



Full wwPDB EM Validation Report ⓘ

Apr 29, 2026 – 04:59 am BST

PDB ID : 9R03 / pdb_00009r03
EMDB ID : EMD-53477
Title : Complex I from *Ovis aries* in presence of D1 inhibitor, Open state
Authors : Sazanov, L.; Petrova, O.
Deposited on : 2025-04-24
Resolution : 3.20 Å (reported)
Based on initial model : 6ZKI

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 : 1.8.4, CSD as541be (2020)
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 EMD 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

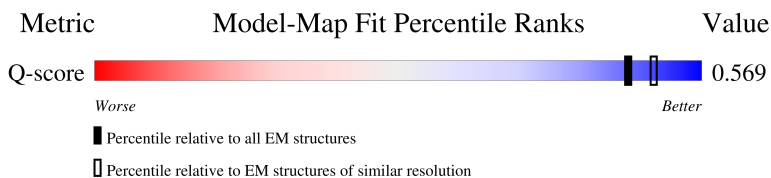
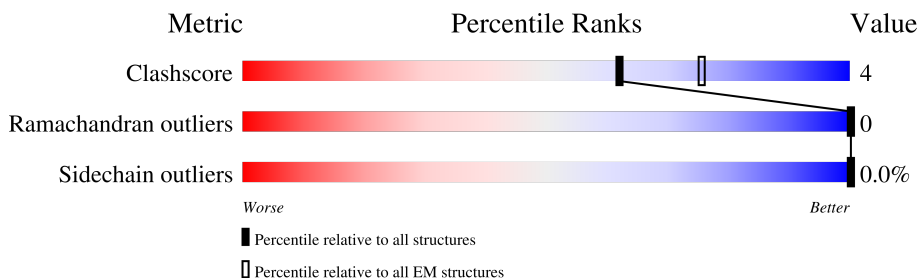
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	4	463	
2	A	115	
3	H	318	
4	6	223	



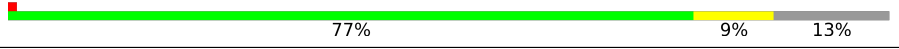



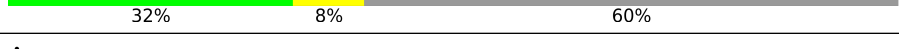
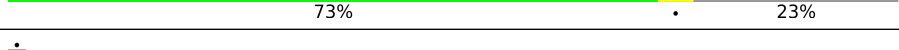
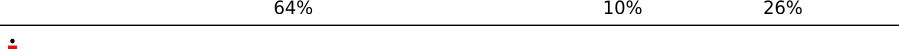
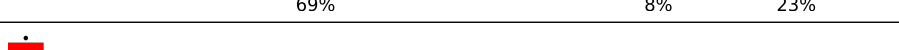

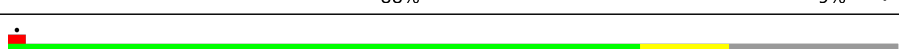

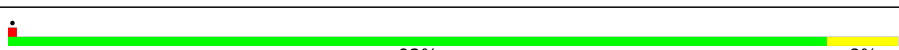
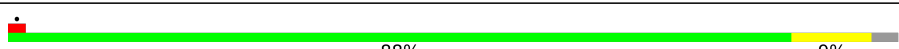

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Mol	Chain	Length	Quality of chain
5	J	175	
6	K	98	
7	L	606	
8	M	459	
9	N	347	
10	V	141	
11	W	189	
12	X	87	
12	j	87	
13	Y	171	
14	Z	175	
15	k	355	
16	l	106	
17	m	84	
18	n	98	
19	o	122	
20	p	130	
21	r	128	
22	s	137	
23	t	179	
24	u	108	
25	v	186	
26	w	154	
27	x	76	
28	y	58	

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Mol	Chain	Length	Quality of chain
29	z	70	
30	1	464	
31	2	246	
32	3	727	
33	5	266	
34	9	217	
35	a	109	
36	b	124	
37	c	170	
38	d	380	
39	e	99	
40	f	116	
41	g	140	
42	h	113	
43	i	145	
44	q	144	

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 66655 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] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4	423	Total	C	N	O	S	0	0
			3409	2177	587	620	25		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	103	Total	C	N	O	S	0	0
			831	565	118	143	5		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	308	Total	C	N	O	S	0	0
			2453	1657	373	404	19		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 6.

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

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	98	Total	C	N	O	S	0	0
			749	490	112	132	15		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	606	Total	C	N	O	S	0	0
			4806	3187	746	829	44		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	459	Total	C	N	O	S	0	0
			3647	2429	571	607	40		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	347	Total	C	N	O	S	0	0
			2723	1808	416	459	40		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	141	Total	C	N	O	S	0	0
			1028	656	175	191	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	0	ACE	-	acetylation	UNP A0A8V6VBD6

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 12 is a protein called Acyl carrier protein.

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

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

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

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

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

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

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

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

- Molecule 21 is a protein called Mitochondrial complex I, B17 subunit.

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

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

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

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

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

8, mitochondrial.

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

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

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

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

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

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

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1	430	Total	C	N	O	S	0	0
			3312	2086	593	613	20		

- Molecule 31 is a protein called Mitochondrial complex I, 24 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	2	213	Total	C	N	O	S	0	0
			1655	1058	278	309	10		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	3	688	Total	C	N	O	S	0	0
			5275	3301	922	1011	41		

- Molecule 33 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	5	208	Total	C	N	O	S	0	0
			1726	1112	296	315	3		

- Molecule 34 is a protein called Complex I-23kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

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

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	293	Total	C	N	O	S	0	0
			2345	1499	427	414	5		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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

- Molecule 41 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

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

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h	96	Total	C	N	O	S	0	0
			763	477	145	138	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	0	ACE	-	acetylation	UNP A0A6P3E9B7

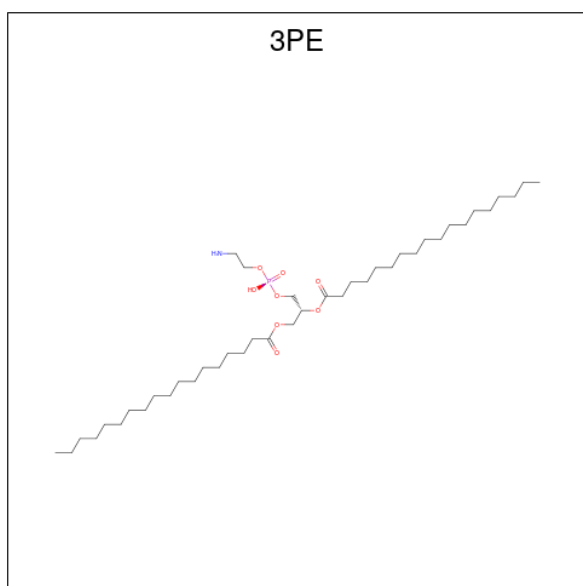
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



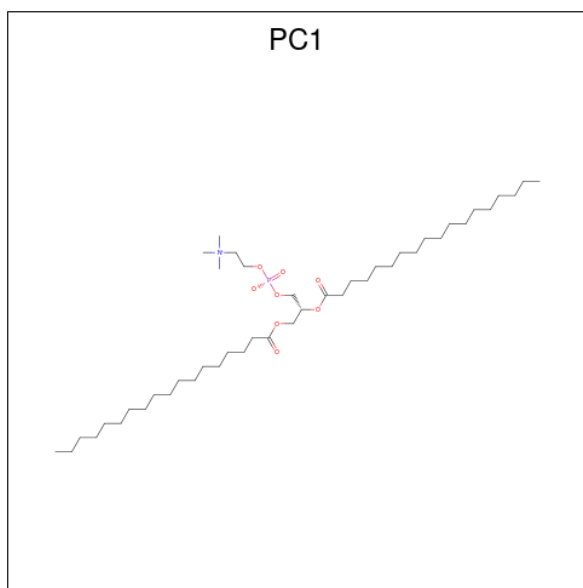
Mol	Chain	Residues	Atoms					AltConf
45	4	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	6	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	K	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	L	1	Total	C	N	O	P	0
			31	21	1	8	1	

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

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



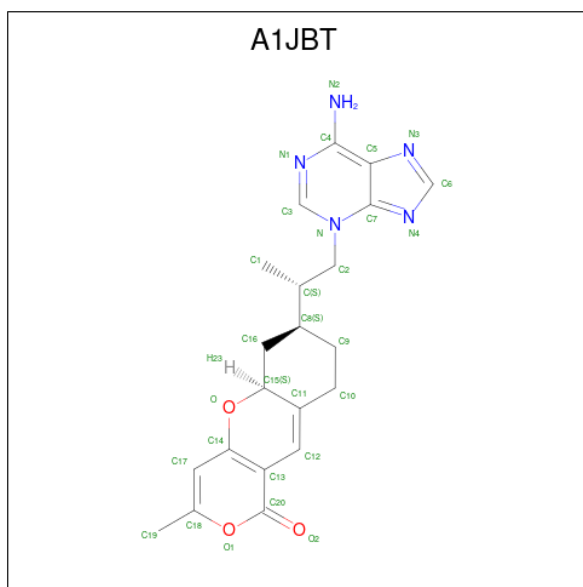
Mol	Chain	Residues	Atoms					AltConf
46	4	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
46	6	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	L	1	Total	C	N	O	P	0
			54	44	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
46	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	M	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 47 is (7 {S})-7-[(2 {S})-1-(6-azanylpurin-3-yl)propan-2-yl]-3-methyl-6,7,8,9-tetrahydro-5 {a} {H}-pyrano[4,3-b]chromen-1-one (CCD ID: A1JBT) (formula: C₂₁H₂₃N₅O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
47	H	1	Total	C	N	O	0
			29	21	5	3	

- Molecule 48 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
48	6	1	Total	Fe	S	0
			8	4	4	
48	1	1	Total	Fe	S	0
			8	4	4	
48	3	1	Total	Fe	S	0
			8	4	4	
48	3	1	Total	Fe	S	0
			8	4	4	
48	9	1	Total	Fe	S	0
			8	4	4	
48	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 49 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
49	k	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 50 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

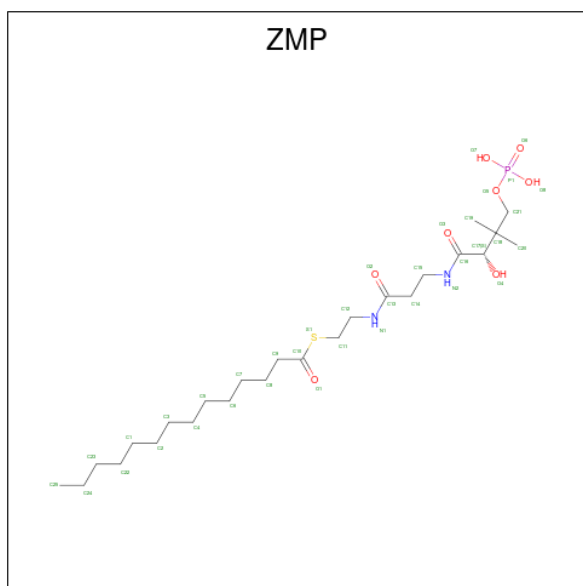
Mol	Chain	Residues	Atoms	AltConf
50	k	1	Total Mg 1 1	0

- Molecule 51 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



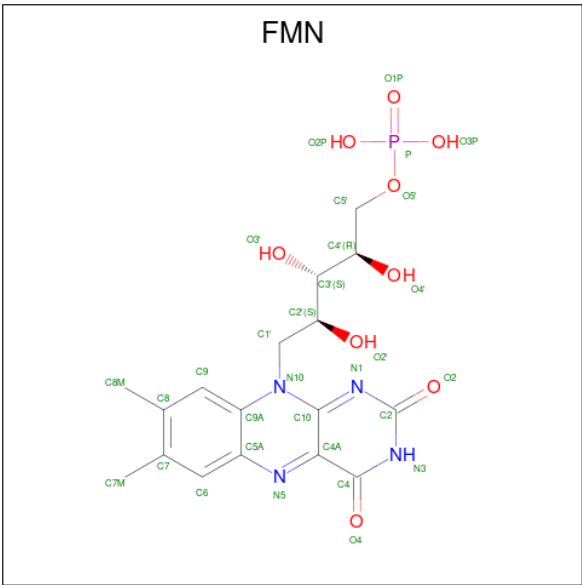
Mol	Chain	Residues	Atoms			AltConf
51	s	1	Total	C	O	0
			15	14	1	

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



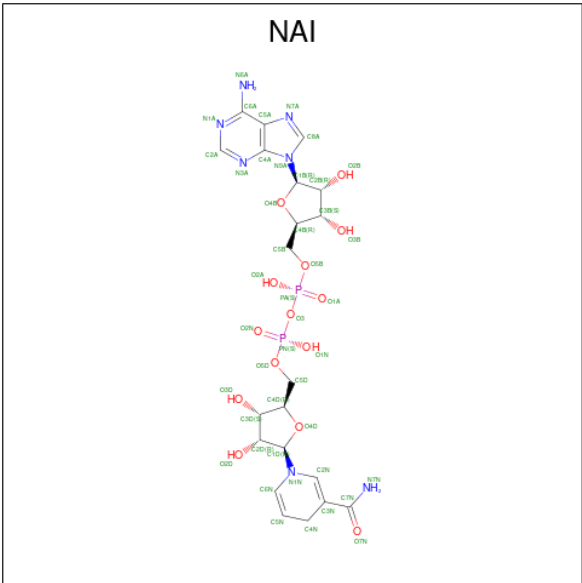
Mol	Chain	Residues	Atoms						AltConf
52	t	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	
52	j	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- Molecule 53 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



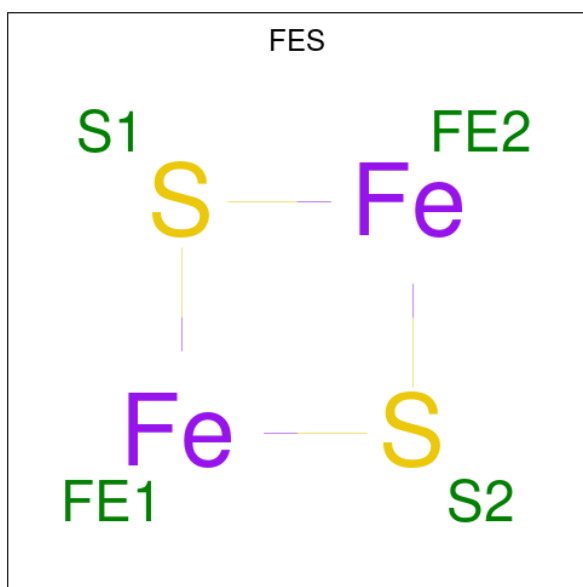
Mol	Chain	Residues	Atoms					AltConf
53	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 54 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
54	1	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 55 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
55	2	1	Total	Fe	S	0
			4	2	2	
55	3	1	Total	Fe	S	0
			4	2	2	

- Molecule 56 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	K	0
			1	1	

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 58 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

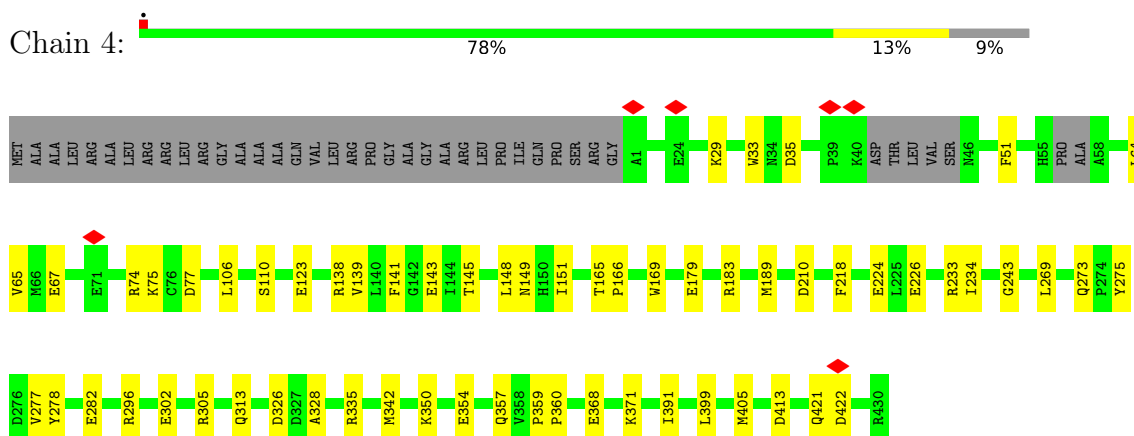


Mol	Chain	Residues	Atoms					AltConf
58	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

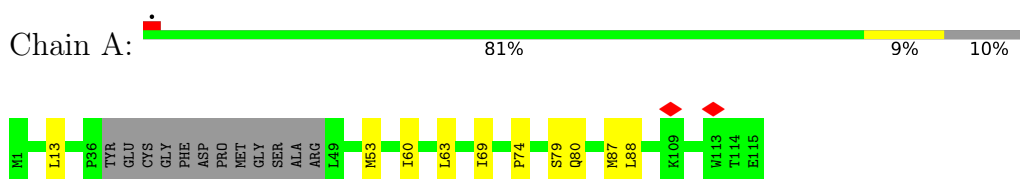
3 Residue-property plots

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.

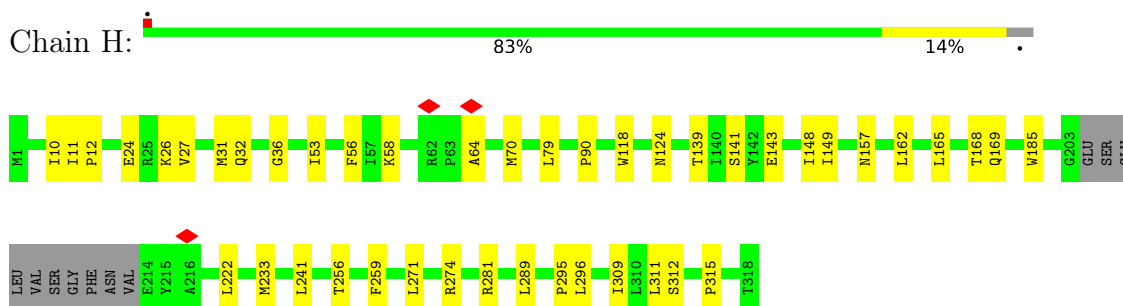
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



- Molecule 2: NADH-ubiquinone oxidoreductase chain 3



- Molecule 3: NADH-ubiquinone oxidoreductase chain 1




- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



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


LYS PRO ALA ALA LEU PRO SER S24 L36 I37 L52 A63 R66 M69 S79 S83 G90 T91 P108 V114 S115 M116 C119 C136 D137 I144 P150 P151 E170 R171 R172 R179

- Molecule 5: NADH-ubiquinone oxidoreductase chain 6

Chain J:  80% 17%

M1 Y4 S10 F13 F17 F20 K23 I27 G38 L45 S50 F51 L52 G53 L54 M55 V56 F57 Y60 V67 Y79 P80 GLU VAL TRP VAL SER N86 L90 I94 K111 K118 G121 W125 Y147 I163 V167 I168

- Molecule 6: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  89% 11%

M1 R23 S24 L40 T46 L55 M59 P60 I61 L63 L73 L93 C98

- Molecule 7: NADH-ubiquinone oxidoreductase chain 5


Chain L:  87% 13%

M1 L7 V10 I113 T16 M17 T26 H27 F29 E60 W66 L69 K75 L76 S77 D83 M88 T97 I100 M101 W106 F118 L125 L129 V132 I142 F152 I172 L173 Y174 M194 T195 Q200 M203 L204

T221 Q226 W232 A245 L246 S249 Q274 M277 L280 Q295 Q309 M313 M314 F326 M338 M341 M359 T370 L373 L374 L375 T396 E397 T416 T419 R425 L431 Q434 P435 R436 F449 L457 L458 Y485

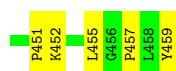
L486 K487 M488 T489 A490 S505 T508 Y515 L526 P530 M544 S548 I556 W557 L558 E559 T560 I561 E606

- Molecule 8: NADH-ubiquinone oxidoreductase chain 4

Chain M:  84% 16%

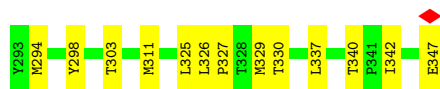
M1 I5 G46 D47 S60 M70 L75 W78 H82 Q103 L104 F105 T109 E114 L115 I116 Y119 L130 I133 Q139 R142 L150 F151 G156 L161 I165 N175 I178 L179 Q180 S191 V221 M229 L231 L231 L231

L248 L249 T254 M257 L277 R278 Q279 T280 D281 L282 K283 S284 S290 H319 S324 K325 E335 R336 K342 L348 L351 P370 I373 I376 I391 T403 A404 L405 Y406 L427 P428 S429 F430 F433 M437 S438 L439 H440 L444 L445 L446



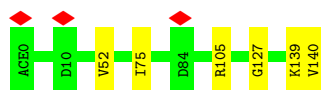
- Molecule 9: NADH-ubiquinone oxidoreductase chain 2

Chain N: 87% 13%



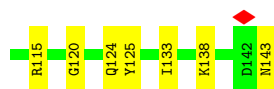
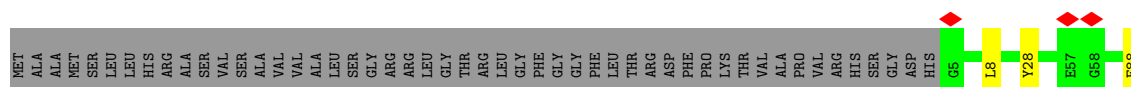
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V: 96%



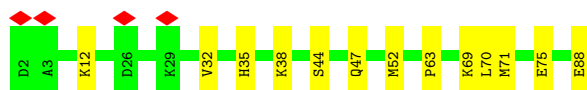
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain W: 68% 5% 26%



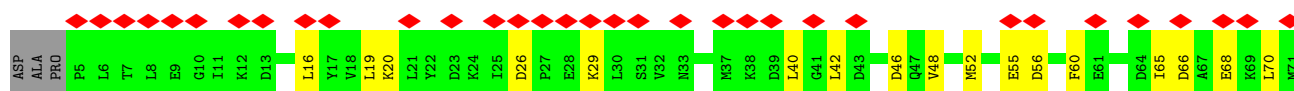
- Molecule 12: Acyl carrier protein

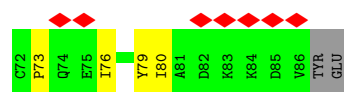
Chain X: 5% 85% 15%



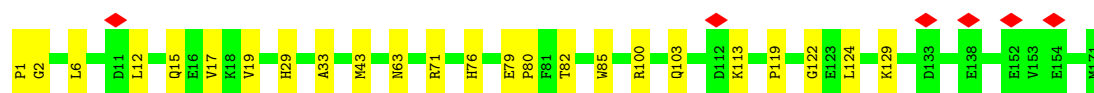
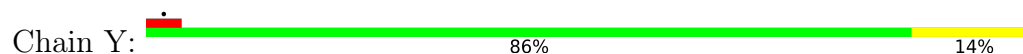
- Molecule 12: Acyl carrier protein

Chain j: 46% 70% 24% 6%

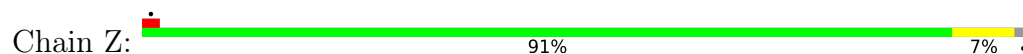




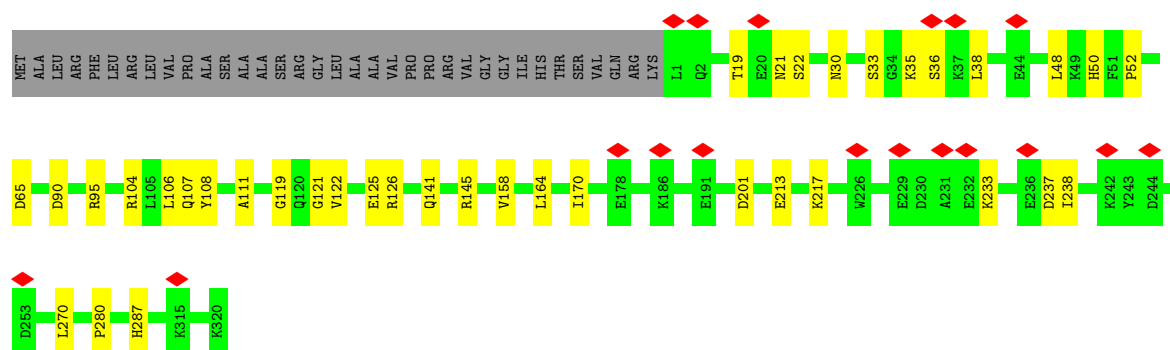
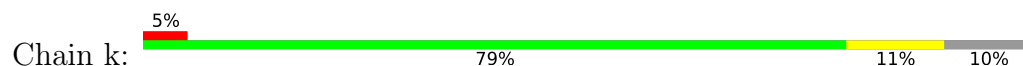
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



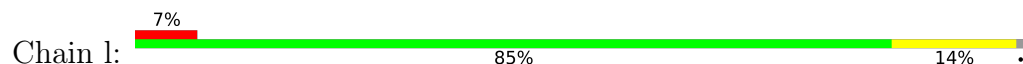
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



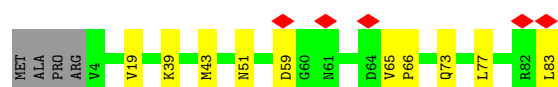
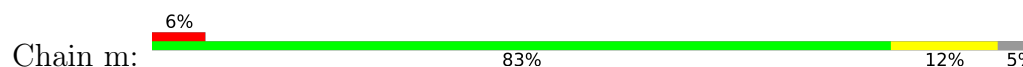
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



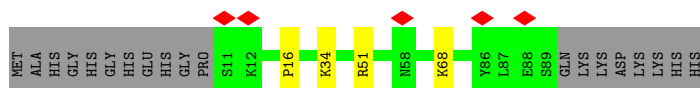
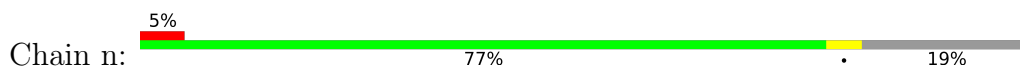
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



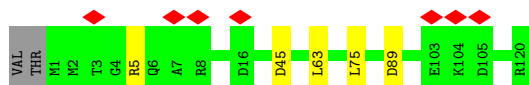
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



- Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



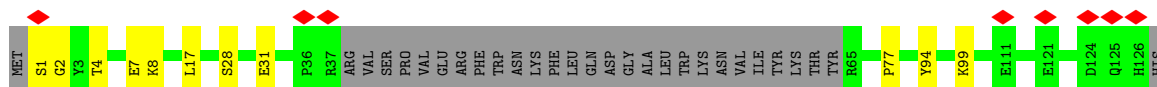
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 subunit C2



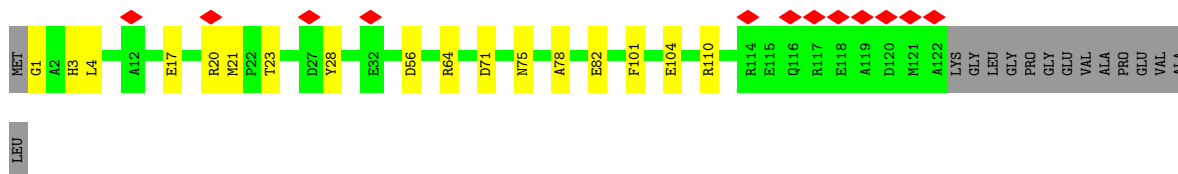
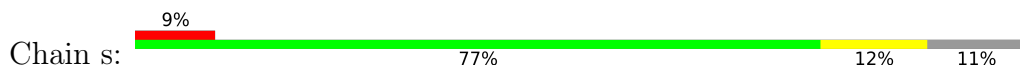
- Molecule 20: NADH:ubiquinone oxidoreductase subunit B4



- Molecule 21: Mitochondrial complex I, B17 subunit



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

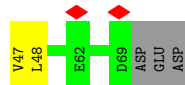
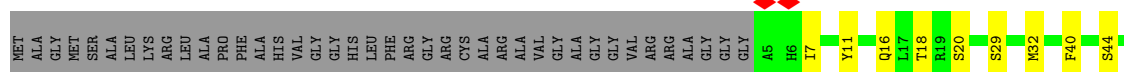


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



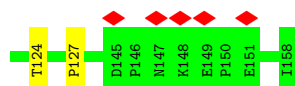
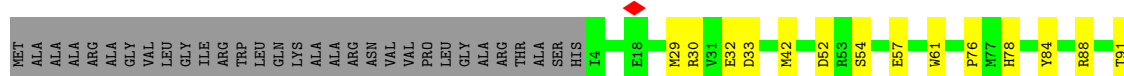
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain u:  50% 10% 40%



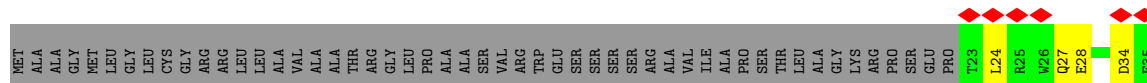
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain v:  75% 9% 17%



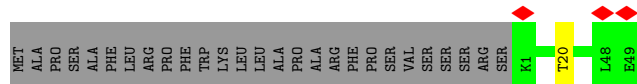
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain w:  6% 57% 8% 34%




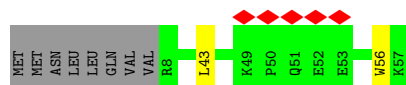
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain x:  63% 36%




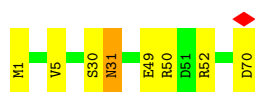
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain y:  9% 83% 14%




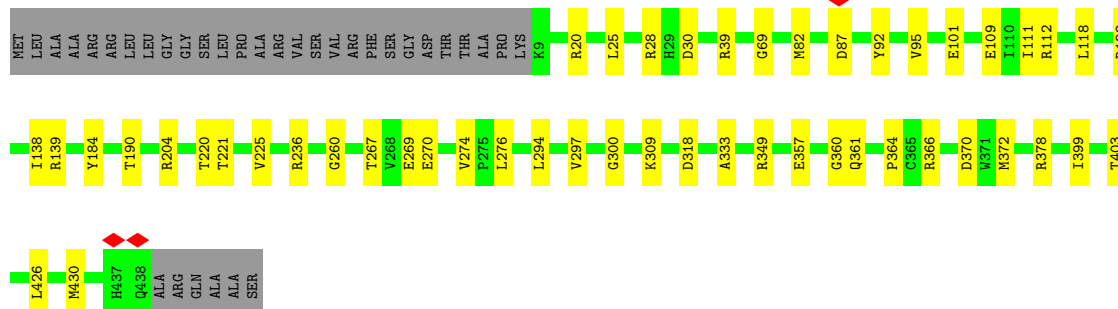
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain z:  89% 10%




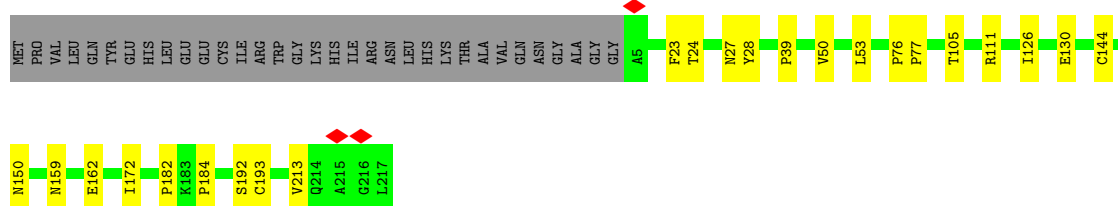
- Molecule 30: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1:  82% 11% 7%




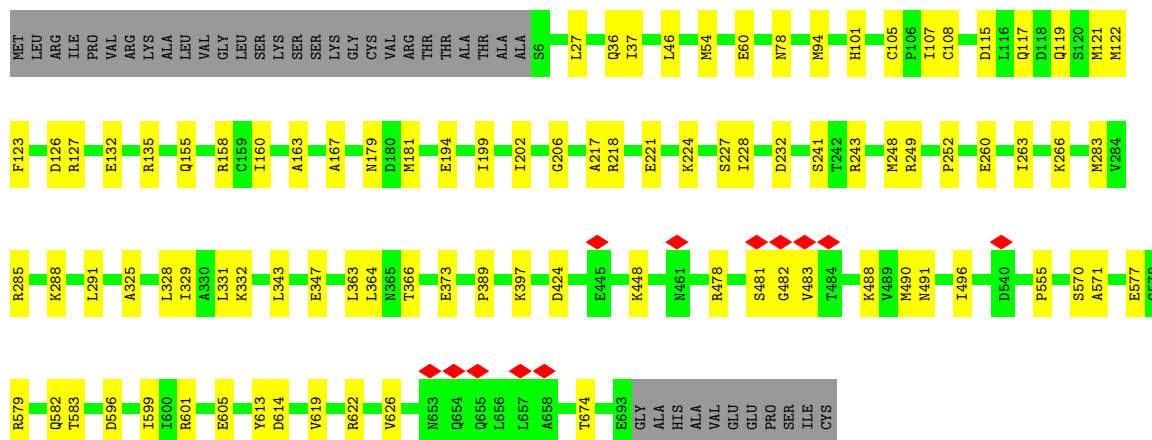
- Molecule 31: Mitochondrial complex I, 24 kDa subunit

Chain 2:  77% 9% 13%



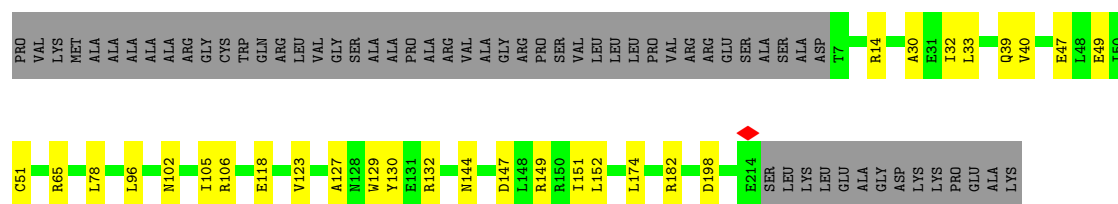
- Molecule 32: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 3:  82% 13% 5%



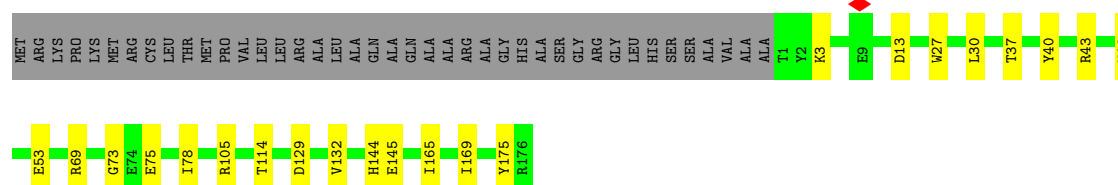
- Molecule 33: NADH:ubiquinone oxidoreductase core subunit S3

Chain 5:  67% 11% 22%



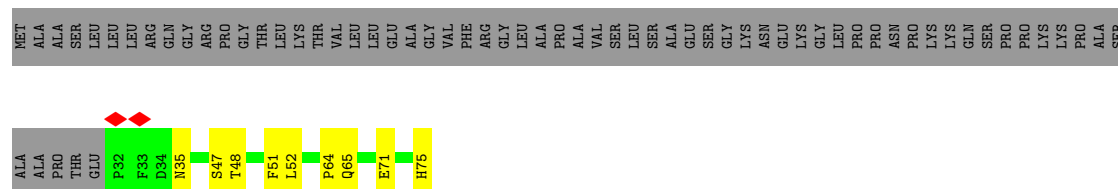
- Molecule 34: Complex I-23kD

Chain 9:  71% 10% 19%



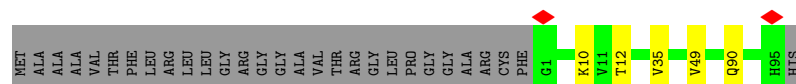
- Molecule 35: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain a:  32% 8% 60%



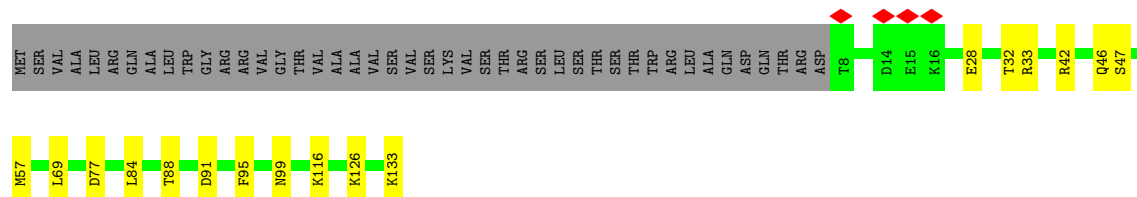
- Molecule 36: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain b:  73% 23%



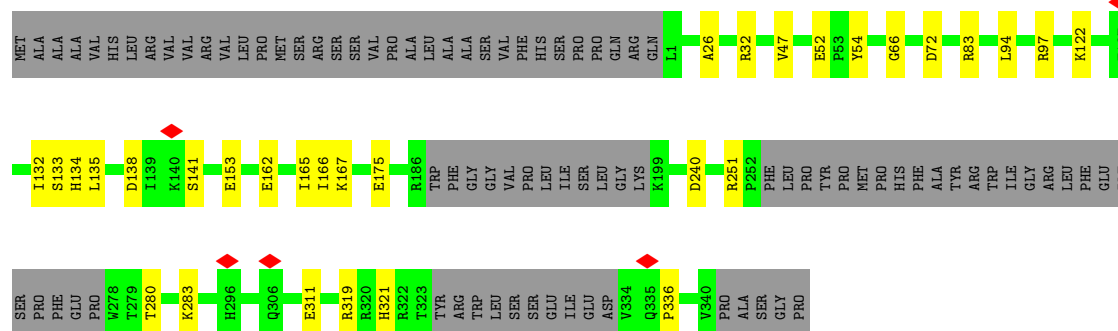
- Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain c:  64% 10% 26%




- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain d:  69% 8% 23%




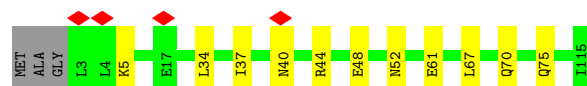
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain e:  75% 12% 13%



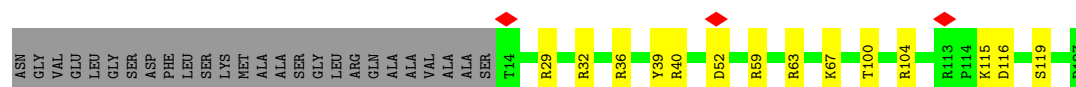
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain f:  88% 9% 3%




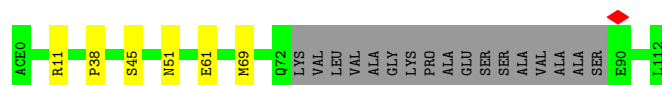
- Molecule 41: NADH:ubiquinone oxidoreductase subunit A6

Chain g:  71% 10% 19%




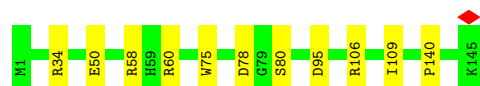
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain h:  80% 5% 15%

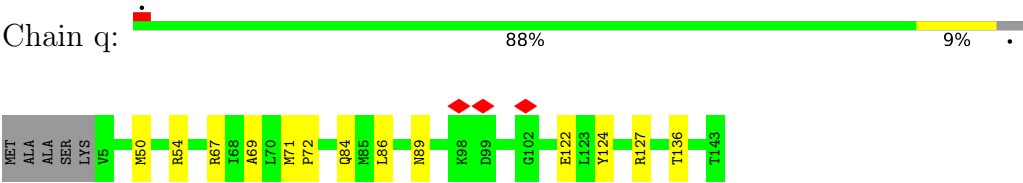


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain i:  92% 8%



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76863	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	90	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.606	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.095	Depositor
Map size (Å)	170.8, 193.98001, 291.58002	wwPDB
Map dimensions	239, 159, 140	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, MG, NAI, A1JBT, FMN, MYR, 2MR, 3PE, FME, ZN, NDP, DGT, SEP, ZMP, K, PC1, SF4, FES

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	4	0.19	0/3484	0.41	0/4716
2	A	0.20	0/852	0.45	0/1167
3	H	0.22	0/2526	0.48	0/3455
4	6	0.18	0/1278	0.39	0/1728
5	J	0.18	0/1324	0.42	0/1790
6	K	0.22	0/749	0.46	0/1014
7	L	0.20	0/4924	0.44	0/6698
8	M	0.22	0/3731	0.46	0/5085
9	N	0.22	0/2787	0.45	0/3795
10	V	0.15	0/1047	0.31	0/1421
11	W	0.16	0/1188	0.33	0/1607
12	X	0.15	0/713	0.36	0/963
12	j	0.20	0/670	0.47	0/902
13	Y	0.15	0/1440	0.37	0/1942
14	Z	0.16	0/1475	0.32	0/1989
15	k	0.14	0/2646	0.32	0/3579
16	l	0.17	0/896	0.43	0/1200
17	m	0.17	0/647	0.42	0/890
18	n	0.16	0/653	0.39	0/882
19	o	0.15	0/1035	0.29	0/1398
20	p	0.15	0/1085	0.33	0/1467
21	r	0.15	0/874	0.36	0/1188
22	s	0.16	0/1072	0.39	0/1436
23	t	0.14	0/1573	0.33	0/2130
24	u	0.14	0/590	0.34	0/810
25	v	0.16	0/1361	0.36	0/1861
26	w	0.17	0/872	0.42	0/1185
27	x	0.15	0/425	0.33	0/576
28	y	0.15	0/449	0.37	0/605
29	z	0.16	0/591	0.37	0/795
30	1	0.16	0/3386	0.36	0/4575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	2	0.16	0/1695	0.40	0/2306
32	3	0.16	0/5362	0.36	0/7266
33	5	0.17	0/1776	0.38	0/2417
34	9	0.19	0/1445	0.41	0/1956
35	a	0.13	0/383	0.28	0/518
36	b	0.17	0/749	0.35	0/1009
37	c	0.15	0/1047	0.34	0/1415
38	d	0.16	0/2397	0.34	0/3241
39	e	0.16	0/702	0.42	0/945
40	f	0.14	0/937	0.32	0/1271
41	g	0.16	0/993	0.32	0/1336
42	h	0.16	0/779	0.35	0/1054
43	i	0.15	0/1250	0.31	0/1698
44	q	0.17	0/1171	0.33	0/1579
All	All	0.18	0/67029	0.39	0/90860

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4	3409	0	3347	43	0
2	A	831	0	874	9	0
3	H	2453	0	2571	36	0
4	6	1247	0	1256	14	0
5	J	1294	0	1317	25	0
6	K	749	0	793	12	0
7	L	4806	0	4945	51	0
8	M	3647	0	3849	46	0
9	N	2723	0	2930	32	0
10	V	1028	0	1036	6	0
11	W	1155	0	1177	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	X	701	0	693	10	0
12	j	660	0	663	17	0
13	Y	1403	0	1392	17	0
14	Z	1441	0	1419	10	0
15	k	2596	0	2559	24	0
16	l	874	0	869	15	0
17	m	626	0	635	8	0
18	n	634	0	616	4	0
19	o	1004	0	995	4	0
20	p	1059	0	1062	9	0
21	r	846	0	864	9	0
22	s	1047	0	1015	11	0
23	t	1520	0	1477	8	0
24	u	563	0	509	7	0
25	v	1307	0	1207	11	0
26	w	846	0	792	13	0
27	x	412	0	411	1	0
28	y	436	0	437	2	0
29	z	576	0	570	7	0
30	1	3312	0	3267	33	0
31	2	1655	0	1668	14	0
32	3	5275	0	5300	61	0
33	5	1726	0	1676	19	0
34	9	1414	0	1371	17	0
35	a	371	0	344	6	0
36	b	737	0	710	3	0
37	c	1024	0	1023	11	0
38	d	2345	0	2375	19	0
39	e	691	0	706	8	0
40	f	917	0	958	8	0
41	g	969	0	980	15	0
42	h	763	0	775	5	0
43	i	1209	0	1182	7	0
44	q	1142	0	1137	11	0
45	4	40	0	54	1	0
45	6	51	0	82	1	0
45	A	51	0	82	3	0
45	H	51	0	82	1	0
45	K	40	0	54	0	0
45	L	82	0	118	2	0
45	M	44	0	65	0	0
45	N	51	0	82	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	V	72	0	92	2	0
45	i	51	0	82	2	0
45	o	31	0	36	0	0
45	p	27	0	27	2	0
46	4	54	0	88	3	0
46	6	46	0	69	3	0
46	A	37	0	48	0	0
46	L	54	0	88	2	0
46	M	108	0	176	3	0
47	H	29	0	0	0	0
48	1	8	0	0	0	0
48	3	16	0	0	1	0
48	6	8	0	0	0	0
48	9	16	0	0	0	0
49	k	31	0	12	2	0
50	k	1	0	0	0	0
51	s	15	0	27	0	0
52	j	34	0	40	0	0
52	t	31	0	34	2	0
53	1	31	0	19	0	0
54	1	44	0	27	2	0
55	2	4	0	0	1	0
55	3	4	0	0	0	0
56	3	1	0	0	0	0
57	b	1	0	0	0	0
58	d	48	0	26	1	0
All	All	66655	0	67262	580	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 4.

All (580) 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)
32:3:570:SER:HA	32:3:583:THR:O	1.74	0.88
8:M:324:SER:HG	8:M:440:HIS:HE2	1.28	0.79
6:K:60:PRO:O	6:K:63:LEU:HB3	1.90	0.72
1:4:326:ASP:OD1	32:3:127:ARG:NH2	2.22	0.72
32:3:228:ILE:HB	32:3:583:THR:HG22	1.76	0.67
1:4:165:THR:HG23	3:H:32:GLN:HG2	1.77	0.67
29:z:30:SER:C	29:z:31:ASN:HD22	2.06	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:336:ARG:HH22	8:M:429:SER:HA	1.62	0.64
1:4:269:LEU:HB2	1:4:368:GLU:HB2	1.79	0.63
30:1:101:GLU:HB2	54:1:503:NAI:H42N	1.78	0.63
11:W:8:LEU:HD21	12:X:88:GLU:HB2	1.80	0.63
9:N:207:ILE:HG22	9:N:211:MET:HE2	1.79	0.62
1:4:65:VAL:HB	1:4:77:ASP:HB3	1.81	0.62
7:L:97:THR:HG21	7:L:125:LEU:HD22	1.82	0.62
5:J:56:VAL:O	5:J:60:TYR:HB3	1.99	0.62
13:Y:15:GLN:O	13:Y:63:ASN:ND2	2.33	0.62
3:H:27:VAL:O	3:H:31:MET:HB2	1.99	0.61
5:J:38:GLY:HA2	5:J:57:PHE:HE1	1.65	0.61
5:J:23:LYS:O	6:K:23:ARG:NH1	2.32	0.61
6:K:73:LEU:HD21	9:N:41:ILE:HG13	1.82	0.61
3:H:58:LYS:HD2	4:6:108:PRO:HB2	1.82	0.61
12:j:40:LEU:HB3	12:j:42:LEU:HD13	1.83	0.61
39:e:26:SER:O	39:e:33:ARG:NH2	2.34	0.61
7:L:221:THR:HG23	7:L:226:GLN:HB2	1.81	0.60
8:M:133:ILE:HD11	8:M:231:LEU:HD11	1.82	0.60
43:i:34:ARG:NH2	43:i:58:ARG:O	2.34	0.60
8:M:46:GLY:H	26:w:85:MET:HE3	1.66	0.60
9:N:130:LEU:HD12	9:N:134:GLN:HG3	1.84	0.60
45:A:202:3PE:H381	3:H:295:PRO:HB3	1.82	0.60
7:L:203:MET:HB2	14:Z:113:GLN:HG3	1.84	0.60
15:k:35:LYS:O	15:k:38:LEU:HB3	2.02	0.60
44:q:67:ARG:NH1	44:q:71:MET:SD	2.75	0.59
33:5:32:ILE:HG22	33:5:33:LEU:HD12	1.85	0.59
35:a:71:GLU:OE2	35:a:75:HIS:ND1	2.35	0.59
2:A:13:LEU:HD22	3:H:10:ILE:HD12	1.85	0.59
11:W:133:ILE:HG23	16:l:21:SER:HB3	1.85	0.59
1:4:342:MET:HE2	32:3:101:HIS:HD2	1.67	0.58
1:4:145:THR:HA	1:4:148:LEU:HD12	1.84	0.58
1:4:328:ALA:HB3	32:3:126:ASP:HB2	1.85	0.58
3:H:149:ILE:HG21	3:H:185:TRP:HB2	1.85	0.58
34:9:69:ARG:NH1	34:9:73:GLY:O	2.37	0.58
31:2:105:THR:OG1	55:2:300:FES:S2	2.61	0.58
32:3:36:GLN:NE2	37:c:47:SER:O	2.37	0.58
12:j:26:ASP:HB3	12:j:29:LYS:HD3	1.85	0.58
30:1:111:ILE:HD12	30:1:138:ILE:HD11	1.86	0.58
34:9:27:TRP:HB3	34:9:30:LEU:HD12	1.86	0.58
8:M:165:ILE:HG21	9:N:268:GLN:HA	1.86	0.58
11:W:88:GLU:OE1	28:y:56:TRP:NE1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:312:SER:HB3	44:q:54:ARG:HH21	1.68	0.57
4:6:52:LEU:HB2	4:6:90:GLY:HA3	1.87	0.57
30:1:139:ARG:NH2	31:2:144:CYS:O	2.35	0.57
33:5:47:GLU:OE1	33:5:106:ARG:NH2	2.37	0.57
17:m:83:LEU:HD21	44:q:54:ARG:HD3	1.86	0.57
41:g:63:ARG:HE	41:g:67:LYS:HZ3	1.53	0.57
1:4:179:GLU:OE2	4:6:66:ARG:NH1	2.33	0.57
2:A:60:ILE:HG21	5:J:168:ILE:HG21	1.87	0.57
7:L:485:TYR:OH	22:s:1:GLY:N	2.38	0.57
8:M:452:LYS:HA	8:M:455:LEU:HD12	1.86	0.56
30:1:20:ARG:NH1	30:1:269:GLU:O	2.38	0.56
1:4:335:ARG:NH2	34:9:129:ASP:OD1	2.38	0.56
9:N:342:ILE:HD11	19:o:75:LEU:HB3	1.87	0.56
30:1:276:LEU:HD11	30:1:297:VAL:HG11	1.86	0.56
7:L:100:ILE:HG21	7:L:246:LEU:HB2	1.88	0.56
46:L:1002:PC1:H32	46:M:503:PC1:H142	1.87	0.56
20:p:47:GLN:HG3	23:t:165:LEU:HD13	1.88	0.56
39:e:68:TYR:HH	39:e:96:SER:HG	1.53	0.56
1:4:273:GLN:NE2	33:5:102:ASN:OD1	2.37	0.56
8:M:325:MET:HE3	8:M:437:MET:HB3	1.88	0.56
12:j:29:LYS:HE3	12:j:40:LEU:HD13	1.89	0.56
6:K:59:MET:HG2	9:N:27:LEU:HD22	1.87	0.55
20:p:39:ARG:NH2	23:t:3:LEU:O	2.39	0.55
1:4:123:GLU:OE2	1:4:138:ARG:NH2	2.37	0.55
7:L:28:LYS:NZ	7:L:29:PHE:O	2.40	0.55
9:N:337:LEU:O	9:N:340:THR:OG1	2.25	0.55
13:Y:12:LEU:O	16:l:104:ARG:NH2	2.37	0.55
31:2:150:ASN:HB3	31:2:162:GLU:HB2	1.88	0.55
32:3:105:CYS:SG	32:3:117:GLN:NE2	2.79	0.55
43:i:60:ARG:HH22	43:i:95:ASP:HA	1.71	0.55
3:H:165:LEU:HD21	3:H:241:LEU:HA	1.89	0.55
7:L:173:LEU:HD12	8:M:405:LEU:HD21	1.88	0.55
1:4:326:ASP:O	32:3:127:ARG:NH2	2.40	0.55
22:s:4:LEU:HD11	25:v:124:THR:HA	1.89	0.55
12:X:12:LYS:HE3	12:X:32:VAL:HG11	1.89	0.55
8:M:60:SER:HB2	8:M:457:PRO:HA	1.89	0.54
8:M:130:LEU:HD22	8:M:150:LEU:HD13	1.89	0.54
41:g:36:ARG:HA	12:j:52:MET:HE2	1.88	0.54
10:V:140:VAL:O	11:W:115:ARG:NH1	2.39	0.54
40:f:5:LYS:NZ	40:f:75:GLN:OE1	2.39	0.54
8:M:105:PHE:O	8:M:109:THR:OG1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:3:199:ILE:HA	32:3:202:ILE:HG12	1.88	0.54
42:h:45:SER:O	42:h:51:ASN:ND2	2.40	0.54
25:v:30:ARG:NH1	25:v:33:ASP:OD2	2.40	0.54
1:4:139:VAL:HG21	1:4:277:VAL:HB	1.90	0.54
33:5:78:LEU:HB3	33:5:130:TYR:HB3	1.90	0.54
33:5:147:ASP:OD2	33:5:149:ARG:NH1	2.41	0.54
9:N:327:PRO:HG3	19:o:45:ASP:HB2	1.88	0.54
32:3:221:GLU:HG3	32:3:243:ARG:HG3	1.90	0.54
32:3:325:ALA:HA	32:3:328:LEU:HD12	1.89	0.54
6:K:23:ARG:HG2	6:K:24:SER:H	1.73	0.53
8:M:282:LEU:HD13	8:M:342:MET:HG3	1.90	0.53
30:1:260:GLY:O	31:2:111:ARG:NH1	2.41	0.53
45:A:202:3PE:H2A2	17:m:19:VAL:HG13	1.89	0.53
32:3:252:PRO:HG3	32:3:263:ILE:HG12	1.90	0.53
39:e:63:LYS:HD3	39:e:75:ASN:HD21	1.73	0.53
1:4:354:GLU:OE2	1:4:357:GLN:NE2	2.41	0.53
44:q:89:ASN:ND2	44:q:122:GLU:O	2.42	0.53
1:4:143:GLU:OE2	1:4:278:TYR:OH	2.24	0.53
1:4:110:SER:OG	1:4:149:ASN:ND2	2.41	0.53
37:c:69:LEU:HD13	38:d:66:GLY:HA3	1.90	0.53
45:i:201:3PE:H281	45:i:201:3PE:H391	1.91	0.53
7:L:75:LYS:NZ	7:L:77:SER:OG	2.41	0.53
19:o:5:ARG:NH1	19:o:89:ASP:OD1	2.42	0.53
11:W:133:ILE:HG21	16:l:37:LYS:HG3	1.90	0.53
14:Z:161:ARG:NH2	26:w:111:ASN:OD1	2.42	0.53
37:c:95:PHE:O	37:c:99:ASN:ND2	2.41	0.53
21:r:17:LEU:HD11	23:t:162:LEU:HD22	1.90	0.53
8:M:139:GLN:O	8:M:142:ARG:NH1	2.42	0.53
8:M:191:SER:HB3	46:M:502:PC1:H31	1.90	0.53
8:M:457:PRO:O	26:w:84:ARG:NH2	2.42	0.53
30:1:270:GLU:HG3	30:1:274:VAL:HG21	1.90	0.53
34:9:145:GLU:OE2	38:d:66:GLY:N	2.41	0.53
41:g:32:ARG:NH1	12:j:68:GLU:OE2	2.42	0.53
15:k:213:GLU:OE2	15:k:217:LYS:NZ	2.41	0.52
5:J:125:TRP:HB2	44:q:136:THR:HG21	1.91	0.52
4:6:37:ILE:HD11	46:6:202:PC1:H381	1.91	0.52
7:L:359:MET:O	7:L:436:ARG:NH2	2.41	0.52
8:M:78:MET:HE1	8:M:439:LEU:HD12	1.90	0.52
9:N:243:LEU:HD22	9:N:330:THR:HG21	1.91	0.52
32:3:424:ASP:OD1	32:3:424:ASP:N	2.42	0.52
36:b:12:THR:HG22	36:b:35:VAL:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:233:ARG:NH1	46:4:502:PC1:O12	2.43	0.52
1:4:413:ASP:OD1	3:H:281:ARG:NH1	2.42	0.52
37:c:42:ARG:NH1	37:c:46:GLN:O	2.43	0.52
31:2:24:THR:OG1	31:2:27:ASN:OD1	2.24	0.52
23:t:34:ASP:OD1	23:t:34:ASP:N	2.41	0.52
32:3:227:SER:OG	32:3:228:ILE:N	2.41	0.52
34:9:43:ARG:HG3	42:h:11:ARG:HD2	1.91	0.52
38:d:311:GLU:HG2	38:d:336:PRO:HB3	1.92	0.52
22:s:28:TYR:OH	22:s:110:ARG:NH1	2.43	0.52
32:3:373:GLU:OE1	32:3:448:LYS:NZ	2.43	0.52
7:L:373:LEU:HD22	7:L:431:LEU:HD11	1.91	0.52
13:Y:129:LYS:HD3	17:m:65:VAL:HG23	1.92	0.52
14:Z:167:LYS:NZ	14:Z:171:GLU:OE1	2.43	0.52
30:1:361:GLN:OE1	37:c:133:LYS:NZ	2.43	0.52
32:3:571:ALA:O	32:3:582:GLN:HA	2.08	0.51
20:p:47:GLN:HA	20:p:50:TYR:HB3	1.92	0.51
32:3:217:ALA:HB2	32:3:248:MET:HE2	1.91	0.51
33:5:14:ARG:NH2	42:h:61:GLU:O	2.43	0.51
33:5:174:LEU:HD21	41:g:104:ARG:HH12	1.76	0.51
38:d:133:SER:OG	38:d:134:HIS:N	2.43	0.51
1:4:243:GLY:O	1:4:296:ARG:NH2	2.43	0.51
3:H:24:GLU:OE2	3:H:274:ARG:NH1	2.42	0.51
13:Y:124:LEU:HD13	44:q:69:ALA:HB2	1.92	0.51
32:3:135:ARG:NH1	32:3:179:ASN:O	2.43	0.51
30:1:118:LEU:HD13	30:1:225:VAL:HG13	1.93	0.51
14:Z:22:GLN:NE2	22:s:71:ASP:OD2	2.43	0.51
30:1:370:ASP:OD2	32:3:179:ASN:ND2	2.42	0.51
9:N:298:TYR:O	9:N:303:THR:OG1	2.27	0.51
32:3:285:ARG:NH2	32:3:555:PRO:O	2.44	0.51
1:4:350:LYS:HG3	32:3:121:MET:HG3	1.93	0.51
4:6:114:VAL:HG22	4:6:144:ILE:HB	1.93	0.51
7:L:370:THR:HG23	7:L:431:LEU:HD13	1.93	0.51
18:n:68:LYS:O	24:u:29:SER:OG	2.29	0.51
32:3:347:GLU:HB2	32:3:496:ILE:HD12	1.92	0.51
7:L:396:ILE:HG21	7:L:490:ALA:HB2	1.91	0.51
32:3:364:LEU:HD12	32:3:491:ASN:HB3	1.92	0.51
2:A:79:SER:HA	2:A:87:MET:HE3	1.93	0.51
21:r:4:THR:OG1	21:r:7:GLU:OE1	2.29	0.51
22:s:64:ARG:HG2	22:s:82:GLU:HG2	1.93	0.51
9:N:173:THR:O	9:N:227:THR:OG1	2.28	0.50
30:1:95:VAL:HG11	30:1:118:LEU:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:426:LEU:O	30:1:430:MET:HG3	2.11	0.50
1:4:275:TYR:OH	1:4:368:GLU:N	2.31	0.50
6:K:55:LEU:HD13	16:l:16:TRP:HE3	1.76	0.50
7:L:375:ILE:HD12	7:L:458:LEU:HD11	1.94	0.50
33:5:127:ALA:HA	33:5:130:TYR:HB2	1.93	0.50
13:Y:79:GLU:HG2	13:Y:80:PRO:HD3	1.93	0.50
32:3:577:GLU:OE2	32:3:579:ARG:NH1	2.45	0.50
30:1:25:LEU:HD21	30:1:267:THR:HG22	1.93	0.50
1:4:234:ILE:HD11	46:4:502:PC1:H341	1.93	0.50
15:k:30:ASN:O	15:k:126:ARG:NH2	2.44	0.50
16:l:104:ARG:NH1	44:q:84:GLN:OE1	2.44	0.50
1:4:67:GLU:HB3	1:4:75:LYS:HB3	1.94	0.50
1:4:405:MET:SD	1:4:421:GLN:NE2	2.84	0.50
10:V:127:GLY:HA3	45:V:202:3PE:H342	1.94	0.50
37:c:28:GLU:O	37:c:32:THR:OG1	2.29	0.50
15:k:233:LYS:NZ	15:k:237:ASP:OD1	2.45	0.49
38:d:319:ARG:NH2	41:g:52:ASP:OD1	2.41	0.49
41:g:40:ARG:NH1	12:j:56:ASP:OD2	2.45	0.49
2:A:63:LEU:HB2	5:J:67:VAL:HG21	1.95	0.49
16:l:101:GLU:HG2	16:l:103:LEU:HD23	1.93	0.49
32:3:622:ARG:NH2	39:e:73:GLU:OE2	2.45	0.49
32:3:481:SER:OG	32:3:482:GLY:N	2.44	0.49
7:L:173:LEU:HD11	45:L:1001:3PE:H292	1.95	0.49
33:5:151:ILE:HG23	33:5:152:LEU:HG	1.94	0.49
15:k:106:LEU:HD13	15:k:270:LEU:HD11	1.94	0.49
30:1:294:LEU:HD23	30:1:309:LYS:HG3	1.93	0.49
33:5:129:TRP:O	33:5:132:ARG:HB3	2.13	0.49
12:j:48:VAL:HG12	12:j:52:MET:HE3	1.93	0.49
8:M:336:ARG:NH1	8:M:427:LEU:O	2.45	0.49
15:k:141:GLN:NE2	15:k:201:ASP:OD2	2.43	0.49
25:v:54:SER:HA	25:v:84:TYR:HB3	1.95	0.49
45:4:501:3PE:H382	8:M:151:PHE:HB3	1.94	0.49
8:M:70:MET:HA	8:M:103:GLN:HE21	1.78	0.49
1:4:226:GLU:OE1	1:4:305:ARG:NH2	2.38	0.49
40:f:37:ILE:O	40:f:44:ARG:NH1	2.40	0.49
25:v:29:MET:HE2	25:v:76:PRO:HG3	1.95	0.48
33:5:39:GLN:HB2	33:5:51:CYS:HB2	1.95	0.48
39:e:15:LEU:HD11	39:e:93:VAL:HG12	1.95	0.48
7:L:195:THR:HG21	7:L:200:GLN:HB3	1.95	0.48
16:l:26:HIS:O	17:m:51:ASN:ND2	2.47	0.48
30:1:372:MET:HE2	30:1:399:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:126:ILE:HB	31:2:130:GLU:HB3	1.94	0.48
32:3:27:LEU:HA	32:3:37:ILE:HD12	1.96	0.48
36:b:49:VAL:HG22	36:b:90:GLN:HG3	1.95	0.48
7:L:485:TYR:O	7:L:489:THR:OG1	2.30	0.48
8:M:459:TYR:HD2	26:w:84:ARG:HD3	1.78	0.48
13:Y:82:THR:HA	13:Y:85:TRP:CD1	2.49	0.48
41:g:29:ARG:HH12	12:j:65:ILE:HD13	1.78	0.48
7:L:397:GLU:OE2	7:L:487:LYS:NZ	2.43	0.48
9:N:24:THR:HG22	16:l:2:PHE:HZ	1.77	0.48
12:X:47:GLN:NE2	12:X:70:LEU:O	2.43	0.48
13:Y:122:GLY:HA3	17:m:77:LEU:HD13	1.94	0.48
15:k:19:THR:HG23	15:k:21:ASN:H	1.78	0.48
22:s:17:GLU:OE2	22:s:20:ARG:NH1	2.46	0.48
32:3:232:ASP:OD1	32:3:232:ASP:N	2.47	0.48
3:H:11:ILE:HG13	3:H:12:PRO:HD3	1.96	0.48
3:H:64:ALA:O	3:H:124:ASN:ND2	2.47	0.48
15:k:170:ILE:HD11	15:k:238:ILE:HD11	1.94	0.48
30:1:300:GLY:HA2	30:1:333:ALA:H	1.78	0.48
3:H:311:LEU:HD22	44:q:50:MET:HE2	1.96	0.48
11:W:138:LYS:HA	16:l:27:ARG:HB3	1.95	0.48
30:1:318:ASP:OD1	30:1:318:ASP:N	2.44	0.48
32:3:108:CYS:O	32:3:218:ARG:NH1	2.45	0.48
15:k:108:TYR:OH	15:k:164:LEU:O	2.22	0.48
38:d:122:LYS:NZ	38:d:162:GLU:OE1	2.46	0.48
43:i:75:TRP:HE1	45:i:201:3PE:H112	1.78	0.48
12:j:66:ASP:OD2	12:j:79:TYR:OH	2.31	0.48
30:1:236:ARG:HG2	31:2:213:VAL:HG22	1.96	0.48
32:3:490:MET:HE3	32:3:491:ASN:H	1.79	0.48
33:5:118:GLU:OE2	33:5:144:ASN:ND2	2.43	0.48
40:f:61:GLU:OE1	40:f:70:GLN:NE2	2.46	0.48
43:i:78:ASP:OD2	43:i:80:SER:OG	2.27	0.48
6:K:73:LEU:HD11	9:N:41:ILE:HG21	1.95	0.47
7:L:129:LEU:HA	7:L:132:VAL:HG22	1.97	0.47
30:1:69:GLY:O	54:1:503:NAI:H2N	2.13	0.47
32:3:54:MET:HE2	32:3:94:MET:HE2	1.96	0.47
33:5:65:ARG:NH1	33:5:123:VAL:O	2.47	0.47
1:4:106:LEU:HD13	1:4:391:ILE:HG21	1.95	0.47
4:6:79:SER:O	4:6:83:SER:OG	2.32	0.47
15:k:52:PRO:O	15:k:107:GLN:NE2	2.46	0.47
30:1:87:ASP:OD1	30:1:87:ASP:N	2.47	0.47
38:d:251:ARG:HH21	38:d:321:HIS:HB3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:36:LEU:HD22	45:6:203:3PE:H392	1.97	0.47
11:W:125:TYR:HB2	16:L:48:SER:HB3	1.95	0.47
13:Y:29:HIS:HB3	13:Y:119:PRO:HD2	1.97	0.47
20:p:30:LYS:O	20:p:34:GLU:HG3	2.14	0.47
32:3:613:TYR:CD2	32:3:619:VAL:HG22	2.49	0.47
3:H:70:MET:HB3	3:H:118:TRP:HB3	1.96	0.47
5:J:167:VAL:HG22	9:N:42:PRO:HG2	1.95	0.47
26:w:34:ASP:OD1	26:w:34:ASP:N	2.46	0.47
38:d:138:ASP:HB3	38:d:141:SER:HB2	1.96	0.47
2:A:88:LEU:HD13	3:H:309:ILE:HD12	1.96	0.47
38:d:52:GLU:HG3	38:d:54:TYR:H	1.79	0.47
15:k:50:HIS:NE2	15:k:125:GLU:OE2	2.41	0.47
32:3:46:LEU:O	37:c:116:LYS:NZ	2.42	0.47
8:M:5:ILE:HG23	8:M:104:LEU:HD11	1.97	0.47
8:M:277:LEU:HD21	8:M:405:LEU:HB3	1.95	0.47
10:V:105:ARG:HD2	10:V:105:ARG:HA	1.78	0.47
32:3:158:ARG:HB3	32:3:202:ILE:HD12	1.96	0.47
3:H:141:SER:HB3	3:H:289:LEU:HD22	1.97	0.47
7:L:7:LEU:HA	7:L:10:VAL:HG12	1.97	0.47
30:1:378:ARG:NH2	32:3:132:GLU:OE2	2.39	0.47
30:1:184:TYR:HB3	30:1:357:GLU:HB3	1.96	0.47
33:5:182:ARG:HG2	41:g:100:THR:HG22	1.96	0.47
8:M:290:SER:HA	8:M:319:HIS:HE2	1.79	0.47
20:p:82:ASN:HA	45:p:201:3PE:H12	1.97	0.46
5:J:10:SER:O	5:J:13:PHE:HB3	2.13	0.46
7:L:106:TRP:HB2	7:L:449:PHE:HB2	1.97	0.46
8:M:403:THR:HA	8:M:406:TYR:CE2	2.50	0.46
22:s:23:THR:OG1	22:s:104:GLU:OE2	2.32	0.46
29:z:31:ASN:HD22	29:z:31:ASN:N	2.12	0.46
30:1:92:TYR:O	30:1:220:THR:HA	2.15	0.46
33:5:49:GLU:OE2	33:5:106:ARG:NH1	2.40	0.46
2:A:80:GLN:NE2	3:H:315:PRO:O	2.42	0.46
45:H:401:3PE:H2G1	5:J:38:GLY:HA3	1.97	0.46
8:M:180:GLN:HA	8:M:248:LEU:HD21	1.97	0.46
30:1:82:MET:SD	30:1:221:THR:OG1	2.70	0.46
1:4:302:GLU:HG2	34:9:3:LYS:HD2	1.98	0.46
3:H:70:MET:HE3	5:J:27:ILE:HG22	1.97	0.46
7:L:245:ALA:O	7:L:249:SER:OG	2.33	0.46
9:N:217:THR:HG23	45:N:401:3PE:H242	1.96	0.46
10:V:52:VAL:HG23	45:V:201:3PE:H371	1.98	0.46
12:X:69:LYS:HA	21:r:2:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:33:ALA:HB2	13:Y:119:PRO:HG3	1.98	0.46
30:1:28:ARG:NH1	35:a:35:ASN:O	2.40	0.46
37:c:57:MET:HE2	37:c:84:LEU:HD12	1.97	0.46
4:6:115:SER:OG	4:6:136:CYS:SG	2.68	0.46
7:L:69:LEU:HD13	8:M:451:PRO:HG2	1.98	0.46
30:1:132:ARG:NH2	35:a:64:PRO:O	2.38	0.46
31:2:50:VAL:O	31:2:53:LEU:HB3	2.15	0.46
32:3:596:ASP:HA	32:3:599:ILE:HD12	1.97	0.46
1:4:51:PHE:HB3	1:4:64:LEU:HB2	1.97	0.46
13:Y:100:ARG:NH1	13:Y:103:GLN:OE1	2.49	0.46
31:2:39:PRO:HA	35:a:65:GLN:HB3	1.98	0.46
4:6:63:ALA:HB2	4:6:69:MET:HE2	1.98	0.46
8:M:373:ILE:HA	8:M:376:ILE:HD12	1.98	0.46
10:V:139:LYS:HG3	10:V:140:VAL:HG13	1.97	0.46
17:m:39:LYS:O	17:m:43:MET:HG2	2.16	0.46
17:m:59:ASP:OD1	17:m:59:ASP:N	2.48	0.46
30:1:364:PRO:HB2	30:1:403:THR:HG22	1.97	0.46
34:9:13:ASP:N	34:9:13:ASP:OD1	2.42	0.46
5:J:52:LEU:HD13	6:K:45:THR:HG23	1.98	0.46
15:k:90:ASP:O	15:k:95:ARG:NH2	2.48	0.46
20:p:84:LYS:HE2	25:v:42:MET:HE2	1.98	0.46
32:3:332:LYS:HA	32:3:343:LEU:HD21	1.98	0.46
40:f:61:GLU:HB3	40:f:67:LEU:HD13	1.98	0.46
5:J:90:LEU:O	5:J:94:ILE:HG12	2.16	0.45
8:M:75:LEU:HB3	8:M:229:MET:HE1	1.98	0.45
8:M:175:ASN:HB3	8:M:178:ILE:HB	1.99	0.45
14:Z:10:PRO:O	21:r:94:TYR:OH	2.32	0.45
32:3:555:PRO:HB3	43:i:140:PRO:HG3	1.98	0.45
7:L:274:GLN:HA	7:L:277:MET:HE3	1.98	0.45
13:Y:71:ARG:NH1	29:z:70:ASP:OD2	2.47	0.45
21:r:99:LYS:HB3	21:r:99:LYS:HE3	1.77	0.45
29:z:49:GLU:OE1	29:z:52:ARG:NH2	2.49	0.45
18:n:16:PRO:HD2	24:u:11:TYR:HD2	1.81	0.45
32:3:478:ARG:HA	32:3:483:VAL:HG21	1.99	0.45
38:d:26:ALA:HB3	38:d:47:VAL:HG13	1.97	0.45
6:K:40:LEU:HD22	9:N:75:ILE:HD12	1.99	0.45
1:4:166:PRO:HA	1:4:169:TRP:HB2	1.99	0.45
7:L:558:LEU:HD13	7:L:561:ILE:HD11	1.97	0.45
15:k:287:HIS:ND1	26:w:28:GLU:OE2	2.40	0.45
7:L:13:ILE:O	7:L:17:MET:HG3	2.16	0.45
7:L:152:PHE:HB2	7:L:172:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:75:GLU:OE2	21:r:8:LYS:NZ	2.46	0.45
33:5:96:LEU:HB2	33:5:105:ILE:HG22	1.98	0.45
43:i:106:ARG:HB2	43:i:109:ILE:HG13	1.99	0.45
1:4:371:LYS:HG2	1:4:422:ASP:HB3	1.99	0.45
38:d:32:ARG:NH1	38:d:175:GLU:OE2	2.45	0.45
41:g:116:ASP:OD1	41:g:119:SER:OG	2.25	0.45
7:L:341:MET:HE3	7:L:457:LEU:HD12	1.99	0.45
15:k:111:ALA:HB1	15:k:122:VAL:HG11	1.98	0.45
25:v:57:GLU:OE2	25:v:91:THR:OG1	2.33	0.45
9:N:20:VAL:HG11	9:N:137:ALA:HB1	1.98	0.45
25:v:52:ASP:HA	25:v:78:HIS:HE2	1.82	0.45
34:9:132:VAL:HG11	34:9:169:ILE:HD11	1.99	0.45
5:J:4:TYR:OH	5:J:111:LYS:NZ	2.50	0.45
5:J:173:ARG:HD2	5:J:175:ASN:HB2	1.99	0.45
26:w:24:LEU:HD11	26:w:27:GLN:HG2	1.99	0.45
3:H:53:ILE:HG12	46:6:202:PC1:H3G1	1.98	0.44
11:W:120:GLY:O	11:W:124:GLN:NE2	2.50	0.44
21:r:1:SER:OG	21:r:2:GLY:N	2.44	0.44
52:t:201:ZMP:H17	52:t:201:ZMP:H15	1.58	0.44
32:3:363:LEU:HD23	32:3:363:LEU:HA	1.85	0.44
33:5:30:ALA:HB2	33:5:40:VAL:HG21	1.98	0.44
3:H:233:MET:HE3	3:H:233:MET:HB3	1.80	0.44
9:N:128:LEU:O	9:N:132:THR:OG1	2.29	0.44
38:d:280:THR:HG23	38:d:283:LYS:H	1.83	0.44
15:k:95:ARG:NH2	26:w:27:GLN:OE1	2.50	0.44
33:5:30:ALA:HB1	42:h:69:MET:HE3	1.99	0.44
14:Z:143:HIS:O	14:Z:157:LYS:NZ	2.44	0.44
32:3:260:GLU:OE2	32:3:397:LYS:NZ	2.44	0.44
3:H:79:LEU:HD11	3:H:222:LEU:HB3	1.99	0.44
8:M:82:HIS:ND1	8:M:335:GLU:OE1	2.50	0.44
24:u:40:PHE:O	24:u:44:SER:OG	2.28	0.44
32:3:366:THR:OG1	32:3:488:LYS:O	2.34	0.44
32:3:601:ARG:NH1	32:3:605:GLU:OE1	2.40	0.44
43:i:50:GLU:HG3	43:i:60:ARG:HG2	2.00	0.44
7:L:280:LEU:HD23	7:L:314:MET:HE2	1.98	0.44
1:4:35:ASP:O	9:N:49:ASN:ND2	2.50	0.44
4:6:170:GLU:OE1	4:6:172:ARG:NE	2.50	0.44
8:M:114:GLU:HG2	8:M:116:ILE:HG22	1.99	0.44
22:s:21:MET:HE1	22:s:101:PHE:HA	1.99	0.44
32:3:119:GLN:HA	32:3:122:MET:HB2	2.00	0.44
37:c:33:ARG:NH1	37:c:77:ASP:OD1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:91:THR:HA	4:6:119:CYS:HB3	2.00	0.44
38:d:72:ASP:O	38:d:83:ARG:NH2	2.50	0.44
38:d:240:ASP:OD1	38:d:240:ASP:N	2.49	0.44
41:g:63:ARG:NH2	12:j:46:ASP:OD1	2.51	0.44
12:j:19:LEU:HD23	12:j:19:LEU:HA	1.86	0.44
1:4:74:ARG:HA	1:4:74:ARG:HD3	1.84	0.43
4:6:116:MET:HE2	4:6:151:PRO:HG2	2.00	0.43
8:M:119:TYR:CZ	8:M:161:LEU:HB2	2.53	0.43
11:W:28:TYR:O	26:w:67:SER:OG	2.34	0.43
15:k:104:ARG:NH2	49:k:401:DGT:N7	2.65	0.43
17:m:66:PRO:HB3	17:m:73:GLN:HG2	2.00	0.43
32:3:119:GLN:HB2	32:3:123:PHE:HD2	1.82	0.43
32:3:155:GLN:NE2	32:3:181:MET:O	2.44	0.43
41:g:100:THR:O	41:g:104:ARG:HG3	2.17	0.43
3:H:26:LYS:HD2	3:H:36:GLY:HA3	1.99	0.43
7:L:200:GLN:HG2	7:L:204:LEU:HD23	1.99	0.43
8:M:254:THR:HA	8:M:257:MET:HB2	2.00	0.43
19:o:63:LEU:HD22	27:x:20:THR:HG23	1.99	0.43
24:u:7:ILE:HG23	24:u:16:GLN:HB3	1.99	0.43
3:H:256:THR:HA	3:H:259:PHE:CE1	2.53	0.43
31:2:172:ILE:HG23	31:2:182:PRO:HG2	2.01	0.43
7:L:338:MET:HE2	7:L:338:MET:HB3	1.82	0.43
9:N:179:MET:HE3	9:N:179:MET:HB3	1.94	0.43
12:X:44:SER:OG	52:t:201:ZMP:O6	2.26	0.43
14:Z:67:PHE:HB3	28:y:43:LEU:HD11	1.99	0.43
32:3:194:GLU:HG3	32:3:389:PRO:HB3	2.00	0.43
1:4:151:ILE:HD11	1:4:218:PHE:CZ	2.54	0.43
3:H:31:MET:SD	34:9:37:THR:HG22	2.58	0.43
25:v:30:ARG:NH2	25:v:32:GLU:OE1	2.52	0.43
40:f:34:LEU:HD23	40:f:48:GLU:HG3	1.99	0.43
45:A:202:3PE:H3C2	45:A:202:3PE:H391	1.87	0.43
4:6:137:ASP:OD2	34:9:144:HIS:ND1	2.52	0.43
5:J:45:LEU:HD23	5:J:50:SER:HA	1.99	0.43
5:J:55:MET:HG2	6:K:61:ILE:HD12	2.01	0.43
9:N:325:LEU:O	9:N:329:MET:HG3	2.17	0.43
29:z:1:MET:HE3	29:z:1:MET:HB3	1.82	0.43
38:d:97:ARG:NH2	58:d:401:NDP:O1A	2.51	0.43
3:H:90:PRO:HD3	3:H:162:LEU:HB3	2.01	0.43
32:3:601:ARG:NH2	32:3:614:ASP:OD1	2.40	0.43
41:g:63:ARG:HE	41:g:67:LYS:NZ	2.15	0.43
3:H:26:LYS:HB3	29:z:5:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:88:MET:HE3	7:L:88:MET:HB3	1.88	0.43
8:M:47:ASP:OD1	8:M:47:ASP:N	2.51	0.43
30:1:30:ASP:O	30:1:39:ARG:NH1	2.43	0.43
7:L:341:MET:HB2	7:L:341:MET:HE2	1.73	0.43
7:L:505:SER:O	7:L:508:THR:OG1	2.36	0.43
12:X:63:PRO:HB3	25:v:61:TRP:CD2	2.54	0.43
15:k:48:LEU:HD22	15:k:121:GLY:HA3	2.01	0.43
30:1:294:LEU:HD11	30:1:297:VAL:HG23	2.01	0.43
41:g:39:TYR:CZ	41:g:59:ARG:HD3	2.53	0.43
3:H:24:GLU:HG3	3:H:271:LEU:HD22	2.01	0.42
6:K:63:LEU:HD12	9:N:30:TRP:CH2	2.54	0.42
15:k:22:SER:OG	15:k:119:GLY:O	2.31	0.42
1:4:183:ARG:NH1	1:4:210:ASP:OD2	2.52	0.42
3:H:56:PHE:HD2	46:6:202:PC1:H3G2	1.83	0.42
9:N:199:THR:HG21	9:N:347:GLU:HG2	2.00	0.42
31:2:159:ASN:HB3	31:2:184:PRO:HB3	2.02	0.42
32:3:60:GLU:HG2	32:3:78:ASN:HB3	2.00	0.42
12:j:70:LEU:HD23	12:j:76:ILE:HG12	2.02	0.42
7:L:515:TYR:OH	23:t:69:GLU:OE2	2.32	0.42
39:e:63:LYS:HB2	39:e:63:LYS:HE2	1.80	0.42
1:4:359:PRO:HA	1:4:360:PRO:HD3	1.95	0.42
1:4:399:LEU:HD12	1:4:399:LEU:HA	1.90	0.42
5:J:56:VAL:O	5:J:60:TYR:CB	2.66	0.42
7:L:60:GLU:HB2	7:L:83:ASP:HA	2.00	0.42
7:L:526:LEU:HD12	7:L:530:PRO:HG2	2.01	0.42
24:u:47:VAL:HG23	24:u:48:LEU:HG	2.01	0.42
26:w:43:ASP:OD1	26:w:43:ASP:N	2.49	0.42
32:3:331:LEU:HD12	32:3:331:LEU:HA	1.93	0.42
46:4:502:PC1:H252	3:H:296:LEU:HD13	1.99	0.42
3:H:24:GLU:HA	3:H:271:LEU:HD13	2.00	0.42
8:M:348:LEU:HD23	8:M:351:LEU:HD12	2.00	0.42
13:Y:17:VAL:O	29:z:50:ARG:NH2	2.52	0.42
32:3:115:ASP:O	32:3:119:GLN:HG2	2.19	0.42
7:L:434:GLN:NE2	18:n:51:ARG:O	2.50	0.42
20:p:83:THR:OG1	45:p:201:3PE:O12	2.34	0.42
7:L:10:VAL:HG23	21:r:77:PRO:HB2	2.00	0.42
40:f:48:GLU:O	40:f:52:ASN:ND2	2.53	0.42
1:4:29:LYS:HE3	1:4:29:LYS:HB2	1.75	0.42
7:L:309:GLN:O	7:L:313:MET:HG3	2.18	0.42
45:L:1001:3PE:H221	25:v:88:ARG:HA	2.01	0.42
9:N:218:LEU:HD13	9:N:244:VAL:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:3:241:SER:OG	32:3:249:ARG:HG2	2.20	0.42
35:a:47:SER:OG	35:a:48:THR:N	2.52	0.42
1:4:33:TRP:HB2	15:k:158:VAL:HG11	2.02	0.42
2:A:69:ILE:HG12	3:H:148:ILE:HD11	2.01	0.42
13:Y:17:VAL:HG12	13:Y:19:VAL:HG22	2.02	0.42
13:Y:76:HIS:HB3	13:Y:113:LYS:HD3	2.01	0.42
30:1:349:ARG:HA	30:1:349:ARG:HD2	1.84	0.42
40:f:34:LEU:HD12	40:f:37:ILE:HD12	2.02	0.42
3:H:165:LEU:HG	3:H:169:GLN:HE21	1.84	0.42
6:K:93:LEU:HD22	9:N:54:GLU:HG2	2.02	0.42
7:L:13:ILE:HA	7:L:16:THR:HG22	2.02	0.42
7:L:375:ILE:HG12	24:u:32:MET:SD	2.60	0.42
26:w:109:GLU:N	26:w:109:GLU:OE1	2.53	0.42
32:3:266:LYS:NZ	32:3:674:THR:OG1	2.41	0.42
34:9:75:GLU:O	34:9:105:ARG:NH1	2.52	0.42
1:4:189:MET:SD	4:6:150:PRO:HG3	2.59	0.41
5:J:163:ILE:HG21	9:N:12:THR:HG21	2.01	0.41
7:L:556:ILE:O	7:L:560:THR:OG1	2.29	0.41
12:X:35:HIS:CD2	12:X:71:MET:HB3	2.55	0.41
31:2:23:PHE:HB2	31:2:28:TYR:CE1	2.55	0.41
32:3:206:GLY:N	48:3:801:SF4:S2	2.89	0.41
32:3:329:ILE:HD11	32:3:626:VAL:HG21	2.02	0.41
41:g:36:ARG:NH2	12:j:55:GLU:OE2	2.52	0.41
41:g:115:LYS:HD3	41:g:115:LYS:HA	1.80	0.41
12:j:16:LEU:O	12:j:20:LYS:HG2	2.20	0.41
12:j:73:PRO:HA	12:j:76:ILE:HD12	2.01	0.41
3:H:139:THR:O	3:H:143:GLU:HG3	2.20	0.41
15:k:145:ARG:HH22	15:k:280:PRO:HD2	1.86	0.41
30:1:109:GLU:OE2	30:1:112:ARG:NH2	2.53	0.41
12:j:60:PHE:HZ	12:j:80:ILE:HG22	1.85	0.41
2:A:74:PRO:HG2	5:J:147:TYR:HE2	1.85	0.41
5:J:54:LEU:HD23	5:J:54:LEU:HA	1.89	0.41
5:J:111:LYS:HA	5:J:121:GLY:HA3	2.01	0.41
16:l:50:ARG:O	16:l:54:GLU:HB2	2.21	0.41
26:w:100:ARG:HG2	26:w:107:LEU:HA	2.02	0.41
31:2:76:PRO:HA	31:2:77:PRO:HD3	1.94	0.41
38:d:132:ILE:HD13	38:d:166:ILE:HB	2.02	0.41
44:q:124:TYR:HA	44:q:127:ARG:HD2	2.01	0.41
1:4:282:GLU:O	1:4:313:GLN:NE2	2.42	0.41
8:M:179:LEU:HD13	8:M:249:LEU:HD11	2.02	0.41
9:N:280:THR:O	9:N:284:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:u:18:THR:HG22	24:u:20:SER:H	1.85	0.41
30:1:360:GLY:HA2	30:1:366:ARG:HB2	2.02	0.41
38:d:94:LEU:HD23	38:d:132:ILE:HG13	2.02	0.41
39:e:54:ILE:O	39:e:55:ARG:NH1	2.46	0.41
9:N:326:LEU:HA	9:N:329:MET:HE2	2.03	0.41
13:Y:6:LEU:HD21	44:q:86:LEU:HB3	2.01	0.41
15:k:233:LYS:HA	15:k:233:LYS:HD2	1.83	0.41
21:r:28:SER:HB2	21:r:31:GLU:HG3	2.02	0.41
22:s:75:ASN:HB3	22:s:78:ALA:HB2	2.03	0.41
32:3:160:ILE:H	32:3:160:ILE:HG13	1.72	0.41
32:3:283:MET:HE3	32:3:291:LEU:HB3	2.03	0.41
32:3:288:LYS:HE2	32:3:288:LYS:HB3	1.81	0.41
40:f:40:ASN:OD1	40:f:40:ASN:N	2.54	0.41
5:J:17:PHE:HA	5:J:20:PHE:CE2	2.55	0.41
7:L:194:ASN:ND2	14:Z:106:GLN:OE1	2.51	0.41
7:L:295:GLN:O	7:L:425:ARG:NH2	2.47	0.41
7:L:544:MET:HG2	7:L:548:SER:HB2	2.02	0.41
8:M:373:ILE:HD11	8:M:444:LEU:HD12	2.01	0.41
35:a:51:PHE:HD2	35:a:52:LEU:HD12	1.85	0.41
36:b:10:LYS:HD2	36:b:35:VAL:HG21	2.03	0.41
2:A:53:MET:HE2	5:J:172:THR:HB	2.03	0.41
10:V:75:ILE:HD13	10:V:75:ILE:HA	1.96	0.41
12:X:38:LYS:HB2	12:X:38:LYS:HE2	1.90	0.41
14:Z:135:VAL:HG11	20:p:124:PHE:HA	2.02	0.41
32:3:163:ALA:HA	32:3:167:ALA:HB3	2.02	0.41
1:4:224:GLU:OE1	34:9:40:TYR:OH	2.20	0.41
3:H:157:ASN:OD1	3:H:168:THR:OG1	2.28	0.41
7:L:88:MET:HB2	7:L:326:PHE:HE2	1.86	0.41
9:N:294:MET:HE3	9:N:294:MET:HB3	1.87	0.41
32:3:107:ILE:HG23	34:9:78:ILE:HD12	2.02	0.41
3:H:27:VAL:O	3:H:31:MET:CB	2.67	0.41
5:J:163:ILE:HD13	5:J:163:ILE:HA	1.92	0.41
8:M:156:GLY:HA2	46:M:502:PC1:H3F1	2.02	0.41
8:M:281:ASP:HB3	8:M:284:SER:HB2	2.03	0.41
8:M:391:ILE:HB	20:p:104:PHE:HE1	1.86	0.41
9:N:289:ASN:HA	9:N:292:PHE:CE2	2.55	0.41
12:X:52:MET:HG2	23:t:24:ARG:HH21	1.86	0.41
14:Z:126:LYS:HE3	14:Z:126:LYS:HB3	1.90	0.41
22:s:56:ASP:OD1	22:s:56:ASP:N	2.54	0.41
34:9:175:TYR:CZ	42:h:38:PRO:HG3	2.56	0.41
37:c:88:THR:OG1	37:c:91:ASP:OD2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:d:135:LEU:HA	38:d:167:LYS:HB3	2.02	0.41
12:j:42:LEU:HD23	12:j:46:ASP:HB3	2.02	0.41
3:H:165:LEU:HD21	3:H:241:LEU:HD12	2.02	0.41
5:J:27:ILE:H	5:J:27:ILE:HG13	1.76	0.41
7:L:66:TRP:HZ3	46:L:1002:PC1:H2B2	1.86	0.41
7:L:142:ILE:HG12	8:M:370:PRO:HB2	2.03	0.41
11:W:143:ASN:HD22	16:l:29:PRO:HB3	1.87	0.41
13:Y:1:PRO:HB2	13:Y:2:GLY:H	1.73	0.41
15:k:65:ASP:OD1	15:k:65:ASP:N	2.49	0.41
30:1:190:THR:HB	30:1:204:ARG:H	1.85	0.41
37:c:126:LYS:HD3	37:c:126:LYS:HA	1.83	0.41
16:l:50:ARG:O	16:l:54:GLU:CB	2.69	0.40
7:L:174:TYR:CD2	7:L:232:TRP:HB3	2.57	0.40
8:M:221:VAL:HA	8:M:283:LYS:HE3	2.02	0.40
8:M:430:PHE:HB2	8:M:433:GLU:HG3	2.03	0.40
8:M:446:LEU:HD23	8:M:446:LEU:HA	1.94	0.40
9:N:202:LEU:HD21	16:l:1:PRO:HD3	2.03	0.40
15:k:126:ARG:HH12	49:k:401:DGT:H2'A	1.85	0.40
16:l:79:LYS:HB3	16:l:79:LYS:HE2	1.88	0.40
23:t:25:HIS:O	23:t:29:ARG:HG2	2.21	0.40
26:w:85:MET:HB2	26:w:88:TRP:HB3	2.02	0.40
31:2:192:SER:OG	31:2:193:CYS:N	2.54	0.40
34:9:49:ASN:O	34:9:53:GLU:N	2.48	0.40
34:9:114:THR:HG21	34:9:144:HIS:CD2	2.56	0.40
1:4:141:PHE:O	1:4:145:THR:OG1	2.39	0.40
7:L:416:THR:O	7:L:419:THR:OG1	2.30	0.40
8:M:279:GLN:HG3	8:M:281:ASP:H	1.85	0.40
8:M:405:LEU:HD23	8:M:405:LEU:HA	1.98	0.40
15:k:30:ASN:N	15:k:33:SER:OG	2.52	0.40
22:s:3:HIS:CE1	25:v:127:PRO:HD3	2.57	0.40
32:3:224:LYS:NZ	33:5:198:ASP:OD2	2.47	0.40
38:d:153:GLU:HG3	38:d:165:ILE:HD13	2.03	0.40
9:N:311:MET:HE2	9:N:311:MET:HB2	1.96	0.40
18:n:34:LYS:HE2	18:n:34:LYS:HB2	1.73	0.40
34:9:132:VAL:HG21	34:9:165:ILE:HG21	2.02	0.40
1:4:350:LYS:HA	1:4:350:LYS:HD2	1.84	0.40
7:L:101:MET:HB3	7:L:118:PHE:HE2	1.86	0.40
13:Y:43:MET:HE2	44:q:72:PRO:HA	2.04	0.40
23:t:9:LEU:HD23	23:t:14:LYS:HG2	2.03	0.40
39:e:96:SER:OG	39:e:97:LYS:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4	416/463 (90%)	403 (97%)	13 (3%)	0	100	100
2	A	99/115 (86%)	96 (97%)	3 (3%)	0	100	100
3	H	304/318 (96%)	299 (98%)	5 (2%)	0	100	100
4	6	154/223 (69%)	150 (97%)	4 (3%)	0	100	100
5	J	165/175 (94%)	153 (93%)	12 (7%)	0	100	100
6	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
7	L	604/606 (100%)	578 (96%)	26 (4%)	0	100	100
8	M	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
9	N	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
10	V	139/141 (99%)	139 (100%)	0	0	100	100
11	W	137/189 (72%)	136 (99%)	1 (1%)	0	100	100
12	X	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
12	j	80/87 (92%)	76 (95%)	4 (5%)	0	100	100
13	Y	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
14	Z	169/175 (97%)	168 (99%)	1 (1%)	0	100	100
15	k	317/355 (89%)	306 (96%)	11 (4%)	0	100	100
16	l	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
17	m	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
18	n	77/98 (79%)	75 (97%)	2 (3%)	0	100	100
19	o	118/122 (97%)	117 (99%)	1 (1%)	0	100	100
20	p	126/130 (97%)	122 (97%)	4 (3%)	0	100	100
21	r	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
22	s	120/137 (88%)	117 (98%)	3 (2%)	0	100	100
23	t	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
24	u	63/108 (58%)	61 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	v	153/186 (82%)	147 (96%)	6 (4%)	0	100	100
26	w	99/154 (64%)	94 (95%)	5 (5%)	0	100	100
27	x	47/76 (62%)	47 (100%)	0	0	100	100
28	y	48/58 (83%)	46 (96%)	2 (4%)	0	100	100
29	z	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
30	1	428/464 (92%)	417 (97%)	11 (3%)	0	100	100
31	2	211/246 (86%)	198 (94%)	13 (6%)	0	100	100
32	3	686/727 (94%)	667 (97%)	19 (3%)	0	100	100
33	5	206/266 (77%)	199 (97%)	7 (3%)	0	100	100
34	9	174/217 (80%)	167 (96%)	7 (4%)	0	100	100
35	a	42/109 (38%)	42 (100%)	0	0	100	100
36	b	93/124 (75%)	92 (99%)	1 (1%)	0	100	100
37	c	124/170 (73%)	121 (98%)	3 (2%)	0	100	100
38	d	285/380 (75%)	278 (98%)	7 (2%)	0	100	100
39	e	84/99 (85%)	81 (96%)	3 (4%)	0	100	100
40	f	111/116 (96%)	109 (98%)	2 (2%)	0	100	100
41	g	112/140 (80%)	106 (95%)	6 (5%)	0	100	100
42	h	92/113 (81%)	90 (98%)	2 (2%)	0	100	100
43	i	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
44	q	137/144 (95%)	134 (98%)	3 (2%)	0	100	100
All	All	8034/9105 (88%)	7798 (97%)	236 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	4	364/391 (93%)	364 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	94/103 (91%)	94 (100%)	0	100	100
3	H	269/278 (97%)	269 (100%)	0	100	100
4	6	132/181 (73%)	132 (100%)	0	100	100
5	J	138/144 (96%)	138 (100%)	0	100	100
6	K	86/86 (100%)	86 (100%)	0	100	100
7	L	538/538 (100%)	538 (100%)	0	100	100
8	M	411/411 (100%)	411 (100%)	0	100	100
9	N	315/315 (100%)	315 (100%)	0	100	100
10	V	101/101 (100%)	101 (100%)	0	100	100
11	W	122/160 (76%)	122 (100%)	0	100	100
12	X	80/80 (100%)	80 (100%)	0	100	100
12	j	76/80 (95%)	76 (100%)	0	100	100
13	Y	154/154 (100%)	154 (100%)	0	100	100
14	Z	155/157 (99%)	155 (100%)	0	100	100
15	k	283/309 (92%)	283 (100%)	0	100	100
16	l	94/95 (99%)	94 (100%)	0	100	100
17	m	69/72 (96%)	69 (100%)	0	100	100
18	n	61/76 (80%)	61 (100%)	0	100	100
19	o	107/109 (98%)	107 (100%)	0	100	100
20	p	114/116 (98%)	114 (100%)	0	100	100
21	r	95/122 (78%)	95 (100%)	0	100	100
22	s	110/120 (92%)	110 (100%)	0	100	100
23	t	159/161 (99%)	159 (100%)	0	100	100
24	u	59/84 (70%)	59 (100%)	0	100	100
25	v	140/160 (88%)	140 (100%)	0	100	100
26	w	92/130 (71%)	92 (100%)	0	100	100
27	x	44/67 (66%)	44 (100%)	0	100	100
28	y	46/54 (85%)	46 (100%)	0	100	100
29	z	59/59 (100%)	58 (98%)	1 (2%)	53	75
30	1	344/368 (94%)	344 (100%)	0	100	100
31	2	183/210 (87%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	3	578/608 (95%)	578 (100%)	0	100	100
33	5	189/230 (82%)	189 (100%)	0	100	100
34	9	151/179 (84%)	151 (100%)	0	100	100
35	a	43/93 (46%)	43 (100%)	0	100	100
36	b	79/97 (81%)	79 (100%)	0	100	100
37	c	113/150 (75%)	113 (100%)	0	100	100
38	d	252/326 (77%)	252 (100%)	0	100	100
39	e	76/82 (93%)	76 (100%)	0	100	100
40	f	101/102 (99%)	101 (100%)	0	100	100
41	g	107/124 (86%)	107 (100%)	0	100	100
42	h	83/94 (88%)	83 (100%)	0	100	100
43	i	131/131 (100%)	131 (100%)	0	100	100
44	q	119/122 (98%)	119 (100%)	0	100	100
All	All	7116/7829 (91%)	7115 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	z	31	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	4	149	ASN
1	4	150	HIS
1	4	217	ASN
1	4	252	ASN
1	4	273	GLN
5	J	175	ASN
6	K	50	ASN
6	K	97	GLN
7	L	23	ASN
7	L	135	ASN
7	L	192	ASN
7	L	199	GLN
7	L	296	ASN

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Mol	Chain	Res	Type
7	L	447	ASN
7	L	479	GLN
8	M	144	ASN
8	M	251	ASN
8	M	304	GLN
8	M	338	HIS
8	M	366	ASN
8	M	422	HIS
9	N	63	GLN
9	N	77	ASN
9	N	289	ASN
9	N	316	GLN
10	V	78	GLN
13	Y	34	GLN
15	k	153	ASN
15	k	288	GLN
20	p	78	ASN
20	p	116	GLN
21	r	66	HIS
21	r	88	HIS
22	s	75	ASN
23	t	52	ASN
25	v	55	GLN
25	v	66	HIS
25	v	99	ASN
25	v	126	GLN
25	v	137	ASN
27	x	46	ASN
28	y	30	ASN
29	z	31	ASN
30	1	116	HIS
30	1	264	ASN
30	1	421	HIS
30	1	438	GLN
31	2	159	ASN
31	2	214	GLN
32	3	237	ASN
32	3	430	GLN
32	3	621	ASN
32	3	629	ASN
32	3	644	GLN
32	3	655	GLN

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Mol	Chain	Res	Type
33	5	95	ASN
33	5	160	HIS
36	b	36	ASN
38	d	36	ASN
38	d	184	ASN
38	d	321	HIS
39	e	47	ASN
40	f	52	ASN
40	f	82	GLN
12	j	35	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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$
1	2MR	4	85	1	10,12,13	0.18	0	5,13,15	0.21	0
6	FME	K	1	6	8,9,10	0.97	0	7,9,11	0.71	0
15	SEP	k	36	15	8,9,10	0.28	0	8,12,14	1.04	1 (12%)
8	FME	M	1	8	8,9,10	0.93	0	7,9,11	0.90	0
7	FME	L	1	7	8,9,10	0.93	0	7,9,11	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MR	4	85	1	-	0/10/13/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FME	K	1	6	-	4/7/9/11	-
15	SEP	k	36	15	-	0/5/8/10	-
8	FME	M	1	8	-	4/7/9/11	-
7	FME	L	1	7	-	1/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	k	36	SEP	P-OG-CB	2.69	125.72	118.30

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	1	FME	O1-CN-N-CA
7	L	1	FME	CA-CB-CG-SD
8	M	1	FME	CB-CA-N-CN
8	M	1	FME	C-CA-CB-CG
8	M	1	FME	O-C-CA-CB
6	K	1	FME	CA-CB-CG-SD
6	K	1	FME	CB-CG-SD-CE
6	K	1	FME	CB-CA-N-CN
8	M	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 3 are monoatomic - leaving 36 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
46	PC1	4	502	-	53,53,53	0.30	0	59,61,61	0.45	0
46	PC1	M	502	-	53,53,53	0.29	0	59,61,61	0.29	0
45	3PE	V	201	-	34,34,50	0.36	0	37,39,55	0.31	0
49	DGT	k	401	50	29,33,33	0.30	0	44,52,52	0.34	0
45	3PE	4	501	-	39,39,50	0.33	0	42,44,55	0.34	0
58	NDP	d	401	-	49,52,52	0.35	0	66,80,80	0.34	0
45	3PE	p	201	-	26,26,50	0.48	0	30,31,55	0.53	1 (3%)
45	3PE	K	101	-	39,39,50	0.34	0	42,44,55	0.36	0
48	SF4	3	801	32	0,12,12	-	-	-		
48	SF4	1	501	30	0,12,12	-	-	-		
48	SF4	9	202	34	0,12,12	-	-	-		
45	3PE	N	401	-	50,50,50	0.32	0	53,55,55	0.47	0
54	NAI	1	503	-	45,48,48	0.33	0	60,73,73	0.37	0
46	PC1	M	503	-	53,53,53	0.29	0	59,61,61	0.34	0
46	PC1	A	201	-	36,36,53	0.37	0	42,44,61	0.53	0
45	3PE	V	202	-	36,36,50	0.35	0	39,41,55	0.32	0
52	ZMP	t	201	-	24,30,36	0.78	1 (4%)	29,37,45	0.88	2 (6%)
45	3PE	H	401	-	50,50,50	0.31	0	53,55,55	0.32	0
46	PC1	L	1002	-	53,53,53	0.31	0	59,61,61	0.55	2 (3%)
55	FES	2	300	31	0,4,4	-	-	-		
48	SF4	3	802	32	0,12,12	-	-	-		
45	3PE	L	1001	-	50,50,50	0.30	0	53,55,55	0.31	0
48	SF4	9	201	34	0,12,12	-	-	-		
52	ZMP	j	201	-	27,33,36	0.65	1 (3%)	32,40,45	1.09	3 (9%)
53	FMN	1	502	-	33,33,33	0.28	0	48,50,50	0.42	0
47	A1JBT	H	402	-	31,33,33	0.27	0	31,49,49	0.60	0
48	SF4	6	201	4	0,12,12	-	-	-		
45	3PE	i	201	-	50,50,50	0.30	0	53,55,55	0.26	0
45	3PE	6	203	-	50,50,50	0.31	0	53,55,55	0.29	0
45	3PE	L	1003	-	30,30,50	0.40	0	33,35,55	0.73	1 (3%)
45	3PE	A	202	-	50,50,50	0.30	0	53,55,55	0.30	0
55	FES	3	803	32	0,4,4	-	-	-		
45	3PE	M	501	-	43,43,50	0.32	0	46,48,55	0.33	0
45	3PE	o	501	-	30,30,50	0.38	0	33,35,55	0.35	0
51	MYR	s	201	22	14,14,15	0.20	0	13,13,15	0.17	0
46	PC1	6	202	-	45,45,53	0.32	0	51,53,61	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PC1	4	502	-	-	10/57/57/57	-
46	PC1	M	502	-	-	14/57/57/57	-
45	3PE	V	201	-	-	6/38/38/54	-
49	DGT	k	401	50	-	1/22/34/34	0/3/3/3
45	3PE	4	501	-	-	8/43/43/54	-
58	NDP	d	401	-	-	6/34/77/77	0/5/5/5
45	3PE	p	201	-	-	3/27/27/54	-
45	3PE	K	101	-	-	6/43/43/54	-
48	SF4	3	801	32	-	-	0/6/5/5
48	SF4	1	501	30	-	-	0/6/5/5
48	SF4	9	202	34	-	-	0/6/5/5
45	3PE	N	401	-	-	11/54/54/54	-
54	NAI	1	503	-	-	5/29/72/72	0/5/5/5
46	PC1	M	503	-	-	6/57/57/57	-
46	PC1	A	201	-	-	11/40/40/57	-
45	3PE	V	202	-	-	8/40/40/54	-
52	ZMP	t	201	-	-	16/35/37/43	-
45	3PE	H	401	-	-	14/54/54/54	-
46	PC1	L	1002	-	-	15/57/57/57	-
55	FES	2	300	31	-	-	0/1/1/1
48	SF4	3	802	32	-	-	0/6/5/5
45	3PE	L	1001	-	-	13/54/54/54	-
48	SF4	9	201	34	-	-	0/6/5/5
52	ZMP	j	201	-	-	4/38/40/43	-
53	FMN	1	502	-	-	8/18/18/18	0/3/3/3
47	A1JBT	H	402	-	-	6/8/29/29	0/5/5/5
48	SF4	6	201	4	-	-	0/6/5/5
45	3PE	i	201	-	-	9/54/54/54	-
45	3PE	6	203	-	-	9/54/54/54	-
45	3PE	L	1003	-	-	8/34/34/54	-
45	3PE	A	202	-	-	16/54/54/54	-
55	FES	3	803	32	-	-	0/1/1/1
45	3PE	M	501	-	-	11/47/47/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	o	501	-	-	6/34/34/54	-
51	MYR	s	201	22	-	1/11/12/13	-
46	PC1	6	202	-	-	9/49/49/57	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	t	201	ZMP	C9-C10	2.58	1.53	1.50
52	j	201	ZMP	C9-C10	2.30	1.53	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	j	201	ZMP	O1-C10-C9	-2.63	120.88	123.99
52	t	201	ZMP	O1-C10-C9	-2.32	121.24	123.99
52	j	201	ZMP	C15-C14-C13	-2.26	108.60	112.36
46	L	1002	PC1	O21-C2-C1	2.23	116.48	108.40
46	L	1002	PC1	C2-O21-C21	2.23	123.27	117.79
45	p	201	3PE	O12-P-O14	2.13	119.04	110.68
52	t	201	ZMP	C15-C14-C13	-2.09	108.87	112.36
45	L	1003	3PE	C2-O21-C21	2.09	122.93	117.79
52	j	201	ZMP	C14-C15-N2	-2.08	107.69	111.90

There are no chirality outliers.

All (240) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	4	501	3PE	C1-O11-P-O12
45	4	501	3PE	C1-O11-P-O13
45	4	501	3PE	C1-O11-P-O14
45	4	501	3PE	C11-O13-P-O12
45	A	202	3PE	C1-O11-P-O12
45	A	202	3PE	C1-O11-P-O14
45	A	202	3PE	C11-O13-P-O12
45	H	401	3PE	C11-O13-P-O14
45	H	401	3PE	O13-C11-C12-N
45	6	203	3PE	C1-O11-P-O12
45	6	203	3PE	C1-O11-P-O14
45	6	203	3PE	C11-O13-P-O12
45	6	203	3PE	C11-O13-P-O14
45	6	203	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
45	K	101	3PE	C1-O11-P-O12
45	K	101	3PE	C1-O11-P-O14
45	K	101	3PE	O13-C11-C12-N
45	L	1001	3PE	C1-O11-P-O12
45	L	1001	3PE	C11-O13-P-O14
45	L	1003	3PE	O13-C11-C12-N
45	M	501	3PE	C1-O11-P-O12
45	M	501	3PE	C1-O11-P-O13
45	M	501	3PE	C1-O11-P-O14
45	N	401	3PE	C1-O11-P-O12
45	V	201	3PE	C11-O13-P-O14
45	o	501	3PE	C11-O13-P-O14
45	o	501	3PE	O13-C11-C12-N
45	i	201	3PE	C1-O11-P-O12
45	i	201	3PE	C1-O11-P-O13
45	i	201	3PE	C1-O11-P-O14
46	4	502	PC1	C11-O13-P-O12
46	4	502	PC1	C1-O11-P-O12
46	A	201	PC1	C11-O13-P-O14
46	6	202	PC1	C11-O13-P-O12
46	6	202	PC1	C1-O11-P-O14
46	L	1002	PC1	C11-O13-P-O14
46	L	1002	PC1	C1-O11-P-O12
46	M	502	PC1	C11-O13-P-O12
46	M	502	PC1	C11-O13-P-O14
47	H	402	A1JBT	C1-C-C2-N
47	H	402	A1JBT	C2-C-C8-C16
47	H	402	A1JBT	C1-C-C8-C16
47	H	402	A1JBT	C2-C-C8-C9
47	H	402	A1JBT	C1-C-C8-C9
52	t	201	ZMP	C16-C17-C18-C21
52	t	201	ZMP	C17-C16-N2-C15
52	j	201	ZMP	S1-C11-C12-N1
52	j	201	ZMP	O1-C10-S1-C11
52	j	201	ZMP	C9-C10-S1-C11
53	1	502	FMN	N10-C1'-C2'-O2'
53	1	502	FMN	N10-C1'-C2'-C3'
53	1	502	FMN	C5'-O5'-P-O1P
53	1	502	FMN	C5'-O5'-P-O2P
53	1	502	FMN	C5'-O5'-P-O3P
54	1	503	NAI	C5B-O5B-PA-O3
52	t	201	ZMP	O3-C16-N2-C15

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Mol	Chain	Res	Type	Atoms
46	L	1002	PC1	C2-C1-O11-P
45	4	501	3PE	C11-O13-P-O11
45	A	202	3PE	C1-O11-P-O13
45	H	401	3PE	C1-O11-P-O13
45	H	401	3PE	C11-O13-P-O11
45	6	203	3PE	C1-O11-P-O13
45	6	203	3PE	C11-O13-P-O11
45	K	101	3PE	C1-O11-P-O13
45	L	1001	3PE	C1-O11-P-O13
45	L	1001	3PE	C11-O13-P-O11
45	L	1003	3PE	C11-O13-P-O11
45	V	201	3PE	C11-O13-P-O11
45	V	202	3PE	C1-O11-P-O13
45	i	201	3PE	C11-O13-P-O11
46	4	502	PC1	C11-O13-P-O11
46	4	502	PC1	C1-O11-P-O13
46	M	502	PC1	C11-O13-P-O11
45	N	401	3PE	C21-C22-C23-C24
45	i	201	3PE	C29-C2A-C2B-C2C
52	t	201	ZMP	C3-C4-C5-C6
46	L	1002	PC1	C38-C39-C3A-C3B
45	M	501	3PE	C32-C33-C34-C35
45	A	202	3PE	C2C-C2D-C2E-C2F
45	6	203	3PE	C23-C24-C25-C26
46	6	202	PC1	C23-C24-C25-C26
45	A	202	3PE	C2E-C2F-C2G-C2H
46	A	201	PC1	C11-C12-N-C13
46	M	502	PC1	C11-C12-N-C14
45	V	201	3PE	C31-C32-C33-C34
46	M	502	PC1	C3A-C3B-C3C-C3D
46	M	503	PC1	C3E-C3F-C3G-C3H
46	A	201	PC1	C11-C12-N-C15
46	6	202	PC1	C1-O11-P-O13
46	L	1002	PC1	C1-O11-P-O13
52	t	201	ZMP	O3-C16-C17-O4
46	M	503	PC1	C28-C29-C2A-C2B
46	A	201	PC1	C11-C12-N-C14
46	M	502	PC1	C11-C12-N-C13
52	t	201	ZMP	C5-C6-C7-C8
45	6	203	3PE	C2A-C2B-C2C-C2D
45	M	501	3PE	O11-C1-C2-C3
45	A	202	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
45	M	501	3PE	O13-C11-C12-N
46	L	1002	PC1	C31-C32-C33-C34
52	t	201	ZMP	S1-C11-C12-N1
46	M	502	PC1	C11-C12-N-C15
45	o	501	3PE	C11-O13-P-O11
46	L	1002	PC1	C11-O13-P-O11
46	M	503	PC1	C2A-C2B-C2C-C2D
46	L	1002	PC1	C3A-C3B-C3C-C3D
45	K	101	3PE	C2-C1-O11-P
45	V	202	3PE	C2-C1-O11-P
46	A	201	PC1	O21-C21-C22-C23
52	t	201	ZMP	O1-C10-S1-C11
46	L	1002	PC1	O11-C1-C2-C3
52	t	201	ZMP	C7-C8-C9-C10
58	d	401	NDP	C2B-O2B-P2B-O1X
46	4	502	PC1	C2A-C2B-C2C-C2D
46	L	1002	PC1	C21-C22-C23-C24
52	t	201	ZMP	C9-C10-S1-C11
45	H	401	3PE	C2-C1-O11-P
45	L	1003	3PE	C2-C1-O11-P
46	L	1002	PC1	O11-C1-C2-O21
52	t	201	ZMP	C16-C17-C18-C20
45	p	201	3PE	C22-C23-C24-C25
46	A	201	PC1	O31-C31-C32-C33
46	M	502	PC1	C25-C26-C27-C28
45	N	401	3PE	C1-O11-P-O13
46	A	201	PC1	C11-O13-P-O11
46	6	202	PC1	C11-O13-P-O11
45	M	501	3PE	C2-C1-O11-P
46	M	502	PC1	C2-C1-O11-P
45	H	401	3PE	C1-O11-P-O12
45	H	401	3PE	C1-O11-P-O14
45	H	401	3PE	C11-O13-P-O12
45	L	1001	3PE	C1-O11-P-O14
45	L	1003	3PE	C11-O13-P-O14
45	N	401	3PE	C1-O11-P-O14
45	V	202	3PE	C1-O11-P-O14
45	o	501	3PE	C11-O13-P-O12
45	i	201	3PE	C11-O13-P-O14
46	6	202	PC1	C11-O13-P-O14
46	L	1002	PC1	C1-O11-P-O14
54	1	503	NAI	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
45	H	401	3PE	C29-C2A-C2B-C2C
45	4	501	3PE	C12-C11-O13-P
45	L	1001	3PE	C12-C11-O13-P
45	V	201	3PE	C12-C11-O13-P
47	H	402	A1JBT	C-C2-N-C7
45	H	401	3PE	O11-C1-C2-O21
45	M	501	3PE	O11-C1-C2-O21
46	A	201	PC1	O11-C1-C2-O21
58	d	401	NDP	O4D-C1D-N1N-C6N
52	j	201	ZMP	C11-C12-N1-C13
46	4	502	PC1	O13-C11-C12-N
46	M	503	PC1	O13-C11-C12-N
51	s	201	MYR	C1-C2-C3-C4
52	t	201	ZMP	O4-C17-C18-C21
46	A	201	PC1	C22-C23-C24-C25
46	M	502	PC1	O31-C31-C32-C33
45	M	501	3PE	C11-O13-P-O11
45	V	202	3PE	C11-O13-P-O11
54	1	503	NAI	O4D-C1D-N1N-C2N
53	1	502	FMN	C2'-C3'-C4'-O4'
53	1	502	FMN	C4'-C5'-O5'-P
46	M	502	PC1	C39-C3A-C3B-C3C
45	N	401	3PE	O13-C11-C12-N
45	L	1003	3PE	O11-C1-C2-O21
45	M	501	3PE	C36-C37-C38-C39
45	H	401	3PE	C2F-C2G-C2H-C2I
45	A	202	3PE	O21-C2-C3-O31
46	6	202	PC1	O31-C31-C32-C33
45	L	1001	3PE	C35-C36-C37-C38
45	A	202	3PE	C1-C2-C3-O31
52	t	201	ZMP	C19-C18-C21-O5
46	4	502	PC1	C22-C23-C24-C25
45	L	1003	3PE	C1-C2-O21-C21
46	4	502	PC1	C3-C2-O21-C21
46	L	1002	PC1	C1-C2-O21-C21
45	L	1001	3PE	C3B-C3C-C3D-C3E
46	L	1002	PC1	C39-C3A-C3B-C3C
52	t	201	ZMP	C12-C11-S1-C10
54	1	503	NAI	C2D-C1D-N1N-C2N
45	K	101	3PE	C38-C39-C3A-C3B
46	M	503	PC1	C37-C38-C39-C3A
45	H	401	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
53	1	502	FMN	O3'-C3'-C4'-O4'
45	M	501	3PE	C31-C32-C33-C34
45	N	401	3PE	C22-C23-C24-C25
45	4	501	3PE	O31-C31-C32-C33
45	N	401	3PE	O31-C31-C32-C33
45	o	501	3PE	O31-C31-C32-C33
45	A	202	3PE	O21-C21-C22-C23
46	M	502	PC1	C3B-C3C-C3D-C3E
45	p	201	3PE	O21-C21-C22-C23
46	L	1002	PC1	O31-C31-C32-C33
45	N	401	3PE	C2C-C2D-C2E-C2F
45	N	401	3PE	C32-C33-C34-C35
45	L	1001	3PE	O31-C31-C32-C33
45	i	201	3PE	O21-C21-C22-C23
46	4	502	PC1	C31-C32-C33-C34
52	t	201	ZMP	C16-C17-C18-C19
45	A	202	3PE	O31-C31-C32-C33
45	L	1001	3PE	O21-C21-C22-C23
45	4	501	3PE	O21-C2-C3-O31
52	t	201	ZMP	O4-C17-C18-C19
58	d	401	NDP	C5D-O5D-PN-O3
45	i	201	3PE	O31-C31-C32-C33
45	V	202	3PE	C25-C26-C27-C28
46	A	201	PC1	O22-C21-C22-C23
45	A	202	3PE	C38-C39-C3A-C3B
45	A	202	3PE	O22-C21-C22-C23
46	6	202	PC1	C3B-C3C-C3D-C3E
49	k	401	DGT	O4'-C4'-C5'-O5'
58	d	401	NDP	O4B-C4B-C5B-O5B
45	V	201	3PE	C22-C23-C24-C25
45	L	1003	3PE	O21-C21-C22-C23
45	V	202	3PE	O31-C31-C32-C33
45	i	201	3PE	O22-C21-C22-C23
45	V	202	3PE	O32-C31-C32-C33
45	A	202	3PE	O32-C31-C32-C33
45	L	1001	3PE	O32-C31-C32-C33
46	M	502	PC1	C36-C37-C38-C39
45	o	501	3PE	O32-C31-C32-C33
45	p	201	3PE	O22-C21-C22-C23
45	H	401	3PE	C26-C27-C28-C29
45	A	202	3PE	C11-O13-P-O14
45	V	202	3PE	C1-O11-P-O12

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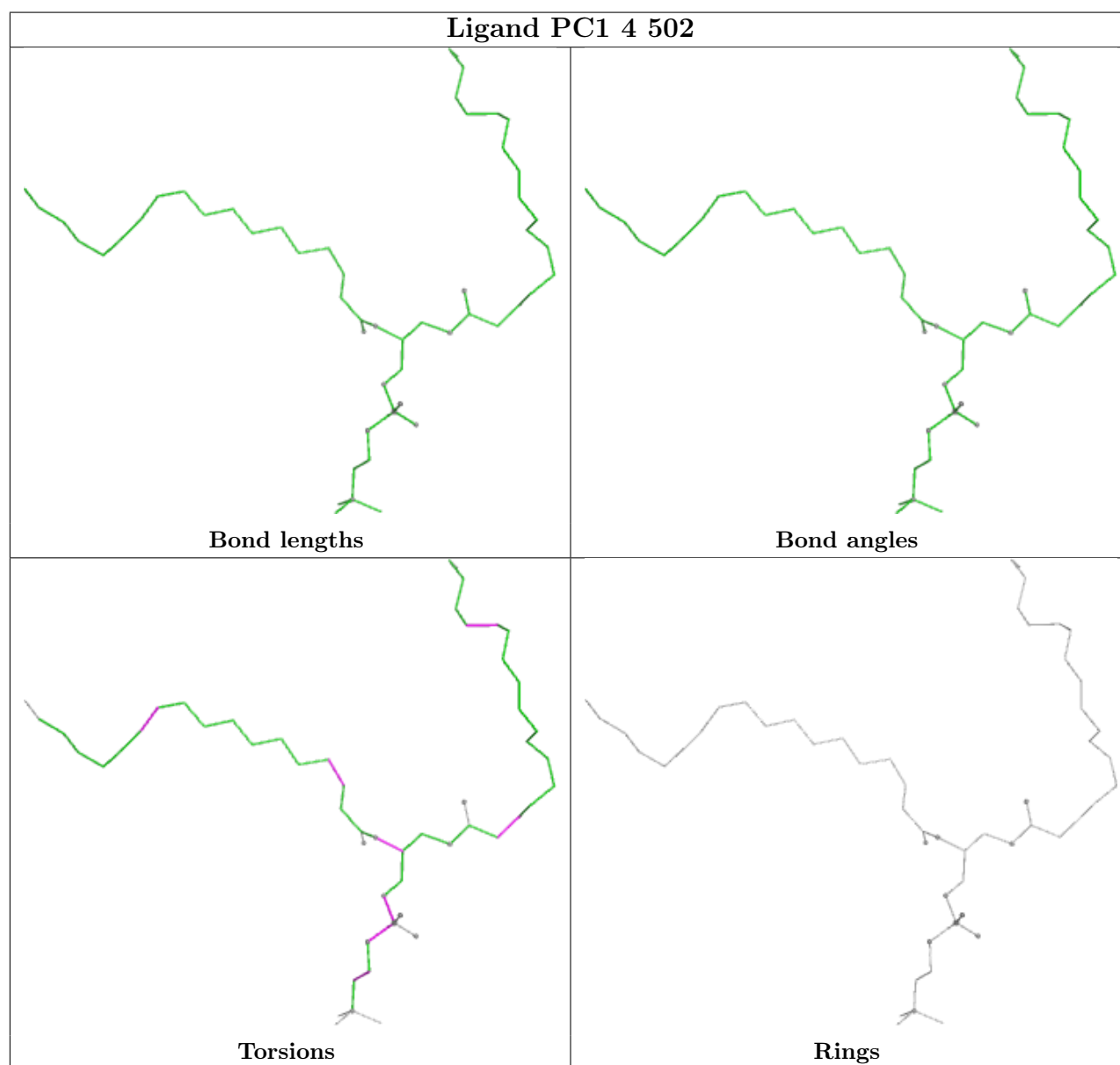
Mol	Chain	Res	Type	Atoms
46	6	202	PC1	C1-O11-P-O12
54	1	503	NAI	C5B-O5B-PA-O1A
58	d	401	NDP	C5D-O5D-PN-O2N
58	d	401	NDP	C2N-C3N-C7N-N7N
46	M	503	PC1	C31-C32-C33-C34
45	L	1001	3PE	O22-C21-C22-C23
45	N	401	3PE	O32-C31-C32-C33
46	M	502	PC1	C28-C29-C2A-C2B
45	V	201	3PE	O31-C31-C32-C33
45	A	202	3PE	C12-C11-O13-P
45	H	401	3PE	C12-C11-O13-P
45	N	401	3PE	C3-C2-O21-C21
46	A	201	PC1	C3-C2-O21-C21
45	L	1001	3PE	C23-C24-C25-C26
45	L	1003	3PE	O22-C21-C22-C23
46	4	502	PC1	C3C-C3D-C3E-C3F

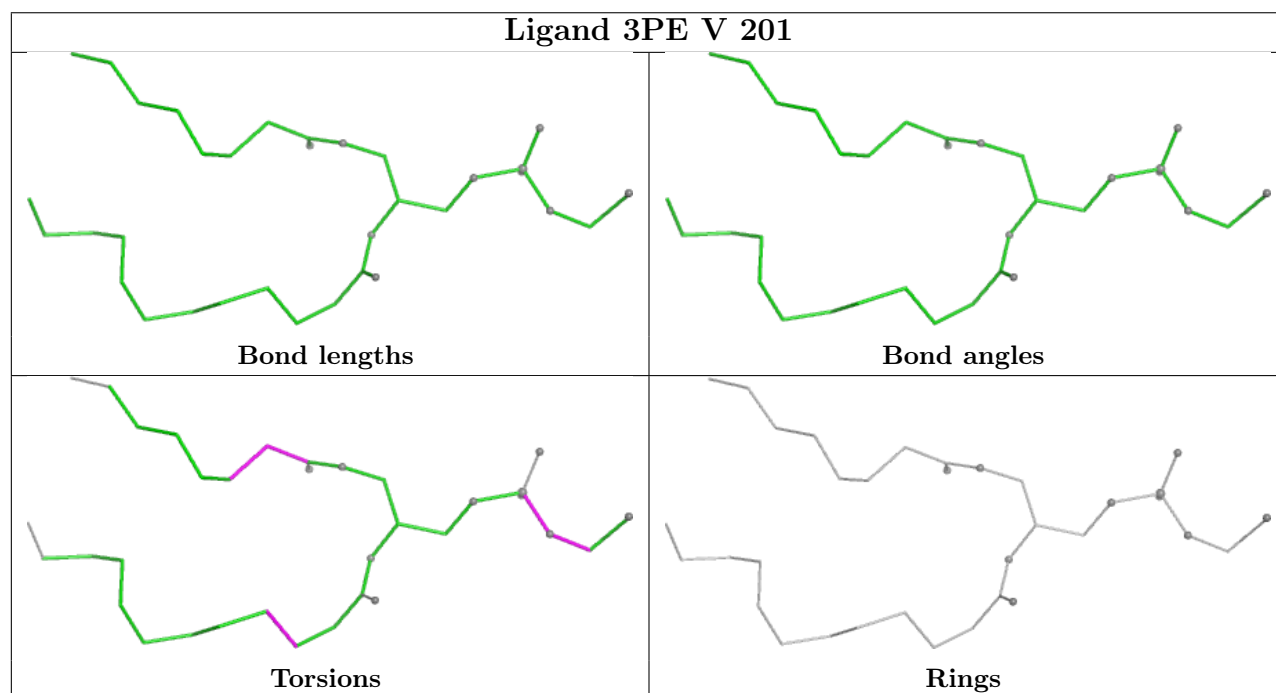
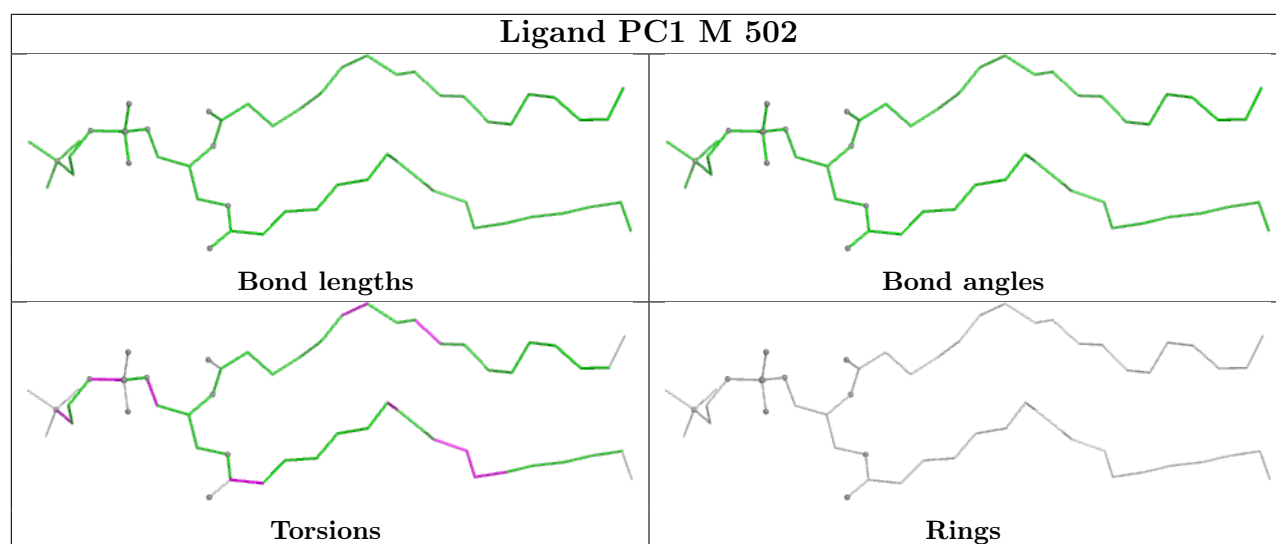
There are no ring outliers.

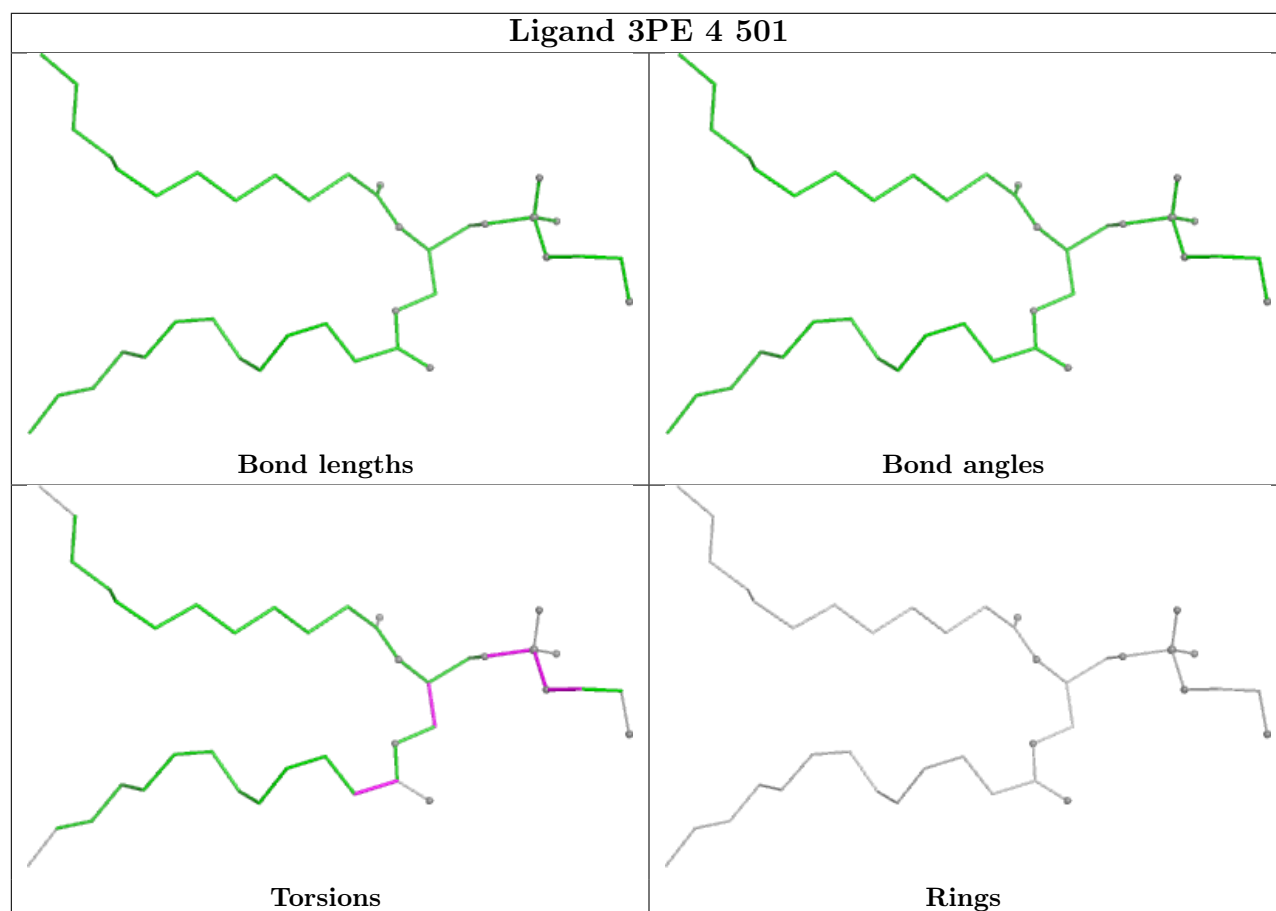
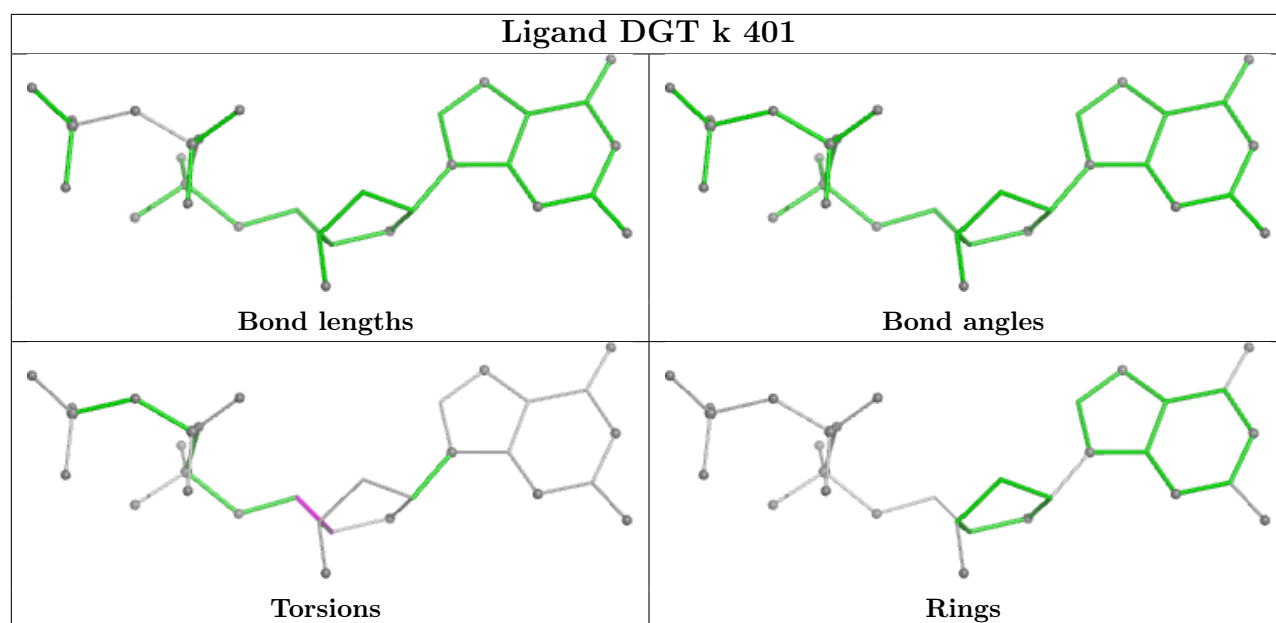
21 monomers are involved in 34 short contacts:

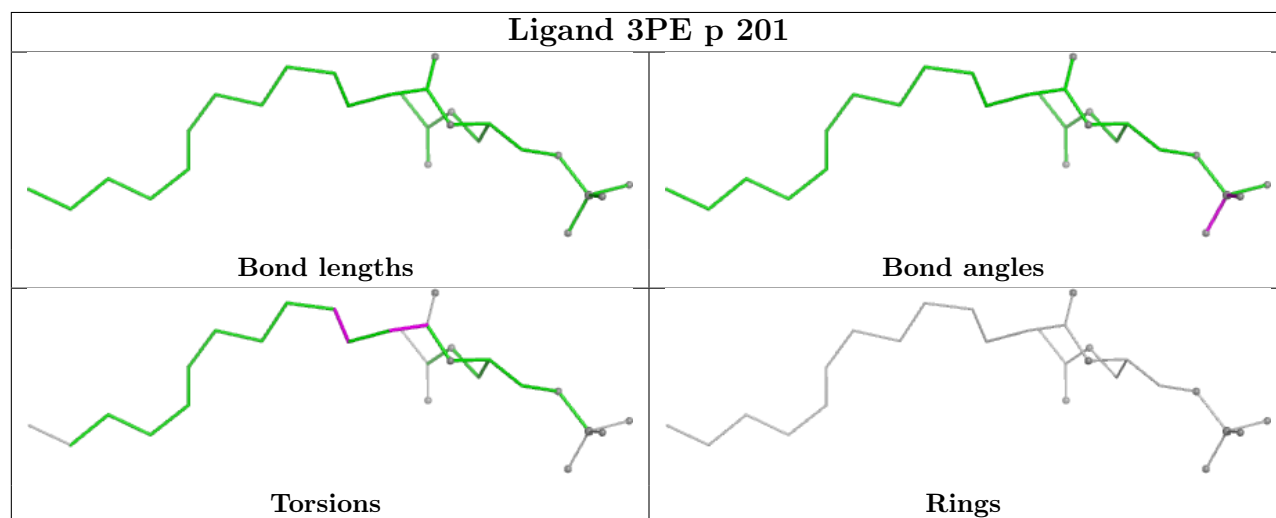
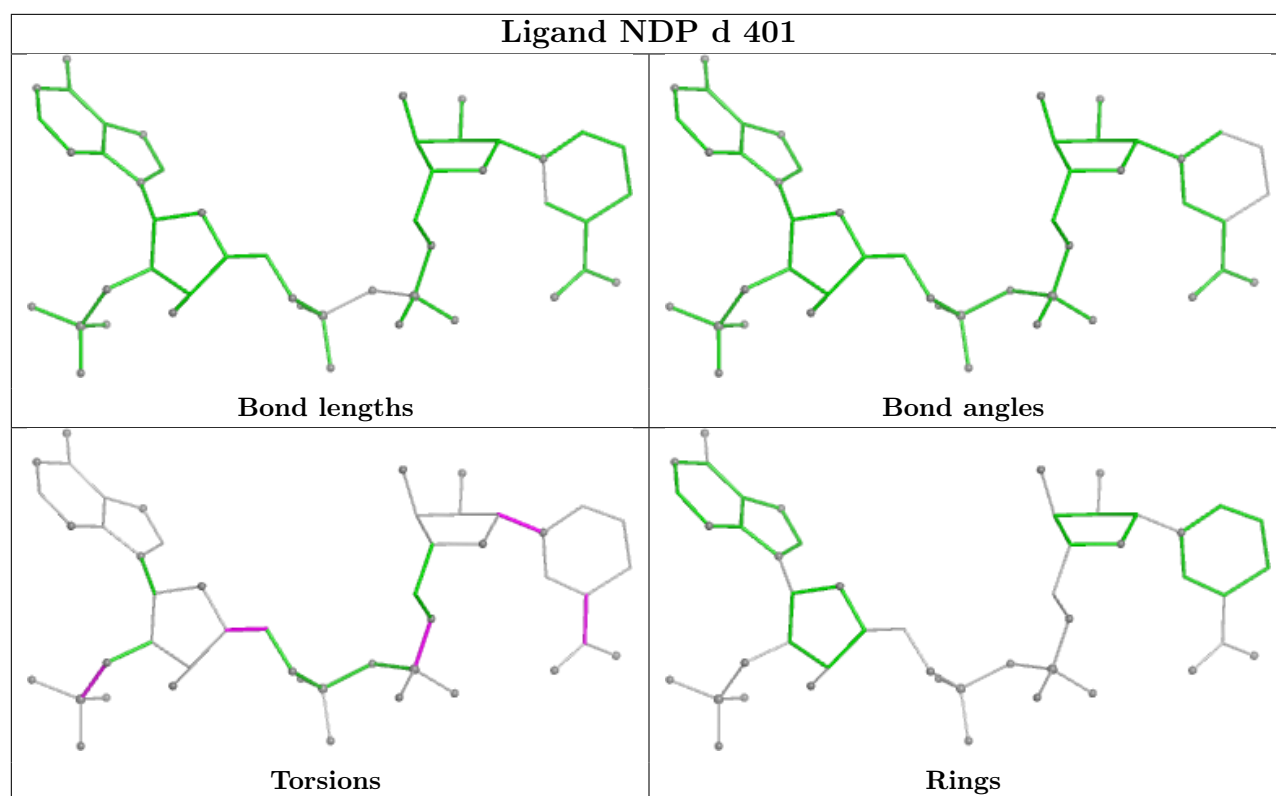
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	4	502	PC1	3	0
46	M	502	PC1	2	0
45	V	201	3PE	1	0
49	k	401	DGT	2	0
45	4	501	3PE	1	0
58	d	401	NDP	1	0
45	p	201	3PE	2	0
48	3	801	SF4	1	0
45	N	401	3PE	1	0
54	1	503	NAI	2	0
46	M	503	PC1	1	0
45	V	202	3PE	1	0
52	t	201	ZMP	2	0
45	H	401	3PE	1	0
46	L	1002	PC1	2	0
55	2	300	FES	1	0
45	L	1001	3PE	2	0
45	i	201	3PE	2	0
45	6	203	3PE	1	0
45	A	202	3PE	3	0
46	6	202	PC1	3	0

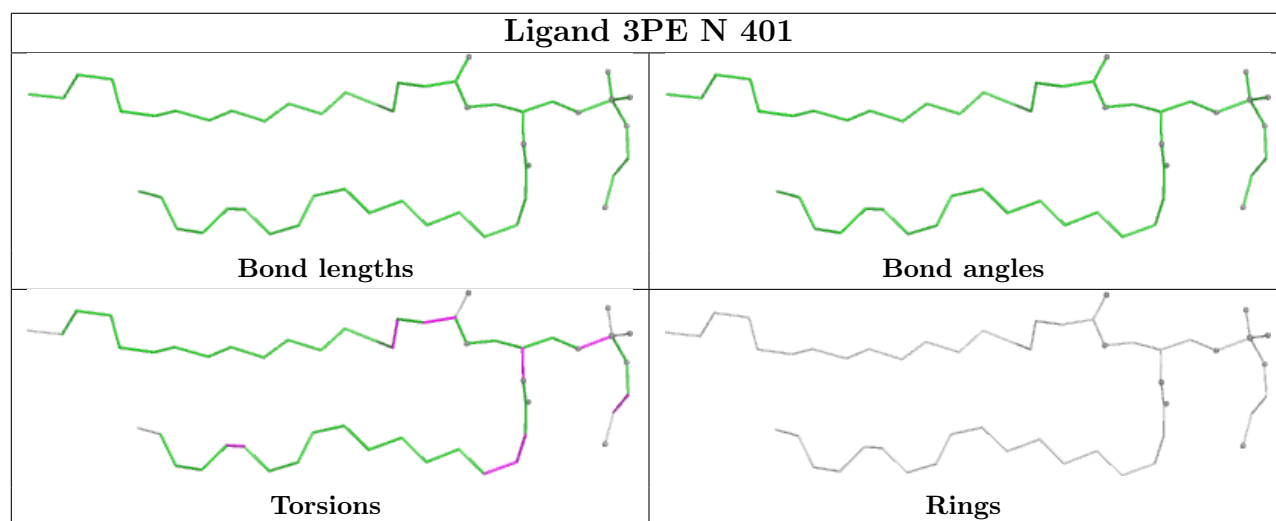
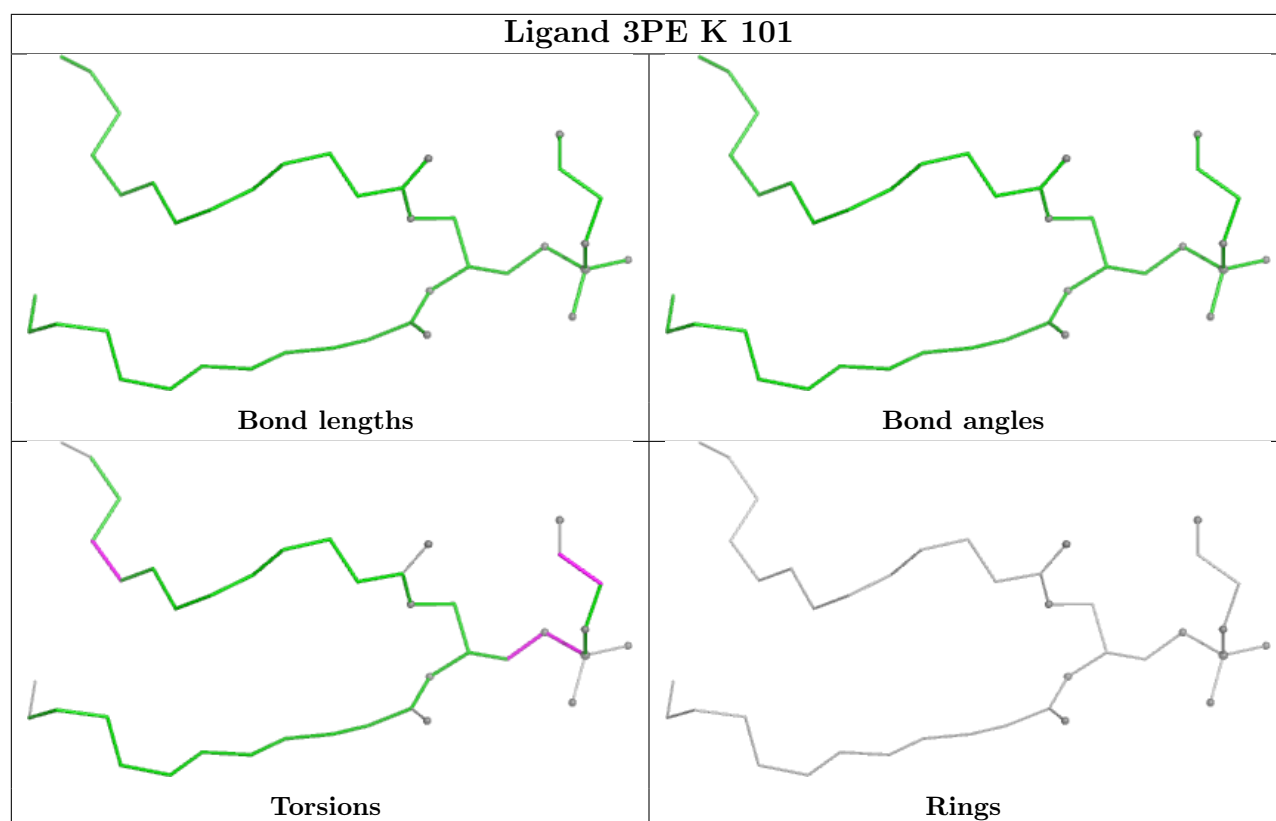
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

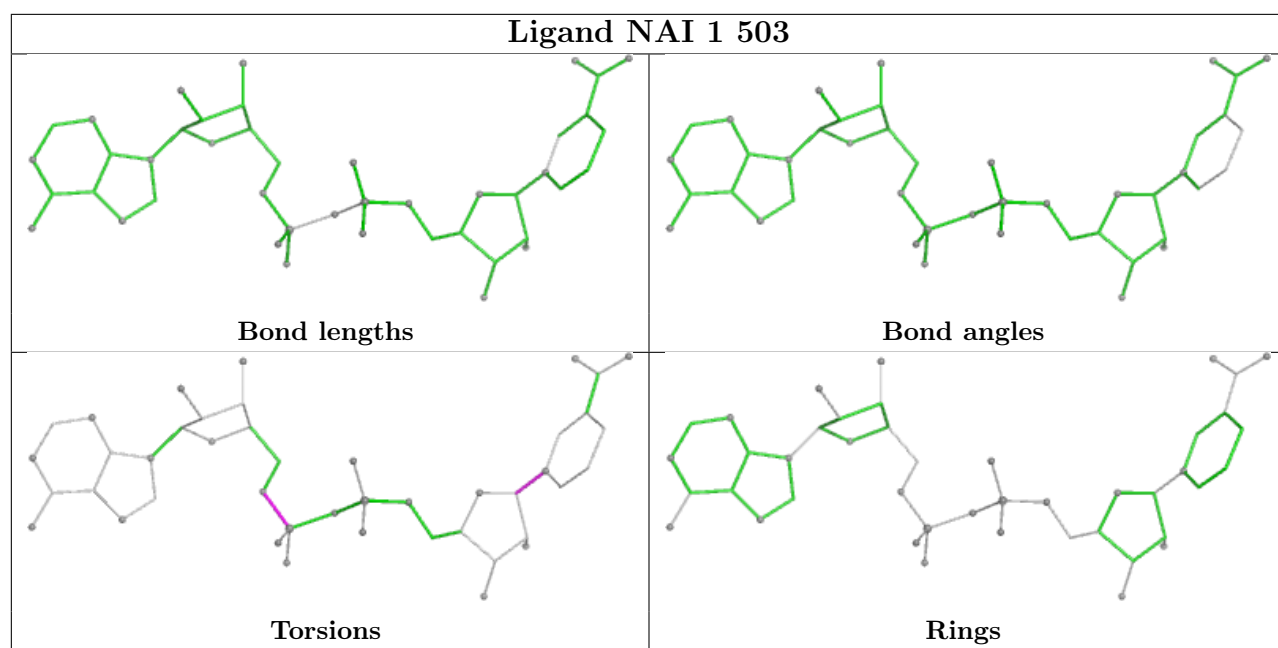


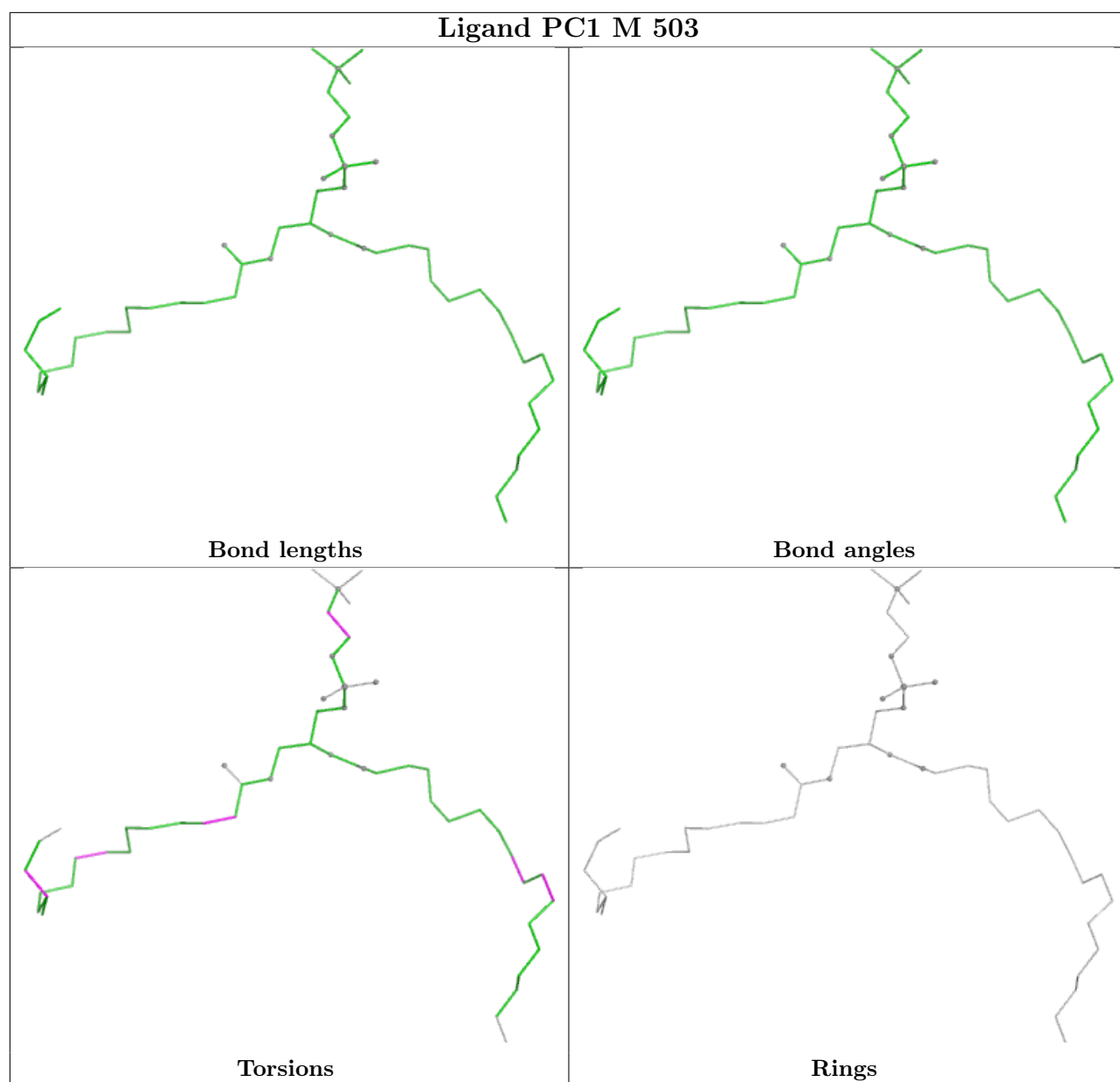


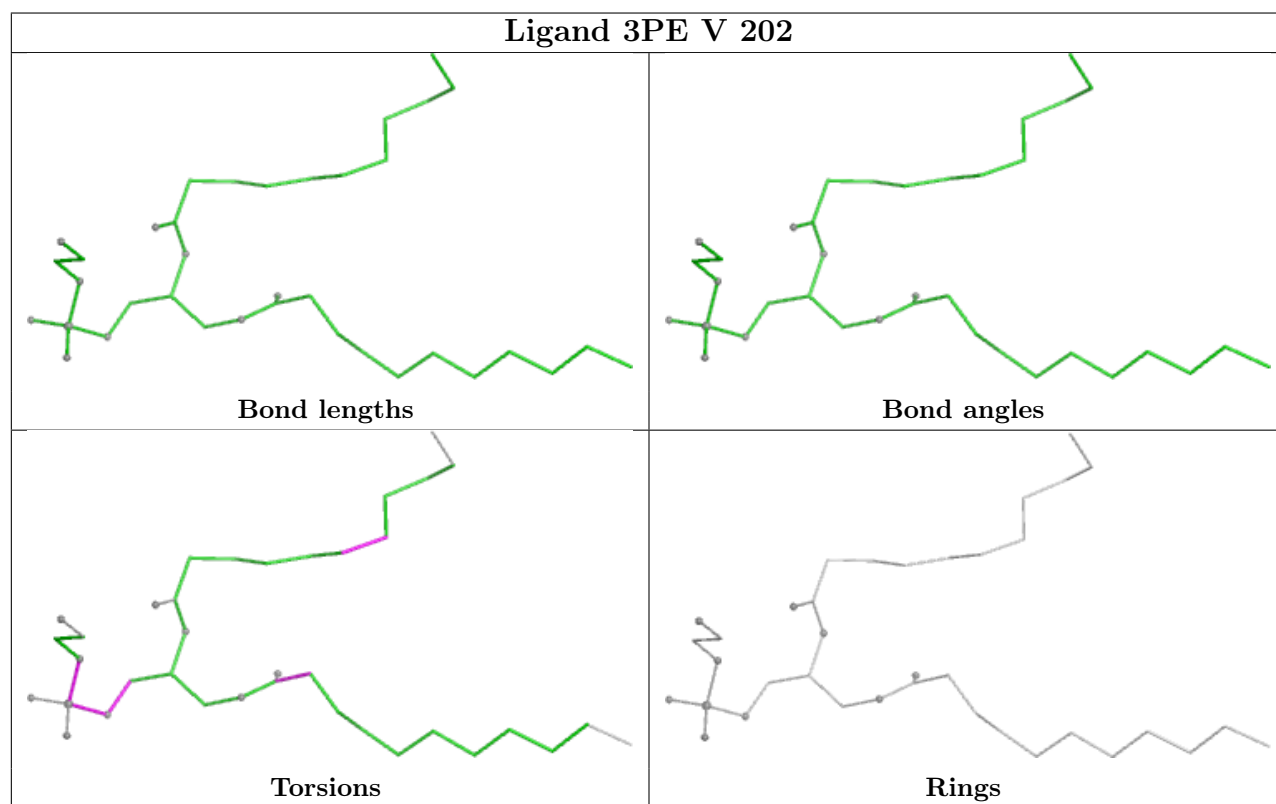
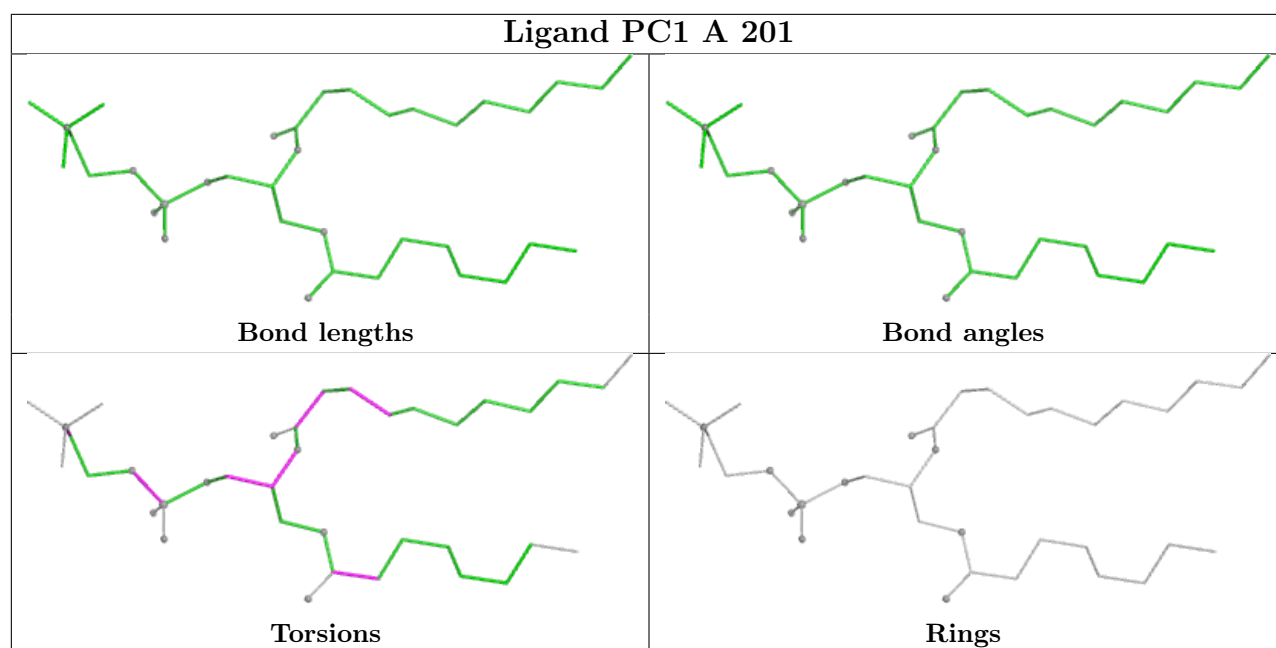


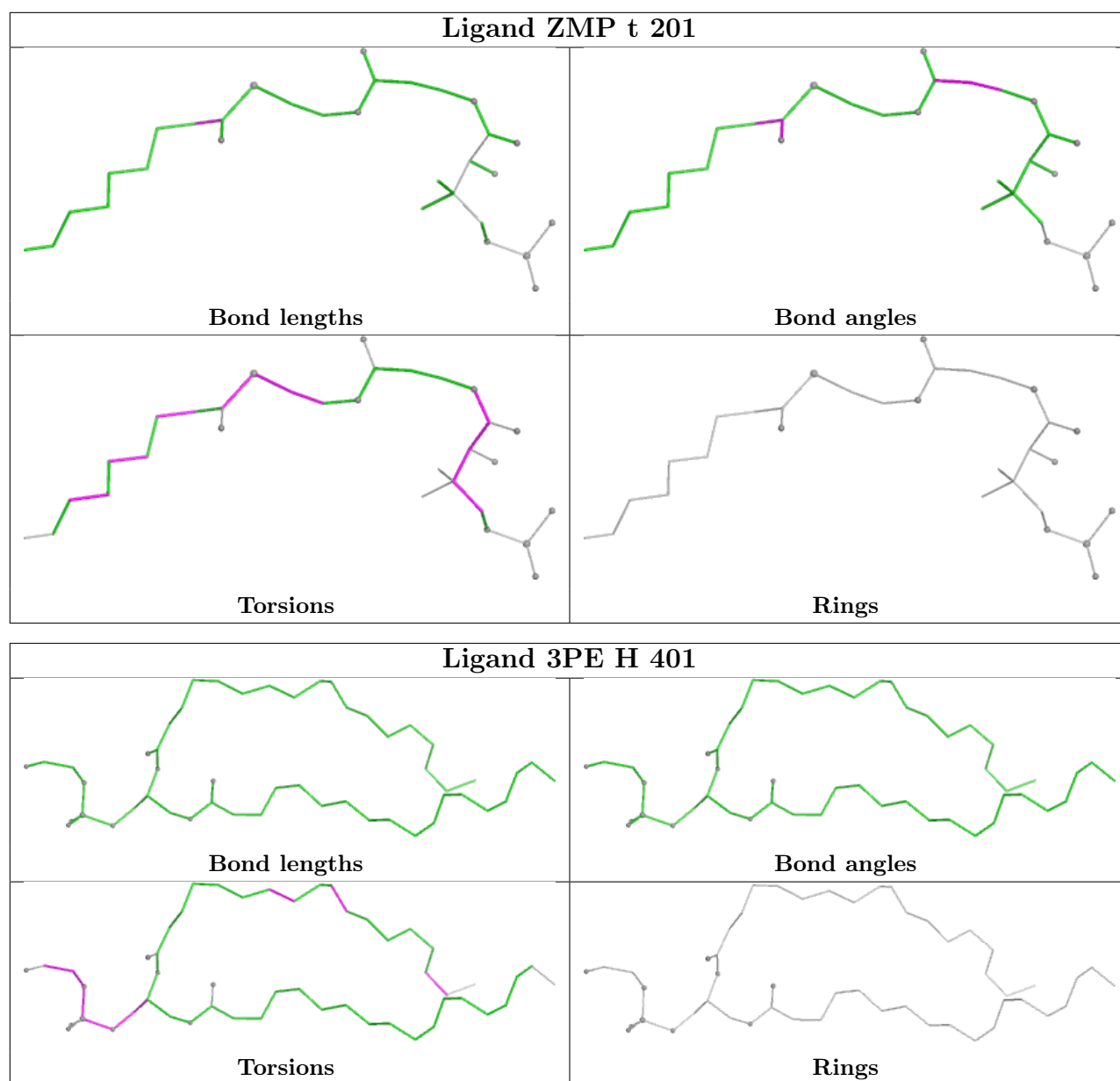


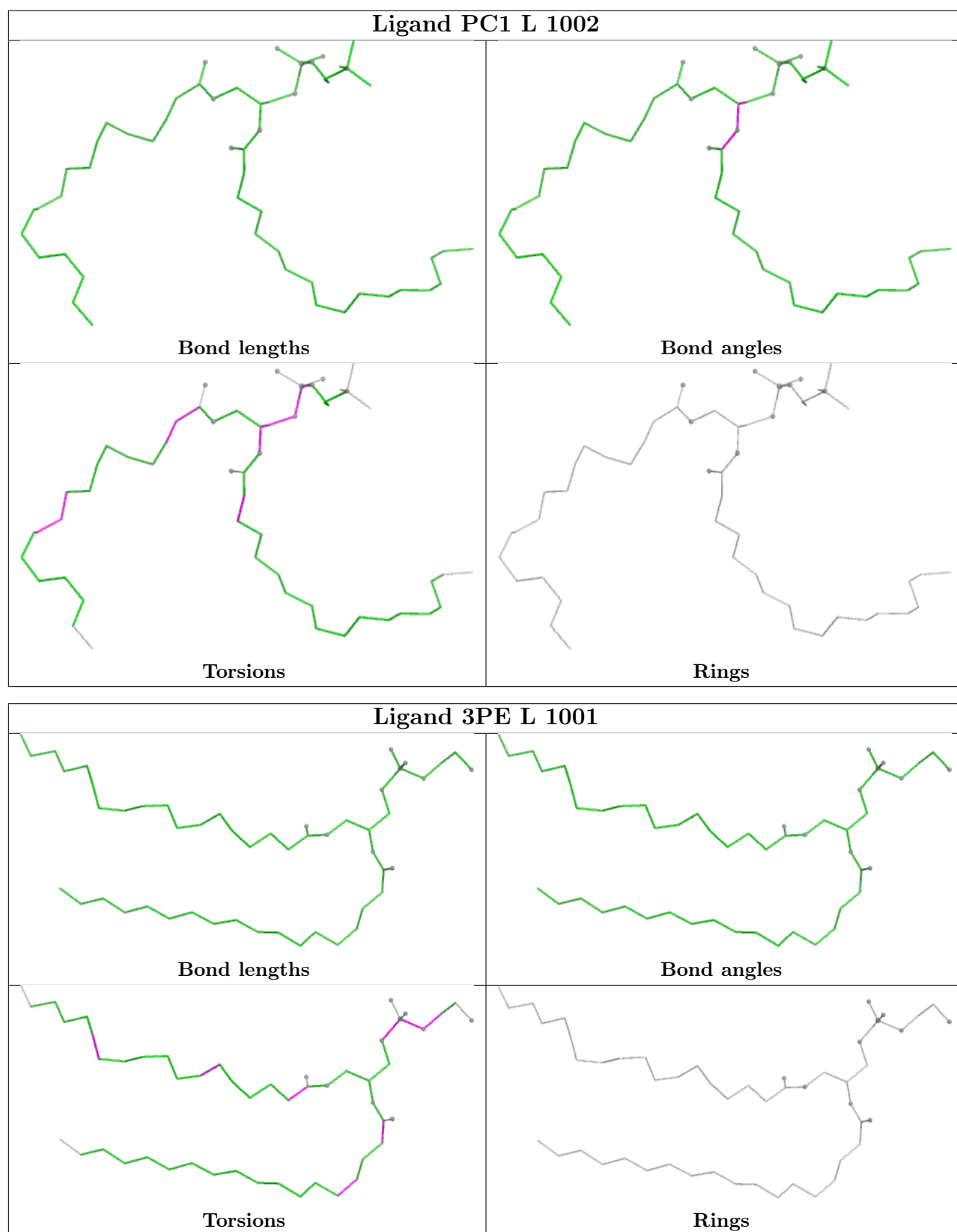


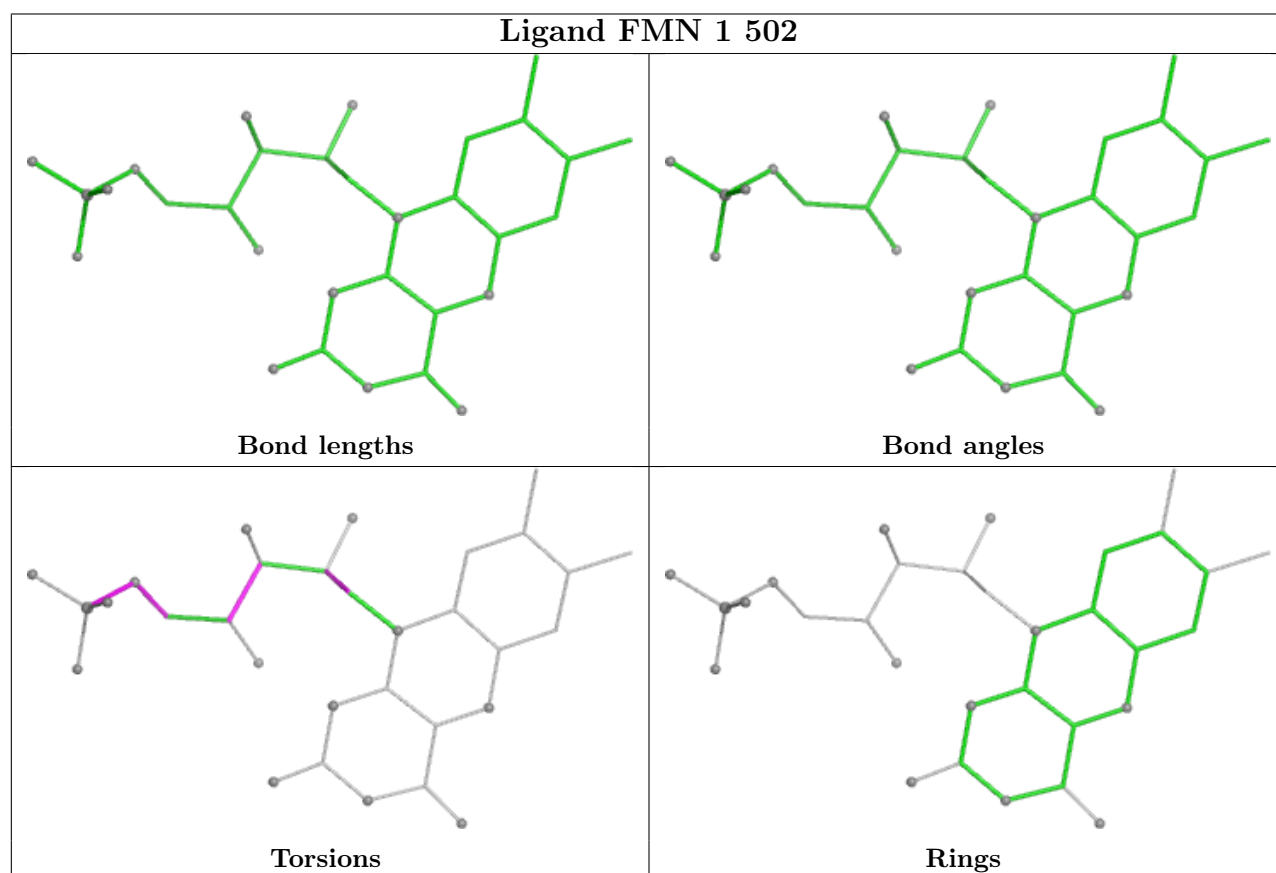
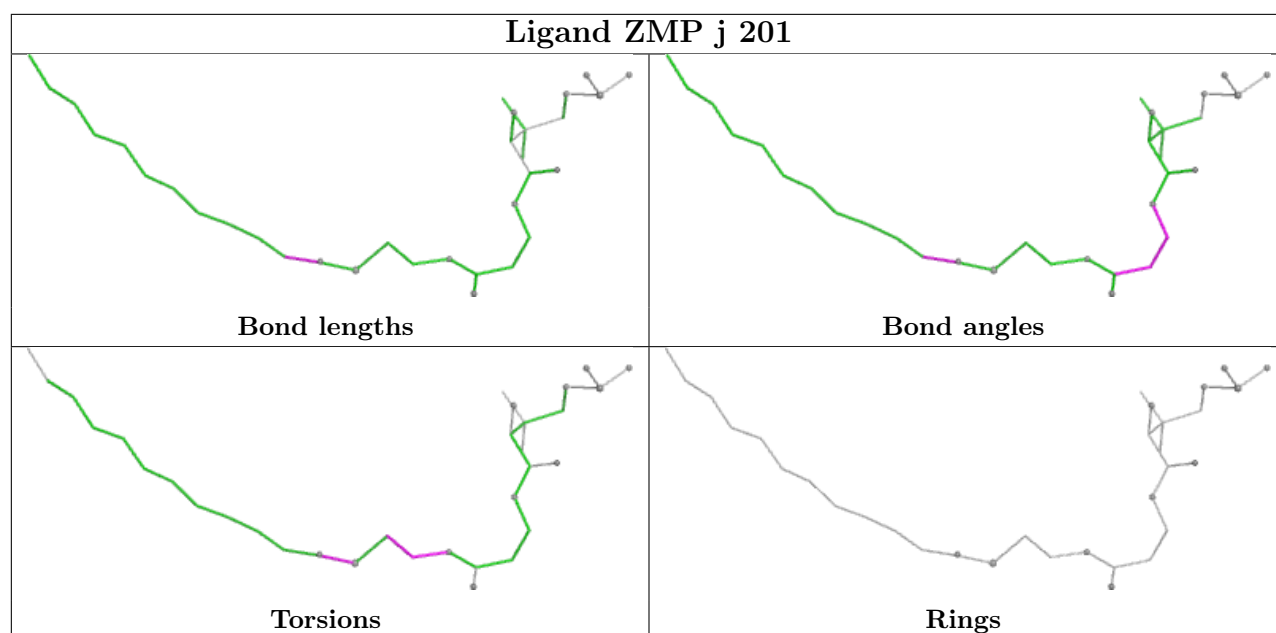


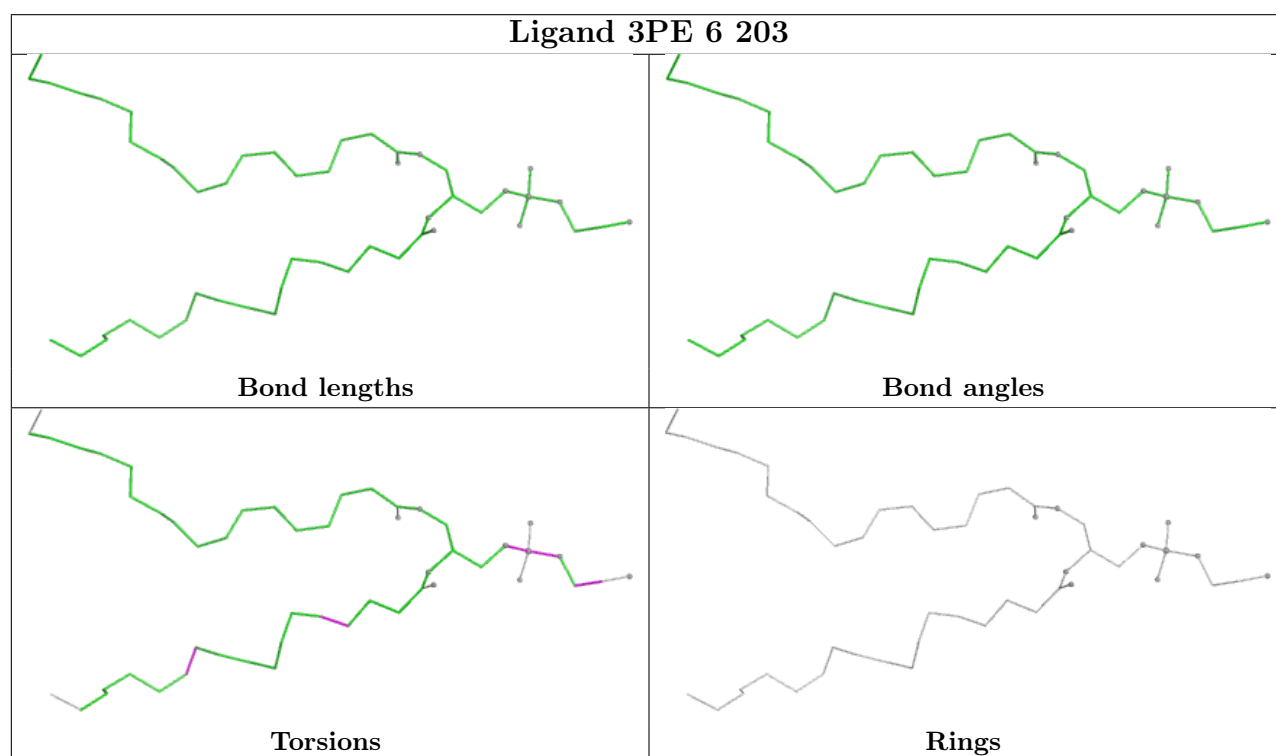
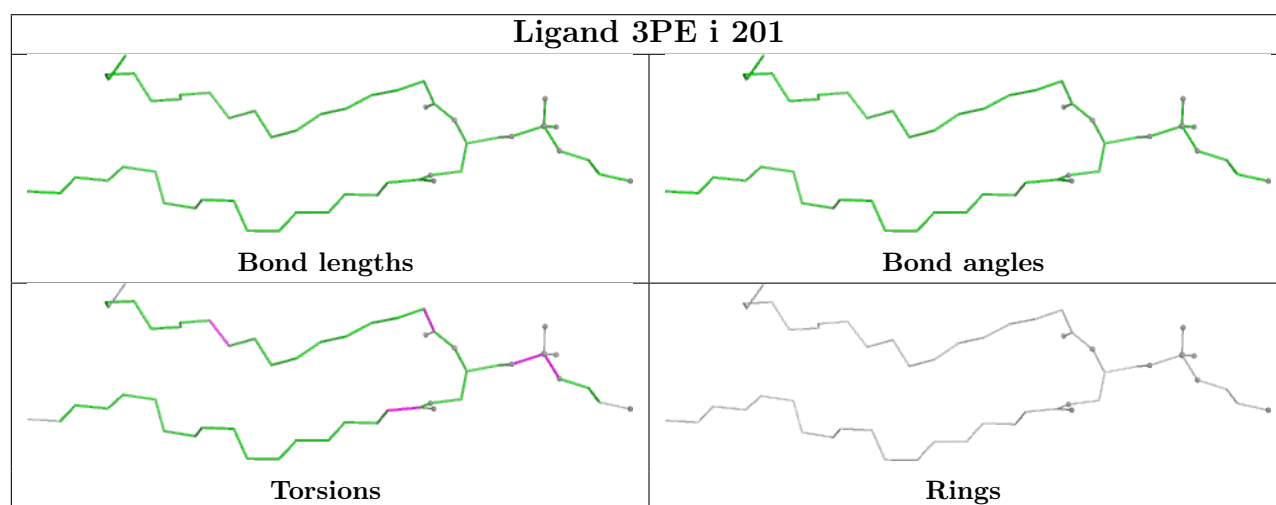
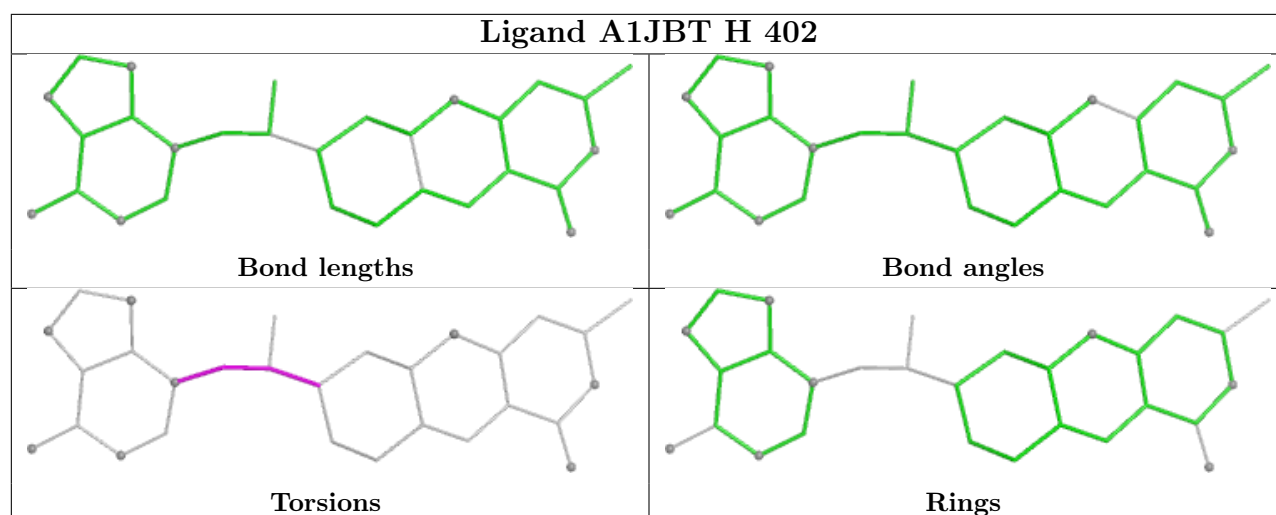


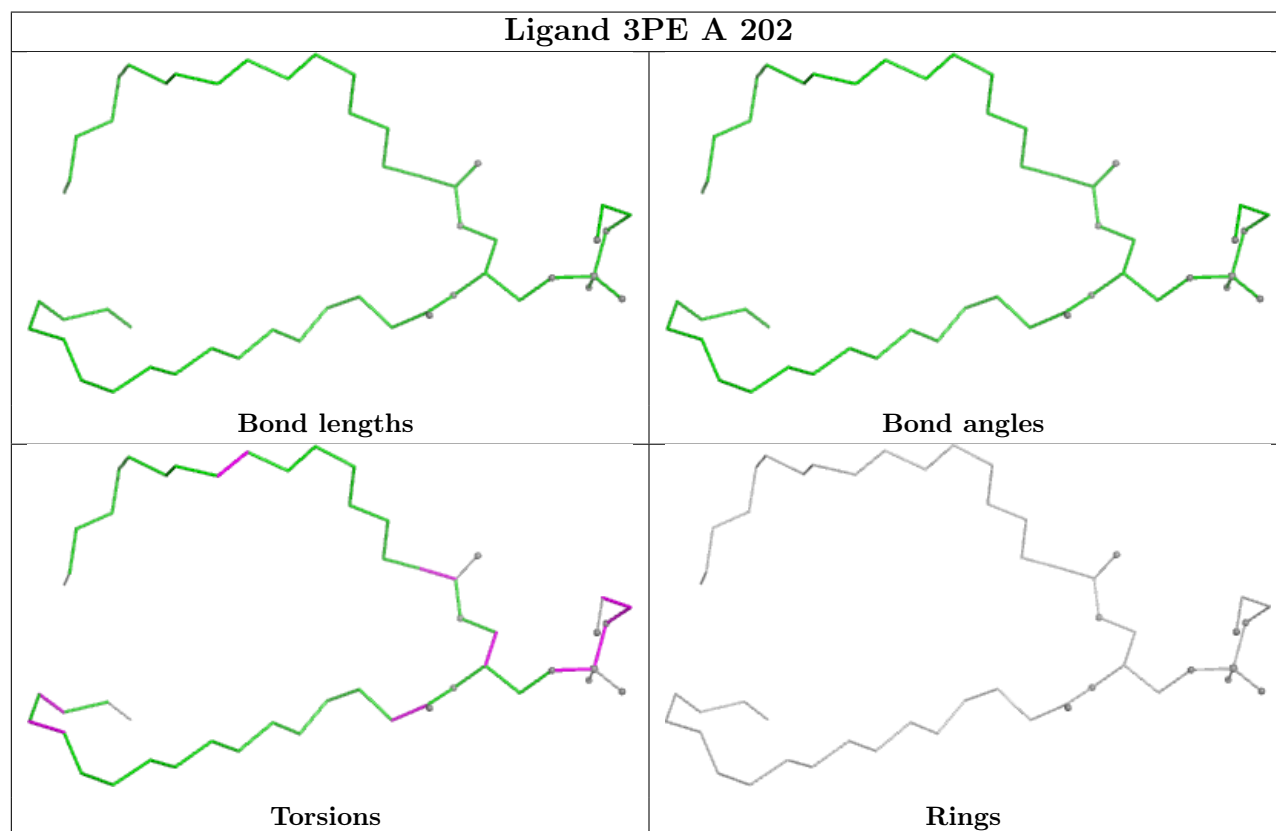
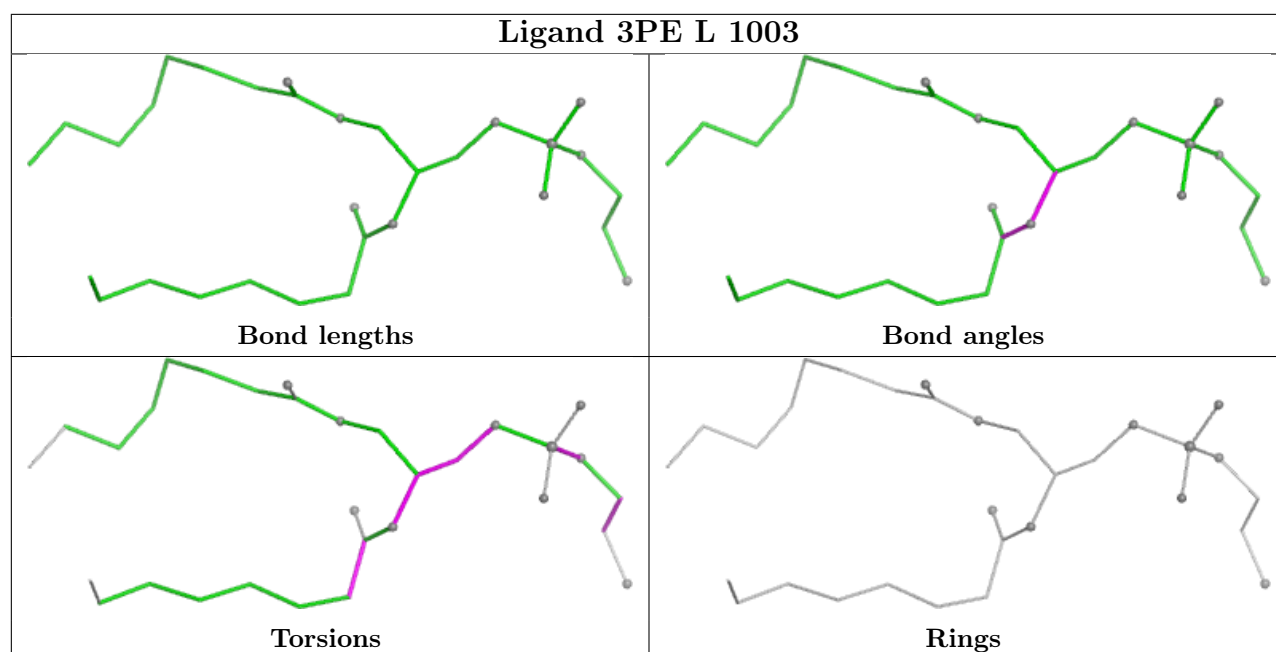


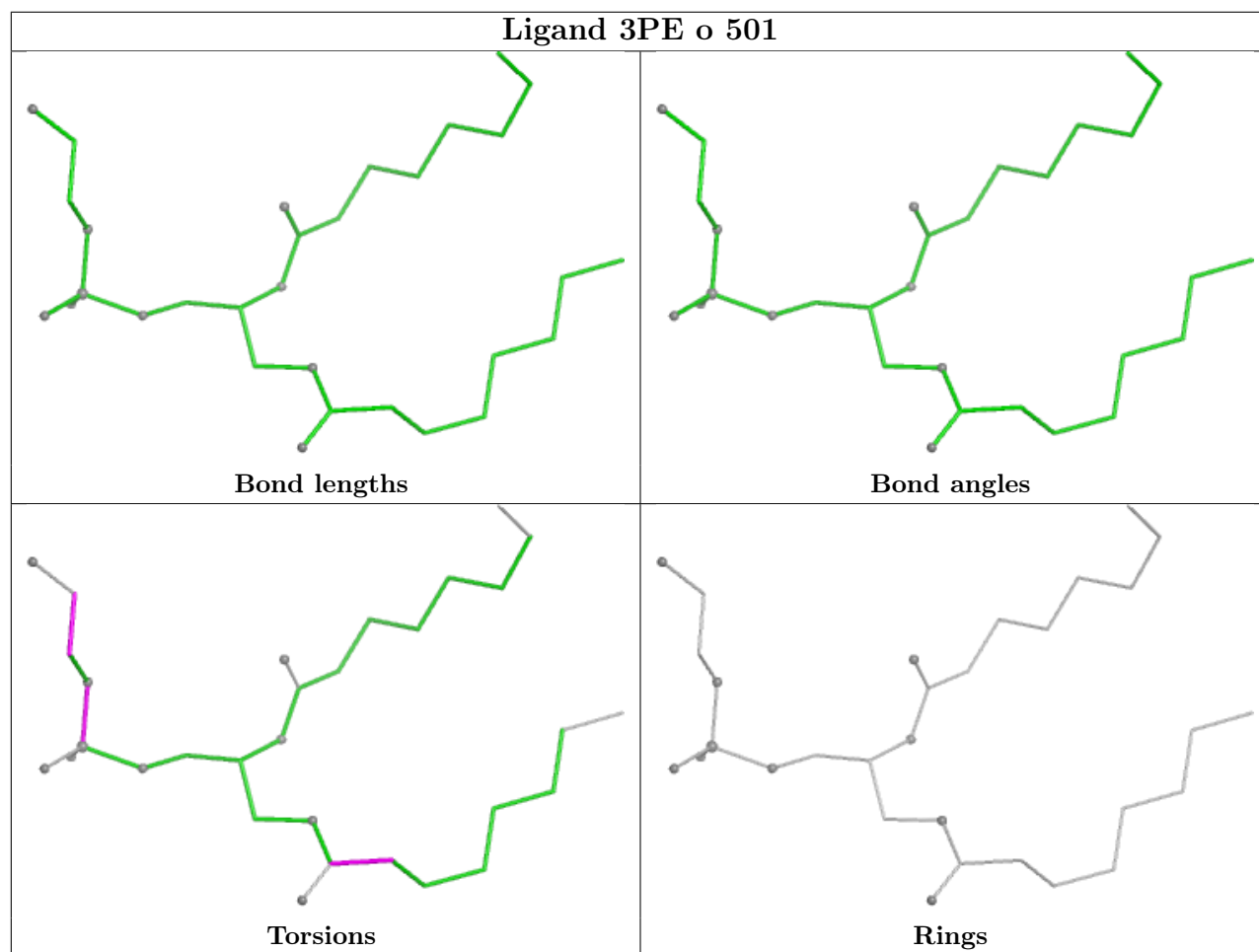
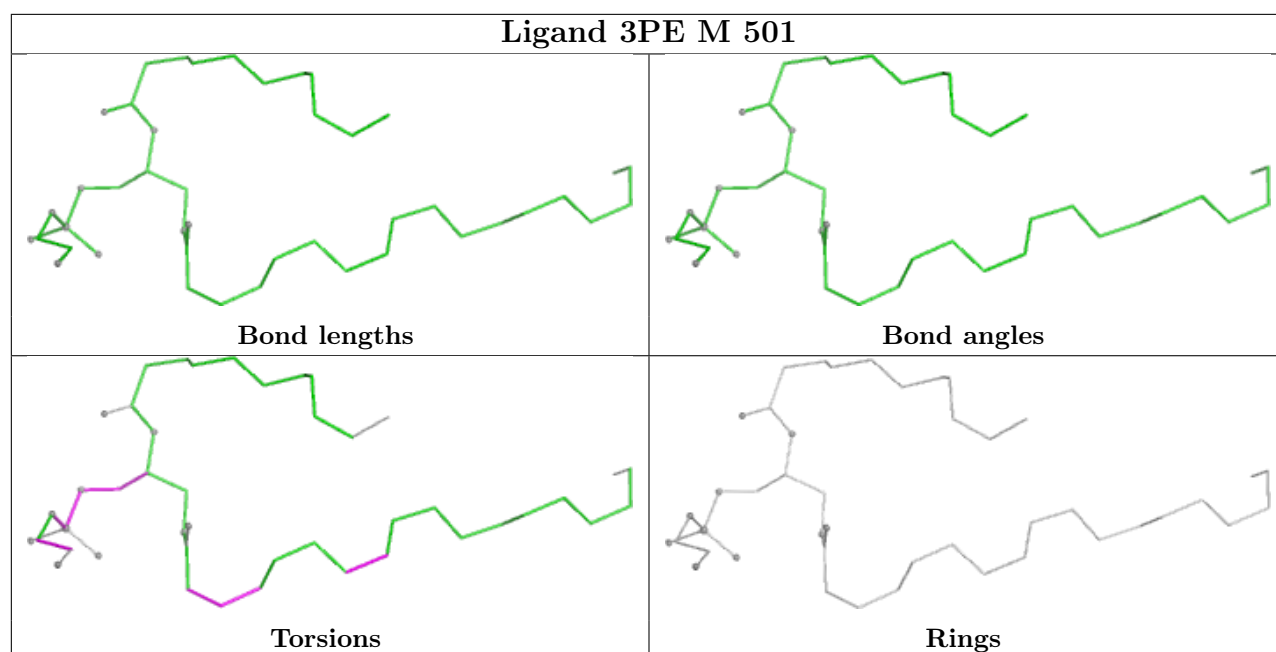


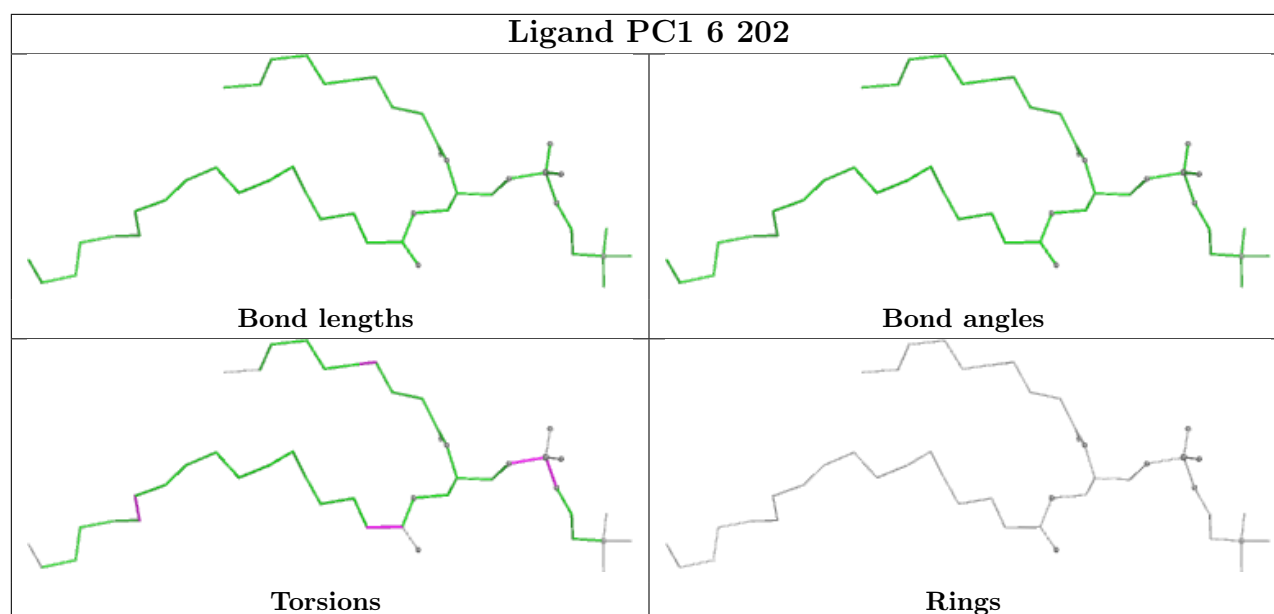












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

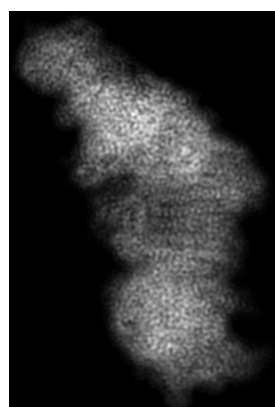
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53477. These allow visual inspection of the internal detail of the map and identification of artifacts.

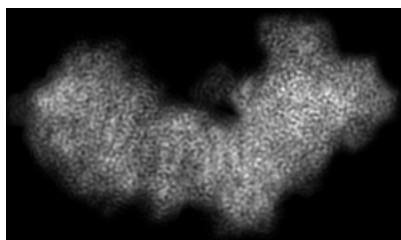
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

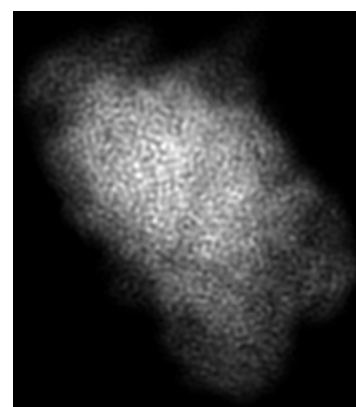
6.1.1 Primary map



X



Y

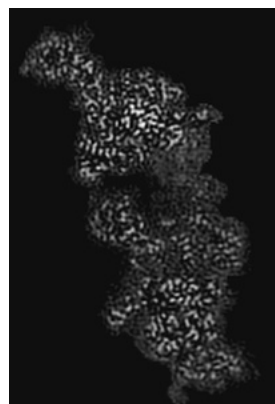


Z

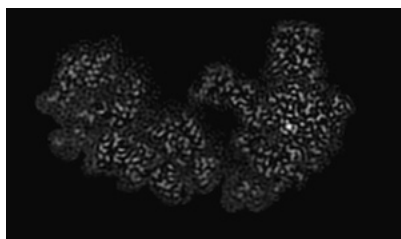
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

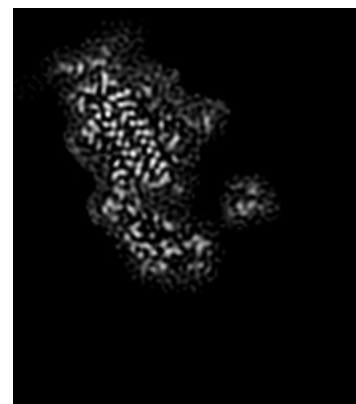
6.2.1 Primary map



X Index: 70



Y Index: 79

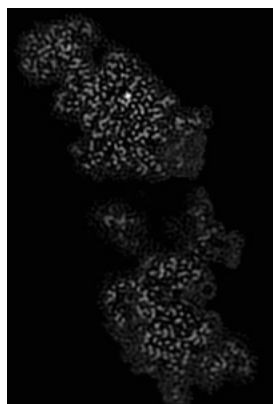


Z Index: 119

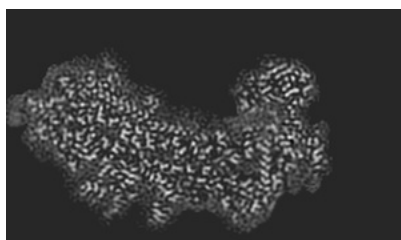
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

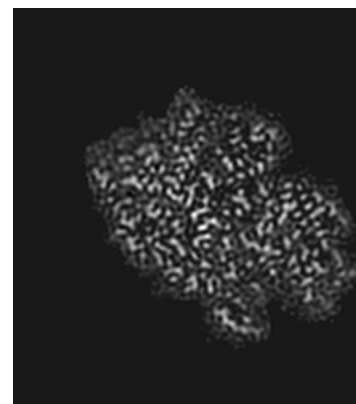
6.3.1 Primary map



X Index: 78



Y Index: 104

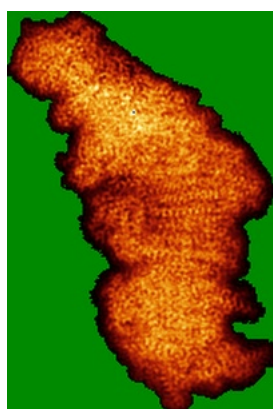


Z Index: 174

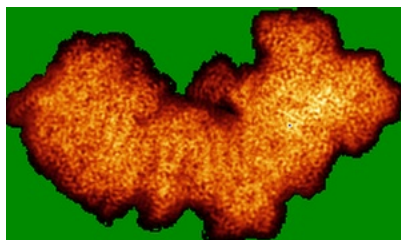
The images above show the largest variance slices of the map in three orthogonal directions.

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

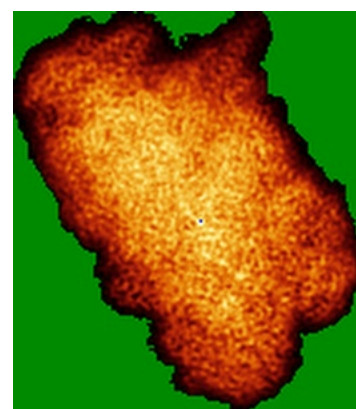
6.4.1 Primary map



X



Y

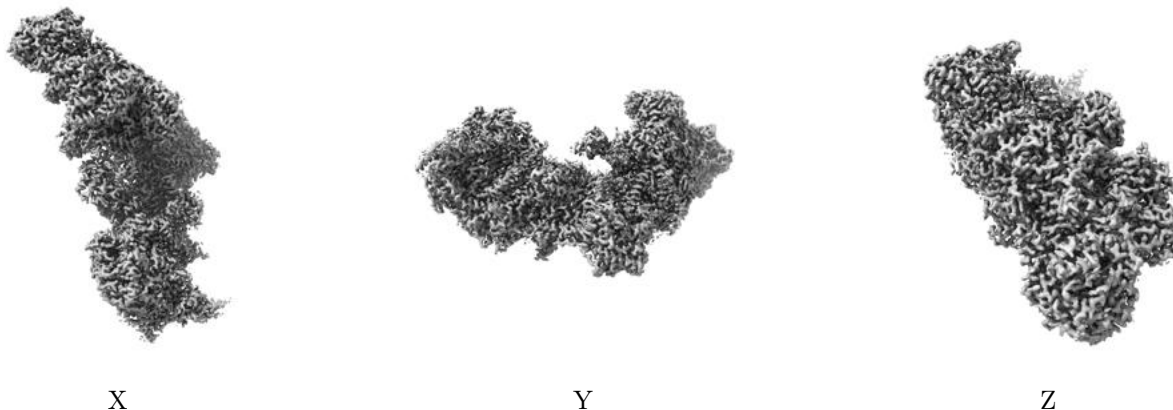


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.095. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

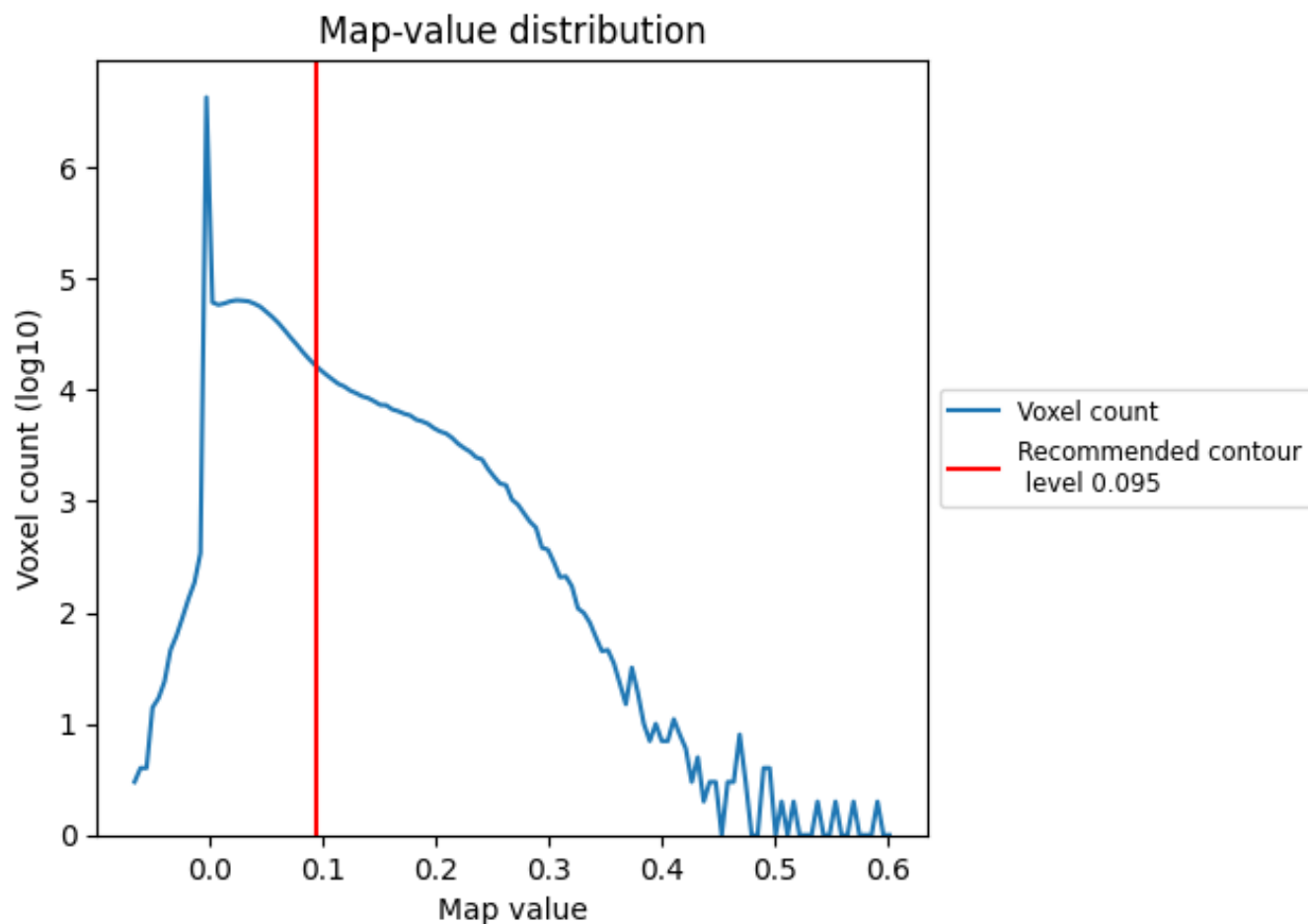
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

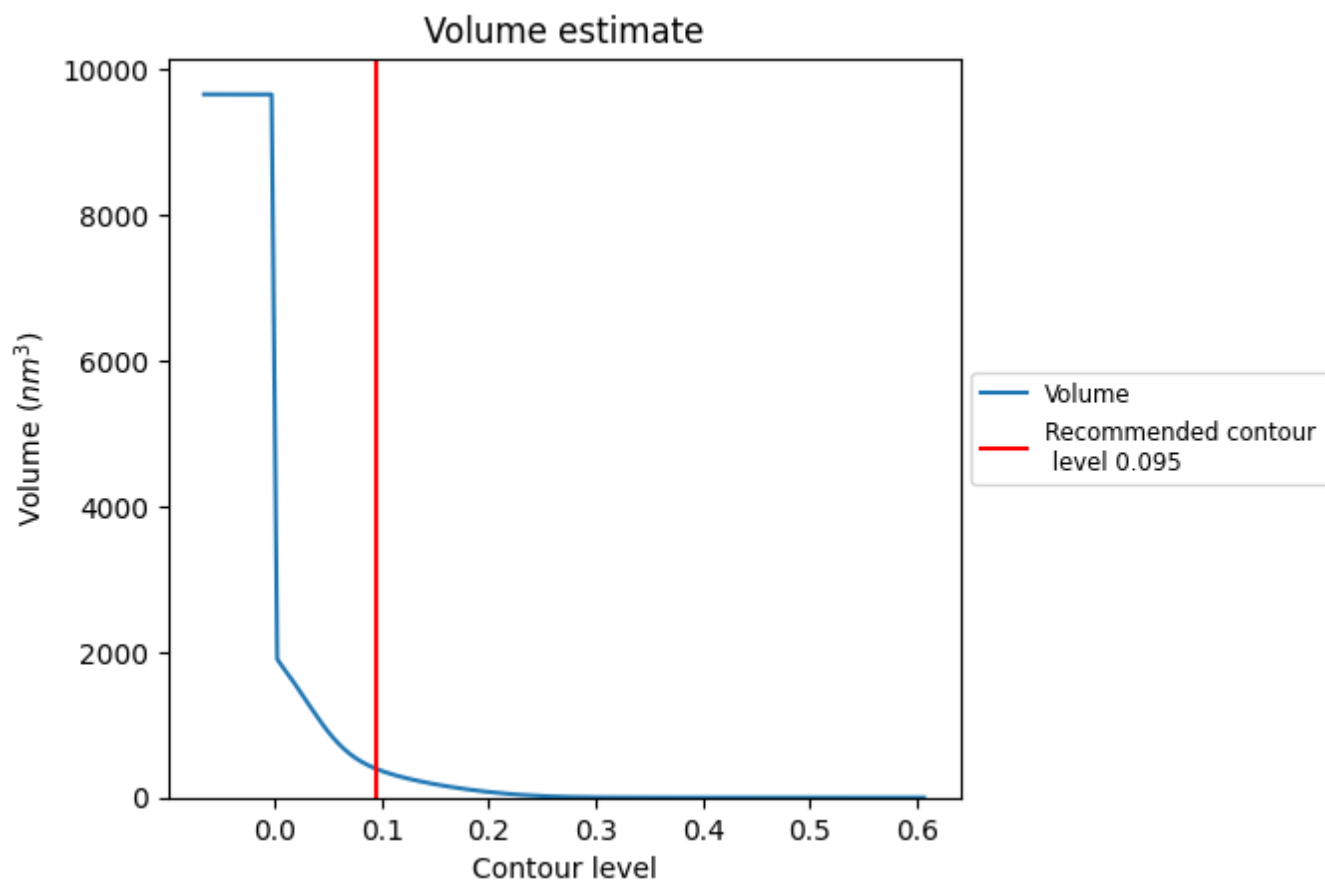
This section contains the results of statistical analysis of the map.

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 394 nm³; this corresponds to an approximate mass of 356 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.

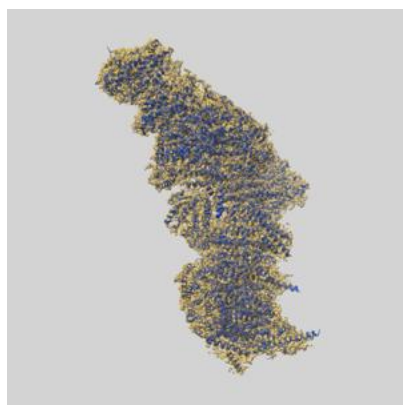
8 Fourier-Shell correlation ⓘ

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

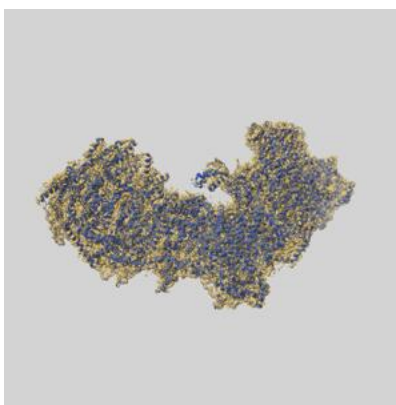
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53477 and PDB model 9R03. Per-residue inclusion information can be found in [section 3](#) on [page 21](#).

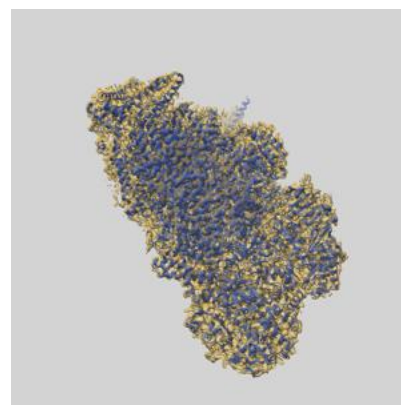
9.1 Map-model overlay [i](#)



X



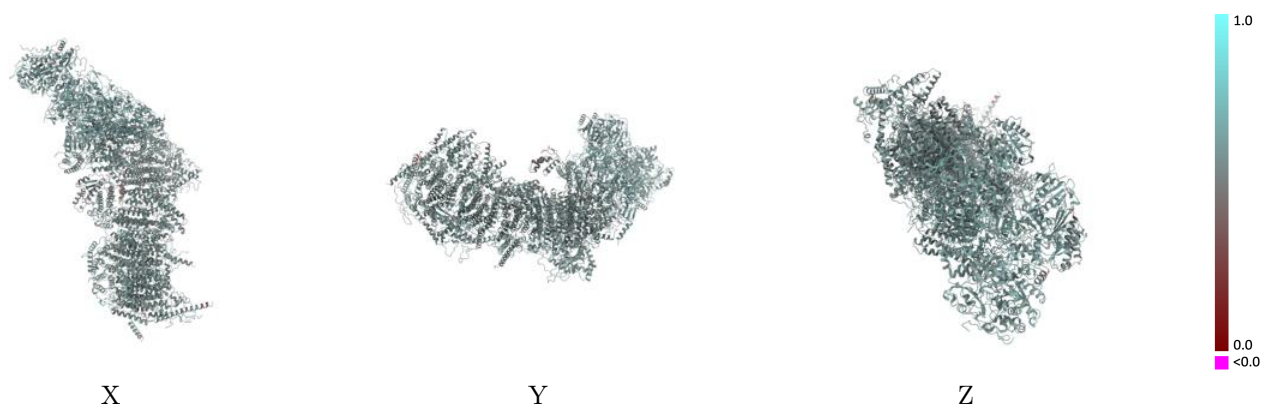
Y



Z

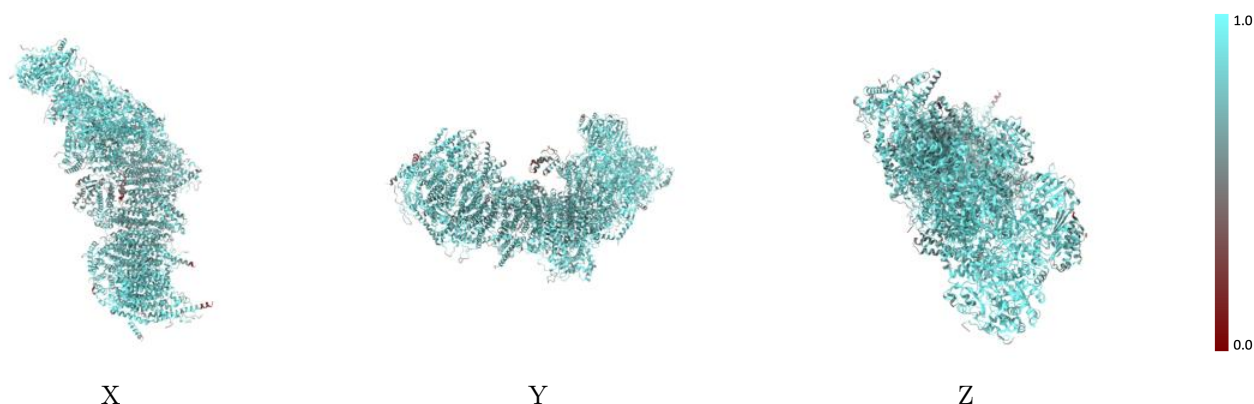
The images above show the 3D surface view of the map at the recommended contour level 0.095 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



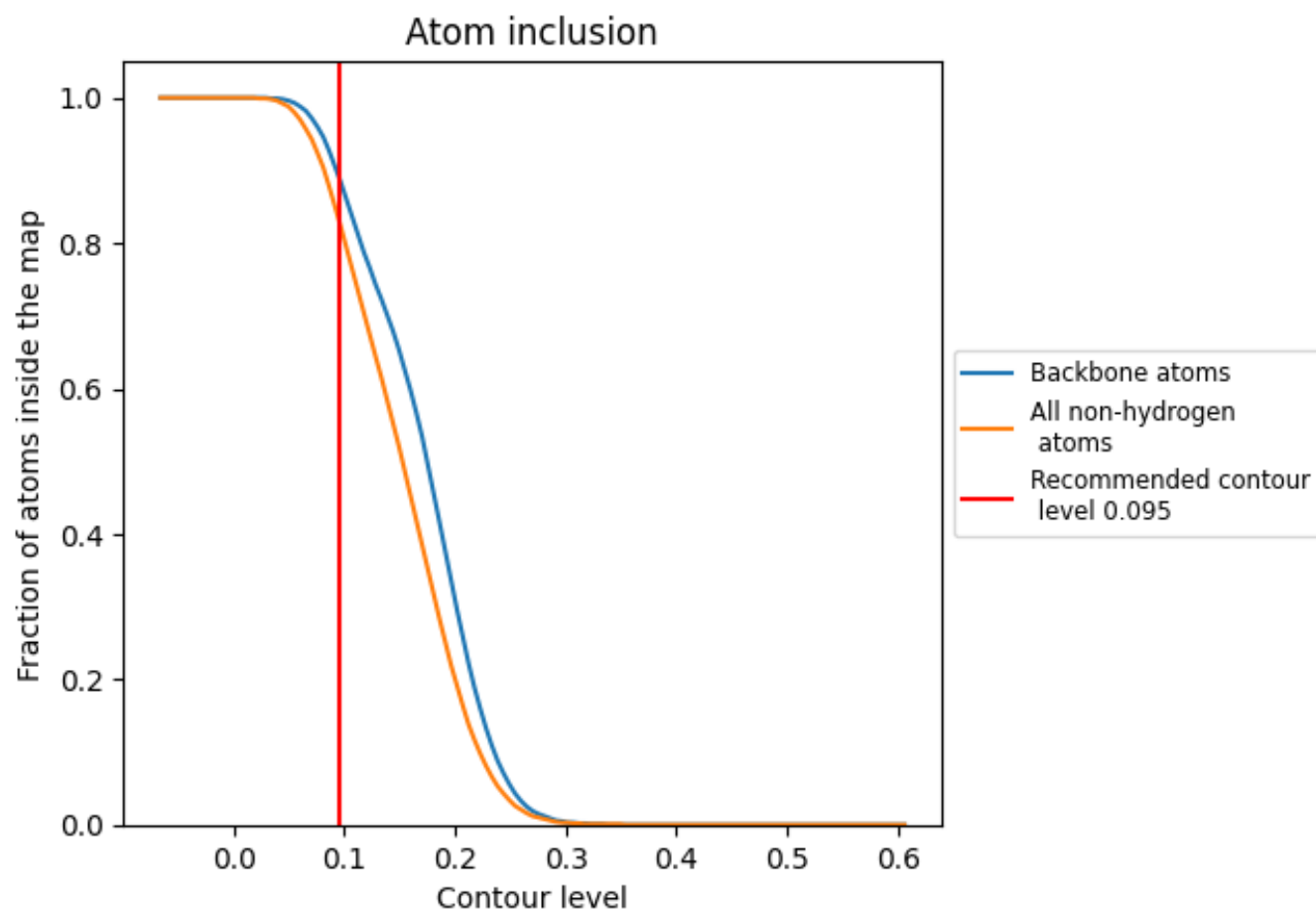
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.095).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 83% 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 (0.095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8340	 0.5690
1	 0.8920	 0.5810
2	 0.8490	 0.5700
3	 0.8780	 0.5890
4	 0.8790	 0.5840
5	 0.9110	 0.6030
6	 0.9150	 0.5880
9	 0.9370	 0.5980
A	 0.7380	 0.5380
H	 0.8410	 0.5530
J	 0.7810	 0.5400
K	 0.8310	 0.5630
L	 0.8670	 0.5620
M	 0.8780	 0.5780
N	 0.8510	 0.5700
V	 0.7310	 0.5450
W	 0.8590	 0.5770
X	 0.7710	 0.5410
Y	 0.7820	 0.5590
Z	 0.8020	 0.5600
a	 0.8540	 0.5700
b	 0.8650	 0.5980
c	 0.8780	 0.6000
d	 0.8400	 0.5790
e	 0.7870	 0.5670
f	 0.7400	 0.5630
g	 0.8050	 0.5770
h	 0.8410	 0.5910
i	 0.8630	 0.5950
j	 0.4890	 0.4820
k	 0.7360	 0.5510
l	 0.7920	 0.5560
m	 0.7570	 0.5450
n	 0.7780	 0.5430
o	 0.8060	 0.5650



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Chain	Atom inclusion	Q-score
p	 0.7940	 0.5600
q	 0.8390	 0.5630
r	 0.7690	 0.5480
s	 0.7790	 0.5380
t	 0.8210	 0.5640
u	 0.8210	 0.5490
v	 0.8210	 0.5630
w	 0.7770	 0.5490
x	 0.7490	 0.5450
y	 0.7590	 0.5500
z	 0.8450	 0.5660