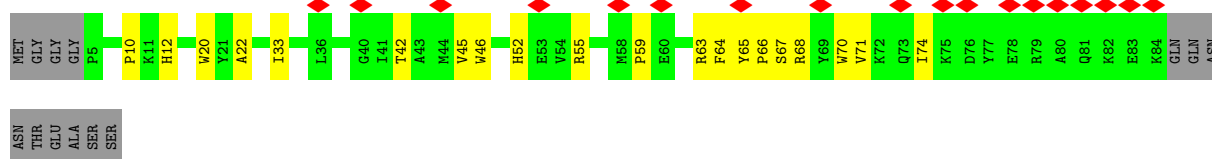
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit

Chain h: 



- Molecule 39: Subunit NDUF6 of NADH-ubiquinone oxidoreductase (Complex I)

Chain i: 



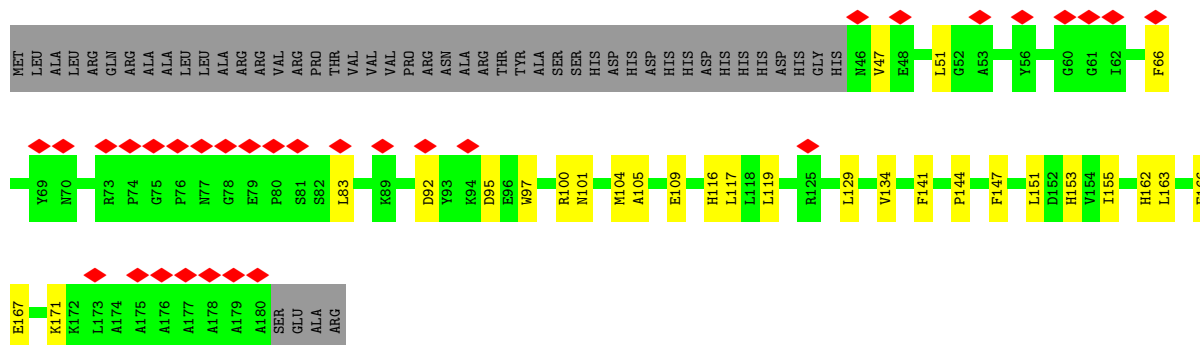
- Molecule 40: Subunit NDUF4 of NADH-ubiquinone oxidoreductase (Complex I)

Chain j: 



- Molecule 41: Subunit NDUF5 of NADH-ubiquinone oxidoreductase (Complex I)

Chain n: 



- Molecule 42: Oxidoreductase-like domain-containing protein

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21989	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.675	Depositor
Minimum map value	-1.374	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.110	Depositor
Recommended contour level	0.12	Depositor
Map size ($\text{\AA}$)	159.03, 221.80501, 319.734	wwPDB
Map dimensions	382, 265, 190	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.837, 0.837, 0.837	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LMN, ZMP, FMN, 3PE, 2MR, FES, ZN, PC1, NDP, SF4, CDL

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	1	0.66	0/2633	0.98	3/3593 (0.1%)
2	2	0.68	3/4562 (0.1%)	0.97	10/6205 (0.2%)
3	3	0.61	0/1053	0.89	0/1428
4	4	0.41	0/4002	0.64	1/5454 (0.0%)
5	5	0.34	1/5414 (0.0%)	0.53	1/7371 (0.0%)
6	6	0.69	0/1479	1.04	2/2017 (0.1%)
7	8	0.20	0/671	0.41	0/896
8	9	0.60	0/824	0.90	1/1112 (0.1%)
9	A	0.46	0/5589	0.66	8/7579 (0.1%)
10	B	0.41	0/3621	0.63	4/4878 (0.1%)
11	C	0.49	1/3542 (0.0%)	0.69	3/4806 (0.1%)
12	D	0.68	0/674	1.04	1/911 (0.1%)
13	E	0.37	0/2807	0.56	0/3807
14	F	0.37	0/1924	0.56	0/2609
15	G	0.40	0/2026	0.58	0/2759
16	H	0.44	2/1737 (0.1%)	0.64	2/2362 (0.1%)
17	I	0.62	0/1527	0.87	0/2070
18	J	0.30	0/1400	0.45	0/1892
19	K	0.57	0/1493	0.87	1/2026 (0.0%)
20	L	0.66	0/677	1.03	1/917 (0.1%)
21	M	0.60	0/961	0.78	0/1309
22	O	0.70	0/640	0.94	0/871
22	Q	0.24	0/676	0.44	0/917
23	P	0.33	0/986	0.50	0/1333
24	R	0.16	0/832	0.37	0/1133
25	S	0.41	0/635	0.55	0/869
26	U	0.79	0/1403	1.15	0/1904
27	W	0.65	0/1001	0.99	0/1354
28	X	0.67	0/1511	1.04	2/2043 (0.1%)
29	Y	0.35	0/1277	0.54	2/1731 (0.1%)
30	Z	0.44	1/1466 (0.1%)	0.62	1/1997 (0.1%)
31	a	0.30	0/1204	0.50	0/1632

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	b	0.38	0/701	0.63	1/939 (0.1%)
33	c	0.19	0/509	0.34	0/691
34	d	0.46	0/840	0.79	1/1130 (0.1%)
35	e	0.24	0/324	0.44	0/440
36	f	0.45	0/731	0.71	0/981
37	g	0.62	0/631	0.81	3/868 (0.3%)
38	h	0.40	0/1158	0.59	0/1577
39	i	0.37	0/706	0.48	0/960
40	j	0.28	0/617	0.42	0/830
41	n	0.62	0/1092	0.90	1/1481 (0.1%)
42	o	0.19	0/262	0.36	0/360
All	All	0.50	8/67818 (0.0%)	0.73	49/92042 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	B	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	122	ILE	C-N	10.49	1.47	1.33
2	2	495	HIS	C-N	7.66	1.44	1.33
5	5	300	LYS	C-N	7.35	1.43	1.33
30	Z	66	ASP	C-N	-6.95	1.26	1.33
16	H	249	PRO	C-N	-6.87	1.24	1.33
2	2	496	GLU	C-N	6.19	1.41	1.33
11	C	342	SER	CA-CB	-6.01	1.46	1.53
16	H	250	MET	C-N	-5.06	1.27	1.33

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	253	PRO	N-CA-C	10.16	123.09	110.70
19	K	100	THR	CB-CA-C	7.88	123.89	111.91
4	4	182	PHE	CA-CB-CG	7.74	121.54	113.80
9	A	83	ASN	N-CA-C	7.64	119.69	111.36
2	2	122	ILE	O-C-N	6.97	131.42	122.77
8	9	57	ALA	N-CA-C	-6.50	104.03	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	30	HIS	N-CA-C	-6.49	103.71	111.69
10	B	252	LYS	CA-C-N	6.47	127.04	120.38
10	B	252	LYS	C-N-CA	6.47	127.04	120.38
2	2	389	PHE	N-CA-C	-6.33	105.86	113.97
5	5	629	THR	CB-CA-C	6.31	121.58	110.85
2	2	494	GLU	N-CA-C	-6.30	105.23	113.17
6	6	105	ASN	N-CA-C	-6.22	105.65	113.18
10	B	254	PRO	N-CA-C	-6.22	101.44	111.03
28	X	63	PRO	N-CA-C	6.16	120.91	111.11
11	C	339	ARG	CB-CA-C	6.13	121.99	109.55
16	H	199	THR	CB-CA-C	6.04	120.58	110.44
9	A	136	ASP	CB-CA-C	-5.99	101.22	111.46
1	1	75	LEU	N-CA-C	5.94	117.76	111.28
20	L	84	ILE	N-CA-C	-5.88	105.65	111.77
32	b	54	ASP	N-CA-C	-5.75	104.62	111.69
2	2	495	HIS	O-C-N	5.74	129.91	123.19
30	Z	67	PRO	N-CA-C	5.71	119.87	110.55
2	2	218	VAL	N-CA-C	-5.62	106.20	111.48
2	2	67	PHE	CB-CA-C	5.62	120.97	110.70
34	d	53	ARG	N-CA-C	-5.59	104.82	111.69
28	X	178	GLU	N-CA-C	-5.54	106.02	112.89
16	H	102	MET	CB-CG-SD	5.50	129.21	112.70
11	C	343	PRO	N-CA-CB	-5.50	98.24	103.19
37	g	65	PRO	CA-C-O	-5.46	116.97	120.90
6	6	6	SER	N-CA-CB	-5.45	107.95	114.17
1	1	179	ARG	N-CA-C	-5.37	106.56	113.01
11	C	339	ARG	N-CA-C	-5.34	106.61	113.23
37	g	48	ARG	N-CA-C	-5.30	105.56	112.23
9	A	128	PHE	CB-CA-C	5.25	119.12	110.88
9	A	104	PRO	CB-CA-C	5.21	117.77	111.46
29	Y	123	ASN	N-CA-C	-5.21	106.70	113.16
2	2	422	PHE	N-CA-C	-5.21	106.43	112.89
2	2	363	THR	N-CA-C	-5.18	105.32	111.69
2	2	357	VAL	N-CA-C	-5.16	100.90	108.54
9	A	181	LYS	O-C-N	5.15	129.18	122.89
1	1	149	ILE	N-CA-C	-5.13	106.33	113.00
41	n	134	VAL	N-CA-C	-5.12	106.34	113.00
29	Y	123	ASN	CB-CA-C	5.11	119.21	110.01
9	A	181	LYS	CA-C-N	-5.06	115.59	122.93
9	A	181	LYS	C-N-CA	-5.06	115.59	122.93
2	2	204	THR	CB-CA-C	5.04	118.41	109.65
9	A	149	GLN	CB-CA-C	-5.03	99.55	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	g	54	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	B	252	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2573	0	2696	67	0
2	2	4456	0	4650	104	0
3	3	1026	0	1049	48	0
4	4	3904	0	4056	130	0
5	5	5272	0	5396	198	0
6	6	1452	0	1542	56	0
7	8	658	0	648	22	0
8	9	807	0	778	27	0
9	A	5476	0	5419	132	0
10	B	3538	0	3477	116	0
11	C	3468	0	3359	108	0
12	D	678	0	642	12	0
13	E	2741	0	2713	81	0
14	F	1884	0	1851	38	0
15	G	1968	0	1935	60	0
16	H	1698	0	1667	54	0
17	I	1487	0	1434	44	0
18	J	1375	0	1386	37	0
19	K	1454	0	1448	42	0
20	L	671	0	737	25	0
21	M	930	0	883	13	0
22	O	631	0	596	8	0
22	Q	666	0	640	20	0
23	P	962	0	941	25	0
24	R	807	0	823	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	S	610	0	557	17	0
26	U	1365	0	1333	20	0
27	W	976	0	990	27	0
28	X	1472	0	1422	45	0
29	Y	1240	0	1204	34	0
30	Z	1432	0	1411	48	0
31	a	1167	0	1104	40	0
32	b	683	0	690	11	0
33	c	490	0	451	12	0
34	d	822	0	812	27	0
35	e	309	0	300	4	0
36	f	717	0	735	15	0
37	g	610	0	620	8	0
38	h	1118	0	1082	14	0
39	i	677	0	653	23	0
40	j	603	0	623	18	0
41	n	1061	0	1022	25	0
42	o	252	0	235	9	0
43	1	77	0	111	8	0
43	4	64	0	76	1	0
43	5	187	0	247	17	0
43	8	36	0	46	1	0
43	E	27	0	28	1	0
43	J	32	0	38	4	0
43	W	74	0	101	7	0
43	g	35	0	44	2	0
43	i	39	0	55	3	0
43	n	39	0	55	5	0
44	1	43	0	60	9	0
44	2	30	0	34	2	0
44	3	49	0	75	5	0
44	4	50	0	77	5	0
44	5	89	0	129	11	0
44	K	34	0	42	1	0
44	S	51	0	76	8	0
45	2	85	0	117	3	0
45	4	83	0	110	2	0
45	X	78	0	103	8	0
45	g	57	0	58	8	0
45	h	65	0	74	1	0
46	2	58	0	77	1	0
46	J	58	0	77	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	j	68	0	83	1	0
47	A	4	0	0	0	0
47	H	4	0	0	0	0
48	A	16	0	0	1	0
48	B	8	0	0	0	0
48	I	16	0	0	0	0
48	K	8	0	0	0	0
49	B	31	0	19	1	0
50	E	48	0	26	0	0
51	M	1	0	0	0	0
52	O	36	0	47	4	0
52	Q	36	0	47	3	0
53	1	90	0	0	3	0
53	2	137	0	0	3	0
53	3	39	0	0	2	0
53	4	56	0	0	5	0
53	5	16	0	0	1	0
53	6	43	0	0	2	0
53	9	14	0	0	0	0
53	A	197	0	0	6	0
53	B	30	0	0	0	0
53	C	166	0	0	5	0
53	D	22	0	0	1	0
53	E	62	0	0	1	0
53	F	29	0	0	0	0
53	G	99	0	0	2	0
53	H	5	0	0	0	0
53	I	84	0	0	3	0
53	K	83	0	0	1	0
53	L	11	0	0	2	0
53	M	34	0	0	0	0
53	P	24	0	0	0	0
53	S	1	0	0	0	0
53	U	38	0	0	0	0
53	W	39	0	0	1	0
53	X	50	0	0	0	0
53	Y	91	0	0	3	0
53	Z	40	0	0	3	0
53	a	4	0	0	0	0
53	b	2	0	0	0	0
53	d	4	0	0	0	0
53	f	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	g	9	0	0	0	0
53	h	46	0	0	0	0
53	j	3	0	0	0	0
53	n	24	0	0	0	0
All	All	69495	0	68142	1575	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 (1575) 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)
5:5:328:HIS:HA	5:5:391:SER:HB2	1.48	0.94
13:E:133:LYS:HD3	43:E:401:3PE:H12	1.51	0.92
24:R:25:ARG:HD3	33:c:43:ARG:HH22	1.32	0.91
1:1:82:PRO:HG3	1:1:228:ILE:HG23	1.52	0.89
3:3:103:VAL:HG22	43:g:102:3PE:H272	1.53	0.89
13:E:210:LEU:HD11	13:E:338:ILE:HD11	1.55	0.89
5:5:261:MET:HE1	5:5:326:LEU:HB2	1.53	0.88
1:1:82:PRO:HG3	1:1:228:ILE:CG2	2.05	0.86
11:C:296:GLU:HG2	17:I:83:VAL:HG21	1.57	0.84
6:6:210:ALA:HA	20:L:69:ILE:HD11	1.59	0.84
1:1:196:ILE:HG12	43:1:401:3PE:H362	1.61	0.81
2:2:553:MET:HE1	46:2:602:LMN:HAW	1.59	0.81
2:2:148:ILE:HD11	2:2:206:LEU:HD11	1.62	0.81
37:g:6:PRO:HB3	37:g:14:LYS:HE2	1.63	0.80
8:9:56:GLU:HB2	27:W:100:VAL:HG11	1.63	0.80
19:K:103:LEU:HB2	19:K:141:GLY:HA3	1.62	0.80
4:4:186:LEU:HD11	4:4:212:THR:HG21	1.65	0.79
4:4:9:ILE:HA	4:4:12:ILE:HD12	1.64	0.79
28:X:158:PHE:O	45:X:201:CDL:HA21	1.84	0.78
1:1:38:MET:HB3	17:I:84:LEU:HD22	1.65	0.78
9:A:463:LEU:HG	9:A:467:LYS:HE2	1.66	0.78
9:A:583:ASP:OD1	9:A:584:ARG:N	2.16	0.78
15:G:280:LEU:CD1	30:Z:129:GLU:OE2	2.32	0.78
8:9:63:LEU:HD22	27:W:113:VAL:HG21	1.65	0.77
36:f:64:TYR:HB2	36:f:68:ARG:HG3	1.67	0.77
18:J:35:ALA:HB1	18:J:55:ASN:HB3	1.66	0.77
12:D:42:VAL:HG13	12:D:46:ASP:HB2	1.64	0.77
2:2:17:LEU:HD21	3:3:108:HIS:HA	1.66	0.76
9:A:197:MET:HE1	9:A:230:SER:HA	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:273:THR:HA	2:2:276:THR:HG22	1.66	0.76
29:Y:154:MET:HE3	29:Y:157:THR:HG21	1.65	0.76
1:1:46:ALA:HA	44:1:403:PC1:H141	1.67	0.76
1:1:205:ALA:HB3	1:1:331:ARG:HG3	1.68	0.76
4:4:92:ILE:HD13	43:n:201:3PE:H371	1.68	0.75
18:J:105:ARG:HG2	18:J:107:PRO:HD2	1.67	0.75
5:5:147:SER:OG	5:5:252:MET:SD	2.43	0.75
2:2:383:ILE:HG21	2:2:432:LEU:HB2	1.69	0.75
10:B:66:GLN:NE2	10:B:82:MET:SD	2.60	0.75
15:G:138:ILE:HB	15:G:190:TYR:HB3	1.68	0.74
36:f:74:LEU:HD22	36:f:82:ILE:HG13	1.68	0.74
6:6:9:LEU:HB3	27:W:118:PRO:HA	1.69	0.74
3:3:68:LEU:HB3	20:L:61:VAL:HG23	1.68	0.74
4:4:248:GLN:HB3	4:4:310:ALA:HB2	1.70	0.74
5:5:68:GLU:HG2	34:d:46:VAL:HG11	1.69	0.74
10:B:158:ARG:NH1	10:B:191:GLU:OE2	2.20	0.74
6:6:10:LEU:HD21	8:9:86:ARG:HD2	1.70	0.73
10:B:424:ARG:NH2	10:B:434:GLU:OE2	2.21	0.73
4:4:471:ARG:NH2	53:4:702:HOH:O	2.22	0.73
5:5:357:ARG:NH1	24:R:69:ASP:O	2.22	0.72
3:3:47:GLN:NE2	11:C:117:THR:H	1.85	0.72
2:2:479:VAL:HG11	44:4:603:PC1:H252	1.71	0.72
11:C:114:ARG:HG2	23:P:7:LYS:NZ	2.04	0.71
4:4:408:GLN:HA	44:5:701:PC1:H131	1.73	0.71
15:G:48:PRO:HG2	15:G:51:ALA:HB3	1.71	0.71
34:d:30:ARG:HH12	34:d:34:ALA:HB2	1.55	0.71
36:f:74:LEU:HD13	36:f:82:ILE:HD11	1.71	0.71
15:G:201:LEU:HD21	23:P:77:GLN:HG2	1.73	0.71
13:E:41:ILE:HD13	13:E:48:LEU:HD12	1.73	0.71
5:5:1:MET:HG3	5:5:42:LEU:HD23	1.73	0.71
2:2:14:SER:HB2	3:3:104:TYR:HA	1.73	0.70
31:a:72:ARG:HG3	31:a:104:LEU:HD11	1.73	0.70
5:5:314:VAL:HA	5:5:317:ILE:HD12	1.72	0.70
11:C:114:ARG:HG2	23:P:7:LYS:HZ1	1.55	0.70
1:1:217:VAL:HG21	3:3:38:PHE:HE2	1.56	0.70
6:6:121:LEU:HA	6:6:124:MET:HG3	1.74	0.70
9:A:273:ARG:NH2	53:A:904:HOH:O	2.25	0.70
4:4:404:ARG:HD3	4:4:476:GLY:HA3	1.72	0.70
36:f:39:MET:HE1	36:f:48:ILE:HG21	1.72	0.70
16:H:163:GLU:OE2	16:H:166:ARG:NH1	2.25	0.69
5:5:167:ALA:HA	5:5:232:TRP:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:O:201:ZMP:H21A	23:P:64:ARG:NH1	2.07	0.69
23:P:123:ARG:HH12	29:Y:136:LYS:H	1.40	0.69
36:f:11:VAL:HG11	36:f:90:VAL:HG12	1.74	0.69
5:5:132:ASN:HB2	5:5:192:LEU:HD12	1.73	0.69
5:5:162:GLN:HB3	44:5:706:PC1:H11	1.73	0.69
14:F:249:PRO:HD3	15:G:99:GLN:HG2	1.75	0.69
11:C:146:ASP:OD2	11:C:148:HIS:NE2	2.26	0.68
43:1:401:3PE:H361	17:I:74:MET:HE1	1.75	0.68
11:C:217:LEU:HD23	11:C:243:ARG:HB2	1.75	0.68
31:a:74:LYS:NZ	31:a:103:ILE:O	2.26	0.68
44:3:201:PC1:H141	13:E:303:TRP:CE3	2.28	0.68
44:3:201:PC1:H261	19:K:84:LEU:HD22	1.75	0.68
9:A:160:GLY:H	11:C:410:ASN:HD21	1.40	0.68
22:Q:79:ASN:OD1	22:Q:80:ASP:N	2.27	0.68
10:B:496:SER:HA	10:B:501:ARG:HH11	1.57	0.67
6:6:198:VAL:HG22	28:X:153:MET:HE1	1.75	0.67
9:A:97:PRO:HG3	9:A:117:LEU:HD21	1.76	0.67
11:C:130:VAL:HG23	19:K:147:MET:HE3	1.75	0.67
16:H:247:ASN:HB3	16:H:259:GLU:HB3	1.76	0.67
17:I:223:ARG:NH1	53:I:401:HOH:O	2.27	0.67
29:Y:195:ASN:HD22	29:Y:198:LEU:HD11	1.58	0.67
2:2:161:LEU:HD21	20:L:69:ILE:HD12	1.76	0.67
4:4:367:GLU:HG2	4:4:522:ILE:HD13	1.76	0.67
9:A:251:ALA:HB2	9:A:282:MET:HE2	1.75	0.67
21:M:113:ARG:NH1	21:M:134:ASP:OD2	2.25	0.67
43:5:704:3PE:H11	43:J:201:3PE:H32	1.77	0.67
9:A:513:ALA:C	9:A:515:ASN:H	2.03	0.67
11:C:382:GLN:HB3	11:C:386:LYS:HZ3	1.60	0.67
4:4:444:LEU:HD12	4:4:448:PRO:HA	1.75	0.67
4:4:2:SER:HB3	4:4:5:TYR:HD2	1.60	0.67
10:B:149:GLY:HA3	10:B:381:ILE:HD11	1.77	0.67
1:1:26:TYR:HA	1:1:29:VAL:HG12	1.74	0.66
5:5:119:LEU:HD22	44:5:701:PC1:H361	1.78	0.66
8:9:17:PHE:CE1	27:W:105:ARG:HD3	2.29	0.66
13:E:109:THR:OG1	13:E:147:ARG:NH2	2.29	0.66
9:A:522:CYS:SG	9:A:674:ARG:NH1	2.65	0.66
26:U:86:ASP:HB3	26:U:127:LEU:HD22	1.76	0.66
28:X:55:LEU:HD23	28:X:75:MET:HE2	1.77	0.66
39:i:63:ARG:O	39:i:68:ARG:NH2	2.29	0.66
13:E:354:TYR:HA	13:E:357:LEU:HD13	1.76	0.66
5:5:338:LEU:HD21	5:5:372:VAL:HB	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:182:THR:HG21	11:C:439:PRO:HD3	1.76	0.66
4:4:11:PRO:HG3	4:4:86:ASN:HD21	1.61	0.66
2:2:514:ASN:HB3	2:2:520:ILE:HD11	1.78	0.66
10:B:188:PHE:HB3	10:B:191:GLU:HB2	1.78	0.66
3:3:47:GLN:HE22	11:C:117:THR:H	1.42	0.66
10:B:291:PHE:HB3	10:B:317:GLU:HG3	1.76	0.66
30:Z:51:ASN:ND2	53:Z:202:HOH:O	2.28	0.66
2:2:181:LEU:HD11	20:L:22:ILE:HG23	1.78	0.66
13:E:134:ASN:OD1	19:K:230:LYS:NZ	2.29	0.65
3:3:103:VAL:HG21	45:g:101:CDL:H551	1.78	0.65
7:8:42:TYR:O	39:i:63:ARG:NH1	2.28	0.65
9:A:129:LEU:HG	10:B:409:THR:HG21	1.78	0.65
9:A:660:PRO:HD3	36:f:17:LEU:HD22	1.77	0.65
9:A:680:GLN:NE2	53:A:908:HOH:O	2.28	0.65
13:E:188:ARG:NH1	13:E:253:GLN:O	2.29	0.65
6:6:170:ILE:HD11	12:D:79:TRP:HB3	1.79	0.65
4:4:268:LEU:HD11	44:4:603:PC1:H3F1	1.77	0.65
11:C:98:LYS:NZ	11:C:106:ASP:OD2	2.29	0.65
1:1:82:PRO:CG	1:1:228:ILE:HG23	2.25	0.65
13:E:69:ARG:HA	13:E:72:ARG:HE	1.60	0.65
3:3:93:ILE:HA	45:X:201:CDL:H241	1.77	0.65
9:A:422:ARG:NH1	9:A:451:GLU:OE1	2.30	0.65
9:A:479:LYS:O	9:A:515:ASN:ND2	2.29	0.65
39:i:65:TYR:HB3	39:i:68:ARG:HE	1.62	0.65
11:C:131:LEU:HB2	11:C:494:PHE:CZ	2.32	0.65
15:G:266:GLN:NE2	53:G:303:HOH:O	2.27	0.65
23:P:6:THR:OG1	23:P:84:GLN:NE2	2.29	0.65
14:F:61:LYS:HA	14:F:70:ARG:HH21	1.62	0.65
5:5:140:TRP:NE1	5:5:175:ASP:OD1	2.30	0.64
7:8:69:ARG:NH1	31:a:148:TYR:O	2.30	0.64
39:i:52:HIS:HE1	43:i:101:3PE:H112	1.62	0.64
22:Q:100:ASP:OD1	24:R:36:ARG:NH1	2.29	0.64
45:X:201:CDL:H761	37:g:37:PRO:HB3	1.80	0.64
24:R:88:VAL:HG21	39:i:10:PRO:HG3	1.80	0.64
4:4:362:THR:HG22	4:4:364:GLN:H	1.63	0.64
13:E:108:ASN:ND2	19:K:65:VAL:O	2.30	0.64
44:4:603:PC1:H241	5:5:610:GLU:HG3	1.79	0.64
5:5:253:VAL:HB	5:5:310:LEU:HD11	1.80	0.64
13:E:166:TYR:CD2	13:E:319:GLN:HG3	2.32	0.64
43:1:401:3PE:H332	17:I:77:MET:HE1	1.79	0.64
11:C:247:MET:HE1	19:K:112:HIS:CE1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:10:PHE:HA	3:3:13:ILE:HG12	1.80	0.64
7:8:14:ARG:NH1	31:a:153:GLU:O	2.31	0.64
19:K:100:THR:HG22	19:K:129:ALA:HA	1.80	0.64
39:i:33:ILE:HD13	41:n:51:LEU:HD11	1.80	0.64
11:C:421:PHE:HD1	17:I:133:VAL:HG21	1.63	0.64
7:8:44:THR:HG21	7:8:50:LYS:HG3	1.80	0.63
6:6:197:ASN:HD21	28:X:142:GLN:HE22	1.45	0.63
11:C:320:LEU:O	15:G:134:GLN:HG2	1.98	0.63
15:G:121:PHE:CZ	15:G:154:TYR:HD2	2.16	0.63
5:5:578:ASN:HA	5:5:582:THR:HG22	1.80	0.63
10:B:351:PRO:HG2	10:B:373:SER:HA	1.80	0.63
40:j:70:ASP:OD1	40:j:71:LEU:N	2.29	0.63
4:4:157:ILE:HG21	43:4:602:3PE:H341	1.81	0.63
4:4:498:PHE:HE1	45:4:601:CDL:H752	1.64	0.63
5:5:79:ASP:H	5:5:82:THR:HG22	1.64	0.62
31:a:145:ARG:NH2	31:a:147:SER:O	2.32	0.62
9:A:271:ASN:ND2	9:A:289:ASN:HD22	1.98	0.62
13:E:203:PHE:HB3	13:E:209:LEU:HD23	1.80	0.62
30:Z:95:ILE:HA	30:Z:99:GLN:NE2	2.14	0.62
2:2:157:TYR:OH	20:L:66:GLU:HB2	1.99	0.62
5:5:257:VAL:O	5:5:261:MET:HG3	2.00	0.62
15:G:81:ASP:OD1	15:G:85:LYS:HE2	2.00	0.62
1:1:65:LYS:HE2	19:K:159:PRO:HB2	1.79	0.62
10:B:60:ASP:OD1	10:B:63:ARG:NH1	2.32	0.62
9:A:382:PHE:HD2	9:A:533:ARG:NH2	1.98	0.62
13:E:235:ASN:ND2	15:G:239:GLU:OE2	2.33	0.62
2:2:91:ILE:HD12	2:2:93:GLU:HB2	1.82	0.62
13:E:302:TRP:HB2	19:K:227:TRP:NE1	2.15	0.62
5:5:171:ASN:ND2	53:5:804:HOH:O	2.28	0.61
11:C:382:GLN:HB3	11:C:386:LYS:NZ	2.14	0.61
14:F:216:ALA:HB3	14:F:222:VAL:HG22	1.81	0.61
28:X:35:TYR:O	28:X:106:ARG:NH2	2.33	0.61
7:8:11:ARG:HD2	7:8:29:SER:HB2	1.80	0.61
5:5:555:LYS:NZ	24:R:21:TRP:O	2.31	0.61
1:1:360:LEU:HD22	37:g:32:ILE:HG23	1.83	0.61
2:2:556:GLU:HB3	32:b:53:ILE:HD11	1.82	0.61
10:B:237:SER:HB2	10:B:249:PRO:HG3	1.82	0.61
11:C:208:THR:HG21	11:C:346:ALA:HB3	1.82	0.61
16:H:268:GLN:HA	16:H:271:THR:HG22	1.81	0.61
5:5:78:TYR:HA	5:5:82:THR:HG21	1.82	0.61
6:6:168:PHE:HB3	12:D:81:VAL:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:505:PRO:HG2	11:C:403:PRO:HG2	1.82	0.61
11:C:349:GLN:NE2	53:C:508:HOH:O	2.31	0.61
19:K:113:LEU:O	19:K:120:GLN:HB2	1.99	0.61
28:X:20:TYR:CE1	28:X:103:GLU:HA	2.36	0.61
32:b:29:ASN:OD1	32:b:32:SER:HB2	2.01	0.61
10:B:139:LEU:HD13	10:B:175:MET:HE1	1.82	0.61
10:B:190:GLN:NE2	16:H:256:ASP:OD1	2.33	0.61
18:J:80:ARG:HH22	18:J:86:VAL:HG13	1.66	0.61
32:b:5:ILE:HD12	32:b:48:TYR:HD1	1.65	0.61
6:6:51:ILE:HB	6:6:81:VAL:HG11	1.82	0.61
13:E:351:PRO:HG2	13:E:354:TYR:HD2	1.66	0.61
15:G:47:LEU:HD23	30:Z:47:LEU:HD22	1.82	0.61
19:K:100:THR:HB	19:K:127:PHE:HB3	1.83	0.61
52:O:201:ZMP:H11	23:P:25:VAL:HG22	1.83	0.61
52:O:201:ZMP:H7	23:P:59:GLU:HB3	1.82	0.61
5:5:611:ARG:HH12	43:J:201:3PE:H121	1.64	0.60
9:A:170:ALA:HB3	21:M:114:ILE:HG12	1.82	0.60
10:B:137:ARG:NH1	10:B:175:MET:O	2.31	0.60
13:E:69:ARG:HG2	13:E:72:ARG:HH21	1.66	0.60
2:2:69:ILE:O	2:2:73:ILE:HD12	2.00	0.60
11:C:404:ARG:NH2	17:I:176:ASP:OD1	2.34	0.60
19:K:222:LYS:HE3	19:K:225:ARG:HB2	1.83	0.60
1:1:159:ILE:O	1:1:163:ILE:HG12	2.02	0.60
5:5:575:PHE:HD1	31:a:112:TYR:HB2	1.65	0.60
13:E:122:VAL:HG23	13:E:157:VAL:HG11	1.83	0.60
31:a:69:ASN:ND2	31:a:99:GLU:OE1	2.35	0.60
10:B:433:ARG:NH1	30:Z:77:ASP:HB2	2.17	0.60
34:d:12:LYS:HE3	34:d:40:ARG:HH22	1.67	0.60
5:5:664:LEU:HB3	18:J:112:PHE:CE1	2.37	0.60
11:C:178:VAL:HG11	11:C:221:MET:HG2	1.84	0.60
1:1:223:GLU:HG2	53:1:514:HOH:O	2.01	0.60
7:8:60:LYS:HZ1	35:e:45:TRP:CG	2.20	0.60
13:E:38:LEU:HD22	13:E:50:GLU:HB3	1.84	0.60
14:F:83:LEU:HD22	14:F:213:LYS:HB3	1.83	0.60
20:L:44:SER:OG	20:L:52:GLY:HA3	2.02	0.60
24:R:25:ARG:HD3	33:c:43:ARG:NH2	2.12	0.60
29:Y:139:ARG:NH1	53:Y:303:HOH:O	2.33	0.60
30:Z:174:ASP:OD1	30:Z:175:VAL:N	2.33	0.60
10:B:270:ASN:OD1	10:B:271:VAL:N	2.35	0.60
17:I:111:GLU:HB3	17:I:186:TYR:CZ	2.37	0.60
4:4:174:ASP:HB3	4:4:234:TYR:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:86:UNK:HA	26:U:4:ARG:NE	2.17	0.60
15:G:121:PHE:CZ	15:G:154:TYR:CD2	2.90	0.60
23:P:8:PHE:HB2	23:P:84:GLN:HG3	1.84	0.60
5:5:95:LEU:HB3	5:5:473:PRO:HB3	1.82	0.59
4:4:371:LEU:HD22	4:4:431:LEU:HD11	1.83	0.59
16:H:111:ASN:OD1	16:H:114:ILE:HD12	2.03	0.59
17:I:91:PRO:HG2	30:Z:45:VAL:HG21	1.84	0.59
1:1:340:ASP:OD1	1:1:341:GLN:N	2.36	0.59
2:2:238:TYR:HB3	2:2:242:PHE:HE2	1.67	0.59
9:A:294:GLU:OE2	9:A:434:LYS:NZ	2.35	0.59
15:G:280:LEU:HD12	30:Z:129:GLU:OE2	2.02	0.59
2:2:63:LEU:HD21	2:2:292:LEU:HD23	1.83	0.59
22:Q:96:LEU:HD12	22:Q:100:ASP:HB3	1.84	0.59
29:Y:114:LYS:NZ	29:Y:115:PRO:O	2.32	0.59
1:1:331:ARG:NH2	53:1:501:HOH:O	2.35	0.59
6:6:8:LEU:HB2	26:U:14:LEU:HB2	1.84	0.59
10:B:155:GLU:OE1	10:B:159:LYS:NZ	2.35	0.59
13:E:58:ALA:HA	13:E:63:GLY:HA3	1.85	0.59
2:2:155:GLN:NE2	53:2:706:HOH:O	2.35	0.59
14:F:28:LEU:HB3	14:F:41:THR:HG21	1.84	0.59
14:F:69:TYR:CZ	14:F:236:MET:HG3	2.38	0.59
26:U:20:PRO:HD2	26:U:23:ILE:HD12	1.84	0.59
9:A:403:SER:OG	9:A:485:MET:HE3	2.02	0.59
24:R:25:ARG:HH11	33:c:43:ARG:HH22	1.50	0.59
34:d:7:GLU:HA	34:d:10:LEU:HD23	1.84	0.59
5:5:202:PRO:HG2	5:5:203:TYR:CE2	2.38	0.58
11:C:96:VAL:HB	11:C:477:GLY:HA3	1.84	0.58
1:1:340:ASP:OD1	1:1:341:GLN:HG3	2.03	0.58
5:5:622:SER:HB2	31:a:40:ARG:HH11	1.68	0.58
9:A:126:MET:HE2	9:A:152:SER:HB2	1.85	0.58
9:A:278:GLY:HA3	29:Y:148:GLN:OE1	2.04	0.58
28:X:76:ARG:HH21	45:g:101:CDL:HA22	1.68	0.58
7:8:86:ASN:HB3	31:a:145:ARG:HD2	1.84	0.58
5:5:208:VAL:HA	5:5:211:ILE:HG22	1.84	0.58
5:5:319:LEU:HD21	5:5:399:ALA:HA	1.86	0.58
10:B:311:PRO:O	16:H:292:ARG:NH2	2.36	0.58
17:I:104:ILE:HG12	38:h:79:SER:HB3	1.86	0.58
34:d:86:LYS:HD3	34:d:88:LYS:HD3	1.84	0.58
9:A:479:LYS:NZ	9:A:512:ASN:OD1	2.36	0.58
7:8:14:ARG:NE	31:a:153:GLU:OE2	2.35	0.58
9:A:57:ALA:HB3	9:A:60:GLN:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:64:ILE:HG21	10:B:276:VAL:HG12	1.84	0.58
11:C:294:THR:HG23	11:C:370:MET:HE1	1.85	0.58
28:X:35:TYR:OH	28:X:114:GLU:OE1	2.20	0.58
5:5:162:GLN:NE2	31:a:108:SER:O	2.37	0.58
5:5:323:ASN:OD1	5:5:324:ILE:HD12	2.04	0.58
27:W:16:TYR:CE1	27:W:17:LYS:HE2	2.39	0.58
9:A:132:ASN:HD21	10:B:416:LYS:HD3	1.69	0.58
9:A:268:LEU:HD11	9:A:425:ALA:HB1	1.84	0.58
1:1:12:GLU:OE2	12:D:29:ARG:HG3	2.03	0.58
6:6:9:LEU:HB2	27:W:115:PRO:HG2	1.86	0.58
14:F:119:GLY:HA2	14:F:129:VAL:HG13	1.86	0.58
19:K:136:VAL:HG22	19:K:163:TRP:HB2	1.86	0.58
27:W:48:LYS:NZ	43:W:202:3PE:O14	2.33	0.58
34:d:14:PRO:HG3	34:d:40:ARG:HG3	1.86	0.58
4:4:142:VAL:O	4:4:492:ARG:HD2	2.04	0.57
9:A:160:GLY:HA3	11:C:410:ASN:OD1	2.04	0.57
10:B:426:GLU:O	10:B:475:ARG:NH1	2.35	0.57
2:2:238:TYR:HB3	2:2:242:PHE:CE2	2.39	0.57
5:5:156:THR:HB	24:R:86:LEU:HD12	1.86	0.57
10:B:324:GLU:HA	10:B:327:GLU:HG2	1.86	0.57
4:4:117:ASP:HB2	4:4:119:TYR:CZ	2.40	0.57
16:H:195:VAL:HG22	16:H:253:ILE:HD12	1.87	0.57
24:R:83:GLU:HB2	24:R:86:LEU:HD11	1.86	0.57
34:d:43:TRP:O	34:d:47:MET:HG2	2.04	0.57
2:2:61:THR:H	2:2:64:THR:HB	1.69	0.57
4:4:404:ARG:HE	4:4:478:VAL:C	2.12	0.57
5:5:321:SER:HB2	5:5:324:ILE:HD13	1.85	0.57
9:A:58:LEU:HD11	9:A:111:VAL:HG21	1.87	0.57
9:A:103:TRP:CE3	10:B:253:PRO:HG3	2.40	0.57
33:c:37:GLU:O	33:c:41:ALA:N	2.38	0.57
10:B:154:ARG:NE	10:B:158:ARG:HH12	2.03	0.57
44:1:403:PC1:H122	38:h:24:LEU:HA	1.85	0.57
10:B:432:PRO:HD2	10:B:486:GLN:NE2	2.20	0.57
11:C:241:GLU:HG2	17:I:93:TYR:CG	2.39	0.57
40:j:12:ASP:HB3	40:j:15:LEU:HB2	1.86	0.57
4:4:88:ILE:O	4:4:92:ILE:HG12	2.04	0.57
5:5:16:SER:HB3	5:5:115:SER:HB3	1.87	0.57
15:G:277:THR:HG23	15:G:278:PHE:HD1	1.69	0.57
2:2:138:PHE:O	2:2:142:THR:HG23	2.05	0.56
9:A:583:ASP:CG	9:A:584:ARG:H	2.12	0.56
30:Z:70:ILE:O	30:Z:74:ASP:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:316:SER:HA	5:5:319:LEU:HD12	1.87	0.56
11:C:241:GLU:HG2	17:I:93:TYR:CD2	2.41	0.56
16:H:207:GLY:HA3	16:H:249:PRO:HD3	1.87	0.56
38:h:26:ILE:HG23	38:h:28:ASP:H	1.70	0.56
1:1:50:TYR:OH	38:h:19:TYR:OH	2.23	0.56
5:5:3:LEU:HD22	39:i:45:VAL:HG13	1.87	0.56
5:5:552:ILE:HD12	24:R:22:THR:HG22	1.87	0.56
6:6:57:VAL:HG11	20:L:34:LEU:HD11	1.87	0.56
13:E:42:GLN:HB2	29:Y:73:THR:HG21	1.88	0.56
15:G:235:ARG:NH1	15:G:237:ASP:OD1	2.39	0.56
31:a:99:GLU:HA	40:j:18:LEU:HD11	1.86	0.56
11:C:411:MET:HE3	11:C:415:ILE:HG13	1.87	0.56
26:U:117:TRP:CD2	26:U:162:PRO:HA	2.40	0.56
31:a:152:PHE:HB3	31:a:156:LEU:HD23	1.87	0.56
35:e:17:THR:O	35:e:21:ALA:N	2.38	0.56
4:4:478:VAL:HG22	24:R:89:PRO:HD2	1.87	0.56
11:C:169:LEU:HD11	11:C:264:ARG:HA	1.86	0.56
22:Q:94:LEU:HG	22:Q:96:LEU:HD23	1.87	0.56
30:Z:15:SER:HB3	30:Z:18:LYS:HZ3	1.71	0.56
4:4:137:MET:HE2	4:4:163:GLU:HB2	1.88	0.56
13:E:291:GLN:OE1	13:E:309:ARG:NH2	2.39	0.56
16:H:262:THR:HG23	16:H:265:THR:H	1.71	0.56
30:Z:16:ILE:HB	30:Z:40:ASN:HA	1.87	0.56
4:4:358:VAL:HA	4:4:366:LEU:HD23	1.88	0.56
5:5:62:PHE:CD2	43:5:703:3PE:H32	2.40	0.56
9:A:518:THR:O	9:A:674:ARG:NH2	2.30	0.56
11:C:181:MET:HE3	11:C:250:TYR:CD1	2.41	0.56
13:E:293:LEU:O	13:E:297:ILE:HD12	2.06	0.56
13:E:301:LEU:HD23	13:E:303:TRP:CZ2	2.40	0.56
15:G:138:ILE:HG12	15:G:154:TYR:CD1	2.41	0.56
33:c:34:ASP:HB3	33:c:37:GLU:OE2	2.06	0.56
9:A:744:GLN:NE2	9:A:746:ALA:O	2.38	0.56
10:B:173:ARG:O	10:B:173:ARG:NH2	2.38	0.56
11:C:163:LYS:HE3	17:I:135:PRO:O	2.05	0.56
11:C:418:PHE:CE2	17:I:129:LEU:HD21	2.41	0.56
45:g:101:CDL:H521	45:g:101:CDL:HA61	1.88	0.56
3:3:47:GLN:HE22	11:C:117:THR:HG22	1.70	0.56
19:K:229:ARG:O	19:K:230:LYS:HB2	2.06	0.56
2:2:361:GLU:HA	2:2:364:GLN:HE21	1.71	0.56
17:I:73:LEU:HD11	27:W:32:LEU:HG	1.88	0.56
26:U:139:ASN:OD1	26:U:139:ASN:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:42:MET:HE2	28:X:93:ARG:HG2	1.88	0.55
4:4:333:THR:HB	4:4:345:TYR:HD2	1.71	0.55
4:4:483:ILE:HD11	40:j:8:LYS:HB3	1.88	0.55
9:A:564:PHE:O	9:A:584:ARG:NH1	2.39	0.55
11:C:69:ILE:HD12	15:G:176:PRO:HG2	1.88	0.55
13:E:133:LYS:HG3	19:K:230:LYS:HZ1	1.70	0.55
30:Z:156:THR:OG1	30:Z:159:LEU:O	2.21	0.55
5:5:94:SER:O	5:5:98:ILE:HG12	2.06	0.55
10:B:154:ARG:HG3	10:B:158:ARG:HH22	1.72	0.55
10:B:164:LEU:HD13	10:B:271:VAL:HG13	1.89	0.55
11:C:128:HIS:NE2	11:C:492:LEU:HB2	2.21	0.55
22:O:90:PHE:HB3	22:O:96:LEU:HD12	1.87	0.55
27:W:17:LYS:NZ	30:Z:183:GLU:OE2	2.39	0.55
14:F:203:THR:O	14:F:206:GLN:N	2.38	0.55
16:H:157:SER:O	16:H:160:VAL:HG12	2.06	0.55
5:5:224:SER:O	5:5:226:GLN:HG2	2.05	0.55
5:5:338:LEU:HD22	5:5:376:ALA:HB2	1.89	0.55
16:H:246:VAL:O	16:H:292:ARG:NH1	2.39	0.55
17:I:62:GLU:O	37:g:21:ARG:NH2	2.33	0.55
17:I:111:GLU:HB3	17:I:186:TYR:CE1	2.41	0.55
8:9:64:GLN:HE21	8:9:68:ARG:NH1	2.05	0.55
14:F:247:GLU:O	15:G:99:GLN:NE2	2.40	0.55
7:8:14:ARG:HH12	31:a:154:GLY:HA3	1.70	0.55
9:A:402:ASN:HB2	9:A:524:TYR:O	2.07	0.55
1:1:24:ILE:HG21	1:1:234:LEU:HD12	1.89	0.55
5:5:634:TYR:CE1	43:5:702:3PE:H32	2.41	0.55
9:A:328:THR:HB	9:A:331:GLN:HG2	1.88	0.55
16:H:129:ILE:HG23	16:H:132:ARG:HH11	1.72	0.55
17:I:75:THR:HA	17:I:78:LEU:HD12	1.89	0.55
26:U:123:VAL:HG13	26:U:127:LEU:HD12	1.89	0.55
2:2:161:LEU:HD13	6:6:213:GLY:HA3	1.88	0.55
2:2:479:VAL:HG21	44:4:603:PC1:H291	1.88	0.55
4:4:77:LYS:HE2	25:S:88:GLY:O	2.07	0.55
5:5:199:SER:HA	34:d:67:HIS:HE1	1.72	0.55
43:J:201:3PE:O22	40:j:31:TRP:NE1	2.37	0.55
4:4:4:LEU:HD23	4:4:120:LEU:HB3	1.89	0.55
13:E:114:GLU:HG2	13:E:117:ARG:NH2	2.22	0.55
30:Z:167:THR:HG22	30:Z:169:VAL:H	1.71	0.55
1:1:217:VAL:HG21	3:3:38:PHE:CE2	2.41	0.55
3:3:10:PHE:O	3:3:14:ILE:HG12	2.06	0.55
4:4:5:TYR:O	4:4:9:ILE:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:85:MET:HE2	5:5:258:TYR:HB2	1.88	0.55
11:C:98:LYS:HZ2	11:C:144:ARG:HH22	1.54	0.55
28:X:20:TYR:CD1	28:X:103:GLU:HA	2.42	0.55
5:5:397:GLU:O	5:5:401:GLY:N	2.35	0.54
11:C:478:HIS:HB3	11:C:482:ASP:HB2	1.89	0.54
4:4:519:HIS:CD2	25:S:117:GLN:HE22	2.25	0.54
10:B:338:ASP:O	10:B:385:LYS:NZ	2.40	0.54
15:G:166:ARG:NH1	53:G:305:HOH:O	2.28	0.54
23:P:124:ASN:ND2	29:Y:73:THR:HA	2.23	0.54
4:4:146:ASN:OD1	4:4:492:ARG:NH2	2.37	0.54
9:A:235:ASP:OD2	9:A:302:ARG:NH1	2.39	0.54
9:A:404:LYS:HE3	9:A:668:VAL:HG21	1.88	0.54
11:C:137:LEU:HD21	11:C:480:LEU:HD13	1.88	0.54
4:4:91:LEU:HD11	25:S:101:LEU:HD23	1.89	0.54
5:5:45:ILE:HG23	39:i:66:PRO:HG2	1.89	0.54
28:X:129:SER:HB2	28:X:160:ASN:O	2.07	0.54
2:2:535:PRO:HA	45:2:601:CDL:H121	1.90	0.54
13:E:205:PHE:HD2	13:E:206:GLU:OE1	1.90	0.54
28:X:107:GLU:OE2	28:X:107:GLU:N	2.40	0.54
9:A:76:GLU:HG2	29:Y:186:ARG:HH21	1.73	0.54
9:A:328:THR:HG22	9:A:330:GLU:H	1.73	0.54
1:1:370:ILE:HG21	27:W:47:VAL:HA	1.89	0.54
30:Z:95:ILE:HA	30:Z:99:GLN:HE22	1.71	0.54
9:A:372:ARG:HG2	36:f:67:GLY:HA3	1.90	0.54
10:B:322:MET:HB2	10:B:363:MET:HE3	1.88	0.54
27:W:50:ILE:HA	27:W:53:GLN:HG2	1.90	0.54
2:2:78:ILE:HG21	2:2:278:PHE:HB2	1.89	0.54
2:2:149:PHE:O	2:2:153:GLU:HG2	2.07	0.54
5:5:69:TRP:CZ3	34:d:49:GLY:HA3	2.43	0.54
6:6:12:GLU:HB3	6:6:16:ASN:HB3	1.89	0.54
6:6:106:SER:HB2	20:L:17:LEU:HD12	1.90	0.54
9:A:106:GLN:HG3	9:A:107:ALA:H	1.73	0.54
9:A:160:GLY:H	11:C:410:ASN:ND2	2.05	0.54
11:C:490:MET:HE3	11:C:492:LEU:HD21	1.89	0.54
22:Q:133:TYR:O	22:Q:137:GLN:NE2	2.41	0.54
8:9:68:ARG:HD3	27:W:116:SER:HB2	1.90	0.53
16:H:272:ALA:HB3	16:H:284:PRO:HG3	1.90	0.53
19:K:50:GLU:HB2	19:K:55:TYR:HB3	1.90	0.53
2:2:507:ASN:ND2	2:2:524:LEU:HB3	2.23	0.53
4:4:17:LEU:O	4:4:21:ILE:HG12	2.07	0.53
5:5:387:THR:HA	5:5:485:GLY:HA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:65:PHE:CD2	10:B:301:LEU:HD11	2.43	0.53
26:U:36:LEU:HD13	27:W:67:LEU:HD13	1.91	0.53
1:1:9:SER:OG	3:3:6:ILE:HD13	2.09	0.53
4:4:92:ILE:HG23	43:n:201:3PE:H321	1.90	0.53
5:5:226:GLN:OE1	5:5:284:THR:HG21	2.08	0.53
18:J:96:GLY:HA2	18:J:99:MET:SD	2.48	0.53
4:4:10:ILE:HG22	4:4:82:THR:HG23	1.90	0.53
4:4:273:LEU:HD21	4:4:345:TYR:HD1	1.72	0.53
5:5:495:LEU:HD22	7:8:58:TYR:HE2	1.73	0.53
16:H:158:ILE:HA	16:H:161:MET:HE3	1.90	0.53
39:i:55:ARG:NH2	39:i:65:TYR:OH	2.41	0.53
1:1:8:ASN:O	1:1:12:GLU:HG3	2.08	0.53
1:1:305:PRO:HG3	12:D:30:HIS:CG	2.43	0.53
5:5:202:PRO:HB3	5:5:269:TYR:CZ	2.43	0.53
9:A:382:PHE:HD2	9:A:533:ARG:HH22	1.55	0.53
10:B:381:ILE:HG12	16:H:202:PRO:HG3	1.91	0.53
13:E:117:ARG:NH2	21:M:85:GLU:OE1	2.36	0.53
13:E:222:SER:HB3	13:E:316:PHE:HE2	1.74	0.53
28:X:20:TYR:HB3	28:X:21:PRO:HD2	1.91	0.53
8:9:57:ALA:O	8:9:61:ARG:HG3	2.08	0.53
1:1:168:SER:O	1:1:169:LEU:HB2	2.08	0.53
9:A:372:ARG:HE	9:A:643:LEU:HD23	1.74	0.53
15:G:256:ASN:ND2	29:Y:156:GLY:O	2.41	0.53
1:1:361:VAL:HG22	43:W:202:3PE:H3F2	1.91	0.53
5:5:205:ASN:O	5:5:209:VAL:HG23	2.08	0.53
9:A:310:THR:HG21	9:A:711:SER:O	2.09	0.53
2:2:18:ARG:HB3	2:2:20:ASP:OD1	2.08	0.53
4:4:144:ASN:HB3	4:4:148:ILE:HG12	1.90	0.53
5:5:123:MET:HE2	5:5:142:GLY:HA3	1.90	0.53
15:G:127:ASN:HB3	15:G:130:ALA:HB3	1.91	0.53
16:H:224:ASN:N	16:H:227:GLU:OE2	2.34	0.53
1:1:77:LEU:HD13	1:1:127:LEU:HD11	1.91	0.53
1:1:130:TRP:CZ2	6:6:44:ILE:HG13	2.44	0.53
5:5:295:GLN:HB2	5:5:301:VAL:HG22	1.91	0.53
25:S:119:TRP:CD1	34:d:12:LYS:HB2	2.44	0.53
30:Z:48:ASN:ND2	38:h:50:GLU:O	2.42	0.53
30:Z:114:VAL:HG23	30:Z:116:LEU:HD12	1.90	0.53
2:2:149:PHE:HE2	20:L:62:VAL:HG21	1.74	0.52
2:2:282:ILE:HB	53:2:744:HOH:O	2.09	0.52
5:5:633:LEU:HD11	6:6:109:LEU:HD11	1.90	0.52
14:F:150:ARG:NH2	45:g:101:CDL:OB4	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:M:64:ARG:HB2	21:M:100:GLU:HG3	1.91	0.52
25:S:75:LEU:O	25:S:78:VAL:HG22	2.08	0.52
2:2:45:SER:OG	28:X:101:MET:HB3	2.09	0.52
18:J:69:TYR:HB2	18:J:95:ALA:HB2	1.91	0.52
24:R:83:GLU:HA	24:R:86:LEU:HD21	1.91	0.52
1:1:9:SER:OG	3:3:3:ALA:HA	2.09	0.52
4:4:219:LEU:HB2	4:4:258:ALA:CB	2.39	0.52
9:A:217:ILE:HG13	48:A:803:SF4:S4	2.49	0.52
28:X:31:ARG:NH2	28:X:111:ASP:OD1	2.43	0.52
30:Z:156:THR:HG21	30:Z:161:PRO:HD3	1.91	0.52
2:2:396:THR:HG21	14:F:167:SER:HB3	1.91	0.52
4:4:118:ILE:HA	4:4:177:LEU:HD11	1.90	0.52
6:6:51:ILE:HD11	6:6:78:ILE:HG12	1.90	0.52
9:A:83:ASN:HB2	10:B:407:GLN:O	2.08	0.52
24:R:48:PRO:HA	24:R:51:GLN:HB3	1.91	0.52
2:2:164:THR:HG22	2:2:164:THR:O	2.09	0.52
4:4:334:LEU:HD21	44:5:706:PC1:H362	1.92	0.52
9:A:41:VAL:HG21	9:A:107:ALA:HA	1.91	0.52
9:A:317:LEU:HB2	9:A:592:VAL:HG22	1.90	0.52
2:2:49:LYS:O	2:2:61:THR:HG23	2.10	0.52
2:2:149:PHE:CE2	20:L:62:VAL:HG21	2.44	0.52
3:3:101:GLY:O	3:3:105:GLU:HG2	2.10	0.52
5:5:144:GLY:HA2	5:5:252:MET:HE1	1.92	0.52
10:B:154:ARG:CZ	10:B:158:ARG:HH12	2.23	0.52
11:C:371:GLU:OE1	30:Z:185:SER:HB3	2.09	0.52
22:Q:106:MET:HG3	24:R:15:LEU:HD11	1.91	0.52
1:1:50:TYR:HB2	1:1:52:LEU:HD23	1.91	0.52
1:1:71:THR:HG23	3:3:35:LEU:O	2.10	0.52
5:5:357:ARG:HA	24:R:23:VAL:HG23	1.90	0.52
5:5:357:ARG:HH11	24:R:67:HIS:CE1	2.27	0.52
9:A:650:GLN:NE2	29:Y:60:ALA:HA	2.23	0.52
9:A:734:PRO:HG2	21:M:70:ARG:HH21	1.75	0.52
2:2:211:ILE:HD11	41:n:129:LEU:HD21	1.90	0.52
4:4:169:VAL:HG11	4:4:294:LEU:HD22	1.91	0.52
5:5:586:LEU:HD12	31:a:103:ILE:HG21	1.91	0.52
10:B:260:GLY:HA3	10:B:266:SER:HB2	1.90	0.52
11:C:337:ASP:OD1	11:C:339:ARG:HG2	2.09	0.52
14:F:83:LEU:O	14:F:86:SER:OG	2.26	0.52
36:f:15:ARG:HG3	36:f:49:LEU:HB2	1.92	0.52
4:4:219:LEU:HD12	4:4:255:ILE:HG12	1.92	0.52
4:4:230:VAL:HG21	4:4:238:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:490:ASP:OD2	7:8:55:ARG:NH1	2.43	0.52
9:A:175:ASN:HB2	9:A:222:GLU:HG3	1.92	0.52
19:K:208:MET:HG3	53:K:481:HOH:O	2.10	0.52
21:M:101:LEU:HA	21:M:104:LYS:HZ3	1.74	0.52
4:4:351:ALA:HA	4:4:354:TYR:CE2	2.45	0.52
4:4:430:THR:HG22	4:4:432:ASN:H	1.75	0.52
9:A:654:ARG:NH1	9:A:657:GLU:OE2	2.43	0.52
10:B:239:ILE:HD12	10:B:261:LEU:HB2	1.91	0.52
11:C:205:PHE:HA	11:C:208:THR:HG22	1.92	0.52
23:P:73:ASP:OD1	23:P:74:VAL:N	2.42	0.52
26:U:1:MET:N	27:W:109:PRO:HD2	2.25	0.52
4:4:9:ILE:O	4:4:13:ILE:HD12	2.09	0.51
11:C:302:ARG:HG2	17:I:77:MET:SD	2.50	0.51
14:F:243:GLU:HB3	14:F:244:PRO:HD2	1.93	0.51
32:b:68:ILE:O	32:b:72:ARG:HG3	2.10	0.51
2:2:317:ILE:HD13	18:J:130:LEU:HD22	1.92	0.51
3:3:57:PHE:HZ	20:L:79:ARG:HH12	1.56	0.51
10:B:96:HIS:HB3	10:B:173:ARG:NH2	2.26	0.51
11:C:157:GLU:OE1	11:C:499:ARG:NH1	2.42	0.51
13:E:107:ARG:HB2	19:K:65:VAL:HG22	1.91	0.51
13:E:164:SER:OG	13:E:198:ARG:HG2	2.10	0.51
3:3:54:ILE:HD13	6:6:86:LEU:HG	1.93	0.51
6:6:7:LEU:HB2	8:9:67:TYR:OH	2.11	0.51
6:6:13:ILE:HG23	6:6:14:TYR:H	1.74	0.51
8:9:80:PRO:HB2	8:9:85:ILE:HD11	1.93	0.51
41:n:95:ASP:N	41:n:95:ASP:OD1	2.43	0.51
5:5:317:ILE:HG23	5:5:322:TYR:CE1	2.45	0.51
9:A:230:SER:O	9:A:233:VAL:HG22	2.10	0.51
1:1:183:TYR:O	1:1:187:LEU:HB2	2.10	0.51
1:1:195:PHE:O	1:1:199:VAL:HG23	2.10	0.51
5:5:206:SER:O	5:5:210:ILE:HD12	2.11	0.51
17:I:46:PRO:HB2	17:I:49:PHE:HB2	1.93	0.51
13:E:69:ARG:HD3	13:E:242:GLU:OE1	2.11	0.51
18:J:95:ALA:O	18:J:98:THR:OG1	2.24	0.51
5:5:218:ILE:HA	5:5:221:MET:SD	2.50	0.51
10:B:111:ARG:C	10:B:270:ASN:HD22	2.18	0.51
10:B:239:ILE:HG23	10:B:261:LEU:HA	1.93	0.51
11:C:240:PHE:CD2	19:K:115:THR:HG21	2.46	0.51
13:E:133:LYS:CG	19:K:230:LYS:HZ1	2.23	0.51
13:E:243:ARG:HB2	13:E:331:LEU:HD12	1.92	0.51
18:J:119:VAL:HG12	18:J:120:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:68:LYS:NZ	29:Y:86:GLU:O	2.37	0.51
38:h:4:PRO:HA	38:h:7:THR:HG22	1.92	0.51
2:2:42:MET:CE	28:X:93:ARG:HG2	2.40	0.51
4:4:200:ASN:HB2	4:4:278:GLU:OE1	2.11	0.51
5:5:421:THR:HA	5:5:424:TYR:CE2	2.46	0.51
9:A:76:GLU:CG	29:Y:186:ARG:HH21	2.24	0.51
16:H:195:VAL:N	16:H:235:THR:O	2.39	0.51
1:1:151:TYR:CE1	1:1:201:GLU:HG2	2.45	0.51
4:4:263:THR:HG21	4:4:355:LEU:HD22	1.92	0.51
10:B:429:MET:HG2	10:B:479:PHE:CE2	2.46	0.51
11:C:180:MET:N	11:C:180:MET:SD	2.84	0.51
15:G:164:ARG:HG3	30:Z:166:GLN:HE22	1.76	0.51
28:X:8:THR:HB	28:X:168:THR:H	1.75	0.51
38:h:38:ASP:HB3	38:h:40:PHE:H	1.76	0.51
4:4:76:LYS:NZ	4:4:145:TRP:O	2.28	0.50
20:L:30:GLU:HB3	53:L:109:HOH:O	2.09	0.50
22:O:97:ASP:OD2	23:P:64:ARG:NH2	2.44	0.50
10:B:327:GLU:HA	10:B:332:GLY:HA2	1.92	0.50
30:Z:168:MET:O	30:Z:168:MET:HG2	2.11	0.50
4:4:219:LEU:HB2	4:4:258:ALA:HB2	1.92	0.50
5:5:575:PHE:HE2	31:a:117:PRO:HB3	1.75	0.50
11:C:355:PRO:HG2	11:C:372:GLU:HG2	1.92	0.50
14:F:211:GLU:HG3	17:I:45:PRO:HG2	1.93	0.50
15:G:280:LEU:HD11	30:Z:129:GLU:OE2	2.11	0.50
18:J:94:PHE:O	18:J:98:THR:HG23	2.10	0.50
2:2:34:ALA:HB1	44:2:603:PC1:H242	1.94	0.50
2:2:57:LEU:HD12	6:6:198:VAL:HB	1.94	0.50
2:2:177:LEU:HD21	20:L:22:ILE:HD13	1.92	0.50
5:5:123:MET:CE	5:5:142:GLY:HA3	2.41	0.50
10:B:137:ARG:HB2	10:B:177:ALA:HA	1.93	0.50
1:1:366:TYR:CE1	3:3:85:ALA:HB2	2.46	0.50
5:5:343:ALA:O	5:5:347:ILE:HG12	2.11	0.50
6:6:22:MET:HE3	6:6:26:LEU:HG	1.94	0.50
8:9:81:THR:O	8:9:85:ILE:HG12	2.12	0.50
11:C:181:MET:HE3	11:C:250:TYR:HD1	1.77	0.50
11:C:404:ARG:NH2	17:I:173:CYS:O	2.44	0.50
13:E:84:GLU:HG2	13:E:87:LYS:HE3	1.92	0.50
15:G:79:LYS:HD3	30:Z:173:TRP:CG	2.47	0.50
2:2:501:LEU:HD23	14:F:182:PHE:HZ	1.75	0.50
5:5:117:LEU:HD12	5:5:246:LEU:HD23	1.94	0.50
5:5:383:PHE:CG	5:5:384:PRO:HD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:535:SER:O	5:5:538:VAL:HG22	2.12	0.50
6:6:197:ASN:HD21	28:X:142:GLN:NE2	2.09	0.50
2:2:2:ILE:HG22	28:X:152:VAL:HA	1.94	0.50
4:4:410:MET:HB3	4:4:413:PHE:HB3	1.93	0.50
6:6:197:ASN:ND2	28:X:142:GLN:HE22	2.09	0.50
10:B:364:ASP:HB3	10:B:367:ALA:HB3	1.92	0.50
16:H:116:PHE:CE2	16:H:160:VAL:HG23	2.46	0.50
1:1:113:TYR:HE1	43:1:402:3PE:H232	1.77	0.50
10:B:433:ARG:HH11	30:Z:77:ASP:HB2	1.77	0.50
13:E:222:SER:OG	13:E:290:LEU:HD23	2.11	0.50
14:F:49:LEU:HD11	14:F:219:ILE:HD11	1.94	0.50
16:H:122:ASN:O	16:H:126:ILE:HG12	2.11	0.50
16:H:292:ARG:NH2	16:H:296:GLU:O	2.40	0.50
45:X:201:CDL:H162	37:g:40:LEU:HD13	1.94	0.50
34:d:79:LEU:HD13	40:j:67:ARG:HH11	1.77	0.50
1:1:92:GLY:HA3	1:1:242:LEU:HD21	1.93	0.50
5:5:641:LEU:HD22	43:5:702:3PE:H3E2	1.93	0.50
9:A:352:VAL:HG21	9:A:366:MET:HE2	1.92	0.50
10:B:158:ARG:HG3	10:B:159:LYS:HD3	1.94	0.50
13:E:257:LEU:HD12	13:E:328:PHE:CE1	2.46	0.50
16:H:111:ASN:HB2	16:H:112:PRO:HD2	1.94	0.50
28:X:156:PHE:HB2	28:X:158:PHE:CE2	2.47	0.50
2:2:418:LEU:HB3	2:2:488:ILE:HD11	1.93	0.49
4:4:498:PHE:CE1	45:4:601:CDL:H752	2.47	0.49
43:5:707:3PE:H231	31:a:126:LEU:HD12	1.92	0.49
13:E:243:ARG:CB	13:E:331:LEU:HD12	2.42	0.49
17:I:151:ARG:NH2	53:I:403:HOH:O	2.45	0.49
18:J:86:VAL:O	18:J:90:ILE:HD12	2.11	0.49
39:i:65:TYR:CE1	39:i:67:SER:HB2	2.47	0.49
2:2:85:TYR:CE1	2:2:115:LYS:HA	2.47	0.49
4:4:103:GLN:HB3	41:n:101:ASN:HD22	1.76	0.49
7:8:67:LYS:HA	7:8:70:VAL:HG12	1.94	0.49
10:B:160:ASP:CG	10:B:163:LYS:HZ3	2.19	0.49
15:G:91:MET:HE2	30:Z:97:GLN:HG3	1.94	0.49
4:4:155:TYR:OH	4:4:159:MET:HE2	2.12	0.49
5:5:1:MET:HB2	39:i:46:TRP:CZ2	2.47	0.49
9:A:633:ARG:HH12	9:A:637:GLU:HG2	1.76	0.49
9:A:672:ALA:HB1	36:f:29:ARG:HD3	1.94	0.49
15:G:211:ILE:HG23	15:G:212:MET:HG2	1.94	0.49
17:I:77:MET:O	17:I:81:MET:HG3	2.12	0.49
17:I:161:THR:HG21	17:I:191:ARG:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:i:64:PHE:CZ	39:i:66:PRO:HG3	2.48	0.49
2:2:313:TYR:O	2:2:317:ILE:HG12	2.13	0.49
4:4:324:ILE:HD11	40:j:50:ILE:HD13	1.94	0.49
4:4:529:ILE:HG23	34:d:92:PHE:HB3	1.93	0.49
14:F:66:HIS:HA	30:Z:146:ALA:HA	1.94	0.49
29:Y:65:VAL:HG21	29:Y:78:PRO:HG2	1.93	0.49
5:5:111:GLN:HE22	39:i:22:ALA:HB3	1.77	0.49
9:A:492:VAL:O	9:A:498:ALA:HB2	2.13	0.49
13:E:205:PHE:CD2	15:G:241:LYS:HE2	2.47	0.49
26:U:146:ARG:HH21	27:W:52:GLU:HG3	1.78	0.49
30:Z:15:SER:HB3	30:Z:18:LYS:NZ	2.27	0.49
4:4:520:TYR:OH	34:d:36:ASP:OD1	2.28	0.49
10:B:63:ARG:HB3	10:B:315:GLU:OE2	2.13	0.49
18:J:162:ILE:HD12	18:J:168:ILE:HG13	1.94	0.49
28:X:4:THR:HG22	28:X:6:THR:H	1.77	0.49
2:2:483:ASN:ND2	53:2:704:HOH:O	2.33	0.49
5:5:556:PHE:HZ	52:Q:201:ZMP:H25	1.78	0.49
10:B:154:ARG:CZ	10:B:158:ARG:NH1	2.76	0.49
10:B:276:VAL:O	10:B:280:ILE:HG12	2.13	0.49
11:C:296:GLU:OE2	17:I:79:ARG:NE	2.38	0.49
13:E:347:LEU:HD12	13:E:350:ARG:HD2	1.94	0.49
16:H:272:ALA:O	16:H:276:SER:OG	2.24	0.49
46:J:202:LMN:HAWA	46:J:202:LMN:HBB	1.95	0.49
2:2:199:VAL:HG13	6:6:126:PRO:HG3	1.95	0.49
2:2:216:SER:HB2	2:2:237:PRO:HG3	1.94	0.49
5:5:199:SER:OG	34:d:56:LEU:HD21	2.13	0.49
5:5:618:LYS:NZ	31:a:49:ASP:OD1	2.46	0.49
6:6:31:VAL:O	6:6:35:ILE:HG12	2.13	0.49
9:A:676:LEU:HD22	36:f:36:TYR:HD2	1.77	0.49
11:C:175:LEU:HD13	11:C:460:ILE:HG21	1.93	0.49
15:G:153:VAL:HG22	15:G:168:LYS:HG2	1.93	0.49
18:J:93:LEU:HD12	18:J:113:ALA:HB1	1.94	0.49
24:R:32:ALA:O	24:R:36:ARG:N	2.37	0.49
28:X:43:HIS:HB3	28:X:89:TYR:HE2	1.78	0.49
30:Z:46:PRO:HD2	38:h:52:PRO:HG2	1.95	0.49
4:4:92:ILE:O	4:4:95:ILE:HG22	2.12	0.49
5:5:143:VAL:HG23	5:5:252:MET:HE3	1.94	0.49
9:A:46:ASP:OD2	9:A:113:THR:OG1	2.30	0.49
9:A:176:ILE:HB	9:A:225:LEU:HG	1.94	0.49
9:A:654:ARG:HD2	9:A:657:GLU:OE2	2.13	0.49
10:B:288:PHE:CZ	10:B:298:GLY:HA3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:103:GLU:OE2	19:K:68:PRO:HD2	2.13	0.49
20:L:78:TYR:HD2	20:L:84:ILE:HG23	1.78	0.49
25:S:124:ALA:HA	25:S:127:ARG:HB2	1.94	0.49
9:A:403:SER:HB3	9:A:522:CYS:O	2.13	0.49
11:C:448:VAL:HB	11:C:457:ARG:HB3	1.94	0.49
14:F:40:GLY:O	14:F:220:GLU:HG2	2.13	0.49
26:U:46:ARG:HD2	26:U:83:VAL:HG13	1.95	0.49
28:X:116:THR:HG21	28:X:174:GLN:HG2	1.95	0.49
29:Y:164:LYS:O	29:Y:168:ILE:HG12	2.12	0.49
30:Z:84:ASP:OD2	30:Z:87:ARG:HD2	2.13	0.49
4:4:218:PHE:HB3	4:4:254:GLY:HA2	1.94	0.48
4:4:237:VAL:HG13	41:n:109:GLU:OE2	2.13	0.48
5:5:317:ILE:HG23	5:5:322:TYR:HE1	1.78	0.48
9:A:210:GLY:HA2	16:H:102:MET:HE2	1.94	0.48
9:A:397:SER:HB3	9:A:671:VAL:HG21	1.94	0.48
14:F:42:HIS:HD2	14:F:44:SER:H	1.60	0.48
21:M:101:LEU:HA	21:M:104:LYS:NZ	2.28	0.48
3:3:86:TYR:HD2	6:6:194:THR:HG22	1.78	0.48
4:4:449:ILE:HG13	4:4:450:ALA:N	2.27	0.48
4:4:461:SER:HA	4:4:464:TYR:CE2	2.47	0.48
8:9:88:LEU:HD12	8:9:97:THR:HG23	1.94	0.48
9:A:409:GLU:OE2	9:A:431:ARG:NH2	2.40	0.48
10:B:164:LEU:HD23	10:B:195:LEU:HD11	1.96	0.48
5:5:205:ASN:O	5:5:208:VAL:HG22	2.13	0.48
10:B:125:MET:SD	10:B:267:THR:OG1	2.67	0.48
10:B:348:SER:HB2	10:B:396:LEU:HD22	1.95	0.48
11:C:184:GLU:OE2	11:C:262:TYR:N	2.47	0.48
18:J:88:ASN:ND2	18:J:124:GLU:HG2	2.28	0.48
18:J:152:ARG:NH2	34:d:93:GLU:O	2.40	0.48
22:Q:99:LEU:HB2	52:Q:201:ZMP:O6	2.12	0.48
33:c:34:ASP:OD2	33:c:36:TRP:HB2	2.14	0.48
4:4:332:SER:HB2	4:4:345:TYR:CE2	2.48	0.48
8:9:11:PRO:HB2	41:n:147:PHE:CZ	2.49	0.48
5:5:84:SER:OG	5:5:326:LEU:HD21	2.12	0.48
5:5:527:LEU:HD23	5:5:531:ILE:HG12	1.94	0.48
6:6:176:ASP:HB2	41:n:144:PRO:HA	1.96	0.48
9:A:210:GLY:CA	16:H:102:MET:HE2	2.43	0.48
11:C:248:GLU:OE1	53:C:501:HOH:O	2.20	0.48
14:F:178:LEU:HD12	14:F:181:ILE:HD13	1.95	0.48
2:2:77:LEU:HD21	45:2:601:CDL:H182	1.96	0.48
4:4:144:ASN:OD1	4:4:282:GLY:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:40:THR:O	5:5:43:SER:OG	2.29	0.48
5:5:124:MET:HE2	5:5:252:MET:HA	1.94	0.48
5:5:216:LEU:HB2	5:5:259:LEU:HD21	1.96	0.48
8:9:10:GLY:HA2	41:n:141:PHE:O	2.14	0.48
11:C:339:ARG:HG3	11:C:352:PHE:CZ	2.48	0.48
11:C:433:TYR:OH	11:C:442:GLU:OE2	2.29	0.48
28:X:20:TYR:CE1	28:X:103:GLU:HG2	2.48	0.48
1:1:204:ARG:HD3	1:1:240:ILE:HD11	1.95	0.48
2:2:9:LEU:HA	28:X:77:LEU:HD21	1.94	0.48
2:2:535:PRO:HD3	45:2:601:CDL:HA32	1.95	0.48
3:3:133:LEU:HG	53:3:322:HOH:O	2.13	0.48
5:5:88:PRO:HG3	5:5:330:VAL:HG22	1.94	0.48
13:E:198:ARG:HB2	13:E:256:GLU:HG2	1.95	0.48
13:E:221:THR:HG22	13:E:223:ASN:O	2.14	0.48
28:X:116:THR:O	28:X:120:LYS:HG2	2.14	0.48
2:2:172:SER:OG	2:2:272:PRO:HD3	2.13	0.48
10:B:445:VAL:HG11	10:B:457:PHE:CZ	2.49	0.48
29:Y:155:GLN:NE2	53:Y:305:HOH:O	2.41	0.48
3:3:117:GLN:HA	11:C:96:VAL:HG21	1.95	0.48
10:B:393:ILE:HG13	10:B:464:LEU:HD13	1.94	0.48
11:C:130:VAL:HG11	11:C:152:LEU:HB2	1.95	0.48
24:R:50:LEU:HD23	24:R:50:LEU:H	1.79	0.48
29:Y:70:ALA:HB3	29:Y:99:PRO:HB3	1.96	0.48
30:Z:186:TYR:HB3	30:Z:190:TYR:HB2	1.95	0.48
2:2:285:ILE:HA	2:2:370:LEU:HD21	1.95	0.48
4:4:273:LEU:HD21	4:4:345:TYR:CD1	2.48	0.48
5:5:186:LEU:HG	5:5:192:LEU:HD23	1.96	0.48
5:5:452:PHE:HA	22:Q:66:GLU:OE2	2.14	0.48
11:C:256:ALA:HB1	53:C:548:HOH:O	2.13	0.48
18:J:15:ASP:HB3	18:J:18:HIS:HB3	1.95	0.48
30:Z:79:PRO:HB2	30:Z:81:TRP:CD1	2.49	0.48
13:E:229:PHE:HE2	13:E:231:PRO:HB3	1.78	0.47
24:R:74:PRO:HA	24:R:80:SER:H	1.79	0.47
2:2:418:LEU:HB3	2:2:488:ILE:CD1	2.43	0.47
9:A:164:GLU:OE2	10:B:424:ARG:NH1	2.47	0.47
9:A:434:LYS:HE2	9:A:434:LYS:HB3	1.65	0.47
12:D:86:UNK:HA	26:U:4:ARG:CZ	2.44	0.47
13:E:278:LYS:HE3	13:E:351:PRO:HD3	1.96	0.47
16:H:122:ASN:HA	16:H:125:ILE:HD12	1.94	0.47
18:J:169:LYS:HD2	18:J:173:TYR:CD2	2.49	0.47
41:n:92:ASP:OD1	41:n:92:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:458:ILE:H	4:4:458:ILE:HD12	1.79	0.47
6:6:8:LEU:HD13	8:9:85:ILE:HD12	1.95	0.47
9:A:378:LEU:HD13	9:A:541:PHE:CD2	2.49	0.47
19:K:90:TRP:CD1	44:K:302:PC1:H31	2.48	0.47
20:L:9:LEU:HA	20:L:12:ILE:HG22	1.96	0.47
26:U:146:ARG:NH2	27:W:52:GLU:HG3	2.28	0.47
2:2:459:LEU:HD11	4:4:221:LEU:HD22	1.95	0.47
4:4:332:SER:HB2	4:4:345:TYR:HE2	1.79	0.47
5:5:214:ILE:O	5:5:218:ILE:HD12	2.14	0.47
9:A:459:LEU:HD13	9:A:469:ALA:HB1	1.94	0.47
9:A:638:PHE:HE1	23:P:116:ILE:HD11	1.80	0.47
10:B:308:VAL:HG13	10:B:382:VAL:HG21	1.96	0.47
28:X:155:TRP:CZ2	45:X:201:CDL:H342	2.49	0.47
4:4:198:SER:HB2	4:4:278:GLU:OE2	2.14	0.47
10:B:154:ARG:HB3	10:B:188:PHE:CE2	2.49	0.47
10:B:200:ASN:ND2	42:o:48:SER:OG	2.48	0.47
10:B:461:ILE:O	10:B:465:ILE:HG12	2.15	0.47
16:H:209:GLY:H	16:H:249:PRO:HG3	1.79	0.47
30:Z:57:GLY:HA3	38:h:81:GLN:O	2.14	0.47
2:2:91:ILE:HD11	2:2:512:ILE:HD11	1.97	0.47
4:4:15:ILE:HG23	4:4:157:ILE:HG12	1.97	0.47
4:4:144:ASN:HD22	4:4:147:SER:HB2	1.80	0.47
4:4:343:ILE:HD13	4:4:383:LEU:HB3	1.97	0.47
5:5:644:ILE:HD13	6:6:120:PHE:CZ	2.50	0.47
7:8:85:SER:OG	31:a:144:ASP:OD1	2.30	0.47
9:A:226:ASP:OD1	9:A:226:ASP:N	2.46	0.47
9:A:530:ALA:HB3	9:A:533:ARG:HG2	1.97	0.47
9:A:606:VAL:HG22	9:A:612:VAL:HG22	1.97	0.47
13:E:81:TYR:CE1	13:E:101:PHE:HB3	2.50	0.47
13:E:154:LYS:HD2	13:E:155:TYR:CE2	2.50	0.47
13:E:169:ASN:O	13:E:178:ARG:HA	2.14	0.47
15:G:142:ASP:OD2	15:G:149:ARG:NH2	2.45	0.47
25:S:100:SER:HA	43:n:201:3PE:H3C1	1.97	0.47
31:a:174:ASP:OD1	31:a:174:ASP:N	2.47	0.47
3:3:49:ARG:HD2	6:6:94:ILE:HG21	1.96	0.47
4:4:415:LEU:O	4:4:419:ILE:HD12	2.14	0.47
5:5:643:LEU:HB3	6:6:120:PHE:CD2	2.49	0.47
6:6:36:CYS:HA	6:6:39:ILE:HG12	1.97	0.47
9:A:256:LEU:HD13	9:A:275:ASP:HB3	1.95	0.47
10:B:432:PRO:HD2	10:B:486:GLN:HE21	1.80	0.47
29:Y:97:GLY:O	53:Y:301:HOH:O	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:92:ASN:HB2	31:a:95:GLU:HB2	1.97	0.47
2:2:37:ILE:HG21	44:2:603:PC1:H251	1.97	0.47
4:4:106:PHE:HA	41:n:97:TRP:CH2	2.50	0.47
8:9:1:MET:N	8:9:12:SER:HB2	2.29	0.47
10:B:126:ASN:OD1	10:B:176:ASN:ND2	2.46	0.47
10:B:497:ARG:NH2	30:Z:64:TYR:O	2.37	0.47
11:C:391:PRO:HA	30:Z:67:PRO:HG2	1.95	0.47
22:Q:112:PHE:HE2	22:Q:134:ILE:HG13	1.79	0.47
4:4:245:TYR:O	4:4:249:LEU:HD23	2.15	0.47
5:5:5:ILE:HD11	5:5:78:TYR:CE2	2.50	0.47
5:5:513:ILE:O	5:5:517:THR:OG1	2.32	0.47
9:A:520:GLU:O	9:A:520:GLU:HG2	2.13	0.47
10:B:339:ASN:O	10:B:385:LYS:N	2.46	0.47
15:G:138:ILE:HB	15:G:190:TYR:CB	2.44	0.47
15:G:253:ALA:HB2	29:Y:150:SER:HB2	1.97	0.47
16:H:105:ARG:NH2	21:M:135:LYS:HG2	2.30	0.47
22:Q:60:GLN:H	22:Q:63:GLU:HB2	1.79	0.47
27:W:43:TRP:HE1	43:W:202:3PE:H3D2	1.79	0.47
27:W:90:GLU:HB3	27:W:97:ASN:OD1	2.15	0.47
5:5:79:ASP:O	5:5:83:VAL:HG22	2.15	0.46
9:A:90:GLU:HB3	9:A:112:LYS:HB2	1.96	0.46
9:A:286:PRO:HB3	9:A:297:ILE:HG23	1.97	0.46
9:A:647:ASP:OD1	9:A:648:VAL:N	2.48	0.46
11:C:279:ASP:CG	15:G:55:ARG:HH12	2.23	0.46
17:I:213:ALA:HB3	38:h:91:LEU:HD13	1.96	0.46
13:E:247:ASP:O	13:E:250:THR:OG1	2.21	0.46
16:H:201:THR:HA	16:H:204:GLN:HG2	1.96	0.46
4:4:151:ASN:HB3	4:4:154:SER:HB2	1.98	0.46
5:5:386:MET:H	5:5:389:PHE:HB3	1.81	0.46
6:6:33:SER:O	6:6:37:VAL:HG23	2.16	0.46
16:H:250:MET:HE2	16:H:250:MET:HB2	1.86	0.46
17:I:108:PHE:HD2	17:I:182:PRO:HA	1.81	0.46
19:K:216:ARG:HG3	19:K:219:ARG:NH1	2.31	0.46
38:h:25:TYR:HH	38:h:63:HIS:HD1	1.60	0.46
41:n:105:ALA:O	41:n:109:GLU:HG2	2.15	0.46
3:3:73:LEU:HD11	3:3:95:ILE:HG12	1.98	0.46
4:4:189:LEU:HD13	4:4:287:LEU:HD21	1.98	0.46
5:5:198:PHE:CG	5:5:265:PRO:HB2	2.50	0.46
5:5:233:LEU:HB3	5:5:234:PRO:HD3	1.96	0.46
8:9:55:LYS:HB3	53:W:326:HOH:O	2.14	0.46
10:B:154:ARG:HD2	16:H:243:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:67:ARG:HD3	22:O:111:GLU:OE1	2.16	0.46
1:1:71:THR:HG23	3:3:35:LEU:HB3	1.96	0.46
2:2:339:LEU:HD11	2:2:480:TYR:CD1	2.50	0.46
10:B:67:ASN:OD1	10:B:71:ARG:N	2.49	0.46
13:E:73:GLN:NE2	13:E:242:GLU:OE2	2.48	0.46
14:F:221:GLU:OE1	17:I:39:ALA:HB3	2.15	0.46
17:I:142:GLU:HB2	17:I:155:ARG:HB3	1.96	0.46
18:J:14:LYS:O	18:J:78:ASN:ND2	2.33	0.46
31:a:48:PRO:HD2	31:a:51:ASP:OD2	2.16	0.46
3:3:25:PHE:CZ	44:3:201:PC1:H3A1	2.51	0.46
5:5:264:SER:HA	5:5:267:ILE:HG12	1.96	0.46
5:5:564:PHE:HE1	43:5:705:3PE:H11	1.81	0.46
5:5:664:LEU:HD13	18:J:112:PHE:CD1	2.51	0.46
6:6:74:LEU:HG	6:6:78:ILE:HD11	1.97	0.46
9:A:70:PRO:HB2	9:A:86:MET:HG3	1.98	0.46
9:A:163:HIS:HB3	10:B:507:MET:HE2	1.97	0.46
10:B:196:GLN:HB2	10:B:223:ILE:HD12	1.97	0.46
10:B:401:ARG:CZ	10:B:416:LYS:HG3	2.46	0.46
16:H:266:ILE:O	16:H:270:LEU:HD23	2.16	0.46
26:U:113:ARG:HG3	26:U:149:GLN:HG3	1.97	0.46
1:1:18:VAL:HB	1:1:19:PRO:HD3	1.98	0.46
1:1:53:LEU:HD11	44:1:403:PC1:H321	1.98	0.46
2:2:68:HIS:HE1	2:2:140:ILE:HB	1.79	0.46
5:5:357:ARG:HH21	24:R:71:TYR:HB2	1.81	0.46
9:A:106:GLN:HG3	9:A:107:ALA:N	2.30	0.46
9:A:513:ALA:C	9:A:515:ASN:N	2.71	0.46
11:C:247:MET:HE1	19:K:112:HIS:NE2	2.29	0.46
14:F:54:HIS:CE1	14:F:81:LEU:HD21	2.50	0.46
20:L:86:ILE:HG22	31:a:32:PHE:HZ	1.78	0.46
23:P:87:MET:HE2	23:P:87:MET:HA	1.98	0.46
1:1:214:SER:O	11:C:126:ALA:HB2	2.15	0.46
5:5:140:TRP:CZ2	5:5:223:LYS:HG3	2.51	0.46
5:5:420:PHE:HZ	43:5:705:3PE:H291	1.81	0.46
28:X:35:TYR:CD1	28:X:110:MET:HE2	2.51	0.46
5:5:133:TYR:HB2	5:5:192:LEU:HD13	1.98	0.46
11:C:431:ASP:OD2	11:C:446:TYR:OH	2.28	0.46
15:G:91:MET:HE1	15:G:100:GLN:HA	1.98	0.46
15:G:176:PRO:HB2	15:G:203:VAL:HG13	1.98	0.46
16:H:213:ILE:HG13	16:H:249:PRO:HB2	1.97	0.46
22:Q:118:ASP:OD1	22:Q:119:LYS:N	2.48	0.46
28:X:159:VAL:HG22	45:X:201:CDL:HA32	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:195:ASN:HA	29:Y:198:LEU:HG	1.98	0.46
30:Z:169:VAL:N	53:Z:208:HOH:O	2.48	0.46
2:2:387:ILE:HG12	2:2:421:TYR:CE2	2.51	0.46
5:5:111:GLN:NE2	39:i:22:ALA:HB3	2.31	0.46
6:6:106:SER:CB	20:L:17:LEU:HD12	2.46	0.46
9:A:175:ASN:HB3	9:A:727:PRO:O	2.15	0.46
2:2:278:PHE:CE2	2:2:282:ILE:HG13	2.50	0.45
3:3:24:ILE:HA	44:3:201:PC1:H132	1.98	0.45
3:3:58:ILE:HG23	6:6:215:ILE:HD12	1.98	0.45
5:5:611:ARG:HG3	31:a:52:TYR:CD1	2.52	0.45
7:8:24:LEU:HD22	34:d:65:VAL:HG13	1.98	0.45
10:B:220:ASP:OD2	10:B:222:TYR:OH	2.28	0.45
16:H:213:ILE:HG13	16:H:249:PRO:CB	2.45	0.45
16:H:246:VAL:HG23	16:H:247:ASN:OD1	2.15	0.45
33:c:43:ARG:O	33:c:48:PHE:HB2	2.16	0.45
1:1:20:SER:O	1:1:24:ILE:HG12	2.16	0.45
3:3:39:GLU:HB3	3:3:42:PHE:O	2.17	0.45
4:4:133:THR:O	4:4:137:MET:HG2	2.16	0.45
4:4:239:LEU:HD22	4:4:305:PRO:HB2	1.97	0.45
4:4:408:GLN:NE2	24:R:86:LEU:O	2.49	0.45
5:5:357:ARG:HH11	24:R:67:HIS:HE1	1.64	0.45
10:B:76:LEU:HD13	10:B:162:HIS:CE1	2.52	0.45
13:E:219:LEU:O	13:E:283:ILE:N	2.29	0.45
23:P:65:TYR:O	29:Y:85:SER:OG	2.26	0.45
24:R:26:ASN:OD1	24:R:27:LEU:N	2.49	0.45
29:Y:192:ALA:HB3	29:Y:195:ASN:OD1	2.15	0.45
35:e:23:MET:HG2	35:e:24:TRP:H	1.81	0.45
43:1:401:3PE:H361	43:1:401:3PE:H392	1.79	0.45
5:5:50:VAL:HB	5:5:83:VAL:HG11	1.99	0.45
5:5:466:GLY:HA3	5:5:470:LEU:HD23	1.99	0.45
5:5:592:ILE:O	5:5:596:LEU:HB2	2.17	0.45
10:B:111:ARG:NH1	10:B:299:THR:O	2.48	0.45
10:B:291:PHE:HD2	10:B:298:GLY:HA2	1.80	0.45
11:C:325:THR:HG21	11:C:442:GLU:HB3	1.98	0.45
16:H:315:ARG:HD3	16:H:315:ARG:N	2.31	0.45
19:K:82:THR:O	19:K:86:ILE:HG12	2.16	0.45
22:O:130:ALA:O	22:O:134:ILE:HG12	2.17	0.45
22:Q:85:THR:H	22:Q:88:ALA:HB2	1.82	0.45
27:W:33:ALA:O	27:W:37:VAL:HG23	2.16	0.45
30:Z:70:ILE:HD13	30:Z:70:ILE:HA	1.85	0.45
1:1:46:ALA:CA	44:1:403:PC1:H141	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:556:GLU:OE2	32:b:4:ARG:HD3	2.17	0.45
4:4:312:LEU:HD23	18:J:162:ILE:HB	1.97	0.45
5:5:112:ARG:HD3	44:5:701:PC1:H2	1.96	0.45
5:5:205:ASN:OD1	5:5:206:SER:N	2.49	0.45
5:5:626:SER:OG	31:a:33:LEU:HB2	2.16	0.45
6:6:93:ASN:HB3	6:6:96:THR:OG1	2.16	0.45
7:8:39:ARG:NE	7:8:43:GLU:OE2	2.42	0.45
8:9:77:GLU:HG2	8:9:78:ASN:H	1.81	0.45
9:A:89:VAL:HA	9:A:118:THR:HG22	1.98	0.45
10:B:89:LYS:O	10:B:93:LEU:HD23	2.16	0.45
26:U:1:MET:H1	27:W:109:PRO:HD2	1.81	0.45
5:5:61:ILE:HG22	5:5:62:PHE:CD2	2.51	0.45
5:5:664:LEU:HB3	18:J:112:PHE:HE1	1.79	0.45
8:9:13:ARG:HG2	20:L:48:ASP:HB3	1.98	0.45
9:A:44:THR:HG22	9:A:49:LYS:HG2	1.99	0.45
9:A:364:VAL:HG21	9:A:655:MET:HG2	1.99	0.45
10:B:88:THR:OG1	10:B:166:GLU:OE2	2.33	0.45
10:B:106:SER:HB2	10:B:288:PHE:HD2	1.81	0.45
13:E:83:GLU:OE1	13:E:86:ALA:N	2.46	0.45
13:E:107:ARG:NH1	13:E:134:ASN:O	2.31	0.45
30:Z:32:ARG:O	30:Z:36:VAL:HG22	2.17	0.45
30:Z:95:ILE:HD13	30:Z:99:GLN:HE22	1.80	0.45
31:a:90:ARG:HD2	31:a:106:MET:SD	2.56	0.45
1:1:104:VAL:HG13	3:3:3:ALA:HB1	1.98	0.45
5:5:8:LEU:HD21	39:i:42:THR:HG23	1.98	0.45
9:A:220:TYR:OH	16:H:187:ARG:HD2	2.16	0.45
16:H:292:ARG:HD2	16:H:296:GLU:N	2.31	0.45
3:3:132:TYR:CZ	3:3:134:GLY:HA2	2.52	0.45
4:4:329:ALA:HA	4:4:345:TYR:CZ	2.52	0.45
5:5:53:ASN:OD1	39:i:63:ARG:HG2	2.17	0.45
5:5:62:PHE:HE2	43:5:703:3PE:H371	1.82	0.45
5:5:614:VAL:HG12	5:5:618:LYS:HE3	1.98	0.45
9:A:208:SER:HB3	9:A:217:ILE:HD13	1.99	0.45
10:B:82:MET:HG2	10:B:163:LYS:NZ	2.32	0.45
11:C:130:VAL:HG22	11:C:151:LEU:HB2	1.97	0.45
13:E:255:PHE:HB3	13:E:257:LEU:CD2	2.47	0.45
15:G:96:LYS:HE2	15:G:97:TYR:CZ	2.51	0.45
39:i:59:PRO:HG3	39:i:65:TYR:CE2	2.52	0.45
40:j:46:VAL:O	40:j:50:ILE:HD12	2.16	0.45
2:2:215:ILE:HG22	8:9:41:ILE:HD13	1.98	0.45
4:4:114:SER:H	4:4:117:ASP:CG	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:677:SER:O	9:A:681:LEU:HB2	2.16	0.45
12:D:38:HIS:HB2	53:D:111:HOH:O	2.16	0.45
13:E:103:GLU:CD	19:K:68:PRO:HD2	2.41	0.45
13:E:205:PHE:CD2	13:E:206:GLU:OE1	2.70	0.45
13:E:343:TYR:CD2	13:E:359:PRO:HG3	2.51	0.45
20:L:24:LEU:HD12	20:L:24:LEU:HA	1.82	0.45
29:Y:142:ASN:ND2	29:Y:143:PRO:HD2	2.32	0.45
31:a:64:ASN:HB2	40:j:21:MET:SD	2.56	0.45
4:4:222:SER:HA	46:J:202:LMN:HBGA	1.98	0.45
4:4:235:PHE:O	4:4:239:LEU:HG	2.17	0.45
4:4:245:TYR:HB2	18:J:161:GLU:CD	2.42	0.45
5:5:409:ALA:HA	31:a:138:VAL:HG11	1.99	0.45
8:9:77:GLU:HG2	8:9:78:ASN:N	2.32	0.45
23:P:124:ASN:HD22	29:Y:73:THR:HA	1.82	0.45
22:Q:75:PHE:HE1	33:c:36:TRP:CH2	2.35	0.45
45:X:201:CDL:H122	45:X:201:CDL:H151	1.84	0.45
34:d:16:VAL:HG21	34:d:30:ARG:NH2	2.32	0.45
2:2:284:LYS:HE2	2:2:344:THR:HG22	1.99	0.45
2:2:419:LYS:HA	2:2:487:GLU:O	2.17	0.45
3:3:129:VAL:HG22	14:F:43:PRO:HB2	1.99	0.45
4:4:196:PHE:HB2	4:4:280:PRO:HG3	1.99	0.45
6:6:62:ILE:HG23	6:6:67:ASN:ND2	2.33	0.45
7:8:44:THR:HG22	7:8:44:THR:O	2.17	0.45
10:B:495:ASP:OD2	10:B:499:LYS:HE2	2.17	0.45
15:G:140:ALA:HB3	15:G:198:PHE:CD2	2.52	0.45
16:H:154:GLY:HA2	42:o:39:VAL:HG21	1.98	0.45
19:K:209:TYR:O	19:K:213:GLN:HG2	2.17	0.45
22:O:75:PHE:HD1	22:O:78:VAL:HG23	1.82	0.45
28:X:176:GLU:O	28:X:180:GLU:N	2.46	0.45
5:5:363:ILE:HD11	5:5:434:LEU:HD12	1.99	0.44
5:5:651:ASP:HB3	5:5:654:TYR:CE2	2.51	0.44
43:5:703:3PE:H31	43:5:703:3PE:H352	1.99	0.44
6:6:42:ASN:HB3	6:6:45:VAL:HG22	1.98	0.44
9:A:199:ASP:OD1	29:Y:206:HIS:NE2	2.50	0.44
9:A:292:VAL:HG22	53:A:909:HOH:O	2.17	0.44
10:B:416:LYS:O	10:B:420:GLN:HG3	2.17	0.44
11:C:300:ASP:O	17:I:76:GLU:HG3	2.17	0.44
13:E:27:SER:OG	13:E:28:ASP:N	2.50	0.44
13:E:257:LEU:HD12	13:E:328:PHE:CZ	2.51	0.44
15:G:101:PHE:HB3	15:G:110:ILE:HD13	1.99	0.44
27:W:23:ARG:HD2	27:W:23:ARG:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:W:202:3PE:H3C1	43:W:202:3PE:H392	1.40	0.44
28:X:118:ARG:HH11	28:X:123:LEU:HB3	1.83	0.44
1:1:53:LEU:HG	44:1:403:PC1:H342	1.98	0.44
2:2:259:PRO:HD2	2:2:260:PHE:CE2	2.52	0.44
4:4:339:VAL:HG23	4:4:398:ARG:O	2.17	0.44
4:4:374:LEU:HD21	44:S:201:PC1:H2F2	1.99	0.44
5:5:120:PHE:CE2	5:5:247:ILE:HG12	2.52	0.44
5:5:294:PHE:HD2	5:5:564:PHE:CD1	2.35	0.44
5:5:664:LEU:HD13	18:J:112:PHE:CE1	2.51	0.44
8:9:17:PHE:CZ	27:W:105:ARG:HD3	2.51	0.44
10:B:203:TYR:CD1	10:B:208:ILE:HG13	2.52	0.44
11:C:469:SER:HB3	15:G:189:TRP:CD2	2.53	0.44
18:J:191:PRO:HB2	40:j:67:ARG:HH21	1.82	0.44
30:Z:16:ILE:HA	30:Z:19:LYS:HD2	2.00	0.44
2:2:261:HIS:CE1	2:2:325:ILE:HG21	2.53	0.44
3:3:45:PHE:CE1	23:P:42:MET:HE2	2.53	0.44
7:8:28:ASP:OD2	31:a:150:ARG:NH1	2.42	0.44
9:A:460:GLY:HA3	9:A:465:ALA:HB1	2.00	0.44
11:C:193:LYS:NZ	15:G:106:ASP:OD1	2.49	0.44
22:Q:87:THR:HA	22:Q:128:ASP:HB2	2.00	0.44
1:1:111:ILE:HD11	1:1:250:LEU:HD21	1.99	0.44
4:4:333:THR:HB	4:4:345:TYR:CD2	2.51	0.44
6:6:173:LYS:HB2	12:D:48:GLN:CD	2.43	0.44
10:B:96:HIS:HB2	10:B:174:ALA:HA	2.00	0.44
11:C:217:LEU:CD2	11:C:243:ARG:HB2	2.42	0.44
16:H:125:ILE:HG12	42:o:50:LEU:HD21	1.98	0.44
18:J:80:ARG:HH22	18:J:86:VAL:CG1	2.28	0.44
19:K:143:LEU:HD11	19:K:148:ALA:HA	1.97	0.44
23:P:84:GLN:O	23:P:88:ASN:ND2	2.51	0.44
36:f:79:ASP:N	36:f:79:ASP:OD1	2.49	0.44
37:g:34:ALA:O	37:g:38:VAL:HG23	2.17	0.44
1:1:368:PHE:HE1	43:W:202:3PE:H232	1.83	0.44
2:2:563:ILE:HD13	32:b:60:MET:HE3	2.00	0.44
3:3:1:MET:HE3	3:3:6:ILE:HD11	1.99	0.44
8:9:16:PRO:HD3	41:n:147:PHE:CZ	2.52	0.44
9:A:142:GLN:O	9:A:142:GLN:HG3	2.18	0.44
10:B:288:PHE:C	10:B:290:SER:H	2.24	0.44
11:C:183:ASN:ND2	11:C:443:MET:SD	2.90	0.44
21:M:64:ARG:HD2	21:M:100:GLU:OE2	2.17	0.44
26:U:72:GLU:HG3	26:U:75:ARG:HH22	1.83	0.44
29:Y:154:MET:O	29:Y:157:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:116:THR:HG22	31:a:118:GLY:H	1.82	0.44
5:5:358:LYS:HD3	24:R:71:TYR:CE1	2.52	0.44
6:6:44:ILE:HA	6:6:47:VAL:HG12	1.99	0.44
9:A:340:TYR:CZ	9:A:373:LEU:HD22	2.52	0.44
10:B:291:PHE:O	10:B:297:HIS:HA	2.18	0.44
13:E:312:VAL:O	13:E:315:GLU:HB3	2.17	0.44
18:J:97:ALA:HA	18:J:109:VAL:HG13	2.00	0.44
24:R:11:TYR:HB2	24:R:39:PHE:CZ	2.53	0.44
26:U:43:ILE:HG12	26:U:83:VAL:HG21	2.00	0.44
31:a:33:LEU:HD23	31:a:33:LEU:HA	1.87	0.44
2:2:79:LEU:HD13	2:2:129:LEU:HD22	1.99	0.44
3:3:115:SER:O	3:3:116:ARG:HG2	2.18	0.44
4:4:252:PHE:CD2	4:4:314:LEU:HD12	2.52	0.44
5:5:264:SER:OG	5:5:265:PRO:HD3	2.17	0.44
5:5:640:ILE:O	5:5:644:ILE:HG12	2.18	0.44
9:A:368:ASP:O	9:A:372:ARG:HG3	2.17	0.44
11:C:381:HIS:HA	11:C:384:LEU:HD12	1.99	0.44
14:F:148:ASP:OD1	14:F:149:GLU:N	2.50	0.44
19:K:52:TYR:CZ	19:K:55:TYR:HD1	2.36	0.44
44:S:201:PC1:H272	44:S:201:PC1:H242	1.75	0.44
1:1:322:ILE:O	1:1:326:VAL:HG23	2.18	0.44
44:1:403:PC1:H133	44:1:403:PC1:H112	1.62	0.44
4:4:309:GLN:NE2	4:4:527:TYR:OH	2.50	0.44
5:5:332:HIS:HA	5:5:335:TYR:CE2	2.53	0.44
5:5:662:LEU:HA	5:5:665:LEU:HG	1.99	0.44
10:B:116:PHE:CD1	10:B:117:PRO:HD2	2.53	0.44
10:B:340:LEU:HD23	10:B:355:LYS:HG2	1.99	0.44
10:B:368:LEU:HD12	10:B:375:LEU:HA	1.99	0.44
14:F:66:HIS:NE2	30:Z:142:GLU:OE1	2.51	0.44
14:F:224:GLN:HA	14:F:227:GLU:HG2	1.99	0.44
15:G:265:ASP:HB2	29:Y:122:LYS:HG3	2.00	0.44
46:J:202:LMN:HBK	46:J:202:LMN:HBEA	1.80	0.44
19:K:96:PHE:HB3	19:K:125:ILE:HG12	1.99	0.44
28:X:55:LEU:HA	28:X:58:MET:HE3	2.00	0.44
2:2:109:ARG:O	2:2:113:ILE:HG12	2.18	0.44
9:A:380:LEU:N	9:A:385:GLY:O	2.46	0.44
10:B:148:PRO:HB2	10:B:348:SER:HB3	1.99	0.44
10:B:200:ASN:OD1	42:o:52:TRP:HD1	2.01	0.44
11:C:244:GLU:HA	11:C:247:MET:HE3	1.99	0.44
26:U:51:ASN:HB3	27:W:69:PRO:HG2	2.00	0.44
26:U:159:TRP:O	26:U:161:ARG:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:n:51:LEU:HD23	41:n:51:LEU:HA	1.91	0.44
3:3:54:ILE:HD12	6:6:90:MET:HB2	2.00	0.43
4:4:141:LEU:O	53:4:701:HOH:O	2.21	0.43
5:5:10:LEU:HD12	5:5:122:PHE:CZ	2.53	0.43
5:5:21:ARG:HD3	5:5:22:LYS:NZ	2.33	0.43
5:5:134:LEU:H	5:5:192:LEU:CD1	2.30	0.43
5:5:350:VAL:HG23	5:5:353:ASN:H	1.82	0.43
5:5:604:PHE:CD1	43:5:704:3PE:H322	2.53	0.43
5:5:611:ARG:HG2	5:5:615:LYS:NZ	2.33	0.43
5:5:639:PHE:O	5:5:643:LEU:HD23	2.18	0.43
6:6:195:ASN:HB3	53:6:318:HOH:O	2.17	0.43
11:C:242:GLU:OE1	11:C:283:TRP:NE1	2.48	0.43
11:C:304:TRP:CZ2	11:C:308:LEU:HD11	2.53	0.43
15:G:160:ARG:HG3	17:I:42:ALA:HB2	2.00	0.43
19:K:68:PRO:HG3	19:K:229:ARG:NE	2.32	0.43
24:R:25:ARG:HH11	33:c:43:ARG:NH2	2.14	0.43
31:a:145:ARG:NH2	31:a:149:PRO:HD3	2.33	0.43
32:b:5:ILE:HD12	32:b:48:TYR:CD1	2.49	0.43
32:b:50:LEU:HD23	32:b:50:LEU:HA	1.79	0.43
39:i:55:ARG:HH22	39:i:71:VAL:HG11	1.82	0.43
4:4:505:VAL:O	4:4:509:ILE:HD12	2.18	0.43
5:5:272:THR:O	5:5:276:LEU:HD12	2.17	0.43
6:6:104:SER:CB	6:6:107:ILE:HG12	2.47	0.43
9:A:494:GLU:OE2	9:A:529:ARG:NH1	2.38	0.43
10:B:143:ALA:HB3	10:B:184:ILE:HD13	1.99	0.43
10:B:158:ARG:HH11	10:B:191:GLU:CD	2.25	0.43
10:B:227:ALA:HB3	16:H:182:TYR:HB3	2.00	0.43
11:C:306:ASN:ND2	53:C:527:HOH:O	2.50	0.43
14:F:64:PRO:HB2	14:F:66:HIS:CE1	2.52	0.43
22:Q:90:PHE:O	22:Q:96:LEU:HB2	2.19	0.43
44:S:201:PC1:H382	44:S:201:PC1:H3B2	1.85	0.43
28:X:144:ARG:HH11	28:X:145:TYR:HD2	1.66	0.43
37:g:23:ARG:HH21	43:g:102:3PE:H111	1.83	0.43
2:2:142:THR:HG22	2:2:147:SER:HB3	1.99	0.43
4:4:481:TYR:HA	40:j:10:ALA:HB3	2.01	0.43
9:A:382:PHE:HB2	9:A:383:PRO:HD2	2.00	0.43
9:A:672:ALA:HB2	36:f:20:GLN:HG3	2.00	0.43
15:G:104:TRP:CZ2	15:G:105:LYS:HD2	2.54	0.43
16:H:191:GLY:H	16:H:235:THR:HG1	1.60	0.43
46:J:202:LMN:HBL	46:J:202:LMN:HBT	1.68	0.43
25:S:104:PHE:HA	43:n:201:3PE:H362	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:43:HIS:HB3	28:X:89:TYR:CE2	2.53	0.43
2:2:119:HIS:CE1	2:2:120:MET:HE2	2.53	0.43
2:2:241:ASN:O	2:2:311:TRP:HB3	2.18	0.43
4:4:516:ASP:OD2	5:5:63:ARG:NH1	2.51	0.43
9:A:359:GLU:OE1	53:A:901:HOH:O	2.21	0.43
10:B:314:VAL:HG21	10:B:329:HIS:CG	2.54	0.43
11:C:246:LEU:HD21	11:C:283:TRP:CZ2	2.54	0.43
13:E:197:VAL:HG13	13:E:257:LEU:HD23	2.00	0.43
13:E:287:LYS:HD3	13:E:316:PHE:CD2	2.54	0.43
14:F:111:ASP:O	14:F:115:VAL:HG22	2.18	0.43
22:O:116:ILE:HG12	22:O:133:TYR:HE2	1.83	0.43
25:S:136:ASP:OD1	25:S:136:ASP:N	2.48	0.43
27:W:7:PRO:HD3	27:W:11:TYR:CZ	2.53	0.43
40:j:29:PHE:CE1	40:j:35:THR:HG21	2.53	0.43
5:5:660:ILE:HG21	18:J:116:THR:HB	1.99	0.43
11:C:169:LEU:HD12	11:C:265:PRO:HD3	2.01	0.43
11:C:281:TYR:O	11:C:285:THR:HG23	2.18	0.43
11:C:361:ASP:OD1	11:C:361:ASP:N	2.51	0.43
11:C:422:THR:CG2	17:I:129:LEU:HD22	2.48	0.43
15:G:196:ASP:OD1	15:G:210:ARG:HB2	2.19	0.43
19:K:78:GLN:O	19:K:82:THR:HG23	2.18	0.43
25:S:133:ILE:HG22	25:S:134:LEU:HD23	1.99	0.43
1:1:257:LEU:HD11	1:1:311:PHE:HB3	2.01	0.43
5:5:615:LYS:HE3	43:5:704:3PE:H111	2.00	0.43
9:A:353:ILE:HG12	9:A:379:ALA:HB3	2.00	0.43
10:B:242:LEU:HD12	10:B:242:LEU:HA	1.88	0.43
15:G:221:PRO:HA	15:G:226:PHE:CG	2.53	0.43
18:J:148:ARG:HH22	41:n:116:HIS:HB2	1.84	0.43
2:2:276:THR:HG21	2:2:337:LYS:HE3	2.01	0.43
4:4:186:LEU:HB3	4:4:209:PHE:CE2	2.53	0.43
5:5:277:CYS:O	5:5:314:VAL:HG12	2.19	0.43
5:5:574:GLU:HA	5:5:577:TYR:HB2	2.00	0.43
6:6:110:THR:HG23	20:L:13:LEU:HD13	2.00	0.43
7:8:73:MET:O	7:8:77:ARG:HG2	2.18	0.43
43:8:101:3PE:H2	43:8:101:3PE:H221	1.73	0.43
10:B:141:VAL:HG21	10:B:168:CYS:SG	2.59	0.43
11:C:242:GLU:OE2	11:C:245:LYS:NZ	2.42	0.43
17:I:121:GLU:HA	21:M:98:ALA:HB1	1.99	0.43
2:2:264:SER:OG	2:2:265:PRO:HD3	2.19	0.43
4:4:370:ILE:HD13	4:4:518:LEU:HD11	2.00	0.43
4:4:488:ASP:CG	4:4:489:LEU:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:120:PHE:CZ	5:5:252:MET:HB2	2.54	0.43
5:5:498:ASN:HB2	5:5:501:VAL:HG11	2.01	0.43
7:8:39:ARG:O	7:8:43:GLU:HG2	2.18	0.43
9:A:249:PHE:CD1	17:I:151:ARG:HD2	2.54	0.43
9:A:721:ALA:O	9:A:725:GLY:N	2.45	0.43
12:D:3:VAL:HG21	45:h:201:CDL:H512	2.00	0.43
17:I:56:ASN:HB3	17:I:59:GLU:HG3	2.01	0.43
17:I:107:ARG:HG2	17:I:219:ASP:OD2	2.19	0.43
34:d:16:VAL:CG2	34:d:17:PRO:HD2	2.49	0.43
1:1:246:LEU:O	1:1:250:LEU:HG	2.19	0.43
1:1:314:LEU:O	1:1:318:VAL:HG23	2.19	0.43
2:2:323:LEU:HB3	2:2:473:THR:HG21	2.01	0.43
2:2:498:ASN:HA	2:2:499:PRO:HD3	1.89	0.43
5:5:41:ILE:O	5:5:44:ILE:HG22	2.18	0.43
6:6:109:LEU:HD12	18:J:37:VAL:HA	2.01	0.43
11:C:277:LEU:HD22	11:C:384:LEU:HD23	2.01	0.43
13:E:161:ILE:HG13	13:E:195:THR:HB	2.01	0.43
17:I:155:ARG:NH2	29:Y:145:MET:O	2.42	0.43
22:O:75:PHE:CD1	22:O:78:VAL:HG23	2.54	0.43
44:S:201:PC1:H152	44:S:201:PC1:H112	1.84	0.43
28:X:35:TYR:CE1	28:X:110:MET:HE2	2.54	0.43
31:a:91:ARG:NH2	40:j:12:ASP:OD2	2.45	0.43
4:4:444:LEU:HD23	5:5:183:PHE:HB3	2.01	0.43
5:5:14:VAL:HG21	43:i:101:3PE:H2F2	2.01	0.43
5:5:254:THR:OG1	5:5:329:LEU:HD11	2.19	0.43
5:5:302:ILE:HG22	5:5:340:PHE:CZ	2.54	0.43
25:S:128:LEU:HD12	34:d:48:MET:HE3	2.01	0.43
28:X:29:PHE:O	28:X:33:ILE:HG12	2.18	0.43
34:d:30:ARG:HG3	34:d:30:ARG:NH1	2.34	0.43
37:g:62:TYR:HA	37:g:63:PRO:HD3	1.89	0.43
41:n:167:GLU:HG2	41:n:171:LYS:HE2	2.01	0.43
1:1:44:PRO:HB3	1:1:54:GLN:HE21	1.82	0.42
1:1:233:PHE:HD1	1:1:233:PHE:HA	1.63	0.42
2:2:14:SER:O	3:3:107:GLY:HA3	2.19	0.42
2:2:390:SER:C	2:2:392:TYR:H	2.27	0.42
2:2:499:PRO:HG2	14:F:170:LEU:HD22	2.01	0.42
5:5:384:PRO:HA	5:5:389:PHE:CD1	2.54	0.42
7:8:69:ARG:HH12	31:a:150:ARG:HG2	1.83	0.42
9:A:447:GLY:O	9:A:458:HIS:NE2	2.39	0.42
11:C:252:ARG:HG2	11:C:273:PRO:HG3	2.01	0.42
13:E:159:ARG:HH21	13:E:195:THR:HG1	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:F:221:GLU:O	14:F:224:GLN:HG2	2.19	0.42
15:G:52:PRO:O	30:Z:20:TYR:OH	2.31	0.42
16:H:191:GLY:N	16:H:235:THR:OG1	2.33	0.42
23:P:69:LEU:HD23	23:P:69:LEU:HA	1.85	0.42
31:a:80:PRO:HG3	31:a:90:ARG:NH2	2.34	0.42
32:b:4:ARG:O	32:b:8:TRP:HD1	2.01	0.42
1:1:211:GLU:HG2	1:1:218:SER:O	2.19	0.42
5:5:53:ASN:HB3	5:5:55:ILE:CD1	2.49	0.42
5:5:339:LEU:HG	5:5:376:ALA:HB1	2.02	0.42
7:8:34:LEU:HB2	7:8:58:TYR:CE1	2.54	0.42
9:A:436:TRP:CE2	29:Y:205:LYS:HE2	2.54	0.42
11:C:151:LEU:HD22	19:K:147:MET:HE2	2.00	0.42
11:C:463:PRO:HD2	11:C:496:GLU:OE1	2.19	0.42
12:D:74:GLU:H	12:D:74:GLU:HG2	1.54	0.42
15:G:229:THR:O	15:G:229:THR:HG22	2.19	0.42
41:n:153:HIS:H	41:n:153:HIS:CD2	2.37	0.42
1:1:71:THR:CG2	3:3:35:LEU:HB3	2.49	0.42
5:5:119:LEU:HD13	44:5:701:PC1:H382	2.02	0.42
10:B:322:MET:SD	10:B:363:MET:HE3	2.59	0.42
16:H:126:ILE:HD12	16:H:145:LEU:HG	2.02	0.42
24:R:69:ASP:N	24:R:69:ASP:OD1	2.50	0.42
28:X:76:ARG:NH2	45:g:101:CDL:HA22	2.33	0.42
45:X:201:CDL:H552	45:X:201:CDL:H321	2.01	0.42
2:2:284:LYS:HE2	2:2:344:THR:CG2	2.49	0.42
2:2:310:SER:HB3	2:2:313:TYR:CE2	2.54	0.42
3:3:94:PHE:O	3:3:98:ILE:HG12	2.19	0.42
4:4:293:LYS:HE2	4:4:373:GLY:O	2.20	0.42
5:5:157:ARG:O	5:5:161:ASN:ND2	2.44	0.42
10:B:140:VAL:O	10:B:268:VAL:HA	2.19	0.42
13:E:130:TYR:OH	53:E:501:HOH:O	2.22	0.42
15:G:50:ASP:H	30:Z:17:THR:HG22	1.83	0.42
16:H:154:GLY:CA	42:o:39:VAL:HG21	2.50	0.42
44:S:201:PC1:H3F1	44:S:201:PC1:H282	2.00	0.42
29:Y:106:THR:HA	29:Y:177:GLU:HB2	2.01	0.42
34:d:98:TRP:CZ2	34:d:100:LYS:HA	2.55	0.42
39:i:67:SER:HA	39:i:70:TRP:CE2	2.55	0.42
39:i:68:ARG:HA	39:i:74:ILE:HD11	2.01	0.42
1:1:355:PHE:HZ	3:3:66:LEU:HD22	1.85	0.42
2:2:10:LEU:HD13	2:2:127:LEU:HD21	2.02	0.42
3:3:51:PRO:HD3	6:6:93:ASN:HA	2.02	0.42
4:4:1:MET:HA	4:4:108:GLN:HE22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:394:ARG:O	40:j:6:HIS:HB2	2.20	0.42
4:4:418:PHE:CD2	44:5:701:PC1:H261	2.55	0.42
5:5:251:THR:O	5:5:254:THR:HG22	2.19	0.42
5:5:297:ASP:HA	5:5:354:GLN:O	2.19	0.42
5:5:327:PHE:O	5:5:331:ASN:ND2	2.53	0.42
5:5:662:LEU:HD22	43:5:702:3PE:H251	2.01	0.42
44:5:706:PC1:H143	44:5:706:PC1:H111	1.71	0.42
6:6:13:ILE:HG12	6:6:14:TYR:CD1	2.55	0.42
9:A:534:ALA:O	9:A:538:GLU:HG2	2.19	0.42
11:C:217:LEU:HD11	11:C:250:TYR:CE2	2.55	0.42
11:C:343:PRO:HB3	11:C:348:ASP:HB3	2.01	0.42
13:E:95:ASP:OD1	13:E:96:LEU:N	2.44	0.42
16:H:229:THR:HG22	16:H:234:PHE:H	1.85	0.42
20:L:51:ILE:HD13	20:L:51:ILE:HA	1.83	0.42
38:h:74:TRP:CG	38:h:86:PRO:HG2	2.54	0.42
1:1:175:VAL:HG11	1:1:255:TYR:CE2	2.55	0.42
1:1:355:PHE:CZ	3:3:66:LEU:HD22	2.54	0.42
2:2:167:ARG:HH22	6:6:219:ILE:N	2.18	0.42
2:2:319:SER:HB3	2:2:352:LEU:CB	2.50	0.42
4:4:4:LEU:HD21	4:4:122:VAL:HG23	2.02	0.42
4:4:423:GLY:HA2	4:4:430:THR:HG21	2.01	0.42
9:A:475:GLY:O	9:A:479:LYS:HG3	2.19	0.42
9:A:703:TYR:O	9:A:709:SER:HB3	2.20	0.42
14:F:110:PHE:O	14:F:112:PRO:HD3	2.20	0.42
22:Q:78:VAL:HG12	22:Q:96:LEU:HD21	2.02	0.42
22:Q:94:LEU:HD23	22:Q:94:LEU:H	1.85	0.42
25:S:98:TRP:CZ3	44:S:201:PC1:H3G2	2.54	0.42
28:X:35:TYR:CD2	28:X:98:PHE:CZ	3.07	0.42
45:g:101:CDL:H521	45:g:101:CDL:OA9	2.20	0.42
38:h:43:LYS:HB2	38:h:59:ASP:HB3	2.01	0.42
1:1:329:TRP:CZ2	17:I:85:LEU:HG	2.55	0.42
2:2:75:SER:O	2:2:79:LEU:HB2	2.19	0.42
44:4:603:PC1:H111	44:4:603:PC1:H143	1.65	0.42
5:5:313:MET:HE2	5:5:329:LEU:HA	2.02	0.42
5:5:356:PHE:HB3	5:5:431:LEU:HD13	2.01	0.42
43:5:702:3PE:H2	43:5:702:3PE:H222	1.45	0.42
9:A:45:ILE:HG12	9:A:111:VAL:HB	2.01	0.42
10:B:125:MET:HE2	10:B:137:ARG:HB3	2.01	0.42
13:E:167:ASN:HD21	13:E:319:GLN:HA	1.85	0.42
16:H:262:THR:OG1	16:H:263:PRO:HD2	2.19	0.42
52:O:201:ZMP:H21A	23:P:64:ARG:HH11	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Q:107:ALA:O	22:Q:111:GLU:HG3	2.19	0.42
27:W:27:ARG:O	27:W:31:LEU:HD23	2.20	0.42
30:Z:119:GLU:OE2	30:Z:123:LYS:NZ	2.52	0.42
39:i:10:PRO:HB3	39:i:12:HIS:NE2	2.35	0.42
43:1:401:3PE:H3F2	43:W:201:3PE:H2I3	2.00	0.42
3:3:39:GLU:O	3:3:39:GLU:HG3	2.20	0.42
5:5:581:ILE:O	5:5:585:ILE:HG12	2.20	0.42
43:5:707:3PE:H382	43:5:707:3PE:H351	1.85	0.42
10:B:319:SER:HA	10:B:364:ASP:HB2	2.01	0.42
14:F:171:GLU:OE2	14:F:171:GLU:N	2.47	0.42
15:G:124:LEU:O	15:G:132:PHE:HB2	2.20	0.42
15:G:132:PHE:CD1	15:G:158:SER:HB2	2.55	0.42
18:J:155:ILE:O	18:J:159:LEU:HG	2.19	0.42
21:M:59:MET:HE3	21:M:59:MET:HB3	1.97	0.42
21:M:110:THR:HG21	21:M:115:VAL:HG11	2.01	0.42
24:R:33:LEU:HD21	33:c:34:ASP:OD1	2.19	0.42
36:f:32:LEU:HD13	36:f:50:LEU:HD22	2.02	0.42
1:1:35:MET:CE	1:1:331:ARG:HE	2.33	0.42
1:1:241:VAL:HG22	1:1:324:ILE:HD11	2.02	0.42
44:1:403:PC1:H381	44:1:403:PC1:H3B1	1.79	0.42
4:4:113:LEU:HD21	41:n:104:MET:HE1	2.02	0.42
44:5:701:PC1:H152	39:i:20:TRP:CH2	2.54	0.42
10:B:85:TRP:CD2	10:B:207:LEU:HD13	2.55	0.42
10:B:200:ASN:OD1	42:o:52:TRP:HA	2.20	0.42
10:B:383:MET:HB3	10:B:387:THR:HG21	2.01	0.42
11:C:176:ASP:OD1	11:C:493:VAL:HG11	2.20	0.42
16:H:116:PHE:HD2	16:H:163:GLU:HG2	1.85	0.42
17:I:217:ARG:NH1	53:I:402:HOH:O	2.27	0.42
30:Z:29:GLU:HA	30:Z:32:ARG:HG2	2.02	0.42
30:Z:186:TYR:CD2	30:Z:192:CYS:HB3	2.55	0.42
31:a:72:ARG:HD2	31:a:98:HIS:CE1	2.55	0.42
40:j:60:LEU:HB2	40:j:75:ARG:NH1	2.34	0.42
1:1:34:THR:O	1:1:38:MET:HG3	2.20	0.42
1:1:366:TYR:CZ	3:3:85:ALA:HB2	2.54	0.42
2:2:427:LEU:HA	2:2:427:LEU:HD12	1.70	0.42
4:4:107:ILE:HD11	41:n:100:ARG:HB3	2.02	0.42
4:4:515:LEU:HD23	4:4:515:LEU:HA	1.88	0.42
5:5:32:THR:O	5:5:36:VAL:HG23	2.20	0.42
5:5:33:CYS:SG	5:5:97:HIS:HB3	2.59	0.42
5:5:603:LEU:O	5:5:608:GLY:HA3	2.20	0.42
9:A:700:GLU:OE1	9:A:700:GLU:N	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:135:LYS:NZ	10:B:264:CYS:HA	2.35	0.42
10:B:151:CYS:SG	16:H:246:VAL:HG22	2.59	0.42
11:C:177:TYR:HB2	19:K:105:CYS:HB3	2.01	0.42
18:J:114:ALA:HB3	43:J:201:3PE:H351	2.02	0.42
24:R:15:LEU:HD13	24:R:28:TRP:HZ2	1.85	0.42
28:X:35:TYR:CE2	28:X:110:MET:HG3	2.55	0.42
41:n:151:LEU:O	41:n:155:ILE:HG12	2.19	0.42
2:2:78:ILE:HD13	2:2:278:PHE:HA	2.01	0.41
5:5:49:GLU:OE2	39:i:65:TYR:CE2	2.73	0.41
5:5:201:ALA:N	5:5:202:PRO:HD2	2.35	0.41
5:5:221:MET:HE2	5:5:229:LEU:HD12	2.01	0.41
5:5:296:GLN:O	5:5:355:ASP:HA	2.20	0.41
43:5:705:3PE:H292	43:5:705:3PE:H2C1	1.83	0.41
16:H:310:GLY:HA3	16:H:311:PRO:HD3	1.94	0.41
46:J:202:LMN:HCH	46:J:202:LMN:HCS	1.71	0.41
30:Z:120:GLU:HG2	30:Z:123:LYS:HD2	2.01	0.41
36:f:17:LEU:O	36:f:58:PRO:HA	2.20	0.41
46:j:101:LMN:HBKA	46:j:101:LMN:HBS	1.77	0.41
43:n:201:3PE:H251	43:n:201:3PE:H221	1.91	0.41
5:5:243:VAL:HG12	5:5:248:HIS:CE1	2.55	0.41
5:5:503:ASN:HB2	34:d:64:GLY:C	2.45	0.41
10:B:414:GLY:O	10:B:418:THR:OG1	2.34	0.41
14:F:52:LEU:HD23	14:F:52:LEU:HA	1.85	0.41
1:1:85:THR:O	1:1:89:SER:OG	2.31	0.41
4:4:94:TYR:HD2	25:S:104:PHE:HZ	1.67	0.41
4:4:117:ASP:HB2	4:4:119:TYR:CE1	2.56	0.41
4:4:394:ARG:NH1	4:4:488:ASP:O	2.50	0.41
5:5:70:PHE:CE2	5:5:186:LEU:HD13	2.56	0.41
5:5:140:TRP:HD1	5:5:141:GLU:OE1	2.03	0.41
7:8:60:LYS:HZ1	35:e:45:TRP:CD1	2.39	0.41
10:B:117:PRO:HB2	10:B:120:LEU:HB3	2.02	0.41
11:C:198:GLU:OE2	11:C:204:LYS:NZ	2.36	0.41
12:D:59:HIS:CE1	12:D:61:ARG:HB2	2.55	0.41
14:F:121:GLU:OE2	14:F:184:ARG:NH2	2.47	0.41
14:F:228:GLY:O	14:F:231:LYS:HG2	2.21	0.41
15:G:96:LYS:HE2	15:G:97:TYR:OH	2.20	0.41
16:H:238:GLU:N	16:H:238:GLU:OE1	2.53	0.41
18:J:16:ALA:HB1	18:J:71:PHE:HD1	1.85	0.41
23:P:49:VAL:HA	23:P:52:ILE:HD12	2.02	0.41
25:S:110:TYR:CZ	41:n:83:LEU:HD23	2.55	0.41
25:S:123:GLU:O	25:S:127:ARG:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:102:ASP:OD1	31:a:102:ASP:N	2.53	0.41
2:2:4:ILE:HD11	28:X:154:PRO:HG3	2.01	0.41
5:5:584:LEU:O	5:5:588:LEU:HD23	2.21	0.41
5:5:616:LEU:HD21	5:5:663:LEU:HD12	2.02	0.41
6:6:92:ILE:O	53:6:301:HOH:O	2.21	0.41
9:A:224:ASN:OD1	9:A:225:LEU:N	2.53	0.41
9:A:254:TRP:HB3	15:G:260:GLY:HA3	2.03	0.41
9:A:509:VAL:HG13	9:A:516:PHE:HB3	2.02	0.41
10:B:260:GLY:N	10:B:264:CYS:O	2.52	0.41
11:C:359:ASN:HB2	11:C:361:ASP:OD1	2.21	0.41
13:E:128:ARG:HD2	13:E:130:TYR:CZ	2.56	0.41
13:E:134:ASN:H	19:K:230:LYS:HE2	1.85	0.41
27:W:39:MET:HE3	43:W:202:3PE:H3D1	2.02	0.41
2:2:171:LEU:HD23	2:2:171:LEU:HA	1.84	0.41
5:5:547:LEU:O	5:5:549:GLU:HG2	2.20	0.41
5:5:618:LYS:O	31:a:40:ARG:NH1	2.54	0.41
8:9:77:GLU:N	8:9:77:GLU:OE1	2.53	0.41
9:A:169:ARG:NH2	53:A:928:HOH:O	2.49	0.41
11:C:322:LEU:HG	15:G:185:MET:HE3	2.02	0.41
13:E:82:ARG:HB3	19:K:226:MET:HE1	2.03	0.41
13:E:272:VAL:O	13:E:276:ILE:HG12	2.20	0.41
15:G:197:MET:HB3	15:G:222:LEU:HD12	2.02	0.41
19:K:109:GLU:HG3	19:K:201:PRO:HB2	2.03	0.41
53:1:571:HOH:O	19:K:100:THR:HG21	2.21	0.41
5:5:585:ILE:HG13	44:5:706:PC1:H3A2	2.02	0.41
9:A:133:HIS:HD2	11:C:411:MET:HE2	1.86	0.41
9:A:227:SER:O	9:A:230:SER:HB2	2.20	0.41
9:A:350:PHE:HB3	9:A:375:SER:HB2	2.02	0.41
49:B:602:FMN:HM73	49:B:602:FMN:HM81	1.90	0.41
13:E:102:MET:HE1	13:E:114:GLU:HB3	2.02	0.41
13:E:114:GLU:HG2	13:E:117:ARG:HH22	1.86	0.41
16:H:98:SER:OG	16:H:99:ASP:N	2.54	0.41
19:K:77:VAL:O	19:K:81:LEU:HG	2.20	0.41
19:K:118:TYR:CD1	19:K:208:MET:HE1	2.55	0.41
24:R:58:THR:O	24:R:61:LEU:HG	2.20	0.41
24:R:97:LEU:HD23	24:R:97:LEU:HA	1.89	0.41
45:g:101:CDL:HB4	45:g:101:CDL:H512	1.75	0.41
1:1:91:LEU:HD11	43:1:402:3PE:H271	2.03	0.41
2:2:9:LEU:HG	2:2:127:LEU:HD12	2.03	0.41
4:4:277:VAL:HA	4:4:340:LYS:HD3	2.02	0.41
8:9:11:PRO:HB2	41:n:147:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:490:MET:HE3	11:C:492:LEU:HD11	2.01	0.41
14:F:96:VAL:HG22	14:F:100:LYS:NZ	2.36	0.41
14:F:219:ILE:HA	14:F:219:ILE:HD12	1.82	0.41
15:G:149:ARG:NH2	15:G:225:ASP:OD1	2.54	0.41
18:J:190:ASN:OD1	18:J:190:ASN:N	2.53	0.41
52:Q:201:ZMP:H3	24:R:61:LEU:HD11	2.01	0.41
29:Y:122:LYS:HE3	29:Y:122:LYS:HB3	1.69	0.41
42:o:39:VAL:HG23	42:o:40:PHE:HD1	1.85	0.41
43:1:401:3PE:H392	17:I:74:MET:HE1	2.03	0.41
44:1:403:PC1:H122	38:h:24:LEU:O	2.20	0.41
2:2:511:ARG:HD2	14:F:189:ASP:OD1	2.21	0.41
4:4:20:THR:O	4:4:23:SER:OG	2.28	0.41
4:4:103:GLN:HB3	41:n:101:ASN:ND2	2.36	0.41
4:4:366:LEU:HD13	4:4:525:VAL:HG23	2.01	0.41
5:5:609:LEU:O	5:5:613:LEU:HB2	2.20	0.41
6:6:213:GLY:O	6:6:216:VAL:HG12	2.21	0.41
9:A:106:GLN:HB3	9:A:109:MET:HE3	2.02	0.41
9:A:129:LEU:HG	10:B:409:THR:CG2	2.49	0.41
20:L:50:ILE:HD12	20:L:50:ILE:HA	1.87	0.41
21:M:110:THR:HG21	21:M:115:VAL:CG1	2.51	0.41
41:n:162:HIS:O	41:n:166:GLU:HG2	2.21	0.41
44:1:403:PC1:H272	44:1:403:PC1:H2A2	1.89	0.41
2:2:292:LEU:HA	2:2:355:LEU:HD11	2.03	0.41
2:2:369:TYR:CD2	2:2:450:ALA:HB1	2.56	0.41
4:4:123:ASP:CG	4:4:301:ARG:HH22	2.29	0.41
4:4:159:MET:HE3	53:4:742:HOH:O	2.20	0.41
4:4:363:ILE:O	4:4:367:GLU:HG3	2.21	0.41
4:4:463:ALA:HA	5:5:169:LEU:HD21	2.02	0.41
5:5:150:LEU:HB3	5:5:243:VAL:HG11	2.02	0.41
5:5:249:ALA:HB2	5:5:340:PHE:CD2	2.55	0.41
5:5:290:LEU:HD13	5:5:567:PHE:HE2	1.85	0.41
5:5:378:LEU:HD23	5:5:378:LEU:HA	1.91	0.41
8:9:73:LYS:HE3	8:9:73:LYS:HB2	1.85	0.41
9:A:165:ILE:HG23	10:B:490:GLY:O	2.21	0.41
10:B:182:ILE:HD11	10:B:221:VAL:HG13	2.03	0.41
11:C:221:MET:HE2	11:C:221:MET:HB2	1.99	0.41
11:C:313:VAL:HA	11:C:360:GLY:O	2.21	0.41
11:C:478:HIS:HB3	11:C:482:ASP:CB	2.51	0.41
13:E:83:GLU:OE2	13:E:85:MET:HB2	2.21	0.41
13:E:109:THR:H	19:K:64:GLU:CD	2.29	0.41
17:I:87:GLN:HA	17:I:90:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:63:ALA:HB1	53:L:111:HOH:O	2.20	0.41
22:Q:96:LEU:HD12	22:Q:100:ASP:CB	2.51	0.41
44:S:201:PC1:H271	44:S:201:PC1:H2A1	1.81	0.41
28:X:176:GLU:HA	28:X:179:LEU:HB2	2.03	0.41
30:Z:14:VAL:CG2	30:Z:19:LYS:HE3	2.51	0.41
32:b:69:LEU:HG	41:n:117:LEU:HD21	2.02	0.41
34:d:42:GLN:O	34:d:46:VAL:HG23	2.21	0.41
36:f:58:PRO:HB2	36:f:74:LEU:HB2	2.03	0.41
43:i:101:3PE:H11	41:n:66:PHE:HE1	1.86	0.41
2:2:8:SER:HG	28:X:80:PHE:HE2	1.66	0.41
4:4:75:TYR:CZ	4:4:153:LYS:NZ	2.89	0.41
4:4:306:ILE:C	4:4:308:PRO:HD3	2.46	0.41
4:4:428:PRO:O	4:4:429:LEU:HB2	2.21	0.41
53:4:747:HOH:O	34:d:33:GLN:HG3	2.21	0.41
5:5:69:TRP:CZ2	34:d:82:LEU:HA	2.55	0.41
5:5:109:HIS:CE1	44:5:701:PC1:H122	2.56	0.41
5:5:488:THR:HA	5:5:491:ILE:HD12	2.03	0.41
5:5:569:GLN:HA	5:5:570:ARG:NH2	2.35	0.41
5:5:600:SER:HB3	40:j:29:PHE:CZ	2.56	0.41
5:5:622:SER:HB2	31:a:40:ARG:NH1	2.36	0.41
5:5:655:LEU:HD22	18:J:130:LEU:HD13	2.03	0.41
9:A:213:ASN:ND2	10:B:412:ARG:O	2.43	0.41
9:A:306:ASP:CG	9:A:713:PRO:HD2	2.46	0.41
10:B:96:HIS:HB2	10:B:174:ALA:O	2.20	0.41
10:B:106:SER:HB2	10:B:288:PHE:CD2	2.56	0.41
11:C:295:GLU:HG2	27:W:20:LEU:HD11	2.02	0.41
13:E:128:ARG:HD2	13:E:130:TYR:CE2	2.56	0.41
16:H:204:GLN:HA	16:H:209:GLY:O	2.21	0.41
17:I:44:PRO:HA	17:I:45:PRO:HD3	1.98	0.41
22:Q:116:ILE:O	24:R:12:ARG:NH2	2.54	0.41
28:X:124:PRO:HG3	28:X:128:GLU:HG3	2.03	0.41
30:Z:98:ALA:O	30:Z:132:GLY:HA3	2.21	0.41
2:2:8:SER:HA	45:g:101:CDL:H152	2.03	0.40
2:2:129:LEU:HD12	2:2:162:LEU:HD11	2.03	0.40
3:3:56:PHE:O	3:3:59:TYR:HB2	2.21	0.40
5:5:347:ILE:HG22	5:5:352:ASP:HA	2.04	0.40
9:A:739:ASP:N	9:A:739:ASP:OD1	2.50	0.40
11:C:169:LEU:HD13	11:C:264:ARG:HG2	2.02	0.40
11:C:169:LEU:CD1	11:C:264:ARG:HA	2.50	0.40
11:C:313:VAL:HG22	11:C:361:ASP:HB3	2.03	0.40
13:E:159:ARG:HD2	13:E:159:ARG:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:G:201:LEU:CD2	23:P:77:GLN:HG2	2.47	0.40
20:L:9:LEU:O	20:L:12:ILE:HG22	2.21	0.40
23:P:30:ARG:HG2	23:P:34:ARG:HH12	1.85	0.40
24:R:26:ASN:HB3	33:c:44:TYR:OH	2.21	0.40
28:X:113:ARG:NE	28:X:117:ASP:OD1	2.54	0.40
29:Y:84:GLY:HA2	29:Y:91:PRO:HG3	2.03	0.40
2:2:199:VAL:CG1	6:6:126:PRO:HD3	2.50	0.40
2:2:379:ASN:HB2	2:2:543:ILE:HG21	2.03	0.40
2:2:427:LEU:HD23	32:b:21:GLY:HA3	2.03	0.40
4:4:170:PHE:CZ	4:4:294:LEU:HD23	2.57	0.40
4:4:194:GLY:HA2	4:4:201:LYS:HD2	2.03	0.40
4:4:244:GLU:HA	18:J:153:ARG:HH12	1.85	0.40
5:5:120:PHE:HZ	5:5:252:MET:HB2	1.86	0.40
5:5:196:THR:HG21	34:d:53:ARG:HD2	2.03	0.40
5:5:383:PHE:O	5:5:389:PHE:HB2	2.21	0.40
9:A:367:LYS:HE3	9:A:539:VAL:O	2.21	0.40
10:B:161:PRO:O	10:B:165:VAL:HG23	2.21	0.40
11:C:136:GLU:OE1	11:C:144:ARG:NH2	2.54	0.40
13:E:107:ARG:HB2	19:K:65:VAL:CG2	2.52	0.40
13:E:224:HIS:HB2	13:E:226:ARG:HE	1.85	0.40
15:G:271:ILE:HB	53:Z:227:HOH:O	2.21	0.40
25:S:108:TYR:CZ	44:S:201:PC1:H132	2.56	0.40
31:a:55:LEU:HD23	31:a:59:GLU:HG3	2.02	0.40
33:c:55:LYS:HB3	33:c:55:LYS:HE2	1.82	0.40
40:j:21:MET:HE3	40:j:21:MET:HB3	1.88	0.40
4:4:510:TYR:CD1	43:5:703:3PE:H222	2.56	0.40
5:5:327:PHE:CD1	5:5:492:PHE:HB2	2.57	0.40
8:9:78:ASN:HA	8:9:79:PRO:HD3	1.93	0.40
9:A:650:GLN:HE22	29:Y:61:PRO:HD2	1.87	0.40
9:A:703:TYR:HE2	9:A:722:LYS:HD3	1.86	0.40
10:B:139:LEU:HD13	10:B:175:MET:CE	2.50	0.40
11:C:320:LEU:HD23	15:G:134:GLN:HE21	1.86	0.40
11:C:335:PRO:O	53:C:502:HOH:O	2.22	0.40
13:E:148:ILE:O	13:E:152:VAL:HG23	2.22	0.40
13:E:214:ALA:O	13:E:280:ARG:NH2	2.54	0.40
13:E:301:LEU:HD23	13:E:303:TRP:CH2	2.56	0.40
15:G:138:ILE:HG23	15:G:154:TYR:CE1	2.56	0.40
22:O:90:PHE:HD2	22:O:101:THR:HG23	1.87	0.40
29:Y:68:ASP:OD1	29:Y:71:THR:HG23	2.21	0.40
1:1:75:LEU:HA	1:1:78:PHE:HB3	2.04	0.40
44:3:201:PC1:H222	44:3:201:PC1:H251	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:389:GLY:HA2	53:4:726:HOH:O	2.21	0.40
43:5:707:3PE:H3A2	43:5:707:3PE:H371	1.72	0.40
6:6:112:LEU:HD11	18:J:32:LEU:HG	2.02	0.40
9:A:327:ALA:HB1	9:A:331:GLN:HG3	2.03	0.40
9:A:380:LEU:HD23	9:A:380:LEU:HA	1.84	0.40
9:A:583:ASP:OD2	9:A:707:VAL:HG12	2.21	0.40
10:B:158:ARG:HD2	10:B:159:LYS:HZ2	1.86	0.40
15:G:135:VAL:HG23	15:G:184:TYR:CD1	2.57	0.40
16:H:157:SER:O	16:H:161:MET:HG3	2.21	0.40
16:H:228:THR:HG21	42:o:29:PHE:CZ	2.57	0.40
2:2:394:TYR:HA	2:2:496:GLU:O	2.22	0.40
2:2:525:LEU:HD22	2:2:529:ASN:ND2	2.36	0.40
3:3:47:GLN:HA	53:3:327:HOH:O	2.20	0.40
3:3:76:PHE:HB2	6:6:193:TYR:CZ	2.56	0.40
4:4:99:PHE:HB2	25:S:114:THR:O	2.22	0.40
4:4:308:PRO:HG2	34:d:95:GLN:HE22	1.85	0.40
5:5:197:VAL:HG23	5:5:198:PHE:CD1	2.57	0.40
5:5:261:MET:HE2	5:5:261:MET:HB3	1.71	0.40
5:5:566:PHE:HD2	5:5:567:PHE:CD1	2.39	0.40
8:9:6:GLY:HA2	20:L:48:ASP:O	2.22	0.40
9:A:127:GLU:HG3	53:A:949:HOH:O	2.22	0.40
11:C:97:GLN:CB	11:C:476:ARG:HD2	2.52	0.40
11:C:176:ASP:HA	11:C:493:VAL:HG11	2.03	0.40
15:G:97:TYR:HD1	15:G:113:CYS:SG	2.45	0.40
17:I:131:GLU:HG3	17:I:139:ILE:O	2.22	0.40
18:J:181:LEU:HD12	40:j:71:LEU:HD12	2.02	0.40
23:P:55:ARG:NH2	23:P:59:GLU:OE2	2.53	0.40
26:U:156:ILE:HA	26:U:157:PRO:HD3	1.90	0.40
42:o:45:PHE:O	42:o:49:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	330/378 (87%)	318 (96%)	12 (4%)	0	100	100
2	2	554/571 (97%)	543 (98%)	11 (2%)	0	100	100
3	3	126/146 (86%)	117 (93%)	9 (7%)	0	100	100
4	4	490/542 (90%)	476 (97%)	14 (3%)	0	100	100
5	5	668/679 (98%)	614 (92%)	53 (8%)	1 (0%)	48	71
6	6	186/224 (83%)	173 (93%)	13 (7%)	0	100	100
7	8	75/86 (87%)	68 (91%)	7 (9%)	0	100	100
8	9	101/785 (13%)	100 (99%)	1 (1%)	0	100	100
9	A	709/749 (95%)	680 (96%)	28 (4%)	1 (0%)	48	71
10	B	454/507 (90%)	437 (96%)	17 (4%)	0	100	100
11	C	438/499 (88%)	417 (95%)	21 (5%)	0	100	100
12	D	79/86 (92%)	77 (98%)	2 (2%)	0	100	100
13	E	335/378 (89%)	319 (95%)	16 (5%)	0	100	100
14	F	236/261 (90%)	224 (95%)	12 (5%)	0	100	100
15	G	240/293 (82%)	231 (96%)	9 (4%)	0	100	100
16	H	219/318 (69%)	207 (94%)	12 (6%)	0	100	100
17	I	183/223 (82%)	178 (97%)	5 (3%)	0	100	100
18	J	184/199 (92%)	178 (97%)	6 (3%)	0	100	100
19	K	180/230 (78%)	171 (95%)	9 (5%)	0	100	100
20	L	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
21	M	115/168 (68%)	110 (96%)	5 (4%)	0	100	100
22	O	80/141 (57%)	78 (98%)	2 (2%)	0	100	100
22	Q	83/141 (59%)	79 (95%)	4 (5%)	0	100	100
23	P	111/124 (90%)	108 (97%)	3 (3%)	0	100	100
24	R	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
25	S	72/143 (50%)	69 (96%)	3 (4%)	0	100	100
26	U	167/186 (90%)	166 (99%)	1 (1%)	0	100	100
27	W	118/121 (98%)	115 (98%)	3 (2%)	0	100	100
28	X	185/191 (97%)	181 (98%)	3 (2%)	1 (0%)	24	43
29	Y	152/210 (72%)	148 (97%)	4 (3%)	0	100	100
30	Z	184/196 (94%)	175 (95%)	9 (5%)	0	100	100
31	a	141/203 (70%)	141 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	b	79/94 (84%)	77 (98%)	2 (2%)	0	100	100
33	c	58/93 (62%)	54 (93%)	4 (7%)	0	100	100
34	d	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
35	e	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
36	f	86/95 (90%)	82 (95%)	4 (5%)	0	100	100
37	g	76/82 (93%)	73 (96%)	3 (4%)	0	100	100
38	h	131/134 (98%)	127 (97%)	4 (3%)	0	100	100
39	i	78/93 (84%)	74 (95%)	4 (5%)	0	100	100
40	j	71/75 (95%)	68 (96%)	3 (4%)	0	100	100
41	n	133/184 (72%)	128 (96%)	5 (4%)	0	100	100
42	o	30/380 (8%)	29 (97%)	1 (3%)	0	100	100
All	All	8251/10547 (78%)	7915 (96%)	333 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	A	672	ALA
28	X	67	GLY
5	5	108	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	284/326 (87%)	275 (97%)	9 (3%)	34	58
2	2	509/518 (98%)	497 (98%)	12 (2%)	43	65
3	3	111/128 (87%)	110 (99%)	1 (1%)	70	82
4	4	431/477 (90%)	431 (100%)	0	100	100
5	5	579/596 (97%)	578 (100%)	1 (0%)	87	95
6	6	162/203 (80%)	156 (96%)	6 (4%)	30	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	8	69/75 (92%)	69 (100%)	0	100	100
8	9	84/687 (12%)	83 (99%)	1 (1%)	63	78
9	A	577/602 (96%)	576 (100%)	1 (0%)	87	95
10	B	366/401 (91%)	366 (100%)	0	100	100
11	C	362/416 (87%)	360 (99%)	2 (1%)	78	88
12	D	68/69 (99%)	67 (98%)	1 (2%)	57	74
13	E	299/335 (89%)	298 (100%)	1 (0%)	86	93
14	F	199/219 (91%)	199 (100%)	0	100	100
15	G	215/257 (84%)	215 (100%)	0	100	100
16	H	190/272 (70%)	189 (100%)	1 (0%)	81	89
17	I	158/191 (83%)	156 (99%)	2 (1%)	61	76
18	J	126/146 (86%)	126 (100%)	0	100	100
19	K	158/191 (83%)	155 (98%)	3 (2%)	50	70
20	L	73/76 (96%)	73 (100%)	0	100	100
21	M	97/135 (72%)	97 (100%)	0	100	100
22	O	68/119 (57%)	65 (96%)	3 (4%)	25	47
22	Q	73/119 (61%)	73 (100%)	0	100	100
23	P	101/110 (92%)	101 (100%)	0	100	100
24	R	87/89 (98%)	87 (100%)	0	100	100
25	S	59/111 (53%)	59 (100%)	0	100	100
26	U	149/167 (89%)	147 (99%)	2 (1%)	61	76
27	W	100/102 (98%)	98 (98%)	2 (2%)	48	69
28	X	143/152 (94%)	140 (98%)	3 (2%)	47	67
29	Y	131/176 (74%)	130 (99%)	1 (1%)	73	84
30	Z	152/155 (98%)	150 (99%)	2 (1%)	61	76
31	a	123/177 (70%)	123 (100%)	0	100	100
32	b	67/74 (90%)	66 (98%)	1 (2%)	57	74
33	c	47/80 (59%)	47 (100%)	0	100	100
34	d	87/94 (93%)	87 (100%)	0	100	100
35	e	29/35 (83%)	29 (100%)	0	100	100
36	f	76/80 (95%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	g	65/69 (94%)	65 (100%)	0	100	100
38	h	117/119 (98%)	116 (99%)	1 (1%)	70	82
39	i	68/78 (87%)	68 (100%)	0	100	100
40	j	63/64 (98%)	63 (100%)	0	100	100
41	n	106/150 (71%)	103 (97%)	3 (3%)	38	61
42	o	26/318 (8%)	26 (100%)	0	100	100
All	All	7054/8958 (79%)	6995 (99%)	59 (1%)	70	84

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	31	GLU
1	1	75	LEU
1	1	120	LEU
1	1	152	GLU
1	1	170	SER
1	1	203	ASN
1	1	217	VAL
1	1	230	VAL
1	1	233	PHE
2	2	23	ILE
2	2	60	ILE
2	2	69	ILE
2	2	109	ARG
2	2	127	LEU
2	2	129	LEU
2	2	170	GLU
2	2	199	VAL
2	2	211	ILE
2	2	294	LEU
2	2	456	SER
2	2	564	LEU
3	3	72	LEU
5	5	189	LEU
6	6	73	TYR
6	6	76	VAL
6	6	126	PRO
6	6	176	ASP
6	6	181	GLU
6	6	198	VAL

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Mol	Chain	Res	Type
8	9	51	LEU
9	A	182	THR
11	C	274	VAL
11	C	391	PRO
12	D	64	THR
13	E	227	GLU
16	H	200	THR
17	I	125	ILE
17	I	185	GLU
19	K	105	CYS
19	K	126	ILE
19	K	142	THR
22	O	99	LEU
22	O	105	VAL
22	O	135	LEU
26	U	130	GLU
26	U	139	ASN
27	W	65	ILE
27	W	103	SER
28	X	90	PHE
28	X	142	GLN
28	X	167	ASP
29	Y	122	LYS
30	Z	62	LEU
30	Z	68	VAL
32	b	53	ILE
38	h	104	VAL
41	n	47	VAL
41	n	119	LEU
41	n	163	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	54	GLN
1	1	72	GLN
1	1	74	ASN
1	1	147	GLN
1	1	203	ASN
2	2	68	HIS
2	2	119	HIS
2	2	200	ASN

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Mol	Chain	Res	Type
2	2	364	GLN
2	2	398	ASN
3	3	29	ASN
3	3	47	GLN
3	3	114	HIS
4	4	200	ASN
4	4	350	HIS
4	4	519	HIS
5	5	109	HIS
5	5	111	GLN
5	5	131	ASN
5	5	162	GLN
5	5	562	ASN
5	5	578	ASN
5	5	591	GLN
5	5	627	HIS
6	6	67	ASN
6	6	93	ASN
6	6	183	ASN
6	6	190	ASN
8	9	64	GLN
9	A	132	ASN
9	A	289	ASN
9	A	525	ASN
10	B	162	HIS
10	B	196	GLN
10	B	197	ASN
10	B	200	ASN
10	B	444	GLN
10	B	448	HIS
10	B	494	HIS
11	C	183	ASN
11	C	306	ASN
11	C	359	ASN
11	C	381	HIS
12	D	44	GLN
12	D	48	GLN
12	D	49	GLN
12	D	59	HIS
13	E	61	GLN
14	F	42	HIS
14	F	54	HIS

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Mol	Chain	Res	Type
14	F	106	HIS
14	F	253	GLN
15	G	252	GLN
15	G	266	GLN
16	H	150	GLN
16	H	268	GLN
16	H	289	GLN
17	I	112	HIS
18	J	18	HIS
18	J	88	ASN
19	K	157	GLN
20	L	46	ASN
21	M	111	HIS
21	M	153	HIS
22	O	123	GLN
23	P	63	HIS
23	P	67	ASN
22	Q	125	HIS
24	R	24	HIS
25	S	85	GLN
26	U	11	HIS
26	U	61	ASN
27	W	15	GLN
27	W	54	ASN
27	W	87	GLN
28	X	10	GLN
28	X	136	GLN
28	X	142	GLN
29	Y	123	ASN
29	Y	142	ASN
29	Y	174	GLN
29	Y	195	ASN
30	Z	23	GLN
30	Z	51	ASN
30	Z	99	GLN
30	Z	166	GLN
31	a	81	HIS
31	a	123	GLN
34	d	67	HIS
35	e	12	HIS
38	h	93	GLN
39	i	12	HIS

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Mol	Chain	Res	Type
39	i	52	HIS
41	n	110	GLN
41	n	153	HIS
41	n	161	GLN

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	$\# Z > 2$
11	2MR	C	154	11	10,12,13	0.29	0	5,13,15	0.94	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	2MR	C	154	11	-	0/10/13/15	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 46 ligands modelled in this entry, 1 is monoatomic - leaving 45 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	SF4	A	803	9	0,12,12	-	-	-		
47	FES	A	801	9	0,4,4	-	-	-		
45	CDL	g	101	-	56,56,99	1.15	7 (12%)	62,68,111	1.27	5 (8%)
47	FES	H	401	16	0,4,4	-	-	-		
48	SF4	I	301	17	0,12,12	-	-	-		
46	LMN	J	202	-	60,60,72	1.75	14 (23%)	74,80,98	0.99	2 (2%)
48	SF4	A	802	9	0,12,12	-	-	-		
46	LMN	2	602	-	60,60,72	0.21	0	74,80,98	0.38	0
48	SF4	K	301	19	0,12,12	-	-	-		
43	3PE	1	402	-	26,26,50	0.34	0	28,30,55	0.56	0
52	ZMP	Q	201	22	30,35,36	0.21	0	34,42,45	0.46	0
45	CDL	2	601	-	84,84,99	0.31	0	90,96,111	0.34	0
44	PC1	S	201	-	50,50,53	0.98	4 (8%)	56,58,61	1.07	2 (3%)
46	LMN	j	101	-	71,71,72	1.65	13 (18%)	91,97,98	1.13	5 (5%)
43	3PE	W	202	-	39,39,50	0.98	4 (10%)	42,44,55	1.14	2 (4%)
44	PC1	2	603	-	29,29,53	1.27	4 (13%)	35,37,61	1.14	2 (5%)
43	3PE	5	703	-	31,31,50	1.08	4 (12%)	34,36,55	1.17	2 (5%)
49	FMN	B	602	-	33,33,33	0.67	0	48,50,50	0.70	1 (2%)
43	3PE	5	705	-	41,41,50	0.95	4 (9%)	44,46,55	1.11	2 (4%)
44	PC1	K	302	-	33,33,53	1.20	4 (12%)	39,41,61	1.14	2 (5%)
43	3PE	J	201	-	31,31,50	1.11	4 (12%)	34,36,55	1.17	2 (5%)
44	PC1	4	603	-	49,49,53	0.99	4 (8%)	55,57,61	1.05	2 (3%)
43	3PE	g	102	-	34,34,50	1.07	4 (11%)	37,39,55	1.25	2 (5%)
50	NDP	E	402	-	51,52,52	0.56	0	71,80,80	0.62	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	ZMP	O	201	22	30,35,36	0.28	0	34,42,45	0.51	0
45	CDL	X	201	-	77,77,99	1.00	7 (9%)	83,89,111	1.12	5 (6%)
45	CDL	h	201	-	64,64,99	0.35	0	70,76,111	0.44	0
44	PC1	5	701	-	45,45,53	1.08	5 (11%)	51,53,61	1.12	2 (3%)
43	3PE	5	704	-	31,31,50	1.08	4 (12%)	34,36,55	1.25	2 (5%)
44	PC1	5	706	-	42,42,53	1.07	4 (9%)	48,50,61	1.05	2 (4%)
44	PC1	1	403	-	42,42,53	1.09	5 (11%)	48,50,61	1.18	2 (4%)
43	3PE	4	602	-	32,32,50	0.38	0	35,37,55	0.56	1 (2%)
43	3PE	5	707	-	40,40,50	0.97	4 (10%)	43,45,55	1.12	2 (4%)
43	3PE	i	101	-	38,38,50	0.99	4 (10%)	41,43,55	1.14	2 (4%)
43	3PE	n	201	-	38,38,50	1.00	4 (10%)	41,43,55	1.13	2 (4%)
45	CDL	4	601	-	82,82,99	0.29	0	88,94,111	0.32	0
44	PC1	3	201	-	48,48,53	0.31	0	54,56,61	0.30	0
48	SF4	I	302	17	0,12,12	-	-	-	-	-
43	3PE	W	201	-	33,33,50	0.95	2 (6%)	34,37,55	1.04	1 (2%)
43	3PE	1	401	-	49,49,50	0.87	4 (8%)	52,54,55	1.14	2 (3%)
43	3PE	8	101	-	35,35,50	1.03	4 (11%)	38,40,55	1.16	2 (5%)
43	3PE	E	401	-	26,26,50	1.18	4 (15%)	29,31,55	1.33	2 (6%)
43	3PE	4	604	-	30,30,50	1.11	4 (13%)	33,35,55	1.15	2 (6%)
43	3PE	5	702	-	39,39,50	0.33	0	42,44,55	0.39	0
48	SF4	B	601	10	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	SF4	A	803	9	-	-	0/6/5/5
47	FES	A	801	9	-	-	0/1/1/1
45	CDL	g	101	-	-	21/67/67/110	-
47	FES	H	401	16	-	-	0/1/1/1
48	SF4	I	301	17	-	-	0/6/5/5
46	LMN	J	202	-	-	27/44/104/130	0/3/3/4
48	SF4	A	802	9	-	-	0/6/5/5
46	LMN	2	602	-	-	16/44/104/130	0/3/3/4
48	SF4	K	301	19	-	-	0/6/5/5
43	3PE	1	402	-	-	9/29/29/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	ZMP	Q	201	22	-	7/40/42/43	-
45	CDL	2	601	-	-	23/95/95/110	-
44	PC1	S	201	-	-	20/54/54/57	-
46	LMN	j	101	-	-	20/49/129/130	0/4/4/4
43	3PE	W	202	-	-	16/43/43/54	-
44	PC1	2	603	-	-	17/33/33/57	-
43	3PE	5	703	-	-	15/35/35/54	-
49	FMN	B	602	-	-	8/18/18/18	0/3/3/3
43	3PE	5	705	-	-	17/45/45/54	-
44	PC1	K	302	-	-	22/37/37/57	-
43	3PE	J	201	-	-	18/35/35/54	-
44	PC1	4	603	-	-	32/53/53/57	-
43	3PE	g	102	-	-	20/38/38/54	-
50	NDP	E	402	-	-	1/34/77/77	0/5/5/5
52	ZMP	O	201	22	-	18/40/42/43	-
45	CDL	X	201	-	-	34/88/88/110	-
45	CDL	h	201	-	-	24/75/75/110	-
44	PC1	5	701	-	-	25/49/49/57	-
43	3PE	5	704	-	-	12/35/35/54	-
44	PC1	5	706	-	-	15/46/46/57	-
44	PC1	1	403	-	-	20/46/46/57	-
43	3PE	4	602	-	-	12/36/36/54	-
43	3PE	5	707	-	-	15/44/44/54	-
43	3PE	i	101	-	-	11/42/42/54	-
43	3PE	n	201	-	-	13/42/42/54	-
45	CDL	4	601	-	-	28/93/93/110	-
44	PC1	3	201	-	-	15/52/52/57	-
48	SF4	I	302	17	-	-	0/6/5/5
43	3PE	W	201	-	-	12/36/36/54	-
43	3PE	1	401	-	-	28/53/53/54	-
43	3PE	8	101	-	-	17/39/39/54	-
43	3PE	E	401	-	-	15/30/30/54	-
43	3PE	4	604	-	-	12/34/34/54	-
43	3PE	5	702	-	-	16/43/43/54	-
48	SF4	B	601	10	-	-	0/6/5/5

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	J	202	LMN	O5-C1	4.70	1.53	1.41
46	j	101	LMN	O5-C1	4.55	1.53	1.41
46	J	202	LMN	CBS-CCM	4.29	1.63	1.53
46	j	101	LMN	CBS-CCM	4.17	1.62	1.53
46	j	101	LMN	CBT-CCM	3.92	1.62	1.53
46	J	202	LMN	CBT-CCM	3.82	1.62	1.53
46	j	101	LMN	CBR-CCM	3.76	1.61	1.54
46	j	101	LMN	O1-C1	-3.74	1.34	1.40
46	J	202	LMN	CBR-CCM	3.72	1.60	1.54
46	J	202	LMN	O1-C1	-3.60	1.34	1.40
46	J	202	LMN	O4-C4	3.32	1.51	1.43
45	g	101	CDL	OB6-CB4	-3.15	1.39	1.46
43	g	102	3PE	O21-C2	-2.99	1.39	1.46
45	X	201	CDL	OA6-CA4	-2.95	1.39	1.46
46	j	101	LMN	O4-C4	2.92	1.51	1.43
44	5	701	PC1	O21-C2	-2.89	1.39	1.46
46	j	101	LMN	OBZ-CCS	2.88	1.49	1.41
46	j	101	LMN	OBY-CCR	2.87	1.49	1.41
43	E	401	3PE	O21-C2	-2.87	1.39	1.46
46	J	202	LMN	OBZ-CCS	2.79	1.49	1.41
44	5	706	PC1	O21-C2	-2.79	1.40	1.46
43	5	705	3PE	O21-C2	-2.72	1.40	1.46
43	W	202	3PE	O21-C2	-2.71	1.40	1.46
43	4	604	3PE	O21-C2	-2.71	1.40	1.46
44	2	603	PC1	O21-C2	-2.70	1.40	1.46
43	W	201	3PE	O21-C2	-2.68	1.40	1.46
44	S	201	PC1	O21-C2	-2.67	1.40	1.46
43	8	101	3PE	O21-C2	-2.66	1.40	1.46
43	i	101	3PE	O21-C2	-2.65	1.40	1.46
43	n	201	3PE	O21-C2	-2.65	1.40	1.46
43	5	707	3PE	O21-C2	-2.65	1.40	1.46
43	1	401	3PE	O21-C2	-2.63	1.40	1.46
44	K	302	PC1	O21-C2	-2.62	1.40	1.46
43	g	102	3PE	O31-C3	-2.61	1.39	1.45
44	1	403	PC1	O21-C2	-2.59	1.40	1.46
43	5	704	3PE	O21-C2	-2.58	1.40	1.46
43	J	201	3PE	O21-C2	-2.58	1.40	1.46
43	5	703	3PE	O21-C2	-2.56	1.40	1.46
44	4	603	PC1	O21-C2	-2.53	1.40	1.46
44	K	302	PC1	O31-C31	2.52	1.40	1.33
46	J	202	LMN	CBQ-CCM	2.50	1.58	1.54
44	5	701	PC1	O31-C3	-2.49	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	J	201	3PE	O31-C31	2.46	1.40	1.33
45	g	101	CDL	OA6-CA4	-2.45	1.40	1.46
43	n	201	3PE	O31-C31	2.44	1.40	1.33
44	S	201	PC1	O31-C31	2.43	1.40	1.33
43	5	703	3PE	O31-C31	2.42	1.40	1.33
44	4	603	PC1	O21-C21	2.41	1.41	1.34
43	4	604	3PE	O31-C31	2.41	1.40	1.33
43	5	707	3PE	O31-C31	2.40	1.40	1.33
44	2	603	PC1	O31-C31	2.40	1.40	1.33
43	i	101	3PE	O31-C31	2.40	1.40	1.33
44	4	603	PC1	O31-C3	-2.39	1.39	1.45
43	8	101	3PE	O31-C31	2.37	1.40	1.33
45	X	201	CDL	OB8-CB7	2.37	1.40	1.33
45	X	201	CDL	OB6-CB4	-2.36	1.41	1.46
45	g	101	CDL	OA6-CA5	2.35	1.40	1.34
43	5	705	3PE	O31-C31	2.35	1.40	1.33
44	5	706	PC1	O31-C31	2.35	1.40	1.33
46	J	202	LMN	C4-C3	-2.33	1.46	1.52
44	1	403	PC1	O31-C3	-2.33	1.40	1.45
46	j	101	LMN	OBX-CCF	2.32	1.50	1.44
44	5	701	PC1	C12-N	-2.32	1.44	1.51
45	g	101	CDL	OB8-CB7	2.32	1.40	1.33
46	J	202	LMN	OBX-CCF	2.31	1.50	1.44
43	5	704	3PE	O31-C3	-2.30	1.40	1.45
43	W	202	3PE	O31-C31	2.29	1.40	1.33
45	X	201	CDL	OA8-CA7	2.29	1.40	1.33
43	E	401	3PE	O31-C31	2.29	1.40	1.33
43	1	401	3PE	O31-C31	2.28	1.40	1.33
43	5	704	3PE	O21-C21	2.27	1.40	1.34
45	X	201	CDL	OA8-CA6	-2.25	1.40	1.45
45	g	101	CDL	OB8-CB6	-2.25	1.40	1.45
43	J	201	3PE	O21-C21	2.24	1.40	1.34
46	j	101	LMN	CBQ-CCM	2.24	1.58	1.54
44	K	302	PC1	O31-C3	-2.24	1.40	1.45
44	5	701	PC1	O31-C31	2.23	1.39	1.33
45	g	101	CDL	OA8-CA7	2.23	1.39	1.33
44	S	201	PC1	O31-C3	-2.23	1.40	1.45
45	g	101	CDL	OA8-CA6	-2.22	1.40	1.45
44	4	603	PC1	O31-C31	2.21	1.39	1.33
44	1	403	PC1	O21-C21	2.21	1.40	1.34
44	5	706	PC1	O21-C21	2.20	1.40	1.34
44	K	302	PC1	O21-C21	2.20	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	W	201	3PE	O21-C21	2.19	1.40	1.34
44	S	201	PC1	O21-C21	2.19	1.40	1.34
45	X	201	CDL	OB8-CB6	-2.19	1.40	1.45
43	5	705	3PE	O31-C3	-2.18	1.40	1.45
43	i	101	3PE	O21-C21	2.17	1.40	1.34
43	n	201	3PE	O21-C21	2.17	1.40	1.34
43	5	707	3PE	O31-C3	-2.17	1.40	1.45
46	J	202	LMN	O5-C5	2.17	1.49	1.44
46	J	202	LMN	OCB-CCQ	2.17	1.49	1.43
43	n	201	3PE	O31-C3	-2.17	1.40	1.45
43	8	101	3PE	O21-C21	2.16	1.40	1.34
44	5	706	PC1	O31-C3	-2.16	1.40	1.45
43	W	202	3PE	O31-C3	-2.16	1.40	1.45
44	2	603	PC1	O31-C3	-2.16	1.40	1.45
43	8	101	3PE	O31-C3	-2.16	1.40	1.45
43	4	604	3PE	O31-C3	-2.15	1.40	1.45
46	j	101	LMN	OBX-CCJ	2.15	1.47	1.41
43	5	707	3PE	O21-C21	2.15	1.40	1.34
43	5	703	3PE	O31-C3	-2.15	1.40	1.45
46	J	202	LMN	OBX-CCJ	2.15	1.47	1.41
43	1	401	3PE	O31-C3	-2.14	1.40	1.45
43	J	201	3PE	O31-C3	-2.14	1.40	1.45
44	5	701	PC1	O21-C21	2.14	1.40	1.34
43	5	704	3PE	O31-C31	2.13	1.39	1.33
43	i	101	3PE	O31-C3	-2.13	1.40	1.45
44	2	603	PC1	O21-C21	2.12	1.40	1.34
46	j	101	LMN	CBQ-CBK	2.12	1.59	1.52
43	5	703	3PE	O21-C21	2.11	1.40	1.34
43	4	604	3PE	O21-C21	2.11	1.40	1.34
44	1	403	PC1	O31-C31	2.09	1.39	1.33
46	j	101	LMN	O5-C5	2.09	1.49	1.44
46	J	202	LMN	CBQ-CBK	2.08	1.59	1.52
43	W	202	3PE	O21-C21	2.08	1.40	1.34
43	E	401	3PE	O31-C3	-2.06	1.40	1.45
44	1	403	PC1	C12-N	-2.06	1.45	1.51
43	5	705	3PE	O21-C21	2.05	1.40	1.34
43	E	401	3PE	O21-C21	2.05	1.40	1.34
45	X	201	CDL	OB6-CB5	2.04	1.40	1.34
43	g	102	3PE	O21-C21	2.02	1.40	1.34
43	g	102	3PE	O31-C31	2.01	1.39	1.33
43	1	401	3PE	O21-C21	2.01	1.39	1.34

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	g	101	CDL	OB6-CB5-C51	4.60	121.43	111.48
43	E	401	3PE	O21-C21-C22	4.52	121.25	111.48
43	5	704	3PE	O21-C21-C22	4.32	120.82	111.48
43	1	401	3PE	O21-C21-C22	4.27	120.71	111.48
44	4	603	PC1	O21-C21-C22	4.23	120.64	111.48
43	i	101	3PE	O21-C21-C22	4.14	120.45	111.48
43	g	102	3PE	O21-C21-C22	4.14	120.44	111.48
44	K	302	PC1	O21-C21-C22	4.12	120.40	111.48
43	J	201	3PE	O21-C21-C22	4.12	120.40	111.48
44	5	701	PC1	O21-C21-C22	4.12	120.39	111.48
44	1	403	PC1	O21-C21-C22	4.09	120.33	111.48
43	5	703	3PE	O21-C21-C22	4.08	120.31	111.48
43	n	201	3PE	O21-C21-C22	4.07	120.28	111.48
43	8	101	3PE	O21-C21-C22	4.05	120.24	111.48
45	X	201	CDL	OB6-CB5-C51	4.03	120.20	111.48
45	X	201	CDL	OA6-CA5-C11	4.03	120.19	111.48
44	S	201	PC1	O21-C21-C22	4.01	120.16	111.48
44	2	603	PC1	O21-C21-C22	3.96	120.04	111.48
43	5	707	3PE	O21-C21-C22	3.95	120.04	111.48
46	j	101	LMN	CCS-OCB-CCQ	-3.95	108.61	117.98
43	W	201	3PE	O21-C21-C22	3.87	119.85	111.48
43	W	202	3PE	O21-C21-C22	3.87	119.85	111.48
43	5	705	3PE	O21-C21-C22	3.87	119.85	111.48
43	4	604	3PE	O21-C21-C22	3.72	119.53	111.48
44	5	706	PC1	O21-C21-C22	3.54	119.13	111.48
46	j	101	LMN	CCR-O4-C4	-3.46	109.78	117.98
43	E	401	3PE	O31-C31-C32	3.09	121.25	111.83
44	K	302	PC1	O31-C31-C32	3.07	121.18	111.83
45	g	101	CDL	OA6-CA5-C11	3.06	118.09	111.48
50	E	402	NDP	P2B-O2B-C2B	-2.97	115.50	123.43
43	1	401	3PE	O31-C31-C32	2.96	120.85	111.83
45	g	101	CDL	OB8-CB7-C71	2.90	119.95	111.15
44	4	603	PC1	O31-C31-C32	2.85	120.52	111.83
45	g	101	CDL	OA8-CA7-C31	2.85	119.79	111.15
45	X	201	CDL	OA8-CA7-C31	2.85	120.51	111.83
43	5	704	3PE	O31-C31-C32	2.84	120.51	111.83
43	W	202	3PE	O31-C31-C32	2.83	120.47	111.83
43	n	201	3PE	O31-C31-C32	2.80	120.38	111.83
44	1	403	PC1	O31-C31-C32	2.80	120.36	111.83
43	J	201	3PE	O31-C31-C32	2.77	120.27	111.83
43	g	102	3PE	O31-C31-C32	2.75	120.21	111.83
43	4	604	3PE	O31-C31-C32	2.74	120.17	111.83
43	8	101	3PE	O31-C31-C32	2.71	120.11	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	5	706	PC1	O31-C31-C32	2.71	120.09	111.83
45	X	201	CDL	OB8-CB7-C71	2.69	120.05	111.83
44	5	701	PC1	O31-C31-C32	2.68	120.01	111.83
43	i	101	3PE	O31-C31-C32	2.67	119.97	111.83
44	S	201	PC1	O31-C31-C32	2.66	119.95	111.83
43	5	707	3PE	O31-C31-C32	2.66	119.93	111.83
46	j	101	LMN	C2-C3-C4	2.64	115.67	109.68
44	2	603	PC1	O31-C31-C32	2.63	119.87	111.83
43	5	703	3PE	O31-C31-C32	2.61	119.79	111.83
43	5	705	3PE	O31-C31-C32	2.61	119.78	111.83
46	J	202	LMN	CCS-OCB-CCQ	-2.53	111.99	117.98
46	j	101	LMN	CBK-CBQ-CCM	-2.39	109.93	117.19
46	j	101	LMN	CBL-CBR-CCM	-2.37	109.99	117.19
43	4	602	3PE	O12-P-O14	2.20	122.69	112.44
49	B	602	FMN	C4-N3-C2	-2.13	121.86	125.64
46	J	202	LMN	CBK-CBQ-CCM	-2.09	110.85	117.19
45	g	101	CDL	C52-C51-CB5	-2.05	106.18	113.69
45	X	201	CDL	CA4-OA6-CA5	-2.01	112.98	117.80

There are no chirality outliers.

All (651) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1	401	3PE	C1-O11-P-O12
43	1	401	3PE	C1-O11-P-O13
43	1	401	3PE	C1-O11-P-O14
43	1	401	3PE	C12-C11-O13-P
43	1	402	3PE	C11-O13-P-O11
43	1	402	3PE	C11-O13-P-O12
43	1	402	3PE	C11-O13-P-O14
43	4	602	3PE	C1-O11-P-O13
43	4	602	3PE	O13-C11-C12-N
43	4	604	3PE	O21-C2-C3-O31
43	5	702	3PE	O13-C11-C12-N
43	5	702	3PE	O22-C21-O21-C2
43	5	702	3PE	C22-C21-O21-C2
43	5	703	3PE	C11-O13-P-O11
43	5	703	3PE	O13-C11-C12-N
43	5	703	3PE	C32-C31-O31-C3
43	5	704	3PE	C1-O11-P-O12
43	5	704	3PE	C1-O11-P-O13
43	5	704	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
43	5	704	3PE	C11-O13-P-O12
43	5	704	3PE	C11-O13-P-O14
43	5	705	3PE	C1-O11-P-O12
43	5	705	3PE	C1-O11-P-O13
43	5	705	3PE	C1-O11-P-O14
43	5	705	3PE	C11-O13-P-O12
43	5	707	3PE	C11-O13-P-O11
43	5	707	3PE	C11-O13-P-O12
43	8	101	3PE	C1-O11-P-O12
43	8	101	3PE	C1-O11-P-O13
43	8	101	3PE	C1-O11-P-O14
43	8	101	3PE	C11-O13-P-O11
43	8	101	3PE	C11-O13-P-O14
43	8	101	3PE	O22-C21-O21-C2
43	8	101	3PE	C22-C21-O21-C2
43	E	401	3PE	C1-O11-P-O12
43	E	401	3PE	C1-O11-P-O13
43	E	401	3PE	C1-O11-P-O14
43	E	401	3PE	C11-O13-P-O11
43	E	401	3PE	O13-C11-C12-N
43	E	401	3PE	O22-C21-O21-C2
43	E	401	3PE	C22-C21-O21-C2
43	J	201	3PE	C11-O13-P-O11
43	J	201	3PE	C11-O13-P-O12
43	J	201	3PE	O13-C11-C12-N
43	W	201	3PE	O32-C31-O31-C3
43	W	202	3PE	C11-O13-P-O11
43	W	202	3PE	C11-O13-P-O12
43	g	102	3PE	C1-O11-P-O13
43	g	102	3PE	C1-O11-P-O14
43	g	102	3PE	O22-C21-O21-C2
43	i	101	3PE	C11-O13-P-O11
43	i	101	3PE	C11-O13-P-O14
43	i	101	3PE	C12-C11-O13-P
43	i	101	3PE	O21-C2-C3-O31
43	i	101	3PE	O22-C21-O21-C2
43	i	101	3PE	C22-C21-O21-C2
43	n	201	3PE	O22-C21-O21-C2
44	1	403	PC1	C11-O13-P-O12
44	1	403	PC1	C11-O13-P-O14
44	1	403	PC1	C11-O13-P-O11
44	1	403	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
44	1	403	PC1	C1-O11-P-O14
44	1	403	PC1	C1-O11-P-O13
44	2	603	PC1	C11-O13-P-O12
44	2	603	PC1	C11-O13-P-O11
44	2	603	PC1	C1-O11-P-O14
44	2	603	PC1	O21-C2-C3-O31
44	2	603	PC1	C22-C21-O21-C2
44	3	201	PC1	O21-C2-C3-O31
44	4	603	PC1	C11-O13-P-O12
44	4	603	PC1	C11-O13-P-O14
44	4	603	PC1	C11-O13-P-O11
44	4	603	PC1	O13-C11-C12-N
44	4	603	PC1	O22-C21-O21-C2
44	5	701	PC1	C11-O13-P-O12
44	5	701	PC1	C11-O13-P-O14
44	5	701	PC1	C11-O13-P-O11
44	5	701	PC1	C12-C11-O13-P
44	5	701	PC1	C22-C21-O21-C2
44	5	706	PC1	O13-C11-C12-N
44	K	302	PC1	C1-O11-P-O12
44	K	302	PC1	C1-O11-P-O13
44	K	302	PC1	O13-C11-C12-N
44	K	302	PC1	C22-C21-O21-C2
44	S	201	PC1	C1-O11-P-O12
44	S	201	PC1	C1-O11-P-O14
44	S	201	PC1	C1-O11-P-O13
45	2	601	CDL	CA2-OA2-PA1-OA3
45	2	601	CDL	CA2-OA2-PA1-OA5
45	4	601	CDL	CA2-OA2-PA1-OA3
45	4	601	CDL	CA2-OA2-PA1-OA5
45	X	201	CDL	CA2-OA2-PA1-OA3
45	X	201	CDL	CA2-OA2-PA1-OA4
45	X	201	CDL	CA2-OA2-PA1-OA5
45	X	201	CDL	OA5-CA3-CA4-OA6
45	X	201	CDL	CB3-OB5-PB2-OB2
45	X	201	CDL	CB3-OB5-PB2-OB3
45	g	101	CDL	O1-C1-CB2-OB2
45	g	101	CDL	CB2-OB2-PB2-OB3
45	g	101	CDL	OB7-CB5-OB6-CB4
45	g	101	CDL	C51-CB5-OB6-CB4
45	h	201	CDL	CA2-OA2-PA1-OA3
45	h	201	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
45	h	201	CDL	CB2-OB2-PB2-OB3
45	h	201	CDL	CB3-OB5-PB2-OB2
46	2	602	LMN	OBX-CCJ-OBV-CBT
46	2	602	LMN	CCL-CCJ-OBV-CBT
46	J	202	LMN	CBK-CBQ-CCM-CBR
46	J	202	LMN	CBK-CBQ-CCM-CBS
46	J	202	LMN	CBK-CBQ-CCM-CBT
46	J	202	LMN	O1-CBS-CCM-CBQ
46	J	202	LMN	O1-CBS-CCM-CBR
46	J	202	LMN	OBV-CBT-CCM-CBQ
46	J	202	LMN	OBV-CBT-CCM-CBR
46	J	202	LMN	OBX-CCJ-OBV-CBT
46	j	101	LMN	CBK-CBQ-CCM-CBR
46	j	101	LMN	CBK-CBQ-CCM-CBS
46	j	101	LMN	CBK-CBQ-CCM-CBT
46	j	101	LMN	O1-CBS-CCM-CBQ
46	j	101	LMN	O1-CBS-CCM-CBR
52	O	201	ZMP	O4-C17-C18-C21
52	O	201	ZMP	O4-C17-C18-C19
52	O	201	ZMP	O4-C17-C18-C20
52	O	201	ZMP	C17-C16-N2-C15
52	O	201	ZMP	C14-C13-N1-C12
52	O	201	ZMP	O2-C13-N1-C12
52	O	201	ZMP	S1-C11-C12-N1
43	5	703	3PE	O32-C31-O31-C3
46	j	101	LMN	O1-CBS-CCM-CBT
46	2	602	LMN	OBZ-CCS-OCB-CCQ
46	j	101	LMN	OBY-CCR-O4-C4
43	n	201	3PE	O32-C31-O31-C3
44	4	603	PC1	O32-C31-O31-C3
46	2	602	LMN	O5-C5-C6-O6
44	2	603	PC1	O22-C21-O21-C2
44	5	701	PC1	O22-C21-O21-C2
45	h	201	CDL	OA7-CA5-OA6-CA4
43	J	201	3PE	C32-C31-O31-C3
44	5	701	PC1	C32-C31-O31-C3
43	g	102	3PE	C22-C21-O21-C2
43	n	201	3PE	C22-C21-O21-C2
44	4	603	PC1	C22-C21-O21-C2
46	J	202	LMN	CCH-CCQ-OCB-CCS
43	n	201	3PE	C32-C31-O31-C3
44	4	603	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
43	8	101	3PE	O32-C31-O31-C3
43	J	201	3PE	O32-C31-O31-C3
44	K	302	PC1	O22-C21-O21-C2
45	X	201	CDL	OA7-CA5-OA6-CA4
46	J	202	LMN	OBV-CBT-CCM-CBS
45	h	201	CDL	O1-C1-CB2-OB2
46	j	101	LMN	OAI-CBM-CCC-OBY
44	5	701	PC1	O32-C31-O31-C3
43	1	402	3PE	C22-C21-O21-C2
43	J	201	3PE	C22-C21-O21-C2
45	X	201	CDL	C11-CA5-OA6-CA4
45	X	201	CDL	C51-CB5-OB6-CB4
46	J	202	LMN	O1-CBS-CCM-CBT
46	j	101	LMN	O5-C5-C6-O6
46	2	602	LMN	C4-C5-C6-O6
43	8	101	3PE	C32-C31-O31-C3
45	4	601	CDL	C31-CA7-OA8-CA6
43	J	201	3PE	O22-C21-O21-C2
45	X	201	CDL	OB7-CB5-OB6-CB4
45	g	101	CDL	CA2-C1-CB2-OB2
46	J	202	LMN	CBE-CBG-CBI-CBK
46	j	101	LMN	C4-C5-C6-O6
45	4	601	CDL	OA9-CA7-OA8-CA6
45	h	201	CDL	C51-CB5-OB6-CB4
46	J	202	LMN	CBI-CBK-CBQ-CCM
43	4	604	3PE	C21-C22-C23-C24
43	1	402	3PE	O22-C21-O21-C2
43	5	702	3PE	C21-C22-C23-C24
43	5	707	3PE	C31-C32-C33-C34
43	J	201	3PE	C31-C32-C33-C34
43	W	202	3PE	C31-C32-C33-C34
44	4	603	PC1	C31-C32-C33-C34
43	5	705	3PE	C21-C22-C23-C24
43	5	707	3PE	C21-C22-C23-C24
45	4	601	CDL	CA5-C11-C12-C13
43	5	702	3PE	C22-C23-C24-C25
46	J	202	LMN	O5-C1-O1-CBS
45	h	201	CDL	CA7-C31-C32-C33
46	j	101	LMN	OAI-CBM-CCC-CCN
45	X	201	CDL	CA7-C31-C32-C33
43	g	102	3PE	C32-C31-O31-C3
43	W	202	3PE	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
45	h	201	CDL	OB7-CB5-OB6-CB4
44	1	403	PC1	C32-C31-O31-C3
52	O	201	ZMP	C1-C22-C23-C24
44	S	201	PC1	C11-C12-N-C15
44	K	302	PC1	C31-C32-C33-C34
46	j	101	LMN	CBB-CBD-CBF-CBH
43	4	602	3PE	C22-C21-O21-C2
43	4	602	3PE	O22-C21-O21-C2
46	J	202	LMN	CBJ-CBL-CBR-CCM
43	5	703	3PE	C31-C32-C33-C34
45	4	601	CDL	C1-CA2-OA2-PA1
43	1	401	3PE	C32-C31-O31-C3
43	g	102	3PE	O32-C31-O31-C3
43	5	704	3PE	C24-C25-C26-C27
44	4	603	PC1	C29-C2A-C2B-C2C
43	E	401	3PE	C31-C32-C33-C34
44	K	302	PC1	C21-C22-C23-C24
43	5	704	3PE	C23-C24-C25-C26
44	4	603	PC1	C23-C24-C25-C26
44	S	201	PC1	C2C-C2D-C2E-C2F
44	1	403	PC1	C3A-C3B-C3C-C3D
46	J	202	LMN	CBA-CBC-CBE-CBG
46	j	101	LMN	CBA-CBC-CBE-CBG
45	2	601	CDL	C77-C78-C79-C80
45	X	201	CDL	C14-C15-C16-C17
46	j	101	LMN	CBH-CBJ-CBL-CBR
45	4	601	CDL	C11-CA5-OA6-CA4
43	5	703	3PE	C21-C22-C23-C24
44	5	701	PC1	C31-C32-C33-C34
44	1	403	PC1	C35-C36-C37-C38
44	5	706	PC1	C24-C25-C26-C27
46	J	202	LMN	CBH-CBJ-CBL-CBR
52	O	201	ZMP	O3-C16-N2-C15
44	1	403	PC1	O32-C31-O31-C3
44	K	302	PC1	C22-C23-C24-C25
45	h	201	CDL	CA2-C1-CB2-OB2
43	J	201	3PE	C36-C37-C38-C39
43	W	201	3PE	C28-C29-C2A-C2B
44	S	201	PC1	C11-C12-N-C13
44	S	201	PC1	C11-C12-N-C14
43	4	604	3PE	C22-C21-O21-C2
43	1	401	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
43	g	102	3PE	C24-C25-C26-C27
44	1	403	PC1	C32-C33-C34-C35
44	4	603	PC1	C2A-C2B-C2C-C2D
43	1	401	3PE	O32-C31-O31-C3
45	g	101	CDL	C51-C52-C53-C54
45	4	601	CDL	OA7-CA5-OA6-CA4
43	n	201	3PE	C35-C36-C37-C38
45	X	201	CDL	C36-C37-C38-C39
45	g	101	CDL	C55-C56-C57-C58
43	5	704	3PE	C22-C23-C24-C25
45	X	201	CDL	C53-C54-C55-C56
44	S	201	PC1	C23-C24-C25-C26
45	X	201	CDL	C15-C16-C17-C18
43	1	401	3PE	C31-C32-C33-C34
44	5	701	PC1	C2D-C2E-C2F-C2G
44	K	302	PC1	C32-C31-O31-C3
43	5	704	3PE	C22-C21-O21-C2
43	5	707	3PE	C22-C21-O21-C2
43	5	707	3PE	O22-C21-O21-C2
43	5	702	3PE	C3A-C3B-C3C-C3D
44	5	706	PC1	C31-C32-C33-C34
43	4	602	3PE	C33-C34-C35-C36
46	2	602	LMN	CBK-CBQ-CCM-CBT
46	J	202	LMN	CBL-CBR-CCM-CBS
45	g	101	CDL	C16-C17-C18-C19
43	4	604	3PE	O22-C21-O21-C2
44	5	706	PC1	O11-C1-C2-O21
45	4	601	CDL	C35-C36-C37-C38
43	5	702	3PE	C33-C34-C35-C36
43	E	401	3PE	C34-C35-C36-C37
44	5	706	PC1	C33-C34-C35-C36
43	1	402	3PE	C23-C24-C25-C26
44	4	603	PC1	C22-C23-C24-C25
46	2	602	LMN	CBC-CBE-CBG-CBI
43	J	201	3PE	C33-C34-C35-C36
44	4	603	PC1	C35-C36-C37-C38
46	J	202	LMN	CBC-CBE-CBG-CBI
43	i	101	3PE	C28-C29-C2A-C2B
44	5	706	PC1	C32-C33-C34-C35
43	W	202	3PE	C22-C23-C24-C25
45	4	601	CDL	C77-C78-C79-C80
43	5	707	3PE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
44	5	701	PC1	C2A-C2B-C2C-C2D
52	O	201	ZMP	O3-C16-C17-O4
44	3	201	PC1	C37-C38-C39-C3A
44	5	701	PC1	C2C-C2D-C2E-C2F
43	1	402	3PE	O11-C1-C2-C3
43	4	602	3PE	O11-C1-C2-C3
44	1	403	PC1	O11-C1-C2-C3
45	X	201	CDL	OA5-CA3-CA4-CA6
43	5	704	3PE	O22-C21-O21-C2
45	g	101	CDL	CB5-C51-C52-C53
46	J	202	LMN	CAW-CAY-CBA-CBC
44	3	201	PC1	C36-C37-C38-C39
43	4	602	3PE	C32-C31-O31-C3
52	O	201	ZMP	C22-C1-C2-C3
52	O	201	ZMP	C3-C4-C5-C6
43	1	401	3PE	C1-C2-C3-O31
43	E	401	3PE	C1-C2-C3-O31
43	i	101	3PE	C1-C2-C3-O31
44	2	603	PC1	C1-C2-C3-O31
44	3	201	PC1	C1-C2-C3-O31
45	X	201	CDL	CA3-CA4-CA6-OA8
44	S	201	PC1	C32-C33-C34-C35
44	5	701	PC1	C23-C24-C25-C26
45	4	601	CDL	C72-C73-C74-C75
45	X	201	CDL	C35-C36-C37-C38
44	K	302	PC1	O32-C31-O31-C3
43	5	707	3PE	C36-C37-C38-C39
44	5	706	PC1	C34-C35-C36-C37
44	S	201	PC1	C32-C31-O31-C3
44	5	701	PC1	C26-C27-C28-C29
43	1	401	3PE	O11-C1-C2-O21
50	E	402	NDP	O4D-C1D-N1N-C6N
44	2	603	PC1	C25-C26-C27-C28
52	Q	201	ZMP	O3-C16-N2-C15
45	2	601	CDL	C18-C19-C20-C21
44	K	302	PC1	O21-C2-C3-O31
44	4	603	PC1	C3C-C3D-C3E-C3F
43	5	702	3PE	C32-C31-O31-C3
43	W	202	3PE	C3A-C3B-C3C-C3D
46	J	202	LMN	CBL-CBR-CCM-CBQ
52	Q	201	ZMP	C17-C16-N2-C15
44	3	201	PC1	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
46	J	202	LMN	CAA-CAW-CAY-CBA
45	2	601	CDL	C31-CA7-OA8-CA6
43	W	201	3PE	C26-C27-C28-C29
45	g	101	CDL	C53-C54-C55-C56
43	8	101	3PE	C23-C24-C25-C26
45	X	201	CDL	C13-C14-C15-C16
45	2	601	CDL	C24-C25-C26-C27
43	1	401	3PE	C24-C25-C26-C27
43	1	401	3PE	C2A-C2B-C2C-C2D
43	5	705	3PE	C34-C35-C36-C37
45	h	201	CDL	C11-C12-C13-C14
43	8	101	3PE	O11-C1-C2-C3
45	2	601	CDL	OA5-CA3-CA4-CA6
45	4	601	CDL	OB5-CB3-CB4-CB6
45	4	601	CDL	C73-C74-C75-C76
43	J	201	3PE	C37-C38-C39-C3A
43	5	703	3PE	C23-C24-C25-C26
44	S	201	PC1	C3E-C3F-C3G-C3H
43	5	703	3PE	C34-C35-C36-C37
46	j	101	LMN	CBG-CBI-CBK-CBQ
43	W	201	3PE	C2A-C2B-C2C-C2D
43	4	602	3PE	O32-C31-O31-C3
44	5	701	PC1	C28-C29-C2A-C2B
44	3	201	PC1	C23-C24-C25-C26
43	5	702	3PE	C1-C2-C3-O31
52	O	201	ZMP	N2-C16-C17-O4
43	1	401	3PE	C2E-C2F-C2G-C2H
43	W	202	3PE	C37-C38-C39-C3A
44	4	603	PC1	C27-C28-C29-C2A
45	h	201	CDL	CA5-C11-C12-C13
46	2	602	LMN	CBA-CBC-CBE-CBG
44	5	701	PC1	C21-C22-C23-C24
43	1	402	3PE	O11-C1-C2-O21
43	4	604	3PE	O11-C1-C2-O21
43	8	101	3PE	O11-C1-C2-O21
43	W	202	3PE	O11-C1-C2-O21
45	2	601	CDL	OA5-CA3-CA4-OA6
52	Q	201	ZMP	O1-C10-S1-C11
44	S	201	PC1	O32-C31-O31-C3
43	5	703	3PE	O21-C2-C3-O31
45	2	601	CDL	OA6-CA4-CA6-OA8
45	g	101	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
43	g	102	3PE	C34-C35-C36-C37
43	n	201	3PE	C38-C39-C3A-C3B
44	5	701	PC1	C2F-C2G-C2H-C2I
44	5	706	PC1	C21-C22-C23-C24
43	g	102	3PE	C26-C27-C28-C29
43	W	202	3PE	C3B-C3C-C3D-C3E
45	X	201	CDL	C71-C72-C73-C74
46	J	202	LMN	CCL-CCJ-OBV-CBT
45	X	201	CDL	C22-C23-C24-C25
43	5	703	3PE	C32-C33-C34-C35
45	X	201	CDL	C54-C55-C56-C57
49	B	602	FMN	C2'-C3'-C4'-O4'
52	Q	201	ZMP	C9-C10-S1-C11
43	1	401	3PE	C29-C2A-C2B-C2C
43	g	102	3PE	C27-C28-C29-C2A
45	2	601	CDL	C52-C53-C54-C55
46	j	101	LMN	CAZ-CBB-CBD-CBF
44	2	603	PC1	O11-C1-C2-C3
44	3	201	PC1	O11-C1-C2-C3
44	4	603	PC1	O11-C1-C2-C3
44	5	706	PC1	O11-C1-C2-C3
44	1	403	PC1	C22-C23-C24-C25
44	4	603	PC1	C28-C29-C2A-C2B
44	5	706	PC1	C32-C31-O31-C3
43	1	401	3PE	C25-C26-C27-C28
43	5	702	3PE	O32-C31-O31-C3
46	J	202	LMN	CAX-CAZ-CBB-CBD
43	E	401	3PE	C21-C22-C23-C24
45	X	201	CDL	CB6-CB4-OB6-CB5
46	J	202	LMN	CBL-CBR-CCM-CBT
52	Q	201	ZMP	O2-C13-C14-C15
44	K	302	PC1	C33-C34-C35-C36
46	J	202	LMN	CCF-CCQ-OCB-CCS
45	2	601	CDL	OA9-CA7-OA8-CA6
43	4	602	3PE	O11-C1-C2-O21
43	J	201	3PE	O11-C1-C2-O21
43	i	101	3PE	O11-C1-C2-O21
44	4	603	PC1	O11-C1-C2-O21
43	g	102	3PE	C2A-C2B-C2C-C2D
43	4	604	3PE	C1-C2-C3-O31
44	K	302	PC1	C1-C2-C3-O31
45	2	601	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
52	Q	201	ZMP	N1-C13-C14-C15
43	4	602	3PE	C12-C11-O13-P
43	5	703	3PE	C12-C11-O13-P
43	W	202	3PE	C12-C11-O13-P
43	g	102	3PE	C12-C11-O13-P
44	2	603	PC1	C12-C11-O13-P
44	4	603	PC1	C12-C11-O13-P
44	S	201	PC1	C12-C11-O13-P
52	O	201	ZMP	C16-C17-C18-C19
45	X	201	CDL	C74-C75-C76-C77
43	5	702	3PE	O21-C2-C3-O31
43	E	401	3PE	O21-C2-C3-O31
43	W	201	3PE	O21-C2-C3-O31
45	h	201	CDL	OA9-CA7-OA8-CA6
44	5	701	PC1	C11-C12-N-C13
44	5	701	PC1	C25-C26-C27-C28
44	2	603	PC1	O13-C11-C12-N
44	5	706	PC1	C26-C27-C28-C29
43	8	101	3PE	C33-C34-C35-C36
44	5	706	PC1	O32-C31-O31-C3
43	E	401	3PE	C35-C36-C37-C38
45	4	601	CDL	C54-C55-C56-C57
44	5	701	PC1	C11-C12-N-C15
45	h	201	CDL	C31-CA7-OA8-CA6
43	n	201	3PE	C36-C37-C38-C39
44	2	603	PC1	C21-C22-C23-C24
43	1	401	3PE	C26-C27-C28-C29
44	3	201	PC1	C26-C27-C28-C29
43	1	401	3PE	O11-C1-C2-C3
43	4	604	3PE	O11-C1-C2-C3
43	W	202	3PE	O11-C1-C2-C3
43	i	101	3PE	O11-C1-C2-C3
44	K	302	PC1	O11-C1-C2-C3
49	B	602	FMN	N10-C1'-C2'-C3'
52	O	201	ZMP	C19-C18-C21-O5
43	1	401	3PE	C23-C24-C25-C26
44	4	603	PC1	C24-C25-C26-C27
45	g	101	CDL	C15-C16-C17-C18
44	S	201	PC1	C3B-C3C-C3D-C3E
44	4	603	PC1	C3B-C3C-C3D-C3E
43	i	101	3PE	C2-C1-O11-P
43	5	702	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
45	X	201	CDL	C37-C38-C39-C40
45	X	201	CDL	C52-C53-C54-C55
44	3	201	PC1	C32-C31-O31-C3
44	2	603	PC1	O11-C1-C2-O21
44	3	201	PC1	O11-C1-C2-O21
44	K	302	PC1	O11-C1-C2-O21
45	4	601	CDL	OA5-CA3-CA4-OA6
45	4	601	CDL	OB5-CB3-CB4-OB6
45	X	201	CDL	C72-C73-C74-C75
43	1	401	3PE	O21-C2-C3-O31
45	X	201	CDL	OA6-CA4-CA6-OA8
44	4	603	PC1	C26-C27-C28-C29
43	5	703	3PE	C1-C2-C3-O31
43	5	704	3PE	C1-C2-C3-O31
43	W	201	3PE	C1-C2-C3-O31
44	5	706	PC1	C1-C2-C3-O31
44	K	302	PC1	C32-C33-C34-C35
46	j	101	LMN	O5-C1-O1-CBS
43	W	201	3PE	C2E-C2F-C2G-C2H
43	5	702	3PE	C36-C37-C38-C39
43	5	705	3PE	C33-C34-C35-C36
43	4	602	3PE	C1-O11-P-O14
43	4	604	3PE	C1-O11-P-O12
43	4	604	3PE	C1-O11-P-O13
43	4	604	3PE	C1-O11-P-O14
43	5	703	3PE	C11-O13-P-O14
43	5	705	3PE	C11-O13-P-O11
43	5	705	3PE	C11-O13-P-O14
43	5	705	3PE	O13-C11-C12-N
43	5	707	3PE	O13-C11-C12-N
43	8	101	3PE	C11-O13-P-O12
43	E	401	3PE	C11-O13-P-O14
43	J	201	3PE	C1-O11-P-O13
43	J	201	3PE	C1-O11-P-O14
43	J	201	3PE	C11-O13-P-O14
43	W	202	3PE	C11-O13-P-O14
43	g	102	3PE	C11-O13-P-O14
43	n	201	3PE	C11-O13-P-O14
44	2	603	PC1	C11-O13-P-O14
44	3	201	PC1	C11-O13-P-O14
44	5	701	PC1	C11-C12-N-C14
44	K	302	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
44	S	201	PC1	C11-O13-P-O12
44	S	201	PC1	C11-O13-P-O14
44	S	201	PC1	C11-O13-P-O11
45	2	601	CDL	CA2-OA2-PA1-OA4
45	2	601	CDL	CA3-OA5-PA1-OA3
45	4	601	CDL	CA2-OA2-PA1-OA4
45	4	601	CDL	CA3-OA5-PA1-OA3
45	X	201	CDL	CB3-OB5-PB2-OB4
45	h	201	CDL	CA3-OA5-PA1-OA4
45	h	201	CDL	CB2-OB2-PB2-OB5
45	h	201	CDL	CB3-OB5-PB2-OB3
44	5	701	PC1	C33-C34-C35-C36
45	4	601	CDL	C74-C75-C76-C77
43	W	201	3PE	C2-C1-O11-P
44	4	603	PC1	C2-C1-O11-P
45	2	601	CDL	C1-CB2-OB2-PB2
45	2	601	CDL	CB4-CB3-OB5-PB2
45	4	601	CDL	CB4-CB3-OB5-PB2
49	B	602	FMN	C4'-C5'-O5'-P
43	5	704	3PE	O31-C31-C32-C33
44	K	302	PC1	C23-C24-C25-C26
44	2	603	PC1	C24-C25-C26-C27
44	1	403	PC1	C31-C32-C33-C34
45	g	101	CDL	CA3-CA4-OA6-CA5
45	h	201	CDL	CA6-CA4-OA6-CA5
43	4	604	3PE	O21-C21-C22-C23
44	S	201	PC1	O31-C31-C32-C33
44	4	603	PC1	C2B-C2C-C2D-C2E
46	j	101	LMN	CAW-CAY-CBA-CBC
45	4	601	CDL	OA5-CA3-CA4-CA6
45	X	201	CDL	C38-C39-C40-C41
44	1	403	PC1	O11-C1-C2-O21
43	n	201	3PE	C37-C38-C39-C3A
44	4	603	PC1	C37-C38-C39-C3A
44	5	701	PC1	O21-C21-C22-C23
43	5	702	3PE	C3B-C3C-C3D-C3E
46	2	602	LMN	CBK-CBQ-CCM-CBR
43	4	602	3PE	C24-C25-C26-C27
45	2	601	CDL	C14-C15-C16-C17
43	E	401	3PE	O31-C31-C32-C33
46	2	602	LMN	CBK-CBQ-CCM-CBS
45	4	601	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
45	h	201	CDL	C55-C56-C57-C58
44	5	701	PC1	C37-C38-C39-C3A
45	h	201	CDL	CA4-CA6-OA8-CA7
45	g	101	CDL	C71-CB7-OB8-CB6
45	g	101	CDL	OB9-CB7-OB8-CB6
44	4	603	PC1	C32-C33-C34-C35
44	1	403	PC1	C39-C3A-C3B-C3C
43	5	707	3PE	C3A-C3B-C3C-C3D
43	W	202	3PE	O21-C2-C3-O31
43	W	202	3PE	C24-C25-C26-C27
43	5	705	3PE	C25-C26-C27-C28
43	W	201	3PE	C2D-C2E-C2F-C2G
43	5	707	3PE	C38-C39-C3A-C3B
45	g	101	CDL	CA5-C11-C12-C13
43	5	707	3PE	C39-C3A-C3B-C3C
45	2	601	CDL	C72-C73-C74-C75
45	4	601	CDL	C71-C72-C73-C74
44	3	201	PC1	O32-C31-O31-C3
44	3	201	PC1	O22-C21-C22-C23
46	2	602	LMN	CBG-CBI-CBK-CBQ
43	1	401	3PE	C22-C23-C24-C25
43	W	201	3PE	C2F-C2G-C2H-C2I
43	4	604	3PE	O31-C31-C32-C33
45	4	601	CDL	CA3-CA4-OA6-CA5
45	h	201	CDL	CB6-CB4-OB6-CB5
49	B	602	FMN	C2'-C3'-C4'-C5'
43	5	702	3PE	C35-C36-C37-C38
43	1	401	3PE	C3A-C3B-C3C-C3D
45	h	201	CDL	OB5-CB3-CB4-OB6
43	1	401	3PE	C33-C34-C35-C36
43	J	201	3PE	O11-C1-C2-C3
43	5	707	3PE	C23-C24-C25-C26
49	B	602	FMN	O3'-C3'-C4'-C5'
43	5	705	3PE	C32-C33-C34-C35
45	2	601	CDL	O1-C1-CA2-OA2
43	1	402	3PE	C21-C22-C23-C24
43	5	707	3PE	C32-C33-C34-C35
43	5	707	3PE	C34-C35-C36-C37
44	1	403	PC1	C2-C1-O11-P
43	5	703	3PE	C35-C36-C37-C38
44	5	701	PC1	C34-C35-C36-C37
45	4	601	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
45	g	101	CDL	OB5-CB3-CB4-OB6
43	5	702	3PE	C37-C38-C39-C3A
43	1	401	3PE	C2B-C2C-C2D-C2E
52	O	201	ZMP	C2-C3-C4-C5
52	Q	201	ZMP	C13-C14-C15-N2
44	4	603	PC1	C3D-C3E-C3F-C3G
45	X	201	CDL	CB2-C1-CA2-OA2
44	5	706	PC1	O21-C2-C3-O31
43	J	201	3PE	C21-C22-C23-C24
44	4	603	PC1	C34-C35-C36-C37
44	K	302	PC1	C35-C36-C37-C38
49	B	602	FMN	O2'-C2'-C3'-C4'
44	5	706	PC1	O31-C31-C32-C33
49	B	602	FMN	O3'-C3'-C4'-O4'
43	g	102	3PE	C28-C29-C2A-C2B
45	4	601	CDL	CA6-CA4-OA6-CA5
45	h	201	CDL	CB3-CB4-OB6-CB5
46	j	101	LMN	CBL-CBR-CCM-CBT
46	j	101	LMN	CAY-CBA-CBC-CBE
43	5	705	3PE	C2-C1-O11-P
43	n	201	3PE	C1-C2-C3-O31
43	W	202	3PE	C35-C36-C37-C38
45	X	201	CDL	C16-C17-C18-C19
44	3	201	PC1	C25-C26-C27-C28
43	n	201	3PE	O21-C2-C3-O31
45	2	601	CDL	OB6-CB4-CB6-OB8
43	5	705	3PE	O31-C31-C32-C33
44	4	603	PC1	C11-C12-N-C14
43	8	101	3PE	C28-C29-C2A-C2B
43	g	102	3PE	C32-C33-C34-C35
44	S	201	PC1	C22-C23-C24-C25
43	g	102	3PE	O31-C31-C32-C33
43	1	401	3PE	O21-C21-C22-C23
44	K	302	PC1	O21-C21-C22-C23
46	2	602	LMN	O1-CBS-CCM-CBQ
46	2	602	LMN	O1-CBS-CCM-CBR
43	J	201	3PE	C34-C35-C36-C37
45	2	601	CDL	C17-C18-C19-C20
43	g	102	3PE	C21-C22-C23-C24
45	X	201	CDL	C31-C32-C33-C34
44	1	403	PC1	O21-C21-C22-C23
45	g	101	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
43	8	101	3PE	O21-C21-C22-C23
43	5	703	3PE	C36-C37-C38-C39
44	K	302	PC1	C34-C35-C36-C37
46	2	602	LMN	O5-C1-O1-CBS
44	2	603	PC1	O31-C31-C32-C33
43	1	401	3PE	C2C-C2D-C2E-C2F
43	g	102	3PE	O21-C21-C22-C23
44	3	201	PC1	C22-C23-C24-C25
44	1	403	PC1	C33-C34-C35-C36
45	2	601	CDL	OB5-CB3-CB4-CB6
49	B	602	FMN	N10-C1'-C2'-O2'
52	O	201	ZMP	C20-C18-C21-O5
52	O	201	ZMP	C16-C17-C18-C21
43	5	705	3PE	C22-C23-C24-C25
44	S	201	PC1	C26-C27-C28-C29
46	2	602	LMN	CBJ-CBL-CBR-CCM
43	5	705	3PE	C2D-C2E-C2F-C2G
44	4	603	PC1	C3A-C3B-C3C-C3D
43	1	401	3PE	O22-C21-C22-C23
43	n	201	3PE	C32-C33-C34-C35
44	4	603	PC1	C11-C12-N-C15
45	4	601	CDL	C72-C71-CB7-OB8
46	J	202	LMN	CBG-CBI-CBK-CBQ
43	1	401	3PE	C3B-C3C-C3D-C3E
43	5	705	3PE	O32-C31-C32-C33
43	g	102	3PE	O32-C31-C32-C33
43	1	401	3PE	C3E-C3F-C3G-C3H
43	8	101	3PE	O22-C21-C22-C23
44	2	603	PC1	O32-C31-C32-C33
44	K	302	PC1	O22-C21-C22-C23
45	g	101	CDL	OA7-CA5-OA6-CA4
43	W	201	3PE	C22-C23-C24-C25
44	1	403	PC1	O22-C21-C22-C23
45	g	101	CDL	C18-C19-C20-C21
45	X	201	CDL	C32-C33-C34-C35
45	g	101	CDL	OB5-CB3-CB4-CB6
45	2	601	CDL	C55-C56-C57-C58
45	4	601	CDL	C72-C71-CB7-OB9
45	h	201	CDL	C12-C11-CA5-OA6
43	W	202	3PE	C3D-C3E-C3F-C3G
43	g	102	3PE	O22-C21-C22-C23
43	n	201	3PE	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
46	2	602	LMN	CBH-CBJ-CBL-CBR
43	W	201	3PE	C2B-C2C-C2D-C2E

There are no ring outliers.

36 monomers are involved in 126 short contacts:

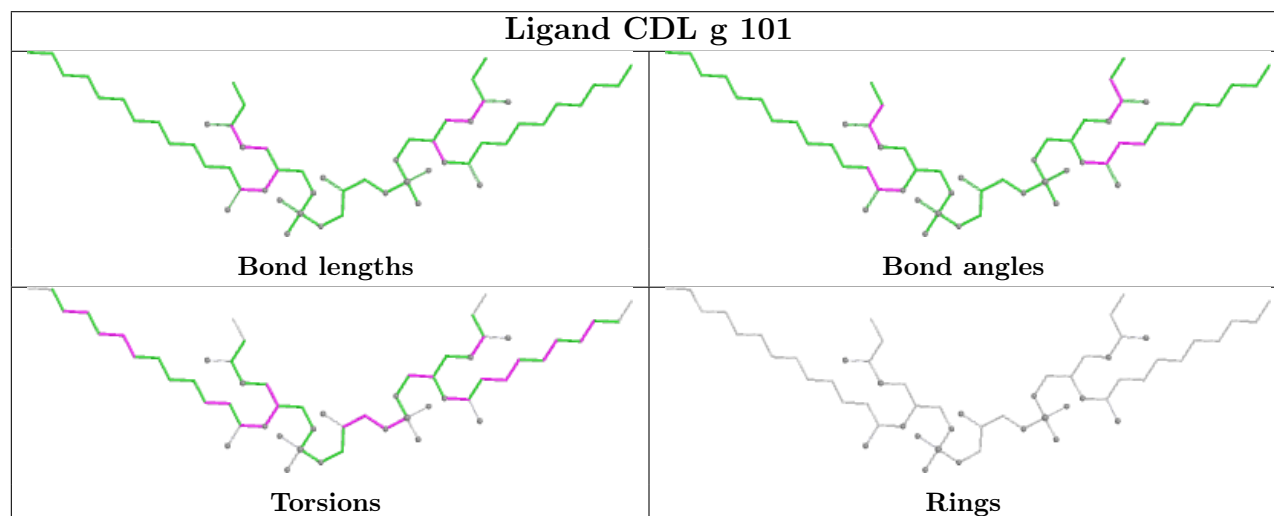
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	A	803	SF4	1	0
45	g	101	CDL	8	0
46	J	202	LMN	5	0
46	2	602	LMN	1	0
43	1	402	3PE	2	0
52	Q	201	ZMP	3	0
45	2	601	CDL	3	0
44	S	201	PC1	8	0
46	j	101	LMN	1	0
43	W	202	3PE	6	0
44	2	603	PC1	2	0
43	5	703	3PE	4	0
49	B	602	FMN	1	0
43	5	705	3PE	3	0
44	K	302	PC1	1	0
43	J	201	3PE	4	0
44	4	603	PC1	5	0
43	g	102	3PE	2	0
52	O	201	ZMP	4	0
45	X	201	CDL	8	0
45	h	201	CDL	1	0
44	5	701	PC1	7	0
43	5	704	3PE	3	0
44	5	706	PC1	4	0
44	1	403	PC1	9	0
43	4	602	3PE	1	0
43	5	707	3PE	3	0
43	i	101	3PE	3	0
43	n	201	3PE	5	0
45	4	601	CDL	2	0
44	3	201	PC1	5	0
43	W	201	3PE	1	0
43	1	401	3PE	6	0
43	8	101	3PE	1	0
43	E	401	3PE	1	0

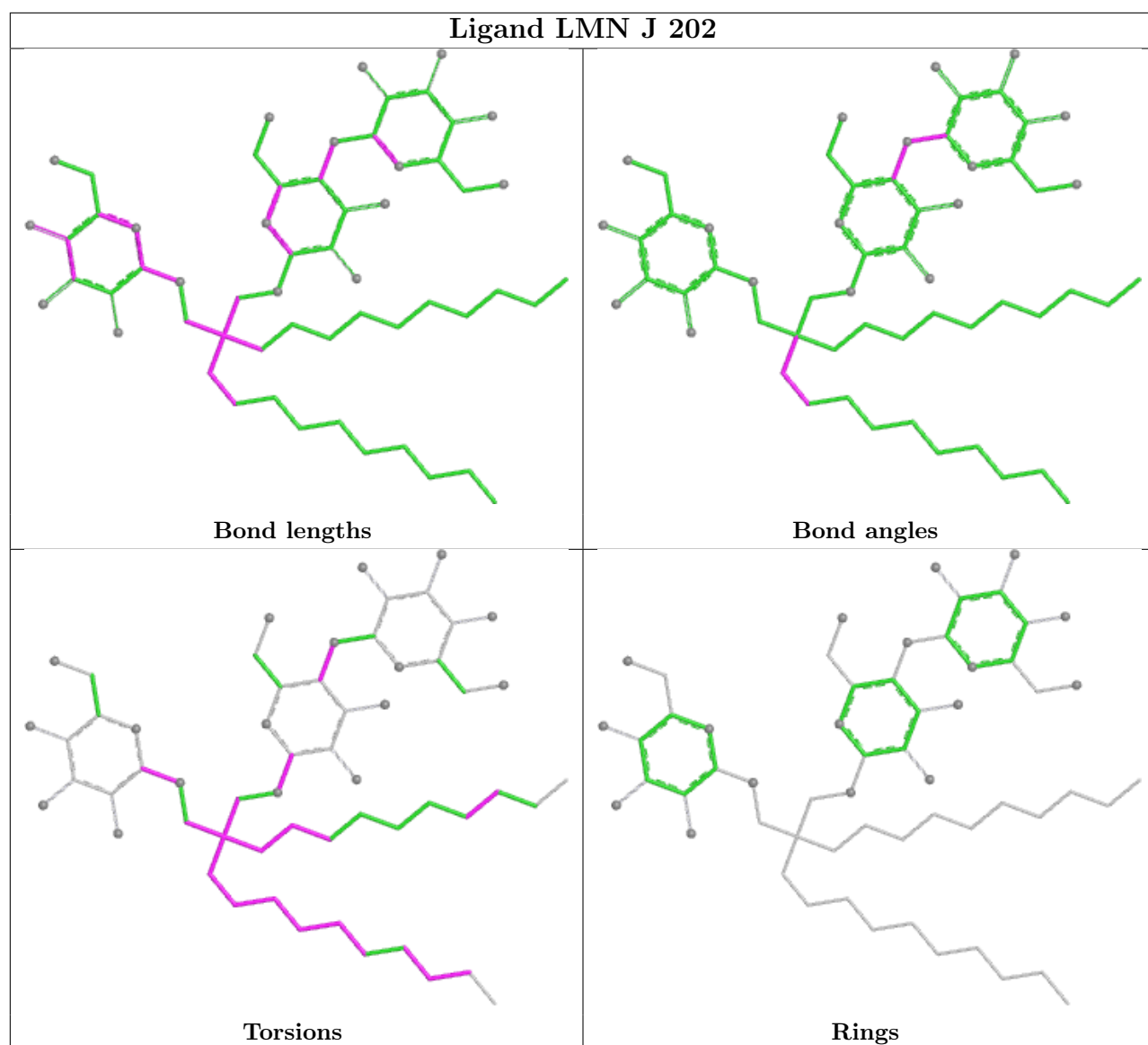
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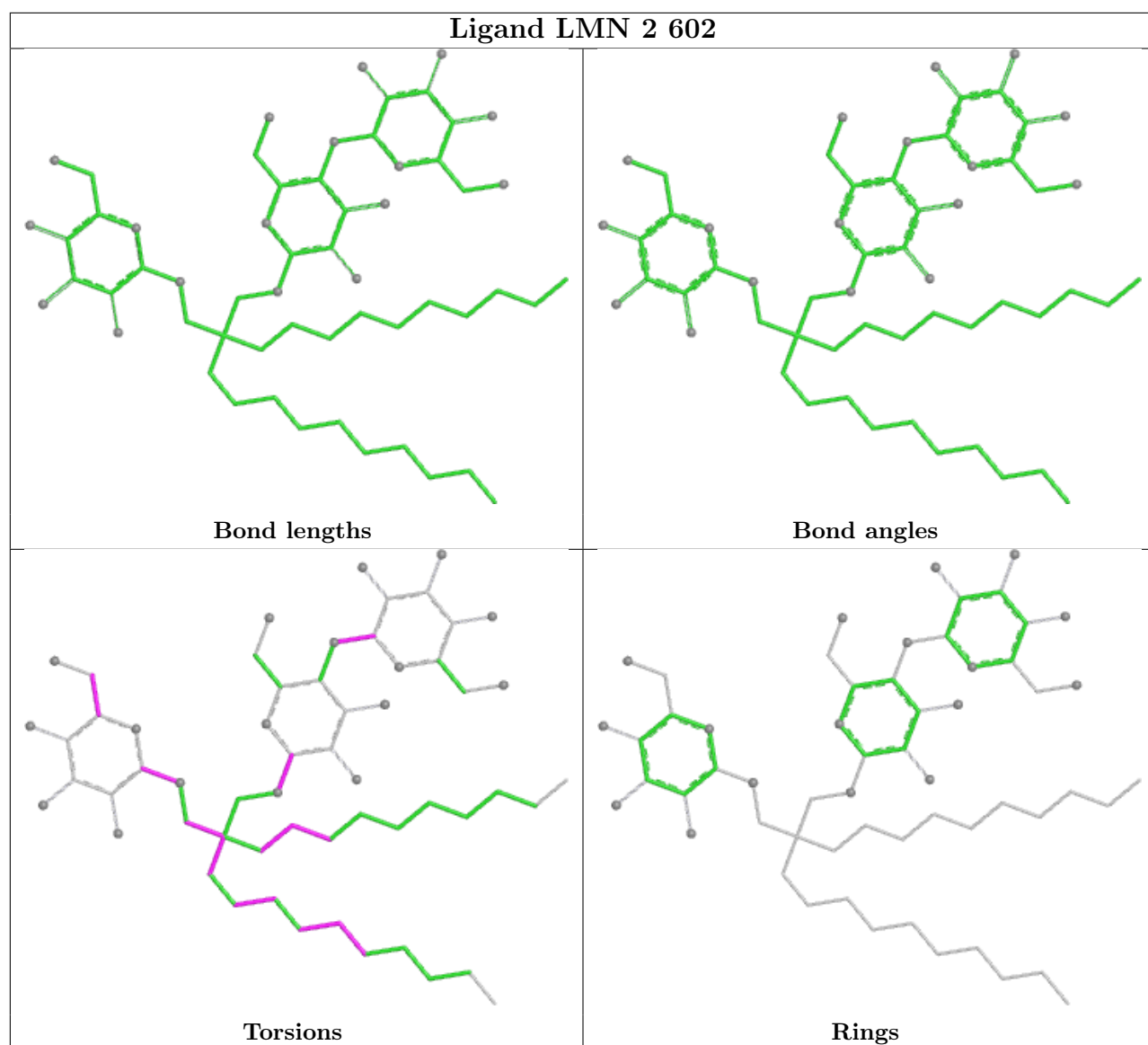
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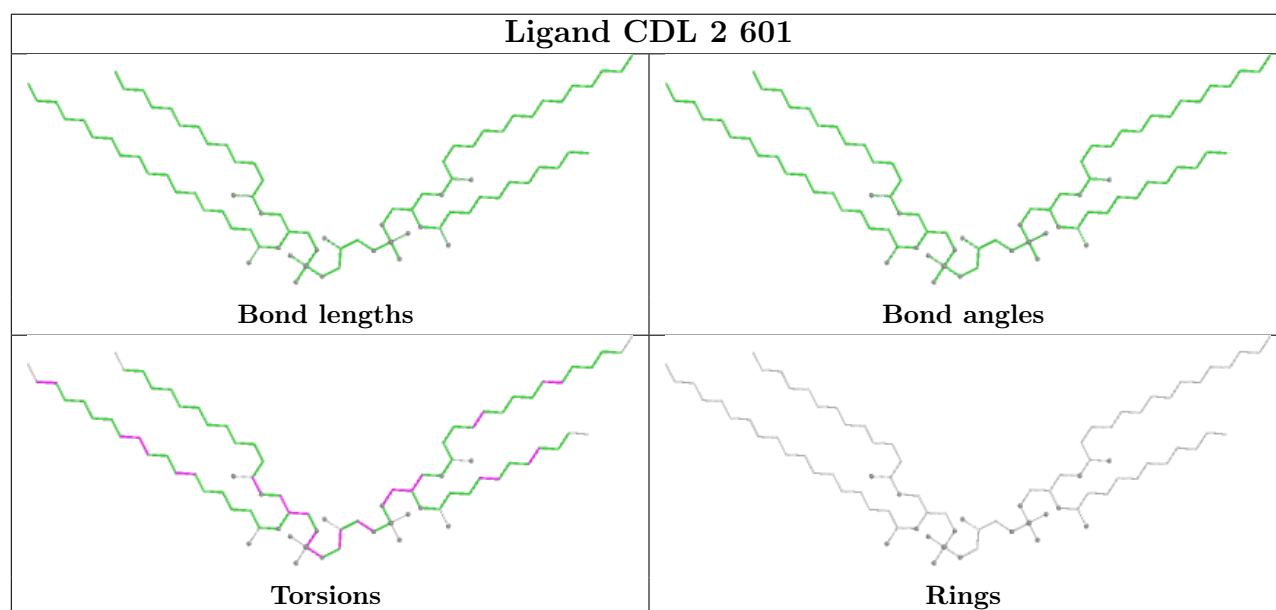
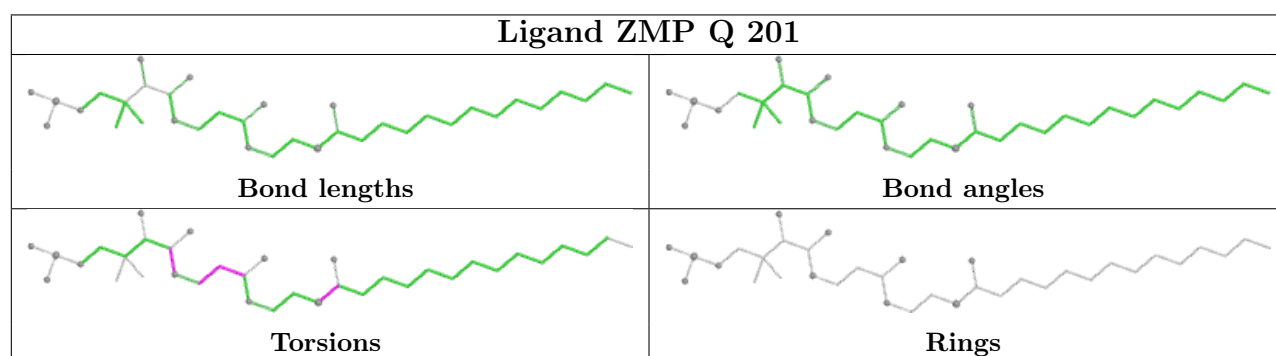
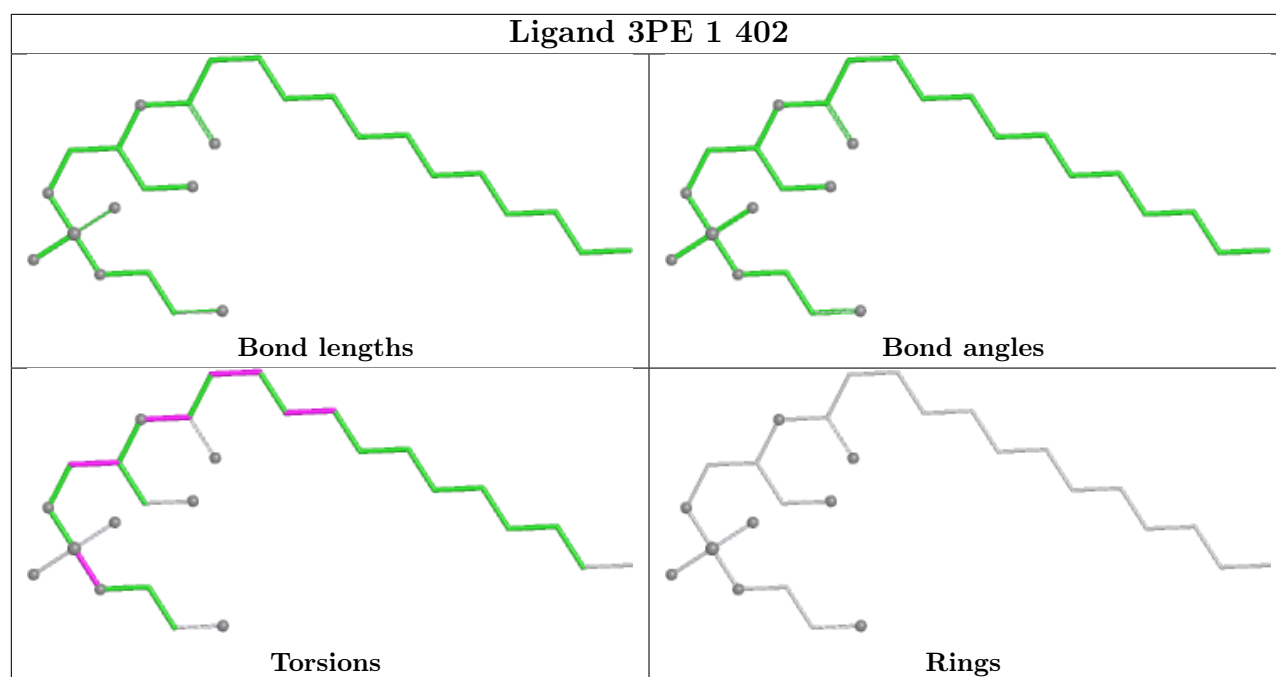
Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	5	702	3PE	4	0

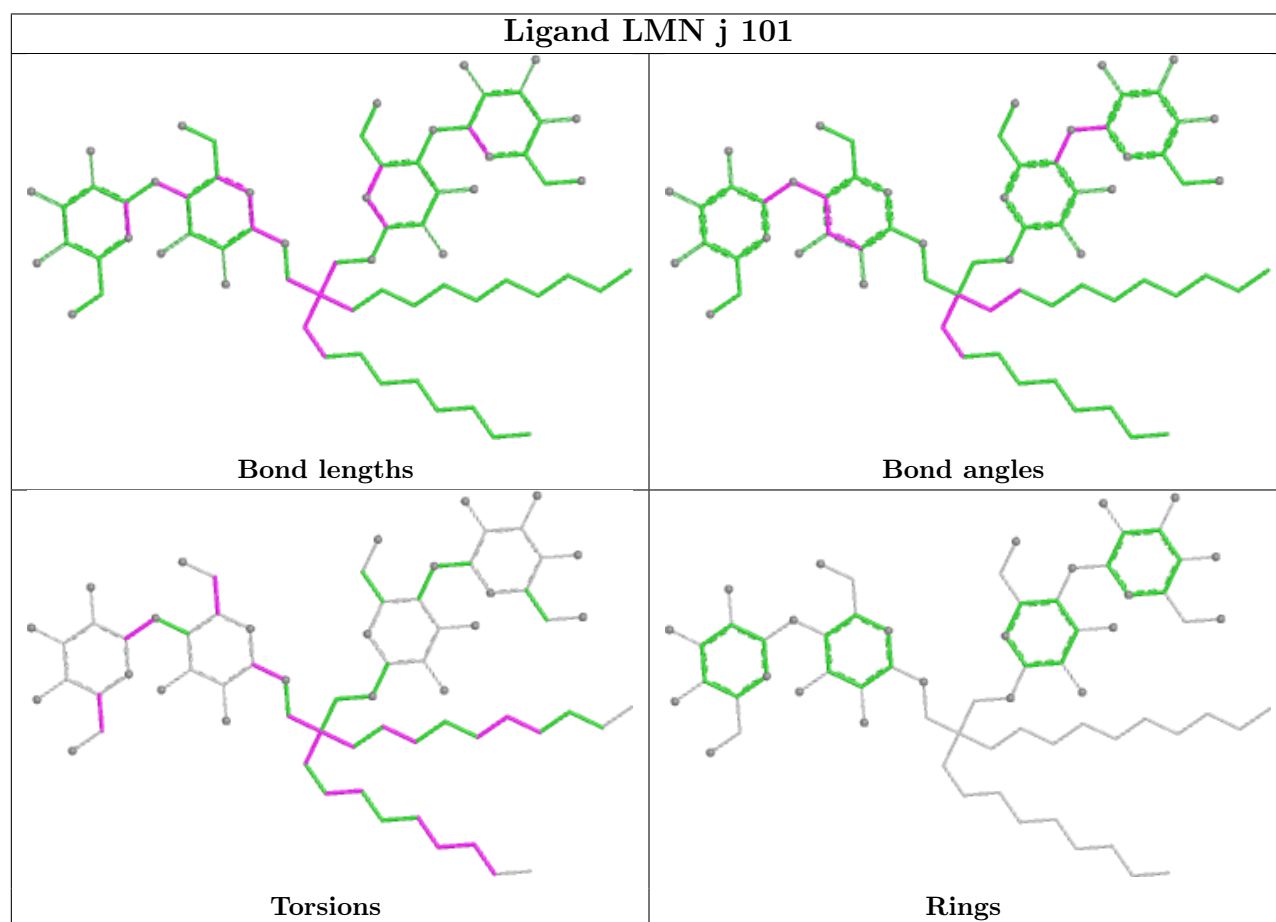
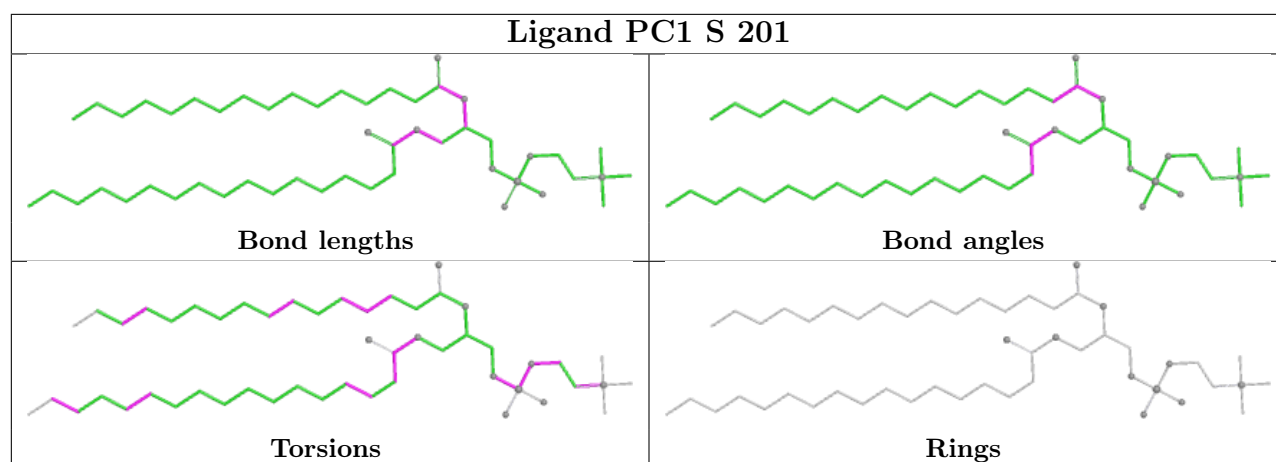
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

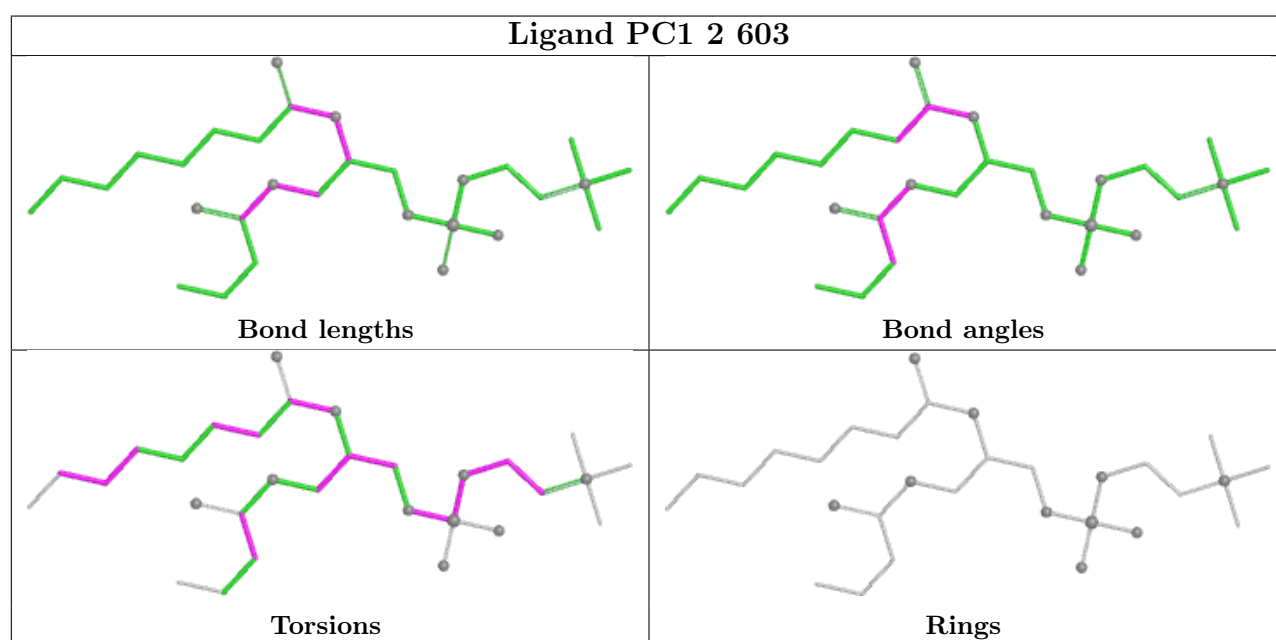
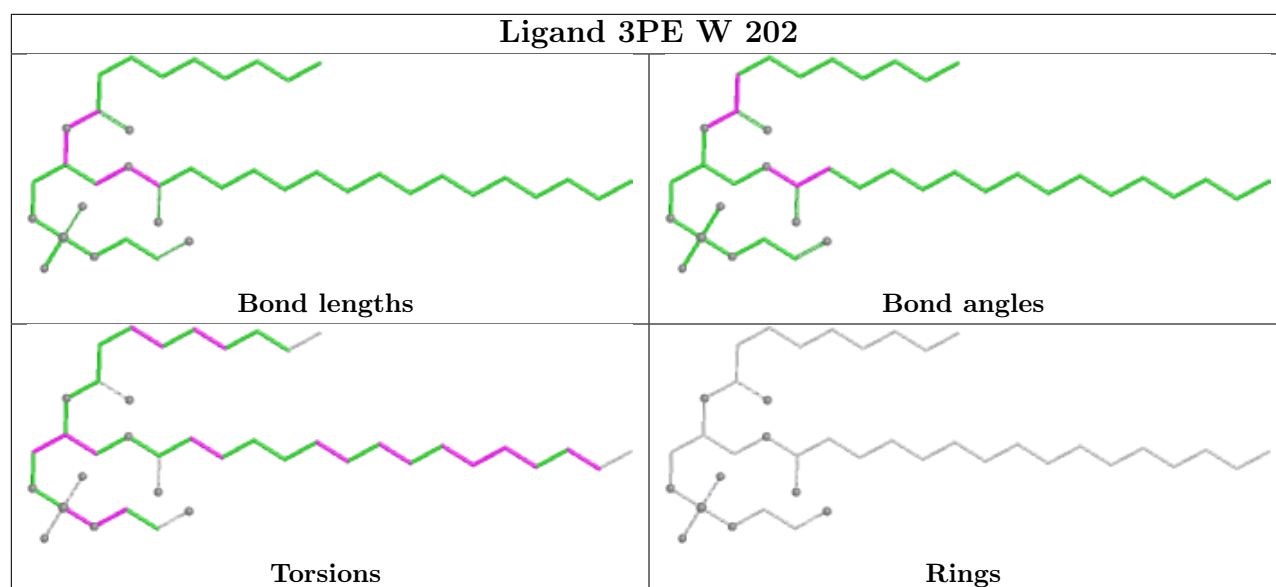


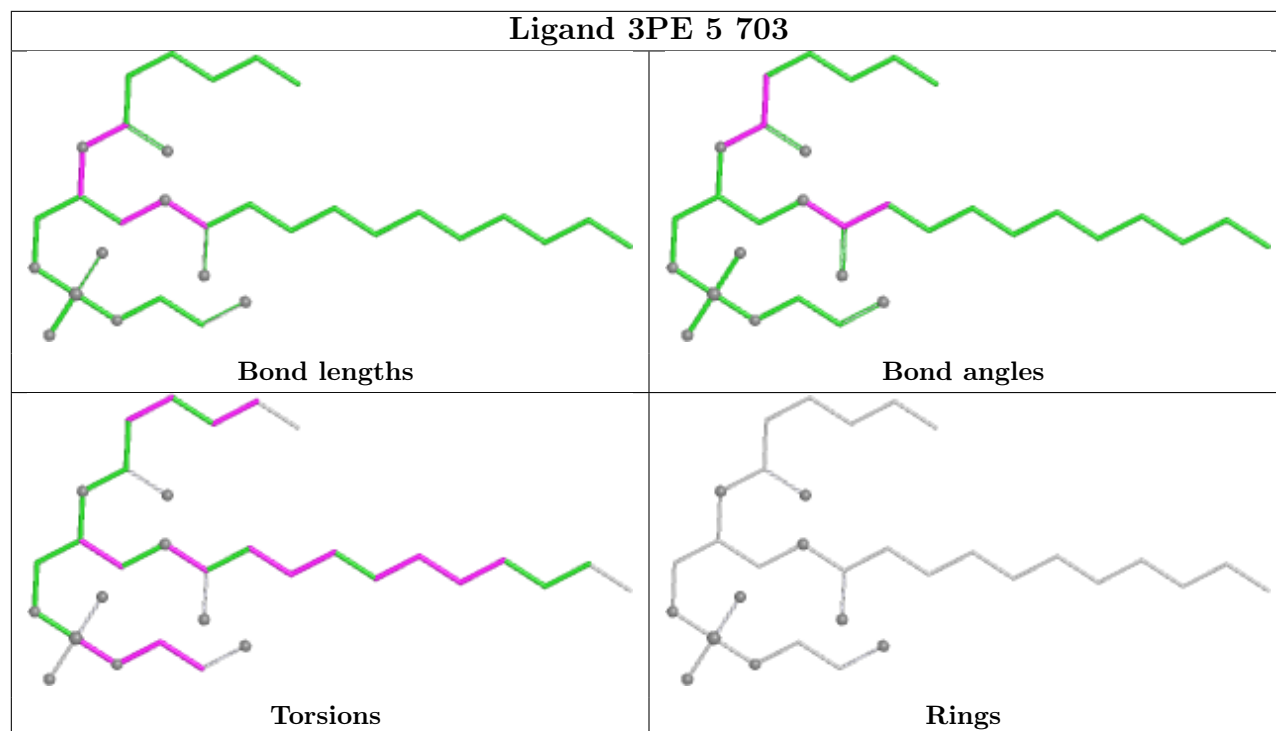


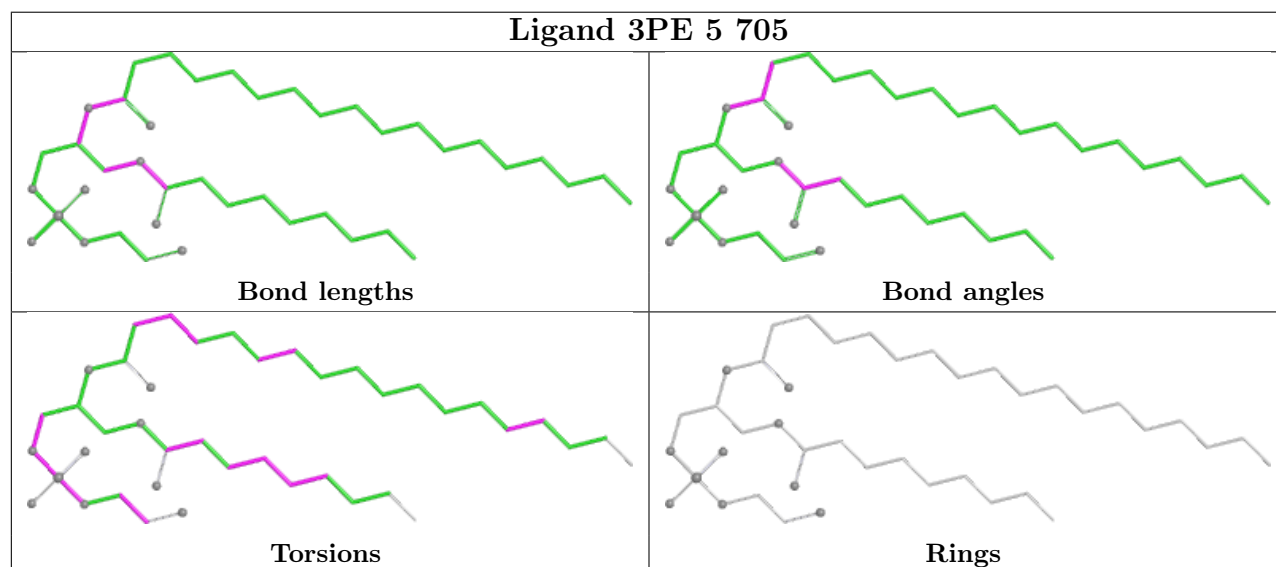
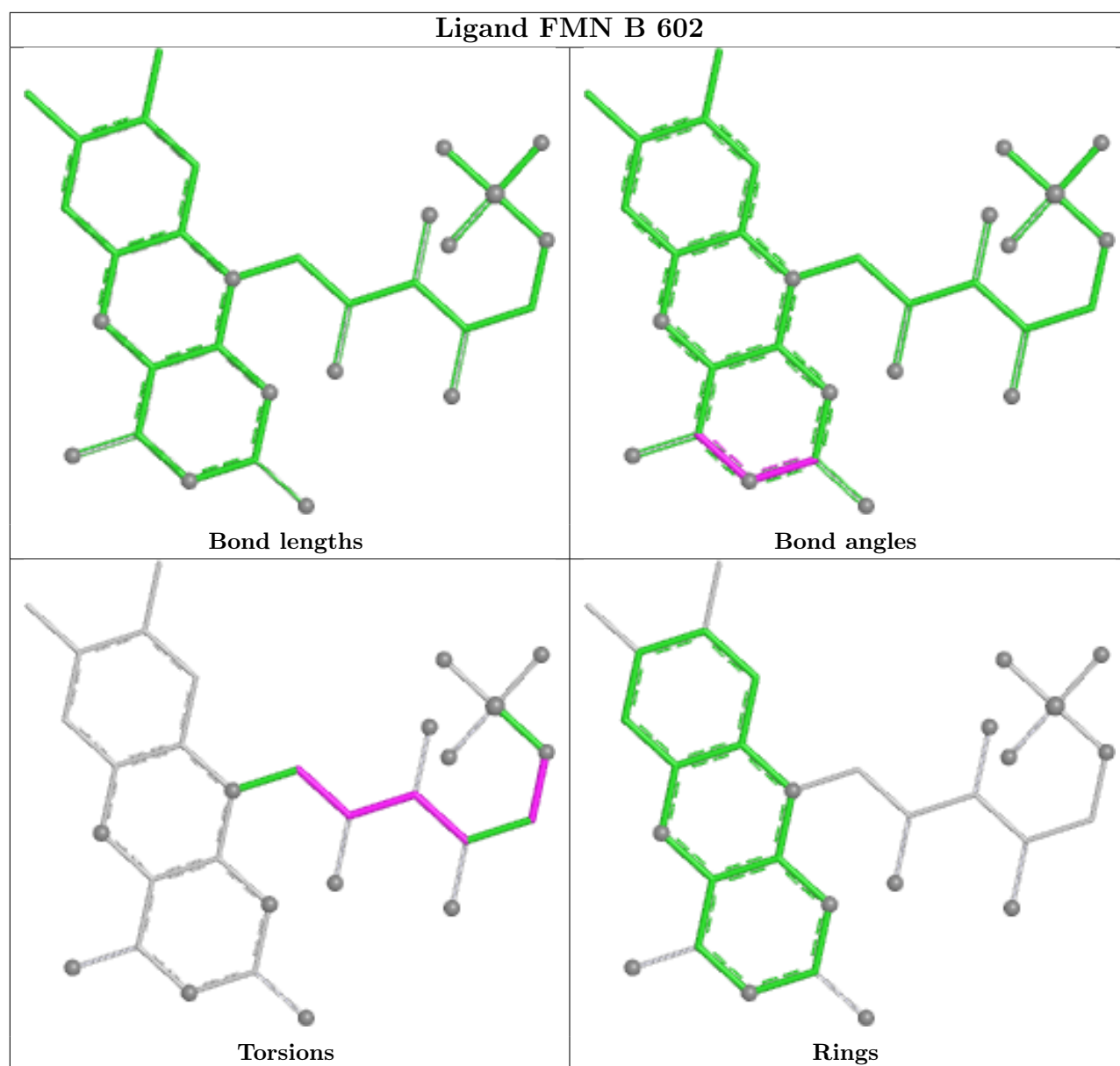


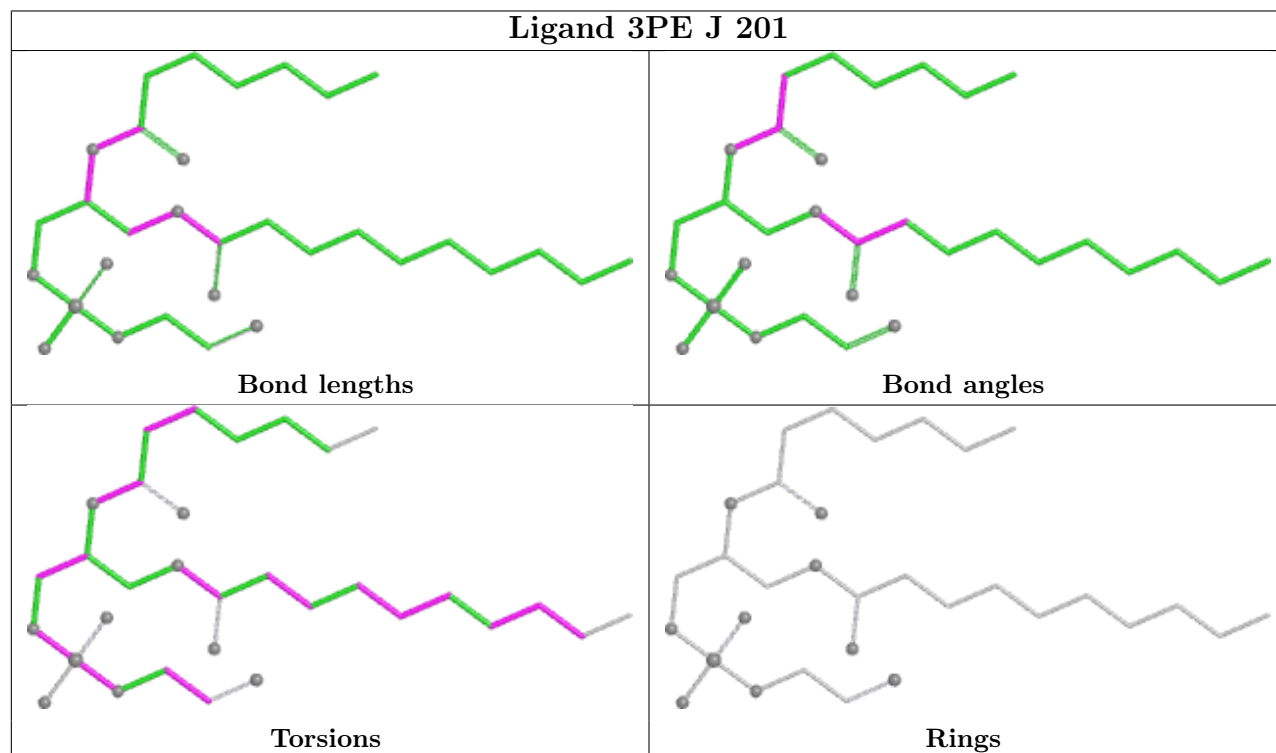
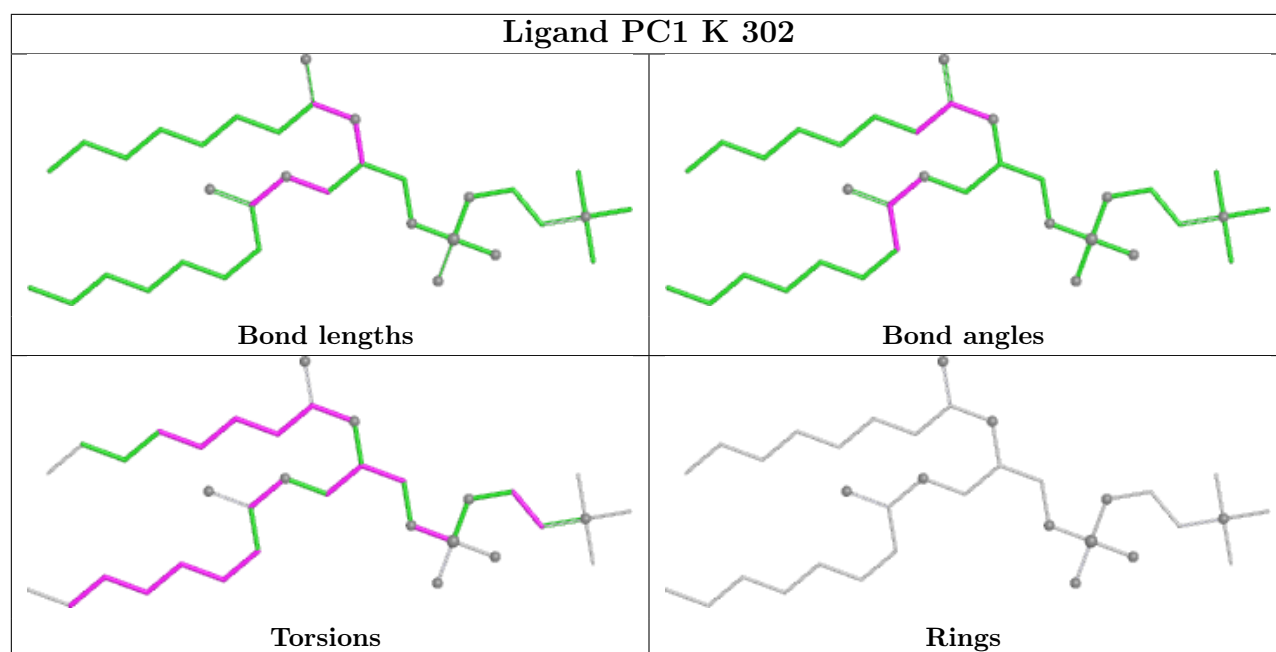


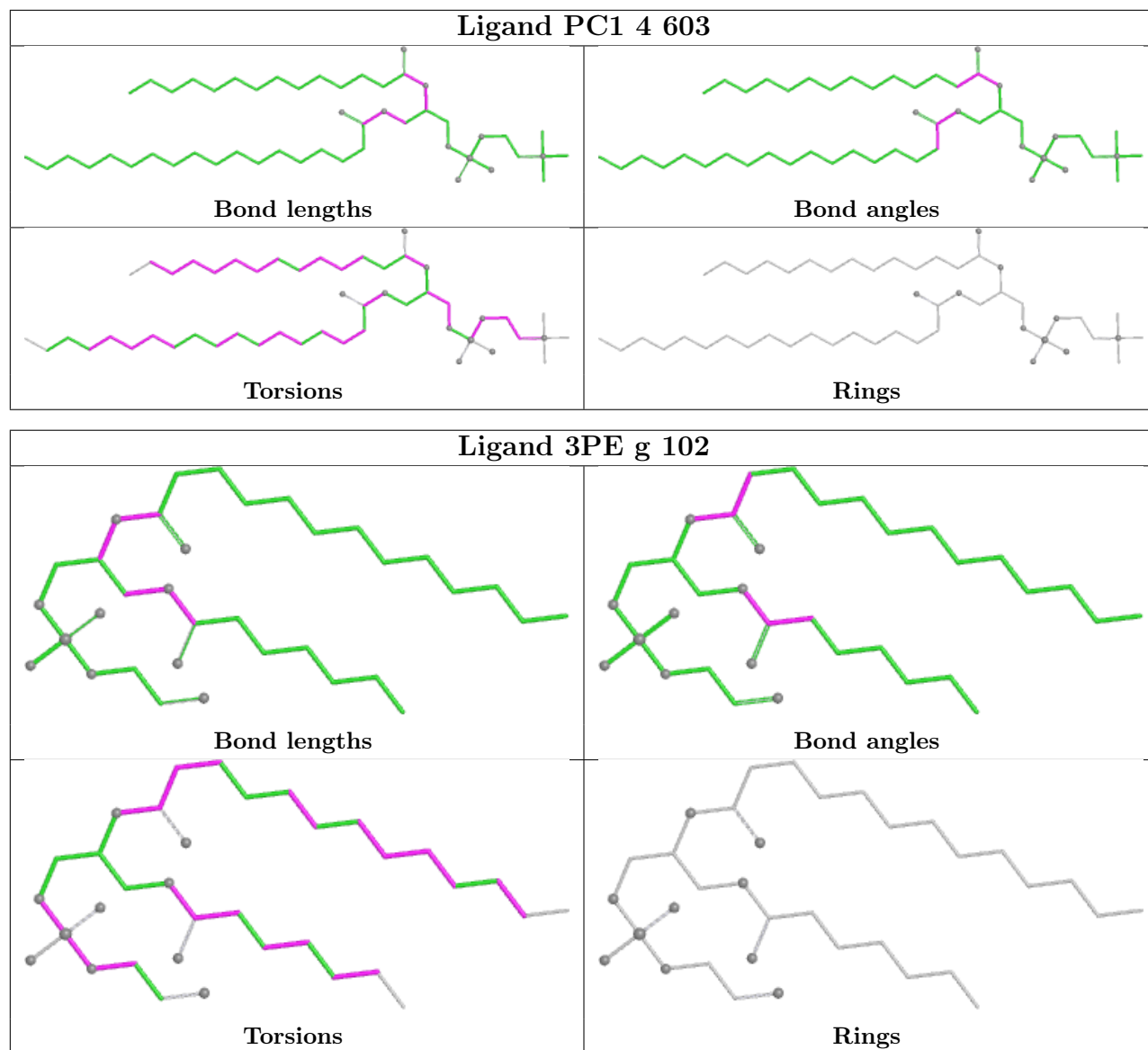


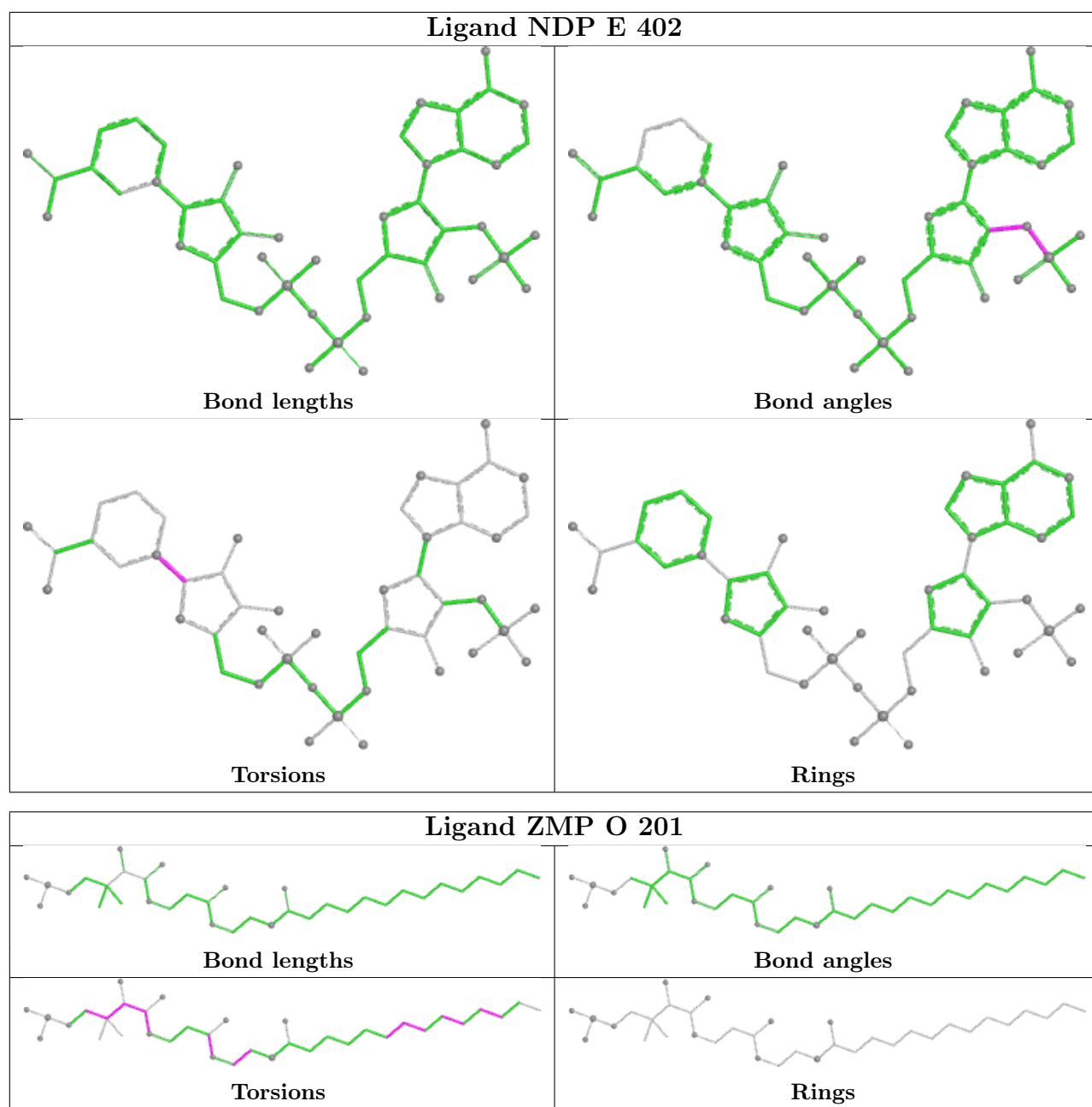


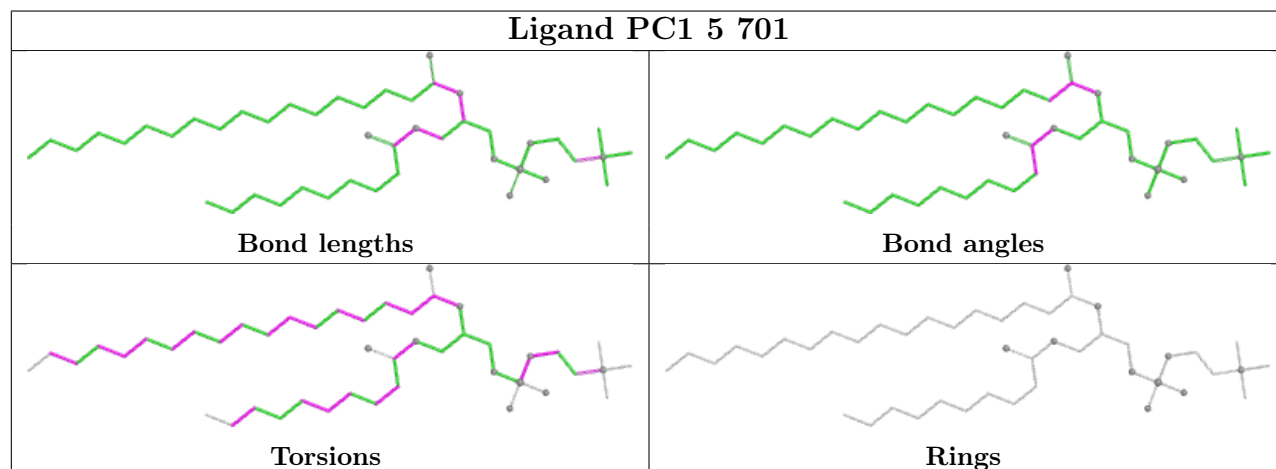
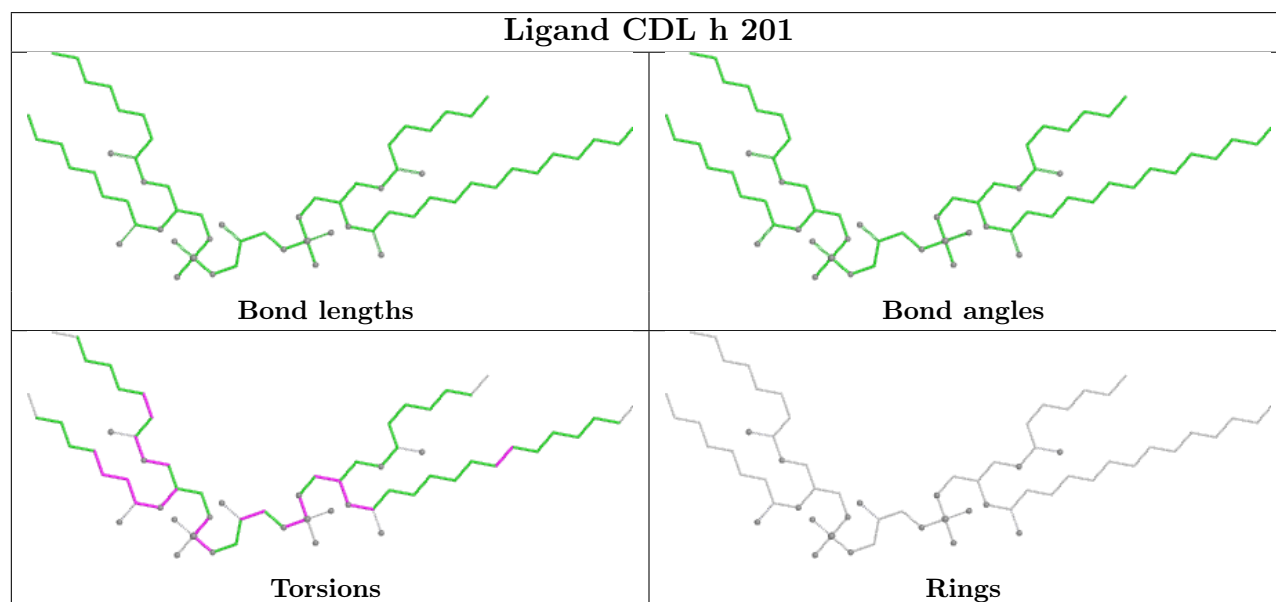
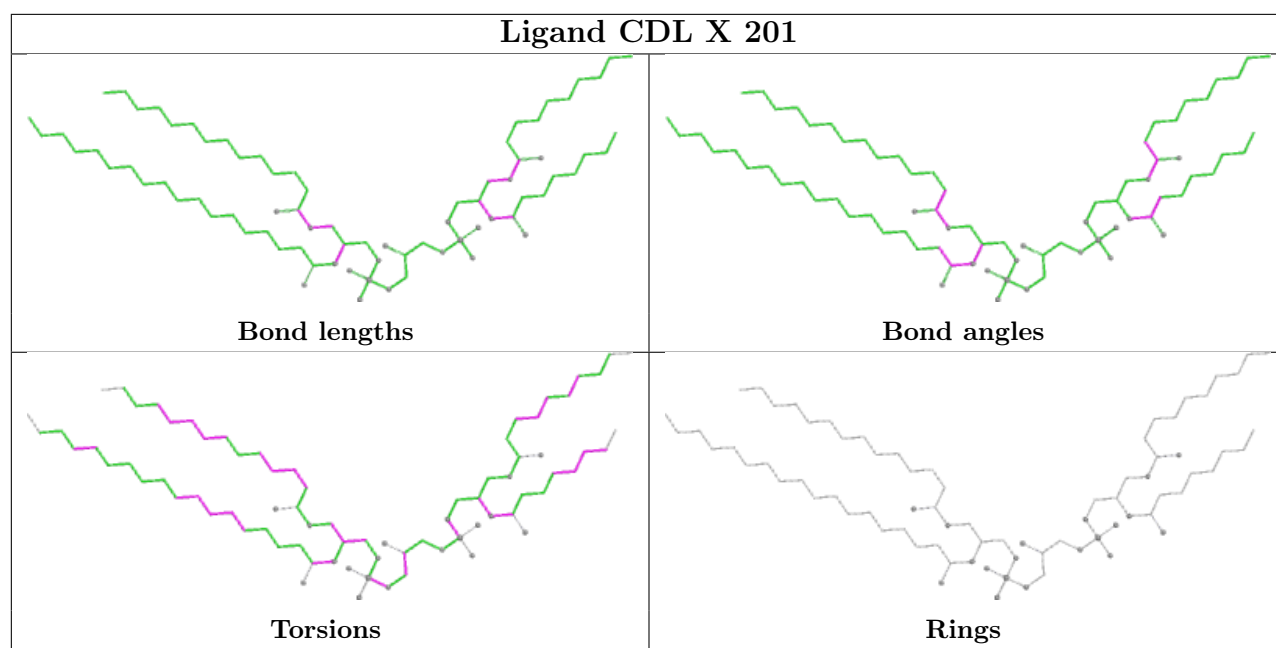


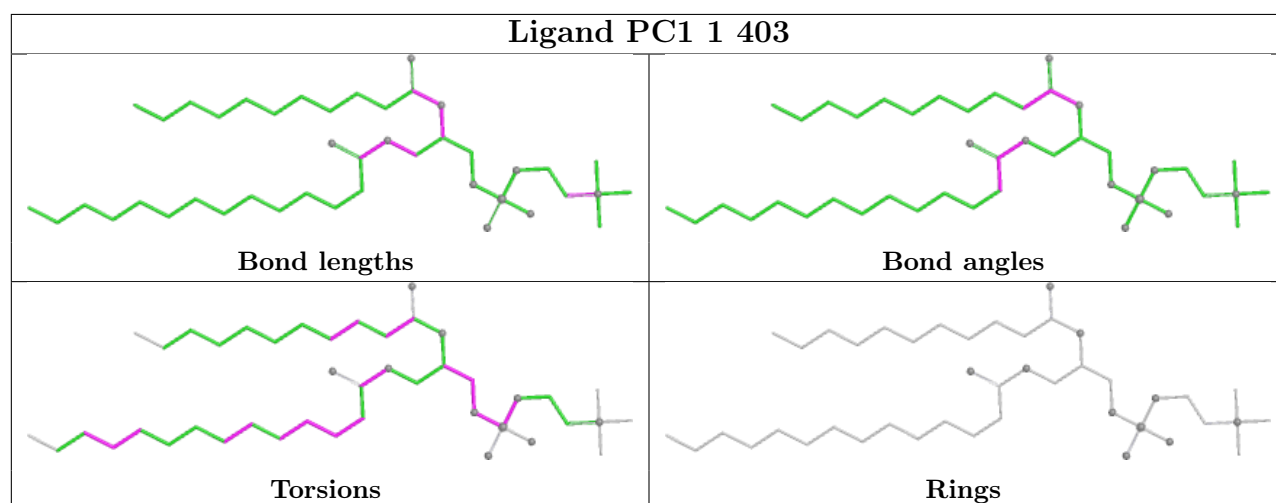
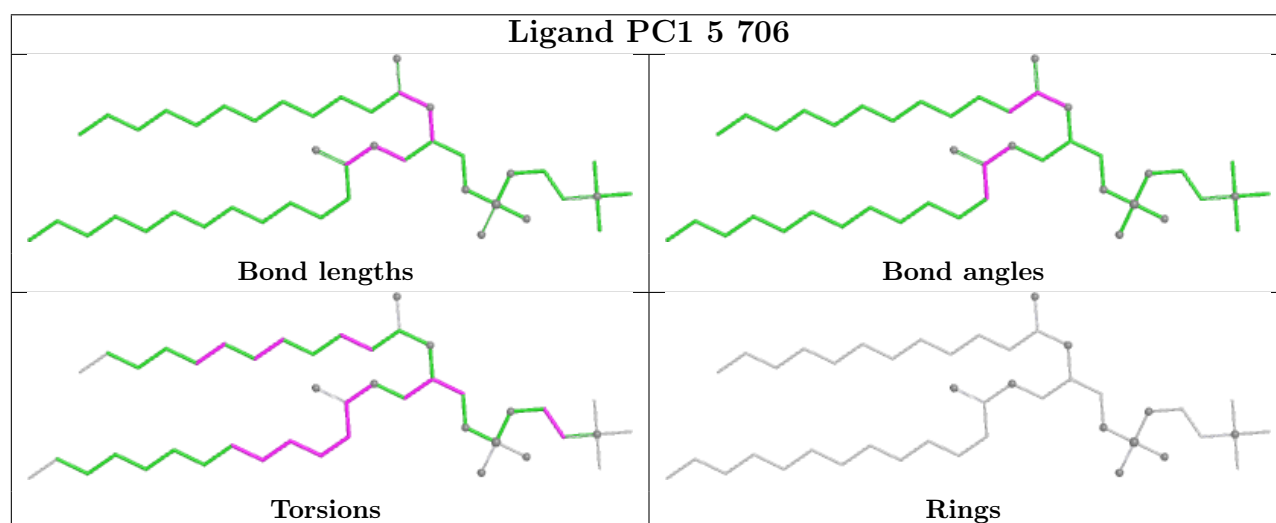
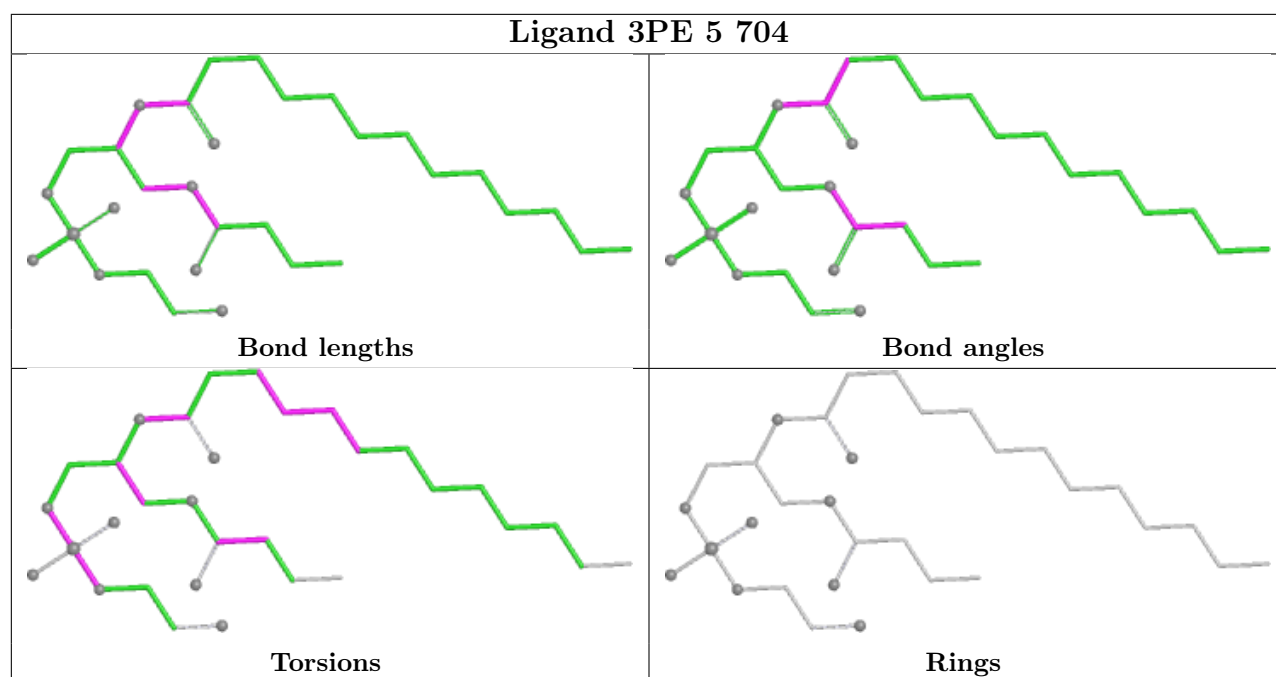


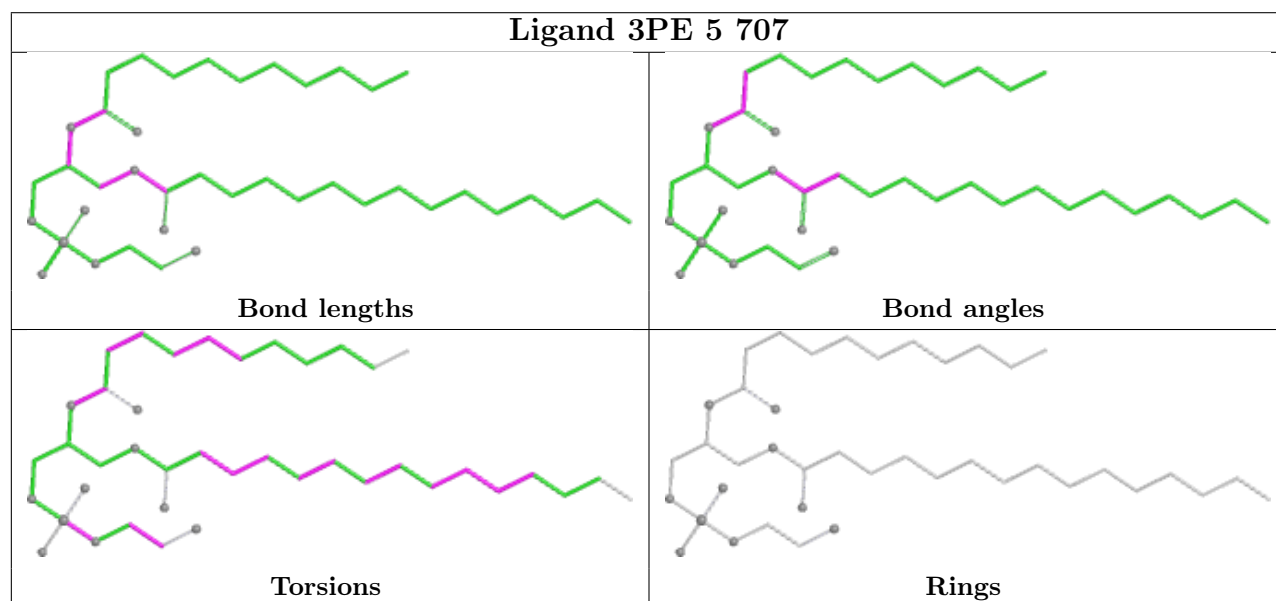
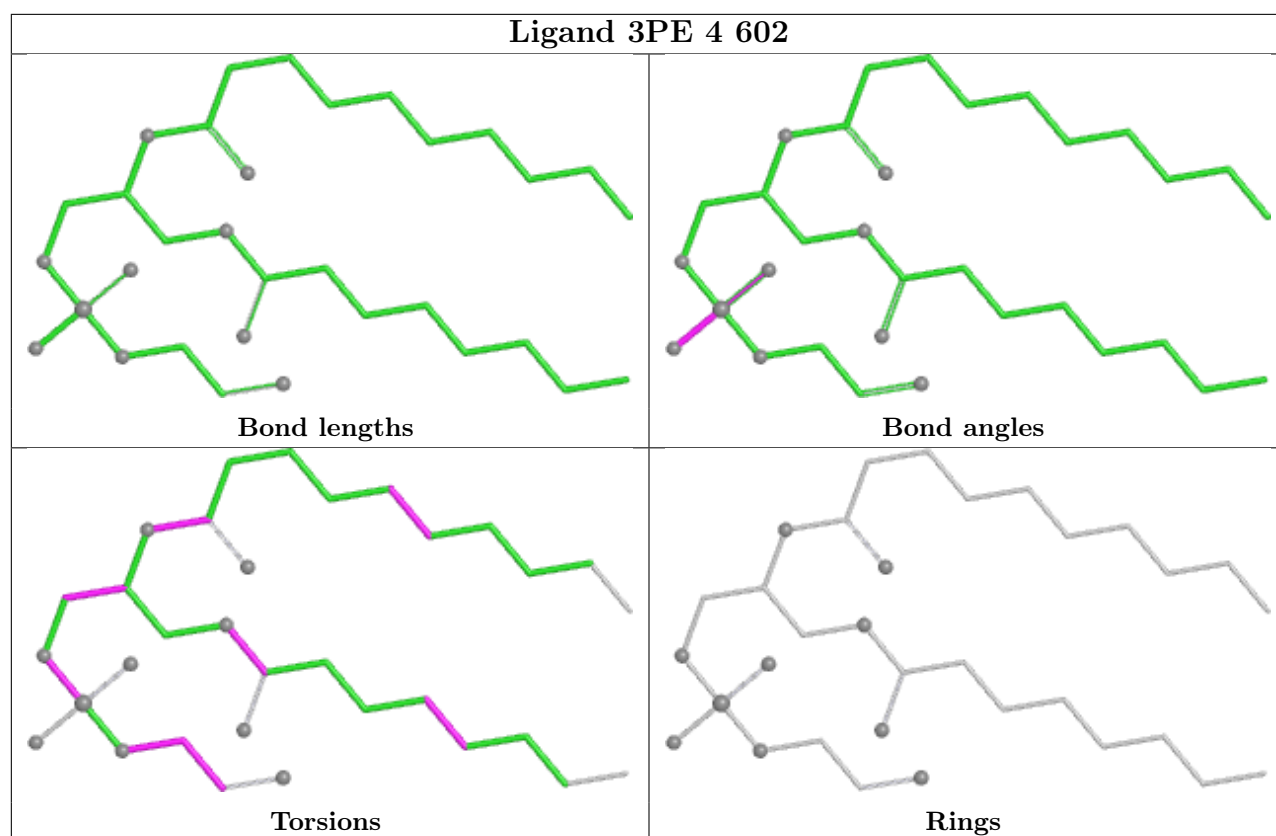


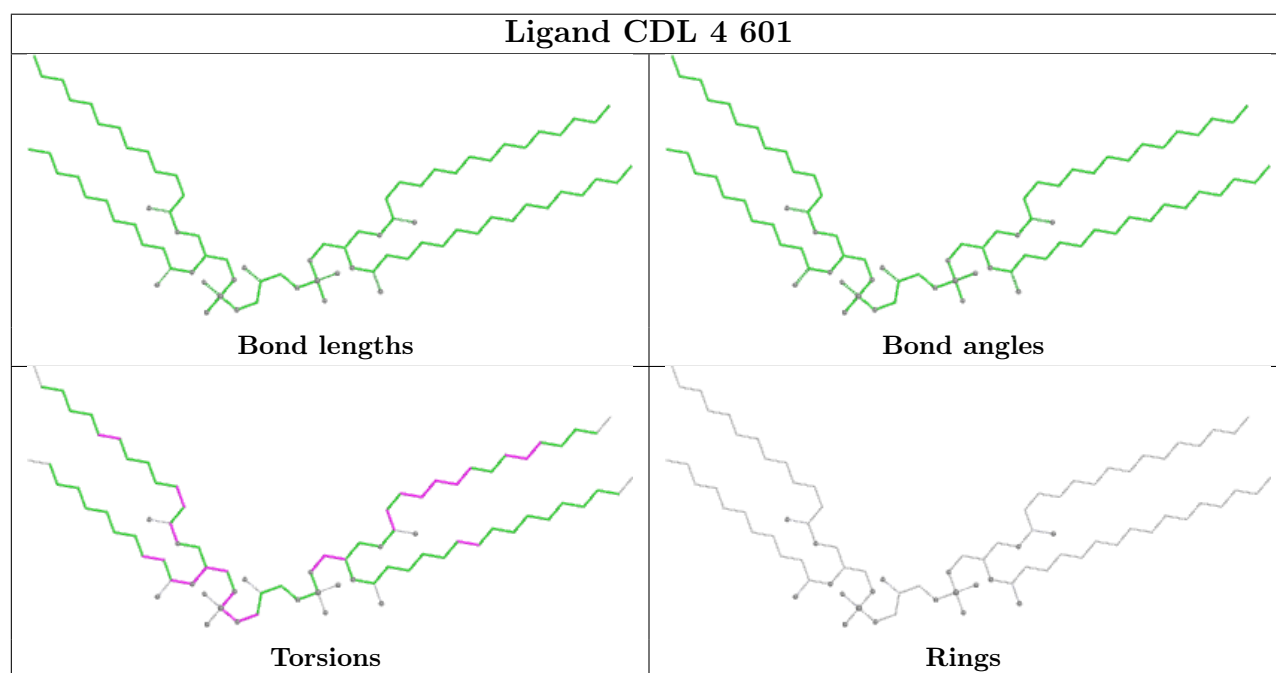
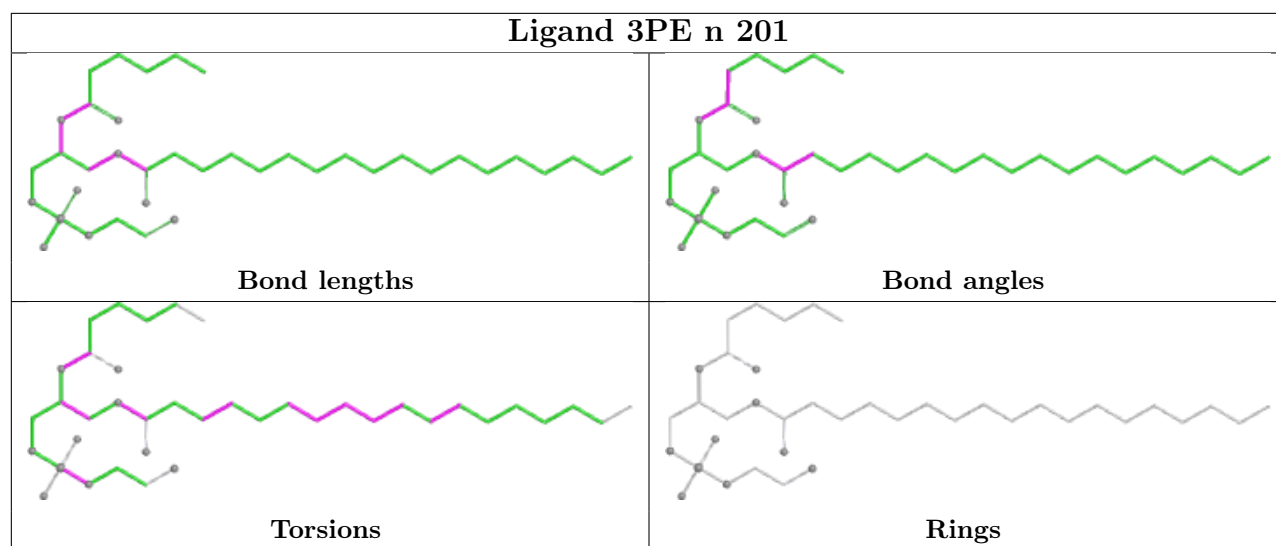
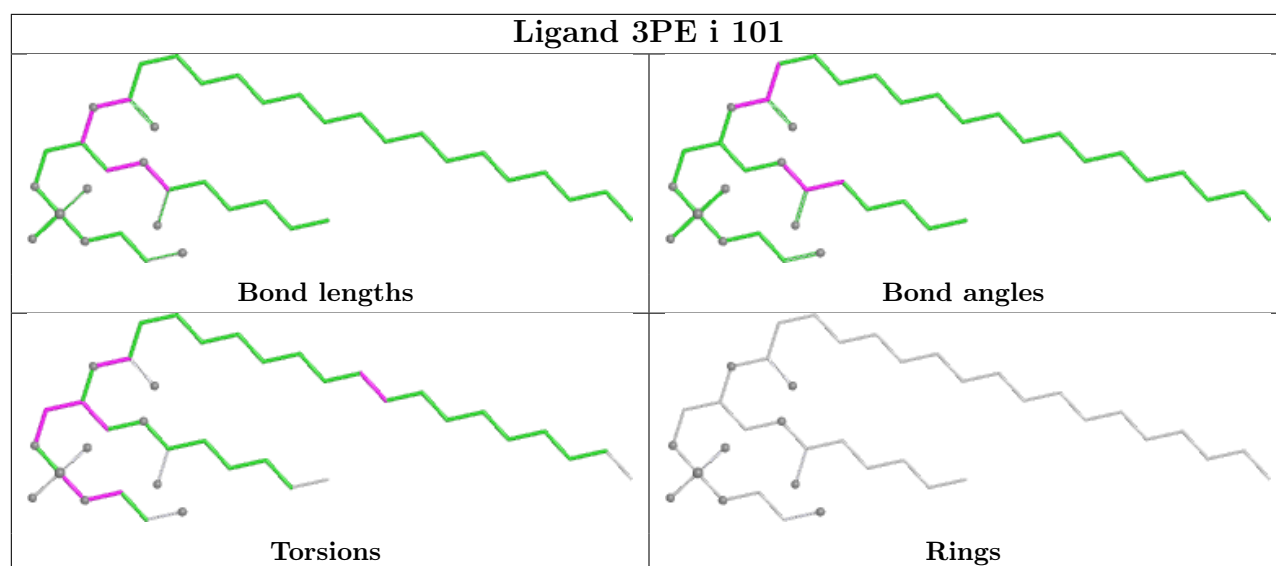


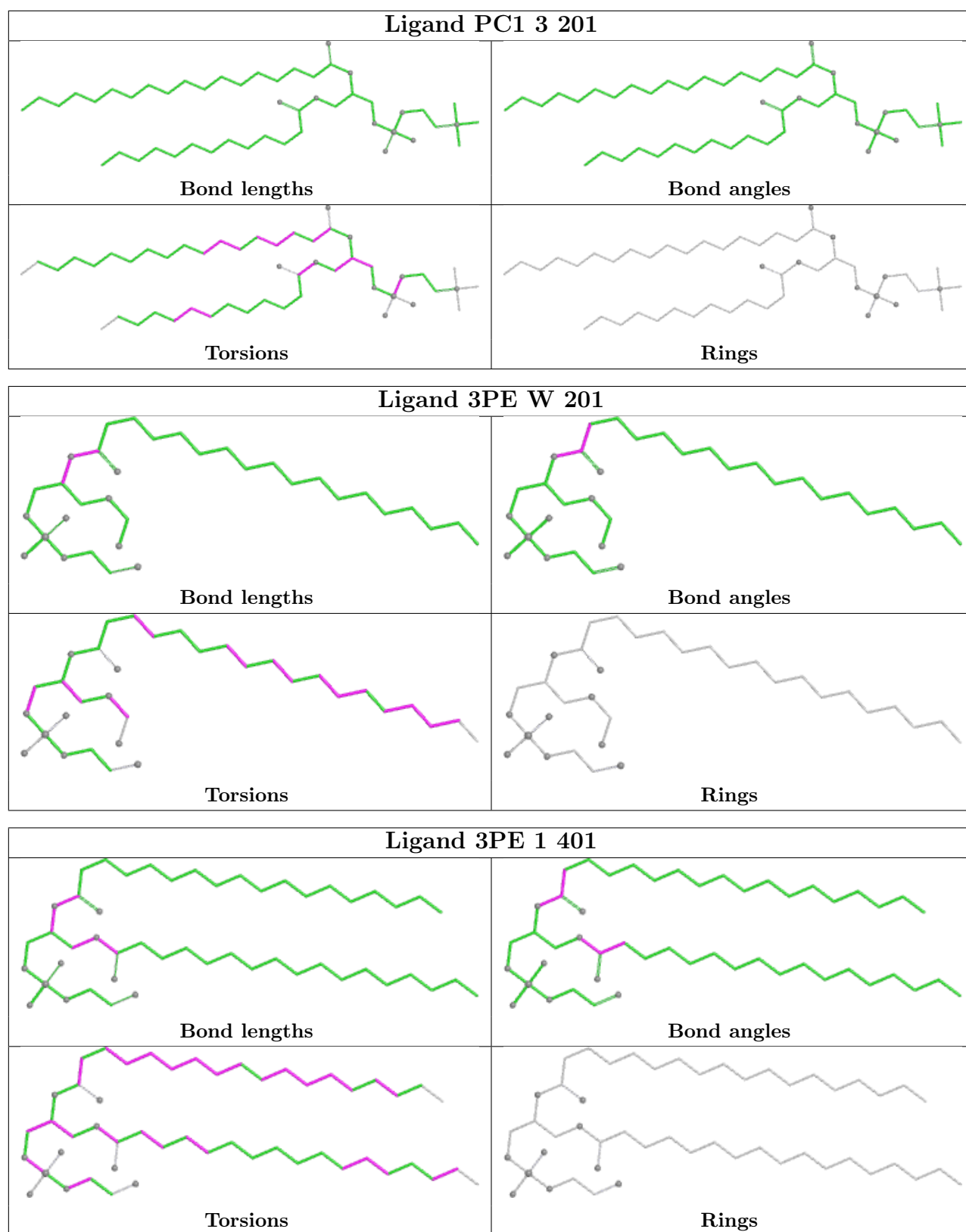




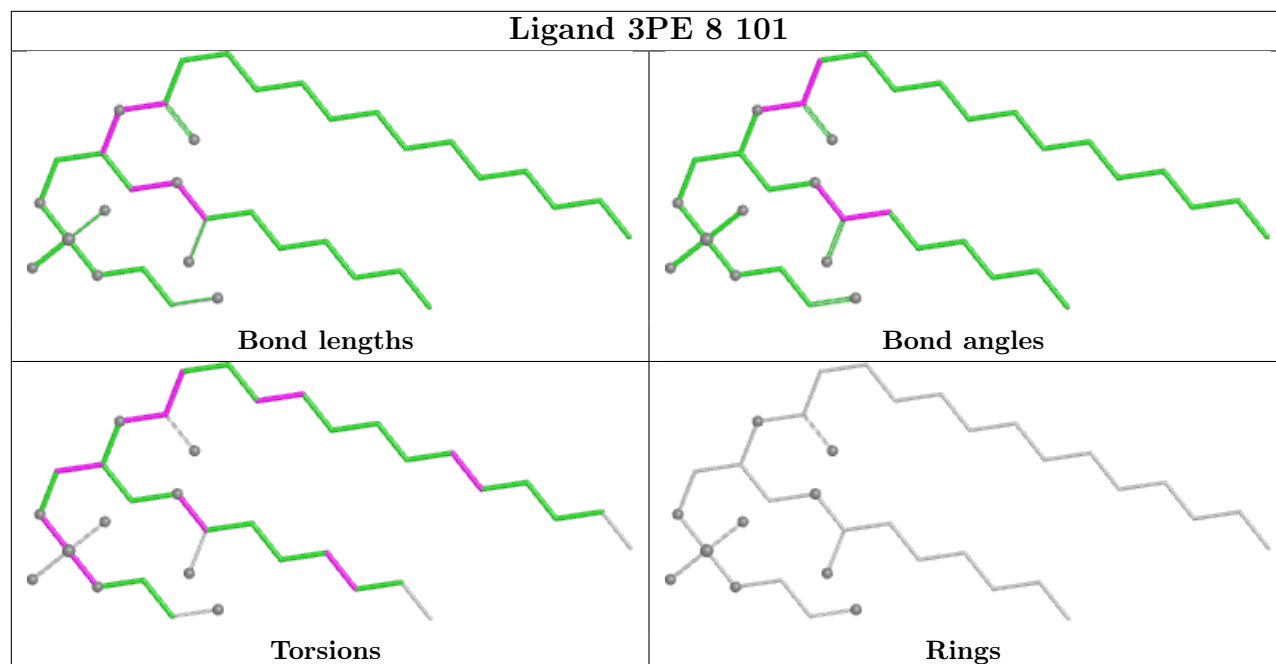




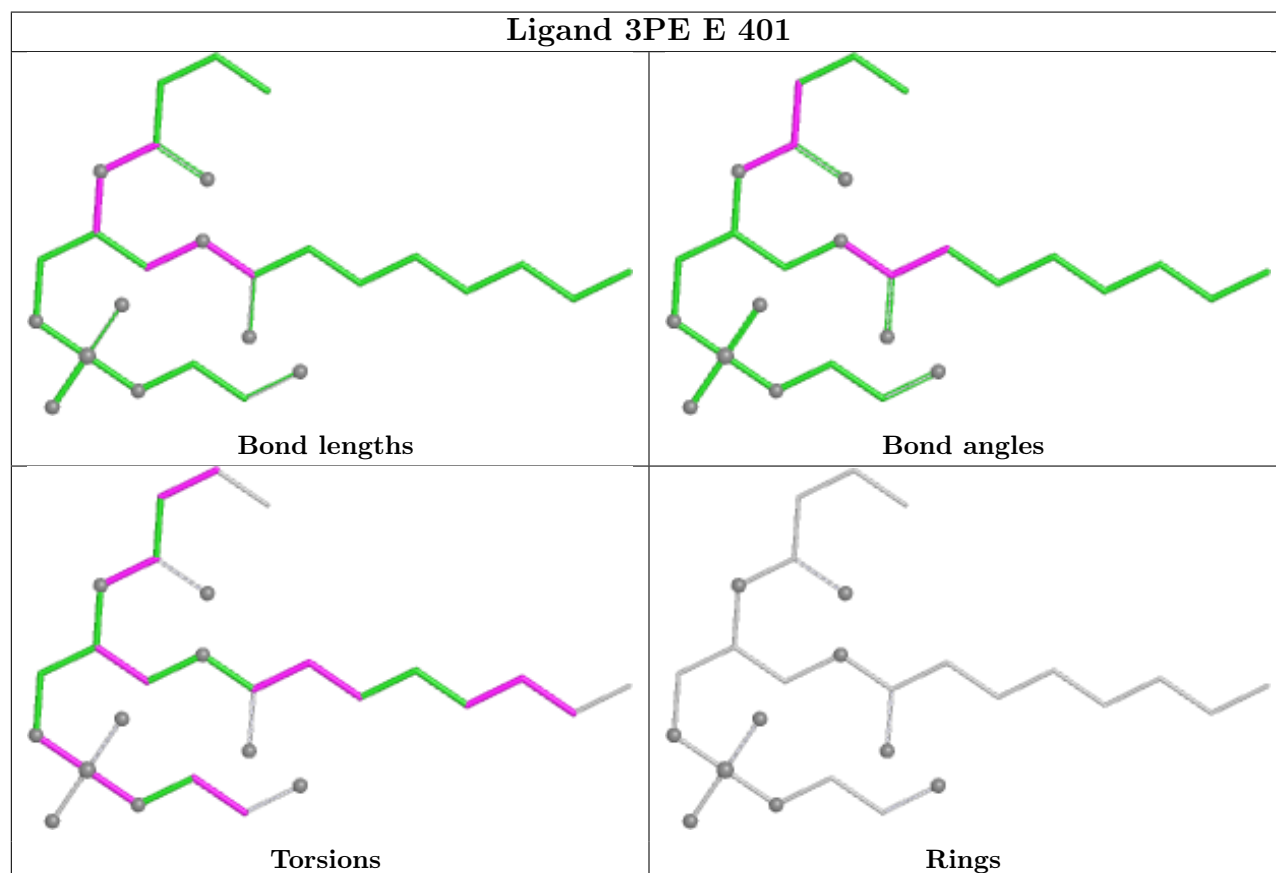


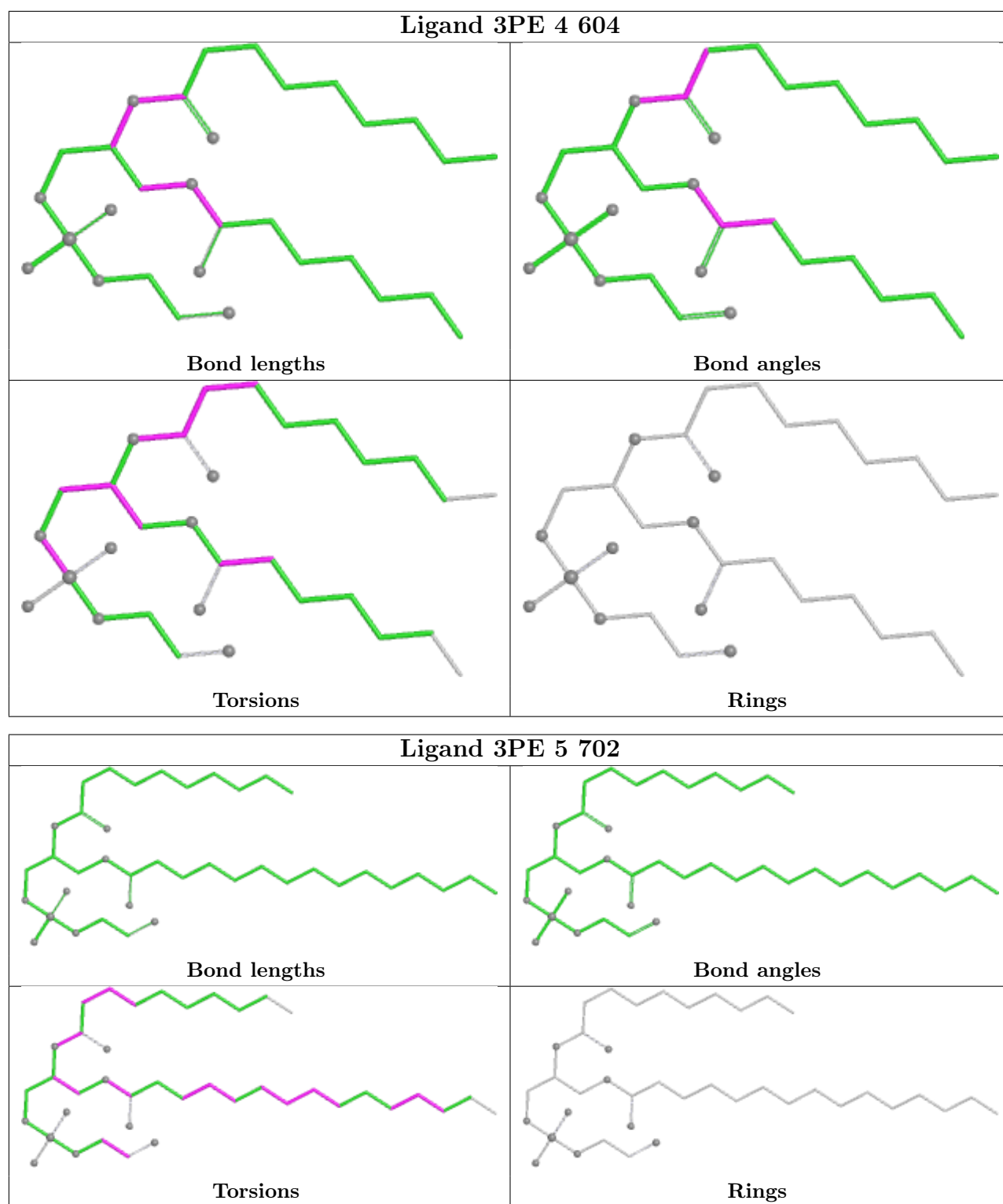


Ligand 3PE 8 101



Ligand 3PE E 401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

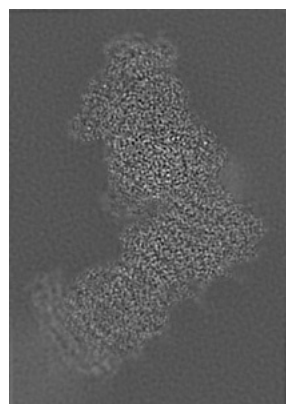
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14794. These allow visual inspection of the internal detail of the map and identification of artifacts.

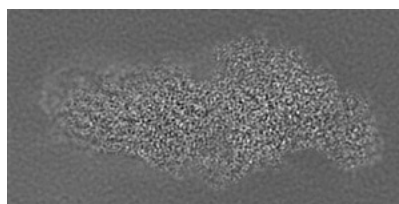
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

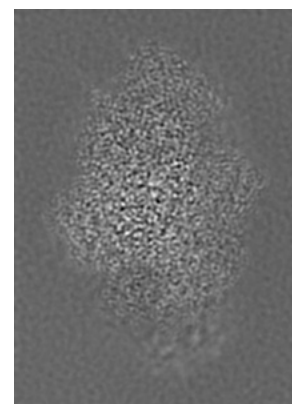
6.1.1 Primary map



X

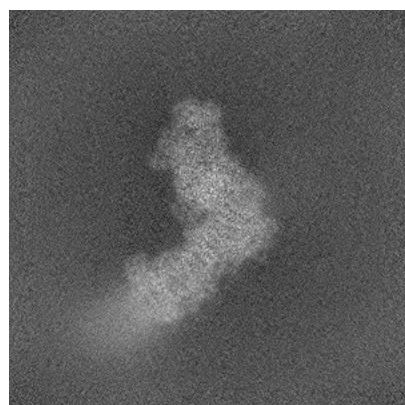


Y

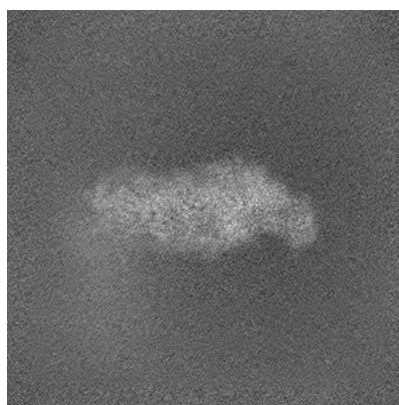


Z

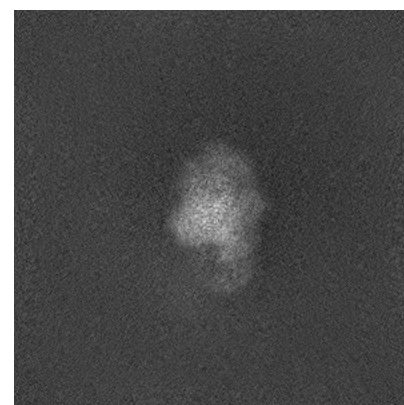
6.1.2 Raw map



X



Y

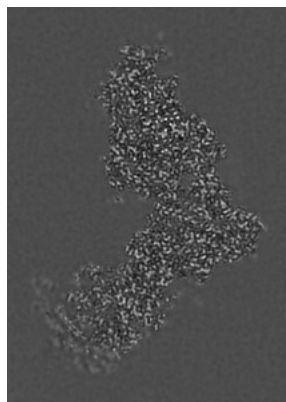


Z

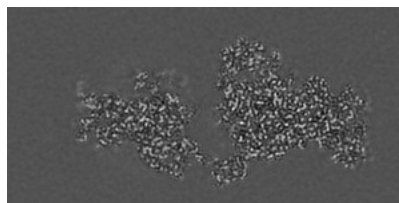
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

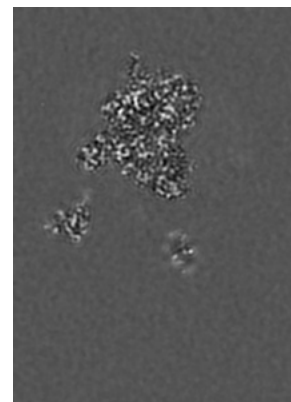
6.2.1 Primary map



X Index: 95

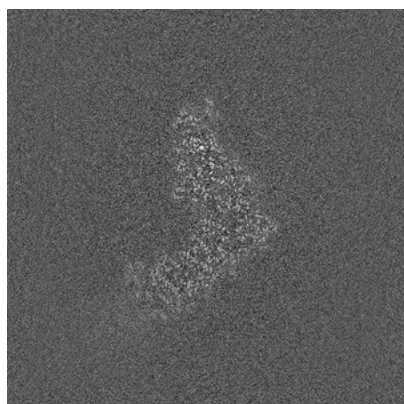


Y Index: 132

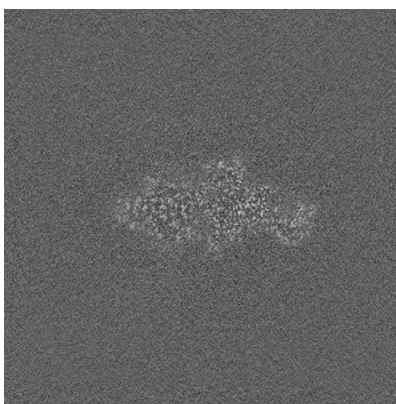


Z Index: 191

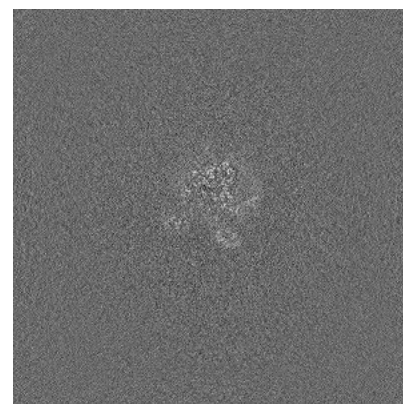
6.2.2 Raw map



X Index: 294



Y Index: 294

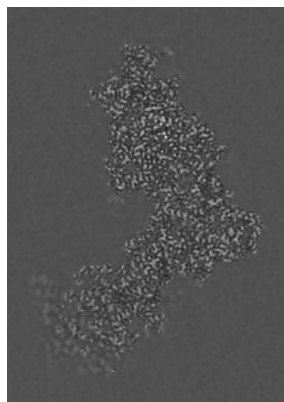


Z Index: 294

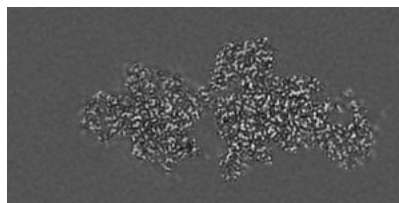
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

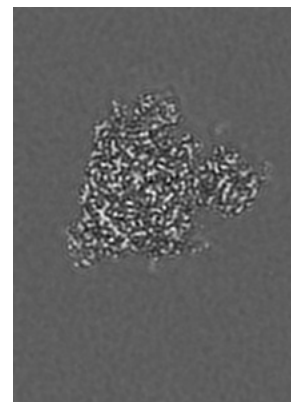
6.3.1 Primary map



X Index: 97

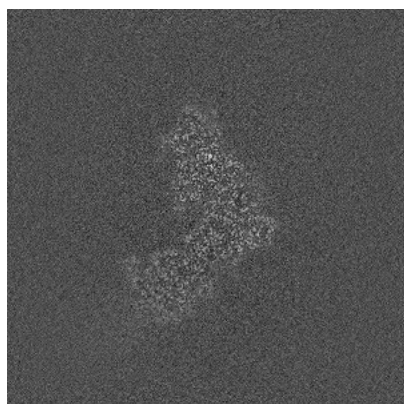


Y Index: 140

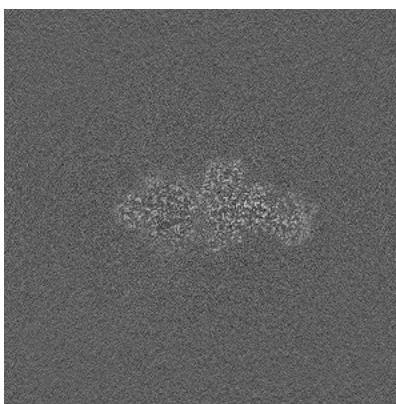


Z Index: 240

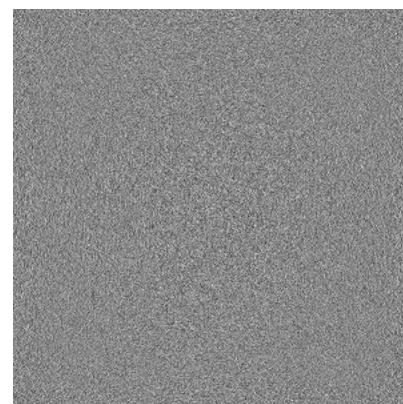
6.3.2 Raw map



X Index: 302



Y Index: 292

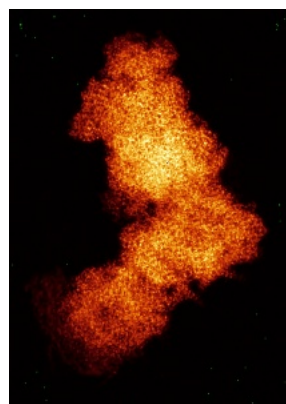


Z Index: 0

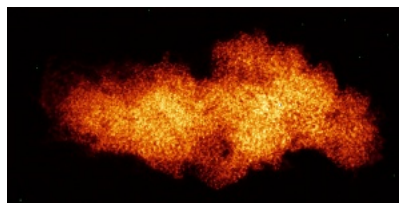
The images above show the largest variance slices of the map in three orthogonal directions.

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

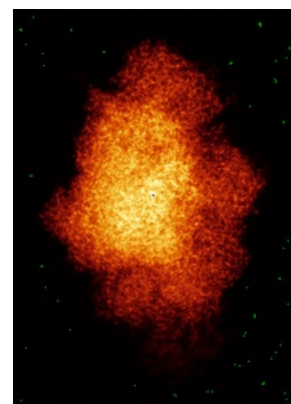
6.4.1 Primary map



X

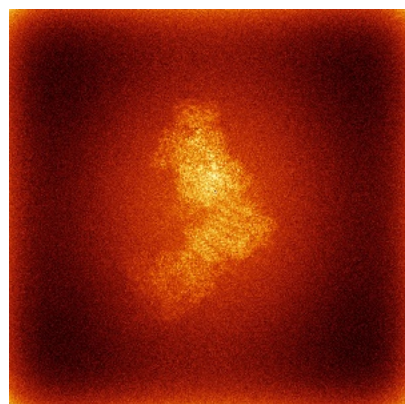


Y

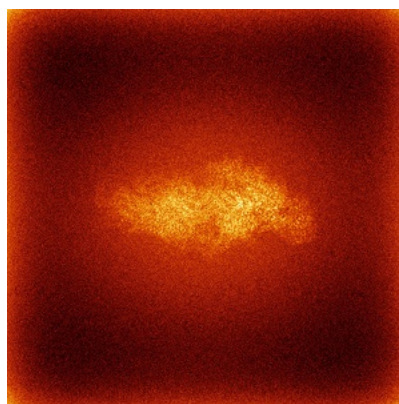


Z

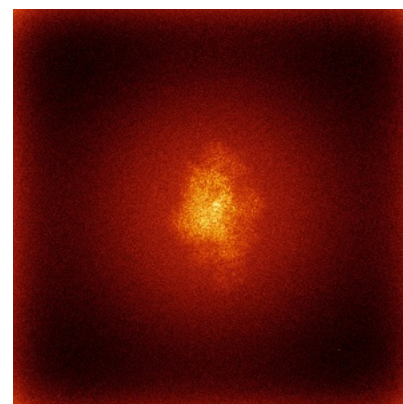
6.4.2 Raw map



X



Y

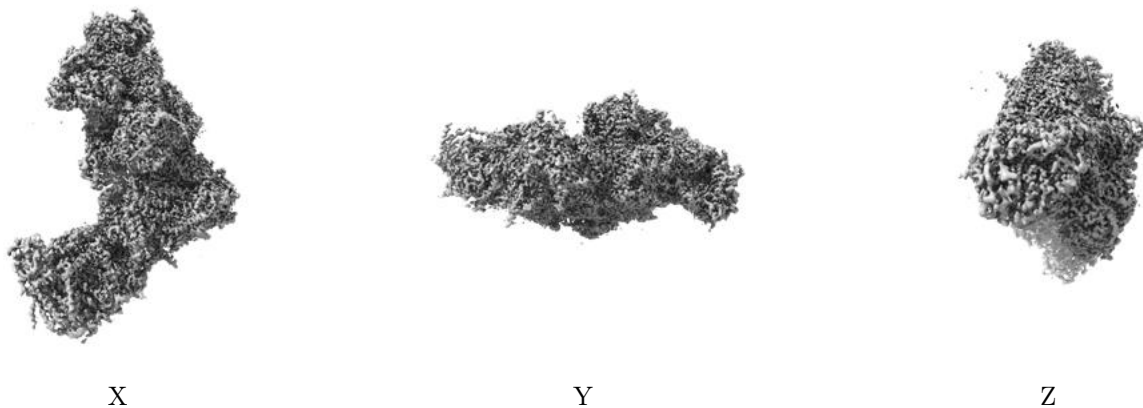


Z

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

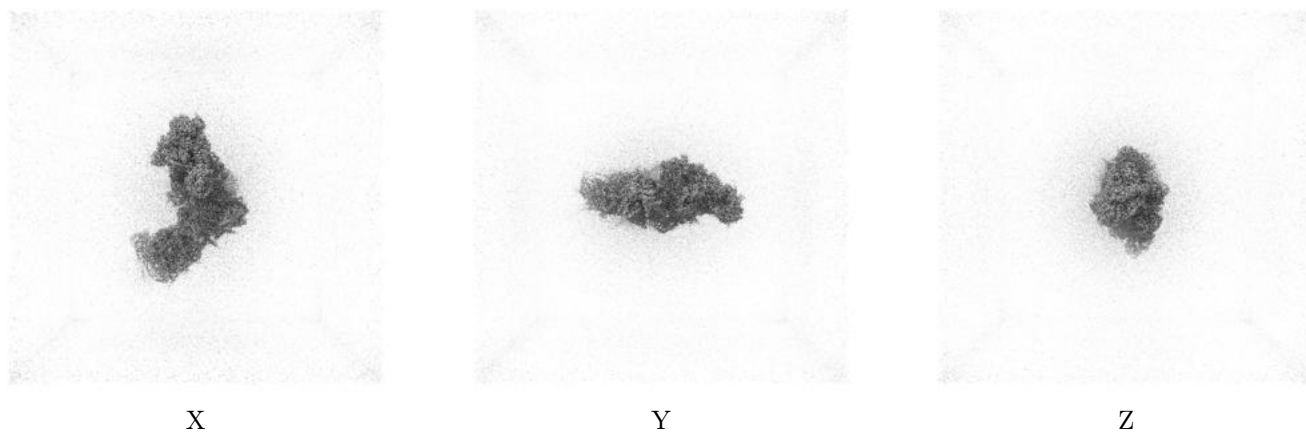
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

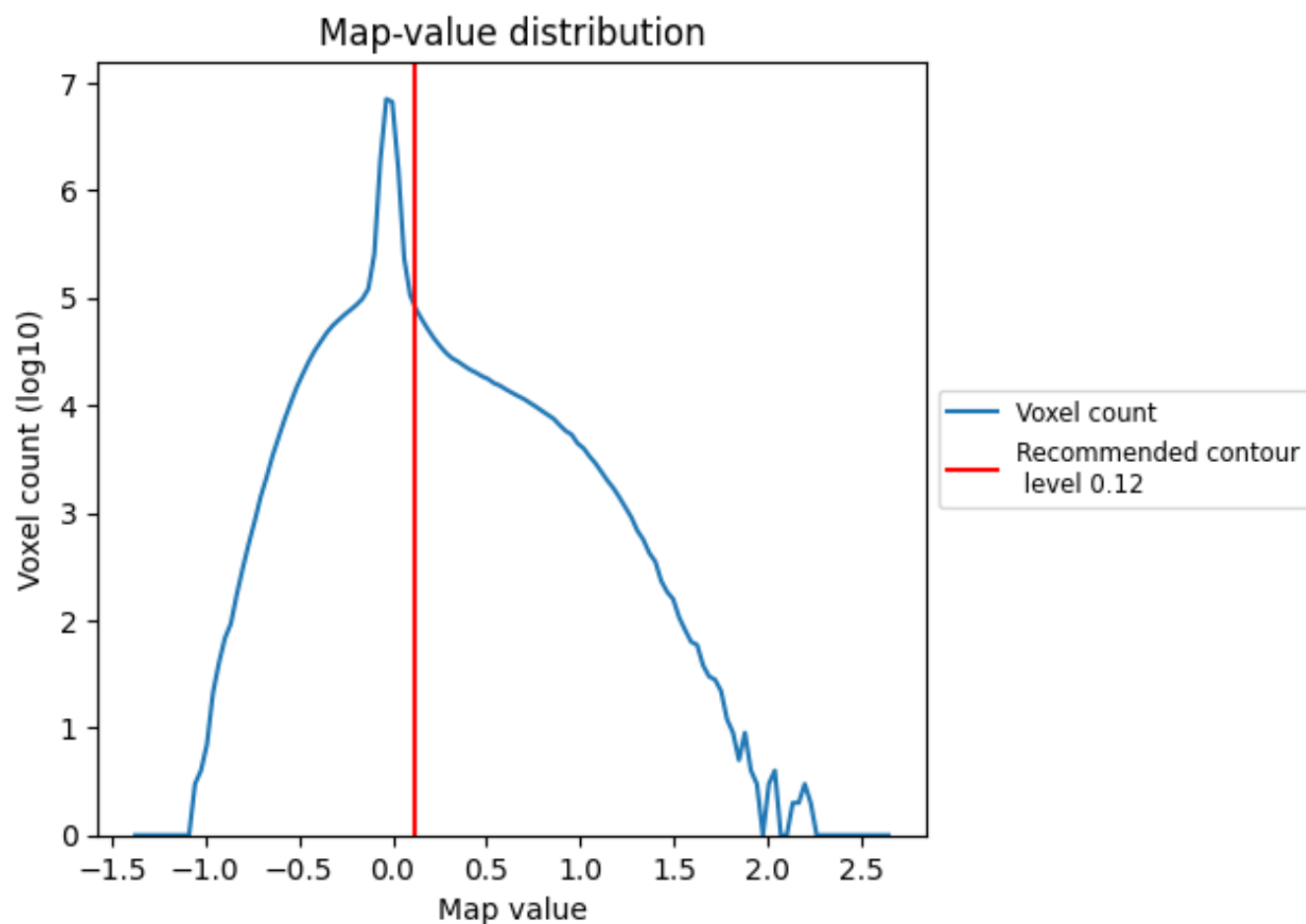
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

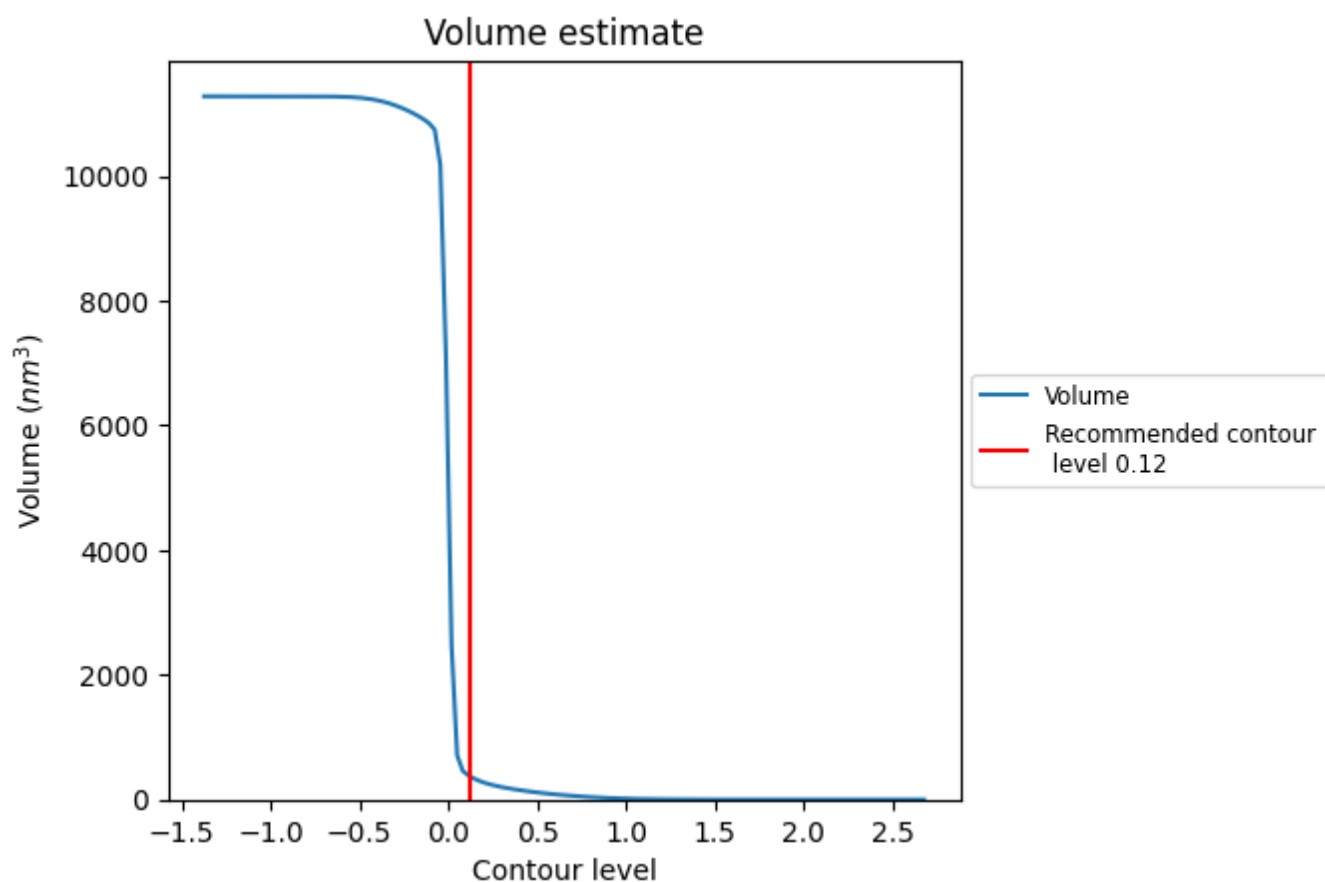
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 375 nm³; this corresponds to an approximate mass of 339 kDa.

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

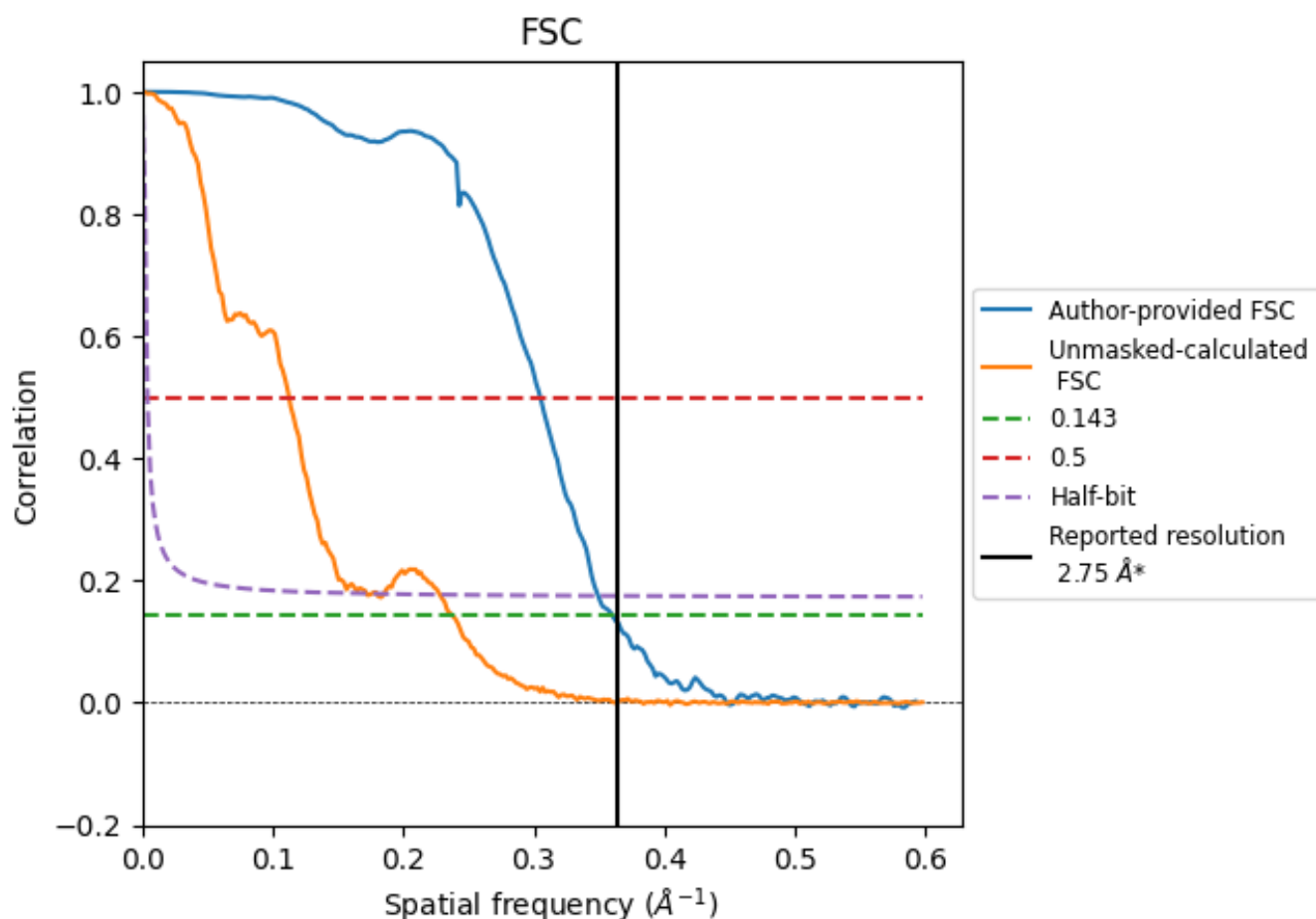
7.3 Rotationally averaged power spectrum [i](#)

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

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.364 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.75	-	-
Author-provided FSC curve	2.78	3.28	2.86
Unmasked-calculated*	4.21	8.90	5.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.21 differs from the reported value 2.75 by more than 10 %

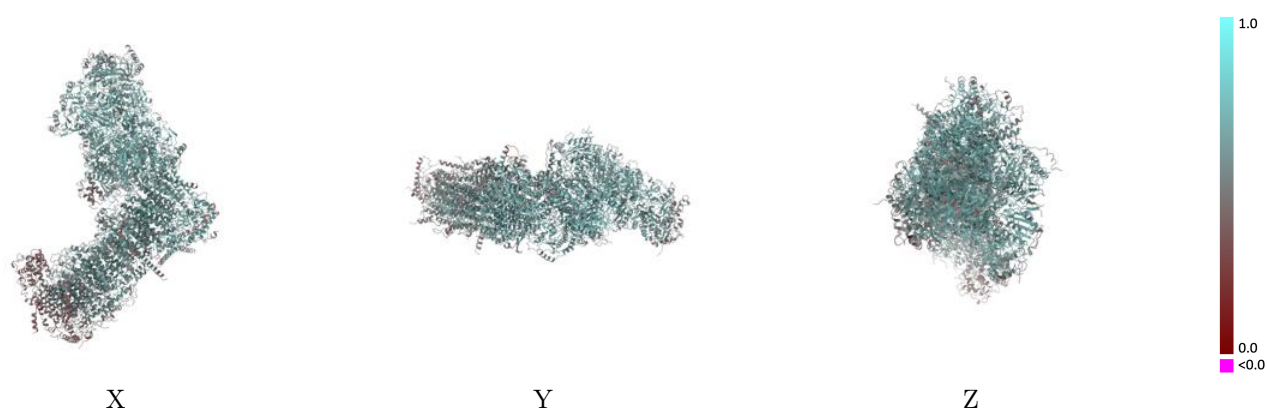
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14794 and PDB model 7ZMB. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay [i](#)

This section was not generated.

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

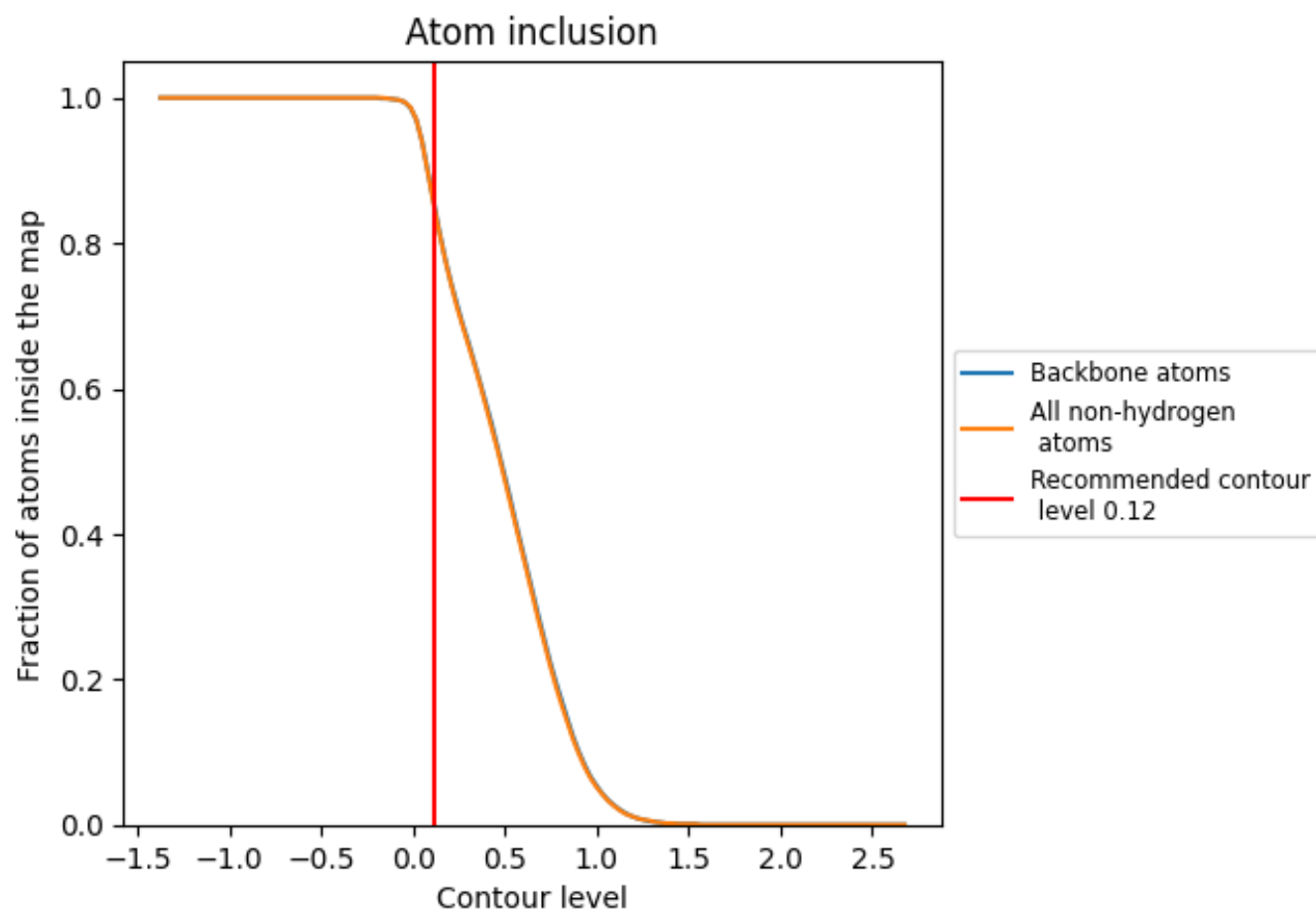


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 84% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8440	 0.5980
1	 0.9530	 0.6590
2	 0.9330	 0.6510
3	 0.9090	 0.6350
4	 0.9070	 0.6290
5	 0.7220	 0.5290
6	 0.8960	 0.6190
8	 0.4190	 0.4030
9	 0.7950	 0.5650
A	 0.9250	 0.6390
B	 0.8610	 0.5790
C	 0.9320	 0.6630
D	 0.9490	 0.6510
E	 0.9010	 0.6200
F	 0.8740	 0.6030
G	 0.9510	 0.6670
H	 0.8200	 0.5640
I	 0.9530	 0.6640
J	 0.6490	 0.5030
K	 0.9210	 0.6430
L	 0.9330	 0.6540
M	 0.9440	 0.6440
O	 0.6260	 0.4410
P	 0.9150	 0.6320
Q	 0.4070	 0.3900
R	 0.5590	 0.4520
S	 0.7450	 0.5330
U	 0.9000	 0.6100
W	 0.8880	 0.6250
X	 0.8980	 0.6280
Y	 0.9130	 0.6460
Z	 0.8500	 0.5860
a	 0.6750	 0.5040
b	 0.8230	 0.5810
c	 0.4270	 0.3900



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Chain	Atom inclusion	Q-score
d	 0.7790	 0.5440
e	 0.4670	 0.4090
f	 0.8200	 0.5560
g	 0.9030	 0.6210
h	 0.9080	 0.6290
i	 0.6180	 0.4950
j	 0.7800	 0.5600
n	 0.6830	 0.5300
o	 0.5770	 0.4630