



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:48 AM UTC

PDB ID : 6ZKA / pdb_00006zka
EMDB ID : EMD-11242
Title : Membrane domain of open complex I during turnover
Authors : Kampjut, D.; Sazanov, L.A.
Deposited on : 2020-06-30
Resolution : 2.50 Å(reported)
Based on initial model : 5LNK

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

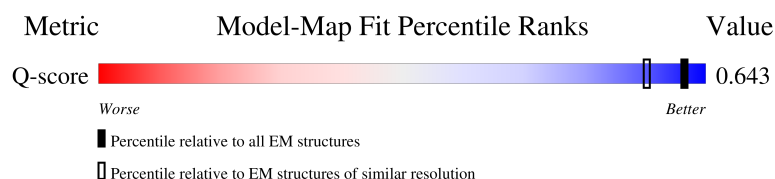
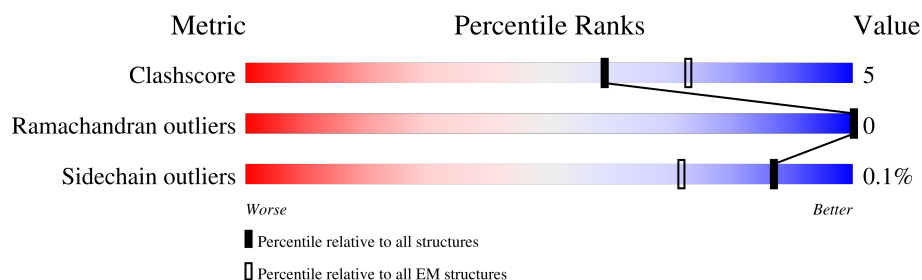
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 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.



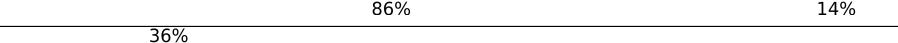
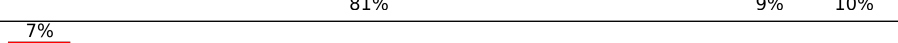
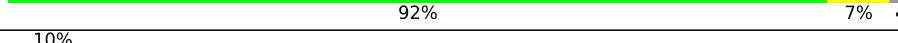
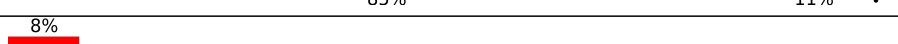
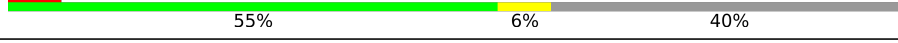
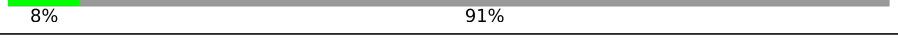
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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

Mol	Chain	Length	Quality of chain
1	A	115	10% 73% 11% 16%
2	H	318	5% 86% 13% .
3	J	175	10% 81% 14% 5%
4	K	98	. 87% 13%

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Mol	Chain	Length	Quality of chain
5	L	606	
6	M	459	
7	N	347	
8	V	141	
9	W	189	
10	X	157	
11	Y	172	
12	Z	175	
13	k	355	
14	l	106	
15	m	84	
16	n	98	
17	o	122	
18	p	130	
19	q	144	
20	r	128	
21	s	137	
22	t	179	
23	u	108	
24	v	186	
25	w	154	
26	x	76	
27	y	58	
28	z	70	
29	4	463	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CDL	L	704	X	-	-	-
33	CDL	V	204	X	-	-	-
33	CDL	Y	201	X	-	-	-
33	CDL	o	502	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 40800 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	97	Total	C	N	O	S	0	0
			787	539	111	132	5		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	313	Total	C	N	O	S	0	0
			2494	1683	379	413	19		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	167	Total	C	N	O	S	0	0
			1273	856	182	222	13		

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

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

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

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

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

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

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 8 is a protein called Mitochondrial complex I, B14.7 subunit.

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

- Molecule 9 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

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

- Molecule 10 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	87	Total	C	N	O	S	0	0
			701	451	103	142	5		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 12 is a protein called Mitochondrial complex I, PDSW subunit.

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

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 14 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

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

- Molecule 15 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

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

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

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

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 18 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

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

- Molecule 19 is a protein called Mitochondrial complex I, B16.6 subunit.

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

- Molecule 20 is a protein called Mitochondrial complex I, B17 subunit.

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

- Molecule 21 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

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

- Molecule 22 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

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

- Molecule 23 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

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

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

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

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

- Molecule 26 is a protein called Mitochondrial complex I, KFYI subunit.

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

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

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

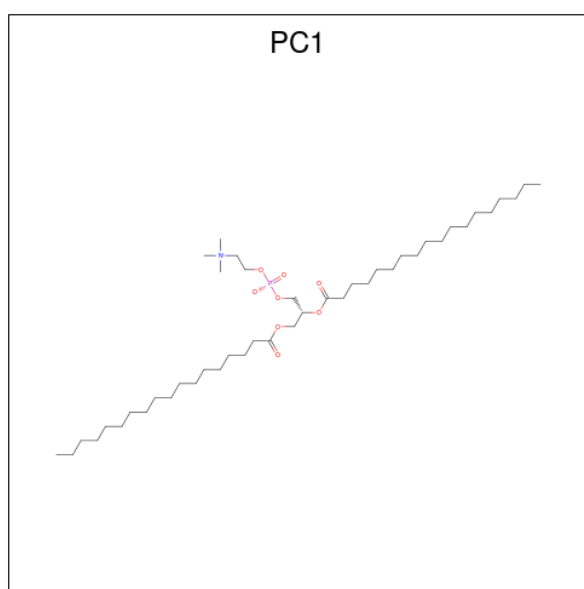
- Molecule 28 is a protein called Mitochondrial complex I, MWFE subunit.

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

- Molecule 29 is a protein called Mitochondrial complex I, ND4L subunit.

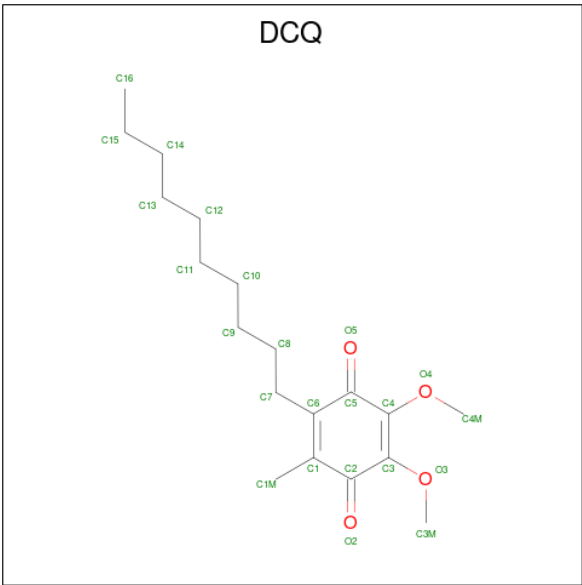
Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	40	Total	C	N	O	S	0	0
			334	217	56	60	1		

- Molecule 30 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



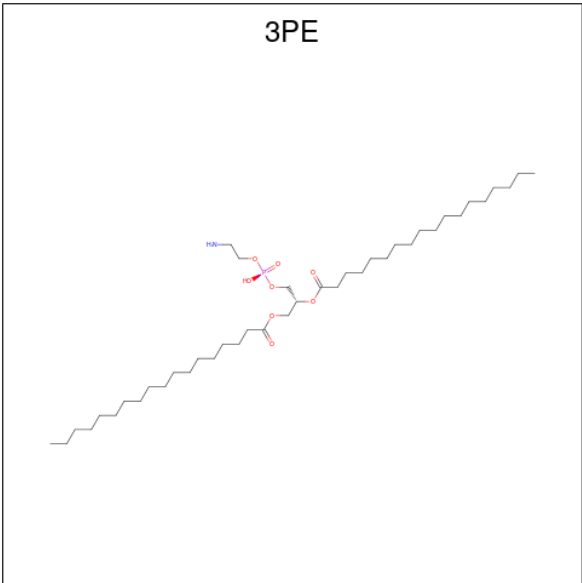
Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
30	H	1	Total	C	N	O	P	0
			54	44	1	8	1	
30	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
30	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
30	w	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 31 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (CCD ID: DCQ) (formula: $C_{19}H_{30}O_4$).



Mol	Chain	Residues	Atoms			AltConf
31	H	1	Total	C	O	0
			23	19	4	

- Molecule 32 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



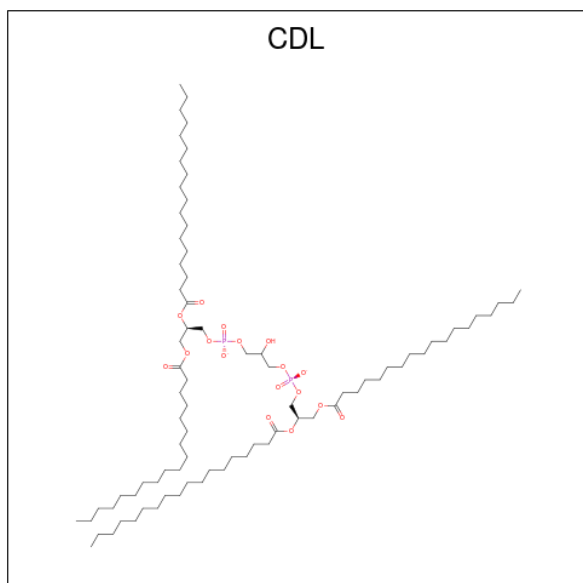
Mol	Chain	Residues	Atoms					AltConf
32	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
32	K	1	Total	C	N	O	P	0
			40	30	1	8	1	

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

- Molecule 33 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



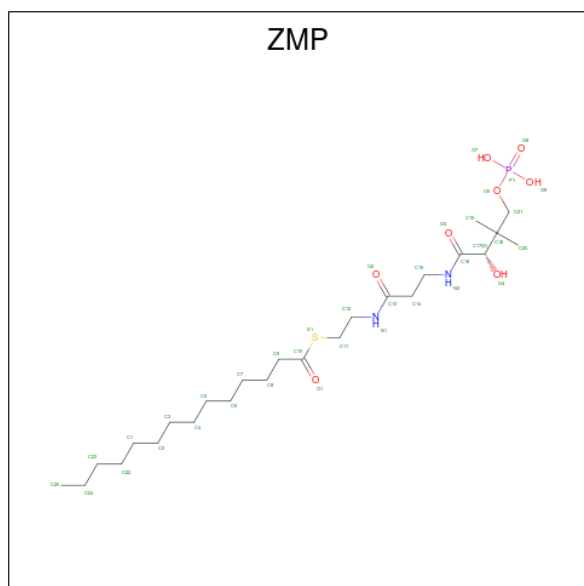
Mol	Chain	Residues	Atoms				AltConf
33	L	1	Total	C	O	P	0
			100	81	17	2	

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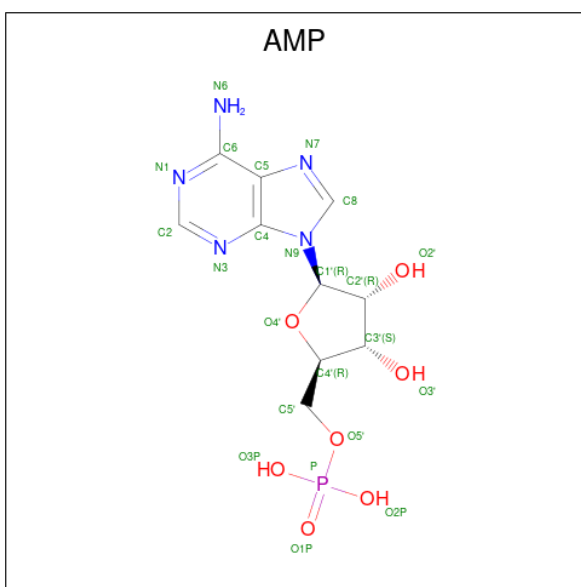
Mol	Chain	Residues	Atoms				AltConf
33	M	1	Total	C	O	P	0
			90	71	17	2	
33	V	1	Total	C	O	P	0
			94	75	17	2	
33	V	1	Total	C	O	P	0
			85	66	17	2	
33	W	1	Total	C	O	P	0
			100	81	17	2	
33	Y	1	Total	C	O	P	0
			100	81	17	2	
33	o	1	Total	C	O	P	0
			75	56	17	2	

- Molecule 34 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



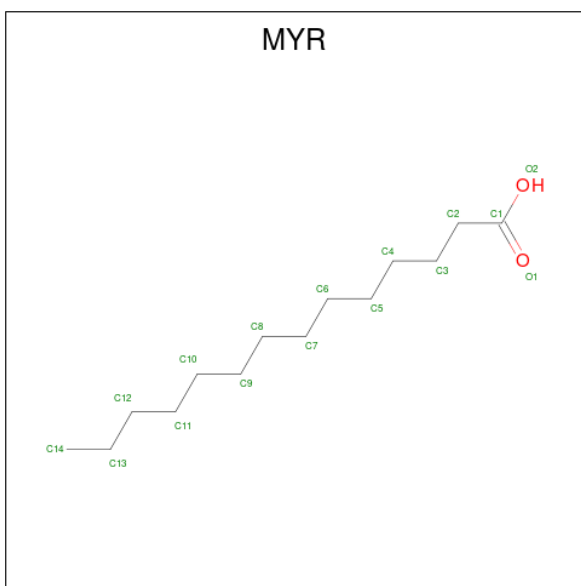
Mol	Chain	Residues	Atoms						AltConf
34	X	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	

- Molecule 35 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

- Molecule 36 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		AltConf
37	A	22	Total 22	O 22	0
37	H	53	Total 53	O 53	0
37	J	44	Total 44	O 44	0
37	K	23	Total 23	O 23	0
37	L	156	Total 156	O 156	0
37	M	184	Total 184	O 184	0
37	N	133	Total 133	O 133	0
37	V	4	Total 4	O 4	0
37	W	75	Total 75	O 75	0
37	X	17	Total 17	O 17	0
37	Y	46	Total 46	O 46	0
37	Z	67	Total 67	O 67	0
37	k	43	Total 43	O 43	0
37	l	45	Total 45	O 45	0
37	m	8	Total 8	O 8	0
37	n	3	Total 3	O 3	0
37	o	59	Total 59	O 59	0
37	p	40	Total 40	O 40	0
37	q	46	Total 46	O 46	0
37	r	20	Total 20	O 20	0
37	s	9	Total 9	O 9	0
37	t	44	Total 44	O 44	0

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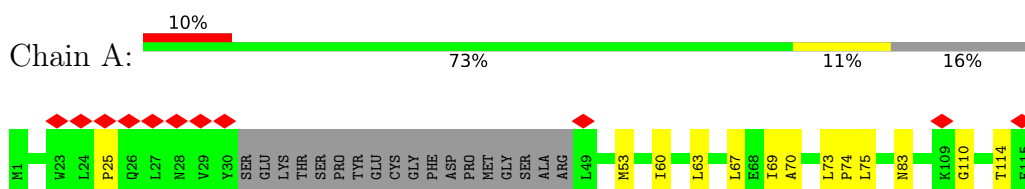
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Mol	Chain	Residues	Atoms		AltConf
37	u	1	Total 1	O 1	0
37	v	41	Total 41	O 41	0
37	w	41	Total 41	O 41	0
37	x	6	Total 6	O 6	0
37	y	21	Total 21	O 21	0
37	z	18	Total 18	O 18	0
37	4	24	Total 24	O 24	0

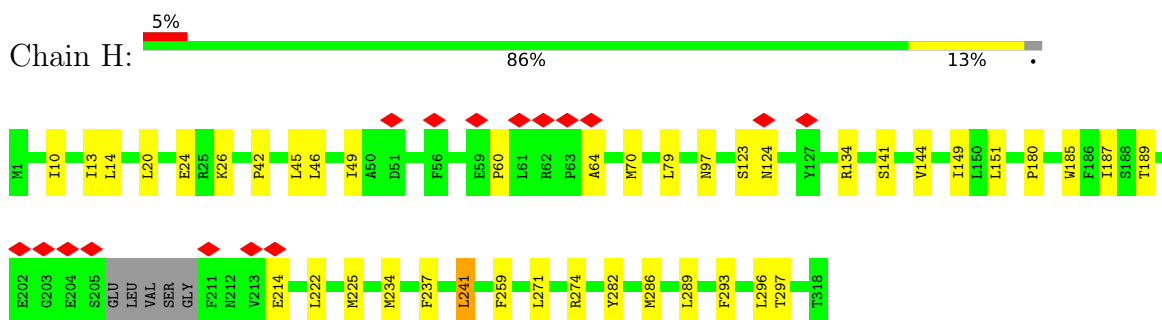
3 Residue-property plots [i](#)

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

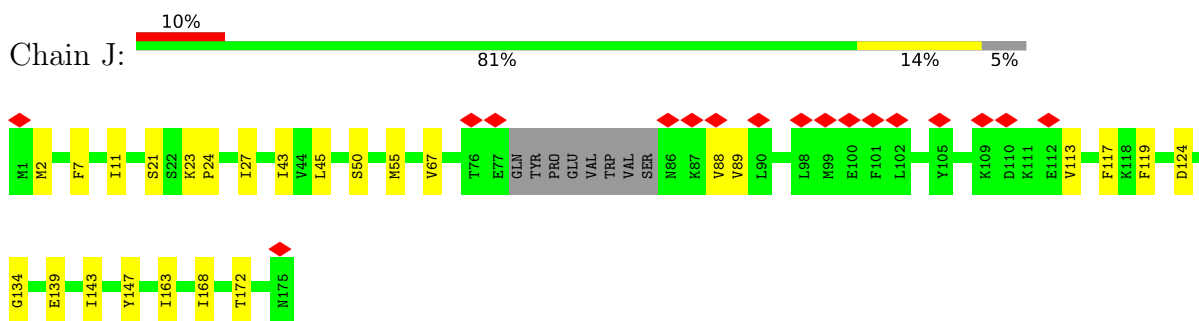
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



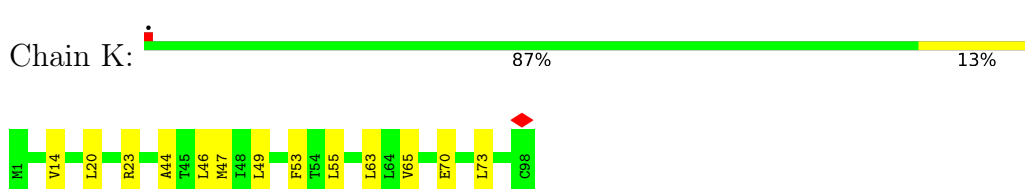
- Molecule 2: NADH-ubiquinone oxidoreductase chain 1



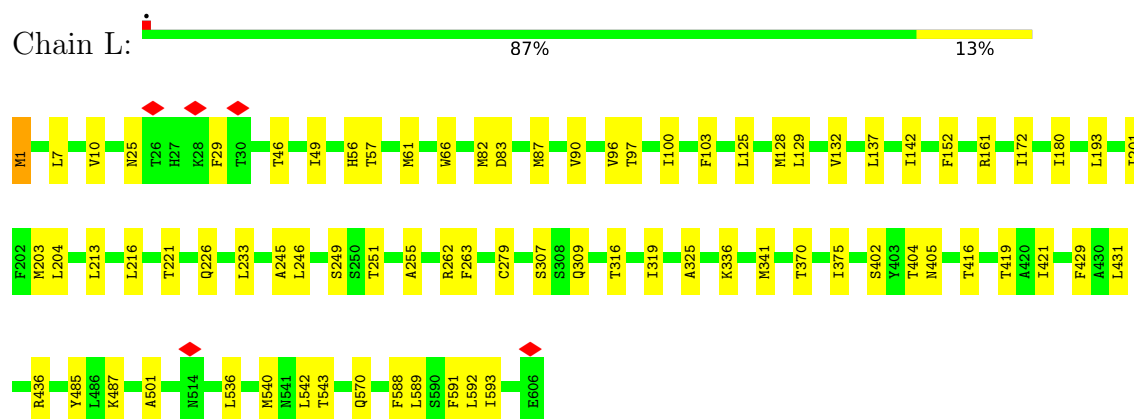
- Molecule 3: NADH-ubiquinone oxidoreductase chain 6



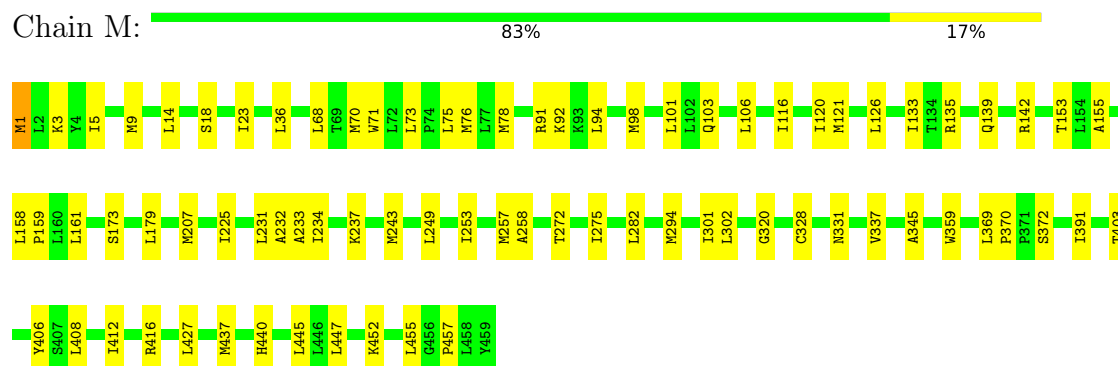
- Molecule 4: NADH-ubiquinone oxidoreductase chain 4L



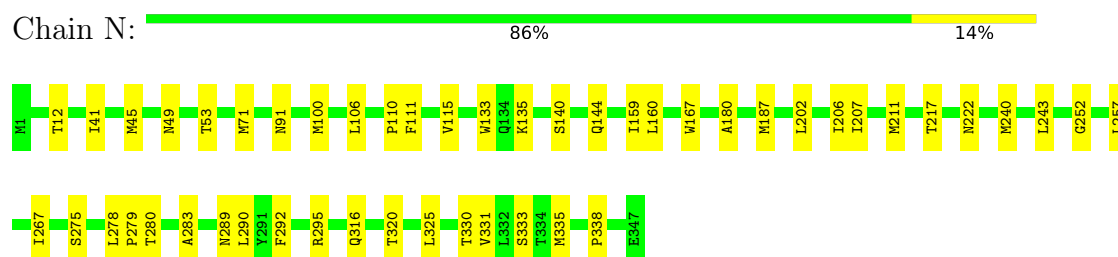
- Molecule 5: NADH-ubiquinone oxidoreductase chain 5



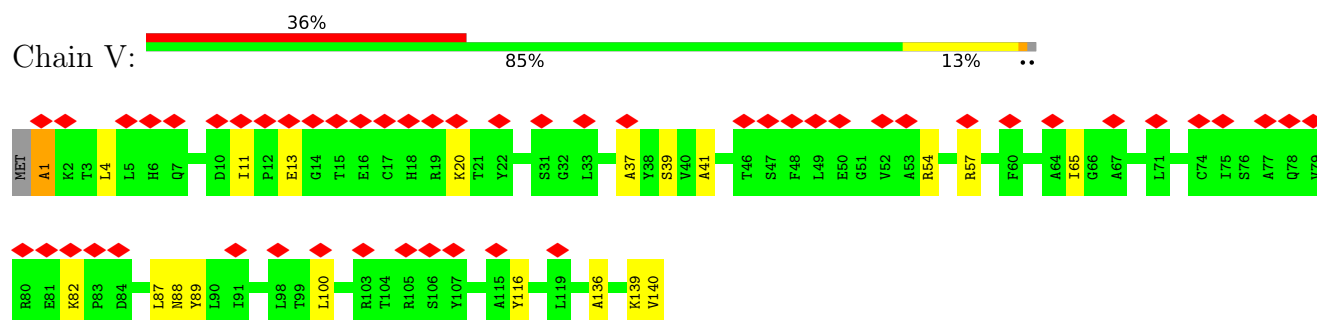
- Molecule 6: NADH-ubiquinone oxidoreductase chain 4



- Molecule 7: NADH-ubiquinone oxidoreductase chain 2

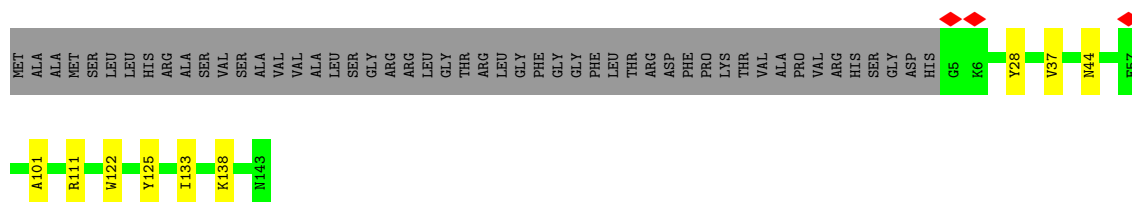


- Molecule 8: Mitochondrial complex I, B14.7 subunit



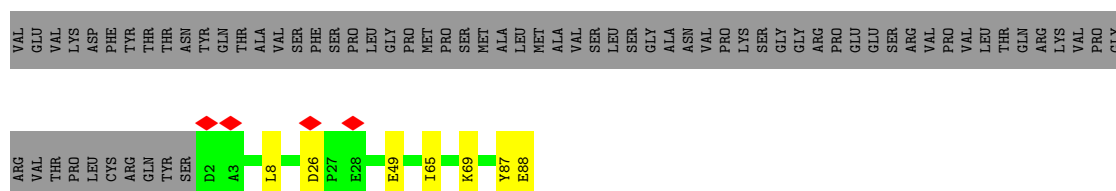
- Molecule 9: NADH:ubiquinone oxidoreductase subunit B5

Chain W: 



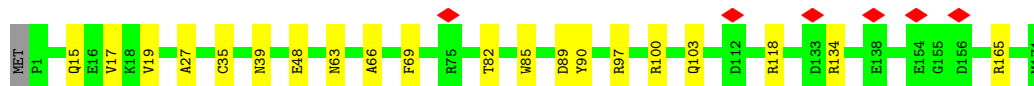
- Molecule 10: Acyl carrier protein

Chain X: 



- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Y: 



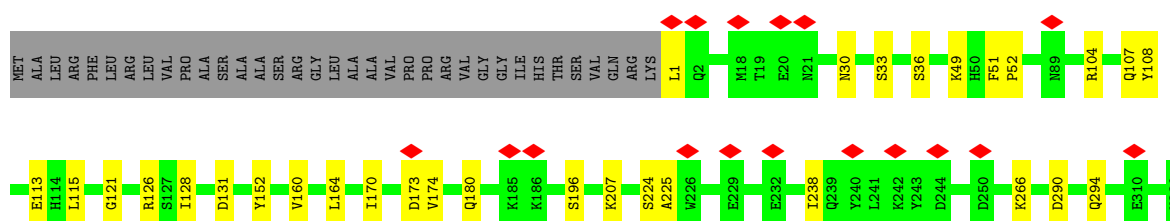
- Molecule 12: Mitochondrial complex I, PDSW subunit

Chain Z: 



- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

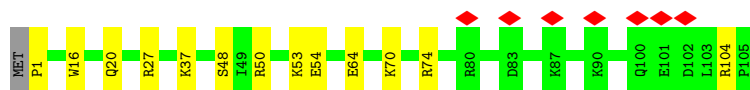
Chain k: 



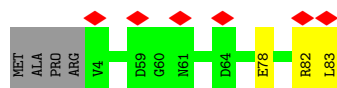
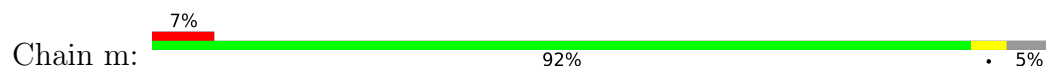
- Molecule 14: NADH:ubiquinone oxidoreductase subunit S5

Chain l: 

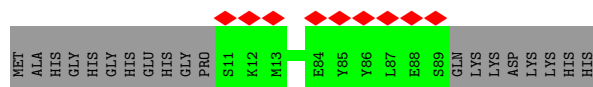
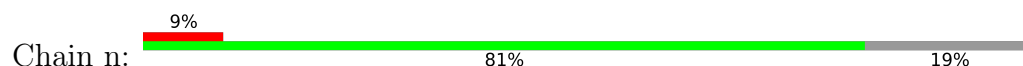




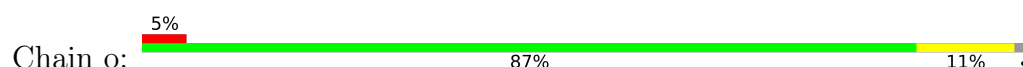
- Molecule 15: NADH:ubiquinone oxidoreductase subunit A3



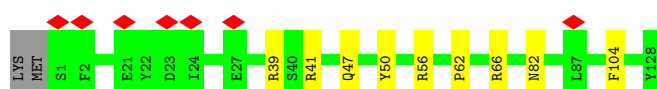
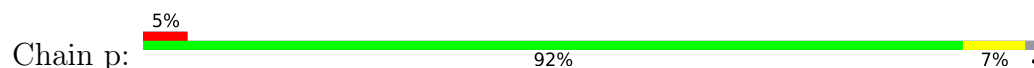
- Molecule 16: NADH:ubiquinone oxidoreductase subunit B3



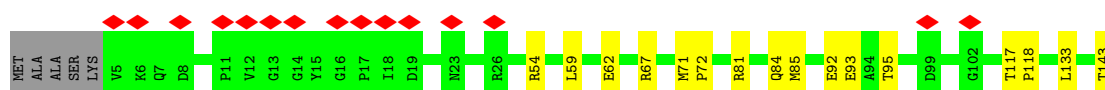
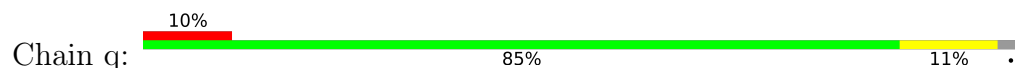
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 subunit C2



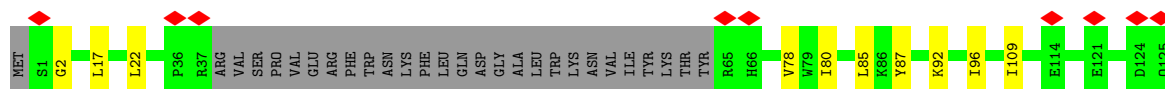
- Molecule 18: NADH:ubiquinone oxidoreductase subunit B4



- Molecule 19: Mitochondrial complex I, B16.6 subunit

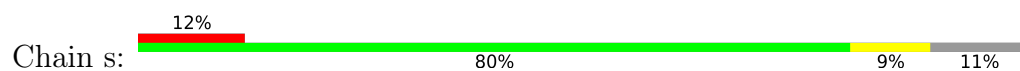


- Molecule 20: Mitochondrial complex I, B17 subunit

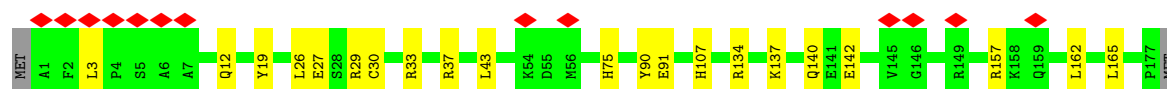
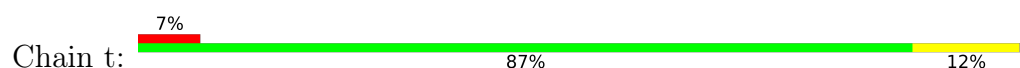




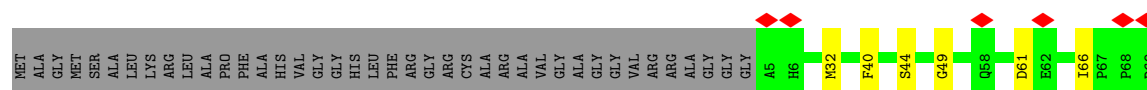
- Molecule 21: NADH:ubiquinone oxidoreductase subunit B7



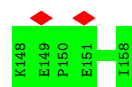
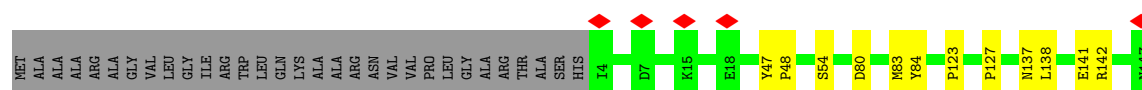
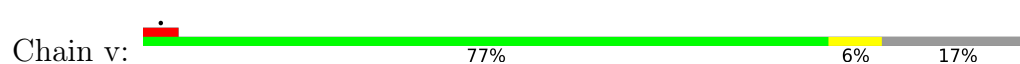
- Molecule 22: NADH:ubiquinone oxidoreductase subunit B9



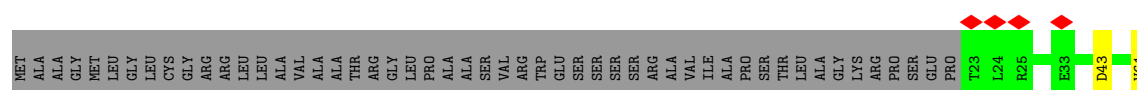
- Molecule 23: NADH:ubiquinone oxidoreductase subunit B2



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



- Molecule 25: Mitochondrial complex I, ESSS subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	315484	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.838	Depositor
Minimum map value	-0.473	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	162.5, 153.5, 249.5	wwPDB
Map dimensions	325, 307, 499	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5, 0.5, 0.5	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, MYR, ZMP, FME, DCQ, AMP, CDL, SEP, PC1, AYA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	1/807 (0.1%)	0.68	0/1106
2	H	0.36	0/2568	0.61	0/3512
3	J	0.32	0/1302	0.60	0/1760
4	K	0.40	0/749	0.65	0/1014
5	L	0.35	0/4924	0.61	0/6698
6	M	0.40	0/3731	0.65	0/5085
7	N	0.40	0/2787	0.62	0/3795
8	V	0.19	0/1041	0.43	0/1412
9	W	0.32	0/1188	0.51	0/1607
10	X	0.26	0/713	0.47	0/963
11	Y	0.29	0/1440	0.54	0/1942
12	Z	0.30	0/1475	0.49	0/1989
13	k	0.28	0/2646	0.47	0/3579
14	l	0.33	0/896	0.57	0/1200
15	m	0.25	0/647	0.46	0/890
16	n	0.22	0/653	0.38	0/882
17	o	0.30	0/1035	0.50	0/1398
18	p	0.27	0/1085	0.49	0/1467
19	q	0.28	0/1171	0.48	0/1579
20	r	0.30	0/874	0.51	0/1188
21	s	0.24	0/1072	0.47	0/1436
22	t	0.28	0/1573	0.55	0/2130
23	u	0.24	0/590	0.46	0/810
24	v	0.28	0/1361	0.50	0/1861
25	w	0.30	0/872	0.58	0/1185
26	x	0.22	0/425	0.40	0/576
27	y	0.30	0/449	0.52	0/605
28	z	0.33	0/591	0.55	0/795
29	4	0.25	0/351	0.43	0/485
All	All	0.33	1/39016 (0.0%)	0.55	0/52949

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	GLY	C-N	-9.46	1.20	1.33

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	A	787	0	831	15	0
2	H	2494	0	2606	27	0
3	J	1273	0	1300	22	0
4	K	749	0	793	15	0
5	L	4806	0	4945	54	0
6	M	3647	0	3849	55	0
7	N	2723	0	2930	38	0
8	V	1028	0	1036	13	0
9	W	1155	0	1177	9	0
10	X	701	0	692	6	0
11	Y	1403	0	1392	16	0
12	Z	1441	0	1419	19	0
13	k	2596	0	2559	19	0
14	l	874	0	869	14	0
15	m	626	0	635	2	0
16	n	634	0	616	0	0
17	o	1004	0	995	11	0
18	p	1059	0	1062	9	0
19	q	1142	0	1137	12	0
20	r	846	0	864	9	0
21	s	1047	0	1015	9	0
22	t	1520	0	1477	17	0
23	u	563	0	509	4	0
24	v	1307	0	1207	9	0
25	w	846	0	792	13	0
26	x	412	0	411	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	y	436	0	437	2	0
28	z	576	0	570	8	0
29	4	334	0	304	2	0
30	A	37	0	48	1	0
30	H	54	0	88	3	0
30	L	54	0	88	3	0
30	M	54	0	88	6	0
30	w	54	0	88	10	0
31	H	23	0	30	0	0
32	H	51	0	82	1	0
32	K	40	0	54	4	0
32	L	122	0	172	1	0
32	M	44	0	65	1	0
32	N	51	0	82	4	0
32	V	72	0	92	1	0
32	m	51	0	82	0	0
32	o	31	0	36	0	0
32	p	27	0	27	1	0
33	L	100	0	156	7	0
33	M	90	0	133	7	0
33	V	179	0	261	6	0
33	W	100	0	156	6	0
33	Y	100	0	156	6	0
33	o	75	0	97	5	0
34	X	31	0	34	3	0
35	k	23	0	12	1	0
36	s	15	0	27	0	0
37	4	24	0	0	0	0
37	A	22	0	0	1	0
37	H	53	0	0	0	0
37	J	44	0	0	0	0
37	K	23	0	0	1	0
37	L	156	0	0	2	0
37	M	184	0	0	1	0
37	N	133	0	0	3	0
37	V	4	0	0	0	0
37	W	75	0	0	1	0
37	X	17	0	0	0	0
37	Y	46	0	0	2	0
37	Z	67	0	0	0	0
37	k	43	0	0	1	0
37	l	45	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	m	8	0	0	0	0
37	n	3	0	0	0	0
37	o	59	0	0	3	0
37	p	40	0	0	2	0
37	q	46	0	0	0	0
37	r	20	0	0	0	0
37	s	9	0	0	0	0
37	t	44	0	0	0	0
37	u	1	0	0	0	0
37	v	41	0	0	0	0
37	w	41	0	0	1	0
37	x	6	0	0	0	0
37	y	21	0	0	0	0
37	z	18	0	0	0	0
All	All	40800	0	40583	370	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (370) 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)
12:Z:119:SER:HB3	21:s:55:ARG:HH22	1.61	0.66
18:p:39:ARG:NH2	22:t:3:LEU:O	2.30	0.65
14:l:50:ARG:HA	14:l:53:LYS:HZ3	1.64	0.63
2:H:141:SER:HB3	2:H:289:LEU:HD22	1.79	0.63
7:N:243:LEU:HD22	7:N:330:THR:HG21	1.81	0.63
11:Y:165:ARG:NH1	17:o:87:ASP:OD1	2.32	0.63
19:q:81:ARG:NH1	19:q:85:MET:SD	2.71	0.62
2:H:237:PHE:O	2:H:241:LEU:HB2	2.00	0.61
3:J:117:PHE:HE1	7:N:91:ASN:HD21	1.49	0.61
30:M:502:PC1:H251	30:M:502:PC1:H372	1.81	0.61
5:L:370:THR:HG23	5:L:431:LEU:HD13	1.84	0.60
6:M:70:MET:HG2	6:M:103:GLN:HE21	1.67	0.60
7:N:320:THR:HB	13:k:1:LEU:HD21	1.83	0.60
5:L:249:SER:HB2	5:L:336:LYS:HG3	1.83	0.59
14:l:27:ARG:NH1	37:l:202:HOH:O	2.36	0.59
8:V:39:SER:OG	8:V:54:ARG:NH2	2.36	0.59
5:L:161:ARG:HA	22:t:91:GLU:HG3	1.85	0.59
7:N:45:MET:HE3	7:N:53:THR:HG22	1.85	0.59
11:Y:89:ASP:OD2	28:z:34:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:w:100:ARG:HB2	25:w:105:LEU:HB2	1.85	0.58
4:K:23:ARG:HG2	32:K:101:3PE:H11	1.86	0.58
15:m:83:LEU:HD13	19:q:54:ARG:HD3	1.86	0.58
17:o:45:ASP:OD2	17:o:51:ARG:NH2	2.36	0.58
4:K:73:LEU:HD11	7:N:41:ILE:HG13	1.85	0.58
18:p:39:ARG:NH1	37:p:304:HOH:O	2.37	0.57
21:s:6:ARG:HH12	21:s:105:ARG:HD2	1.69	0.57
5:L:103:PHE:HB2	5:L:341:MET:HE3	1.86	0.57
8:V:11:ILE:HB	8:V:20:LYS:HD3	1.84	0.57
5:L:100:ILE:HG21	5:L:246:LEU:HB2	1.85	0.57
12:Z:67:PHE:HD1	27:y:43:LEU:HD21	1.69	0.57
5:L:570:GLN:OE1	7:N:167:TRP:NE1	2.35	0.57
2:H:26:LYS:HB3	28:z:5:VAL:HG12	1.86	0.57
6:M:133:ILE:HD11	6:M:231:LEU:HD11	1.87	0.56
2:H:10:ILE:HA	2:H:13:ILE:HD12	1.87	0.56
18:p:47:GLN:HG3	22:t:165:LEU:HD13	1.86	0.56
18:p:62:PRO:O	18:p:66:ARG:HB2	2.06	0.56
9:W:133:ILE:HD13	14:l:37:LYS:HG2	1.87	0.56
33:L:704:CDL:H431	30:w:801:PC1:H291	1.87	0.56
33:M:503:CDL:H352	33:M:503:CDL:H612	1.88	0.55
1:A:60:ILE:HG21	3:J:168:ILE:HG21	1.88	0.55
15:m:78:GLU:OE1	15:m:82:ARG:NH1	2.39	0.55
7:N:106:LEU:HD22	7:N:187:MET:HE2	1.86	0.55
11:Y:66:ALA:O	11:Y:69:PHE:HB3	2.07	0.55
5:L:90:VAL:HG22	5:L:129:LEU:HD22	1.89	0.55
5:L:10:VAL:HG21	20:r:78:VAL:HG22	1.88	0.54
17:o:86:ARG:NH1	37:o:603:HOH:O	2.40	0.54
5:L:161:ARG:NH2	22:t:90:TYR:O	2.37	0.54
32:H:502:3PE:H2B2	32:H:502:3PE:H352	1.90	0.54
32:M:501:3PE:H221	8:V:87:LEU:HB2	1.90	0.54
5:L:316:THR:HA	5:L:319:ILE:HG12	1.89	0.54
5:L:536:LEU:HG	5:L:540:MET:HE2	1.90	0.54
2:H:24:GLU:OE2	2:H:274:ARG:NH1	2.41	0.54
7:N:331:VAL:HG13	7:N:335:MET:HE3	1.90	0.54
13:k:294:GLN:NE2	37:k:605:HOH:O	2.41	0.54
25:w:114:ASP:HB3	25:w:117:LYS:HG2	1.89	0.54
14:l:104:ARG:NH1	19:q:84:GLN:OE1	2.41	0.53
7:N:338:PRO:HG3	33:Y:201:CDL:H792	1.90	0.53
5:L:128:MET:HG2	5:L:251:THR:HG22	1.90	0.53
6:M:457:PRO:O	25:w:84:ARG:NH1	2.37	0.53
24:v:137:ASN:O	24:v:142:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:211:MET:HG2	7:N:333:SER:HB2	1.90	0.53
24:v:54:SER:HA	24:v:84:TYR:HB3	1.91	0.53
5:L:309:GLN:NE2	37:L:827:HOH:O	2.40	0.53
5:L:543:THR:HG23	24:v:83:MET:HE1	1.91	0.53
6:M:36:LEU:HB2	25:w:69:VAL:HG22	1.90	0.53
2:H:134:ARG:HH11	2:H:282:TYR:HB2	1.74	0.53
33:V:204:CDL:H362	33:V:204:CDL:H542	1.91	0.52
13:k:173:ASP:OD1	13:k:207:LYS:NZ	2.41	0.52
22:t:29:ARG:HD2	22:t:75:HIS:CD2	2.45	0.52
6:M:155:ALA:HB1	30:M:502:PC1:H2H2	1.92	0.52
5:L:279:CYS:SG	5:L:405:ASN:ND2	2.83	0.52
6:M:5:ILE:HG22	6:M:9:MET:HE2	1.92	0.52
7:N:252:GLY:HA3	7:N:290:LEU:HD13	1.91	0.52
5:L:193:LEU:HD23	5:L:201:ILE:HA	1.92	0.52
7:N:217:THR:HG23	32:N:401:3PE:H242	1.91	0.52
13:k:170:ILE:HD11	13:k:238:ILE:HD11	1.92	0.52
6:M:116:ILE:HD11	6:M:161:LEU:HD12	1.92	0.51
6:M:173:SER:HB2	9:W:101:ALA:HB2	1.92	0.51
1:A:53:MET:HE2	3:J:172:THR:HB	1.93	0.51
4:K:70:GLU:OE1	37:K:201:HOH:O	2.19	0.51
17:o:45:ASP:OD1	17:o:49:ARG:NH2	2.43	0.51
30:L:703:PC1:H3A1	20:r:80:ILE:HG23	1.93	0.51
33:L:704:CDL:H631	6:M:445:LEU:HD22	1.93	0.51
33:V:203:CDL:H512	33:V:204:CDL:H121	1.93	0.51
30:L:703:PC1:H32	30:w:801:PC1:H142	1.91	0.51
8:V:139:LYS:HG3	8:V:140:VAL:HG13	1.91	0.51
4:K:14:VAL:HG22	32:K:101:3PE:H2B2	1.93	0.51
2:H:149:ILE:HG21	2:H:185:TRP:HB2	1.92	0.51
23:u:40:PHE:O	23:u:44:SER:OG	2.26	0.51
2:H:180:PRO:HB3	30:H:503:PC1:H261	1.93	0.51
37:L:817:HOH:O	20:r:92:LYS:NZ	2.44	0.51
6:M:416:ARG:NH2	37:M:630:HOH:O	2.43	0.51
11:Y:35:CYS:O	11:Y:39:ASN:ND2	2.44	0.51
6:M:232:ALA:O	6:M:237:LYS:NZ	2.44	0.50
2:H:14:LEU:HD22	2:H:225:MET:HE2	1.94	0.50
33:V:203:CDL:HB31	33:V:204:CDL:H122	1.93	0.50
5:L:213:LEU:HD23	5:L:216:LEU:HD12	1.94	0.50
6:M:91:ARG:NH2	13:k:290:ASP:OD2	2.44	0.50
6:M:101:LEU:HD21	33:M:503:CDL:H841	1.93	0.50
33:o:502:CDL:H732	33:o:502:CDL:HB4	1.93	0.50
5:L:542:LEU:HB2	24:v:83:MET:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:k:128:ILE:HD12	13:k:160:VAL:HG23	1.94	0.50
5:L:593:ILE:HD12	8:V:41:ALA:HB2	1.94	0.49
7:N:159:ILE:HG21	7:N:278:LEU:HD11	1.93	0.49
33:L:704:CDL:H562	33:L:704:CDL:H642	1.94	0.49
21:s:7:ARG:HH21	21:s:17:GLU:HG3	1.77	0.49
7:N:207:ILE:HG22	7:N:211:MET:HE2	1.95	0.49
12:Z:5:ASP:HB3	12:Z:8:VAL:HG12	1.94	0.49
13:k:173:ASP:HB2	13:k:224:SER:HA	1.95	0.49
26:x:41:GLU:OE2	26:x:44:ARG:NH2	2.40	0.49
1:A:67:LEU:HD22	4:K:65:VAL:HA	1.94	0.49
34:X:101:ZMP:H5A	22:t:43:LEU:HD11	1.95	0.49
13:k:51:PHE:HB3	13:k:107:GLN:HE21	1.78	0.49
1:A:114:THR:HB	2:H:286:MET:HG3	1.93	0.49
6:M:9:MET:HE1	33:Y:201:CDL:H162	1.94	0.49
9:W:111:ARG:NH2	37:W:312:HOH:O	2.46	0.49
6:M:328:CYS:HB3	6:M:437:MET:HE1	1.94	0.49
3:J:21:SER:O	3:J:23:LYS:NZ	2.45	0.49
5:L:129:LEU:HA	5:L:132:VAL:HG22	1.94	0.48
11:Y:97:ARG:HD3	19:q:59:LEU:HD13	1.94	0.48
7:N:325:LEU:HD11	33:o:502:CDL:H722	1.94	0.48
1:A:73:LEU:HD13	3:J:55:MET:HE1	1.95	0.48
6:M:408:LEU:O	6:M:412:ILE:N	2.44	0.48
9:W:125:TYR:HB2	14:l:48:SER:HB3	1.95	0.48
11:Y:48:GLU:OE1	11:Y:134:ARG:NH2	2.43	0.48
12:Z:5:ASP:OD2	25:w:98:LYS:NZ	2.45	0.48
14:l:64:GLU:HG3	14:l:70:LYS:HD2	1.96	0.48
32:K:101:3PE:H3C2	5:L:592:LEU:HD21	1.96	0.48
12:Z:159:LYS:HE2	25:w:118:ILE:HG23	1.96	0.48
6:M:94:LEU:HD21	33:M:503:CDL:H551	1.95	0.48
34:X:101:ZMP:O6	22:t:12:GLN:NE2	2.44	0.48
3:J:45:LEU:HD23	3:J:50:SER:HA	1.95	0.48
12:Z:136:LYS:NZ	12:Z:140:ASP:OD2	2.42	0.48
6:M:179:LEU:HD13	6:M:249:LEU:HD11	1.94	0.48
7:N:202:LEU:HD21	14:l:1:PRO:HD3	1.96	0.48
22:t:27:GLU:OE2	22:t:33:ARG:NH1	2.46	0.48
3:J:124:ASP:OD1	3:J:124:ASP:N	2.47	0.48
33:M:503:CDL:H821	33:M:503:CDL:H851	1.60	0.48
12:Z:26:PRO:HB2	12:Z:31:TYR:HE2	1.79	0.48
18:p:41:ARG:NH1	37:p:309:HOH:O	2.46	0.48
1:A:67:LEU:HB3	4:K:65:VAL:HG13	1.96	0.47
1:A:70:ALA:HA	1:A:73:LEU:HD12	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:8:LEU:H	10:X:87:TYR:HE2	1.62	0.47
2:H:97:ASN:H	19:q:143:THR:HG22	1.78	0.47
6:M:369:LEU:HD12	6:M:370:PRO:HD2	1.96	0.47
6:M:73:LEU:HA	6:M:76:MET:HE3	1.97	0.47
10:X:88:GLU:HA	20:r:22:LEU:HB3	1.95	0.47
11:Y:165:ARG:NH2	37:Y:309:HOH:O	2.48	0.47
13:k:113:GLU:OE1	13:k:266:LYS:NZ	2.43	0.47
1:A:63:LEU:HB2	3:J:67:VAL:HG21	1.95	0.47
2:H:20:LEU:HD13	28:z:12:MET:HE1	1.96	0.47
2:H:46:LEU:HD13	2:H:49:ILE:HD13	1.96	0.47
5:L:221:THR:HG23	5:L:226:GLN:HB2	1.96	0.47
19:q:92:GLU:HA	19:q:95:THR:HG22	1.96	0.47
21:s:21:MET:HE1	21:s:101:PHE:HA	1.95	0.47
14:l:53:LYS:HG3	14:l:54:GLU:HG3	1.96	0.47
2:H:296:LEU:HD13	30:H:503:PC1:H252	1.97	0.47
33:L:704:CDL:H621	6:M:372:SER:HB3	1.97	0.46
19:q:67:ARG:NE	19:q:71:MET:SD	2.88	0.46
5:L:1:FME:HG3	5:L:61:MET:HE1	1.97	0.46
5:L:233:LEU:HD23	5:L:307:SER:HB3	1.96	0.46
5:L:487:LYS:HE3	23:u:49:GLY:HA2	1.98	0.46
6:M:78:MET:HE2	25:w:61:VAL:HG22	1.96	0.46
10:X:65:ILE:HD13	22:t:3:LEU:HD22	1.96	0.46
5:L:56:HIS:ND1	5:L:57:THR:HG23	2.30	0.46
7:N:144:GLN:NE2	37:N:521:HOH:O	2.47	0.46
12:Z:145:LEU:HD22	12:Z:153:LYS:HB3	1.96	0.46
20:r:17:LEU:HD11	22:t:162:LEU:HD22	1.97	0.46
33:M:503:CDL:H873	7:N:257:LEU:HD11	1.96	0.46
3:J:43:ILE:HG22	4:K:46:LEU:HD21	1.96	0.46
3:J:88:VAL:HG11	32:K:101:3PE:H2	1.98	0.46
7:N:115:VAL:HG12	7:N:180:ALA:HB1	1.97	0.46
6:M:106:LEU:HD13	6:M:234:ILE:HG21	1.98	0.46
33:W:201:CDL:H112	12:Z:51:ILE:HD11	1.97	0.46
13:k:108:TYR:OH	13:k:164:LEU:O	2.31	0.46
5:L:429:PHE:O	5:L:436:ARG:NH2	2.48	0.46
5:L:203:MET:HB2	12:Z:113:GLN:HG3	1.98	0.46
20:r:85:LEU:HD22	20:r:96:ILE:HD11	1.98	0.46
21:s:6:ARG:NH1	21:s:15:GLU:OE2	2.49	0.46
5:L:83:ASP:OD2	5:L:262:ARG:NH1	2.49	0.46
11:Y:39:ASN:ND2	37:Y:310:HOH:O	2.48	0.46
33:L:704:CDL:H801	30:w:801:PC1:H2F2	1.97	0.45
6:M:23:ILE:HD11	6:M:92:LYS:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:452:LYS:NZ	37:w:902:HOH:O	2.41	0.45
12:Z:98:ASP:OD2	12:Z:142:TYR:OH	2.34	0.45
2:H:42:PRO:HD2	2:H:46:LEU:HD23	1.97	0.45
6:M:447:LEU:HD11	30:w:801:PC1:H3F1	1.96	0.45
7:N:49:ASN:ND2	29:4:35:ASP:O	2.49	0.45
33:Y:201:CDL:H641	33:Y:201:CDL:H872	1.99	0.45
12:Z:3:SER:OG	12:Z:4:TRP:N	2.49	0.45
18:p:82:ASN:HA	32:p:201:3PE:H12	1.98	0.45
6:M:233:ALA:HA	6:M:320:GLY:HA2	1.99	0.45
33:W:201:CDL:HB62	30:w:801:PC1:H153	1.99	0.45
6:M:98:MET:HE1	33:M:503:CDL:H822	1.98	0.45
14:l:74:ARG:NH2	19:q:93:GLU:OE2	2.49	0.45
6:M:91:ARG:HD3	6:M:135:ARG:HH21	1.82	0.45
13:k:30:ASN:N	13:k:33:SER:OG	2.47	0.45
18:p:47:GLN:HA	18:p:50:TYR:HB3	1.99	0.45
1:A:83:ASN:ND2	30:A:201:PC1:O14	2.39	0.45
22:t:33:ARG:O	22:t:37:ARG:HB2	2.16	0.45
2:H:24:GLU:HG3	2:H:271:LEU:HD22	1.99	0.45
3:J:113:VAL:HG12	3:J:119:PHE:HB2	1.98	0.45
6:M:18:SER:HB2	6:M:23:ILE:HG22	1.98	0.45
11:Y:118:ARG:NH2	19:q:62:GLU:OE2	2.49	0.45
11:Y:27:ALA:HB1	11:Y:69:PHE:HE2	1.82	0.45
5:L:97:THR:HG21	5:L:125:LEU:HD22	1.98	0.45
5:L:137:LEU:HD21	5:L:263:PHE:HZ	1.81	0.45
5:L:416:THR:O	5:L:419:THR:OG1	2.33	0.45
33:M:503:CDL:HA61	17:o:53:VAL:HG21	1.98	0.45
8:V:65:ILE:HD11	8:V:100:LEU:HD23	1.99	0.45
10:X:69:LYS:HA	20:r:2:GLY:HA2	1.98	0.45
5:L:128:MET:HE1	5:L:255:ALA:HB2	1.97	0.44
3:J:139:GLU:HG3	4:K:49:LEU:HD21	2.00	0.44
8:V:1:AYA:HA	8:V:4:LEU:HD23	1.98	0.44
14:l:20:GLN:NE2	37:l:209:HOH:O	2.49	0.44
22:t:137:LYS:HA	22:t:140:GLN:HG2	1.99	0.44
6:M:14:LEU:O	6:M:18:SER:OG	2.31	0.44
6:M:75:LEU:HD23	6:M:440:HIS:CE1	2.53	0.44
6:M:139:GLN:O	6:M:142:ARG:NH1	2.50	0.44
6:M:159:PRO:HG2	30:M:502:PC1:H3D2	1.98	0.44
6:M:272:THR:HA	6:M:275:ILE:HD12	1.98	0.44
7:N:289:ASN:HA	7:N:292:PHE:CE1	2.52	0.44
9:W:44:ASN:ND2	33:W:201:CDL:OB4	2.45	0.44
8:V:116:TYR:HB2	33:V:204:CDL:H372	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:PRO:HB2	2:H:60:PRO:HD3	2.00	0.44
1:A:69:ILE:HD11	2:H:144:VAL:HG13	1.99	0.44
2:H:45:LEU:HD21	28:z:7:PRO:HB2	2.00	0.44
13:k:174:VAL:HG22	13:k:225:ALA:HB2	1.98	0.44
6:M:427:LEU:HD21	18:p:56:ARG:HH12	1.83	0.44
33:Y:201:CDL:H632	33:Y:201:CDL:H601	1.83	0.44
21:s:102:GLU:OE2	21:s:105:ARG:NH2	2.50	0.44
21:s:8:TYR:OH	24:v:123:PRO:O	2.33	0.44
6:M:126:LEU:HD21	6:M:153:THR:HG21	2.00	0.44
12:Z:15:ARG:HB3	20:r:109:ILE:HD12	2.00	0.44
2:H:70:MET:HE1	3:J:27:ILE:HG22	2.00	0.43
7:N:133:TRP:HE3	32:N:401:3PE:H3A2	1.82	0.43
22:t:107:HIS:NE2	25:w:43:ASP:OD1	2.40	0.43
6:M:403:THR:HA	6:M:406:TYR:CE1	2.53	0.43
5:L:180:ILE:HD13	32:L:702:3PE:H2H2	2.00	0.43
5:L:485:TYR:OH	21:s:1:GLY:N	2.42	0.43
9:W:28:TYR:O	25:w:67:SER:OG	2.31	0.43
5:L:402:SER:OG	5:L:404:THR:OG1	2.34	0.43
30:L:703:PC1:H262	33:W:201:CDL:H621	2.01	0.43
6:M:36:LEU:HD23	25:w:69:VAL:HA	1.99	0.43
8:V:13:GLU:OE2	8:V:89:TYR:OH	2.32	0.43
33:W:201:CDL:H841	33:W:201:CDL:H812	1.82	0.43
28:z:34:ARG:NH2	28:z:61:TYR:O	2.32	0.43
4:K:53:PHE:CG	14:l:20:GLN:HG2	2.53	0.43
6:M:243:MET:HB3	6:M:301:ILE:HG21	2.01	0.43
7:N:110:PRO:HD3	7:N:160:LEU:HD23	2.00	0.43
22:t:134:ARG:HA	22:t:137:LYS:HE3	2.01	0.43
2:H:293:PHE:O	2:H:297:THR:OG1	2.29	0.43
5:L:245:ALA:O	5:L:249:SER:OG	2.36	0.43
23:u:61:ASP:HB3	23:u:66:ILE:HB	2.01	0.43
4:K:55:LEU:HD13	14:l:16:TRP:HE3	1.83	0.43
7:N:206:ILE:HG23	32:N:401:3PE:H2I2	2.00	0.43
12:Z:81:VAL:HG23	12:Z:82:LEU:HD22	1.99	0.43
22:t:26:LEU:O	22:t:30:CYS:HB2	2.18	0.43
5:L:66:TRP:NE1	30:w:801:PC1:O12	2.39	0.43
9:W:138:LYS:HA	14:l:27:ARG:HB3	2.01	0.43
17:o:8:ARG:NH1	37:o:608:HOH:O	2.52	0.43
2:H:189:THR:HG22	2:H:234:MET:HE3	2.01	0.42
5:L:82:MET:HB3	5:L:87:MET:HE3	2.00	0.42
30:M:502:PC1:H221	30:M:502:PC1:H252	1.93	0.42
27:y:8:ARG:HG3	27:y:10:HIS:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:79:LEU:HD11	2:H:222:LEU:HD22	2.00	0.42
6:M:120:ILE:HG22	6:M:121:MET:HE2	2.01	0.42
33:V:203:CDL:H412	33:V:203:CDL:H441	1.85	0.42
6:M:337:VAL:HG11	6:M:345:ALA:HB2	2.01	0.42
10:X:49:GLU:OE2	22:t:19:TYR:OH	2.35	0.42
11:Y:15:GLN:O	11:Y:63:ASN:ND2	2.52	0.42
17:o:52:PRO:HG2	17:o:56:ALA:HB2	2.01	0.42
5:L:7:LEU:HD22	5:L:46:THR:HG23	2.02	0.42
6:M:258:ALA:HB1	6:M:302:LEU:HB3	2.01	0.42
33:Y:201:CDL:H571	33:Y:201:CDL:H152	2.01	0.42
14:l:16:TRP:H	14:l:16:TRP:CD1	2.37	0.42
1:A:75:LEU:HD12	2:H:151:LEU:HD21	2.02	0.42
3:J:163:ILE:HG21	7:N:12:THR:HG21	2.02	0.42
11:Y:39:ASN:HB3	19:q:72:PRO:HG2	2.02	0.42
21:s:3:HIS:CE1	24:v:127:PRO:HD3	2.55	0.42
3:J:7:PHE:O	3:J:11:ILE:HG12	2.20	0.42
9:W:122:TRP:CD1	17:o:2:MET:HG2	2.53	0.42
11:Y:82:THR:HA	11:Y:85:TRP:CD1	2.55	0.42
33:Y:201:CDL:H571	33:Y:201:CDL:H171	2.01	0.42
17:o:8:ARG:NH2	37:o:607:HOH:O	2.52	0.42
24:v:138:LEU:HB3	24:v:141:GLU:HB2	2.02	0.42
3:J:24:PRO:HB3	3:J:89:VAL:HG11	2.01	0.42
13:k:131:ASP:OD2	13:k:152:TYR:OH	2.33	0.42
5:L:1:FME:HE2	5:L:1:FME:HB2	1.73	0.42
33:L:704:CDL:H671	33:L:704:CDL:H401	2.00	0.42
6:M:71:TRP:CG	30:w:801:PC1:H3C2	2.55	0.42
11:Y:17:VAL:HG12	11:Y:19:VAL:HG22	2.02	0.42
13:k:104:ARG:NH1	13:k:126:ARG:O	2.53	0.42
33:o:502:CDL:H132	33:o:502:CDL:H522	2.01	0.42
7:N:222:ASN:HD21	7:N:240:MET:HB3	1.85	0.41
11:Y:90:TYR:HA	28:z:34:ARG:HG2	2.02	0.41
24:v:80:ASP:HB3	24:v:83:MET:HB3	2.02	0.41
5:L:49:ILE:HG12	12:Z:32:LEU:HD13	2.01	0.41
6:M:1:FME:O1	6:M:3:LYS:NZ	2.51	0.41
30:M:502:PC1:H262	30:M:502:PC1:H292	1.92	0.41
7:N:135:LYS:NZ	37:N:525:HOH:O	2.53	0.41
12:Z:141:ARG:HG3	25:w:112:CYS:HB2	2.01	0.41
13:k:49:LYS:HE3	13:k:51:PHE:HE1	1.85	0.41
13:k:52:PRO:O	13:k:107:GLN:NE2	2.53	0.41
25:w:78:ALA:HB2	30:w:801:PC1:H31	2.03	0.41
28:z:51:ASP:HA	28:z:54:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:207:MET:HE3	6:M:294:MET:HB3	2.02	0.41
2:H:123:SER:HB2	2:H:214:GLU:HG3	2.03	0.41
5:L:316:THR:HG23	5:L:325:ALA:HB2	2.02	0.41
7:N:275:SER:HB3	8:V:136:ALA:HB3	2.03	0.41
11:Y:100:ARG:NH1	11:Y:103:GLN:OE1	2.46	0.41
13:k:115:LEU:HD13	13:k:121:GLY:HA2	2.02	0.41
3:J:24:PRO:HA	3:J:89:VAL:HG21	2.03	0.41
6:M:391:ILE:HB	18:p:104:PHE:HE1	1.86	0.41
30:M:502:PC1:H371	7:N:280:THR:HG21	2.02	0.41
32:N:401:3PE:H2E1	32:N:401:3PE:H2H1	1.88	0.41
3:J:23:LYS:HE2	4:K:23:ARG:HG3	2.02	0.41
5:L:96:VAL:O	5:L:100:ILE:HG12	2.20	0.41
5:L:204:LEU:HD23	5:L:204:LEU:HA	1.89	0.41
7:N:316:GLN:NE2	37:N:512:HOH:O	2.53	0.41
17:o:39:TYR:HD1	17:o:65:ILE:HD11	1.84	0.41
33:o:502:CDL:H311	33:o:502:CDL:H511	2.03	0.41
2:H:187:ILE:HD12	30:H:503:PC1:H351	2.02	0.41
8:V:82:LYS:O	8:V:88:ASN:ND2	2.54	0.41
9:W:37:VAL:HG21	33:W:201:CDL:H811	2.02	0.41
10:X:26:ASP:OD1	10:X:26:ASP:N	2.53	0.41
1:A:53:MET:N	37:A:305:HOH:O	2.54	0.41
2:H:64:ALA:O	2:H:124:ASN:ND2	2.42	0.41
4:K:44:ALA:HA	4:K:47:MET:HE3	2.02	0.41
12:Z:81:VAL:HA	12:Z:84:MET:HG2	2.02	0.41
5:L:25:ASN:HD22	5:L:29:PHE:HE2	1.68	0.41
5:L:142:ILE:HG12	6:M:370:PRO:HB2	2.03	0.41
5:L:152:PHE:HB2	5:L:172:ILE:HD11	2.02	0.41
7:N:295:ARG:NH2	29:4:20:TYR:OH	2.53	0.41
12:Z:48:ARG:HG2	20:r:87:TYR:CE1	2.56	0.41
22:t:142:GLU:OE2	22:t:157:ARG:NH2	2.54	0.41
30:w:801:PC1:H282	30:w:801:PC1:H2B1	1.85	0.41
4:K:63:LEU:HD13	7:N:71:MET:HE3	2.02	0.41
5:L:7:LEU:HD23	5:L:7:LEU:HA	1.93	0.41
6:M:452:LYS:HA	6:M:455:LEU:HD12	2.02	0.41
7:N:325:LEU:HD21	33:o:502:CDL:H731	2.03	0.41
13:k:180:GLN:NE2	13:k:196:SER:OG	2.40	0.41
19:q:117:THR:HA	19:q:118:PRO:HD3	1.97	0.41
4:K:20:LEU:HD13	5:L:588:PHE:HD1	1.85	0.40
4:K:55:LEU:HA	4:K:55:LEU:HD23	1.90	0.40
5:L:375:ILE:HG12	23:u:32:MET:SD	2.61	0.40
6:M:68:LEU:HB2	30:w:801:PC1:H3G1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:225:ILE:HD13	6:M:331:ASN:HB2	2.03	0.40
7:N:267:ILE:HG12	7:N:279:PRO:HB2	2.03	0.40
8:V:37:ALA:HA	32:V:201:3PE:H2A1	2.03	0.40
13:k:104:ARG:HH21	35:k:501:AMP:H8	1.69	0.40
1:A:74:PRO:HB3	3:J:143:ILE:HG22	2.02	0.40
3:J:134:GLY:HA2	28:z:43:TYR:HB2	2.03	0.40
5:L:402:SER:HG	5:L:404:THR:HG1	1.68	0.40
7:N:100:MET:HE1	33:V:203:CDL:H272	2.03	0.40
34:X:101:ZMP:H15	34:X:101:ZMP:H17	1.65	0.40
17:o:46:ASN:ND2	17:o:61:GLN:HE21	2.19	0.40
5:L:421:ILE:HG12	5:L:501:ALA:HB2	2.03	0.40
33:L:704:CDL:H512	33:L:704:CDL:H541	1.90	0.40
6:M:282:LEU:HD21	6:M:359:TRP:HH2	1.87	0.40
8:V:54:ARG:HG2	8:V:57:ARG:HH22	1.85	0.40
5:L:591:PHE:CE1	7:N:111:PHE:HA	2.56	0.40
6:M:158:LEU:HD23	7:N:283:ALA:HB1	2.03	0.40
7:N:140:SER:O	7:N:144:GLN:HG3	2.22	0.40
12:Z:162:MET:HE2	25:w:120:LEU:HD21	2.02	0.40
24:v:47:TYR:HA	24:v:48:PRO:HD3	1.97	0.40
1:A:74:PRO:HG2	3:J:147:TYR:HE2	1.87	0.40
3:J:2:MET:HB3	19:q:133:LEU:HD11	2.03	0.40
6:M:207:MET:HE3	6:M:207:MET:HB3	1.94	0.40
6:M:253:ILE:HG12	6:M:257:MET:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	93/115 (81%)	89 (96%)	4 (4%)	0	100	100
2	H	309/318 (97%)	304 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	163/175 (93%)	156 (96%)	7 (4%)	0	100	100
4	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
5	L	604/606 (100%)	583 (96%)	21 (4%)	0	100	100
6	M	457/459 (100%)	452 (99%)	5 (1%)	0	100	100
7	N	345/347 (99%)	336 (97%)	9 (3%)	0	100	100
8	V	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
9	W	137/189 (72%)	137 (100%)	0	0	100	100
10	X	85/157 (54%)	83 (98%)	2 (2%)	0	100	100
11	Y	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
12	Z	169/175 (97%)	167 (99%)	2 (1%)	0	100	100
13	k	317/355 (89%)	309 (98%)	8 (2%)	0	100	100
14	l	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
15	m	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
16	n	77/98 (79%)	76 (99%)	1 (1%)	0	100	100
17	o	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
18	p	126/130 (97%)	123 (98%)	3 (2%)	0	100	100
19	q	137/144 (95%)	135 (98%)	2 (2%)	0	100	100
20	r	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
21	s	120/137 (88%)	116 (97%)	4 (3%)	0	100	100
22	t	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
23	u	63/108 (58%)	61 (97%)	2 (3%)	0	100	100
24	v	153/186 (82%)	147 (96%)	6 (4%)	0	100	100
25	w	99/154 (64%)	94 (95%)	5 (5%)	0	100	100
26	x	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
27	y	48/58 (83%)	48 (100%)	0	0	100	100
28	z	68/70 (97%)	68 (100%)	0	0	100	100
29	4	38/463 (8%)	36 (95%)	2 (5%)	0	100	100
All	All	4627/5550 (83%)	4511 (98%)	116 (2%)	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	A	88/103 (85%)	88 (100%)	0	100	100
2	H	274/278 (99%)	272 (99%)	2 (1%)	76	89
3	J	136/144 (94%)	136 (100%)	0	100	100
4	K	86/86 (100%)	86 (100%)	0	100	100
5	L	538/538 (100%)	537 (100%)	1 (0%)	87	95
6	M	411/411 (100%)	411 (100%)	0	100	100
7	N	315/315 (100%)	315 (100%)	0	100	100
8	V	101/102 (99%)	101 (100%)	0	100	100
9	W	122/160 (76%)	122 (100%)	0	100	100
10	X	80/141 (57%)	80 (100%)	0	100	100
11	Y	154/155 (99%)	154 (100%)	0	100	100
12	Z	155/157 (99%)	155 (100%)	0	100	100
13	k	283/309 (92%)	283 (100%)	0	100	100
14	l	94/95 (99%)	94 (100%)	0	100	100
15	m	69/72 (96%)	69 (100%)	0	100	100
16	n	61/76 (80%)	61 (100%)	0	100	100
17	o	107/109 (98%)	107 (100%)	0	100	100
18	p	114/116 (98%)	114 (100%)	0	100	100
19	q	119/122 (98%)	119 (100%)	0	100	100
20	r	95/122 (78%)	95 (100%)	0	100	100
21	s	110/120 (92%)	110 (100%)	0	100	100
22	t	159/161 (99%)	159 (100%)	0	100	100
23	u	59/84 (70%)	59 (100%)	0	100	100
24	v	140/160 (88%)	140 (100%)	0	100	100
25	w	92/130 (71%)	92 (100%)	0	100	100
26	x	44/67 (66%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	y	46/54 (85%)	46 (100%)	0	100	100
28	z	59/59 (100%)	59 (100%)	0	100	100
29	4	34/392 (9%)	34 (100%)	0	100	100
All	All	4145/4838 (86%)	4142 (100%)	3 (0%)	87	96

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

Mol	Chain	Res	Type
2	H	241	LEU
2	H	259	PHE
5	L	589	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	235	ASN
2	H	317	GLN
5	L	135	ASN
5	L	192	ASN
5	L	199	GLN
5	L	269	ASN
5	L	405	ASN
5	L	434	GLN
5	L	446	ASN
5	L	471	ASN
5	L	506	ASN
6	M	82	HIS
6	M	138	ASN
6	M	144	ASN
6	M	169	ASN
6	M	338	HIS
6	M	374	ASN
6	M	415	GLN
7	N	48	HIS
7	N	134	GLN
7	N	144	GLN
7	N	197	ASN
8	V	18	HIS
9	W	124	GLN
11	Y	76	HIS

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Mol	Chain	Res	Type
11	Y	142	HIS
12	Z	106	GLN
13	k	251	GLN
14	l	100	GLN
17	o	12	GLN
17	o	61	GLN
19	q	23	ASN
22	t	50	HIS
22	t	72	HIS
24	v	55	GLN
24	v	87	ASN
25	w	27	GLN
26	x	9	HIS
26	x	34	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
13	SEP	k	36	13	8,9,10	1.61	1 (12%)	7,12,14	1.13	1 (14%)
6	FME	M	1	6	8,9,10	1.01	1 (12%)	8,9,11	0.97	0
5	FME	L	1	5	8,9,10	0.96	0	8,9,11	1.35	2 (25%)
8	AYA	V	1	8	6,7,8	1.27	1 (16%)	6,8,10	1.83	2 (33%)
4	FME	K	1	4	8,9,10	0.97	0	8,9,11	0.84	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
13	SEP	k	36	13	-	3/6/8/10	-
6	FME	M	1	6	-	2/7/9/11	-
5	FME	L	1	5	-	3/7/9/11	-
8	AYA	V	1	8	-	3/5/6/8	-
4	FME	K	1	4	-	3/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	k	36	SEP	P-O1P	3.54	1.61	1.50
8	V	1	AYA	CA-N	-2.30	1.44	1.46
6	M	1	FME	CA-N	-2.10	1.43	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	1	AYA	CA-N-CT	2.98	125.35	121.50
8	V	1	AYA	CB-CA-N	2.87	112.92	109.68
5	L	1	FME	C-CA-N	2.65	114.61	109.50
5	L	1	FME	CA-N-CN	2.41	126.53	122.82
13	k	36	SEP	OG-CB-CA	2.22	110.31	108.14

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	1	FME	O1-CN-N-CA
6	M	1	FME	C-CA-CB-CG
8	V	1	AYA	O-C-CA-CB
13	k	36	SEP	CB-OG-P-O1P
13	k	36	SEP	CB-OG-P-O2P
13	k	36	SEP	CB-OG-P-O3P
8	V	1	AYA	OT-CT-N-CA
8	V	1	AYA	CM-CT-N-CA
5	L	1	FME	CA-CB-CG-SD
4	K	1	FME	CA-CB-CG-SD
5	L	1	FME	N-CA-CB-CG
6	M	1	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
5	L	1	FME	CB-CG-SD-CE
4	K	1	FME	CB-CG-SD-CE

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	1	FME	1	0
5	L	1	FME	2	0
8	V	1	AYA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

28 ligands 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	$\# Z > 2$
32	3PE	M	501	-	43,43,50	0.32	0	46,48,55	0.57	2 (4%)
32	3PE	m	101	-	50,50,50	0.31	0	53,55,55	0.43	0
33	CDL	o	502	-	74,74,99	0.34	0	80,86,111	0.52	1 (1%)
32	3PE	H	502	-	50,50,50	0.31	0	53,55,55	0.44	1 (1%)
32	3PE	L	702	-	50,50,50	0.31	0	53,55,55	0.37	0
36	MYR	s	201	21	13,14,15	0.15	0	12,13,15	0.16	0
32	3PE	N	401	-	50,50,50	0.31	0	53,55,55	0.53	2 (3%)
31	DCQ	H	501	-	23,23,23	0.16	0	27,29,29	0.66	0
33	CDL	M	503	-	89,89,99	0.31	0	95,101,111	0.42	0
33	CDL	L	704	-	99,99,99	0.29	0	105,111,111	0.41	1 (0%)
32	3PE	V	202	-	36,36,50	0.34	0	39,41,55	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	3PE	V	201	-	34,34,50	0.36	0	37,39,55	0.30	0
30	PC1	A	201	-	36,36,53	0.37	0	42,44,61	0.63	2 (4%)
32	3PE	L	705	-	30,30,50	0.41	0	33,35,55	0.81	2 (6%)
32	3PE	L	701	-	39,39,50	0.34	0	42,44,55	0.36	0
35	AMP	k	501	-	25,25,25	1.42	4 (16%)	37,38,38	1.93	7 (18%)
30	PC1	H	503	-	53,53,53	0.31	0	59,61,61	0.51	0
32	3PE	p	201	-	26,26,50	0.48	0	29,31,55	0.50	1 (3%)
32	3PE	o	501	-	30,30,50	0.38	0	33,35,55	0.46	0
30	PC1	w	801	-	53,53,53	0.32	0	59,61,61	0.39	0
33	CDL	V	203	-	93,93,99	0.25	0	99,105,111	0.27	0
33	CDL	Y	201	-	99,99,99	0.27	0	105,111,111	0.40	1 (0%)
33	CDL	V	204	-	84,84,99	0.27	0	90,96,111	0.29	0
33	CDL	W	201	-	99,99,99	0.30	0	105,111,111	0.35	0
30	PC1	M	502	-	53,53,53	0.31	0	59,61,61	0.40	0
34	ZMP	X	101	10	25,30,36	0.85	2 (8%)	29,37,45	1.05	3 (10%)
30	PC1	L	703	-	53,53,53	0.32	0	59,61,61	0.64	2 (3%)
32	3PE	K	101	-	39,39,50	0.35	0	42,44,55	0.42	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
32	3PE	M	501	-	-	16/47/47/54	-
33	CDL	o	502	-	2/2/9/9	18/85/85/110	-
32	3PE	m	101	-	-	14/54/54/54	-
32	3PE	H	502	-	-	19/54/54/54	-
32	3PE	L	702	-	-	7/54/54/54	-
36	MYR	s	201	21	-	2/12/12/13	-
32	3PE	N	401	-	-	15/54/54/54	-
31	DCQ	H	501	-	-	4/14/38/38	0/1/1/1
33	CDL	M	503	-	-	34/100/100/110	-
33	CDL	L	704	-	1/1/9/9	27/110/110/110	-
32	3PE	V	202	-	-	11/40/40/54	-
32	3PE	V	201	-	-	2/38/38/54	-
30	PC1	A	201	-	-	8/40/40/57	-
32	3PE	L	705	-	-	11/34/34/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	3PE	L	701	-	-	9/43/43/54	-
35	AMP	k	501	-	-	6/10/26/26	0/3/3/3
30	PC1	H	503	-	-	21/57/57/57	-
32	3PE	p	201	-	-	7/27/27/54	-
32	3PE	o	501	-	-	4/34/34/54	-
30	PC1	w	801	-	-	14/57/57/57	-
33	CDL	V	203	-	-	37/104/104/110	-
33	CDL	Y	201	-	1/1/9/9	27/110/110/110	-
33	CDL	V	204	-	1/1/9/9	33/95/95/110	-
33	CDL	W	201	-	-	26/110/110/110	-
30	PC1	M	502	-	-	19/57/57/57	-
34	ZMP	X	101	10	-	12/35/37/43	-
30	PC1	L	703	-	-	21/57/57/57	-
32	3PE	K	101	-	-	7/43/43/54	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	k	501	AMP	C5-C4	4.84	1.47	1.39
34	X	101	ZMP	C9-C10	2.63	1.53	1.50
35	k	501	AMP	C5-C6	2.53	1.48	1.41
35	k	501	AMP	C5-N7	-2.50	1.34	1.39
34	X	101	ZMP	C10-S1	-2.20	1.71	1.76
35	k	501	AMP	C8-N7	2.12	1.35	1.31

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	k	501	AMP	C5-C4-N3	-6.14	118.26	126.72
35	k	501	AMP	N3-C4-N9	5.14	135.91	127.17
35	k	501	AMP	C2-N3-C4	3.79	121.10	111.83
35	k	501	AMP	N3-C2-N1	-3.26	123.65	128.58
35	k	501	AMP	C4-C5-N7	-2.96	107.19	110.58
30	L	703	PC1	C2-O21-C21	2.75	124.38	117.80
32	L	705	3PE	C2-O21-C21	2.47	123.70	117.80
34	X	101	ZMP	O1-C10-C9	-2.45	121.16	123.98
35	k	501	AMP	C4-N9-C8	2.42	108.28	105.74
30	A	201	PC1	O21-C2-C3	2.41	116.98	108.34
32	M	501	3PE	O21-C2-C3	-2.31	100.07	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	Y	201	CDL	OA8-CA6-CA4	2.30	115.02	108.40
35	k	501	AMP	C5-N7-C8	2.26	107.01	103.45
32	H	502	3PE	O31-C3-C2	2.25	114.88	108.40
34	X	101	ZMP	C9-C10-S1	2.25	116.08	113.40
30	A	201	PC1	C2-O21-C21	2.24	123.16	117.80
30	L	703	PC1	O21-C2-C1	2.23	116.35	108.34
32	N	401	3PE	C2-O21-C21	2.15	122.94	117.80
32	N	401	3PE	O21-C2-C1	2.14	116.03	108.34
32	M	501	3PE	O31-C3-C2	2.14	114.55	108.40
32	L	705	3PE	O21-C2-C1	2.11	115.93	108.34
32	p	201	3PE	O12-P-O14	2.10	119.00	110.83
33	o	502	CDL	CB4-OB6-CB5	2.07	122.74	117.80
34	X	101	ZMP	C15-C14-C13	-2.05	108.98	112.39
33	L	704	CDL	OA8-CA6-CA4	-2.04	102.50	108.40

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	L	704	CDL	CB4
33	V	204	CDL	CB4
33	Y	201	CDL	CB4
33	o	502	CDL	CB4
33	o	502	CDL	CA4

All (431) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	H	503	PC1	C11-O13-P-O14
30	H	503	PC1	C11-O13-P-O11
30	L	703	PC1	C1-O11-P-O12
30	M	502	PC1	C11-O13-P-O11
30	M	502	PC1	C1-O11-P-O12
30	w	801	PC1	C11-O13-P-O14
30	w	801	PC1	O13-C11-C12-N
32	H	502	3PE	C11-O13-P-O11
32	H	502	3PE	C11-O13-P-O12
32	H	502	3PE	C11-O13-P-O14
32	H	502	3PE	O13-C11-C12-N
32	K	101	3PE	C1-O11-P-O12
32	K	101	3PE	C1-O11-P-O13
32	K	101	3PE	C1-O11-P-O14
32	L	701	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
32	L	701	3PE	C1-O11-P-O13
32	L	701	3PE	C11-O13-P-O11
32	L	701	3PE	C11-O13-P-O12
32	L	705	3PE	C1-O11-P-O12
32	L	705	3PE	C1-O11-P-O13
32	L	705	3PE	C1-O11-P-O14
32	L	705	3PE	C11-O13-P-O12
32	L	705	3PE	O13-C11-C12-N
32	M	501	3PE	C1-O11-P-O13
32	M	501	3PE	C1-O11-P-O14
32	M	501	3PE	C11-O13-P-O11
32	M	501	3PE	C11-O13-P-O12
32	M	501	3PE	C11-O13-P-O14
32	N	401	3PE	C1-O11-P-O12
32	N	401	3PE	C1-O11-P-O13
32	N	401	3PE	C1-O11-P-O14
32	V	201	3PE	O13-C11-C12-N
32	V	202	3PE	C1-O11-P-O12
32	V	202	3PE	C1-O11-P-O13
32	V	202	3PE	C11-O13-P-O11
32	V	202	3PE	C11-O13-P-O12
32	V	202	3PE	C11-O13-P-O14
32	V	202	3PE	O13-C11-C12-N
32	m	101	3PE	C11-O13-P-O11
32	m	101	3PE	C11-O13-P-O12
32	m	101	3PE	C11-O13-P-O14
32	o	501	3PE	O13-C11-C12-N
32	p	201	3PE	C1-O11-P-O12
32	p	201	3PE	C1-O11-P-O13
33	L	704	CDL	CA2-C1-CB2-OB2
33	L	704	CDL	CA2-OA2-PA1-OA3
33	L	704	CDL	CA3-OA5-PA1-OA2
33	L	704	CDL	CA3-OA5-PA1-OA4
33	L	704	CDL	CB2-OB2-PB2-OB3
33	L	704	CDL	CB2-OB2-PB2-OB5
33	M	503	CDL	O1-C1-CB2-OB2
33	M	503	CDL	C1-CA2-OA2-PA1
33	M	503	CDL	CA2-OA2-PA1-OA3
33	M	503	CDL	CA2-OA2-PA1-OA5
33	M	503	CDL	CA3-OA5-PA1-OA3
33	M	503	CDL	CB2-OB2-PB2-OB3
33	M	503	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
33	M	503	CDL	CB3-OB5-PB2-OB3
33	V	203	CDL	CB2-OB2-PB2-OB3
33	V	203	CDL	CB2-OB2-PB2-OB4
33	V	203	CDL	CB2-OB2-PB2-OB5
33	V	203	CDL	CB3-OB5-PB2-OB2
33	V	203	CDL	CB3-OB5-PB2-OB3
33	V	203	CDL	CB3-OB5-PB2-OB4
33	V	204	CDL	O1-C1-CB2-OB2
33	V	204	CDL	CA2-OA2-PA1-OA3
33	V	204	CDL	CA2-OA2-PA1-OA4
33	V	204	CDL	CA2-OA2-PA1-OA5
33	V	204	CDL	CB2-OB2-PB2-OB3
33	V	204	CDL	CB3-OB5-PB2-OB2
33	V	204	CDL	CB3-OB5-PB2-OB3
33	Y	201	CDL	O1-C1-CB2-OB2
33	Y	201	CDL	CB3-OB5-PB2-OB2
33	Y	201	CDL	CB3-OB5-PB2-OB3
33	o	502	CDL	O1-C1-CB2-OB2
34	X	101	ZMP	C19-C18-C21-O5
34	X	101	ZMP	C20-C18-C21-O5
34	X	101	ZMP	C17-C18-C21-O5
34	X	101	ZMP	C16-C17-C18-C21
34	X	101	ZMP	C17-C16-N2-C15
35	k	501	AMP	C5'-O5'-P-O2P
35	k	501	AMP	C5'-O5'-P-O3P
31	H	501	DCQ	C6-C7-C8-C9
34	X	101	ZMP	O3-C16-N2-C15
33	M	503	CDL	CA2-C1-CB2-OB2
33	W	201	CDL	CB2-C1-CA2-OA2
33	W	201	CDL	CA2-C1-CB2-OB2
33	o	502	CDL	CA2-C1-CB2-OB2
30	M	502	PC1	C11-C12-N-C14
33	W	201	CDL	O1-C1-CA2-OA2
33	W	201	CDL	O1-C1-CB2-OB2
35	k	501	AMP	C3'-C4'-C5'-O5'
33	L	704	CDL	CB5-C51-C52-C53
30	M	502	PC1	C11-C12-N-C15
32	V	201	3PE	C31-C32-C33-C34
33	L	704	CDL	CB7-C71-C72-C73
33	L	704	CDL	O1-C1-CB2-OB2
30	w	801	PC1	C21-C22-C23-C24
33	Y	201	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
33	V	204	CDL	CA2-C1-CB2-OB2
33	M	503	CDL	C82-C83-C84-C85
32	L	705	3PE	C2-C1-O11-P
32	N	401	3PE	C21-C22-C23-C24
33	M	503	CDL	C78-C79-C80-C81
33	L	704	CDL	C21-C22-C23-C24
32	m	101	3PE	C38-C39-C3A-C3B
33	V	203	CDL	C52-C53-C54-C55
33	V	204	CDL	C71-C72-C73-C74
33	W	201	CDL	C72-C73-C74-C75
32	N	401	3PE	C32-C33-C34-C35
33	L	704	CDL	C56-C57-C58-C59
33	Y	201	CDL	C63-C64-C65-C66
33	V	203	CDL	CA7-C31-C32-C33
33	W	201	CDL	CA5-C11-C12-C13
33	L	704	CDL	C77-C78-C79-C80
33	L	704	CDL	C41-C42-C43-C44
33	Y	201	CDL	C52-C53-C54-C55
32	K	101	3PE	C24-C25-C26-C27
33	V	203	CDL	C40-C41-C42-C43
33	W	201	CDL	C35-C36-C37-C38
33	Y	201	CDL	C80-C81-C82-C83
33	Y	201	CDL	C11-C12-C13-C14
33	V	203	CDL	C20-C21-C22-C23
31	H	501	DCQ	C10-C11-C12-C13
33	W	201	CDL	CB5-C51-C52-C53
30	H	503	PC1	C3B-C3C-C3D-C3E
30	L	703	PC1	C37-C38-C39-C3A
30	L	703	PC1	C38-C39-C3A-C3B
32	K	101	3PE	C34-C35-C36-C37
32	m	101	3PE	C2C-C2D-C2E-C2F
32	m	101	3PE	C2E-C2F-C2G-C2H
33	V	203	CDL	C38-C39-C40-C41
30	w	801	PC1	C3A-C3B-C3C-C3D
33	V	204	CDL	C14-C15-C16-C17
33	L	704	CDL	C17-C18-C19-C20
33	V	203	CDL	C31-C32-C33-C34
32	L	702	3PE	C3B-C3C-C3D-C3E
33	V	203	CDL	C79-C80-C81-C82
33	L	704	CDL	C82-C83-C84-C85
30	w	801	PC1	C2D-C2E-C2F-C2G
30	L	703	PC1	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
30	H	503	PC1	C3C-C3D-C3E-C3F
30	M	502	PC1	C31-C32-C33-C34
33	M	503	CDL	C51-C52-C53-C54
33	M	503	CDL	C56-C57-C58-C59
30	L	703	PC1	C36-C37-C38-C39
35	k	501	AMP	O4'-C4'-C5'-O5'
30	M	502	PC1	C11-C12-N-C13
33	Y	201	CDL	C14-C15-C16-C17
32	N	401	3PE	O11-C1-C2-O21
33	Y	201	CDL	C81-C82-C83-C84
30	H	503	PC1	C22-C21-O21-C2
33	W	201	CDL	C82-C83-C84-C85
33	V	203	CDL	OB6-CB4-CB6-OB8
33	Y	201	CDL	C15-C16-C17-C18
30	L	703	PC1	C2-C1-O11-P
33	V	204	CDL	C1-CA2-OA2-PA1
33	Y	201	CDL	CA2-C1-CB2-OB2
33	V	204	CDL	C34-C35-C36-C37
33	M	503	CDL	C64-C65-C66-C67
32	L	705	3PE	C21-C22-C23-C24
33	o	502	CDL	CA7-C31-C32-C33
33	L	704	CDL	C34-C35-C36-C37
33	M	503	CDL	C73-C74-C75-C76
34	X	101	ZMP	O3-C16-C17-O4
33	L	704	CDL	C35-C36-C37-C38
32	H	502	3PE	O11-C1-C2-C3
33	L	704	CDL	OB5-CB3-CB4-CB6
33	V	203	CDL	OA5-CA3-CA4-CA6
33	W	201	CDL	OA5-CA3-CA4-CA6
32	L	702	3PE	C26-C27-C28-C29
33	V	204	CDL	C51-C52-C53-C54
33	Y	201	CDL	CA3-CA4-CA6-OA8
33	Y	201	CDL	C37-C38-C39-C40
33	W	201	CDL	C31-C32-C33-C34
30	w	801	PC1	C39-C3A-C3B-C3C
33	Y	201	CDL	C12-C13-C14-C15
33	L	704	CDL	C22-C23-C24-C25
33	M	503	CDL	C53-C54-C55-C56
32	H	502	3PE	C33-C34-C35-C36
33	M	503	CDL	C81-C82-C83-C84
30	w	801	PC1	C23-C24-C25-C26
33	Y	201	CDL	C79-C80-C81-C82

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Mol	Chain	Res	Type	Atoms
33	V	204	CDL	OA6-CA4-CA6-OA8
30	w	801	PC1	C3E-C3F-C3G-C3H
30	L	703	PC1	C3F-C3G-C3H-C3I
30	M	502	PC1	C3B-C3C-C3D-C3E
33	V	204	CDL	C1-CB2-OB2-PB2
35	k	501	AMP	C4'-C5'-O5'-P
30	A	201	PC1	C22-C23-C24-C25
33	W	201	CDL	CA7-C31-C32-C33
33	V	204	CDL	C52-C53-C54-C55
32	L	701	3PE	C31-C32-C33-C34
30	L	703	PC1	O11-C1-C2-C3
30	M	502	PC1	O11-C1-C2-C3
32	N	401	3PE	O11-C1-C2-C3
32	N	401	3PE	C31-C32-C33-C34
33	V	204	CDL	C15-C16-C17-C18
32	L	702	3PE	C37-C38-C39-C3A
32	H	502	3PE	C2D-C2E-C2F-C2G
32	p	201	3PE	C22-C23-C24-C25
33	M	503	CDL	C19-C20-C21-C22
30	L	703	PC1	C21-C22-C23-C24
33	V	203	CDL	CB3-CB4-CB6-OB8
33	W	201	CDL	CA3-CA4-CA6-OA8
34	X	101	ZMP	N2-C16-C17-O4
33	V	203	CDL	C11-C12-C13-C14
33	L	704	CDL	OB5-CB3-CB4-OB6
33	V	203	CDL	OA5-CA3-CA4-OA6
33	V	203	CDL	OB5-CB3-CB4-OB6
33	W	201	CDL	OA5-CA3-CA4-OA6
32	H	502	3PE	C2-C1-O11-P
32	V	202	3PE	C2-C1-O11-P
30	M	502	PC1	C3A-C3B-C3C-C3D
32	H	502	3PE	C28-C29-C2A-C2B
33	V	204	CDL	OB6-CB4-CB6-OB8
33	W	201	CDL	OA6-CA4-CA6-OA8
30	H	503	PC1	O22-C21-O21-C2
30	H	503	PC1	C2D-C2E-C2F-C2G
32	M	501	3PE	C3B-C3C-C3D-C3E
33	L	704	CDL	C61-C62-C63-C64
32	L	702	3PE	C35-C36-C37-C38
32	L	701	3PE	C37-C38-C39-C3A
30	M	502	PC1	C32-C33-C34-C35
30	A	201	PC1	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
30	L	703	PC1	O11-C1-C2-O21
30	L	703	PC1	C3A-C3B-C3C-C3D
33	o	502	CDL	C71-C72-C73-C74
33	V	204	CDL	CB3-CB4-CB6-OB8
33	o	502	CDL	CB3-CB4-CB6-OB8
32	p	201	3PE	C21-C22-C23-C24
30	H	503	PC1	C12-C11-O13-P
32	H	502	3PE	C12-C11-O13-P
32	L	701	3PE	C12-C11-O13-P
33	Y	201	CDL	C59-C60-C61-C62
32	N	401	3PE	O21-C2-C3-O31
33	M	503	CDL	C71-C72-C73-C74
33	Y	201	CDL	C57-C58-C59-C60
30	L	703	PC1	C23-C24-C25-C26
33	M	503	CDL	C83-C84-C85-C86
30	H	503	PC1	O13-C11-C12-N
33	M	503	CDL	C72-C73-C74-C75
36	s	201	MYR	C1-C2-C3-C4
33	L	704	CDL	C58-C59-C60-C61
34	X	101	ZMP	C6-C7-C8-C9
30	H	503	PC1	C2B-C2C-C2D-C2E
32	o	501	3PE	C25-C26-C27-C28
30	L	703	PC1	C2A-C2B-C2C-C2D
33	o	502	CDL	C15-C16-C17-C18
33	M	503	CDL	CB4-CB3-OB5-PB2
30	M	502	PC1	O11-C1-C2-O21
32	H	502	3PE	O11-C1-C2-O21
32	L	702	3PE	O11-C1-C2-O21
32	L	705	3PE	O11-C1-C2-O21
33	o	502	CDL	OB5-CB3-CB4-OB6
32	N	401	3PE	C38-C39-C3A-C3B
32	o	501	3PE	C22-C23-C24-C25
30	w	801	PC1	C28-C29-C2A-C2B
36	s	201	MYR	C11-C10-C9-C8
30	w	801	PC1	O21-C2-C3-O31
30	w	801	PC1	C1-C2-C3-O31
33	V	204	CDL	CA3-CA4-CA6-OA8
30	A	201	PC1	C11-O13-P-O14
30	A	201	PC1	C11-C12-N-C13
30	H	503	PC1	C11-O13-P-O12
30	L	703	PC1	C1-O11-P-O14
30	L	703	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
30	M	502	PC1	C11-O13-P-O14
32	H	502	3PE	C1-O11-P-O13
32	L	701	3PE	C1-O11-P-O14
32	M	501	3PE	C1-O11-P-O12
32	V	202	3PE	C1-O11-P-O14
32	o	501	3PE	C11-O13-P-O14
33	L	704	CDL	CA2-OA2-PA1-OA5
33	L	704	CDL	CA3-OA5-PA1-OA3
33	M	503	CDL	CA2-OA2-PA1-OA4
33	M	503	CDL	CA3-OA5-PA1-OA2
33	M	503	CDL	CB2-OB2-PB2-OB4
33	V	204	CDL	CB3-OB5-PB2-OB4
33	Y	201	CDL	CB2-OB2-PB2-OB3
33	o	502	CDL	CA2-OA2-PA1-OA3
33	o	502	CDL	CA2-OA2-PA1-OA5
33	o	502	CDL	CA3-OA5-PA1-OA2
33	o	502	CDL	CB3-OB5-PB2-OB3
34	X	101	ZMP	O4-C17-C18-C21
30	L	703	PC1	C39-C3A-C3B-C3C
33	V	203	CDL	C77-C78-C79-C80
33	L	704	CDL	CA4-CA3-OA5-PA1
33	W	201	CDL	C1-CA2-OA2-PA1
33	V	203	CDL	C41-C42-C43-C44
30	M	502	PC1	C2D-C2E-C2F-C2G
32	H	502	3PE	C31-C32-C33-C34
32	L	702	3PE	O11-C1-C2-C3
33	V	203	CDL	OB5-CB3-CB4-CB6
33	o	502	CDL	CB2-C1-CA2-OA2
33	Y	201	CDL	C32-C33-C34-C35
33	W	201	CDL	C81-C82-C83-C84
30	H	503	PC1	C22-C23-C24-C25
31	H	501	DCQ	C5-C4-O4-C4M
30	M	502	PC1	C2B-C2C-C2D-C2E
30	M	502	PC1	C2-C1-O11-P
33	M	503	CDL	OA6-CA4-CA6-OA8
33	V	203	CDL	OA6-CA4-CA6-OA8
33	W	201	CDL	OB6-CB4-CB6-OB8
33	Y	201	CDL	OA6-CA4-CA6-OA8
32	N	401	3PE	C37-C38-C39-C3A
33	W	201	CDL	C79-C80-C81-C82
33	V	204	CDL	C23-C24-C25-C26
30	L	703	PC1	C3E-C3F-C3G-C3H

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Mol	Chain	Res	Type	Atoms
33	M	503	CDL	CB5-C51-C52-C53
33	o	502	CDL	CB7-C71-C72-C73
30	M	502	PC1	C2F-C2G-C2H-C2I
32	H	502	3PE	C32-C31-O31-C3
32	K	101	3PE	C2-C1-O11-P
30	A	201	PC1	O31-C31-C32-C33
32	H	502	3PE	C3A-C3B-C3C-C3D
32	M	501	3PE	C32-C31-O31-C3
33	M	503	CDL	C63-C64-C65-C66
30	A	201	PC1	C11-C12-N-C14
33	V	203	CDL	O1-C1-CB2-OB2
32	M	501	3PE	C31-C32-C33-C34
33	V	204	CDL	CA5-C11-C12-C13
33	V	204	CDL	C21-C22-C23-C24
32	M	501	3PE	C2-C1-O11-P
30	H	503	PC1	C2C-C2D-C2E-C2F
32	M	501	3PE	C32-C33-C34-C35
33	V	203	CDL	CA2-C1-CB2-OB2
30	M	502	PC1	C25-C26-C27-C28
30	H	503	PC1	C3-C2-O21-C21
30	L	703	PC1	C1-C2-O21-C21
32	L	705	3PE	C1-C2-O21-C21
32	N	401	3PE	C3-C2-O21-C21
33	L	704	CDL	C80-C81-C82-C83
33	W	201	CDL	C53-C54-C55-C56
33	W	201	CDL	OB5-CB3-CB4-OB6
33	o	502	CDL	O1-C1-CA2-OA2
32	N	401	3PE	C2C-C2D-C2E-C2F
32	H	502	3PE	C36-C37-C38-C39
30	A	201	PC1	C11-C12-N-C15
34	X	101	ZMP	C3-C4-C5-C6
31	H	501	DCQ	C7-C8-C9-C10
33	V	203	CDL	C78-C79-C80-C81
33	V	203	CDL	C37-C38-C39-C40
32	m	101	3PE	C35-C36-C37-C38
30	w	801	PC1	C2C-C2D-C2E-C2F
33	M	503	CDL	CA3-CA4-CA6-OA8
33	W	201	CDL	C58-C59-C60-C61
33	V	203	CDL	C71-C72-C73-C74
33	V	203	CDL	CA5-C11-C12-C13
30	A	201	PC1	O21-C21-C22-C23
30	M	502	PC1	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
30	M	502	PC1	O31-C31-C32-C33
32	K	101	3PE	O31-C31-C32-C33
30	w	801	PC1	C2F-C2G-C2H-C2I
33	M	503	CDL	OB5-CB3-CB4-CB6
30	H	503	PC1	C2-C1-O11-P
30	L	703	PC1	C28-C29-C2A-C2B
32	M	501	3PE	O32-C31-O31-C3
35	k	501	AMP	C5'-O5'-P-O1P
30	L	703	PC1	C2C-C2D-C2E-C2F
33	V	204	CDL	C31-C32-C33-C34
33	M	503	CDL	CB3-CB4-OB6-CB5
30	H	503	PC1	C34-C35-C36-C37
30	H	503	PC1	C3A-C3B-C3C-C3D
33	V	203	CDL	CA4-CA3-OA5-PA1
33	W	201	CDL	C15-C16-C17-C18
32	N	401	3PE	C1-C2-C3-O31
33	W	201	CDL	CB3-CB4-CB6-OB8
33	V	203	CDL	C32-C31-CA7-OA8
33	M	503	CDL	C84-C85-C86-C87
32	H	502	3PE	O32-C31-O31-C3
32	m	101	3PE	C12-C11-O13-P
34	X	101	ZMP	C16-C17-C18-C20
32	m	101	3PE	C3A-C3B-C3C-C3D
32	L	701	3PE	C24-C25-C26-C27
32	m	101	3PE	O21-C2-C3-O31
32	L	702	3PE	C34-C35-C36-C37
32	V	202	3PE	O31-C31-C32-C33
33	Y	201	CDL	C12-C11-CA5-OA6
33	W	201	CDL	OB5-CB3-CB4-CB6
33	Y	201	CDL	OB5-CB3-CB4-CB6
33	V	204	CDL	C77-C78-C79-C80
30	H	503	PC1	C3D-C3E-C3F-C3G
33	V	203	CDL	C72-C71-CB7-OB8
33	V	204	CDL	C52-C51-CB5-OB6
30	w	801	PC1	C31-C32-C33-C34
33	M	503	CDL	C52-C53-C54-C55
33	o	502	CDL	C73-C74-C75-C76
32	L	705	3PE	O21-C21-C22-C23
32	M	501	3PE	O21-C21-C22-C23
32	m	101	3PE	O21-C21-C22-C23
33	o	502	CDL	C72-C71-CB7-OB8
32	p	201	3PE	C26-C27-C28-C29

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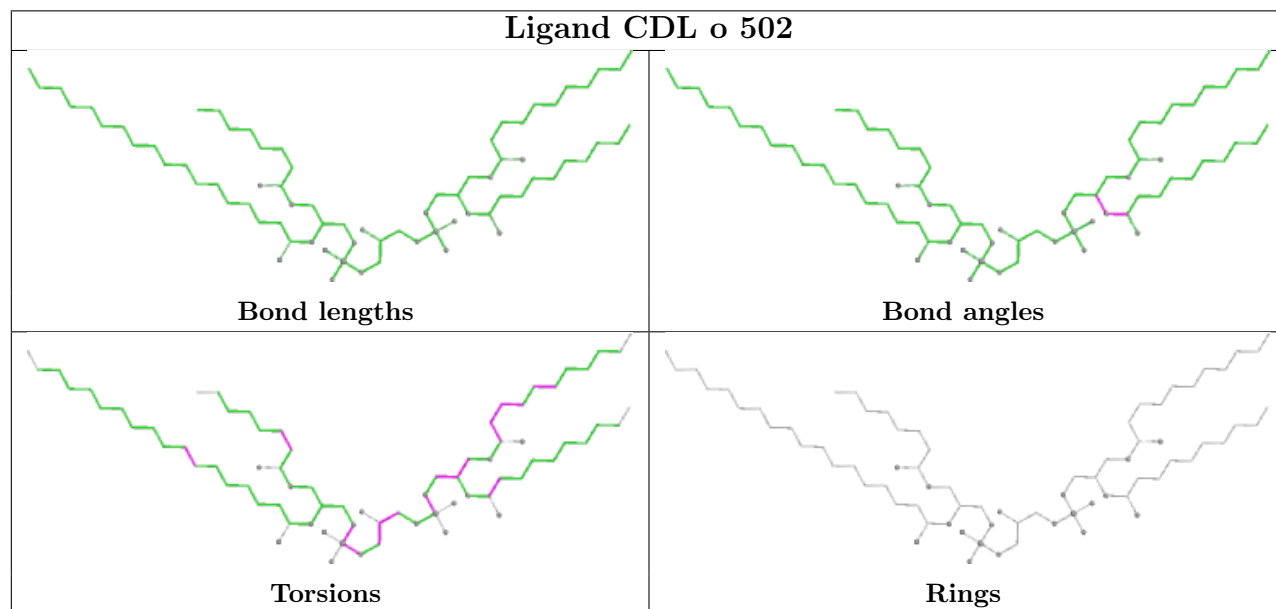
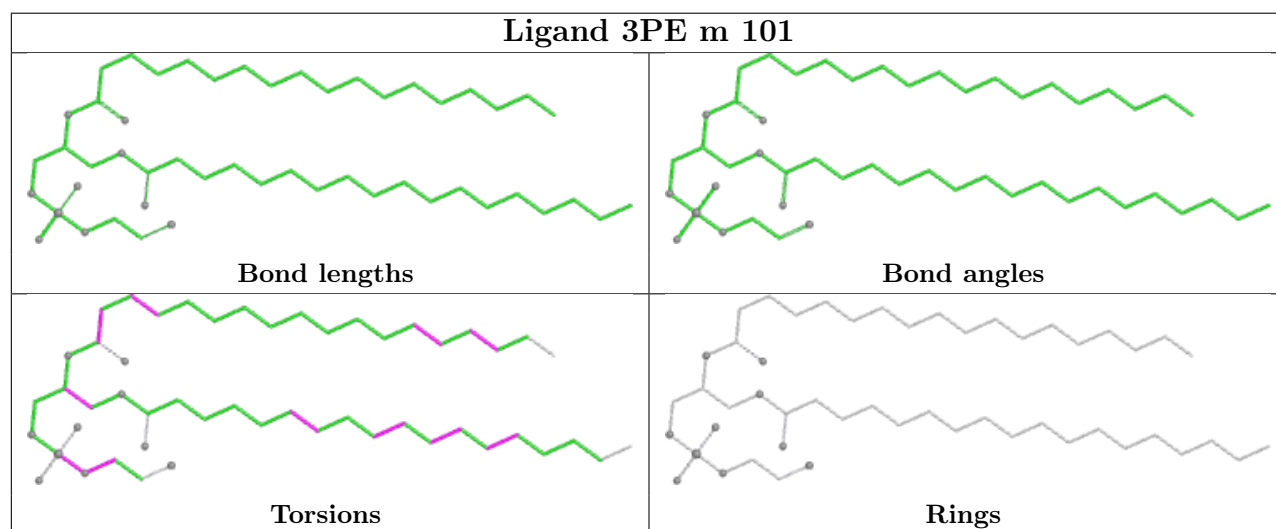
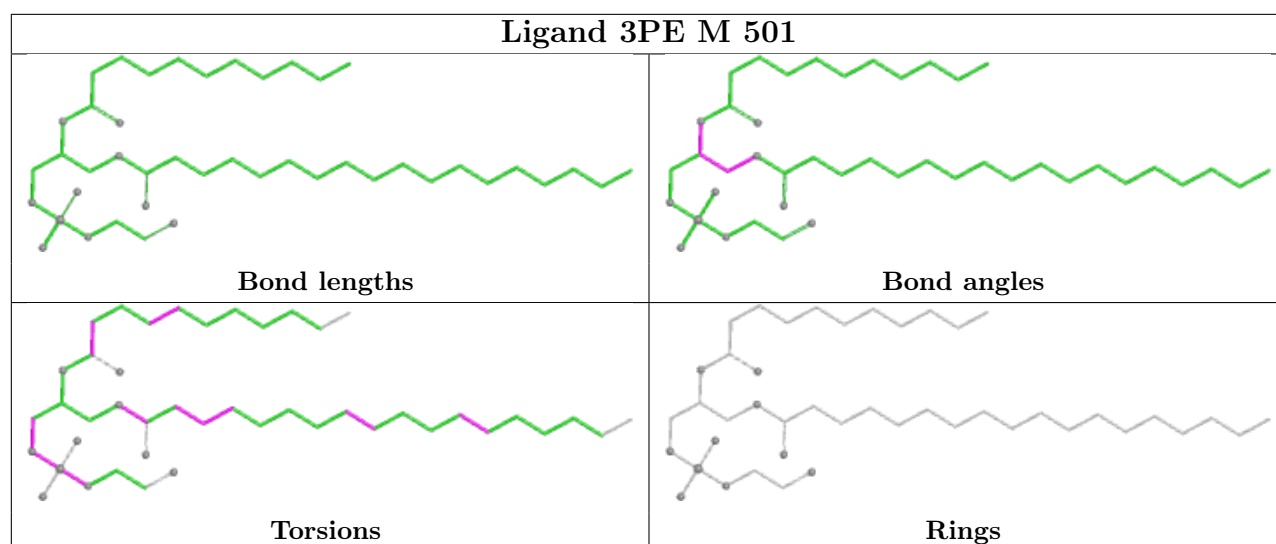
Mol	Chain	Res	Type	Atoms
32	H	502	3PE	C3C-C3D-C3E-C3F
33	V	204	CDL	C32-C31-CA7-OA8
30	H	503	PC1	C11-C12-N-C14
32	m	101	3PE	C22-C23-C24-C25
32	p	201	3PE	O21-C21-C22-C23
33	Y	201	CDL	C52-C51-CB5-OB6
33	V	203	CDL	C72-C71-CB7-OB9
33	Y	201	CDL	C1-CB2-OB2-PB2
32	M	501	3PE	C23-C24-C25-C26
33	M	503	CDL	C31-C32-C33-C34
32	M	501	3PE	C37-C38-C39-C3A
33	V	203	CDL	C80-C81-C82-C83
33	V	204	CDL	C32-C31-CA7-OA9
33	Y	201	CDL	C12-C11-CA5-OA7
30	H	503	PC1	C31-C32-C33-C34
33	V	204	CDL	C12-C11-CA5-OA6
32	M	501	3PE	O22-C21-C22-C23
32	V	202	3PE	O32-C31-C32-C33
33	V	203	CDL	C32-C31-CA7-OA9
33	V	204	CDL	C52-C51-CB5-OB7
33	V	204	CDL	CB2-C1-CA2-OA2
32	H	502	3PE	C26-C27-C28-C29
32	m	101	3PE	C3C-C3D-C3E-C3F
33	L	704	CDL	C11-C12-C13-C14
30	H	503	PC1	C3F-C3G-C3H-C3I
32	V	202	3PE	O11-C1-C2-C3
32	N	401	3PE	C2E-C2F-C2G-C2H
33	V	203	CDL	C13-C14-C15-C16
32	L	705	3PE	O22-C21-C22-C23
32	m	101	3PE	O22-C21-C22-C23
33	Y	201	CDL	C52-C51-CB5-OB7
33	o	502	CDL	C72-C71-CB7-OB9
30	L	703	PC1	O31-C31-C32-C33
33	W	201	CDL	C12-C11-CA5-OA6
33	o	502	CDL	C52-C51-CB5-OB6
32	p	201	3PE	O22-C21-C22-C23
33	V	204	CDL	C72-C71-CB7-OB8
33	V	203	CDL	C43-C44-C45-C46

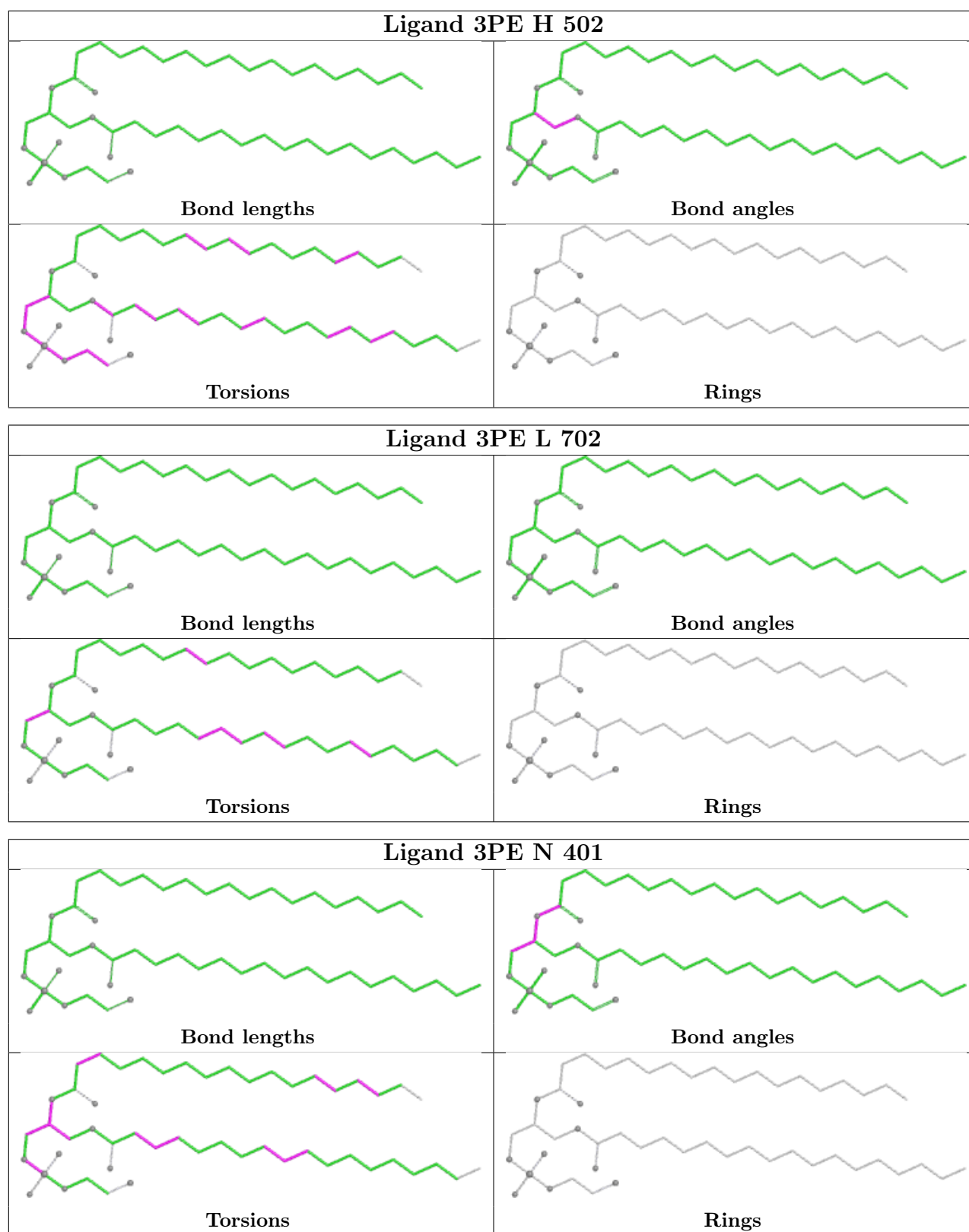
There are no ring outliers.

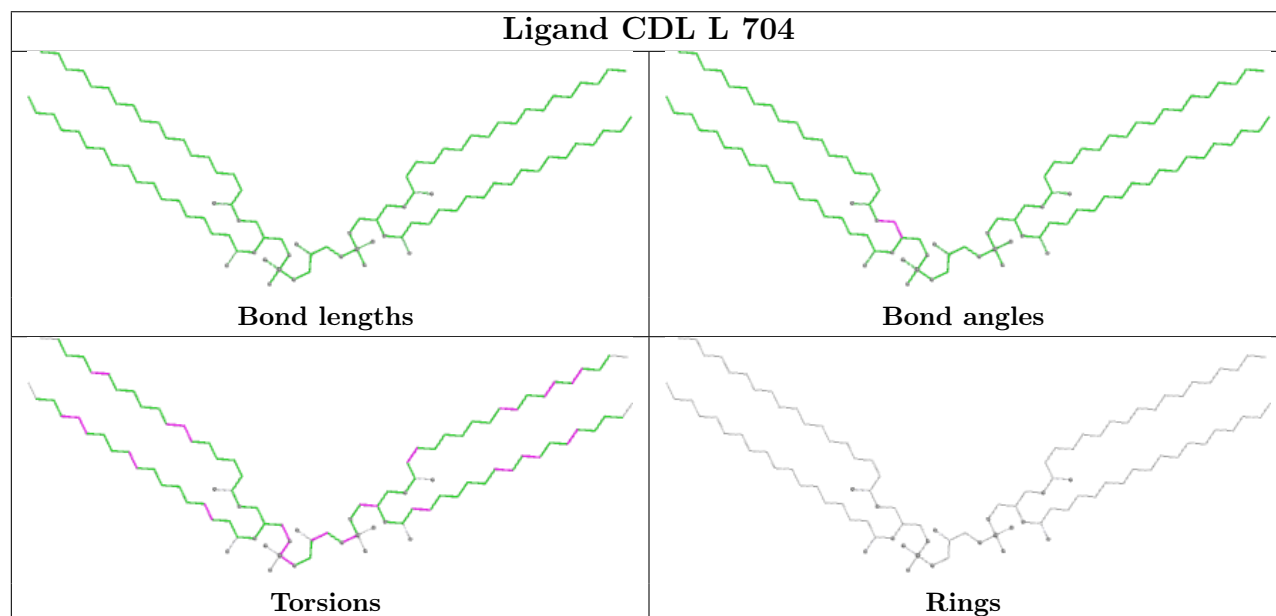
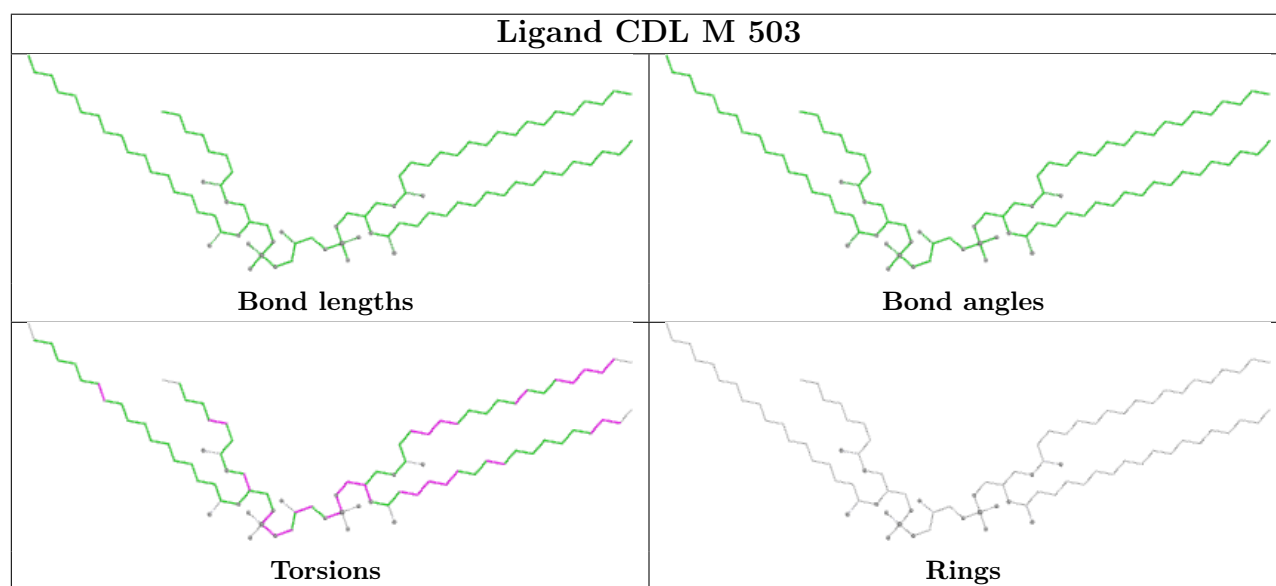
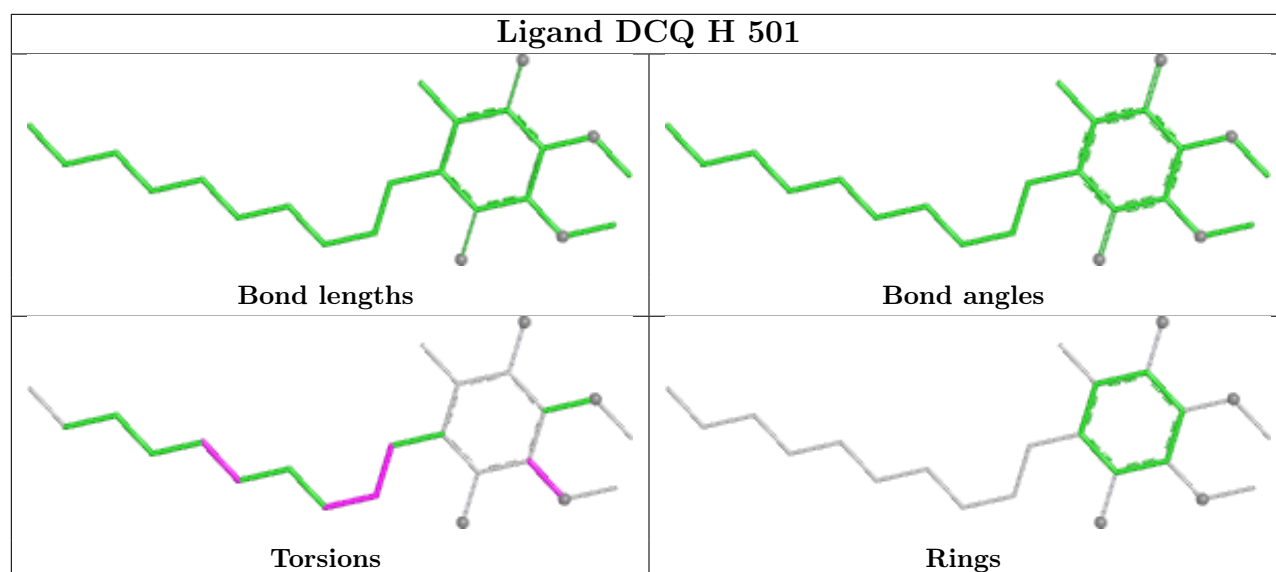
21 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	M	501	3PE	1	0
33	o	502	CDL	5	0
32	H	502	3PE	1	0
32	L	702	3PE	1	0
32	N	401	3PE	4	0
33	M	503	CDL	7	0
33	L	704	CDL	7	0
32	V	201	3PE	1	0
30	A	201	PC1	1	0
35	k	501	AMP	1	0
30	H	503	PC1	3	0
32	p	201	3PE	1	0
30	w	801	PC1	10	0
33	V	203	CDL	4	0
33	Y	201	CDL	6	0
33	V	204	CDL	4	0
33	W	201	CDL	6	0
30	M	502	PC1	6	0
34	X	101	ZMP	3	0
30	L	703	PC1	3	0
32	K	101	3PE	4	0

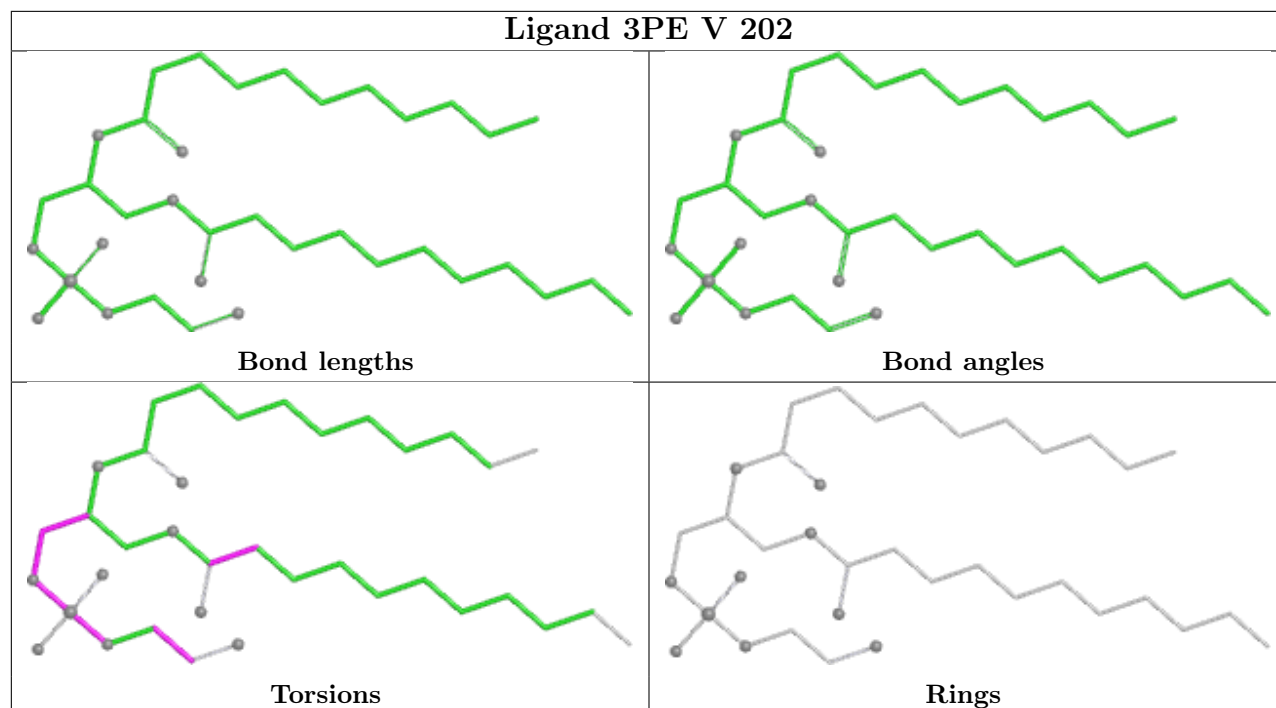
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



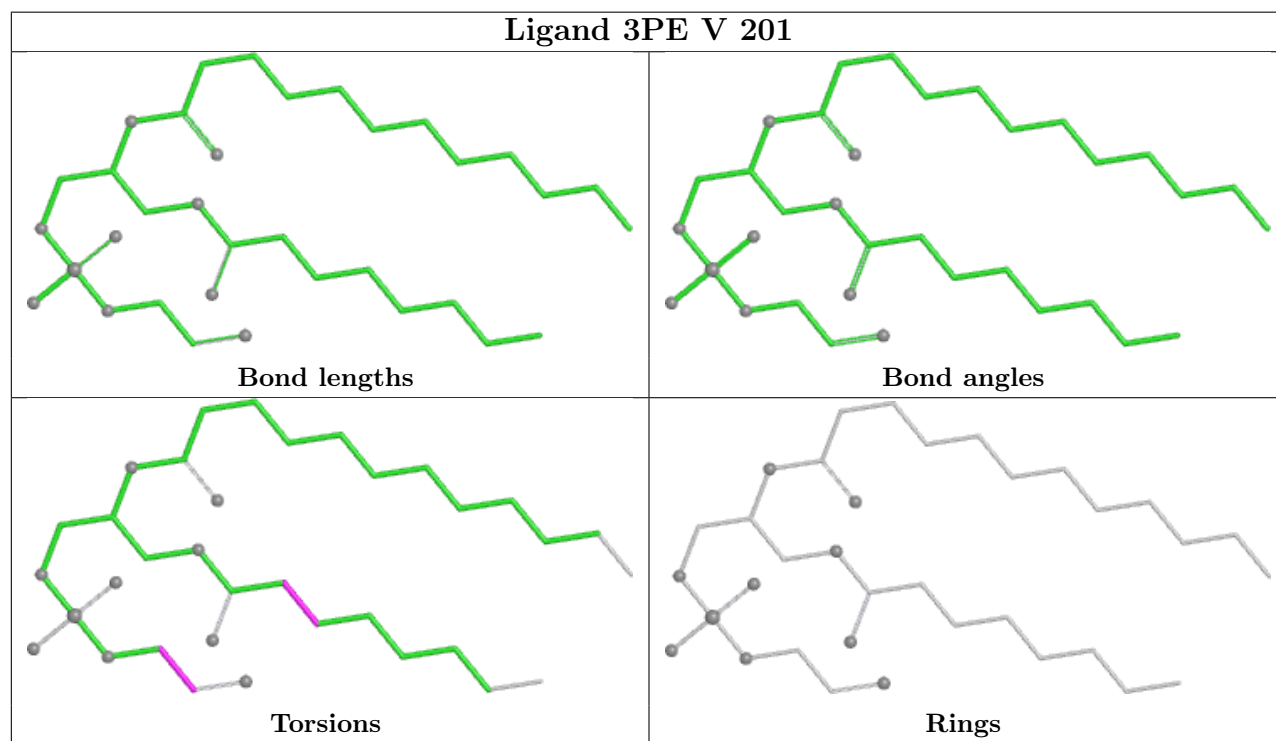


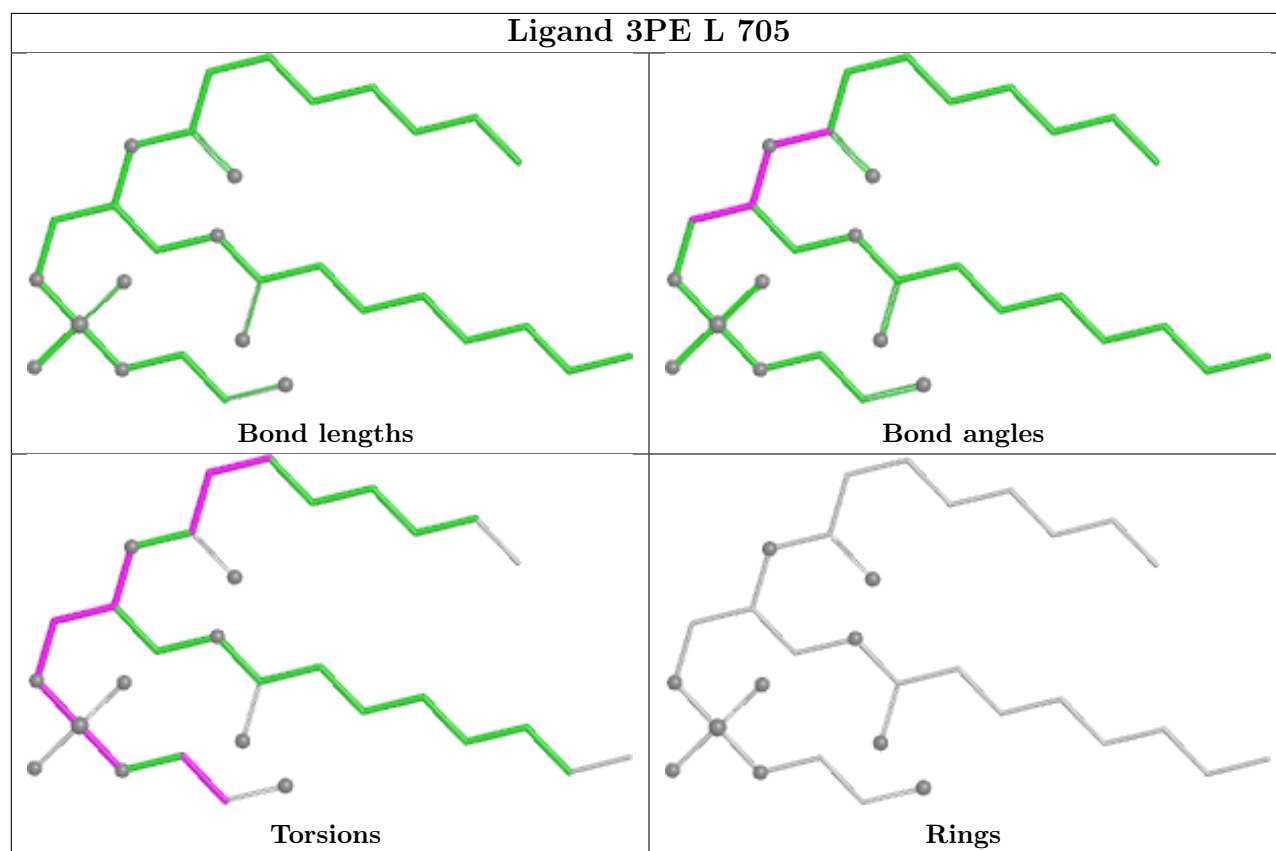
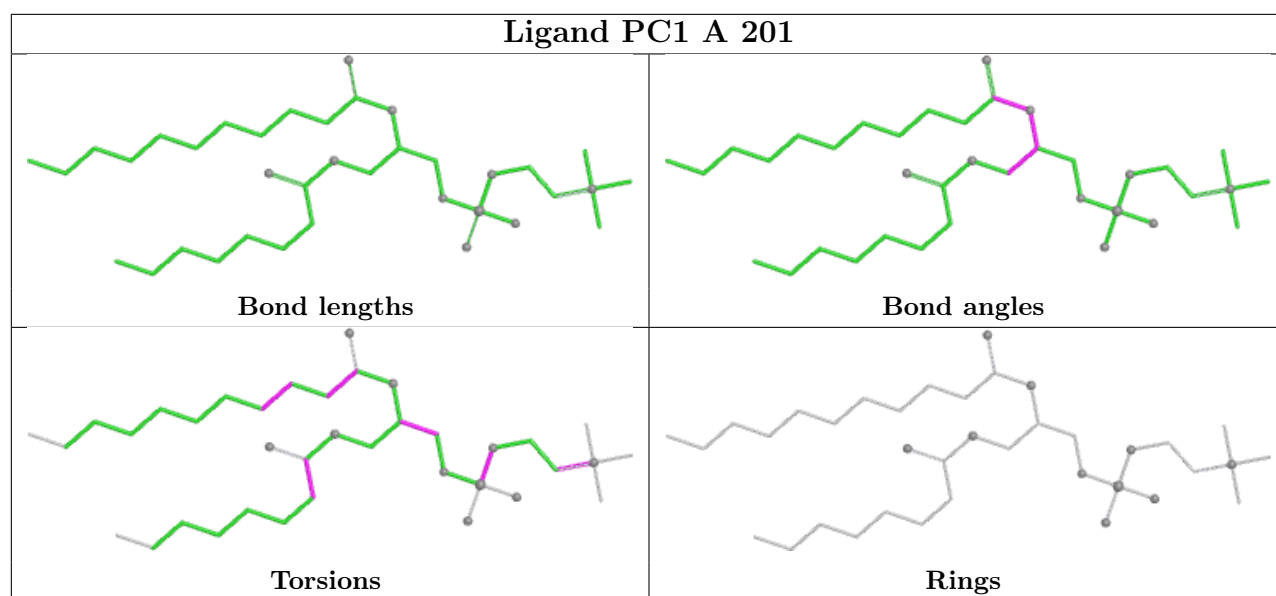


Ligand 3PE V 202

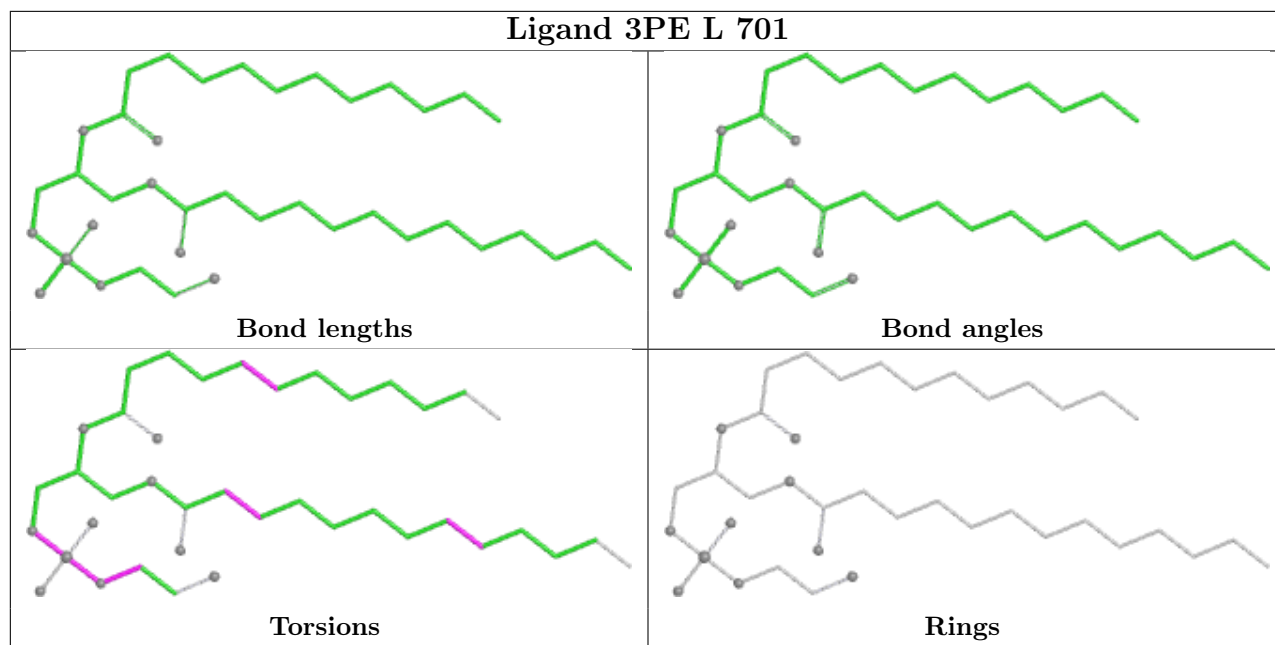


Ligand 3PE V 201

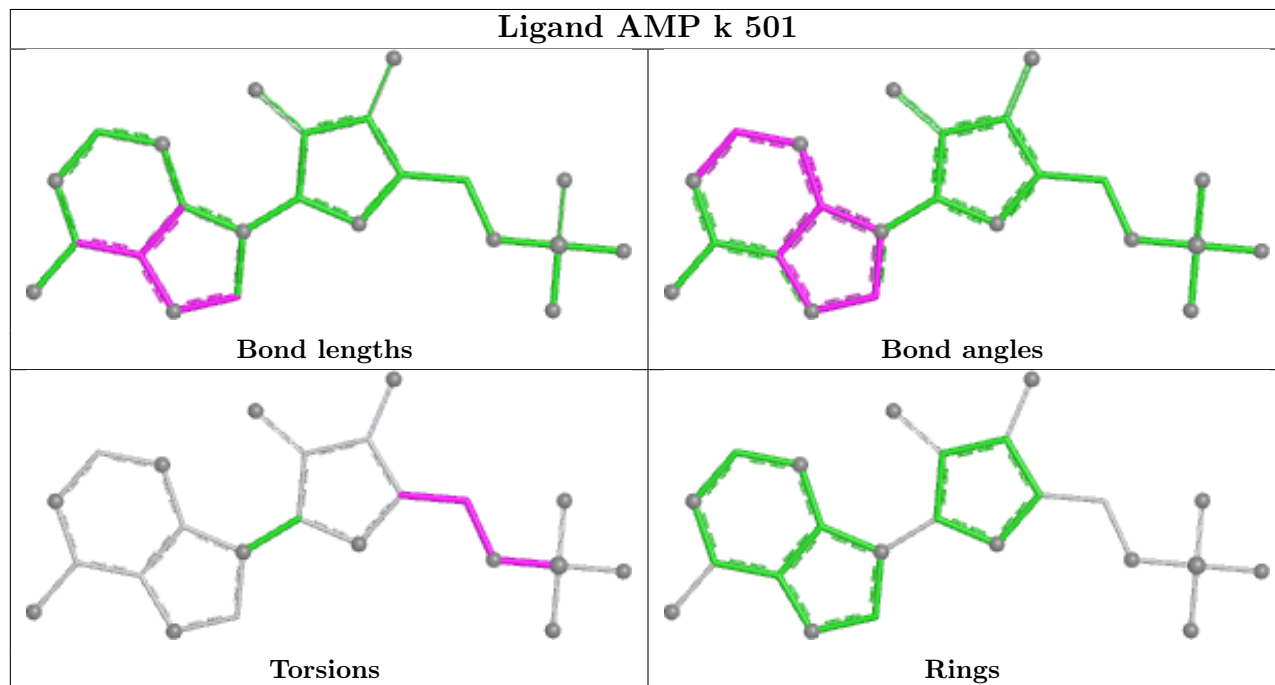




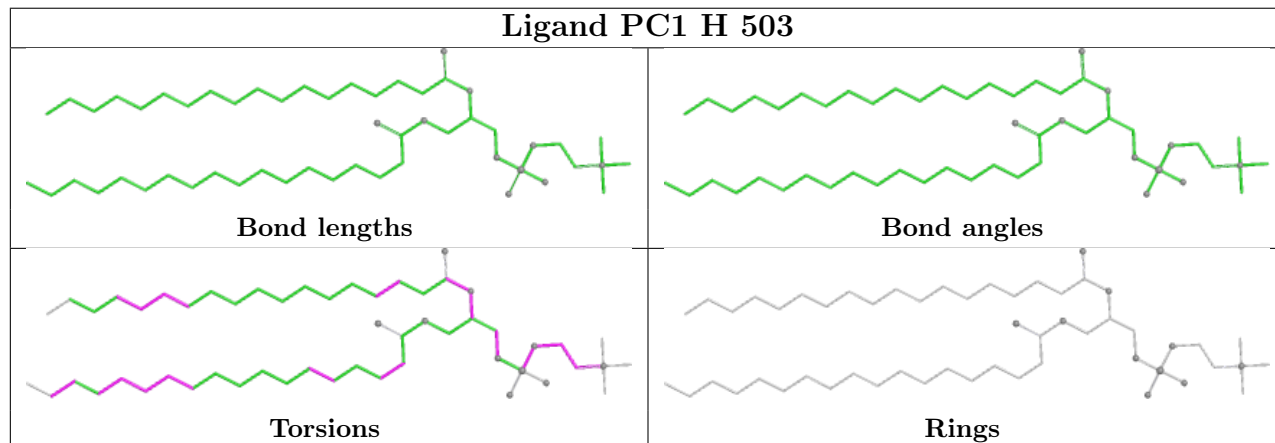
Ligand 3PE L 701

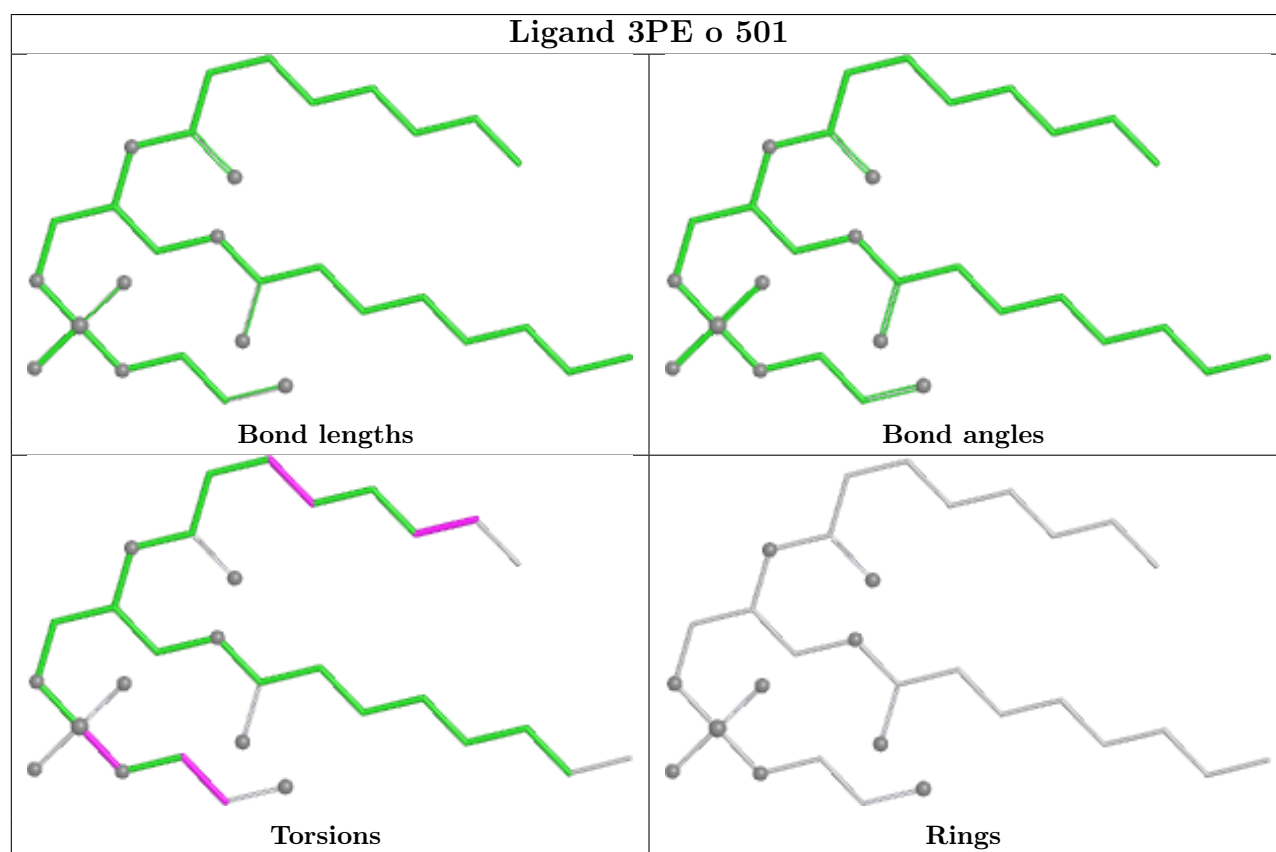
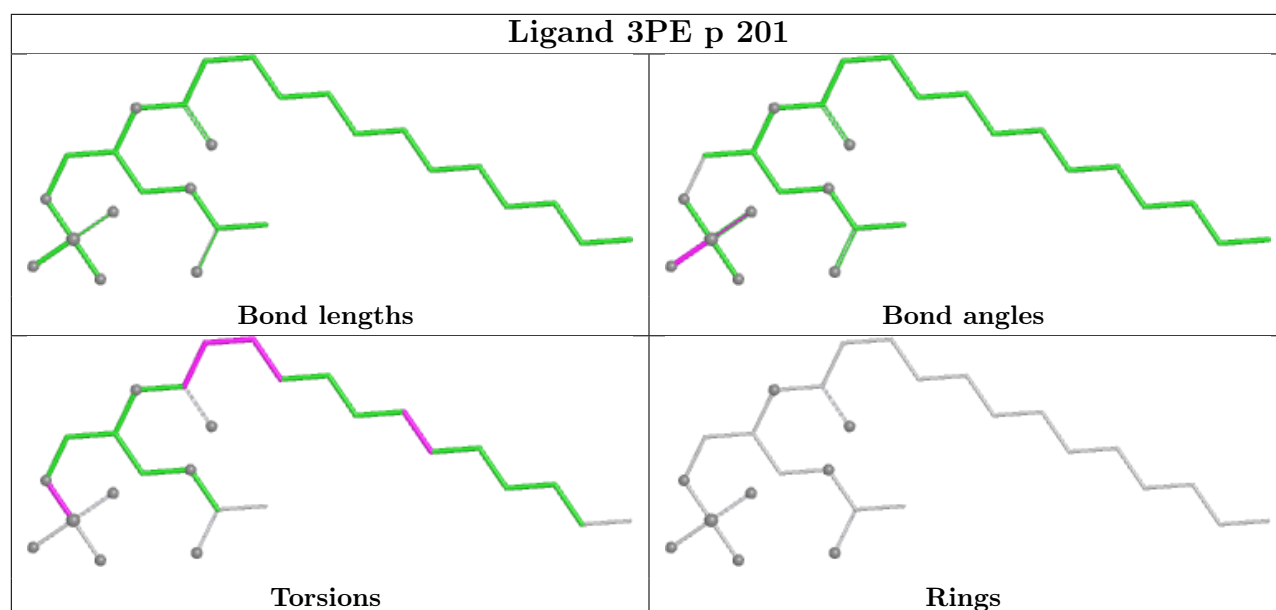


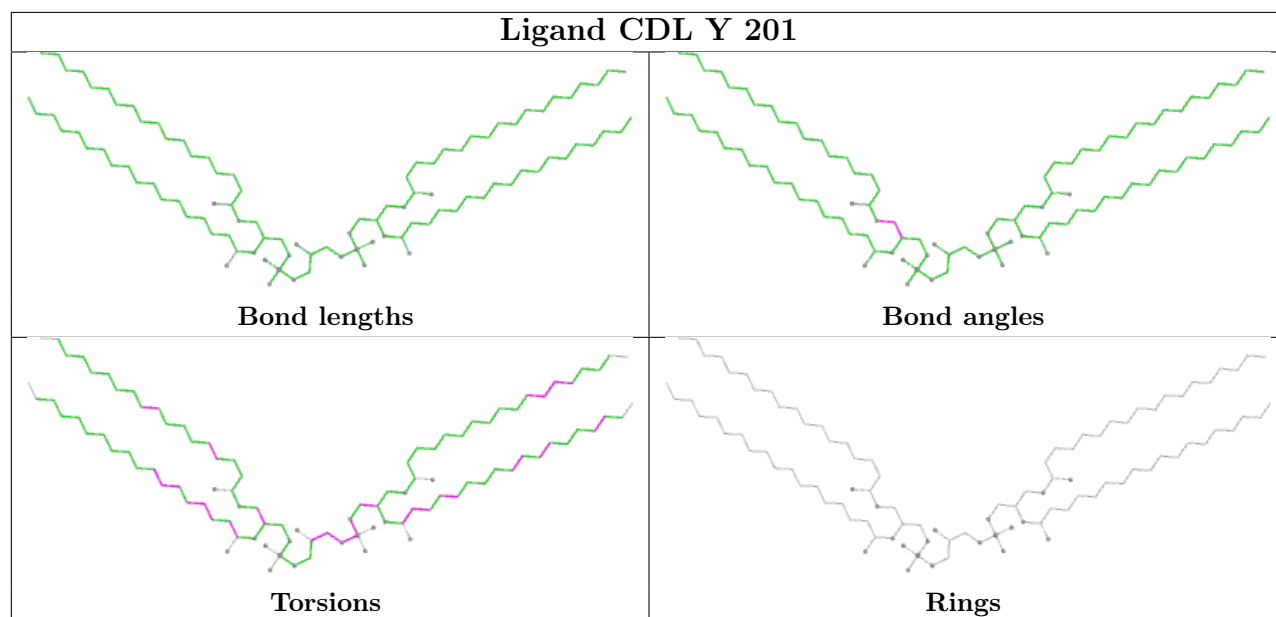
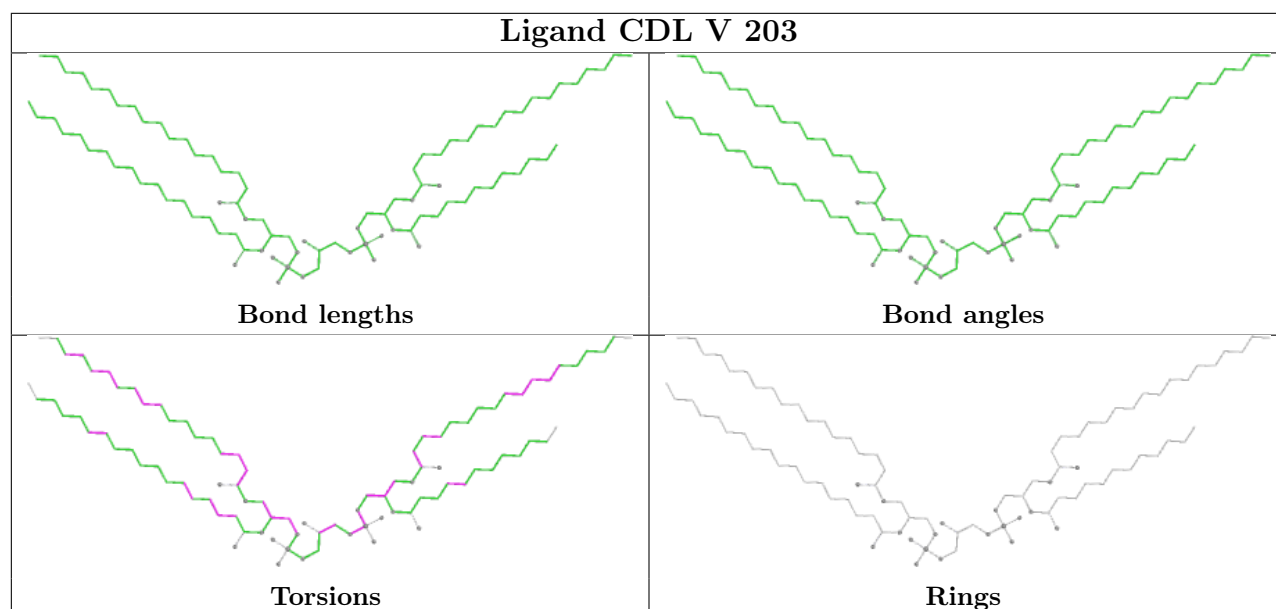
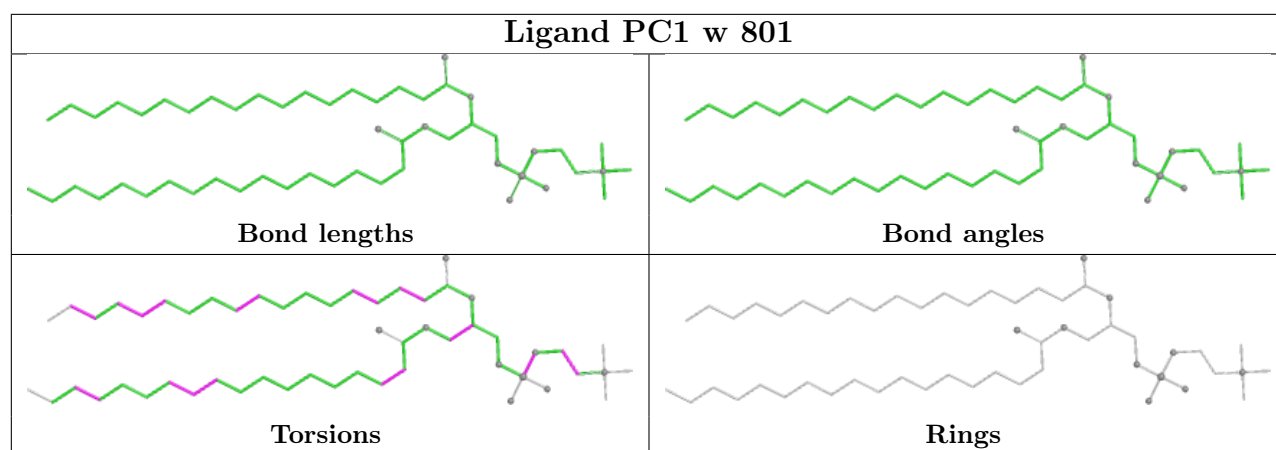
Ligand AMP k 501

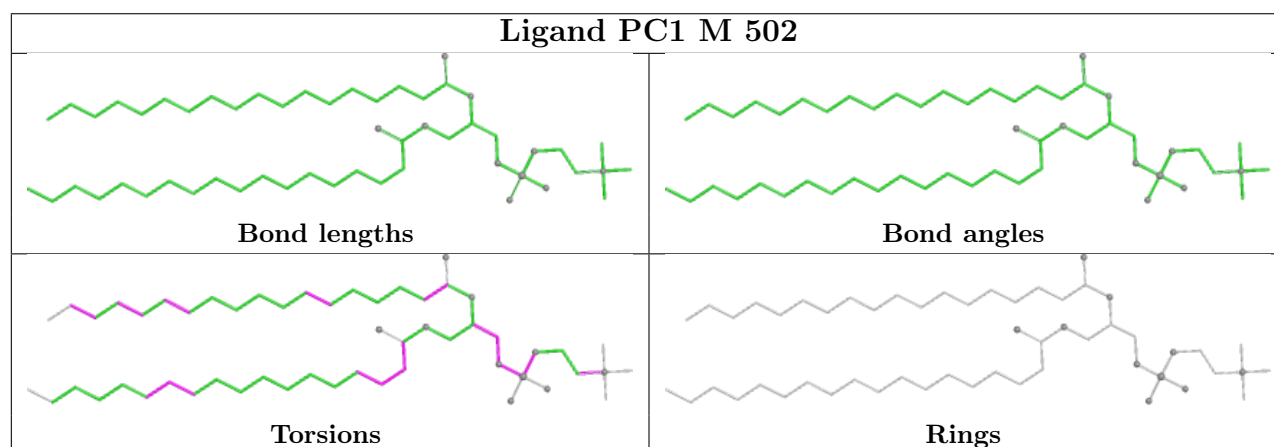
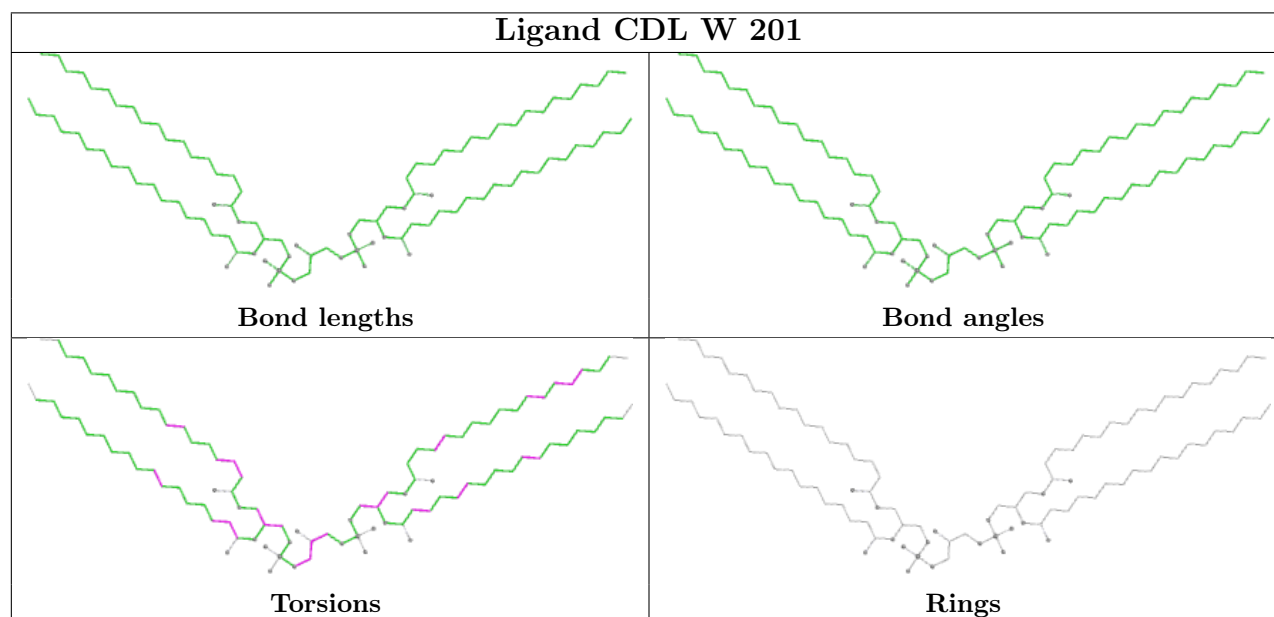
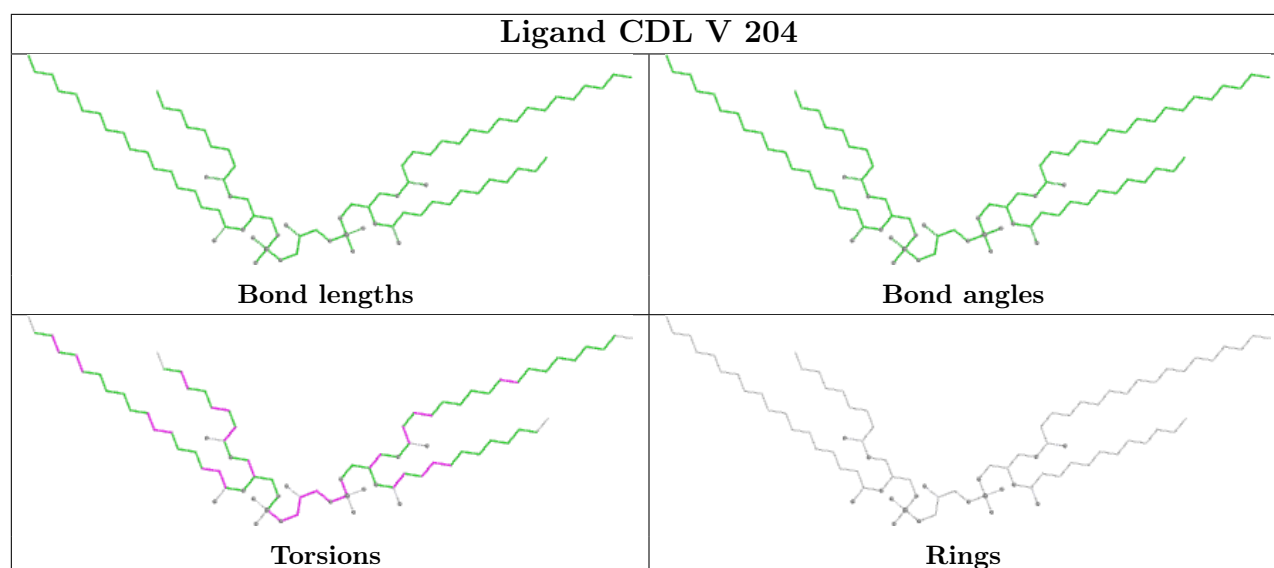


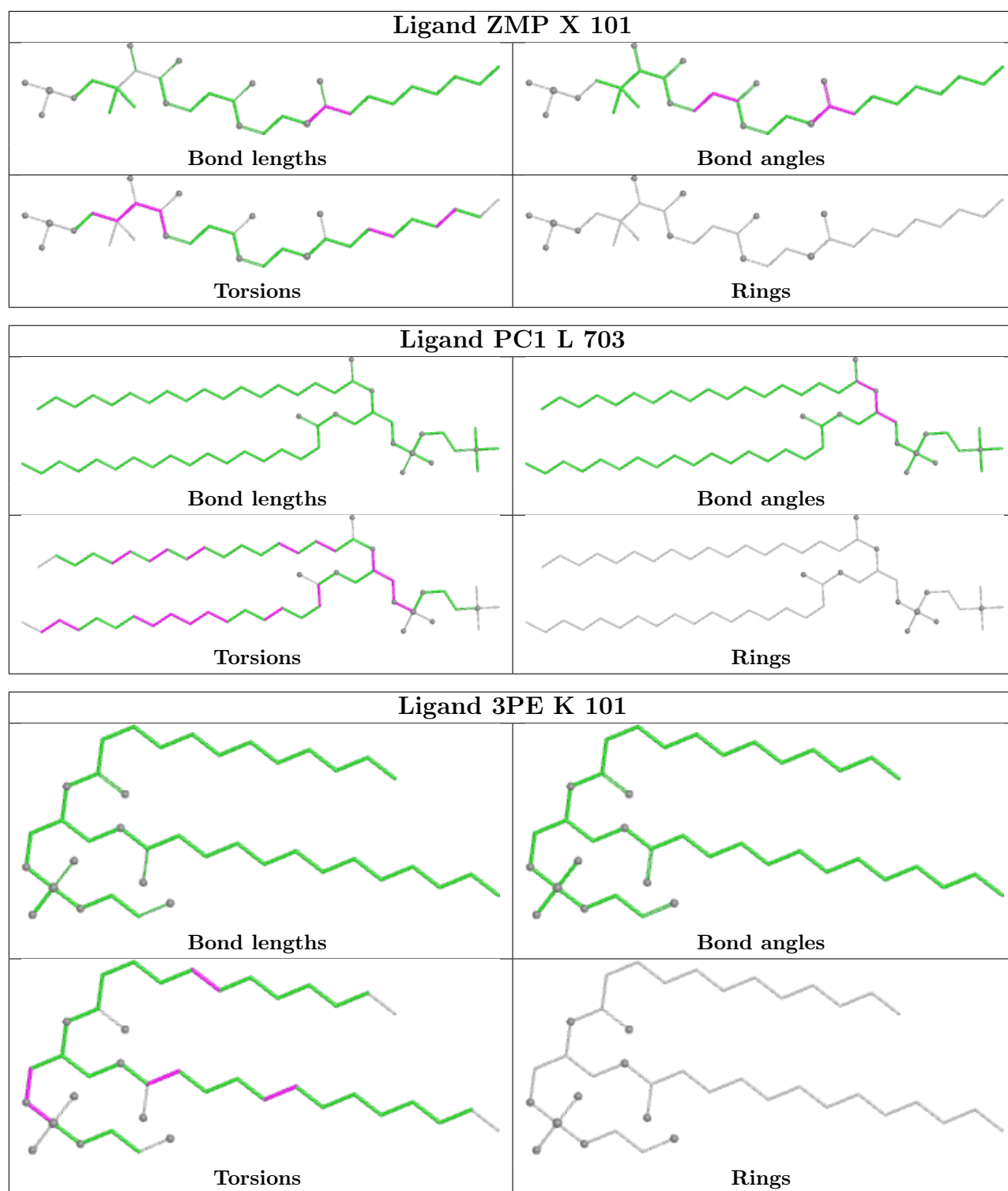
Ligand PC1 H 503











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

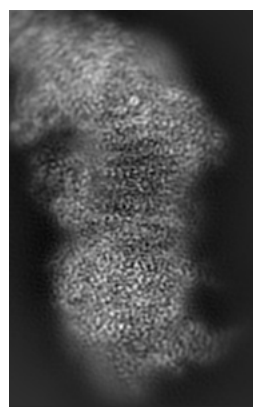
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11242. These allow visual inspection of the internal detail of the map and identification of artifacts.

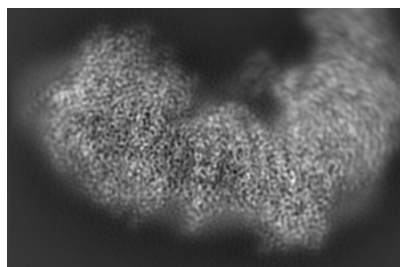
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

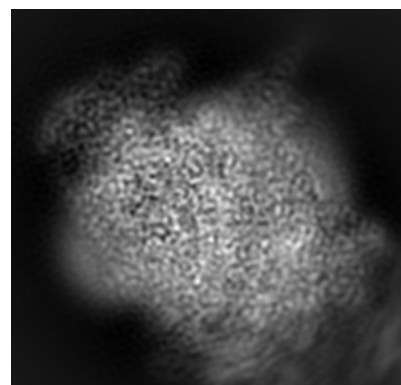
6.1.1 Primary map



X



Y

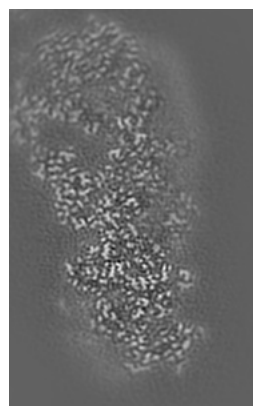


Z

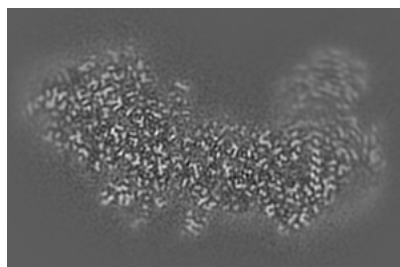
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

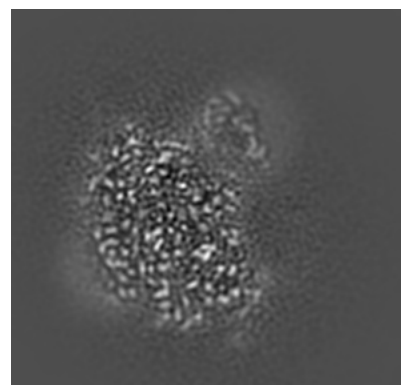
6.2.1 Primary map



X Index: 162



Y Index: 153

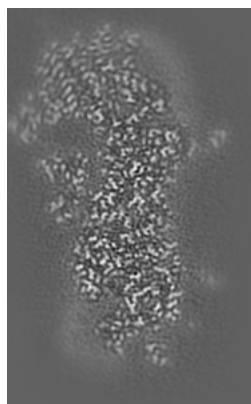


Z Index: 249

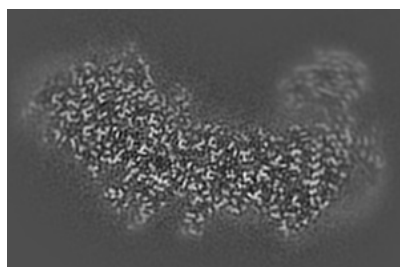
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

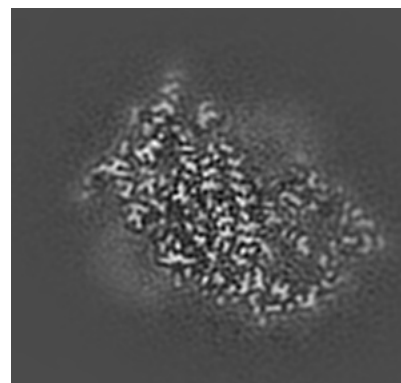
6.3.1 Primary map



X Index: 137



Y Index: 157

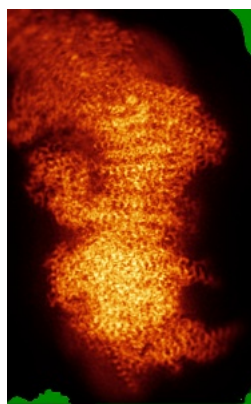


Z Index: 163

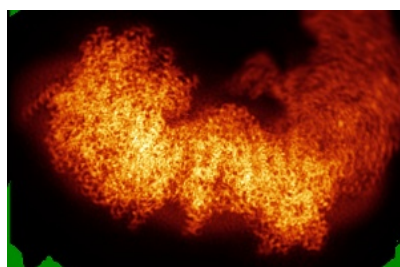
The images above show the largest variance slices of the map in three orthogonal directions.

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

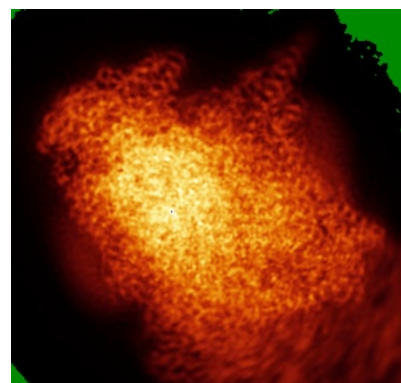
6.4.1 Primary map



X



Y

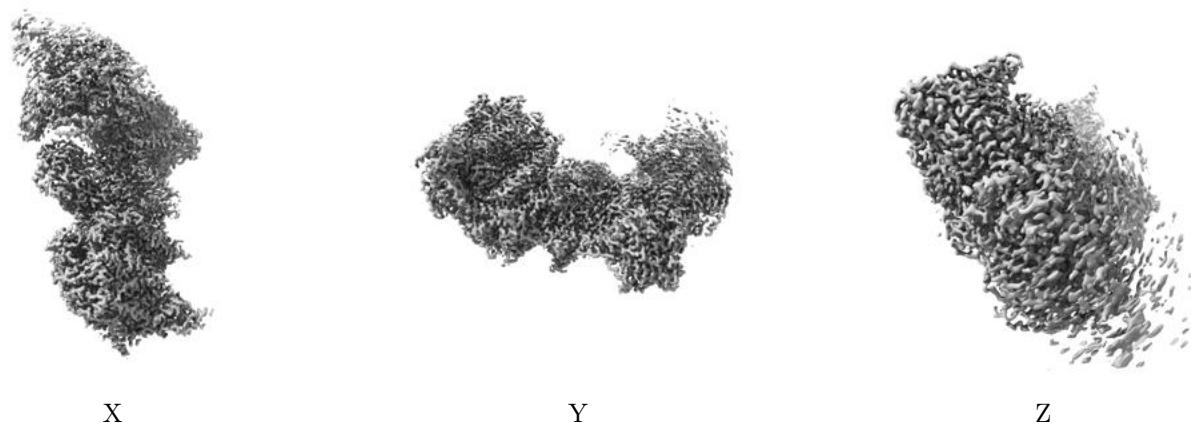


Z

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 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

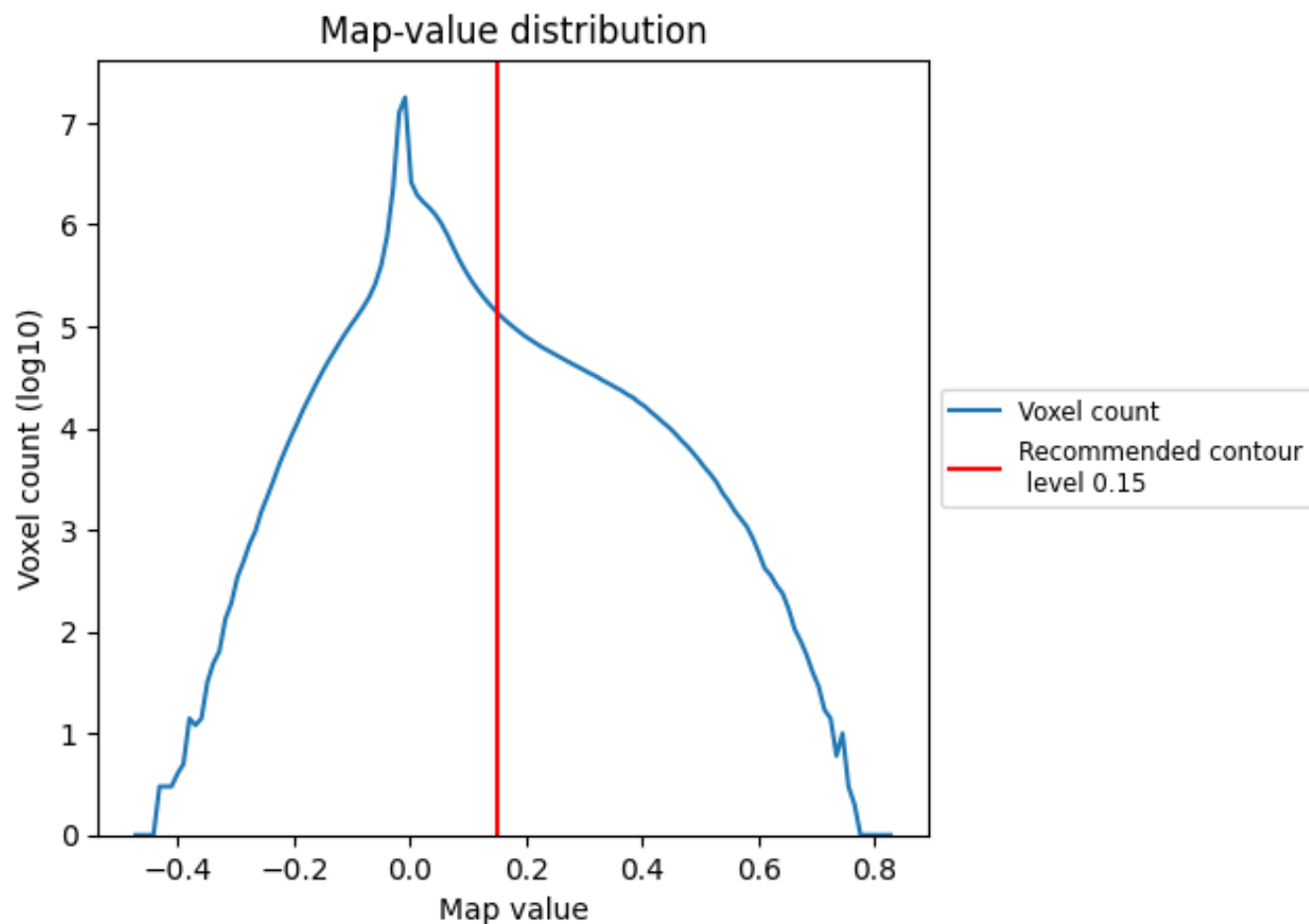
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

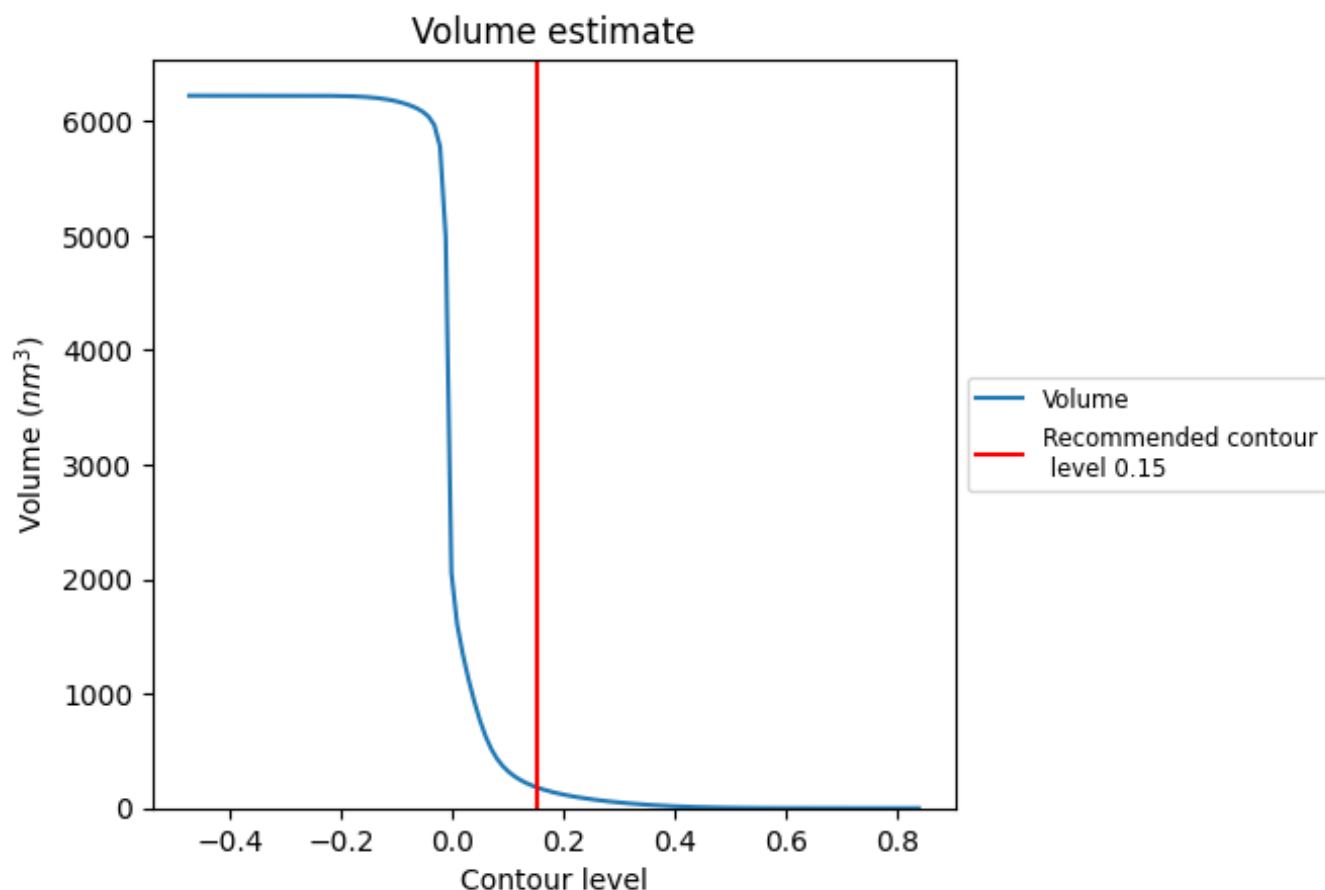
This section contains the results of statistical analysis of the map.

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 184 nm³; this corresponds to an approximate mass of 166 kDa.

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

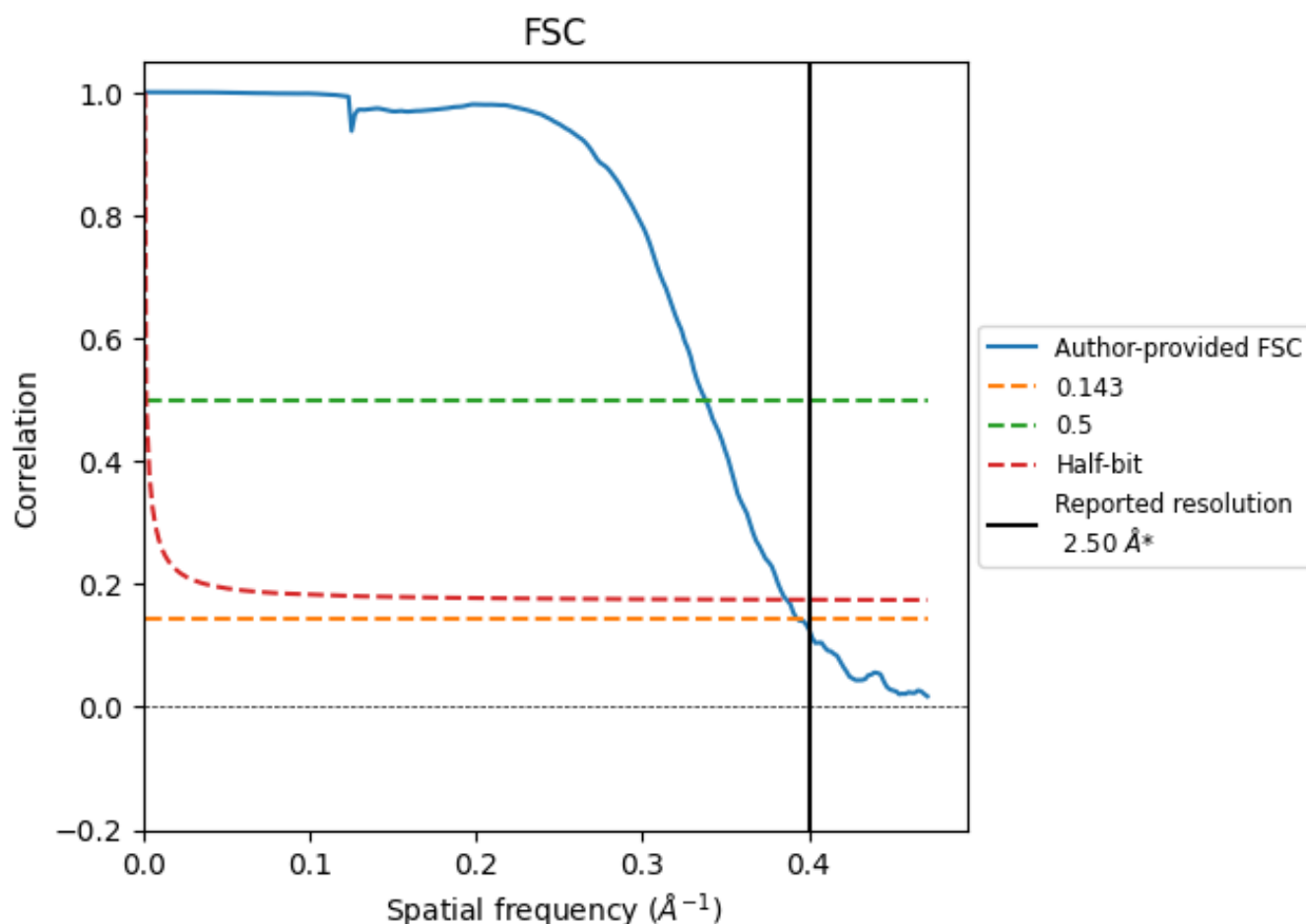
7.3 Rotationally averaged power spectrum [i](#)

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

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

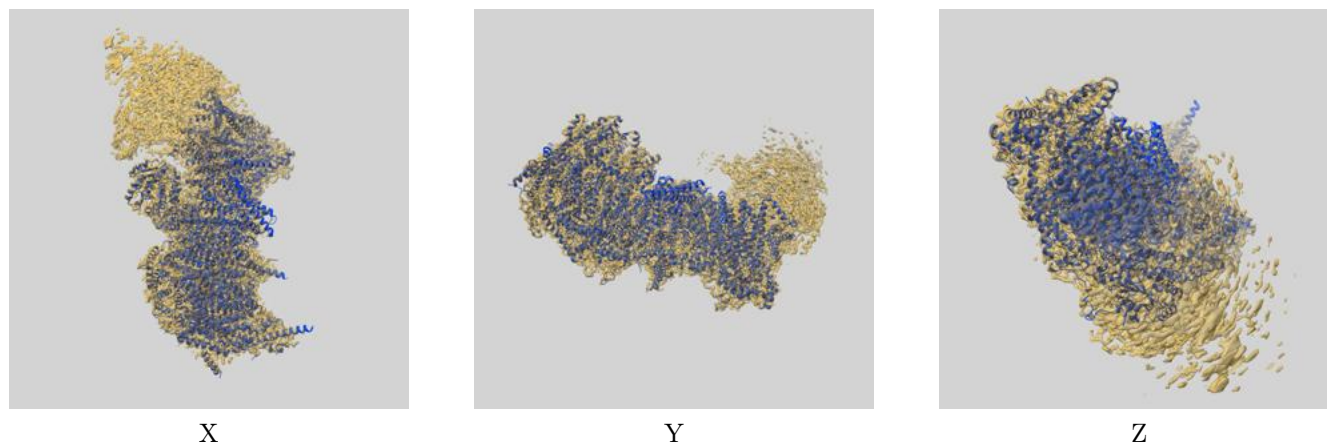
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.54	2.96	2.59
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

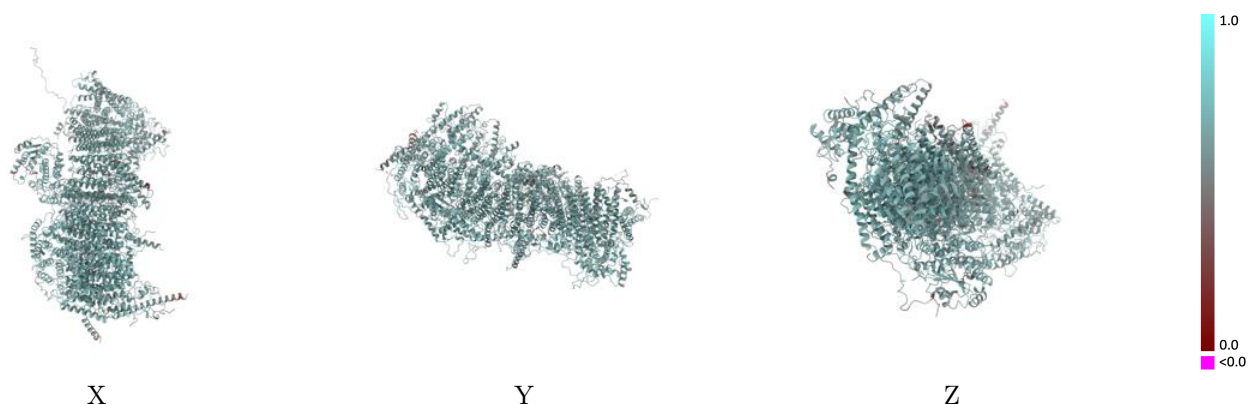
This section contains information regarding the fit between EMDB map EMD-11242 and PDB model 6ZKA. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



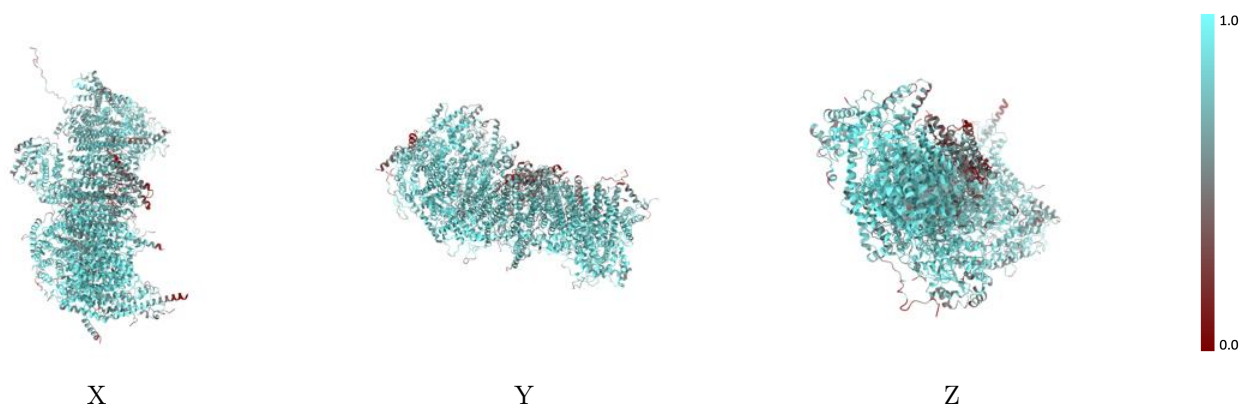
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



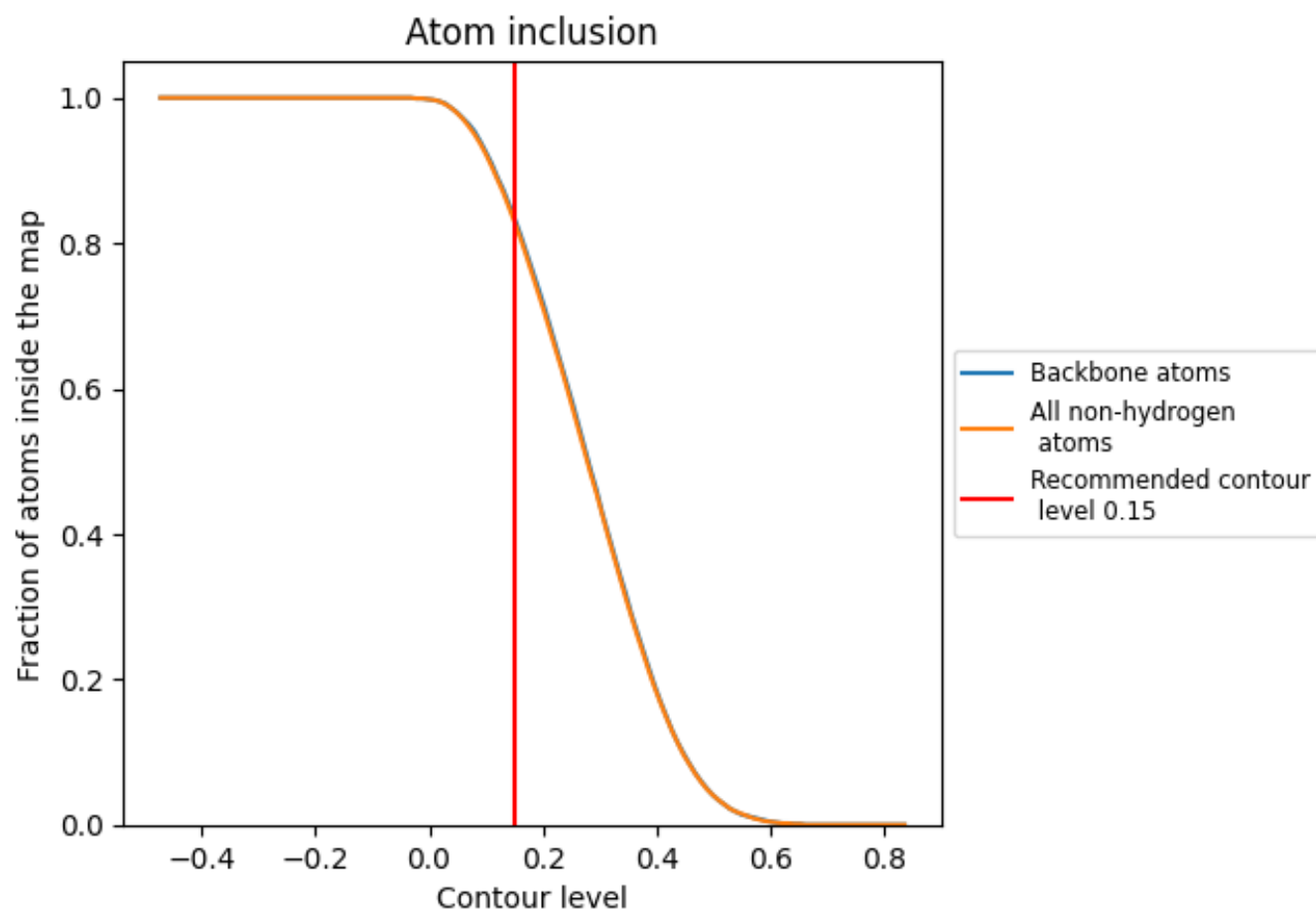
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8300	 0.6430
4	 0.7330	 0.6170
A	 0.7680	 0.6240
H	 0.8360	 0.6380
J	 0.8120	 0.6390
K	 0.9020	 0.6780
L	 0.8980	 0.6630
M	 0.9460	 0.6940
N	 0.9550	 0.6940
V	 0.4360	 0.5750
W	 0.8950	 0.6650
X	 0.7960	 0.6150
Y	 0.8100	 0.6270
Z	 0.8550	 0.6420
k	 0.8000	 0.6250
l	 0.8280	 0.6260
m	 0.7750	 0.6090
n	 0.7020	 0.5770
o	 0.8620	 0.6500
p	 0.7800	 0.6330
q	 0.7890	 0.6220
r	 0.7900	 0.6220
s	 0.7170	 0.5870
t	 0.8180	 0.6310
u	 0.7770	 0.5990
v	 0.8400	 0.6390
w	 0.8460	 0.6380
x	 0.7270	 0.6080
y	 0.8010	 0.6250
z	 0.8390	 0.6360

