



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 04:30 PM UTC

PDB ID : 7QSD / pdb_00007qsd
EMDB ID : EMD-14127
Title : Bovine complex I in the active state at 3.1 Å
Authors : Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.
Deposited on : 2022-01-13
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

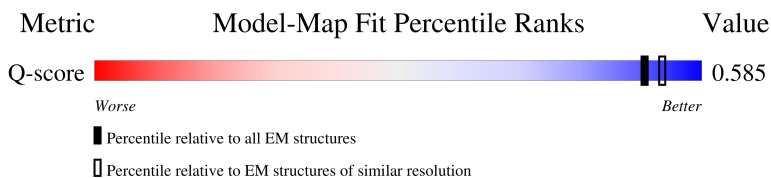
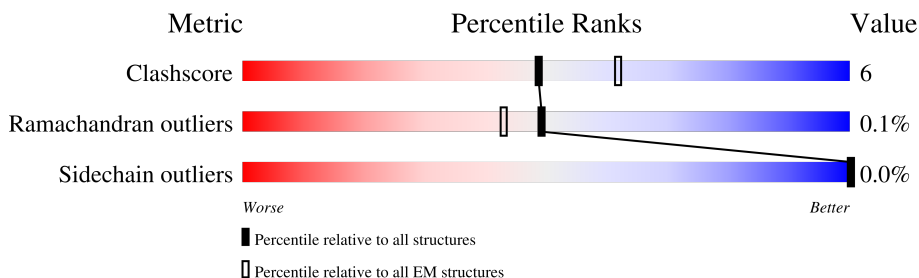
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	A	115	 8% 84% 15% .
2	B	216	 61% 11% 28%
3	C	266	 69% 9% 22%
4	D	463	 78% 15% 7%

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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	

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Mol	Chain	Length	Quality of chain
29	d	120	
30	e	106	
31	f	57	
32	g	154	
33	h	189	
34	i	127	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
47	SF4	F	502	-	-	X	-

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 67258 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 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	S	0	0
			921	622	133	159	7		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	155	Total	C	N	O	S	0	0
			1241	792	224	211	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	207	Total	C	N	O	S	0	0
			1721	1111	296	311	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	430	Total	C	N	O	S	0	0
			3459	2209	596	629	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1655	1057	277	311	10		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	431	Total	C	N	O	S	0	0
			3319	2091	593	615	20		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	688	Total	C	N	O	S	0	0
			5279	3307	920	1013	39		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2509	1681	385	420	23		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	174	Total	C	N	O	S	0	0
			1337	902	189	234	12		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			745	486	112	131	16		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4802	3195	737	827	43		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3654	2436	570	609	39		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	347	Total	C	N	O	S	0	0
			2733	1817	416	457	43		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2589	1662	429	488	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	variant	UNP P34942

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	341	Total	C	N	O	S	0	0
			2747	1777	486	479	5		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	125	Total	C	N	O	S	0	0
			1016	641	181	191	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	95	Total	C	N	O	S	0	0
			730	448	137	142	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	84	Total	C	N	O	S	0	0
			677	425	126	124	2		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	76	Total	C	N	O	S	0	0
			612	393	90	124	5		
20	U	86	Total	C	N	O	S	0	0
			692	447	102	138	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	113	Total	C	N	O	S	0	0
			919	595	155	166	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			971	622	180	165	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1402	887	253	252	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	140	Total	C	N	O	S	0	0
			1030	657	176	191	6		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	141	Total	C	N	O	S	0	0
			1152	740	201	202	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	70	Total	C	N	O	S	0	0
			569	365	104	95	5		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			651	425	109	115	2		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	48	Total	C	N	O	0	0
			405	268	69	68		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	120	Total	C	N	O	S	0	0
			993	647	169	172	5		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	97	Total	C	N	O	S	0	0
			819	518	156	139	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	50	Total	C	N	O	S	0	0
			437	286	77	73	1		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	98	Total	C	N	O	S	0	0
			824	529	137	154	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	138	Total	C	N	O	S	0	0
			1154	759	196	197	2		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	107	Total	C	N	O	S	0	0
			920	605	158	156	1		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	64	Total	C	N	O	S	0	0
			556	367	90	98	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	80	Total	C	N	O	S	0	0
			644	421	108	113	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	155	Total	C	N	O	S	0	0
			1304	844	213	239	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	127	Total	C	N	O	S	0	0
			1061	681	187	193			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	172	Total	C	N	O	S	0	0
			1492	955	273	257	7		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	122	Total	C	N	O	S	0	0
			1048	653	201	185	9		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	171	Total	C	N	O	S	0	0
			1443	904	266	265	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	144	Total	C	N	O	S	0	0
			1201	773	215	209	4		

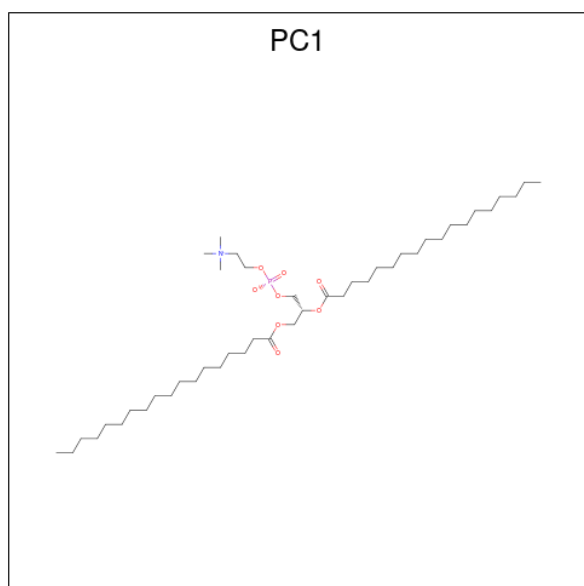
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	94	Total	C	N	O	S	0	0
			767	485	143	136	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

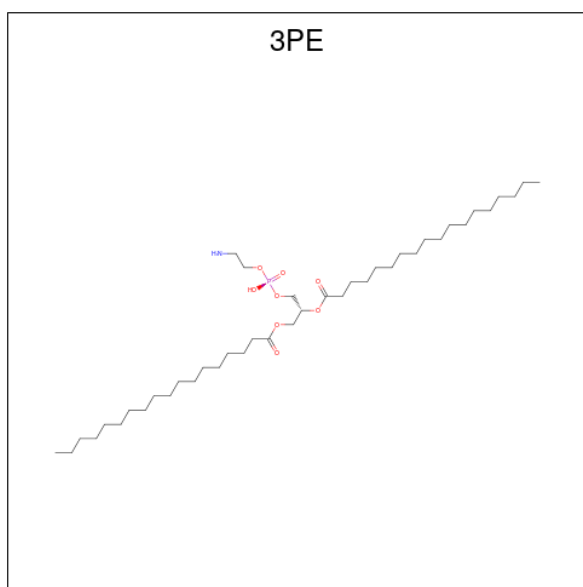
Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 45 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



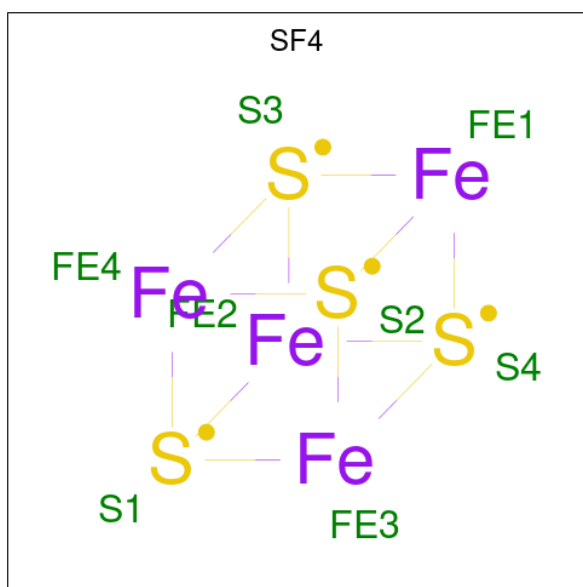
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			21	11	1	8	1	
45	B	1	Total	C	N	O	P	0
			43	33	1	8	1	
45	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	d	1	Total	C	N	O	P	0
			26	16	1	8	1	
45	g	1	Total	C	N	O	P	0
			49	39	1	8	1	

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



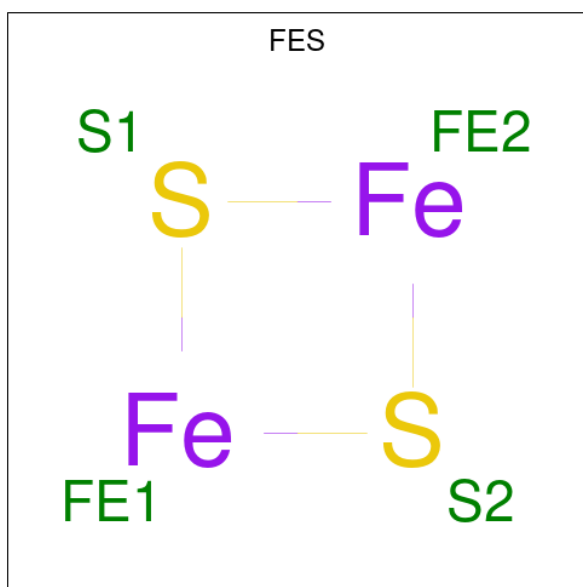
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	I	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	J	1	Total	C	N	O	P	0
			28	18	1	8	1	
46	K	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	L	1	Total	C	N	O	P	0
			38	28	1	8	1	
46	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
46	L	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	M	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	M	1	Total	C	N	O	P	0
			40	30	1	8	1	
46	N	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	N	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	X	1	Total	C	N	O	P	0
			31	21	1	8	1	
46	c	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



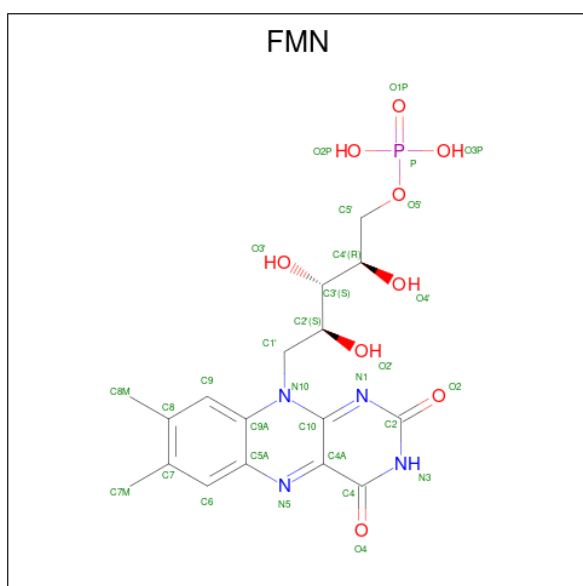
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



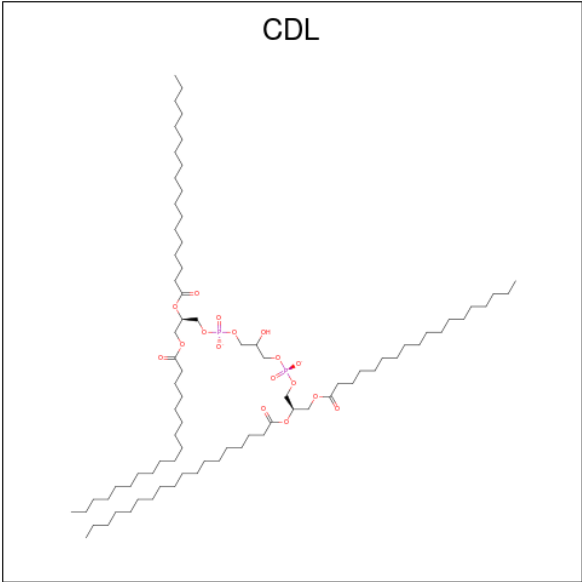
Mol	Chain	Residues	Atoms			AltConf
48	E	1	Total	Fe	S	0
			4	2	2	
48	G	1	Total	Fe	S	0
			4	2	2	

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



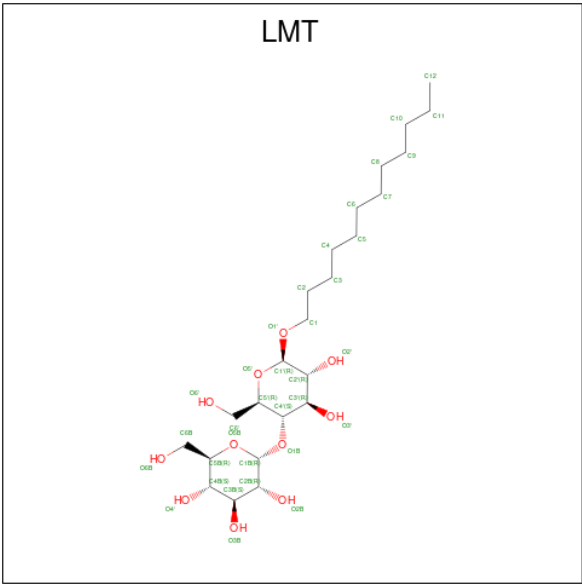
Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



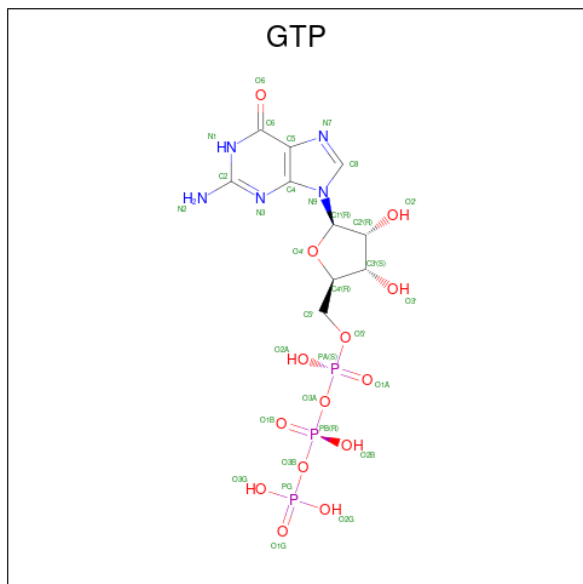
Mol	Chain	Residues	Atoms				AltConf
50	L	1	Total	C	O	P	0
			62	43	17	2	
50	Y	1	Total	C	O	P	0
			50	31	17	2	
50	h	1	Total	C	O	P	0
			64	45	17	2	
50	q	1	Total	C	O	P	0
			69	50	17	2	

- Molecule 51 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
51	M	1	Total	C	O	0
			35	24	11	
51	N	1	Total	C	O	0
			35	24	11	
51	b	1	Total	C	O	0
			35	24	11	

- Molecule 52 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

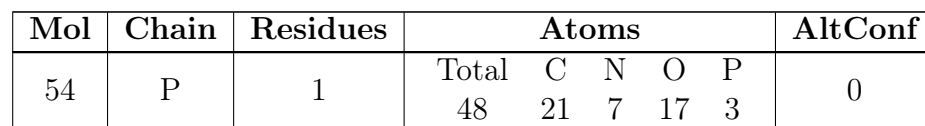


Mol	Chain	Residues	Atoms					AltConf
52	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	O	1	Total	Mg	0
			1	1	

- Molecule 54 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 |
|-----|-------|----------|-----------------|---------|
| 55 | R | 1 | Total Zn
1 1 | 0 |

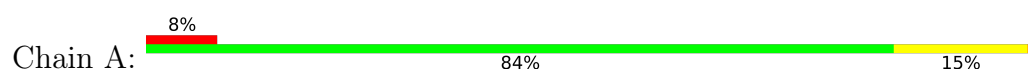
- # EHZ
-
- The chemical structure of EHZ (Ergosterol) is shown. It features a long hydrocarbon side chain (C1-C17) attached to a steroid nucleus. The side chain is a long, straight alkyl chain. The steroid nucleus consists of four fused rings (A, B, C, D) with various functional groups. A hydroxyl group (OH) is attached to C3. A double bond is present between C5 and C6. A side chain is attached to C17, which includes a ketone group (C18=O), a hydroxyl group (C19-OH), and a phosphate group (C20-PO4). The phosphate group is shown as a phosphorus atom (P1) bonded to four oxygen atoms (O1, O2, O3, O4). The structure is labeled with atom numbers (C1-C19, O1-O4, P1) and bond types (single, double, triple).

Mol	Chain	Residues	Atoms						AltConf
56	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
56	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

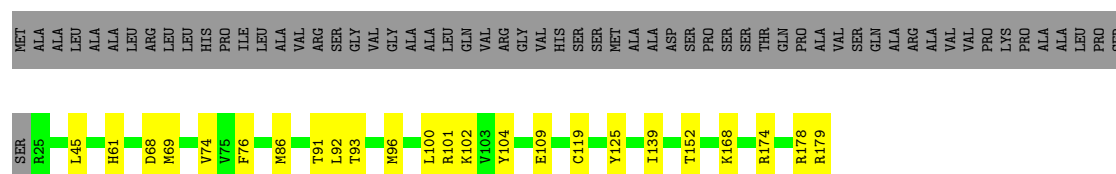
3 Residue-property plots [i](#)

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.

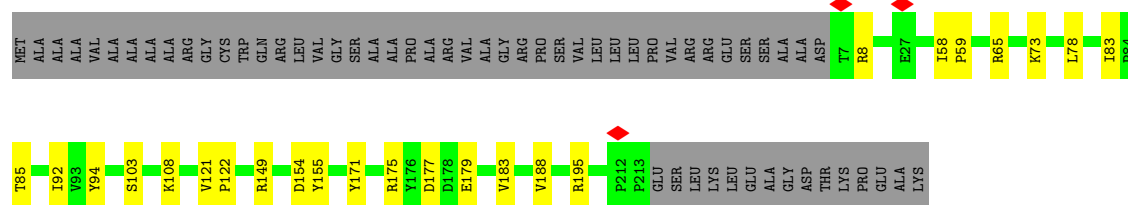
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



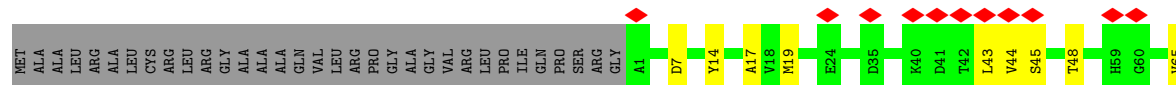
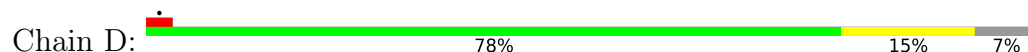
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

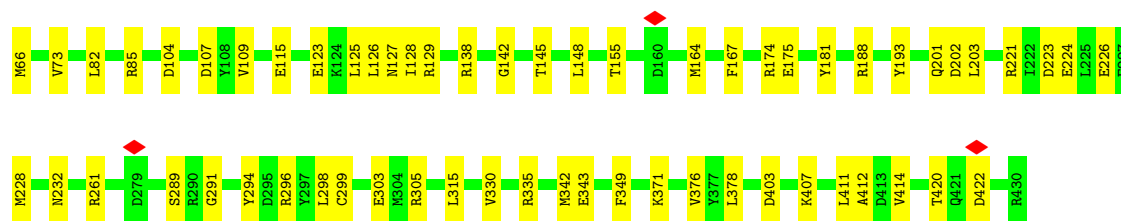


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

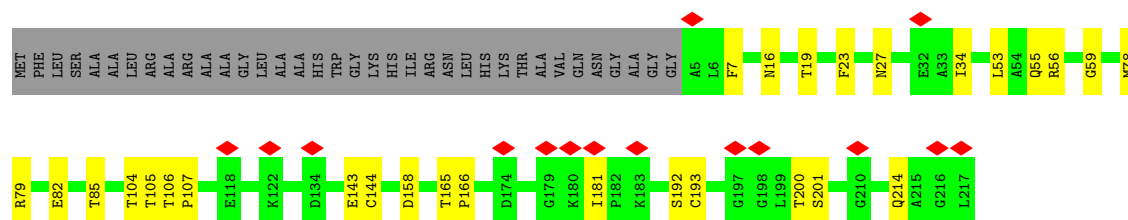
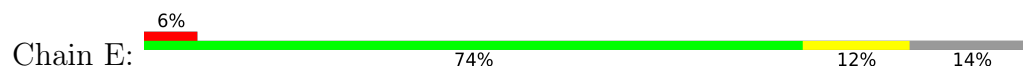


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

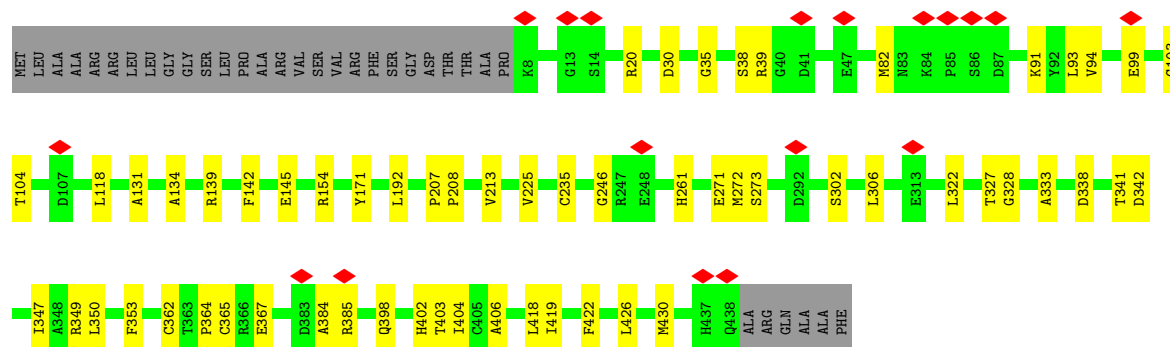
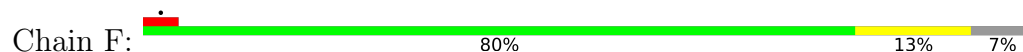




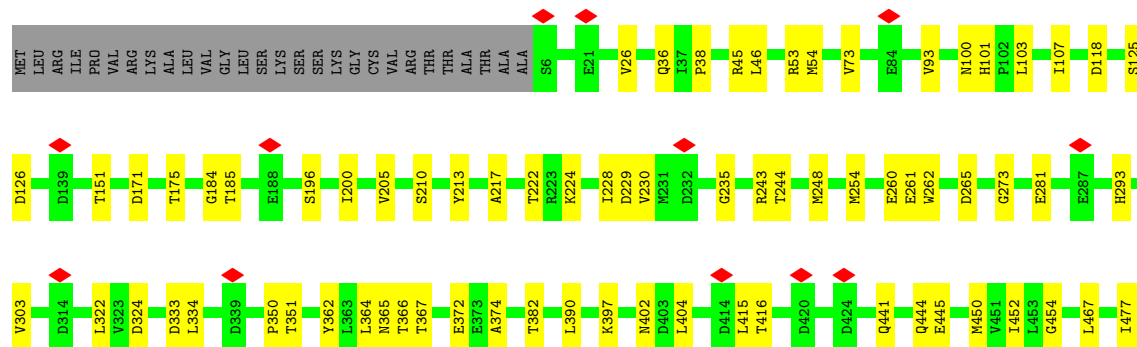
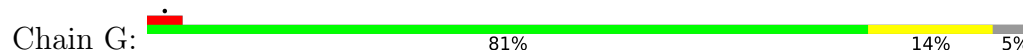
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

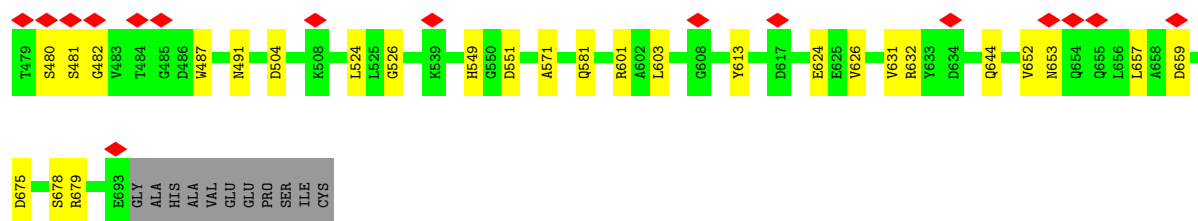


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

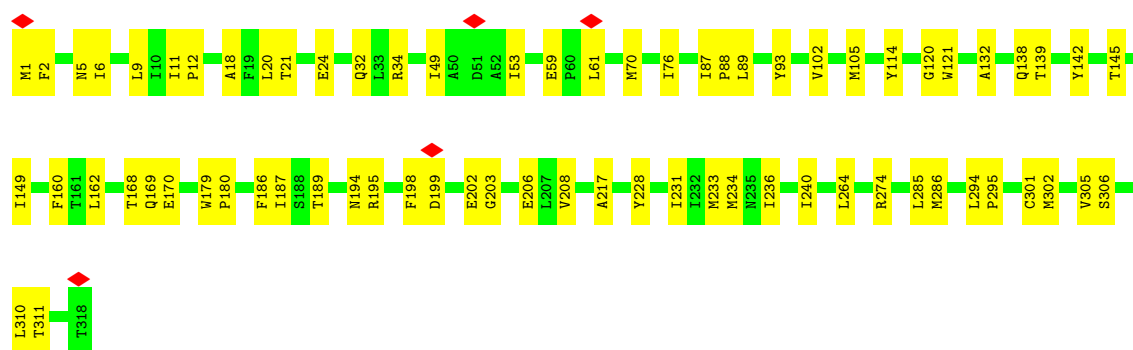
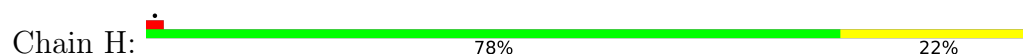


- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

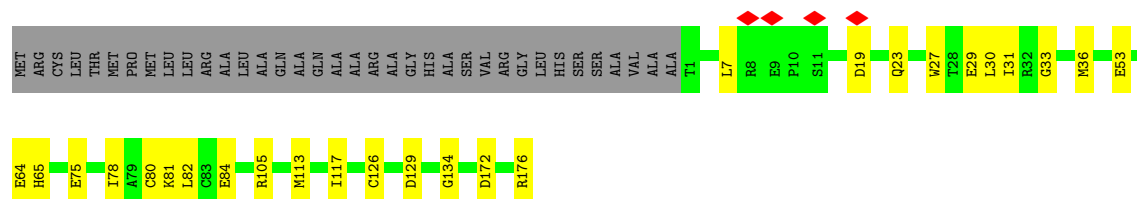




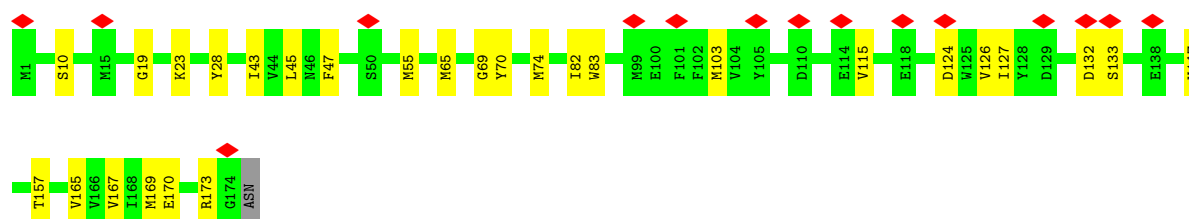
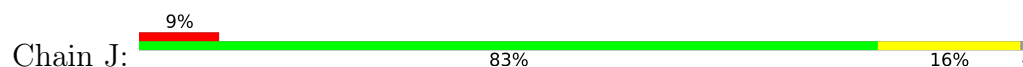
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



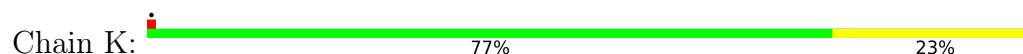
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

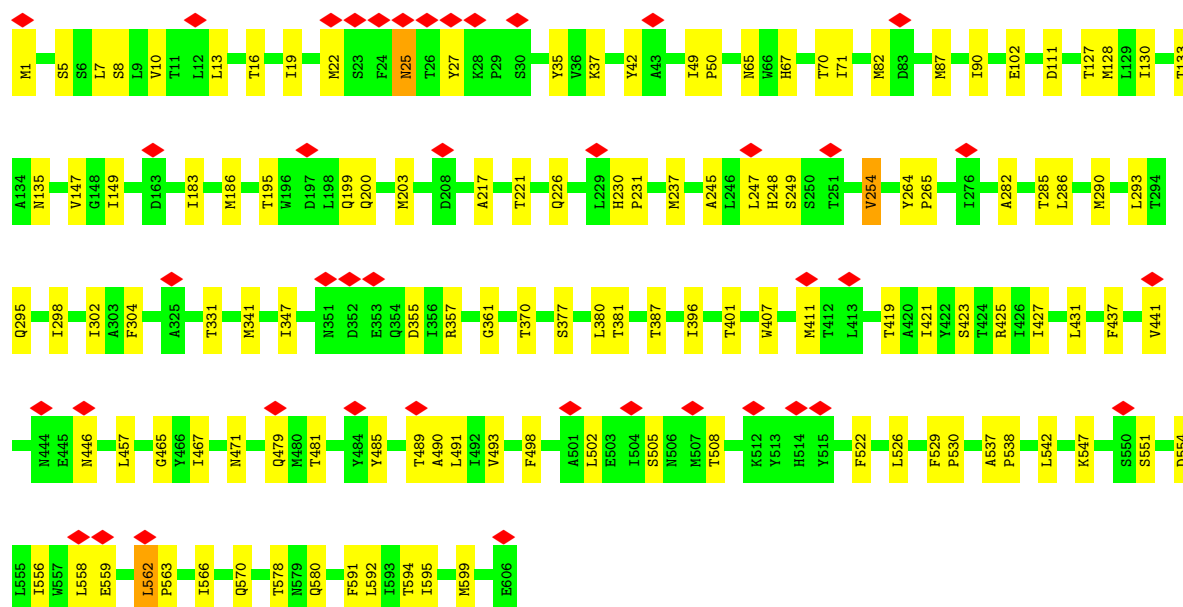
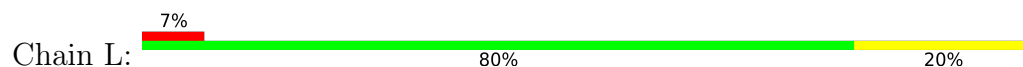


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

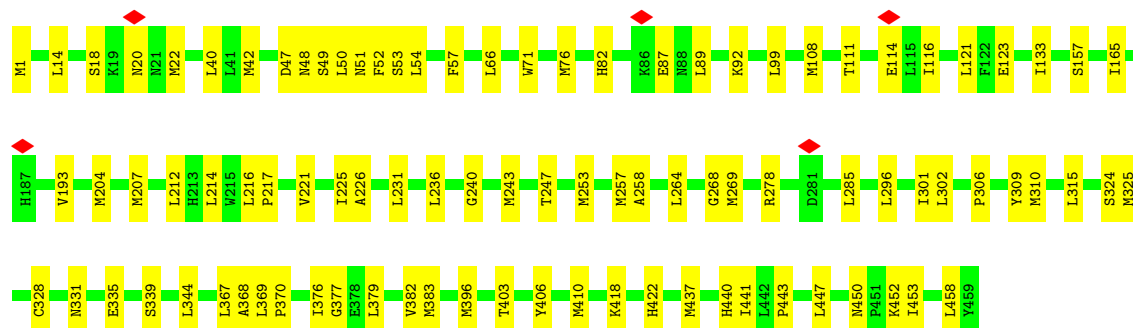
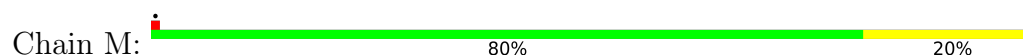




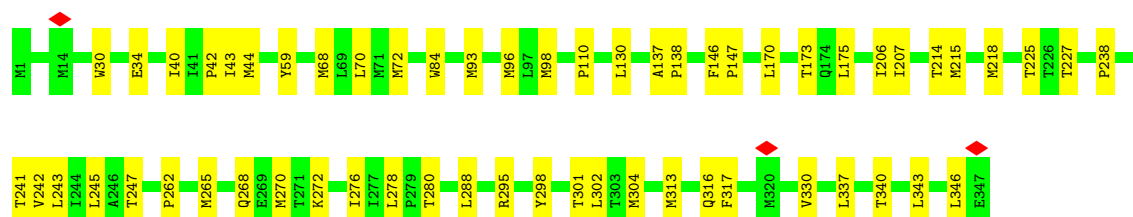
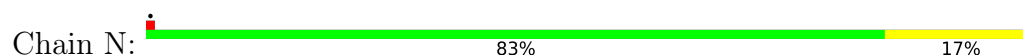
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



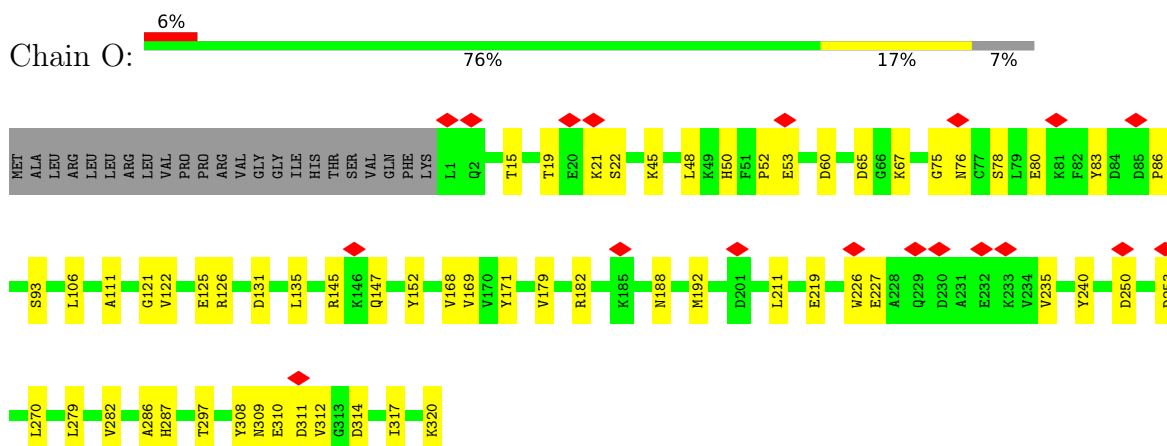
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



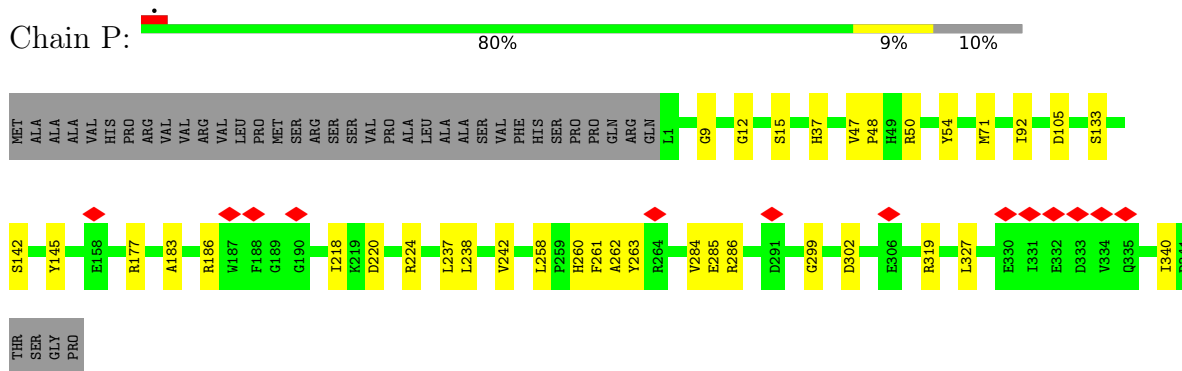
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



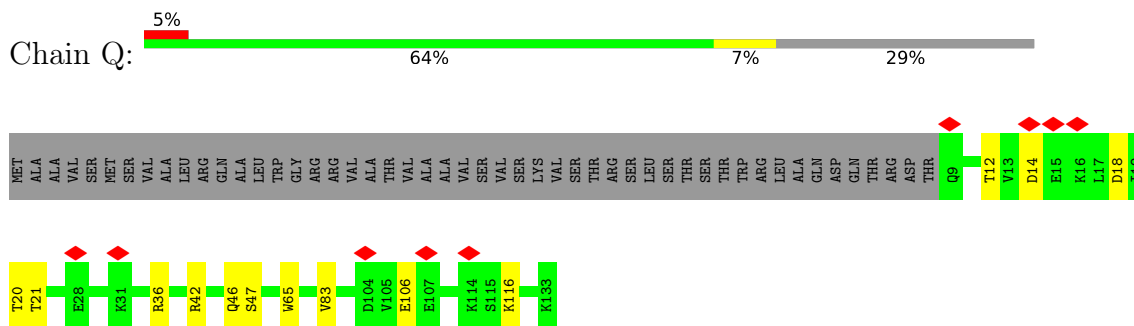
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



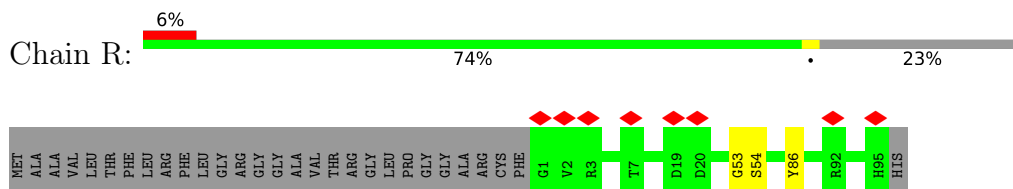
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



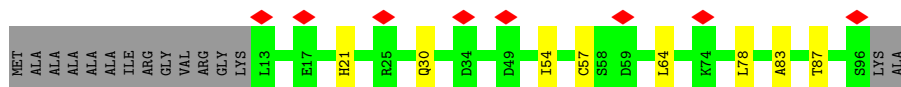
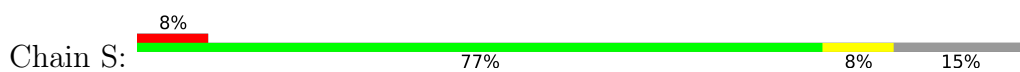
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



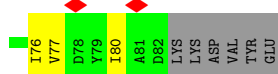
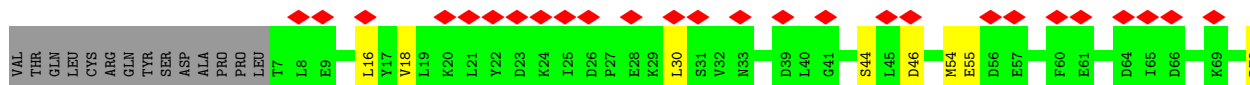
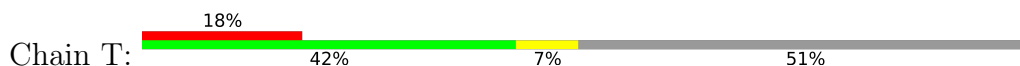
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



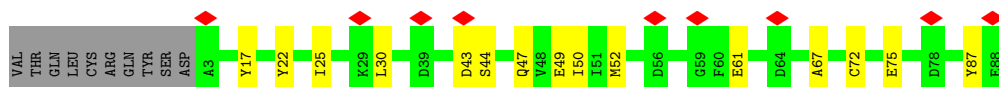
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



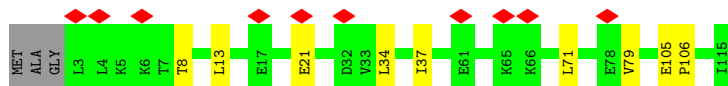
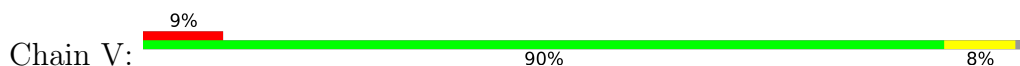
- Molecule 20: Acyl carrier protein, mitochondrial



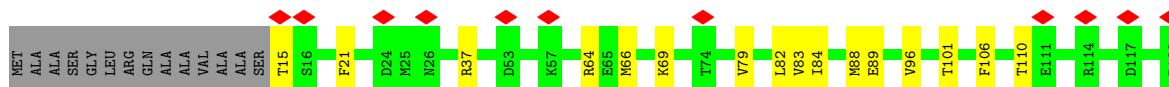
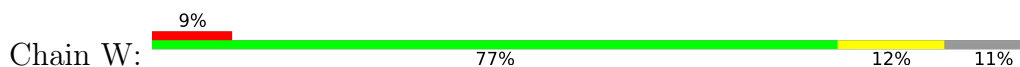
- Molecule 20: Acyl carrier protein, mitochondrial



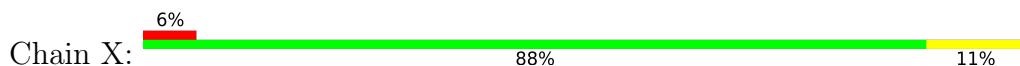
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

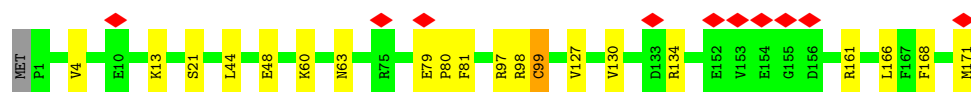


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

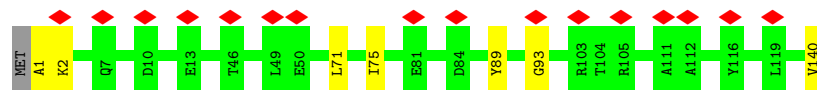


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

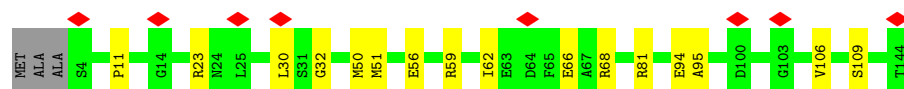
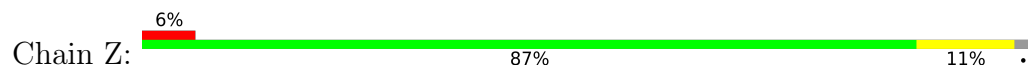




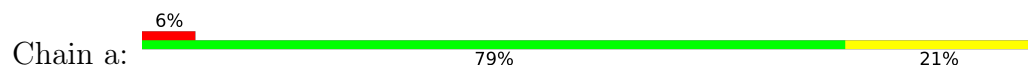
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



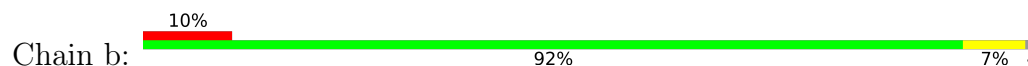
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



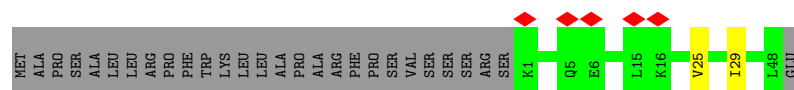
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



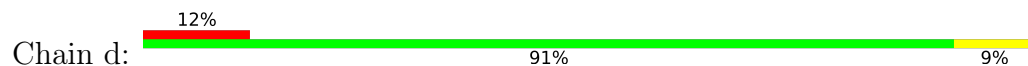
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



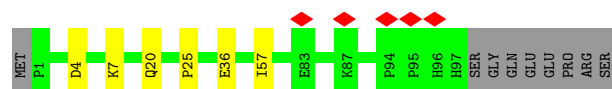
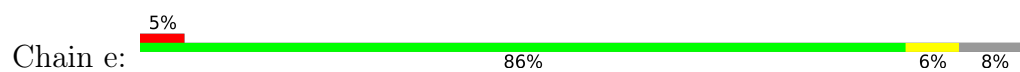
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



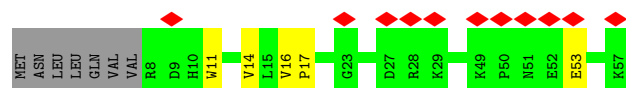
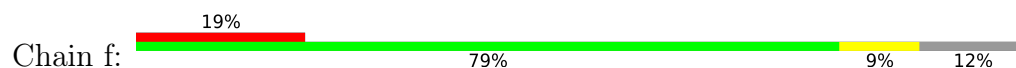
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



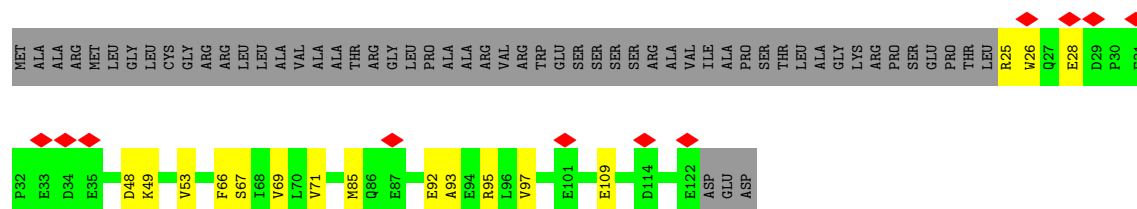
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



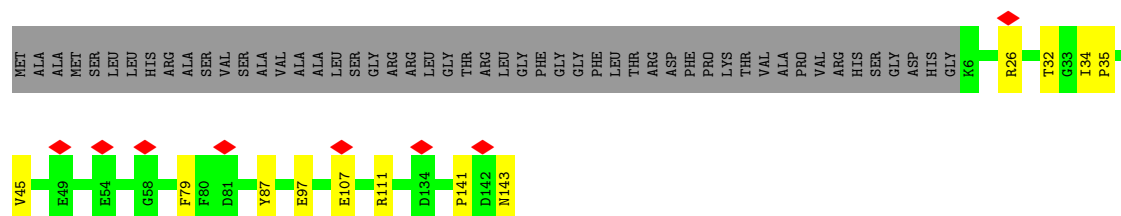
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



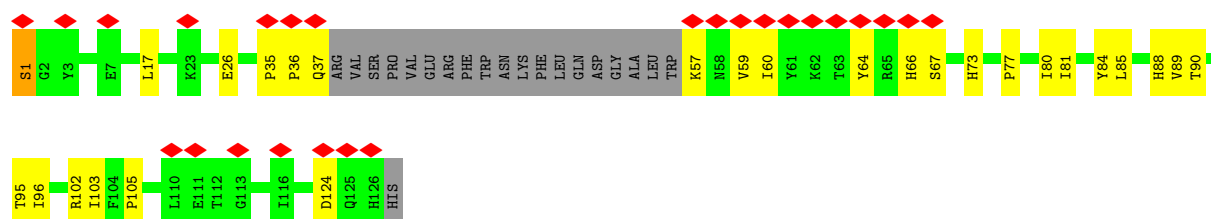
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



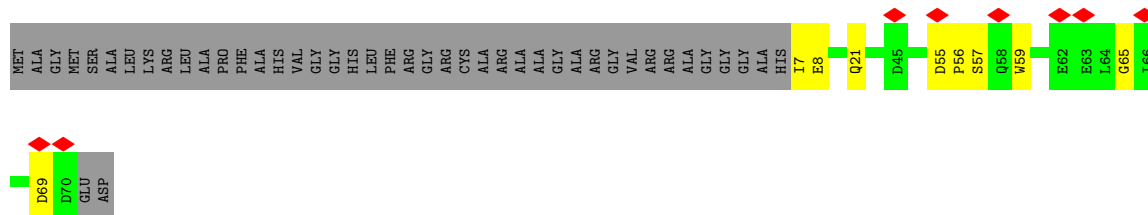
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



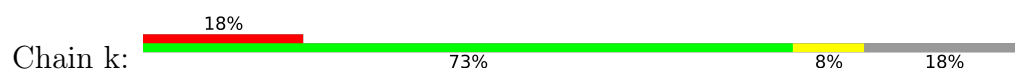
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



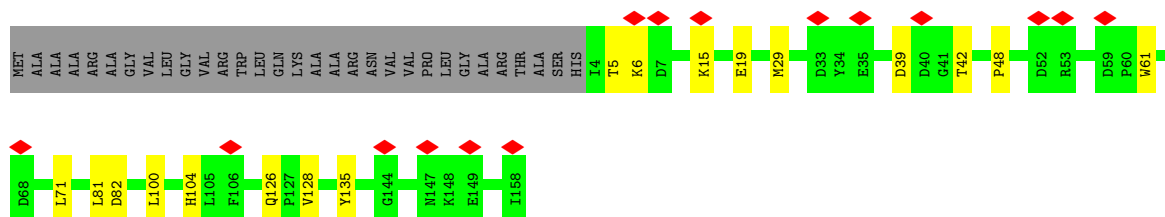
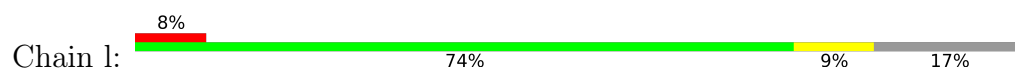
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



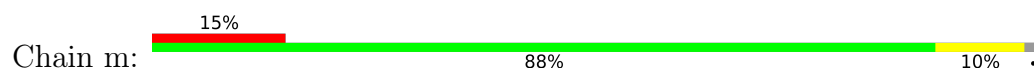
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



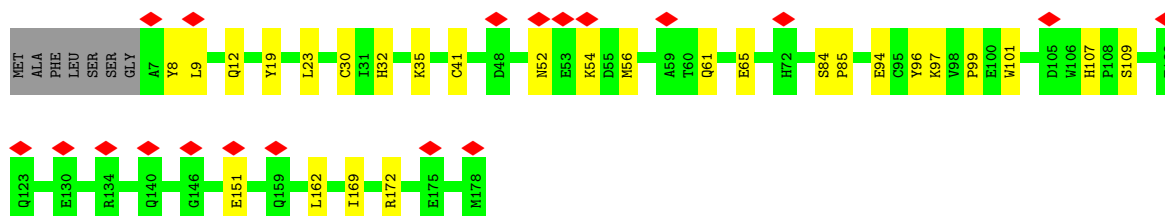
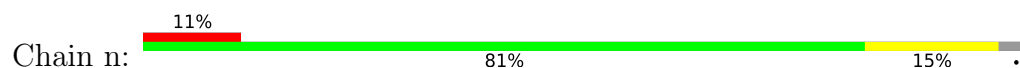
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



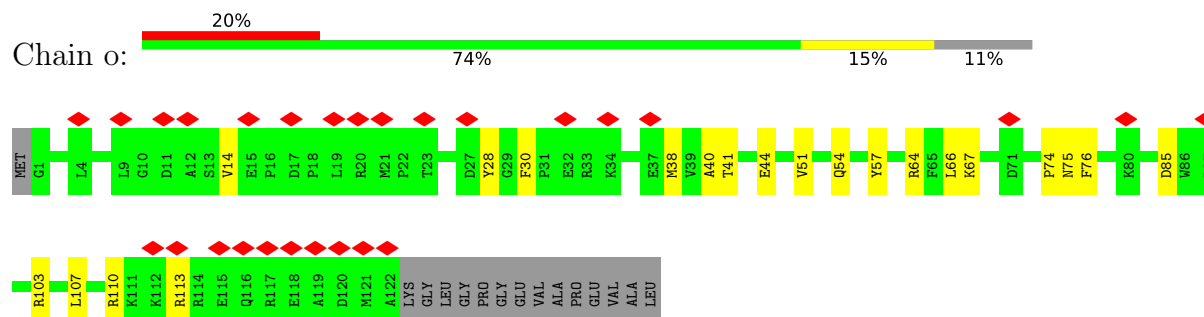
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



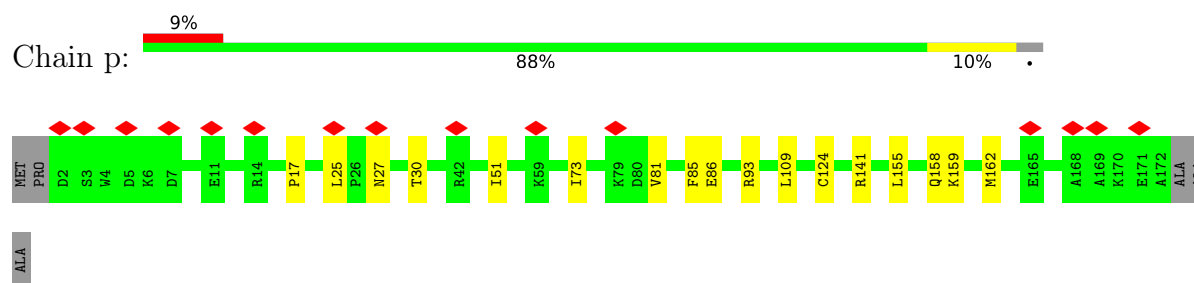
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



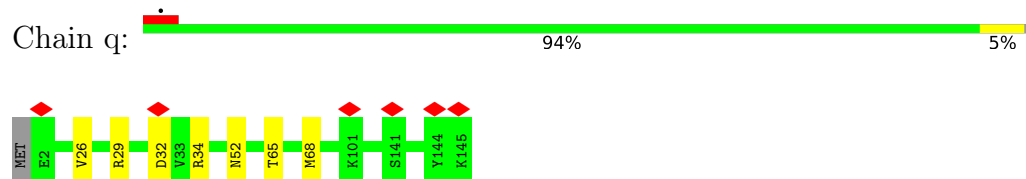
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



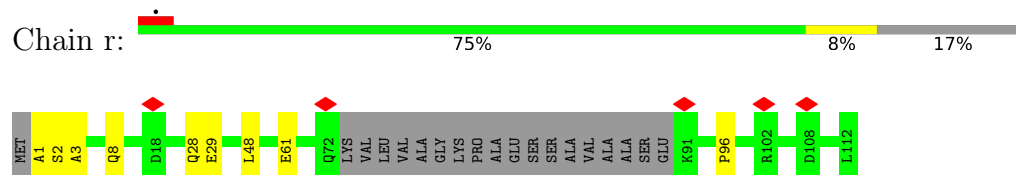
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



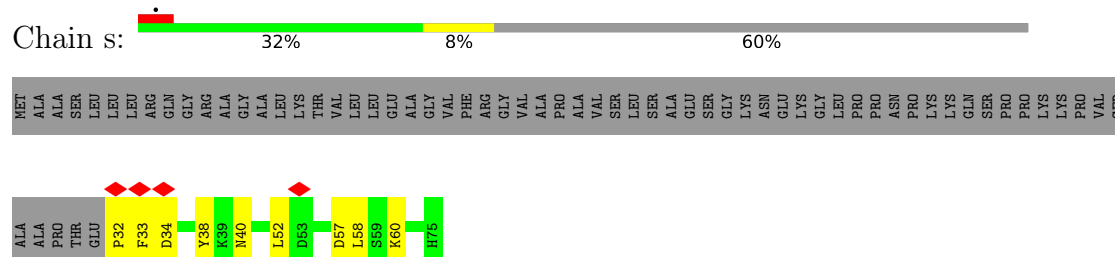
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18231	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	27.341	Depositor
Minimum map value	-13.287	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.973	Depositor
Recommended contour level	5.08	Depositor
Map size (Å)	475.2, 475.2, 475.2	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AYA, PC1, FMN, CDL, SF4, EHZ, MG, FES, 2MR, ZN, AME, SAC, FME, NDP, 3PE, LMT, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.28	0/936	0.30	0/1281
2	B	0.35	0/1272	0.41	0/1720
3	C	0.32	0/1772	0.33	0/2413
4	D	0.32	0/3537	0.33	0/4794
5	E	0.27	0/1695	0.33	0/2307
6	F	0.28	0/3393	0.38	0/4584
7	G	0.29	0/5367	0.34	0/7274
8	H	0.31	0/2571	0.37	1/3513 (0.0%)
9	I	0.35	0/1445	0.37	0/1956
10	J	0.28	0/1362	0.30	0/1848
11	K	0.31	0/745	0.32	0/1008
12	L	0.27	0/4920	0.32	0/6694
13	M	0.31	0/3738	0.33	0/5097
14	N	0.30	0/2792	0.32	0/3800
15	O	0.26	0/2651	0.30	0/3587
16	P	0.28	0/2824	0.33	0/3831
17	Q	0.29	0/1039	0.31	0/1404
18	R	0.30	0/742	0.31	0/999
19	S	0.25	0/688	0.31	0/927
20	T	0.21	0/621	0.33	0/837
20	U	0.26	0/704	0.34	0/950
21	V	0.26	0/939	0.30	0/1272
22	W	0.28	0/995	0.32	0/1337
23	X	0.28	0/1439	0.37	0/1942
24	Y	0.23	0/1042	0.28	0/1414
25	Z	0.28	0/1181	0.31	0/1592
26	a	0.29	0/584	0.33	0/786
27	b	0.25	0/672	0.32	0/923
28	c	0.24	0/418	0.26	0/567
29	d	0.29	0/1012	0.31	0/1368
30	e	0.28	0/840	0.33	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.23	0/450	0.36	0/606
32	g	0.27	0/850	0.31	0/1154
33	h	0.28	0/1188	0.31	0/1607
34	i	0.23	0/941	0.37	0/1279
35	j	0.25	0/582	0.29	0/799
36	k	0.21	0/663	0.31	0/895
37	l	0.26	0/1358	0.33	0/1858
38	m	0.25	0/1088	0.33	0/1472
39	n	0.25	0/1545	0.32	0/2092
40	o	0.23	0/1073	0.35	0/1437
41	p	0.27	0/1476	0.31	0/1990
42	q	0.29	0/1242	0.35	0/1688
43	r	0.28	0/780	0.30	0/1056
44	s	0.25	0/383	0.37	0/518
All	All	0.28	0/67555	0.33	1/91599 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	217	ALA	CB-CA-C	-5.01	110.82	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	921	0	952	21	0
2	B	1241	0	1251	20	0
3	C	1721	0	1675	16	0
4	D	3459	0	3404	55	0
5	E	1655	0	1661	25	0
6	F	3319	0	3274	44	0
7	G	5279	0	5301	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	2509	0	2621	54	0
9	I	1414	0	1370	23	0
10	J	1337	0	1346	31	0
11	K	745	0	785	26	0
12	L	4802	0	4960	100	0
13	M	3654	0	3852	68	0
14	N	2733	0	2912	51	0
15	O	2589	0	2566	39	0
16	P	2747	0	2766	25	0
17	Q	1016	0	1014	13	0
18	R	730	0	707	2	0
19	S	677	0	688	6	0
20	T	612	0	604	9	0
20	U	692	0	688	10	0
21	V	919	0	961	5	0
22	W	971	0	989	13	0
23	X	1402	0	1381	20	0
24	Y	1030	0	1039	5	0
25	Z	1152	0	1151	14	0
26	a	569	0	568	13	0
27	b	651	0	662	7	0
28	c	405	0	409	1	0
29	d	993	0	977	9	0
30	e	819	0	821	7	0
31	f	437	0	435	3	0
32	g	824	0	772	16	0
33	h	1154	0	1168	11	0
34	i	920	0	939	23	0
35	j	556	0	501	6	0
36	k	644	0	626	6	0
37	l	1304	0	1203	14	0
38	m	1061	0	1059	9	0
39	n	1492	0	1438	24	0
40	o	1048	0	1020	15	0
41	p	1443	0	1415	13	0
42	q	1201	0	1170	5	0
43	r	767	0	776	7	0
44	s	371	0	344	9	0
45	A	21	0	18	0	0
45	B	78	0	104	2	0
45	d	26	0	26	0	0
45	g	49	0	75	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	A	39	0	52	0	0
46	I	42	0	58	4	0
46	J	28	0	30	1	0
46	K	39	0	52	0	0
46	L	118	0	161	0	0
46	M	86	0	123	2	0
46	N	85	0	121	4	0
46	X	31	0	36	1	0
46	c	38	0	53	1	0
47	B	8	0	0	0	0
47	F	8	0	0	2	0
47	G	16	0	0	1	0
47	I	16	0	0	0	0
48	E	4	0	0	0	0
48	G	4	0	0	0	0
49	F	31	0	19	1	0
50	L	62	0	68	0	0
50	Y	50	0	44	1	0
50	h	64	0	75	2	0
50	q	69	0	82	1	0
51	M	35	0	46	1	0
51	N	35	0	46	0	0
51	b	35	0	46	0	0
52	O	32	0	12	3	0
53	O	1	0	0	0	0
54	P	48	0	26	4	0
55	R	1	0	0	0	0
56	T	37	0	0	0	0
56	U	37	0	0	1	0
All	All	67258	0	67594	786	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 6.

All (786) 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)
20:T:46:ASP:OD1	22:W:64:ARG:NH2	1.96	0.99
1:A:71:LEU:O	10:J:147:TYR:OH	1.83	0.96
4:D:403:ASP:OD2	4:D:407:LYS:NZ	2.01	0.93
3:C:65:ARG:O	3:C:73:LYS:NZ	2.02	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:GLU:OE1	16:P:54:TYR:OH	1.91	0.89
7:G:362:TYR:OH	7:G:504:ASP:OD1	1.91	0.88
17:Q:42:ARG:NH1	17:Q:46:GLN:O	2.08	0.87
4:D:145:THR:HG1	4:D:181:TYR:HH	1.01	0.86
46:X:401:3PE:O14	46:X:401:3PE:N	2.09	0.86
7:G:415:LEU:O	7:G:416:THR:OG1	1.94	0.85
11:K:37:MET:HE3	11:K:67:ALA:HB2	1.59	0.84
17:Q:36:ARG:NE	17:Q:106:GLU:OE2	2.08	0.84
7:G:366:THR:O	7:G:367:THR:OG1	1.96	0.84
4:D:261:ARG:NH1	4:D:303:GLU:OE2	2.12	0.82
10:J:103:MET:HE2	10:J:115:VAL:HG11	1.60	0.81
12:L:505:SER:O	12:L:508:THR:OG1	1.99	0.81
41:p:158:GLN:HG2	41:p:162:MET:HE3	1.63	0.80
20:T:55:GLU:OE2	22:W:37:ARG:NH2	2.15	0.80
3:C:8:ARG:NH2	43:r:61:GLU:OE1	2.14	0.80
3:C:175:ARG:NH2	3:C:177:ASP:OD1	2.15	0.79
32:g:92:GLU:OE2	32:g:95:ARG:NH2	2.16	0.79
15:O:131:ASP:OD1	15:O:152:TYR:OH	2.00	0.79
2:B:174:ARG:O	2:B:178:ARG:NE	2.15	0.78
12:L:485:TYR:O	12:L:489:THR:OG1	2.01	0.78
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.16	0.78
34:i:105:PRO:O	40:o:67:LYS:NZ	2.17	0.77
16:P:183:ALA:O	16:P:186:ARG:NH1	2.17	0.77
15:O:78:SER:OG	15:O:80:GLU:OE1	2.01	0.77
15:O:309:ASN:N	15:O:314:ASP:OD1	2.18	0.77
19:S:83:ALA:O	19:S:87:THR:OG1	2.02	0.77
44:s:57:ASP:OD1	44:s:60:LYS:NZ	2.18	0.76
4:D:228:MET:O	4:D:232:ASN:ND2	2.19	0.76
8:H:93:TYR:OH	26:a:35:GLU:OE2	2.04	0.76
12:L:71:ILE:HG23	13:M:310:MET:HE1	1.65	0.76
7:G:632:ARG:NH1	19:S:57:CYS:SG	2.60	0.75
8:H:32:GLN:OE1	8:H:34:ARG:NH1	2.19	0.75
4:D:164:MET:HE2	8:H:32:GLN:HE22	1.52	0.75
6:F:261:HIS:ND1	6:F:338:ASP:OD1	2.20	0.75
15:O:83:TYR:OH	52:O:401:GTP:O3'	2.02	0.74
16:P:299:GLY:N	16:P:302:ASP:OD2	2.21	0.74
37:l:5:THR:HG22	37:l:6:LYS:H	1.52	0.74
37:l:71:LEU:HD11	37:l:81:LEU:HD11	1.68	0.74
7:G:626:VAL:O	19:S:21:HIS:NE2	2.21	0.73
14:N:170:LEU:HD11	14:N:288:LEU:HD22	1.69	0.73
20:U:49:GLU:OE1	39:n:19:TYR:OH	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:94:GLU:OE2	39:n:97:LYS:NZ	2.21	0.72
39:n:52:ASN:O	39:n:54:LYS:NZ	2.21	0.72
12:L:446:ASN:ND2	35:j:21:GLN:OE1	2.22	0.72
34:i:1:SAC:OAC	34:i:1:SAC:OG	2.07	0.71
12:L:130:ILE:HD11	50:h:1001:CDL:H273	1.73	0.71
13:M:309:TYR:HB2	13:M:458:LEU:HD12	1.73	0.70
14:N:243:LEU:HD22	14:N:330:VAL:HG21	1.73	0.70
22:W:66:MET:SD	22:W:69:LYS:NZ	2.65	0.70
14:N:265:MET:HE1	23:X:166:LEU:HD21	1.73	0.69
7:G:644:GLN:N	7:G:644:GLN:OE1	2.24	0.69
23:X:171:MET:HE3	29:d:28:ASP:OD2	1.92	0.69
15:O:19:THR:HG23	15:O:21:LYS:H	1.55	0.69
12:L:65:ASN:O	34:i:84:TYR:OH	2.09	0.69
7:G:118:ASP:OD2	17:Q:46:GLN:NE2	2.26	0.69
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.74	0.69
38:m:105:LYS:NZ	38:m:109:ASP:OD2	2.24	0.69
7:G:675:ASP:OD1	7:G:678:SER:OG	2.06	0.69
5:E:53:LEU:HD13	44:s:52:LEU:CD1	2.23	0.68
12:L:341:MET:HE2	12:L:457:LEU:HD12	1.73	0.68
12:L:13:LEU:HD22	34:i:81:ILE:HD11	1.74	0.68
26:a:34:LYS:NZ	26:a:61:TYR:O	2.26	0.68
32:g:109:GLU:O	41:p:141:ARG:NH2	2.25	0.68
14:N:265:MET:HE3	14:N:343:LEU:HD21	1.73	0.68
26:a:66:LEU:O	26:a:69:ILE:HG22	1.92	0.68
29:d:110:GLY:O	41:p:159:LYS:NZ	2.21	0.68
2:B:86:MET:HE1	2:B:104:TYR:HB2	1.74	0.68
15:O:219:GLU:N	15:O:219:GLU:OE1	2.27	0.68
5:E:214:GLN:NE2	6:F:235:CYS:O	2.27	0.67
4:D:66:MET:HE1	4:D:411:LEU:HD13	1.76	0.67
12:L:591:PHE:O	12:L:595:ILE:HD12	1.93	0.67
33:h:45:VAL:HG22	41:p:51:ILE:HD12	1.76	0.67
10:J:45:LEU:HD21	46:J:401:3PE:H222	1.75	0.67
10:J:133:SER:O	25:Z:68:ARG:NH2	2.28	0.67
4:D:14:TYR:HD1	4:D:19:MET:HE1	1.60	0.67
29:d:28:ASP:OD1	29:d:30:ARG:NH2	2.28	0.67
5:E:105:THR:HG22	5:E:106:THR:H	1.61	0.66
9:I:65:HIS:ND1	9:I:113:MET:HE1	2.09	0.66
15:O:50:HIS:NE2	15:O:125:GLU:OE1	2.27	0.66
12:L:341:MET:CE	12:L:457:LEU:HD12	2.24	0.66
8:H:24:GLU:OE1	8:H:274:ARG:NH1	2.29	0.66
13:M:306:PRO:HA	13:M:458:LEU:HD13	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:10:VAL:HG12	34:i:81:ILE:HD13	1.78	0.66
4:D:14:TYR:CD1	4:D:19:MET:HE1	2.31	0.66
12:L:149:ILE:HG13	13:M:369:LEU:HD13	1.78	0.65
15:O:171:TYR:CD2	15:O:211:LEU:HD11	2.32	0.65
32:g:48:ASP:OD1	32:g:49:LYS:N	2.29	0.65
15:O:145:ARG:NH2	15:O:147:GLN:OE1	2.30	0.65
13:M:443:PRO:O	13:M:447:LEU:HD23	1.97	0.65
15:O:86:PRO:O	15:O:93:SER:OG	2.14	0.65
24:Y:2:LYS:NZ	50:Y:701:CDL:OA4	2.28	0.65
6:F:99:GLU:OE2	6:F:104:THR:HG22	1.96	0.65
9:I:27:TRP:HB3	9:I:30:LEU:HD12	1.79	0.65
1:A:101:SER:OG	10:J:165:VAL:HG21	1.96	0.64
7:G:107:ILE:HG23	9:I:78:ILE:HD12	1.79	0.64
13:M:285:LEU:HD22	13:M:410:MET:HE2	1.78	0.64
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.27	0.64
14:N:206:ILE:CD1	14:N:346:LEU:HD21	2.26	0.64
37:l:29:MET:HE1	37:l:48:PRO:HB3	1.80	0.64
6:F:118:LEU:HD13	6:F:225:VAL:HG13	1.81	0.63
10:J:157:THR:HG22	11:K:66:PHE:HE1	1.62	0.63
29:d:45:ASP:OD1	29:d:49:ARG:NH1	2.31	0.63
5:E:79:ARG:NH1	5:E:82:GLU:OE2	2.30	0.63
34:i:85:LEU:O	34:i:90:THR:HG23	1.98	0.63
8:H:18:ALA:O	8:H:21:THR:OG1	2.17	0.63
12:L:295:GLN:O	12:L:425:ARG:NH2	2.32	0.63
8:H:24:GLU:OE2	8:H:228:TYR:OH	2.07	0.63
36:k:32:GLN:NE2	36:k:42:ASP:OD1	2.31	0.63
6:F:99:GLU:O	6:F:139:ARG:NH2	2.33	0.62
12:L:599:MET:HE2	14:N:93:MET:HE1	1.81	0.62
7:G:303:VAL:CG1	7:G:603:LEU:HD11	2.30	0.62
10:J:23:LYS:NZ	11:K:18:GLY:O	2.30	0.62
10:J:157:THR:HG22	11:K:66:PHE:CE1	2.35	0.62
13:M:76:MET:CE	13:M:99:LEU:HD22	2.28	0.62
16:P:177:ARG:NH2	54:P:501:NDP:O2N	2.32	0.62
10:J:157:THR:HG21	11:K:62:ILE:HD12	1.80	0.62
1:A:68:GLU:HG3	1:A:98:LEU:HD13	1.81	0.62
8:H:145:THR:HG22	8:H:149:ILE:HD12	1.82	0.62
34:i:35:PRO:O	34:i:37:GLN:NE2	2.32	0.62
8:H:311:THR:HB	25:Z:51:MET:HE2	1.81	0.61
23:X:48:GLU:OE2	23:X:134:ARG:NH2	2.33	0.61
23:X:81:PHE:HD2	26:a:66:LEU:HD11	1.64	0.61
17:Q:18:ASP:OD2	17:Q:20:THR:OG1	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:53:PHE:CE2	11:K:56:ALA:HB2	2.36	0.61
14:N:265:MET:HE3	14:N:343:LEU:CD2	2.29	0.61
7:G:217:ALA:HB2	7:G:248:MET:HE2	1.81	0.61
12:L:237:MET:HE3	12:L:248:HIS:CE1	2.35	0.61
13:M:87:GLU:O	13:M:92:LYS:NZ	2.33	0.61
1:A:33:LYS:NZ	8:H:59:GLU:OE2	2.26	0.61
8:H:195:ARG:HD3	8:H:231:ILE:HD11	1.82	0.61
13:M:66:LEU:HD11	13:M:111:THR:HG23	1.83	0.61
13:M:1:FME:HE3	13:M:111:THR:HG21	1.83	0.61
23:X:63:ASN:OD1	25:Z:81:ARG:NH2	2.33	0.61
5:E:16:ASN:OD1	5:E:19:THR:OG1	2.06	0.60
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.36	0.60
42:q:52:ASN:O	43:r:28:GLN:NE2	2.35	0.60
13:M:207:MET:O	13:M:236:LEU:HD22	2.00	0.60
11:K:43:MET:SD	14:N:72:MET:HE1	2.40	0.60
1:A:105:GLU:HA	10:J:169:MET:HE1	1.83	0.60
12:L:387:THR:HG23	12:L:465:GLY:N	2.17	0.60
14:N:238:PRO:O	14:N:241:THR:OG1	2.20	0.60
14:N:40:ILE:HD12	14:N:43:ILE:HD11	1.84	0.60
15:O:311:ASP:OD1	15:O:312:VAL:HG13	2.02	0.59
25:Z:94:GLU:OE2	25:Z:106:VAL:HG13	2.02	0.59
4:D:193:TYR:OH	4:D:201:GLN:O	2.14	0.59
40:o:41:THR:OG1	40:o:44:GLU:OE1	2.08	0.59
24:Y:89:TYR:O	24:Y:93:GLY:N	2.35	0.59
56:U:101:EHZ:O4	39:n:12:GLN:NE2	2.35	0.59
7:G:444:GLN:NE2	7:G:480:SER:O	2.35	0.59
12:L:467:ILE:O	12:L:471:ASN:ND2	2.35	0.59
14:N:206:ILE:HD12	14:N:346:LEU:HD21	1.83	0.59
12:L:135:ASN:ND2	12:L:199:GLN:OE1	2.34	0.59
15:O:48:LEU:HD22	15:O:121:GLY:HA3	1.85	0.59
6:F:103:GLY:O	6:F:333:ALA:HB1	2.02	0.59
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.33	0.59
23:X:134:ARG:O	27:b:57:ARG:NH2	2.36	0.59
2:B:69:MET:HE3	2:B:74:VAL:HG12	1.84	0.59
12:L:5:SER:O	12:L:8:SER:OG	2.13	0.59
16:P:92:ILE:HD11	16:P:218:ILE:HD11	1.83	0.59
33:h:87:TYR:OH	41:p:86:GLU:OE1	2.17	0.59
3:C:154:ASP:OD1	3:C:155:TYR:N	2.36	0.59
14:N:317:PHE:HZ	15:O:106:LEU:HD21	1.68	0.59
4:D:291:GLY:O	4:D:296:ARG:NH1	2.35	0.58
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:53:SER:OG	13:M:54:LEU:N	2.35	0.58
20:U:52:MET:HE1	39:n:23:LEU:HB3	1.85	0.58
6:F:367:GLU:OE1	7:G:100:ASN:ND2	2.37	0.58
25:Z:95:ALA:HB2	25:Z:106:VAL:HG11	1.84	0.58
7:G:107:ILE:CG2	9:I:78:ILE:HD12	2.34	0.58
16:P:237:LEU:HG	16:P:340:ILE:HD11	1.86	0.58
3:C:183:VAL:O	22:W:101:THR:OG1	2.15	0.58
5:E:53:LEU:HD13	44:s:52:LEU:HD13	1.84	0.58
12:L:387:THR:HG23	12:L:465:GLY:H	1.67	0.58
14:N:276:ILE:O	14:N:280:THR:OG1	2.14	0.58
40:o:103:ARG:NH2	40:o:107:LEU:HD11	2.19	0.58
7:G:450:MET:SD	7:G:452:ILE:HD11	2.44	0.57
1:A:58:VAL:HG11	8:H:286:MET:HE3	1.85	0.57
5:E:7:PHE:HB3	7:G:175:THR:HG22	1.84	0.57
32:g:67:SER:OG	33:h:32:THR:OG1	2.12	0.57
15:O:308:TYR:OH	15:O:320:LYS:O	2.15	0.57
7:G:372:GLU:OE1	7:G:397:LYS:NZ	2.27	0.57
13:M:82:HIS:ND1	13:M:335:GLU:OE1	2.37	0.57
13:M:22:MET:CE	32:g:53:VAL:HG22	2.34	0.57
37:l:15:LYS:N	37:l:19:GLU:OE2	2.37	0.57
1:A:95:ILE:HG21	8:H:302:MET:HG3	1.86	0.57
19:S:64:LEU:HB2	19:S:78:LEU:HD11	1.85	0.57
5:E:85:THR:HG21	7:G:175:THR:HG23	1.85	0.57
6:F:385:ARG:NH2	43:r:48:LEU:HD11	2.20	0.57
12:L:203:MET:HG2	41:p:109:LEU:HD11	1.87	0.57
34:i:77:PRO:O	34:i:81:ILE:HD12	2.05	0.57
39:n:65:GLU:N	39:n:65:GLU:OE1	2.38	0.57
6:F:384:ALA:HB3	6:F:430:MET:HE3	1.87	0.56
7:G:230:VAL:HG23	7:G:322:LEU:HD22	1.87	0.56
13:M:269:MET:HE1	13:M:296:LEU:HD23	1.88	0.56
14:N:265:MET:HE2	14:N:340:THR:CG2	2.35	0.56
17:Q:12:THR:HG23	22:W:15:THR:HB	1.88	0.56
40:o:64:ARG:NH2	40:o:85:ASP:OD2	2.38	0.56
9:I:7:LEU:HD23	9:I:7:LEU:O	2.06	0.56
5:E:201:SER:OG	6:F:20:ARG:NE	2.38	0.56
13:M:22:MET:HE2	32:g:53:VAL:HG22	1.87	0.56
7:G:26:VAL:HG22	7:G:73:VAL:HG12	1.87	0.56
7:G:303:VAL:HG12	7:G:603:LEU:HD11	1.87	0.56
12:L:559:GLU:HG2	13:M:214:LEU:HD23	1.88	0.56
27:b:73:GLN:N	27:b:73:GLN:OE1	2.39	0.56
2:B:125:TYR:HB2	9:I:117:ILE:CG2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:228:MET:HA	4:D:228:MET:HE2	1.88	0.55
14:N:337:LEU:O	14:N:340:THR:OG1	2.18	0.55
8:H:9:LEU:HD12	26:a:19:PRO:HB3	1.88	0.55
12:L:370:THR:OG1	12:L:431:LEU:HD13	2.06	0.55
12:L:508:THR:O	39:n:35:LYS:NZ	2.34	0.55
4:D:342:MET:HE2	7:G:101:HIS:HD2	1.72	0.55
15:O:310:GLU:OE2	15:O:317:ILE:HD12	2.06	0.55
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.40	0.55
12:L:90:ILE:HD11	12:L:133:THR:HG21	1.88	0.55
17:Q:21:THR:HG22	22:W:82:LEU:HD21	1.89	0.55
12:L:195:THR:HG21	12:L:200:GLN:HB3	1.88	0.55
7:G:624:GLU:HG3	7:G:631:VAL:HG21	1.88	0.55
37:l:100:LEU:HD11	37:l:104:HIS:NE2	2.22	0.55
7:G:624:GLU:CG	7:G:631:VAL:HG21	2.36	0.55
8:H:302:MET:HE1	27:b:25:ALA:HB1	1.89	0.55
14:N:44:MET:HE3	14:N:130:LEU:HD13	1.88	0.55
39:n:61:GLN:NE2	39:n:65:GLU:OE2	2.40	0.55
39:n:169:ILE:O	39:n:172:ARG:NH1	2.40	0.55
7:G:365:ASN:N	7:G:491:ASN:OD1	2.40	0.54
14:N:173:THR:O	14:N:227:THR:OG1	2.21	0.54
34:i:102:ARG:HH21	40:o:66:LEU:HD13	1.72	0.54
12:L:396:ILE:HG21	12:L:490:ALA:HB2	1.90	0.54
15:O:83:TYR:OH	52:O:401:GTP:O2'	2.11	0.54
15:O:135:LEU:HD22	15:O:152:TYR:CG	2.42	0.54
7:G:46:LEU:O	17:Q:116:LYS:NZ	2.39	0.54
7:G:171:ASP:O	7:G:185:THR:HG22	2.07	0.54
13:M:50:LEU:HD23	13:M:52:PHE:CZ	2.43	0.54
22:W:96:VAL:HG12	22:W:96:VAL:O	2.07	0.54
2:B:61:HIS:ND1	4:D:175:GLU:OE2	2.39	0.54
4:D:226:GLU:OE1	25:Z:23:ARG:NE	2.41	0.54
20:T:18:VAL:HB	20:T:54:MET:HE1	1.89	0.54
8:H:105:MET:HE3	8:H:162:LEU:HD11	1.90	0.54
10:J:10:SER:HA	10:J:43:ILE:HD11	1.88	0.54
10:J:47:PHE:CD2	11:K:46:LEU:HD22	2.42	0.54
10:J:74:MET:HE1	11:K:79:VAL:HG22	1.89	0.54
14:N:170:LEU:HD11	14:N:288:LEU:CD2	2.37	0.54
12:L:489:THR:O	12:L:493:VAL:HG12	2.08	0.54
17:Q:12:THR:HG22	17:Q:14:ASP:OD1	2.08	0.54
37:l:126:GLN:O	37:l:128:VAL:N	2.40	0.54
25:Z:56:GLU:OE1	25:Z:59:ARG:NH2	2.41	0.53
12:L:217:ALA:O	12:L:221:THR:OG1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:551:SER:O	12:L:556:ILE:HD12	2.08	0.53
13:M:42:MET:HE1	13:M:453:ILE:HB	1.90	0.53
23:X:13:LYS:O	23:X:60:LYS:NZ	2.41	0.53
28:c:25:VAL:HG12	28:c:29:ILE:HD12	1.90	0.53
7:G:477:ILE:HG22	7:G:477:ILE:O	2.09	0.53
9:I:75:GLU:O	9:I:105:ARG:NH1	2.41	0.53
13:M:450:ASN:OD1	13:M:452:LYS:NZ	2.41	0.53
37:l:42:THR:O	37:l:42:THR:HG22	2.08	0.53
4:D:128:ILE:HD13	4:D:330:VAL:HG11	1.89	0.53
1:A:53:MET:HE1	10:J:69:GLY:HA3	1.89	0.53
2:B:168:LYS:NZ	45:B:203:PC1:O12	2.41	0.53
11:K:53:PHE:CE1	30:e:20:GLN:HA	2.44	0.53
12:L:67:HIS:HE2	12:L:70:THR:HG1	1.53	0.53
13:M:76:MET:HE2	13:M:99:LEU:HD22	1.89	0.53
22:W:21:PHE:CE2	22:W:84:ILE:HD11	2.44	0.53
37:l:5:THR:HG22	37:l:6:LYS:N	2.20	0.53
6:F:364:PRO:HB2	6:F:403:THR:HG22	1.91	0.53
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.91	0.53
15:O:15:THR:HG23	15:O:253:ASP:OD1	2.09	0.53
20:U:17:TYR:OH	36:k:21:TRP:NE1	2.33	0.53
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.43	0.53
14:N:298:TYR:HD1	14:N:302:LEU:HD12	1.74	0.53
39:n:94:GLU:CD	39:n:97:LYS:HZ2	2.13	0.53
1:A:58:VAL:HG11	8:H:286:MET:CE	2.39	0.52
4:D:335:ARG:NH2	9:I:129:ASP:OD1	2.42	0.52
9:I:172:ASP:OD2	9:I:176:ARG:NE	2.38	0.52
12:L:71:ILE:HG22	12:L:71:ILE:O	2.09	0.52
12:L:554:ASP:OD1	12:L:558:LEU:HD12	2.09	0.52
14:N:70:LEU:HD12	14:N:98:MET:HG3	1.90	0.52
12:L:42:TYR:OH	34:i:66:HIS:ND1	2.36	0.52
12:L:128:MET:HE2	12:L:147:VAL:HG11	1.92	0.52
12:L:127:THR:OG1	12:L:147:VAL:HG12	2.08	0.52
34:i:17:LEU:HD11	39:n:162:LEU:HD22	1.92	0.52
34:i:64:TYR:O	34:i:67:SER:OG	2.18	0.52
5:E:181:ILE:HG23	5:E:181:ILE:O	2.09	0.52
7:G:364:LEU:HD12	7:G:491:ASN:HB3	1.91	0.52
4:D:228:MET:HE1	9:I:33:GLY:O	2.09	0.52
34:i:89:VAL:O	34:i:95:THR:OG1	2.25	0.52
5:E:105:THR:HG22	5:E:106:THR:N	2.24	0.52
11:K:43:MET:HE1	14:N:72:MET:HE1	1.92	0.52
12:L:566:ILE:O	12:L:570:GLN:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:170:LEU:O	14:N:295:ARG:NH1	2.33	0.52
21:V:34:LEU:HD23	21:V:37:ILE:HD12	1.92	0.52
13:M:114:GLU:CD	13:M:116:ILE:HG22	2.35	0.51
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.40	0.51
20:U:25:ILE:HG21	20:U:30:LEU:HD13	1.91	0.51
40:o:75:ASN:HB2	41:p:25:LEU:HD12	1.92	0.51
7:G:273:GLY:O	7:G:549:HIS:NE2	2.40	0.51
12:L:90:ILE:HD11	12:L:133:THR:CG2	2.41	0.51
13:M:216:LEU:HB3	13:M:217:PRO:HD3	1.93	0.51
39:n:56:MET:SD	39:n:56:MET:N	2.84	0.51
6:F:30:ASP:O	6:F:39:ARG:NH1	2.42	0.51
12:L:286:LEU:HD22	12:L:411:MET:SD	2.51	0.51
20:U:22:TYR:CE2	20:U:50:ILE:HD11	2.45	0.51
14:N:242:VAL:HG11	46:N:902:3PE:H332	1.92	0.51
15:O:65:ASP:OD2	15:O:67:LYS:NZ	2.43	0.51
3:C:8:ARG:O	4:D:129:ARG:NH2	2.44	0.51
11:K:59:MET:HE2	14:N:84:TRP:HH2	1.75	0.51
12:L:111:ASP:OD1	39:n:96:TYR:OH	2.23	0.51
4:D:138:ARG:O	4:D:142:GLY:N	2.44	0.51
10:J:170:GLU:OE2	10:J:173:ARG:NH1	2.44	0.51
3:C:149:ARG:HA	22:W:88:MET:HE2	1.93	0.51
7:G:222:THR:O	7:G:224:LYS:NZ	2.43	0.51
13:M:14:LEU:O	13:M:18:SER:OG	2.24	0.51
13:M:204:MET:HE2	13:M:243:MET:SD	2.51	0.51
20:T:16:LEU:HG	20:T:30:LEU:HD22	1.93	0.51
12:L:380:LEU:HD23	12:L:380:LEU:O	2.11	0.51
7:G:333:ASP:OD2	7:G:613:TYR:OH	2.25	0.50
4:D:104:ASP:OD1	4:D:115:GLU:OE2	2.29	0.50
7:G:551:ASP:OD2	7:G:679:ARG:NH2	2.43	0.50
12:L:381:THR:HG21	12:L:498:PHE:CZ	2.47	0.50
14:N:272:LYS:HB3	24:Y:140:VAL:HG21	1.94	0.50
15:O:188:ASN:H	15:O:192:MET:HE3	1.75	0.50
4:D:109:VAL:O	4:D:109:VAL:HG12	2.11	0.50
4:D:223:ASP:OD1	4:D:305:ARG:NH2	2.43	0.50
20:U:61:GLU:OE1	39:n:84:SER:OG	2.16	0.50
40:o:51:VAL:O	40:o:54:GLN:N	2.41	0.50
4:D:221:ARG:NH1	4:D:224:GLU:OE2	2.39	0.50
12:L:479:GLN:NE2	12:L:481:THR:O	2.42	0.50
4:D:296:ARG:HH21	4:D:420:THR:HG21	1.76	0.50
12:L:599:MET:HE3	14:N:96:MET:HE1	1.94	0.50
22:W:110:THR:O	22:W:110:THR:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:k:42:ASP:OD1	36:k:42:ASP:N	2.44	0.50
50:q:201:CDL:O1	43:r:2:SER:O	2.30	0.50
1:A:73:LEU:HD12	10:J:55:MET:HE1	1.94	0.50
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.93	0.50
32:g:85:MET:O	32:g:85:MET:HG3	2.12	0.50
42:q:65:THR:HG21	42:q:68:MET:HB2	1.93	0.50
4:D:44:VAL:O	4:D:44:VAL:HG13	2.12	0.49
13:M:207:MET:SD	13:M:240:GLY:N	2.85	0.49
20:T:76:ILE:HG22	20:T:80:ILE:HD11	1.93	0.49
6:F:306:LEU:HD23	6:F:347:ILE:HD11	1.95	0.49
7:G:196:SER:OG	7:G:265:ASP:OD1	2.30	0.49
7:G:200:ILE:HD13	7:G:210:SER:HB3	1.94	0.49
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.93	0.49
11:K:1:FME:SD	11:K:9:MET:HE1	2.52	0.49
22:W:89:GLU:OE2	22:W:106:PHE:CZ	2.65	0.49
35:j:7:ILE:HG22	35:j:7:ILE:O	2.11	0.49
9:I:29:GLU:OE1	9:I:29:GLU:N	2.43	0.49
10:J:132:ASP:OD1	10:J:133:SER:N	2.45	0.49
11:K:82:SER:O	11:K:86:GLY:N	2.40	0.49
3:C:171:TYR:C	3:C:188:VAL:HG23	2.38	0.49
4:D:43:LEU:O	4:D:45:SER:N	2.46	0.49
7:G:366:THR:C	7:G:367:THR:HG1	2.11	0.49
14:N:265:MET:HE2	14:N:340:THR:HG22	1.94	0.49
14:N:316:GLN:NE2	15:O:60:ASP:OD1	2.42	0.49
15:O:226:TRP:CE2	15:O:227:GLU:HG3	2.48	0.49
25:Z:62:ILE:HG22	25:Z:66:GLU:OE1	2.12	0.49
6:F:99:GLU:OE2	6:F:104:THR:CG2	2.60	0.49
8:H:208:VAL:O	8:H:208:VAL:HG12	2.12	0.49
12:L:87:MET:HA	12:L:87:MET:HE2	1.95	0.49
16:P:260:HIS:NE2	16:P:285:GLU:OE2	2.36	0.49
15:O:126:ARG:NH1	52:O:401:GTP:O2A	2.45	0.49
15:O:188:ASN:N	15:O:192:MET:HE3	2.28	0.49
5:E:55:GLN:O	5:E:59:GLY:N	2.41	0.49
7:G:334:LEU:HD21	7:G:603:LEU:HD22	1.95	0.49
12:L:290:MET:HE1	12:L:522:PHE:CE2	2.48	0.49
8:H:306:SER:OG	27:b:28:ALA:O	2.30	0.48
19:S:30:GLN:O	19:S:30:GLN:NE2	2.41	0.48
2:B:91:THR:HA	2:B:119:CYS:HB3	1.94	0.48
5:E:200:THR:HG22	5:E:200:THR:O	2.12	0.48
8:H:89:LEU:CD2	8:H:105:MET:HE1	2.43	0.48
12:L:35:TYR:OH	34:i:73:HIS:NE2	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:478:ARG:NH1	7:G:487:TRP:O	2.46	0.48
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.48
10:J:167:VAL:HG22	14:N:42:PRO:HG3	1.95	0.48
32:g:93:ALA:O	32:g:97:VAL:HG23	2.12	0.48
9:I:19:ASP:OD1	25:Z:32:GLY:N	2.40	0.48
23:X:127:VAL:HG13	27:b:54:VAL:O	2.12	0.48
4:D:343:GLU:OE2	4:D:343:GLU:N	2.45	0.48
7:G:254:MET:HA	7:G:260:GLU:O	2.14	0.48
7:G:260:GLU:OE2	7:G:397:LYS:HE2	2.14	0.48
8:H:301:CYS:O	8:H:305:VAL:HG23	2.13	0.48
12:L:13:LEU:CD2	34:i:81:ILE:HD11	2.41	0.48
29:d:90:MET:HE1	33:h:107:GLU:HB2	1.96	0.48
43:r:3:ALA:O	43:r:8:GLN:NE2	2.45	0.48
7:G:601:ARG:NE	7:G:613:TYR:O	2.46	0.48
30:e:57:ILE:HD12	30:e:57:ILE:H	1.79	0.48
12:L:49:ILE:HB	12:L:50:PRO:HD3	1.95	0.48
12:L:355:ASP:OD2	12:L:357:ARG:NH2	2.42	0.48
46:c:301:3PE:H3G1	29:d:34:VAL:HG13	1.94	0.48
9:I:27:TRP:NE1	46:I:201:3PE:O22	2.47	0.48
12:L:599:MET:CE	14:N:93:MET:HE1	2.42	0.48
13:M:217:PRO:O	13:M:221:VAL:HG23	2.13	0.48
6:F:35:GLY:O	6:F:38:SER:OG	2.24	0.47
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.94	0.47
13:M:264:LEU:O	13:M:268:GLY:N	2.47	0.47
20:U:87:TYR:OH	34:i:26:GLU:OE1	2.29	0.47
4:D:125:LEU:HD12	4:D:378:LEU:HD23	1.97	0.47
8:H:187:ILE:HD12	46:I:201:3PE:H262	1.95	0.47
16:P:105:ASP:OD1	16:P:105:ASP:C	2.56	0.47
17:Q:83:VAL:O	17:Q:83:VAL:HG23	2.14	0.47
21:V:8:THR:OG1	21:V:13:LEU:O	2.27	0.47
16:P:319:ARG:NH1	16:P:327:LEU:O	2.47	0.47
20:T:16:LEU:HD23	20:T:16:LEU:O	2.13	0.47
20:T:76:ILE:HG22	20:T:80:ILE:CD1	2.44	0.47
13:M:193:VAL:HG22	13:M:253:MET:HE1	1.95	0.47
12:L:264:TYR:N	12:L:265:PRO:CD	2.77	0.47
14:N:207:ILE:HD13	14:N:262:PRO:HD3	1.96	0.47
2:B:69:MET:HE1	2:B:76:PHE:CD2	2.49	0.47
4:D:123:GLU:OE1	4:D:138:ARG:NH2	2.39	0.47
33:h:141:PRO:O	33:h:143:ASN:N	2.43	0.47
34:i:59:VAL:HG12	34:i:59:VAL:O	2.14	0.47
2:B:68:ASP:OD2	8:H:34:ARG:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:MET:HE1	2:B:76:PHE:CE2	2.50	0.47
4:D:66:MET:HE1	4:D:411:LEU:CD1	2.44	0.47
4:D:73:VAL:HG21	4:D:414:VAL:HG21	1.97	0.47
4:D:148:LEU:HD23	4:D:174:ARG:HG2	1.97	0.47
8:H:168:THR:HG23	25:Z:50:MET:HE1	1.97	0.47
8:H:310:LEU:HD12	8:H:311:THR:HG23	1.97	0.47
12:L:423:SER:O	12:L:427:ILE:HD12	2.15	0.47
13:M:20:ASN:OD1	13:M:89:LEU:HD22	2.13	0.47
13:M:324:SER:HG	13:M:440:HIS:HE2	1.62	0.47
14:N:270:MET:CE	14:N:278:LEU:HD23	2.45	0.47
31:f:53:GLU:OE2	31:f:53:GLU:N	2.47	0.47
8:H:20:LEU:HA	26:a:12:MET:CE	2.45	0.47
14:N:313:MET:HG2	15:O:270:LEU:HD13	1.96	0.47
29:d:5:ARG:CZ	29:d:85:VAL:HG13	2.45	0.47
29:d:90:MET:HE2	33:h:107:GLU:HA	1.96	0.47
5:E:143:GLU:O	5:E:144:CYS:C	2.57	0.47
16:P:220:ASP:O	16:P:224:ARG:NH1	2.48	0.47
40:o:14:VAL:O	40:o:14:VAL:HG22	2.15	0.47
6:F:142:PHE:HB3	6:F:145:GLU:HB2	1.97	0.47
8:H:120:GLY:HA3	8:H:132:ALA:HB2	1.97	0.47
12:L:254:VAL:HG23	12:L:254:VAL:O	2.15	0.47
12:L:183:ILE:HG21	13:M:382:VAL:HG11	1.97	0.46
16:P:258:LEU:HD23	16:P:263:TYR:CD1	2.50	0.46
18:R:53:GLY:O	18:R:54:SER:OG	2.24	0.46
20:T:73:PRO:O	20:T:77:VAL:HG23	2.15	0.46
3:C:58:ILE:HB	3:C:59:PRO:HD3	1.96	0.46
12:L:82:MET:SD	12:L:87:MET:HE3	2.55	0.46
12:L:502:LEU:HD13	36:k:62:PHE:CD2	2.50	0.46
8:H:105:MET:HE3	8:H:162:LEU:CD1	2.45	0.46
12:L:547:LYS:O	12:L:551:SER:OG	2.33	0.46
4:D:202:ASP:OD1	4:D:203:LEU:N	2.48	0.46
5:E:106:THR:HB	5:E:107:PRO:HD3	1.96	0.46
6:F:362:CYS:HB3	6:F:404:ILE:HD12	1.97	0.46
13:M:212:LEU:HD22	51:M:602:LMT:H123	1.98	0.46
46:M:603:3PE:N	46:N:902:3PE:O12	2.34	0.46
6:F:302:SER:HB2	6:F:350:LEU:HD22	1.98	0.46
6:F:347:ILE:HG13	6:F:418:LEU:HD13	1.97	0.46
7:G:441:GLN:O	7:G:445:GLU:OE1	2.33	0.46
46:I:201:3PE:H3C1	27:b:24:ILE:HD11	1.96	0.46
12:L:245:ALA:O	12:L:249:SER:OG	2.29	0.46
42:q:26:VAL:HG12	42:q:32:ASP:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:230:HIS:N	12:L:231:PRO:CD	2.79	0.46
12:L:491:LEU:HD12	12:L:491:LEU:O	2.15	0.46
13:M:165:ILE:HG21	14:N:268:GLN:HA	1.96	0.46
16:P:12:GLY:N	16:P:15:SER:OG	2.46	0.46
23:X:161:ARG:HH11	23:X:161:ARG:HG2	1.81	0.46
5:E:34:ILE:HD11	44:s:52:LEU:HD22	1.98	0.46
8:H:139:THR:HG21	10:J:65:MET:SD	2.56	0.46
32:g:95:ARG:HG2	32:g:95:ARG:HH11	1.80	0.46
44:s:33:PHE:O	44:s:34:ASP:C	2.59	0.46
2:B:179:ARG:NH1	54:P:501:NDP:O2X	2.49	0.46
11:K:37:MET:SD	14:N:68:MET:HE1	2.56	0.46
4:D:17:ALA:HB1	11:K:98:CYS:SG	2.56	0.46
11:K:5:TYR:HB3	11:K:9:MET:HE2	1.99	0.46
4:D:289:SER:OG	9:I:7:LEU:HD12	2.15	0.45
6:F:385:ARG:O	6:F:430:MET:HE1	2.17	0.45
7:G:351:THR:HG22	7:G:351:THR:O	2.15	0.45
12:L:377:SER:O	12:L:381:THR:HG23	2.15	0.45
12:L:542:LEU:O	13:M:278:ARG:NH1	2.48	0.45
13:M:20:ASN:OD1	13:M:89:LEU:HD13	2.16	0.45
13:M:367:LEU:O	13:M:368:ALA:HB3	2.16	0.45
46:M:603:3PE:O12	46:N:902:3PE:N	2.43	0.45
14:N:265:MET:CE	23:X:166:LEU:HD21	2.44	0.45
12:L:290:MET:HE1	12:L:522:PHE:HE2	1.81	0.45
13:M:278:ARG:NE	37:l:82:ASP:OD2	2.40	0.45
13:M:339:SER:HB3	13:M:344:LEU:HD23	1.98	0.45
36:k:35:LEU:HD21	39:n:41:CYS:SG	2.57	0.45
14:N:343:LEU:C	14:N:343:LEU:HD12	2.40	0.45
44:s:32:PRO:HB2	44:s:34:ASP:OD2	2.17	0.45
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.98	0.45
7:G:36:GLN:NE2	17:Q:47:SER:O	2.46	0.45
7:G:235:GLY:O	7:G:581:GLN:NE2	2.49	0.45
16:P:50:ARG:NH1	54:P:501:NDP:O2X	2.49	0.45
32:g:85:MET:HE1	41:p:93:ARG:HG2	1.99	0.45
1:A:18:VAL:HG21	8:H:76:ILE:HG13	1.97	0.45
12:L:298:ILE:CG2	12:L:347:ILE:HD11	2.47	0.45
13:M:403:THR:HA	13:M:406:TYR:CE1	2.52	0.45
15:O:240:TYR:OH	21:V:21:GLU:OE1	2.35	0.45
23:X:98:ARG:O	23:X:99:CYS:HB3	2.16	0.45
1:A:44:MET:HE3	4:D:48:THR:HG22	1.97	0.45
4:D:335:ARG:NH2	9:I:126:CYS:O	2.38	0.45
7:G:372:GLU:O	7:G:402:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:269:MET:HE1	13:M:296:LEU:CD2	2.46	0.45
14:N:44:MET:CE	14:N:130:LEU:HD13	2.47	0.45
40:o:38:MET:HE1	40:o:57:TYR:C	2.41	0.45
12:L:302:ILE:O	12:L:302:ILE:HG22	2.17	0.45
12:L:401:THR:O	12:L:401:THR:HG23	2.16	0.45
12:L:401:THR:HG21	12:L:479:GLN:HG2	1.98	0.45
14:N:214:THR:HG22	14:N:218:MET:HE2	1.98	0.45
39:n:107:HIS:CE1	39:n:109:SER:HG	2.23	0.45
2:B:152:THR:HG22	4:D:188:ARG:HD3	1.97	0.45
16:P:238:LEU:O	16:P:242:VAL:HG23	2.17	0.45
24:Y:140:VAL:HG23	33:h:111:ARG:NH2	2.32	0.45
31:f:11:TRP:O	31:f:14:VAL:HG22	2.17	0.45
12:L:25:ASN:OD1	33:h:26:ARG:NH2	2.50	0.45
10:J:19:GLY:O	10:J:83:TRP:NE1	2.47	0.45
12:L:230:HIS:N	12:L:231:PRO:HD3	2.32	0.45
2:B:69:MET:HE3	2:B:74:VAL:CG1	2.47	0.44
3:C:195:ARG:NH1	9:I:84:GLU:OE2	2.50	0.44
7:G:281:GLU:OE1	7:G:293:HIS:ND1	2.50	0.44
39:n:107:HIS:HD1	39:n:109:SER:HG	0.55	0.44
3:C:83:ILE:HG22	3:C:85:THR:HG22	1.99	0.44
4:D:412:ALA:HB2	8:H:206:GLU:OE2	2.16	0.44
7:G:374:ALA:O	7:G:404:LEU:HD13	2.17	0.44
7:G:657:LEU:O	7:G:659:ASP:N	2.48	0.44
11:K:37:MET:CE	11:K:67:ALA:HB2	2.41	0.44
20:U:22:TYR:CD2	20:U:50:ILE:HD11	2.53	0.44
23:X:79:GLU:HB3	23:X:80:PRO:HD3	1.99	0.44
6:F:398:GLN:O	6:F:402:HIS:ND1	2.51	0.44
8:H:114:TYR:OH	10:J:65:MET:N	2.50	0.44
13:M:133:ILE:HD11	13:M:231:LEU:HD11	2.00	0.44
34:i:35:PRO:HB2	34:i:36:PRO:HD2	2.00	0.44
5:E:192:SER:OG	5:E:193:CYS:N	2.50	0.44
13:M:328:CYS:HB3	13:M:437:MET:HE1	2.00	0.44
14:N:304:MET:HE3	15:O:286:ALA:HB1	1.99	0.44
16:P:263:TYR:CE2	16:P:284:VAL:HG13	2.52	0.44
25:Z:68:ARG:HG3	26:a:43:TYR:CZ	2.52	0.44
38:m:50:TYR:HA	38:m:59:ILE:HD11	1.98	0.44
1:A:42:ASP:OD1	2:B:102:LYS:NZ	2.49	0.44
6:F:341:THR:HG22	6:F:342:ASP:N	2.33	0.44
10:J:70:TYR:HE2	11:K:79:VAL:HG23	1.83	0.44
13:M:225:ILE:HG23	13:M:226:ALA:N	2.33	0.44
38:m:72:SER:OG	38:m:73:ALA:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:294:TYR:CE2	4:D:298:LEU:HD11	2.53	0.44
8:H:198:PHE:CD1	8:H:285:LEU:HD13	2.53	0.44
13:M:253:MET:HE3	13:M:257:MET:HG3	1.99	0.44
4:D:299:CYS:O	4:D:303:GLU:HG3	2.17	0.44
6:F:93:LEU:O	6:F:134:ALA:HA	2.18	0.44
6:F:419:ILE:HG22	6:F:419:ILE:O	2.16	0.44
8:H:199:ASP:OD2	8:H:199:ASP:N	2.48	0.44
13:M:225:ILE:HD13	13:M:331:ASN:HB2	1.99	0.44
30:e:4:ASP:OD2	30:e:7:LYS:HB2	2.18	0.44
44:s:57:ASP:O	44:s:60:LYS:NZ	2.44	0.44
4:D:155:THR:HB	4:D:167:PHE:HA	2.00	0.44
4:D:228:MET:HE3	9:I:36:MET:HB3	1.99	0.44
12:L:203:MET:HE1	41:p:124:CYS:CB	2.47	0.44
7:G:481:SER:OG	7:G:482:GLY:N	2.51	0.44
35:j:55:ASP:OD1	35:j:57:SER:OG	2.36	0.44
37:l:61:TRP:CZ2	39:n:85:PRO:HD2	2.53	0.44
12:L:361:GLY:N	12:L:431:LEU:O	2.51	0.43
23:X:21:SER:N	26:a:51:ASP:OD1	2.50	0.43
23:X:98:ARG:O	23:X:99:CYS:CB	2.66	0.43
33:h:34:ILE:HB	33:h:35:PRO:HD3	2.00	0.43
39:n:8:TYR:O	39:n:9:LEU:HB2	2.17	0.43
1:A:44:MET:HE1	4:D:65:VAL:HG13	2.00	0.43
2:B:92:LEU:HD13	2:B:100:LEU:HD13	2.00	0.43
8:H:2:PHE:O	8:H:5:ASN:N	2.51	0.43
12:L:381:THR:HG21	12:L:498:PHE:HZ	1.83	0.43
12:L:437:PHE:HE2	12:L:441:VAL:HG22	1.83	0.43
16:P:47:VAL:HG12	16:P:47:VAL:O	2.18	0.43
1:A:96:ILE:O	1:A:100:VAL:HG23	2.18	0.43
3:C:121:VAL:N	3:C:122:PRO:CD	2.81	0.43
40:o:103:ARG:CZ	40:o:107:LEU:HD11	2.49	0.43
6:F:213:VAL:O	6:F:213:VAL:HG12	2.17	0.43
12:L:237:MET:HE3	12:L:248:HIS:NE2	2.33	0.43
12:L:562:LEU:CB	12:L:563:PRO:CD	2.96	0.43
13:M:114:GLU:OE1	23:X:168:PHE:HB3	2.18	0.43
13:M:418:LYS:NZ	39:n:94:GLU:OE1	2.49	0.43
6:F:246:GLY:N	6:F:271:GLU:OE2	2.47	0.43
7:G:350:PRO:HG2	7:G:467:LEU:HD22	2.01	0.43
8:H:89:LEU:HD23	8:H:105:MET:HE1	2.01	0.43
12:L:7:LEU:HA	12:L:10:VAL:HG22	2.01	0.43
12:L:128:MET:HE2	12:L:128:MET:HA	1.99	0.43
12:L:282:ALA:O	12:L:285:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:331:THR:HB	12:L:387:THR:HG22	1.99	0.43
12:L:407:TRP:CZ2	12:L:411:MET:HE3	2.53	0.43
13:M:47:ASP:OD1	13:M:48:ASN:N	2.49	0.43
13:M:296:LEU:CD2	13:M:396:MET:HE1	2.48	0.43
14:N:30:TRP:CZ2	14:N:34:GLU:OE1	2.71	0.43
16:P:263:TYR:CE2	16:P:284:VAL:HG22	2.53	0.43
31:f:16:VAL:HB	31:f:17:PRO:HD3	2.00	0.43
12:L:13:LEU:O	12:L:16:THR:OG1	2.26	0.43
12:L:578:THR:O	12:L:580:GLN:N	2.47	0.43
20:U:72:CYS:HB2	20:U:75:GLU:HG3	2.00	0.43
12:L:293:LEU:HD22	12:L:421:ILE:HG21	2.01	0.43
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.53	0.43
38:m:11:SER:O	38:m:11:SER:OG	2.32	0.43
38:m:39:ARG:NH1	39:n:151:GLU:OE1	2.46	0.43
45:B:203:PC1:H133	42:q:29:ARG:O	2.18	0.43
3:C:78:LEU:HD13	3:C:94:TYR:CD2	2.53	0.43
6:F:327:THR:OG1	6:F:328:GLY:N	2.50	0.43
15:O:287:HIS:HB2	32:g:28:GLU:OE2	2.19	0.43
16:P:133:SER:O	54:P:501:NDP:H6N	2.19	0.43
21:V:71:LEU:HD13	21:V:79:VAL:HG11	2.00	0.43
2:B:45:LEU:O	2:B:74:VAL:HA	2.18	0.43
10:J:28:TYR:CE2	10:J:82:ILE:HG22	2.54	0.43
11:K:20:LEU:HD12	12:L:592:LEU:HD13	2.01	0.43
14:N:242:VAL:HG11	46:N:902:3PE:C33	2.48	0.43
14:N:245:LEU:HD22	14:N:301:THR:HG21	2.00	0.43
26:a:37:ARG:HG2	26:a:48:MET:HE2	2.01	0.43
2:B:101:ARG:NH1	2:B:139:ILE:O	2.46	0.43
6:F:349:ARG:O	6:F:349:ARG:NH2	2.51	0.43
6:F:403:THR:HB	47:F:502:SF4:S4	2.59	0.43
6:F:406:ALA:HB3	49:F:501:FMN:HM82	2.01	0.43
7:G:524:LEU:O	7:G:526:GLY:N	2.51	0.43
12:L:427:ILE:HD12	12:L:427:ILE:H	1.84	0.43
14:N:146:PHE:N	14:N:147:PRO:CD	2.82	0.43
15:O:179:VAL:O	15:O:182:ARG:N	2.51	0.43
40:o:74:PRO:O	40:o:76:PHE:N	2.52	0.43
41:p:81:VAL:O	41:p:85:PHE:N	2.45	0.43
1:A:73:LEU:N	1:A:74:PRO:CD	2.82	0.42
4:D:349:PHE:CE2	9:I:82:LEU:HD11	2.53	0.42
5:E:104:THR:HG22	5:E:104:THR:O	2.19	0.42
6:F:365:CYS:HB3	47:F:502:SF4:S3	2.59	0.42
8:H:87:ILE:N	8:H:88:PRO:CD	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:57:PHE:O	13:M:57:PHE:CG	2.72	0.42
23:X:48:GLU:OE1	27:b:57:ARG:NE	2.51	0.42
23:X:81:PHE:CD2	26:a:66:LEU:HD11	2.51	0.42
8:H:233:MET:HE1	8:H:234:MET:HE3	2.01	0.42
8:H:264:LEU:HD21	26:a:16:LEU:HD12	2.00	0.42
13:M:214:LEU:N	13:M:214:LEU:HD12	2.34	0.42
13:M:379:LEU:O	13:M:383:MET:HG2	2.19	0.42
34:i:90:THR:HG22	34:i:96:ILE:HD12	2.01	0.42
34:i:103:ILE:HD13	41:p:17:PRO:HG3	2.01	0.42
35:j:69:ASP:OD1	40:o:113:ARG:NH2	2.52	0.42
4:D:342:MET:CE	7:G:101:HIS:HD2	2.32	0.42
5:E:56:ARG:NH2	5:E:158:ASP:OD1	2.53	0.42
6:F:131:ALA:O	6:F:171:TYR:OH	2.20	0.42
7:G:652:VAL:HG12	7:G:653:ASN:N	2.34	0.42
10:J:126:VAL:HG23	10:J:127:ILE:HG23	2.01	0.42
15:O:168:VAL:HG12	15:O:169:VAL:N	2.35	0.42
15:O:297:THR:O	15:O:297:THR:HG22	2.18	0.42
20:U:47:GLN:NE2	20:U:67:ALA:O	2.52	0.42
22:W:79:VAL:O	22:W:83:VAL:HG23	2.19	0.42
24:Y:71:LEU:HG	24:Y:75:ILE:HD12	2.00	0.42
1:A:73:LEU:CD1	10:J:55:MET:HE1	2.49	0.42
4:D:126:LEU:O	4:D:127:ASN:CB	2.67	0.42
4:D:315:LEU:O	25:Z:11:PRO:HG3	2.20	0.42
4:D:371:LYS:HG2	4:D:422:ASP:OD2	2.19	0.42
7:G:151:THR:O	7:G:151:THR:HG22	2.19	0.42
7:G:415:LEU:O	7:G:416:THR:CB	2.68	0.42
8:H:138:GLN:NE2	8:H:194:ASN:OD1	2.51	0.42
11:K:43:MET:CE	14:N:72:MET:HE1	2.49	0.42
15:O:22:SER:O	15:O:22:SER:OG	2.35	0.42
32:g:25:ARG:CG	32:g:26:TRP:N	2.81	0.42
3:C:103:SER:OG	43:r:96:PRO:HB2	2.20	0.42
12:L:529:PHE:HB3	12:L:530:PRO:HD3	2.01	0.42
16:P:258:LEU:CD2	16:P:263:TYR:HB2	2.50	0.42
1:A:53:MET:HE1	10:J:69:GLY:CA	2.48	0.42
7:G:243:ARG:O	7:G:244:THR:OG1	2.32	0.42
15:O:45:LYS:HB2	15:O:235:VAL:HG21	2.00	0.42
21:V:105:GLU:HG2	21:V:106:PRO:HD2	2.01	0.42
35:j:56:PRO:HA	35:j:59:TRP:CE3	2.55	0.42
35:j:65:GLY:HA3	40:o:30:PHE:CE1	2.55	0.42
37:l:135:TYR:OH	40:o:40:ALA:O	2.33	0.42
7:G:303:VAL:HG11	7:G:603:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:142:SER:OG	16:P:285:GLU:OE1	2.24	0.42
39:n:30:CYS:O	39:n:32:HIS:N	2.52	0.42
5:E:23:PHE:HB3	5:E:27:ASN:HB2	2.01	0.42
6:F:426:LEU:O	6:F:430:MET:HG3	2.20	0.42
17:Q:18:ASP:CG	17:Q:20:THR:HG1	2.24	0.42
23:X:44:LEU:HD22	23:X:130:VAL:CG2	2.50	0.42
26:a:14:VAL:O	26:a:14:VAL:HG12	2.19	0.42
39:n:61:GLN:O	39:n:65:GLU:OE1	2.38	0.42
4:D:107:ASP:CG	4:D:371:LYS:HZ3	2.28	0.42
37:l:29:MET:HE1	37:l:48:PRO:CB	2.48	0.42
8:H:49:ILE:O	8:H:53:ILE:HD12	2.20	0.42
12:L:186:MET:HB2	13:M:383:MET:HE1	2.02	0.42
12:L:293:LEU:HD22	12:L:421:ILE:CG2	2.50	0.42
12:L:380:LEU:CD2	12:L:419:THR:HG23	2.50	0.42
15:O:250:ASP:O	15:O:250:ASP:OD2	2.37	0.42
23:X:4:VAL:HG23	25:Z:109:SER:HB2	2.01	0.42
26:a:6:LEU:N	26:a:7:PRO:CD	2.83	0.42
8:H:202:GLU:O	8:H:203:GLY:C	2.63	0.41
13:M:40:LEU:HD22	33:h:79:PHE:HB3	2.02	0.41
16:P:261:PHE:CG	16:P:262:ALA:N	2.88	0.41
29:d:103:GLU:O	29:d:103:GLU:HG3	2.20	0.41
30:e:20:GLN:HG3	30:e:36:GLU:OE1	2.19	0.41
5:E:181:ILE:O	5:E:181:ILE:CG2	2.68	0.41
7:G:230:VAL:CG2	7:G:322:LEU:HD22	2.50	0.41
8:H:70:MET:HE1	8:H:121:TRP:CE3	2.56	0.41
8:H:169:GLN:NE2	8:H:240:ILE:O	2.49	0.41
13:M:369:LEU:HD12	13:M:370:PRO:HD2	2.03	0.41
13:M:422:HIS:HB2	38:m:59:ILE:HD12	2.02	0.41
3:C:92:ILE:O	3:C:108:LYS:HA	2.19	0.41
9:I:80:CYS:O	9:I:81:LYS:HB2	2.19	0.41
14:N:146:PHE:CD1	14:N:147:PRO:HD3	2.56	0.41
14:N:175:LEU:N	14:N:225:THR:O	2.40	0.41
25:Z:30:LEU:HD12	25:Z:30:LEU:N	2.36	0.41
1:A:33:LYS:HG2	8:H:61:LEU:HD13	2.02	0.41
5:E:143:GLU:HG2	6:F:353:PHE:HD1	1.84	0.41
5:E:201:SER:OG	6:F:20:ARG:CZ	2.68	0.41
6:F:82:MET:O	6:F:91:LYS:NZ	2.50	0.41
7:G:103:LEU:O	18:R:86:TYR:OH	2.38	0.41
7:G:382:THR:HB	7:G:454:GLY:HA3	2.02	0.41
10:J:103:MET:HE2	10:J:115:VAL:CG1	2.41	0.41
11:K:59:MET:HB3	11:K:60:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:49:SER:OG	13:M:51:ASN:OD1	2.38	0.41
13:M:123:GLU:OE2	13:M:157:SER:OG	2.37	0.41
13:M:243:MET:O	13:M:247:THR:HG23	2.20	0.41
37:l:39:ASP:O	38:m:80:ARG:NH2	2.54	0.41
7:G:45:ARG:NE	7:G:261:GLU:OE1	2.41	0.41
8:H:11:ILE:HB	8:H:12:PRO:HD3	2.02	0.41
32:g:26:TRP:CD1	32:g:28:GLU:HB2	2.55	0.41
1:A:1:FME:O1	1:A:4:MET:SD	2.78	0.41
4:D:7:ASP:HB2	32:g:26:TRP:CH2	2.55	0.41
6:F:154:ARG:HA	44:s:58:LEU:HD21	2.02	0.41
8:H:142:TYR:C	8:H:142:TYR:CD2	2.99	0.41
8:H:187:ILE:HD12	46:I:201:3PE:C26	2.51	0.41
12:L:594:THR:HG21	14:N:110:PRO:HG2	2.01	0.41
16:P:9:GLY:HA2	17:Q:65:TRP:CZ3	2.56	0.41
17:Q:21:THR:CG2	22:W:82:LEU:HD21	2.49	0.41
32:g:66:PHE:O	32:g:71:VAL:HG23	2.21	0.41
40:o:28:TYR:OH	40:o:110:ARG:NH2	2.54	0.41
41:p:73:ILE:HG23	41:p:155:LEU:HD22	2.03	0.41
2:B:93:THR:OG1	4:D:82:LEU:O	2.31	0.41
7:G:53:ARG:O	7:G:93:VAL:HG21	2.20	0.41
7:G:125:SER:OG	7:G:126:ASP:N	2.54	0.41
9:I:64:GLU:O	9:I:134:GLY:N	2.38	0.41
30:e:20:GLN:CG	30:e:36:GLU:OE1	2.68	0.41
34:i:77:PRO:O	34:i:80:ILE:N	2.52	0.41
37:l:71:LEU:HD11	37:l:81:LEU:CD1	2.44	0.41
38:m:123:THR:HG23	38:m:124:PHE:N	2.35	0.41
1:A:44:MET:CE	4:D:48:THR:HG22	2.50	0.41
6:F:306:LEU:C	6:F:306:LEU:HD12	2.45	0.41
7:G:38:PRO:HB2	7:G:54:MET:HG3	2.03	0.41
8:H:186:PHE:O	8:H:189:THR:OG1	2.32	0.41
12:L:16:THR:O	12:L:19:ILE:N	2.54	0.41
12:L:37:LYS:HD2	12:L:102:GLU:CG	2.51	0.41
13:M:315:LEU:HG	13:M:377:GLY:HA3	2.01	0.41
43:r:29:GLU:OE2	43:r:29:GLU:N	2.47	0.41
3:C:179:GLU:OE2	16:P:37:HIS:NE2	2.53	0.41
6:F:272:MET:O	6:F:273:SER:HB2	2.20	0.41
7:G:213:TYR:O	7:G:213:TYR:CG	2.74	0.41
8:H:170:GLU:OE1	23:X:97:ARG:NH2	2.54	0.41
11:K:16:LEU:HA	11:K:36:MET:HE2	2.02	0.41
12:L:7:LEU:HD12	12:L:49:ILE:HG21	2.02	0.41
12:L:22:MET:HA	12:L:27:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:247:LEU:HD23	12:L:248:HIS:HD2	1.86	0.41
14:N:215:MET:HE1	14:N:247:THR:HB	2.03	0.41
36:k:81:ILE:HG13	36:k:82:GLY:N	2.36	0.41
41:p:27:ASN:O	41:p:30:THR:HG22	2.20	0.41
2:B:96:MET:SD	4:D:82:LEU:HD23	2.61	0.41
5:E:78:MET:HE2	7:G:184:GLY:O	2.21	0.41
13:M:108:MET:CB	13:M:121:LEU:HD13	2.51	0.41
13:M:376:ILE:H	13:M:376:ILE:HD12	1.86	0.41
15:O:75:GLY:O	15:O:76:ASN:HB3	2.21	0.41
19:S:54:ILE:O	19:S:54:ILE:HG22	2.20	0.41
33:h:97:GLU:HA	33:h:97:GLU:OE1	2.20	0.41
4:D:376:VAL:O	4:D:376:VAL:HG23	2.22	0.40
7:G:228:ILE:HG22	7:G:229:ASP:N	2.36	0.40
10:J:43:ILE:HG22	11:K:46:LEU:HD21	2.02	0.40
6:F:322:LEU:HB3	6:F:327:THR:HG23	2.02	0.40
20:T:76:ILE:CG2	20:T:80:ILE:HD11	2.51	0.40
34:i:57:LYS:HD3	34:i:60:ILE:HD11	2.03	0.40
44:s:38:TYR:CE1	44:s:40:ASN:HB3	2.55	0.40
9:I:23:GLN:O	9:I:27:TRP:N	2.54	0.40
13:M:258:ALA:HB1	13:M:302:LEU:HB3	2.03	0.40
13:M:325:MET:HE1	13:M:441:ILE:HB	2.03	0.40
15:O:52:PRO:O	15:O:53:GLU:C	2.64	0.40
16:P:48:PRO:HA	16:P:71:MET:O	2.21	0.40
5:E:165:THR:HB	5:E:166:PRO:HD2	2.02	0.40
6:F:104:THR:OG1	6:F:333:ALA:HB2	2.21	0.40
6:F:207:PRO:HA	6:F:208:PRO:C	2.46	0.40
6:F:306:LEU:HD13	6:F:422:PHE:HE2	1.87	0.40
8:H:102:VAL:HG23	8:H:160:PHE:O	2.21	0.40
9:I:27:TRP:O	9:I:31:ILE:HG12	2.21	0.40
10:J:45:LEU:HD23	10:J:45:LEU:C	2.45	0.40
10:J:124:ASP:OD2	11:K:4:VAL:HB	2.21	0.40
11:K:55:LEU:HD21	30:e:25:PRO:HD3	2.03	0.40
13:M:243:MET:HE2	13:M:301:ILE:HG21	2.04	0.40
38:m:76:TYR:N	38:m:77:PRO:CD	2.84	0.40
39:n:99:PRO:HB2	39:n:101:TRP:CD1	2.56	0.40
7:G:205:VAL:HB	47:G:801:SF4:S2	2.61	0.40
8:H:89:LEU:HD13	8:H:236:ILE:HG21	2.03	0.40
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.03	0.40
10:J:65:MET:HE2	10:J:65:MET:HB3	1.98	0.40
14:N:44:MET:HE1	14:N:59:TYR:CG	2.57	0.40
15:O:279:LEU:HB2	15:O:282:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:145:TYR:CD2	16:P:286:ARG:HD3	2.56	0.40
30:e:7:LYS:N	30:e:7:LYS:CD	2.84	0.40
50:h:1001:CDL:OB4	34:i:88:HIS:NE2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
2	B	153/216 (71%)	145 (95%)	8 (5%)	0	100	100
3	C	205/266 (77%)	199 (97%)	6 (3%)	0	100	100
4	D	427/463 (92%)	397 (93%)	30 (7%)	0	100	100
5	E	211/249 (85%)	192 (91%)	19 (9%)	0	100	100
6	F	429/464 (92%)	410 (96%)	19 (4%)	0	100	100
7	G	686/727 (94%)	642 (94%)	44 (6%)	0	100	100
8	H	316/318 (99%)	293 (93%)	23 (7%)	0	100	100
9	I	174/212 (82%)	165 (95%)	9 (5%)	0	100	100
10	J	172/175 (98%)	160 (93%)	12 (7%)	0	100	100
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	557 (92%)	44 (7%)	3 (0%)	24	57
13	M	457/459 (100%)	443 (97%)	14 (3%)	0	100	100
14	N	345/347 (99%)	333 (96%)	12 (4%)	0	100	100
15	O	318/343 (93%)	300 (94%)	18 (6%)	0	100	100
16	P	339/380 (89%)	318 (94%)	21 (6%)	0	100	100
17	Q	123/175 (70%)	117 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	93/124 (75%)	88 (95%)	5 (5%)	0	100	100
19	S	82/99 (83%)	76 (93%)	6 (7%)	0	100	100
20	T	74/156 (47%)	71 (96%)	3 (4%)	0	100	100
20	U	84/156 (54%)	82 (98%)	1 (1%)	1 (1%)	10	37
21	V	111/116 (96%)	108 (97%)	3 (3%)	0	100	100
22	W	112/128 (88%)	106 (95%)	6 (5%)	0	100	100
23	X	169/172 (98%)	154 (91%)	14 (8%)	1 (1%)	21	52
24	Y	138/141 (98%)	133 (96%)	5 (4%)	0	100	100
25	Z	139/144 (96%)	129 (93%)	10 (7%)	0	100	100
26	a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
27	b	81/84 (96%)	73 (90%)	8 (10%)	0	100	100
28	c	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
29	d	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
30	e	95/106 (90%)	92 (97%)	3 (3%)	0	100	100
31	f	48/57 (84%)	44 (92%)	4 (8%)	0	100	100
32	g	96/154 (62%)	89 (93%)	7 (7%)	0	100	100
33	h	136/189 (72%)	131 (96%)	5 (4%)	0	100	100
34	i	103/127 (81%)	92 (89%)	10 (10%)	1 (1%)	12	41
35	j	62/108 (57%)	59 (95%)	2 (3%)	1 (2%)	7	30
36	k	78/98 (80%)	72 (92%)	5 (6%)	1 (1%)	9	35
37	l	153/186 (82%)	142 (93%)	11 (7%)	0	100	100
38	m	125/129 (97%)	115 (92%)	10 (8%)	0	100	100
39	n	170/179 (95%)	157 (92%)	13 (8%)	0	100	100
40	o	120/137 (88%)	107 (89%)	13 (11%)	0	100	100
41	p	169/176 (96%)	165 (98%)	4 (2%)	0	100	100
42	q	142/145 (98%)	141 (99%)	1 (1%)	0	100	100
43	r	90/113 (80%)	82 (91%)	8 (9%)	0	100	100
44	s	42/109 (38%)	38 (90%)	4 (10%)	0	100	100
All	All	8112/9212 (88%)	7640 (94%)	464 (6%)	8 (0%)	49	78

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	X	99	CYS
12	L	562	LEU
20	U	43	ASP
35	j	8	GLU
12	L	25	ASN
34	i	124	ASP
36	k	17	ASP
12	L	254	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/100 (100%)	100 (100%)	0	100	100
2	B	131/175 (75%)	131 (100%)	0	100	100
3	C	188/228 (82%)	188 (100%)	0	100	100
4	D	370/392 (94%)	370 (100%)	0	100	100
5	E	183/205 (89%)	183 (100%)	0	100	100
6	F	345/368 (94%)	345 (100%)	0	100	100
7	G	578/608 (95%)	578 (100%)	0	100	100
8	H	274/274 (100%)	274 (100%)	0	100	100
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	140/141 (99%)	140 (100%)	0	100	100
11	K	85/85 (100%)	85 (100%)	0	100	100
12	L	533/533 (100%)	533 (100%)	0	100	100
13	M	412/412 (100%)	412 (100%)	0	100	100
14	N	315/315 (100%)	315 (100%)	0	100	100
15	O	283/303 (93%)	283 (100%)	0	100	100
16	P	295/327 (90%)	295 (100%)	0	100	100
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	78/97 (80%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	S	75/82 (92%)	75 (100%)	0	100	100
20	T	70/135 (52%)	69 (99%)	1 (1%)	59	76
20	U	79/135 (58%)	78 (99%)	1 (1%)	61	77
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	107/114 (94%)	107 (100%)	0	100	100
23	X	154/155 (99%)	154 (100%)	0	100	100
24	Y	101/102 (99%)	101 (100%)	0	100	100
25	Z	120/121 (99%)	120 (100%)	0	100	100
26	a	59/59 (100%)	59 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	44/68 (65%)	44 (100%)	0	100	100
29	d	104/105 (99%)	104 (100%)	0	100	100
30	e	88/96 (92%)	88 (100%)	0	100	100
31	f	47/54 (87%)	47 (100%)	0	100	100
32	g	89/131 (68%)	89 (100%)	0	100	100
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	102/120 (85%)	102 (100%)	0	100	100
35	j	59/84 (70%)	59 (100%)	0	100	100
36	k	62/76 (82%)	62 (100%)	0	100	100
37	l	139/159 (87%)	139 (100%)	0	100	100
38	m	113/115 (98%)	113 (100%)	0	100	100
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	110/120 (92%)	110 (100%)	0	100	100
41	p	155/157 (99%)	155 (100%)	0	100	100
42	q	130/131 (99%)	130 (100%)	0	100	100
43	r	84/97 (87%)	84 (100%)	0	100	100
44	s	43/92 (47%)	43 (100%)	0	100	100
All	All	7156/7892 (91%)	7154 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	T	44	SER

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Mol	Chain	Res	Type
20	U	44	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	162	GLN
3	C	160	HIS
3	C	192	GLN
4	D	13	GLN
4	D	46	ASN
4	D	273	GLN
5	E	58	ASN
5	E	150	ASN
5	E	159	ASN
6	F	283	HIS
6	F	421	HIS
6	F	432	GLN
7	G	365	ASN
7	G	401	HIS
7	G	546	GLN
7	G	643	GLN
10	J	120	ASN
12	L	113	ASN
12	L	248	HIS
12	L	295	GLN
12	L	348	HIS
12	L	354	GLN
13	M	251	ASN
13	M	304	GLN
13	M	390	ASN
14	N	91	ASN
14	N	120	GLN
14	N	232	HIS
14	N	235	ASN
14	N	268	GLN
15	O	154	GLN
15	O	180	GLN
16	P	49	HIS
16	P	93	ASN
16	P	131	HIS
17	Q	50	ASN
19	S	75	ASN

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Mol	Chain	Res	Type
22	W	48	HIS
22	W	108	HIS
23	X	162	HIS
25	Z	24	ASN
28	c	9	HIS
29	d	79	GLN
29	d	117	HIS
30	e	69	GLN
31	f	13	HIS
33	h	124	HIS
34	i	12	GLN
36	k	90	GLN
37	l	132	GLN
39	n	77	GLN
40	o	46	ASN
40	o	49	GLN
41	p	77	GLN
43	r	107	GLN
44	s	43	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	H	1	8	8,9,10	0.94	0	8,9,11	1.04	1 (12%)
11	FME	K	1	11	8,9,10	1.01	0	8,9,11	0.81	0
4	2MR	D	85	4	10,12,13	2.48	2 (20%)	5,13,15	1.29	0
24	AYA	Y	1	24	6,7,8	1.29	1 (16%)	6,8,10	1.37	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	A	1	1	8,9,10	1.06	1 (12%)	8,9,11	0.79	0
43	AYA	r	1	43	6,7,8	1.40	1 (16%)	6,8,10	0.88	0
12	FME	L	1	12	8,9,10	1.04	1 (12%)	8,9,11	0.77	0
29	AME	d	1	29	9,10,11	1.55	1 (11%)	9,11,13	1.33	1 (11%)
34	SAC	i	1	34	7,8,9	0.94	0	7,9,11	1.16	1 (14%)
14	FME	N	1	14	8,9,10	0.99	0	8,9,11	0.93	0
10	FME	J	1	10	8,9,10	0.95	0	8,9,11	0.92	0
13	FME	M	1	13	8,9,10	0.98	0	8,9,11	1.03	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	H	1	8	-	3/7/9/11	-
11	FME	K	1	11	-	2/7/9/11	-
4	2MR	D	85	4	-	1/10/13/15	-
24	AYA	Y	1	24	-	0/5/6/8	-
1	FME	A	1	1	-	0/7/9/11	-
43	AYA	r	1	43	-	0/5/6/8	-
12	FME	L	1	12	-	2/7/9/11	-
29	AME	d	1	29	-	7/9/10/12	-
34	SAC	i	1	34	-	2/7/8/10	-
14	FME	N	1	14	-	3/7/9/11	-
10	FME	J	1	10	-	3/7/9/11	-
13	FME	M	1	13	-	0/7/9/11	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.61	1.45	1.33
4	D	85	2MR	CZ-NE	4.92	1.44	1.34
29	d	1	AME	CT1-N	3.60	1.46	1.34
43	r	1	AYA	CA-N	-2.92	1.43	1.46
24	Y	1	AYA	CA-N	-2.60	1.43	1.46
1	A	1	FME	CA-N	-2.33	1.43	1.46
12	L	1	FME	CA-N	-2.19	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	1	AYA	CB-CA-N	3.18	113.27	109.68
29	d	1	AME	CT2-CT1-N	2.40	120.10	116.12
34	i	1	SAC	OG-CB-CA	-2.13	105.27	111.13
8	H	1	FME	C-CA-N	2.06	113.48	109.50

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	85	2MR	O-C-CA-CB
8	H	1	FME	O-C-CA-CB
10	J	1	FME	O1-CN-N-CA
12	L	1	FME	O1-CN-N-CA
14	N	1	FME	O1-CN-N-CA
14	N	1	FME	CB-CA-N-CN
29	d	1	AME	O-C-CA-CB
29	d	1	AME	CB-CA-N-CT1
34	i	1	SAC	C-CA-N-C1A
34	i	1	SAC	CB-CA-N-C1A
12	L	1	FME	CA-CB-CG-SD
29	d	1	AME	CA-CB-CG-SD
8	H	1	FME	C-CA-CB-CG
10	J	1	FME	N-CA-CB-CG
14	N	1	FME	N-CA-CB-CG
29	d	1	AME	N-CA-CB-CG
11	K	1	FME	CB-CG-SD-CE
29	d	1	AME	CB-CG-SD-CE
10	J	1	FME	CB-CG-SD-CE
11	K	1	FME	CA-CB-CG-SD
29	d	1	AME	C-CA-N-CT1
29	d	1	AME	C-CA-CB-CG
8	H	1	FME	CB-CA-N-CN

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	1	FME	1	0
1	A	1	FME	1	0
34	i	1	SAC	1	0
13	M	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 2 are monoatomic - leaving 38 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
46	3PE	L	701	-	37,37,50	1.03	4 (10%)	40,42,55	1.14	2 (5%)
45	PC1	g	1501	-	48,48,53	1.02	4 (8%)	54,56,61	1.10	2 (3%)
51	LMT	M	602	-	36,36,36	1.15	2 (5%)	47,47,47	1.03	1 (2%)
52	GTP	O	401	53	33,34,34	3.25	14 (42%)	50,54,54	1.87	14 (28%)
46	3PE	K	101	-	38,38,50	1.02	4 (10%)	41,43,55	1.13	2 (4%)
48	FES	E	301	5	0,4,4	-	-	-	-	-
50	CDL	L	702	-	61,61,99	1.13	8 (13%)	67,73,111	1.16	5 (7%)
47	SF4	B	201	2	0,12,12	-	-	-	-	-
50	CDL	h	1001	-	63,63,99	1.11	8 (12%)	69,75,111	1.24	5 (7%)
46	3PE	X	401	-	30,30,50	1.11	3 (10%)	33,35,55	1.25	2 (6%)
46	3PE	L	704	-	34,34,50	1.05	4 (11%)	37,39,55	1.17	2 (5%)
46	3PE	N	903	-	40,40,50	0.96	4 (10%)	43,45,55	1.21	2 (4%)
46	3PE	I	201	-	41,41,50	0.94	3 (7%)	44,46,55	1.19	2 (4%)
47	SF4	G	801	7	0,12,12	-	-	-	-	-
47	SF4	I	203	9	0,12,12	-	-	-	-	-
51	LMT	N	901	-	36,36,36	1.13	2 (5%)	47,47,47	1.18	3 (6%)
56	EHZ	U	101	20	31,36,37	1.52	5 (16%)	36,44,47	1.39	4 (11%)
46	3PE	L	703	-	44,44,50	0.92	4 (9%)	47,49,55	1.15	3 (6%)
45	PC1	B	203	-	34,34,53	1.21	4 (11%)	40,42,61	1.11	2 (5%)
47	SF4	I	202	9	0,12,12	-	-	-	-	-
46	3PE	N	902	-	43,43,50	0.93	3 (6%)	46,48,55	1.05	2 (4%)
50	CDL	q	201	-	68,68,99	1.05	8 (11%)	74,80,111	1.12	4 (5%)
54	NDP	P	501	-	51,52,52	2.13	6 (11%)	71,80,80	1.53	15 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	3PE	M	601	-	45,45,50	0.93	4 (8%)	48,50,55	1.23	2 (4%)
46	3PE	c	301	-	37,37,50	1.01	4 (10%)	40,42,55	0.99	2 (5%)
46	3PE	J	401	-	27,27,50	1.10	3 (11%)	30,32,55	1.11	1 (3%)
51	LMT	b	301	-	36,36,36	1.19	3 (8%)	47,47,47	1.35	5 (10%)
45	PC1	d	501	-	25,25,53	1.39	4 (16%)	31,33,61	0.99	2 (6%)
46	3PE	M	603	-	39,39,50	0.98	4 (10%)	42,44,55	1.07	2 (4%)
45	PC1	A	701	-	20,20,53	1.80	3 (15%)	24,27,61	1.15	1 (4%)
49	FMN	F	501	-	33,33,33	1.09	2 (6%)	48,50,50	1.30	6 (12%)
50	CDL	Y	701	-	49,49,99	1.22	8 (16%)	55,61,111	1.34	4 (7%)
56	EHZ	T	101	20	31,36,37	1.58	5 (16%)	36,44,47	1.79	8 (22%)
48	FES	G	803	7	0,4,4	-	-	-	-	-
46	3PE	A	702	-	38,38,50	1.00	4 (10%)	41,43,55	1.12	2 (4%)
45	PC1	B	202	-	42,42,53	1.07	4 (9%)	48,50,61	1.05	2 (4%)
47	SF4	F	502	6	0,12,12	-	-	-	-	-
47	SF4	G	802	7	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
46	3PE	L	701	-	-	19/41/41/54	-
45	PC1	g	1501	-	-	23/52/52/57	-
51	LMT	M	602	-	-	6/21/61/61	0/2/2/2
52	GTP	O	401	53	-	1/22/38/38	0/3/3/3
46	3PE	K	101	-	-	19/42/42/54	-
48	FES	E	301	5	-	-	0/1/1/1
50	CDL	L	702	-	-	35/72/72/110	-
47	SF4	B	201	2	-	-	0/6/5/5
50	CDL	h	1001	-	-	26/74/74/110	-
46	3PE	X	401	-	-	15/34/34/54	-
46	3PE	L	704	-	-	19/38/38/54	-
46	3PE	N	903	-	-	18/44/44/54	-
46	3PE	I	201	-	-	17/45/45/54	-
47	SF4	G	801	7	-	-	0/6/5/5
47	SF4	I	203	9	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	LMT	N	901	-	-	5/21/61/61	0/2/2/2
56	EHZ	U	101	20	-	7/42/44/45	-
46	3PE	L	703	-	-	22/48/48/54	-
45	PC1	B	203	-	-	12/38/38/57	-
54	NDP	P	501	-	-	9/34/77/77	0/5/5/5
46	3PE	N	902	-	-	24/47/47/54	-
50	CDL	q	201	-	-	34/79/79/110	-
47	SF4	I	202	9	-	-	0/6/5/5
46	3PE	M	601	-	-	19/49/49/54	-
46	3PE	c	301	-	-	22/41/41/54	-
46	3PE	J	401	-	-	11/30/30/54	-
51	LMT	b	301	-	-	8/21/61/61	0/2/2/2
45	PC1	d	501	-	-	11/29/29/57	-
46	3PE	M	603	-	-	20/43/43/54	-
45	PC1	A	701	-	-	12/22/22/57	-
49	FMN	F	501	-	-	3/18/18/18	0/3/3/3
50	CDL	Y	701	-	-	21/59/59/110	-
56	EHZ	T	101	20	-	9/42/44/45	-
48	FES	G	803	7	-	-	0/1/1/1
46	3PE	A	702	-	-	17/42/42/54	-
45	PC1	B	202	-	-	20/46/46/57	-
47	SF4	F	502	6	-	-	0/6/5/5
47	SF4	G	802	7	-	-	0/6/5/5

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	P	501	NDP	P2B-O2B	11.67	1.80	1.59
52	O	401	GTP	O6-C6	8.70	1.40	1.23
52	O	401	GTP	C5-N7	6.63	1.52	1.39
56	T	101	EHZ	C12-N1	5.07	1.45	1.33
52	O	401	GTP	C2-N1	4.99	1.49	1.37
45	A	701	PC1	O21-C2	-4.97	1.40	1.46
52	O	401	GTP	PA-O3A	4.91	1.64	1.59
52	O	401	GTP	PB-O3A	4.80	1.64	1.59
56	U	101	EHZ	C15-N2	4.79	1.44	1.33
56	U	101	EHZ	C12-N1	4.79	1.44	1.33
52	O	401	GTP	C2-N2	4.62	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	T	101	EHZ	C15-N2	4.58	1.44	1.33
52	O	401	GTP	PB-O3B	4.58	1.64	1.59
52	O	401	GTP	C2-N3	4.51	1.44	1.33
52	O	401	GTP	C8-N9	-4.38	1.27	1.37
52	O	401	GTP	C4-N9	-3.94	1.28	1.38
54	P	501	NDP	PN-O5D	3.60	1.73	1.59
54	P	501	NDP	O2B-C2B	-3.51	1.32	1.44
51	b	301	LMT	O5B-C1B	3.41	1.50	1.41
54	P	501	NDP	PA-O3	3.31	1.63	1.59
51	M	602	LMT	O5B-C1B	3.27	1.50	1.41
45	A	701	PC1	O21-C21	3.19	1.40	1.33
51	N	901	LMT	O5B-C1B	3.19	1.50	1.41
51	b	301	LMT	O5'-C1'	3.11	1.49	1.41
50	h	1001	CDL	OA6-CA4	-2.95	1.39	1.46
46	L	701	3PE	O21-C2	-2.95	1.39	1.46
50	L	702	CDL	OA6-CA4	-2.93	1.39	1.46
50	L	702	CDL	OB6-CB4	-2.90	1.39	1.46
45	B	203	PC1	O21-C2	-2.90	1.39	1.46
50	q	201	CDL	OA6-CA4	-2.89	1.39	1.46
46	X	401	3PE	O21-C2	-2.89	1.39	1.46
46	L	704	3PE	O21-C2	-2.88	1.39	1.46
45	g	1501	PC1	O21-C2	-2.86	1.39	1.46
46	I	201	3PE	O21-C2	-2.84	1.39	1.46
54	P	501	NDP	C7N-C3N	-2.83	1.42	1.48
45	B	202	PC1	O21-C2	-2.80	1.40	1.46
52	O	401	GTP	O4'-C1'	2.79	1.48	1.42
46	A	702	3PE	O21-C2	-2.78	1.40	1.46
51	M	602	LMT	O5'-C1'	2.78	1.49	1.41
50	h	1001	CDL	OB6-CB4	-2.76	1.40	1.46
51	N	901	LMT	O5'-C1'	2.76	1.48	1.41
46	L	703	3PE	O21-C2	-2.76	1.40	1.46
46	N	902	3PE	O21-C2	-2.76	1.40	1.46
45	d	501	PC1	O21-C2	-2.74	1.40	1.46
49	F	501	FMN	C4A-N5	2.72	1.36	1.30
46	c	301	3PE	O21-C2	-2.72	1.40	1.46
56	T	101	EHZ	O3-C12	-2.70	1.17	1.23
46	J	401	3PE	O21-C2	-2.68	1.40	1.46
50	q	201	CDL	OB6-CB4	-2.68	1.40	1.46
46	M	603	3PE	O21-C2	-2.64	1.40	1.46
46	M	601	3PE	O21-C2	-2.64	1.40	1.46
46	K	101	3PE	O31-C31	2.63	1.41	1.33
46	K	101	3PE	O21-C2	-2.61	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	Y	701	CDL	OA6-CA4	-2.60	1.40	1.46
56	T	101	EHZ	O4-C15	-2.59	1.18	1.23
46	L	701	3PE	O31-C3	-2.56	1.39	1.45
46	N	903	3PE	O21-C2	-2.56	1.40	1.46
50	L	702	CDL	OB8-CB7	2.56	1.40	1.33
56	U	101	EHZ	O4-C15	-2.55	1.18	1.23
50	Y	701	CDL	OB6-CB4	-2.53	1.40	1.46
50	h	1001	CDL	OB8-CB7	2.50	1.40	1.33
50	L	702	CDL	OA8-CA7	2.49	1.40	1.33
52	O	401	GTP	C2'-C3'	-2.49	1.46	1.53
46	c	301	3PE	O31-C31	2.47	1.40	1.33
45	d	501	PC1	O31-C31	2.46	1.40	1.33
50	h	1001	CDL	OA8-CA7	2.46	1.40	1.33
46	L	704	3PE	O31-C31	2.45	1.40	1.33
46	I	201	3PE	O31-C3	-2.44	1.39	1.45
46	M	603	3PE	O31-C31	2.44	1.40	1.33
46	L	703	3PE	O31-C3	-2.42	1.39	1.45
54	P	501	NDP	O5D-C5D	-2.42	1.35	1.44
50	q	201	CDL	OA8-CA7	2.42	1.40	1.33
50	Y	701	CDL	OA8-CA7	2.40	1.40	1.33
56	T	101	EHZ	C9-S1	2.39	1.81	1.76
45	g	1501	PC1	O31-C3	-2.37	1.39	1.45
45	B	203	PC1	O31-C31	2.37	1.40	1.33
50	Y	701	CDL	OB8-CB7	2.36	1.40	1.33
56	U	101	EHZ	O3-C12	-2.36	1.18	1.23
50	Y	701	CDL	OB6-CB5	2.35	1.40	1.35
46	M	601	3PE	O31-C3	-2.35	1.39	1.45
52	O	401	GTP	PG-O2G	-2.32	1.46	1.54
50	h	1001	CDL	OB6-CB5	2.31	1.40	1.34
50	q	201	CDL	OB8-CB7	2.31	1.40	1.33
46	J	401	3PE	O31-C3	-2.31	1.40	1.45
45	B	202	PC1	O31-C31	2.30	1.40	1.33
46	N	902	3PE	O31-C31	2.29	1.40	1.33
46	N	903	3PE	O31-C3	-2.28	1.40	1.45
46	A	702	3PE	O31-C31	2.28	1.40	1.33
46	X	401	3PE	O31-C31	2.27	1.40	1.33
52	O	401	GTP	PG-O3G	-2.27	1.46	1.54
46	c	301	3PE	O31-C3	-2.26	1.40	1.45
46	N	903	3PE	O31-C31	2.25	1.39	1.33
45	d	501	PC1	O31-C3	-2.25	1.40	1.45
45	g	1501	PC1	O31-C31	2.24	1.39	1.33
46	N	902	3PE	O31-C3	-2.23	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	A	702	3PE	O31-C3	-2.22	1.40	1.45
50	h	1001	CDL	OB8-CB6	-2.21	1.40	1.45
46	M	601	3PE	O31-C31	2.20	1.39	1.33
50	L	702	CDL	OA8-CA6	-2.20	1.40	1.45
56	U	101	EHZ	C9-S1	2.20	1.81	1.76
46	L	701	3PE	O31-C31	2.20	1.39	1.33
46	K	101	3PE	O21-C21	2.20	1.40	1.34
46	A	702	3PE	O21-C21	2.19	1.40	1.34
50	q	201	CDL	OB8-CB6	-2.19	1.40	1.45
46	N	903	3PE	O21-C21	2.18	1.40	1.34
46	M	601	3PE	O21-C21	2.18	1.40	1.34
45	B	202	PC1	O31-C3	-2.17	1.40	1.45
46	X	401	3PE	O31-C3	-2.17	1.40	1.45
50	q	201	CDL	OA8-CA6	-2.17	1.40	1.45
50	L	702	CDL	OB8-CB6	-2.17	1.40	1.45
50	Y	701	CDL	OB8-CB6	-2.16	1.40	1.45
45	A	701	PC1	O31-C3	-2.16	1.40	1.45
46	J	401	3PE	O21-C21	2.16	1.40	1.34
50	q	201	CDL	OB6-CB5	2.15	1.40	1.34
46	L	703	3PE	O31-C31	2.15	1.39	1.33
46	I	201	3PE	O31-C31	2.15	1.39	1.33
46	M	603	3PE	O21-C21	2.14	1.40	1.34
45	B	203	PC1	O31-C3	-2.13	1.40	1.45
50	h	1001	CDL	OA8-CA6	-2.13	1.40	1.45
46	M	603	3PE	O31-C3	-2.12	1.40	1.45
50	Y	701	CDL	OA8-CA6	-2.12	1.40	1.45
50	q	201	CDL	OA6-CA5	2.11	1.40	1.34
51	b	301	LMT	O5B-C5B	2.10	1.49	1.44
50	L	702	CDL	OB6-CB5	2.10	1.40	1.34
45	d	501	PC1	O21-C21	2.08	1.40	1.34
46	L	704	3PE	O31-C3	-2.08	1.40	1.45
46	K	101	3PE	O31-C3	-2.08	1.40	1.45
45	g	1501	PC1	C12-N	-2.07	1.45	1.51
45	B	203	PC1	O21-C21	2.07	1.40	1.34
50	h	1001	CDL	OA6-CA5	2.06	1.40	1.34
45	B	202	PC1	O21-C21	2.06	1.40	1.34
49	F	501	FMN	C10-N1	2.06	1.37	1.33
46	L	703	3PE	O21-C21	2.05	1.40	1.34
50	L	702	CDL	OA6-CA5	2.02	1.40	1.34
46	L	704	3PE	O21-C21	2.02	1.40	1.34
46	L	701	3PE	O21-C21	2.02	1.40	1.34
50	Y	701	CDL	OA6-CA5	2.01	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	c	301	3PE	O21-C21	2.01	1.40	1.34

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	O	401	GTP	C8-N9-C4	7.54	120.16	106.03
56	T	101	EHZ	C8-C9-S1	6.14	121.31	113.56
50	Y	701	CDL	OB6-CB5-C51	5.72	121.29	111.09
56	U	101	EHZ	C8-C9-S1	5.01	119.89	113.56
50	h	1001	CDL	OB6-CB5-C51	5.00	122.30	111.48
46	M	601	3PE	O21-C21-C22	4.74	121.74	111.48
46	N	903	3PE	O21-C21-C22	4.53	121.28	111.48
45	A	701	PC1	O21-C21-O22	-4.40	120.05	125.70
46	I	201	3PE	O21-C21-C22	4.30	120.78	111.48
46	L	703	3PE	O21-C21-C22	4.15	120.46	111.48
54	P	501	NDP	P2B-O2B-C2B	-4.13	112.40	123.43
46	X	401	3PE	O21-C21-C22	4.12	120.40	111.48
46	A	702	3PE	O21-C21-C22	4.08	120.31	111.48
46	L	704	3PE	O21-C21-C22	4.07	120.29	111.48
45	g	1501	PC1	O21-C21-C22	4.06	120.27	111.48
50	L	702	CDL	OA6-CA5-C11	4.06	120.27	111.48
50	q	201	CDL	OB6-CB5-C51	4.05	120.24	111.48
46	L	701	3PE	O21-C21-C22	4.00	120.13	111.48
45	B	203	PC1	O21-C21-C22	3.91	119.94	111.48
46	K	101	3PE	O21-C21-C22	3.89	119.90	111.48
45	B	202	PC1	O21-C21-C22	3.89	119.89	111.48
46	J	401	3PE	O21-C21-C22	3.87	119.84	111.48
54	P	501	NDP	O2B-P2B-O1X	-3.82	95.72	109.33
50	h	1001	CDL	OA6-CA5-C11	3.81	119.72	111.48
46	M	603	3PE	O21-C21-C22	3.80	119.70	111.48
50	L	702	CDL	OB6-CB5-C51	3.80	119.69	111.48
50	Y	701	CDL	OA6-CA5-C11	3.78	119.66	111.48
50	q	201	CDL	OA6-CA5-C11	3.67	119.42	111.48
56	T	101	EHZ	C10-S1-C9	3.60	112.47	101.84
49	F	501	FMN	C4-N3-C2	-3.52	119.39	125.64
51	b	301	LMT	C1'-C2'-C3'	3.42	117.21	110.01
46	K	101	3PE	O31-C31-C32	3.42	122.27	111.83
54	P	501	NDP	O3-PA-O1A	-3.30	100.78	110.70
56	T	101	EHZ	O2-C9-C8	-3.22	118.68	123.74
46	N	902	3PE	O21-C21-C22	3.15	118.29	111.48
46	X	401	3PE	O31-C31-C32	3.15	121.43	111.83
50	h	1001	CDL	OB8-CB7-C71	3.11	121.31	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	T	101	EHZ	C13-C12-N1	3.10	121.98	116.34
52	O	401	GTP	C2-N1-C6	-3.08	119.52	125.11
46	c	301	3PE	O21-C21-C22	3.08	118.15	111.48
46	N	903	3PE	O31-C31-C32	3.05	121.13	111.83
49	F	501	FMN	C4A-C10-N10	3.03	120.83	116.48
46	N	902	3PE	O31-C31-C32	3.02	121.03	111.83
45	B	203	PC1	O31-C31-C32	3.01	121.03	111.83
45	d	501	PC1	O31-C31-C32	2.93	120.78	111.83
49	F	501	FMN	O4-C4-C4A	-2.92	118.83	126.53
54	P	501	NDP	PA-O5B-C5B	-2.90	104.73	121.35
50	h	1001	CDL	OA8-CA7-C31	2.89	120.65	111.83
45	g	1501	PC1	O31-C31-C32	2.89	120.64	111.83
46	L	704	3PE	O31-C31-C32	2.88	120.62	111.83
45	B	202	PC1	O31-C31-C32	2.87	120.59	111.83
52	O	401	GTP	O2G-PG-O3B	2.83	114.12	104.64
51	N	901	LMT	C1B-O1B-C4'	-2.81	111.31	117.98
46	A	702	3PE	O31-C31-C32	2.78	120.31	111.83
50	Y	701	CDL	OB8-CB7-C71	2.76	120.25	111.83
52	O	401	GTP	O3G-PG-O3B	2.75	113.85	104.64
54	P	501	NDP	PN-O5D-C5D	-2.71	105.82	121.35
50	q	201	CDL	OA8-CA7-C31	2.70	120.07	111.83
51	b	301	LMT	C3B-C4B-C5B	2.68	115.09	110.23
52	O	401	GTP	O6-C6-C5	-2.67	119.48	126.53
46	M	601	3PE	O31-C31-C32	2.66	119.95	111.83
46	L	703	3PE	O31-C31-C32	2.66	119.94	111.83
46	M	603	3PE	O31-C31-C32	2.65	119.91	111.83
51	b	301	LMT	O5'-C1'-C2'	2.64	115.79	110.37
46	I	201	3PE	O31-C31-C32	2.63	119.86	111.83
50	q	201	CDL	OB8-CB7-C71	2.62	119.83	111.83
50	L	702	CDL	OB8-CB7-C71	2.62	119.83	111.83
54	P	501	NDP	O3X-P2B-O2X	2.58	117.49	107.80
49	F	501	FMN	C4A-C4-N3	2.58	119.82	113.25
50	L	702	CDL	OA8-CA7-C31	2.58	119.69	111.83
46	c	301	3PE	O31-C31-C32	2.57	119.66	111.83
54	P	501	NDP	C2A-N1A-C6A	-2.53	114.57	118.73
50	Y	701	CDL	OA8-CA7-C31	2.52	119.53	111.83
46	L	701	3PE	O31-C31-C32	2.49	119.43	111.83
54	P	501	NDP	O2N-PN-O3	2.45	113.91	107.27
52	O	401	GTP	O2B-PB-O1B	-2.44	101.09	112.44
52	O	401	GTP	C1'-N9-C8	-2.44	119.81	126.73
56	T	101	EHZ	C13-C14-N2	-2.42	106.85	112.00
54	P	501	NDP	N3A-C4A-N9A	2.42	131.28	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	O	401	GTP	C5-C4-N9	-2.42	101.33	105.66
56	U	101	EHZ	C10-S1-C9	2.41	108.95	101.84
54	P	501	NDP	O2N-PN-O1N	2.40	123.63	112.44
54	P	501	NDP	C5B-C4B-C3B	-2.36	106.72	115.21
54	P	501	NDP	O4B-C4B-C3B	2.36	109.83	105.15
51	N	901	LMT	C1B-C2B-C3B	2.35	114.96	110.01
52	O	401	GTP	C5-C6-N1	2.32	119.17	113.25
51	b	301	LMT	C1B-C2B-C3B	2.29	114.83	110.01
56	T	101	EHZ	C19-C17-C20	2.29	112.00	108.22
56	T	101	EHZ	C14-N2-C15	-2.28	118.46	122.55
52	O	401	GTP	C8-N7-C5	-2.26	100.23	104.26
54	P	501	NDP	C5A-C4A-N3A	-2.25	123.61	126.72
52	O	401	GTP	O2A-PA-O1A	-2.24	102.03	112.44
56	U	101	EHZ	O2-C9-S1	-2.22	119.86	122.68
56	U	101	EHZ	O2-C9-C8	-2.22	120.25	123.74
45	d	501	PC1	O21-C21-C22	2.20	119.00	110.93
49	F	501	FMN	C4-C4A-C10	2.19	120.69	116.93
52	O	401	GTP	C1'-N9-C4	-2.19	120.02	126.49
51	M	602	LMT	C3B-C4B-C5B	2.17	114.17	110.23
52	O	401	GTP	C3'-C2'-C1'	2.17	105.57	101.46
50	h	1001	CDL	OB6-CB5-OB7	-2.17	118.64	123.70
49	F	501	FMN	C4A-C10-N1	-2.16	119.30	124.59
52	O	401	GTP	C2'-C3'-C4'	2.14	106.74	102.61
51	b	301	LMT	O5B-C1B-C2B	2.13	114.75	110.37
56	T	101	EHZ	O2-C9-S1	-2.10	120.01	122.68
51	N	901	LMT	C4B-C3B-C2B	2.09	114.50	110.83
46	L	703	3PE	C2-O21-C21	-2.07	112.85	117.80
50	L	702	CDL	OA6-CA5-OA7	-2.05	118.92	123.70
54	P	501	NDP	O3X-P2B-O2B	-2.03	97.95	105.85
54	P	501	NDP	O5D-PN-O1N	-2.01	100.95	108.94

There are no chirality outliers.

All (484) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	701	PC1	C11-O13-P-O12
45	A	701	PC1	C1-O11-P-O14
45	A	701	PC1	C1-O11-P-O13
45	A	701	PC1	O13-C11-C12-N
45	A	701	PC1	C1-C2-O21-C21
45	A	701	PC1	O22-C21-O21-C2
45	B	202	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
45	B	202	PC1	C11-O13-P-O11
45	B	202	PC1	C1-O11-P-O14
45	B	202	PC1	O13-C11-C12-N
45	B	203	PC1	C11-O13-P-O12
45	B	203	PC1	C11-O13-P-O11
45	d	501	PC1	C11-O13-P-O12
45	d	501	PC1	C11-O13-P-O14
45	d	501	PC1	C11-O13-P-O11
45	d	501	PC1	O13-C11-C12-N
45	g	1501	PC1	C1-O11-P-O14
45	g	1501	PC1	O13-C11-C12-N
46	A	702	3PE	C1-O11-P-O12
46	A	702	3PE	C1-O11-P-O13
46	A	702	3PE	O13-C11-C12-N
46	A	702	3PE	C22-C21-O21-C2
46	I	201	3PE	C1-O11-P-O12
46	I	201	3PE	C1-O11-P-O13
46	J	401	3PE	C11-O13-P-O11
46	J	401	3PE	C11-O13-P-O12
46	J	401	3PE	C11-O13-P-O14
46	J	401	3PE	O21-C2-C3-O31
46	K	101	3PE	O13-C11-C12-N
46	L	701	3PE	C11-O13-P-O11
46	L	701	3PE	C11-O13-P-O12
46	L	701	3PE	C11-O13-P-O14
46	L	701	3PE	O13-C11-C12-N
46	L	701	3PE	C22-C21-O21-C2
46	L	703	3PE	O13-C11-C12-N
46	L	704	3PE	O22-C21-O21-C2
46	L	704	3PE	C22-C21-O21-C2
46	M	601	3PE	C1-O11-P-O13
46	M	601	3PE	C12-C11-O13-P
46	M	601	3PE	O13-C11-C12-N
46	M	601	3PE	C22-C21-O21-C2
46	M	603	3PE	C1-O11-P-O12
46	M	603	3PE	C1-O11-P-O13
46	M	603	3PE	C1-O11-P-O14
46	M	603	3PE	C11-O13-P-O11
46	M	603	3PE	C11-O13-P-O12
46	M	603	3PE	C11-O13-P-O14
46	N	902	3PE	C1-O11-P-O12
46	N	902	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
46	N	902	3PE	C1-O11-P-O14
46	N	902	3PE	C11-O13-P-O11
46	N	902	3PE	C11-O13-P-O14
46	N	903	3PE	C1-O11-P-O12
46	N	903	3PE	C1-O11-P-O13
46	N	903	3PE	C2-C1-O11-P
46	N	903	3PE	O22-C21-O21-C2
46	N	903	3PE	C22-C21-O21-C2
46	X	401	3PE	C11-O13-P-O11
46	X	401	3PE	C11-O13-P-O12
46	X	401	3PE	C11-O13-P-O14
46	X	401	3PE	C12-C11-O13-P
46	X	401	3PE	O13-C11-C12-N
46	X	401	3PE	O22-C21-O21-C2
46	c	301	3PE	C1-O11-P-O12
46	c	301	3PE	C1-O11-P-O13
46	c	301	3PE	C11-O13-P-O11
46	c	301	3PE	C11-O13-P-O14
46	c	301	3PE	C22-C21-O21-C2
49	F	501	FMN	C5'-O5'-P-O1P
49	F	501	FMN	C5'-O5'-P-O2P
50	L	702	CDL	CA2-OA2-PA1-OA3
50	L	702	CDL	CA2-OA2-PA1-OA5
50	L	702	CDL	CA3-OA5-PA1-OA3
50	L	702	CDL	OA7-CA5-OA6-CA4
50	L	702	CDL	C11-CA5-OA6-CA4
50	L	702	CDL	OA9-CA7-OA8-CA6
50	L	702	CDL	CB2-OB2-PB2-OB3
50	L	702	CDL	CB2-OB2-PB2-OB5
50	Y	701	CDL	CA2-OA2-PA1-OA3
50	Y	701	CDL	CA2-OA2-PA1-OA5
50	Y	701	CDL	CB2-OB2-PB2-OB3
50	Y	701	CDL	CB2-OB2-PB2-OB5
50	Y	701	CDL	C51-CB5-OB6-CB4
50	h	1001	CDL	CB3-OB5-PB2-OB2
50	h	1001	CDL	CB3-OB5-PB2-OB3
50	h	1001	CDL	CB3-OB5-PB2-OB4
50	h	1001	CDL	OB7-CB5-OB6-CB4
50	h	1001	CDL	C51-CB5-OB6-CB4
50	q	201	CDL	CA2-C1-CB2-OB2
50	q	201	CDL	CA3-OA5-PA1-OA2
50	q	201	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
50	q	201	CDL	CB2-OB2-PB2-OB5
51	N	901	LMT	C2-C1-O1'-C1'
54	P	501	NDP	C5B-O5B-PA-O1A
54	P	501	NDP	C5B-O5B-PA-O2A
54	P	501	NDP	C5B-O5B-PA-O3
54	P	501	NDP	O4B-C4B-C5B-O5B
56	T	101	EHZ	C16-C17-C20-O6
56	T	101	EHZ	C18-C17-C20-O6
56	T	101	EHZ	C19-C17-C20-O6
56	T	101	EHZ	O2-C9-S1-C10
56	T	101	EHZ	C8-C9-S1-C10
56	U	101	EHZ	C5-C6-C7-C8
56	U	101	EHZ	O2-C9-S1-C10
56	U	101	EHZ	C8-C9-S1-C10
50	Y	701	CDL	OB7-CB5-OB6-CB4
45	g	1501	PC1	O32-C31-O31-C3
46	K	101	3PE	O32-C31-O31-C3
46	L	703	3PE	O32-C31-O31-C3
46	N	903	3PE	O32-C31-O31-C3
46	K	101	3PE	C32-C31-O31-C3
46	N	903	3PE	C32-C31-O31-C3
50	L	702	CDL	C31-CA7-OA8-CA6
45	d	501	PC1	O32-C31-O31-C3
46	L	704	3PE	O32-C31-O31-C3
50	h	1001	CDL	OB9-CB7-OB8-CB6
46	J	401	3PE	C32-C31-O31-C3
46	L	701	3PE	O22-C21-O21-C2
46	M	601	3PE	O22-C21-O21-C2
46	c	301	3PE	O22-C21-O21-C2
45	d	501	PC1	C32-C31-O31-C3
45	g	1501	PC1	C32-C31-O31-C3
46	L	703	3PE	C32-C31-O31-C3
46	L	704	3PE	C32-C31-O31-C3
46	N	902	3PE	C32-C31-O31-C3
46	X	401	3PE	C22-C21-O21-C2
45	A	701	PC1	O32-C31-O31-C3
46	M	603	3PE	C32-C31-O31-C3
50	h	1001	CDL	C71-CB7-OB8-CB6
46	J	401	3PE	O32-C31-O31-C3
46	N	902	3PE	O32-C31-O31-C3
46	A	702	3PE	O22-C21-O21-C2
45	A	701	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
50	L	702	CDL	O1-C1-CA2-OA2
50	L	702	CDL	O1-C1-CB2-OB2
51	M	602	LMT	O5'-C5'-C6'-O6'
51	b	301	LMT	O5'-C5'-C6'-O6'
46	M	603	3PE	C22-C21-O21-C2
46	M	603	3PE	O32-C31-O31-C3
51	N	901	LMT	O5B-C5B-C6B-O6B
51	b	301	LMT	C4'-C5'-C6'-O6'
54	P	501	NDP	C3B-C4B-C5B-O5B
54	P	501	NDP	O4D-C4D-C5D-O5D
50	Y	701	CDL	C1-CB2-OB2-PB2
51	M	602	LMT	C4'-C5'-C6'-O6'
50	Y	701	CDL	OB9-CB7-OB8-CB6
50	Y	701	CDL	C71-CB7-OB8-CB6
45	B	203	PC1	C32-C31-O31-C3
46	L	701	3PE	C32-C31-O31-C3
51	N	901	LMT	C4B-C5B-C6B-O6B
45	B	203	PC1	O32-C31-O31-C3
50	q	201	CDL	O1-C1-CB2-OB2
46	L	701	3PE	O32-C31-O31-C3
51	b	301	LMT	C5'-C4'-O1B-C1B
50	Y	701	CDL	OA5-CA3-CA4-OA6
50	Y	701	CDL	C11-CA5-OA6-CA4
50	h	1001	CDL	C31-CA7-OA8-CA6
46	M	603	3PE	O22-C21-O21-C2
45	g	1501	PC1	C21-C22-C23-C24
50	L	702	CDL	CA5-C11-C12-C13
50	L	702	CDL	CB5-C51-C52-C53
45	B	203	PC1	C22-C21-O21-C2
46	M	601	3PE	C21-C22-C23-C24
46	N	902	3PE	C21-C22-C23-C24
50	q	201	CDL	CA7-C31-C32-C33
50	q	201	CDL	O1-C1-CA2-OA2
50	q	201	CDL	CA5-C11-C12-C13
46	I	201	3PE	C22-C21-O21-C2
45	B	203	PC1	O22-C21-O21-C2
46	I	201	3PE	O22-C21-O21-C2
50	Y	701	CDL	OA7-CA5-OA6-CA4
50	q	201	CDL	CB2-C1-CA2-OA2
50	L	702	CDL	C71-CB7-OB8-CB6
50	q	201	CDL	C31-CA7-OA8-CA6
46	N	902	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
51	M	602	LMT	C2'-C1'-O1'-C1
50	h	1001	CDL	OA9-CA7-OA8-CA6
56	U	101	EHZ	C5-C6-C7-O1
51	N	901	LMT	O1'-C1-C2-C3
46	K	101	3PE	C22-C21-O21-C2
50	L	702	CDL	OB9-CB7-OB8-CB6
45	B	202	PC1	C25-C26-C27-C28
46	K	101	3PE	C35-C36-C37-C38
46	M	601	3PE	C2E-C2F-C2G-C2H
50	L	702	CDL	C53-C54-C55-C56
46	L	704	3PE	C35-C36-C37-C38
46	N	902	3PE	C37-C38-C39-C3A
46	N	902	3PE	C28-C29-C2A-C2B
50	h	1001	CDL	C22-C23-C24-C25
50	q	201	CDL	C52-C53-C54-C55
46	K	101	3PE	O22-C21-O21-C2
46	L	704	3PE	C31-C32-C33-C34
50	h	1001	CDL	C11-CA5-OA6-CA4
46	K	101	3PE	C32-C33-C34-C35
46	c	301	3PE	C3E-C3F-C3G-C3H
50	Y	701	CDL	C31-C32-C33-C34
50	q	201	CDL	OA9-CA7-OA8-CA6
50	h	1001	CDL	CB7-C71-C72-C73
46	N	902	3PE	O22-C21-O21-C2
50	L	702	CDL	CA2-C1-CB2-OB2
46	L	701	3PE	C33-C34-C35-C36
46	M	601	3PE	C34-C35-C36-C37
46	M	603	3PE	C33-C34-C35-C36
46	N	902	3PE	C2D-C2E-C2F-C2G
45	g	1501	PC1	C29-C2A-C2B-C2C
50	L	702	CDL	C59-C60-C61-C62
50	L	702	CDL	C54-C55-C56-C57
51	b	301	LMT	C3'-C4'-O1B-C1B
46	N	902	3PE	C31-C32-C33-C34
46	J	401	3PE	C22-C23-C24-C25
50	h	1001	CDL	OA7-CA5-OA6-CA4
45	g	1501	PC1	C23-C24-C25-C26
45	g	1501	PC1	C34-C35-C36-C37
46	I	201	3PE	C33-C34-C35-C36
46	L	704	3PE	C32-C33-C34-C35
50	L	702	CDL	C52-C53-C54-C55
46	L	701	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
46	N	902	3PE	C2A-C2B-C2C-C2D
50	h	1001	CDL	C16-C17-C18-C19
46	N	903	3PE	C33-C34-C35-C36
46	L	701	3PE	C35-C36-C37-C38
46	M	603	3PE	C35-C36-C37-C38
45	d	501	PC1	C22-C21-O21-C2
46	L	703	3PE	C22-C21-O21-C2
45	g	1501	PC1	C26-C27-C28-C29
45	B	202	PC1	C3A-C3B-C3C-C3D
46	M	603	3PE	C22-C23-C24-C25
50	q	201	CDL	C37-C38-C39-C40
45	B	202	PC1	C22-C21-O21-C2
46	L	704	3PE	C34-C35-C36-C37
56	T	101	EHZ	C2-C1-C21-C22
46	L	704	3PE	C21-C22-C23-C24
50	h	1001	CDL	CA5-C11-C12-C13
45	g	1501	PC1	C38-C39-C3A-C3B
45	g	1501	PC1	C27-C28-C29-C2A
46	L	703	3PE	C34-C35-C36-C37
50	L	702	CDL	C34-C35-C36-C37
51	M	602	LMT	C5-C6-C7-C8
46	A	702	3PE	C27-C28-C29-C2A
46	L	703	3PE	O22-C21-O21-C2
46	M	601	3PE	C26-C27-C28-C29
45	g	1501	PC1	C22-C21-O21-C2
51	N	901	LMT	C4-C5-C6-C7
45	B	202	PC1	O11-C1-C2-C3
46	K	101	3PE	O11-C1-C2-C3
46	L	704	3PE	O11-C1-C2-C3
46	N	902	3PE	O11-C1-C2-C3
50	Y	701	CDL	OA5-CA3-CA4-CA6
46	N	903	3PE	C38-C39-C3A-C3B
45	g	1501	PC1	C32-C33-C34-C35
46	M	603	3PE	C32-C33-C34-C35
50	q	201	CDL	C71-C72-C73-C74
46	c	301	3PE	C33-C34-C35-C36
50	Y	701	CDL	C12-C13-C14-C15
45	B	202	PC1	C36-C37-C38-C39
46	L	703	3PE	C33-C34-C35-C36
45	B	203	PC1	C1-C2-C3-O31
46	J	401	3PE	C1-C2-C3-O31
46	K	101	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
46	L	704	3PE	C1-C2-C3-O31
46	I	201	3PE	C26-C27-C28-C29
51	b	301	LMT	O5B-C5B-C6B-O6B
46	K	101	3PE	C29-C2A-C2B-C2C
56	U	101	EHZ	C3-C4-C5-C6
46	I	201	3PE	C37-C38-C39-C3A
46	M	601	3PE	C38-C39-C3A-C3B
50	Y	701	CDL	CA6-CA4-OA6-CA5
46	N	902	3PE	C35-C36-C37-C38
46	X	401	3PE	C22-C23-C24-C25
54	P	501	NDP	O4D-C1D-N1N-C6N
46	A	702	3PE	C32-C33-C34-C35
46	J	401	3PE	C24-C25-C26-C27
45	d	501	PC1	O21-C2-C3-O31
50	h	1001	CDL	C72-C73-C74-C75
45	g	1501	PC1	C2F-C2G-C2H-C2I
46	L	701	3PE	C37-C38-C39-C3A
46	X	401	3PE	C36-C37-C38-C39
46	L	704	3PE	C3B-C3C-C3D-C3E
45	d	501	PC1	O22-C21-O21-C2
46	M	601	3PE	C28-C29-C2A-C2B
56	T	101	EHZ	C21-C22-C23-C24
46	L	701	3PE	C32-C33-C34-C35
46	M	603	3PE	C28-C29-C2A-C2B
46	A	702	3PE	O11-C1-C2-C3
46	N	903	3PE	C2A-C2B-C2C-C2D
46	L	703	3PE	C31-C32-C33-C34
54	P	501	NDP	C3D-C4D-C5D-O5D
46	N	903	3PE	C36-C37-C38-C39
50	L	702	CDL	CB2-C1-CA2-OA2
46	c	301	3PE	C22-C23-C24-C25
46	I	201	3PE	C32-C31-O31-C3
46	N	902	3PE	C25-C26-C27-C28
50	L	702	CDL	CB3-CB4-CB6-OB8
46	c	301	3PE	C3A-C3B-C3C-C3D
46	K	101	3PE	C28-C29-C2A-C2B
45	g	1501	PC1	C24-C25-C26-C27
45	B	202	PC1	O22-C21-O21-C2
46	N	902	3PE	O11-C1-C2-O21
46	c	301	3PE	O11-C1-C2-O21
50	L	702	CDL	C35-C36-C37-C38
45	B	202	PC1	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
45	g	1501	PC1	C2-C1-O11-P
46	N	902	3PE	C32-C33-C34-C35
45	B	203	PC1	O21-C2-C3-O31
46	K	101	3PE	O21-C2-C3-O31
46	L	704	3PE	O21-C2-C3-O31
46	N	903	3PE	O21-C2-C3-O31
50	L	702	CDL	OB6-CB4-CB6-OB8
50	Y	701	CDL	OB6-CB4-CB6-OB8
50	q	201	CDL	OA6-CA4-CA6-OA8
46	M	601	3PE	C31-C32-C33-C34
46	c	301	3PE	C39-C3A-C3B-C3C
56	U	101	EHZ	C2-C1-C21-C22
50	L	702	CDL	C60-C61-C62-C63
46	M	601	3PE	C32-C31-O31-C3
46	N	903	3PE	O11-C1-C2-C3
46	X	401	3PE	O11-C1-C2-C3
46	L	703	3PE	C37-C38-C39-C3A
46	c	301	3PE	C32-C33-C34-C35
46	I	201	3PE	O32-C31-O31-C3
49	F	501	FMN	C5'-O5'-P-O3P
50	q	201	CDL	C11-CA5-OA6-CA4
45	g	1501	PC1	O22-C21-O21-C2
50	h	1001	CDL	CA6-CA4-OA6-CA5
45	g	1501	PC1	C2A-C2B-C2C-C2D
46	L	703	3PE	C39-C3A-C3B-C3C
46	A	702	3PE	O11-C1-C2-O21
46	L	704	3PE	O11-C1-C2-O21
46	N	903	3PE	O11-C1-C2-O21
46	X	401	3PE	O11-C1-C2-O21
46	X	401	3PE	C34-C35-C36-C37
50	Y	701	CDL	CB3-CB4-CB6-OB8
50	Y	701	CDL	C13-C14-C15-C16
45	B	202	PC1	C12-C11-O13-P
46	A	702	3PE	C12-C11-O13-P
46	L	703	3PE	C12-C11-O13-P
50	q	201	CDL	OA7-CA5-OA6-CA4
45	B	203	PC1	O13-C11-C12-N
46	I	201	3PE	C39-C3A-C3B-C3C
46	M	601	3PE	O32-C31-O31-C3
45	A	701	PC1	O11-C1-C2-C3
46	L	701	3PE	O11-C1-C2-C3
46	c	301	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
46	M	601	3PE	C2-C1-O11-P
50	h	1001	CDL	CB4-CB3-OB5-PB2
50	q	201	CDL	CB4-CB3-OB5-PB2
46	L	703	3PE	C32-C33-C34-C35
45	B	203	PC1	C23-C24-C25-C26
45	B	202	PC1	O11-C1-C2-O21
46	K	101	3PE	O11-C1-C2-O21
46	L	701	3PE	O11-C1-C2-O21
50	L	702	CDL	C57-C58-C59-C60
46	N	902	3PE	C27-C28-C29-C2A
45	g	1501	PC1	O21-C2-C3-O31
45	g	1501	PC1	C1-C2-C3-O31
50	q	201	CDL	CA3-CA4-CA6-OA8
46	L	701	3PE	C24-C25-C26-C27
46	K	101	3PE	C26-C27-C28-C29
45	A	701	PC1	C11-O13-P-O11
45	A	701	PC1	C1-O11-P-O12
45	B	202	PC1	C11-O13-P-O12
45	g	1501	PC1	C1-O11-P-O13
46	A	702	3PE	C11-O13-P-O11
46	A	702	3PE	C11-O13-P-O12
46	A	702	3PE	C11-O13-P-O14
46	I	201	3PE	C1-O11-P-O14
46	K	101	3PE	C1-O11-P-O14
46	L	703	3PE	C1-O11-P-O14
46	L	703	3PE	C11-O13-P-O11
46	L	703	3PE	C11-O13-P-O12
46	L	703	3PE	C11-O13-P-O14
46	L	704	3PE	C11-O13-P-O11
46	L	704	3PE	C11-O13-P-O12
46	M	601	3PE	C1-O11-P-O14
46	N	903	3PE	C1-O11-P-O14
46	c	301	3PE	C1-O11-P-O14
50	L	702	CDL	CA2-OA2-PA1-OA4
50	L	702	CDL	CA3-OA5-PA1-OA2
50	Y	701	CDL	CB2-OB2-PB2-OB4
50	q	201	CDL	CA3-OA5-PA1-OA3
50	q	201	CDL	CB2-OB2-PB2-OB3
50	q	201	CDL	CB3-OB5-PB2-OB2
50	q	201	CDL	CB3-OB5-PB2-OB3
50	q	201	CDL	CB3-OB5-PB2-OB4
46	L	704	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
46	M	603	3PE	C2-C1-O11-P
46	c	301	3PE	C31-C32-C33-C34
50	h	1001	CDL	O1-C1-CB2-OB2
50	q	201	CDL	C51-C52-C53-C54
45	A	701	PC1	O11-C1-C2-O21
50	h	1001	CDL	OA6-CA4-CA6-OA8
46	K	101	3PE	C37-C38-C39-C3A
46	M	603	3PE	C23-C24-C25-C26
46	L	703	3PE	C28-C29-C2A-C2B
45	d	501	PC1	C1-C2-C3-O31
46	X	401	3PE	C31-C32-C33-C34
50	h	1001	CDL	C31-C32-C33-C34
54	P	501	NDP	C2B-O2B-P2B-O2X
50	q	201	CDL	C73-C74-C75-C76
56	T	101	EHZ	S1-C10-C11-N1
46	L	701	3PE	C23-C24-C25-C26
46	X	401	3PE	C32-C33-C34-C35
46	A	702	3PE	C37-C38-C39-C3A
45	B	203	PC1	C22-C23-C24-C25
46	K	101	3PE	C27-C28-C29-C2A
46	M	601	3PE	C32-C33-C34-C35
51	M	602	LMT	O5'-C1'-O1'-C1
51	b	301	LMT	O5'-C1'-O1'-C1
50	q	201	CDL	CA4-CA3-OA5-PA1
45	B	202	PC1	C35-C36-C37-C38
50	q	201	CDL	C15-C16-C17-C18
46	I	201	3PE	C23-C24-C25-C26
46	L	703	3PE	C1-C2-O21-C21
46	L	703	3PE	C3-C2-O21-C21
50	Y	701	CDL	CB6-CB4-OB6-CB5
56	T	101	EHZ	C5-C6-C7-O1
46	L	703	3PE	O31-C31-C32-C33
46	M	603	3PE	C31-C32-C33-C34
46	A	702	3PE	C29-C2A-C2B-C2C
46	I	201	3PE	C22-C23-C24-C25
46	L	704	3PE	C33-C34-C35-C36
46	I	201	3PE	C24-C25-C26-C27
51	M	602	LMT	O1'-C1-C2-C3
46	M	601	3PE	C2A-C2B-C2C-C2D
50	q	201	CDL	C38-C39-C40-C41
46	L	703	3PE	C36-C37-C38-C39
46	N	903	3PE	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
45	B	202	PC1	C2-C1-O11-P
46	N	902	3PE	C2-C1-O11-P
46	X	401	3PE	C2-C1-O11-P
50	h	1001	CDL	CA4-CA3-OA5-PA1
50	q	201	CDL	OB5-CB3-CB4-OB6
51	b	301	LMT	O1'-C1-C2-C3
46	N	902	3PE	C34-C35-C36-C37
46	I	201	3PE	C38-C39-C3A-C3B
46	M	603	3PE	C37-C38-C39-C3A
46	L	704	3PE	C38-C39-C3A-C3B
46	M	601	3PE	O21-C2-C3-O31
50	L	702	CDL	OA6-CA4-CA6-OA8
46	L	703	3PE	C21-C22-C23-C24
45	B	202	PC1	C33-C34-C35-C36
46	L	701	3PE	C34-C35-C36-C37
50	h	1001	CDL	C12-C13-C14-C15
56	U	101	EHZ	C21-C22-C23-C24
46	J	401	3PE	C21-C22-C23-C24
46	c	301	3PE	C3-C2-O21-C21
46	L	701	3PE	C38-C39-C3A-C3B
46	N	903	3PE	C32-C33-C34-C35
46	M	603	3PE	C34-C35-C36-C37
46	N	903	3PE	C1-C2-C3-O31
50	h	1001	CDL	C52-C53-C54-C55
46	K	101	3PE	C2A-C2B-C2C-C2D
50	q	201	CDL	C36-C37-C38-C39
50	L	702	CDL	OB7-CB5-OB6-CB4
50	h	1001	CDL	C15-C16-C17-C18
46	N	902	3PE	C36-C37-C38-C39
51	b	301	LMT	C4-C5-C6-C7
46	c	301	3PE	C36-C37-C38-C39
50	L	702	CDL	C51-CB5-OB6-CB4
46	I	201	3PE	C2B-C2C-C2D-C2E
46	I	201	3PE	C34-C35-C36-C37
45	B	202	PC1	O31-C31-C32-C33
45	g	1501	PC1	O31-C31-C32-C33
50	q	201	CDL	C72-C71-CB7-OB8
45	B	202	PC1	O21-C21-C22-C23
50	h	1001	CDL	CA3-CA4-CA6-OA8
46	c	301	3PE	C38-C39-C3A-C3B
46	K	101	3PE	C31-C32-C33-C34
46	c	301	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
46	c	301	3PE	C1-C2-O21-C21
50	L	702	CDL	CB4-CB6-OB8-CB7
45	d	501	PC1	O21-C21-C22-C23
46	c	301	3PE	O32-C31-O31-C3
50	L	702	CDL	OA5-CA3-CA4-OA6
46	J	401	3PE	C28-C29-C2A-C2B
45	g	1501	PC1	O32-C31-C32-C33
50	q	201	CDL	C72-C71-CB7-OB9
46	A	702	3PE	C2A-C2B-C2C-C2D
45	B	203	PC1	C35-C36-C37-C38
45	B	202	PC1	O32-C31-C32-C33
50	L	702	CDL	OA5-CA3-CA4-CA6
50	q	201	CDL	C32-C31-CA7-OA8
52	O	401	GTP	PA-O3A-PB-O2B
46	A	702	3PE	C34-C35-C36-C37

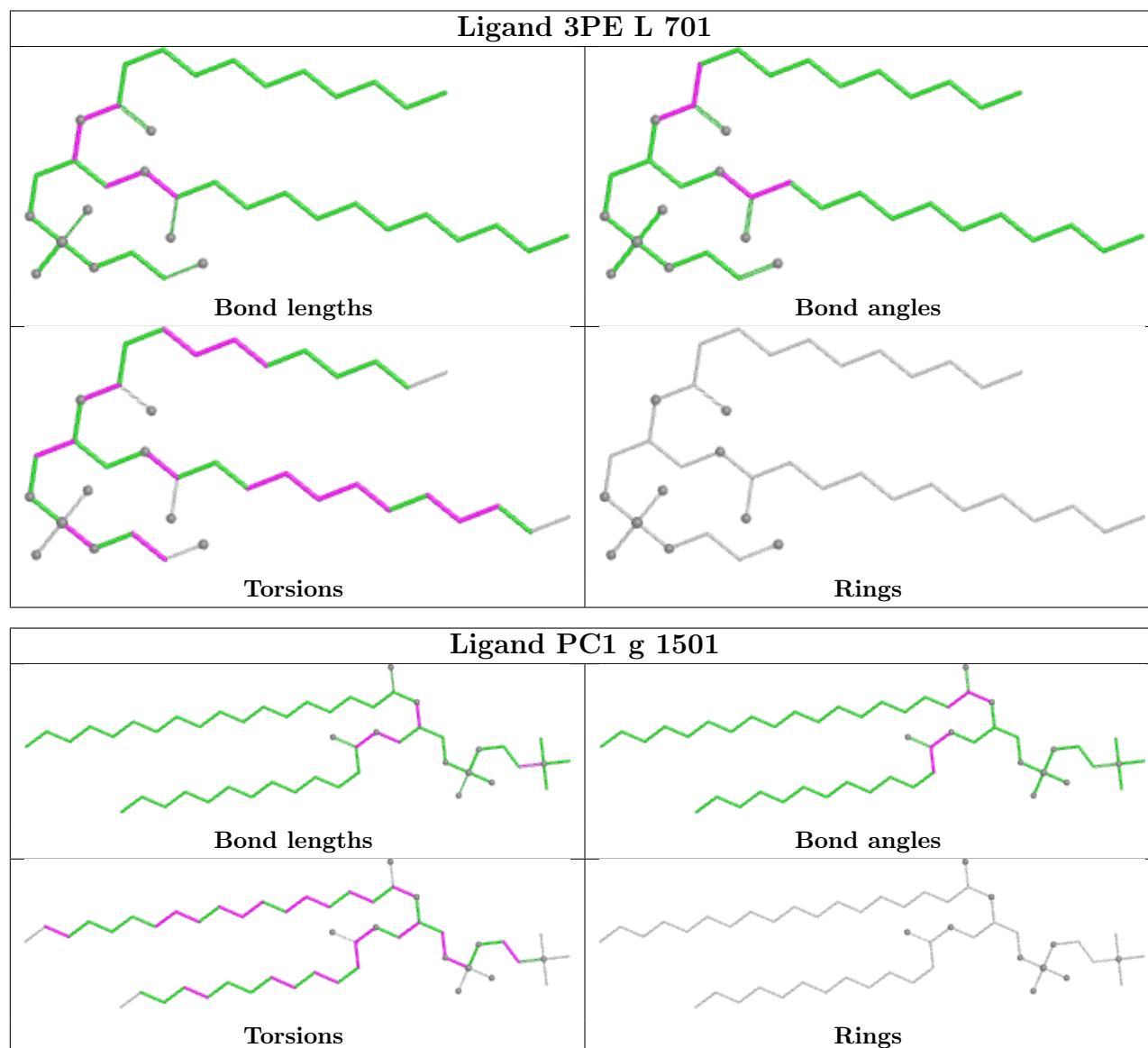
There are no ring outliers.

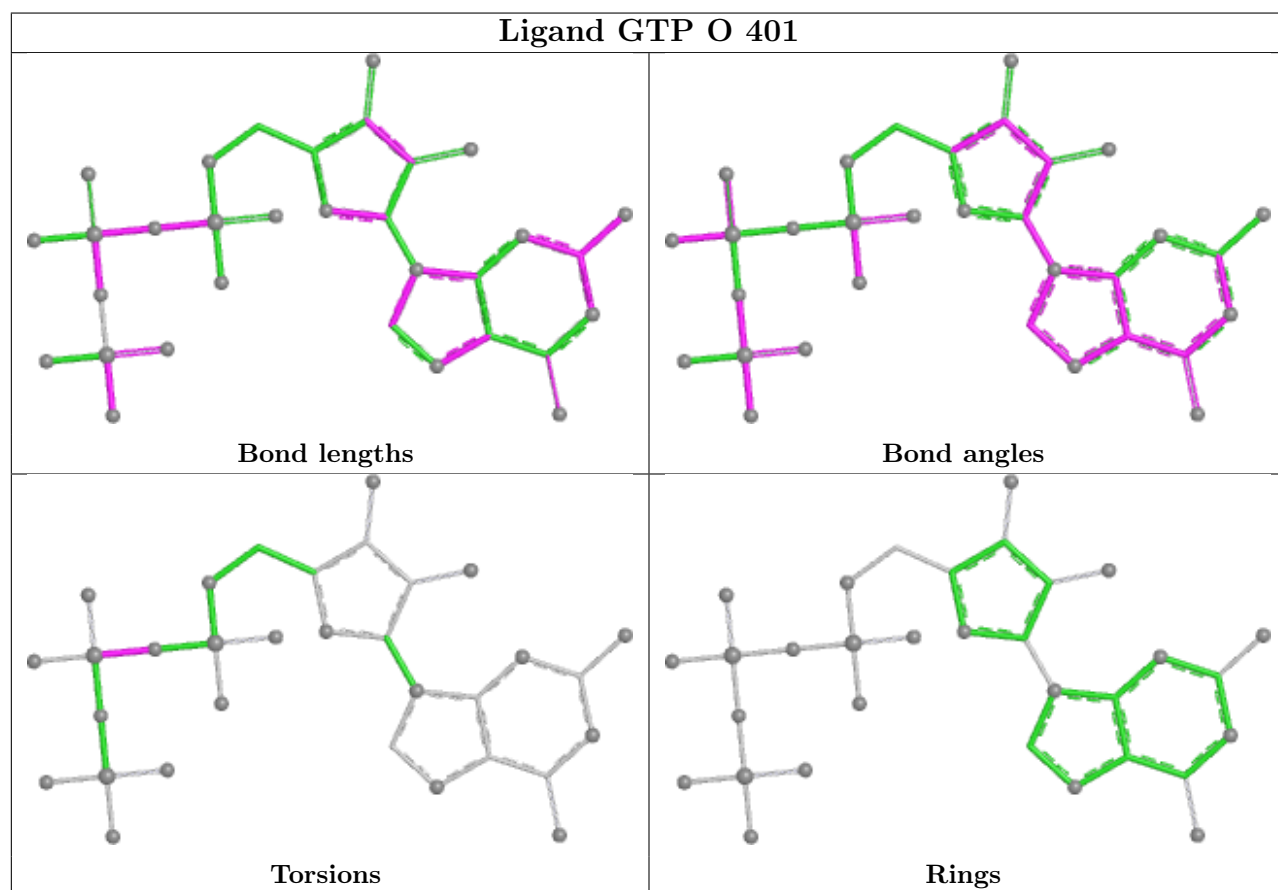
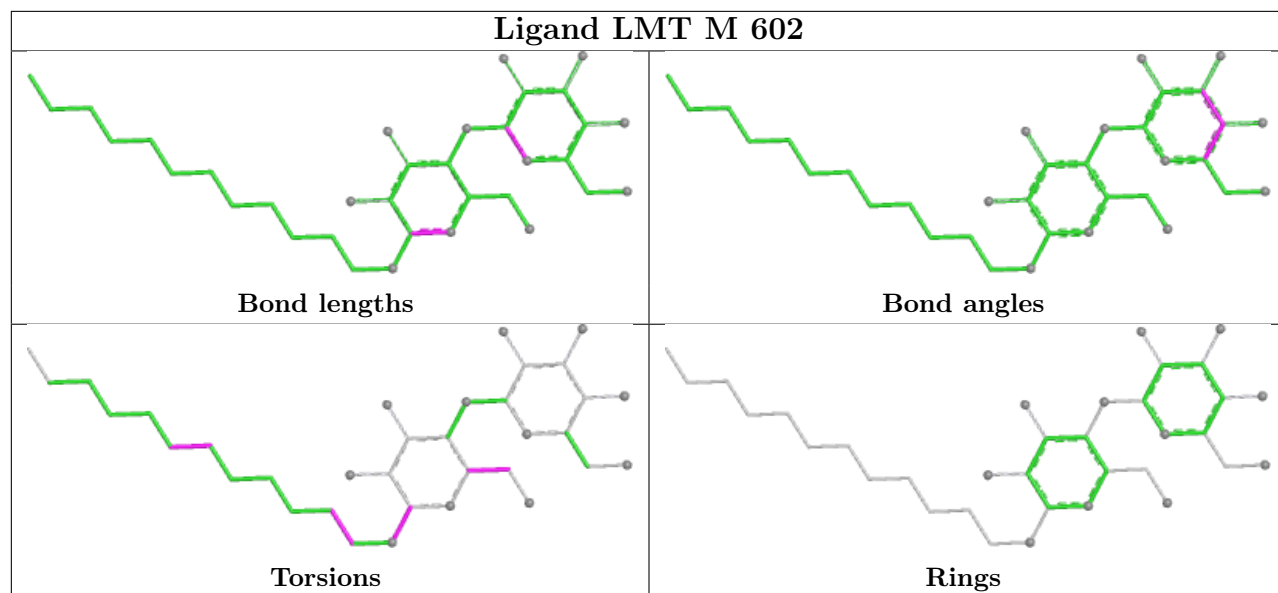
17 monomers are involved in 30 short contacts:

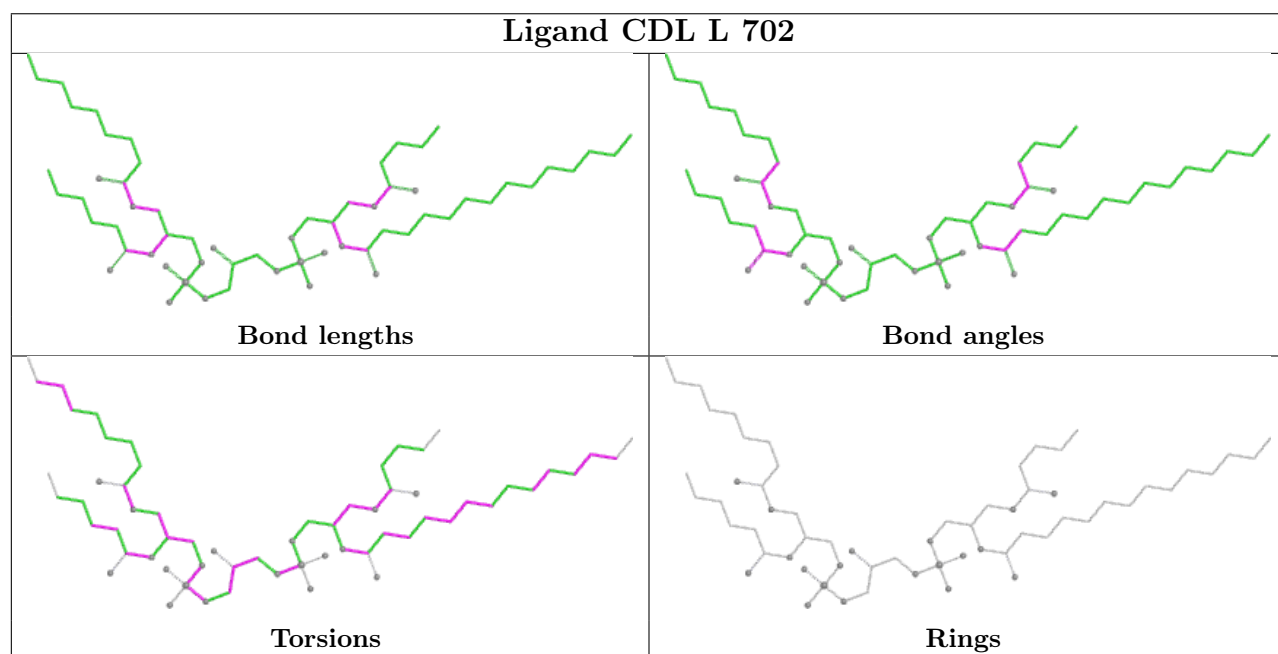
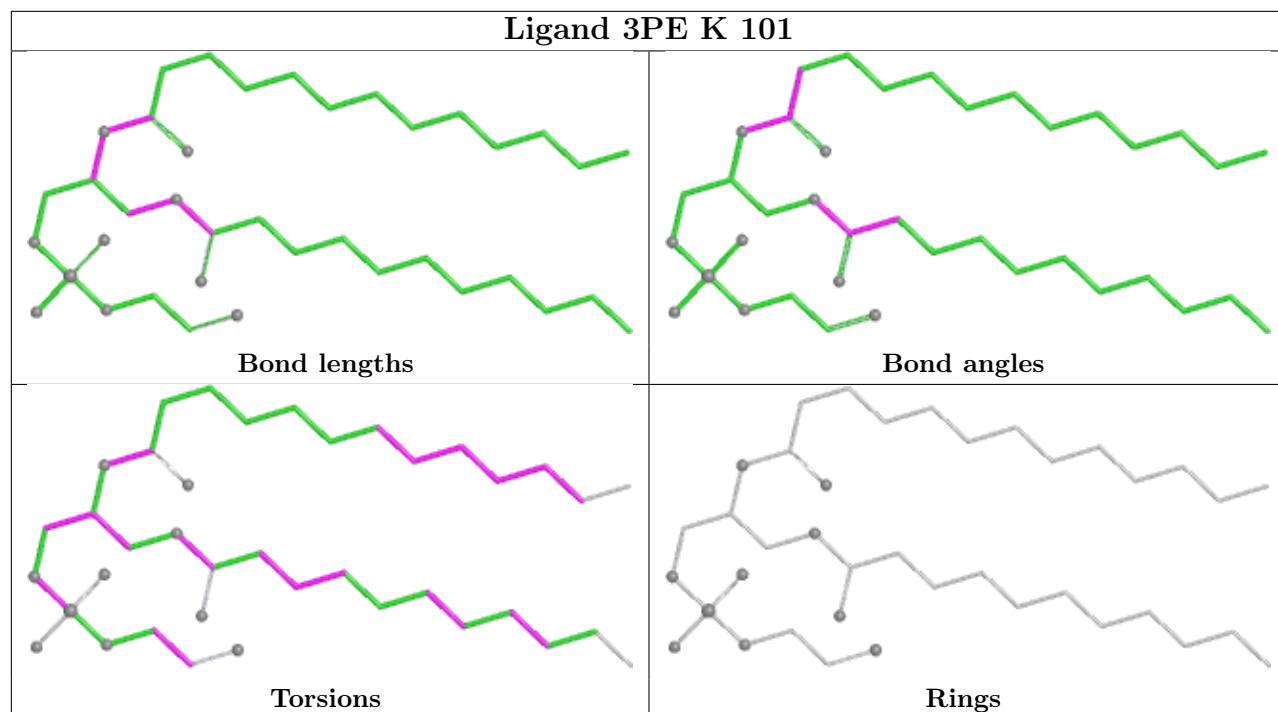
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	M	602	LMT	1	0
52	O	401	GTP	3	0
50	h	1001	CDL	2	0
46	X	401	3PE	1	0
46	I	201	3PE	4	0
47	G	801	SF4	1	0
56	U	101	EHZ	1	0
45	B	203	PC1	2	0
46	N	902	3PE	4	0
50	q	201	CDL	1	0
54	P	501	NDP	4	0
46	c	301	3PE	1	0
46	J	401	3PE	1	0
46	M	603	3PE	2	0
49	F	501	FMN	1	0
50	Y	701	CDL	1	0
47	F	502	SF4	2	0

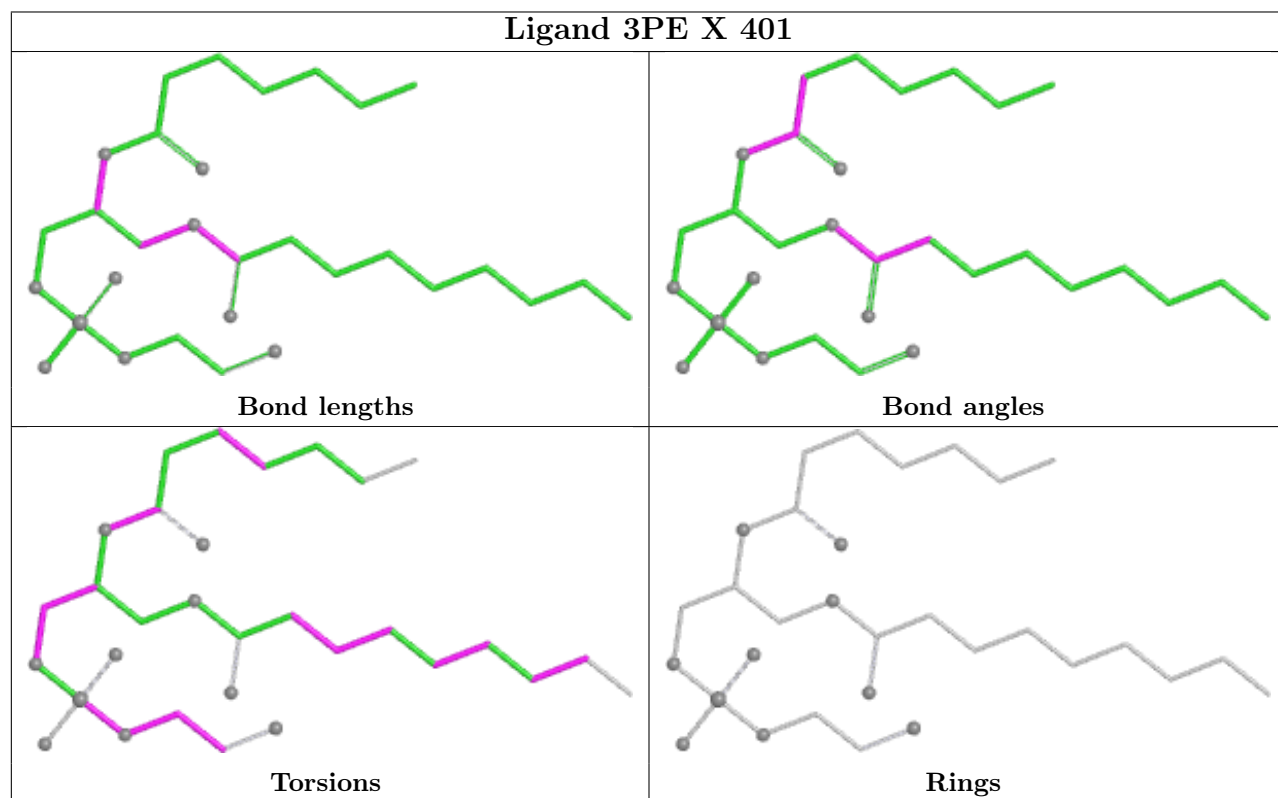
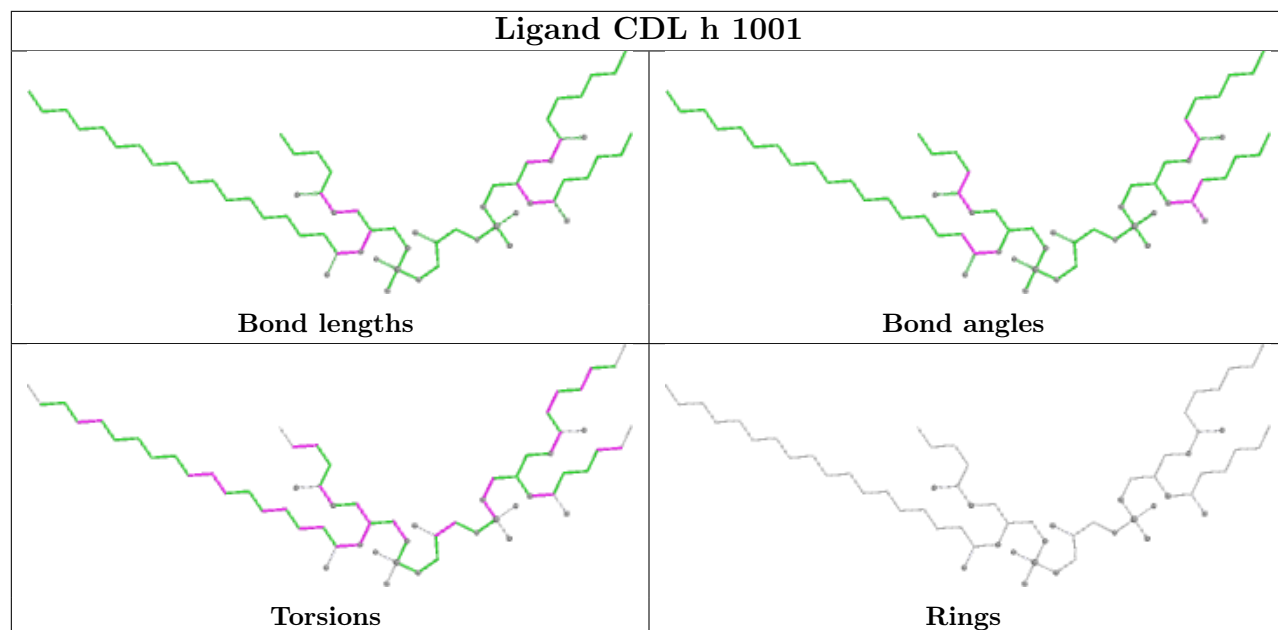
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

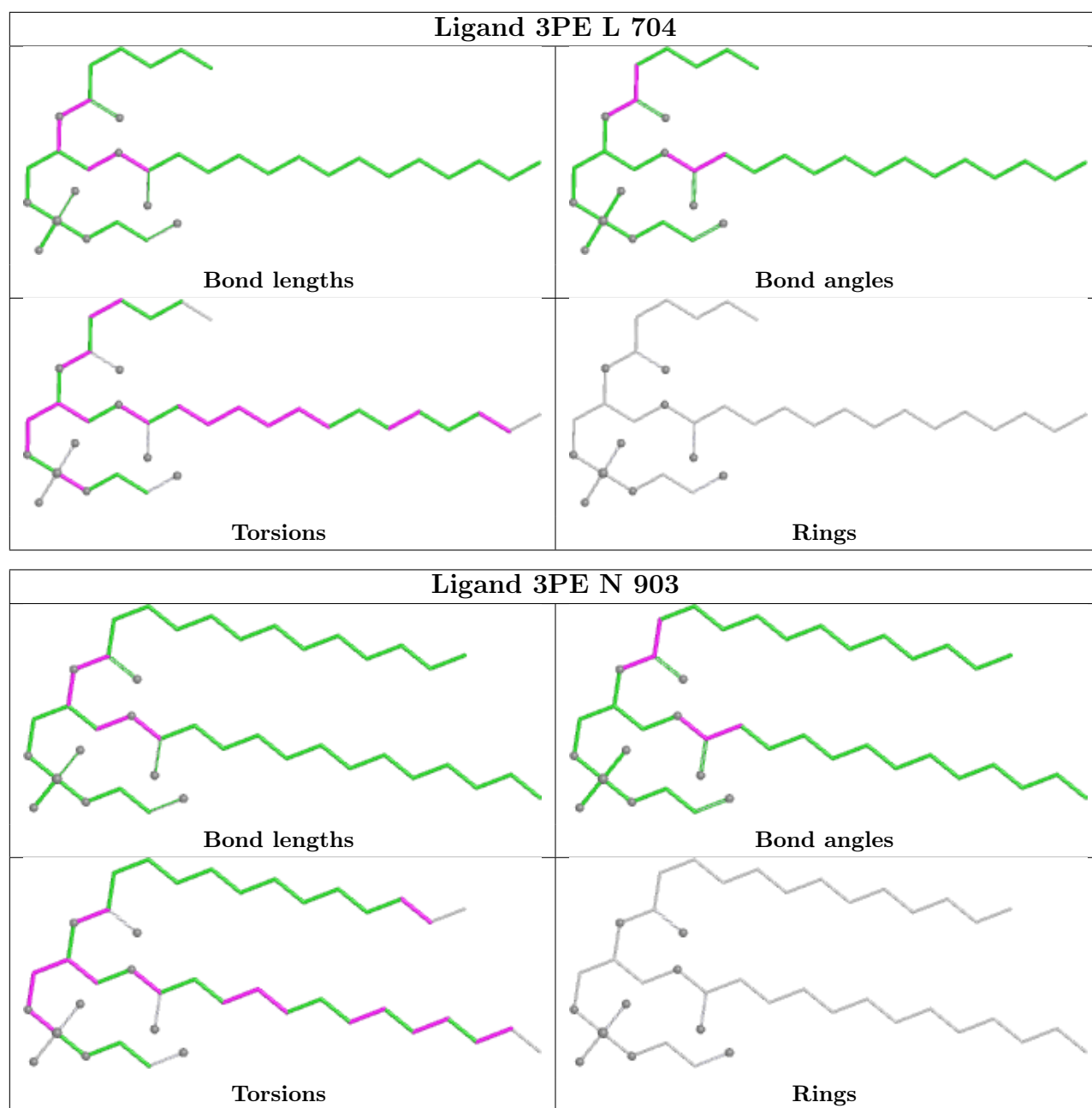
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

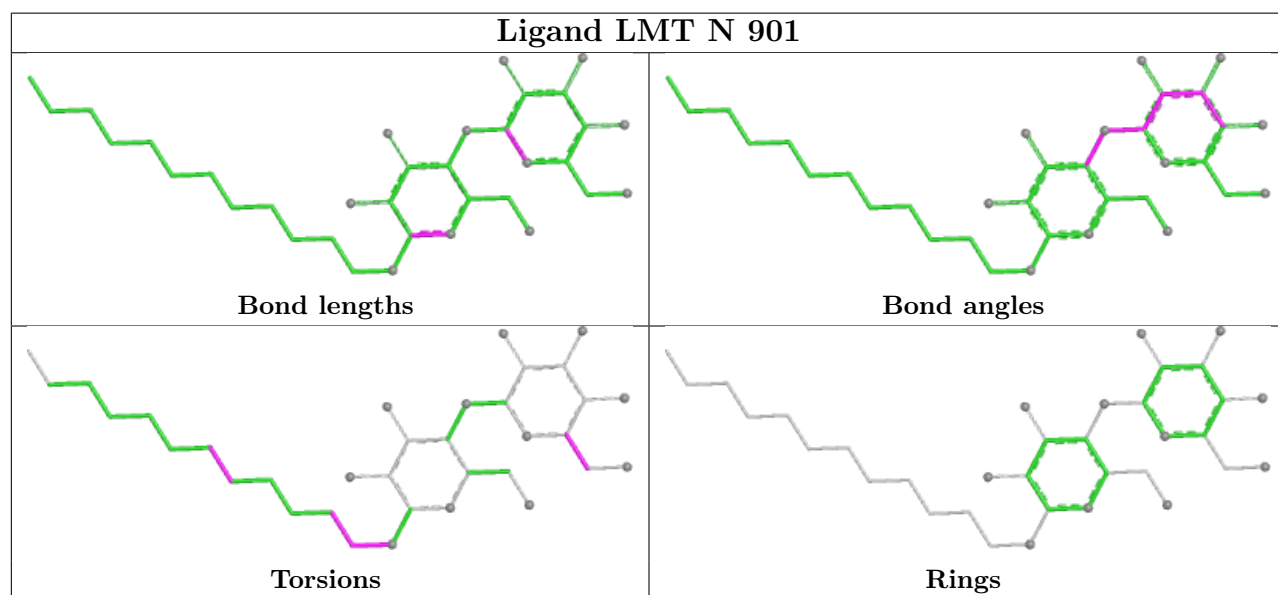
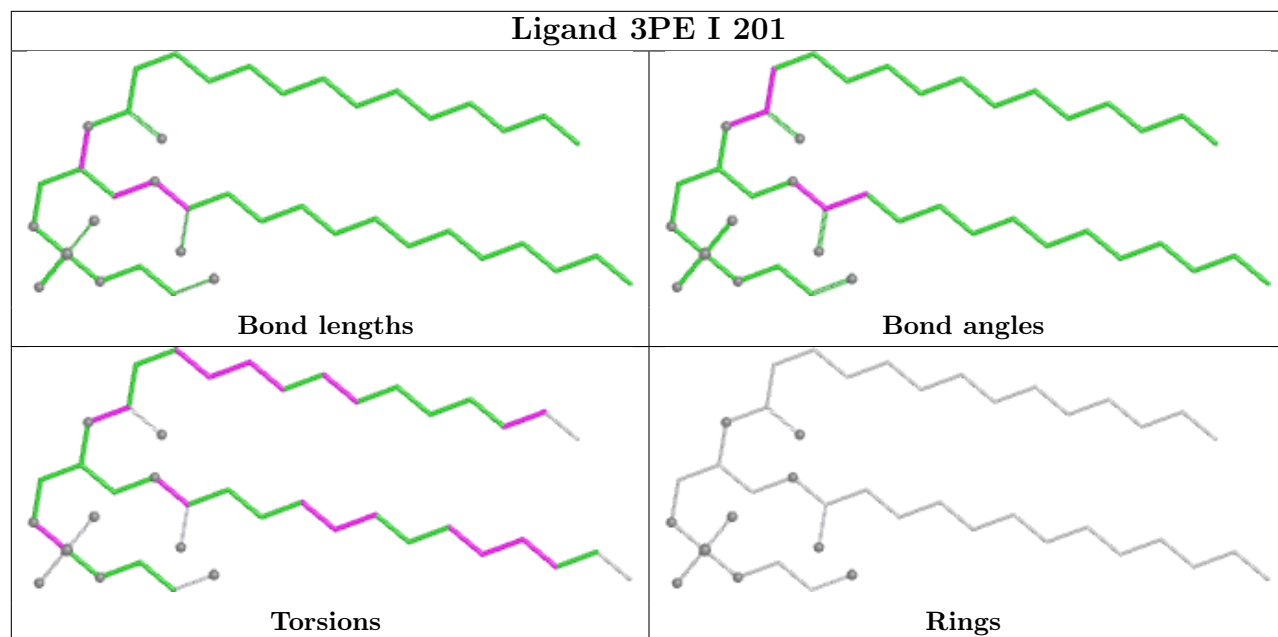


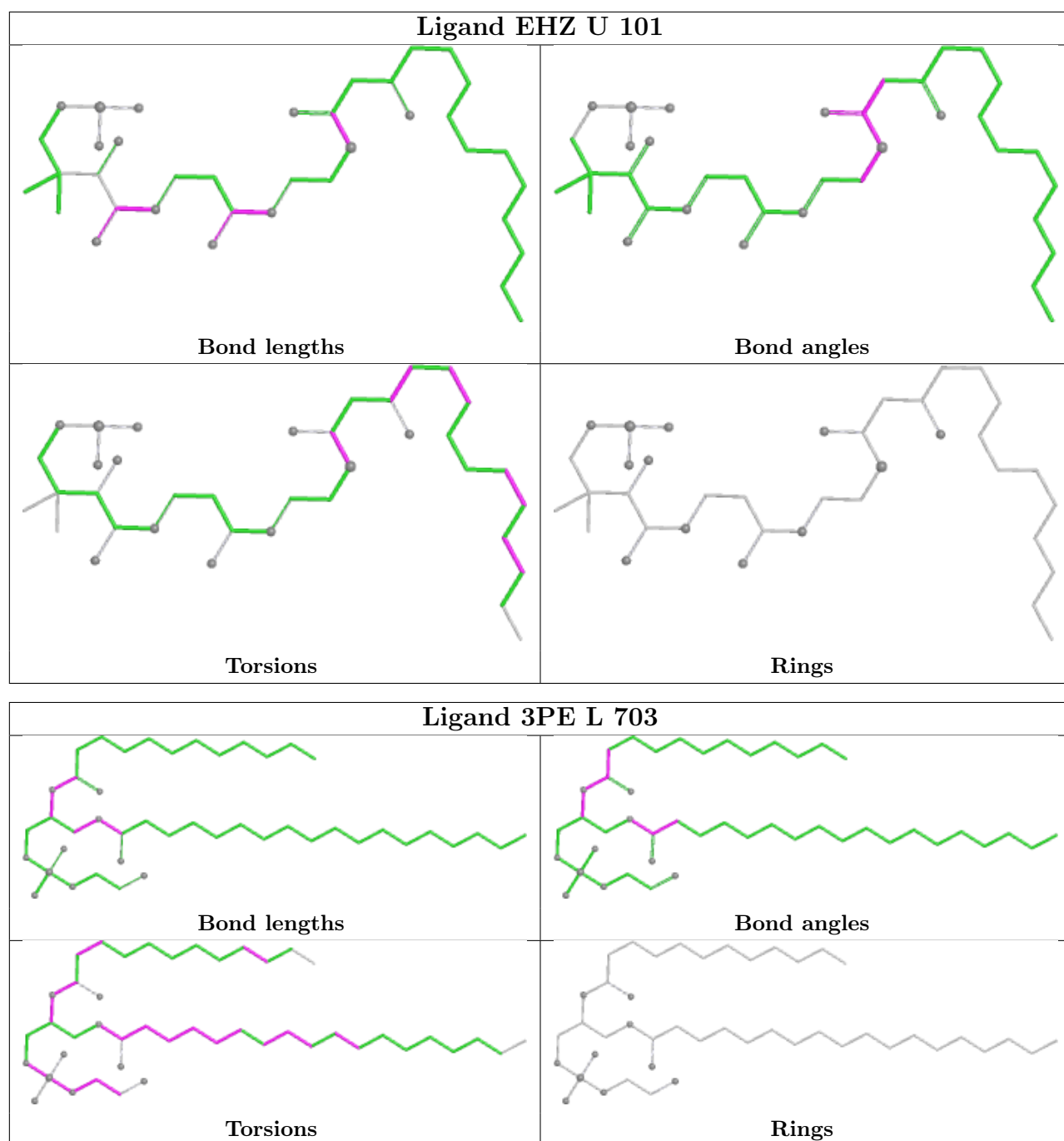


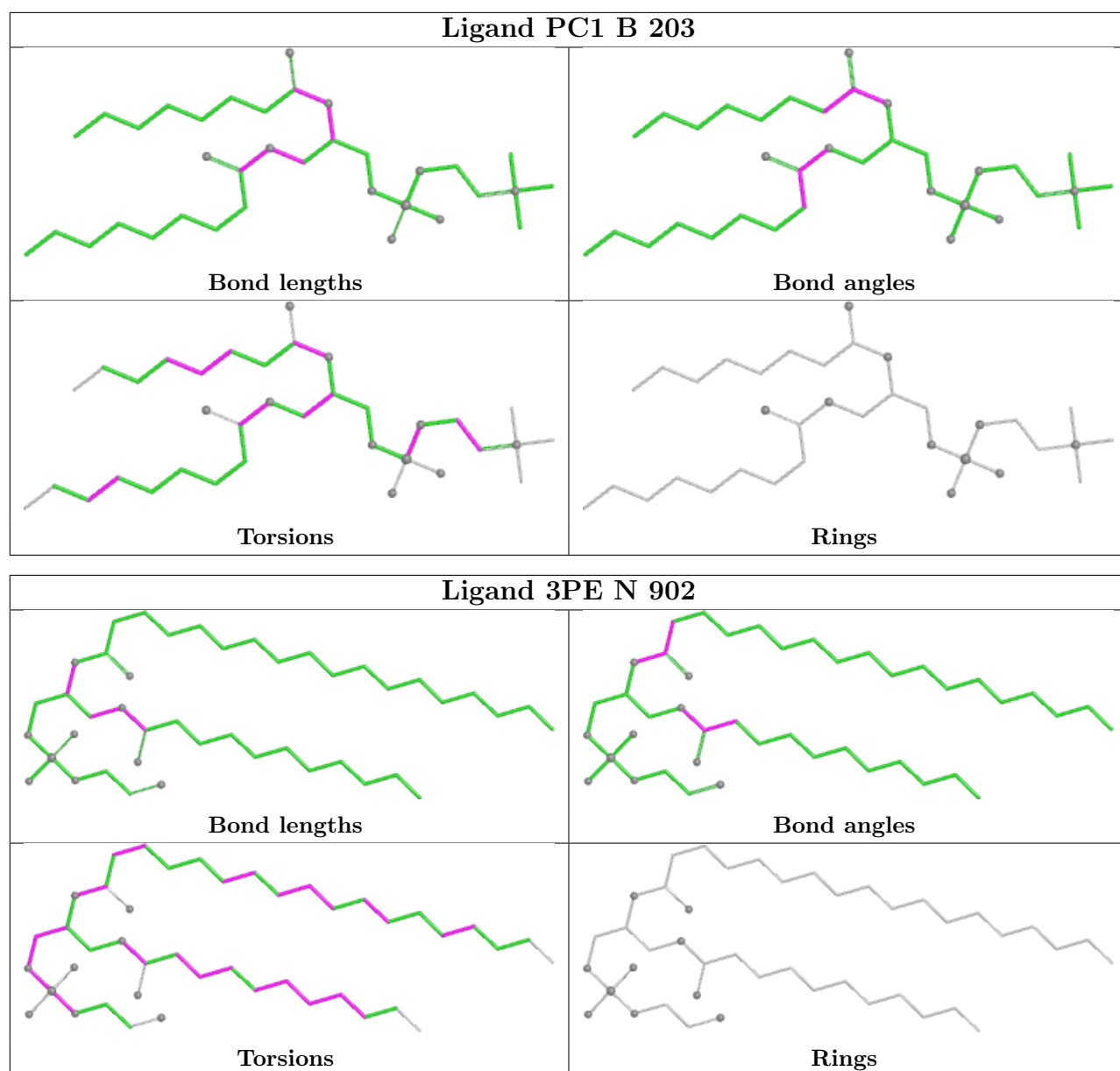


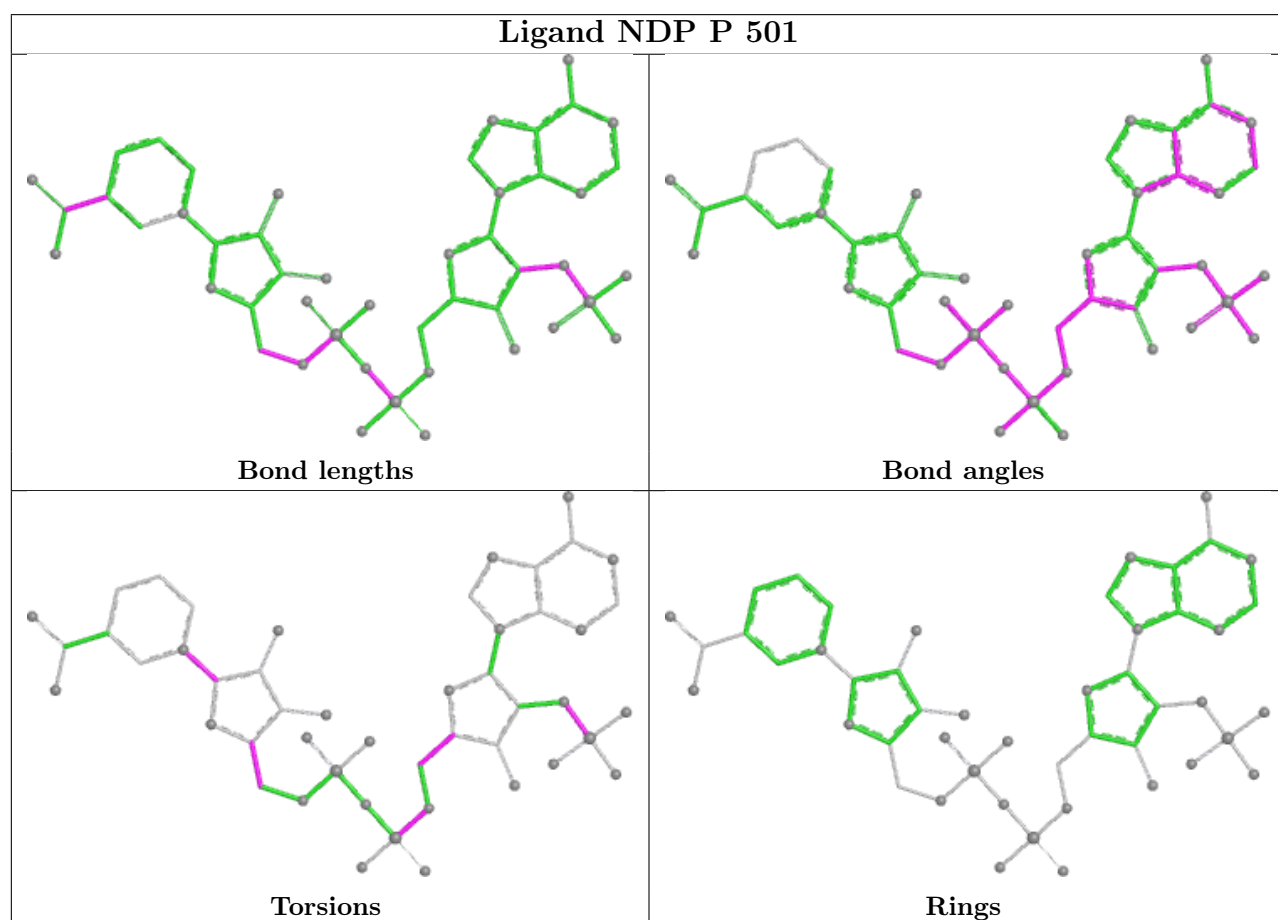
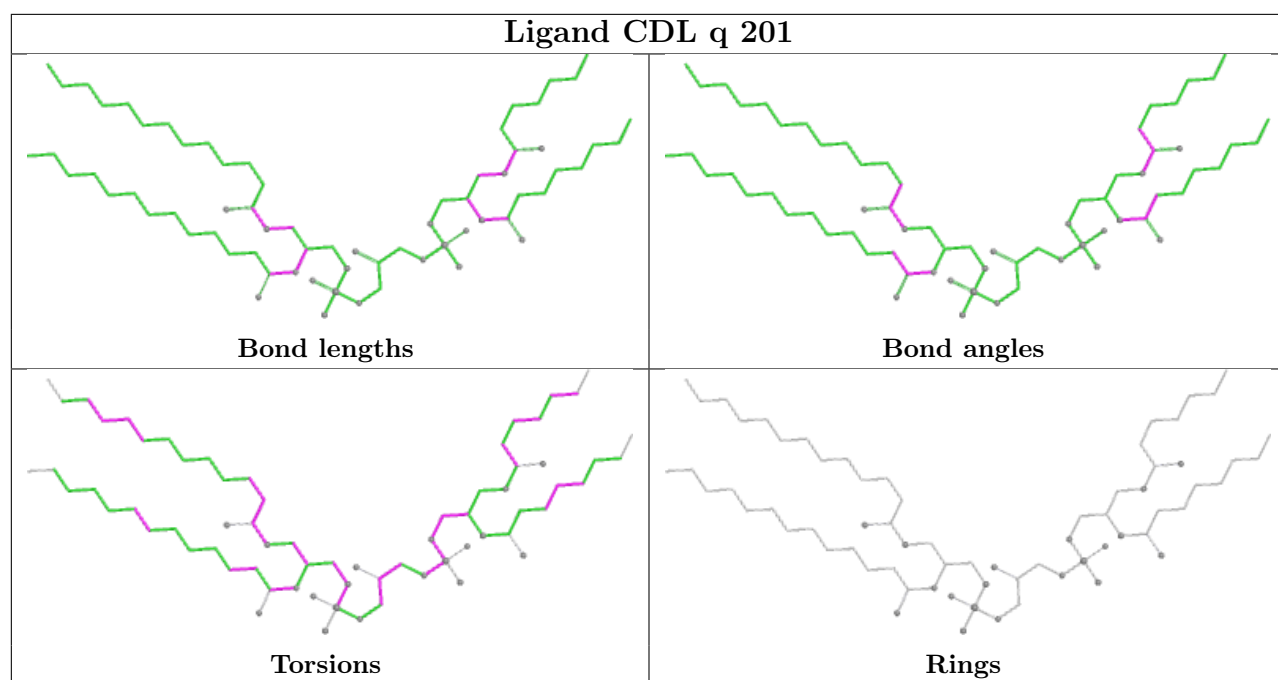


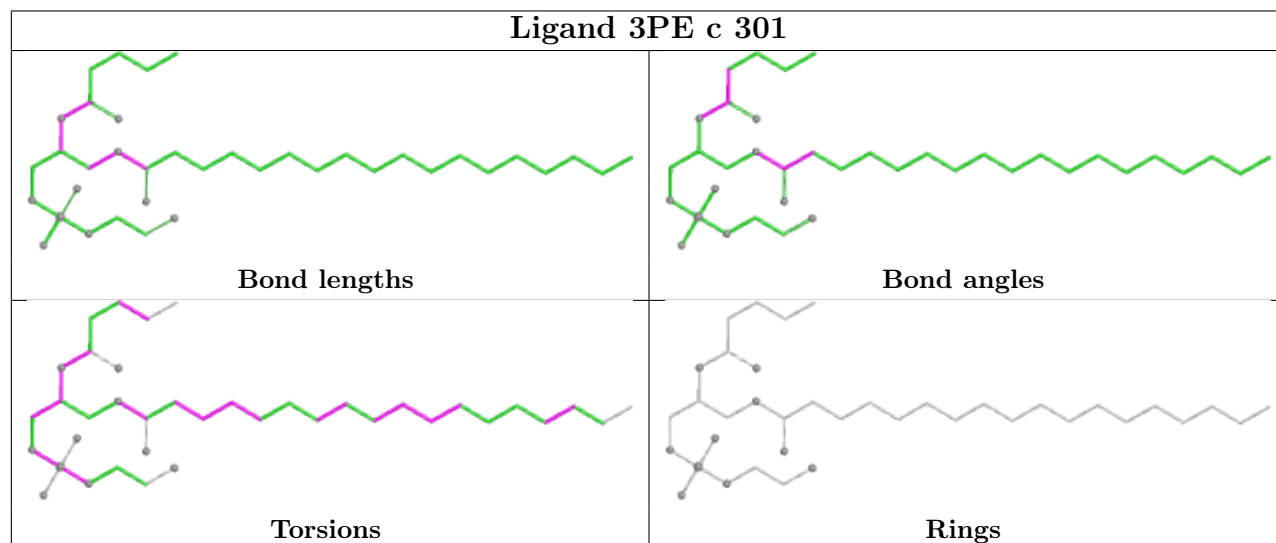
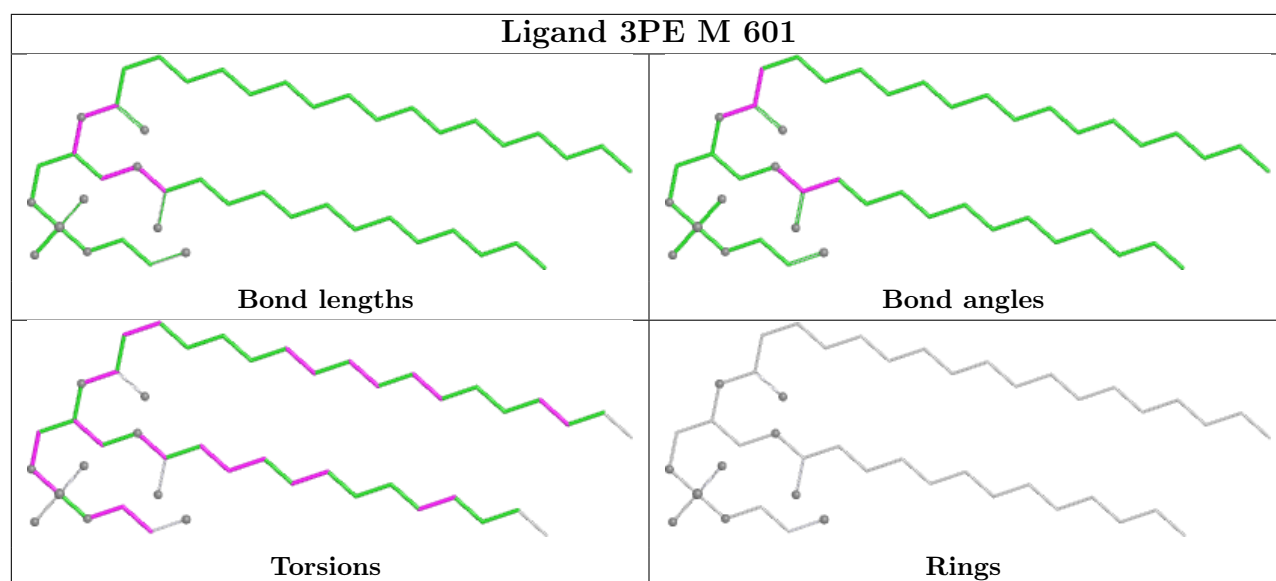


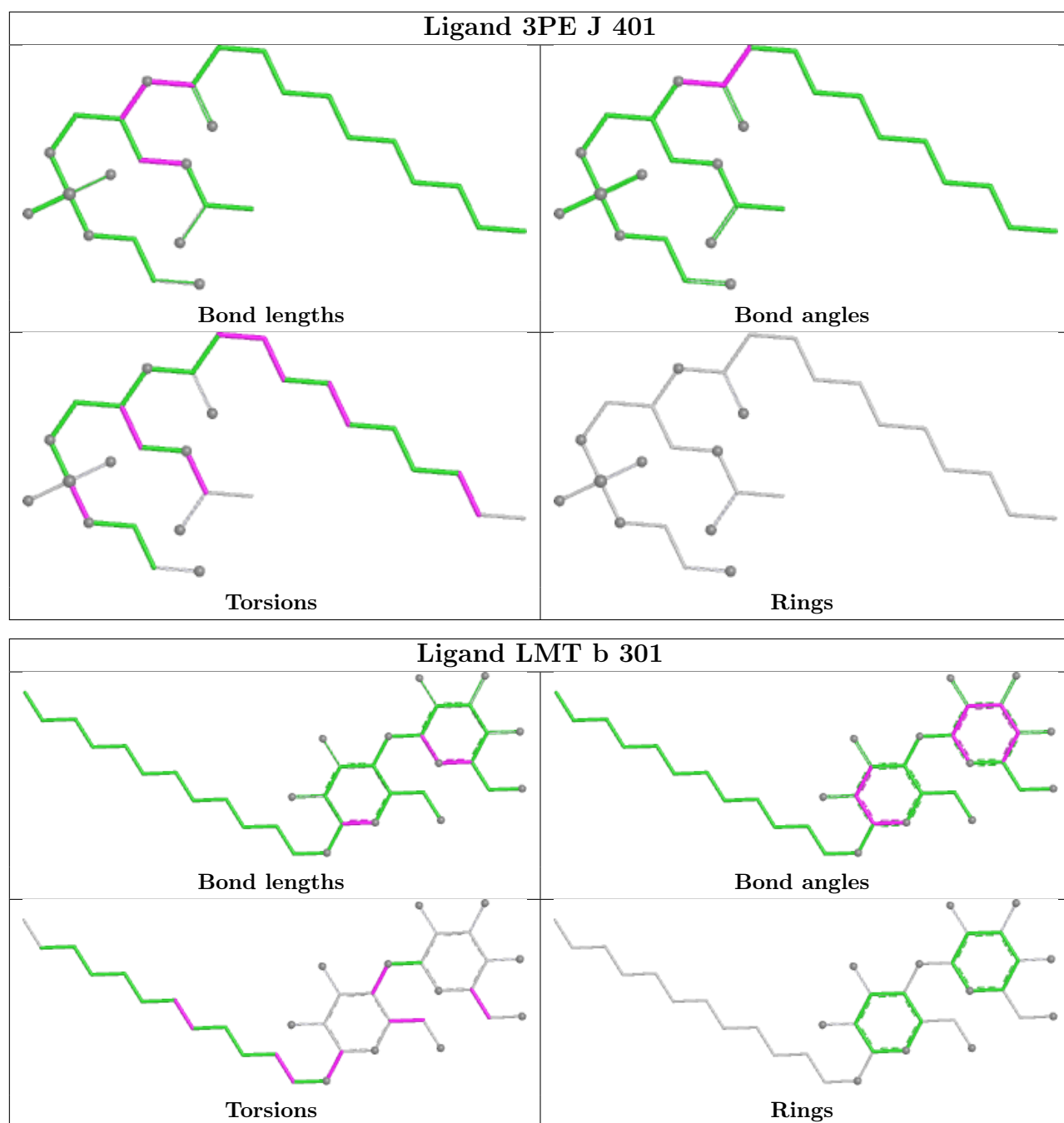


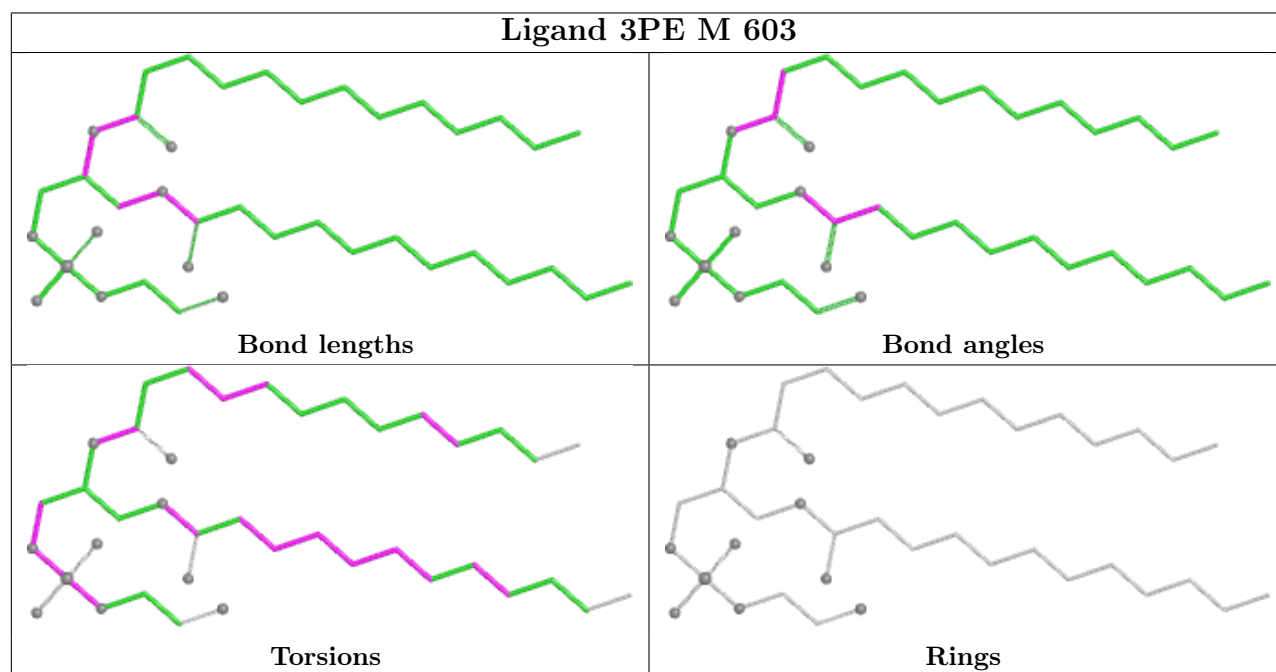
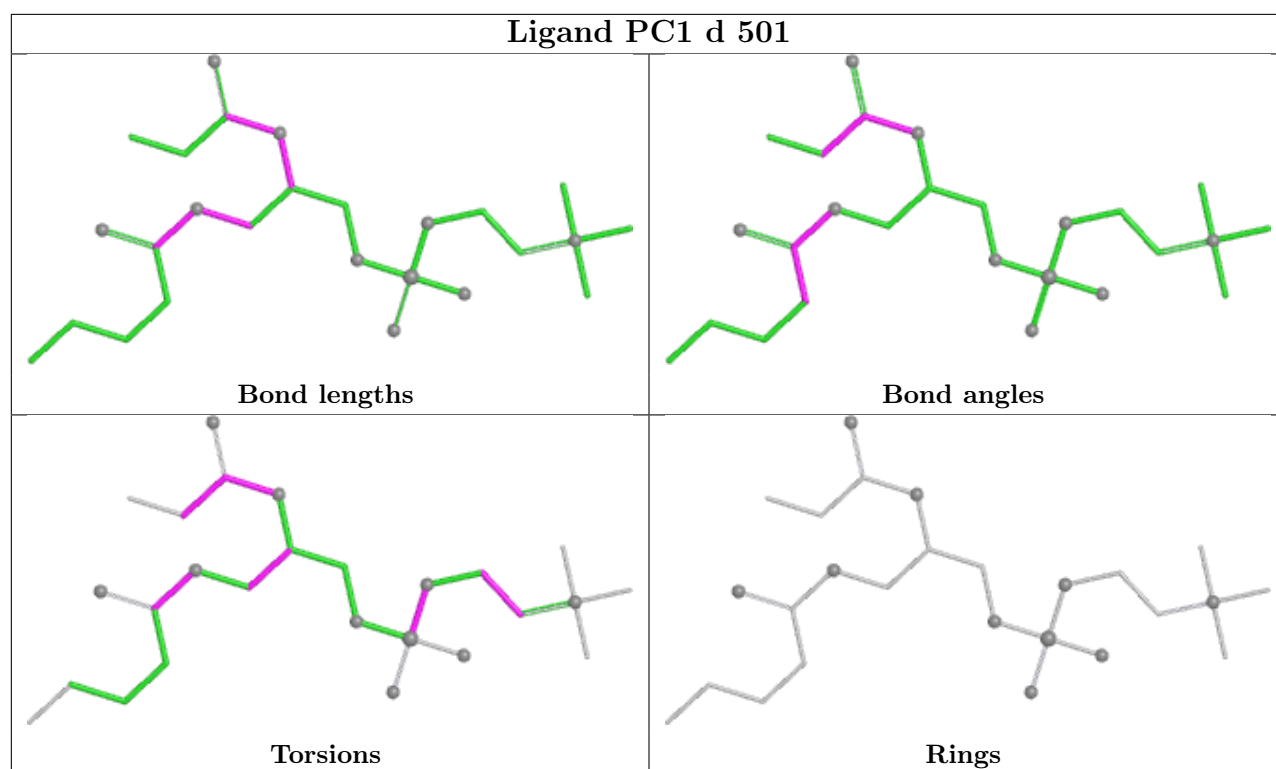


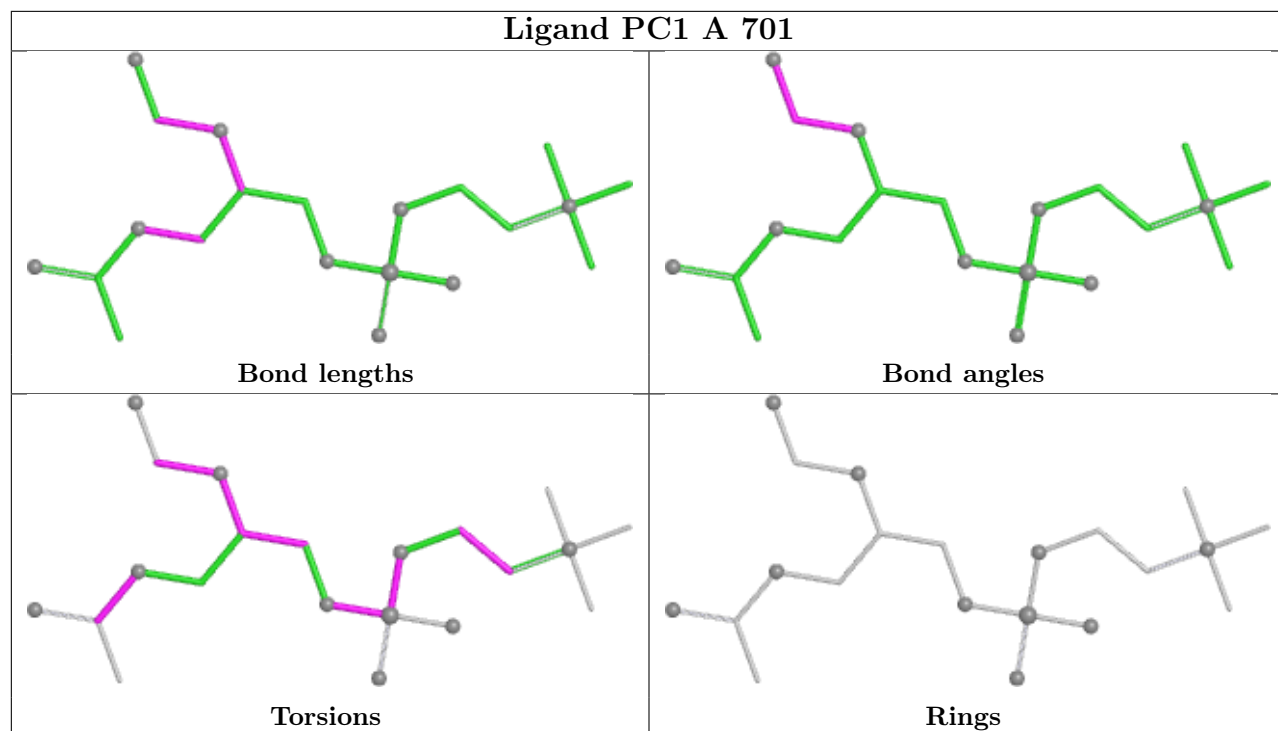


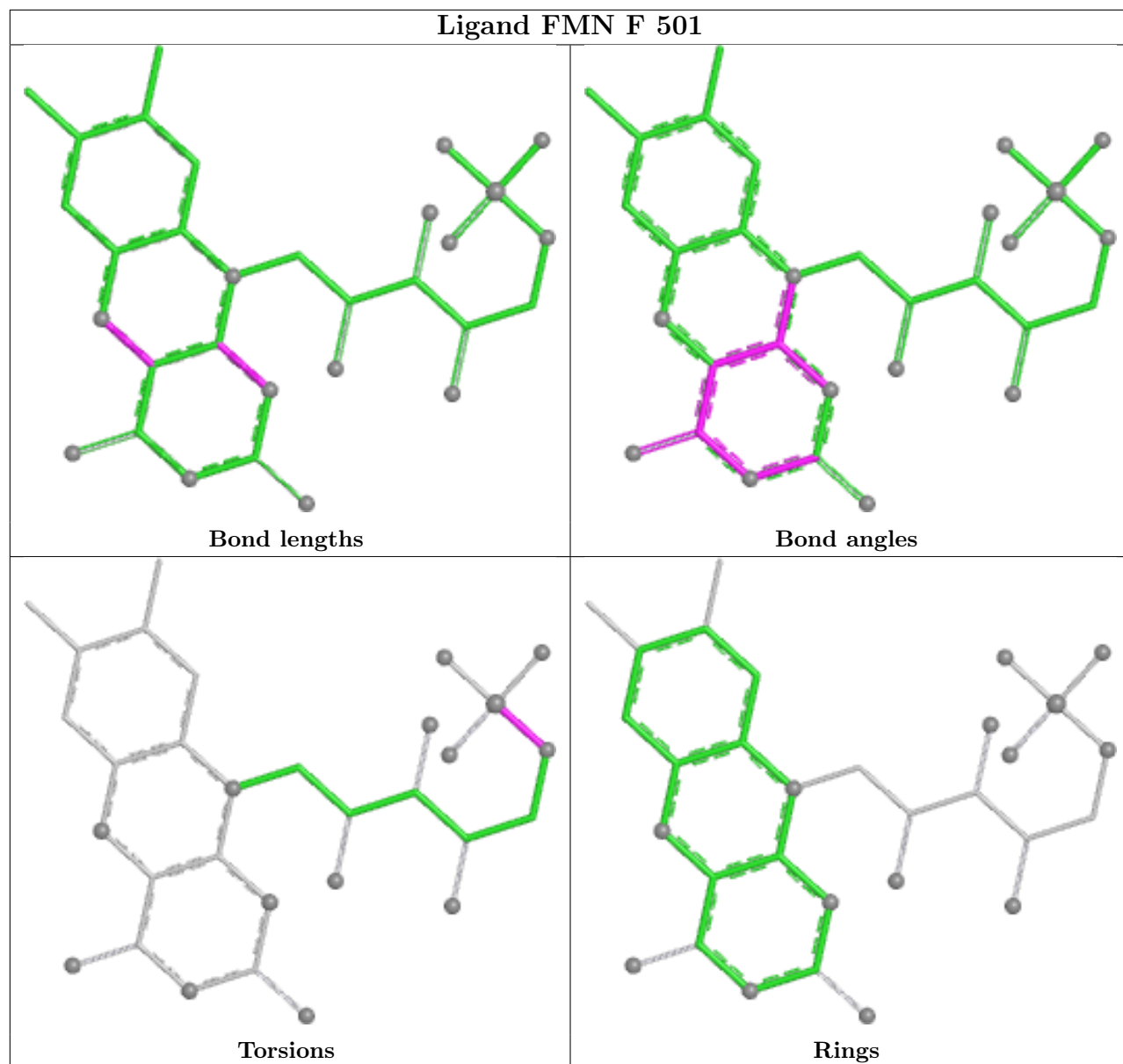


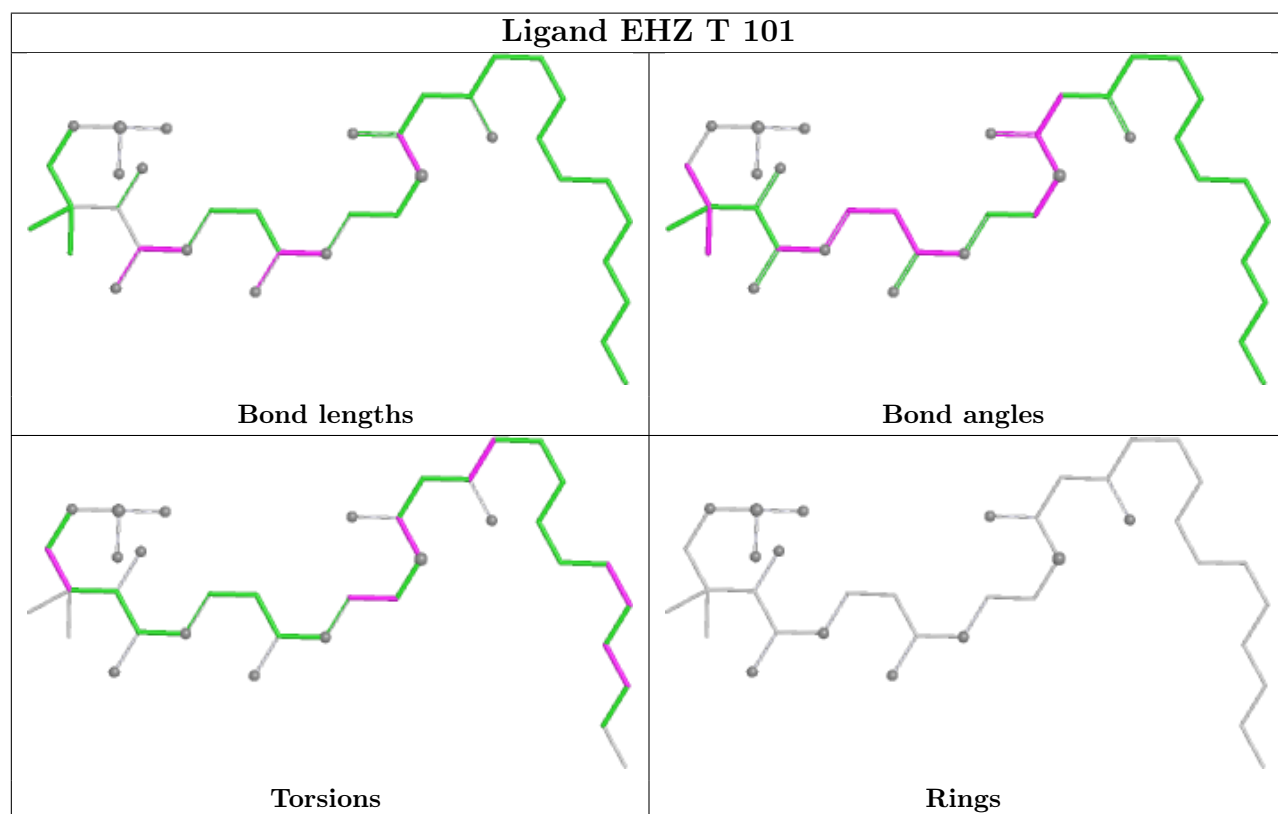
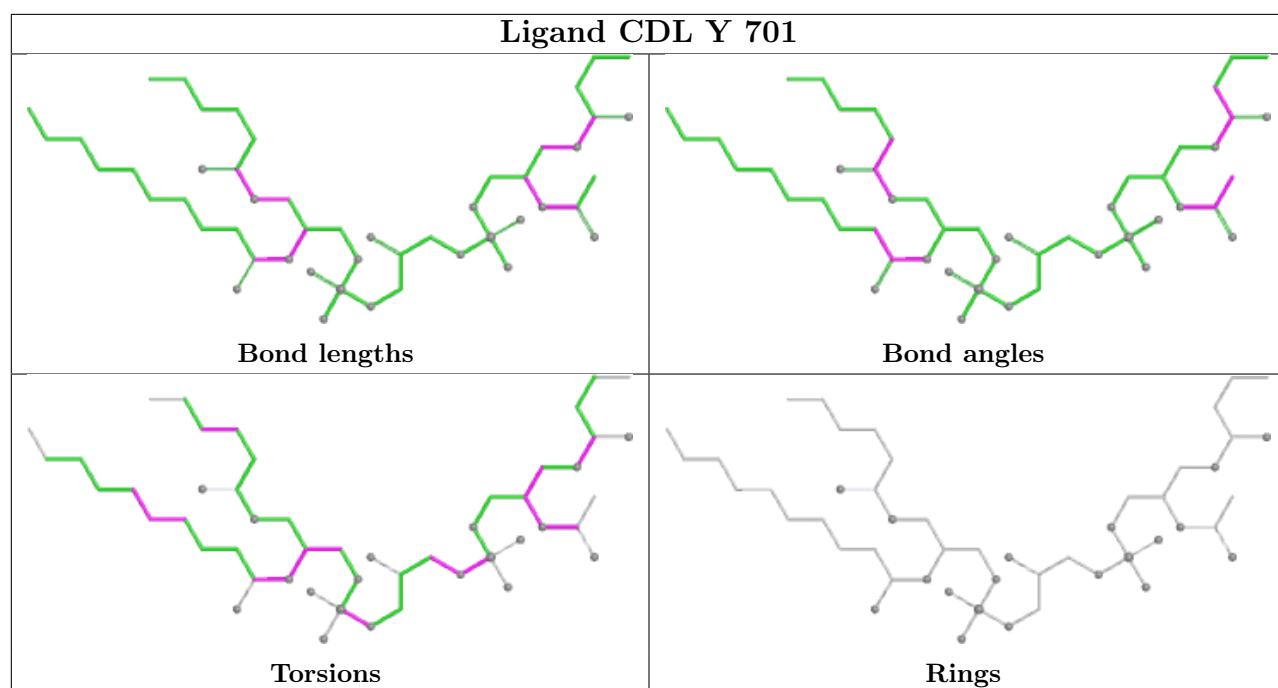


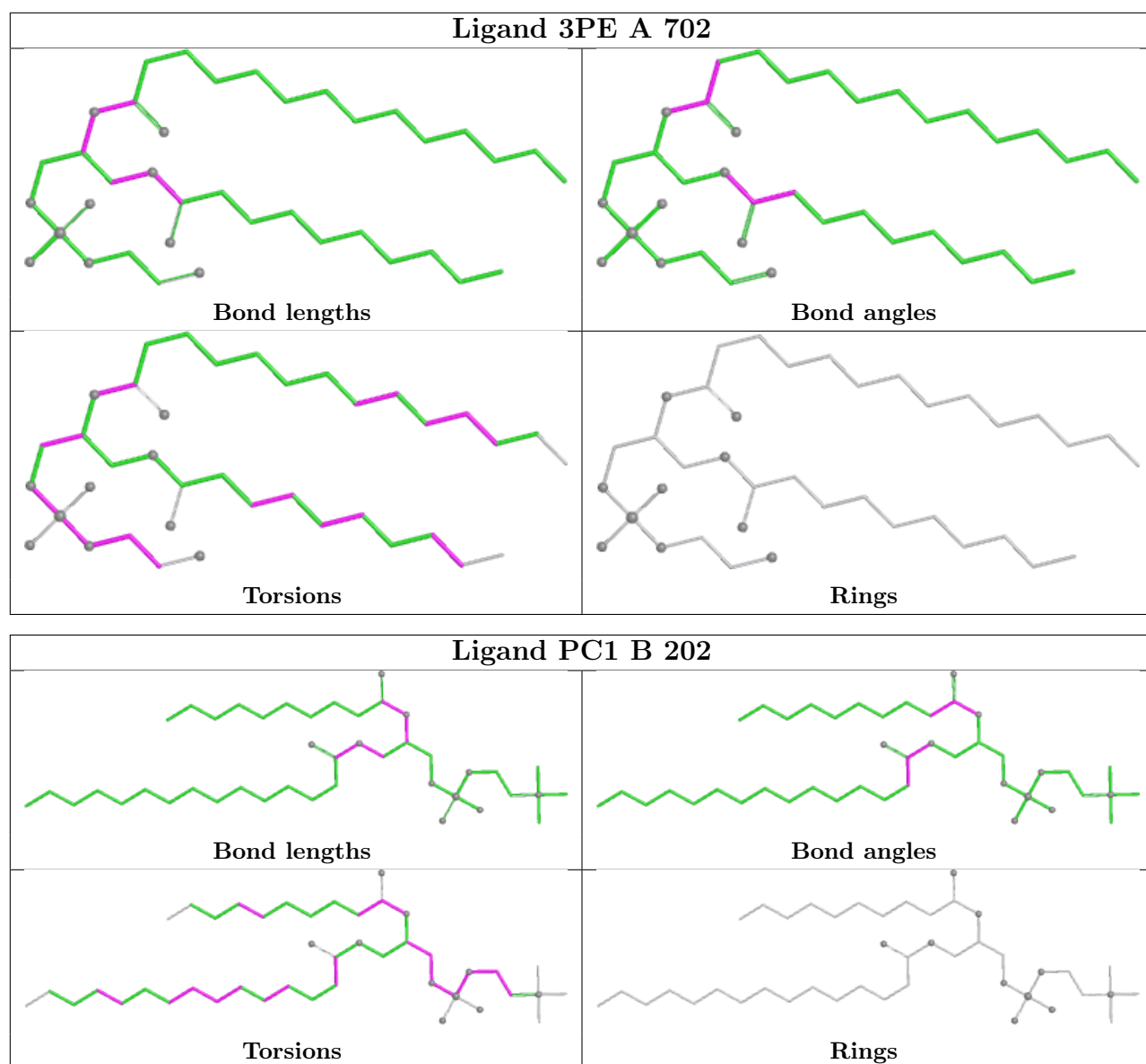












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

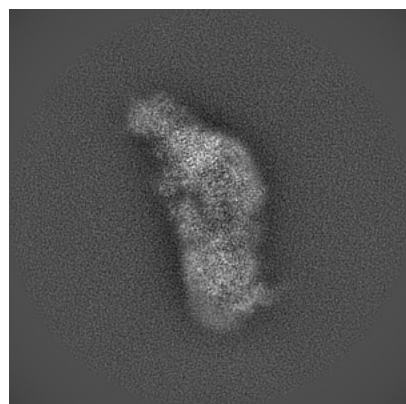
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14127. These allow visual inspection of the internal detail of the map and identification of artifacts.

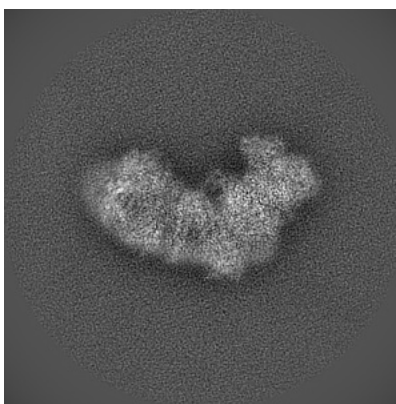
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

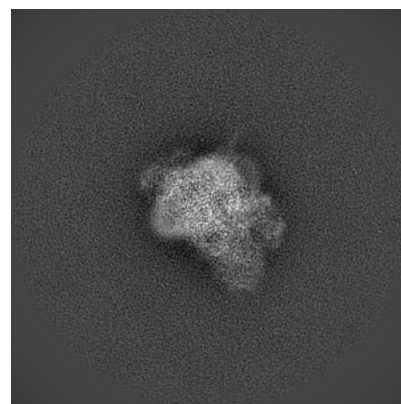
6.1.1 Primary map



X

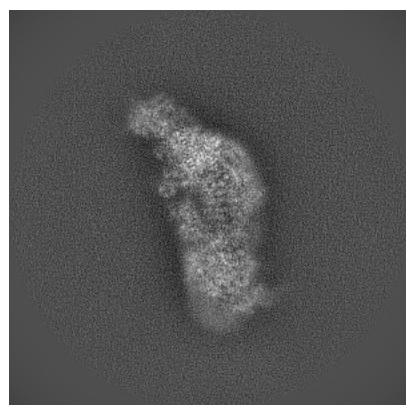


Y

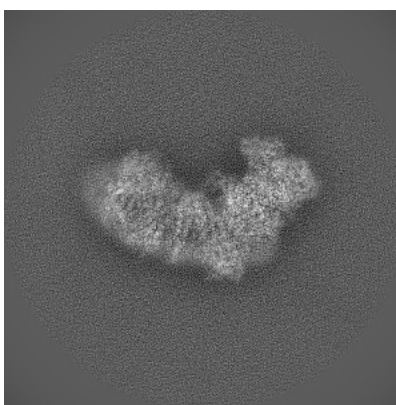


Z

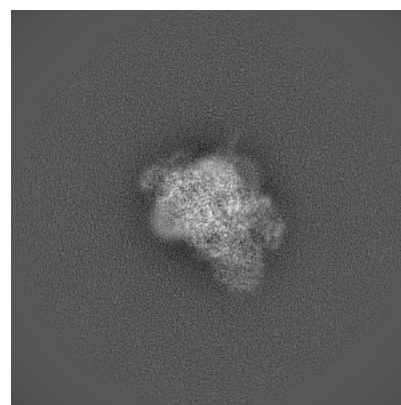
6.1.2 Raw map



X



Y

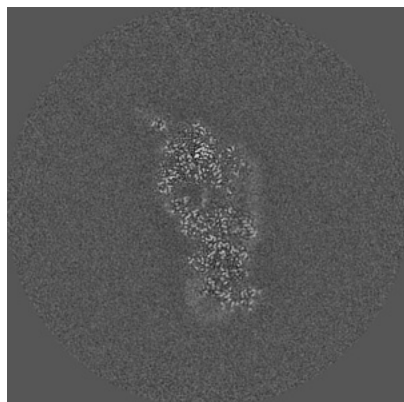


Z

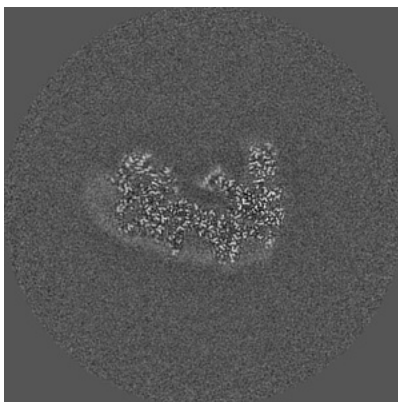
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

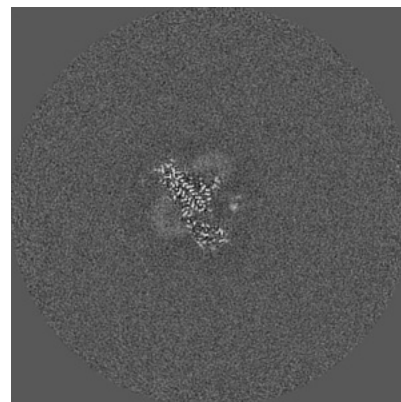
6.2.1 Primary map



X Index: 225

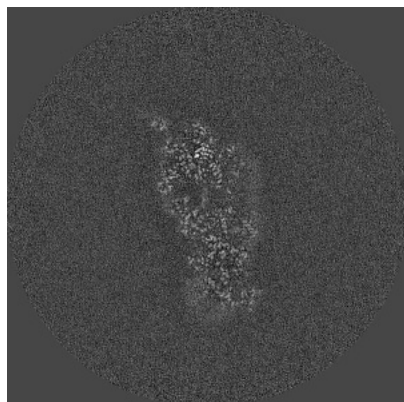


Y Index: 225

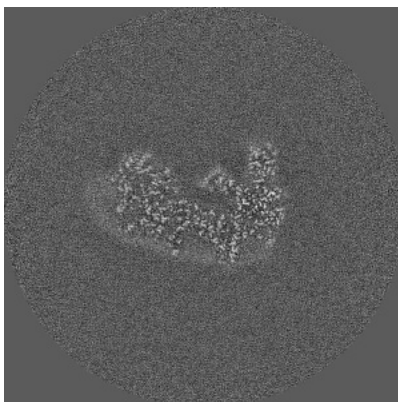


Z Index: 225

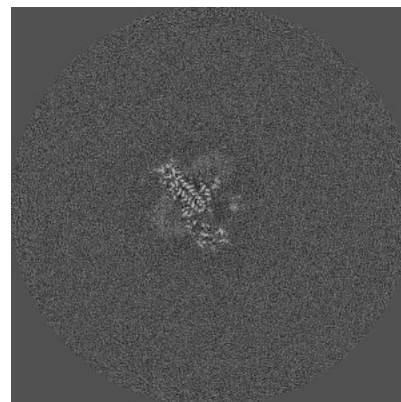
6.2.2 Raw map



X Index: 225



Y Index: 225

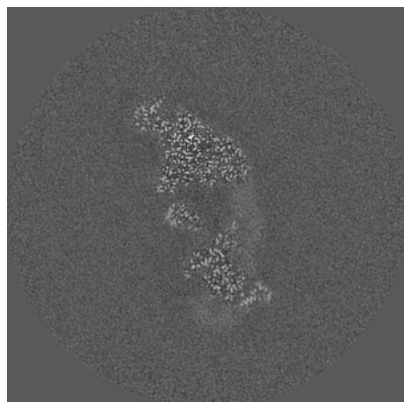


Z Index: 225

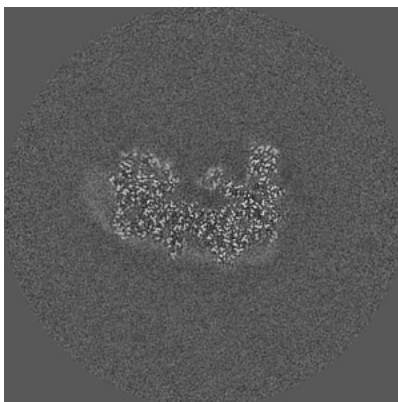
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

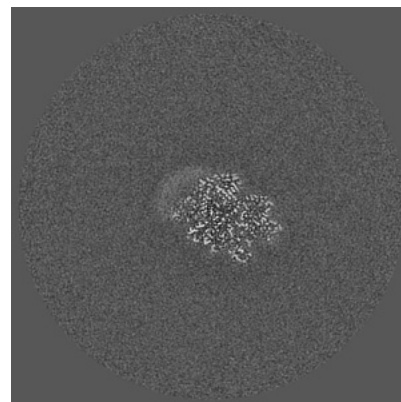
6.3.1 Primary map



X Index: 238

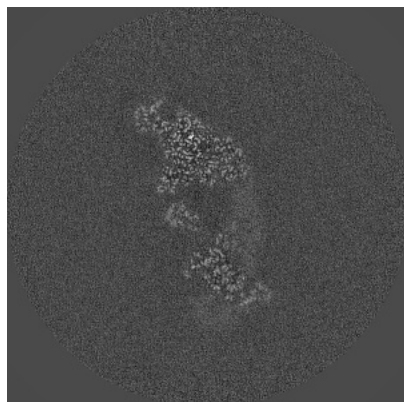


Y Index: 229

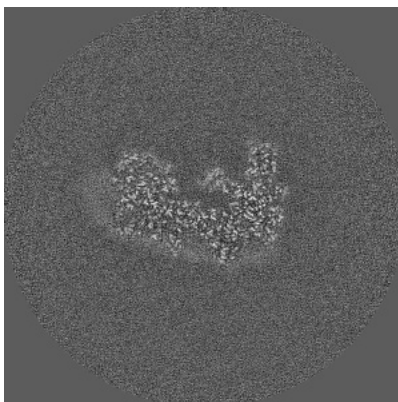


Z Index: 290

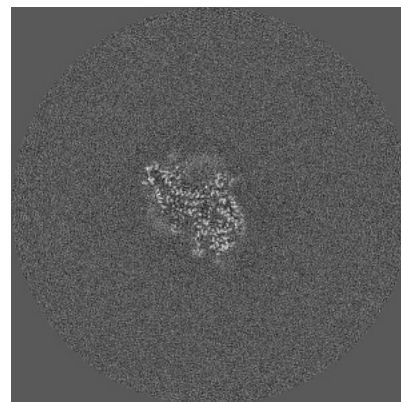
6.3.2 Raw map



X Index: 238



Y Index: 227

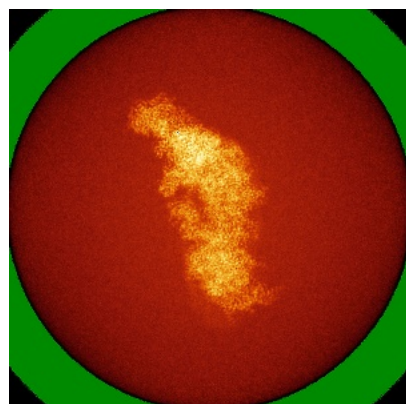


Z Index: 254

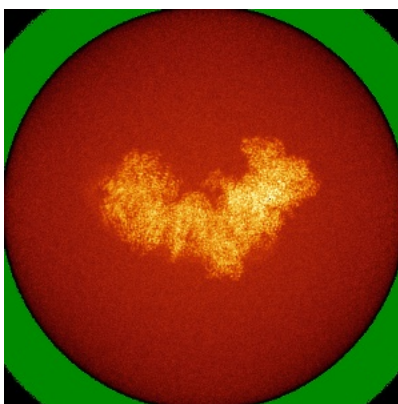
The images above show the largest variance slices of the map in three orthogonal directions.

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

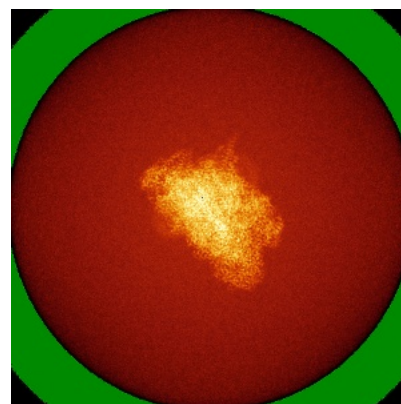
6.4.1 Primary map



X

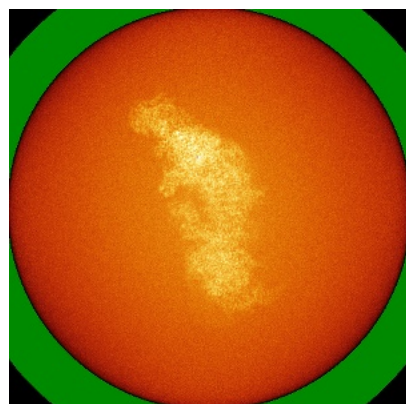


Y

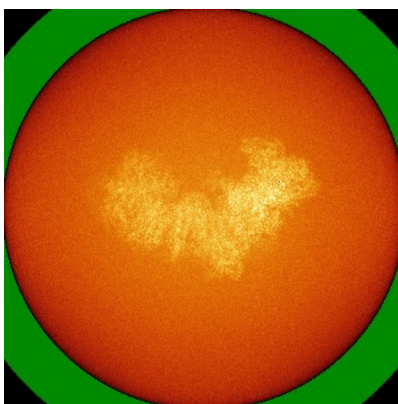


Z

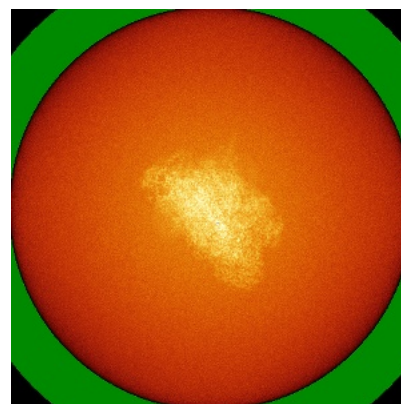
6.4.2 Raw map



X



Y

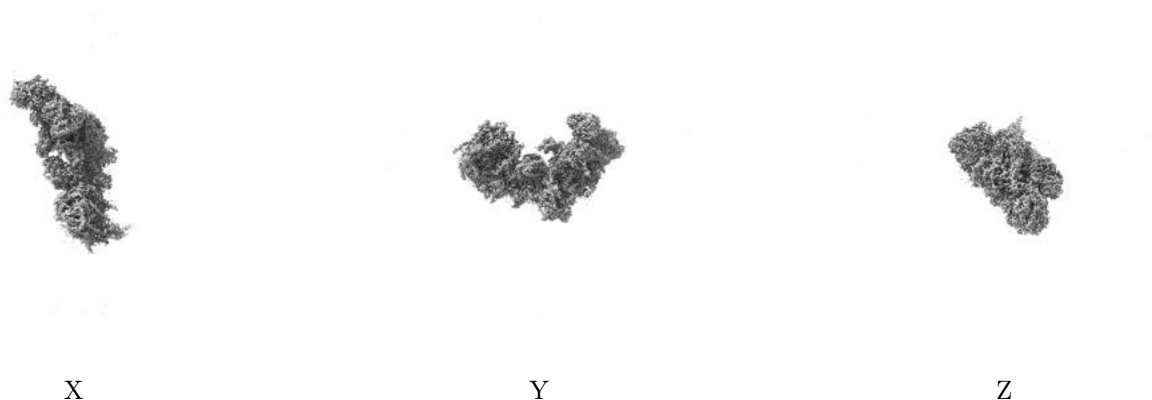


Z

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

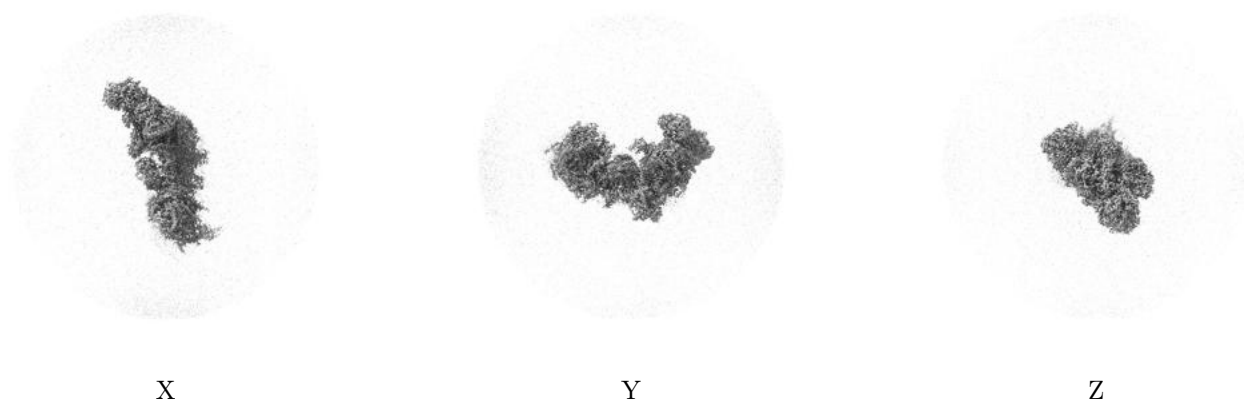
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

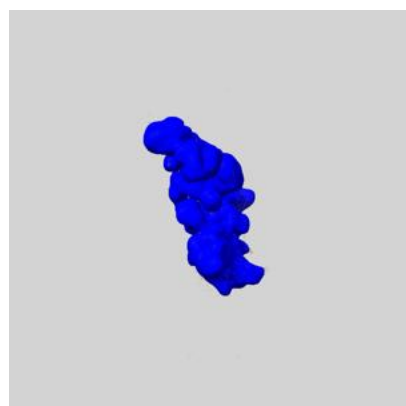
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

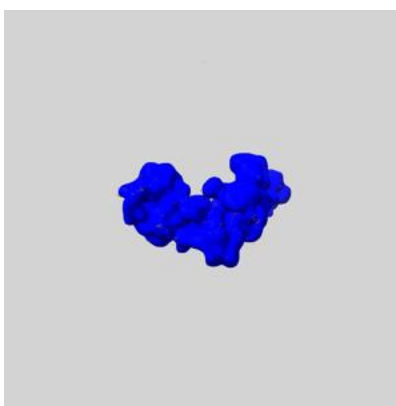
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

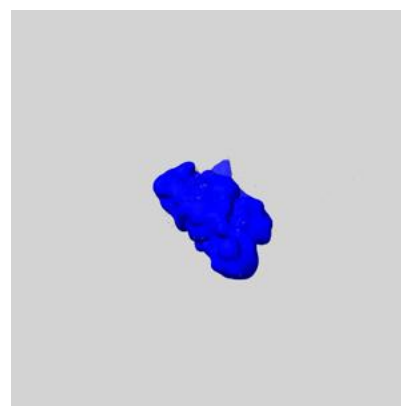
6.6.1 emd_14127_msk_1.map [i](#)



X



Y

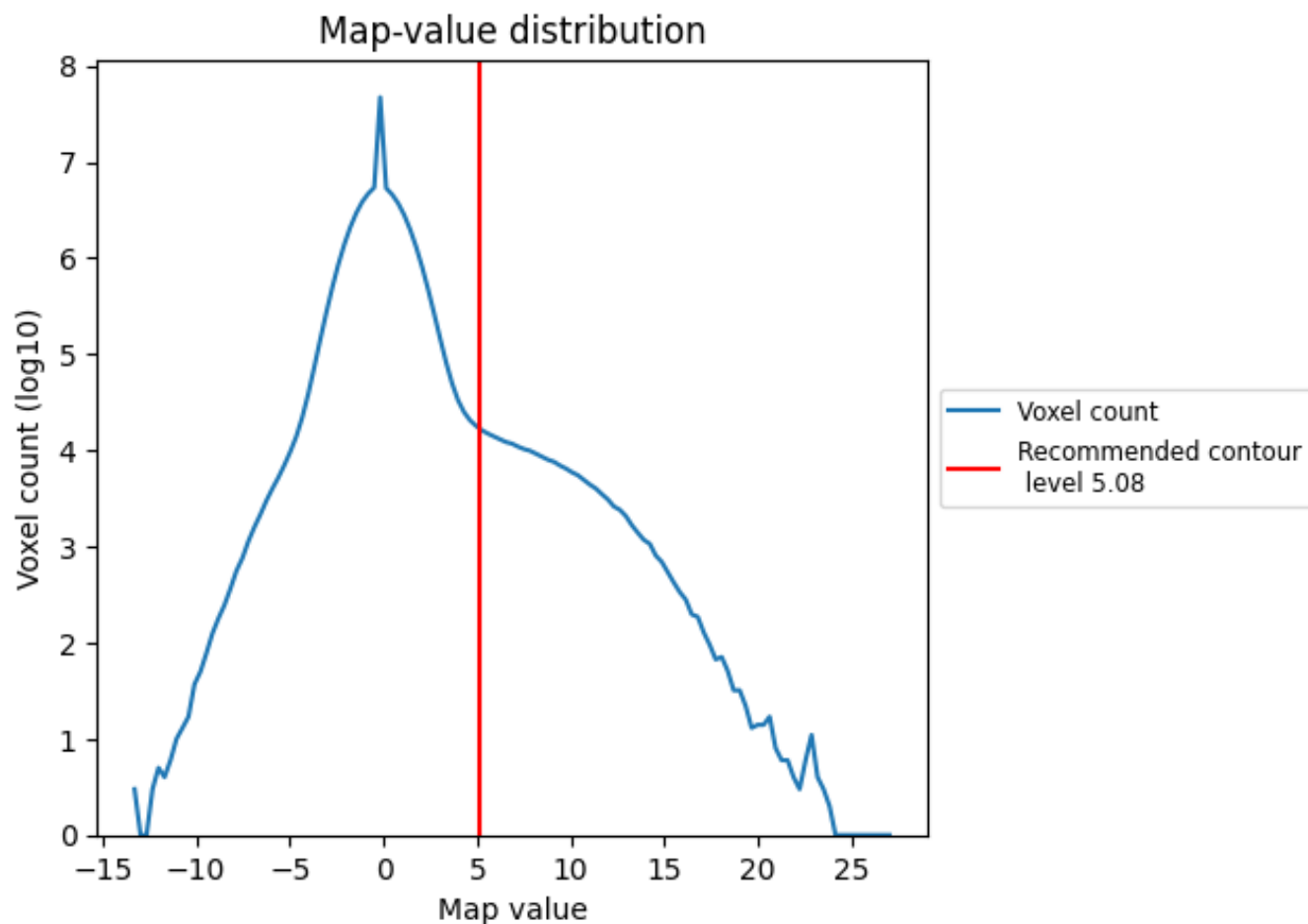


Z

7 Map analysis [i](#)

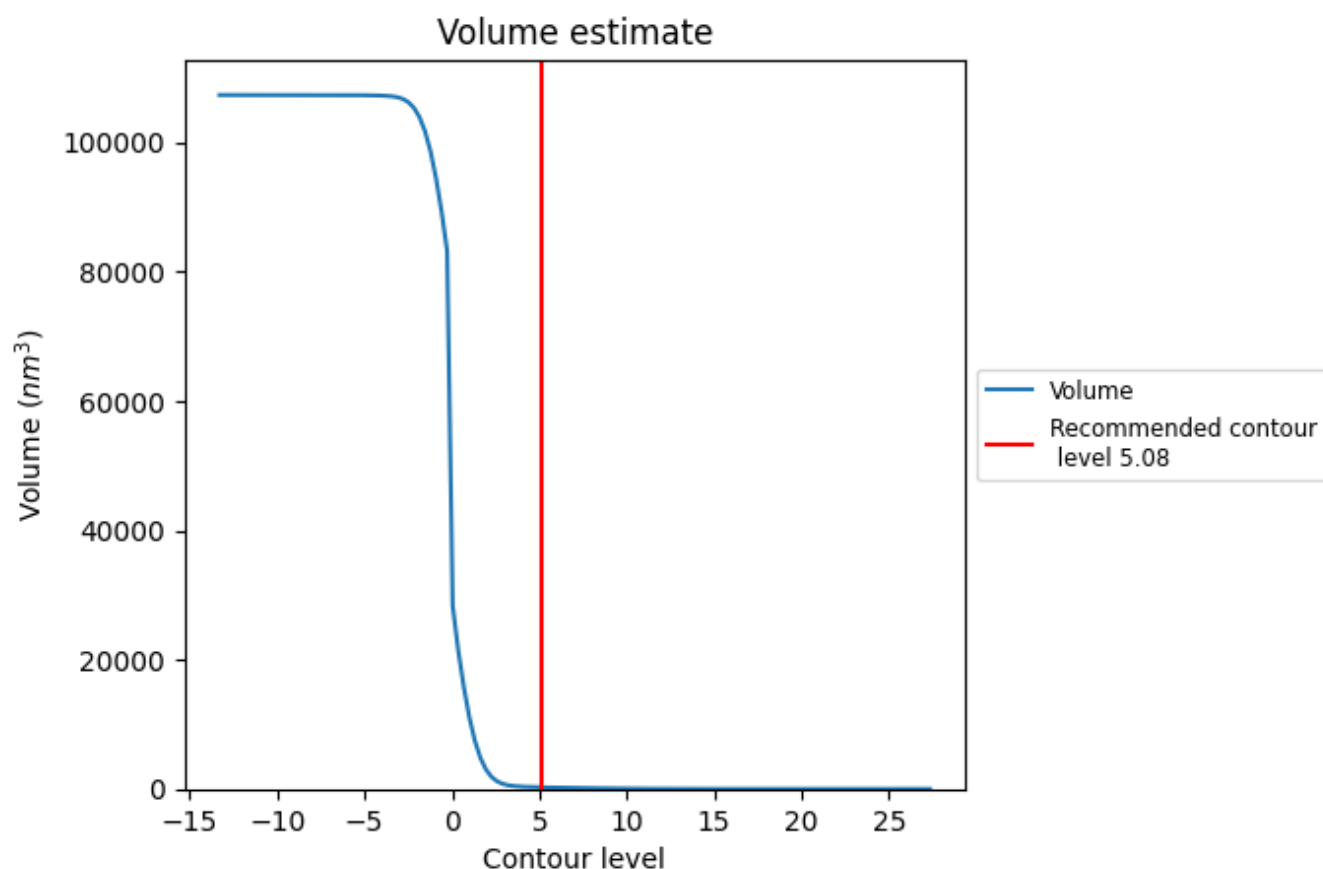
This section contains the results of statistical analysis of the map.

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.

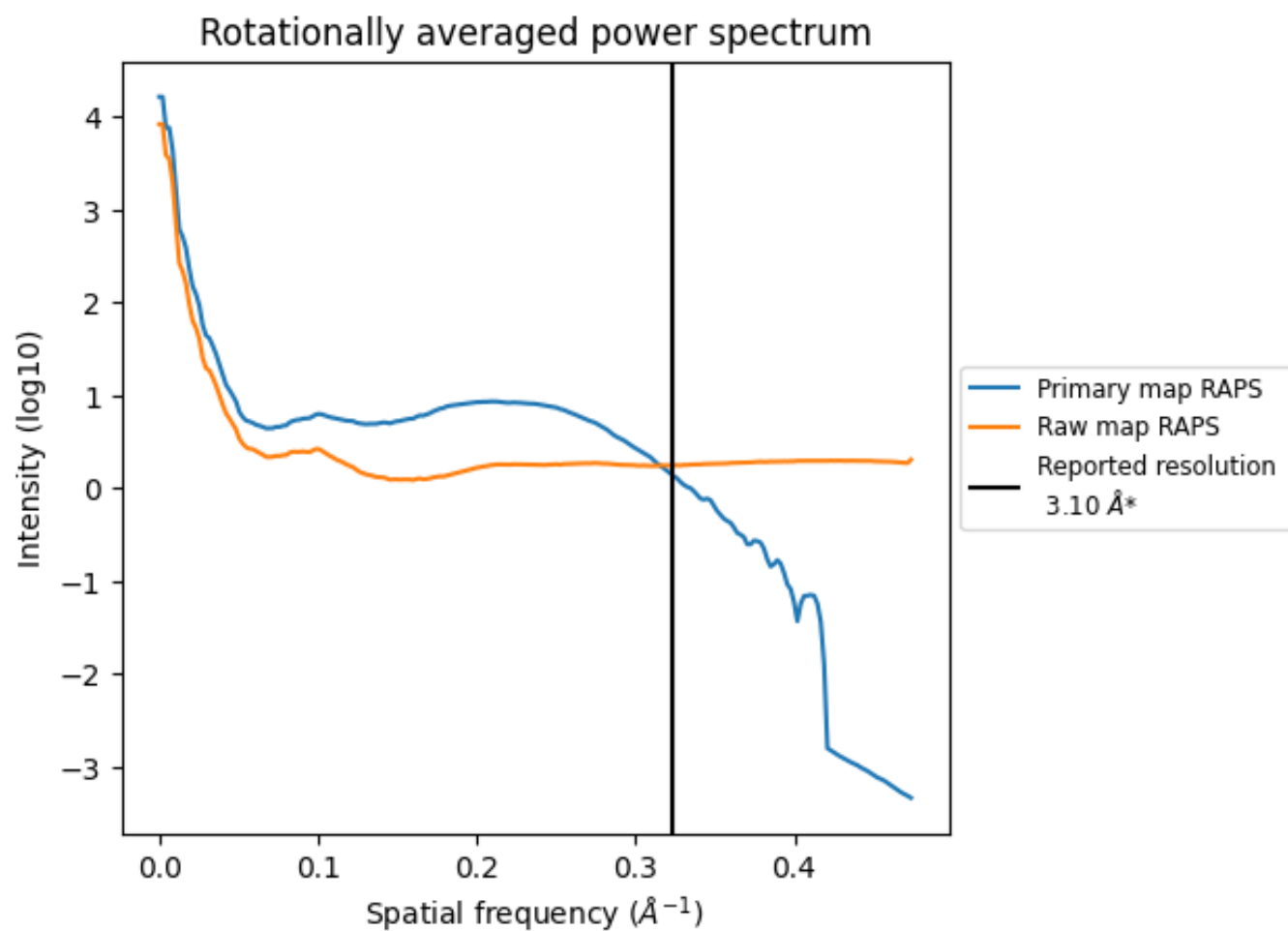
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 257 nm^3 ; this corresponds to an approximate mass of 232 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

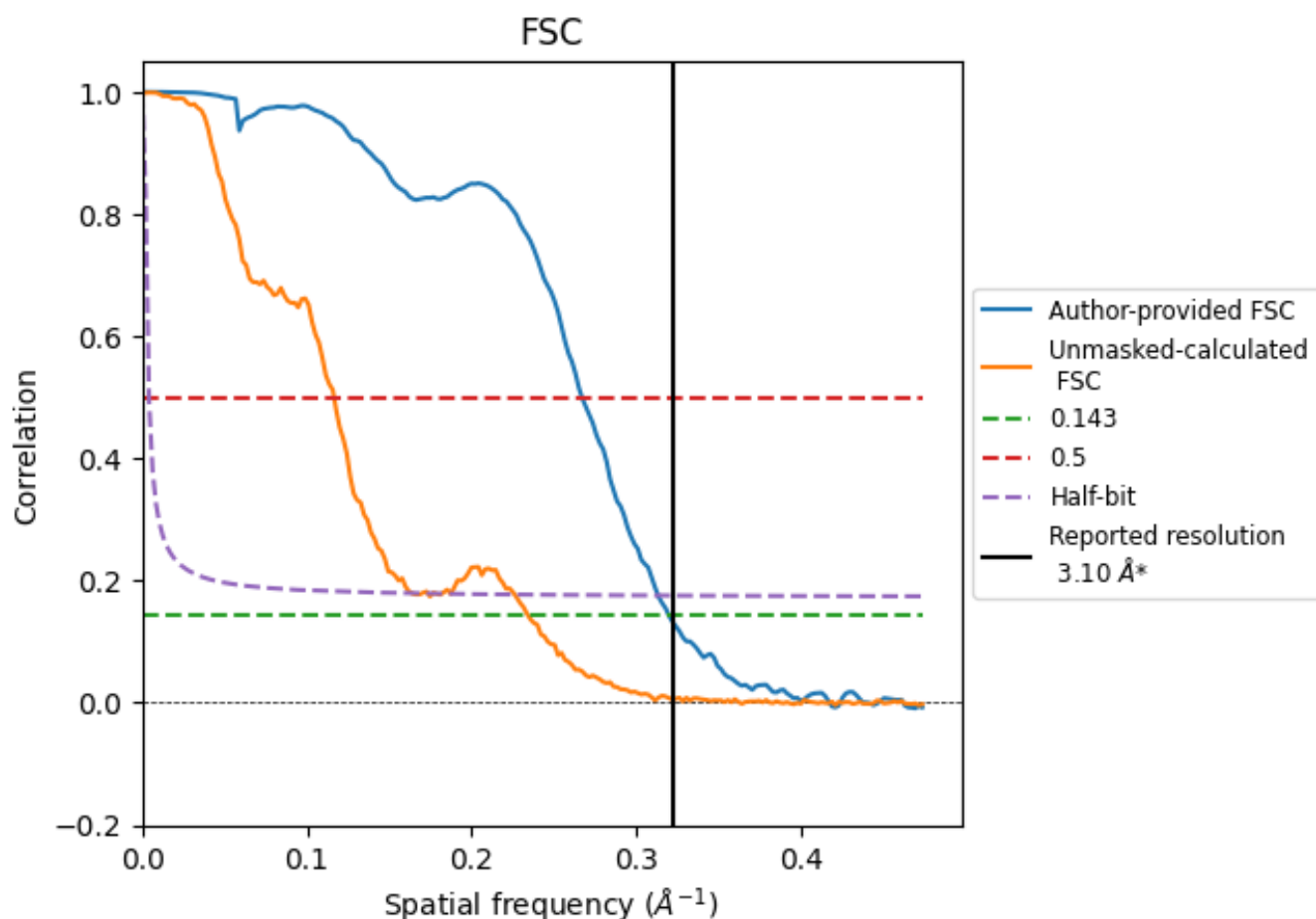


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

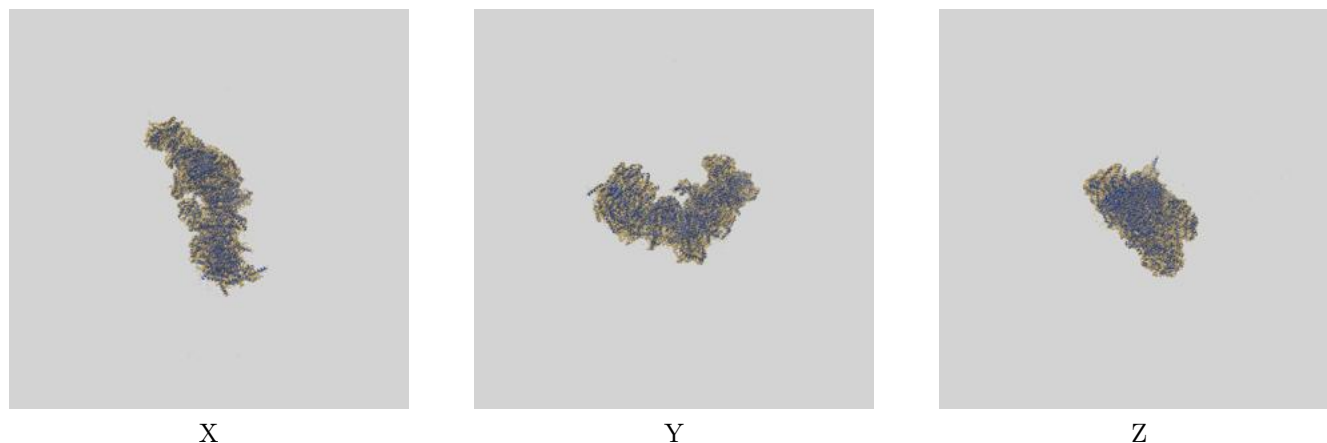
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.13	3.75	3.19
Unmasked-calculated*	4.27	8.58	6.11

*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 4.27 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

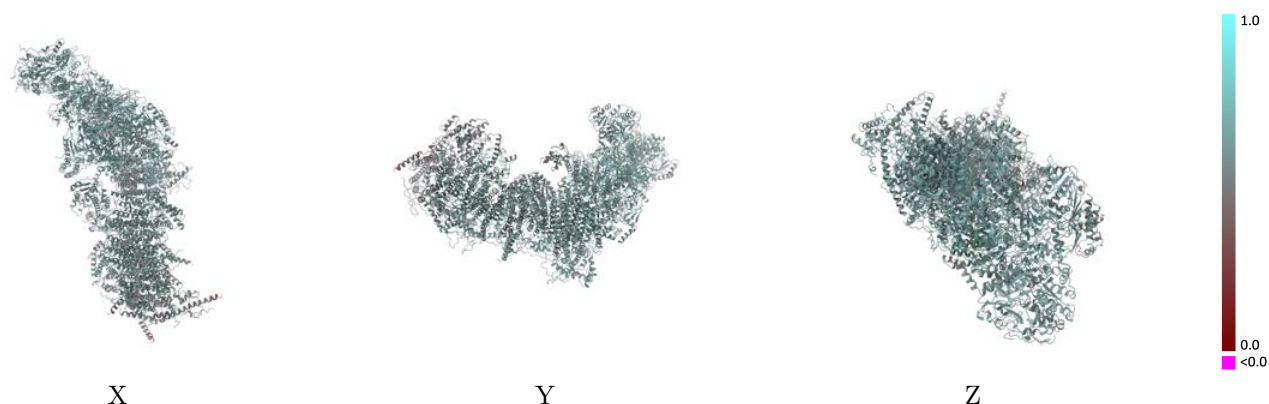
This section contains information regarding the fit between EMDB map EMD-14127 and PDB model 7QSD. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



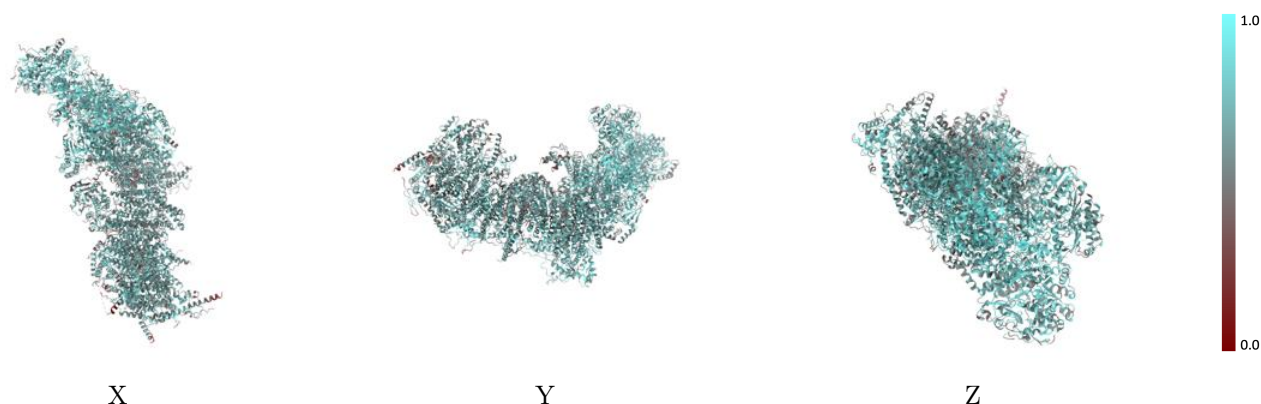
The images above show the 3D surface view of the map at the recommended contour level 5.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



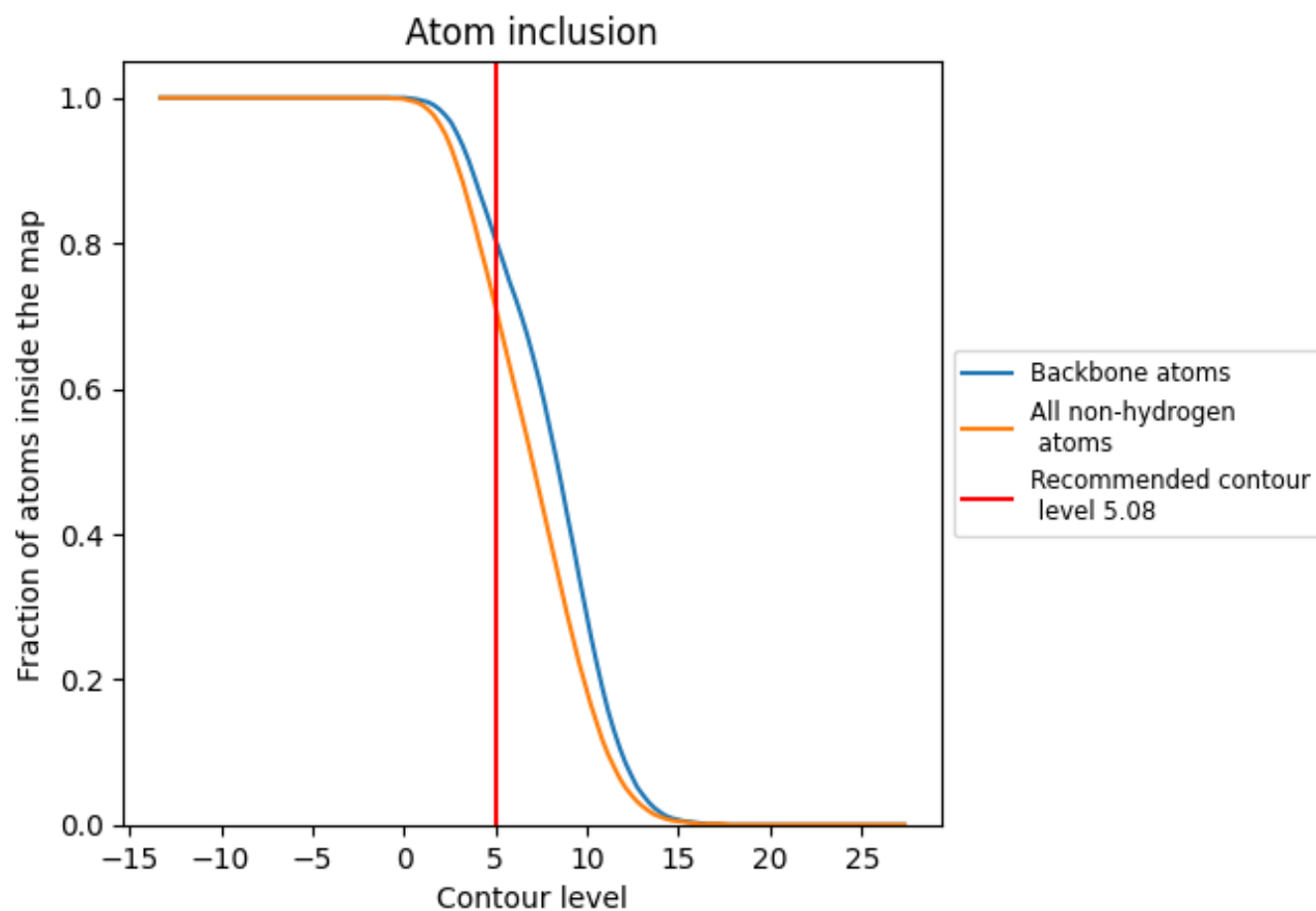
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 70% 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 (5.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7050	 0.5850
A	 0.6560	 0.6000
B	 0.8020	 0.6320
C	 0.8130	 0.6290
D	 0.7960	 0.6240
E	 0.7060	 0.5780
F	 0.7350	 0.5800
G	 0.7550	 0.6010
H	 0.7600	 0.6190
I	 0.8280	 0.6280
J	 0.6710	 0.5910
K	 0.7290	 0.6090
L	 0.6540	 0.5670
M	 0.7200	 0.6070
N	 0.7340	 0.6140
O	 0.6700	 0.5660
P	 0.7400	 0.5960
Q	 0.7260	 0.6120
R	 0.7290	 0.6020
S	 0.6780	 0.5550
T	 0.5030	 0.4900
U	 0.5770	 0.5180
V	 0.6660	 0.5880
W	 0.6810	 0.5940
X	 0.6940	 0.5780
Y	 0.5820	 0.5510
Z	 0.7110	 0.5910
a	 0.7320	 0.5980
b	 0.6580	 0.5660
c	 0.5590	 0.5550
d	 0.6750	 0.5830
e	 0.6900	 0.5810
f	 0.5900	 0.5460
g	 0.6540	 0.5720
h	 0.7050	 0.5920



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Chain	Atom inclusion	Q-score
i	 0.5530	 0.5260
j	 0.6450	 0.4950
k	 0.5800	 0.4990
l	 0.6750	 0.5440
m	 0.6390	 0.5500
n	 0.6750	 0.5500
o	 0.5890	 0.4930
p	 0.6780	 0.5610
q	 0.7310	 0.6020
r	 0.7320	 0.6020
s	 0.6550	 0.5530