



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:57 AM UTC

PDB ID : 6ZKH / pdb_00006zkh
EMDB ID : EMD-11249
Title : Complex I with NADH, open1
Authors : Kampjut, D.; Sazanov, L.A.
Deposited on : 2020-06-30
Resolution : 3.00 Å (reported)
Based on initial model : 5LNK

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

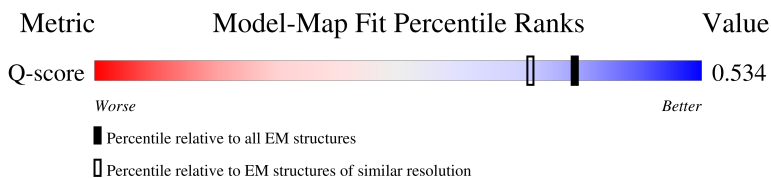
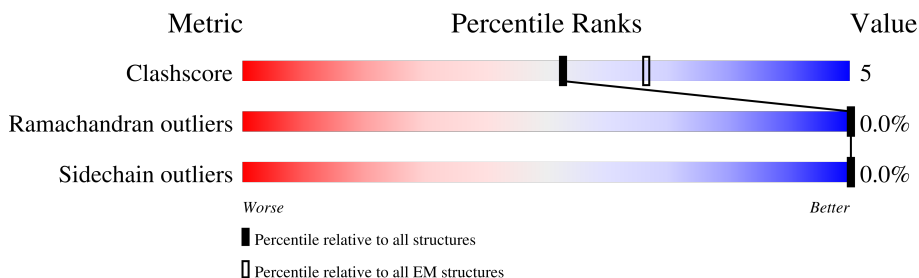
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	1	464	 80% 13% 7%
2	2	246	 72% 15% 13%
3	3	727	 78% 17% 5%
4	4	463	 76% 16% 8%

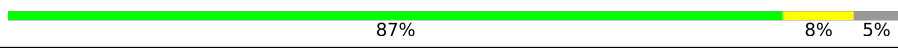
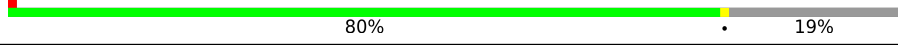
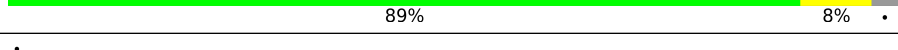
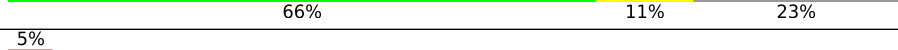
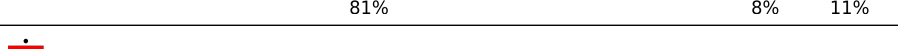
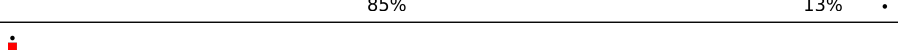
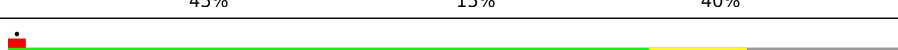
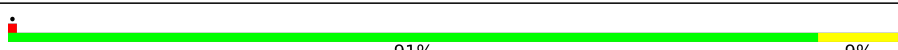
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Mol	Chain	Length	Quality of chain
5	5	266	
6	6	223	
7	9	217	
8	A	115	
9	H	318	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	V	141	
16	W	189	
17	X	157	
17	j	157	
18	Y	172	
19	Z	175	
20	a	109	
21	b	124	
22	c	170	
23	d	380	
24	e	99	
25	f	116	
26	g	140	
27	h	114	
28	i	145	

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Mol	Chain	Length	Quality of chain
29	k	355	
30	l	106	
31	m	84	
32	n	98	
33	o	122	
34	p	130	
35	q	144	
36	r	128	
37	s	137	
38	t	179	
39	u	108	
40	v	186	
41	w	154	
42	x	76	
43	y	58	
44	z	70	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	1	501	-	-	X	-
53	CDL	L	1003	X	-	-	-
53	CDL	V	204	X	-	-	-
53	CDL	Y	201	X	-	-	-
53	CDL	o	502	X	-	-	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 67479 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	430	Total	C	N	O	S	0	0
			3312	2086	593	613	20		

- Molecule 2 is a protein called Mitochondrial complex I, 24 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	213	Total	C	N	O	S	0	0
			1655	1058	278	309	10		

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	688	Total	C	N	O	S	0	0
			5275	3301	922	1011	41		

- Molecule 4 is a protein called Mitochondrial complex I, 49 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	426	Total	C	N	O	S	0	0
			3427	2188	590	624	25		

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	208	Total	C	N	O	S	0	0
			1726	1112	296	315	3		

- Molecule 6 is a protein called Mitochondrial complex I, PSST subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

- Molecule 7 is a protein called Mitochondrial complex I, TYKY subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	104	Total	C	N	O	S	0	0
			842	571	122	144	5		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	318	Total	C	N	O	S	0	0
			2528	1704	384	421	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	169	Total	C	N	O	S	0	0
			1294	870	185	226	13		

- 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
			749	490	112	132	15		

- 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
			4806	3187	746	829	44		

- 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
			3647	2429	571	607	40		

- 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
			2723	1808	416	459	40		

- Molecule 15 is a protein called Mitochondrial complex I, B14.7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	140	Total	C	N	O	S	0	0
			1028	656	175	191	6		

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	139	Total	C	N	O	S	0	0
			1155	761	194	198	2		

- Molecule 17 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	87	Total	C	N	O	S	0	0
			701	451	103	142	5		
17	j	82	Total	C	N	O	S	0	0
			660	425	98	132	5		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	171	Total	C	N	O	S	0	0
			1403	889	253	251	10		

- Molecule 19 is a protein called Mitochondrial complex I, PDSW subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	171	Total	C	N	O	S	0	0
			1441	905	266	262	8		

- Molecule 20 is a protein called Mitochondrial complex I, 10 kDa subunit.

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

- Molecule 21 is a protein called Mitochondrial complex I, 13 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	126	Total	C	N	O	S	0	0
			1024	646	182	193	3		

- Molecule 23 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	297	Total	C	N	O	S	0	0
			2372	1516	432	419	5		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 25 is a protein called Mitochondrial complex I, B13 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	113	Total	C	N	O	S	0	0
			917	595	153	167	2		

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

- Molecule 27 is a protein called Mitochondrial complex I, B14.5a subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	h	96	Total	C	N	O	S	0	0
			769	480	146	140	3		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	i	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	k	320	Total	C	N	O	P S	0	0
			2596	1659	432	494	1 10		

- Molecule 30 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	l	105	Total	C	N	O	S	0	0
			874	551	164	153	6		

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	m	80	Total	C	N	O	S	0	0
			626	411	103	110	2		

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	n	79	Total	C	N	O	S	0	0
			634	415	106	111	2		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	o	120	Total	C	N	O	S	0	0
			1004	652	175	172	5		

- Molecule 34 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	p	128	Total	C	N	O	S	0	0
			1059	675	189	194	1		

- Molecule 35 is a protein called Mitochondrial complex I, B16.6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	q	139	Total	C	N	O	S	0	0
			1142	733	200	200	9		

- Molecule 36 is a protein called Mitochondrial complex I, B17 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	r	99	Total	C	N	O	S	0	0
			846	554	149	142	1		

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	s	122	Total	C	N	O	S	0	0
			1047	653	199	186	9		

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	t	177	Total	C	N	O	S	0	0
			1520	973	279	262	6		

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	u	65	Total	C	N	O	S	0	0
			563	372	93	97	1		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	v	155	Total	C	N	O	S	0	0
			1307	846	213	239	9		

- Molecule 41 is a protein called Mitochondrial complex I, ESSS subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	w	101	Total	C	N	O	S	0	0
			846	542	140	160	4		

- Molecule 42 is a protein called Mitochondrial complex I, KFYI subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	x	49	Total	C	N	O	0	0
			412	271	70	71		

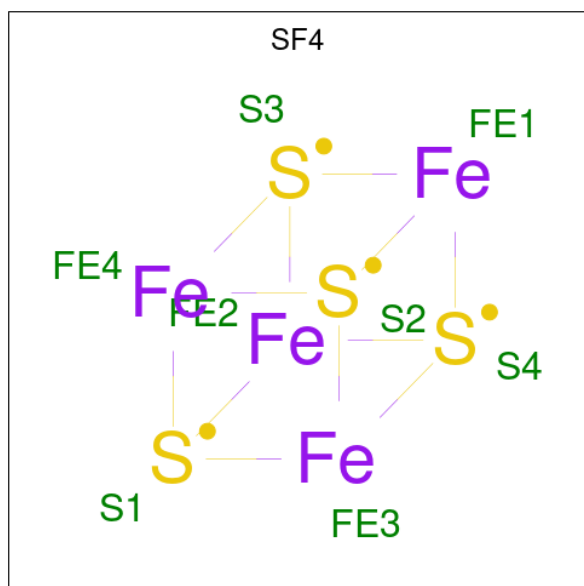
- Molecule 43 is a protein called Mitochondrial complex I, MNLL subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	y	50	Total	C	N	O	0	0
			436	287	77	72		

- Molecule 44 is a protein called Mitochondrial complex I, MWFE subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	z	70	Total	C	N	O	S	0	0
			576	369	106	96	5		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



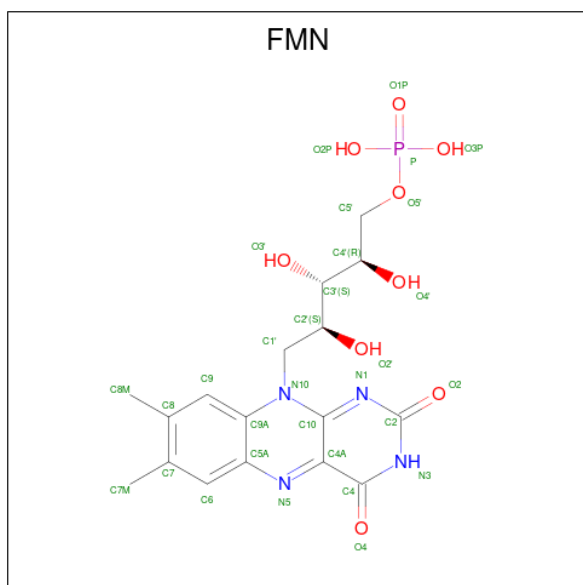
Mol	Chain	Residues	Atoms			AltConf
45	1	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	6	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
45	9	1	Total	Fe	S	0
			8	4	4	
45	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

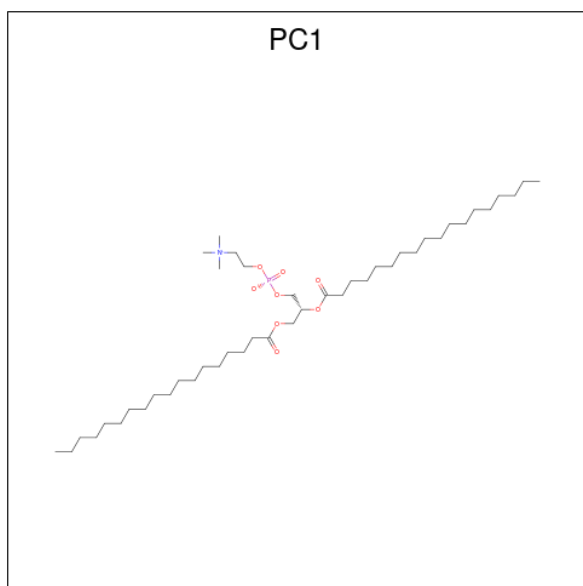


Mol	Chain	Residues	Atoms					AltConf
46	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).

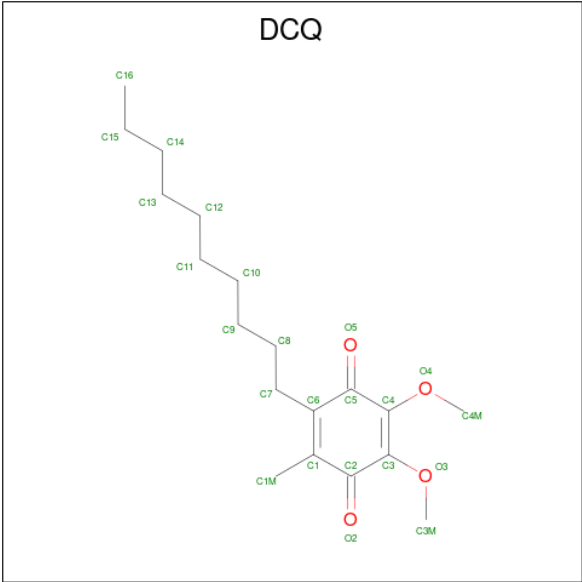
Mol	Chain	Residues	Atoms		AltConf
49	3	1	Total	K	0
			1	1	

- Molecule 50 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



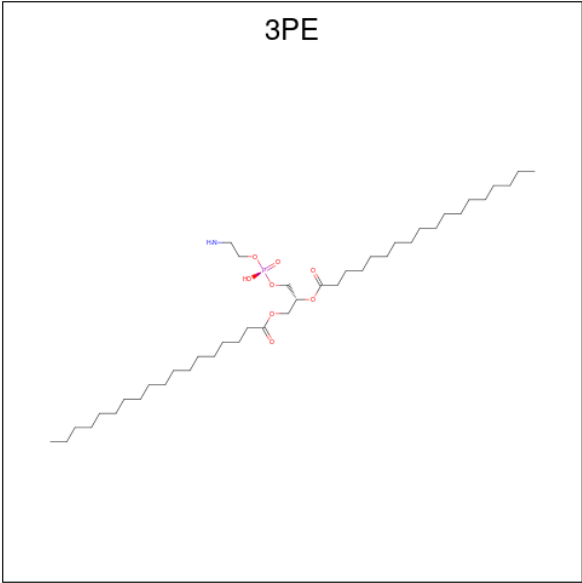
Mol	Chain	Residues	Atoms					AltConf
50	6	1	Total	C	N	O	P	0
			46	36	1	8	1	
50	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
50	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
50	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
50	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
50	M	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 51 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (CCD ID: DCQ) (formula: $C_{19}H_{30}O_4$).



Mol	Chain	Residues	Atoms			AltConf
51	6	1	Total	C	O	0
			23	19	4	

- Molecule 52 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



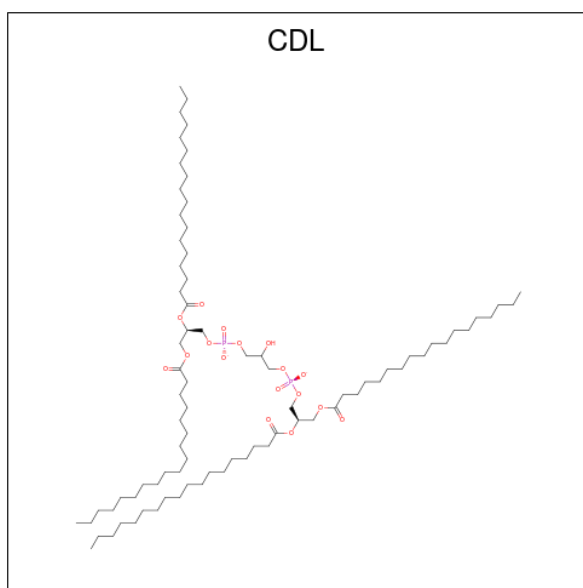
Mol	Chain	Residues	Atoms					AltConf
52	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	H	1	Total	C	N	O	P	0
			51	41	1	8	1	

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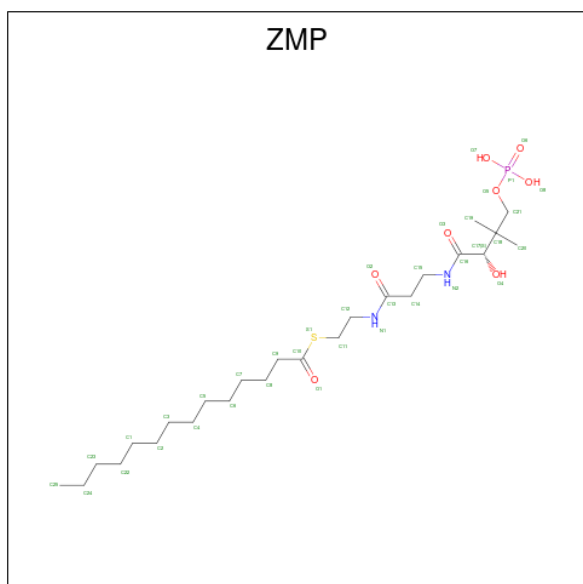
Mol	Chain	Residues	Atoms					AltConf
52	K	1	Total	C	N	O	P	0
			40	30	1	8	1	
52	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
52	M	1	Total	C	N	O	P	0
			40	30	1	8	1	
52	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
52	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	V	1	Total	C	N	O	P	0
			35	25	1	8	1	
52	V	1	Total	C	N	O	P	0
			37	27	1	8	1	
52	V	1	Total	C	O	P		0
			27	18	8	1		
52	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	o	1	Total	C	N	O	P	0
			31	21	1	8	1	

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
53	L	1	Total	C	O	P	0
			100	81	17	2	
53	M	1	Total	C	O	P	0
			90	71	17	2	
53	V	1	Total	C	O	P	0
			94	75	17	2	
53	V	1	Total	C	O	P	0
			85	66	17	2	
53	W	1	Total	C	O	P	0
			100	81	17	2	
53	Y	1	Total	C	O	P	0
			100	81	17	2	
53	o	1	Total	C	O	P	0
			75	56	17	2	
53	z	1	Total	C	O	P	0
			58	39	17	2	

- Molecule 54 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).

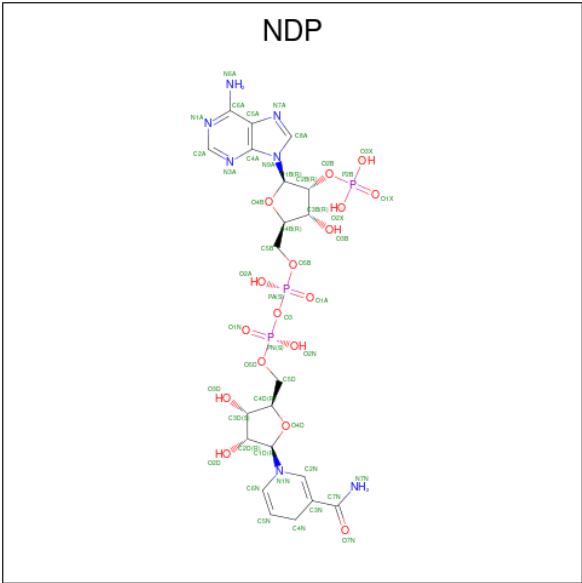


Mol	Chain	Residues	Atoms						AltConf
54	X	1	Total 31	C 20	N 2	O 7	P 1	S 1	0
54	g	1	Total 34	C 23	N 2	O 7	P 1	S 1	0

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

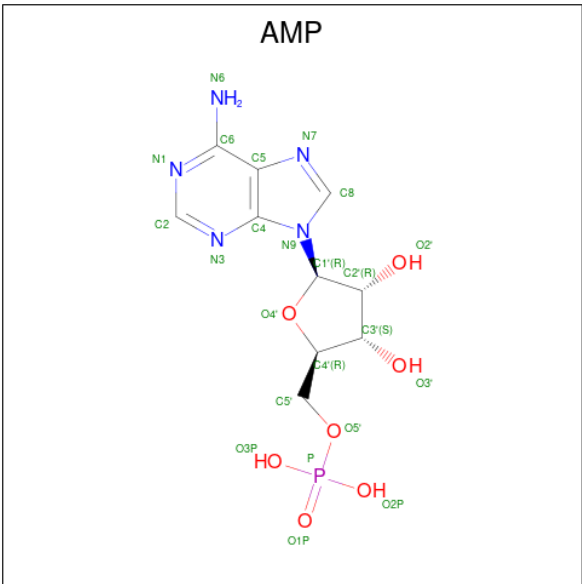
Mol	Chain	Residues	Atoms		AltConf
55	b	1	Total	Zn	0
			1	1	

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



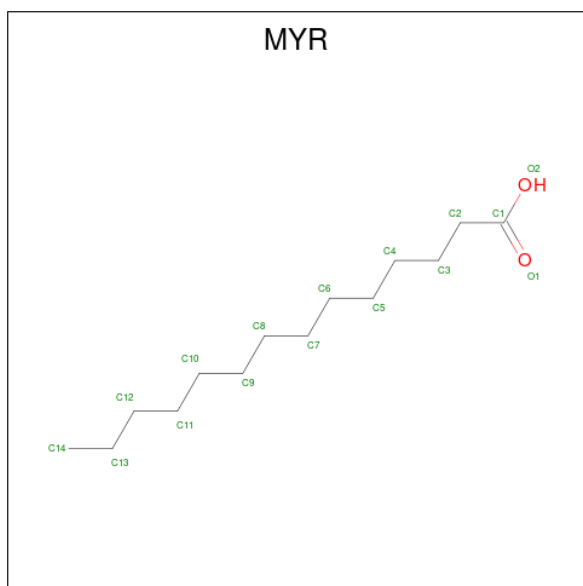
Mol	Chain	Residues	Atoms					AltConf
56	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					AltConf
57	k	1	Total	C	N	O	P	0
			23	10	5	7	1	

- Molecule 58 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).

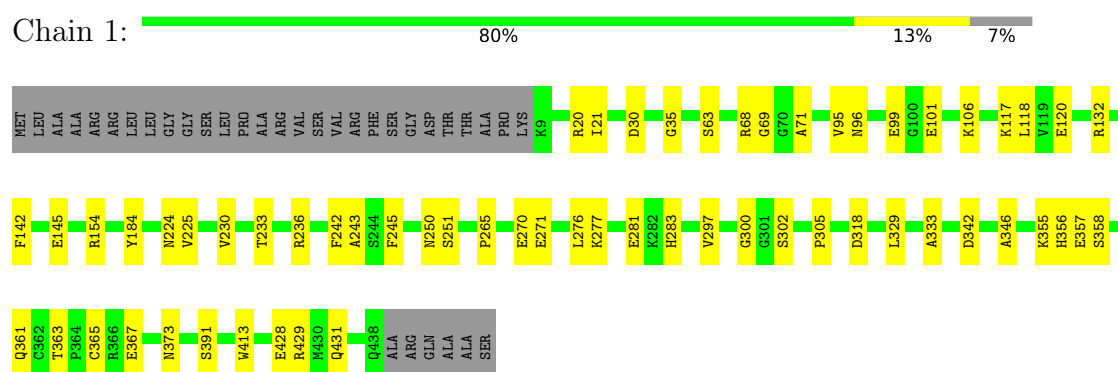


Mol	Chain	Residues	Atoms			AltConf
58	s	1	Total	C	O	0
			15	14	1	

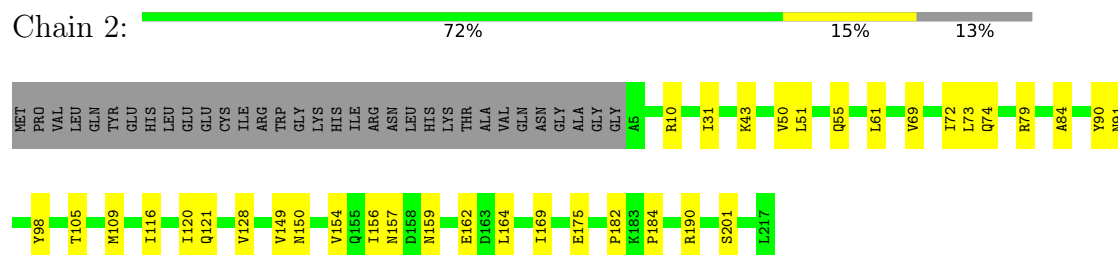
3 Residue-property plots

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

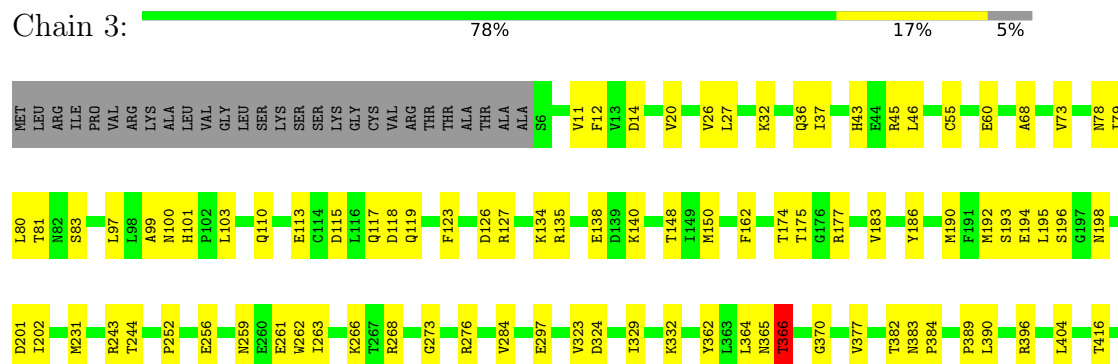
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

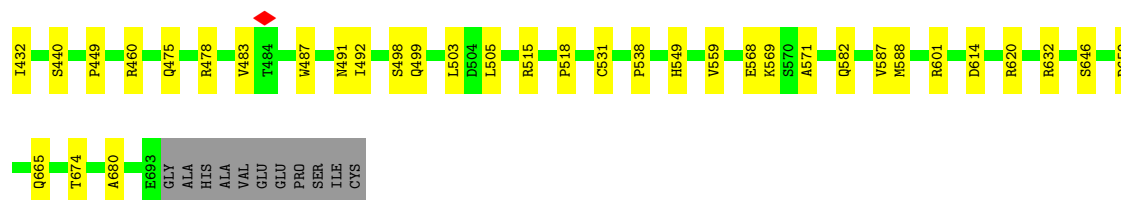


- Molecule 2: Mitochondrial complex I, 24 kDa subunit

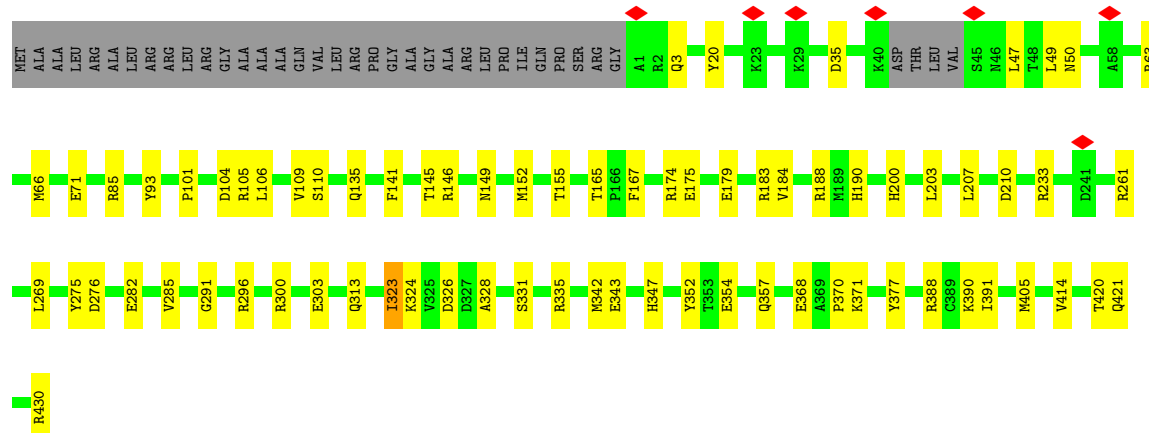
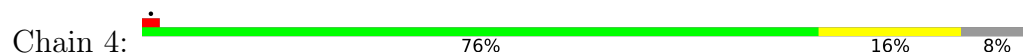


- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

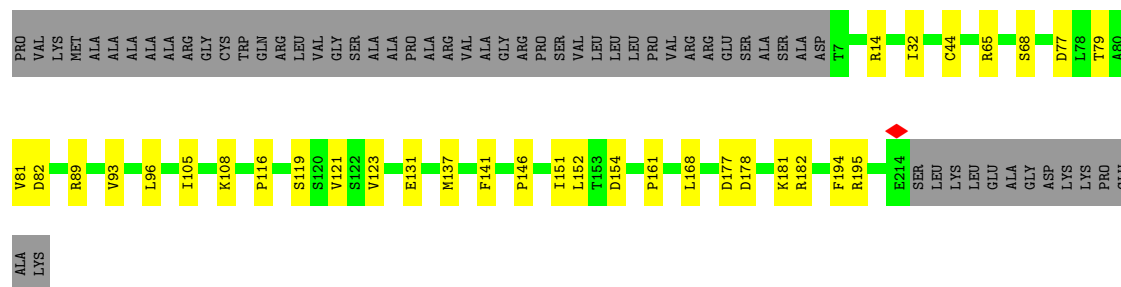




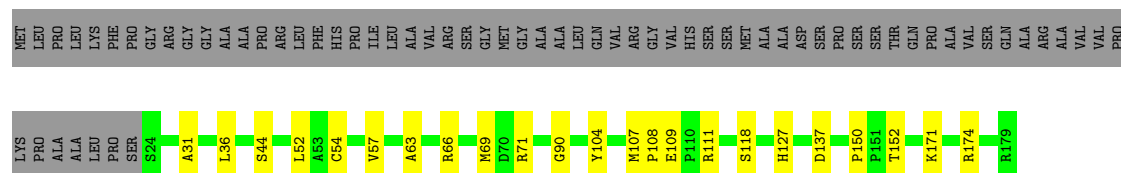
• Molecule 4: Mitochondrial complex I, 49 kDa subunit



• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

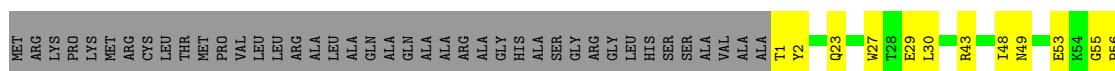


• Molecule 6: Mitochondrial complex I, PSST subunit

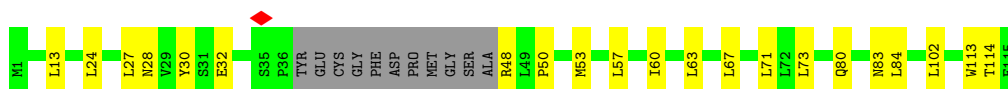


• Molecule 7: Mitochondrial complex I, TYKY subunit

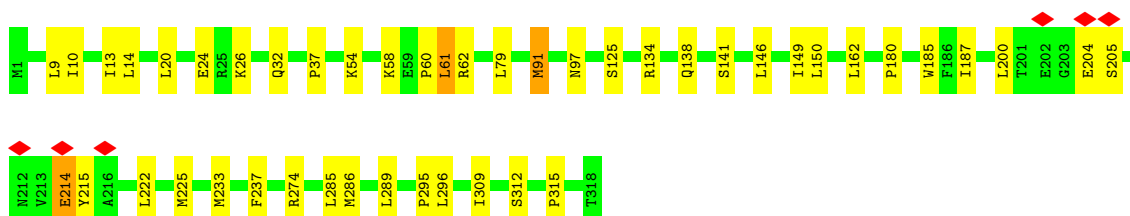
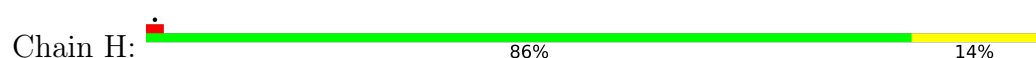




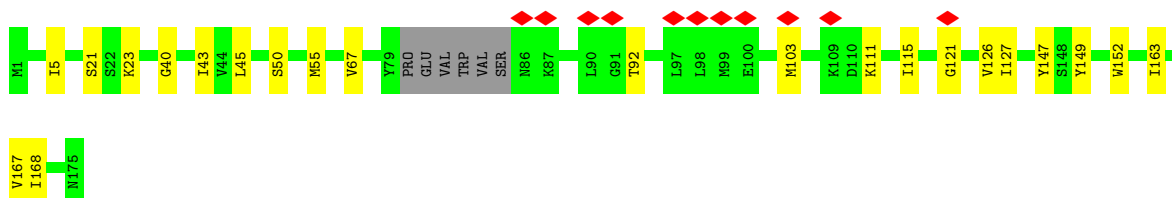
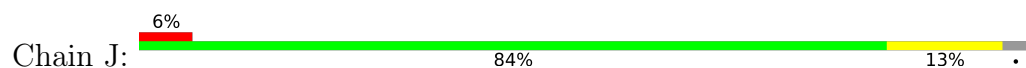
- Molecule 8: NADH-ubiquinone oxidoreductase chain 3



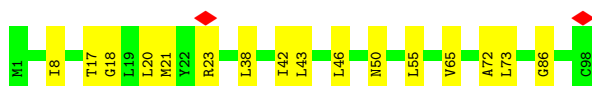
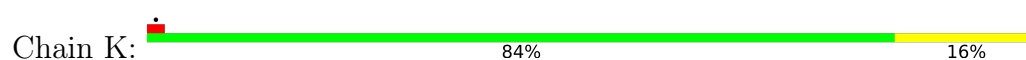
- Molecule 9: NADH-ubiquinone oxidoreductase chain 1



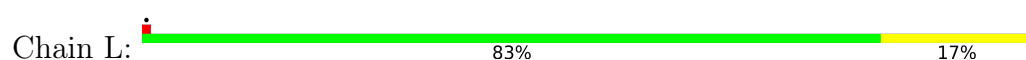
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

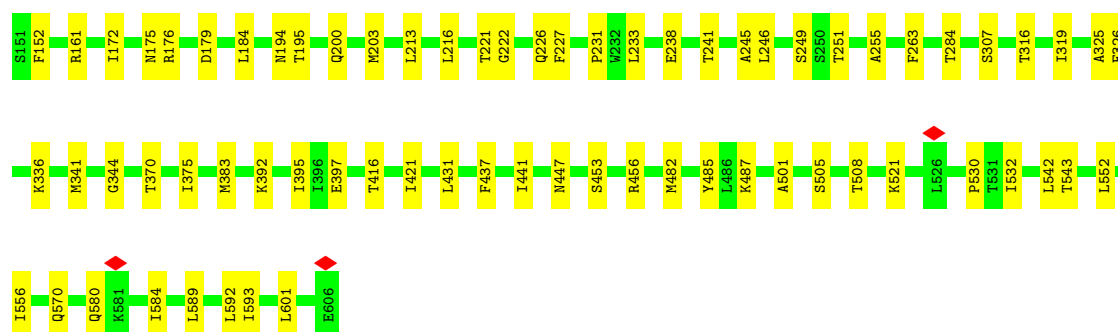


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5





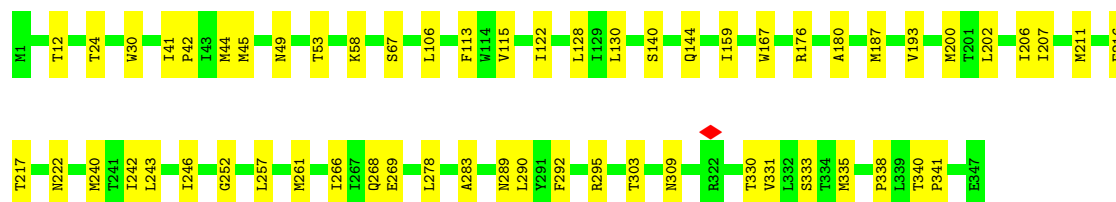
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M: 80% 20%



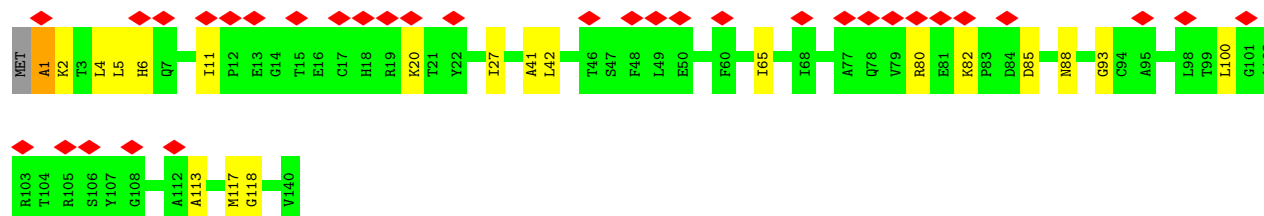
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 83% 17%



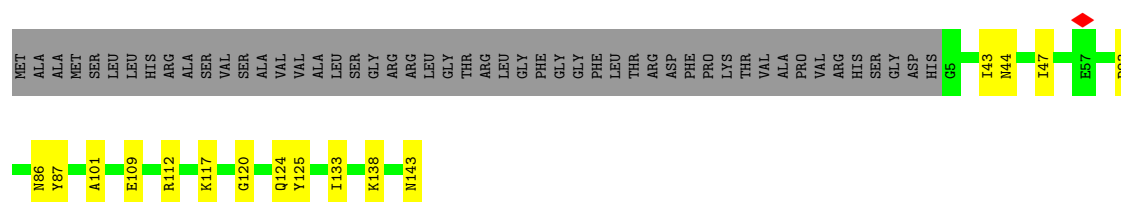
• Molecule 15: Mitochondrial complex I, B14.7 subunit

Chain V: 23% 85% 13%

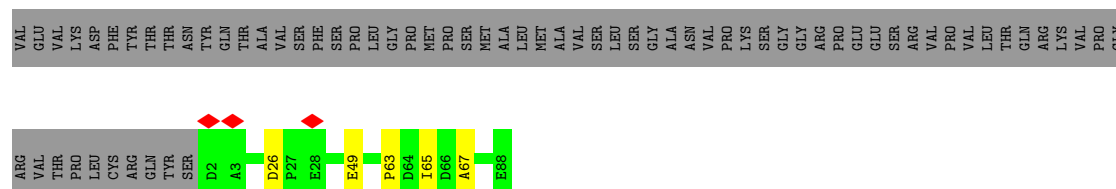


• Molecule 16: NADH:ubiquinone oxidoreductase subunit B5

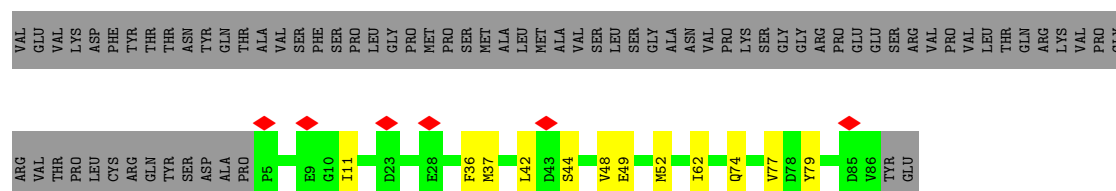
Chain W: 65% 8% 26%



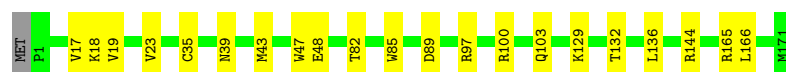
- Molecule 17: Acyl carrier protein



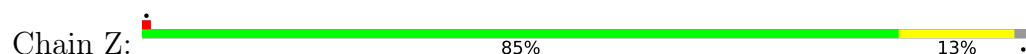
- Molecule 17: Acyl carrier protein



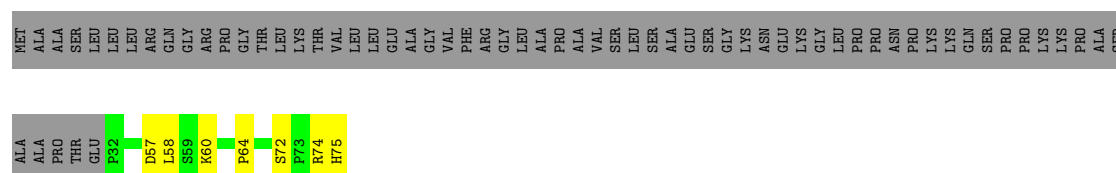
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 19: Mitochondrial complex I, PDSW subunit

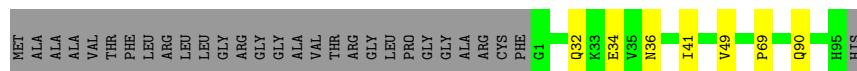


- Molecule 20: Mitochondrial complex I, 10 kDa subunit



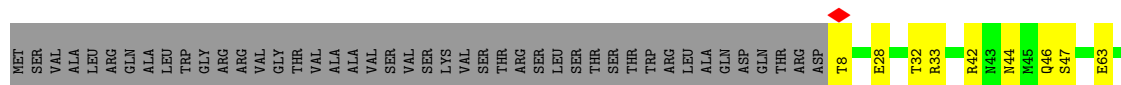
- Molecule 21: Mitochondrial complex I, 13 kDa subunit

Chain b:  71% 6% 23%



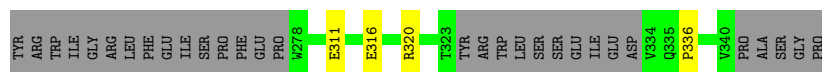
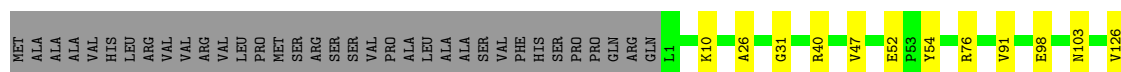
- Molecule 22: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain c:  65% 9% 26%



- Molecule 23: NADH:ubiquinone oxidoreductase subunit A9

Chain d:  68% 10% 22%



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain e:  74% 13% 13%



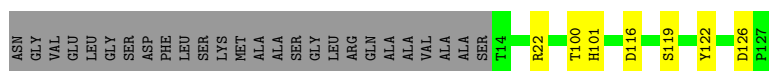
- Molecule 25: Mitochondrial complex I, B13 subunit

Chain f:  87% 10% 3%

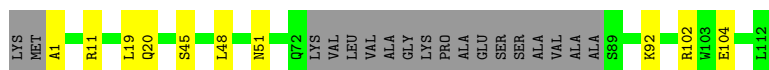


- Molecule 26: NADH:ubiquinone oxidoreductase subunit A6

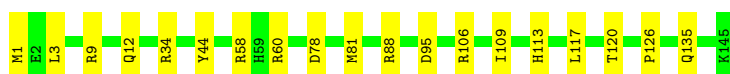
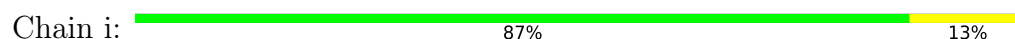
Chain g:  76% 5% 19%



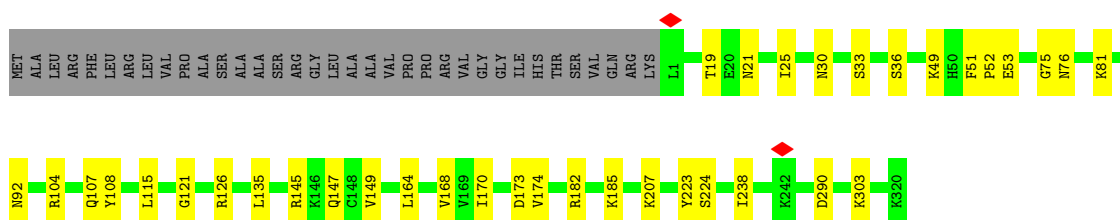
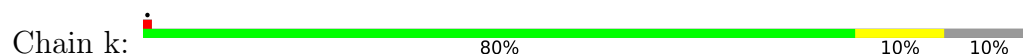
- Molecule 27: Mitochondrial complex I, B14.5a subunit



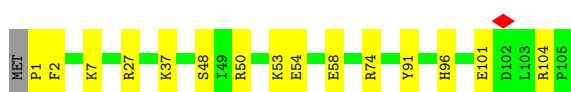
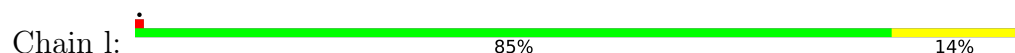
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



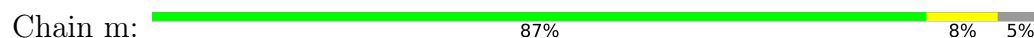
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



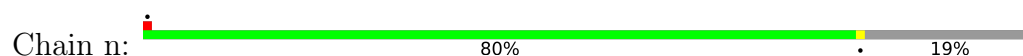
- Molecule 30: NADH:ubiquinone oxidoreductase subunit S5

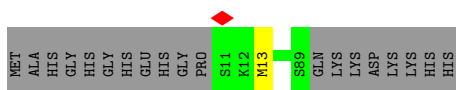


- Molecule 31: NADH:ubiquinone oxidoreductase subunit A3

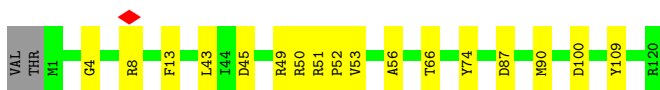
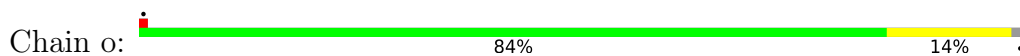


- Molecule 32: NADH:ubiquinone oxidoreductase subunit B3

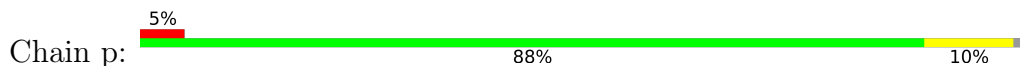




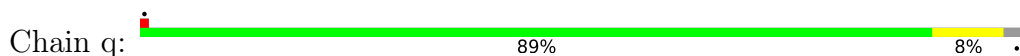
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2



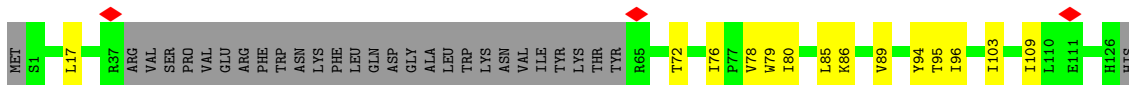
- Molecule 34: NADH:ubiquinone oxidoreductase subunit B4



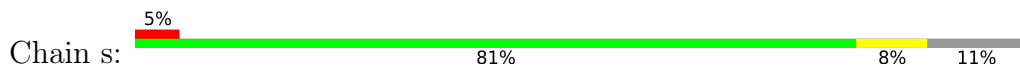
- Molecule 35: Mitochondrial complex I, B16.6 subunit



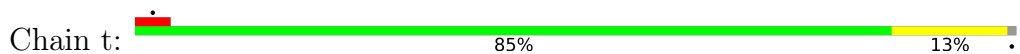
- Molecule 36: Mitochondrial complex I, B17 subunit



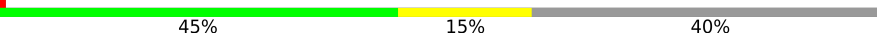
- Molecule 37: NADH:ubiquinone oxidoreductase subunit B7

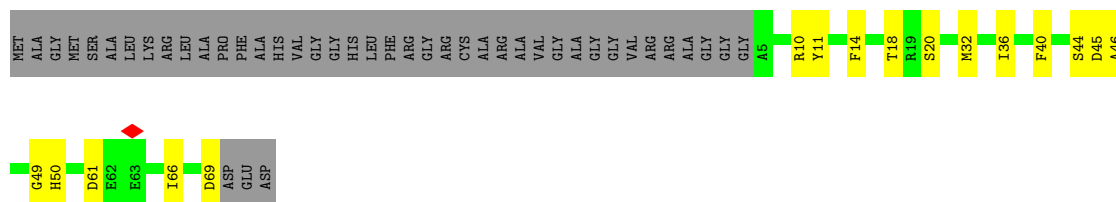


- Molecule 38: NADH:ubiquinone oxidoreductase subunit B9



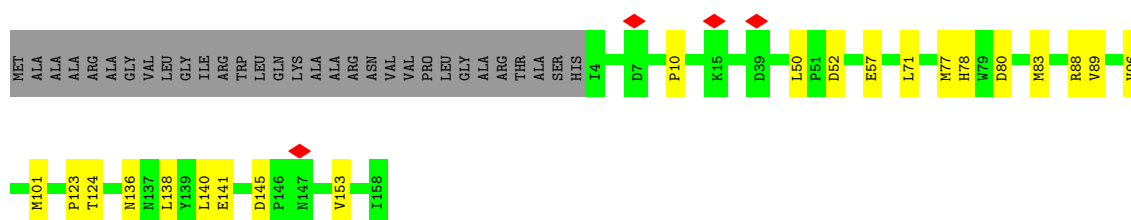
- Molecule 39: NADH:ubiquinone oxidoreductase subunit B2

Chain u: 



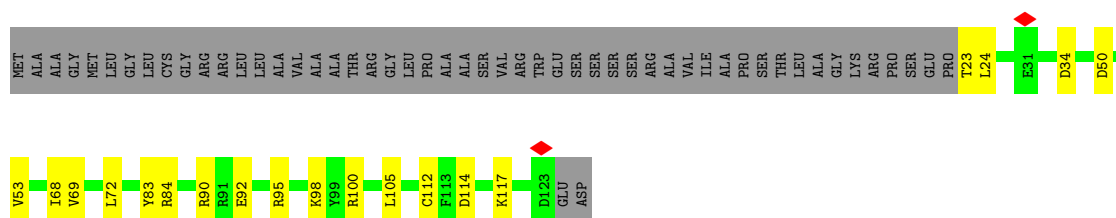
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain v: 



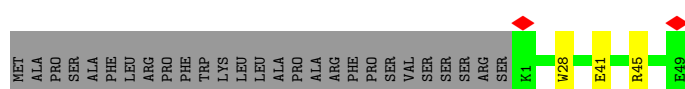
- Molecule 41: Mitochondrial complex I, ESSS subunit

Chain w: 



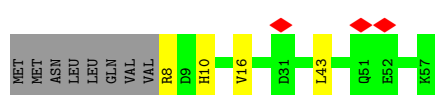
- Molecule 42: Mitochondrial complex I, KFYI subunit

Chain x: 

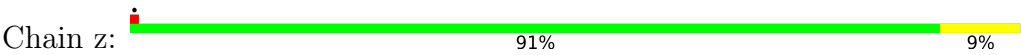


- Molecule 43: Mitochondrial complex I, MNLL subunit

Chain y: 



- Molecule 44: Mitochondrial complex I, MWFE subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28253	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 ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.464	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	171.882, 194.163, 286.47	wwPDB
Map dimensions	270, 183, 162	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, NAI, AYA, 2MR, FMN, CDL, FES, PC1, SEP, K, ZN, DCQ, 3PE, MYR, ZMP, AMP, SF4, FME

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.32	0/3386	0.56	0/4575
2	2	0.31	0/1695	0.57	2/2306 (0.1%)
3	3	0.32	0/5362	0.54	2/7266 (0.0%)
4	4	0.36	0/3504	0.54	0/4746
5	5	0.34	0/1776	0.53	0/2417
6	6	0.37	0/1278	0.54	0/1728
7	9	0.39	0/1445	0.57	0/1956
8	A	0.30	0/863	0.56	0/1181
9	H	0.35	0/2603	0.66	4/3561 (0.1%)
10	J	0.29	0/1324	0.60	0/1790
11	K	0.31	0/749	0.59	0/1014
12	L	0.28	0/4924	0.57	0/6698
13	M	0.33	0/3731	0.57	0/5085
14	N	0.34	0/2787	0.56	0/3795
15	V	0.19	0/1041	0.42	0/1412
16	W	0.26	0/1188	0.51	0/1607
17	X	0.19	0/713	0.43	0/963
17	j	0.22	0/670	0.47	0/902
18	Y	0.26	0/1440	0.53	0/1942
19	Z	0.24	0/1475	0.46	0/1989
20	a	0.22	0/383	0.42	0/518
21	b	0.28	0/749	0.44	0/1009
22	c	0.30	0/1047	0.45	0/1415
23	d	0.27	0/2424	0.47	0/3276
24	e	0.23	0/702	0.47	0/945
25	f	0.27	0/937	0.50	0/1271
26	g	0.28	0/993	0.50	0/1336
27	h	0.30	0/779	0.54	0/1053
28	i	0.29	0/1250	0.44	0/1698
29	k	0.23	0/2646	0.42	0/3579
30	l	0.27	0/896	0.53	0/1200

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	m	0.25	0/647	0.48	0/890
32	n	0.21	0/653	0.39	0/882
33	o	0.25	0/1035	0.46	0/1398
34	p	0.22	0/1085	0.46	0/1467
35	q	0.26	0/1171	0.50	0/1579
36	r	0.25	0/874	0.50	0/1188
37	s	0.20	0/1072	0.46	0/1436
38	t	0.22	0/1573	0.51	0/2130
39	u	0.20	0/590	0.44	0/810
40	v	0.20	0/1361	0.46	0/1861
41	w	0.25	0/872	0.49	0/1185
42	x	0.19	0/425	0.38	0/576
43	y	0.24	0/449	0.49	0/605
44	z	0.33	0/591	0.52	0/795
All	All	0.29	0/67158	0.52	8/91035 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	3	0	2
4	4	0	1
8	A	0	1
9	H	0	2
All	All	0	6

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	366	THR	CA-C-N	6.17	133.32	121.54
3	3	366	THR	C-N-CA	6.17	133.32	121.54
9	H	215	TYR	CA-CB-CG	5.90	124.52	113.90
9	H	91	MET	CA-C-N	5.46	140.12	127.00
9	H	91	MET	C-N-CA	5.46	140.12	127.00
2	2	156	ILE	CA-C-N	5.40	131.85	121.54
2	2	156	ILE	C-N-CA	5.40	131.85	121.54
9	H	91	MET	C-N-CD	-5.06	109.47	120.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	259	ASN	Peptide
3	3	366	THR	Peptide
4	4	275	TYR	Peptide
8	A	113	TRP	Peptide
9	H	60	PRO	Peptide
9	H	61	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3312	0	3269	42	0
2	2	1655	0	1668	22	0
3	3	5275	0	5300	80	0
4	4	3427	0	3365	54	0
5	5	1726	0	1676	22	0
6	6	1247	0	1259	20	0
7	9	1414	0	1371	30	0
8	A	842	0	887	19	0
9	H	2528	0	2641	33	0
10	J	1294	0	1317	19	0
11	K	749	0	793	16	0
12	L	4806	0	4945	75	0
13	M	3647	0	3849	66	0
14	N	2723	0	2930	44	0
15	V	1028	0	1036	13	0
16	W	1155	0	1177	13	0
17	X	701	0	692	4	0
17	j	660	0	663	7	0
18	Y	1403	0	1392	17	0
19	Z	1441	0	1419	20	0
20	a	371	0	344	5	0
21	b	737	0	710	5	0
22	c	1024	0	1023	14	0
23	d	2372	0	2407	23	0
24	e	691	0	706	7	0
25	f	917	0	958	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	g	969	0	980	6	0
27	h	769	0	780	8	0
28	i	1209	0	1182	12	0
29	k	2596	0	2559	24	0
30	l	874	0	869	15	0
31	m	626	0	635	9	0
32	n	634	0	616	1	0
33	o	1004	0	995	14	0
34	p	1059	0	1062	12	0
35	q	1142	0	1137	11	0
36	r	846	0	864	13	0
37	s	1047	0	1015	9	0
38	t	1520	0	1477	21	0
39	u	563	0	509	11	0
40	v	1307	0	1207	18	0
41	w	846	0	792	14	0
42	x	412	0	411	2	0
43	y	436	0	437	4	0
44	z	576	0	570	6	0
45	1	8	0	0	3	0
45	3	16	0	0	1	0
45	6	8	0	0	1	0
45	9	16	0	0	0	0
46	1	31	0	19	1	0
47	1	44	0	27	3	0
48	2	4	0	0	1	0
48	3	4	0	0	0	0
49	3	1	0	0	0	0
50	6	46	0	69	2	0
50	9	54	0	88	4	0
50	A	37	0	48	2	0
50	L	54	0	88	7	0
50	M	108	0	176	6	0
51	6	23	0	30	0	0
52	A	51	0	82	3	0
52	H	51	0	82	0	0
52	K	40	0	54	4	0
52	L	82	0	118	1	0
52	M	84	0	119	2	0
52	N	51	0	82	2	0
52	V	99	0	119	3	0
52	i	102	0	164	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	o	31	0	36	0	0
53	L	100	0	156	5	0
53	M	90	0	133	12	0
53	V	179	0	261	5	0
53	W	100	0	156	10	0
53	Y	100	0	156	6	0
53	o	75	0	97	1	0
53	z	58	0	60	0	0
54	X	31	0	34	3	0
54	g	34	0	40	0	0
55	b	1	0	0	0	0
56	d	48	0	26	1	0
57	k	23	0	12	0	0
58	s	15	0	27	0	0
All	All	67479	0	68453	719	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 5.

All (719) 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)
11:K:46:LEU:O	11:K:50:ASN:HB2	1.83	0.79
4:4:50:ASN:HD21	4:4:63:ARG:HE	1.41	0.68
24:e:19:ARG:HB2	24:e:65:TRP:HB2	1.76	0.67
3:3:118:ASP:OD2	22:c:46:GLN:NE2	2.29	0.66
18:Y:165:ARG:NH1	33:o:87:ASP:OD1	2.29	0.65
44:z:34:ARG:NH2	44:z:61:TYR:O	2.26	0.65
11:K:21:MET:HG2	12:L:589:LEU:HD23	1.77	0.64
14:N:243:LEU:HD22	14:N:330:THR:HG21	1.79	0.64
4:4:377:TYR:HB3	4:4:390:LYS:HB3	1.79	0.64
7:9:43:ARG:HG2	27:h:11:ARG:HD2	1.80	0.64
1:1:355:LYS:HD3	1:1:373:ASN:HD22	1.63	0.63
9:H:200:LEU:HD11	9:H:285:LEU:HD21	1.80	0.62
8:A:60:ILE:HG21	10:J:168:ILE:HG21	1.81	0.62
2:2:74:GLN:O	20:a:74:ARG:NH2	2.32	0.62
2:2:98:TYR:HA	2:2:157:ASN:HD21	1.64	0.62
4:4:405:MET:SD	4:4:421:GLN:NE2	2.71	0.62
35:q:81:ARG:NH1	35:q:85:MET:SD	2.73	0.62
30:l:96:HIS:HA	30:l:101:GLU:HG2	1.80	0.62
23:d:167:LYS:HB2	23:d:229:ALA:HA	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:L:1003:CDL:H642	53:L:1003:CDL:H562	1.82	0.61
7:9:92:ILE:HG12	7:9:111:ILE:HG12	1.82	0.61
11:K:73:LEU:HD11	14:N:41:ILE:HG13	1.82	0.61
12:L:69:LEU:HD13	13:M:451:PRO:HG2	1.82	0.60
14:N:106:LEU:HD22	14:N:187:MET:HE2	1.83	0.60
14:N:45:MET:HE3	14:N:53:THR:HG22	1.83	0.60
4:4:66:MET:HE1	4:4:414:VAL:HG11	1.83	0.60
6:6:36:LEU:HD13	52:i:501:3PE:H392	1.84	0.60
36:r:103:ILE:HB	37:s:47:ASP:HB3	1.81	0.60
4:4:183:ARG:NH1	4:4:210:ASP:OD2	2.33	0.60
2:2:150:ASN:HB3	2:2:162:GLU:HB3	1.83	0.60
1:1:101:GLU:HB2	47:1:503:NAI:H42N	1.83	0.60
25:f:69:GLU:HG3	27:h:102:ARG:HH12	1.67	0.60
24:e:23:CYS:SG	24:e:24:GLN:N	2.75	0.59
5:5:151:ILE:HG23	5:5:152:LEU:HG	1.84	0.59
12:L:241:THR:HG21	12:L:344:GLY:HA3	1.83	0.59
3:3:46:LEU:O	22:c:116:LYS:NZ	2.35	0.59
3:3:126:ASP:HB2	4:4:328:ALA:HB3	1.84	0.59
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.84	0.59
54:X:101:ZMP:H5A	38:t:43:LEU:HD11	1.85	0.59
34:p:47:GLN:HA	34:p:50:TYR:HB3	1.84	0.59
3:3:127:ARG:NH2	4:4:326:ASP:O	2.34	0.59
4:4:49:LEU:HB3	4:4:66:MET:HB2	1.83	0.59
12:L:106:TRP:HD1	12:L:447:ASN:HD22	1.51	0.59
53:M:505:CDL:H352	53:M:505:CDL:H612	1.85	0.59
1:1:132:ARG:NH2	20:a:64:PRO:O	2.36	0.58
3:3:329:ILE:HD13	3:3:505:LEU:HD22	1.85	0.58
22:c:42:ARG:NH1	22:c:46:GLN:O	2.36	0.58
36:r:85:LEU:HD22	36:r:96:ILE:HD11	1.85	0.58
3:3:194:GLU:HG3	3:3:389:PRO:HB3	1.86	0.58
9:H:26:LYS:HB3	44:z:5:VAL:HG12	1.84	0.58
12:L:161:ARG:NH2	38:t:90:TYR:O	2.36	0.58
19:Z:67:PHE:HD1	43:y:43:LEU:HD21	1.68	0.58
3:3:396:ARG:NH1	3:3:416:THR:O	2.37	0.58
3:3:515:ARG:NH2	3:3:531:CYS:O	2.37	0.58
6:6:171:LYS:HG2	6:6:174:ARG:HH11	1.66	0.58
13:M:50:LEU:HA	16:W:86:ASN:HD21	1.69	0.58
53:Y:201:CDL:H311	53:Y:201:CDL:H562	1.86	0.58
3:3:198:ASN:OD1	3:3:268:ARG:NH2	2.36	0.58
9:H:141:SER:HB3	9:H:289:LEU:HD22	1.86	0.58
11:K:20:LEU:HB3	12:L:592:LEU:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:110:SER:OG	4:4:149:ASN:ND2	2.37	0.57
4:4:233:ARG:NH2	7:9:23:GLN:O	2.35	0.57
13:M:243:MET:HB3	13:M:301:ILE:HG21	1.85	0.57
13:M:158:LEU:HD23	14:N:283:ALA:HB1	1.84	0.57
14:N:140:SER:HA	30:l:1:PRO:HD2	1.86	0.57
3:3:632:ARG:HH12	24:e:59:ASP:H	1.52	0.57
14:N:211:MET:HG2	14:N:333:SER:HB2	1.86	0.57
16:W:133:ILE:HD13	30:l:37:LYS:HG2	1.86	0.57
25:f:34:LEU:HD12	25:f:37:ILE:HD12	1.86	0.57
4:4:388:ARG:HG2	5:5:81:VAL:HG22	1.85	0.57
12:L:100:ILE:HG21	12:L:246:LEU:HB2	1.86	0.57
1:1:30:ASP:HB3	1:1:35:GLY:HA3	1.87	0.57
4:4:343:GLU:O	4:4:347:HIS:ND1	2.33	0.57
12:L:184:LEU:HD13	13:M:393:ILE:HG21	1.86	0.57
53:Y:201:CDL:H571	53:Y:201:CDL:H152	1.87	0.57
12:L:67:HIS:HB3	50:L:1002:PC1:H111	1.87	0.56
30:l:104:ARG:NH1	35:q:84:GLN:OE1	2.38	0.56
12:L:487:LYS:HE3	39:u:49:GLY:HA2	1.87	0.56
19:Z:5:ASP:OD2	41:w:98:LYS:NZ	2.35	0.56
19:Z:136:LYS:NZ	19:Z:140:ASP:OD2	2.38	0.56
1:1:365:CYS:HB3	45:1:501:SF4:S3	2.46	0.56
8:A:48:ARG:NH2	11:K:86:GLY:O	2.38	0.56
11:K:23:ARG:HG2	52:K:101:3PE:H11	1.86	0.56
17:X:65:ILE:HD13	38:t:3:LEU:HD22	1.87	0.56
28:i:34:ARG:NH2	28:i:58:ARG:O	2.37	0.56
6:6:108:PRO:HB2	9:H:58:LYS:HD2	1.88	0.56
17:j:48:VAL:HG12	17:j:52:MET:HE2	1.86	0.56
12:L:249:SER:HB2	12:L:336:LYS:HG3	1.86	0.56
14:N:252:GLY:HA3	14:N:290:LEU:HD13	1.88	0.56
2:2:79:ARG:HE	22:c:131:SER:HG	1.53	0.56
3:3:252:PRO:HG3	3:3:263:ILE:HG12	1.86	0.56
9:H:10:ILE:HA	9:H:13:ILE:HD12	1.87	0.56
12:L:570:GLN:OE1	14:N:167:TRP:NE1	2.39	0.56
4:4:109:VAL:HG11	4:4:152:MET:HG2	1.88	0.56
6:6:44:SER:O	9:H:54:LYS:NZ	2.38	0.56
18:Y:89:ASP:OD2	44:z:34:ARG:NH1	2.39	0.56
41:w:92:GLU:OE2	41:w:95:ARG:NH2	2.38	0.56
2:2:10:ARG:NH2	3:3:138:GLU:OE2	2.38	0.56
3:3:262:TRP:HB2	3:3:390:LEU:HD21	1.88	0.56
12:L:90:VAL:HG22	12:L:129:LEU:HD22	1.88	0.56
3:3:382:THR:HG23	3:3:384:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:118:SER:N	45:6:201:SF4:S4	2.79	0.55
12:L:103:PHE:HB2	12:L:341:MET:HE3	1.88	0.55
13:M:167:ILE:HD13	13:M:249:LEU:HD13	1.88	0.55
17:j:37:MET:HE1	17:j:44:SER:HA	1.89	0.55
3:3:175:THR:HG21	3:3:186:TYR:HB2	1.88	0.55
10:J:21:SER:O	10:J:23:LYS:NZ	2.39	0.55
38:t:100:GLU:O	38:t:121:ARG:NH1	2.40	0.55
3:3:261:GLU:OE1	22:c:42:ARG:NH2	2.40	0.55
8:A:80:GLN:NE2	9:H:315:PRO:O	2.38	0.55
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.88	0.55
18:Y:43:MET:HE3	18:Y:47:TRP:HZ3	1.71	0.55
23:d:138:ASP:HB3	23:d:141:SER:HB2	1.89	0.55
13:M:179:LEU:HD13	13:M:249:LEU:HD11	1.88	0.55
3:3:101:HIS:HD2	4:4:342:MET:HE2	1.72	0.55
13:M:204:MET:HE1	13:M:302:LEU:HD11	1.88	0.55
13:M:343:ILE:O	13:M:346:ARG:NH1	2.40	0.55
18:Y:132:THR:OG1	31:m:57:ARG:NH1	2.39	0.55
25:f:71:LEU:HD13	25:f:79:VAL:HG11	1.88	0.55
38:t:169:ILE:O	38:t:172:ARG:NH1	2.39	0.55
4:4:354:GLU:OE2	4:4:357:GLN:NE2	2.39	0.55
2:2:121:GLN:HE21	2:2:128:VAL:HG23	1.72	0.54
10:J:163:ILE:HG21	14:N:12:THR:HG21	1.88	0.54
4:4:335:ARG:NH2	7:9:129:ASP:OD1	2.40	0.54
29:k:52:PRO:O	29:k:107:GLN:NE2	2.40	0.54
2:2:50:VAL:HG12	2:2:69:VAL:HG22	1.89	0.54
37:s:7:ARG:HH21	37:s:17:GLU:HG3	1.71	0.54
13:M:165:ILE:HG21	14:N:268:GLN:HA	1.90	0.54
31:m:83:LEU:HD13	35:q:54:ARG:HD3	1.89	0.54
12:L:203:MET:HB2	19:Z:113:GLN:HG3	1.89	0.54
54:X:101:ZMP:O6	38:t:12:GLN:NE2	2.40	0.54
18:Y:35:CYS:O	18:Y:39:ASN:ND2	2.41	0.54
29:k:108:TYR:OH	29:k:164:LEU:O	2.25	0.54
2:2:105:THR:OG1	48:2:300:FES:S2	2.65	0.54
50:M:503:PC1:H251	53:W:201:CDL:H381	1.90	0.54
3:3:174:THR:HG22	3:3:183:VAL:HG22	1.89	0.54
29:k:145:ARG:NH1	29:k:147:GLN:OE1	2.41	0.54
9:H:162:LEU:HD21	9:H:237:PHE:HE1	1.73	0.54
12:L:97:THR:HG21	12:L:125:LEU:HD22	1.90	0.54
15:V:11:ILE:HB	15:V:20:LYS:HD3	1.89	0.54
6:6:137:ASP:OD2	7:9:144:HIS:ND1	2.41	0.54
28:i:60:ARG:HH22	28:i:95:ASP:HA	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:A:201:PC1:H292	10:J:152:TRP:HZ3	1.71	0.53
13:M:133:ILE:HD11	13:M:231:LEU:HD11	1.90	0.53
23:d:176:ASP:OD1	23:d:180:ASN:ND2	2.41	0.53
5:5:195:ARG:HH12	7:9:93:THR:HA	1.73	0.53
1:1:71:ALA:HB2	47:1:503:NAI:H4D	1.91	0.53
3:3:364:LEU:HD12	3:3:491:ASN:HB3	1.91	0.53
12:L:106:TRP:CD1	12:L:447:ASN:HD22	2.27	0.53
13:M:7:PRO:HB3	43:y:16:VAL:HG13	1.91	0.53
16:W:43:ILE:HG12	16:W:47:ILE:HD12	1.91	0.53
22:c:8:THR:OG1	26:g:22:ARG:NH1	2.42	0.53
34:p:62:PRO:O	34:p:66:ARG:HB2	2.08	0.53
4:4:233:ARG:NH1	50:9:401:PC1:O12	2.41	0.53
13:M:418:LYS:HD3	38:t:94:GLU:HB3	1.89	0.53
30:l:74:ARG:NH2	35:q:93:GLU:OE2	2.42	0.53
1:1:265:PRO:O	2:2:190:ARG:NH1	2.41	0.53
7:9:132:VAL:HG21	7:9:165:ILE:HG21	1.91	0.53
14:N:331:VAL:HG13	14:N:335:MET:HE3	1.90	0.53
22:c:33:ARG:NH1	22:c:77:ASP:OD1	2.40	0.53
41:w:100:ARG:HB2	41:w:105:LEU:HB2	1.91	0.53
37:s:110:ARG:NH1	39:u:69:ASP:OD2	2.42	0.53
9:H:24:GLU:OE2	9:H:274:ARG:NH1	2.42	0.53
6:6:71:ARG:NH2	7:9:48:ILE:O	2.36	0.53
12:L:231:PRO:HB3	12:L:530:PRO:HG3	1.91	0.53
40:v:80:ASP:HB3	40:v:83:MET:HB3	1.91	0.53
1:1:428:GLU:HA	1:1:431:GLN:HG2	1.91	0.52
7:9:145:GLU:HA	7:9:148:LEU:HD13	1.91	0.52
7:9:155:LEU:HB3	21:b:36:ASN:HD22	1.73	0.52
28:i:78:ASP:HB3	28:i:81:MET:HG3	1.90	0.52
40:v:71:LEU:HD21	40:v:77:MET:HG2	1.90	0.52
1:1:300:GLY:HA2	1:1:333:ALA:H	1.75	0.52
6:6:63:ALA:HB2	6:6:69:MET:HE3	1.90	0.52
10:J:40:GLY:HA2	10:J:43:ILE:HD12	1.92	0.52
14:N:159:ILE:HG21	14:N:278:LEU:HD11	1.90	0.52
14:N:207:ILE:HG22	14:N:211:MET:HE2	1.91	0.52
22:c:42:ARG:NH2	22:c:44:ASN:OD1	2.43	0.52
4:4:203:LEU:HD22	4:4:207:LEU:HD23	1.92	0.52
19:Z:141:ARG:HG3	41:w:112:CYS:HB2	1.91	0.52
1:1:356:HIS:O	3:3:177:ARG:NH2	2.42	0.52
52:V:205:3PE:H222	34:p:81:PRO:HB2	1.92	0.52
7:9:64:GLU:OE1	7:9:136:ASN:ND2	2.42	0.52
1:1:391:SER:HB2	27:h:48:LEU:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:300:ARG:NH2	4:4:420:THR:O	2.42	0.52
10:J:23:LYS:O	11:K:23:ARG:NH1	2.43	0.52
12:L:316:THR:HA	12:L:319:ILE:HG12	1.92	0.52
53:V:203:CDL:H202	53:V:203:CDL:H372	1.91	0.52
29:k:30:ASN:O	29:k:126:ARG:NH2	2.42	0.52
53:L:1003:CDL:H851	53:W:201:CDL:H671	1.91	0.52
37:s:6:ARG:HH12	37:s:105:ARG:HD2	1.75	0.52
1:1:21:ILE:O	1:1:117:LYS:NZ	2.36	0.52
13:M:60:SER:HB2	13:M:457:PRO:HA	1.91	0.52
16:W:44:ASN:ND2	53:W:201:CDL:OB4	2.40	0.51
53:Y:201:CDL:H841	53:Y:201:CDL:H662	1.92	0.51
25:f:112:LYS:NZ	25:f:115:ILE:O	2.42	0.51
28:i:1:MET:HG3	28:i:3:LEU:H	1.75	0.51
4:4:71:GLU:OE2	9:H:134:ARG:NH1	2.39	0.51
4:4:101:PRO:O	4:4:105:ARG:NH1	2.41	0.51
4:4:141:PHE:O	4:4:145:THR:OG1	2.28	0.51
12:L:9:LEU:HD11	12:L:63:ILE:HG21	1.92	0.51
14:N:115:VAL:HG12	14:N:180:ALA:HB1	1.91	0.51
1:1:21:ILE:HG12	1:1:233:THR:HG21	1.93	0.51
1:1:118:LEU:HD13	1:1:225:VAL:HG13	1.92	0.51
23:d:246:PHE:HD1	23:d:251:ARG:HB2	1.75	0.51
27:h:11:ARG:NH2	27:h:20:GLN:OE1	2.43	0.51
29:k:173:ASP:OD1	29:k:207:LYS:NZ	2.43	0.51
5:5:65:ARG:NH1	5:5:123:VAL:O	2.42	0.51
13:M:337:VAL:HG11	13:M:345:ALA:HB2	1.92	0.51
21:b:32:GLN:HE22	21:b:34:GLU:HB2	1.75	0.51
3:3:193:SER:H	3:3:196:SER:HB3	1.75	0.51
4:4:179:GLU:OE2	6:6:66:ARG:NH1	2.39	0.51
13:M:64:PRO:HB3	13:M:454:ILE:HG22	1.92	0.51
13:M:301:ILE:HA	13:M:309:TYR:HE1	1.75	0.51
15:V:65:ILE:HD11	15:V:100:LEU:HD23	1.92	0.51
8:A:67:LEU:HD22	11:K:65:VAL:HA	1.92	0.51
19:Z:10:PRO:O	36:r:94:TYR:OH	2.29	0.51
3:3:190:MET:HG2	3:3:192:MET:HG2	1.92	0.51
3:3:273:GLY:O	3:3:549:HIS:NE2	2.37	0.51
7:9:164:GLU:HG3	28:i:88:ARG:HG3	1.93	0.51
9:H:9:LEU:HD13	9:H:91:MET:HE1	1.92	0.51
12:L:10:VAL:HG21	36:r:78:VAL:HG22	1.92	0.51
15:V:27:ILE:HG23	53:V:203:CDL:H473	1.93	0.51
3:3:201:ASP:OD2	3:3:268:ARG:NH2	2.39	0.51
20:a:57:ASP:OD1	20:a:60:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:r:17:LEU:HD11	38:t:162:LEU:HD22	1.92	0.51
4:4:47:LEU:HD13	8:A:50:PRO:HG2	1.93	0.51
4:4:190:HIS:CD2	6:6:150:PRO:HD3	2.46	0.51
4:4:269:LEU:HB2	4:4:368:GLU:HB2	1.93	0.51
12:L:75:LYS:NZ	12:L:77:SER:OG	2.43	0.51
1:1:270:GLU:OE1	1:1:283:HIS:NE2	2.44	0.50
1:1:342:ASP:OD1	1:1:429:ARG:NH2	2.43	0.50
3:3:194:GLU:HG2	3:3:195:LEU:HG	1.92	0.50
9:H:312:SER:HB3	35:q:54:ARG:HH21	1.76	0.50
12:L:233:LEU:HD23	12:L:307:SER:HB3	1.92	0.50
19:Z:15:ARG:HB3	36:r:109:ILE:HD12	1.94	0.50
33:o:45:ASP:OD1	33:o:49:ARG:NH2	2.44	0.50
1:1:243:ALA:HA	1:1:251:SER:HB3	1.94	0.50
5:5:32:ILE:HG23	25:f:43:TYR:HB2	1.92	0.50
12:L:161:ARG:HA	38:t:91:GLU:HG3	1.93	0.50
3:3:362:TYR:HA	3:3:492:ILE:HD12	1.92	0.50
3:3:601:ARG:NH2	3:3:614:ASP:OD1	2.43	0.50
4:4:35:ASP:O	14:N:49:ASN:ND2	2.44	0.50
9:H:20:LEU:HD13	44:z:12:MET:HE1	1.92	0.50
13:M:328:CYS:HB3	13:M:437:MET:HE1	1.94	0.50
35:q:92:GLU:HA	35:q:95:THR:HG22	1.93	0.50
12:L:128:MET:HG2	12:L:251:THR:HG22	1.93	0.50
3:3:36:GLN:NE2	22:c:47:SER:O	2.44	0.50
3:3:140:LYS:HB2	3:3:148:THR:HG21	1.93	0.50
9:H:14:LEU:HD22	9:H:225:MET:HE2	1.93	0.50
23:d:91:VAL:HG23	23:d:126:VAL:HG11	1.93	0.50
6:6:52:LEU:HB2	6:6:90:GLY:HA3	1.94	0.50
7:9:132:VAL:HG11	7:9:169:ILE:HD11	1.92	0.50
50:L:1002:PC1:H341	53:W:201:CDL:H512	1.93	0.50
23:d:127:GLU:O	23:d:224:ARG:NH1	2.42	0.50
8:A:83:ASN:ND2	50:A:201:PC1:O14	2.38	0.50
23:d:10:LYS:NZ	26:g:126:ASP:OD2	2.43	0.50
5:5:121:VAL:HG21	5:5:146:PRO:HD3	1.93	0.50
5:5:178:ASP:O	5:5:181:LYS:NZ	2.41	0.50
12:L:75:LYS:HD2	41:w:90:ARG:HH22	1.76	0.50
53:M:505:CDL:HA61	33:o:53:VAL:HG21	1.93	0.50
7:9:69:ARG:NH1	7:9:73:GLY:O	2.43	0.50
13:M:101:LEU:HD21	53:M:505:CDL:H841	1.93	0.50
3:3:100:ASN:HB3	3:3:135:ARG:HG2	1.94	0.49
3:3:588:MET:HG3	22:c:63:GLU:HA	1.94	0.49
13:M:36:LEU:HB2	41:w:69:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:40:VAL:HG13	36:r:79:TRP:HD1	1.77	0.49
23:d:52:GLU:HG3	23:d:54:TYR:H	1.77	0.49
33:o:45:ASP:OD2	33:o:51:ARG:NH2	2.45	0.49
2:2:149:VAL:O	2:2:190:ARG:NH2	2.38	0.49
53:W:201:CDL:H192	19:Z:47:VAL:HG21	1.93	0.49
21:b:49:VAL:HG22	21:b:90:GLN:HG3	1.93	0.49
1:1:96:ASN:ND2	46:1:502:FMN:O4'	2.46	0.49
3:3:99:ALA:O	3:3:134:LYS:NZ	2.44	0.49
3:3:244:THR:HB	22:c:73:ALA:HB2	1.95	0.49
4:4:352:TYR:HD1	7:9:86:VAL:HG21	1.77	0.49
12:L:13:ILE:HD11	53:W:201:CDL:H622	1.92	0.49
13:M:179:LEU:HD22	13:M:249:LEU:HD21	1.95	0.49
16:W:124:GLN:HB2	33:o:4:GLY:HA3	1.94	0.49
29:k:170:ILE:HD11	29:k:238:ILE:HD11	1.95	0.49
29:k:173:ASP:HB2	29:k:224:SER:HA	1.95	0.49
32:n:13:MET:HE2	39:u:11:TYR:HB2	1.95	0.49
1:1:367:GLU:OE1	3:3:100:ASN:ND2	2.44	0.49
53:W:201:CDL:OA3	19:Z:48:ARG:NH1	2.45	0.49
19:Z:140:ASP:O	19:Z:161:ARG:NH1	2.45	0.49
12:L:421:ILE:HG12	12:L:501:ALA:HB2	1.93	0.49
18:Y:100:ARG:NH1	18:Y:103:GLN:OE1	2.43	0.49
3:3:148:THR:HG23	3:3:150:MET:HE3	1.93	0.49
12:L:601:LEU:O	15:V:1:AYA:N	2.44	0.49
13:M:41:LEU:HD13	13:M:66:LEU:HD13	1.93	0.49
22:c:28:GLU:O	22:c:32:THR:OG1	2.25	0.49
12:L:1:FME:HA	12:L:61:MET:HE1	1.94	0.49
10:J:103:MET:HE3	10:J:115:ILE:HG13	1.94	0.49
50:M:503:PC1:H153	53:W:201:CDL:HB62	1.95	0.49
14:N:261:MET:HG3	14:N:340:THR:HG23	1.95	0.49
28:i:44:TYR:OH	28:i:113:HIS:N	2.46	0.49
29:k:51:PHE:HB3	29:k:107:GLN:HE21	1.77	0.49
34:p:51:ASN:HD22	38:t:165:LEU:HD22	1.77	0.49
37:s:4:LEU:HD11	40:v:124:THR:HA	1.93	0.49
8:A:71:LEU:O	10:J:147:TYR:OH	2.28	0.49
9:H:204:GLU:HG3	9:H:205:SER:H	1.77	0.49
13:M:144:ASN:ND2	52:M:501:3PE:O32	2.46	0.49
3:3:460:ARG:NH1	3:3:659:ASP:O	2.46	0.48
6:6:71:ARG:HA	9:H:37:PRO:HA	1.95	0.48
14:N:44:MET:HE2	14:N:130:LEU:HD12	1.95	0.48
14:N:122:ILE:O	14:N:176:ARG:NH1	2.46	0.48
14:N:217:THR:HG23	52:N:401:3PE:H242	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:p:47:GLN:HG3	38:t:165:LEU:HD13	1.95	0.48
1:1:120:GLU:OE2	1:1:236:ARG:NH1	2.46	0.48
3:3:377:VAL:HG23	3:3:404:LEU:HD11	1.94	0.48
4:4:261:ARG:NH2	4:4:303:GLU:OE2	2.47	0.48
12:L:136:ASN:HD21	50:L:1002:PC1:H2I1	1.79	0.48
12:L:485:TYR:OH	37:s:1:GLY:N	2.42	0.48
13:M:91:ARG:HD3	13:M:135:ARG:HH21	1.78	0.48
38:t:27:GLU:OE2	38:t:33:ARG:NH1	2.46	0.48
3:3:55:CYS:SG	3:3:68:ALA:N	2.87	0.48
4:4:149:ASN:HD21	4:4:371:LYS:HG3	1.79	0.48
7:9:143:THR:HB	7:9:146:GLU:HG3	1.95	0.48
10:J:126:VAL:HG23	10:J:127:ILE:HG23	1.95	0.48
19:Z:3:SER:OG	19:Z:4:TRP:N	2.45	0.48
29:k:115:LEU:HD13	29:k:121:GLY:HA2	1.95	0.48
30:l:7:LYS:NZ	33:o:8:ARG:O	2.44	0.48
36:r:89:VAL:O	36:r:95:THR:OG1	2.30	0.48
4:4:146:ARG:NH2	4:4:368:GLU:O	2.43	0.48
11:K:17:THR:HG22	12:L:592:LEU:HD11	1.95	0.48
30:l:53:LYS:HG3	30:l:54:GLU:HG3	1.95	0.48
10:J:45:LEU:HD23	10:J:50:SER:HA	1.95	0.48
13:M:282:LEU:HD21	13:M:359:TRP:HH2	1.78	0.48
14:N:30:TRP:NE1	14:N:67:SER:OG	2.47	0.48
40:v:136:ASN:HA	40:v:153:VAL:HB	1.94	0.48
41:w:114:ASP:HB3	41:w:117:LYS:HG2	1.94	0.48
1:1:184:TYR:HB3	1:1:357:GLU:HB3	1.94	0.48
3:3:43:HIS:NE2	3:3:261:GLU:OE2	2.46	0.48
12:L:176:ARG:HH21	13:M:400:MET:HB3	1.79	0.48
50:L:1002:PC1:H3A2	36:r:80:ILE:HG12	1.96	0.48
53:M:505:CDL:H862	14:N:257:LEU:HD21	1.95	0.48
4:4:3:GLN:NE2	13:M:135:ARG:O	2.40	0.48
7:9:27:TRP:HB3	7:9:30:LEU:HD12	1.96	0.48
13:M:447:LEU:HD11	50:M:503:PC1:H3F1	1.96	0.48
53:Y:201:CDL:H622	53:Y:201:CDL:H251	1.96	0.48
1:1:95:VAL:HG11	1:1:118:LEU:HD11	1.96	0.48
3:3:27:LEU:HA	3:3:37:ILE:HD12	1.96	0.48
3:3:110:GLN:NE2	3:3:113:GLU:O	2.44	0.48
3:3:332:LYS:NZ	3:3:505:LEU:O	2.38	0.48
2:2:175:GLU:HG3	2:2:182:PRO:HG3	1.96	0.48
3:3:366:THR:HG22	3:3:370:GLY:HA3	1.95	0.48
5:5:116:PRO:HB3	5:5:141:PHE:HD2	1.79	0.48
12:L:129:LEU:HA	12:L:132:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:18:SER:HB2	13:M:23:ILE:HG22	1.95	0.48
12:L:50:PRO:HA	12:L:53:MET:HG2	1.96	0.47
12:L:552:LEU:HA	12:L:556:ILE:HD12	1.95	0.47
1:1:245:PHE:HB3	1:1:271:GLU:HG3	1.96	0.47
3:3:449:PRO:O	3:3:487:TRP:NE1	2.35	0.47
29:k:25:ILE:HG12	29:k:168:VAL:HB	1.95	0.47
30:l:50:ARG:HG2	30:l:53:LYS:HZ1	1.79	0.47
31:m:49:PRO:HB2	35:q:68:ILE:HD11	1.96	0.47
40:v:52:ASP:OD1	40:v:78:HIS:NE2	2.40	0.47
5:5:82:ASP:OD2	5:5:89:ARG:NH2	2.44	0.47
12:L:72:GLN:NE2	13:M:458:LEU:O	2.48	0.47
12:L:383:MET:HE2	39:u:36:ILE:HD13	1.96	0.47
13:M:155:ALA:HB1	50:M:504:PC1:H2H2	1.96	0.47
28:i:117:LEU:O	28:i:120:THR:OG1	2.31	0.47
29:k:30:ASN:N	29:k:33:SER:OG	2.47	0.47
13:M:232:ALA:O	13:M:237:LYS:NZ	2.47	0.47
27:h:11:ARG:HG2	27:h:19:LEU:HD12	1.96	0.47
36:r:72:THR:HA	36:r:76:ILE:HD12	1.95	0.47
43:y:8:ARG:HG3	43:y:10:HIS:H	1.79	0.47
4:4:149:ASN:HD22	4:4:370:PRO:HB2	1.79	0.47
12:L:453:SER:HA	12:L:456:ARG:HH21	1.79	0.47
27:h:45:SER:O	27:h:51:ASN:ND2	2.35	0.47
40:v:138:LEU:HB3	40:v:141:GLU:HB2	1.95	0.47
8:A:114:THR:HB	9:H:286:MET:HG3	1.97	0.47
34:p:12:SER:OG	40:v:57:GLU:OE2	2.32	0.47
1:1:21:ILE:HG21	1:1:230:VAL:HG12	1.95	0.47
1:1:363:THR:HG21	3:3:97:LEU:HG	1.97	0.47
4:4:282:GLU:HB3	4:4:313:GLN:HE22	1.79	0.47
4:4:323:ILE:HD12	4:4:324:LYS:HG3	1.95	0.47
50:9:401:PC1:H252	9:H:296:LEU:HD13	1.95	0.47
23:d:135:LEU:HA	23:d:167:LYS:HB3	1.97	0.47
29:k:19:THR:HG23	29:k:21:ASN:H	1.80	0.47
1:1:20:ARG:HH12	2:2:201:SER:HB2	1.80	0.47
7:9:162:GLU:HB3	28:i:109:ILE:HG12	1.97	0.47
12:L:487:LYS:NZ	39:u:46:ALA:O	2.48	0.47
18:Y:165:ARG:HH12	33:o:90:MET:HE1	1.79	0.47
23:d:145:TYR:HH	56:d:401:NDP:HO2N	1.63	0.47
23:d:157:ARG:NH1	23:d:226:LYS:O	2.48	0.47
17:j:11:ILE:HG22	17:j:77:VAL:HG23	1.97	0.47
50:9:401:PC1:H351	9:H:187:ILE:HD12	1.97	0.47
12:L:172:ILE:HG21	13:M:408:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:532:ILE:HD11	40:v:101:MET:HB3	1.97	0.47
19:Z:68:ARG:NH1	43:y:43:LEU:O	2.48	0.47
34:p:39:ARG:NH2	38:t:3:LEU:O	2.47	0.47
40:v:50:LEU:HB2	40:v:78:HIS:HD2	1.79	0.47
1:1:358:SER:OG	1:1:365:CYS:SG	2.66	0.47
8:A:63:LEU:HB2	10:J:67:VAL:HG21	1.97	0.47
53:V:203:CDL:H512	53:V:204:CDL:H121	1.97	0.47
23:d:26:ALA:HA	23:d:31:GLY:HA3	1.95	0.47
23:d:76:ARG:NH2	23:d:103:ASN:O	2.44	0.47
12:L:593:ILE:HD12	15:V:41:ALA:HB2	1.96	0.46
13:M:201:MET:HG3	50:M:504:PC1:H3C1	1.97	0.46
53:M:505:CDL:H661	14:N:335:MET:HG2	1.96	0.46
38:t:29:ARG:HD2	38:t:75:HIS:CD2	2.50	0.46
12:L:397:GLU:HB3	12:L:482:MET:HE1	1.97	0.46
13:M:119:TYR:HE1	13:M:157:SER:HB2	1.79	0.46
23:d:167:LYS:O	23:d:230:PHE:N	2.44	0.46
23:d:174:ARG:NH2	23:d:316:GLU:OE2	2.48	0.46
39:u:10:ARG:NH1	39:u:14:PHE:O	2.47	0.46
2:2:120:ILE:HD11	2:2:169:ILE:HG12	1.96	0.46
4:4:391:ILE:O	4:4:430:ARG:NH1	2.48	0.46
53:M:505:CDL:H652	53:M:505:CDL:H842	1.98	0.46
29:k:53:GLU:HG3	29:k:104:ARG:HH12	1.80	0.46
1:1:69:GLY:O	47:1:503:NAI:H2N	2.15	0.46
3:3:569:LYS:HG3	3:3:571:ALA:HB2	1.96	0.46
4:4:20:TYR:OH	14:N:295:ARG:NH2	2.48	0.46
10:J:111:LYS:HA	10:J:121:GLY:HA3	1.97	0.46
16:W:109:GLU:OE2	16:W:112:ARG:NH2	2.41	0.46
39:u:18:THR:HG22	39:u:20:SER:H	1.80	0.46
23:d:26:ALA:HB3	23:d:47:VAL:HG13	1.96	0.46
26:g:116:ASP:OD1	26:g:119:SER:OG	2.26	0.46
1:1:142:PHE:HB3	1:1:145:GLU:HB2	1.98	0.46
1:1:277:LYS:NZ	1:1:281:GLU:OE2	2.40	0.46
13:M:258:ALA:HB1	13:M:302:LEU:HB3	1.96	0.46
18:Y:144:ARG:NE	30:l:58:GLU:OE2	2.46	0.46
1:1:276:LEU:HD21	1:1:297:VAL:HG11	1.98	0.46
12:L:56:HIS:ND1	12:L:57:THR:HG23	2.30	0.46
3:3:26:VAL:HG13	3:3:79:ILE:HD13	1.98	0.46
3:3:276:ARG:NH1	3:3:680:ALA:O	2.48	0.46
13:M:122:PHE:HZ	13:M:206:LYS:HG3	1.81	0.46
29:k:81:LYS:HD2	29:k:92:ASN:HD22	1.81	0.46
12:L:161:ARG:NE	12:L:238:GLU:OE2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:316:THR:HG23	12:L:325:ALA:HB2	1.97	0.46
15:V:113:ALA:O	15:V:117:MET:HB2	2.16	0.46
29:k:135:LEU:HD21	29:k:149:VAL:HA	1.98	0.46
2:2:61:LEU:HD12	2:2:90:TYR:HB3	1.98	0.46
4:4:188:ARG:HH21	6:6:152:THR:HB	1.81	0.46
13:M:91:ARG:NH2	29:k:290:ASP:OD2	2.48	0.46
7:9:114:THR:HG21	7:9:144:HIS:CD2	2.50	0.45
9:H:97:ASN:H	35:q:143:THR:HG22	1.81	0.45
36:r:85:LEU:HA	36:r:89:VAL:HB	1.98	0.45
9:H:149:ILE:HG21	9:H:185:TRP:HB2	1.97	0.45
13:M:452:LYS:HE2	41:w:83:TYR:HB3	1.98	0.45
39:u:61:ASP:HB3	39:u:66:ILE:HB	1.98	0.45
1:1:305:PRO:HG3	1:1:413:TRP:HB3	1.98	0.45
2:2:116:ILE:HG23	2:2:169:ILE:HG21	1.98	0.45
5:5:119:SER:OG	5:5:131:GLU:OE2	2.27	0.45
25:f:5:LYS:NZ	25:f:68:GLU:OE2	2.50	0.45
16:W:138:LYS:HA	30:l:27:ARG:HB3	1.97	0.45
19:Z:64:HIS:NE2	41:w:92:GLU:OE1	2.37	0.45
3:3:12:PHE:HB2	3:3:78:ASN:HA	1.97	0.45
8:A:84:LEU:HD11	31:m:45:ASN:HD22	1.81	0.45
18:Y:48:GLU:OE1	31:m:57:ARG:NH2	2.47	0.45
19:Z:145:LEU:HD22	19:Z:153:LYS:HB3	1.99	0.45
3:3:323:VAL:H	3:3:498:SER:HB3	1.82	0.45
4:4:155:THR:HB	4:4:167:PHE:HA	1.98	0.45
7:9:49:ASN:O	7:9:53:GLU:N	2.46	0.45
8:A:13:LEU:HD21	9:H:14:LEU:HD11	1.98	0.45
13:M:5:ILE:HG22	13:M:9:MET:HE2	1.99	0.45
3:3:231:MET:HB3	3:3:266:LYS:HD2	1.98	0.45
4:4:200:HIS:NE2	7:9:124:GLU:OE1	2.49	0.45
6:6:127:HIS:CD2	7:9:115:LYS:HE2	2.51	0.45
9:H:146:LEU:O	9:H:150:LEU:HB2	2.17	0.45
13:M:126:LEU:HD13	13:M:150:LEU:HD12	1.98	0.45
17:X:26:ASP:OD1	17:X:26:ASP:N	2.47	0.45
3:3:266:LYS:NZ	3:3:674:THR:OG1	2.46	0.45
5:5:194:PHE:O	22:c:81:ASN:ND2	2.49	0.45
6:6:31:ALA:HA	6:6:174:ARG:HH21	1.82	0.45
11:K:21:MET:HE1	52:K:101:3PE:H331	1.99	0.45
12:L:144:TRP:NE1	12:L:179:ASP:OD1	2.44	0.45
13:M:116:ILE:HD11	13:M:161:LEU:HD12	1.99	0.45
18:Y:97:ARG:HD3	35:q:59:LEU:HD13	1.98	0.45
18:Y:129:LYS:NZ	31:m:65:VAL:O	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:136:LEU:HD23	31:m:57:ARG:HE	1.81	0.45
20:a:72:SER:OG	20:a:75:HIS:ND1	2.34	0.45
13:M:173:SER:HB2	16:W:101:ALA:HB2	1.98	0.45
13:M:352:LEU:HB3	13:M:355:MET:HB3	1.98	0.45
13:M:369:LEU:HD12	13:M:370:PRO:HD2	1.98	0.45
8:A:32:GLU:HG3	23:d:320:ARG:HH22	1.82	0.44
14:N:309:ASN:HD21	29:k:76:ASN:HB3	1.83	0.44
19:Z:119:SER:HB3	37:s:55:ARG:HH22	1.81	0.44
2:2:159:ASN:HB3	2:2:184:PRO:HB3	1.99	0.44
4:4:93:TYR:HE2	5:5:168:LEU:HB2	1.82	0.44
13:M:266:LEU:HB3	13:M:395:LEU:HD13	1.99	0.44
52:V:205:3PE:H12	34:p:82:ASN:HA	2.00	0.44
16:W:117:LYS:NZ	33:o:100:ASP:OD2	2.46	0.44
1:1:101:GLU:OE2	1:1:302:SER:N	2.50	0.44
53:L:1003:CDL:H532	53:L:1003:CDL:H362	1.98	0.44
13:M:403:THR:HA	13:M:406:TYR:CE1	2.53	0.44
23:d:98:GLU:HG3	23:d:177:ARG:HE	1.81	0.44
29:k:104:ARG:NH1	29:k:126:ARG:O	2.50	0.44
3:3:103:LEU:HD23	21:b:69:PRO:HB3	1.99	0.44
3:3:243:ARG:HH12	7:9:81:LYS:HE2	1.81	0.44
3:3:518:PRO:HB2	3:3:538:PRO:HD3	2.00	0.44
5:5:93:VAL:HG22	5:5:108:LYS:HG2	2.00	0.44
53:M:505:CDL:H562	14:N:242:ILE:HG21	1.97	0.44
14:N:338:PRO:HG3	53:Y:201:CDL:H792	1.99	0.44
39:u:40:PHE:O	39:u:44:SER:OG	2.28	0.44
24:e:13:LEU:HD22	24:e:16:ARG:HH22	1.82	0.44
34:p:17:LEU:HD11	38:t:71:TRP:CG	2.52	0.44
37:s:8:TYR:OH	40:v:123:PRO:O	2.30	0.44
3:3:46:LEU:HD11	3:3:202:ILE:HD12	1.99	0.44
3:3:162:PHE:HB2	3:3:202:ILE:HD11	1.99	0.44
3:3:568:GLU:HG2	3:3:587:VAL:HG23	1.99	0.44
4:4:106:LEU:HD13	4:4:391:ILE:HG21	1.99	0.44
10:J:92:THR:HG21	52:K:101:3PE:H231	1.99	0.44
28:i:9:ARG:HA	28:i:12:GLN:HG2	1.98	0.44
5:5:68:SER:HB2	25:f:50:ILE:HD12	2.00	0.44
10:J:167:VAL:HG22	14:N:42:PRO:HG2	2.00	0.44
13:M:139:GLN:O	13:M:142:ARG:NH1	2.50	0.44
15:V:2:LYS:HE3	15:V:6:HIS:HE1	1.83	0.44
15:V:5:LEU:HD23	52:V:202:3PE:H231	1.98	0.44
1:1:63:SER:HB2	1:1:242:PHE:HB3	2.00	0.44
1:1:300:GLY:HA3	1:1:329:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:119:GLN:HB2	3:3:123:PHE:HD2	1.82	0.44
3:3:478:ARG:HG3	3:3:483:VAL:HG11	1.99	0.44
7:9:1:THR:N	27:h:104:GLU:O	2.41	0.44
12:L:123:LEU:HB2	12:L:150:MET:HE2	2.00	0.44
13:M:126:LEU:HD21	13:M:153:THR:HG21	1.99	0.44
50:M:504:PC1:H251	50:M:504:PC1:H372	2.00	0.44
17:j:74:GLN:HA	17:j:77:VAL:HG12	1.99	0.44
1:1:346:ALA:HA	2:2:109:MET:HE1	2.00	0.44
4:4:291:GLY:O	4:4:296:ARG:NH1	2.48	0.44
6:6:109:GLU:HG2	6:6:111:ARG:HD3	2.00	0.44
14:N:341:PRO:HG3	18:Y:166:LEU:HD23	2.00	0.44
54:X:101:ZMP:H17	54:X:101:ZMP:H15	1.62	0.44
18:Y:82:THR:HA	18:Y:85:TRP:CD1	2.53	0.44
22:c:69:LEU:HD11	28:i:126:PRO:HG2	2.00	0.44
3:3:284:VAL:HG12	3:3:559:VAL:HG22	2.00	0.43
5:5:154:ASP:OD1	26:g:101:HIS:NE2	2.45	0.43
12:L:195:THR:HG21	12:L:200:GLN:HB3	2.00	0.43
23:d:153:GLU:HG3	23:d:165:ILE:HD13	2.00	0.43
38:t:137:LYS:HA	38:t:140:GLN:HG2	1.99	0.43
4:4:135:GLN:HB3	4:4:276:ASP:HB3	1.99	0.43
8:A:102:LEU:HD23	52:A:202:3PE:H372	2.00	0.43
3:3:117:GLN:NE2	45:3:801:SF4:S3	2.90	0.43
3:3:324:ASP:HB3	3:3:571:ALA:HB1	2.00	0.43
4:4:184:VAL:O	7:9:60:ARG:NH1	2.50	0.43
5:5:77:ASP:OD2	5:5:79:THR:OG1	2.35	0.43
12:L:128:MET:HE1	12:L:255:ALA:HB2	1.98	0.43
12:L:245:ALA:O	12:L:249:SER:OG	2.36	0.43
13:M:143:LEU:HD11	14:N:303:THR:HG21	2.01	0.43
14:N:309:ASN:ND2	29:k:75:GLY:O	2.50	0.43
41:w:50:ASP:HB3	41:w:53:VAL:HB	2.00	0.43
52:A:202:3PE:H381	9:H:295:PRO:HB3	1.99	0.43
15:V:1:AYA:HA	15:V:4:LEU:HD23	2.00	0.43
34:p:70:ALA:HB2	40:v:10:PRO:HG2	2.01	0.43
2:2:51:LEU:HD21	2:2:84:ALA:HB2	2.00	0.43
4:4:93:TYR:HD2	5:5:168:LEU:HD22	1.84	0.43
8:A:63:LEU:HD23	11:K:72:ALA:HB2	1.99	0.43
29:k:173:ASP:N	29:k:223:TYR:O	2.38	0.43
37:s:42:GLN:HE22	40:v:140:LEU:HD12	1.84	0.43
38:t:29:ARG:HD2	38:t:75:HIS:HD2	1.84	0.43
41:w:34:ASP:OD1	41:w:34:ASP:N	2.51	0.43
5:5:177:ASP:OD1	23:d:40:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:88:MET:HB2	12:L:326:PHE:HE2	1.83	0.43
12:L:137:LEU:HD21	12:L:263:PHE:HZ	1.82	0.43
53:L:1003:CDL:H621	13:M:372:SER:HB3	2.00	0.43
14:N:200:MET:HG3	14:N:269:GLU:HG3	2.01	0.43
16:W:83:PRO:O	16:W:87:TYR:HB2	2.18	0.43
1:1:365:CYS:HB2	45:1:501:SF4:S3	2.57	0.43
3:3:11:VAL:HG11	3:3:73:VAL:HB	2.00	0.43
12:L:437:PHE:HE2	12:L:441:ILE:HG13	1.84	0.43
40:v:145:ASP:OD1	40:v:145:ASP:N	2.52	0.43
1:1:154:ARG:HA	20:a:58:LEU:HD21	2.01	0.43
3:3:45:ARG:NH2	3:3:256:GLU:OE2	2.37	0.43
50:6:202:PC1:H3C1	50:6:202:PC1:H3F2	1.87	0.43
12:L:392:LYS:HZ1	12:L:416:THR:HG23	1.82	0.43
12:L:543:THR:HG23	40:v:83:MET:HE1	2.00	0.43
3:3:365:ASN:N	3:3:491:ASN:OD1	2.52	0.43
9:H:79:LEU:HD11	9:H:222:LEU:HD22	2.00	0.43
14:N:338:PRO:HG3	53:Y:201:CDL:H762	2.01	0.43
24:e:57:CYS:SG	24:e:58:SER:N	2.92	0.43
30:l:91:TYR:OH	35:q:92:GLU:OE1	2.32	0.43
3:3:60:GLU:HG2	3:3:78:ASN:HB3	2.01	0.43
7:9:172:ASP:OD2	7:9:176:ARG:NE	2.47	0.43
13:M:106:LEU:HD13	13:M:234:ILE:HG21	2.00	0.43
13:M:426:ILE:HB	38:t:101:TRP:HH2	1.84	0.43
15:V:82:LYS:O	15:V:88:ASN:ND2	2.52	0.43
6:6:104:TYR:O	6:6:111:ARG:NH1	2.52	0.42
9:H:138:GLN:HA	9:H:286:MET:HE1	2.00	0.42
14:N:206:ILE:HG23	52:N:401:3PE:H2I2	2.01	0.42
4:4:324:LYS:HD3	4:4:331:SER:HB3	2.01	0.42
14:N:222:ASN:HD21	14:N:240:MET:HB3	1.84	0.42
4:4:175:GLU:OE2	4:4:188:ARG:NH1	2.52	0.42
8:A:13:LEU:HD22	9:H:10:ILE:HD12	2.00	0.42
17:X:63:PRO:O	17:X:67:ALA:N	2.52	0.42
29:k:182:ARG:HA	29:k:185:LYS:HZ1	1.85	0.42
33:o:66:THR:OG1	42:x:28:TRP:NE1	2.52	0.42
1:1:99:GLU:OE2	1:1:106:LYS:N	2.52	0.42
53:M:505:CDL:H321	33:o:43:LEU:HB3	2.01	0.42
3:3:276:ARG:HA	28:i:135:GLN:HB2	2.02	0.42
4:4:149:ASN:ND2	4:4:370:PRO:HB2	2.34	0.42
15:V:93:GLY:HA3	15:V:118:GLY:HA2	2.00	0.42
17:j:36:PHE:HB3	17:j:42:LEU:HD12	2.01	0.42
38:t:48:ASP:HA	38:t:51:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:t:134:ARG:HA	38:t:137:LYS:HE3	2.01	0.42
3:3:475:GLN:HG3	3:3:646:SER:HB2	2.02	0.42
10:J:43:ILE:HG22	11:K:46:LEU:HD21	2.01	0.42
16:W:120:GLY:O	16:W:124:GLN:NE2	2.53	0.42
40:v:88:ARG:HB3	40:v:89:VAL:H	1.67	0.42
3:3:383:ASN:ND2	3:3:665:GLN:O	2.39	0.42
5:5:182:ARG:HD2	26:g:100:THR:HA	2.02	0.42
11:K:8:ILE:HB	11:K:43:LEU:HD13	2.01	0.42
12:L:227:PHE:N	12:L:284:THR:OG1	2.51	0.42
13:M:325:MET:HE3	13:M:437:MET:HB3	2.02	0.42
14:N:128:LEU:HD13	14:N:216:PHE:HB2	2.01	0.42
19:Z:159:LYS:NZ	33:o:109:TYR:O	2.41	0.42
28:i:106:ARG:HB2	28:i:109:ILE:HG13	2.01	0.42
17:j:62:ILE:HG12	17:j:79:TYR:HE2	1.84	0.42
1:1:361:GLN:N	45:1:501:SF4:S4	2.91	0.42
5:5:14:ARG:HH22	5:5:44:CYS:HB2	1.83	0.42
6:6:107:MET:HA	6:6:108:PRO:HD3	1.93	0.42
50:9:401:PC1:H261	9:H:180:PRO:HB3	2.00	0.42
10:J:5:ILE:HG21	35:q:141:TRP:HZ2	1.84	0.42
34:p:66:ARG:HG3	40:v:10:PRO:HD3	2.02	0.42
1:1:68:ARG:C	1:1:224:ASN:HD22	2.28	0.42
3:3:20:VAL:HG21	3:3:73:VAL:HG21	2.00	0.42
10:J:149:TYR:HD2	11:K:55:LEU:HD21	1.84	0.42
12:L:152:PHE:HB2	12:L:172:ILE:HD11	2.01	0.42
12:L:375:ILE:HG12	39:u:32:MET:SD	2.60	0.42
12:L:584:ILE:HG12	14:N:58:LYS:HE2	2.02	0.42
15:V:80:ARG:NH1	15:V:85:ASP:OD2	2.48	0.42
16:W:125:TYR:HB2	30:l:48:SER:HB3	2.02	0.42
2:2:55:GLN:NE2	2:2:91:ASN:OD1	2.52	0.42
3:3:14:ASP:OD2	3:3:81:THR:OG1	2.35	0.42
3:3:80:LEU:HB3	3:3:83:SER:HB3	2.02	0.42
34:p:74:ASN:OD1	34:p:78:ASN:ND2	2.53	0.42
3:3:20:VAL:HG12	3:3:32:LYS:HD3	2.02	0.41
4:4:104:ASP:HB3	4:4:190:HIS:ND1	2.34	0.41
7:9:55:GLY:HA2	7:9:56:PRO:HD3	1.88	0.41
13:M:122:PHE:CZ	13:M:206:LYS:HG3	2.55	0.41
13:M:457:PRO:O	41:w:84:ARG:NH1	2.53	0.41
14:N:193:VAL:HG11	14:N:266:ILE:HG12	2.02	0.41
1:1:250:ASN:ND2	1:1:318:ASP:OD2	2.54	0.41
2:2:43:LYS:HE2	2:2:73:LEU:HA	2.02	0.41
50:L:1002:PC1:H3H2	53:W:201:CDL:H422	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:L:1003:CDL:H512	53:L:1003:CDL:H541	1.81	0.41
39:u:45:ASP:HB3	39:u:50:HIS:HA	2.02	0.41
3:3:329:ILE:HD12	3:3:329:ILE:HA	1.90	0.41
12:L:542:LEU:HB2	40:v:83:MET:HE3	2.03	0.41
18:Y:23:VAL:HG21	44:z:65:GLY:HA2	2.03	0.41
19:Z:8:VAL:HA	19:Z:108:ARG:HH21	1.86	0.41
23:d:311:GLU:HG2	23:d:336:PRO:HB3	2.03	0.41
29:k:33:SER:HA	29:k:174:VAL:HG21	2.02	0.41
33:o:13:PHE:HE2	33:o:74:TYR:HB3	1.85	0.41
33:o:52:PRO:HG2	33:o:56:ALA:HB2	2.01	0.41
3:3:432:ILE:HA	3:3:440:SER:HB2	2.03	0.41
5:5:96:LEU:HB2	5:5:105:ILE:HG22	2.01	0.41
11:K:18:GLY:HA2	52:K:101:3PE:H241	2.01	0.41
12:L:68:TRP:CD2	50:L:1002:PC1:H2G1	2.55	0.41
13:M:23:ILE:HD11	13:M:92:LYS:HD2	2.01	0.41
13:M:180:GLN:HA	13:M:248:LEU:HD21	2.01	0.41
13:M:216:LEU:HD23	13:M:287:ALA:HB1	2.02	0.41
53:M:505:CDL:H871	14:N:246:ILE:HG22	2.03	0.41
7:9:100:ALA:HB3	21:b:41:ILE:HD11	2.01	0.41
12:L:1:FME:HB2	12:L:1:FME:HE2	1.76	0.41
12:L:213:LEU:HD23	12:L:216:LEU:HD12	2.02	0.41
19:Z:41:ASP:OD1	36:r:86:LYS:NZ	2.42	0.41
11:K:38:LEU:O	11:K:42:ILE:HG12	2.20	0.41
12:L:580:GLN:HE22	15:V:42:LEU:HB3	1.85	0.41
23:d:166:ILE:HG22	23:d:168:PRO:HD3	2.03	0.41
24:e:64:LEU:HB3	24:e:76:VAL:HB	2.00	0.41
12:L:521:LYS:HD3	40:v:96:VAL:HG22	2.02	0.41
13:M:70:MET:HA	13:M:103:GLN:HE21	1.85	0.41
14:N:24:THR:HG22	30:l:2:PHE:HZ	1.86	0.41
25:f:49:GLN:HE22	27:h:92:LYS:HA	1.85	0.41
3:3:499:GLN:HE21	3:3:503:LEU:HD11	1.86	0.41
9:H:233:MET:HB3	9:H:233:MET:HE3	1.88	0.41
12:L:73:THR:HB	12:L:194:ASN:HD21	1.84	0.41
13:M:151:PHE:HB3	52:M:501:3PE:H382	2.03	0.41
14:N:144:GLN:HE21	30:l:2:PHE:HB2	1.85	0.41
16:W:138:LYS:HB2	16:W:143:ASN:HD21	1.86	0.41
18:Y:18:LYS:O	44:z:68:ASN:ND2	2.54	0.41
2:2:154:VAL:HG22	2:2:164:LEU:HD11	2.03	0.41
3:3:115:ASP:O	3:3:119:GLN:HG2	2.20	0.41
3:3:297:GLU:HG3	26:g:122:TYR:CZ	2.56	0.41
17:X:49:GLU:OE2	38:t:19:TYR:OH	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:k:303:LYS:O	33:o:50:ARG:NH1	2.54	0.41
41:w:23:THR:OG1	41:w:24:LEU:N	2.54	0.41
4:4:165:THR:HG23	9:H:32:GLN:HG2	2.03	0.41
4:4:285:VAL:H	7:9:2:TYR:HA	1.86	0.41
5:5:137:MET:HA	5:5:161:PRO:HD2	2.03	0.41
9:H:309:ILE:HG22	31:m:38:THR:HG23	2.03	0.41
12:L:505:SER:O	12:L:508:THR:OG1	2.35	0.41
13:M:94:LEU:HD21	53:M:505:CDL:H551	2.03	0.41
13:M:379:LEU:O	13:M:383:MET:HG2	2.20	0.41
14:N:202:LEU:HD21	30:l:1:PRO:HD3	2.03	0.41
19:Z:40:VAL:HG11	36:r:78:VAL:HG12	2.03	0.41
2:2:31:ILE:HG21	2:2:72:ILE:HD12	2.02	0.40
4:4:174:ARG:HH12	6:6:57:VAL:HG13	1.86	0.40
4:4:233:ARG:NE	7:9:29:GLU:OE2	2.43	0.40
8:A:73:LEU:HD13	10:J:55:MET:HE1	2.04	0.40
12:L:175:ASN:ND2	12:L:222:GLY:O	2.54	0.40
53:M:505:CDL:H572	53:M:505:CDL:H311	2.03	0.40
53:V:203:CDL:HB31	53:V:204:CDL:H122	2.03	0.40
53:o:502:CDL:H732	53:o:502:CDL:HB4	2.03	0.40
3:3:582:GLN:OE1	3:3:620:ARG:NH1	2.54	0.40
8:A:28:ASN:ND2	8:A:30:TYR:OH	2.54	0.40
52:L:1001:3PE:H261	13:M:405:LEU:HD13	2.02	0.40
50:L:1002:PC1:H3I1	53:W:201:CDL:H452	2.03	0.40
13:M:225:ILE:HD13	13:M:331:ASN:HB2	2.03	0.40
13:M:397:GLY:HA2	13:M:400:MET:HE3	2.03	0.40
53:M:505:CDL:H531	53:M:505:CDL:CA7	2.51	0.40
14:N:289:ASN:HA	14:N:292:PHE:CE1	2.56	0.40
24:e:63:LYS:HD3	24:e:77:SER:HA	2.04	0.40
42:x:41:GLU:OE2	42:x:45:ARG:NE	2.54	0.40
6:6:44:SER:OG	9:H:54:LYS:NZ	2.40	0.40
50:6:202:PC1:H143	50:6:202:PC1:H112	1.88	0.40
9:H:125:SER:HB2	9:H:214:GLU:HG3	2.03	0.40
12:L:7:LEU:HA	12:L:10:VAL:HB	2.03	0.40
23:d:133:SER:OG	23:d:134:HIS:N	2.53	0.40
17:j:49:GLU:HA	17:j:52:MET:HE3	2.03	0.40
41:w:68:ILE:O	41:w:72:LEU:HB2	2.21	0.40
8:A:24:LEU:HD12	8:A:27:LEU:HD12	2.02	0.40
14:N:113:PHE:HZ	53:V:203:CDL:H131	1.87	0.40
8:A:53:MET:HG3	8:A:57:LEU:HD23	2.03	0.40
52:A:202:3PE:H281	31:m:22:PHE:HB2	2.03	0.40
10:J:163:ILE:HD13	10:J:163:ILE:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:316:THR:HB	12:L:395:ILE:HG23	2.03	0.40
18:Y:17:VAL:HG12	18:Y:19:VAL:HG22	2.04	0.40
29:k:49:LYS:HE3	29:k:51:PHE:HE1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	428/464 (92%)	409 (96%)	19 (4%)	0	100	100
2	2	211/246 (86%)	195 (92%)	16 (8%)	0	100	100
3	3	686/727 (94%)	658 (96%)	28 (4%)	0	100	100
4	4	421/463 (91%)	403 (96%)	18 (4%)	0	100	100
5	5	206/266 (77%)	197 (96%)	9 (4%)	0	100	100
6	6	154/223 (69%)	149 (97%)	5 (3%)	0	100	100
7	9	174/217 (80%)	166 (95%)	8 (5%)	0	100	100
8	A	100/115 (87%)	94 (94%)	6 (6%)	0	100	100
9	H	316/318 (99%)	299 (95%)	14 (4%)	3 (1%)	14	48
10	J	165/175 (94%)	153 (93%)	12 (7%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	604/606 (100%)	566 (94%)	38 (6%)	0	100	100
13	M	457/459 (100%)	445 (97%)	12 (3%)	0	100	100
14	N	345/347 (99%)	337 (98%)	8 (2%)	0	100	100
15	V	138/141 (98%)	133 (96%)	5 (4%)	0	100	100
16	W	137/189 (72%)	134 (98%)	3 (2%)	0	100	100
17	X	85/157 (54%)	82 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	j	80/157 (51%)	77 (96%)	3 (4%)	0	100	100
18	Y	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
19	Z	169/175 (97%)	166 (98%)	3 (2%)	0	100	100
20	a	42/109 (38%)	41 (98%)	1 (2%)	0	100	100
21	b	93/124 (75%)	89 (96%)	4 (4%)	0	100	100
22	c	124/170 (73%)	119 (96%)	5 (4%)	0	100	100
23	d	289/380 (76%)	280 (97%)	9 (3%)	0	100	100
24	e	84/99 (85%)	82 (98%)	2 (2%)	0	100	100
25	f	111/116 (96%)	110 (99%)	1 (1%)	0	100	100
26	g	112/140 (80%)	107 (96%)	5 (4%)	0	100	100
27	h	92/114 (81%)	88 (96%)	4 (4%)	0	100	100
28	i	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
29	k	317/355 (89%)	303 (96%)	14 (4%)	0	100	100
30	l	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
31	m	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
32	n	77/98 (79%)	75 (97%)	2 (3%)	0	100	100
33	o	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
34	p	126/130 (97%)	121 (96%)	5 (4%)	0	100	100
35	q	137/144 (95%)	134 (98%)	3 (2%)	0	100	100
36	r	95/128 (74%)	89 (94%)	6 (6%)	0	100	100
37	s	120/137 (88%)	118 (98%)	2 (2%)	0	100	100
38	t	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
39	u	63/108 (58%)	61 (97%)	2 (3%)	0	100	100
40	v	153/186 (82%)	144 (94%)	9 (6%)	0	100	100
41	w	99/154 (64%)	94 (95%)	5 (5%)	0	100	100
42	x	47/76 (62%)	47 (100%)	0	0	100	100
43	y	48/58 (83%)	45 (94%)	3 (6%)	0	100	100
44	z	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
All	All	8055/9247 (87%)	7729 (96%)	323 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	H	61	LEU
9	H	214	GLU
9	H	62	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	344/368 (94%)	344 (100%)	0	100	100
2	2	183/210 (87%)	183 (100%)	0	100	100
3	3	578/608 (95%)	578 (100%)	0	100	100
4	4	366/391 (94%)	365 (100%)	1 (0%)	86	91
5	5	189/230 (82%)	189 (100%)	0	100	100
6	6	132/181 (73%)	131 (99%)	1 (1%)	73	86
7	9	151/179 (84%)	150 (99%)	1 (1%)	76	86
8	A	95/103 (92%)	95 (100%)	0	100	100
9	H	278/278 (100%)	278 (100%)	0	100	100
10	J	138/144 (96%)	138 (100%)	0	100	100
11	K	86/86 (100%)	86 (100%)	0	100	100
12	L	538/538 (100%)	538 (100%)	0	100	100
13	M	411/411 (100%)	411 (100%)	0	100	100
14	N	315/315 (100%)	315 (100%)	0	100	100
15	V	101/102 (99%)	101 (100%)	0	100	100
16	W	122/160 (76%)	122 (100%)	0	100	100
17	X	80/141 (57%)	80 (100%)	0	100	100
17	j	76/141 (54%)	76 (100%)	0	100	100
18	Y	154/155 (99%)	154 (100%)	0	100	100
19	Z	155/157 (99%)	155 (100%)	0	100	100
20	a	43/93 (46%)	43 (100%)	0	100	100
21	b	79/97 (81%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	c	113/150 (75%)	113 (100%)	0	100	100
23	d	255/326 (78%)	255 (100%)	0	100	100
24	e	76/82 (93%)	76 (100%)	0	100	100
25	f	101/102 (99%)	101 (100%)	0	100	100
26	g	107/124 (86%)	107 (100%)	0	100	100
27	h	84/96 (88%)	84 (100%)	0	100	100
28	i	131/131 (100%)	131 (100%)	0	100	100
29	k	283/309 (92%)	283 (100%)	0	100	100
30	l	94/95 (99%)	94 (100%)	0	100	100
31	m	69/72 (96%)	69 (100%)	0	100	100
32	n	61/76 (80%)	61 (100%)	0	100	100
33	o	107/109 (98%)	107 (100%)	0	100	100
34	p	114/116 (98%)	114 (100%)	0	100	100
35	q	119/122 (98%)	119 (100%)	0	100	100
36	r	95/122 (78%)	95 (100%)	0	100	100
37	s	110/120 (92%)	110 (100%)	0	100	100
38	t	159/161 (99%)	159 (100%)	0	100	100
39	u	59/84 (70%)	59 (100%)	0	100	100
40	v	140/160 (88%)	140 (100%)	0	100	100
41	w	92/130 (71%)	92 (100%)	0	100	100
42	x	44/67 (66%)	44 (100%)	0	100	100
43	y	46/54 (85%)	46 (100%)	0	100	100
44	z	59/59 (100%)	59 (100%)	0	100	100
All	All	7132/7955 (90%)	7129 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	4	323	ILE
6	6	54	CYS
7	9	78	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	24	ASN
1	1	148	ASN
1	1	150	GLN
1	1	250	ASN
1	1	293	ASN
1	1	373	ASN
2	2	121	GLN
2	2	155	GLN
3	3	117	GLN
3	3	654	GLN
4	4	149	ASN
4	4	252	ASN
5	5	19	HIS
5	5	71	GLN
5	5	144	ASN
5	5	160	HIS
6	6	94	ASN
6	6	106	GLN
9	H	247	HIS
10	J	175	ASN
11	K	7	ASN
12	L	175	ASN
12	L	323	HIS
12	L	434	GLN
12	L	580	GLN
13	M	81	GLN
13	M	138	ASN
13	M	144	ASN
13	M	169	ASN
13	M	338	HIS
13	M	374	ASN
13	M	390	ASN
13	M	399	ASN
13	M	415	GLN
14	N	316	GLN
15	V	18	HIS
16	W	143	ASN
18	Y	29	HIS
18	Y	63	ASN
19	Z	77	HIS
19	Z	106	GLN
19	Z	123	ASN
20	a	40	ASN

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Mol	Chain	Res	Type
21	b	36	ASN
22	c	43	ASN
23	d	87	HIS
23	d	131	HIS
23	d	148	ASN
23	d	180	ASN
23	d	184	ASN
24	e	21	HIS
24	e	47	ASN
25	f	49	GLN
28	i	69	ASN
28	i	72	ASN
28	i	112	ASN
29	k	97	GLN
29	k	141	GLN
29	k	200	GLN
29	k	204	ASN
29	k	288	GLN
30	l	81	GLN
30	l	97	HIS
30	l	100	GLN
33	o	61	GLN
33	o	97	HIS
34	p	51	ASN
34	p	78	ASN
38	t	25	HIS
38	t	50	HIS
38	t	77	GLN
40	v	55	GLN
40	v	66	HIS
40	v	87	ASN
40	v	126	GLN
42	x	34	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 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$
13	FME	M	1	13	8,9,10	0.93	0	8,9,11	0.96	0
12	FME	L	1	12	8,9,10	0.94	0	8,9,11	1.33	2 (25%)
27	AYA	h	1	27	6,7,8	1.40	1 (16%)	6,8,10	1.31	1 (16%)
4	2MR	4	85	4	10,12,13	2.49	3 (30%)	5,13,15	1.16	0
11	FME	K	1	11	8,9,10	0.98	0	8,9,11	0.88	0
15	AYA	V	1	15	6,7,8	1.31	1 (16%)	6,8,10	1.78	2 (33%)
29	SEP	k	36	29	8,9,10	1.64	1 (12%)	7,12,14	1.54	1 (14%)

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
13	FME	M	1	13	-	5/7/9/11	-
12	FME	L	1	12	-	3/7/9/11	-
27	AYA	h	1	27	-	0/5/6/8	-
4	2MR	4	85	4	-	3/10/13/15	-
11	FME	K	1	11	-	4/7/9/11	-
15	AYA	V	1	15	-	2/5/6/8	-
29	SEP	k	36	29	-	4/6/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	85	2MR	CZ-NE	5.10	1.45	1.34
4	4	85	2MR	CZ-NH2	5.03	1.43	1.33
29	k	36	SEP	P-O1P	3.58	1.61	1.50
27	h	1	AYA	CA-N	-2.93	1.43	1.46
15	V	1	AYA	CA-N	-2.44	1.43	1.46
4	4	85	2MR	CQ1-NH1	-2.23	1.41	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	k	36	SEP	OG-CB-CA	3.55	111.60	108.14
15	V	1	AYA	CB-CA-N	3.07	113.14	109.68
27	h	1	AYA	CB-CA-N	3.00	113.07	109.68
12	L	1	FME	C-CA-N	2.55	114.43	109.50
15	V	1	AYA	CA-N-CT	2.43	124.64	121.50
12	L	1	FME	CA-N-CN	2.33	126.41	122.82

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	1	FME	O1-CN-N-CA
13	M	1	FME	C-CA-CB-CG
13	M	1	FME	O-C-CA-CB
29	k	36	SEP	CB-OG-P-O1P
29	k	36	SEP	CB-OG-P-O2P
29	k	36	SEP	CB-OG-P-O3P
4	4	85	2MR	C-CA-CB-CG
12	L	1	FME	CA-CB-CG-SD
15	V	1	AYA	OT-CT-N-CA
15	V	1	AYA	CM-CT-N-CA
11	K	1	FME	CA-CB-CG-SD
11	K	1	FME	CB-CG-SD-CE
12	L	1	FME	N-CA-CB-CG
4	4	85	2MR	CA-CB-CG-CD
29	k	36	SEP	CA-CB-OG-P
4	4	85	2MR	NE-CD-CG-CB
13	M	1	FME	N-CA-CB-CG
13	M	1	FME	CB-CG-SD-CE
11	K	1	FME	CB-CA-N-CN
13	M	1	FME	CB-CA-N-CN
12	L	1	FME	CB-CG-SD-CE

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	1	FME	2	0
15	V	1	AYA	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 2 are monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
52	3PE	L	1004	-	30,30,50	0.41	0	33,35,55	0.75	2 (6%)
52	3PE	o	501	-	30,30,50	0.38	0	33,35,55	0.41	0
57	AMP	k	501	-	25,25,25	1.42	4 (16%)	37,38,38	1.95	7 (18%)
52	3PE	V	201	-	34,34,50	0.36	0	37,39,55	0.32	0
52	3PE	M	501	-	39,39,50	0.33	0	42,44,55	0.42	0
53	CDL	M	505	-	89,89,99	0.29	0	95,101,111	0.41	1 (1%)
52	3PE	i	502	-	50,50,50	0.31	0	53,55,55	0.29	0
52	3PE	M	502	-	43,43,50	0.33	0	46,48,55	0.45	0
53	CDL	z	101	-	57,57,99	0.36	0	63,69,111	0.31	0
50	PC1	A	201	-	36,36,53	0.38	0	42,44,61	0.61	1 (2%)
50	PC1	9	401	-	53,53,53	0.32	0	59,61,61	0.56	1 (1%)
45	SF4	9	402	7	0,12,12	-	-	-	-	-
52	3PE	V	202	-	36,36,50	0.34	0	39,41,55	0.33	0
54	ZMP	X	101	17	25,30,36	0.70	1 (4%)	29,37,45	1.05	2 (6%)
50	PC1	L	1002	-	53,53,53	0.32	0	59,61,61	0.59	2 (3%)
53	CDL	W	201	-	99,99,99	0.27	0	105,111,111	0.30	0
53	CDL	Y	201	-	99,99,99	0.26	0	105,111,111	0.31	0
46	FMN	1	502	-	33,33,33	1.12	3 (9%)	48,50,50	1.40	8 (16%)
48	FES	3	803	3	0,4,4	-	-	-	-	-
45	SF4	1	501	1	0,12,12	-	-	-	-	-
52	3PE	A	202	-	50,50,50	0.30	0	53,55,55	0.38	0
50	PC1	M	503	-	53,53,53	0.29	0	59,61,61	0.40	0
52	3PE	N	401	-	50,50,50	0.31	0	53,55,55	0.54	1 (1%)
50	PC1	6	202	-	45,45,53	0.31	0	51,53,61	0.36	0
45	SF4	9	403	7	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SF4	6	201	6	0,12,12	-	-	-		
52	3PE	K	101	-	39,39,50	0.35	0	42,44,55	0.32	0
45	SF4	3	802	3	0,12,12	-	-	-		
52	3PE	i	501	-	50,50,50	0.30	0	53,55,55	0.31	0
53	CDL	V	203	-	93,93,99	0.26	0	99,105,111	0.24	0
56	NDP	d	401	-	51,52,52	0.40	0	71,80,80	0.42	0
48	FES	2	300	2	0,4,4	-	-	-		
50	PC1	M	504	-	53,53,53	0.30	0	59,61,61	0.36	0
45	SF4	3	801	3	0,12,12	-	-	-		
52	3PE	V	205	-	26,26,50	0.49	0	29,31,55	0.52	1 (3%)
52	3PE	L	1001	-	50,50,50	0.30	0	53,55,55	0.36	0
52	3PE	H	401	-	50,50,50	0.30	0	53,55,55	0.40	0
53	CDL	V	204	-	84,84,99	0.28	0	90,96,111	0.25	0
53	CDL	L	1003	-	99,99,99	0.25	0	105,111,111	0.31	0
54	ZMP	g	201	-	28,33,36	0.63	0	32,40,45	1.19	3 (9%)
47	NAI	1	503	-	47,48,48	0.41	0	64,73,73	1.80	4 (6%)
58	MYR	s	201	37	13,14,15	0.17	0	12,13,15	0.14	0
51	DCQ	6	203	-	23,23,23	0.23	0	27,29,29	0.50	0
53	CDL	o	502	-	74,74,99	0.31	0	80,86,111	0.46	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	3PE	L	1004	-	-	9/34/34/54	-
52	3PE	o	501	-	-	8/34/34/54	-
57	AMP	k	501	-	-	6/10/26/26	0/3/3/3
52	3PE	V	201	-	-	10/38/38/54	-
52	3PE	M	501	-	-	7/43/43/54	-
53	CDL	M	505	-	-	32/100/100/110	-
52	3PE	i	502	-	-	9/54/54/54	-
52	3PE	M	502	-	-	12/47/47/54	-
53	CDL	z	101	-	-	17/68/68/110	-
50	PC1	9	401	-	-	19/57/57/57	-
50	PC1	A	201	-	-	9/40/40/57	-
52	3PE	V	202	-	-	9/40/40/54	-
45	SF4	9	402	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	ZMP	X	101	17	-	16/35/37/43	-
53	CDL	Y	201	-	1/1/9/9	26/110/110/110	-
50	PC1	L	1002	-	-	18/57/57/57	-
53	CDL	W	201	-	-	20/110/110/110	-
46	FMN	1	502	-	-	10/18/18/18	0/3/3/3
48	FES	3	803	3	-	-	0/1/1/1
45	SF4	1	501	1	-	-	0/6/5/5
52	3PE	A	202	-	-	12/54/54/54	-
50	PC1	M	503	-	-	12/57/57/57	-
52	3PE	N	401	-	-	11/54/54/54	-
50	PC1	6	202	-	-	7/49/49/57	-
45	SF4	6	201	6	-	-	0/6/5/5
45	SF4	9	403	7	-	-	0/6/5/5
52	3PE	K	101	-	-	8/43/43/54	-
45	SF4	3	802	3	-	-	0/6/5/5
52	3PE	i	501	-	-	14/54/54/54	-
53	CDL	V	203	-	-	37/104/104/110	-
56	NDP	d	401	-	-	8/34/77/77	0/5/5/5
50	PC1	M	504	-	-	17/57/57/57	-
48	FES	2	300	2	-	-	0/1/1/1
45	SF4	3	801	3	-	-	0/6/5/5
52	3PE	V	205	-	-	4/27/27/54	-
52	3PE	L	1001	-	-	6/54/54/54	-
52	3PE	H	401	-	-	13/54/54/54	-
53	CDL	V	204	-	1/1/9/9	33/95/95/110	-
53	CDL	L	1003	-	1/1/9/9	34/110/110/110	-
54	ZMP	g	201	-	-	15/38/40/43	-
47	NAI	1	503	-	-	12/29/72/72	0/5/5/5
58	MYR	s	201	37	-	2/12/12/13	-
51	DCQ	6	203	-	-	3/14/38/38	0/1/1/1
53	CDL	o	502	-	2/2/9/9	18/85/85/110	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	k	501	AMP	C5-C4	4.70	1.47	1.39
46	1	502	FMN	C4A-N5	2.83	1.36	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	k	501	AMP	C5-C6	2.69	1.48	1.41
57	k	501	AMP	C5-N7	-2.47	1.34	1.39
57	k	501	AMP	C8-N7	2.18	1.35	1.31
54	X	101	ZMP	C9-C10	2.13	1.53	1.50
46	1	502	FMN	C4A-C10	-2.03	1.38	1.44
46	1	502	FMN	C10-N1	2.02	1.37	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	1	503	NAI	O5B-PA-O1A	-9.49	71.32	108.94
47	1	503	NAI	O2A-PA-O1A	-8.50	72.90	112.44
57	k	501	AMP	C5-C4-N3	-6.53	117.72	126.72
47	1	503	NAI	O3-PA-O1A	-5.81	93.22	110.70
57	k	501	AMP	N3-C4-N9	5.25	136.10	127.17
46	1	502	FMN	C4-N3-C2	-3.98	118.58	125.64
57	k	501	AMP	C2-N3-C4	3.85	121.24	111.83
57	k	501	AMP	C4-C5-N7	-3.28	106.83	110.58
46	1	502	FMN	C4A-C10-N10	3.01	120.79	116.48
57	k	501	AMP	N3-C2-N1	-2.91	124.18	128.58
46	1	502	FMN	O4-C4-C4A	-2.90	118.88	126.53
54	g	201	ZMP	O1-C10-C9	-2.87	120.67	123.98
54	g	201	ZMP	C14-C15-N2	-2.85	105.94	112.00
46	1	502	FMN	C4A-C4-N3	2.76	120.29	113.25
54	g	201	ZMP	C15-C14-C13	-2.65	107.98	112.39
54	X	101	ZMP	O1-C10-C9	-2.64	120.93	123.98
46	1	502	FMN	C4A-C10-N1	-2.59	118.23	124.59
50	L	1002	PC1	C2-O21-C21	2.59	123.99	117.80
47	1	503	NAI	O2A-PA-O5B	2.57	119.22	107.57
54	X	101	ZMP	C15-C14-C13	-2.50	108.24	112.39
52	L	1004	3PE	C2-O21-C21	2.47	123.71	117.80
52	N	401	3PE	O21-C2-C1	2.40	116.94	108.34
57	k	501	AMP	C5-N7-C8	2.38	107.19	103.45
46	1	502	FMN	C4-C4A-C10	2.36	120.99	116.93
50	A	201	PC1	C2-O21-C21	2.30	123.30	117.80
57	k	501	AMP	C4-N9-C8	2.25	108.10	105.74
46	1	502	FMN	C10-C4A-N5	-2.21	120.29	124.81
50	9	401	PC1	C2-O21-C21	2.14	122.91	117.80
52	V	205	3PE	O12-P-O14	2.13	119.13	110.83
46	1	502	FMN	C4'-C3'-C2'	-2.11	110.06	113.57
52	L	1004	3PE	O21-C2-C1	2.04	115.67	108.34
50	L	1002	PC1	O21-C2-C1	2.01	115.56	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	M	505	CDL	CB4-OB6-CB5	2.01	122.60	117.80
53	o	502	CDL	CB4-OB6-CB5	2.01	122.60	117.80

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	L	1003	CDL	CB4
53	V	204	CDL	CB4
53	Y	201	CDL	CB4
53	o	502	CDL	CB4
53	o	502	CDL	CA4

All (503) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1	502	FMN	C5'-O5'-P-O2P
46	1	502	FMN	C5'-O5'-P-O3P
47	1	503	NAI	C5B-O5B-PA-O1A
47	1	503	NAI	C5D-O5D-PN-O1N
50	6	202	PC1	C11-O13-P-O12
50	6	202	PC1	C11-O13-P-O11
50	9	401	PC1	C11-O13-P-O12
50	9	401	PC1	C11-O13-P-O14
50	9	401	PC1	C11-O13-P-O11
50	9	401	PC1	C1-O11-P-O12
50	9	401	PC1	O13-C11-C12-N
50	L	1002	PC1	C1-O11-P-O12
50	L	1002	PC1	O13-C11-C12-N
50	M	503	PC1	C11-O13-P-O14
50	M	503	PC1	C11-O13-P-O11
50	M	503	PC1	O13-C11-C12-N
50	M	504	PC1	C11-O13-P-O11
52	A	202	3PE	C11-O13-P-O11
52	A	202	3PE	C11-O13-P-O12
52	A	202	3PE	C11-O13-P-O14
52	A	202	3PE	O13-C11-C12-N
52	H	401	3PE	C1-O11-P-O13
52	H	401	3PE	C11-O13-P-O11
52	H	401	3PE	C11-O13-P-O14
52	H	401	3PE	O13-C11-C12-N
52	K	101	3PE	C1-O11-P-O14
52	K	101	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
52	L	1004	3PE	C1-O11-P-O13
52	L	1004	3PE	C11-O13-P-O11
52	L	1004	3PE	O13-C11-C12-N
52	M	501	3PE	C1-O11-P-O12
52	M	501	3PE	C1-O11-P-O13
52	M	501	3PE	C1-O11-P-O14
52	M	501	3PE	C11-O13-P-O11
52	M	501	3PE	C11-O13-P-O14
52	M	502	3PE	C1-O11-P-O13
52	M	502	3PE	C1-O11-P-O14
52	M	502	3PE	C11-O13-P-O11
52	M	502	3PE	C11-O13-P-O14
52	M	502	3PE	O13-C11-C12-N
52	N	401	3PE	C11-O13-P-O14
52	V	201	3PE	C1-O11-P-O13
52	V	201	3PE	C11-O13-P-O11
52	V	201	3PE	C11-O13-P-O12
52	V	201	3PE	O13-C11-C12-N
52	V	202	3PE	C11-O13-P-O14
52	i	501	3PE	C1-O11-P-O12
52	i	501	3PE	C11-O13-P-O11
52	i	502	3PE	C1-O11-P-O12
52	o	501	3PE	C11-O13-P-O11
52	o	501	3PE	C11-O13-P-O14
52	o	501	3PE	O13-C11-C12-N
53	L	1003	CDL	CA3-OA5-PA1-OA2
53	L	1003	CDL	CA3-OA5-PA1-OA4
53	L	1003	CDL	CB2-OB2-PB2-OB5
53	M	505	CDL	O1-C1-CB2-OB2
53	M	505	CDL	CA2-OA2-PA1-OA3
53	M	505	CDL	CA2-OA2-PA1-OA4
53	M	505	CDL	CA2-OA2-PA1-OA5
53	M	505	CDL	CB2-OB2-PB2-OB3
53	M	505	CDL	CB2-OB2-PB2-OB4
53	M	505	CDL	CB2-OB2-PB2-OB5
53	M	505	CDL	CB3-OB5-PB2-OB3
53	V	203	CDL	CA2-OA2-PA1-OA4
53	V	203	CDL	CB2-OB2-PB2-OB3
53	V	203	CDL	CB2-OB2-PB2-OB5
53	V	203	CDL	CB3-OB5-PB2-OB3
53	V	203	CDL	CB3-OB5-PB2-OB4
53	V	204	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
53	V	204	CDL	CA2-OA2-PA1-OA4
53	V	204	CDL	CA2-OA2-PA1-OA5
53	V	204	CDL	CA3-OA5-PA1-OA2
53	V	204	CDL	CA3-OA5-PA1-OA4
53	V	204	CDL	CB2-OB2-PB2-OB3
53	V	204	CDL	CB2-OB2-PB2-OB5
53	V	204	CDL	CB3-OB5-PB2-OB2
53	V	204	CDL	CB3-OB5-PB2-OB3
53	W	201	CDL	CB2-OB2-PB2-OB4
53	W	201	CDL	CB2-OB2-PB2-OB5
53	Y	201	CDL	CA2-OA2-PA1-OA3
53	Y	201	CDL	CA2-OA2-PA1-OA5
53	Y	201	CDL	CB3-OB5-PB2-OB3
53	o	502	CDL	CA2-OA2-PA1-OA3
53	o	502	CDL	CA2-OA2-PA1-OA5
53	o	502	CDL	CA3-OA5-PA1-OA4
53	o	502	CDL	CB2-OB2-PB2-OB4
53	o	502	CDL	CB2-OB2-PB2-OB5
53	z	101	CDL	CB2-OB2-PB2-OB3
53	z	101	CDL	CB2-OB2-PB2-OB4
53	z	101	CDL	CB2-OB2-PB2-OB5
53	z	101	CDL	CB3-OB5-PB2-OB2
53	z	101	CDL	CB3-OB5-PB2-OB3
54	X	101	ZMP	O4-C17-C18-C21
54	X	101	ZMP	C16-C17-C18-C21
54	X	101	ZMP	O4-C17-C18-C19
54	X	101	ZMP	C16-C17-C18-C19
54	X	101	ZMP	C16-C17-C18-C20
54	X	101	ZMP	C17-C16-N2-C15
54	X	101	ZMP	C7-C8-C9-C10
54	g	201	ZMP	S1-C11-C12-N1
54	g	201	ZMP	C12-C11-S1-C10
54	g	201	ZMP	C7-C8-C9-C10
56	d	401	NDP	C2N-C3N-C7N-O7N
57	k	501	AMP	C5'-O5'-P-O1P
57	k	501	AMP	C5'-O5'-P-O2P
57	k	501	AMP	C5'-O5'-P-O3P
53	V	204	CDL	O1-C1-CB2-OB2
53	Y	201	CDL	O1-C1-CB2-OB2
53	o	502	CDL	O1-C1-CB2-OB2
54	X	101	ZMP	O3-C16-N2-C15
50	L	1002	PC1	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
52	L	1004	3PE	C2-C1-O11-P
53	M	505	CDL	CA2-C1-CB2-OB2
53	V	203	CDL	CA2-C1-CB2-OB2
53	V	203	CDL	O1-C1-CB2-OB2
50	M	504	PC1	C11-C12-N-C14
53	o	502	CDL	CA7-C31-C32-C33
52	V	205	3PE	C21-C22-C23-C24
53	L	1003	CDL	CB7-C71-C72-C73
53	W	201	CDL	O1-C1-CA2-OA2
53	W	201	CDL	O1-C1-CB2-OB2
52	N	401	3PE	C21-C22-C23-C24
53	W	201	CDL	CA2-C1-CB2-OB2
50	M	504	PC1	C11-C12-N-C15
52	V	202	3PE	C2-C1-O11-P
53	z	101	CDL	CB4-CB3-OB5-PB2
53	M	505	CDL	CB5-C51-C52-C53
53	L	1003	CDL	C22-C23-C24-C25
53	L	1003	CDL	C56-C57-C58-C59
52	K	101	3PE	C34-C35-C36-C37
53	L	1003	CDL	C77-C78-C79-C80
50	9	401	PC1	C3C-C3D-C3E-C3F
52	i	501	3PE	C3C-C3D-C3E-C3F
53	Y	201	CDL	C63-C64-C65-C66
52	i	502	3PE	C29-C2A-C2B-C2C
53	L	1003	CDL	C21-C22-C23-C24
53	L	1003	CDL	C82-C83-C84-C85
53	M	505	CDL	C78-C79-C80-C81
53	V	204	CDL	C71-C72-C73-C74
53	Y	201	CDL	C52-C53-C54-C55
50	6	202	PC1	C31-C32-C33-C34
53	W	201	CDL	C35-C36-C37-C38
57	k	501	AMP	C3'-C4'-C5'-O5'
53	V	203	CDL	C52-C53-C54-C55
53	L	1003	CDL	C41-C42-C43-C44
50	6	202	PC1	C3B-C3C-C3D-C3E
50	L	1002	PC1	C23-C24-C25-C26
52	M	502	3PE	C3B-C3C-C3D-C3E
53	M	505	CDL	C81-C82-C83-C84
50	M	504	PC1	C3A-C3B-C3C-C3D
50	M	504	PC1	C11-C12-N-C13
53	W	201	CDL	C72-C73-C74-C75
53	Y	201	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
53	W	201	CDL	CB5-C51-C52-C53
53	Y	201	CDL	CB5-C51-C52-C53
50	L	1002	PC1	C3A-C3B-C3C-C3D
53	V	203	CDL	C79-C80-C81-C82
50	M	504	PC1	C31-C32-C33-C34
52	A	202	3PE	C2E-C2F-C2G-C2H
53	V	203	CDL	C39-C40-C41-C42
53	Y	201	CDL	C81-C82-C83-C84
52	A	202	3PE	C2C-C2D-C2E-C2F
53	Y	201	CDL	C15-C16-C17-C18
52	A	202	3PE	C38-C39-C3A-C3B
52	L	1001	3PE	C24-C25-C26-C27
50	9	401	PC1	C3B-C3C-C3D-C3E
53	M	505	CDL	C56-C57-C58-C59
52	K	101	3PE	C23-C24-C25-C26
54	X	101	ZMP	C3-C4-C5-C6
50	M	503	PC1	C39-C3A-C3B-C3C
53	V	203	CDL	OB6-CB4-CB6-OB8
54	g	201	ZMP	C1-C2-C3-C4
53	V	204	CDL	C14-C15-C16-C17
47	1	503	NAI	C2D-C1D-N1N-C2N
47	1	503	NAI	C2D-C1D-N1N-C6N
51	6	203	DCQ	C6-C7-C8-C9
53	V	204	CDL	CA2-C1-CB2-OB2
53	o	502	CDL	CA2-C1-CB2-OB2
54	X	101	ZMP	O3-C16-C17-O4
53	V	204	CDL	CA5-C11-C12-C13
50	L	1002	PC1	O11-C1-C2-C3
50	M	504	PC1	O11-C1-C2-C3
53	L	1003	CDL	C17-C18-C19-C20
53	V	203	CDL	CA7-C31-C32-C33
53	o	502	CDL	CB7-C71-C72-C73
46	1	502	FMN	O3'-C3'-C4'-C5'
53	M	505	CDL	CA3-CA4-CA6-OA8
53	V	203	CDL	CB3-CB4-CB6-OB8
53	V	204	CDL	CB3-CB4-CB6-OB8
53	W	201	CDL	C31-C32-C33-C34
50	L	1002	PC1	C38-C39-C3A-C3B
50	9	401	PC1	C3A-C3B-C3C-C3D
46	1	502	FMN	C5'-O5'-P-O1P
53	Y	201	CDL	C32-C33-C34-C35
53	Y	201	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
53	W	201	CDL	CB2-C1-CA2-OA2
52	H	401	3PE	O11-C1-C2-O21
52	V	201	3PE	O11-C1-C2-O21
53	o	502	CDL	OB5-CB3-CB4-OB6
53	Y	201	CDL	C59-C60-C61-C62
53	L	1003	CDL	C37-C38-C39-C40
53	V	204	CDL	OA6-CA4-CA6-OA8
53	M	505	CDL	C19-C20-C21-C22
50	9	401	PC1	C22-C23-C24-C25
53	V	203	CDL	C31-C32-C33-C34
54	X	101	ZMP	O4-C17-C18-C20
54	g	201	ZMP	O4-C17-C18-C19
54	g	201	ZMP	O4-C17-C18-C20
52	M	502	3PE	C31-C32-C33-C34
52	M	502	3PE	C32-C33-C34-C35
53	Y	201	CDL	C37-C38-C39-C40
50	M	503	PC1	C3E-C3F-C3G-C3H
52	M	502	3PE	C2-C1-O11-P
53	z	101	CDL	C1-CB2-OB2-PB2
53	Y	201	CDL	C14-C15-C16-C17
53	Y	201	CDL	CA5-C11-C12-C13
53	V	203	CDL	OA5-CA3-CA4-CA6
53	W	201	CDL	OA5-CA3-CA4-CA6
50	9	401	PC1	C2B-C2C-C2D-C2E
53	z	101	CDL	CA2-C1-CB2-OB2
52	N	401	3PE	C1-C2-C3-O31
53	Y	201	CDL	CA3-CA4-CA6-OA8
53	z	101	CDL	CA3-CA4-CA6-OA8
54	g	201	ZMP	N2-C16-C17-O4
53	M	505	CDL	C84-C85-C86-C87
53	V	204	CDL	C34-C35-C36-C37
52	N	401	3PE	O11-C1-C2-O21
53	V	203	CDL	OB5-CB3-CB4-OB6
53	L	1003	CDL	CA4-CA3-OA5-PA1
53	M	505	CDL	C1-CA2-OA2-PA1
50	L	1002	PC1	C31-C32-C33-C34
54	X	101	ZMP	O1-C10-S1-C11
53	V	204	CDL	C52-C53-C54-C55
53	V	203	CDL	C40-C41-C42-C43
53	M	505	CDL	OA6-CA4-CA6-OA8
53	V	203	CDL	OA6-CA4-CA6-OA8
53	V	204	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
53	Y	201	CDL	OA6-CA4-CA6-OA8
56	d	401	NDP	C2N-C3N-C7N-N7N
53	M	505	CDL	C64-C65-C66-C67
52	V	202	3PE	C21-C22-C23-C24
52	i	501	3PE	C33-C34-C35-C36
47	1	503	NAI	PN-O3-PA-O5B
46	1	502	FMN	C2'-C3'-C4'-O4'
54	X	101	ZMP	C9-C10-S1-C11
53	Y	201	CDL	CA2-C1-CB2-OB2
52	N	401	3PE	C32-C33-C34-C35
53	V	203	CDL	OB5-CB3-CB4-CB6
53	V	204	CDL	OA5-CA3-CA4-CA6
50	9	401	PC1	C22-C21-O21-C2
50	M	504	PC1	O11-C1-C2-O21
53	V	203	CDL	OA5-CA3-CA4-OA6
53	V	204	CDL	OA5-CA3-CA4-OA6
53	Y	201	CDL	C57-C58-C59-C60
53	V	204	CDL	C15-C16-C17-C18
54	g	201	ZMP	C16-C17-C18-C20
47	1	503	NAI	O4D-C1D-N1N-C2N
46	1	502	FMN	C4'-C5'-O5'-P
53	z	101	CDL	O1-C1-CB2-OB2
58	s	201	MYR	C1-C2-C3-C4
53	z	101	CDL	C52-C53-C54-C55
53	M	505	CDL	C71-C72-C73-C74
52	H	401	3PE	O11-C1-C2-C3
46	1	502	FMN	O3'-C3'-C4'-O4'
52	i	501	3PE	C36-C37-C38-C39
46	1	502	FMN	N10-C1'-C2'-O2'
46	1	502	FMN	N10-C1'-C2'-C3'
54	X	101	ZMP	C19-C18-C21-O5
54	g	201	ZMP	C16-C17-C18-C21
53	L	1003	CDL	C34-C35-C36-C37
57	k	501	AMP	O4'-C4'-C5'-O5'
51	6	203	DCQ	C11-C10-C9-C8
53	M	505	CDL	CB4-CB3-OB5-PB2
50	9	401	PC1	O22-C21-O21-C2
50	A	201	PC1	O11-C1-C2-O21
53	L	1003	CDL	OB5-CB3-CB4-OB6
53	W	201	CDL	OA5-CA3-CA4-OA6
52	i	501	3PE	C2D-C2E-C2F-C2G
53	L	1003	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
53	M	505	CDL	C23-C24-C25-C26
53	V	203	CDL	C37-C38-C39-C40
47	1	503	NAI	O4D-C1D-N1N-C6N
53	z	101	CDL	OA6-CA4-CA6-OA8
52	A	202	3PE	C24-C25-C26-C27
53	o	502	CDL	CB3-CB4-CB6-OB8
53	M	505	CDL	C83-C84-C85-C86
50	L	1002	PC1	C34-C35-C36-C37
53	M	505	CDL	C31-C32-C33-C34
52	N	401	3PE	C2C-C2D-C2E-C2F
50	M	504	PC1	O31-C31-C32-C33
47	1	503	NAI	C5B-O5B-PA-O3
47	1	503	NAI	C5D-O5D-PN-O3
47	1	503	NAI	C5D-O5D-PN-O2N
50	6	202	PC1	C11-O13-P-O14
50	A	201	PC1	C11-O13-P-O14
50	L	1002	PC1	C1-O11-P-O14
50	L	1002	PC1	C1-O11-P-O13
50	M	504	PC1	C11-O13-P-O14
52	H	401	3PE	C11-O13-P-O12
52	K	101	3PE	C11-O13-P-O11
52	K	101	3PE	C11-O13-P-O12
52	K	101	3PE	C11-O13-P-O14
52	L	1001	3PE	C1-O11-P-O14
52	L	1004	3PE	C1-O11-P-O14
52	L	1004	3PE	C11-O13-P-O14
52	M	501	3PE	C11-O13-P-O12
52	M	502	3PE	C1-O11-P-O12
52	V	201	3PE	C1-O11-P-O14
52	V	202	3PE	C1-O11-P-O12
52	V	202	3PE	C1-O11-P-O13
52	V	202	3PE	C1-O11-P-O14
52	i	501	3PE	C1-O11-P-O13
52	i	501	3PE	C1-O11-P-O14
52	i	501	3PE	C11-O13-P-O14
52	i	502	3PE	C1-O11-P-O13
52	i	502	3PE	C1-O11-P-O14
52	i	502	3PE	C11-O13-P-O14
52	o	501	3PE	C11-O13-P-O12
53	L	1003	CDL	CA2-OA2-PA1-OA3
53	L	1003	CDL	CA2-OA2-PA1-OA4
53	L	1003	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
53	L	1003	CDL	CA3-OA5-PA1-OA3
53	L	1003	CDL	CB2-OB2-PB2-OB3
53	L	1003	CDL	CB3-OB5-PB2-OB2
53	M	505	CDL	CA3-OA5-PA1-OA3
53	V	203	CDL	CA2-OA2-PA1-OA3
53	V	203	CDL	CA2-OA2-PA1-OA5
53	V	203	CDL	CB2-OB2-PB2-OB4
53	V	203	CDL	CB3-OB5-PB2-OB2
53	V	204	CDL	CB2-OB2-PB2-OB4
53	V	204	CDL	CB3-OB5-PB2-OB4
53	W	201	CDL	CA2-OA2-PA1-OA3
53	Y	201	CDL	CA2-OA2-PA1-OA4
53	Y	201	CDL	CB3-OB5-PB2-OB2
53	o	502	CDL	CA2-OA2-PA1-OA4
53	o	502	CDL	CA3-OA5-PA1-OA2
53	o	502	CDL	CA3-OA5-PA1-OA3
53	z	101	CDL	CA3-OA5-PA1-OA2
53	z	101	CDL	CA3-OA5-PA1-OA3
53	z	101	CDL	CA3-OA5-PA1-OA4
53	z	101	CDL	CB3-OB5-PB2-OB4
54	g	201	ZMP	O4-C17-C18-C21
50	M	504	PC1	C2-C1-O11-P
52	H	401	3PE	C2-C1-O11-P
52	V	201	3PE	C2-C1-O11-P
53	V	204	CDL	C1-CA2-OA2-PA1
53	V	204	CDL	C1-CB2-OB2-PB2
52	M	502	3PE	C25-C26-C27-C28
53	M	505	CDL	C72-C73-C74-C75
53	V	203	CDL	CA5-C11-C12-C13
56	d	401	NDP	C2D-C1D-N1N-C6N
52	H	401	3PE	C2D-C2E-C2F-C2G
53	M	505	CDL	CA5-C11-C12-C13
52	H	401	3PE	C27-C28-C29-C2A
50	A	201	PC1	C11-C12-N-C13
52	V	201	3PE	O11-C1-C2-C3
53	L	1003	CDL	OB5-CB3-CB4-CB6
52	M	501	3PE	C31-C32-C33-C34
54	g	201	ZMP	C2-C1-C22-C23
50	M	504	PC1	C36-C37-C38-C39
53	L	1003	CDL	C1-CA2-OA2-PA1
53	V	204	CDL	C75-C76-C77-C78
53	V	204	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
54	g	201	ZMP	C5-C6-C7-C8
50	L	1002	PC1	C29-C2A-C2B-C2C
53	W	201	CDL	C83-C84-C85-C86
53	V	203	CDL	C1-CA2-OA2-PA1
53	Y	201	CDL	C1-CB2-OB2-PB2
50	M	503	PC1	O11-C1-C2-O21
53	V	203	CDL	C43-C44-C45-C46
46	1	502	FMN	C2'-C3'-C4'-C5'
53	V	203	CDL	C80-C81-C82-C83
52	i	502	3PE	C28-C29-C2A-C2B
50	L	1002	PC1	C39-C3A-C3B-C3C
56	d	401	NDP	O4D-C1D-N1N-C6N
50	9	401	PC1	C2C-C2D-C2E-C2F
50	9	401	PC1	C2-C1-O11-P
57	k	501	AMP	C4'-C5'-O5'-P
52	L	1001	3PE	C3B-C3C-C3D-C3E
50	M	504	PC1	C39-C3A-C3B-C3C
52	o	501	3PE	C22-C23-C24-C25
50	9	401	PC1	C3-C2-O21-C21
52	H	401	3PE	C26-C27-C28-C29
52	L	1001	3PE	C35-C36-C37-C38
50	M	504	PC1	C25-C26-C27-C28
50	M	503	PC1	C28-C29-C2A-C2B
50	L	1002	PC1	O11-C1-C2-O21
52	N	401	3PE	C2B-C2C-C2D-C2E
52	K	101	3PE	C2-C1-O11-P
52	i	501	3PE	C23-C24-C25-C26
53	L	1003	CDL	C11-C12-C13-C14
53	V	203	CDL	C78-C79-C80-C81
53	L	1003	CDL	OA6-CA4-CA6-OA8
53	W	201	CDL	OB6-CB4-CB6-OB8
47	1	503	NAI	C2N-C3N-C7N-N7N
52	N	401	3PE	C22-C23-C24-C25
52	A	202	3PE	C23-C24-C25-C26
50	L	1002	PC1	C28-C29-C2A-C2B
52	V	205	3PE	C22-C23-C24-C25
50	9	401	PC1	C2D-C2E-C2F-C2G
50	L	1002	PC1	C3D-C3E-C3F-C3G
53	M	505	CDL	CA4-CA3-OA5-PA1
50	L	1002	PC1	C2A-C2B-C2C-C2D
52	M	502	3PE	C36-C37-C38-C39
53	L	1003	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
50	9	401	PC1	C34-C35-C36-C37
58	s	201	MYR	C11-C10-C9-C8
50	9	401	PC1	C3F-C3G-C3H-C3I
52	i	501	3PE	C32-C33-C34-C35
52	A	202	3PE	O21-C2-C3-O31
50	A	201	PC1	O31-C31-C32-C33
51	6	203	DCQ	C7-C8-C9-C10
53	L	1003	CDL	C81-C82-C83-C84
53	W	201	CDL	CA5-C11-C12-C13
53	L	1003	CDL	CB5-C51-C52-C53
50	A	201	PC1	O21-C21-C22-C23
50	L	1002	PC1	C1-C2-O21-C21
52	L	1004	3PE	C1-C2-O21-C21
50	A	201	PC1	C32-C33-C34-C35
53	Y	201	CDL	C58-C59-C60-C61
47	1	503	NAI	C4D-C5D-O5D-PN
53	V	203	CDL	C13-C14-C15-C16
52	L	1004	3PE	O11-C1-C2-O21
52	i	501	3PE	O11-C1-C2-O21
52	V	202	3PE	C31-C32-C33-C34
50	A	201	PC1	C11-C12-N-C14
50	6	202	PC1	C3C-C3D-C3E-C3F
50	M	503	PC1	C31-C32-C33-C34
53	L	1003	CDL	CA7-C31-C32-C33
50	6	202	PC1	C23-C24-C25-C26
54	g	201	ZMP	C16-C17-C18-C19
52	V	201	3PE	C31-C32-C33-C34
52	V	202	3PE	O31-C31-C32-C33
53	M	505	CDL	C82-C83-C84-C85
53	V	204	CDL	C12-C13-C14-C15
50	A	201	PC1	C11-C12-N-C15
50	M	504	PC1	C3B-C3C-C3D-C3E
52	H	401	3PE	C31-C32-C33-C34
50	M	504	PC1	O21-C21-C22-C23
52	i	502	3PE	O21-C21-C22-C23
53	L	1003	CDL	C32-C33-C34-C35
54	X	101	ZMP	C2-C3-C4-C5
53	M	505	CDL	C80-C81-C82-C83
52	o	501	3PE	O31-C31-C32-C33
53	V	203	CDL	C44-C45-C46-C47
52	N	401	3PE	O31-C31-C32-C33
54	g	201	ZMP	O3-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
56	d	401	NDP	C2D-C1D-N1N-C2N
53	V	204	CDL	C32-C31-CA7-OA8
50	M	503	PC1	C3A-C3B-C3C-C3D
53	o	502	CDL	C71-C72-C73-C74
52	L	1004	3PE	C33-C34-C35-C36
53	W	201	CDL	CB3-CB4-CB6-OB8
50	M	504	PC1	C23-C24-C25-C26
50	M	503	PC1	C27-C28-C29-C2A
52	A	202	3PE	O21-C21-C22-C23
52	L	1001	3PE	O31-C31-C32-C33
53	V	203	CDL	C32-C33-C34-C35
53	W	201	CDL	C19-C20-C21-C22
50	A	201	PC1	C21-C22-C23-C24
53	V	203	CDL	C73-C74-C75-C76
52	N	401	3PE	C3-C2-O21-C21
53	M	505	CDL	CB3-CB4-OB6-CB5
53	o	502	CDL	CB6-CB4-OB6-CB5
50	M	503	PC1	C2E-C2F-C2G-C2H
56	d	401	NDP	O4B-C4B-C5B-O5B
54	g	201	ZMP	N2-C16-C17-C18
53	Y	201	CDL	C72-C71-CB7-OB8
52	i	501	3PE	C25-C26-C27-C28
53	L	1003	CDL	CB4-CB3-OB5-PB2
56	d	401	NDP	O4D-C1D-N1N-C2N
56	d	401	NDP	C2B-O2B-P2B-O1X
52	H	401	3PE	C29-C2A-C2B-C2C
53	z	101	CDL	C52-C51-CB5-OB6
52	V	205	3PE	C26-C27-C28-C29
53	Y	201	CDL	C16-C17-C18-C19
52	A	202	3PE	O22-C21-C22-C23
53	W	201	CDL	C58-C59-C60-C61
50	9	401	PC1	C31-C32-C33-C34
53	L	1003	CDL	C39-C40-C41-C42
52	o	501	3PE	O32-C31-C32-C33
53	M	505	CDL	C72-C71-CB7-OB8
52	V	205	3PE	O21-C21-C22-C23
52	i	502	3PE	O22-C21-C22-C23
53	V	204	CDL	C23-C24-C25-C26
52	i	501	3PE	C2F-C2G-C2H-C2I
52	V	202	3PE	O32-C31-C32-C33
53	V	203	CDL	CA3-CA4-CA6-OA8
53	W	201	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
54	X	101	ZMP	N2-C16-C17-O4
53	V	204	CDL	C32-C31-CA7-OA9
53	L	1003	CDL	C60-C61-C62-C63
53	V	203	CDL	C32-C31-CA7-OA8
52	N	401	3PE	O32-C31-C32-C33
52	o	501	3PE	C31-C32-C33-C34
53	o	502	CDL	OB5-CB3-CB4-CB6
50	M	503	PC1	C37-C38-C39-C3A
52	i	502	3PE	O31-C31-C32-C33
53	V	204	CDL	C12-C11-CA5-OA6
53	V	203	CDL	C72-C71-CB7-OB8
53	o	502	CDL	C72-C71-CB7-OB8
52	V	201	3PE	C25-C26-C27-C28
52	L	1001	3PE	O32-C31-C32-C33

There are no ring outliers.

29 monomers are involved in 84 short contacts:

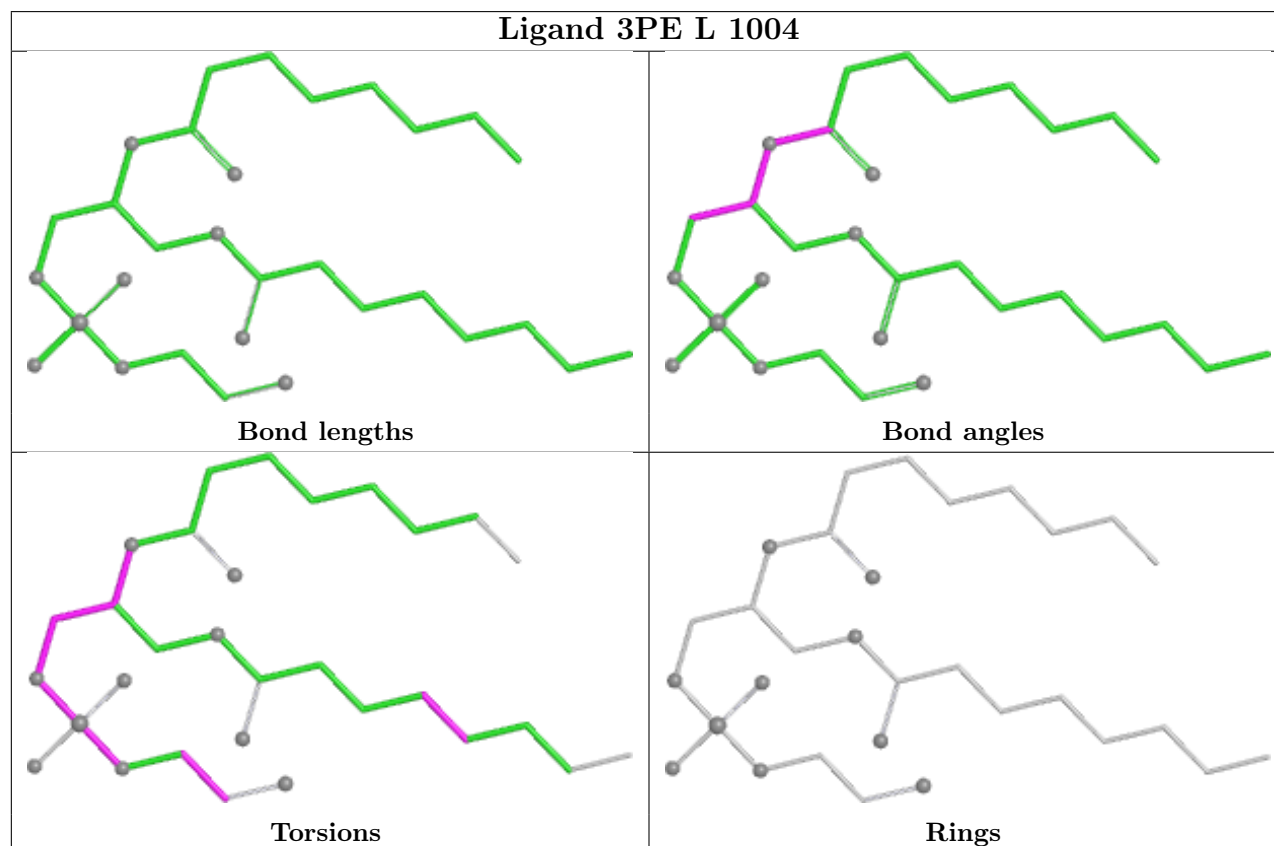
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	M	501	3PE	2	0
53	M	505	CDL	12	0
50	A	201	PC1	2	0
50	9	401	PC1	4	0
52	V	202	3PE	1	0
54	X	101	ZMP	3	0
50	L	1002	PC1	7	0
53	W	201	CDL	10	0
53	Y	201	CDL	6	0
46	1	502	FMN	1	0
45	1	501	SF4	3	0
52	A	202	3PE	3	0
50	M	503	PC1	3	0
52	N	401	3PE	2	0
50	6	202	PC1	2	0
45	6	201	SF4	1	0
52	K	101	3PE	4	0
52	i	501	3PE	1	0
53	V	203	CDL	5	0
56	d	401	NDP	1	0
48	2	300	FES	1	0
50	M	504	PC1	3	0
45	3	801	SF4	1	0

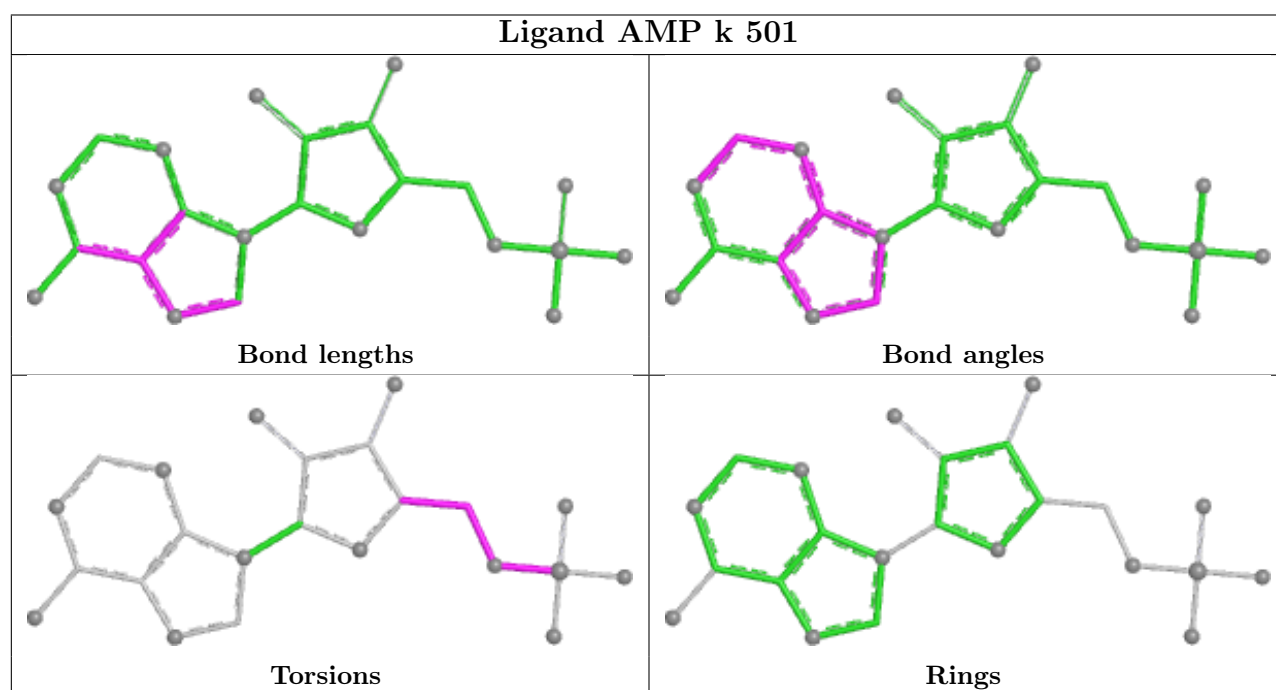
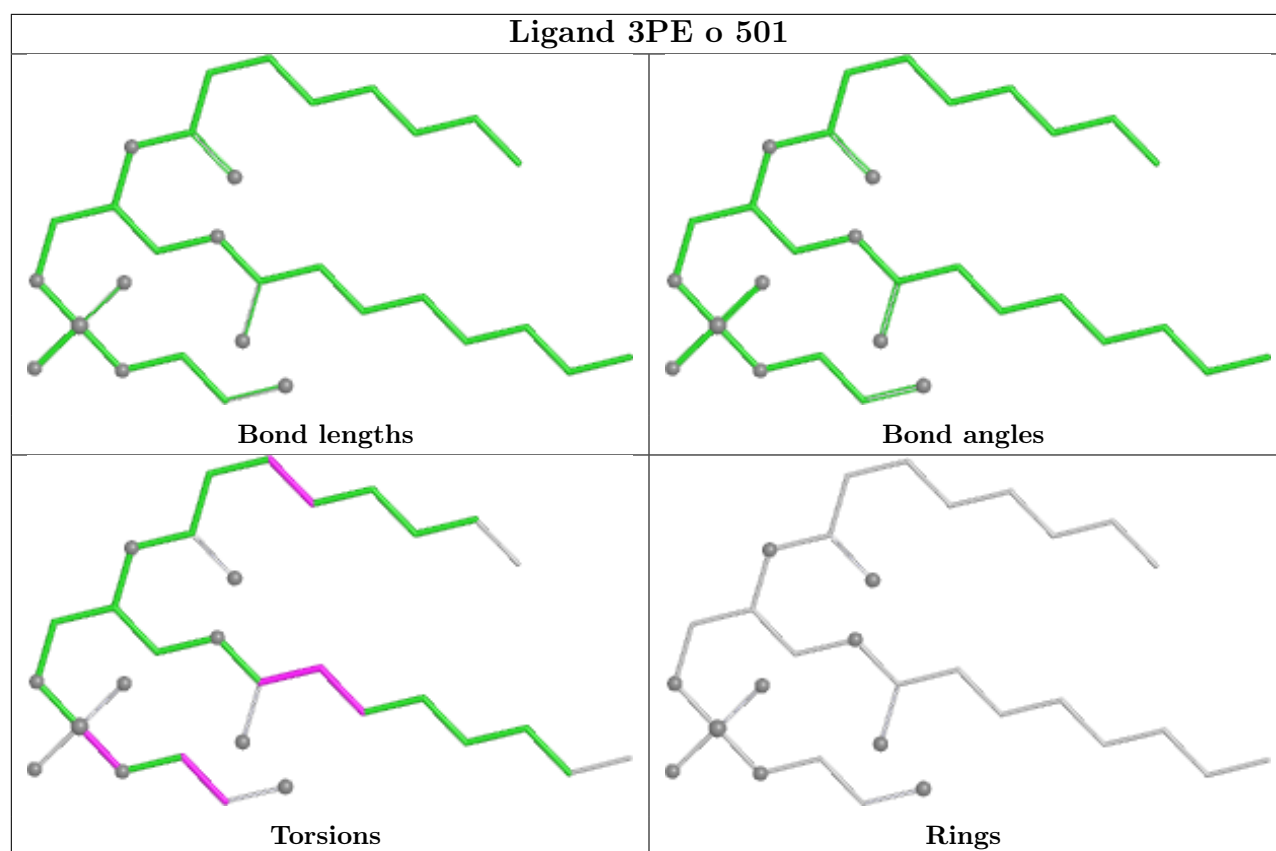
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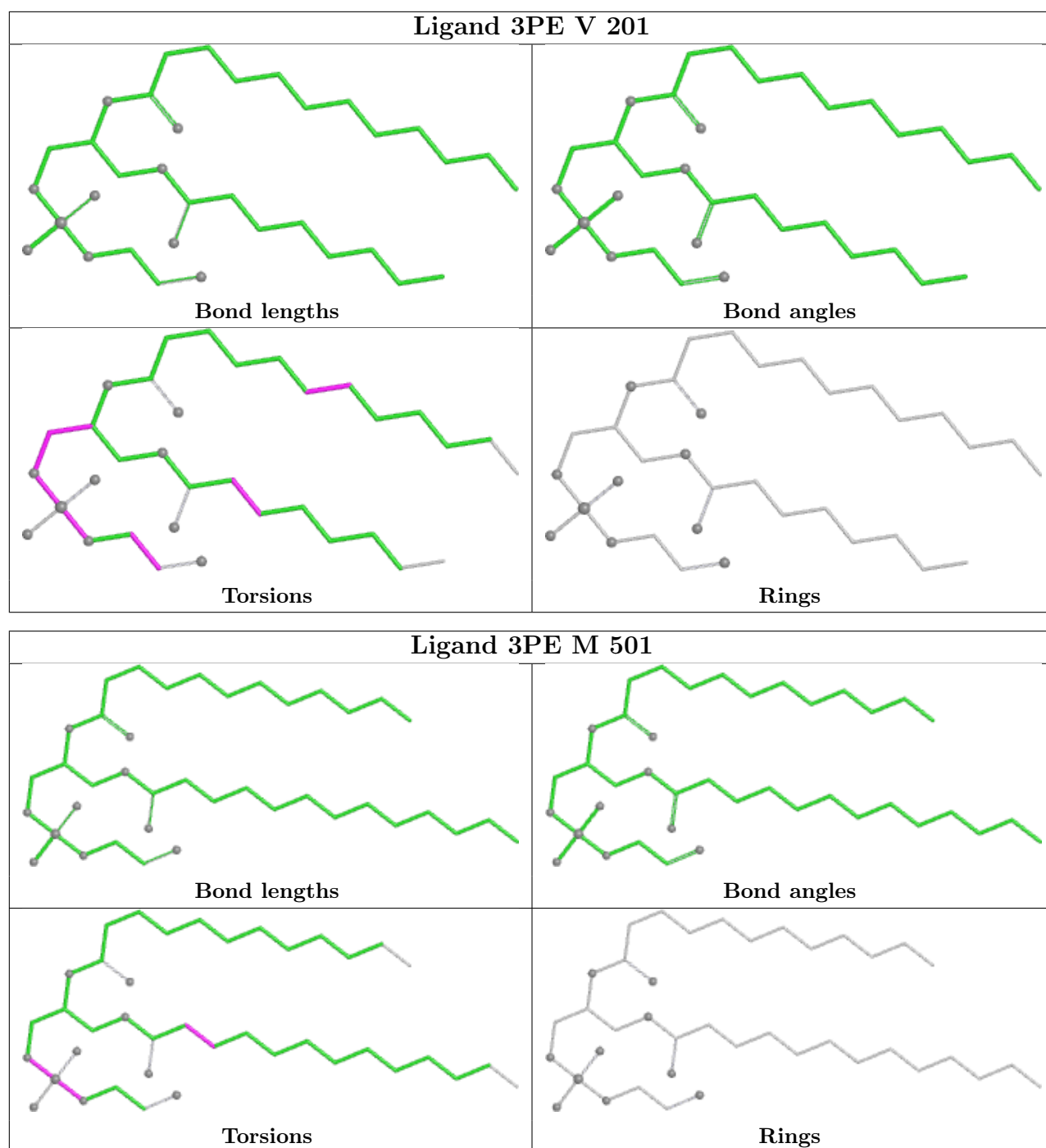
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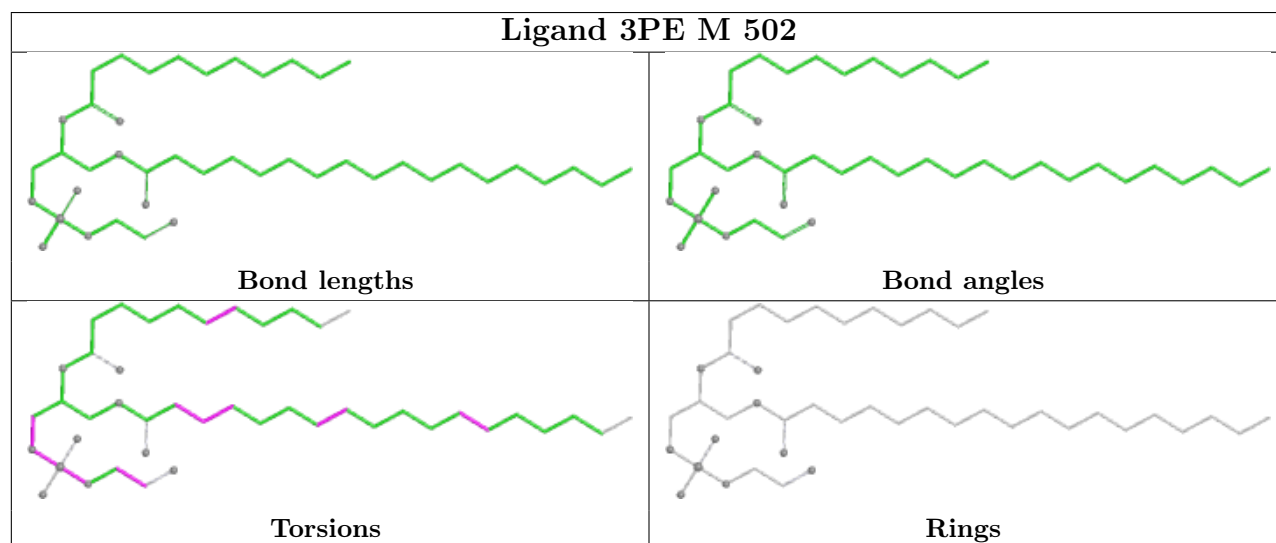
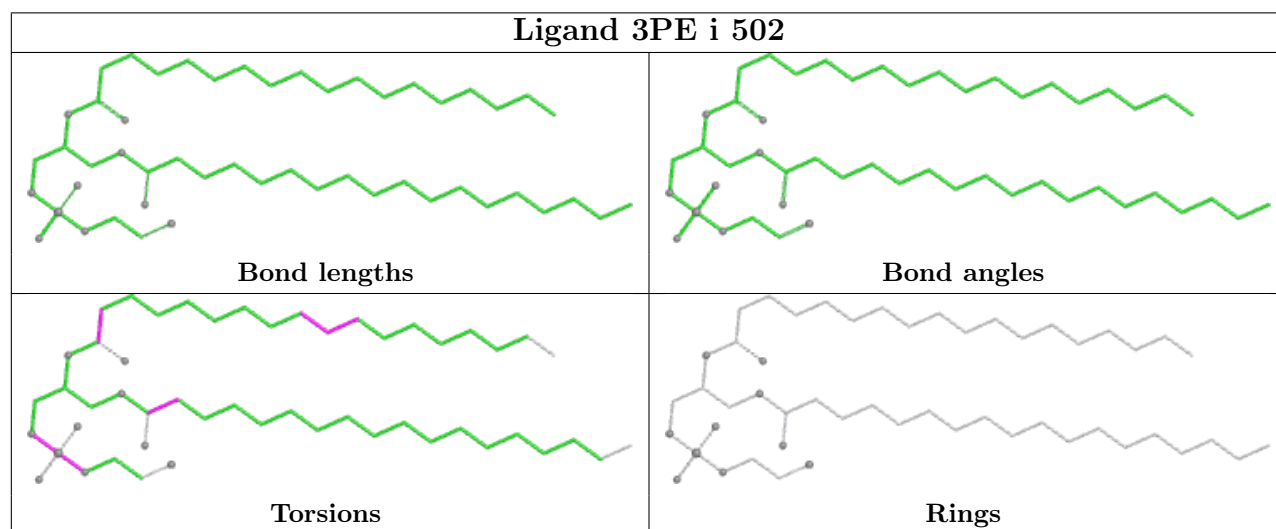
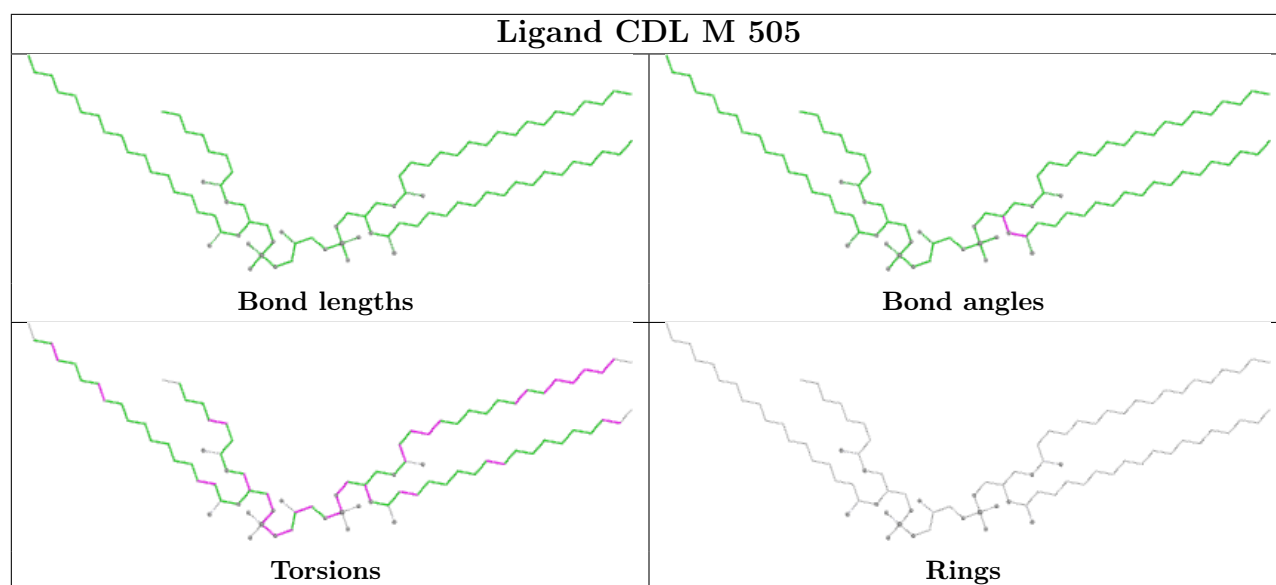
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	V	205	3PE	2	0
52	L	1001	3PE	1	0
53	V	204	CDL	2	0
53	L	1003	CDL	5	0
47	1	503	NAI	3	0
53	o	502	CDL	1	0

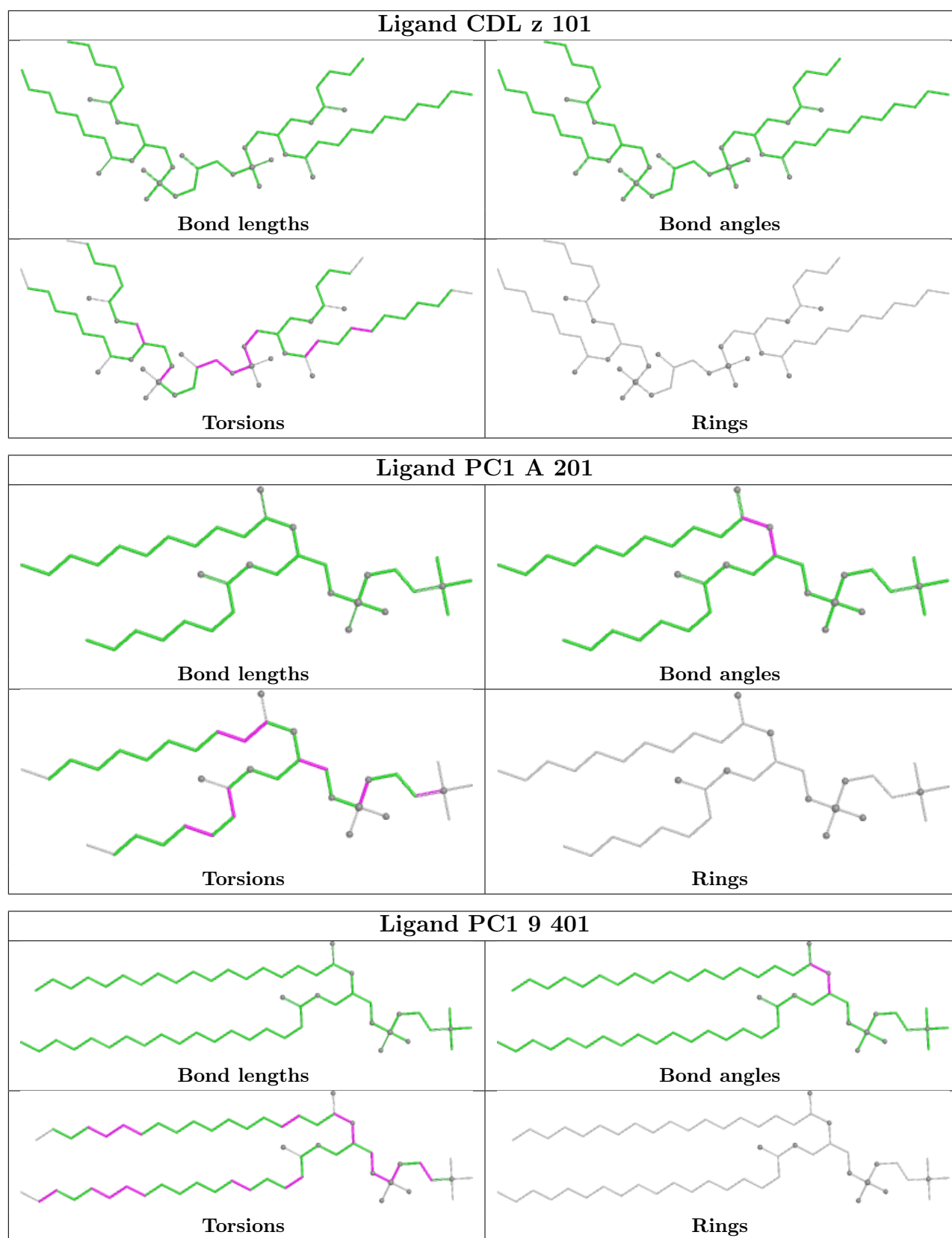
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

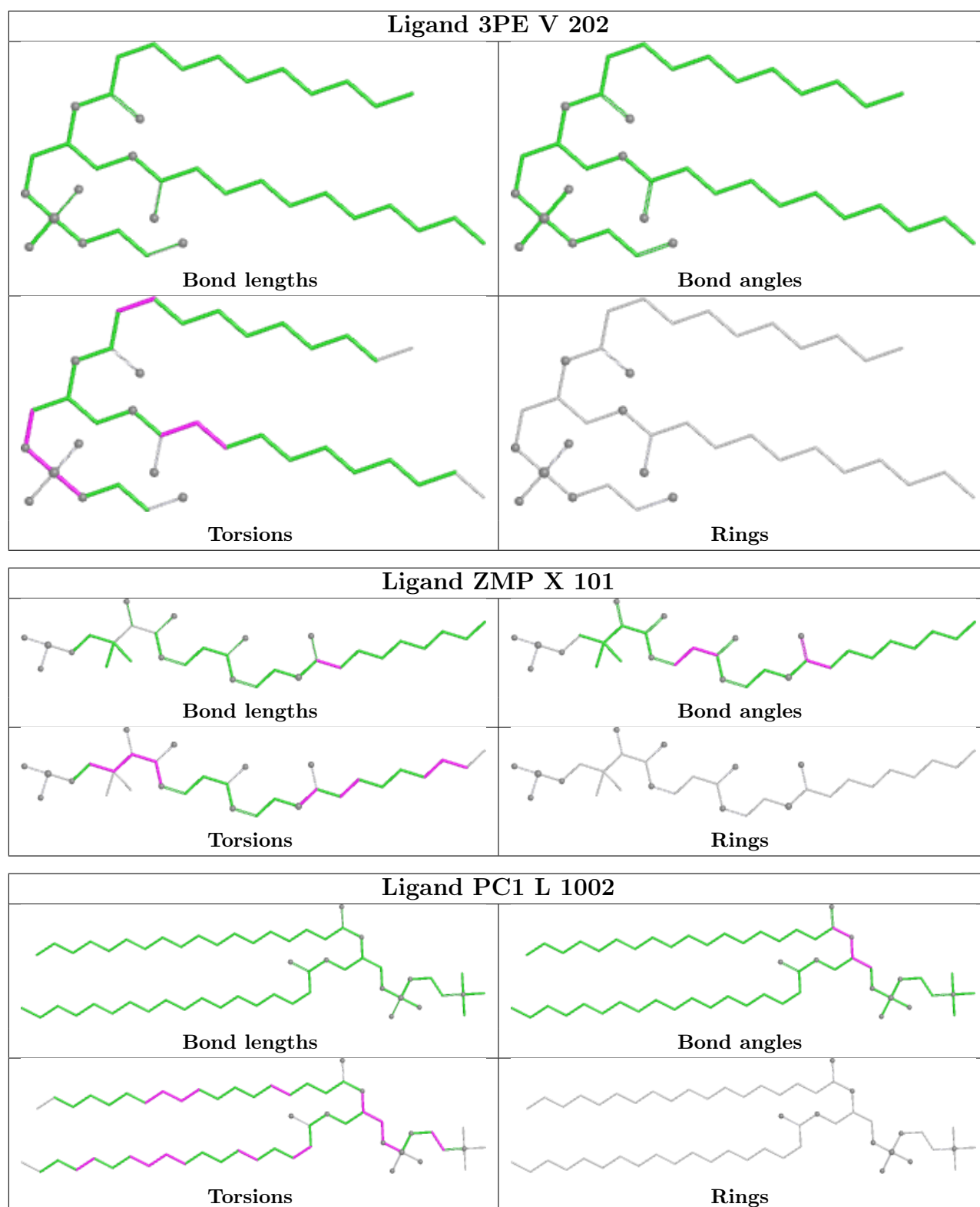


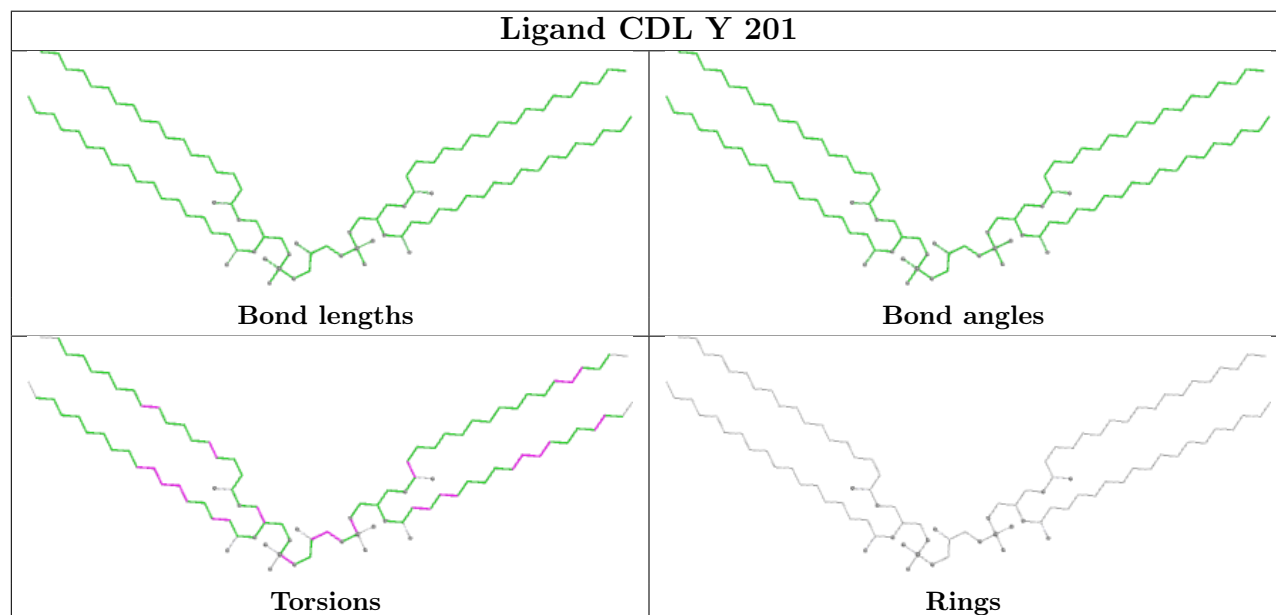
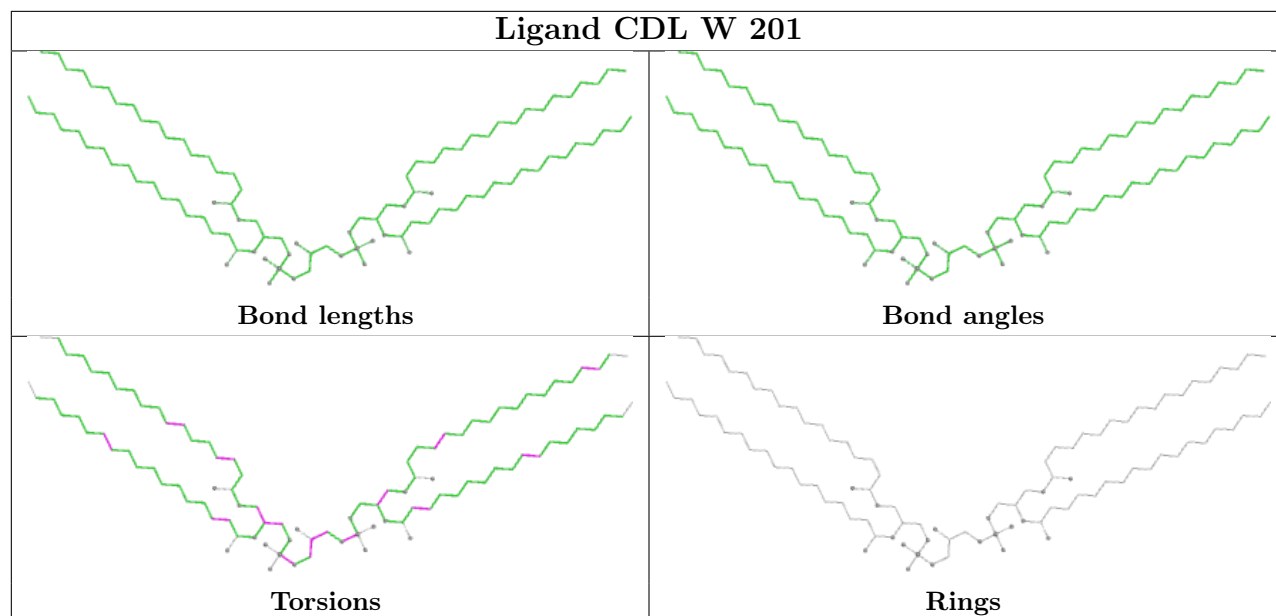


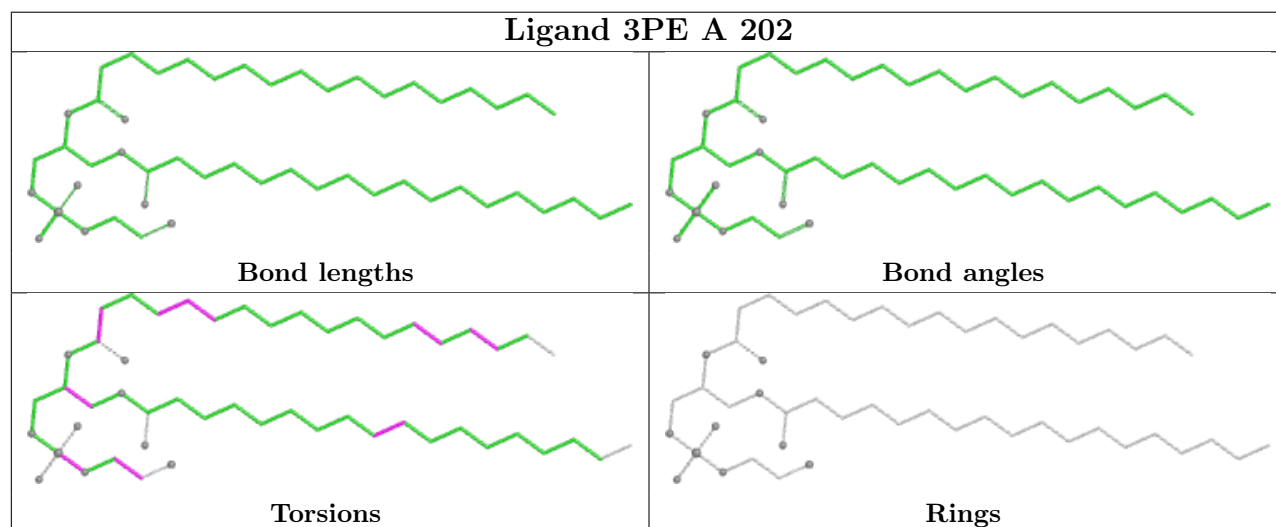
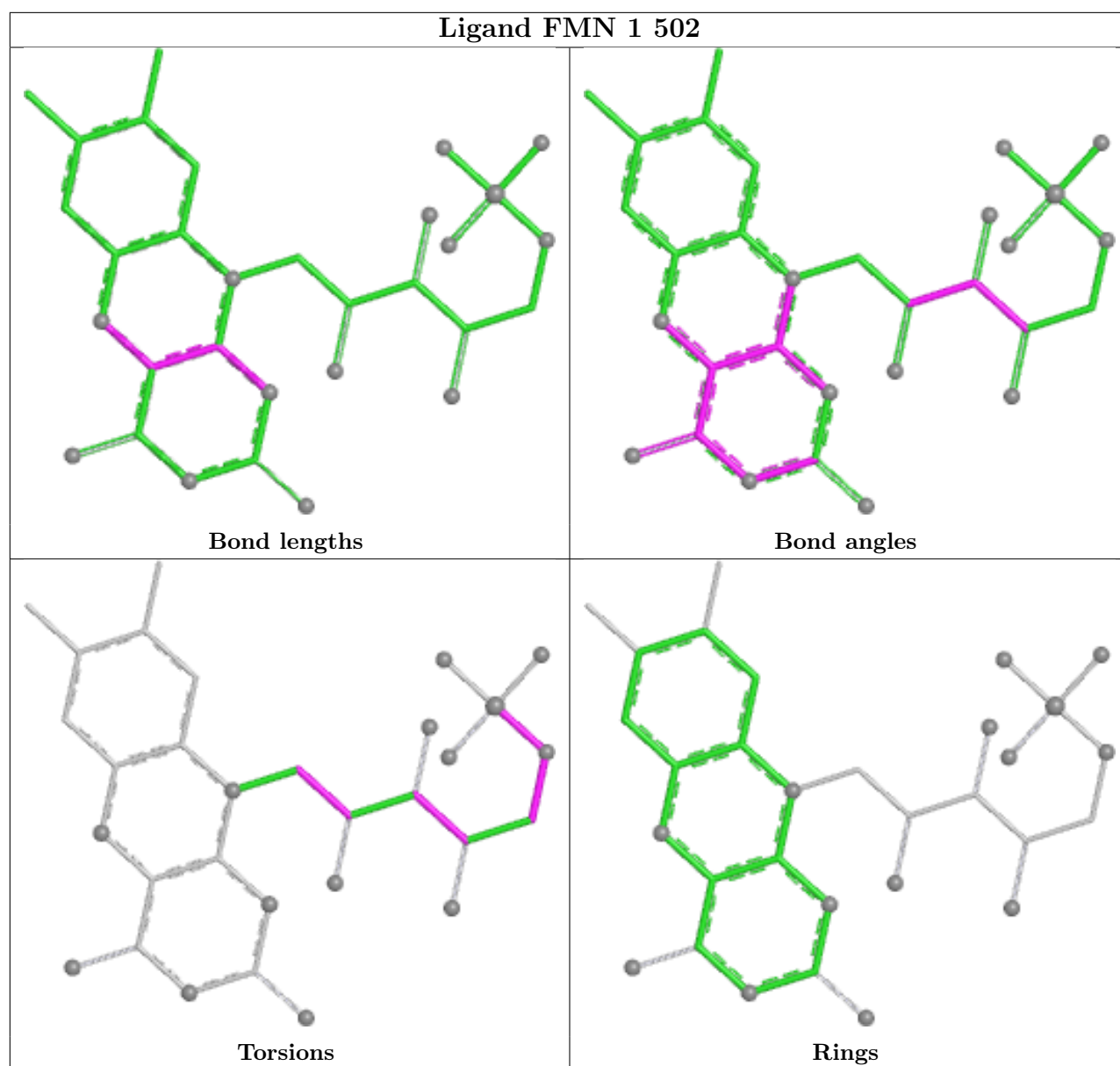


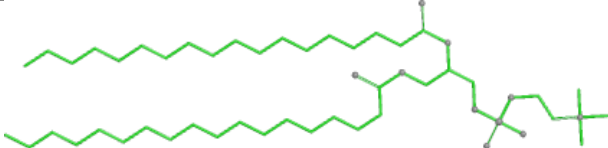
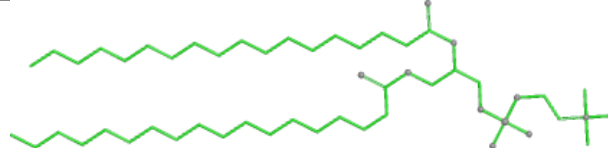
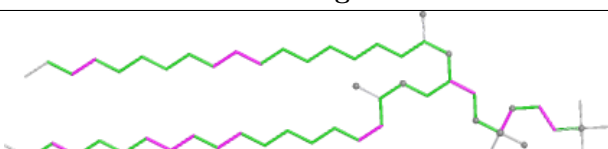
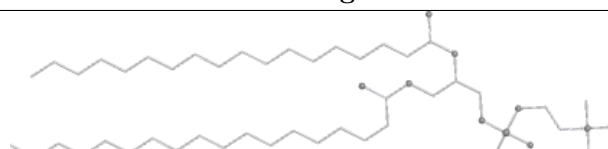
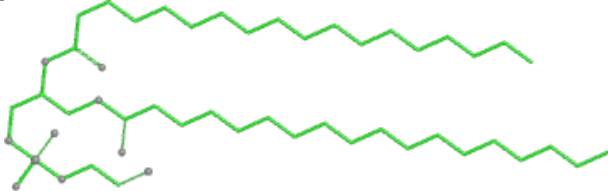
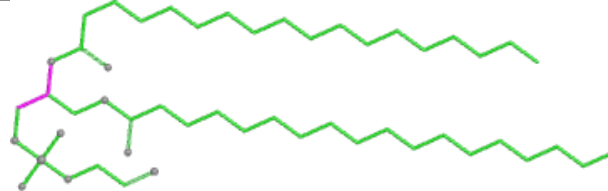
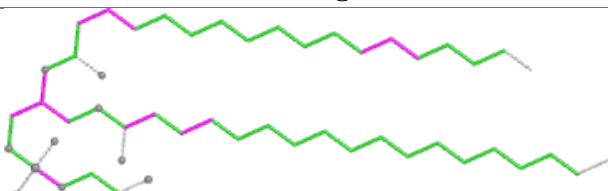
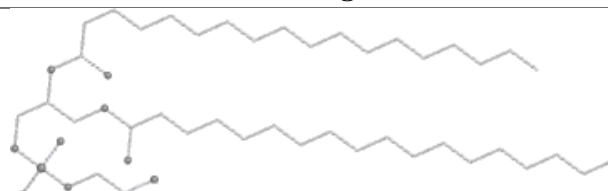
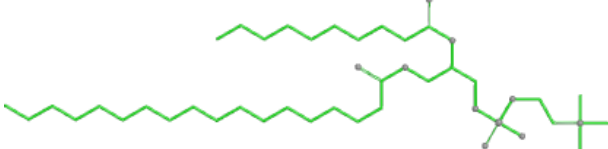
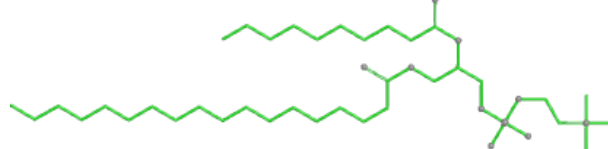
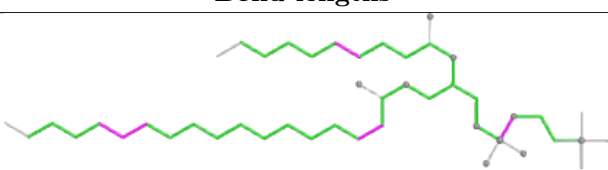
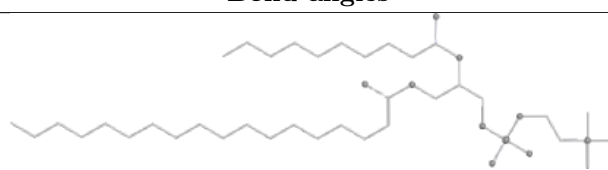


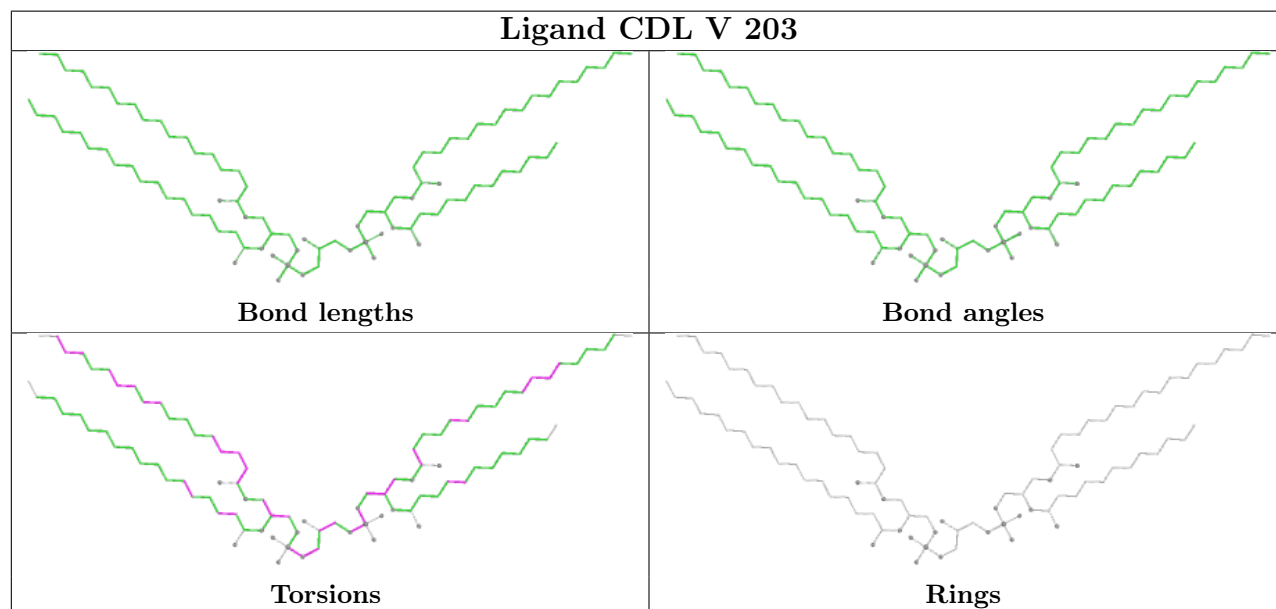
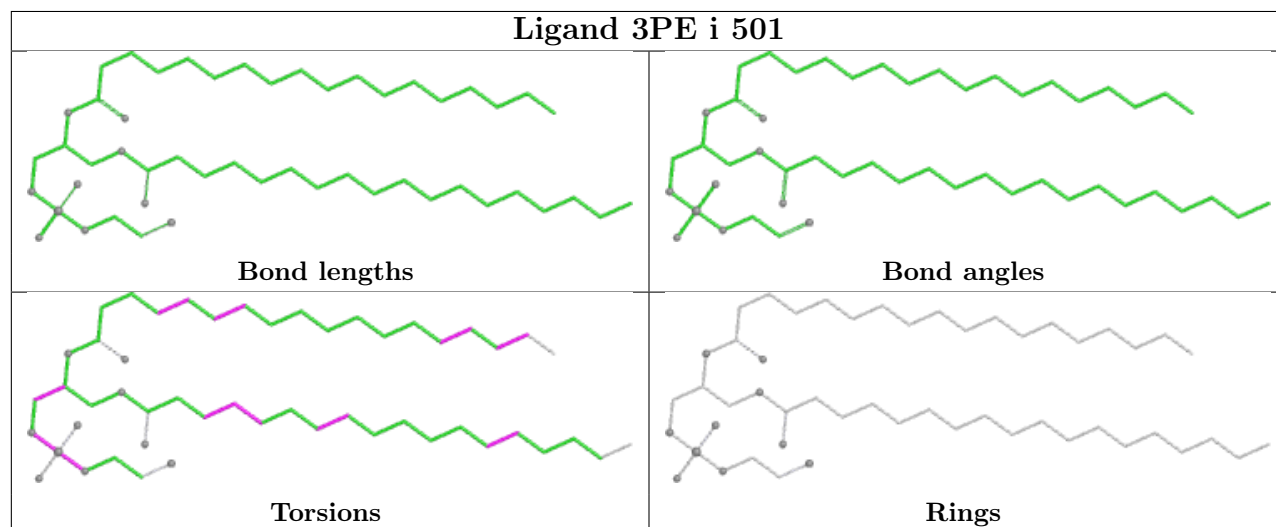
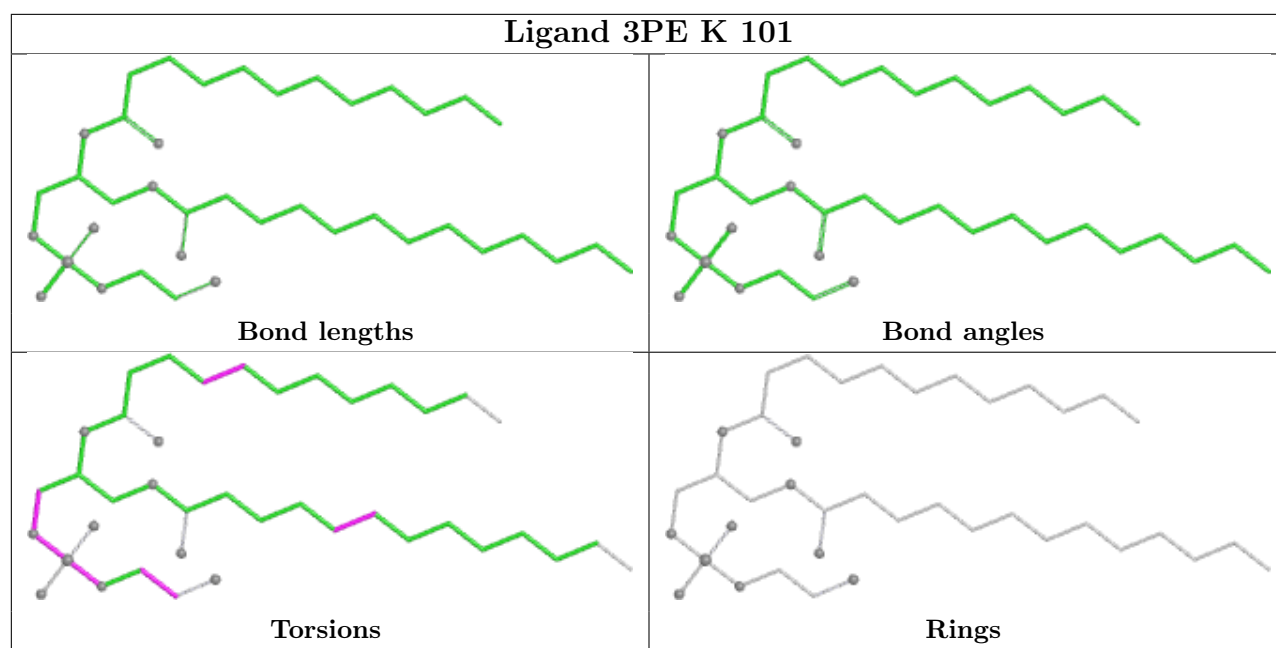


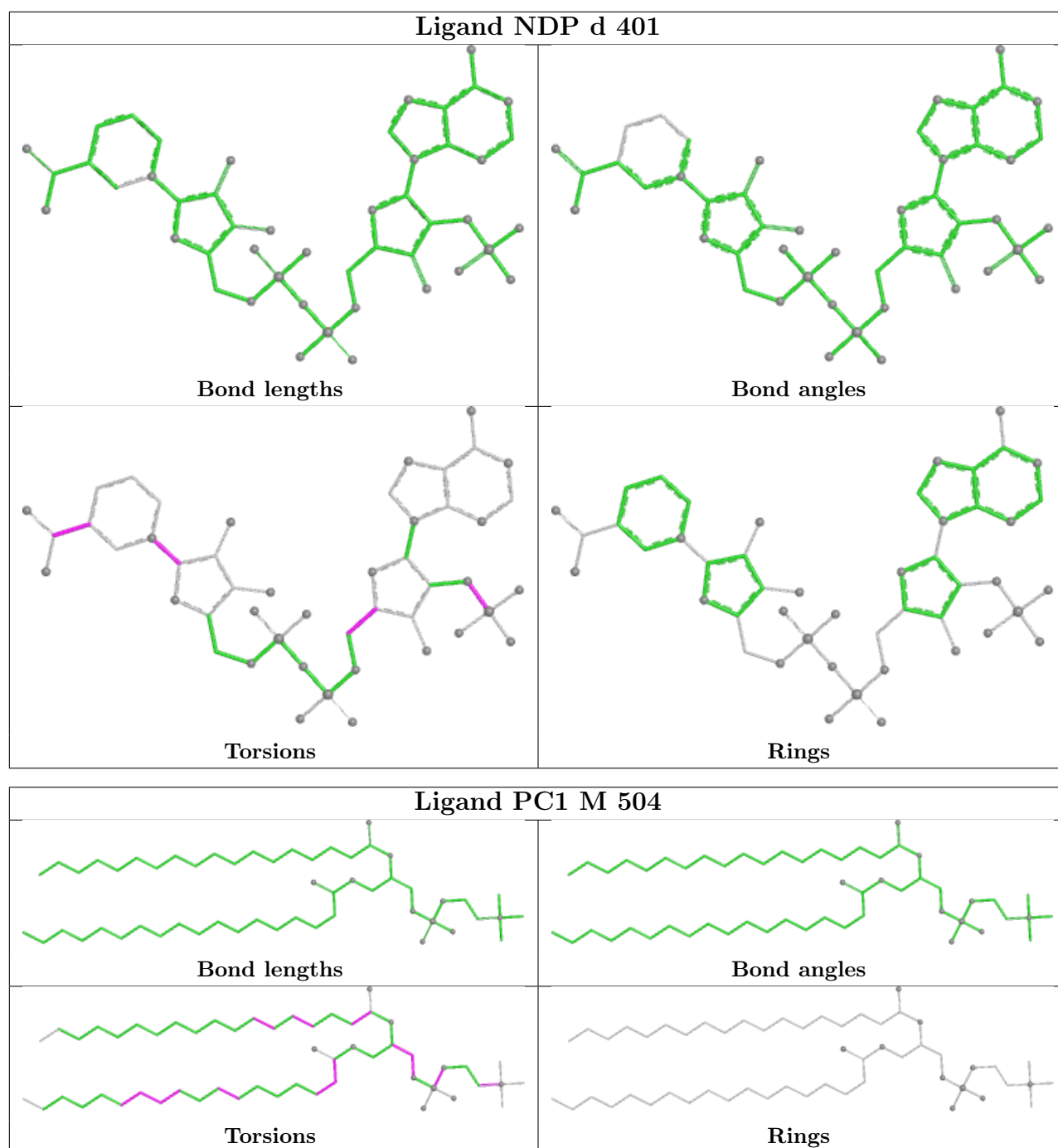


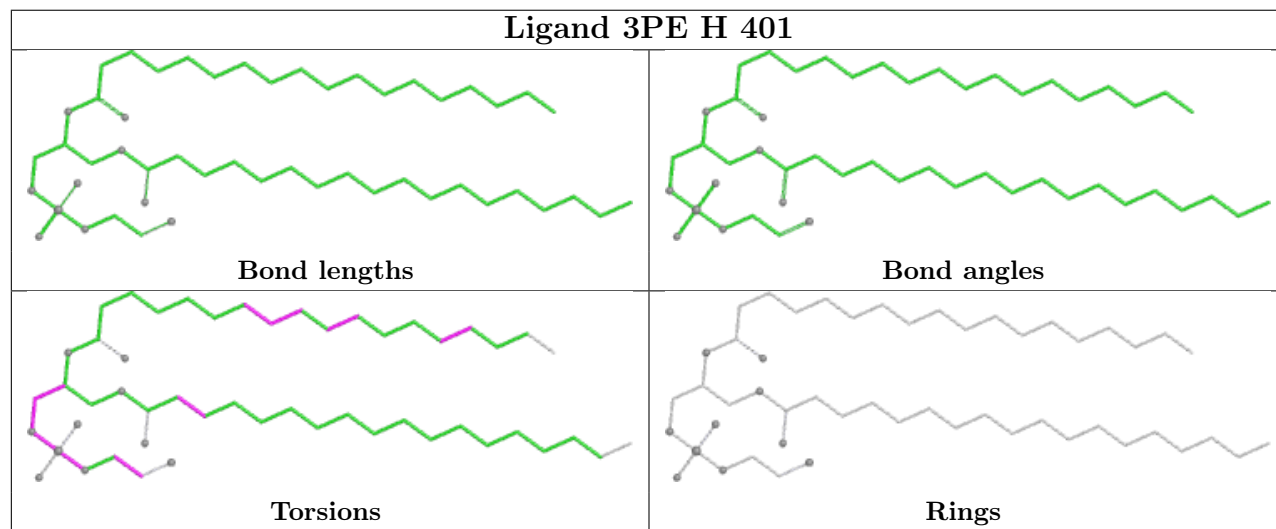
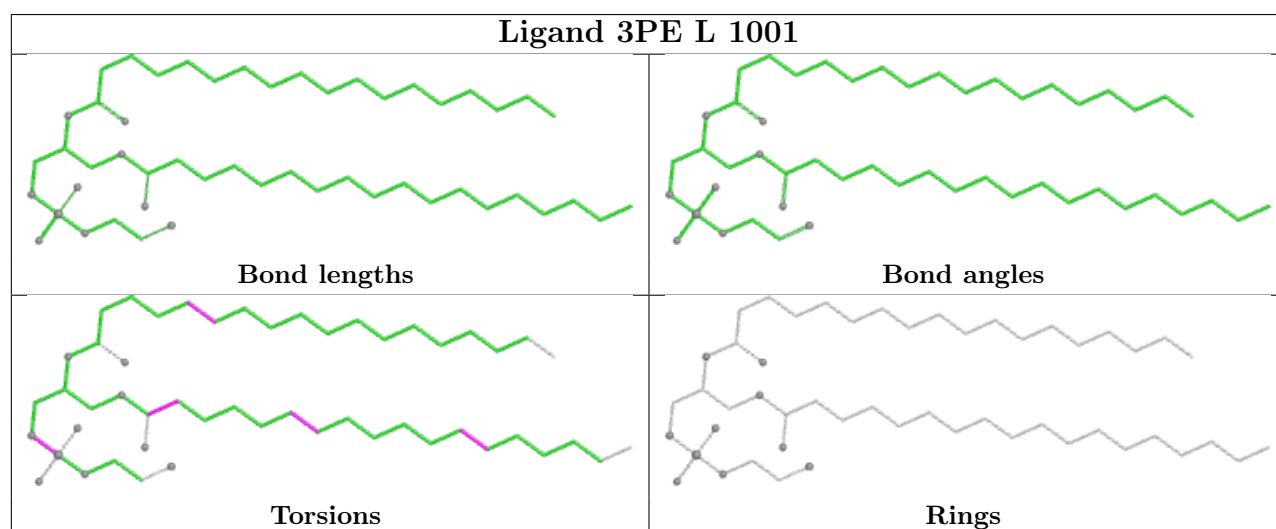
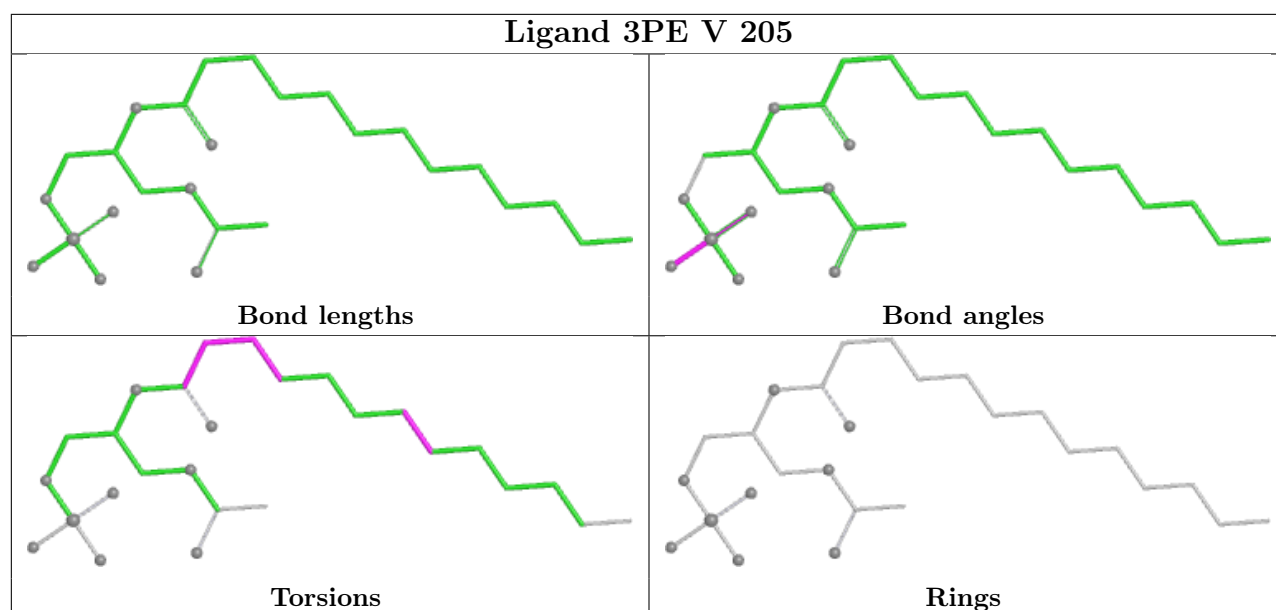


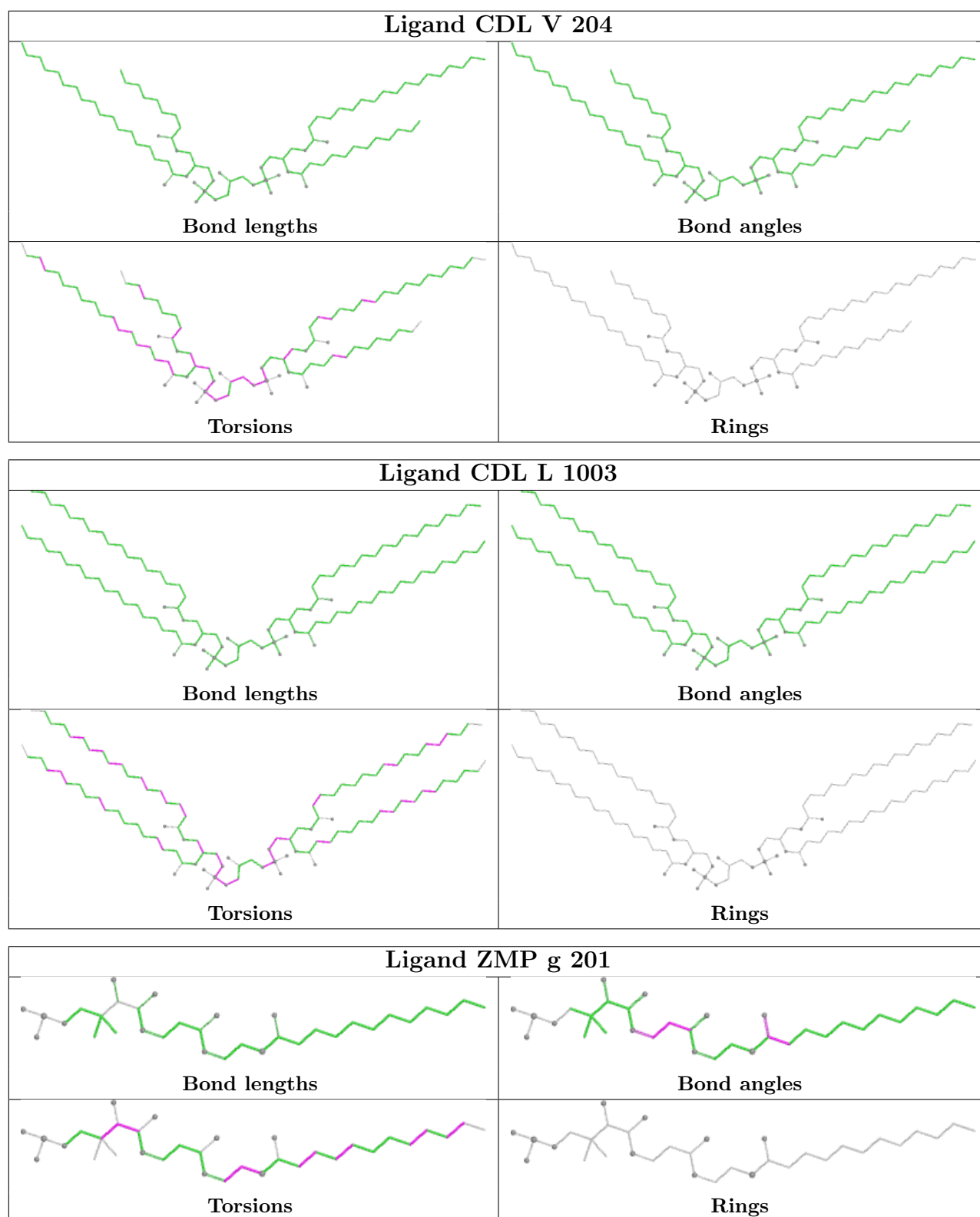


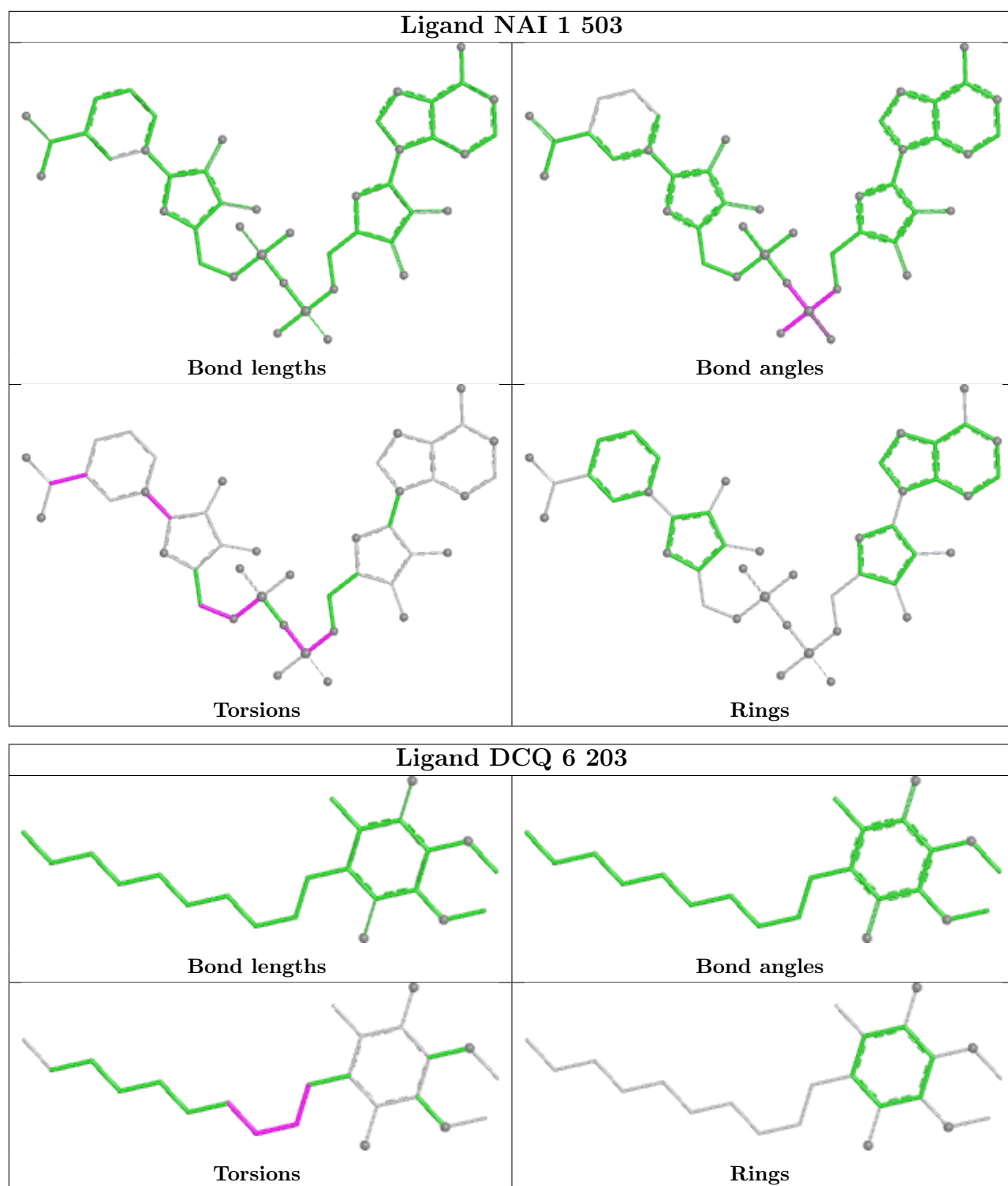
Ligand PC1 M 503	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand 3PE N 401	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 6 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

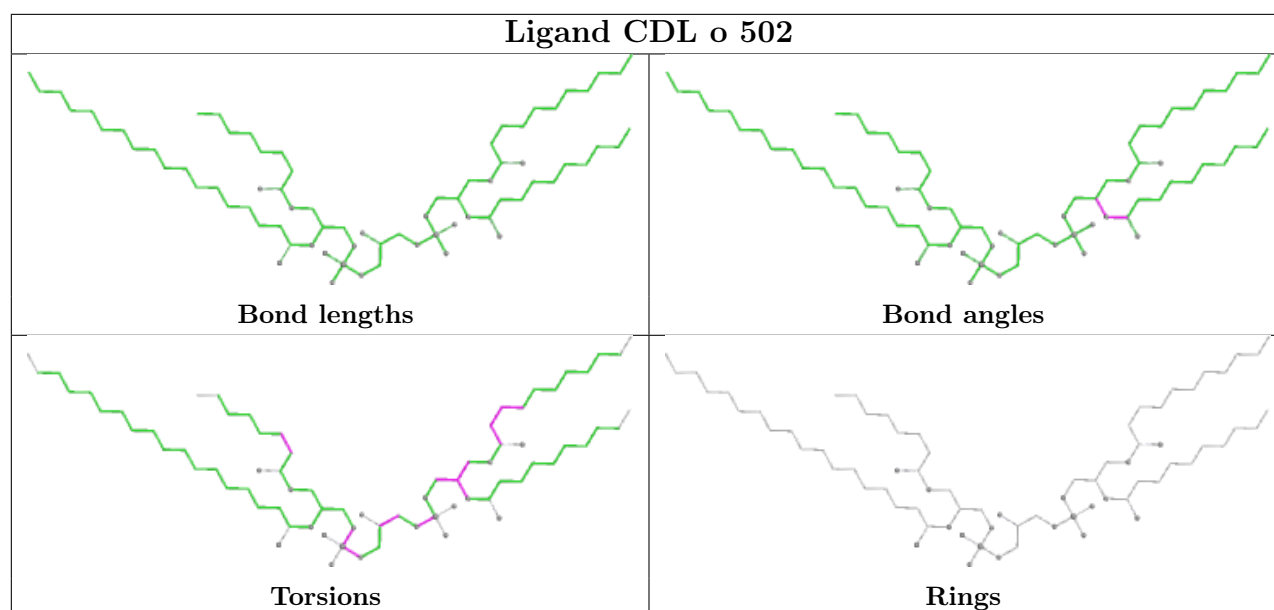












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

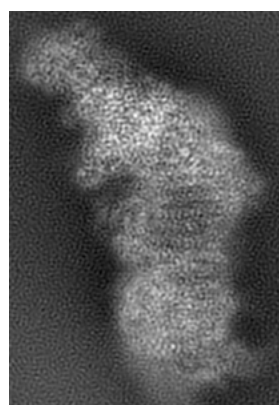
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11249. These allow visual inspection of the internal detail of the map and identification of artifacts.

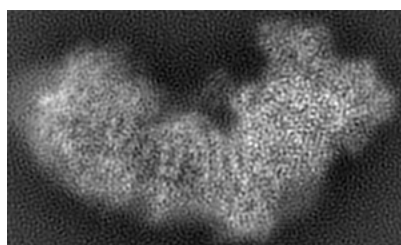
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

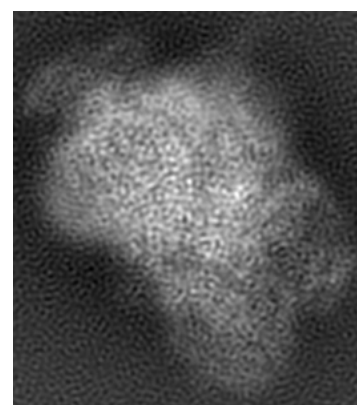
6.1.1 Primary map



X



Y

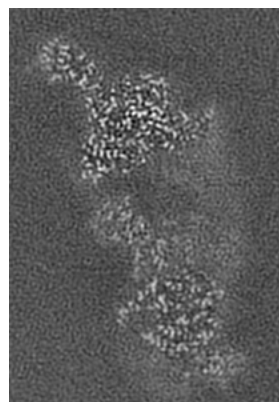


Z

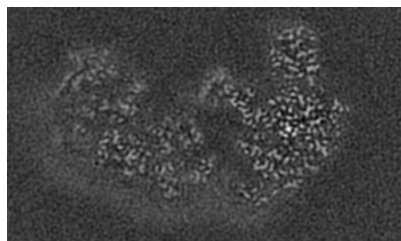
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 81



Y Index: 91

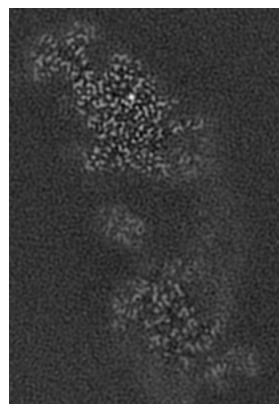


Z Index: 135

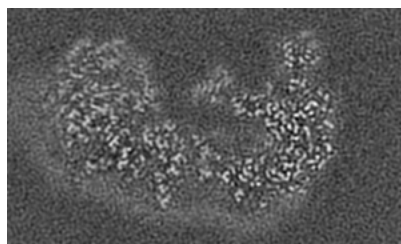
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

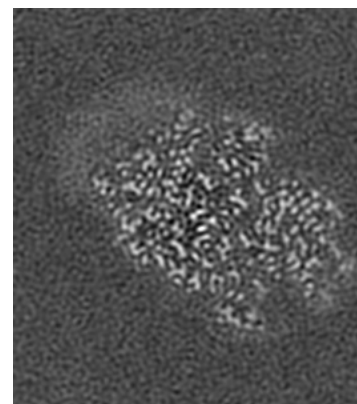
6.3.1 Primary map



X Index: 90



Y Index: 100

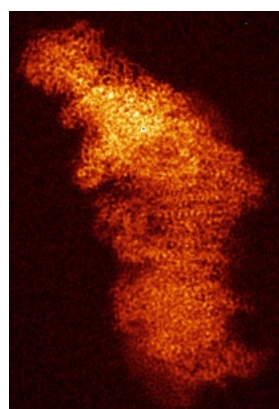


Z Index: 196

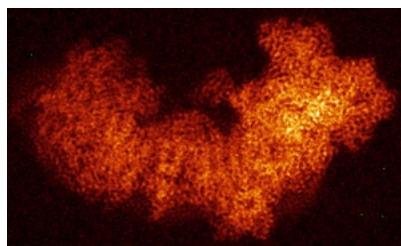
The images above show the largest variance slices of the map in three orthogonal directions.

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

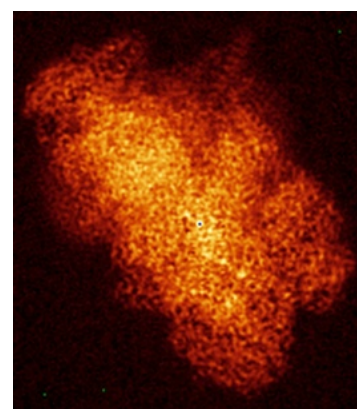
6.4.1 Primary map



X



Y



Z

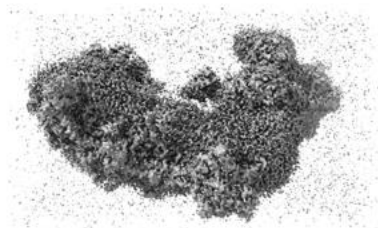
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

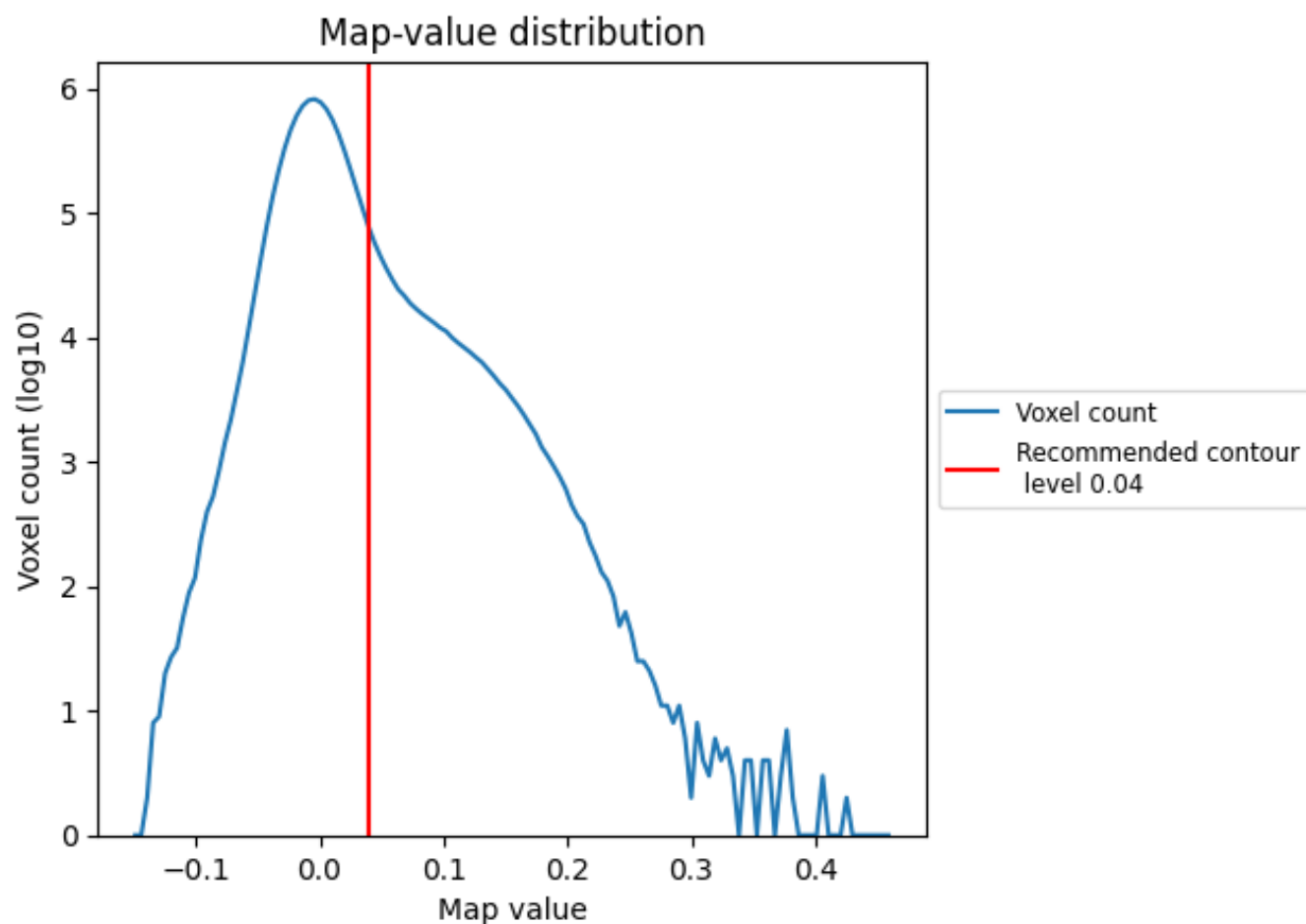
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

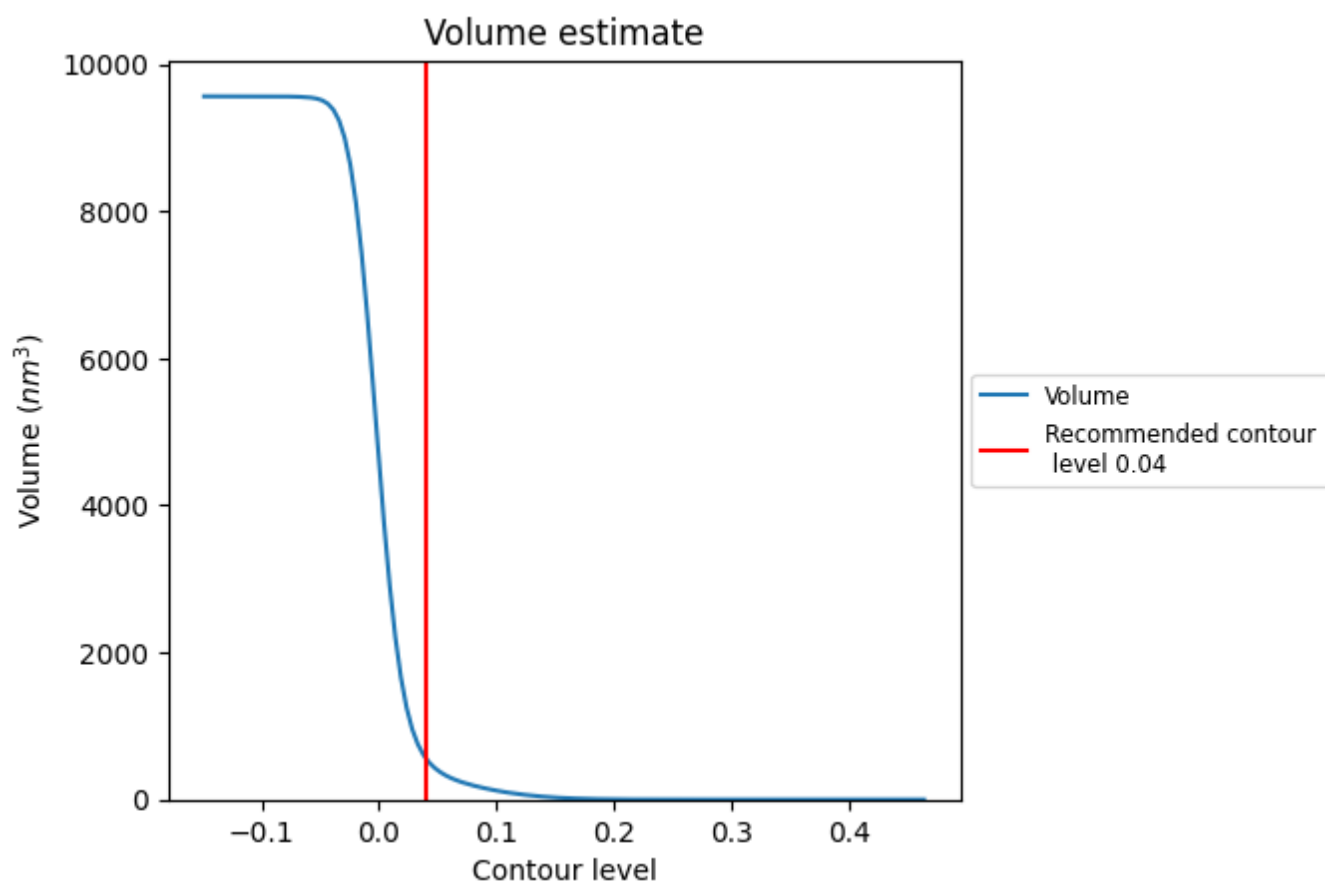
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 561 nm³; this corresponds to an approximate mass of 507 kDa.

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

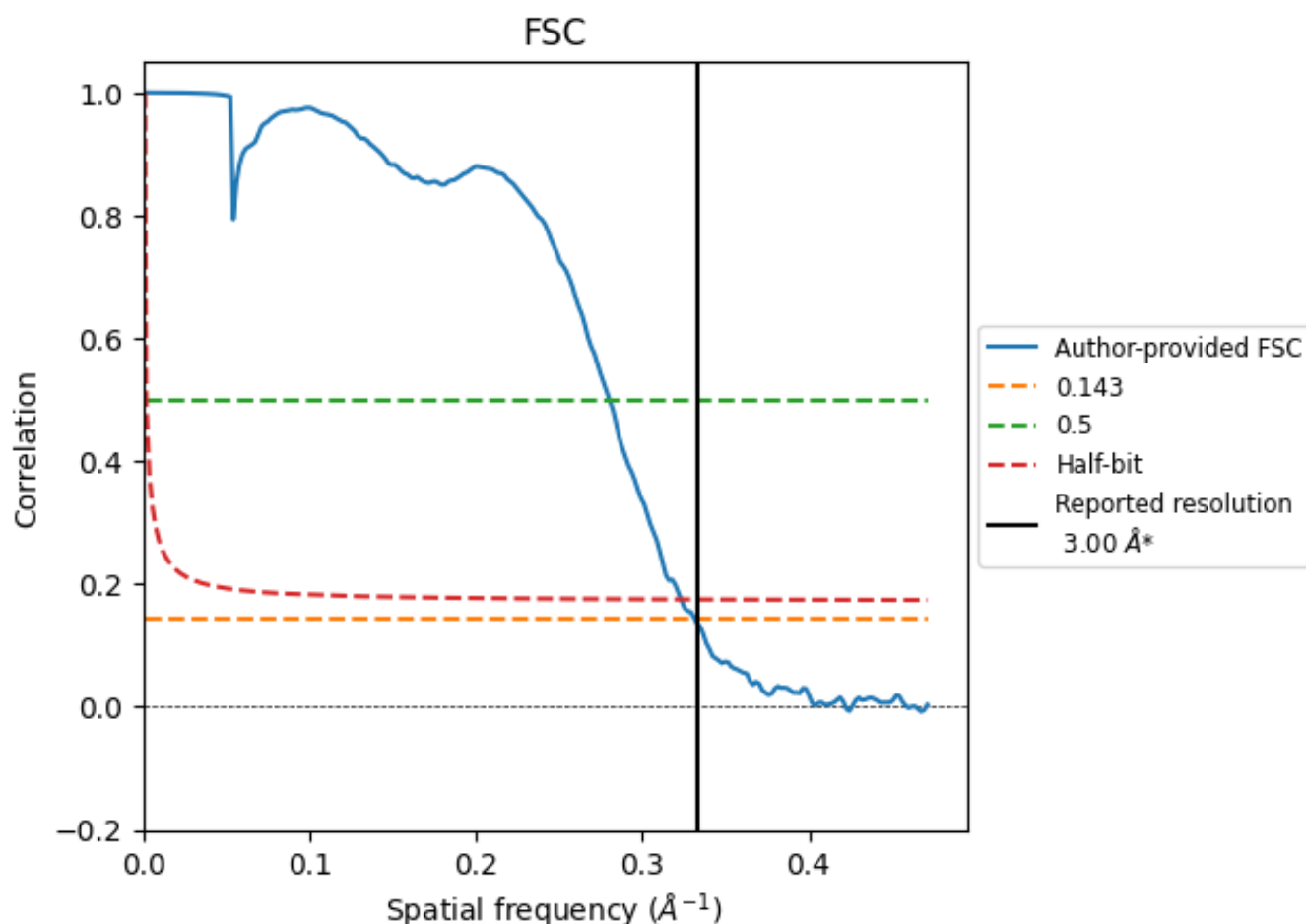
7.3 Rotationally averaged power spectrum [i](#)

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

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

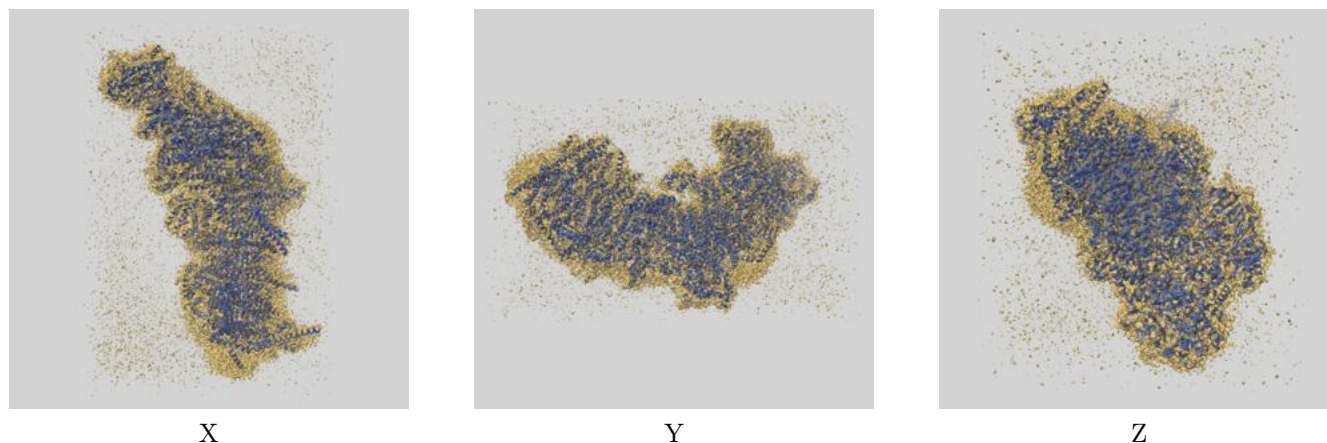
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.02	3.57	3.09
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

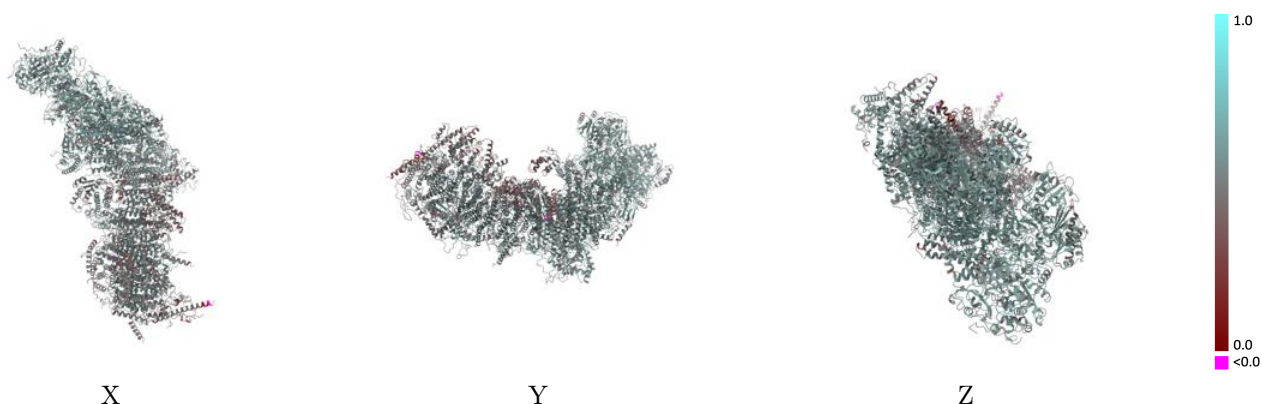
This section contains information regarding the fit between EMDB map EMD-11249 and PDB model 6ZKH. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



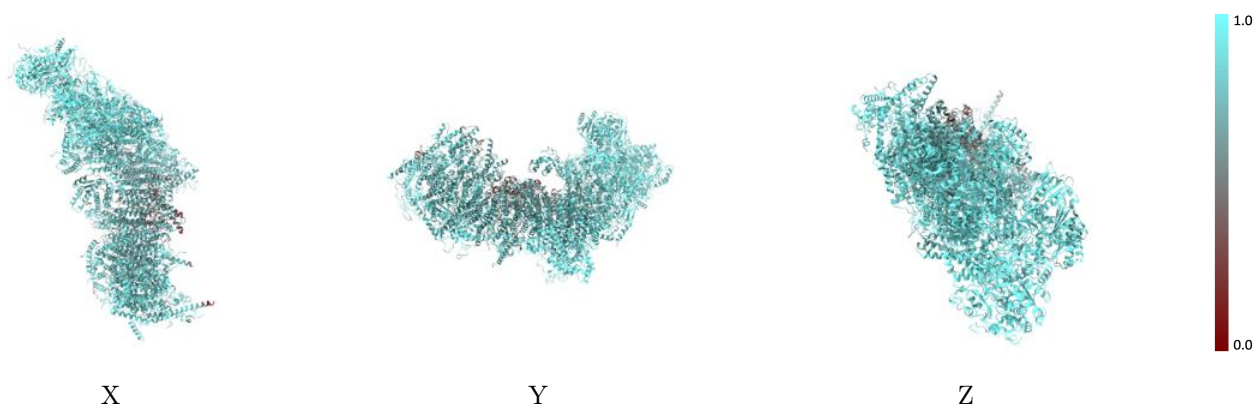
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



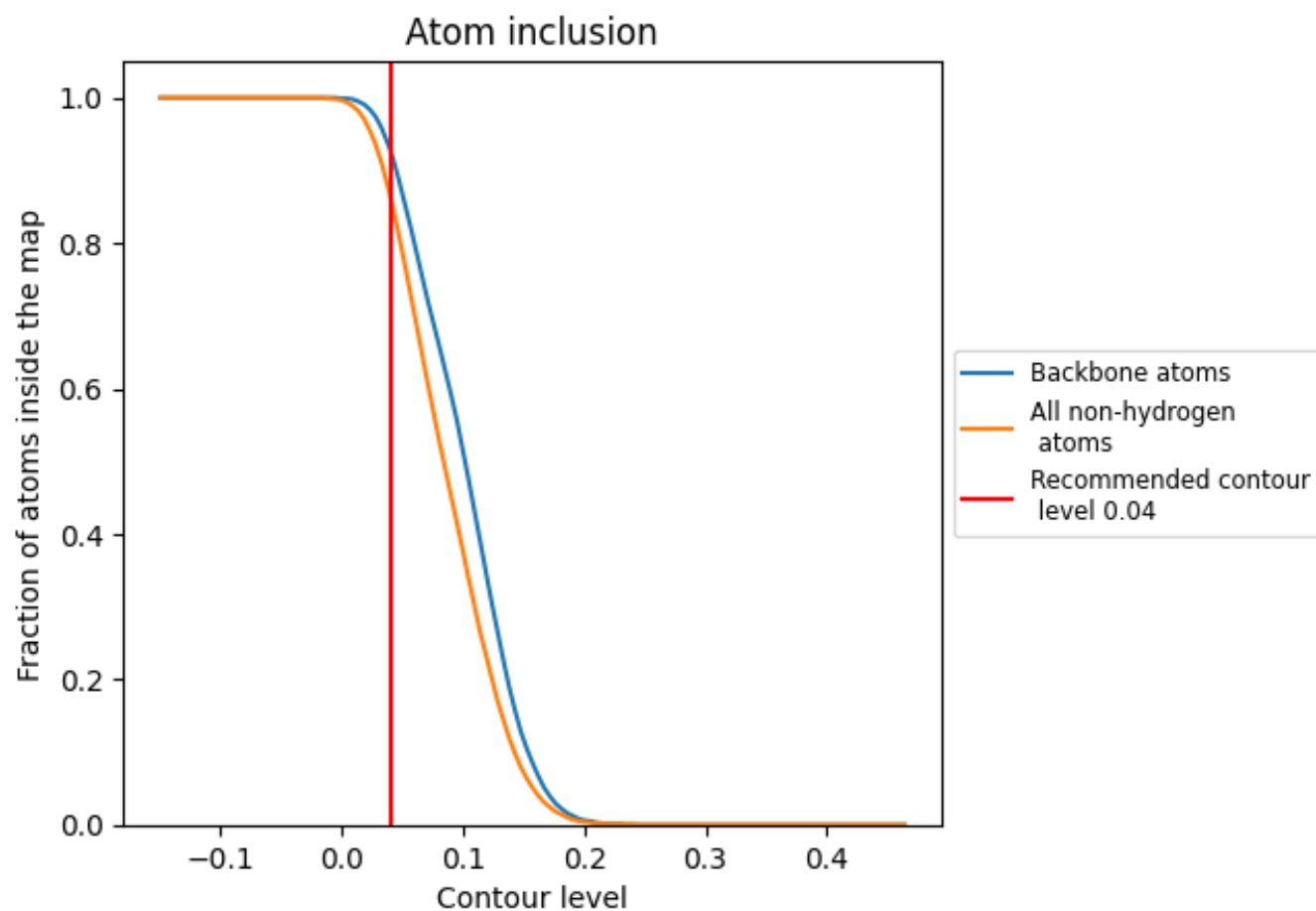
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8670	 0.5340
1	 0.9370	 0.5620
2	 0.9110	 0.5460
3	 0.9230	 0.5680
4	 0.9110	 0.5790
5	 0.9430	 0.5950
6	 0.9170	 0.5730
9	 0.9440	 0.5920
A	 0.7910	 0.5260
H	 0.8860	 0.5580
J	 0.7940	 0.4880
K	 0.8340	 0.5440
L	 0.8210	 0.5150
M	 0.8740	 0.5590
N	 0.8910	 0.5670
V	 0.5120	 0.3960
W	 0.8640	 0.5470
X	 0.7690	 0.4440
Y	 0.8830	 0.5370
Z	 0.8430	 0.4970
a	 0.9280	 0.5460
b	 0.9290	 0.5750
c	 0.9160	 0.5770
d	 0.8900	 0.5430
e	 0.8870	 0.5180
f	 0.8870	 0.5480
g	 0.8900	 0.5590
h	 0.9100	 0.5630
i	 0.9060	 0.5740
j	 0.7630	 0.4100
k	 0.8490	 0.5200
l	 0.8660	 0.5260
m	 0.8880	 0.5280
n	 0.7910	 0.4200
o	 0.8640	 0.5380



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Chain	Atom inclusion	Q-score
p	 0.7890	 0.4770
q	 0.9100	 0.5510
r	 0.8170	 0.4660
s	 0.7990	 0.4190
t	 0.8000	 0.4470
u	 0.8560	 0.4650
v	 0.8210	 0.4720
w	 0.8250	 0.5010
x	 0.8060	 0.5000
y	 0.8080	 0.4870
z	 0.8940	 0.5560