



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:10 PM UTC

PDB ID : 7ZM7 / pdb_00007zm7
EMDB ID : EMD-14791
Title : CryoEM structure of mitochondrial complex I from *Chaetomium thermophilum* (inhibited by DDM)
Authors : Laube, E.; Kuehlbrandt, W.
Deposited on : 2022-04-19
Resolution : 2.77 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:

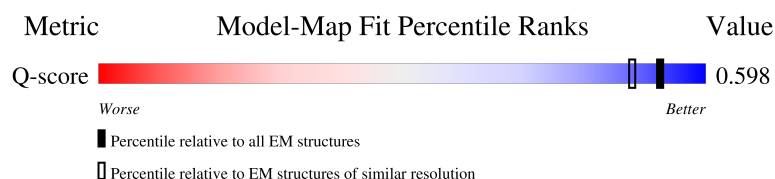
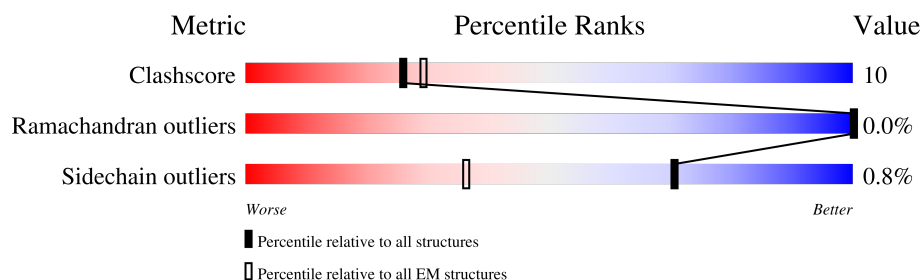
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.77 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.



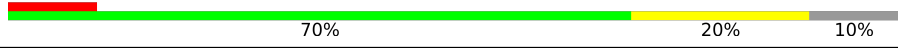
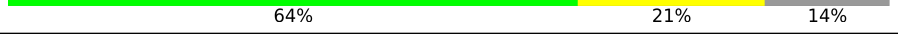
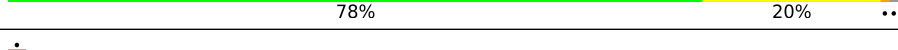
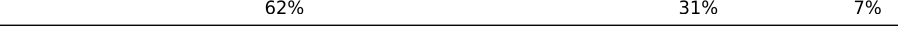
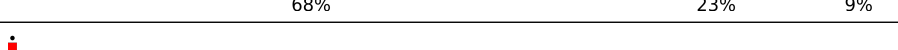
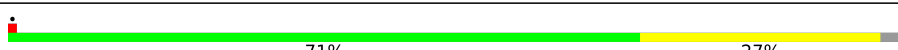
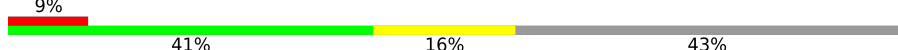
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10695 (2.27 - 3.27)

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	11% 78% 21% .
2	2	571	72% 25% ..
3	3	146	53% 26% 21%
4	4	542	66% 24% 9%

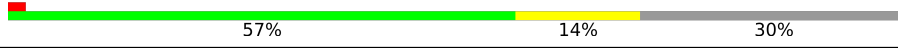
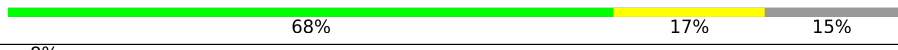
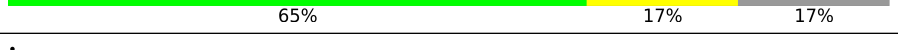
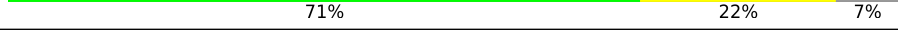
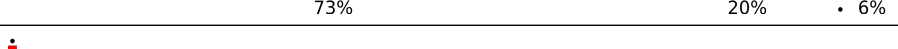
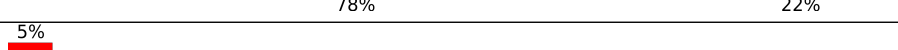
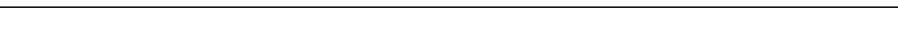
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Mol	Chain	Length	Quality of chain
5	5	679	
6	6	224	
7	8	86	
8	9	785	
9	A	749	
10	B	507	
11	C	499	
12	D	86	
13	E	378	
14	F	261	
15	G	293	
16	H	318	
17	I	223	
18	J	199	
19	K	230	
20	L	89	
21	M	168	
22	O	141	
22	Q	141	
23	P	124	
24	R	99	
25	S	143	
26	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 69157 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	378	Total	C	N	O	S	0	0
			2852	1916	430	496	10		

- 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	116	Total	C	N	O	S	0	0
			897	608	134	153	2		

- 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
			5276	3552	793	906	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	189	Total	C	N	O	S	0	0
			1460	985	219	250	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
			654	405	125	118	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	102	Total	C	N	O	S	0	0
			802	497	146	153	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	427	Total	C	N	O	S	0	0
			3376	2152	585	620	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	353	Total	C	N	O	S	0	0
			2866	1816	510	530	10		

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	237	Total	C	N	O	S	0	0
			1877	1185	328	363	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	220	Total	C	N	O	S	0	0
			1695	1069	288	324	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	188	Total	C	N	O	S	0	0
			1408	892	263	251	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
			1439	916	253	255	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	87	Total	C	N	O	S	0	0
			673	453	102	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	118	Total	C	N	O	S	0	0
			937	585	178	169	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	80	Total	C	N	O	S	0	0
			617	389	100	127	1		
22	Q	85	Total	C	N	O	S	0	0
			670	421	109	139	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	122	Total	C	N	O	S	0	0
			1035	658	197	177	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	72	Total	C	N	O	0	0
			598	393	96	109		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	167	Total	C	N	O	S	0	0
			1353	852	252	240	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	186	Total	C	N	O	S	0	0
			1467	934	266	259	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	80	Total	C	N	O	S	0	0
			675	440	124	109	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	64	Total	C	N	O	S	0	0
			510	332	90	86	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	100	Total	C	N	O	S	0	0
			827	526	146	151	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	38	Total	C	N	O	S	0	0
			320	217	58	44	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	77	Total	C	N	O	S	0	0
			604	395	104	104	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
			1124	726	197	200	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	81	Total	C	N	O	S	0	0
			686	453	119	112	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
			1068	683	189	195	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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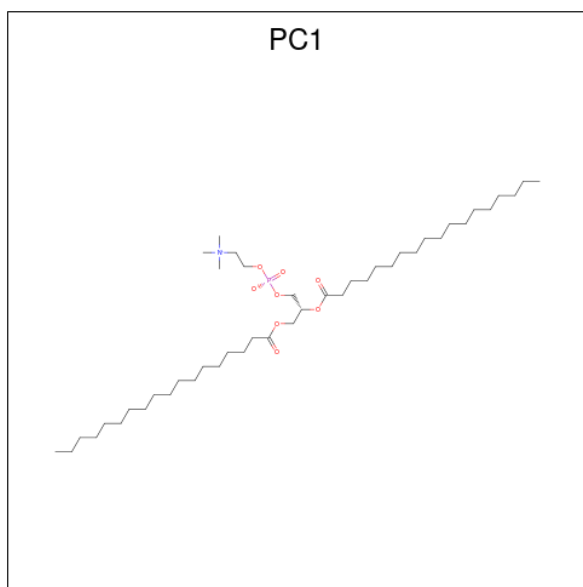
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Chain	Residue	Modelled	Actual	Comment	Reference
n	44	GLY	-	insertion	UNP G0S086
n	45	HIS	-	insertion	UNP G0S086
n	46	ASN	-	insertion	UNP G0S086
n	47	VAL	-	insertion	UNP G0S086
n	48	GLU	-	insertion	UNP G0S086
n	49	GLU	-	insertion	UNP G0S086
n	50	PRO	-	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-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



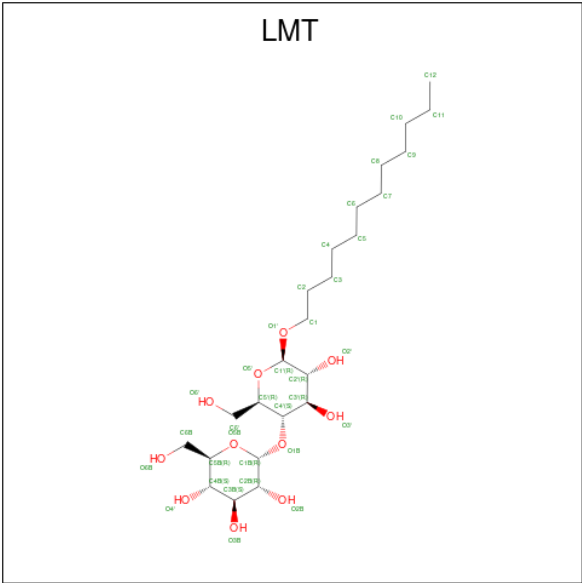
Mol	Chain	Residues	Atoms					AltConf
43	1	1	Total	C	N	O	P	0
			33	23	1	8	1	
43	2	1	Total	C	N	O	P	0
			45	35	1	8	1	
43	5	1	Total	C	N	O	P	0
			40	30	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
43	5	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 44 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



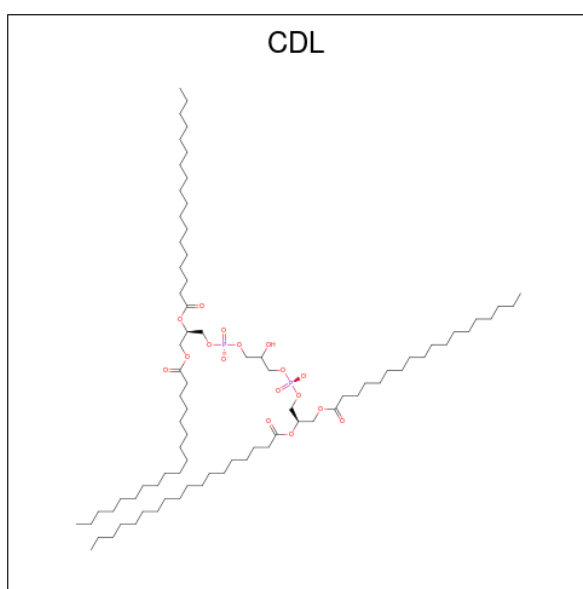
Mol	Chain	Residues	Atoms			AltConf
44	1	1	Total	C	O	0
			35	24	11	
44	1	1	Total	C	O	0
			35	24	11	
44	2	1	Total	C	O	0
			35	24	11	
44	2	1	Total	C	O	0
			33	22	11	
44	2	1	Total	C	O	0
			35	24	11	
44	3	1	Total	C	O	0
			35	24	11	
44	3	1	Total	C	O	0
			35	24	11	
44	4	1	Total	C	O	0
			35	24	11	
44	5	1	Total	C	O	0
			35	24	11	
44	J	1	Total	C	O	0
			31	20	11	

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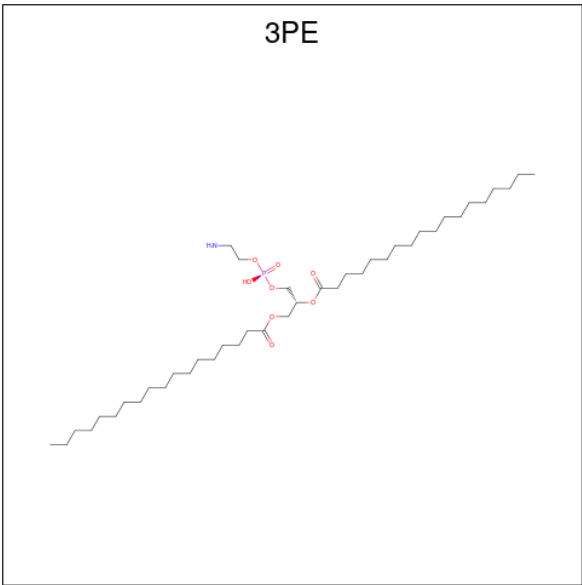
Mol	Chain	Residues	Atoms			AltConf
44	X	1	Total	C	O	0
			35	24	11	
44	a	1	Total	C	O	0
			35	24	11	
44	g	1	Total	C	O	0
			34	23	11	
44	j	1	Total	C	O	0
			35	24	11	

- Molecule 45 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



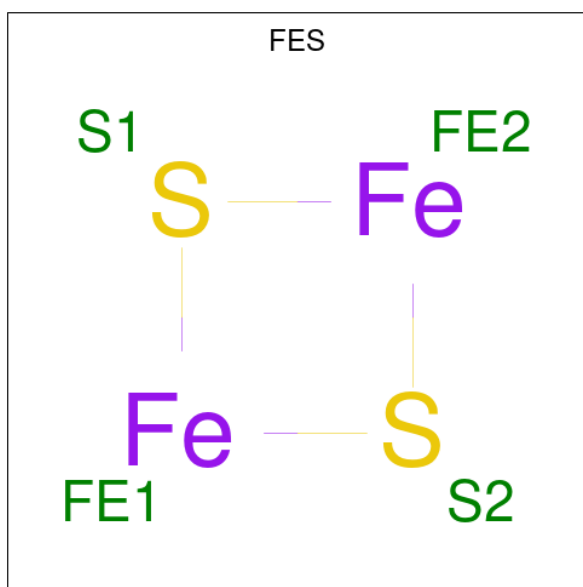
Mol	Chain	Residues	Atoms				AltConf
45	2	1	Total	C	O	P	0
			68	49	17	2	
45	D	1	Total	C	O	P	0
			59	40	17	2	
45	S	1	Total	C	O	P	0
			61	42	17	2	
45	X	1	Total	C	O	P	0
			52	33	17	2	
45	X	1	Total	C	O	P	0
			76	57	17	2	

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



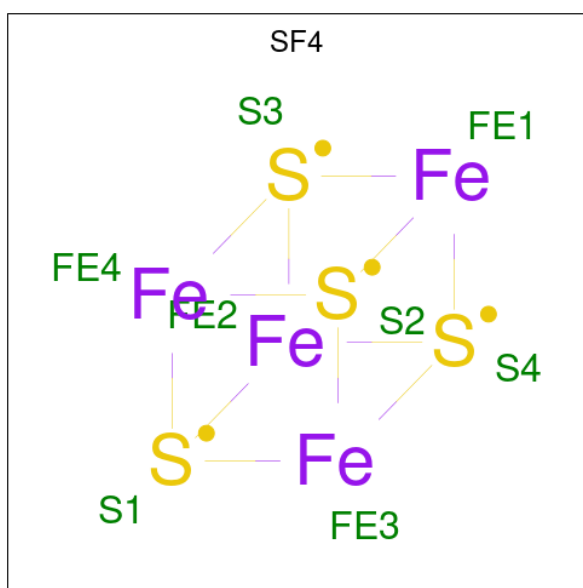
Mol	Chain	Residues	Atoms					AltConf
46	5	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	E	1	Total	C	N	O	P	0
			29	19	1	8	1	
46	I	1	Total	C	N	O	P	0
			37	27	1	8	1	
46	W	1	Total	C	N	O	P	0
			40	30	1	8	1	
46	W	1	Total	C	N	O	P	0
			32	22	1	8	1	
46	i	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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).



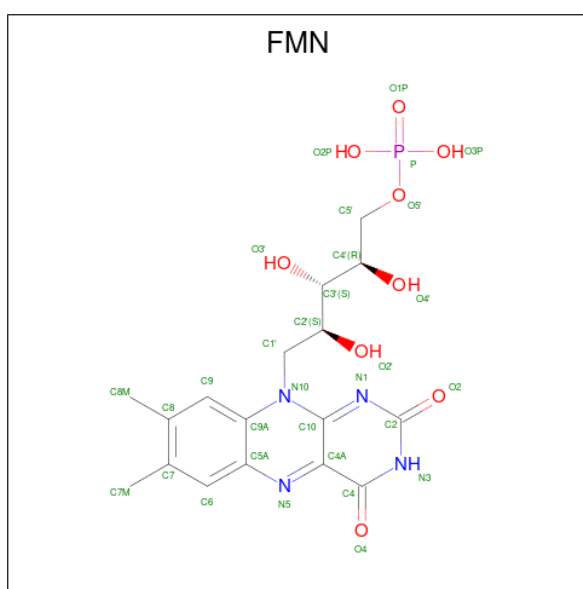
Mol	Chain	Residues	Atoms			AltConf
48	A	1	Total	Fe	S	0
			8	4	4	
48	A	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 50 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 51 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- 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	45	Total	O	0
			45	45	
53	2	115	Total	O	0
			115	115	
53	3	9	Total	O	0
			9	9	
53	4	79	Total	O	0
			79	79	
53	5	34	Total	O	0
			34	34	
53	6	21	Total	O	0
			21	21	
53	9	24	Total	O	0
			24	24	
53	A	123	Total	O	0
			123	123	
53	B	25	Total	O	0
			25	25	
53	C	114	Total	O	0
			114	114	
53	D	24	Total	O	0
			24	24	
53	E	31	Total	O	0
			31	31	
53	F	37	Total	O	0
			37	37	
53	G	76	Total	O	0
			76	76	
53	H	11	Total	O	0
			11	11	
53	I	68	Total	O	0
			68	68	
53	J	2	Total	O	0
			2	2	
53	K	38	Total	O	0
			38	38	

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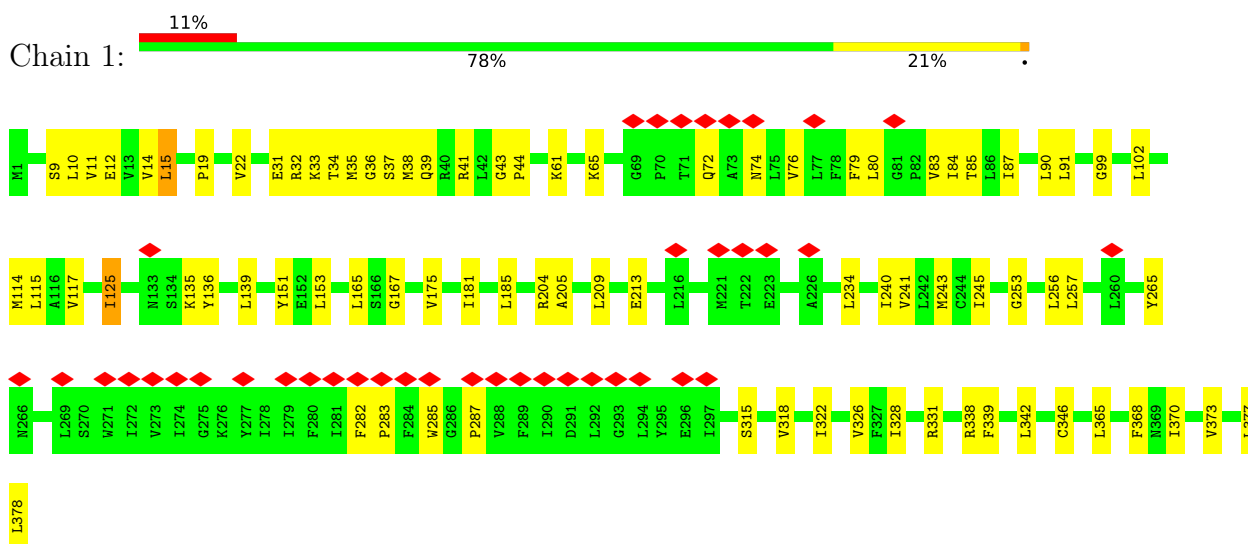
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Mol	Chain	Residues	Atoms		AltConf
53	L	5	Total 5	O 5	0
53	M	26	Total 26	O 26	0
53	P	20	Total 20	O 20	0
53	R	2	Total 2	O 2	0
53	U	23	Total 23	O 23	0
53	W	41	Total 41	O 41	0
53	X	41	Total 41	O 41	0
53	Y	60	Total 60	O 60	0
53	Z	35	Total 35	O 35	0
53	a	5	Total 5	O 5	0
53	b	6	Total 6	O 6	0
53	d	14	Total 14	O 14	0
53	f	2	Total 2	O 2	0
53	g	2	Total 2	O 2	0
53	h	26	Total 26	O 26	0
53	i	1	Total 1	O 1	0
53	j	7	Total 7	O 7	0
53	n	27	Total 27	O 27	0

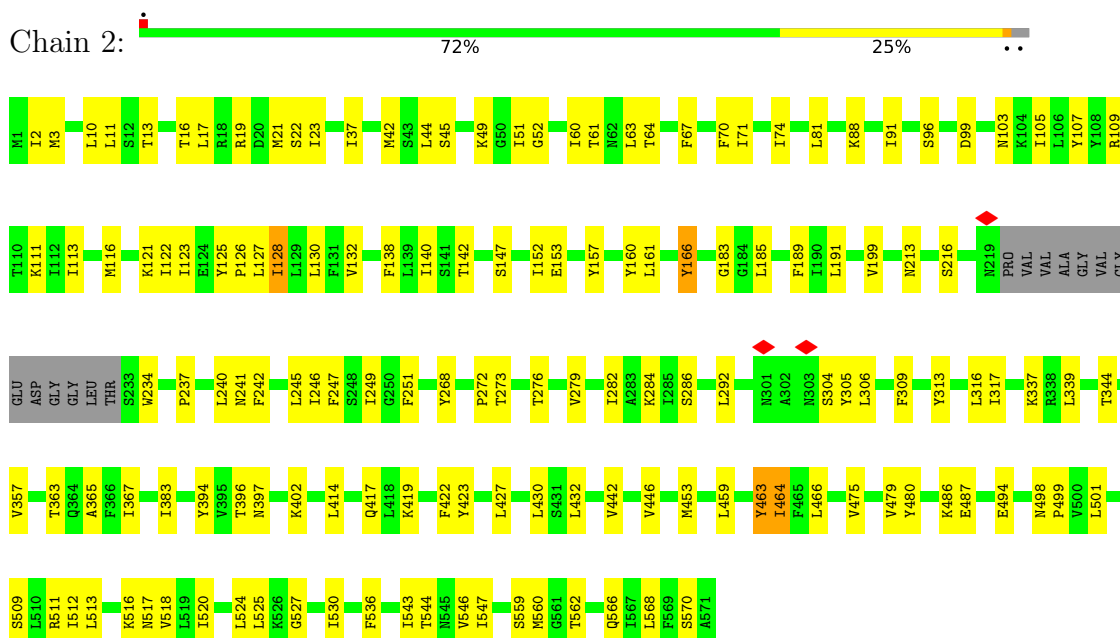
3 Residue-property plots

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.

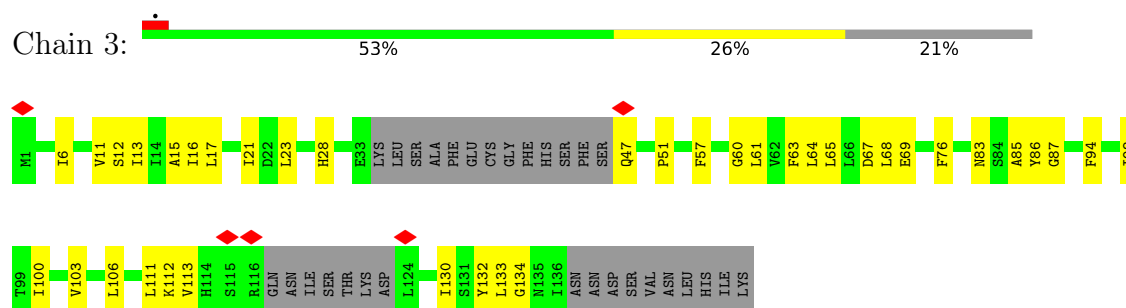
• Molecule 1: NADH-ubiquinone oxidoreductase chain 1



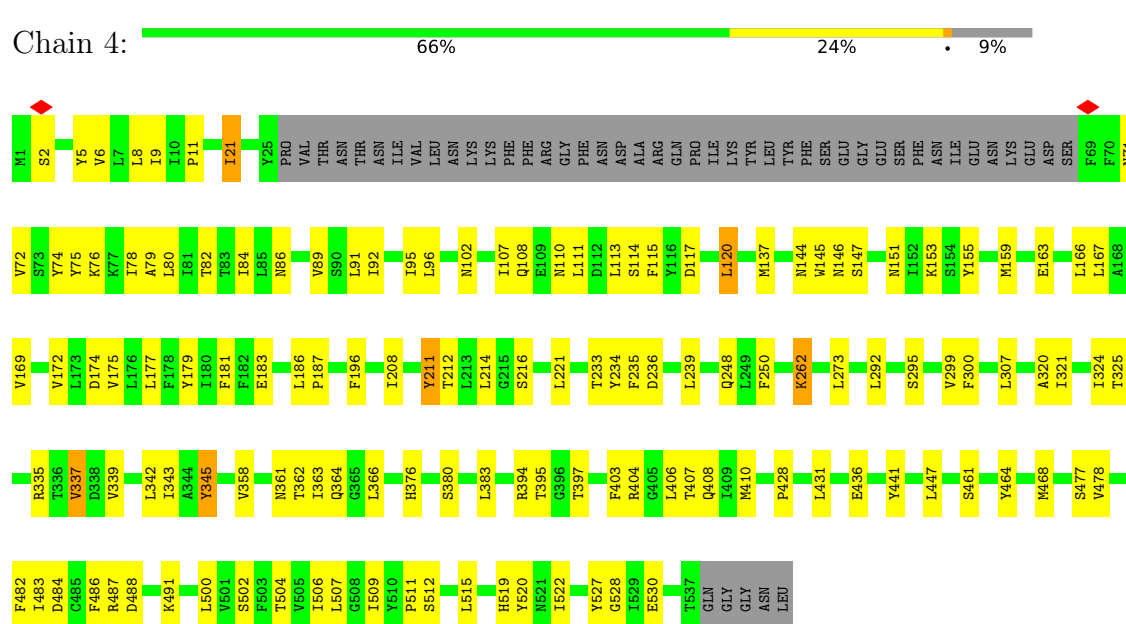
• Molecule 2: NADH dehydrogenase subunit 2



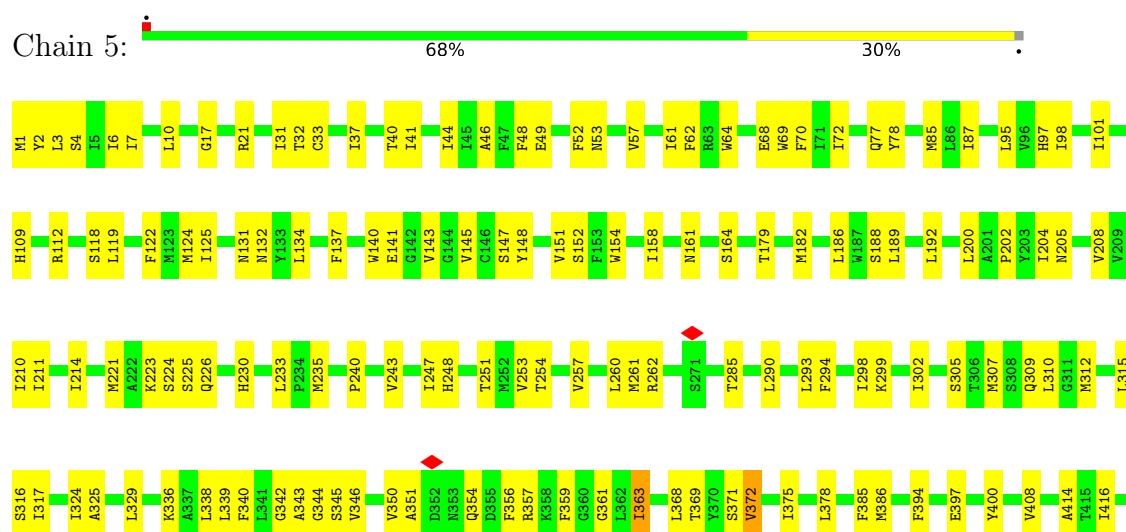
- Molecule 3: NADH-ubiquinone oxidoreductase chain 3

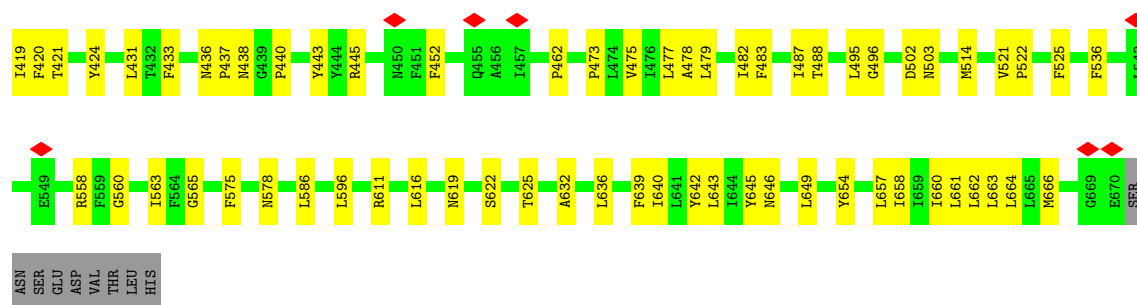


- Molecule 4: NADH-ubiquinone oxidoreductase chain 4

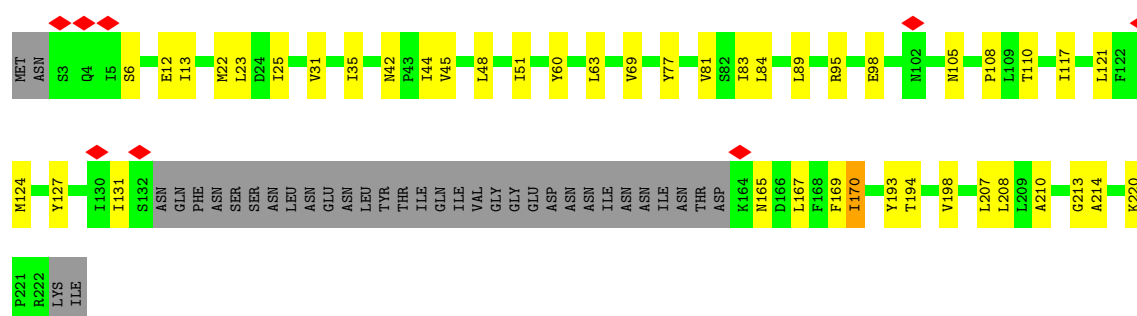


- Molecule 5: NADH-ubiquinone oxidoreductase chain 5

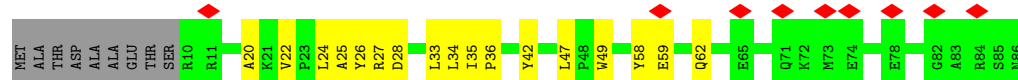




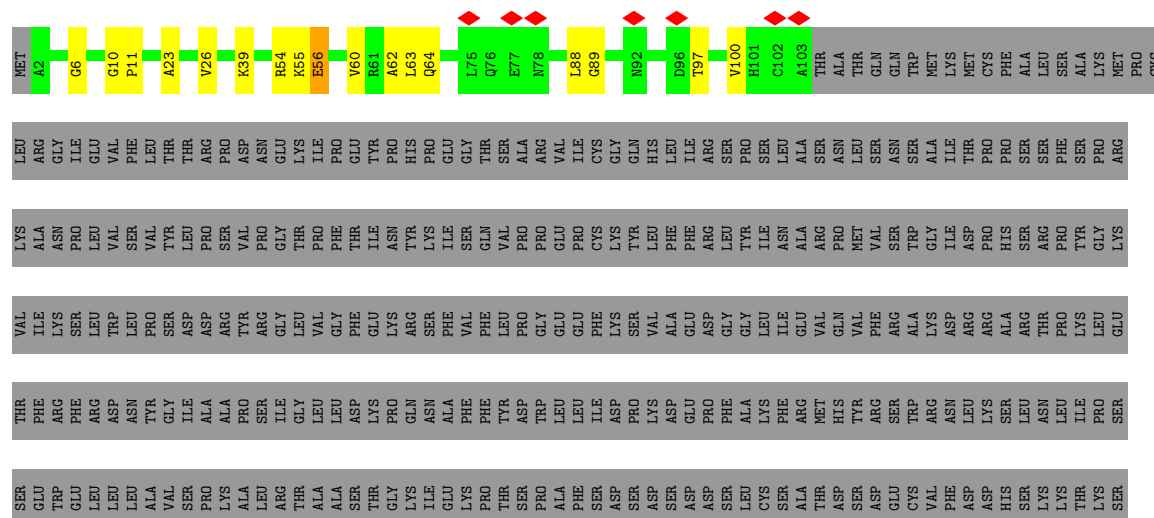
• Molecule 6: NADH-ubiquinone oxidoreductase chain 6



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

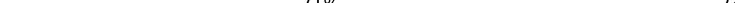


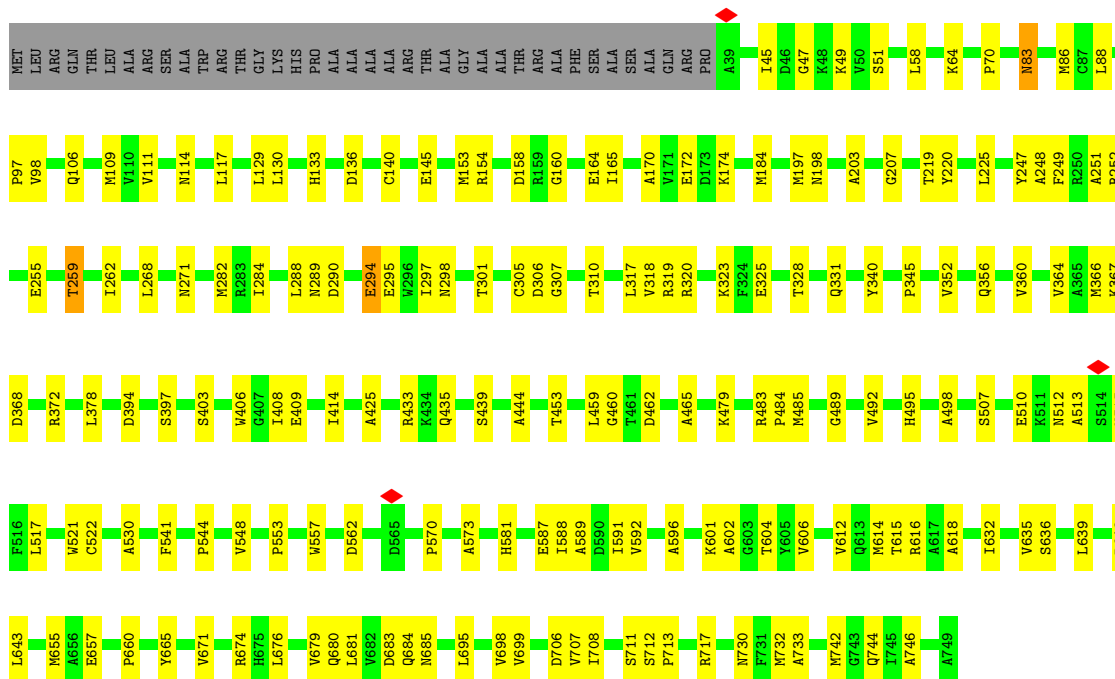
• Molecule 8: Subunit NDUF5 of NADH-ubiquinone oxidoreductase (Complex I)



[illegible]

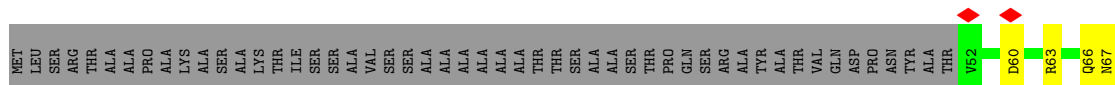
- Molecule 9: NADH-ubiquinone oxidoreductase-like protein

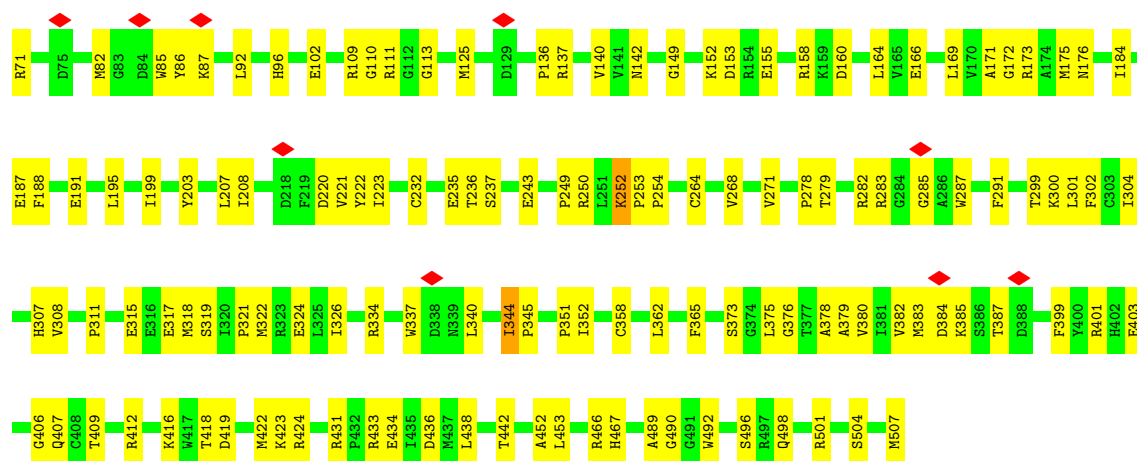
Chain A:  71% 23% 5%



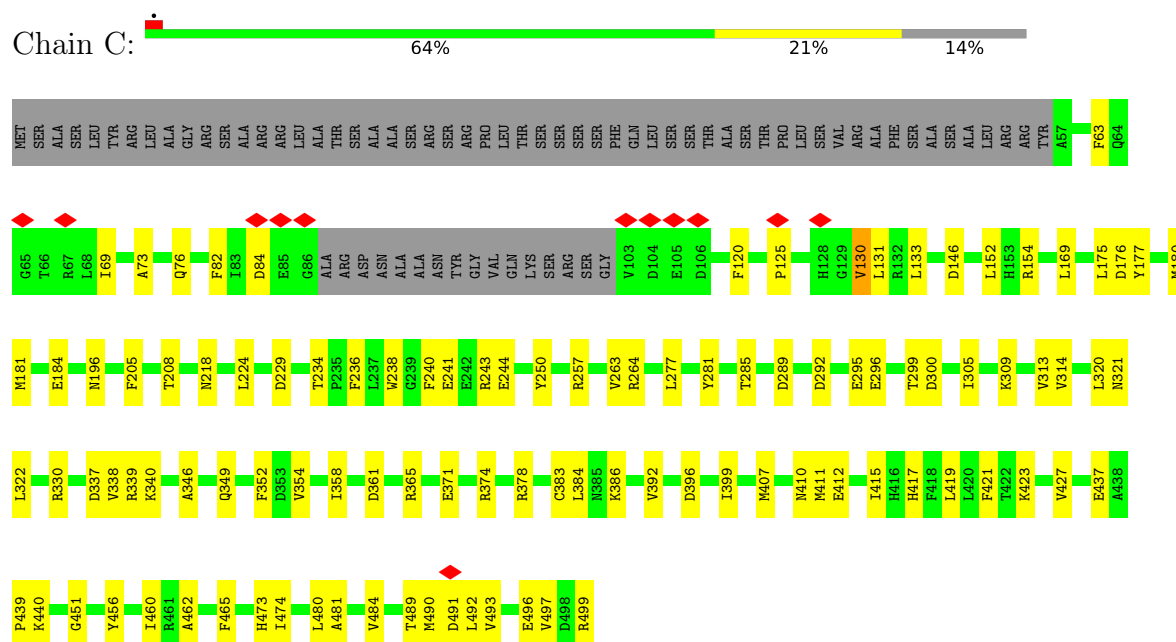
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain B:  63% 26% 10%

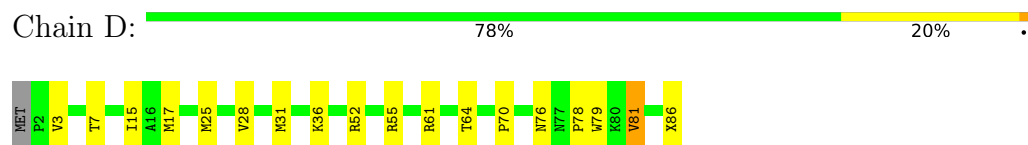




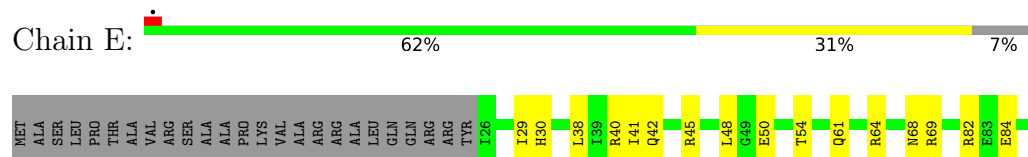
- Molecule 11: NADH-ubiquinone oxidoreductase 49 kDa subunit-like protein

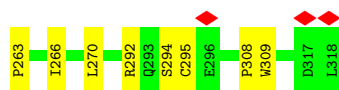


- Molecule 12: Subunit NDUFA1 of NADH-ubiquinone oxidoreductase (Complex I)



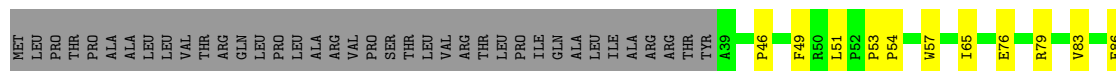
- Molecule 13: NADH dehydrogenase (Ubiquinone)-like protein





- Molecule 17: Oxidoreductase-like protein

Chain I: 63% 20% 17%



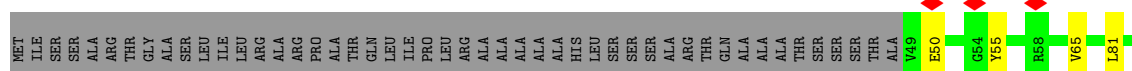
- Molecule 18: NADH-ubiquinone oxidoreductase-like protein

Chain J: 9% 76% 18% 6%



- Molecule 19: NADH-ubiquinone oxidoreductase-like protein

Chain K: 60% 19% 21%



- Molecule 20: NADH-ubiquinone oxidoreductase chain 4L

Chain L: 71% 27%

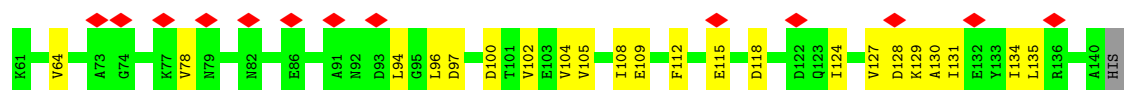
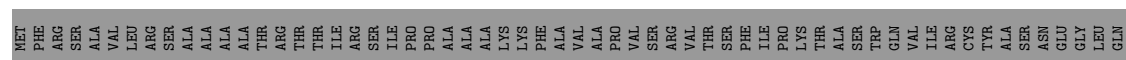


- Molecule 21: NADH-ubiquinone oxidoreductase-like protein

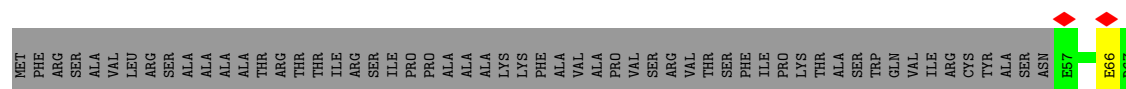
Chain M: 55% 15% 30%



- Molecule 22: Acyl carrier protein



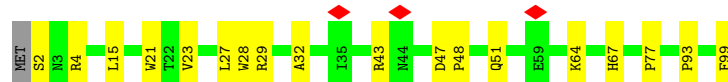
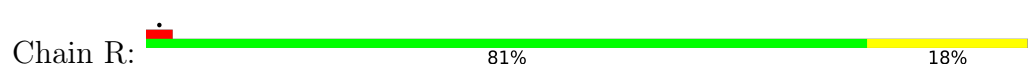
- Molecule 22: Acyl carrier protein



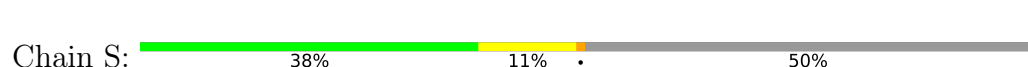
- Molecule 23: NADH-ubiquinone oxidoreductase B14 subunit-like protein



- Molecule 24: Complex I-B22



- Molecule 25: Complex I-ESSS



MET ASP GLY GLY PRO PRO THR PHE ALA PHE ARG PRO THR ALA ARG ALA PRO PRO GLY LYS LEU SER SER ALA VAL THR THR ARG LEU ALA ALA ALA LEU SER ARG ALA THR THR VAL SER SER LYS ALA LEU THR PRO ALA ARG PHE ARG PHE PHE THR THR GLN ARG ARG

ALA GLY HIS MET Q67 P70 P71 P72 G73 G74 L75 L76 G77 E82 W98 I102 Q117 E122 E123 A124 R125 R126 E131 G132 I133 N138 PRO THR LYS LYS GLU

- Molecule 26: NADH-ubiquinone oxidoreductase

Chain U: 76% 13% 10%

M1 V12 V16 T17 P18 L19 P20 I23 S32 S33 F42 A45 K48 N51 E66 K71 R75 V76 T77 R78 C91 R96 N105 Q108 Q111 E116 I133 P134 D135 Q136 P158 Q167 PRO GLU PRO PRO LEU PRO ALA GLY ILE

GLU ILE PRO GLU TYR LYS ASN GLN SER

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

Chain W: 73% 26% ..

MET P2 Y16 K17 R18 N19 L20 P21 G24 R27 P30 L31 L32 A35 M39 L40 Y41 Y44 K45 L46 Y47 R51 M61 I65 P69 Y80 R81 R82 Y83 Q87 A88 R89 K99 Y100 Y101 R108 P109 T110 F111 A112 V113 K117 Q120

E121

- Molecule 28: NADH-ubiquinone oxidoreductase-like protein

Chain X: 75% 22% ..

MET SER ASN T4 F11 P12 S13 Y20 P21 L22 I23 D24 N25 H28 V32 H43 L55 M58 P63 S64 Q65 R68 F71 A72 K73 A74 M75 Y89 R93 L96 R97 M101 N104 M112 M115 R118 V119 P124 L125 E128

R144 Y145 L148 V152 W155 N162 Q163 H164 G165 A169 K170 Y171 Y172 Q173 Q174 R186 E187 Q188 A189 GLN GLN

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

Chain Y: 61% 12% 27%

MET SER LEU ARG PRO ALA THR ALA ARG ALA LEU LEU ARG ASN SER THR ALA SER ARG ALA THR VAL VAL MET PRO CYS ARG ALA ALA HIS ASN ILE HIS VAL PRO VAL GLN LYS GLU ARG THR LYS ASP SER PRO LEU ALA THR LEU P57 R58 D62

V65 P78 K79 Q82 L94 L102 Q103 T106 K114 P115 V133 W140 S149 M154 K162 T163 K164 E177 V180 R186 Y193 L204 K205 H206 I207 T209 K210

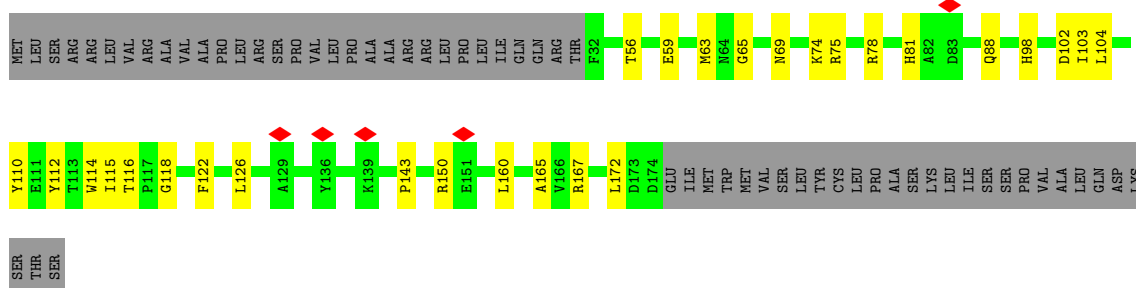
- Molecule 30: NADH-ubiquinone oxidoreductase-like protein

Chain Z: 



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

Chain a: 



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

Chain b: 



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

Chain c: 



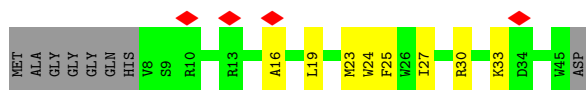
- Molecule 34: Subunit NDUFB10 of NADH-ubiquinone oxidoreductase (Complex I)

Chain d: 



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

Chain e: 



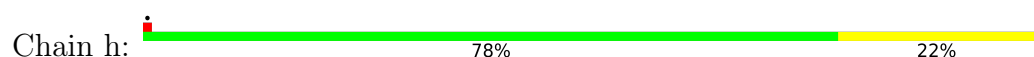
- Molecule 36: NADH dehydrogenase-like protein



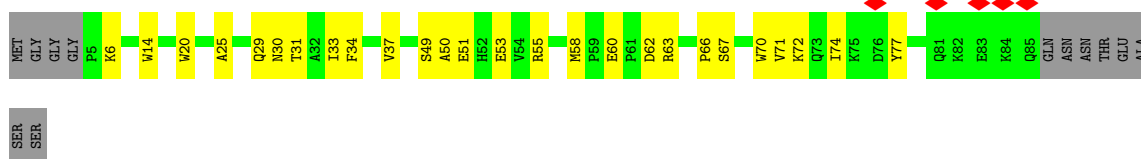
- Molecule 37: Subunit NDUFA3 of NADH-ubiquinone oxidoreductase (Complex I)



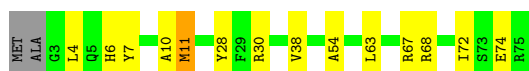
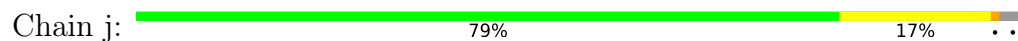
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit



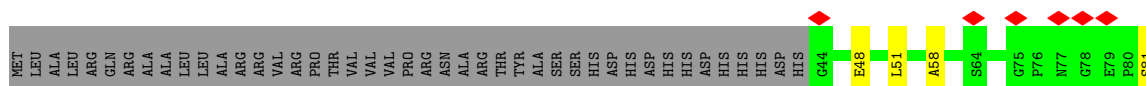
- Molecule 39: Subunit NDUFB6 of NADH-ubiquinone oxidoreductase (Complex I)



- Molecule 40: Subunit NDUFB4 of NADH-ubiquinone oxidoreductase (Complex I)

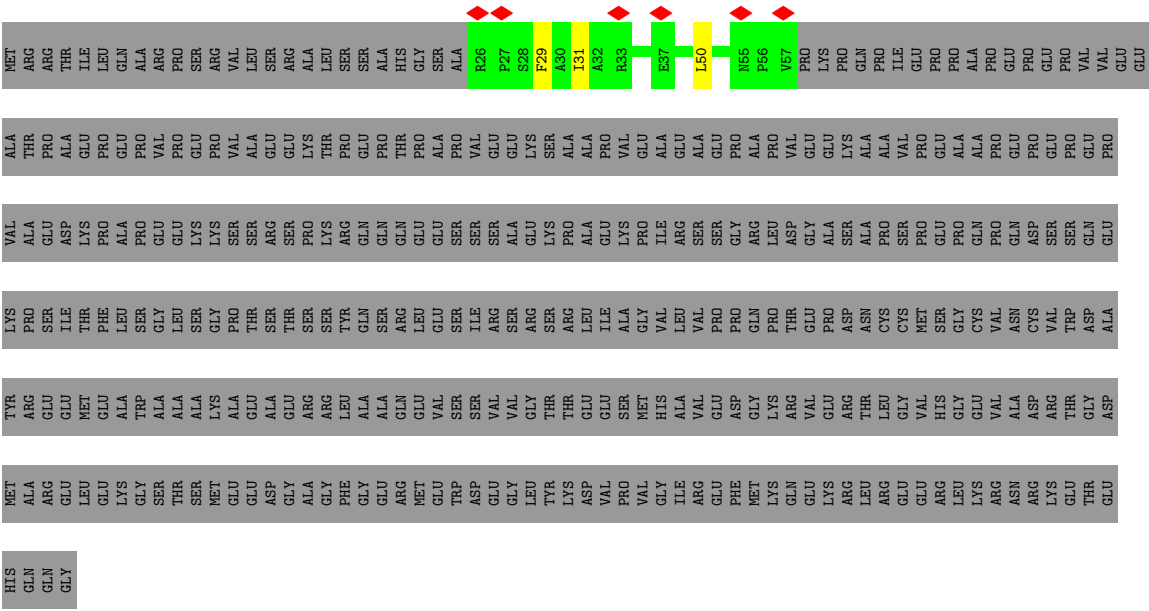


- Molecule 41: Subunit NDUFB5 of NADH-ubiquinone oxidoreductase (Complex I)





• Molecule 42: Oxidoreductase-like domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37767	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)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.497	Depositor
Minimum map value	-1.728	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.108	Depositor
Recommended contour level	0.12	Depositor
Map size ($\text{\AA}$)	154.48529, 228.63824, 305.8809	wwPDB
Map dimensions	297, 222, 150	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.029902, 1.029902, 1.029902	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.68	1/2921 (0.0%)	0.96	7/3996 (0.2%)
2	2	0.77	2/4562 (0.0%)	1.06	8/6205 (0.1%)
3	3	0.56	0/918	0.75	0/1249
4	4	0.68	2/4002 (0.0%)	0.85	3/5454 (0.1%)
5	5	0.54	0/5418	0.72	3/7376 (0.0%)
6	6	0.66	0/1487	0.80	1/2026 (0.0%)
7	8	0.40	0/667	0.61	0/892
8	9	0.68	0/819	0.99	1/1105 (0.1%)
9	A	0.57	0/5589	0.76	3/7579 (0.0%)
10	B	0.49	0/3621	0.69	6/4878 (0.1%)
11	C	0.60	0/3447	0.74	1/4675 (0.0%)
12	D	0.73	0/674	1.09	1/911 (0.1%)
13	E	0.53	0/2932	0.69	0/3973
14	F	0.46	0/1916	0.57	0/2596
15	G	0.57	0/2026	0.73	2/2759 (0.1%)
16	H	0.49	0/1734	0.66	2/2358 (0.1%)
17	I	0.65	0/1527	0.81	1/2070 (0.0%)
18	J	0.49	0/1435	0.74	2/1940 (0.1%)
19	K	0.64	0/1478	0.90	2/2009 (0.1%)
20	L	0.72	0/680	1.03	1/921 (0.1%)
21	M	0.64	0/968	0.79	2/1319 (0.2%)
22	O	0.27	0/626	0.40	0/852
22	Q	0.23	0/680	0.37	0/922
23	P	0.59	0/1062	0.84	1/1432 (0.1%)
24	R	0.55	0/832	0.68	0/1133
25	S	0.66	0/622	0.97	2/850 (0.2%)
26	U	0.85	0/1390	1.23	4/1885 (0.2%)
27	W	0.76	0/1001	1.14	5/1354 (0.4%)
28	X	0.75	0/1506	1.08	2/2036 (0.1%)
29	Y	0.64	0/1277	0.78	0/1731
30	Z	0.49	0/1466	0.62	0/1997
31	a	0.46	0/1204	0.58	0/1632

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	b	0.67	0/693	1.09	2/929 (0.2%)
33	c	0.37	0/529	0.57	0/720
34	d	0.56	0/845	0.89	1/1137 (0.1%)
35	e	0.54	0/335	0.73	0/454
36	f	0.42	0/731	0.60	0/981
37	g	0.67	0/624	0.87	0/857
38	h	0.53	0/1164	0.66	0/1584
39	i	0.53	0/715	0.76	0/971
40	j	0.61	0/617	0.83	0/830
41	n	0.67	0/1100	0.97	1/1491 (0.1%)
42	o	0.41	0/262	0.39	0/360
All	All	0.60	5/68102 (0.0%)	0.82	64/92429 (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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	113	LEU	C-N	-11.55	1.23	1.33
4	4	436	GLU	C-N	-7.01	1.25	1.33
2	2	394	TYR	C-N	-6.48	1.25	1.33
2	2	122	ILE	C-N	5.81	1.41	1.33
1	1	167	GLY	C-N	5.25	1.40	1.33

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	253	PRO	N-CA-C	8.45	121.00	110.70
10	B	453	LEU	N-CA-C	-8.11	103.39	113.28
1	1	125	ILE	N-CA-C	-7.17	105.79	112.96
26	U	45	ALA	N-CA-C	-7.13	103.55	112.90
4	4	113	LEU	CA-C-N	7.06	131.48	122.16
4	4	113	LEU	C-N-CA	7.06	131.48	122.16
26	U	66	GLU	N-CA-C	-6.82	103.92	111.36
23	P	60	PHE	N-CA-C	-6.75	105.17	113.41
1	1	115	LEU	N-CA-C	-6.73	105.19	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	W	21	PRO	N-CA-C	6.69	121.01	110.50
1	1	377	LEU	N-CA-C	-6.68	99.17	109.52
25	S	70	PRO	N-CA-CB	-6.67	99.75	103.22
2	2	67	PHE	CB-CA-C	6.66	122.18	110.85
18	J	169	LYS	CB-CA-C	6.57	117.49	110.65
20	L	84	ILE	N-CA-C	-6.49	106.40	112.83
11	C	392	VAL	N-CA-C	-6.42	106.26	112.29
1	1	85	THR	N-CA-C	-6.39	104.40	111.82
5	5	363	ILE	N-CA-C	-6.09	105.13	111.58
41	n	125	ARG	N-CA-C	-6.08	105.16	113.30
27	W	65	ILE	N-CA-C	5.99	116.65	110.36
26	U	42	PHE	CB-CA-C	5.99	120.28	110.88
5	5	211	ILE	N-CA-C	-5.88	105.99	111.45
27	W	51	ARG	CB-CA-C	5.87	120.18	110.90
2	2	166	TYR	CB-CA-C	5.71	121.28	111.68
16	H	258	TYR	CB-CA-C	5.67	119.59	110.29
2	2	544	THR	CB-CA-C	5.67	120.19	110.79
10	B	232	CYS	N-CA-C	-5.66	106.97	112.97
18	J	165	GLY	CA-C-O	-5.63	117.12	122.13
10	B	345	PRO	N-CA-C	5.62	120.94	113.40
21	M	92	GLN	CB-CA-C	5.54	118.12	109.42
2	2	494	GLU	N-CA-C	-5.52	106.13	112.92
10	B	252	LYS	CA-C-N	5.44	125.98	120.38
10	B	252	LYS	C-N-CA	5.44	125.98	120.38
28	X	124	PRO	N-CA-C	-5.43	102.67	111.14
2	2	423	TYR	CB-CA-C	5.42	120.06	110.85
2	2	357	VAL	CA-C-N	-5.35	115.42	122.85
2	2	357	VAL	C-N-CA	-5.35	115.42	122.85
8	9	39	LYS	N-CA-C	-5.34	106.77	113.28
1	1	32	ARG	N-CA-C	-5.33	105.92	112.90
12	D	52	ARG	N-CA-C	-5.30	105.55	112.23
34	d	83	ALA	N-CA-C	-5.30	107.37	113.88
26	U	134	PRO	N-CA-C	5.29	119.79	111.38
21	M	104	LYS	N-CA-C	-5.28	106.61	113.16
1	1	234	LEU	N-CA-C	-5.26	105.60	112.23
27	W	80	VAL	N-CA-C	-5.26	105.27	111.00
1	1	243	MET	N-CA-C	-5.24	106.40	112.89
28	X	23	ILE	N-CA-C	-5.24	107.31	111.81
27	W	108	ARG	CB-CA-C	5.21	117.79	109.62
15	G	106	ASP	N-CA-C	-5.20	106.18	112.88
2	2	463	TYR	CB-CA-C	5.18	119.47	111.13
15	G	219	GLY	CA-C-O	-5.18	118.59	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	H	246	VAL	N-CA-C	-5.18	106.03	113.07
19	K	100	THR	CA-CB-OG1	-5.17	101.84	109.60
4	4	21	ILE	N-CA-C	-5.16	107.37	111.81
9	A	83	ASN	N-CA-C	5.14	116.97	111.36
17	I	187	ALA	N-CA-C	-5.14	103.36	110.35
9	A	294	GLU	N-CA-CB	-5.12	103.66	111.74
5	5	502	ASP	N-CA-C	-5.11	106.89	112.72
32	b	5	ILE	N-CA-C	-5.09	105.58	110.72
6	6	13	ILE	N-CA-C	5.08	115.85	110.72
32	b	27	PHE	CA-CB-CG	5.07	118.87	113.80
9	A	618	ALA	N-CA-C	-5.04	107.26	113.41
19	K	168	GLY	CA-C-O	-5.04	118.21	122.29
25	S	70	PRO	CB-CA-C	-5.03	106.44	111.17

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	2852	0	2895	62	0
2	2	4456	0	4650	113	0
3	3	897	0	912	35	0
4	4	3904	0	4056	98	0
5	5	5276	0	5403	166	0
6	6	1460	0	1567	38	0
7	8	654	0	637	12	0
8	9	802	0	773	19	0
9	A	5476	0	5419	123	0
10	B	3538	0	3477	93	0
11	C	3376	0	3286	88	0
12	D	678	0	643	17	0
13	E	2866	0	2825	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	F	1877	0	1851	51	0
15	G	1968	0	1935	54	0
16	H	1695	0	1673	40	0
17	I	1487	0	1434	40	0
18	J	1408	0	1411	28	0
19	K	1439	0	1413	34	0
20	L	673	0	742	25	0
21	M	937	0	890	21	0
22	O	617	0	588	15	0
22	Q	670	0	644	12	0
23	P	1035	0	1018	27	0
24	R	807	0	823	15	0
25	S	598	0	548	15	0
26	U	1353	0	1324	12	0
27	W	976	0	990	31	0
28	X	1467	0	1420	37	0
29	Y	1240	0	1204	19	0
30	Z	1432	0	1411	52	0
31	a	1167	0	1104	25	0
32	b	675	0	678	11	0
33	c	510	0	458	10	0
34	d	827	0	814	18	0
35	e	320	0	313	12	0
36	f	717	0	735	17	0
37	g	604	0	614	13	0
38	h	1124	0	1093	27	0
39	i	686	0	666	25	0
40	j	603	0	623	17	0
41	n	1068	0	1026	14	0
42	o	252	0	235	3	0
43	1	33	0	40	1	0
43	2	45	0	67	13	0
43	5	85	0	118	11	0
44	1	70	0	92	3	0
44	2	103	0	131	6	0
44	3	70	0	92	3	0
44	4	35	0	46	4	0
44	5	35	0	46	3	0
44	J	31	0	35	0	0
44	X	35	0	46	3	0
44	a	35	0	46	2	0
44	g	34	0	41	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	j	35	0	46	4	0
45	2	68	0	80	2	0
45	D	59	0	62	3	0
45	S	61	0	66	3	0
45	X	128	0	144	3	0
46	5	125	0	175	3	0
46	E	29	0	32	1	0
46	I	37	0	48	2	0
46	W	72	0	95	4	0
46	i	38	0	50	1	0
47	A	4	0	0	0	0
47	H	4	0	0	0	0
48	A	16	0	0	0	0
48	B	8	0	0	0	0
48	I	16	0	0	0	0
48	K	8	0	0	1	0
49	B	31	0	19	2	0
50	E	48	0	26	2	0
51	M	1	0	0	0	0
52	O	36	0	47	1	0
52	Q	36	0	47	3	0
53	1	45	0	0	0	0
53	2	115	0	0	0	0
53	3	9	0	0	0	0
53	4	79	0	0	1	0
53	5	34	0	0	3	0
53	6	21	0	0	0	0
53	9	24	0	0	1	0
53	A	123	0	0	1	0
53	B	25	0	0	0	0
53	C	114	0	0	1	0
53	D	24	0	0	1	0
53	E	31	0	0	2	0
53	F	37	0	0	4	0
53	G	76	0	0	0	0
53	H	11	0	0	0	0
53	I	68	0	0	6	0
53	J	2	0	0	0	0
53	K	38	0	0	0	0
53	L	5	0	0	0	0
53	M	26	0	0	3	0
53	P	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	R	2	0	0	0	0
53	U	23	0	0	0	0
53	W	41	0	0	0	0
53	X	41	0	0	2	0
53	Y	60	0	0	1	0
53	Z	35	0	0	3	0
53	a	5	0	0	1	0
53	b	6	0	0	0	0
53	d	14	0	0	0	0
53	f	2	0	0	0	0
53	g	2	0	0	0	0
53	h	26	0	0	1	0
53	i	1	0	0	0	0
53	j	7	0	0	0	0
53	n	27	0	0	0	0
All	All	69157	0	67958	1384	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 10.

All (1384) 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)
2:2:19:ARG:HA	2:2:123:ILE:HD11	1.28	1.09
2:2:546:VAL:HG21	43:2:605:PC1:C3I	1.99	0.92
8:9:63:LEU:HD22	27:W:113:VAL:HG21	1.55	0.88
9:A:366:MET:HE2	9:A:632:ILE:HG12	1.54	0.87
4:4:408:GLN:HA	43:5:702:PC1:H131	1.57	0.84
10:B:498:GLN:HG2	30:Z:62:LEU:HD21	1.60	0.83
30:Z:79:PRO:HG2	30:Z:82:LYS:HD3	1.61	0.82
43:2:605:PC1:H3G1	43:2:605:PC1:H3C1	1.61	0.81
2:2:42:MET:HE1	28:X:93:ARG:HA	1.61	0.80
9:A:544:PRO:HD2	9:A:548:VAL:HG11	1.63	0.80
36:f:78:THR:HG22	36:f:81:GLN:HG3	1.64	0.80
23:P:114:ASN:HD21	23:P:116:ILE:HG22	1.47	0.80
5:5:350:VAL:HG23	5:5:351:ALA:H	1.46	0.79
25:S:75:LEU:HD21	45:S:201:CDL:HB32	1.63	0.79
10:B:308:VAL:HG13	10:B:382:VAL:HG11	1.63	0.79
26:U:78:ARG:HE	37:g:80:GLU:HG2	1.47	0.78
4:4:483:ILE:HD11	40:j:10:ALA:HB2	1.65	0.78
5:5:657:LEU:HD21	18:J:120:LEU:HD21	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:375:ILE:HD13	35:e:23:MET:HE3	1.65	0.78
10:B:184:ILE:HD11	10:B:195:LEU:HD23	1.66	0.77
10:B:504:SER:H	10:B:507:MET:HE3	1.50	0.77
45:X:202:CDL:HB32	45:X:202:CDL:H1	1.68	0.76
4:4:175:VAL:HG22	4:4:233:THR:HB	1.67	0.76
3:3:85:ALA:HB1	45:X:202:CDL:H511	1.68	0.75
7:8:25:ALA:O	31:a:150:ARG:NH1	2.20	0.75
11:C:218:ASN:HD22	11:C:439:PRO:HB2	1.51	0.75
13:E:233:HIS:HB3	13:E:236:GLU:OE1	1.87	0.75
17:I:155:ARG:NH2	53:I:401:HOH:O	2.20	0.75
22:O:118:ASP:OD1	23:P:30:ARG:NH2	2.20	0.74
5:5:619:ASN:ND2	5:5:666:MET:O	2.20	0.74
10:B:300:LYS:NZ	10:B:301:LEU:O	2.20	0.74
13:E:175:GLU:OE1	13:E:178:ARG:NH1	2.21	0.74
19:K:113:LEU:HB3	19:K:120:GLN:HE21	1.51	0.73
2:2:42:MET:HE2	28:X:96:LEU:HD12	1.70	0.73
9:A:698:VAL:HG23	9:A:699:VAL:HG23	1.70	0.73
10:B:164:LEU:HD12	10:B:271:VAL:HG13	1.70	0.73
11:C:84:ASP:O	14:F:142:ARG:NH1	2.22	0.73
2:2:509:SER:HB2	2:2:511:ARG:HH22	1.52	0.73
3:3:47:GLN:NE2	13:E:357:LEU:HD21	2.04	0.73
2:2:292:LEU:HD11	2:2:363:THR:HG23	1.69	0.73
4:4:174:ASP:HB2	4:4:177:LEU:HB2	1.71	0.73
19:K:113:LEU:HD11	19:K:208:MET:HG3	1.70	0.73
39:i:58:MET:HE1	39:i:74:ILE:HA	1.69	0.73
1:1:257:LEU:HG	1:1:315:SER:HB2	1.70	0.72
10:B:109:ARG:HE	10:B:365:PHE:HD2	1.37	0.72
12:D:55:ARG:NH1	53:D:201:HOH:O	2.23	0.72
10:B:384:ASP:OD1	10:B:385:LYS:N	2.22	0.72
16:H:122:ASN:ND2	16:H:152:GLN:OE1	2.23	0.72
6:6:170:ILE:HD12	12:D:81:VAL:HG12	1.73	0.71
2:2:546:VAL:HG21	43:2:605:PC1:H3I3	1.72	0.71
5:5:254:THR:HG23	5:5:329:LEU:HD11	1.73	0.71
24:R:27:LEU:HD21	33:c:28:THR:HB	1.72	0.71
29:Y:82:GLN:H	29:Y:103:GLN:HE22	1.36	0.71
4:4:404:ARG:NH2	53:4:701:HOH:O	2.22	0.71
16:H:125:ILE:HG12	42:o:50:LEU:HD11	1.73	0.71
11:C:257:ARG:NH2	19:K:109:GLU:OE2	2.22	0.70
16:H:107:THR:HG22	16:H:109:GLU:H	1.56	0.70
28:X:119:VAL:HG23	28:X:125:LEU:HD21	1.73	0.70
4:4:102:ASN:O	34:d:32:LYS:NZ	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:208:THR:HG21	11:C:346:ALA:HB3	1.74	0.69
14:F:239:ALA:O	15:G:96:LYS:NZ	2.25	0.69
9:A:160:GLY:HA3	11:C:410:ASN:HD21	1.58	0.69
9:A:553:PRO:HD2	9:A:570:PRO:HG3	1.75	0.69
53:F:330:HOH:O	29:Y:162:LYS:HE2	1.92	0.69
5:5:386:MET:HE3	35:e:27:ILE:HD11	1.75	0.69
13:E:64:ARG:NH1	53:E:501:HOH:O	2.25	0.69
16:H:138:LYS:HE2	16:H:168:LEU:HA	1.74	0.69
25:S:133:ILE:HG21	34:d:52:VAL:HG22	1.74	0.69
38:h:30:LYS:NZ	38:h:50:GLU:OE2	2.26	0.69
2:2:19:ARG:HE	2:2:121:LYS:HE2	1.58	0.69
5:5:400:TYR:HD2	5:5:521:VAL:HG12	1.57	0.68
2:2:22:SER:HB3	2:2:123:ILE:HD13	1.74	0.68
10:B:188:PHE:HB3	10:B:191:GLU:HB2	1.74	0.68
13:E:30:HIS:HB2	13:E:40:ARG:HH11	1.58	0.68
13:E:228:LYS:HB3	13:E:262:GLN:HE21	1.59	0.68
10:B:321:PRO:HG2	10:B:324:GLU:HB2	1.75	0.67
2:2:140:ILE:HD11	2:2:286:SER:HA	1.77	0.67
5:5:243:VAL:HG13	5:5:247:ILE:HD12	1.76	0.67
5:5:475:VAL:HG23	35:e:19:LEU:HD11	1.74	0.67
9:A:172:GLU:OE1	16:H:105:ARG:NH2	2.28	0.67
2:2:546:VAL:HG21	43:2:605:PC1:H3I2	1.77	0.67
29:Y:102:LEU:HD11	29:Y:154:MET:HE3	1.75	0.67
23:P:63:HIS:HD2	29:Y:94:LEU:HD11	1.59	0.67
29:Y:164:LYS:HD2	29:Y:180:VAL:HG11	1.77	0.67
11:C:296:GLU:OE2	17:I:79:ARG:NH1	2.28	0.67
13:E:228:LYS:HB3	13:E:262:GLN:NE2	2.10	0.67
10:B:431:ARG:HD3	10:B:489:ALA:HB2	1.77	0.66
11:C:499:ARG:NH1	15:G:193:GLU:OE2	2.27	0.66
13:E:40:ARG:HD2	13:E:42:GLN:HE21	1.60	0.66
15:G:127:ASN:HB3	15:G:130:ALA:HB3	1.78	0.66
5:5:436:ASN:CG	33:c:53:ARG:HH22	2.03	0.66
21:M:73:ARG:NH2	53:M:301:HOH:O	2.28	0.66
36:f:13:GLU:OE2	36:f:63:ARG:NH2	2.28	0.66
12:D:36:LYS:HD2	12:D:61:ARG:HB3	1.76	0.66
2:2:237:PRO:HG2	2:2:306:LEU:HD11	1.78	0.66
5:5:421:THR:HA	5:5:424:TYR:CE2	2.30	0.66
11:C:69:ILE:HG12	23:P:14:GLN:HE22	1.59	0.66
5:5:48:PHE:HA	5:5:52:PHE:HD2	1.58	0.66
10:B:66:GLN:HB2	10:B:82:MET:HE3	1.77	0.66
13:E:61:GLN:HA	13:E:64:ARG:NH2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:112:PRO:HD3	23:P:124:ASN:HB2	1.78	0.66
10:B:71:ARG:HH11	16:H:308:PRO:HG3	1.60	0.66
6:6:210:ALA:HA	20:L:69:ILE:HD11	1.78	0.66
15:G:233:GLU:CD	15:G:248:LEU:HA	2.21	0.66
11:C:462:ALA:HB1	11:C:496:GLU:HG2	1.77	0.65
6:6:31:VAL:O	6:6:35:ILE:HG12	1.96	0.65
19:K:120:GLN:HB3	19:K:125:ILE:HB	1.78	0.65
36:f:20:GLN:HG3	36:f:52:GLU:HG3	1.79	0.65
3:3:28:HIS:HB2	44:3:201:LMT:H2'	1.78	0.65
19:K:81:LEU:HA	19:K:84:LEU:HD12	1.79	0.65
19:K:113:LEU:O	19:K:120:GLN:HG3	1.96	0.65
4:4:8:LEU:HD11	4:4:120:LEU:HD11	1.78	0.65
6:6:60:TYR:CD2	20:L:38:PHE:HZ	2.14	0.65
5:5:560:GLY:HA2	5:5:563:ILE:HG22	1.78	0.65
11:C:184:GLU:HG3	11:C:263:VAL:HB	1.79	0.65
2:2:430:LEU:HD11	44:2:604:LMT:H72	1.78	0.65
9:A:268:LEU:HD11	9:A:425:ALA:HB1	1.79	0.65
2:2:216:SER:HB2	2:2:237:PRO:HG3	1.79	0.64
4:4:11:PRO:HG3	4:4:86:ASN:HD21	1.61	0.64
4:4:410:MET:HG2	4:4:488:ASP:HA	1.79	0.64
13:E:167:ASN:HD21	13:E:319:GLN:HA	1.62	0.64
11:C:456:TYR:CZ	15:G:224:LYS:HE3	2.33	0.64
1:1:65:LYS:HE3	19:K:159:PRO:HG2	1.79	0.64
17:I:223:ARG:NH1	53:I:405:HOH:O	2.30	0.64
38:h:6:ARG:NH1	38:h:29:THR:O	2.31	0.64
2:2:273:THR:HA	2:2:276:THR:HG22	1.78	0.64
13:E:235:ASN:ND2	15:G:239:GLU:OE2	2.31	0.64
19:K:103:LEU:HB2	19:K:141:GLY:HA3	1.78	0.64
9:A:513:ALA:C	9:A:515:ASN:H	2.06	0.64
20:L:18:ASN:ND2	20:L:21:ASN:O	2.21	0.64
44:3:202:LMT:H62	37:g:26:LEU:HD22	1.79	0.64
5:5:350:VAL:HG21	5:5:359:PHE:HE1	1.63	0.64
9:A:154:ARG:O	9:A:154:ARG:NH2	2.30	0.64
40:j:63:LEU:HD11	44:j:101:LMT:H101	1.79	0.64
9:A:328:THR:HG22	13:E:29:ILE:HB	1.80	0.64
5:5:44:ILE:HD13	5:5:87:ILE:HD12	1.80	0.63
13:E:64:ARG:HD3	15:G:238:GLU:OE2	1.99	0.63
5:5:487:ILE:HG23	5:5:488:THR:HG23	1.79	0.63
10:B:326:ILE:HD11	10:B:337:TRP:HZ3	1.62	0.63
10:B:307:HIS:CD2	10:B:334:ARG:HH21	2.17	0.63
2:2:2:ILE:HD11	28:X:152:VAL:HG13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:12:GLU:HG2	26:U:12:VAL:HG23	1.80	0.63
11:C:289:ASP:OD2	30:Z:19:LYS:NZ	2.25	0.63
15:G:233:GLU:OE1	15:G:248:LEU:HD12	1.99	0.63
5:5:134:LEU:HB2	5:5:192:LEU:HD11	1.80	0.63
5:5:225:SER:HB3	5:5:307:MET:HE2	1.80	0.63
10:B:351:PRO:HD2	10:B:373:SER:HA	1.81	0.63
12:D:3:VAL:HG21	45:D:101:CDL:H111	1.80	0.63
16:H:261:LEU:HD13	16:H:266:ILE:HD13	1.79	0.63
1:1:209:LEU:HD23	1:1:338:ARG:HA	1.81	0.63
10:B:92:LEU:HD11	10:B:169:LEU:HD21	1.80	0.63
22:O:115:GLU:HG3	23:P:34:ARG:NH1	2.13	0.63
30:Z:21:THR:HG21	30:Z:42:SER:HB2	1.82	0.62
4:4:397:THR:HB	40:j:11:MET:HE1	1.80	0.62
11:C:295:GLU:OE2	27:W:18:ARG:NE	2.30	0.62
1:1:34:THR:HG22	1:1:38:MET:HE2	1.82	0.62
15:G:284:LYS:HD2	30:Z:117:ILE:HG22	1.81	0.62
30:Z:168:MET:HG3	30:Z:173:TRP:CD2	2.34	0.62
2:2:276:THR:HA	2:2:279:VAL:HG22	1.81	0.62
2:2:464:ILE:HG23	18:J:126:ALA:HB1	1.80	0.62
31:a:63:MET:HE2	40:j:30:ARG:HB2	1.81	0.62
5:5:260:LEU:HB2	5:5:317:ILE:HD13	1.82	0.62
17:I:121:GLU:HA	21:M:98:ALA:HB1	1.81	0.62
44:4:601:LMT:H123	44:5:705:LMT:H71	1.81	0.62
13:E:250:THR:HA	13:E:253:GLN:NE2	2.14	0.62
5:5:253:VAL:HB	5:5:310:LEU:HD11	1.80	0.62
15:G:50:ASP:HB3	30:Z:17:THR:HG22	1.81	0.62
9:A:433:ARG:NH1	9:A:453:THR:O	2.30	0.61
9:A:294:GLU:O	9:A:295:GLU:HB2	1.98	0.61
30:Z:99:GLN:HB2	53:Z:234:HOH:O	1.99	0.61
7:8:42:TYR:O	39:i:63:ARG:NH1	2.33	0.61
11:C:218:ASN:ND2	11:C:439:PRO:HB2	2.16	0.61
13:E:45:ARG:HG2	13:E:95:ASP:HB2	1.81	0.61
5:5:221:MET:HB2	5:5:226:GLN:HB2	1.83	0.61
5:5:33:CYS:O	5:5:37:ILE:HG12	2.01	0.61
23:P:48:PRO:HG2	23:P:51:HIS:HB2	1.83	0.61
18:J:70:ASP:OD1	18:J:73:ARG:NH1	2.33	0.61
5:5:17:GLY:HA3	43:5:702:PC1:H341	1.82	0.61
9:A:507:SER:HA	9:A:510:GLU:HG2	1.81	0.61
27:W:24:GLY:HA2	27:W:27:ARG:HE	1.66	0.61
9:A:460:GLY:HA3	9:A:465:ALA:HB1	1.82	0.61
4:4:406:LEU:HD22	4:4:410:MET:HE2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:565:GLY:HA3	31:a:114:TRP:CZ2	2.36	0.60
2:2:213:ASN:HB2	2:2:240:LEU:HD22	1.82	0.60
5:5:158:ILE:HA	5:5:161:ASN:HD22	1.66	0.60
3:3:60:GLY:HA3	6:6:84:LEU:HD13	1.83	0.60
5:5:257:VAL:HG12	5:5:261:MET:HE2	1.82	0.60
6:6:207:LEU:HD21	20:L:61:VAL:HG13	1.83	0.60
11:C:130:VAL:HG21	11:C:152:LEU:HB2	1.84	0.60
18:J:88:ASN:HD22	18:J:124:GLU:HB2	1.66	0.60
18:J:181:LEU:HD12	18:J:189:ILE:HD11	1.81	0.60
31:a:75:ARG:HA	31:a:78:ARG:HG3	1.83	0.60
43:2:605:PC1:H3C1	43:2:605:PC1:C3G	2.30	0.60
9:A:70:PRO:HB2	9:A:86:MET:HG3	1.81	0.60
9:A:364:VAL:HG21	9:A:655:MET:HG2	1.83	0.60
1:1:365:LEU:HA	1:1:370:ILE:HG13	1.81	0.60
2:2:242:PHE:CD1	6:6:124:MET:HG3	2.37	0.60
10:B:291:PHE:HB3	10:B:317:GLU:HG3	1.84	0.60
11:C:224:LEU:HB3	11:C:236:PHE:HA	1.82	0.60
16:H:189:PRO:HG3	42:o:31:ILE:HD11	1.84	0.60
14:F:232:LEU:HD11	14:F:236:MET:HE3	1.84	0.59
18:J:154:PRO:HG2	18:J:157:GLU:HB2	1.84	0.59
28:X:63:PRO:HB2	28:X:65:GLN:NE2	2.16	0.59
4:4:295:SER:O	4:4:299:VAL:HG23	2.01	0.59
6:6:42:ASN:ND2	6:6:44:ILE:HB	2.18	0.59
9:A:197:MET:HE2	9:A:225:LEU:HD22	1.84	0.59
9:A:602:ALA:HB1	9:A:614:MET:HE2	1.84	0.59
10:B:86:TYR:CD2	10:B:87:LYS:HG2	2.37	0.59
10:B:433:ARG:NH2	10:B:436:ASP:OD2	2.36	0.59
18:J:11:TYR:HE1	18:J:81:GLU:HA	1.68	0.59
36:f:52:GLU:OE2	36:f:52:GLU:N	2.35	0.59
9:A:588:ILE:O	38:h:134:ARG:NH1	2.35	0.59
22:O:105:VAL:O	22:O:109:GLU:N	2.36	0.59
24:R:77:PRO:HG2	31:a:81:HIS:NE2	2.18	0.59
3:3:12:SER:O	3:3:16:ILE:HG12	2.03	0.59
10:B:326:ILE:HD11	10:B:337:TRP:CZ3	2.37	0.59
20:L:21:ASN:CG	20:L:24:LEU:HD13	2.27	0.59
9:A:106:GLN:H	9:A:109:MET:HE3	1.68	0.59
9:A:403:SER:HB3	9:A:522:CYS:O	2.02	0.59
2:2:479:VAL:HG11	44:a:301:LMT:H41	1.85	0.59
3:3:94:PHE:O	3:3:98:ILE:HG12	2.03	0.59
4:4:76:LYS:NZ	4:4:145:TRP:O	2.35	0.59
30:Z:144:LYS:HB2	30:Z:148:GLU:OE2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:371:SER:O	5:5:375:ILE:HG12	2.02	0.58
9:A:317:LEU:HB2	9:A:592:VAL:HB	1.85	0.58
18:J:177:ARG:HH21	40:j:74:GLU:HA	1.68	0.58
40:j:72:ILE:HB	44:j:101:LMT:H12	1.84	0.58
13:E:223:ASN:HB3	13:E:315:GLU:HG3	1.86	0.58
13:E:38:LEU:HD22	13:E:50:GLU:HG3	1.84	0.58
14:F:250:ARG:HH22	15:G:148:MET:HG2	1.68	0.58
18:J:155:ILE:HG21	34:d:98:TRP:HD1	1.68	0.58
19:K:137:MET:HE1	19:K:155:TYR:HB2	1.85	0.58
5:5:342:GLY:O	5:5:345:SER:OG	2.22	0.58
2:2:45:SER:HB2	28:X:101:MET:HB3	1.85	0.58
2:2:157:TYR:OH	20:L:66:GLU:HB3	2.02	0.58
10:B:208:ILE:HG21	10:B:221:VAL:HG23	1.84	0.58
11:C:205:PHE:HA	11:C:208:THR:HG22	1.84	0.58
14:F:87:VAL:HG21	14:F:210:LEU:HD13	1.83	0.58
17:I:86:GLU:OE1	30:Z:36:VAL:HG22	2.03	0.58
7:8:47:LEU:HD12	7:8:49:TRP:CH2	2.39	0.58
17:I:91:PRO:HG2	30:Z:45:VAL:HG21	1.86	0.58
1:1:125:ILE:HD11	44:1:402:LMT:H4'	1.84	0.58
5:5:357:ARG:HG2	24:R:23:VAL:HG12	1.86	0.58
30:Z:135:LYS:HB2	30:Z:139:LYS:HB2	1.85	0.58
3:3:68:LEU:HD22	20:L:61:VAL:HG22	1.85	0.58
4:4:335:ARG:NH1	5:5:586:LEU:O	2.35	0.58
5:5:340:PHE:O	5:5:344:GLY:N	2.36	0.58
8:9:88:LEU:HD22	12:D:76:ASN:HB3	1.84	0.58
10:B:171:ALA:O	10:B:175:MET:HG2	2.04	0.58
22:O:102:VAL:HG12	23:P:33:ILE:HD11	1.86	0.57
44:4:601:LMT:H82	44:a:301:LMT:H101	1.85	0.57
18:J:88:ASN:ND2	18:J:124:GLU:OE2	2.37	0.57
1:1:265:TYR:HB3	26:U:158:PRO:HD3	1.87	0.57
32:b:49:TRP:O	32:b:53:ILE:HG12	2.04	0.57
2:2:161:LEU:HD13	6:6:213:GLY:HA3	1.86	0.57
43:5:702:PC1:H133	39:i:20:TRP:CZ2	2.38	0.57
10:B:63:ARG:HB3	10:B:315:GLU:OE2	2.04	0.57
30:Z:70:ILE:O	30:Z:74:ASP:HB2	2.04	0.57
2:2:19:ARG:HA	2:2:123:ILE:CD1	2.20	0.57
5:5:632:ALA:HB1	20:L:15:PHE:CD2	2.39	0.57
6:6:42:ASN:HD21	6:6:44:ILE:HB	1.69	0.57
14:F:250:ARG:NH2	15:G:148:MET:HG2	2.20	0.57
1:1:31:GLU:HG3	1:1:328:ILE:HG12	1.86	0.57
5:5:312:MET:HE1	5:5:414:ALA:HB1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:368:ASP:O	9:A:372:ARG:HG2	2.05	0.57
10:B:304:ILE:HD13	10:B:380:VAL:HB	1.86	0.57
11:C:146:ASP:OD1	15:G:209:ARG:NH2	2.35	0.57
13:E:239:GLU:CD	13:E:333:MET:HE3	2.30	0.57
13:E:272:VAL:O	13:E:276:ILE:HG12	2.03	0.57
5:5:132:ASN:HB2	5:5:192:LEU:HD12	1.85	0.57
28:X:63:PRO:HB2	28:X:65:GLN:HE21	1.68	0.57
38:h:7:THR:O	38:h:11:LEU:HD23	2.04	0.57
2:2:191:LEU:HG	20:L:36:ILE:HG21	1.86	0.57
3:3:130:ILE:HD12	14:F:48:ALA:HA	1.86	0.57
5:5:208:VAL:HG22	40:j:63:LEU:HD22	1.86	0.57
9:A:356:GLN:HB2	9:A:530:ALA:HB1	1.86	0.57
10:B:60:ASP:OD1	10:B:63:ARG:NH1	2.38	0.57
13:E:69:ARG:HD3	13:E:242:GLU:OE1	2.04	0.57
24:R:28:TRP:O	24:R:32:ALA:N	2.38	0.57
10:B:452:ALA:HB3	49:B:602:FMN:HM82	1.87	0.57
41:n:81:SER:HB3	41:n:84:HIS:HD2	1.70	0.57
2:2:414:LEU:HB2	2:2:417:GLN:HG3	1.86	0.57
4:4:447:LEU:HD21	40:j:54:ALA:HB1	1.87	0.56
12:D:55:ARG:HD2	12:D:78:PRO:HD3	1.86	0.56
13:E:167:ASN:HD21	13:E:320:VAL:H	1.52	0.56
22:O:127:VAL:O	22:O:131:ILE:HG12	2.05	0.56
9:A:679:VAL:HG21	36:f:36:TYR:CE2	2.40	0.56
11:C:340:LYS:NZ	11:C:352:PHE:O	2.36	0.56
13:E:212:LYS:O	13:E:216:VAL:HG22	2.05	0.56
14:F:143:LEU:HD12	14:F:144:PRO:HD2	1.87	0.56
27:W:61:MET:HA	27:W:61:MET:HE2	1.85	0.56
2:2:459:LEU:HD11	4:4:221:LEU:HD22	1.88	0.56
5:5:226:GLN:O	5:5:230:HIS:HB3	2.05	0.56
10:B:111:ARG:NH2	10:B:299:THR:O	2.36	0.56
11:C:314:VAL:HB	11:C:474:ILE:HD11	1.87	0.56
13:E:243:ARG:NH1	53:E:504:HOH:O	2.36	0.56
15:G:65:ILE:HG22	30:Z:69:THR:HG22	1.88	0.56
15:G:131:GLU:HG2	15:G:160:ARG:HH11	1.69	0.56
30:Z:119:GLU:HG3	30:Z:120:GLU:H	1.70	0.56
2:2:499:PRO:HD2	14:F:170:LEU:HD13	1.87	0.56
5:5:368:LEU:HA	35:e:16:ALA:HB2	1.88	0.56
39:i:30:ASN:ND2	41:n:51:LEU:HG	2.21	0.56
2:2:88:LYS:HD3	45:2:601:CDL:HA22	1.87	0.56
5:5:285:THR:HG21	5:5:312:MET:HE3	1.87	0.56
9:A:408:ILE:HG12	9:A:485:MET:HE1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:444:ALA:HB1	9:A:459:LEU:HD23	1.88	0.56
22:O:128:ASP:OD1	22:O:129:LYS:N	2.39	0.56
4:4:248:GLN:HA	4:4:307:LEU:HD22	1.88	0.56
4:4:361:ASN:HD21	4:4:527:TYR:HB3	1.71	0.56
13:E:166:TYR:CD2	13:E:319:GLN:HG3	2.41	0.56
2:2:509:SER:HB2	2:2:511:ARG:NH2	2.21	0.56
9:A:47:GLY:O	9:A:49:LYS:NZ	2.38	0.56
9:A:606:VAL:HG22	9:A:612:VAL:HG22	1.88	0.56
10:B:237:SER:HB2	10:B:249:PRO:HG3	1.88	0.56
14:F:103:LEU:HD22	14:F:130:LYS:HD3	1.88	0.56
17:I:111:GLU:HB3	17:I:186:TYR:CZ	2.40	0.56
17:I:122:GLU:O	17:I:152:ARG:NH1	2.39	0.56
5:5:112:ARG:HD3	43:5:702:PC1:H2	1.87	0.56
5:5:632:ALA:HB1	20:L:15:PHE:HD2	1.69	0.56
22:Q:103:GLU:OE2	24:R:29:ARG:NH2	2.39	0.56
25:S:98:TRP:O	25:S:102:ILE:HD12	2.05	0.56
5:5:147:SER:O	5:5:151:VAL:HG22	2.05	0.56
14:F:96:VAL:O	14:F:100:LYS:HG2	2.06	0.56
18:J:80:ARG:NH2	18:J:84:ASP:OD1	2.39	0.56
1:1:135:LYS:HE2	1:1:139:LEU:HD11	1.88	0.55
2:2:10:LEU:HD21	6:6:208:LEU:HD11	1.87	0.55
9:A:58:LEU:HD11	9:A:111:VAL:HG21	1.87	0.55
30:Z:119:GLU:O	30:Z:120:GLU:HG3	2.06	0.55
38:h:30:LYS:HD3	38:h:57:TRP:CD2	2.40	0.55
28:X:25:ASN:ND2	28:X:165:GLY:HA3	2.21	0.55
2:2:105:ILE:HG22	2:2:512:ILE:HD13	1.87	0.55
2:2:546:VAL:CG2	43:2:605:PC1:C3I	2.81	0.55
5:5:375:ILE:HG23	5:5:482:ILE:HD11	1.88	0.55
13:E:227:GLU:OE2	13:E:315:GLU:HA	2.05	0.55
2:2:11:LEU:HD13	3:3:100:ILE:HG23	1.89	0.55
10:B:283:ARG:HH11	10:B:287:TRP:NE1	2.05	0.55
27:W:19:ASN:ND2	30:Z:38:ASP:OD2	2.39	0.55
5:5:452:PHE:HA	22:Q:66:GLU:OE1	2.06	0.55
9:A:435:GLN:O	9:A:439:SER:OG	2.25	0.55
28:X:71:PHE:CZ	28:X:75:MET:HE3	2.42	0.55
2:2:543:ILE:HG12	43:2:605:PC1:H3H1	1.89	0.55
4:4:407:THR:HG22	43:5:702:PC1:H141	1.89	0.55
9:A:164:GLU:OE2	10:B:424:ARG:NH1	2.39	0.55
23:P:99:PHE:O	23:P:101:LYS:NZ	2.40	0.55
2:2:249:ILE:HG21	5:5:639:PHE:CD1	2.41	0.55
44:2:602:LMT:O1B	32:b:60:MET:HE1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:21:ARG:NH1	25:S:72:THR:O	2.35	0.55
9:A:219:THR:HA	16:H:173:MET:HE2	1.88	0.55
16:H:105:ARG:HH12	21:M:135:LYS:HG2	1.71	0.55
8:9:88:LEU:HD12	8:9:100:VAL:HG11	1.89	0.55
2:2:446:VAL:HG12	2:2:547:ILE:HG23	1.89	0.55
10:B:140:VAL:HB	10:B:268:VAL:HG22	1.88	0.55
11:C:177:TYR:HB2	19:K:105:CYS:HB3	1.88	0.54
11:C:338:VAL:HB	11:C:437:GLU:HB2	1.89	0.54
11:C:499:ARG:HH12	15:G:193:GLU:CD	2.15	0.54
13:E:301:LEU:HD13	13:E:303:TRP:CZ2	2.42	0.54
39:i:49:SER:O	39:i:53:GLU:HG3	2.07	0.54
1:1:12:GLU:HB3	12:D:25:MET:HE3	1.88	0.54
2:2:81:LEU:HA	2:2:536:PHE:HE1	1.72	0.54
4:4:363:ILE:HG21	5:5:68:GLU:HG3	1.88	0.54
6:6:45:VAL:HA	6:6:48:LEU:HD12	1.88	0.54
11:C:358:ILE:HD12	17:I:51:LEU:HD11	1.88	0.54
13:E:175:GLU:O	13:E:179:THR:OG1	2.20	0.54
13:E:223:ASN:HD22	13:E:316:PHE:HA	1.73	0.54
10:B:85:TRP:CD2	10:B:207:LEU:HD13	2.43	0.54
43:2:605:PC1:H371	44:X:203:LMT:H61	1.90	0.54
10:B:365:PHE:CE1	10:B:375:LEU:HD23	2.42	0.54
32:b:38:LEU:O	32:b:42:VAL:HG23	2.08	0.54
1:1:153:LEU:HD11	3:3:63:PHE:HA	1.89	0.54
4:4:6:VAL:HA	4:4:9:ILE:HG12	1.90	0.54
5:5:77:GLN:HB2	5:5:131:ASN:ND2	2.22	0.54
9:A:596:ALA:O	9:A:601:LYS:NZ	2.34	0.54
22:Q:109:GLU:HG3	22:Q:116:ILE:HG12	1.89	0.54
28:X:112:MET:HG3	28:X:174:GLN:OE1	2.06	0.54
2:2:216:SER:CB	2:2:237:PRO:HG3	2.38	0.54
4:4:235:PHE:O	4:4:239:LEU:HG	2.07	0.54
9:A:136:ASP:O	9:A:140:CYS:HB2	2.08	0.54
11:C:407:MET:HE2	11:C:417:HIS:CE1	2.43	0.54
25:S:124:ALA:HB1	34:d:48:MET:HG3	1.89	0.54
4:4:395:THR:HG21	4:4:403:PHE:CE1	2.43	0.54
22:O:124:ILE:HD12	22:O:130:ALA:HA	1.88	0.54
2:2:2:ILE:HG12	28:X:152:VAL:HA	1.88	0.54
5:5:1:MET:HE1	5:5:46:ALA:HB2	1.90	0.54
2:2:546:VAL:CG2	43:2:605:PC1:H3I3	2.38	0.54
5:5:646:ASN:ND2	53:5:803:HOH:O	2.41	0.54
9:A:158:ASP:OD1	30:Z:83:ARG:NH1	2.41	0.54
11:C:120:PHE:CD1	11:C:133:LEU:HD21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:120:PHE:CD2	11:C:480:LEU:HD11	2.43	0.53
11:C:423:LYS:HG2	15:G:260:GLY:O	2.08	0.53
23:P:81:ALA:O	23:P:85:GLU:HG2	2.08	0.53
2:2:396:THR:HG21	14:F:167:SER:HB3	1.90	0.53
3:3:112:LYS:HE3	13:E:376:ASP:O	2.08	0.53
5:5:189:LEU:HD21	5:5:204:ILE:HD11	1.91	0.53
9:A:288:LEU:HD11	29:Y:186:ARG:HG2	1.88	0.53
34:d:59:CYS:O	34:d:63:GLU:HG2	2.09	0.53
11:C:125:PRO:HG2	11:C:229:ASP:OD1	2.09	0.53
28:X:124:PRO:HG3	28:X:128:GLU:HG2	1.90	0.53
35:e:23:MET:C	35:e:25:PHE:H	2.16	0.53
4:4:484:ASP:OD1	4:4:484:ASP:N	2.40	0.53
9:A:170:ALA:HB3	21:M:114:ILE:HG12	1.89	0.53
1:1:80:LEU:HD13	1:1:83:VAL:HG11	1.89	0.53
9:A:318:VAL:HG12	9:A:320:ARG:HG3	1.90	0.53
9:A:328:THR:OG1	9:A:331:GLN:HG3	2.08	0.53
11:C:120:PHE:HD1	11:C:133:LEU:HD21	1.73	0.53
13:E:107:ARG:HB2	19:K:65:VAL:HG22	1.89	0.53
13:E:224:HIS:CD2	13:E:284:ASN:HD21	2.26	0.53
5:5:661:LEU:HD22	18:J:62:PHE:CZ	2.43	0.53
15:G:79:LYS:HB3	30:Z:173:TRP:CD1	2.44	0.53
2:2:241:ASN:HB3	2:2:309:PHE:O	2.09	0.53
3:3:133:LEU:HD11	14:F:139:VAL:HG23	1.91	0.53
3:3:133:LEU:HD12	14:F:137:VAL:HG12	1.91	0.53
23:P:78:GLN:NE2	53:P:204:HOH:O	2.30	0.53
1:1:282:PHE:CG	1:1:283:PRO:HD3	2.43	0.53
9:A:319:ARG:NH2	9:A:587:GLU:O	2.39	0.53
9:A:657:GLU:O	36:f:17:LEU:HD11	2.09	0.53
2:2:245:LEU:O	2:2:249:ILE:HG12	2.09	0.53
5:5:32:THR:HG23	5:5:118:SER:OG	2.09	0.53
6:6:167:LEU:HD22	27:W:111:PHE:HB3	1.91	0.53
34:d:29:LYS:HG3	41:n:98:GLU:OE2	2.09	0.53
2:2:138:PHE:O	2:2:142:THR:HG23	2.09	0.53
3:3:17:LEU:O	3:3:21:ILE:HD12	2.09	0.53
4:4:80:LEU:O	4:4:84:ILE:HG12	2.09	0.53
4:4:166:LEU:O	4:4:169:VAL:HG12	2.09	0.53
9:A:570:PRO:HG2	9:A:573:ALA:HB2	1.90	0.53
11:C:180:MET:N	11:C:180:MET:SD	2.82	0.53
4:4:428:PRO:HG2	5:5:141:GLU:HG3	1.92	0.52
16:H:226:GLY:HA2	16:H:237:ILE:HG22	1.89	0.52
2:2:99:ASP:HA	2:2:103:ASN:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:10:LEU:HB2	5:5:122:PHE:CD1	2.44	0.52
18:J:20:GLY:HA3	18:J:71:PHE:HB2	1.90	0.52
16:H:126:ILE:HD12	16:H:145:LEU:HG	1.90	0.52
5:5:140:TRP:CZ2	5:5:223:LYS:HG3	2.43	0.52
52:Q:201:ZMP:O7	24:R:43:ARG:NH1	2.43	0.52
26:U:71:LYS:HE3	26:U:75:ARG:HH11	1.75	0.52
36:f:62:ALA:HB3	36:f:89:LEU:HD12	1.90	0.52
10:B:301:LEU:HD23	10:B:315:GLU:HB3	1.91	0.52
17:I:181:SER:HB3	17:I:212:LEU:HD21	1.92	0.52
22:O:105:VAL:HA	22:O:108:ILE:HB	1.91	0.52
6:6:23:LEU:HD22	6:6:60:TYR:CE1	2.45	0.52
9:A:83:ASN:HB2	10:B:407:GLN:O	2.10	0.52
20:L:33:LEU:O	20:L:37:THR:HG22	2.09	0.52
22:Q:88:ALA:O	22:Q:126:SER:HB2	2.09	0.52
9:A:489:GLY:O	9:A:492:VAL:HG22	2.10	0.52
19:K:119:ASP:O	19:K:122:ARG:HG2	2.09	0.52
27:W:19:ASN:ND2	30:Z:13:ALA:HB2	2.24	0.52
6:6:105:ASN:O	6:6:108:PRO:HD2	2.10	0.52
10:B:322:MET:SD	10:B:358:CYS:HB2	2.50	0.52
11:C:490:MET:HE2	11:C:492:LEU:HD11	1.92	0.52
12:D:64:THR:H	26:U:32:SER:HB3	1.74	0.52
23:P:8:PHE:HB2	23:P:84:GLN:HG3	1.90	0.52
5:5:4:SER:HA	5:5:7:ILE:HG22	1.91	0.52
11:C:295:GLU:OE1	11:C:374:ARG:NH2	2.37	0.52
13:E:82:ARG:HD3	50:E:402:NDP:C2A	2.39	0.52
34:d:34:ALA:O	34:d:38:ILE:HD12	2.10	0.52
1:1:99:GLY:HA3	1:1:102:LEU:HD12	1.92	0.51
5:5:316:SER:HB3	5:5:325:ALA:HB2	1.92	0.51
9:A:717:ARG:HA	9:A:732:MET:HE2	1.91	0.51
11:C:378:ARG:HD2	27:W:16:TYR:CZ	2.45	0.51
11:C:465:PHE:HA	11:C:497:VAL:HG13	1.91	0.51
13:E:184:GLU:HG2	13:E:196:ILE:HD12	1.91	0.51
19:K:222:LYS:HB2	19:K:226:MET:HG2	1.92	0.51
26:U:108:GLN:HB2	26:U:111:GLN:HG3	1.91	0.51
2:2:249:ILE:HG21	5:5:639:PHE:HD1	1.75	0.51
10:B:419:ASP:OD1	10:B:423:LYS:NZ	2.30	0.51
11:C:82:PHE:O	14:F:142:ARG:NH2	2.43	0.51
31:a:65:GLY:HA2	40:j:28:TYR:CD2	2.45	0.51
4:4:477:SER:H	31:a:88:GLN:HE22	1.59	0.51
11:C:322:LEU:HD23	15:G:185:MET:HB2	1.92	0.51
15:G:191:GLU:HG2	15:G:202:PHE:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:J:86:VAL:O	18:J:90:ILE:HD12	2.11	0.51
35:e:24:TRP:H	35:e:27:ILE:HG12	1.76	0.51
1:1:125:ILE:HD11	44:1:402:LMT:H1B	1.91	0.51
13:E:287:LYS:HB2	13:E:316:PHE:HZ	1.76	0.51
28:X:119:VAL:CG2	28:X:125:LEU:HD21	2.38	0.51
37:g:23:ARG:HH21	44:g:101:LMT:H5'	1.75	0.51
37:g:79:THR:O	37:g:80:GLU:C	2.52	0.51
1:1:165:LEU:HG	27:W:46:LEU:HD21	1.93	0.51
2:2:189:PHE:HE2	5:5:639:PHE:CG	2.28	0.51
15:G:67:GLN:O	30:Z:71:PRO:HG2	2.11	0.51
1:1:35:MET:HE1	1:1:331:ARG:HE	1.76	0.51
2:2:10:LEU:HD13	2:2:127:LEU:HD21	1.93	0.51
2:2:107:TYR:CZ	2:2:109:ARG:HG2	2.46	0.51
2:2:242:PHE:CE1	2:2:246:ILE:HD11	2.46	0.51
5:5:188:SER:HA	40:j:63:LEU:O	2.11	0.51
29:Y:79:LYS:NZ	29:Y:177:GLU:OE1	2.43	0.51
39:i:51:GLU:HA	39:i:72:LYS:HG2	1.91	0.51
10:B:191:GLU:OE1	10:B:191:GLU:N	2.38	0.51
11:C:349:GLN:O	11:C:386:LYS:NZ	2.43	0.51
11:C:419:LEU:HD22	11:C:423:LYS:HD2	1.92	0.51
13:E:159:ARG:NH1	13:E:244:MET:O	2.35	0.51
14:F:111:ASP:OD2	14:F:113:THR:OG1	2.29	0.51
17:I:121:GLU:OE2	17:I:122:GLU:N	2.44	0.51
21:M:107:VAL:HG22	21:M:147:PRO:HB2	1.91	0.51
41:n:92:ASP:OD1	41:n:93:TYR:N	2.40	0.51
2:2:13:THR:HG23	2:2:123:ILE:HG22	1.92	0.51
14:F:219:ILE:HG13	14:F:220:GLU:N	2.26	0.51
1:1:84:ILE:HG22	1:1:87:ILE:HD12	1.93	0.51
2:2:109:ARG:O	2:2:113:ILE:HG12	2.11	0.51
43:2:605:PC1:H121	44:X:203:LMT:H4'	1.93	0.51
5:5:3:LEU:HD11	5:5:61:ILE:HD11	1.91	0.51
5:5:37:ILE:O	5:5:41:ILE:HD12	2.10	0.51
5:5:350:VAL:HG23	5:5:351:ALA:N	2.19	0.51
22:Q:119:LYS:HD2	22:Q:120:ASP:OD1	2.11	0.51
1:1:19:PRO:HA	1:1:22:VAL:HG22	1.93	0.51
9:A:220:TYR:CE2	16:H:104:HIS:HB2	2.46	0.51
1:1:114:MET:HA	1:1:117:VAL:HG22	1.93	0.50
2:2:317:ILE:HD11	5:5:645:TYR:CE2	2.46	0.50
2:2:339:LEU:HD11	2:2:480:TYR:CD1	2.47	0.50
9:A:129:LEU:HG	10:B:409:THR:HG21	1.93	0.50
2:2:560:MET:HG3	44:2:602:LMT:H21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:376:HIS:O	4:4:380:SER:OG	2.29	0.50
6:6:22:MET:HA	6:6:25:ILE:HD12	1.93	0.50
13:E:223:ASN:HB2	13:E:316:PHE:CE1	2.47	0.50
19:K:149:PRO:O	19:K:153:GLN:HG3	2.10	0.50
24:R:99:PHE:HE2	40:j:7:TYR:CE2	2.29	0.50
39:i:58:MET:HE2	39:i:77:TYR:CB	2.40	0.50
3:3:83:ASN:HB3	3:3:87:GLY:HA3	1.92	0.50
4:4:75:TYR:CZ	4:4:153:LYS:HD2	2.46	0.50
5:5:658:ILE:O	5:5:662:LEU:HG	2.11	0.50
8:9:60:VAL:HG13	27:W:113:VAL:HG23	1.93	0.50
10:B:321:PRO:HG2	10:B:324:GLU:CB	2.42	0.50
13:E:227:GLU:O	13:E:264:SER:HA	2.11	0.50
2:2:397:ASN:O	2:2:402:LYS:NZ	2.45	0.50
3:3:65:LEU:O	3:3:69:GLU:HG3	2.10	0.50
5:5:324:ILE:HD11	5:5:514:MET:HE1	1.93	0.50
13:E:136:SER:O	13:E:139:ASP:N	2.44	0.50
28:X:118:ARG:NH1	28:X:124:PRO:O	2.44	0.50
38:h:104:VAL:HG22	38:h:107:ARG:HH12	1.77	0.50
1:1:153:LEU:HD21	3:3:67:ASP:HB2	1.93	0.50
8:9:63:LEU:CD2	27:W:113:VAL:HG21	2.36	0.50
13:E:87:LYS:HD2	13:E:101:PHE:CD1	2.47	0.50
23:P:42:MET:HB3	23:P:89:PHE:HE1	1.76	0.50
1:1:9:SER:HB2	3:3:6:ILE:HD12	1.93	0.50
4:4:11:PRO:HG3	4:4:86:ASN:ND2	2.26	0.50
13:E:114:GLU:HA	13:E:117:ARG:HG3	1.93	0.50
4:4:339:VAL:HG13	4:4:468:MET:HE2	1.94	0.50
4:4:343:ILE:HD12	4:4:383:LEU:HB3	1.94	0.50
13:E:88:ARG:NH2	19:K:162:ARG:O	2.42	0.50
13:E:109:THR:O	13:E:113:GLU:HG2	2.11	0.50
13:E:183:ALA:HA	13:E:186:VAL:HG22	1.94	0.50
15:G:233:GLU:OE2	15:G:247:PRO:O	2.29	0.50
16:H:195:VAL:HG22	16:H:253:ILE:HD12	1.93	0.50
17:I:57:TRP:CH2	37:g:18:TRP:HB2	2.47	0.50
4:4:114:SER:HB3	4:4:117:ASP:OD1	2.11	0.50
5:5:363:ILE:HB	5:5:433:PHE:HB3	1.94	0.50
6:6:60:TYR:CD2	20:L:38:PHE:CZ	2.99	0.50
22:O:96:LEU:HD13	22:O:104:VAL:HG21	1.93	0.50
1:1:90:LEU:HD12	3:3:11:VAL:HG13	1.93	0.50
1:1:370:ILE:HD13	27:W:47:VAL:HG22	1.93	0.50
3:3:13:ILE:O	3:3:17:LEU:HD23	2.12	0.50
8:9:11:PRO:HB2	41:n:147:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:328:THR:H	9:A:331:GLN:NE2	2.10	0.50
16:H:214:VAL:HG13	16:H:236:PHE:HZ	1.77	0.50
19:K:214:LEU:O	19:K:218:MET:HG3	2.11	0.50
37:g:62:TYR:HD1	37:g:64:ILE:HG13	1.76	0.50
5:5:124:MET:SD	5:5:143:VAL:HG11	2.52	0.49
5:5:495:LEU:HD22	7:8:59:GLU:HG2	1.94	0.49
9:A:198:ASN:ND2	29:Y:209:THR:HG22	2.27	0.49
10:B:125:MET:HG2	10:B:137:ARG:NH1	2.27	0.49
14:F:257:PHE:O	14:F:259:ARG:NH1	2.45	0.49
16:H:109:GLU:N	16:H:109:GLU:OE1	2.45	0.49
28:X:145:TYR:HB3	28:X:148:LEU:HD12	1.94	0.49
1:1:175:VAL:HG13	1:1:253:GLY:O	2.13	0.49
39:i:67:SER:O	39:i:71:VAL:HG22	2.12	0.49
4:4:363:ILE:HG21	5:5:68:GLU:CG	2.42	0.49
10:B:149:GLY:C	10:B:379:ALA:HB1	2.38	0.49
11:C:320:LEU:O	15:G:134:GLN:HG2	2.12	0.49
17:I:208:TRP:O	17:I:212:LEU:HG	2.13	0.49
45:2:601:CDL:H322	28:X:58:MET:HG3	1.94	0.49
5:5:440:PRO:HD2	5:5:443:TYR:CE2	2.47	0.49
13:E:102:MET:HE1	21:M:86:GLN:HB2	1.94	0.49
22:O:112:PHE:CD2	22:O:134:ILE:HG12	2.48	0.49
24:R:48:PRO:HA	24:R:51:GLN:HB3	1.93	0.49
32:b:66:GLN:O	32:b:70:GLU:HG2	2.13	0.49
6:6:42:ASN:HD22	6:6:45:VAL:HG23	1.78	0.49
7:8:34:LEU:HB2	7:8:58:TYR:CE1	2.48	0.49
10:B:66:GLN:HE21	16:H:309:TRP:NE1	2.11	0.49
11:C:177:TYR:CZ	11:C:493:VAL:HG13	2.47	0.49
52:Q:201:ZMP:O6	24:R:4:ARG:NH1	2.46	0.49
39:i:25:ALA:HB3	41:n:48:GLU:HG2	1.95	0.49
5:5:137:PHE:CD1	5:5:182:MET:HE1	2.48	0.49
5:5:575:PHE:HD1	31:a:112:TYR:HB2	1.78	0.49
38:h:71:GLU:CD	38:h:72:PRO:HD2	2.37	0.49
1:1:11:VAL:HG12	1:1:15:LEU:HD12	1.93	0.49
1:1:204:ARG:HD3	1:1:240:ILE:HD11	1.93	0.49
9:A:297:ILE:HB	9:A:301:THR:CG2	2.42	0.49
9:A:517:LEU:HD23	9:A:674:ARG:HE	1.77	0.49
10:B:418:THR:O	10:B:422:MET:HG2	2.13	0.49
14:F:207:VAL:CG1	14:F:219:ILE:HD13	2.43	0.49
14:F:221:GLU:OE2	15:G:160:ARG:NH2	2.45	0.49
16:H:119:THR:HG23	16:H:152:GLN:CD	2.38	0.49
16:H:139:LYS:HZ2	29:Y:207:ILE:HG23	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:U:51:ASN:HB3	27:W:69:PRO:HG2	1.93	0.49
34:d:9:PHE:O	34:d:10:LEU:HD22	2.12	0.49
36:f:58:PRO:HB2	36:f:74:LEU:HB2	1.95	0.49
1:1:285:TRP:O	1:1:287:PRO:HD3	2.12	0.49
4:4:491:LYS:HE2	25:S:76:TRP:CD1	2.47	0.49
5:5:649:LEU:HD23	5:5:649:LEU:O	2.12	0.49
21:M:73:ARG:NH1	21:M:77:GLU:O	2.45	0.49
22:O:97:ASP:H	22:O:100:ASP:HB2	1.77	0.49
23:P:88:ASN:O	23:P:90:TRP:N	2.44	0.49
34:d:29:LYS:CG	41:n:98:GLU:OE2	2.61	0.49
6:6:69:VAL:HG12	20:L:57:ILE:HD11	1.95	0.49
9:A:248:ALA:HB3	53:I:455:HOH:O	2.12	0.49
21:M:113:ARG:NH1	21:M:134:ASP:OD2	2.40	0.49
25:S:123:GLU:HB2	34:d:9:PHE:CZ	2.47	0.49
9:A:51:SER:O	9:A:64:LYS:NZ	2.28	0.49
13:E:372:LEU:HD22	20:L:79:ARG:HG2	1.95	0.49
52:O:201:ZMP:H22A	23:P:56:ILE:HG12	1.94	0.49
2:2:268:TYR:O	2:2:337:LYS:HE2	2.13	0.48
13:E:298:ASN:HD22	13:E:308:SER:HB2	1.77	0.48
14:F:244:PRO:HG2	30:Z:139:LYS:HE2	1.94	0.48
25:S:82:GLU:OE2	25:S:82:GLU:N	2.34	0.48
45:S:201:CDL:HB62	39:i:14:TRP:CH2	2.47	0.48
39:i:29:GLN:O	39:i:33:ILE:HG12	2.14	0.48
39:i:50:ALA:HB1	39:i:70:TRP:O	2.12	0.48
5:5:361:GLY:O	5:5:433:PHE:HA	2.13	0.48
10:B:300:LYS:NZ	10:B:378:ALA:HB3	2.27	0.48
14:F:180:LYS:HB3	14:F:184:ARG:NH1	2.29	0.48
1:1:33:LYS:HG2	1:1:43:GLY:HA3	1.95	0.48
15:G:197:MET:HB3	15:G:222:LEU:HD12	1.96	0.48
18:J:154:PRO:HG2	18:J:157:GLU:CB	2.43	0.48
22:O:64:VAL:HG21	22:O:135:LEU:HD21	1.95	0.48
41:n:99:THR:O	41:n:102:THR:HG22	2.13	0.48
21:M:60:GLN:OE1	21:M:74:PRO:HA	2.14	0.48
52:Q:201:ZMP:H12	52:Q:201:ZMP:H14A	1.57	0.48
30:Z:156:THR:OG1	30:Z:159:LEU:O	2.31	0.48
34:d:18:PRO:HG3	34:d:41:GLU:HG3	1.96	0.48
39:i:71:VAL:HG23	39:i:74:ILE:HB	1.94	0.48
4:4:500:LEU:O	4:4:504:THR:HG23	2.13	0.48
4:4:512:SER:HA	4:4:515:LEU:HB2	1.95	0.48
15:G:95:PRO:HB3	30:Z:137:VAL:CG2	2.44	0.48
28:X:112:MET:HE3	28:X:174:GLN:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:5:706:3PE:H341	44:j:101:LMT:H31	1.94	0.48
7:8:28:ASP:OD2	7:8:62:GLN:NE2	2.46	0.48
9:A:130:LEU:HD12	11:C:412:GLU:HG3	1.96	0.48
23:P:80:ASN:N	23:P:80:ASN:HD22	2.12	0.48
2:2:157:TYR:CZ	20:L:66:GLU:HB3	2.49	0.48
44:2:603:LMT:H12	4:4:250:PHE:HB3	1.96	0.48
3:3:51:PRO:HB2	13:E:375:LEU:HG	1.94	0.48
5:5:375:ILE:HA	35:e:23:MET:CE	2.44	0.48
5:5:558:ARG:HH12	24:R:64:LYS:HG2	1.78	0.48
10:B:504:SER:N	10:B:507:MET:HE3	2.24	0.48
19:K:93:GLN:OE1	19:K:219:ARG:HG3	2.14	0.48
9:A:249:PHE:CG	17:I:151:ARG:HG3	2.49	0.48
15:G:238:GLU:O	15:G:241:LYS:HD3	2.13	0.48
10:B:136:PRO:O	10:B:264:CYS:HB3	2.13	0.48
15:G:162:ASN:HD22	30:Z:175:VAL:HA	1.79	0.48
2:2:427:LEU:HD22	32:b:21:GLY:HA3	1.96	0.47
4:4:144:ASN:OD1	4:4:147:SER:HB2	2.13	0.47
4:4:431:LEU:HD13	4:4:507:LEU:HB3	1.96	0.47
5:5:98:ILE:HA	5:5:101:ILE:HD12	1.97	0.47
5:5:221:MET:HE3	5:5:226:GLN:HB2	1.96	0.47
5:5:299:LYS:HD3	5:5:354:GLN:OE1	2.14	0.47
10:B:102:GLU:OE2	10:B:285:GLY:N	2.35	0.47
16:H:221:LEU:HD21	16:H:270:LEU:HD13	1.95	0.47
2:2:475:VAL:HG21	4:4:214:LEU:HD12	1.96	0.47
4:4:186:LEU:HB3	4:4:187:PRO:HD3	1.96	0.47
5:5:109:HIS:CE1	43:5:702:PC1:H121	2.49	0.47
5:5:338:LEU:HD13	5:5:477:LEU:HB2	1.96	0.47
5:5:416:ILE:O	5:5:419:ILE:HG22	2.14	0.47
9:A:259:THR:HG23	9:A:616:ARG:HB3	1.95	0.47
16:H:155:PHE:CE2	16:H:189:PRO:HD3	2.50	0.47
30:Z:174:ASP:OD1	30:Z:175:VAL:N	2.46	0.47
31:a:167:ARG:HH22	31:a:172:LEU:HD11	1.79	0.47
38:h:30:LYS:HD3	38:h:57:TRP:CE3	2.48	0.47
9:A:340:TYR:CE1	9:A:345:PRO:HG2	2.49	0.47
10:B:311:PRO:O	16:H:292:ARG:NH2	2.45	0.47
19:K:81:LEU:HD22	19:K:224:THR:HB	1.96	0.47
4:4:89:VAL:HA	4:4:92:ILE:HD12	1.97	0.47
5:5:33:CYS:SG	5:5:97:HIS:HB3	2.55	0.47
5:5:68:GLU:O	5:5:69:TRP:HB2	2.14	0.47
10:B:172:GLY:O	10:B:176:ASN:N	2.47	0.47
10:B:187:GLU:HG2	16:H:242:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:295:GLU:HG3	11:C:299:THR:OG1	2.14	0.47
13:E:269:ALA:HB1	13:E:280:ARG:HH12	1.78	0.47
29:Y:65:VAL:HG11	29:Y:78:PRO:HG2	1.96	0.47
2:2:21:MET:HE1	28:X:74:ALA:HB2	1.96	0.47
2:2:166:TYR:CD1	2:2:272:PRO:HG2	2.49	0.47
2:2:422:PHE:HE1	44:2:604:LMT:H12	1.77	0.47
3:3:111:LEU:HB3	3:3:113:VAL:HG23	1.97	0.47
5:5:346:VAL:HG13	5:5:369:THR:HG21	1.95	0.47
8:9:88:LEU:HA	8:9:97:THR:HG22	1.95	0.47
9:A:397:SER:HB3	9:A:671:VAL:HG11	1.97	0.47
14:F:83:LEU:HD13	14:F:213:LYS:HB3	1.95	0.47
2:2:125:TYR:N	2:2:126:PRO:HD2	2.30	0.47
9:A:207:GLY:HA3	16:H:173:MET:HE3	1.97	0.47
10:B:235:GLU:OE2	10:B:236:THR:HG23	2.14	0.47
14:F:211:GLU:HG3	14:F:219:ILE:HG23	1.96	0.47
16:H:128:GLN:O	16:H:131:LYS:HG2	2.14	0.47
1:1:181:ILE:HD11	1:1:185:LEU:HD12	1.96	0.47
2:2:383:ILE:HG21	2:2:432:LEU:HB2	1.96	0.47
4:4:153:LYS:HE2	4:4:153:LYS:HB3	1.66	0.47
5:5:179:THR:HA	5:5:182:MET:HE3	1.97	0.47
5:5:357:ARG:O	5:5:438:ASN:HB3	2.14	0.47
43:5:703:PC1:H231	43:5:703:PC1:H3A2	1.97	0.47
6:6:117:ILE:HG23	6:6:121:LEU:HD12	1.97	0.47
9:A:251:ALA:HB2	9:A:282:MET:HE2	1.96	0.47
11:C:440:LYS:HD3	11:C:491:ASP:O	2.15	0.47
14:F:60:LEU:O	14:F:70:ARG:NE	2.44	0.47
18:J:85:TRP:HA	18:J:124:GLU:HG2	1.94	0.47
23:P:6:THR:HG21	23:P:90:TRP:HH2	1.79	0.47
26:U:32:SER:OG	26:U:33:SER:N	2.48	0.47
5:5:496:GLY:HA2	7:8:26:TYR:CE2	2.49	0.47
9:A:153:MET:HE3	53:C:569:HOH:O	2.13	0.47
9:A:676:LEU:HD13	36:f:36:TYR:CD2	2.50	0.47
13:E:117:ARG:NH2	21:M:85:GLU:OE2	2.47	0.47
20:L:44:SER:OG	20:L:52:GLY:HA3	2.15	0.47
53:M:320:HOH:O	38:h:119:THR:HG23	2.13	0.47
23:P:97:MET:SD	23:P:103:GLU:HG2	2.55	0.47
39:i:58:MET:HE2	39:i:77:TYR:CG	2.49	0.47
1:1:241:VAL:O	1:1:245:ILE:HG13	2.15	0.47
2:2:37:ILE:HG22	43:2:605:PC1:H232	1.96	0.47
2:2:70:PHE:O	2:2:74:ILE:HG12	2.15	0.47
9:A:679:VAL:O	9:A:684:GLN:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:G:95:PRO:HB2	30:Z:138:ALA:HB2	1.95	0.47
15:G:255:ARG:NH1	53:I:402:HOH:O	2.48	0.47
16:H:206:GLY:HA3	16:H:248:ALA:HB3	1.97	0.47
20:L:29:ILE:O	20:L:33:LEU:HG	2.14	0.47
2:2:153:GLU:HG3	20:L:62:VAL:HG11	1.97	0.47
4:4:74:TYR:CE2	4:4:78:ILE:HD11	2.50	0.47
5:5:293:LEU:HD23	5:5:294:PHE:CE1	2.50	0.47
14:F:76:VAL:HG11	15:G:128:THR:HG21	1.97	0.47
16:H:221:LEU:HD12	16:H:229:THR:HG21	1.97	0.47
22:Q:86:GLU:OE1	22:Q:86:GLU:N	2.48	0.47
4:4:406:LEU:HD21	4:4:482:PHE:HE2	1.79	0.46
9:A:45:ILE:HG12	9:A:111:VAL:HB	1.97	0.46
9:A:394:ASP:OD2	9:A:680:GLN:NE2	2.48	0.46
17:I:108:PHE:HD2	17:I:182:PRO:HA	1.80	0.46
19:K:113:LEU:HB3	19:K:120:GLN:NE2	2.24	0.46
19:K:167:MET:HG3	19:K:207:LEU:HD13	1.97	0.46
45:S:201:CDL:H572	41:n:58:ALA:HB2	1.97	0.46
1:1:213:GLU:OE2	11:C:481:ALA:HB2	2.15	0.46
2:2:61:THR:HG22	2:2:63:LEU:H	1.80	0.46
4:4:8:LEU:CD1	4:4:120:LEU:HD11	2.42	0.46
4:4:364:GLN:NE2	5:5:68:GLU:O	2.48	0.46
44:4:601:LMT:H101	44:4:601:LMT:H71	1.63	0.46
9:A:298:ASN:OD1	9:A:301:THR:HG22	2.15	0.46
11:C:176:ASP:OD1	11:C:493:VAL:HB	2.15	0.46
14:F:250:ARG:HH22	15:G:148:MET:CG	2.28	0.46
41:n:104:MET:HG3	41:n:108:LEU:HD12	1.97	0.46
1:1:33:LYS:HA	1:1:43:GLY:HA3	1.96	0.46
4:4:96:LEU:HD22	41:n:91:SER:HB3	1.98	0.46
5:5:95:LEU:HD22	5:5:473:PRO:HA	1.97	0.46
5:5:578:ASN:HD22	31:a:112:TYR:HE1	1.63	0.46
9:A:614:MET:HB2	9:A:665:TYR:CE1	2.50	0.46
17:I:57:TRP:CZ2	37:g:14:LYS:HE2	2.51	0.46
23:P:6:THR:HG22	23:P:7:LYS:H	1.80	0.46
1:1:205:ALA:HB3	1:1:331:ARG:HG3	1.97	0.46
4:4:110:ASN:C	4:4:111:LEU:HD23	2.40	0.46
10:B:220:ASP:OD2	10:B:222:TYR:OH	2.32	0.46
19:K:120:GLN:HE22	19:K:127:PHE:HE1	1.62	0.46
28:X:162:ASN:HB3	53:X:324:HOH:O	2.15	0.46
4:4:2:SER:HB2	4:4:108:GLN:HB2	1.97	0.46
10:B:140:VAL:O	10:B:268:VAL:HA	2.15	0.46
24:R:47:ASP:OD1	24:R:47:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:324:ILE:HD13	5:5:394:PHE:HD2	1.80	0.46
44:5:705:LMT:H22	44:5:705:LMT:H51	1.80	0.46
9:A:513:ALA:C	9:A:515:ASN:N	2.74	0.46
12:D:79:TRP:CZ2	27:W:82:ARG:HD3	2.51	0.46
13:E:41:ILE:HD12	13:E:48:LEU:HD12	1.96	0.46
21:M:103:HIS:O	21:M:166:PRO:HD3	2.16	0.46
26:U:19:LEU:HG	27:W:81:ARG:HB2	1.97	0.46
28:X:115:MET:HE1	28:X:125:LEU:HB3	1.98	0.46
2:2:249:ILE:HD11	5:5:642:TYR:CD2	2.51	0.46
2:2:501:LEU:HD12	2:2:527:GLY:HA3	1.97	0.46
5:5:61:ILE:HG22	5:5:62:PHE:HD1	1.80	0.46
9:A:460:GLY:HA3	9:A:465:ALA:CB	2.45	0.46
17:I:182:PRO:HG2	17:I:211:GLU:OE2	2.16	0.46
46:I:303:3PE:H322	46:I:303:3PE:H32	1.53	0.46
23:P:39:ILE:HD12	23:P:86:THR:HG22	1.98	0.46
5:5:235:MET:HE3	43:5:703:PC1:H153	1.98	0.46
5:5:298:ILE:O	5:5:302:ILE:HG13	2.15	0.46
8:9:62:ALA:O	53:9:801:HOH:O	2.21	0.46
9:A:635:VAL:HG22	9:A:639:LEU:HD13	1.96	0.46
10:B:199:ILE:HD12	10:B:223:ILE:HD11	1.98	0.46
10:B:254:PRO:HG2	29:Y:193:TYR:HD2	1.80	0.46
10:B:406:GLY:HA2	10:B:412:ARG:HB2	1.96	0.46
13:E:135:PHE:HB3	13:E:140:VAL:HG23	1.98	0.46
13:E:152:VAL:HG13	13:E:157:VAL:HB	1.98	0.46
2:2:516:LYS:O	2:2:518:VAL:HG23	2.16	0.46
3:3:100:ILE:O	3:3:103:VAL:HG22	2.16	0.46
5:5:224:SER:HB3	5:5:226:GLN:HE21	1.81	0.46
11:C:131:LEU:HG	11:C:133:LEU:HD22	1.96	0.46
11:C:240:PHE:CD2	19:K:115:THR:HG21	2.51	0.46
11:C:277:LEU:HD22	11:C:384:LEU:HD23	1.98	0.46
14:F:211:GLU:OE2	14:F:218:LEU:HA	2.15	0.46
15:G:51:ALA:HB1	30:Z:20:TYR:CZ	2.50	0.46
25:S:67:GLN:O	39:i:6:LYS:NZ	2.44	0.46
39:i:55:ARG:HH11	39:i:71:VAL:HG21	1.81	0.46
1:1:79:PHE:HE2	3:3:23:LEU:HD11	1.81	0.46
1:1:136:TYR:CZ	11:C:480:LEU:HD23	2.50	0.46
1:1:339:PHE:O	1:1:342:LEU:HG	2.16	0.46
4:4:321:ILE:O	4:4:325:THR:HG22	2.16	0.46
9:A:636:SER:OG	9:A:643:LEU:HG	2.16	0.46
29:Y:204:LEU:HD23	29:Y:204:LEU:HA	1.73	0.46
3:3:76:PHE:HB2	6:6:193:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:262:ARG:NH1	53:5:805:HOH:O	2.50	0.45
5:5:305:SER:HB3	5:5:336:LYS:HZ1	1.80	0.45
5:5:356:PHE:HB3	5:5:431:LEU:HD13	1.98	0.45
9:A:636:SER:HB3	9:A:642:PRO:HA	1.98	0.45
10:B:489:ALA:N	10:B:507:MET:O	2.37	0.45
11:C:208:THR:HG23	11:C:383:CYS:SG	2.57	0.45
19:K:188:ASP:HA	19:K:191:VAL:O	2.16	0.45
36:f:19:CYS:HB2	36:f:56:THR:H	1.80	0.45
1:1:368:PHE:HE1	46:W:202:3PE:H232	1.80	0.45
5:5:636:LEU:O	5:5:640:ILE:HG12	2.16	0.45
9:A:306:ASP:OD1	9:A:712:SER:OG	2.32	0.45
11:C:238:TRP:CZ2	17:I:87:GLN:HG3	2.51	0.45
27:W:99:LYS:HG3	27:W:101:TYR:O	2.16	0.45
4:4:441:TYR:CZ	5:5:70:PHE:HZ	2.34	0.45
5:5:143:VAL:HG23	5:5:223:LYS:HZ1	1.80	0.45
5:5:290:LEU:HD11	46:5:701:3PE:H3A2	1.97	0.45
5:5:654:TYR:O	5:5:658:ILE:HD12	2.16	0.45
9:A:307:GLY:O	9:A:581:HIS:NE2	2.48	0.45
10:B:203:TYR:OH	10:B:220:ASP:HB2	2.16	0.45
14:F:80:ARG:NH1	53:F:303:HOH:O	2.49	0.45
29:Y:62:ASP:HB3	29:Y:65:VAL:HG13	1.99	0.45
2:2:42:MET:CE	28:X:93:ARG:HA	2.41	0.45
4:4:2:SER:HB3	4:4:5:TYR:CD2	2.51	0.45
4:4:114:SER:OG	4:4:115:PHE:N	2.49	0.45
4:4:408:GLN:HB2	4:4:478:VAL:HG23	1.97	0.45
4:4:511:PRO:HD2	5:5:64:TRP:O	2.16	0.45
5:5:261:MET:HE1	5:5:329:LEU:HD13	1.98	0.45
9:A:462:ASP:OD1	9:A:462:ASP:N	2.46	0.45
10:B:111:ARG:HB3	10:B:152:LYS:NZ	2.31	0.45
10:B:496:SER:HA	10:B:501:ARG:HD2	1.98	0.45
11:C:330:ARG:HD3	11:C:354:VAL:HG12	1.98	0.45
13:E:54:THR:HB	13:E:122:VAL:HG22	1.98	0.45
13:E:113:GLU:OE1	13:E:154:LYS:HD3	2.17	0.45
13:E:220:PHE:CE1	13:E:283:ILE:HG13	2.52	0.45
17:I:211:GLU:HG3	38:h:76:ALA:HB2	1.97	0.45
25:S:133:ILE:CG2	34:d:52:VAL:HG22	2.45	0.45
26:U:20:PRO:HD2	26:U:23:ILE:HD12	1.98	0.45
30:Z:100:GLN:HG2	30:Z:104:LEU:HD13	1.97	0.45
34:d:79:LEU:HD13	40:j:67:ARG:HD3	1.99	0.45
36:f:53:ALA:O	36:f:56:THR:OG1	2.29	0.45
4:4:234:TYR:CE2	4:4:236:ASP:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:519:HIS:CD2	25:S:117:GLN:HE22	2.35	0.45
9:A:406:TRP:CE3	9:A:409:GLU:HG3	2.52	0.45
19:K:50:GLU:OE2	19:K:55:TYR:HB3	2.16	0.45
30:Z:143:GLU:OE2	30:Z:144:LYS:HG3	2.17	0.45
31:a:160:LEU:C	34:d:68:LEU:HD22	2.41	0.45
35:e:30:ARG:HH22	35:e:33:LYS:HD3	1.80	0.45
6:6:95:ARG:HB2	6:6:98:GLU:OE1	2.16	0.45
10:B:142:ASN:O	10:B:271:VAL:HG23	2.16	0.45
10:B:166:GLU:HG3	10:B:278:PRO:HG3	1.99	0.45
10:B:279:THR:HA	10:B:282:ARG:HG2	1.98	0.45
11:C:281:TYR:O	11:C:285:THR:HG23	2.17	0.45
15:G:69:LEU:HD13	30:Z:83:ARG:HB3	1.97	0.45
21:M:78:ALA:HB1	38:h:117:TYR:CD1	2.52	0.45
22:Q:106:MET:HE1	24:R:15:LEU:HB3	1.99	0.45
28:X:28:HIS:O	28:X:32:VAL:HG23	2.16	0.45
39:i:50:ALA:HA	39:i:71:VAL:HG12	1.99	0.45
2:2:96:SER:HA	32:b:34:TRP:HE1	1.82	0.45
2:2:559:SER:HA	2:2:562:THR:HG22	1.99	0.45
4:4:146:ASN:O	40:j:4:LEU:HD21	2.16	0.45
4:4:262:LYS:HA	4:4:262:LYS:HD2	1.74	0.45
9:A:495:HIS:CD2	9:A:695:LEU:HD23	2.52	0.45
11:C:321:ASN:OD1	15:G:184:TYR:HA	2.16	0.45
13:E:270:GLU:HA	13:E:273:ASP:HB2	1.98	0.45
16:H:231:ASP:OD1	16:H:231:ASP:N	2.45	0.45
17:I:211:GLU:OE1	38:h:72:PRO:O	2.35	0.45
23:P:80:ASN:HD22	23:P:80:ASN:H	1.64	0.45
33:c:20:ASP:OD1	33:c:21:MET:N	2.49	0.45
2:2:527:GLY:HA2	2:2:530:ILE:HD12	1.99	0.45
5:5:408:VAL:HG21	31:a:143:PRO:HD2	1.99	0.45
11:C:73:ALA:HA	11:C:76:GLN:HG2	1.98	0.45
14:F:111:ASP:HB3	14:F:114:LYS:HB2	1.99	0.45
14:F:207:VAL:HG13	14:F:219:ILE:HD13	1.97	0.45
18:J:154:PRO:HD2	18:J:157:GLU:OE1	2.17	0.45
6:6:131:ILE:HG12	6:6:169:PHE:CZ	2.52	0.45
13:E:188:ARG:HA	13:E:191:PHE:O	2.17	0.45
35:e:30:ARG:NH2	35:e:33:LYS:HD3	2.32	0.45
36:f:85:THR:O	36:f:89:LEU:HD23	2.16	0.45
38:h:30:LYS:HG2	38:h:57:TRP:CZ2	2.52	0.45
2:2:419:LYS:HA	2:2:487:GLU:O	2.17	0.45
5:5:616:LEU:HD21	5:5:663:LEU:HD12	1.98	0.45
6:6:6:SER:HB2	27:W:89:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:165:ILE:HG22	10:B:492:TRP:CD2	2.52	0.45
9:A:284:ILE:HD12	9:A:305:CYS:HB3	1.98	0.45
21:M:91:ALA:HB1	38:h:107:ARG:HD3	1.99	0.45
1:1:61:LYS:HD3	19:K:95:SER:HB3	1.98	0.44
3:3:64:LEU:HD11	6:6:81:VAL:HG22	1.98	0.44
4:4:117:ASP:O	4:4:177:LEU:HD11	2.17	0.44
5:5:385:PHE:O	5:5:386:MET:HE2	2.16	0.44
5:5:625:THR:O	5:5:625:THR:HG22	2.17	0.44
9:A:197:MET:HE3	9:A:203:ALA:HB3	1.99	0.44
17:I:79:ARG:O	17:I:83:VAL:HG23	2.17	0.44
17:I:148:ASP:OD1	17:I:148:ASP:N	2.47	0.44
23:P:69:LEU:HD12	23:P:69:LEU:HA	1.78	0.44
27:W:41:TYR:O	27:W:45:LYS:HG2	2.17	0.44
28:X:115:MET:HE3	28:X:125:LEU:HD22	1.98	0.44
2:2:160:TYR:OH	2:2:183:GLY:HA3	2.16	0.44
2:2:313:TYR:O	2:2:317:ILE:HG13	2.18	0.44
5:5:205:ASN:HB3	5:5:208:VAL:HG23	1.98	0.44
7:8:24:LEU:HD23	7:8:24:LEU:HA	1.74	0.44
7:8:42:TYR:OH	39:i:60:GLU:HG3	2.16	0.44
9:A:323:LYS:HD2	9:A:325:GLU:OE2	2.17	0.44
11:C:374:ARG:HD3	27:W:16:TYR:O	2.17	0.44
16:H:228:THR:HG21	42:o:29:PHE:CE1	2.53	0.44
19:K:130:SER:O	19:K:134:SER:OG	2.35	0.44
35:e:23:MET:HB2	35:e:24:TRP:CD1	2.52	0.44
5:5:186:LEU:HG	5:5:192:LEU:HD23	1.98	0.44
5:5:437:PRO:HD2	33:c:43:ARG:O	2.17	0.44
9:A:378:LEU:HD23	9:A:541:PHE:HA	2.00	0.44
10:B:109:ARG:NE	10:B:365:PHE:HD2	2.11	0.44
11:C:169:LEU:HD13	11:C:264:ARG:HG2	1.98	0.44
14:F:223:ILE:O	14:F:227:GLU:HG2	2.18	0.44
18:J:80:ARG:HH22	18:J:84:ASP:CG	2.26	0.44
30:Z:139:LYS:O	30:Z:143:GLU:HG3	2.16	0.44
37:g:44:PRO:HB2	37:g:45:PRO:HD3	1.99	0.44
38:h:4:PRO:HA	38:h:7:THR:HG22	1.97	0.44
11:C:411:MET:HE3	11:C:415:ILE:HG13	2.00	0.44
13:E:137:LEU:HD12	13:E:137:LEU:H	1.81	0.44
13:E:167:ASN:ND2	13:E:319:GLN:HA	2.30	0.44
14:F:45:PRO:CB	14:F:219:ILE:HD12	2.47	0.44
14:F:203:THR:HB	53:F:309:HOH:O	2.17	0.44
15:G:51:ALA:HB1	30:Z:20:TYR:CE2	2.53	0.44
20:L:26:LEU:HD23	20:L:26:LEU:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:11:PHE:CD2	28:X:163:GLN:HG2	2.53	0.44
28:X:155:TRP:HA	45:X:202:CDL:H782	1.99	0.44
32:b:69:LEU:HD23	32:b:69:LEU:HA	1.84	0.44
36:f:7:PHE:HB3	36:f:11:VAL:HG11	2.00	0.44
38:h:104:VAL:HG22	38:h:107:ARG:NH1	2.32	0.44
4:4:155:TYR:OH	4:4:159:MET:HE2	2.17	0.44
10:B:67:ASN:O	10:B:67:ASN:CG	2.60	0.44
12:D:36:LYS:HE2	12:D:36:LYS:HB3	1.75	0.44
14:F:49:LEU:HG	14:F:53:TYR:CE2	2.52	0.44
16:H:218:LYS:HE3	16:H:218:LYS:HB2	1.74	0.44
28:X:55:LEU:HD23	28:X:75:MET:HE2	2.00	0.44
31:a:74:LYS:HB3	53:a:405:HOH:O	2.17	0.44
1:1:204:ARG:HD3	1:1:240:ILE:CD1	2.48	0.44
5:5:372:VAL:HG22	5:5:478:ALA:HB2	1.99	0.44
5:5:445:ARG:O	5:5:462:PRO:HB3	2.17	0.44
6:6:23:LEU:HD23	6:6:63:LEU:HD23	1.98	0.44
13:E:301:LEU:HD12	13:E:305:THR:HG21	1.99	0.44
14:F:209:GLU:HG2	14:F:213:LYS:NZ	2.33	0.44
17:I:79:ARG:NH2	27:W:21:PRO:O	2.50	0.44
19:K:226:MET:HE3	19:K:226:MET:HB3	1.82	0.44
31:a:75:ARG:HG2	31:a:78:ARG:NE	2.33	0.44
38:h:33:GLU:O	38:h:45:TYR:HA	2.17	0.44
1:1:11:VAL:HG11	12:D:28:VAL:HG11	1.98	0.44
2:2:49:LYS:NZ	2:2:568:LEU:O	2.51	0.44
3:3:61:LEU:HD11	6:6:214:ALA:CB	2.48	0.44
5:5:233:LEU:HD11	5:5:248:HIS:O	2.18	0.44
9:A:414:ILE:HG12	9:A:485:MET:HB3	2.00	0.44
10:B:401:ARG:HD2	10:B:416:LYS:HA	1.99	0.44
13:E:205:PHE:C	13:E:206:GLU:HG2	2.42	0.44
17:I:111:GLU:HG2	17:I:183:ASN:HB3	2.00	0.44
19:K:109:GLU:HG2	19:K:202:PRO:O	2.16	0.44
1:1:36:GLY:HA2	1:1:41:ARG:HG3	2.00	0.44
2:2:71:ILE:HG23	2:2:282:ILE:HD11	2.00	0.44
4:4:183:GLU:OE1	4:4:186:LEU:HD22	2.18	0.44
4:4:362:THR:HG22	4:4:364:GLN:H	1.83	0.44
5:5:437:PRO:HG2	33:c:48:PHE:CD2	2.53	0.44
5:5:660:ILE:HD11	18:J:119:VAL:HG11	2.00	0.44
9:A:252:ARG:O	9:A:255:GLU:HG2	2.18	0.44
14:F:54:HIS:CE1	14:F:136:ARG:HE	2.35	0.44
21:M:59:MET:HG3	21:M:65:ALA:HA	2.00	0.44
30:Z:97:GLN:O	30:Z:101:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:137:MET:HE2	4:4:163:GLU:HB2	1.99	0.44
5:5:619:ASN:O	5:5:622:SER:OG	2.27	0.44
6:6:127:TYR:CG	8:9:54:ARG:HG2	2.52	0.44
9:A:403:SER:OG	9:A:485:MET:HE2	2.18	0.44
45:D:101:CDL:OA4	45:D:101:CDL:HA62	2.18	0.44
13:E:64:ARG:HD2	13:E:206:GLU:OE2	2.18	0.44
17:I:46:PRO:HB2	17:I:49:PHE:HB2	2.00	0.44
21:M:147:PRO:HG3	21:M:165:TYR:CD1	2.53	0.44
22:O:78:VAL:HG22	22:O:94:LEU:HD23	1.99	0.44
1:1:79:PHE:CE2	3:3:23:LEU:HD11	2.53	0.43
2:2:51:ILE:HG22	28:X:144:ARG:NH2	2.33	0.43
4:4:212:THR:HG23	4:4:262:LYS:HD3	2.00	0.43
9:A:174:LYS:HD2	9:A:184:MET:HG3	2.00	0.43
9:A:310:THR:HG23	9:A:711:SER:HB2	1.99	0.43
10:B:344:ILE:HG12	10:B:352:ILE:HD13	2.00	0.43
13:E:170:PRO:HB3	13:E:182:ILE:HD13	2.00	0.43
22:Q:103:GLU:CD	33:c:36:TRP:HE1	2.25	0.43
1:1:76:VAL:O	1:1:80:LEU:N	2.48	0.43
2:2:52:GLY:O	28:X:144:ARG:NH2	2.51	0.43
2:2:185:LEU:O	2:2:189:PHE:HD1	2.00	0.43
4:4:21:ILE:HD11	4:4:75:TYR:CD1	2.54	0.43
4:4:110:ASN:O	4:4:111:LEU:HD23	2.18	0.43
5:5:312:MET:O	5:5:315:LEU:HB3	2.18	0.43
5:5:338:LEU:HD13	5:5:477:LEU:CB	2.48	0.43
19:K:111:MET:O	19:K:115:THR:HG23	2.18	0.43
22:O:96:LEU:HD22	22:O:100:ASP:HB3	2.01	0.43
25:S:122:GLU:HG2	25:S:126:ARG:NH2	2.33	0.43
27:W:44:TYR:HA	46:W:202:3PE:H332	2.00	0.43
29:Y:106:THR:HA	29:Y:177:GLU:HB2	1.99	0.43
30:Z:143:GLU:CD	30:Z:144:LYS:HG3	2.43	0.43
36:f:7:PHE:H	36:f:43:ASN:ND2	2.16	0.43
1:1:83:VAL:HG23	3:3:15:ALA:HB1	2.00	0.43
5:5:2:TYR:HB3	5:5:78:TYR:CE1	2.53	0.43
5:5:372:VAL:O	5:5:375:ILE:HB	2.18	0.43
5:5:639:PHE:O	5:5:643:LEU:HD23	2.18	0.43
9:A:706:ASP:OD2	9:A:708:ILE:HB	2.18	0.43
13:E:167:ASN:ND2	13:E:320:VAL:H	2.16	0.43
14:F:69:TYR:CZ	14:F:236:MET:HG3	2.53	0.43
17:I:65:ILE:HD12	17:I:65:ILE:H	1.83	0.43
17:I:131:GLU:OE1	53:I:402:HOH:O	2.21	0.43
24:R:93:PRO:HB3	25:S:74:TRP:CH2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:S:131:GLU:H	25:S:131:GLU:HG3	1.66	0.43
46:W:202:3PE:H221	37:g:50:ILE:HD11	2.00	0.43
36:f:17:LEU:O	36:f:58:PRO:HA	2.19	0.43
1:1:256:LEU:HD23	1:1:256:LEU:HA	1.78	0.43
5:5:154:TRP:CH2	5:5:240:PRO:HG3	2.54	0.43
11:C:196:ASN:OD1	15:G:72:PRO:HG2	2.19	0.43
13:E:188:ARG:HH22	13:E:196:ILE:HG13	1.83	0.43
15:G:242:ARG:CZ	15:G:244:VAL:HG12	2.48	0.43
18:J:93:LEU:HD12	18:J:117:GLY:HA3	2.01	0.43
23:P:42:MET:HB3	23:P:89:PHE:CE1	2.53	0.43
31:a:74:LYS:HD2	31:a:104:LEU:HA	1.99	0.43
4:4:172:VAL:HG11	4:4:181:PHE:CE2	2.54	0.43
4:4:502:SER:O	4:4:506:ILE:HD12	2.18	0.43
5:5:3:LEU:HB3	39:i:49:SER:OG	2.18	0.43
11:C:240:PHE:HA	11:C:243:ARG:HB3	2.00	0.43
11:C:300:ASP:O	17:I:76:GLU:HG3	2.18	0.43
11:C:421:PHE:CD1	17:I:172:SER:HB3	2.53	0.43
28:X:97:ARG:HB3	28:X:104:ASN:HB3	2.00	0.43
2:2:105:ILE:HG22	2:2:512:ILE:CD1	2.49	0.43
2:2:161:LEU:HD21	20:L:69:ILE:HD12	2.01	0.43
2:2:304:SER:OG	2:2:305:TYR:N	2.52	0.43
5:5:350:VAL:HG21	5:5:359:PHE:CE1	2.48	0.43
9:A:360:VAL:HG23	9:A:604:THR:O	2.17	0.43
9:A:562:ASP:OD2	9:A:707:VAL:HG11	2.18	0.43
9:A:744:GLN:NE2	9:A:746:ALA:O	2.50	0.43
10:B:110:GLY:HA3	49:B:602:FMN:O2P	2.19	0.43
10:B:321:PRO:HA	10:B:362:LEU:HA	2.01	0.43
13:E:176:PHE:CE1	13:E:180:LYS:HD2	2.53	0.43
13:E:247:ASP:HB3	13:E:250:THR:HG23	2.01	0.43
15:G:221:PRO:HA	15:G:226:PHE:CD1	2.54	0.43
27:W:35:ALA:HB2	46:W:201:3PE:H2D1	1.99	0.43
31:a:69:ASN:OD1	31:a:98:HIS:CD2	2.72	0.43
44:3:201:LMT:H12	44:3:201:LMT:H42	1.89	0.43
4:4:406:LEU:HD22	4:4:410:MET:CE	2.48	0.43
5:5:57:VAL:HB	5:5:78:TYR:HB2	2.00	0.43
5:5:302:ILE:HD13	5:5:339:LEU:HB3	2.01	0.43
8:9:23:ALA:HB1	41:n:153:HIS:CE1	2.54	0.43
10:B:300:LYS:HZ1	10:B:378:ALA:HB3	1.84	0.43
10:B:438:LEU:O	10:B:442:THR:HG23	2.19	0.43
15:G:48:PRO:O	30:Z:17:THR:HG23	2.19	0.43
17:I:142:GLU:OE1	38:h:123:LYS:NZ	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:140:TRP:CE2	29:Y:149:SER:HB2	2.53	0.43
3:3:86:TYR:HD2	6:6:194:THR:HG22	1.84	0.43
5:5:148:TYR:CD1	5:5:164:SER:HB2	2.53	0.43
5:5:189:LEU:HA	5:5:189:LEU:HD23	1.80	0.43
5:5:479:LEU:HD23	5:5:479:LEU:HA	1.89	0.43
10:B:383:MET:HB2	10:B:387:THR:HG21	2.00	0.43
11:C:305:ILE:O	11:C:309:LYS:HG2	2.19	0.43
12:D:86:UNK:O	20:L:46:ASN:HA	2.19	0.43
13:E:205:PHE:CD1	15:G:241:LYS:HE2	2.54	0.43
22:Q:78:VAL:HG12	22:Q:96:LEU:HD11	2.00	0.43
31:a:56:THR:HG22	31:a:59:GLU:CD	2.44	0.43
34:d:69:GLU:OE2	34:d:70:LYS:HB2	2.18	0.43
1:1:318:VAL:HG22	12:D:15:ILE:HD13	2.00	0.43
2:2:44:LEU:O	44:2:602:LMT:H1B	2.18	0.43
2:2:189:PHE:HE2	5:5:639:PHE:CD1	2.36	0.43
43:2:605:PC1:H31	43:2:605:PC1:H321	1.24	0.43
5:5:119:LEU:HD12	5:5:119:LEU:HA	1.86	0.43
6:6:110:THR:HG23	20:L:13:LEU:HD22	2.00	0.43
14:F:207:VAL:HG13	14:F:219:ILE:HG21	2.01	0.43
46:I:303:3PE:H382	46:I:303:3PE:H3B1	1.86	0.43
18:J:139:ASP:OD2	32:b:72:ARG:NH2	2.50	0.43
23:P:73:ASP:OD1	23:P:74:VAL:N	2.52	0.43
1:1:39:GLN:HG2	11:C:234:THR:HG23	2.00	0.43
2:2:152:ILE:HD12	2:2:152:ILE:HA	1.84	0.43
4:4:358:VAL:HA	4:4:366:LEU:HD23	2.01	0.43
5:5:293:LEU:HD22	5:5:420:PHE:HD1	1.84	0.43
9:A:290:ASP:OD1	9:A:294:GLU:HG3	2.19	0.43
10:B:109:ARG:O	10:B:111:ARG:HD2	2.18	0.43
10:B:318:MET:HE3	10:B:318:MET:HB3	1.90	0.43
13:E:295:GLU:O	13:E:299:ARG:HG2	2.19	0.43
15:G:77:GLN:HG3	15:G:273:ARG:HH11	1.84	0.43
15:G:101:PHE:HB3	15:G:110:ILE:HD13	2.00	0.43
30:Z:95:ILE:HG23	30:Z:99:GLN:HB3	2.00	0.43
38:h:3:TYR:CZ	38:h:6:ARG:HB2	2.54	0.43
1:1:37:SER:OG	12:D:7:THR:HG21	2.19	0.42
3:3:57:PHE:CZ	3:3:61:LEU:HD12	2.54	0.42
4:4:337:VAL:HG12	31:a:102:ASP:OD2	2.19	0.42
5:5:309:GLN:O	5:5:312:MET:HB2	2.19	0.42
5:5:586:LEU:HD12	31:a:103:ILE:HG21	2.01	0.42
13:E:84:GLU:O	13:E:87:LYS:HG2	2.18	0.42
15:G:207:ASP:HB2	23:P:5:PRO:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:82:GLN:N	29:Y:103:GLN:HE22	2.10	0.42
29:Y:204:LEU:O	29:Y:205:LYS:HG2	2.19	0.42
30:Z:49:PRO:HD3	53:h:221:HOH:O	2.19	0.42
5:5:664:LEU:HD13	18:J:112:PHE:CD2	2.54	0.42
9:A:318:VAL:HG22	9:A:591:ILE:CD1	2.49	0.42
14:F:66:HIS:CD2	30:Z:142:GLU:HA	2.54	0.42
21:M:91:ALA:HA	38:h:107:ARG:NH2	2.34	0.42
30:Z:15:SER:HA	30:Z:40:ASN:OD1	2.20	0.42
5:5:151:VAL:HG23	5:5:164:SER:HB3	2.01	0.42
5:5:522:PRO:HG2	5:5:525:PHE:HD2	1.84	0.42
6:6:44:ILE:HD13	6:6:89:LEU:HB3	2.01	0.42
8:9:56:GLU:OE1	27:W:110:THR:HG22	2.19	0.42
9:A:483:ARG:HG3	9:A:521:TRP:CD2	2.55	0.42
9:A:484:PRO:HG3	9:A:515:ASN:OD1	2.18	0.42
9:A:557:TRP:CH2	9:A:635:VAL:HG11	2.55	0.42
9:A:713:PRO:O	9:A:717:ARG:HG3	2.19	0.42
13:E:106:LEU:O	13:E:147:ARG:HD2	2.19	0.42
13:E:141:HIS:O	13:E:183:ALA:HB2	2.19	0.42
13:E:267:GLN:O	13:E:270:GLU:HG3	2.20	0.42
14:F:225:VAL:HB	53:F:303:HOH:O	2.19	0.42
14:F:246:GLU:OE2	15:G:96:LYS:HE3	2.20	0.42
22:O:97:ASP:N	22:O:100:ASP:HB2	2.34	0.42
22:Q:68:ILE:HG21	22:Q:131:ILE:HD11	2.01	0.42
32:b:34:TRP:C	32:b:37:PRO:HD2	2.44	0.42
4:4:21:ILE:HD13	4:4:78:ILE:CD1	2.49	0.42
4:4:91:LEU:O	4:4:95:ILE:HG12	2.19	0.42
4:4:394:ARG:O	40:j:6:HIS:HB2	2.20	0.42
5:5:6:ILE:HA	5:5:125:ILE:HG21	2.01	0.42
5:5:31:ILE:HD11	39:i:31:THR:HG23	2.00	0.42
8:9:10:GLY:HA2	41:n:141:PHE:O	2.18	0.42
8:9:89:GLY:O	12:D:70:PRO:HG2	2.20	0.42
10:B:155:GLU:OE2	10:B:158:ARG:NH1	2.52	0.42
10:B:337:TRP:CZ3	10:B:340:LEU:HD22	2.54	0.42
10:B:344:ILE:HG12	10:B:352:ILE:CD1	2.50	0.42
11:C:427:VAL:O	11:C:451:GLY:HA2	2.18	0.42
18:J:81:GLU:O	18:J:81:GLU:HG3	2.19	0.42
29:Y:114:LYS:NZ	29:Y:115:PRO:O	2.52	0.42
38:h:73:MET:HG3	38:h:86:PRO:HG3	2.01	0.42
1:1:151:TYR:CZ	1:1:346:CYS:HB2	2.55	0.42
2:2:142:THR:HG22	2:2:147:SER:HB3	2.01	0.42
3:3:132:TYR:CZ	3:3:134:GLY:HA2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:102:ASN:HB3	4:4:520:TYR:HE2	1.85	0.42
6:6:48:LEU:HA	6:6:51:ILE:HD12	2.01	0.42
7:8:22:VAL:HG13	7:8:27:ARG:HG2	2.02	0.42
8:9:64:GLN:HG3	27:W:113:VAL:HG13	2.01	0.42
12:D:28:VAL:HA	12:D:31:MET:HE2	2.01	0.42
14:F:218:LEU:O	14:F:222:VAL:HG23	2.19	0.42
15:G:124:LEU:O	15:G:132:PHE:HB2	2.20	0.42
17:I:167:GLY:O	17:I:171:GLU:HG3	2.20	0.42
2:2:111:LYS:HG2	14:F:163:GLU:OE2	2.20	0.42
4:4:167:LEU:HA	4:4:167:LEU:HD23	1.76	0.42
5:5:49:GLU:OE2	39:i:66:PRO:HD2	2.19	0.42
5:5:200:LEU:HD11	34:d:78:TYR:CE2	2.55	0.42
46:5:704:3PE:H382	46:i:101:3PE:H32	2.01	0.42
10:B:111:ARG:O	10:B:152:LYS:NZ	2.50	0.42
11:C:419:LEU:HD23	11:C:419:LEU:HA	1.89	0.42
13:E:82:ARG:O	19:K:226:MET:HE1	2.19	0.42
28:X:20:TYR:HB3	28:X:21:PRO:HD2	2.01	0.42
38:h:8:LEU:O	38:h:12:ARG:HG3	2.20	0.42
39:i:62:ASP:OD1	39:i:62:ASP:N	2.53	0.42
44:j:101:LMT:H1'	44:j:101:LMT:H22	1.27	0.42
1:1:76:VAL:HG13	1:1:80:LEU:HB2	2.02	0.42
3:3:133:LEU:HD13	14:F:103:LEU:HD11	2.01	0.42
4:4:11:PRO:CG	4:4:86:ASN:HD21	2.27	0.42
4:4:300:PHE:CE1	4:4:366:LEU:HD22	2.54	0.42
43:5:703:PC1:H111	31:a:110:TYR:HB2	2.01	0.42
16:H:203:CYS:HA	16:H:248:ALA:HB1	2.00	0.42
19:K:81:LEU:O	19:K:224:THR:OG1	2.37	0.42
21:M:91:ALA:HA	38:h:107:ARG:HH21	1.84	0.42
33:c:63:ILE:HD12	33:c:63:ILE:H	1.85	0.42
39:i:34:PHE:HA	39:i:37:VAL:HG12	2.02	0.42
45:D:101:CDL:HB62	30:Z:31:ILE:HG22	2.02	0.42
22:Q:109:GLU:HG2	22:Q:114:ILE:O	2.19	0.42
31:a:114:TRP:CD1	31:a:115:ILE:HG23	2.54	0.42
36:f:12:LYS:HZ2	36:f:65:GLU:HA	1.84	0.42
2:2:16:THR:HB	28:X:73:LYS:HE2	2.02	0.42
2:2:566:GLN:O	2:2:570:SER:HB3	2.20	0.42
4:4:79:ALA:O	4:4:82:THR:HG22	2.19	0.42
4:4:487:ARG:HH11	25:S:77:GLY:HA3	1.83	0.42
10:B:319:SER:HB3	10:B:362:LEU:HD23	2.01	0.42
13:E:68:ASN:HD22	15:G:239:GLU:HB2	1.84	0.42
13:E:142:ILE:HA	13:E:142:ILE:HD13	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:190:VAL:HG21	16:H:194:HIS:CD2	2.55	0.42
17:I:119:SER:O	53:I:403:HOH:O	2.21	0.42
19:K:141:GLY:HA2	48:K:301:SF4:S2	2.59	0.42
44:1:403:LMT:H71	44:1:403:LMT:H102	1.81	0.42
2:2:234:TRP:CD2	8:9:55:LYS:HG2	2.55	0.42
5:5:343:ALA:HA	5:5:346:VAL:HG22	2.02	0.42
9:A:114:ASN:OD1	9:A:114:ASN:N	2.53	0.42
9:A:679:VAL:HA	9:A:683:ASP:HB2	2.02	0.42
10:B:466:ARG:HD2	10:B:467:HIS:NE2	2.35	0.42
13:E:160:PHE:HB3	13:E:191:PHE:CE2	2.54	0.42
16:H:244:ALA:HB3	16:H:250:MET:HG2	2.02	0.42
27:W:35:ALA:O	27:W:39:MET:HG3	2.19	0.42
37:g:36:GLY:O	37:g:39:THR:HG22	2.20	0.42
38:h:46:GLU:HA	38:h:55:THR:O	2.20	0.42
1:1:114:MET:HB2	1:1:114:MET:HE3	1.67	0.41
43:1:401:PC1:H132	43:1:401:PC1:H112	1.88	0.41
2:2:116:MET:HG3	14:F:154:TRP:CH2	2.55	0.41
2:2:247:PHE:CZ	2:2:251:PHE:HE2	2.37	0.41
4:4:151:ASN:HB2	4:4:196:PHE:HE1	1.85	0.41
4:4:211:TYR:CE2	44:4:601:LMT:H102	2.55	0.41
4:4:273:LEU:HD11	4:4:345:TYR:CE2	2.55	0.41
5:5:72:ILE:HG23	5:5:132:ASN:CG	2.45	0.41
6:6:77:TYR:CE2	20:L:60:ILE:HG23	2.55	0.41
9:A:88:LEU:HA	9:A:98:VAL:O	2.20	0.41
9:A:444:ALA:HB1	9:A:459:LEU:CD2	2.50	0.41
9:A:479:LYS:HG2	9:A:512:ASN:OD1	2.20	0.41
11:C:337:ASP:OD2	11:C:339:ARG:HB2	2.20	0.41
17:I:95:ILE:HG23	17:I:100:GLU:HB2	2.00	0.41
1:1:91:LEU:HD23	1:1:91:LEU:HA	1.92	0.41
1:1:185:LEU:O	27:W:39:MET:HA	2.20	0.41
2:2:11:LEU:HD12	2:2:11:LEU:HA	1.80	0.41
2:2:284:LYS:HE2	2:2:344:THR:HG21	2.02	0.41
2:2:316:LEU:HD11	2:2:463:TYR:HE2	1.85	0.41
7:8:20:ALA:HB3	7:8:35:ILE:HD12	2.03	0.41
9:A:297:ILE:HB	9:A:301:THR:HG23	2.02	0.41
9:A:310:THR:HG21	9:A:711:SER:O	2.20	0.41
11:C:313:VAL:HG22	11:C:361:ASP:HB3	2.01	0.41
14:F:232:LEU:HG	14:F:236:MET:HG2	2.02	0.41
30:Z:60:PRO:HB2	30:Z:63:GLU:HG2	2.02	0.41
37:g:45:PRO:O	37:g:48:ARG:HG2	2.20	0.41
4:4:71:ASN:OD1	4:4:72:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:172:VAL:HG11	4:4:181:PHE:HE2	1.85	0.41
5:5:596:LEU:HD21	40:j:38:VAL:HG12	2.01	0.41
7:8:33:LEU:C	7:8:36:PRO:HD2	2.45	0.41
13:E:128:ARG:HE	50:E:402:NDP:H8A	1.85	0.41
13:E:302:TRP:HB3	46:E:401:3PE:O22	2.21	0.41
15:G:229:THR:HG21	15:G:250:LEU:HD21	2.01	0.41
16:H:212:ALA:HB1	16:H:263:PRO:HG3	2.03	0.41
18:J:17:VAL:O	18:J:21:LEU:HG	2.19	0.41
21:M:83:ARG:HD2	53:M:313:HOH:O	2.20	0.41
28:X:170:LYS:HG3	28:X:171:TYR:N	2.34	0.41
31:a:122:PHE:CZ	31:a:126:LEU:HD21	2.56	0.41
31:a:165:ALA:HA	40:j:68:ARG:NH1	2.35	0.41
2:2:498:ASN:HB3	2:2:501:LEU:HD23	2.01	0.41
4:4:528:GLY:HA2	18:J:168:ILE:HD13	2.02	0.41
4:4:530:GLU:HG2	34:d:88:LYS:HG3	2.01	0.41
6:6:220:LYS:HB2	13:E:376:ASP:CG	2.45	0.41
9:A:372:ARG:HG2	9:A:372:ARG:H	1.69	0.41
13:E:184:GLU:OE1	13:E:196:ILE:HG21	2.20	0.41
18:J:181:LEU:HD22	18:J:185:TYR:HD1	1.85	0.41
27:W:32:LEU:HD23	27:W:32:LEU:HA	1.87	0.41
33:c:58:LEU:HB3	33:c:61:PHE:HB2	2.02	0.41
35:e:23:MET:C	35:e:25:PHE:N	2.78	0.41
3:3:106:LEU:HD23	3:3:106:LEU:HA	1.83	0.41
5:5:248:HIS:HA	53:5:819:HOH:O	2.20	0.41
5:5:394:PHE:HA	5:5:397:GLU:HG2	2.02	0.41
5:5:419:ILE:HD11	5:5:536:PHE:CE1	2.54	0.41
5:5:611:ARG:HH11	44:5:705:LMT:H2B	1.85	0.41
6:6:44:ILE:CD1	6:6:89:LEU:HB3	2.51	0.41
8:9:6:GLY:HA2	20:L:48:ASP:O	2.20	0.41
8:9:64:GLN:HB2	27:W:113:VAL:HG22	2.02	0.41
11:C:396:ASP:OD1	30:Z:80:TYR:HE1	2.03	0.41
13:E:118:HIS:NE2	21:M:85:GLU:OE2	2.32	0.41
13:E:145:THR:O	13:E:149:VAL:HG12	2.20	0.41
16:H:190:VAL:HG22	16:H:191:GLY:H	1.86	0.41
18:J:19:LEU:HB3	18:J:70:ASP:OD2	2.20	0.41
27:W:83:TYR:O	27:W:87:GLN:HG2	2.21	0.41
30:Z:119:GLU:C	30:Z:121:GLY:H	2.28	0.41
31:a:116:THR:HG22	31:a:118:GLY:H	1.85	0.41
4:4:397:THR:CB	40:j:11:MET:HE1	2.49	0.41
4:4:461:SER:HA	4:4:464:TYR:CZ	2.56	0.41
5:5:189:LEU:HD22	5:5:200:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:202:PRO:HG2	34:d:68:LEU:HD21	2.02	0.41
9:A:310:THR:HA	38:h:125:GLN:HB2	2.03	0.41
10:B:113:GLY:HA2	10:B:376:GLY:O	2.21	0.41
11:C:181:MET:HE3	11:C:250:TYR:CE1	2.55	0.41
11:C:330:ARG:HD3	11:C:354:VAL:CG1	2.51	0.41
13:E:221:THR:O	13:E:284:ASN:HA	2.20	0.41
14:F:250:ARG:HB2	14:F:251:PRO:HD2	2.01	0.41
18:J:103:THR:HG21	18:J:108:ARG:HD2	2.01	0.41
21:M:156:TYR:CZ	21:M:160:LEU:HD21	2.55	0.41
28:X:43:HIS:HB3	28:X:89:TYR:CE2	2.56	0.41
1:1:10:LEU:O	1:1:14:VAL:HG13	2.21	0.41
2:2:284:LYS:HE2	2:2:344:THR:CG2	2.51	0.41
5:5:141:GLU:O	5:5:145:VAL:HG23	2.21	0.41
9:A:133:HIS:HD2	11:C:411:MET:HE2	1.86	0.41
9:A:165:ILE:HG23	10:B:490:GLY:O	2.20	0.41
10:B:434:GLU:OE1	10:B:489:ALA:HA	2.20	0.41
11:C:175:LEU:HD13	11:C:460:ILE:HG21	2.02	0.41
15:G:118:ILE:HB	15:G:119:PRO:HD3	2.03	0.41
17:I:190:THR:OG1	17:I:193:GLU:HG3	2.21	0.41
30:Z:24:SER:HA	53:Z:218:HOH:O	2.20	0.41
33:c:34:ASP:HB3	33:c:37:GLU:HB2	2.03	0.41
2:2:520:ILE:HD13	2:2:520:ILE:HA	1.90	0.41
4:4:179:TYR:HE2	4:4:216:SER:O	2.04	0.41
5:5:148:TYR:O	5:5:152:SER:OG	2.24	0.41
5:5:251:THR:O	5:5:254:THR:HB	2.21	0.41
9:A:352:VAL:HG23	9:A:378:LEU:HA	2.02	0.41
9:A:367:LYS:HG3	9:A:378:LEU:HD21	2.01	0.41
11:C:176:ASP:OD2	11:C:440:LYS:HE3	2.20	0.41
11:C:292:ASP:O	11:C:296:GLU:HG2	2.21	0.41
11:C:371:GLU:OE1	30:Z:185:SER:HB2	2.21	0.41
17:I:183:ASN:HB2	17:I:208:TRP:CZ2	2.56	0.41
29:Y:210:LYS:HD3	53:Y:360:HOH:O	2.20	0.41
2:2:363:THR:O	2:2:367:ILE:HG12	2.21	0.41
2:2:513:LEU:HD12	2:2:517:ASN:C	2.46	0.41
4:4:292:LEU:HD23	4:4:292:LEU:HA	1.90	0.41
9:A:262:ILE:HB	9:A:615:THR:HG22	2.03	0.41
9:A:271:ASN:OD1	9:A:289:ASN:ND2	2.54	0.41
9:A:589:ALA:HB1	9:A:591:ILE:O	2.21	0.41
9:A:681:LEU:O	9:A:685:ASN:HB2	2.20	0.41
9:A:730:ASN:HA	9:A:733:ALA:HB3	2.02	0.41
10:B:243:GLU:OE2	10:B:250:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:399:PHE:O	10:B:403:GLU:HG2	2.20	0.41
11:C:63:PHE:CG	23:P:68:LYS:HG3	2.55	0.41
11:C:365:ARG:HH21	11:C:489:THR:HG21	1.85	0.41
11:C:396:ASP:OD2	11:C:399:ILE:HD12	2.21	0.41
13:E:96:LEU:HD21	17:I:191:ARG:HG3	2.02	0.41
13:E:136:SER:C	13:E:138:ALA:N	2.79	0.41
17:I:122:GLU:HG3	21:M:98:ALA:HB2	2.03	0.41
26:U:133:ILE:HD12	26:U:136:GLN:NE2	2.36	0.41
27:W:27:ARG:O	27:W:30:PRO:HD2	2.21	0.41
28:X:13:SER:HB3	53:X:318:HOH:O	2.21	0.41
28:X:125:LEU:HD23	28:X:125:LEU:HA	1.71	0.41
37:g:11:THR:HB	37:g:14:LYS:HB3	2.03	0.41
41:n:95:ASP:OD1	41:n:95:ASP:N	2.54	0.41
1:1:83:VAL:CG2	3:3:15:ALA:HB1	2.51	0.41
5:5:109:HIS:ND1	43:5:702:PC1:H112	2.36	0.41
5:5:254:THR:HG21	5:5:329:LEU:HD21	2.03	0.41
9:A:660:PRO:HD3	36:f:17:LEU:HD22	2.03	0.41
11:C:322:LEU:HD11	11:C:473:HIS:CD2	2.55	0.41
13:E:301:LEU:HD23	13:E:301:LEU:HA	1.85	0.41
15:G:64:GLU:OE1	30:Z:70:ILE:HD11	2.20	0.41
24:R:21:TRP:CZ2	24:R:67:HIS:HA	2.55	0.41
30:Z:193:ARG:NH1	53:Z:202:HOH:O	2.27	0.41
35:e:23:MET:O	35:e:25:PHE:N	2.54	0.41
38:h:54:ARG:HE	38:h:54:ARG:HB3	1.75	0.41
2:2:3:MET:HE3	2:2:138:PHE:CE2	2.55	0.40
2:2:91:ILE:HG21	2:2:525:LEU:HD21	2.03	0.40
43:2:605:PC1:H392	44:X:203:LMT:H102	2.02	0.40
43:5:703:PC1:H111	31:a:110:TYR:CB	2.51	0.40
6:6:165:ASN:HB2	8:9:64:GLN:OE1	2.21	0.40
9:A:742:MET:SD	9:A:742:MET:N	2.82	0.40
13:E:198:ARG:HD2	13:E:256:GLU:OE2	2.21	0.40
16:H:196:GLN:HB3	16:H:239:VAL:HG11	2.03	0.40
17:I:53:PRO:HA	17:I:54:PRO:HD3	1.96	0.40
27:W:45:LYS:HE3	27:W:45:LYS:HB3	1.88	0.40
32:b:50:LEU:HD23	32:b:50:LEU:HA	1.91	0.40
1:1:22:VAL:HG23	12:D:17:MET:HG3	2.02	0.40
1:1:44:PRO:HA	19:K:122:ARG:HA	2.04	0.40
5:5:40:THR:O	5:5:44:ILE:HG12	2.22	0.40
9:A:492:VAL:O	9:A:498:ALA:HB2	2.20	0.40
10:B:96:HIS:HB3	10:B:173:ARG:NH2	2.36	0.40
10:B:300:LYS:HE3	10:B:302:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:241:GLU:HG2	17:I:93:TYR:CZ	2.56	0.40
14:F:245:LEU:HD23	14:F:248:GLN:OE1	2.21	0.40
15:G:100:GLN:HG3	15:G:111:TYR:CD2	2.56	0.40
16:H:250:MET:HE2	16:H:250:MET:HB2	1.73	0.40
20:L:18:ASN:OD1	20:L:21:ASN:HB2	2.22	0.40
23:P:29:TYR:O	23:P:33:ILE:HG12	2.21	0.40
24:R:2:SER:C	24:R:4:ARG:H	2.29	0.40
30:Z:153:LEU:HD23	30:Z:158:GLY:O	2.21	0.40
1:1:39:GLN:CG	11:C:234:THR:HG23	2.51	0.40
1:1:322:ILE:O	1:1:326:VAL:HG23	2.21	0.40
4:4:320:ALA:O	4:4:324:ILE:HG12	2.20	0.40
5:5:85:MET:HE1	5:5:254:THR:CG2	2.52	0.40
5:5:210:ILE:O	5:5:214:ILE:HG12	2.22	0.40
5:5:482:ILE:HG22	5:5:483:PHE:CD1	2.56	0.40
6:6:83:ILE:HD13	6:6:83:ILE:HA	1.99	0.40
8:9:89:GLY:H	8:9:97:THR:HG22	1.85	0.40
9:A:97:PRO:HG3	9:A:117:LEU:HD21	2.04	0.40
9:A:247:TYR:HE1	9:A:282:MET:HB3	1.87	0.40
10:B:300:LYS:HZ2	10:B:300:LYS:HG2	1.68	0.40
14:F:70:ARG:NH1	14:F:74:GLU:OE2	2.55	0.40
14:F:148:ASP:CG	14:F:150:ARG:HE	2.30	0.40
15:G:66:LYS:HG2	30:Z:70:ILE:HB	2.02	0.40
26:U:105:ASN:HB3	26:U:111:GLN:HB2	2.04	0.40
28:X:169:ALA:O	28:X:173:GLN:HG3	2.21	0.40
32:b:47:GLY:HA2	32:b:50:LEU:HB2	2.03	0.40
39:i:55:ARG:HH11	39:i:71:VAL:HG11	1.85	0.40
1:1:125:ILE:HD13	1:1:125:ILE:HA	1.86	0.40
2:2:19:ARG:C	2:2:21:MET:H	2.29	0.40
2:2:128:ILE:O	2:2:132:VAL:HG23	2.21	0.40
4:4:509:ILE:C	4:4:511:PRO:HD3	2.46	0.40
5:5:53:ASN:OD1	39:i:63:ARG:HD2	2.22	0.40
10:B:153:ASP:OD1	10:B:271:VAL:HB	2.22	0.40
10:B:160:ASP:OD1	10:B:160:ASP:N	2.55	0.40
11:C:218:ASN:HD21	11:C:440:LYS:HE2	1.86	0.40
11:C:480:LEU:O	11:C:484:VAL:HG13	2.22	0.40
13:E:112:ILE:HD13	13:E:148:ILE:HG13	2.03	0.40
15:G:82:ASN:HA	15:G:85:LYS:HB2	2.02	0.40
15:G:91:MET:HG3	30:Z:100:GLN:OE1	2.22	0.40
16:H:211:ASP:OD1	16:H:211:ASP:N	2.52	0.40
16:H:214:VAL:HG13	16:H:236:PHE:CZ	2.55	0.40
22:Q:75:PHE:CE1	33:c:36:TRP:CE2	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:72:GLN:C	1:1:74:ASN:H	2.30	0.40
2:2:60:ILE:CD1	28:X:148:LEU:HB3	2.52	0.40
2:2:365:ALA:HA	2:2:453:MET:HE2	2.03	0.40
4:4:395:THR:HG22	4:4:486:PHE:CE2	2.56	0.40
9:A:130:LEU:CD1	11:C:412:GLU:HG3	2.52	0.40
9:A:145:GLU:HB3	53:A:1021:HOH:O	2.21	0.40
11:C:181:MET:HA	11:C:184:GLU:HG2	2.04	0.40
11:C:244:GLU:OE2	19:K:117:ARG:HD2	2.22	0.40
13:E:152:VAL:HG11	13:E:160:PHE:HB2	2.02	0.40
16:H:294:SER:OG	16:H:295:CYS:N	2.54	0.40
17:I:154:THR:HG22	38:h:120:THR:HG22	2.04	0.40
30:Z:115:GLU:HG2	30:Z:116:LEU:N	2.37	0.40
37:g:27:PHE:O	37:g:31:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	376/378 (100%)	357 (95%)	19 (5%)	0	100	100
2	2	554/571 (97%)	541 (98%)	13 (2%)	0	100	100
3	3	110/146 (75%)	107 (97%)	3 (3%)	0	100	100
4	4	490/542 (90%)	472 (96%)	18 (4%)	0	100	100
5	5	668/679 (98%)	632 (95%)	36 (5%)	0	100	100
6	6	185/224 (83%)	175 (95%)	10 (5%)	0	100	100
7	8	75/86 (87%)	72 (96%)	3 (4%)	0	100	100
8	9	100/785 (13%)	98 (98%)	2 (2%)	0	100	100
9	A	709/749 (95%)	680 (96%)	29 (4%)	0	100	100
10	B	454/507 (90%)	434 (96%)	20 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	C	422/499 (85%)	404 (96%)	18 (4%)	0	100	100
12	D	79/86 (92%)	76 (96%)	3 (4%)	0	100	100
13	E	351/378 (93%)	337 (96%)	13 (4%)	1 (0%)	36	63
14	F	235/261 (90%)	232 (99%)	3 (1%)	0	100	100
15	G	240/293 (82%)	233 (97%)	7 (3%)	0	100	100
16	H	218/318 (69%)	205 (94%)	13 (6%)	0	100	100
17	I	183/223 (82%)	179 (98%)	4 (2%)	0	100	100
18	J	186/199 (94%)	182 (98%)	4 (2%)	0	100	100
19	K	180/230 (78%)	172 (96%)	7 (4%)	1 (1%)	21	47
20	L	85/89 (96%)	85 (100%)	0	0	100	100
21	M	39/168 (23%)	39 (100%)	0	0	100	100
22	O	32/141 (23%)	31 (97%)	1 (3%)	0	100	100
22	Q	83/141 (59%)	81 (98%)	2 (2%)	0	100	100
23	P	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
24	R	96/99 (97%)	91 (95%)	5 (5%)	0	100	100
25	S	40/143 (28%)	36 (90%)	4 (10%)	0	100	100
27	W	40/121 (33%)	40 (100%)	0	0	100	100
28	X	184/191 (96%)	179 (97%)	5 (3%)	0	100	100
29	Y	152/210 (72%)	144 (95%)	8 (5%)	0	100	100
30	Z	184/196 (94%)	174 (95%)	10 (5%)	0	100	100
31	a	141/203 (70%)	133 (94%)	8 (6%)	0	100	100
32	b	78/94 (83%)	77 (99%)	1 (1%)	0	100	100
33	c	62/93 (67%)	59 (95%)	3 (5%)	0	100	100
34	d	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
35	e	36/46 (78%)	34 (94%)	2 (6%)	0	100	100
36	f	86/95 (90%)	83 (96%)	3 (4%)	0	100	100
37	g	75/82 (92%)	71 (95%)	4 (5%)	0	100	100
38	h	131/134 (98%)	127 (97%)	4 (3%)	0	100	100
39	i	79/93 (85%)	75 (95%)	4 (5%)	0	100	100
40	j	71/75 (95%)	70 (99%)	1 (1%)	0	100	100
41	n	133/184 (72%)	127 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	o	30/380 (8%)	29 (97%)	1 (3%)	0	100	100
All	All	7890/10361 (76%)	7583 (96%)	305 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	E	286	PRO
19	K	102	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	298/326 (91%)	295 (99%)	3 (1%)	68	86
2	2	509/518 (98%)	498 (98%)	11 (2%)	45	75
3	3	95/128 (74%)	95 (100%)	0	100	100
4	4	431/477 (90%)	422 (98%)	9 (2%)	47	76
5	5	581/596 (98%)	578 (100%)	3 (0%)	81	92
6	6	167/203 (82%)	165 (99%)	2 (1%)	63	84
7	8	68/75 (91%)	68 (100%)	0	100	100
8	9	84/687 (12%)	82 (98%)	2 (2%)	43	74
9	A	577/602 (96%)	576 (100%)	1 (0%)	87	96
10	B	366/401 (91%)	365 (100%)	1 (0%)	86	94
11	C	354/416 (85%)	353 (100%)	1 (0%)	86	94
12	D	68/69 (99%)	67 (98%)	1 (2%)	57	81
13	E	311/335 (93%)	310 (100%)	1 (0%)	86	94
14	F	198/219 (90%)	198 (100%)	0	100	100
15	G	215/257 (84%)	213 (99%)	2 (1%)	70	87
16	H	190/272 (70%)	189 (100%)	1 (0%)	81	92
17	I	158/191 (83%)	156 (99%)	2 (1%)	61	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	J	131/146 (90%)	131 (100%)	0	100	100
19	K	154/191 (81%)	152 (99%)	2 (1%)	61	83
20	L	74/76 (97%)	73 (99%)	1 (1%)	59	82
21	M	98/135 (73%)	98 (100%)	0	100	100
22	O	67/119 (56%)	67 (100%)	0	100	100
22	Q	74/119 (62%)	74 (100%)	0	100	100
23	P	109/110 (99%)	106 (97%)	3 (3%)	38	70
24	R	87/89 (98%)	87 (100%)	0	100	100
25	S	58/111 (52%)	57 (98%)	1 (2%)	53	80
26	U	148/167 (89%)	141 (95%)	7 (5%)	23	54
27	W	100/102 (98%)	99 (99%)	1 (1%)	68	86
28	X	143/152 (94%)	143 (100%)	0	100	100
29	Y	131/176 (74%)	130 (99%)	1 (1%)	73	89
30	Z	152/155 (98%)	152 (100%)	0	100	100
31	a	123/177 (70%)	123 (100%)	0	100	100
32	b	66/74 (89%)	66 (100%)	0	100	100
33	c	47/80 (59%)	47 (100%)	0	100	100
34	d	87/94 (93%)	86 (99%)	1 (1%)	65	85
35	e	30/35 (86%)	30 (100%)	0	100	100
36	f	76/80 (95%)	76 (100%)	0	100	100
37	g	65/69 (94%)	64 (98%)	1 (2%)	57	81
38	h	118/119 (99%)	118 (100%)	0	100	100
39	i	69/78 (88%)	69 (100%)	0	100	100
40	j	63/64 (98%)	62 (98%)	1 (2%)	55	81
41	n	108/150 (72%)	107 (99%)	1 (1%)	70	87
42	o	26/318 (8%)	26 (100%)	0	100	100
All	All	7074/8958 (79%)	7014 (99%)	60 (1%)	70	89

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	15	LEU
1	1	373	VAL

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Mol	Chain	Res	Type
1	1	378	LEU
2	2	17	LEU
2	2	23	ILE
2	2	64	THR
2	2	128	ILE
2	2	130	LEU
2	2	199	VAL
2	2	442	VAL
2	2	464	ILE
2	2	466	LEU
2	2	486	LYS
2	2	524	LEU
4	4	107	ILE
4	4	120	LEU
4	4	208	ILE
4	4	211	TYR
4	4	262	LYS
4	4	337	VAL
4	4	342	LEU
4	4	345	TYR
4	4	522	ILE
5	5	372	VAL
5	5	378	LEU
5	5	503	ASN
6	6	170	ILE
6	6	198	VAL
8	9	26	VAL
8	9	56	GLU
9	A	259	THR
10	B	344	ILE
11	C	130	VAL
12	D	81	VAL
13	E	104	PHE
15	G	107	GLU
15	G	229	THR
16	H	250	MET
17	I	125	ILE
17	I	173	CYS
19	K	105	CYS
19	K	176	TYR
20	L	51	ILE
23	P	80	ASN

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Mol	Chain	Res	Type
23	P	94	SER
23	P	99	PHE
25	S	131	GLU
26	U	17	THR
26	U	19	LEU
26	U	48	LYS
26	U	76	VAL
26	U	91	CYS
26	U	96	ARG
26	U	116	GLU
27	W	40	LEU
29	Y	133	VAL
34	d	31	LEU
37	g	50	ILE
40	j	11	MET
41	n	119	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	8	ASN
1	1	54	GLN
1	1	147	GLN
2	2	26	ASN
2	2	68	HIS
2	2	80	GLN
2	2	119	HIS
2	2	155	GLN
2	2	200	ASN
2	2	299	ASN
2	2	364	GLN
2	2	409	ASN
3	3	47	GLN
3	3	53	ASN
3	3	83	ASN
4	4	86	ASN
4	4	151	ASN
4	4	248	GLN
4	4	519	HIS
5	5	131	ASN
5	5	171	ASN
5	5	295	GLN

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Mol	Chain	Res	Type
5	5	296	GLN
5	5	503	ASN
5	5	583	ASN
6	6	49	HIS
6	6	182	ASN
6	6	183	ASN
8	9	28	ASN
8	9	38	ASN
9	A	142	GLN
9	A	216	GLN
9	A	289	ASN
9	A	423	HIS
9	A	429	ASN
10	B	66	GLN
10	B	67	ASN
10	B	96	HIS
10	B	142	ASN
10	B	176	ASN
10	B	190	GLN
10	B	309	ASN
11	C	60	GLN
11	C	123	GLN
11	C	218	ASN
11	C	269	HIS
11	C	270	GLN
11	C	359	ASN
11	C	410	ASN
12	D	33	ASN
12	D	48	GLN
13	E	42	GLN
13	E	134	ASN
13	E	162	GLN
13	E	167	ASN
13	E	223	ASN
13	E	284	ASN
13	E	291	GLN
13	E	298	ASN
14	F	42	HIS
14	F	62	GLN
14	F	106	HIS
15	G	77	GLN
15	G	155	ASN

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Mol	Chain	Res	Type
15	G	161	HIS
15	G	220	HIS
15	G	266	GLN
16	H	104	HIS
16	H	122	ASN
16	H	128	GLN
16	H	153	HIS
17	I	87	GLN
18	J	45	ASN
19	K	120	GLN
21	M	153	HIS
22	O	92	ASN
23	P	63	HIS
23	P	114	ASN
25	S	86	ASN
26	U	51	ASN
26	U	107	GLN
26	U	144	HIS
28	X	65	GLN
29	Y	64	ASN
29	Y	103	GLN
29	Y	181	GLN
29	Y	184	ASN
29	Y	195	ASN
30	Z	51	ASN
30	Z	78	ASN
30	Z	166	GLN
31	a	88	GLN
31	a	101	HIS
32	b	29	ASN
33	c	39	HIS
34	d	28	ASN
34	d	45	GLN
34	d	67	HIS
36	f	42	HIS
38	h	121	GLN
41	n	84	HIS
41	n	110	GLN
41	n	126	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	0.44	0	5,13,15	1.05	1 (20%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	154	2MR	NE-CZ-NH2	-2.20	117.46	119.48

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 44 ligands modelled in this entry, 1 is monoatomic - leaving 43 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
44	LMT	2	602	-	36,36,36	0.48	0	47,47,47	0.98	3 (6%)
46	3PE	5	704	-	41,41,50	0.31	0	44,46,55	0.37	0
45	CDL	S	201	-	60,60,99	0.33	0	66,72,111	0.44	0
44	LMT	3	202	-	36,36,36	0.41	0	47,47,47	0.94	3 (6%)
44	LMT	1	403	-	36,36,36	0.36	0	47,47,47	0.62	0
48	SF4	I	301	17	0,12,12	-	-	-	-	-
46	3PE	W	202	-	31,31,50	0.37	0	34,36,55	0.39	0
48	SF4	K	301	19	0,12,12	-	-	-	-	-
44	LMT	g	101	-	35,35,36	1.10	2 (5%)	46,46,47	1.08	1 (2%)
47	FES	A	801	9	0,4,4	-	-	-	-	-
45	CDL	X	202	-	75,75,99	0.34	0	81,87,111	0.38	0
52	ZMP	Q	201	22	30,35,36	0.20	0	34,42,45	0.41	0
43	PC1	2	605	-	44,44,53	0.29	0	50,52,61	0.53	0
43	PC1	5	703	-	44,44,53	0.30	0	50,52,61	0.33	0
45	CDL	2	601	-	67,67,99	0.33	0	73,79,111	0.42	0
46	3PE	i	101	-	37,37,50	0.32	0	40,42,55	0.36	0
46	3PE	I	303	-	36,36,50	0.35	0	39,41,55	0.56	0
52	ZMP	O	201	22	30,35,36	0.26	0	34,42,45	0.45	0
46	3PE	5	701	-	40,40,50	0.29	0	43,45,55	0.32	0
47	FES	H	401	16	0,4,4	-	-	-	-	-
44	LMT	4	601	-	36,36,36	1.10	2 (5%)	47,47,47	1.11	3 (6%)
43	PC1	1	401	-	32,32,53	0.33	0	38,40,61	0.35	0
44	LMT	X	203	-	36,36,36	0.38	0	47,47,47	0.70	0
49	FMN	B	602	-	33,33,33	0.69	0	48,50,50	0.71	1 (2%)
48	SF4	I	302	17	0,12,12	-	-	-	-	-
44	LMT	5	705	-	36,36,36	0.34	0	47,47,47	1.15	4 (8%)
44	LMT	2	603	-	34,34,36	0.37	0	45,45,47	0.84	1 (2%)
43	PC1	5	702	-	39,39,53	0.36	0	45,47,61	0.51	0
48	SF4	A	802	9	0,12,12	-	-	-	-	-
46	3PE	5	706	-	41,41,50	0.95	4 (9%)	44,46,55	1.11	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	LMT	1	402	-	36,36,36	0.35	0	47,47,47	0.82	1 (2%)
44	LMT	j	101	-	36,36,36	0.39	0	47,47,47	0.95	3 (6%)
45	CDL	X	201	-	51,51,99	0.38	0	57,63,111	0.51	0
48	SF4	A	803	9	0,12,12	-	-	-		
46	3PE	W	201	-	39,39,50	0.30	0	42,44,55	0.35	0
44	LMT	3	201	-	36,36,36	0.33	0	47,47,47	0.85	0
44	LMT	2	604	-	36,36,36	0.42	0	47,47,47	0.71	0
44	LMT	J	201	-	32,32,36	0.40	0	43,43,47	0.70	1 (2%)
44	LMT	a	301	-	36,36,36	0.39	0	47,47,47	0.79	2 (4%)
46	3PE	E	401	-	28,28,50	0.37	0	31,33,55	0.48	0
50	NDP	E	402	-	51,52,52	0.52	0	71,80,80	0.77	1 (1%)
45	CDL	D	101	-	58,58,99	0.35	0	64,70,111	0.42	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
44	LMT	2	602	-	-	7/21/61/61	0/2/2/2
46	3PE	5	704	-	-	17/45/45/54	-
45	CDL	S	201	-	-	20/70/70/110	-
44	LMT	3	202	-	-	9/21/61/61	0/2/2/2
44	LMT	1	403	-	-	2/21/61/61	0/2/2/2
48	SF4	I	301	17	-	-	0/6/5/5
46	3PE	W	202	-	-	7/35/35/54	-
48	SF4	K	301	19	-	-	0/6/5/5
44	LMT	g	101	-	-	11/20/60/61	0/2/2/2
47	FES	A	801	9	-	-	0/1/1/1
45	CDL	X	202	-	-	35/86/86/110	-
52	ZMP	Q	201	22	-	17/40/42/43	-
43	PC1	2	605	-	-	8/48/48/57	-
43	PC1	5	703	-	-	7/48/48/57	-
45	CDL	2	601	-	-	18/78/78/110	-
46	3PE	i	101	-	-	7/41/41/54	-
46	3PE	I	303	-	-	14/40/40/54	-
52	ZMP	O	201	22	-	10/40/42/43	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	5	701	-	-	9/44/44/54	-
47	FES	H	401	16	-	-	0/1/1/1
44	LMT	4	601	-	-	8/21/61/61	0/2/2/2
43	PC1	1	401	-	-	10/36/36/57	-
44	LMT	X	203	-	-	3/21/61/61	0/2/2/2
49	FMN	B	602	-	-	5/18/18/18	0/3/3/3
48	SF4	I	302	17	-	-	0/6/5/5
44	LMT	5	705	-	-	6/21/61/61	0/2/2/2
44	LMT	2	603	-	-	7/19/59/61	0/2/2/2
43	PC1	5	702	-	-	18/43/43/57	-
48	SF4	A	802	9	-	-	0/6/5/5
46	3PE	5	706	-	-	14/45/45/54	-
44	LMT	1	402	-	-	3/21/61/61	0/2/2/2
44	LMT	j	101	-	-	6/21/61/61	0/2/2/2
45	CDL	X	201	-	-	23/62/62/110	-
48	SF4	A	803	9	-	-	0/6/5/5
46	3PE	W	201	-	-	13/43/43/54	-
44	LMT	3	201	-	-	3/21/61/61	0/2/2/2
44	LMT	2	604	-	-	9/21/61/61	0/2/2/2
44	LMT	J	201	-	-	6/17/57/61	0/2/2/2
44	LMT	a	301	-	-	6/21/61/61	0/2/2/2
46	3PE	E	401	-	-	7/32/32/54	-
50	NDP	E	402	-	-	7/34/77/77	0/5/5/5
45	CDL	D	101	-	-	25/69/69/110	-
48	SF4	B	601	10	-	-	0/6/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	4	601	LMT	O5B-C1B	3.25	1.50	1.41
44	g	101	LMT	O5B-C1B	3.15	1.49	1.41
44	g	101	LMT	O5'-C1'	3.10	1.49	1.41
44	4	601	LMT	O5'-C1'	2.76	1.48	1.41
46	5	706	3PE	O21-C2	-2.62	1.40	1.46
46	5	706	3PE	O31-C31	2.35	1.40	1.33
46	5	706	3PE	O31-C3	-2.23	1.40	1.45
46	5	706	3PE	O21-C21	2.13	1.40	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	E	402	NDP	P2B-O2B-C2B	-4.92	110.29	123.43
46	5	706	3PE	O21-C21-C22	3.86	119.82	111.48
44	4	601	LMT	C1B-O1B-C4'	-3.62	109.40	117.98
44	5	705	LMT	O1'-C1'-C2'	3.46	113.53	108.27
44	5	705	LMT	C1-O1'-C1'	-3.20	108.22	113.68
44	2	602	LMT	C1B-O1B-C4'	-2.87	111.17	117.98
44	g	101	LMT	C1B-O1B-C4'	-2.83	111.28	117.98
44	j	101	LMT	C1-O1'-C1'	-2.76	108.97	113.68
44	a	301	LMT	C1B-O1B-C4'	-2.72	111.53	117.98
44	3	202	LMT	O1B-C4'-C3'	2.72	114.13	107.23
44	1	402	LMT	C4B-C3B-C2B	-2.62	106.24	110.83
44	j	101	LMT	O1'-C1'-C2'	2.59	112.20	108.27
44	2	603	LMT	C1-O1'-C1'	-2.58	109.27	113.68
46	5	706	3PE	O31-C31-C32	2.42	119.22	111.83
44	2	602	LMT	C3B-C4B-C5B	-2.38	105.92	110.23
44	5	705	LMT	C1'-O5'-C5'	-2.33	109.17	113.72
44	2	602	LMT	O5B-C5B-C6B	2.29	112.12	106.44
44	5	705	LMT	O5'-C1'-C2'	-2.20	105.85	110.37
44	4	601	LMT	C1'-C2'-C3'	2.16	114.56	110.01
44	3	202	LMT	O1B-C4'-C5'	-2.15	103.85	109.48
44	j	101	LMT	C1'-O5'-C5'	-2.14	109.54	113.72
44	J	201	LMT	C1B-O1B-C4'	-2.12	112.96	117.98
49	B	602	FMN	C4-N3-C2	-2.09	121.94	125.64
44	4	601	LMT	C2'-C3'-C4'	2.04	114.31	109.68
44	3	202	LMT	C1'-C2'-C3'	2.03	114.29	110.01
44	a	301	LMT	C1'-O5'-C5'	-2.00	109.81	113.72

There are no chirality outliers.

All (377) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1	401	PC1	C11-O13-P-O14
43	1	401	PC1	C11-O13-P-O11
43	1	401	PC1	C1-O11-P-O12
43	1	401	PC1	C1-O11-P-O14
43	1	401	PC1	C1-O11-P-O13
43	1	401	PC1	C22-C21-O21-C2
43	2	605	PC1	C22-C21-O21-C2
43	2	605	PC1	O32-C31-O31-C3
43	2	605	PC1	C32-C31-O31-C3
43	5	702	PC1	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
43	5	702	PC1	C11-O13-P-O14
43	5	702	PC1	C11-O13-P-O11
43	5	702	PC1	C1-O11-P-O12
43	5	702	PC1	C1-O11-P-O14
44	2	602	LMT	C2'-C1'-O1'-C1
44	2	602	LMT	O5'-C1'-O1'-C1
44	3	202	LMT	C2'-C1'-O1'-C1
44	4	601	LMT	O5'-C1'-O1'-C1
44	J	201	LMT	O5'-C1'-O1'-C1
44	J	201	LMT	C2-C1-O1'-C1'
44	a	301	LMT	C2'-C1'-O1'-C1
44	a	301	LMT	O5'-C1'-O1'-C1
44	g	101	LMT	O5B-C1B-O1B-C4'
44	j	101	LMT	C2-C1-O1'-C1'
45	2	601	CDL	CA2-OA2-PA1-OA4
45	2	601	CDL	CA2-OA2-PA1-OA5
45	2	601	CDL	CA3-OA5-PA1-OA2
45	2	601	CDL	CA3-OA5-PA1-OA3
45	2	601	CDL	OB7-CB5-OB6-CB4
45	D	101	CDL	CA3-OA5-PA1-OA2
45	D	101	CDL	CA3-OA5-PA1-OA3
45	D	101	CDL	CA3-OA5-PA1-OA4
45	D	101	CDL	CB2-OB2-PB2-OB4
45	D	101	CDL	CB2-OB2-PB2-OB5
45	D	101	CDL	CB3-OB5-PB2-OB3
45	S	201	CDL	C1-CA2-OA2-PA1
45	S	201	CDL	CA2-OA2-PA1-OA4
45	S	201	CDL	CA2-OA2-PA1-OA5
45	S	201	CDL	CB2-OB2-PB2-OB3
45	S	201	CDL	CB2-OB2-PB2-OB4
45	S	201	CDL	CB2-OB2-PB2-OB5
45	S	201	CDL	CB3-OB5-PB2-OB3
45	S	201	CDL	OB6-CB4-CB6-OB8
45	X	201	CDL	C11-CA5-OA6-CA4
45	X	201	CDL	OB7-CB5-OB6-CB4
45	X	202	CDL	CA2-C1-CB2-OB2
45	X	202	CDL	CA3-OA5-PA1-OA2
45	X	202	CDL	CB2-OB2-PB2-OB3
45	X	202	CDL	CB2-OB2-PB2-OB5
46	5	701	3PE	C11-O13-P-O11
46	5	701	3PE	C11-O13-P-O14
46	5	704	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
46	5	704	3PE	C11-O13-P-O11
46	5	706	3PE	C1-O11-P-O12
46	5	706	3PE	C1-O11-P-O13
46	5	706	3PE	C1-O11-P-O14
46	5	706	3PE	C11-O13-P-O11
46	5	706	3PE	C11-O13-P-O14
46	5	706	3PE	O13-C11-C12-N
46	5	706	3PE	O21-C2-C3-O31
46	E	401	3PE	C1-O11-P-O13
46	I	303	3PE	C11-O13-P-O11
46	I	303	3PE	C11-O13-P-O12
46	I	303	3PE	C11-O13-P-O14
46	W	201	3PE	C1-O11-P-O12
46	W	201	3PE	C2-C1-O11-P
46	i	101	3PE	C11-O13-P-O14
52	O	201	ZMP	O4-C17-C18-C21
52	O	201	ZMP	O4-C17-C18-C19
52	Q	201	ZMP	O3-C16-C17-C18
52	Q	201	ZMP	N2-C16-C17-C18
52	Q	201	ZMP	O3-C16-C17-O4
52	Q	201	ZMP	N2-C16-C17-O4
52	Q	201	ZMP	O1-C10-S1-C11
52	Q	201	ZMP	C9-C10-S1-C11
44	2	603	LMT	O5B-C1B-O1B-C4'
44	5	705	LMT	O5B-C1B-O1B-C4'
44	J	201	LMT	O5B-C1B-O1B-C4'
44	2	603	LMT	C2B-C1B-O1B-C4'
46	I	303	3PE	O32-C31-O31-C3
46	I	303	3PE	C32-C31-O31-C3
43	1	401	PC1	O22-C21-O21-C2
43	2	605	PC1	O22-C21-O21-C2
45	X	201	CDL	OA7-CA5-OA6-CA4
46	5	704	3PE	O22-C21-O21-C2
45	2	601	CDL	C51-CB5-OB6-CB4
45	X	201	CDL	C51-CB5-OB6-CB4
46	5	704	3PE	C22-C21-O21-C2
52	Q	201	ZMP	C14-C13-N1-C12
44	3	202	LMT	C3'-C4'-O1B-C1B
46	I	303	3PE	O22-C21-O21-C2
45	X	201	CDL	O1-C1-CA2-OA2
45	X	202	CDL	O1-C1-CA2-OA2
45	X	202	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
46	I	303	3PE	C22-C21-O21-C2
44	3	202	LMT	O5'-C1'-O1'-C1
52	Q	201	ZMP	O2-C13-N1-C12
44	2	604	LMT	O5'-C5'-C6'-O6'
45	X	201	CDL	CB2-C1-CA2-OA2
45	X	202	CDL	CB2-C1-CA2-OA2
44	J	201	LMT	C2'-C1'-O1'-C1
45	X	201	CDL	OB5-CB3-CB4-OB6
45	S	201	CDL	C11-CA5-OA6-CA4
44	2	602	LMT	C4B-C5B-C6B-O6B
44	2	603	LMT	O5'-C5'-C6'-O6'
44	g	101	LMT	O5'-C5'-C6'-O6'
44	4	601	LMT	C7-C8-C9-C10
46	5	704	3PE	C21-C22-C23-C24
44	2	603	LMT	C4'-C5'-C6'-O6'
45	D	101	CDL	CB5-C51-C52-C53
44	2	603	LMT	C3-C4-C5-C6
45	X	202	CDL	CB7-C71-C72-C73
45	S	201	CDL	OA7-CA5-OA6-CA4
44	2	602	LMT	O5B-C5B-C6B-O6B
45	D	101	CDL	C51-CB5-OB6-CB4
45	D	101	CDL	OB7-CB5-OB6-CB4
43	5	702	PC1	C11-C12-N-C13
43	5	702	PC1	C11-C12-N-C14
46	I	303	3PE	C21-C22-C23-C24
46	E	401	3PE	C22-C21-O21-C2
44	2	604	LMT	C2'-C1'-O1'-C1
44	g	101	LMT	C2'-C1'-O1'-C1
45	D	101	CDL	CA4-CA3-OA5-PA1
46	i	101	3PE	C2-C1-O11-P
44	2	604	LMT	O5B-C1B-O1B-C4'
44	1	402	LMT	O5'-C1'-O1'-C1
44	2	604	LMT	O5'-C1'-O1'-C1
46	W	202	3PE	C22-C21-O21-C2
43	5	703	PC1	C32-C33-C34-C35
46	5	704	3PE	C33-C34-C35-C36
46	E	401	3PE	O22-C21-O21-C2
44	1	402	LMT	C2-C1-O1'-C1'
44	1	403	LMT	C1-C2-C3-C4
46	W	201	3PE	C31-C32-C33-C34
46	i	101	3PE	C31-C32-C33-C34
45	X	201	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
44	g	101	LMT	C7-C8-C9-C10
44	J	201	LMT	C4-C5-C6-C7
43	5	702	PC1	C11-C12-N-C15
46	I	303	3PE	C2-C1-O11-P
44	3	202	LMT	C4-C5-C6-C7
46	W	202	3PE	O22-C21-O21-C2
44	4	601	LMT	C3-C4-C5-C6
44	3	201	LMT	O5B-C5B-C6B-O6B
44	5	705	LMT	C3-C4-C5-C6
43	5	702	PC1	C22-C21-O21-C2
45	2	601	CDL	C11-CA5-OA6-CA4
45	D	101	CDL	C11-CA5-OA6-CA4
44	g	101	LMT	C1-C2-C3-C4
46	5	704	3PE	C23-C24-C25-C26
44	2	603	LMT	O5B-C5B-C6B-O6B
45	X	201	CDL	OA9-CA7-OA8-CA6
44	2	604	LMT	O5B-C5B-C6B-O6B
45	X	202	CDL	CA7-C31-C32-C33
44	5	705	LMT	C2-C3-C4-C5
43	5	702	PC1	O22-C21-O21-C2
44	3	202	LMT	C5'-C4'-O1B-C1B
45	2	601	CDL	O1-C1-CA2-OA2
44	a	301	LMT	O5'-C5'-C6'-O6'
44	X	203	LMT	O5'-C5'-C6'-O6'
45	X	201	CDL	CA7-C31-C32-C33
45	X	201	CDL	OB5-CB3-CB4-CB6
46	E	401	3PE	O11-C1-C2-C3
44	2	604	LMT	C11-C10-C9-C8
45	X	202	CDL	C75-C76-C77-C78
44	4	601	LMT	C11-C10-C9-C8
46	I	303	3PE	C22-C23-C24-C25
45	S	201	CDL	C73-C74-C75-C76
43	1	401	PC1	C32-C31-O31-C3
44	1	403	LMT	O5B-C5B-C6B-O6B
45	S	201	CDL	CB3-CB4-CB6-OB8
52	O	201	ZMP	C22-C1-C2-C3
44	4	601	LMT	O5B-C5B-C6B-O6B
44	j	101	LMT	O5'-C5'-C6'-O6'
44	2	604	LMT	C4'-C5'-C6'-O6'
44	4	601	LMT	C4-C5-C6-C7
43	2	605	PC1	C1-C2-O21-C21
45	X	201	CDL	CB6-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
45	X	202	CDL	C31-C32-C33-C34
46	i	101	3PE	C26-C27-C28-C29
45	2	601	CDL	C31-CA7-OA8-CA6
52	Q	201	ZMP	C17-C16-N2-C15
52	O	201	ZMP	O4-C17-C18-C20
45	X	202	CDL	C51-CB5-OB6-CB4
43	1	401	PC1	O32-C31-O31-C3
52	O	201	ZMP	O3-C16-C17-C18
44	4	601	LMT	C2-C1-O1'-C1'
45	S	201	CDL	CA4-CA3-OA5-PA1
45	X	201	CDL	C1-CB2-OB2-PB2
45	X	202	CDL	C1-CB2-OB2-PB2
46	E	401	3PE	C2-C1-O11-P
46	I	303	3PE	C23-C24-C25-C26
52	Q	201	ZMP	O3-C16-N2-C15
45	D	101	CDL	C52-C51-CB5-OB6
45	X	202	CDL	C72-C71-CB7-OB8
45	X	202	CDL	CA5-C11-C12-C13
43	5	702	PC1	C1-C2-C3-O31
46	5	706	3PE	C1-C2-C3-O31
45	D	101	CDL	C13-C14-C15-C16
45	X	202	CDL	OB5-CB3-CB4-OB6
44	g	101	LMT	C4-C5-C6-C7
46	W	201	3PE	C2B-C2C-C2D-C2E
46	5	704	3PE	O21-C2-C3-O31
45	2	601	CDL	OA7-CA5-OA6-CA4
52	Q	201	ZMP	C3-C4-C5-C6
44	5	705	LMT	C4-C5-C6-C7
45	2	601	CDL	CB5-C51-C52-C53
45	X	202	CDL	C76-C77-C78-C79
45	X	201	CDL	C32-C31-CA7-OA8
43	5	702	PC1	C24-C25-C26-C27
45	X	201	CDL	OA5-CA3-CA4-CA6
45	S	201	CDL	C51-C52-C53-C54
43	5	703	PC1	C25-C26-C27-C28
45	2	601	CDL	OA9-CA7-OA8-CA6
45	D	101	CDL	OA7-CA5-OA6-CA4
45	X	202	CDL	OB7-CB5-OB6-CB4
45	D	101	CDL	C32-C31-CA7-OA8
45	D	101	CDL	OA5-CA3-CA4-OA6
44	g	101	LMT	O5'-C1'-O1'-C1
46	5	701	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
46	i	101	3PE	C12-C11-O13-P
52	Q	201	ZMP	C16-C17-C18-C20
52	Q	201	ZMP	C2-C3-C4-C5
43	1	401	PC1	O13-C11-C12-N
50	E	402	NDP	PN-O3-PA-O2A
46	5	706	3PE	C32-C31-O31-C3
44	2	602	LMT	C1-C2-C3-C4
45	X	202	CDL	OB5-CB3-CB4-CB6
46	W	202	3PE	C25-C26-C27-C28
52	Q	201	ZMP	C20-C18-C21-O5
52	Q	201	ZMP	C16-C17-C18-C21
43	5	702	PC1	C2A-C2B-C2C-C2D
45	D	101	CDL	C71-C72-C73-C74
45	X	201	CDL	OA5-CA3-CA4-OA6
44	3	202	LMT	C7-C8-C9-C10
44	2	602	LMT	C5-C6-C7-C8
46	5	706	3PE	C33-C34-C35-C36
44	a	301	LMT	C5-C6-C7-C8
43	5	702	PC1	O21-C2-C3-O31
45	X	201	CDL	OA6-CA4-CA6-OA8
46	I	303	3PE	O21-C2-C3-O31
45	X	202	CDL	CA3-CA4-CA6-OA8
46	I	303	3PE	C1-C2-C3-O31
44	3	202	LMT	O5B-C1B-O1B-C4'
52	O	201	ZMP	C1-C2-C3-C4
46	5	706	3PE	O32-C31-O31-C3
43	5	702	PC1	C1-O11-P-O13
45	2	601	CDL	CA3-OA5-PA1-OA4
45	D	101	CDL	CA2-OA2-PA1-OA3
45	D	101	CDL	CB3-OB5-PB2-OB2
45	D	101	CDL	CB3-OB5-PB2-OB4
45	S	201	CDL	CB3-OB5-PB2-OB2
45	X	201	CDL	CB2-OB2-PB2-OB4
45	X	202	CDL	CA2-OA2-PA1-OA3
45	X	202	CDL	CA3-OA5-PA1-OA3
45	X	202	CDL	CB2-OB2-PB2-OB4
46	5	701	3PE	C1-O11-P-O14
46	5	701	3PE	C11-O13-P-O12
46	5	704	3PE	C1-O11-P-O12
46	5	704	3PE	C1-O11-P-O13
46	5	704	3PE	C11-O13-P-O14
46	E	401	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
46	W	201	3PE	C1-O11-P-O13
46	W	201	3PE	C1-O11-P-O14
46	W	201	3PE	C11-O13-P-O14
46	i	101	3PE	C11-O13-P-O11
45	X	201	CDL	C72-C73-C74-C75
45	X	202	CDL	C51-C52-C53-C54
43	2	605	PC1	C31-C32-C33-C34
44	4	601	LMT	C1-C2-C3-C4
44	3	202	LMT	C3-C4-C5-C6
45	S	201	CDL	CA6-CA4-OA6-CA5
45	X	202	CDL	C32-C31-CA7-OA8
44	3	202	LMT	C2B-C1B-O1B-C4'
45	D	101	CDL	OB5-CB3-CB4-CB6
46	W	201	3PE	O11-C1-C2-C3
46	W	201	3PE	C2C-C2D-C2E-C2F
45	2	601	CDL	CB2-C1-CA2-OA2
46	E	401	3PE	O11-C1-C2-O21
45	X	202	CDL	CA4-CA3-OA5-PA1
45	X	202	CDL	C11-CA5-OA6-CA4
50	E	402	NDP	C2D-C1D-N1N-C6N
44	5	705	LMT	C5-C6-C7-C8
46	5	704	3PE	C1-C2-C3-O31
52	O	201	ZMP	C2-C3-C4-C5
49	B	602	FMN	C2'-C3'-C4'-O4'
44	g	101	LMT	C5-C6-C7-C8
44	2	602	LMT	C2-C1-O1'-C1'
44	2	603	LMT	C2-C1-O1'-C1'
44	3	201	LMT	C2-C1-O1'-C1'
45	X	202	CDL	C31-CA7-OA8-CA6
45	X	202	CDL	C72-C73-C74-C75
46	5	701	3PE	O11-C1-C2-O21
43	5	702	PC1	C25-C26-C27-C28
50	E	402	NDP	O4B-C4B-C5B-O5B
46	5	701	3PE	C24-C25-C26-C27
45	X	202	CDL	OA9-CA7-OA8-CA6
44	g	101	LMT	C4'-C5'-C6'-O6'
44	3	201	LMT	C3-C4-C5-C6
46	W	202	3PE	C2-C1-O11-P
52	O	201	ZMP	C5-C6-C7-C8
46	5	704	3PE	C24-C25-C26-C27
44	2	604	LMT	C7-C8-C9-C10
45	2	601	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
45	X	201	CDL	CA3-CA4-CA6-OA8
52	O	201	ZMP	N2-C16-C17-O4
43	5	702	PC1	C28-C29-C2A-C2B
46	i	101	3PE	C27-C28-C29-C2A
45	D	101	CDL	OA5-CA3-CA4-CA6
45	X	202	CDL	OA7-CA5-OA6-CA4
45	S	201	CDL	OA6-CA4-CA6-OA8
50	E	402	NDP	O4D-C1D-N1N-C6N
50	E	402	NDP	C2D-C1D-N1N-C2N
44	2	604	LMT	C1-C2-C3-C4
45	X	202	CDL	C71-CB7-OB8-CB6
50	E	402	NDP	PN-O3-PA-O1A
46	5	704	3PE	C36-C37-C38-C39
44	j	101	LMT	O5B-C1B-O1B-C4'
43	5	703	PC1	C3D-C3E-C3F-C3G
43	5	703	PC1	C21-C22-C23-C24
45	X	202	CDL	C35-C36-C37-C38
45	2	601	CDL	CA3-CA4-CA6-OA8
46	W	201	3PE	O11-C1-C2-O21
44	X	203	LMT	C2-C3-C4-C5
45	D	101	CDL	C52-C51-CB5-OB7
45	D	101	CDL	C72-C73-C74-C75
46	W	201	3PE	C33-C34-C35-C36
45	2	601	CDL	C54-C55-C56-C57
49	B	602	FMN	C4'-C5'-O5'-P
46	I	303	3PE	C38-C39-C3A-C3B
44	1	402	LMT	C1-C2-C3-C4
45	X	202	CDL	C72-C71-CB7-OB9
45	2	601	CDL	C56-C57-C58-C59
44	j	101	LMT	C2B-C1B-O1B-C4'
44	J	201	LMT	C2-C3-C4-C5
46	W	202	3PE	O11-C1-C2-O21
46	5	701	3PE	C34-C35-C36-C37
46	5	706	3PE	C12-C11-O13-P
52	Q	201	ZMP	C16-C17-C18-C19
46	W	201	3PE	C24-C25-C26-C27
45	X	202	CDL	OB9-CB7-OB8-CB6
46	W	202	3PE	O11-C1-C2-C3
45	S	201	CDL	OB7-CB5-OB6-CB4
46	5	706	3PE	C34-C35-C36-C37
44	5	705	LMT	O1'-C1-C2-C3
43	5	703	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
45	S	201	CDL	C51-CB5-OB6-CB4
44	a	301	LMT	C7-C8-C9-C10
49	B	602	FMN	O3'-C3'-C4'-C5'
45	S	201	CDL	C54-C55-C56-C57
44	X	203	LMT	O5'-C1'-O1'-C1
43	5	703	PC1	C38-C39-C3A-C3B
46	5	704	3PE	C35-C36-C37-C38
49	B	602	FMN	N10-C1'-C2'-O2'
52	Q	201	ZMP	C19-C18-C21-O5
45	X	201	CDL	C71-C72-C73-C74
45	X	201	CDL	C32-C31-CA7-OA9
46	W	201	3PE	C32-C33-C34-C35
43	5	702	PC1	C26-C27-C28-C29
45	D	101	CDL	C32-C31-CA7-OA9
46	W	202	3PE	C32-C33-C34-C35
46	5	704	3PE	C32-C33-C34-C35
52	O	201	ZMP	O3-C16-N2-C15
44	j	101	LMT	C6-C7-C8-C9
44	g	101	LMT	C11-C10-C9-C8
50	E	402	NDP	O4D-C1D-N1N-C2N
43	2	605	PC1	C38-C39-C3A-C3B
46	5	704	3PE	C26-C27-C28-C29
46	5	701	3PE	O11-C1-C2-C3
49	B	602	FMN	C2'-C3'-C4'-C5'
46	5	706	3PE	O31-C31-C32-C33
44	g	101	LMT	C2-C3-C4-C5
45	X	201	CDL	C72-C71-CB7-OB8
44	a	301	LMT	C9-C10-C11-C12
43	5	703	PC1	C22-C21-O21-C2
43	2	605	PC1	C23-C24-C25-C26
44	j	101	LMT	C11-C10-C9-C8

There are no ring outliers.

34 monomers are involved in 78 short contacts:

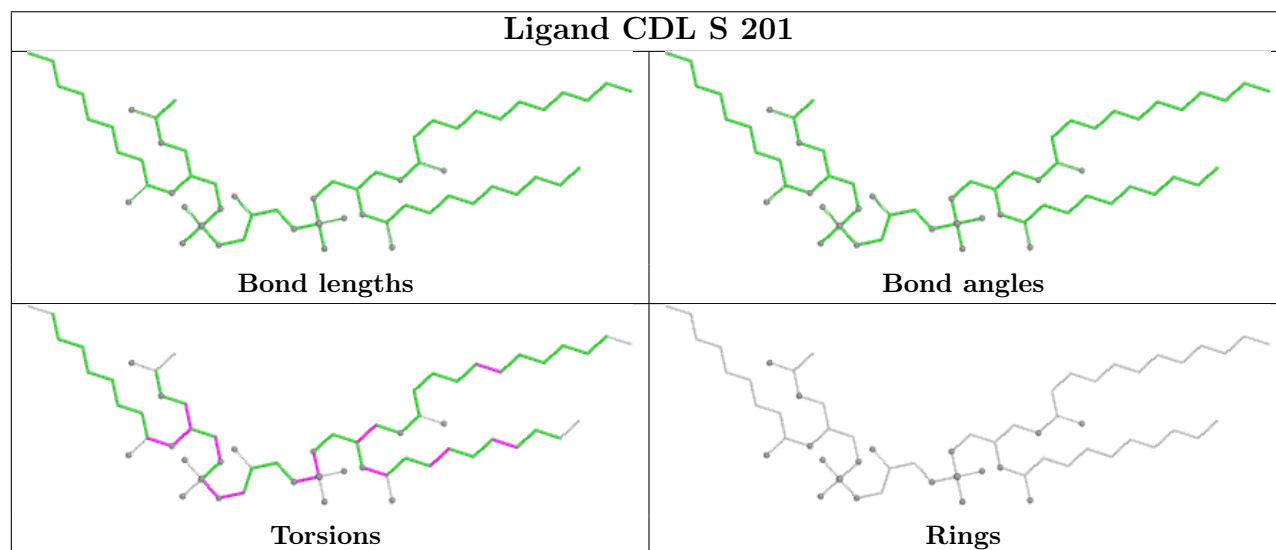
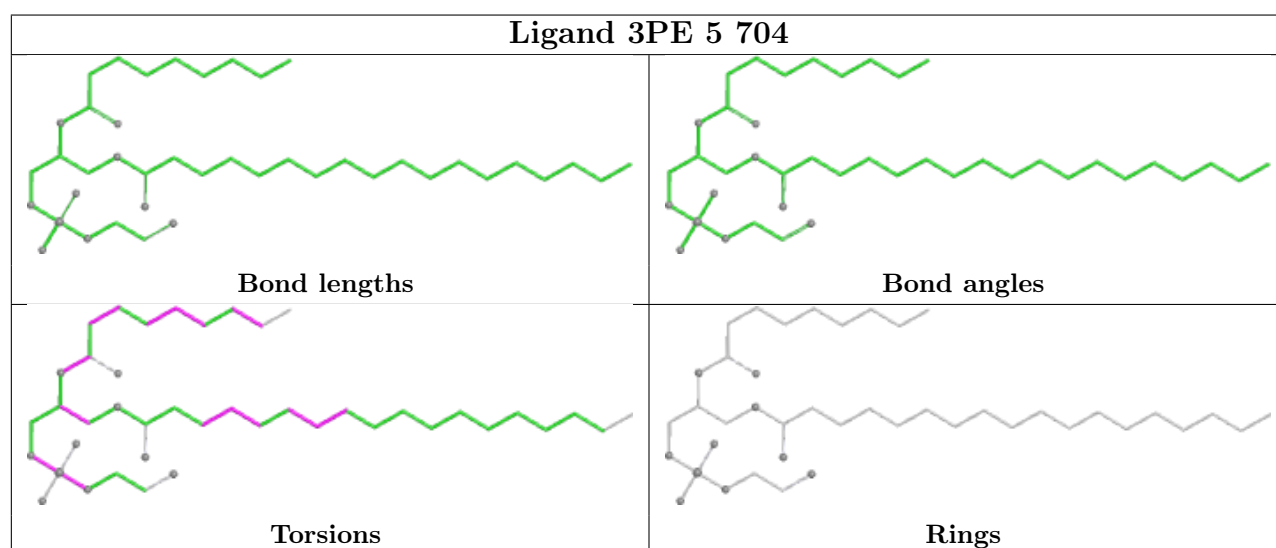
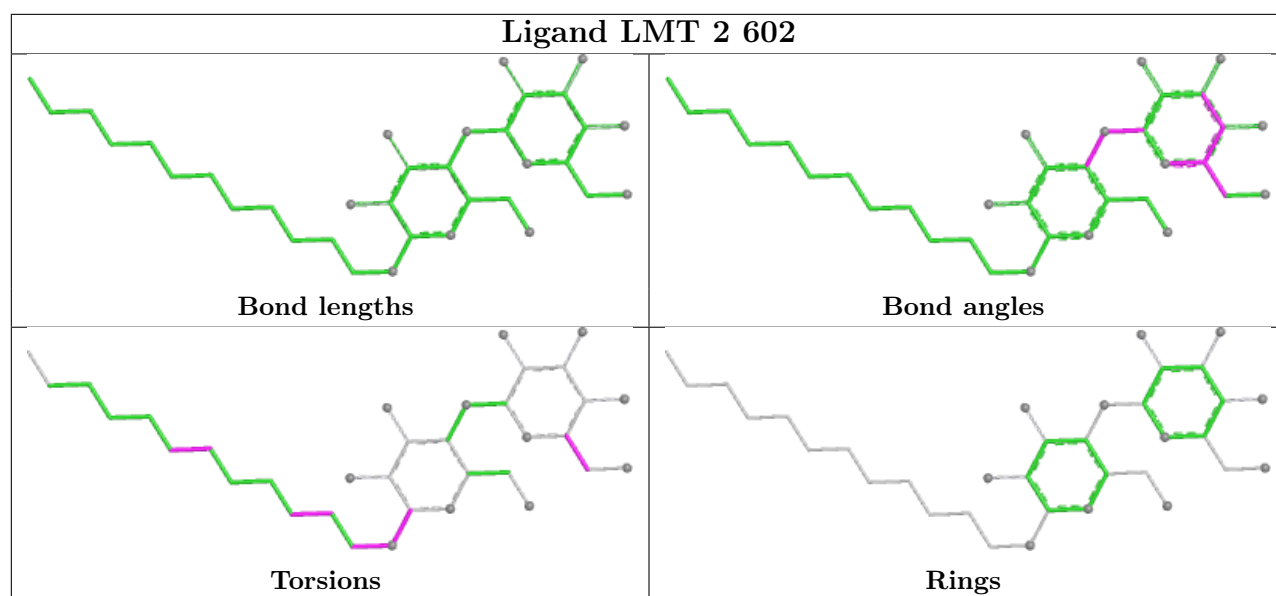
Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	2	602	LMT	3	0
46	5	704	3PE	1	0
45	S	201	CDL	3	0
44	3	202	LMT	1	0
44	1	403	LMT	1	0
46	W	202	3PE	3	0

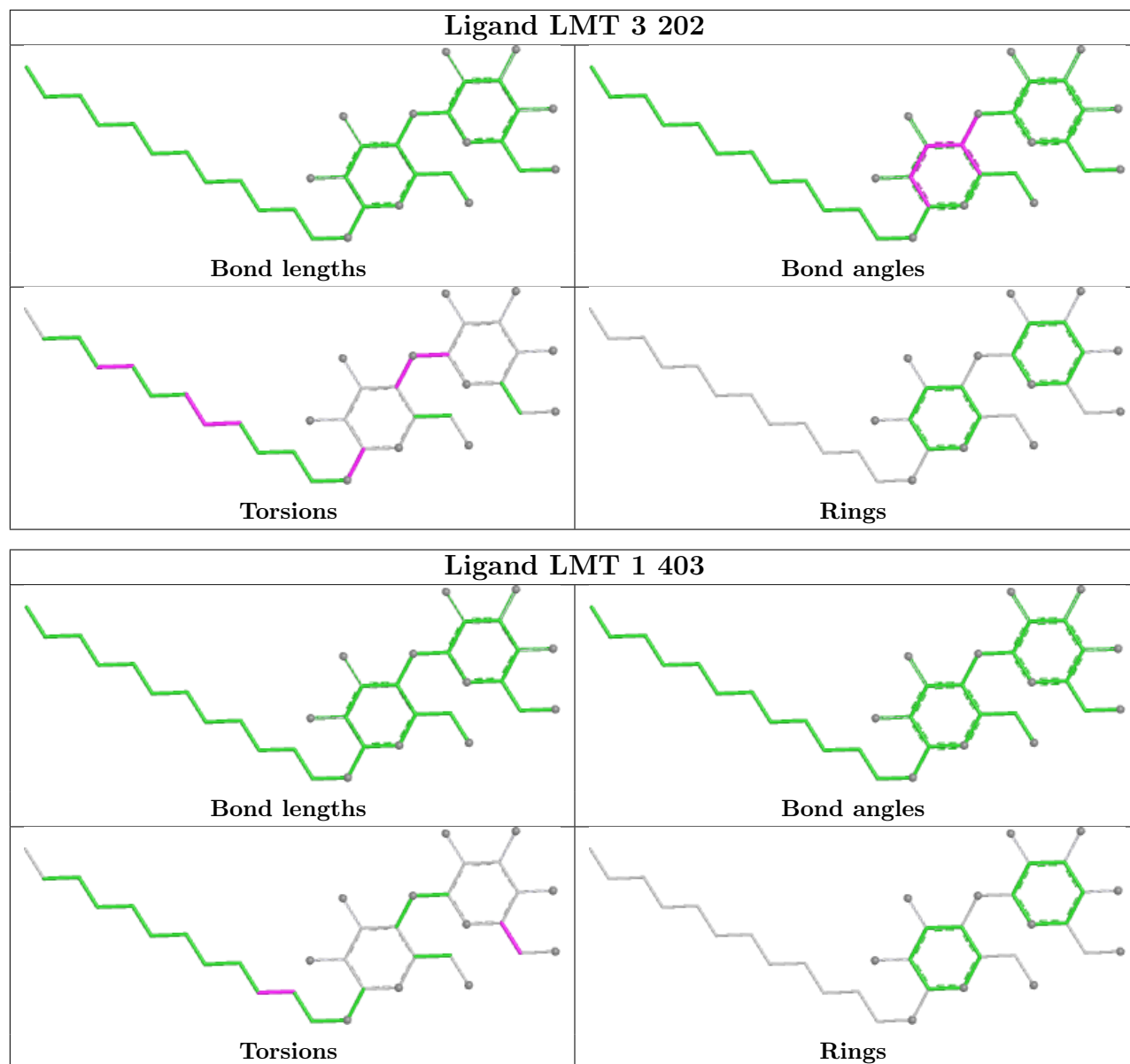
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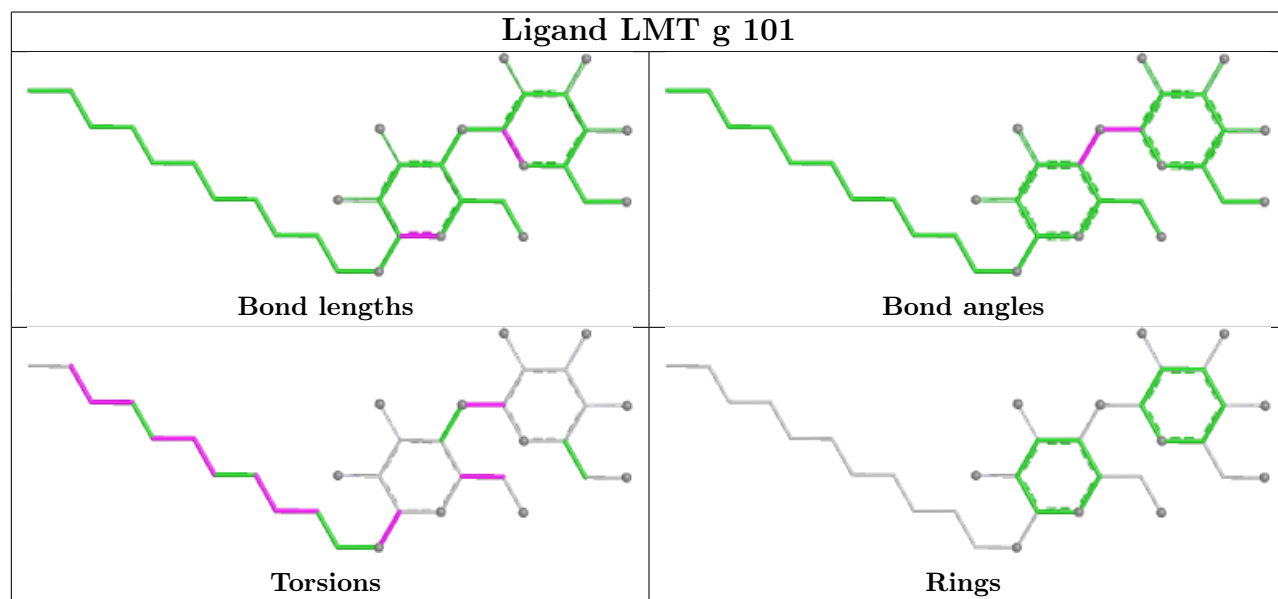
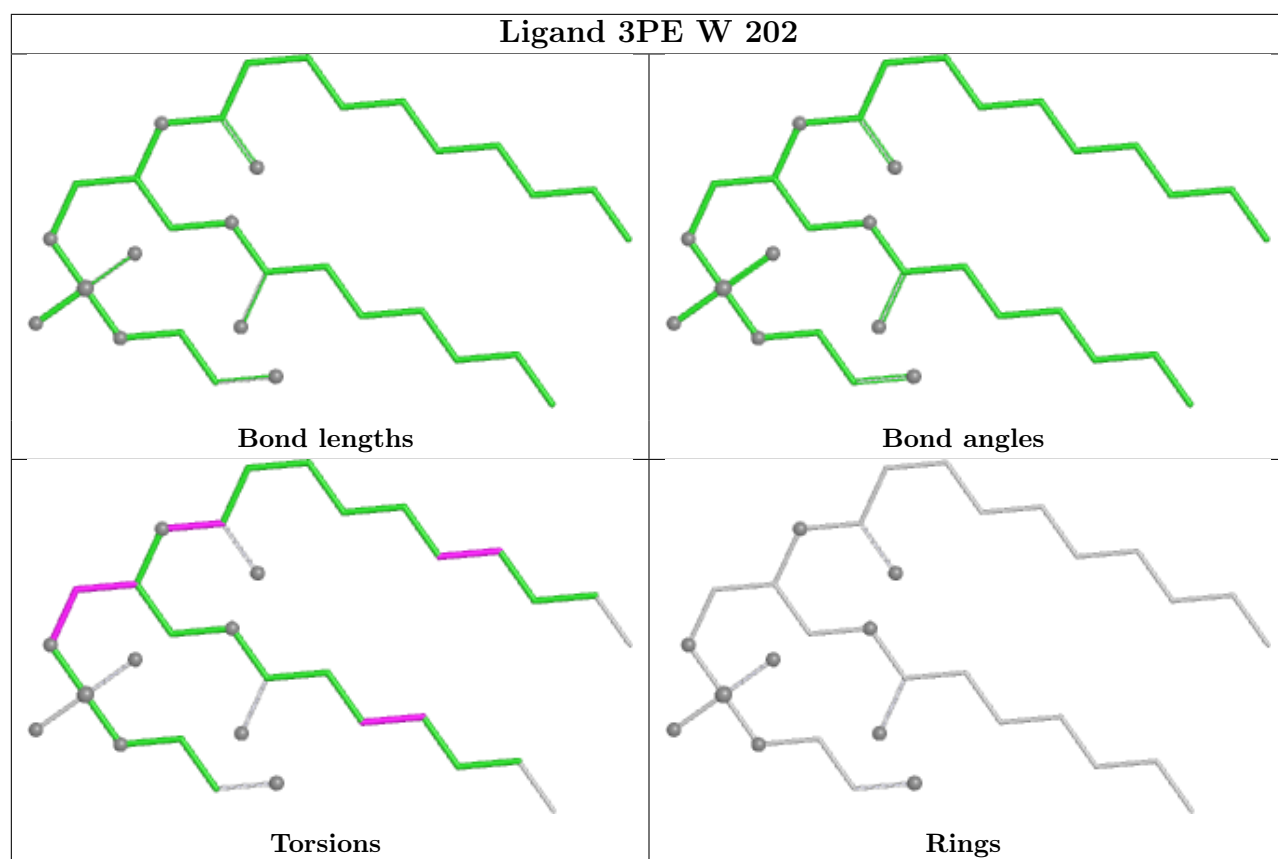
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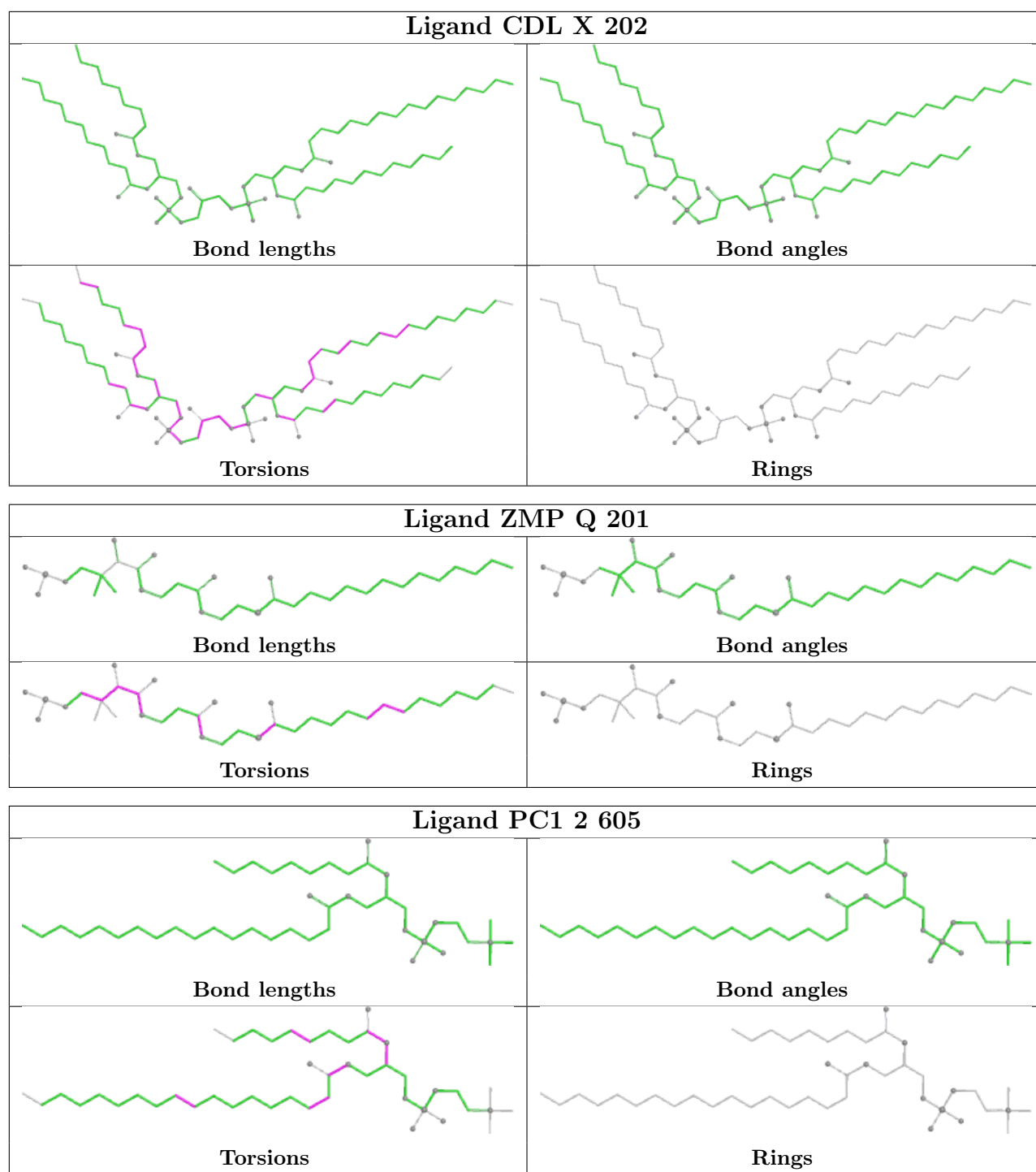
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	K	301	SF4	1	0
44	g	101	LMT	1	0
45	X	202	CDL	3	0
52	Q	201	ZMP	3	0
43	2	605	PC1	13	0
43	5	703	PC1	4	0
45	2	601	CDL	2	0
46	i	101	3PE	1	0
46	I	303	3PE	2	0
52	O	201	ZMP	1	0
46	5	701	3PE	1	0
44	4	601	LMT	4	0
43	1	401	PC1	1	0
44	X	203	LMT	3	0
49	B	602	FMN	2	0
44	5	705	LMT	3	0
44	2	603	LMT	1	0
43	5	702	PC1	7	0
46	5	706	3PE	1	0
44	1	402	LMT	2	0
44	j	101	LMT	4	0
46	W	201	3PE	1	0
44	3	201	LMT	2	0
44	2	604	LMT	2	0
44	a	301	LMT	2	0
46	E	401	3PE	1	0
50	E	402	NDP	2	0
45	D	101	CDL	3	0

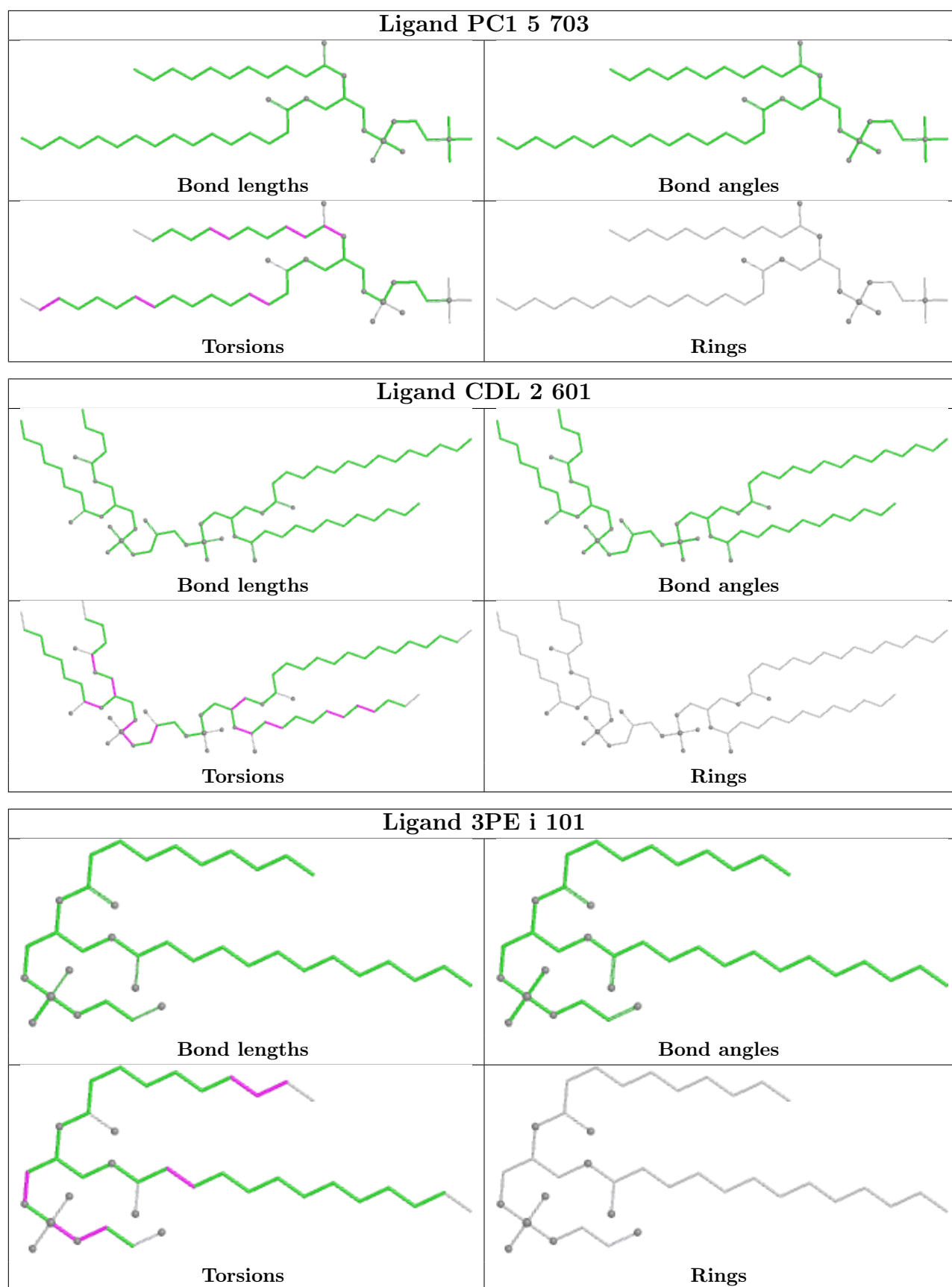
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



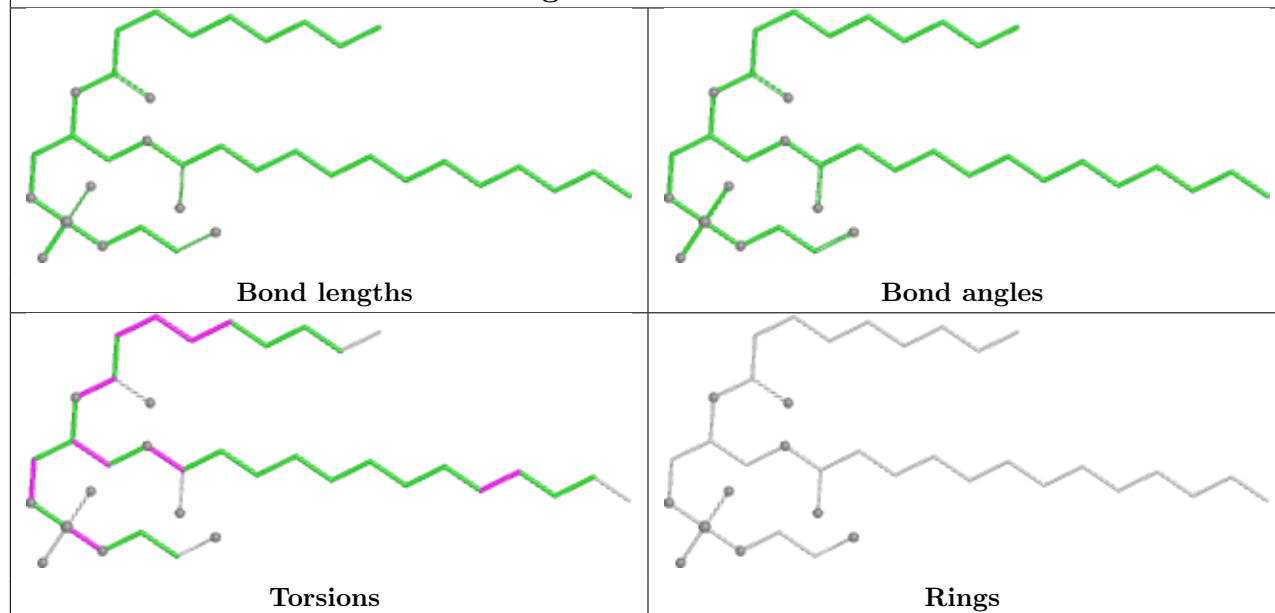




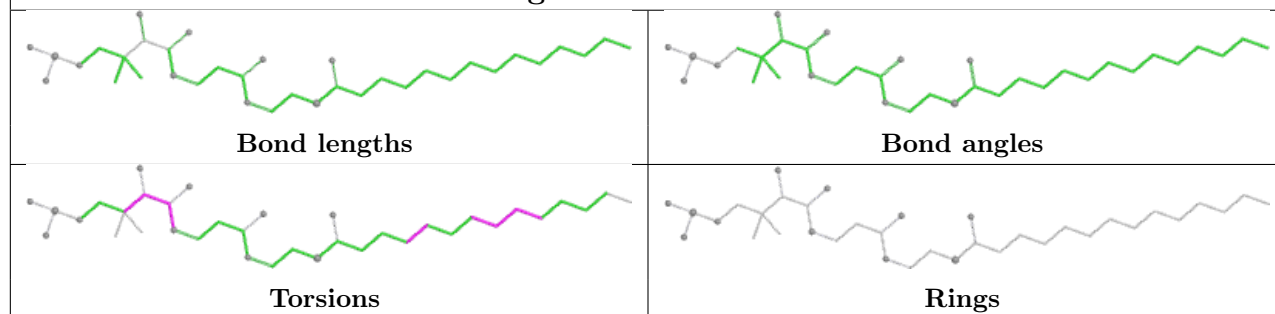




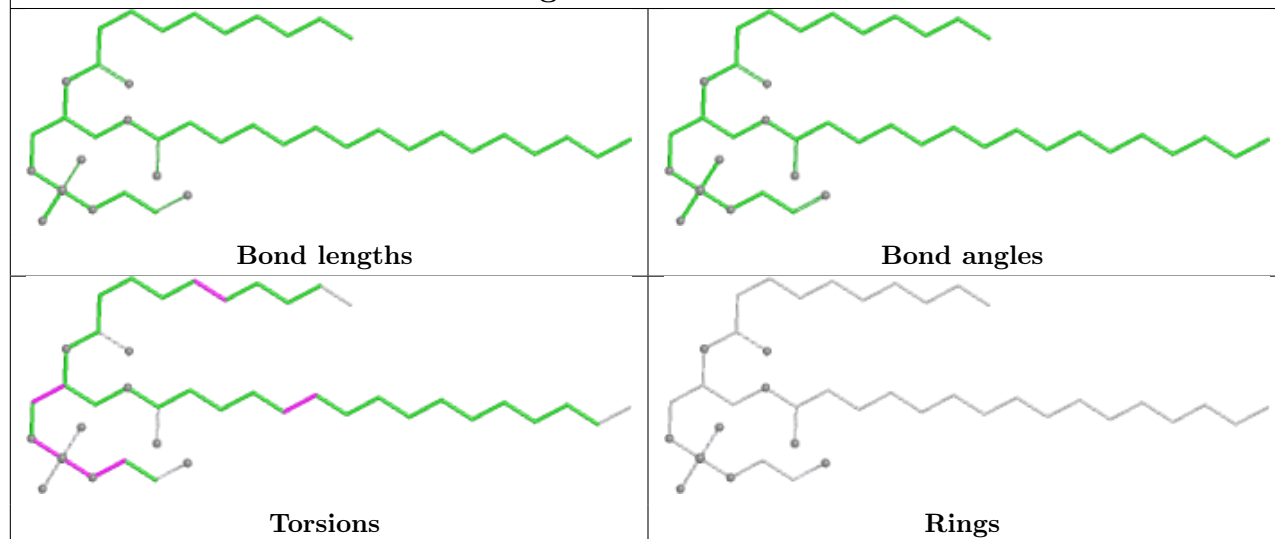
Ligand 3PE I 303

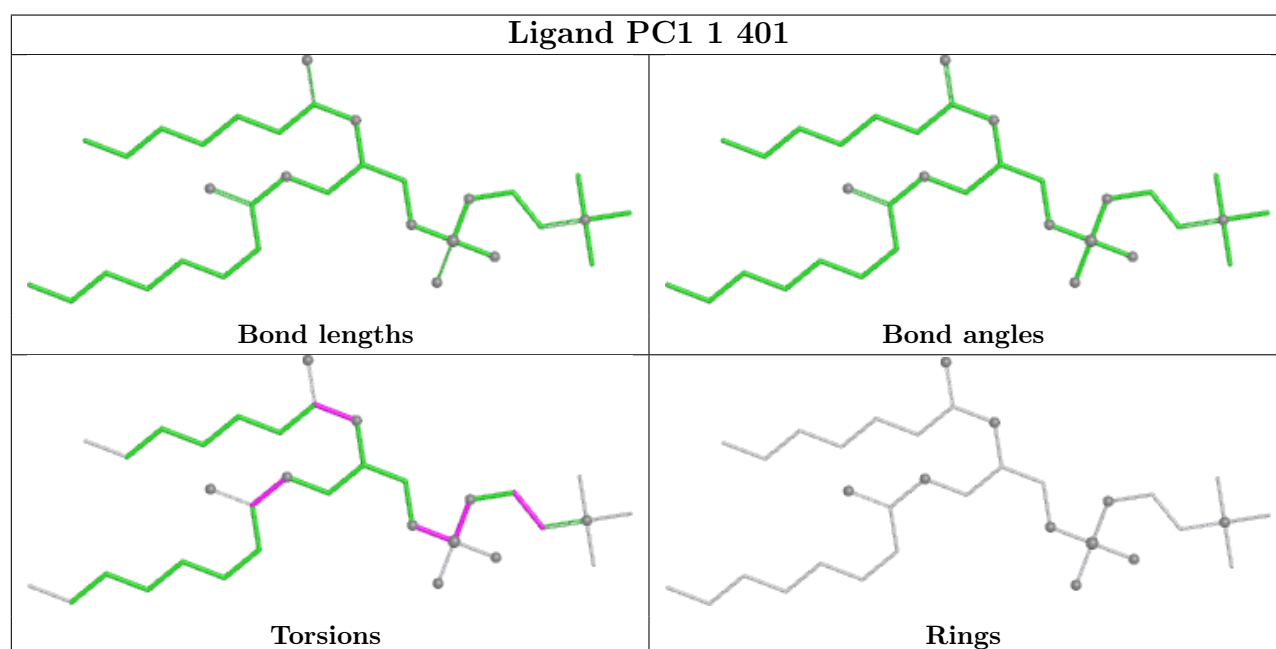
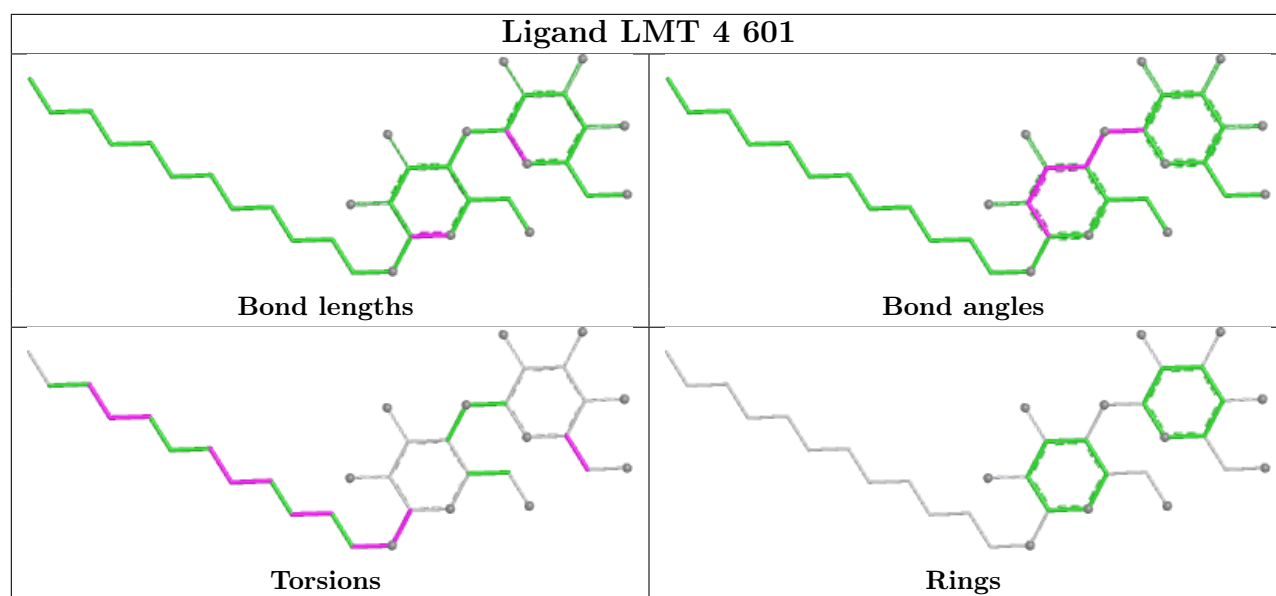


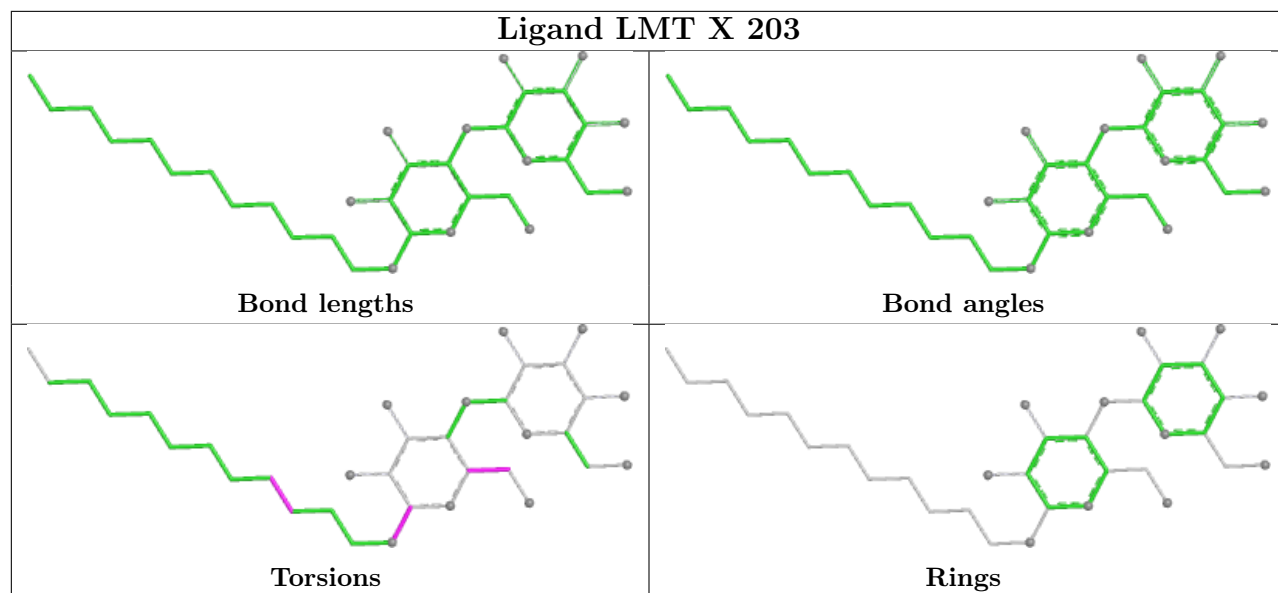
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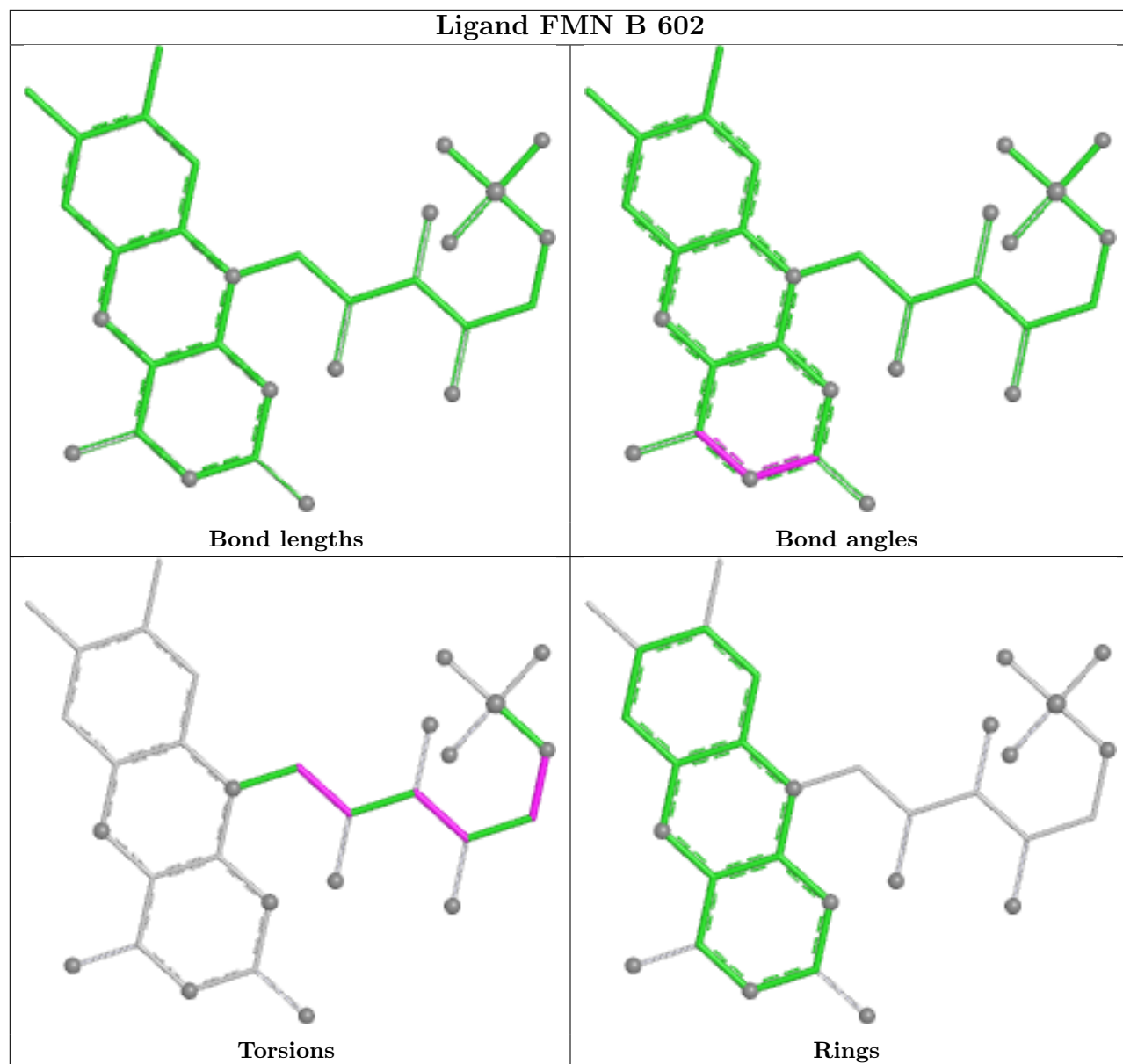


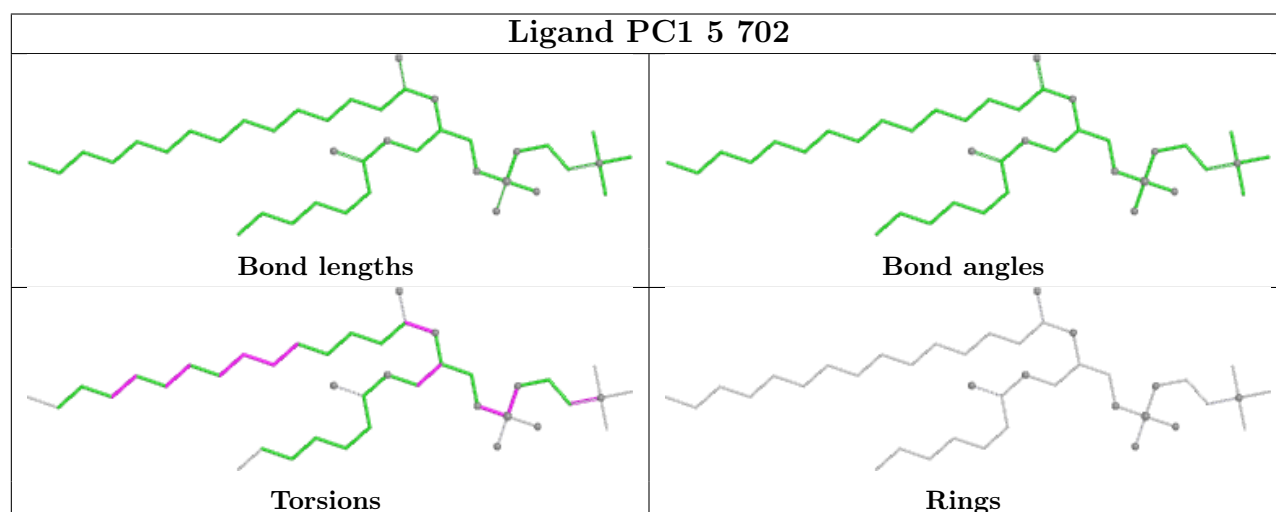
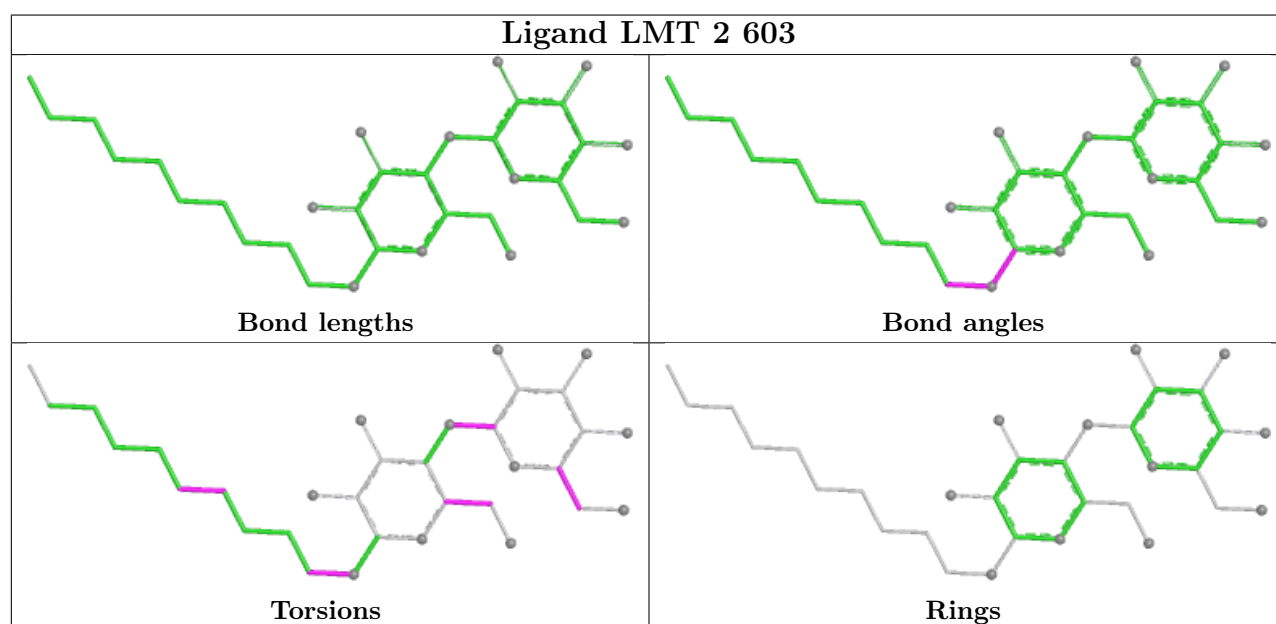
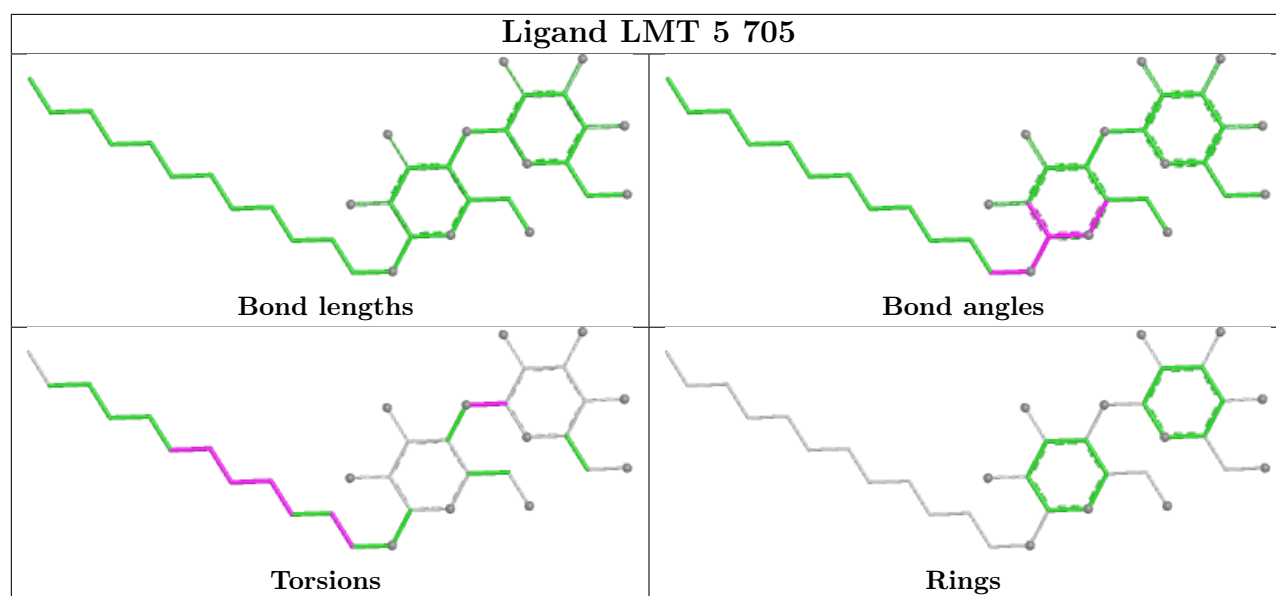
Ligand 3PE 5 701

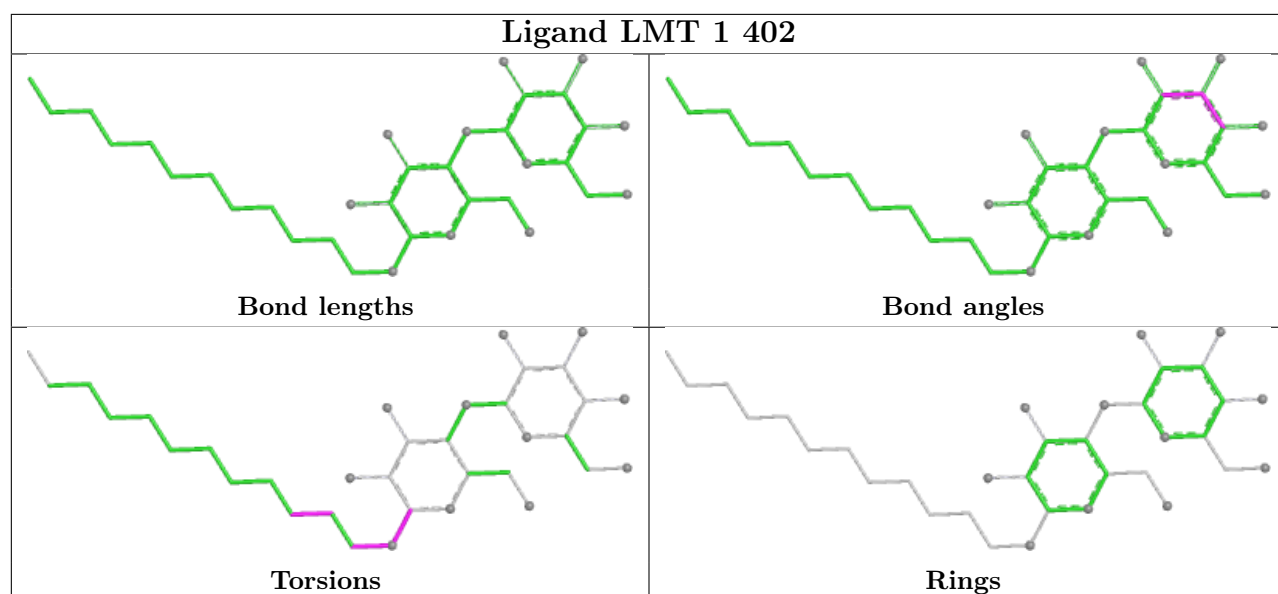
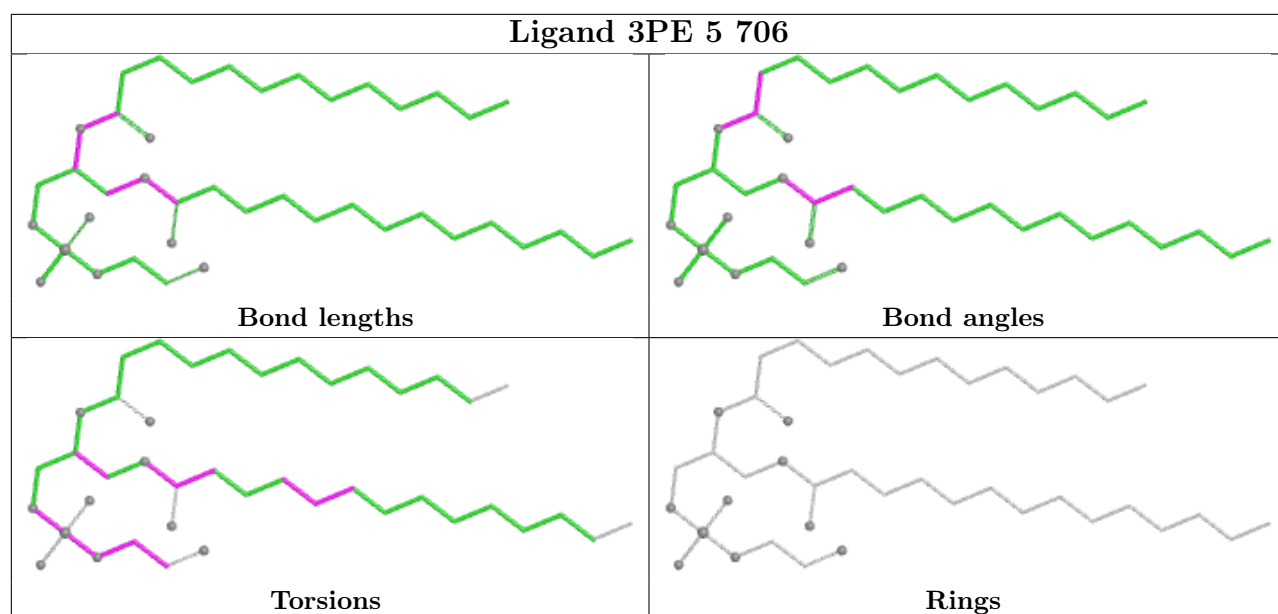


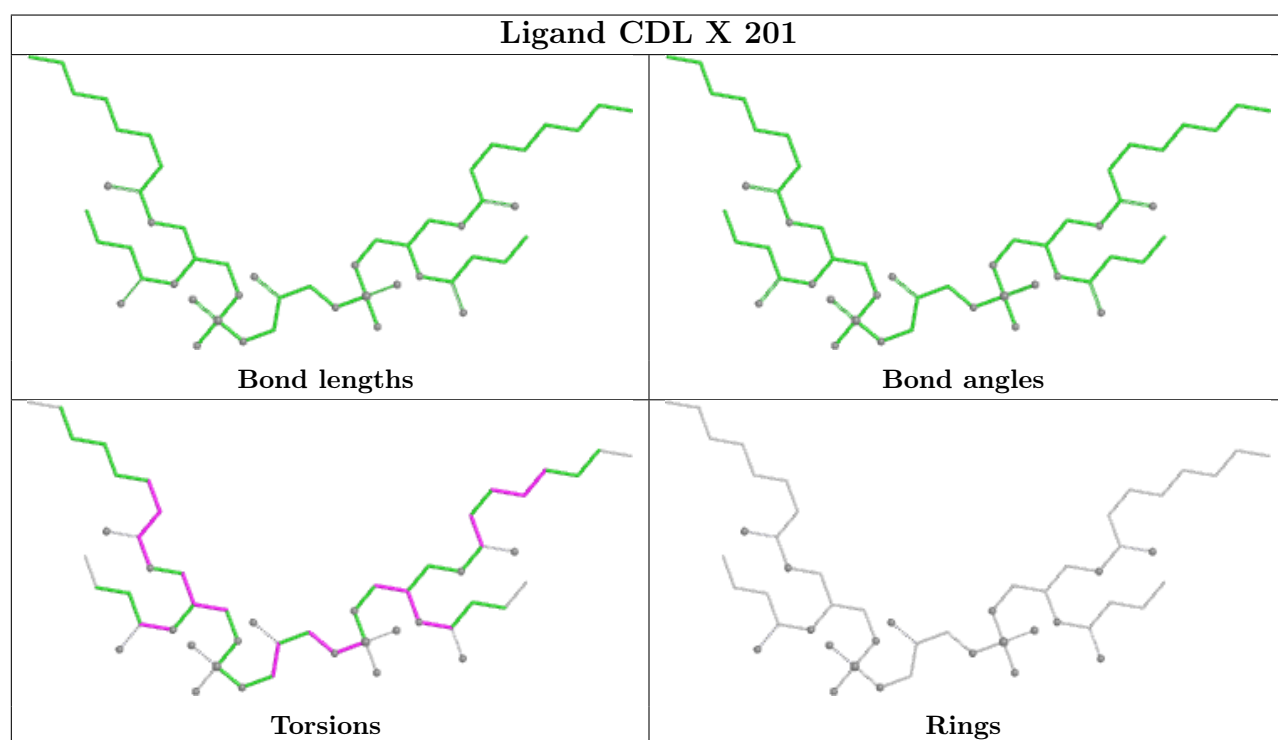
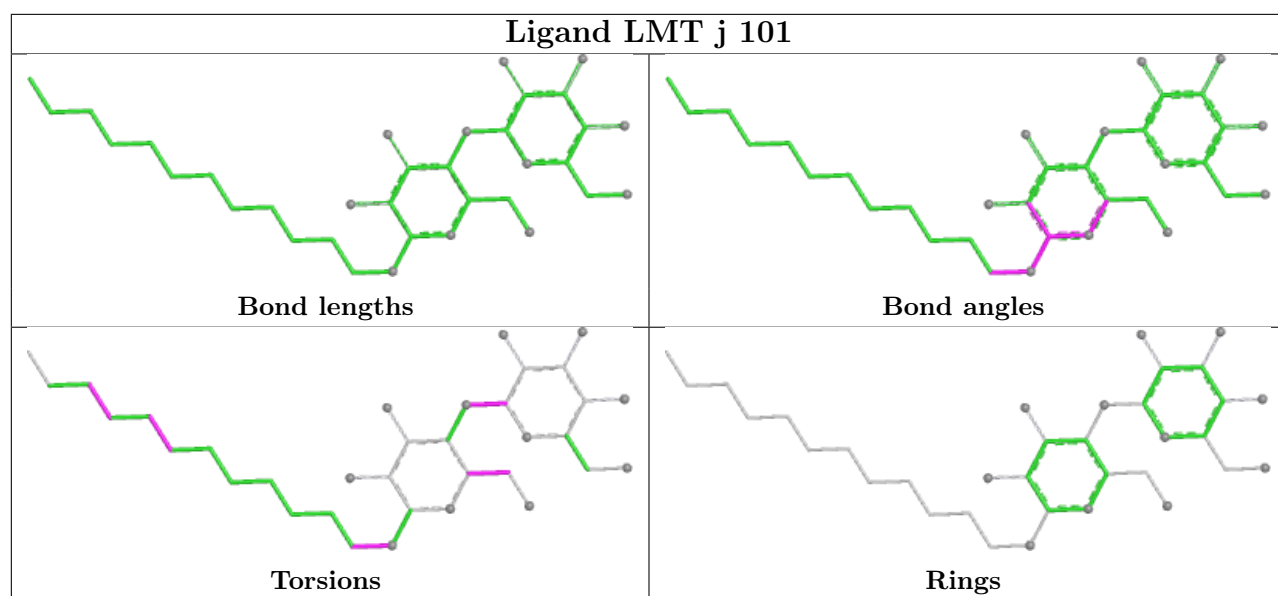


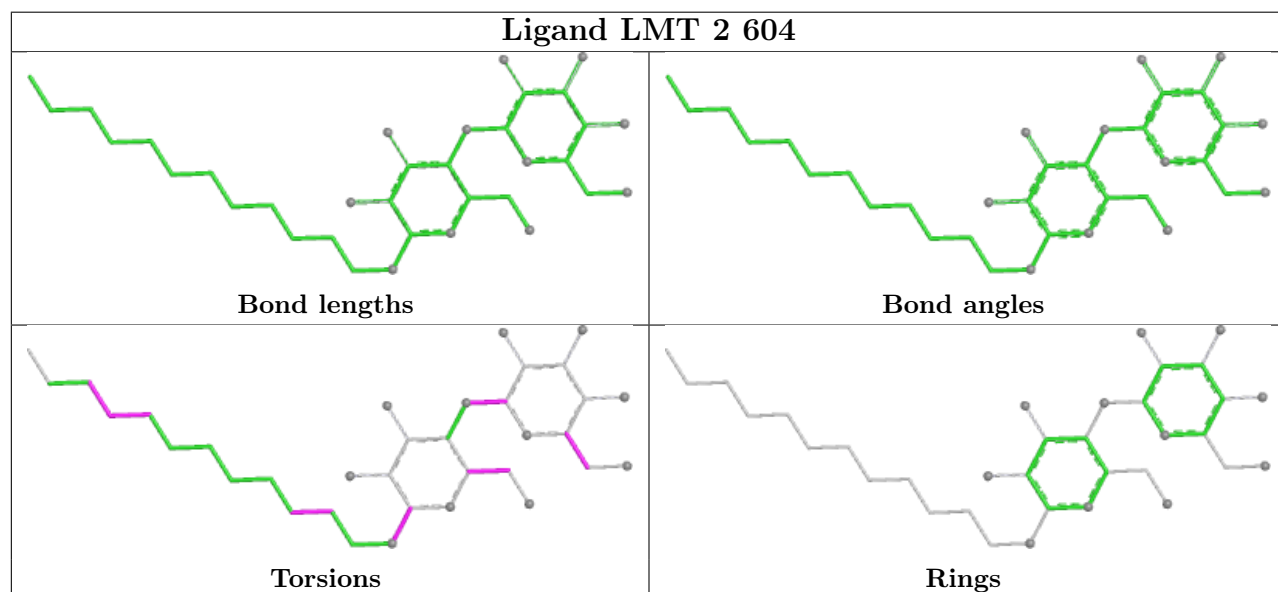
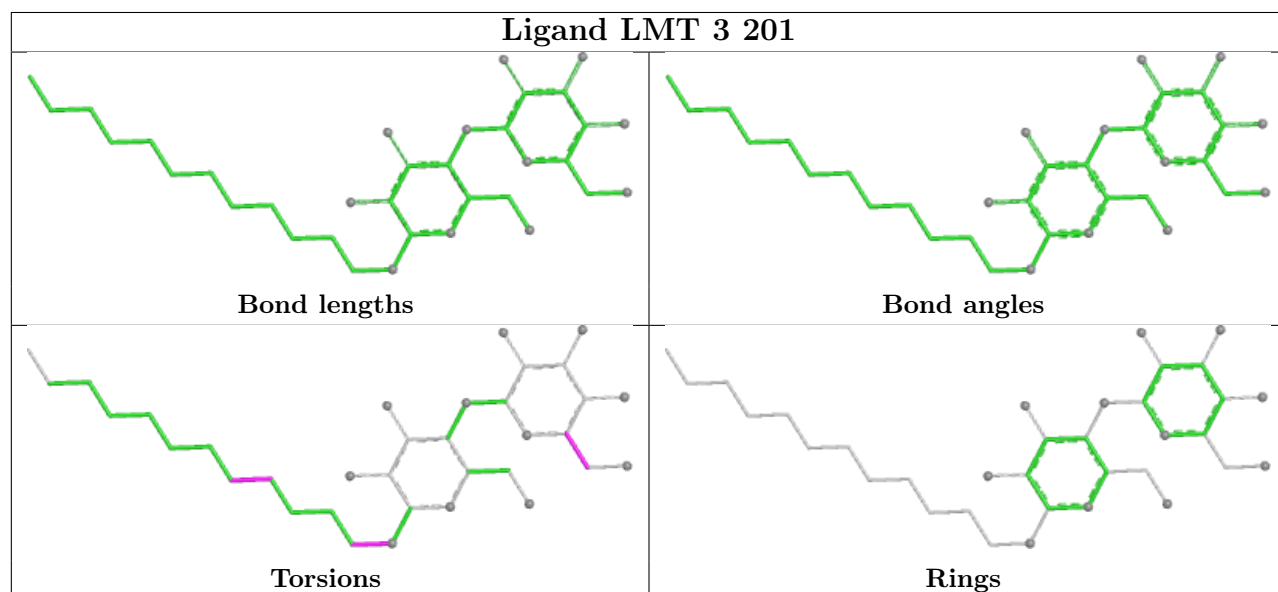
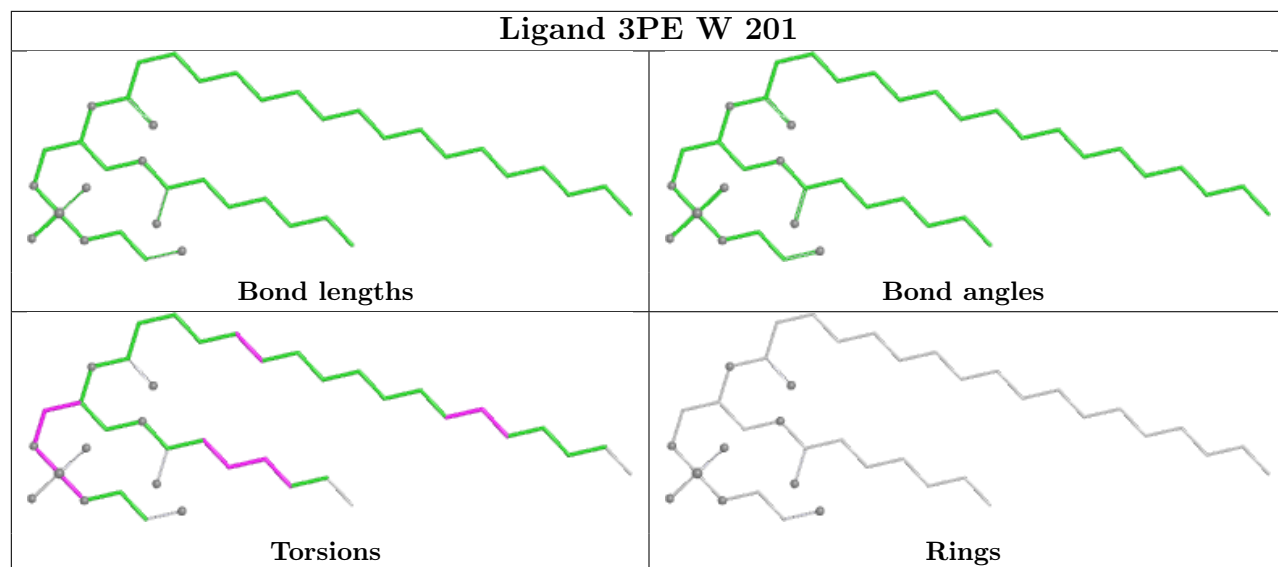


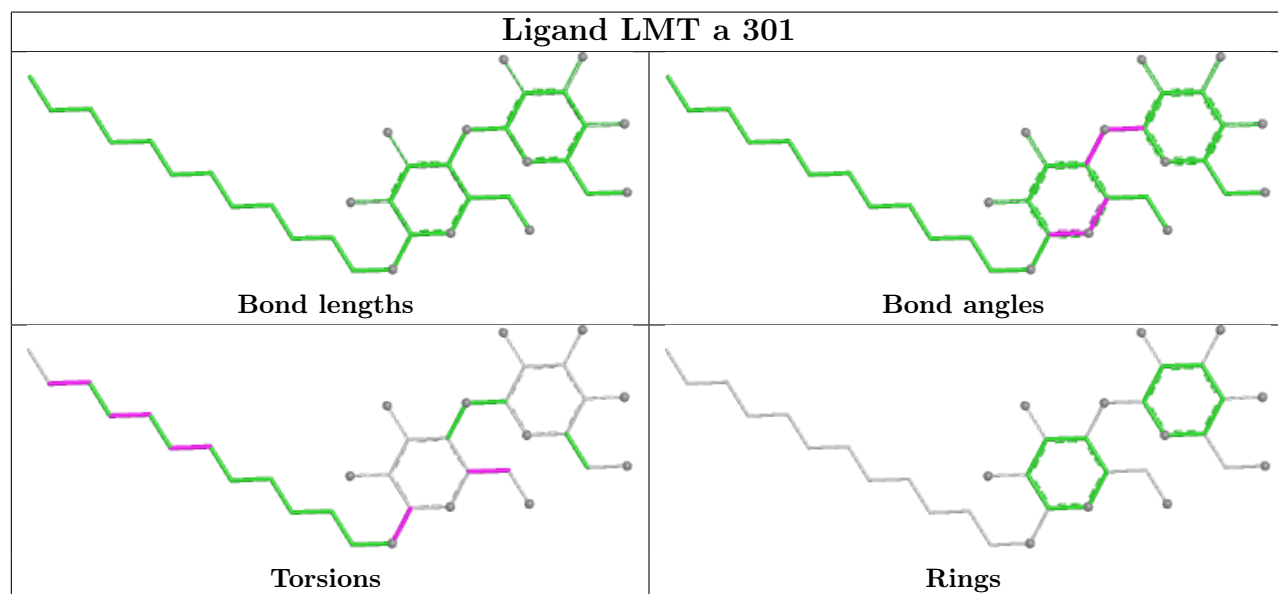
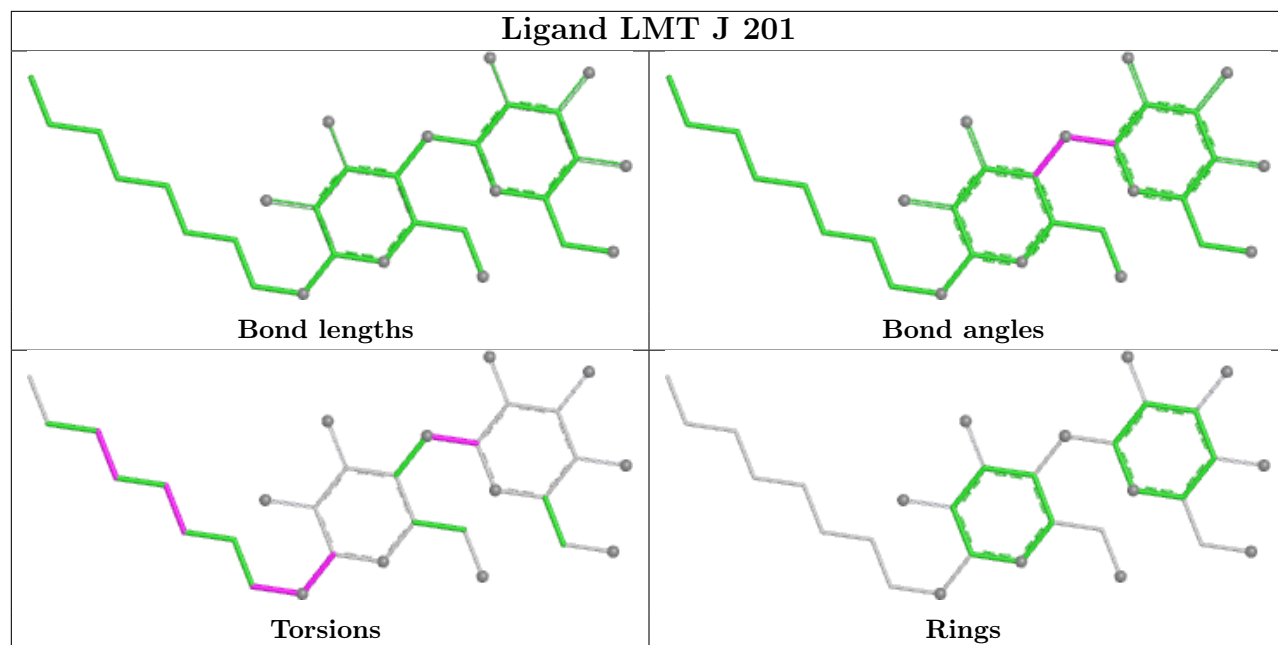




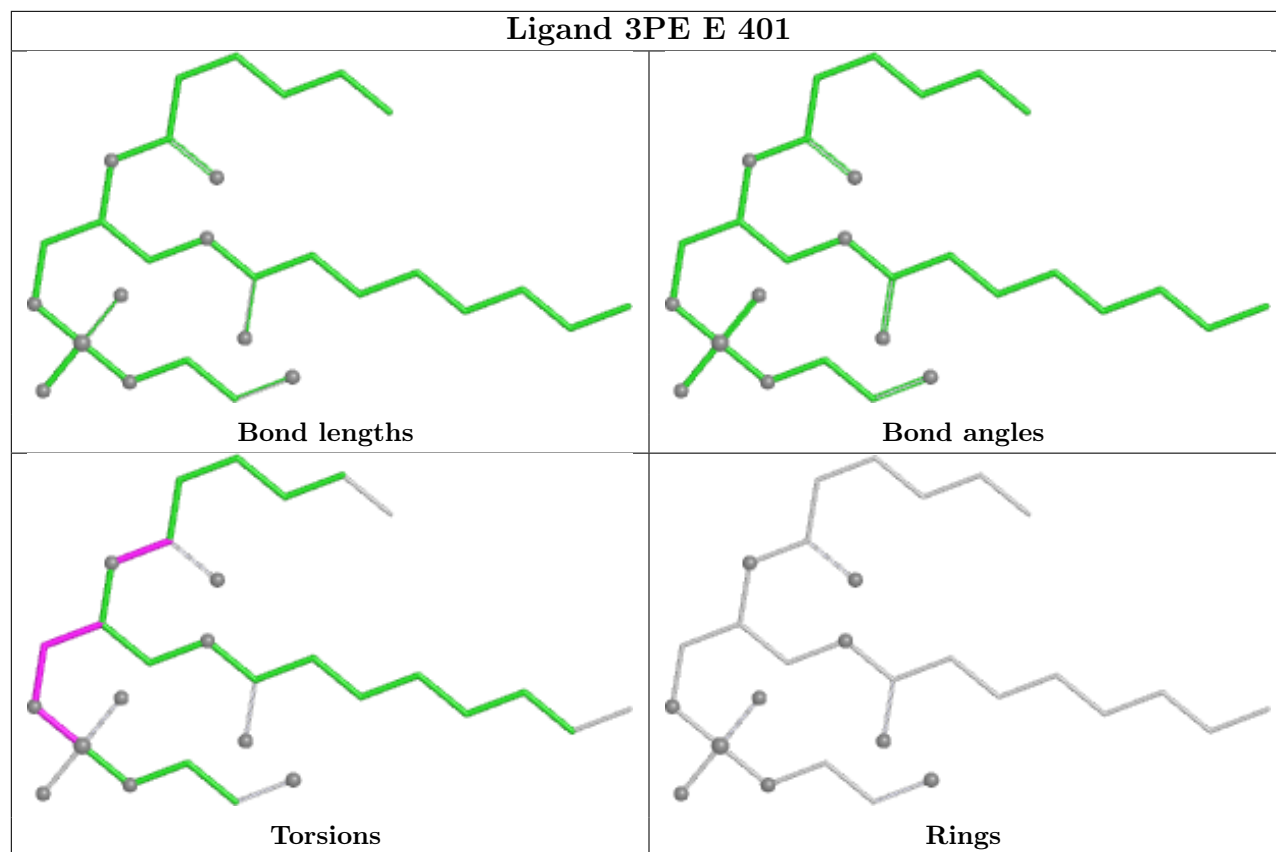




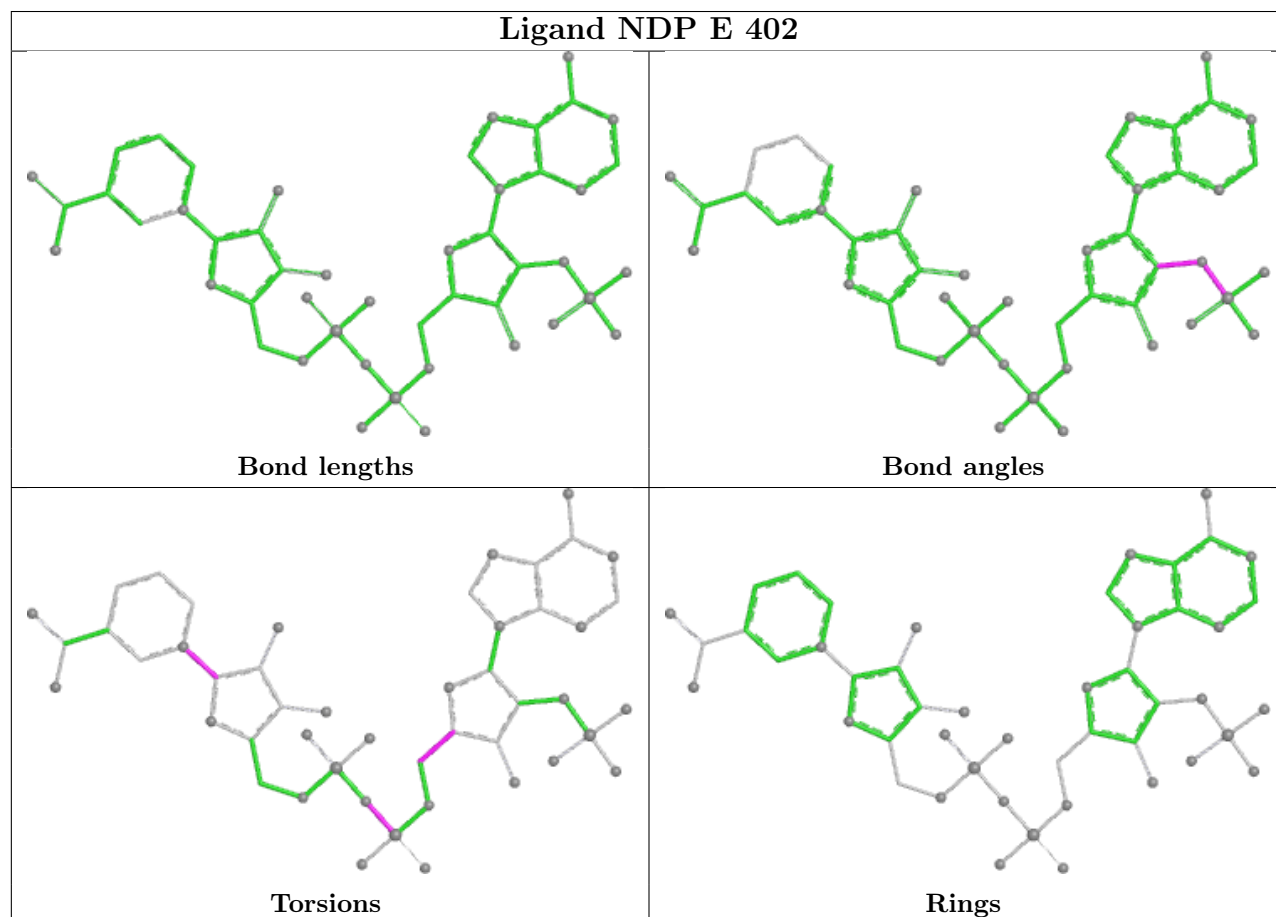


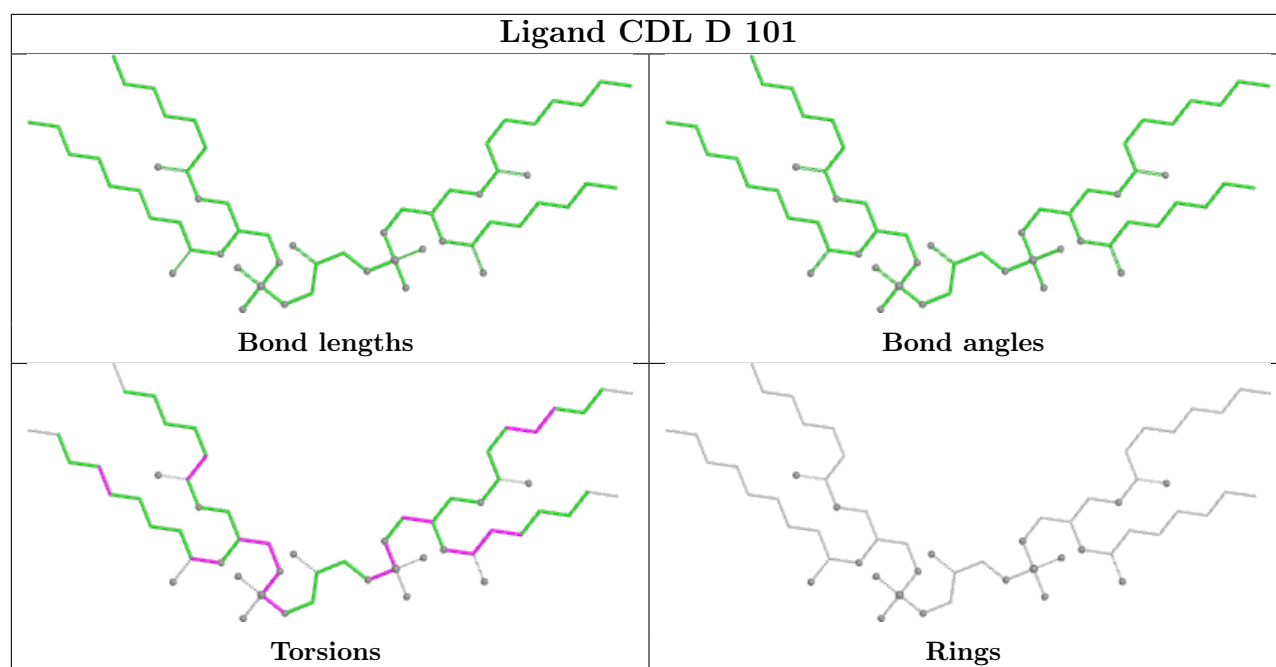


Ligand 3PE E 401



Ligand NDP E 402





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

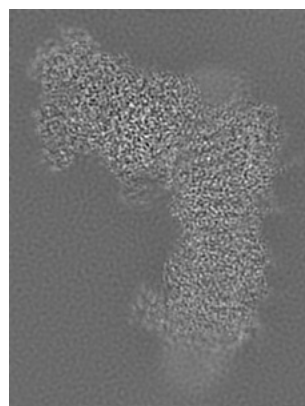
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14791. These allow visual inspection of the internal detail of the map and identification of artifacts.

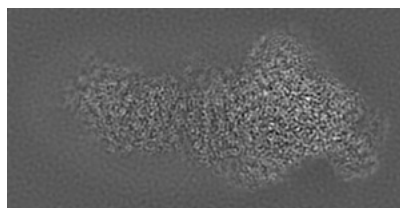
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

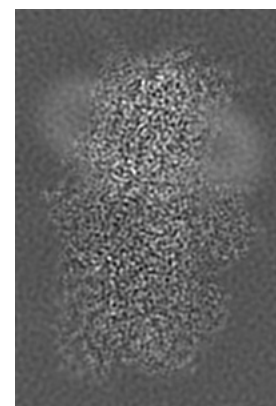
6.1.1 Primary map



X

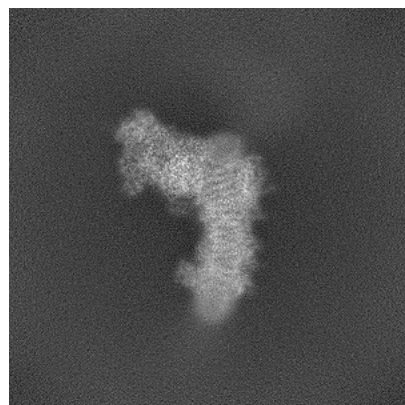


Y

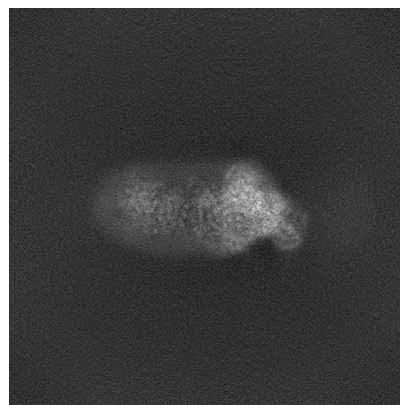


Z

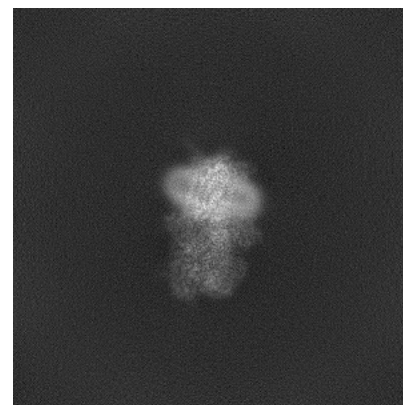
6.1.2 Raw map



X



Y

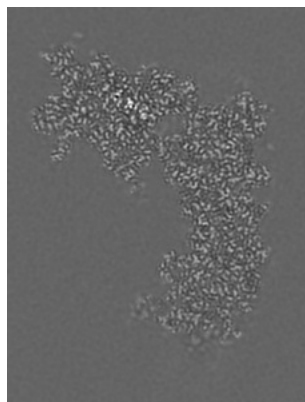


Z

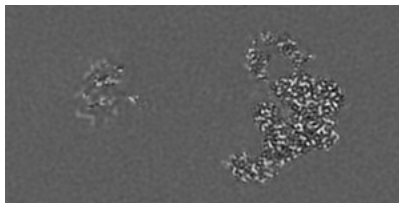
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

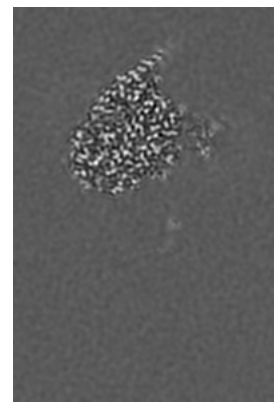
6.2.1 Primary map



X Index: 75

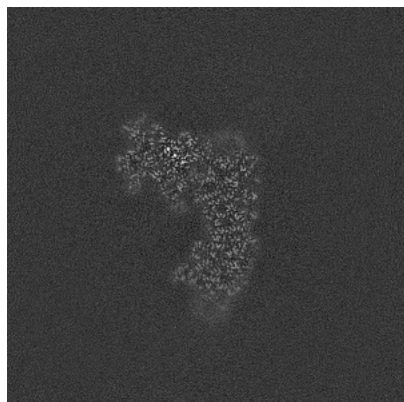


Y Index: 111

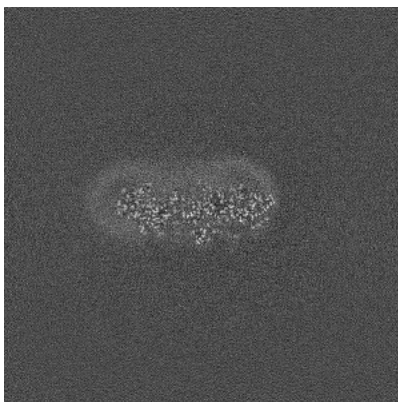


Z Index: 148

6.2.2 Raw map



X Index: 256



Y Index: 256

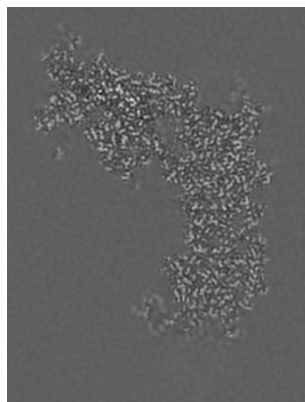


Z Index: 256

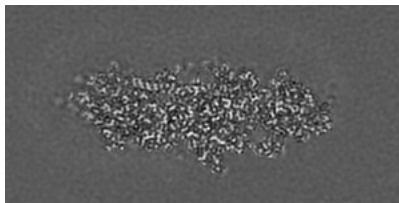
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

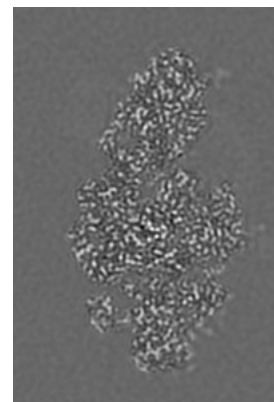
6.3.1 Primary map



X Index: 71

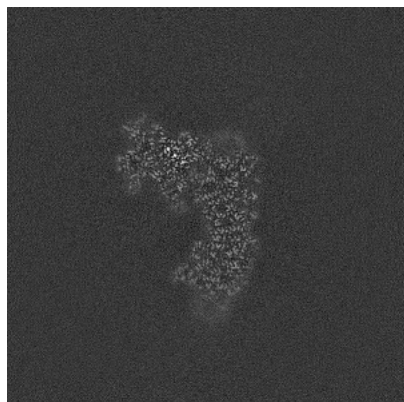


Y Index: 139

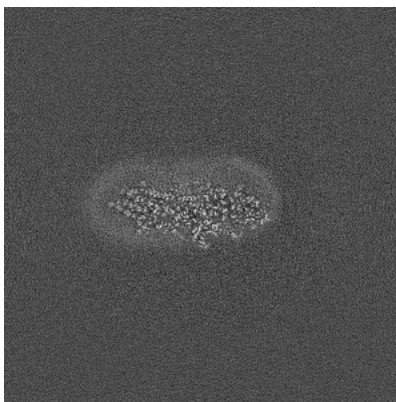


Z Index: 214

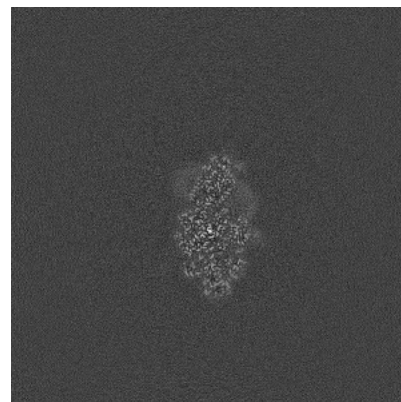
6.3.2 Raw map



X Index: 256



Y Index: 262

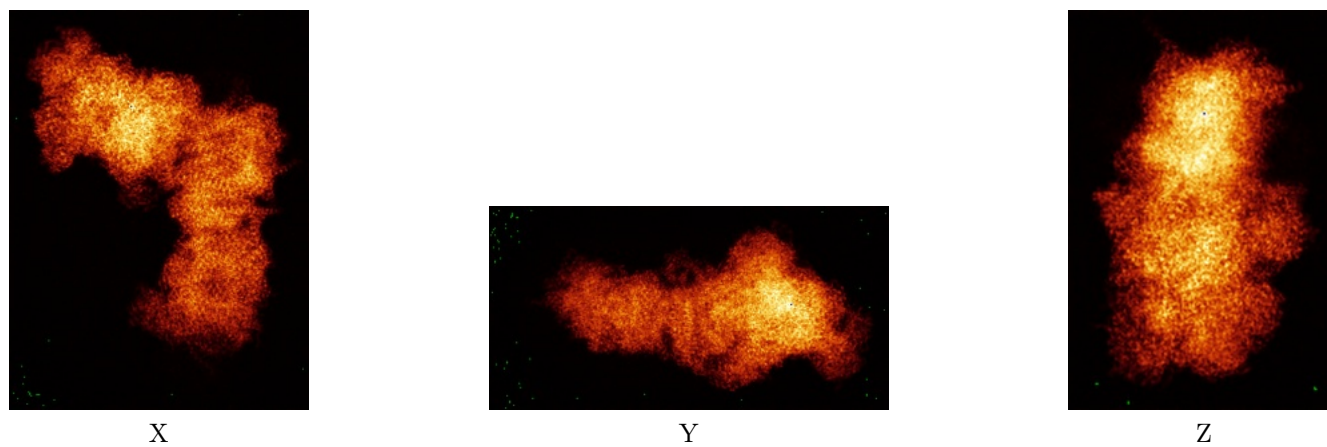


Z Index: 312

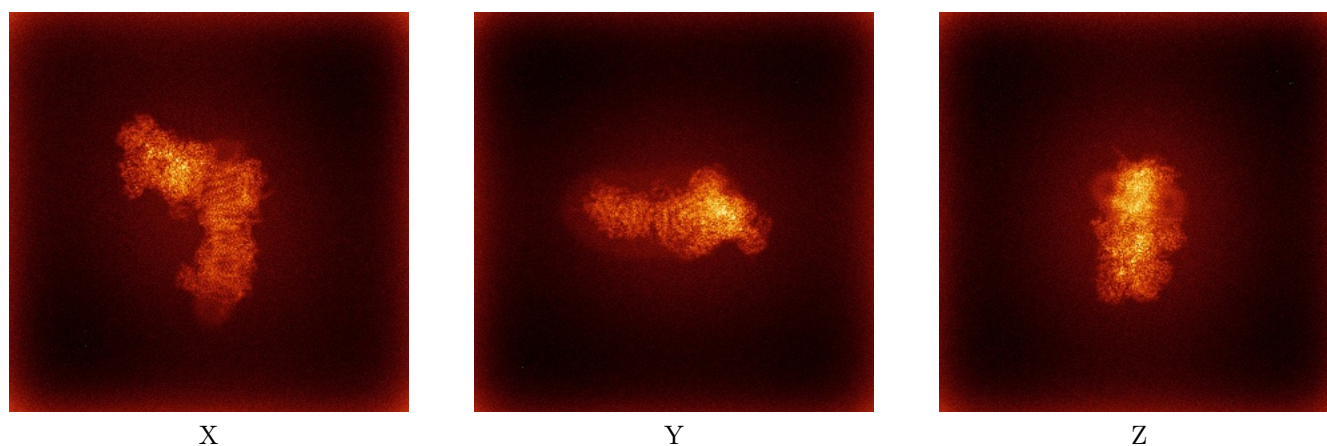
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

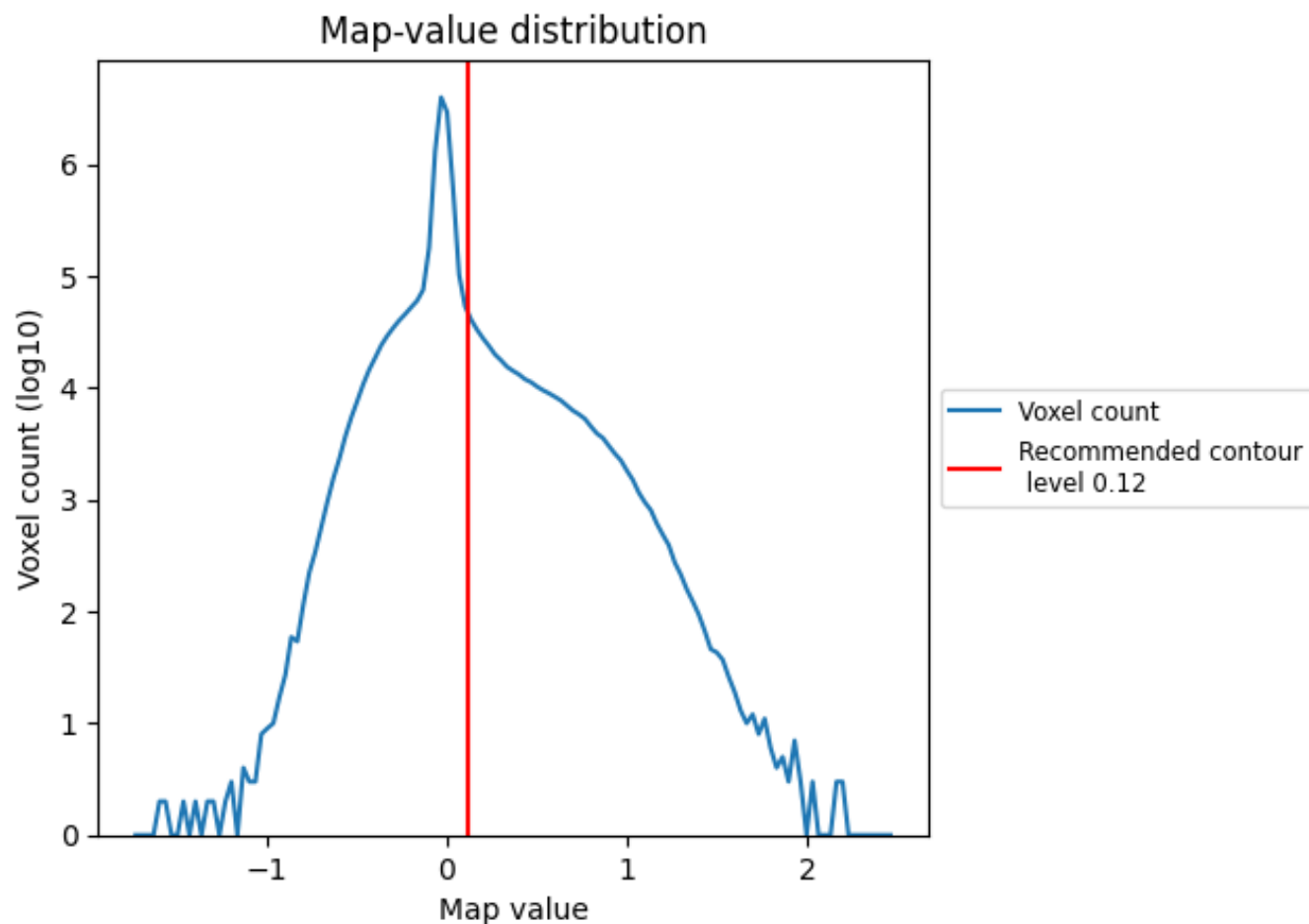
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

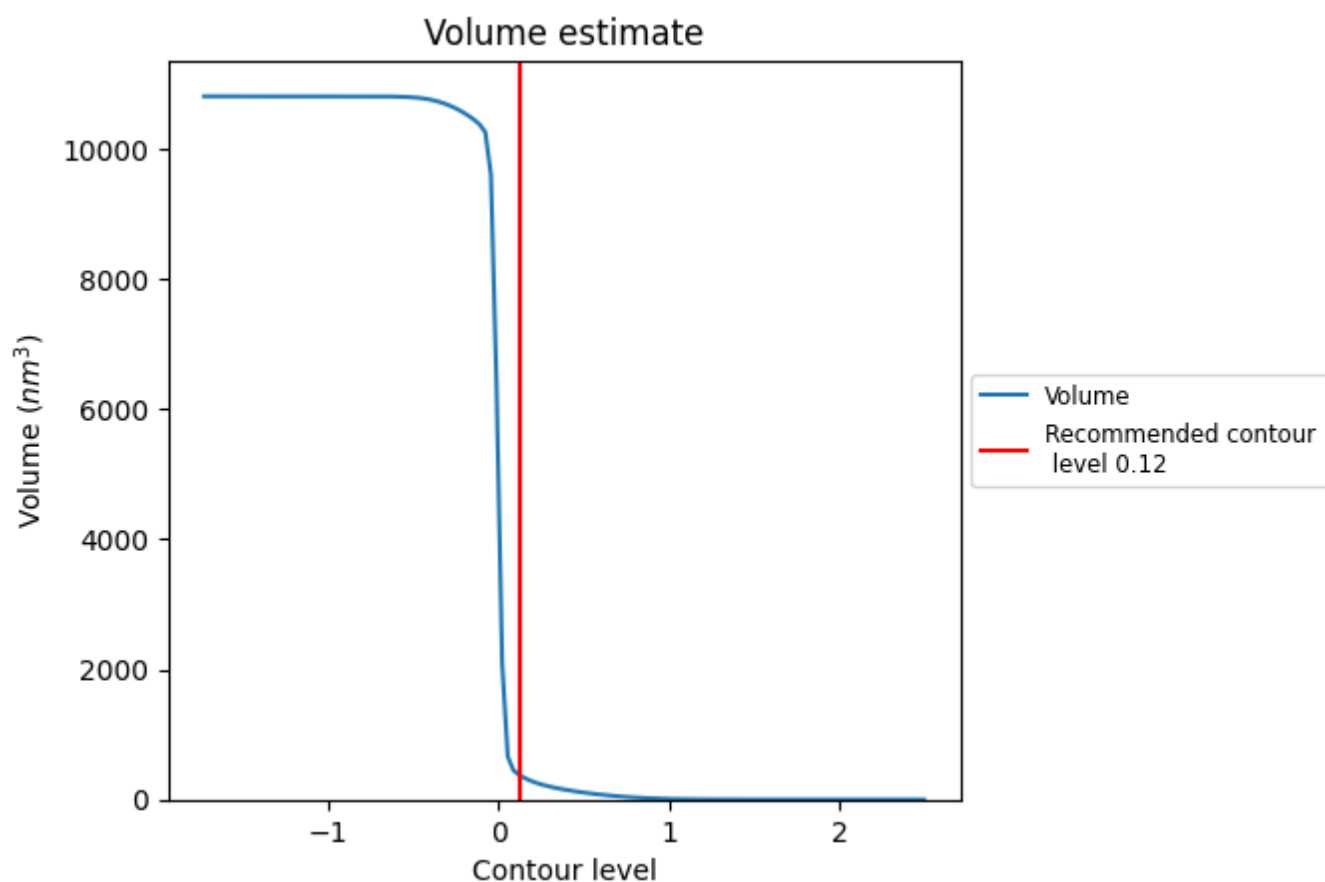
This section contains the results of statistical analysis of the map.

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 382 nm³; this corresponds to an approximate mass of 345 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.

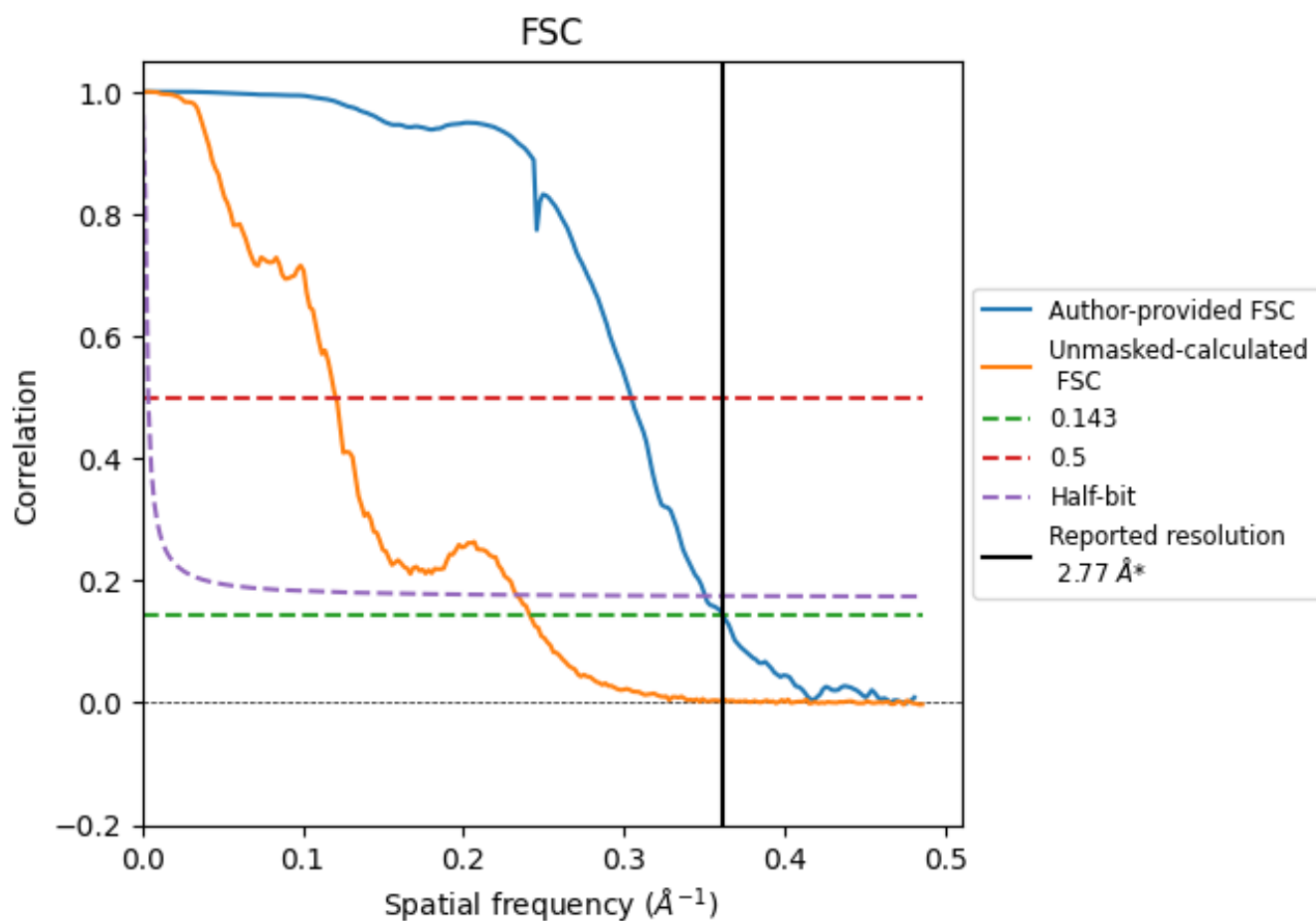
7.3 Rotationally averaged power spectrum [i](#)

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 0.361 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

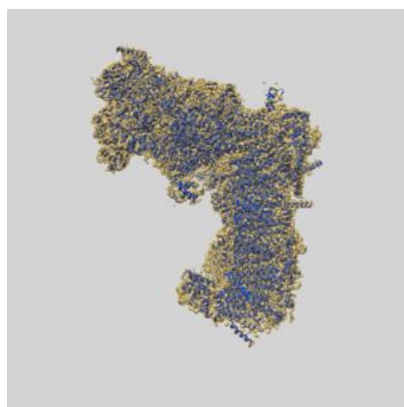
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	2.77	3.29	2.85
Unmasked-calculated*	4.14	8.30	4.29

*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 4.14 differs from the reported value 2.77 by more than 10 %

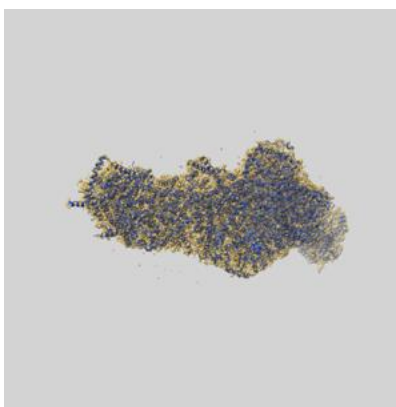
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14791 and PDB model 7ZM7. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

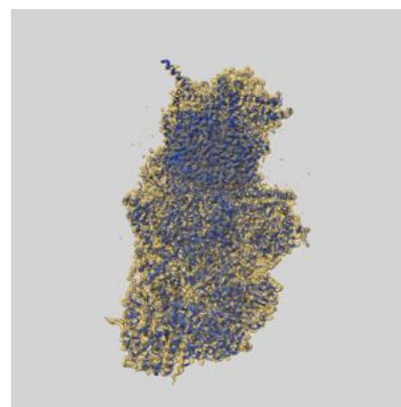
9.1 Map-model overlay [i](#)



X



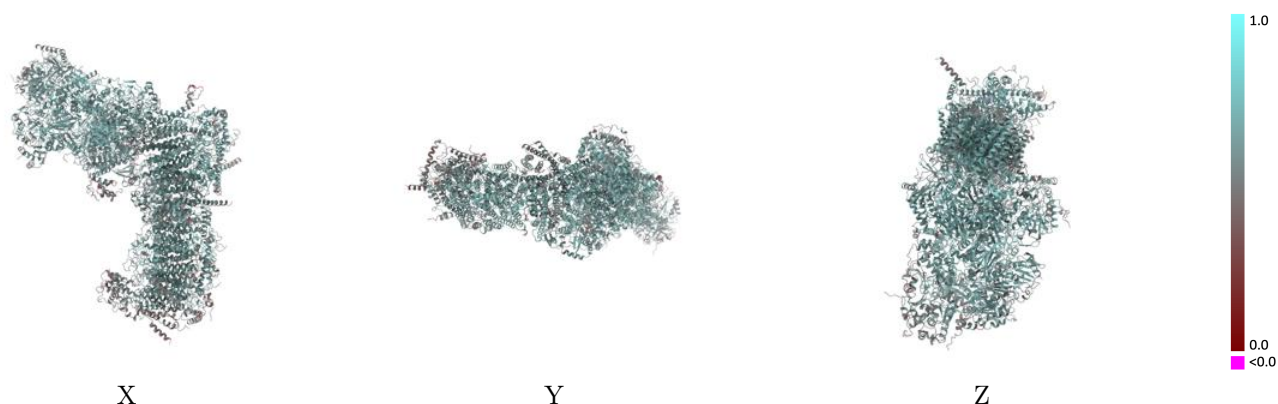
Y



Z

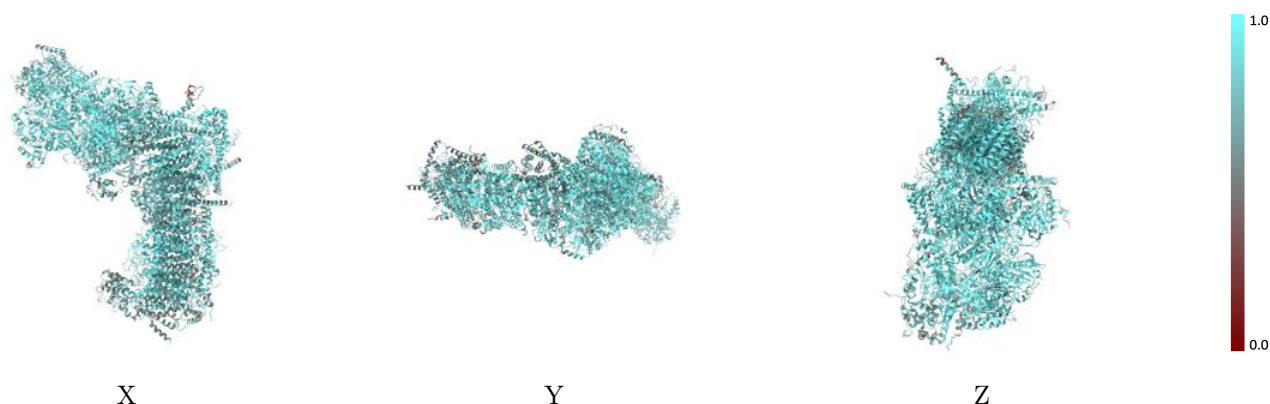
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



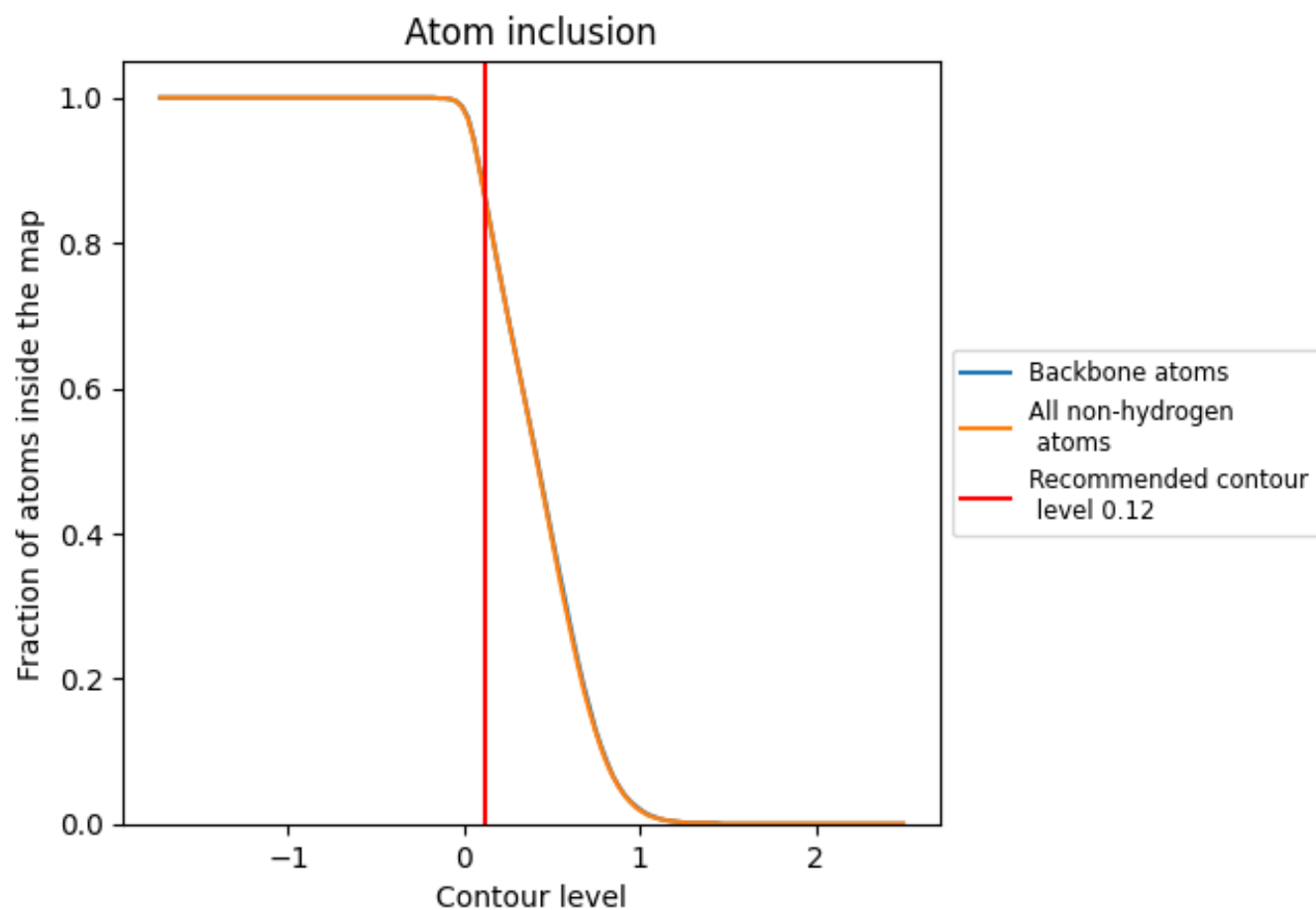
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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	 0.8610	 0.5980
1	 0.8390	 0.5950
2	 0.9270	 0.6390
3	 0.8270	 0.5880
4	 0.9500	 0.6400
5	 0.8450	 0.5820
6	 0.8710	 0.6040
8	 0.6820	 0.4830
9	 0.8110	 0.5780
A	 0.9100	 0.6200
B	 0.8300	 0.5650
C	 0.9330	 0.6490
D	 0.9230	 0.6350
E	 0.8580	 0.5840
F	 0.8550	 0.5930
G	 0.9410	 0.6580
H	 0.8300	 0.5630
I	 0.9450	 0.6540
J	 0.7010	 0.5290
K	 0.9260	 0.6300
L	 0.9200	 0.6260
M	 0.9120	 0.6240
O	 0.6440	 0.4590
P	 0.8830	 0.5880
Q	 0.6160	 0.4750
R	 0.7400	 0.5230
S	 0.8520	 0.5770
U	 0.9030	 0.6110
W	 0.8530	 0.6070
X	 0.8960	 0.6180
Y	 0.9230	 0.6330
Z	 0.8610	 0.5970
a	 0.7730	 0.5380
b	 0.8510	 0.5980
c	 0.6430	 0.4690



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Chain	Atom inclusion	Q-score
d	 0.8680	 0.5980
e	 0.6410	 0.4690
f	 0.8140	 0.5510
g	 0.8450	 0.5910
h	 0.9100	 0.6340
i	 0.7690	 0.5560
j	 0.8400	 0.5850
n	 0.7880	 0.5660
o	 0.5890	 0.5030