



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 08:39 PM UTC

PDB ID : 8ZXZ / pdb_00008zxz
EMDB ID : EMD-60550
Title : Complex I form respirasome closed state bound by proguanil (SC-ProgC)
Authors : Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.
Deposited on : 2024-06-15
Resolution : 3.14 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

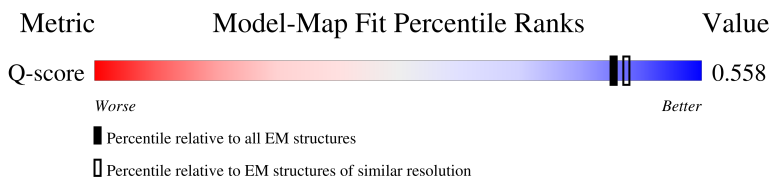
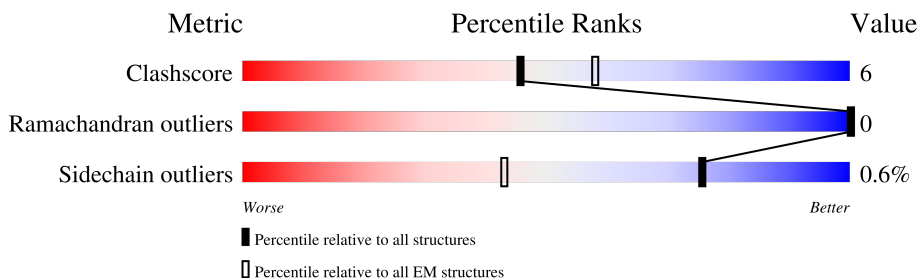
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.14 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	14483 (2.64 - 3.64)

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	4L	98	
2	A1	70	
3	A2	85	
4	A3	83	

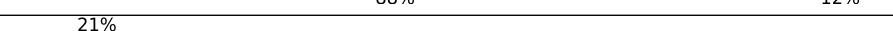
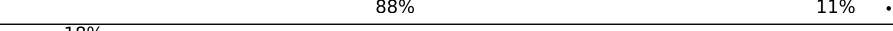
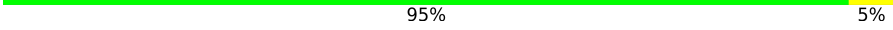
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Mol	Chain	Length	Quality of chain
5	A5	112	
6	A6	114	
7	A7	112	
8	A8	171	
9	A9	341	
10	AB	87	
10	AC	87	
11	AK	321	
12	AL	140	
13	AM	144	
14	AN	142	
15	B1	56	
16	B2	67	
17	B3	80	
18	B4	128	
19	B5	138	
20	B6	126	
21	B7	125	
22	B8	156	
23	B9	178	
24	BK	176	
25	BL	102	
26	CA	49	
27	CB	121	
28	N1	318	

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Mol	Chain	Length	Quality of chain
29	N2	347	
30	N3	115	
31	N4	459	
32	N5	603	
33	N6	174	
34	S1	689	
35	S2	430	
36	S3	208	
37	S4	124	
38	S5	105	
39	S6	96	
40	S7	156	
41	S8	176	
42	V1	431	
43	V2	217	
44	V3	42	

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
52	XEW	N1	402	-	X	-	-
52	XEW	S2	501	-	X	-	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 68568 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 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4L	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A1	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A2	85	Total	C	N	O	S	0	0
			686	431	128	125	2		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A3	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A5	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A6	114	Total	C	N	O	S	0	0
			967	617	178	167	5		

- Molecule 7 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A7	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A8	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A9	341	Total	C	N	O	S	0	0
			2743	1777	480	477	9		

- Molecule 10 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AB	77	Total	C	N	O	S	0	0
			624	402	93	124	5		
10	AC	87	Total	C	N	O	S	0	0
			702	452	103	142	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	321	Total	C	N	O	S	0	0
			2601	1655	444	492	10		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	144	Total	C	N	O	S	0	0
			1204	770	218	212	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	142	Total	C	N	O	S	0	0
			1173	755	203	206	9		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	B1	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	B2	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B3	80	Total	C	N	O	S	0	0
			641	418	108	114	1		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	B4	128	Total	C	N	O	0	0
			1062	691	182	189		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	B5	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B6	103	Total	C	N	O	S	0	0
			882	577	156	148	1		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B7	125	Total	C	N	O	S	0	0
			1068	663	204	190	11		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B8	156	Total	C	N	O	S	0	0
			1315	853	213	241	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B9	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BK	174	Total	C	N	O	S	0	0
			1456	913	264	271	8		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BL	99	Total	C	N	O	S	0	0
			828	531	137	156	4		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	CA	49	Total	C	N	O	0	0
			417	276	71	70		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CB	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 28 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	N1	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

- Molecule 29 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	N2	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 30 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	N3	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

- Molecule 31 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	N4	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	N5	603	Total	C	N	O	S	0	0
			4785	3173	741	820	51		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	N6	174	Total	C	N	O	S	0	0
			1329	892	189	236	12		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	S1	689	Total	C	N	O	S	0	0
			5290	3317	922	1012	39		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	S2	430	Total	C	N	O	S	0	0
			3459	2212	594	629	24		

- Molecule 36 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	S3	208	Total	C	N	O	S	0	0
			1738	1124	298	314	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	S4	124	Total	C	N	O	S	0	0
			1007	637	179	188	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	S5	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	S6	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	S7	156	Total	C	N	O	S	0	0
			1248	794	227	213	14		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	S8	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	V1	431	Total	C	N	O	S	0	0
			3316	2092	592	612	20		

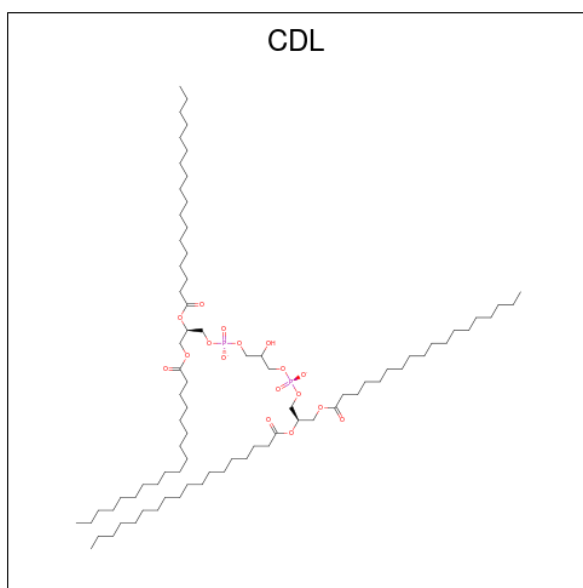
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	V2	217	Total	C	N	O	S	0	0
			1671	1065	281	315	10		

- Molecule 44 is a protein called NADH:ubiquinone oxidoreductase subunit V3.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	V3	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

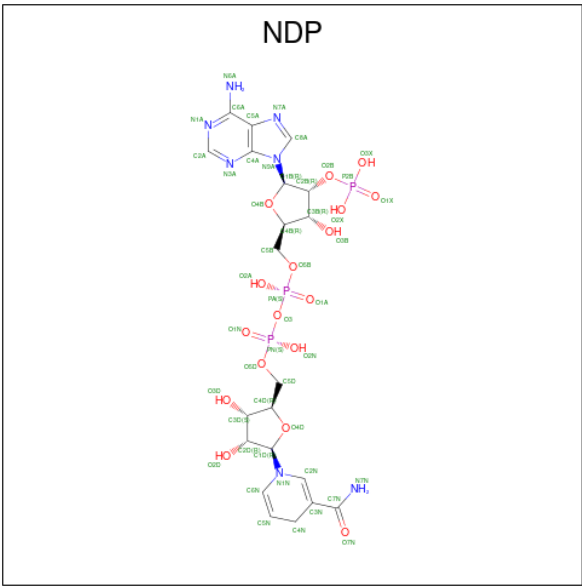
- Molecule 45 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
45	4L	1	Total	C	O	P	0
			92	73	17	2	
45	A7	1	Total	C	O	P	0
			51	32	17	2	
45	A8	1	Total	C	O	P	0
			83	64	17	2	
45	AL	1	Total	C	O	P	0
			94	75	17	2	
45	B4	1	Total	C	O	P	0
			80	61	17	2	
45	B4	1	Total	C	O	P	0
			62	43	17	2	
45	B5	1	Total	C	O	P	0
			100	81	17	2	
45	N1	1	Total	C	O	P	0
			78	59	17	2	
45	N2	1	Total	C	O	P	0
			68	49	17	2	
45	N4	1	Total	C	O	P	0
			100	81	17	2	
45	N5	1	Total	C	O	P	0
			89	70	17	2	
45	N5	1	Total	C	O	P	0
			100	81	17	2	

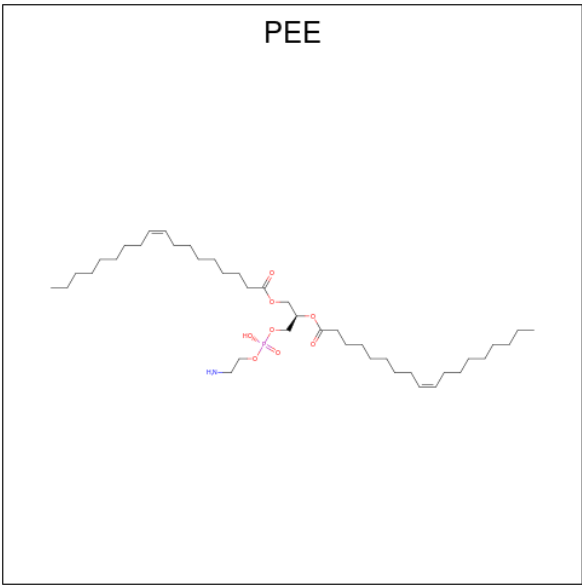
- Molecule 46 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					AltConf
46	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 47 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P).



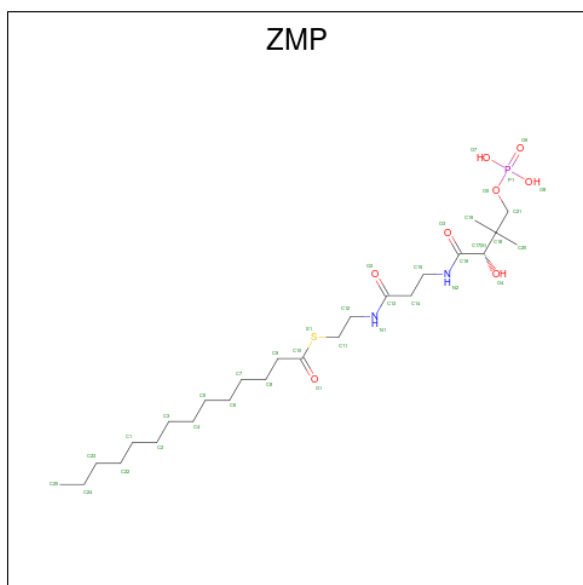
Mol	Chain	Residues	Atoms					AltConf
47	A9	1	Total	C	N	O	P	0
			39	29	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
47	BL	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	N1	1	Total	C	N	O	P	0
			31	21	1	8	1	
47	N1	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	N2	1	Total	C	N	O	P	0
			48	38	1	8	1	
47	N3	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	N4	1	Total	C	N	O	P	0
			49	39	1	8	1	
47	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
47	N5	1	Total	C	N	O	P	0
			40	30	1	8	1	
47	N5	1	Total	C	N	O	P	0
			51	41	1	8	1	

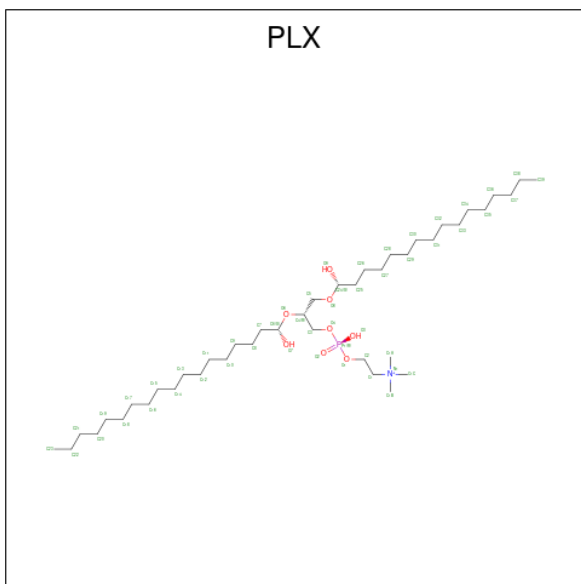
- Molecule 48 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



Mol	Chain	Residues	Atoms						AltConf
48	AB	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	
48	AC	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- # ADP

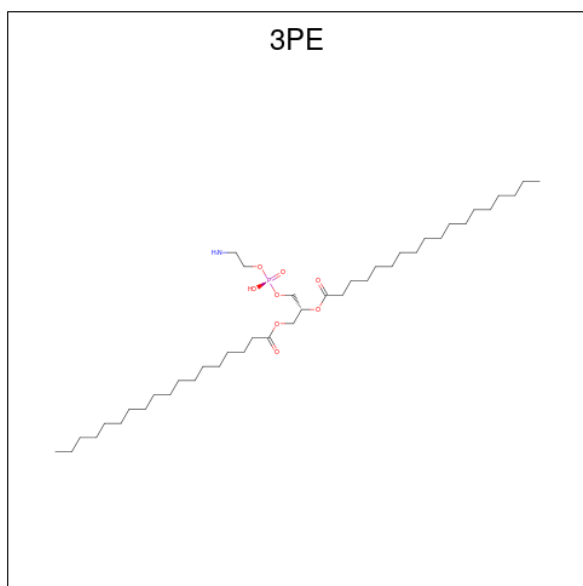
- Molecule 50 is (9R,11S)-9-([[(1S)-1-HYDROXYHEXADECYL]OXY]METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$).



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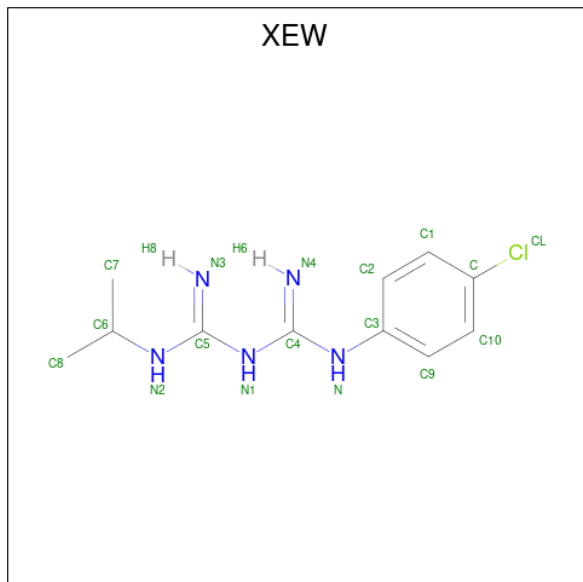
Mol	Chain	Residues	Atoms					AltConf
50	B5	1	Total	C	N	O	P	0
			52	42	1	8	1	
50	CB	1	Total	C	N	O	P	0
			52	42	1	8	1	
50	N3	1	Total	C	N	O	P	0
			52	42	1	8	1	
50	N4	1	Total	C	N	O	P	0
			47	37	1	8	1	
50	N4	1	Total	C	N	O	P	0
			49	39	1	8	1	
50	S7	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 51 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



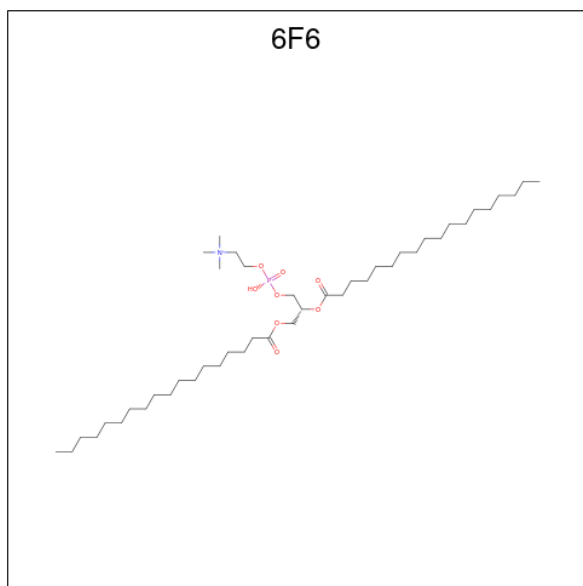
Mol	Chain	Residues	Atoms					AltConf
51	B8	1	Total	C	N	O	P	0
			32	22	1	8	1	
51	CA	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	CB	1	Total	C	N	O	P	0
			46	36	1	8	1	
51	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
51	S7	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 52 is N-(4-chlorophenyl)-N'-(propan-2-yl)triimidodicarbonic diamide (CCD ID: XEW) (formula: $C_{11}H_{16}ClN_5$).



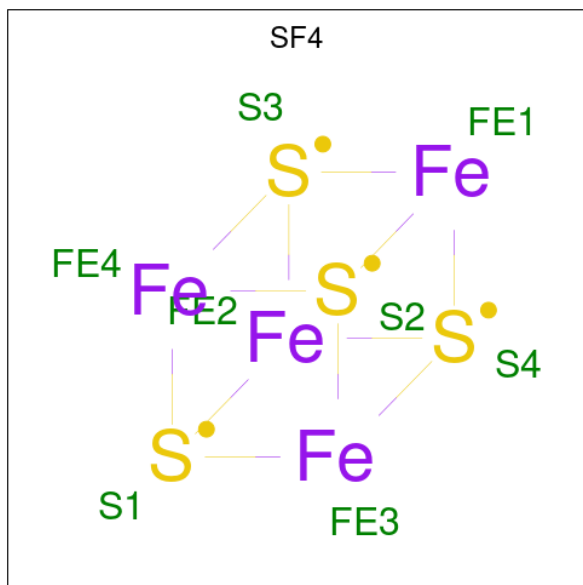
Mol	Chain	Residues	Atoms				AltConf
			Total	C	Cl	N	
52	N1	1	17	11	1	5	0
52	S2	1	17	11	1	5	0

- Molecule 53 is (4S,7R)-4-hydroxy-N,N,N-trimethyl-7-(octadecanoyloxy)-4,10-dioxo-3,5,9-tri-oxa-4lambda 5 -phosphaheptacosan-1-aminium (CCD ID: 6F6) (formula: $C_{44}H_{89}NO_8P$).



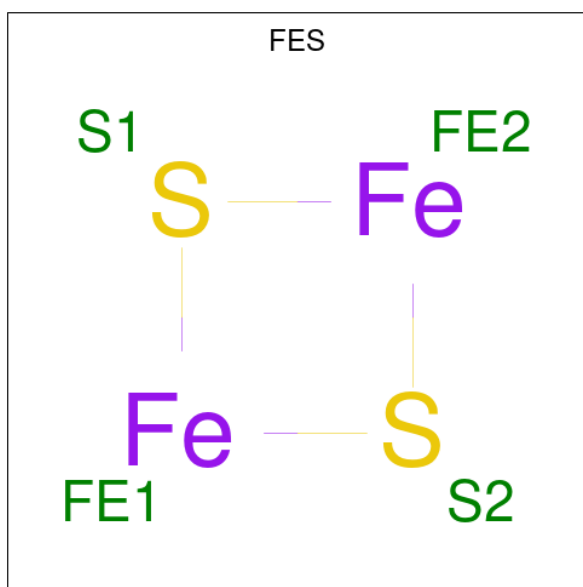
Mol	Chain	Residues	Atoms					AltConf
53	N3	1	Total	C	N	O	P	0
			54	44	1	8	1	
53	N6	1	Total	C	N	O	P	0
			48	38	1	8	1	

- Molecule 54 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
54	S1	1	Total	Fe	S	0
			8	4	4	
54	S1	1	Total	Fe	S	0
			8	4	4	
54	S7	1	Total	Fe	S	0
			8	4	4	
54	S8	1	Total	Fe	S	0
			8	4	4	
54	S8	1	Total	Fe	S	0
			8	4	4	
54	V1	1	Total	Fe	S	0
			8	4	4	

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



Mol	Chain	Residues	Atoms			AltConf
55	S1	1	Total	Fe	S	0
			4	2	2	
55	V2	1	Total	Fe	S	0
			4	2	2	

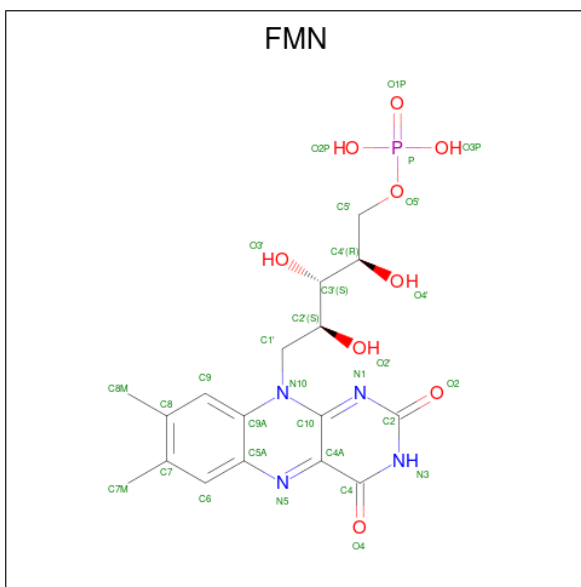
- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	S1	1	Total	Mg	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
57	S6	1	Total	Zn	0
			1	1	

- Molecule 58 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).

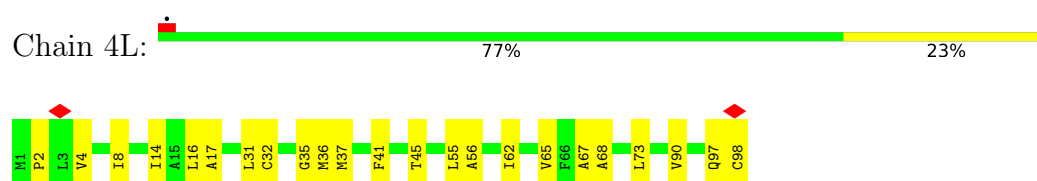


Mol	Chain	Residues	Atoms					AltConf
58	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

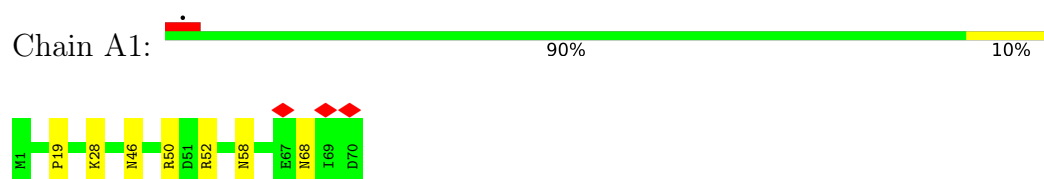
3 Residue-property plots [i](#)

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

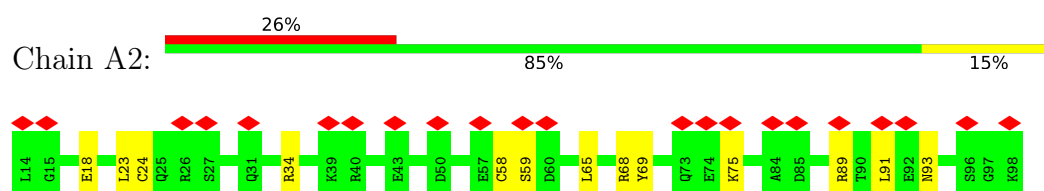
- Molecule 1: NADH-ubiquinone oxidoreductase chain 4L



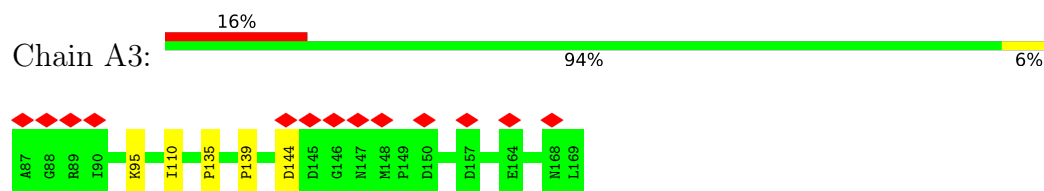
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



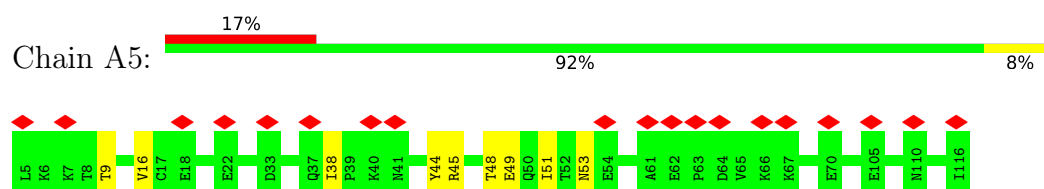
- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



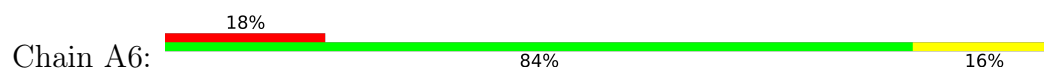
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



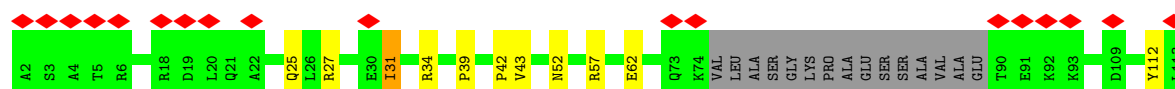
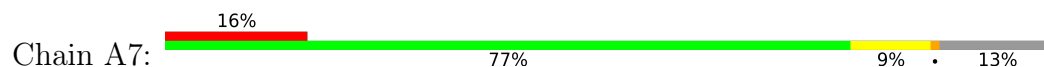
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



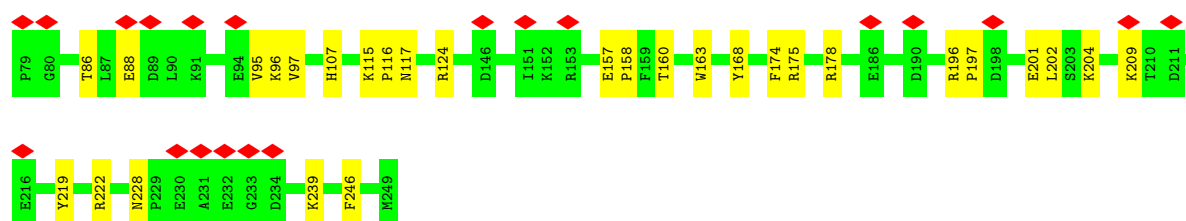
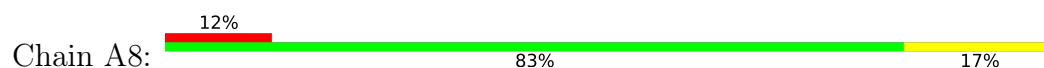
- Molecule 6: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



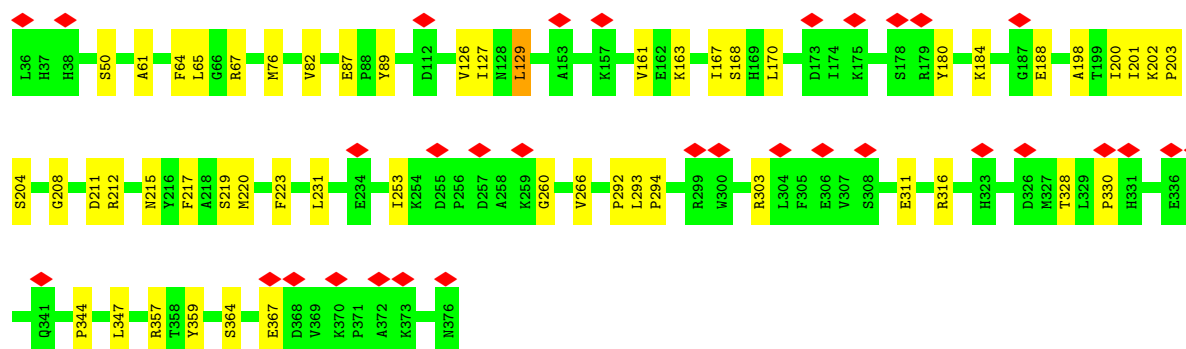
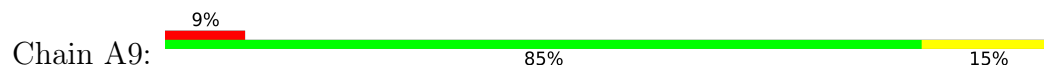
- Molecule 7: Complex I-B14.5a



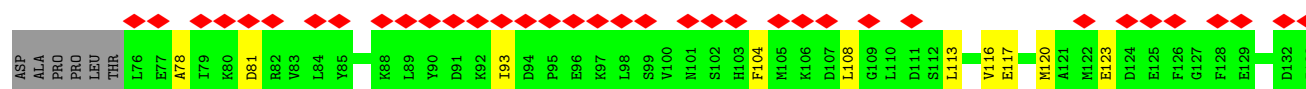
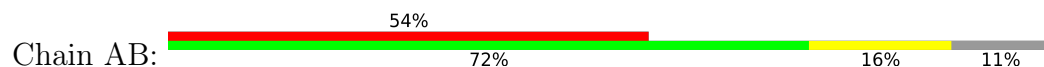
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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

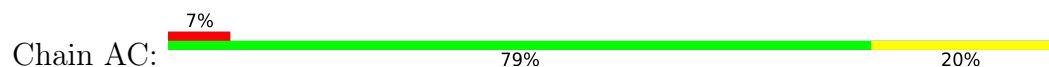


- Molecule 10: Acyl carrier protein

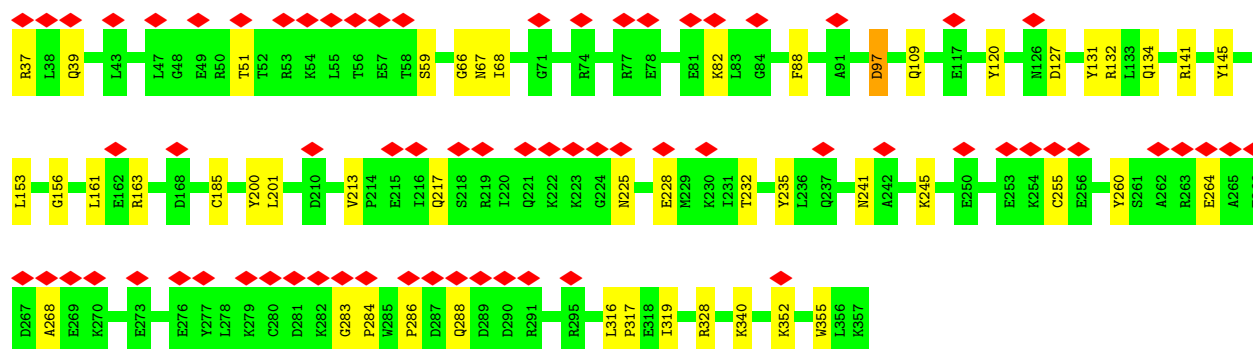
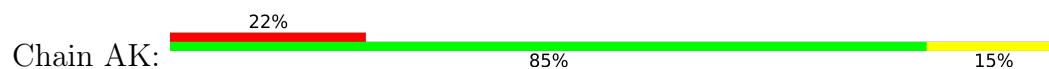




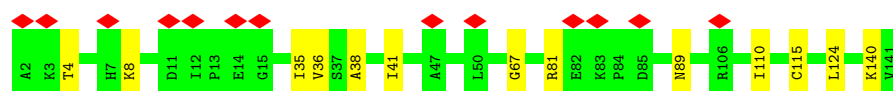
- Molecule 10: Acyl carrier protein



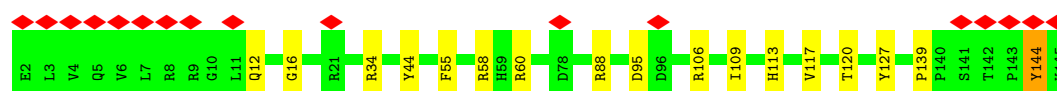
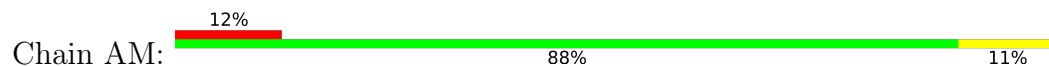
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



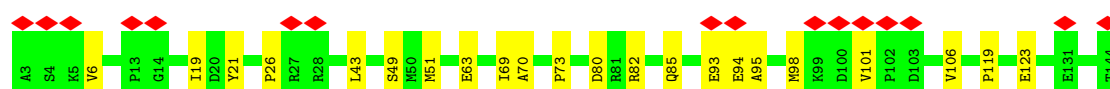
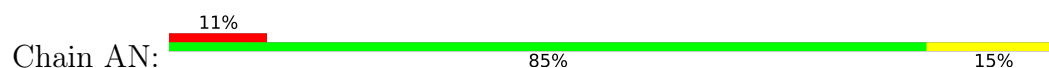
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



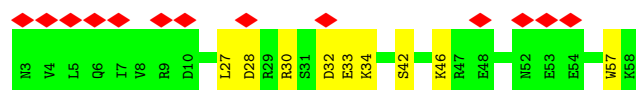
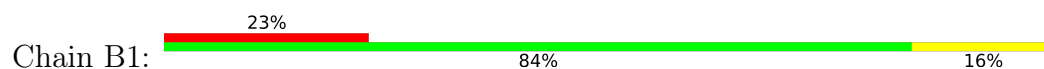
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



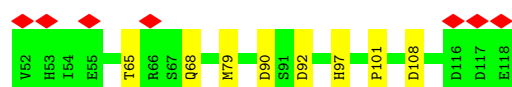
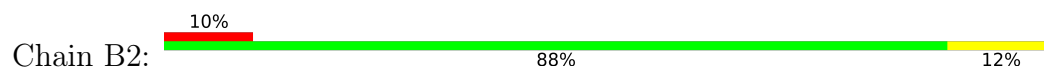
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



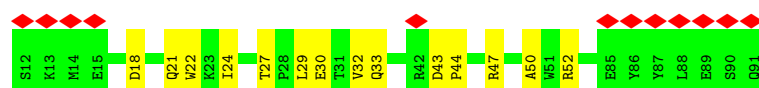
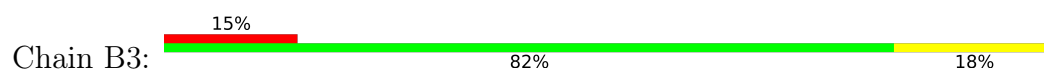
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



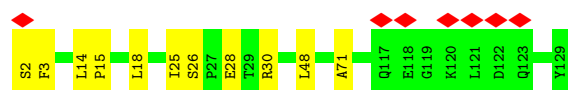
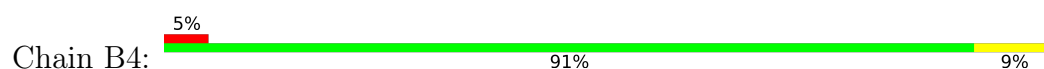
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



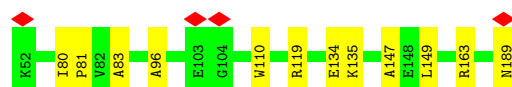
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



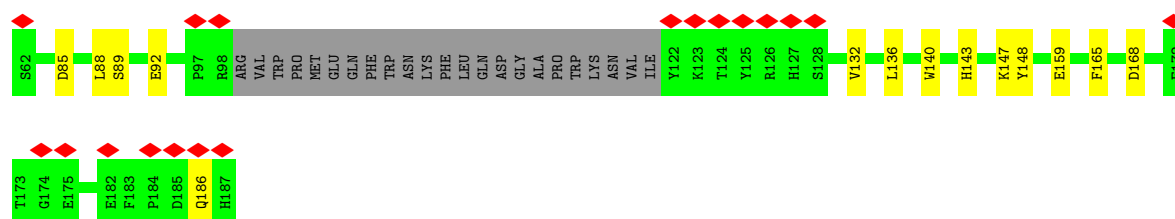
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



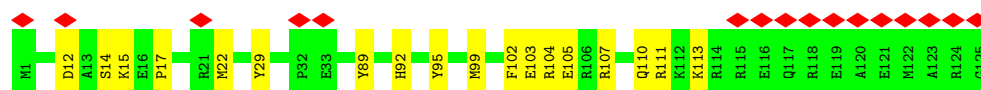
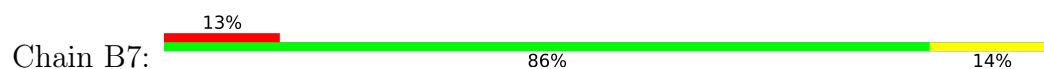
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



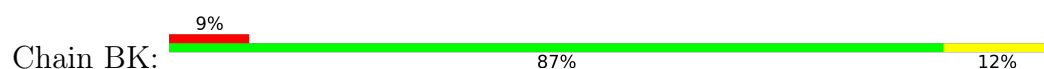
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



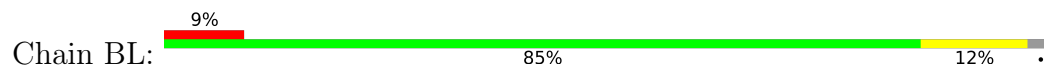
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



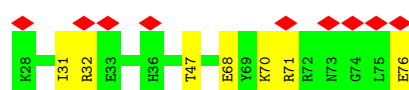
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

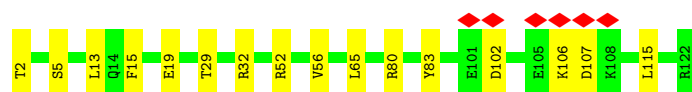


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

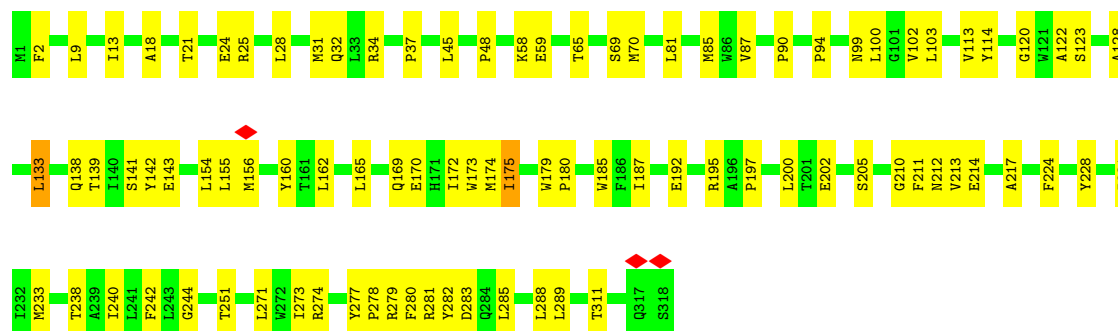


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C2

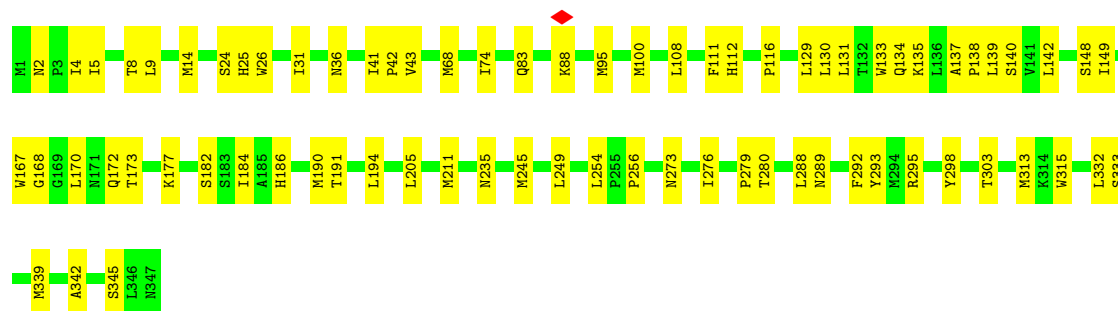
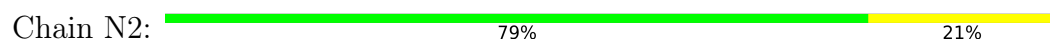




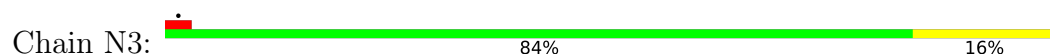
- Molecule 28: NADH-ubiquinone oxidoreductase chain 1



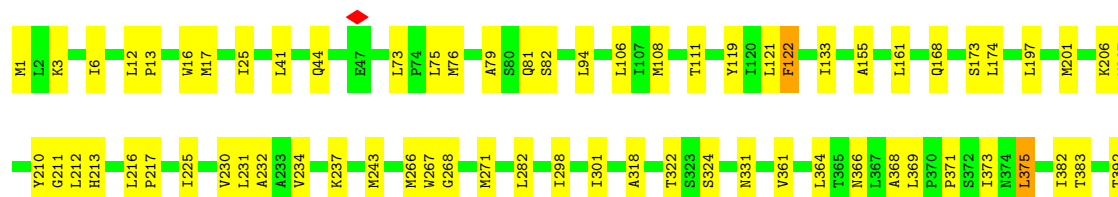
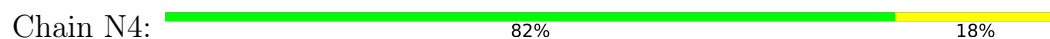
- Molecule 29: NADH-ubiquinone oxidoreductase chain 2

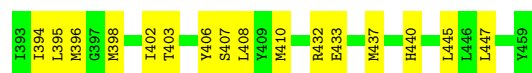


- Molecule 30: NADH-ubiquinone oxidoreductase chain 3



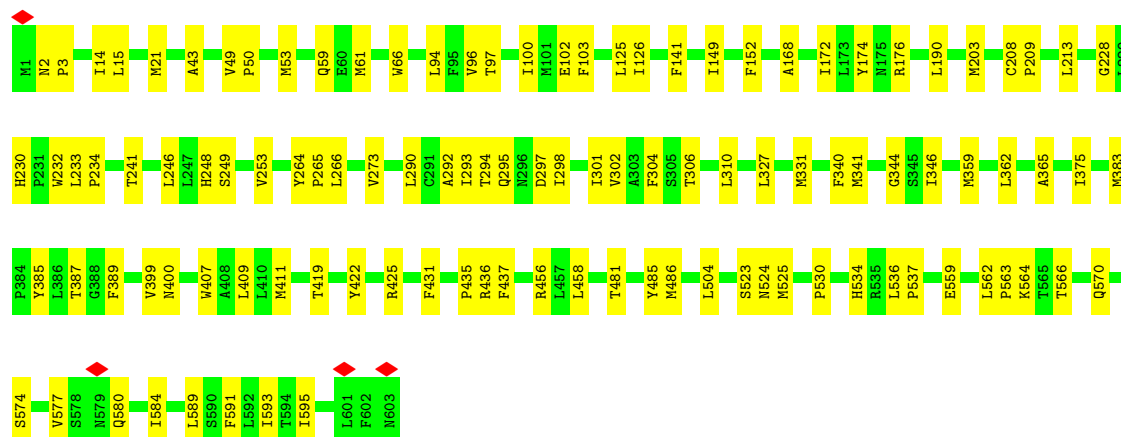
- Molecule 31: NADH-ubiquinone oxidoreductase chain 4





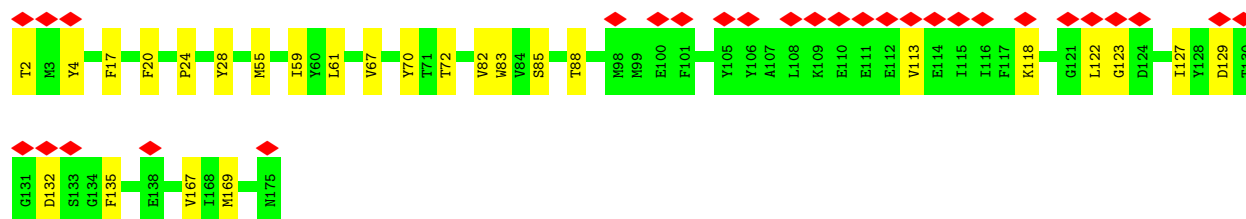
• Molecule 32: NADH-ubiquinone oxidoreductase chain 5

Chain N5: 82% 18%



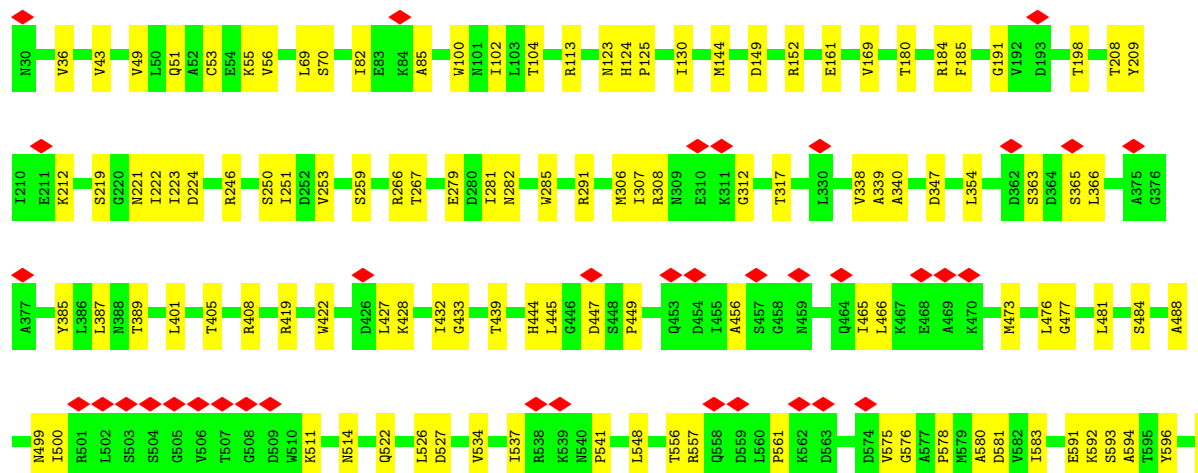
• Molecule 33: NADH-ubiquinone oxidoreductase chain 6

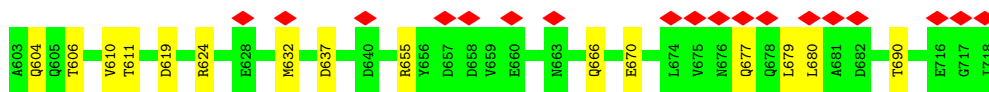
Chain N6: 17% 85% 15%



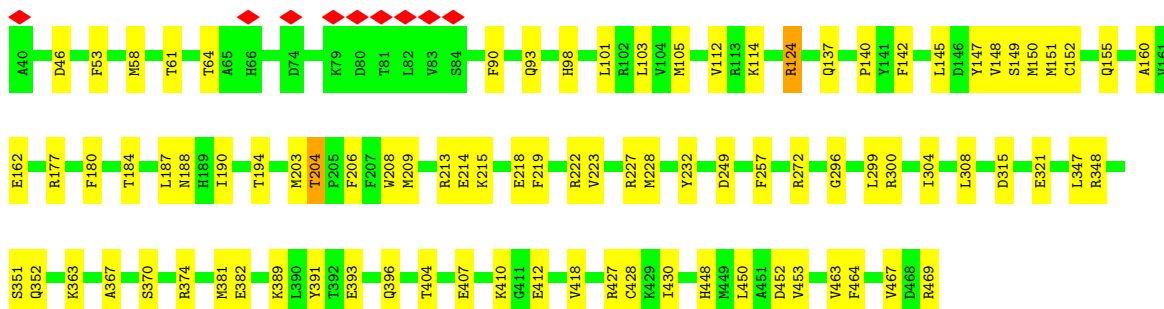
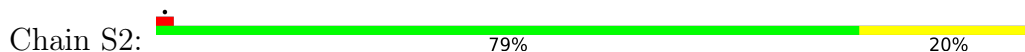
• Molecule 34: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain S1: 8% 81% 19%

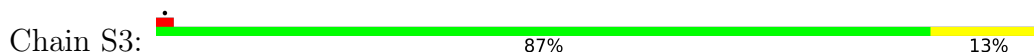




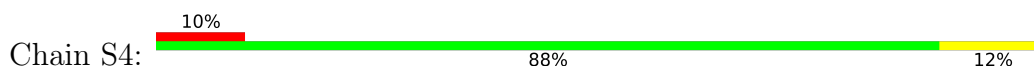
- Molecule 35: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



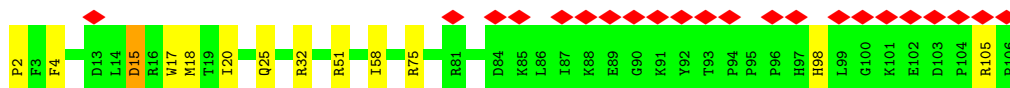
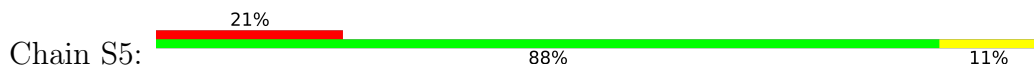
- Molecule 36: Complex I-30kD



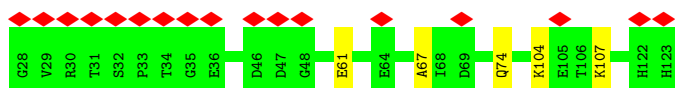
- Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



- Molecule 38: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

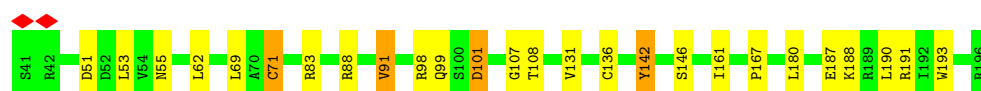


- Molecule 39: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



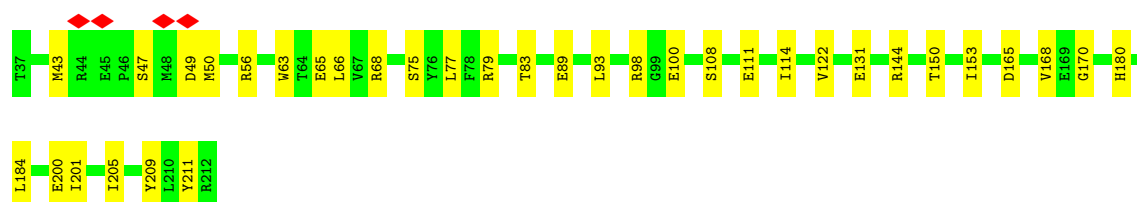
- Molecule 40: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain S7:  83% 14%



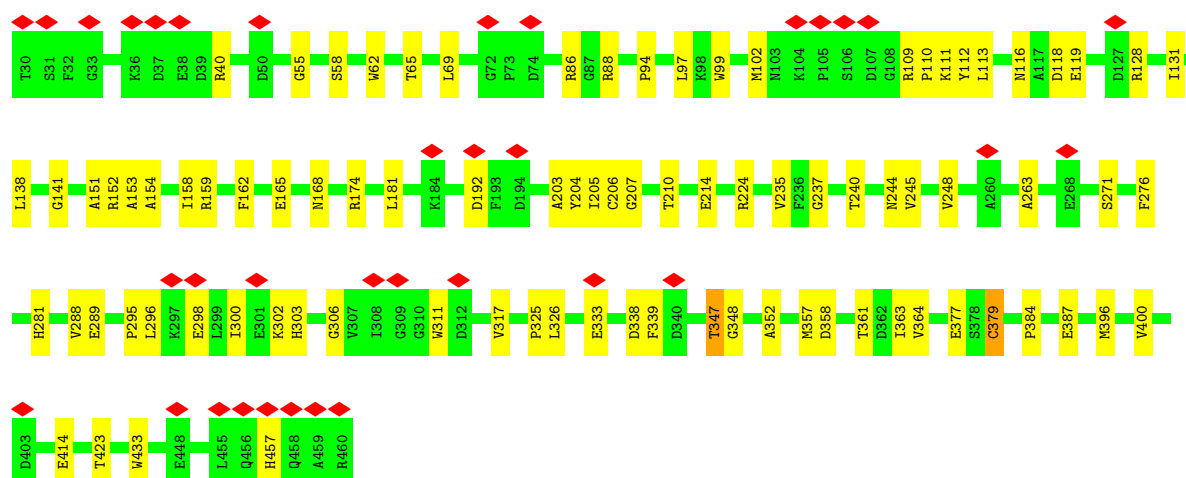
- Molecule 41: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain S8:  80% 20%



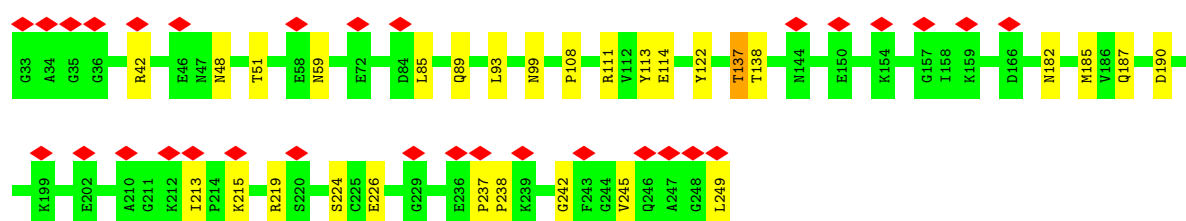
- Molecule 42: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain V1:  8% 80% 20%



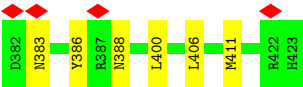
- Molecule 43: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain V2:  14% 86% 13%



- Molecule 44: NADH:ubiquinone oxidoreductase subunit V3

Chain V3:  10% 86% 14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92003	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 ($e^-/\text{\AA}^2$)	51.9	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	10500	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	53.044	Depositor
Minimum map value	-19.428	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	7	Depositor
Map size (Å)	576.0, 576.0, 576.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, PLX, ZMP, XEW, 6F6, SF4, PEE, MG, 2MR, FMN, CDL, ADP, FES, NDP, ZN

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	4L	0.13	0/759	0.27	0/1029
2	A1	0.11	0/577	0.25	0/777
3	A2	0.10	0/697	0.26	0/938
4	A3	0.10	0/664	0.23	0/912
5	A5	0.11	0/929	0.22	0/1258
6	A6	0.11	0/991	0.25	0/1335
7	A7	0.10	0/798	0.22	0/1079
8	A8	0.10	0/1436	0.24	0/1938
9	A9	0.11	0/2820	0.24	0/3823
10	AB	0.07	0/633	0.20	0/851
10	AC	0.12	0/714	0.23	0/965
11	AK	0.10	0/2661	0.28	2/3602 (0.1%)
12	AL	0.11	0/1042	0.21	0/1411
13	AM	0.11	0/1245	0.23	0/1694
14	AN	0.12	0/1204	0.25	0/1624
15	B1	0.11	0/491	0.23	0/663
16	B2	0.12	0/610	0.25	0/836
17	B3	0.12	0/660	0.23	0/892
18	B4	0.13	0/1092	0.25	0/1481
19	B5	0.14	0/1184	0.25	0/1603
20	B6	0.14	0/910	0.31	0/1237
21	B7	0.12	0/1092	0.23	0/1459
22	B8	0.13	0/1371	0.25	0/1875
23	B9	0.13	0/1590	0.26	0/2155
24	BK	0.13	0/1489	0.23	0/2008
25	BL	0.13	0/851	0.26	0/1155
26	CA	0.10	0/430	0.21	0/581
27	CB	0.13	0/1031	0.24	0/1394
28	N1	0.17	0/2581	0.33	0/3529
29	N2	0.17	0/2773	0.32	0/3768
30	N3	0.14	0/938	0.25	0/1281
31	N4	0.17	0/3723	0.30	0/5078

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	N5	0.16	0/4914	0.33	0/6683
33	N6	0.12	0/1364	0.27	0/1850
34	S1	0.14	0/5378	0.29	0/7287
35	S2	0.15	0/3538	0.27	0/4796
36	S3	0.13	0/1789	0.25	0/2436
37	S4	0.12	0/1030	0.25	0/1391
38	S5	0.10	0/889	0.21	0/1190
39	S6	0.11	0/755	0.26	0/1018
40	S7	0.15	0/1279	0.27	0/1730
41	S8	0.15	0/1443	0.26	0/1952
42	V1	0.14	0/3391	0.29	0/4583
43	V2	0.13	0/1711	0.28	0/2328
44	V3	0.09	0/365	0.25	0/493
All	All	0.13	0/67832	0.27	2/91968 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AK	200	TYR	CA-C-N	5.29	130.98	120.94
11	AK	200	TYR	C-N-CA	5.29	130.98	120.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4L	748	0	799	24	0
2	A1	562	0	557	6	0
3	A2	686	0	699	7	0
4	A3	643	0	642	5	0
5	A5	910	0	950	5	0
6	A6	967	0	972	17	0
7	A7	780	0	808	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A8	1398	0	1372	24	0
9	A9	2743	0	2762	34	0
10	AB	624	0	625	9	0
10	AC	702	0	694	12	0
11	AK	2601	0	2566	29	0
12	AL	1021	0	1025	12	0
13	AM	1204	0	1162	11	0
14	AN	1173	0	1166	20	0
15	B1	479	0	486	8	0
16	B2	584	0	529	7	0
17	B3	641	0	620	9	0
18	B4	1062	0	1072	7	0
19	B5	1151	0	1164	10	0
20	B6	882	0	899	13	0
21	B7	1068	0	1043	15	0
22	B8	1315	0	1208	5	0
23	B9	1534	0	1470	18	0
24	BK	1456	0	1426	17	0
25	BL	828	0	788	11	0
26	CA	417	0	422	4	0
27	CB	1000	0	994	14	0
28	N1	2508	0	2607	65	0
29	N2	2710	0	2874	58	0
30	N3	914	0	951	15	0
31	N4	3631	0	3839	60	0
32	N5	4785	0	4933	80	0
33	N6	1329	0	1326	28	0
34	S1	5290	0	5321	82	0
35	S2	3459	0	3396	68	0
36	S3	1738	0	1693	18	0
37	S4	1007	0	1008	12	0
38	S5	867	0	871	15	0
39	S6	741	0	701	4	0
40	S7	1248	0	1254	22	0
41	S8	1412	0	1363	28	0
42	V1	3316	0	3272	54	0
43	V2	1671	0	1673	16	0
44	V3	355	0	329	6	0
45	4L	92	0	137	10	0
45	A7	51	0	46	0	0
45	A8	83	0	113	6	0
45	AL	94	0	138	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	B4	142	0	175	3	0
45	B5	100	0	156	4	0
45	N1	78	0	103	5	0
45	N2	68	0	80	0	0
45	N4	100	0	156	8	0
45	N5	189	0	284	16	0
46	A9	48	0	26	1	0
47	A9	39	0	52	4	0
47	BL	51	0	82	2	0
47	N1	82	0	118	8	0
47	N2	48	0	73	7	0
47	N3	51	0	82	2	0
47	N4	49	0	75	6	0
47	N5	137	0	205	4	0
48	AB	36	0	47	2	0
48	AC	36	0	47	2	0
49	AK	27	0	12	4	0
50	AM	52	0	88	6	0
50	B5	52	0	88	0	0
50	CB	52	0	88	4	0
50	N3	52	0	88	1	0
50	N4	96	0	154	4	0
50	S7	52	0	88	4	0
51	B8	32	0	38	1	0
51	CA	51	0	82	2	0
51	CB	46	0	69	0	0
51	N5	46	0	69	2	0
51	S7	51	0	82	3	0
52	N1	17	0	0	0	0
52	S2	17	0	0	0	0
53	N3	54	0	0	0	0
53	N6	48	0	0	1	0
54	S1	16	0	0	1	0
54	S7	8	0	0	0	0
54	S8	16	0	0	1	0
54	V1	8	0	0	0	0
55	S1	4	0	0	0	0
55	V2	4	0	0	0	0
56	S1	1	0	0	0	0
57	S6	1	0	0	0	0
58	V1	31	0	19	1	0
All	All	68568	0	69491	860	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (860) 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)
21:B7:92:HIS:HD1	32:N5:481:THR:HG1	1.12	0.94
24:BK:140:GLN:O	24:BK:144:SER:HB2	1.70	0.90
9:A9:198:ALA:O	9:A9:260:GLY:HA2	1.74	0.88
1:4L:37:MET:HG2	1:4L:67:ALA:HB2	1.59	0.82
20:B6:88:LEU:HD22	20:B6:92:GLU:HG2	1.61	0.81
11:AK:120:TYR:HH	49:AK:401:ADP:HO2'	1.30	0.79
34:S1:149:ASP:HB2	35:S2:367:ALA:HB3	1.66	0.78
17:B3:27:THR:HG22	17:B3:29:LEU:H	1.49	0.77
45:N5:703:CDL:HA4	45:N5:703:CDL:H551	1.66	0.75
1:4L:68:ALA:HB3	30:N3:67:LEU:HD11	1.68	0.74
29:N2:88:LYS:HG3	29:N2:148:SER:HB3	1.70	0.74
28:N1:139:THR:O	28:N1:143:GLU:HB2	1.89	0.73
47:N2:402:PEE:H37	47:N4:501:PEE:H46	1.71	0.71
34:S1:433:GLY:HA2	34:S1:447:ASP:HA	1.71	0.71
1:4L:14:ILE:HG12	45:4L:201:CDL:H781	1.73	0.71
34:S1:250:SER:HB2	34:S1:606:THR:HG23	1.72	0.70
42:V1:235:VAL:HG12	42:V1:240:THR:HG21	1.73	0.70
13:AM:34:ARG:NH2	41:S8:89:GLU:OE2	2.23	0.70
12:AL:140:LYS:O	29:N2:273:ASN:ND2	2.24	0.70
42:V1:40:ARG:NH1	42:V1:289:GLU:O	2.25	0.70
31:N4:369:LEU:HD21	32:N5:149:ILE:HD13	1.74	0.69
2:A1:46:ASN:ND2	33:N6:132:ASP:OD2	2.25	0.69
9:A9:129:LEU:HD23	9:A9:167:ILE:HG13	1.74	0.69
28:N1:87:VAL:HG11	30:N3:6:THR:HG21	1.74	0.69
30:N3:37:TYR:OH	35:S2:93:GLN:NE2	2.25	0.69
42:V1:205:ILE:HG12	42:V1:379:CYS:HB3	1.73	0.69
3:A2:59:SER:HB2	34:S1:655:ARG:HD3	1.75	0.68
45:4L:201:CDL:H521	33:N6:88:THR:HG23	1.75	0.68
35:S2:374:ARG:NH2	41:S8:165:ASP:OD1	2.27	0.67
40:S7:188:LYS:HB2	40:S7:191:ARG:HB2	1.75	0.67
3:A2:24:CYS:N	3:A2:58:CYS:SG	2.67	0.67
17:B3:33:GLN:NE2	17:B3:43:ASP:OD1	2.27	0.67
8:A8:174:PHE:HB3	8:A8:178:ARG:HH12	1.60	0.67
34:S1:338:VAL:O	34:S1:365:SER:HB2	1.96	0.66
42:V1:94:PRO:HB2	42:V1:97:LEU:HB2	1.77	0.66
6:A6:89:VAL:HG22	48:AB:201:ZMP:H2A	1.78	0.66
35:S2:124:2MR:O	40:S7:146:SER:OG	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AC:201:ZMP:H14	23:B9:102:ALA:HB1	1.78	0.65
12:AL:140:LYS:H	29:N2:273:ASN:HD22	1.41	0.65
9:A9:188:GLU:HG3	9:A9:200:ILE:HD13	1.78	0.65
8:A8:246:PHE:HE1	45:A8:301:CDL:H341	1.62	0.65
10:AB:116:VAL:HG12	10:AB:120:MET:HE2	1.78	0.65
1:4L:31:LEU:HD21	33:N6:67:VAL:HG11	1.79	0.65
45:N5:703:CDL:H591	45:N5:703:CDL:H642	1.79	0.65
31:N4:371:PRO:HD2	45:N5:703:CDL:H391	1.77	0.64
35:S2:308:LEU:HB2	35:S2:407:GLU:HB2	1.79	0.64
32:N5:530:PRO:O	32:N5:534:HIS:HB2	1.98	0.64
29:N2:108:LEU:HD11	29:N2:191:THR:HG21	1.80	0.64
33:N6:113:VAL:HG13	33:N6:118:LYS:HG2	1.77	0.64
27:CB:2:THR:HB	27:CB:5:SER:HB3	1.80	0.64
6:A6:88:LYS:NZ	6:A6:132:PHE:O	2.30	0.63
35:S2:155:GLN:NE2	35:S2:315:ASP:OD2	2.29	0.63
42:V1:325:PRO:HG3	42:V1:433:TRP:HB3	1.81	0.63
45:N1:401:CDL:HB31	33:N6:82:VAL:HG21	1.81	0.62
29:N2:42:PRO:HG2	33:N6:167:VAL:HG22	1.81	0.62
42:V1:111:LYS:HB2	42:V1:151:ALA:HA	1.79	0.62
31:N4:375:LEU:HD11	32:N5:141:PHE:HE2	1.65	0.62
42:V1:112:TYR:HB2	42:V1:240:THR:HG22	1.81	0.62
9:A9:87:GLU:HG3	9:A9:89:TYR:H	1.64	0.62
20:B6:147:LYS:NZ	24:BK:42:ASP:OD1	2.32	0.62
40:S7:55:ASN:ND2	40:S7:187:GLU:O	2.33	0.62
43:V2:111:ARG:NH1	43:V2:114:GLU:OE2	2.32	0.62
43:V2:108:PRO:HB2	43:V2:111:ARG:HG2	1.81	0.62
34:S1:266:ARG:HD2	34:S1:267:THR:HG23	1.82	0.62
34:S1:282:ASN:ND2	34:S1:285:TRP:O	2.33	0.62
34:S1:456:ALA:O	34:S1:499:ASN:ND2	2.33	0.62
35:S2:222:ARG:NH1	35:S2:249:ASP:OD2	2.19	0.62
11:AK:145:TYR:OH	11:AK:201:LEU:O	2.17	0.61
42:V1:110:PRO:HB3	42:V1:152:ARG:HD3	1.81	0.61
45:N4:504:CDL:H251	45:N4:504:CDL:H851	1.82	0.61
41:S8:47:SER:O	41:S8:56:ARG:NH2	2.33	0.61
32:N5:293:ILE:HD12	45:N5:704:CDL:H521	1.81	0.61
24:BK:2:PRO:O	24:BK:7:LYS:NZ	2.33	0.61
11:AK:141:ARG:NH2	49:AK:401:ADP:N7	2.48	0.61
21:B7:29:TYR:O	21:B7:104:ARG:NH2	2.33	0.61
39:S6:104:LYS:HG2	39:S6:107:LYS:HG2	1.83	0.61
8:A8:239:LYS:HD3	19:B5:149:LEU:HD11	1.83	0.61
20:B6:132:VAL:O	20:B6:136:LEU:HB3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:V2:182:ASN:HB3	43:V2:194:GLU:HB3	1.83	0.61
14:AN:51:MET:HE2	28:N1:311:THR:HB	1.82	0.60
32:N5:100:ILE:HG21	32:N5:246:LEU:HB2	1.83	0.60
34:S1:246:ARG:HH22	37:S4:123:ASN:HD21	1.47	0.60
5:A5:49:GLU:O	5:A5:53:ASN:ND2	2.34	0.60
40:S7:53:LEU:HB2	50:S7:302:PLX:H301	1.82	0.60
28:N1:173:TRP:HB3	28:N1:175:ILE:HG22	1.84	0.60
34:S1:49:VAL:HG13	34:S1:102:ILE:HD13	1.82	0.60
37:S4:75:ARG:NH1	37:S4:119:ASP:OD1	2.29	0.60
40:S7:69:LEU:HB2	40:S7:107:GLY:HA3	1.83	0.60
45:A8:301:CDL:H572	45:A8:301:CDL:H532	1.84	0.60
28:N1:141:SER:HB2	28:N1:289:LEU:HD12	1.83	0.60
6:A6:67:ARG:NH2	10:AB:123:GLU:OE1	2.35	0.60
32:N5:362:LEU:HA	32:N5:365:ALA:HB3	1.83	0.60
31:N4:361:VAL:HG22	45:N5:703:CDL:H311	1.84	0.59
34:S1:123:ASN:ND2	42:V1:387:GLU:OE1	2.30	0.59
43:V2:187:GLN:HE21	43:V2:190:ASP:HA	1.65	0.59
31:N4:403:THR:HA	31:N4:406:TYR:CE2	2.37	0.59
45:A8:301:CDL:H112	27:CB:32:ARG:HG2	1.84	0.59
47:N1:404:PEE:H2	35:S2:272:ARG:HH11	1.67	0.59
2:A1:19:PRO:HB3	28:N1:9:LEU:HD12	1.82	0.59
7:A7:62:GLU:OE2	36:S3:44:ARG:NH1	2.35	0.59
28:N1:205:SER:OG	28:N1:279:ARG:NH1	2.36	0.59
34:S1:124:HIS:HD2	35:S2:381:MET:HE2	1.68	0.59
34:S1:433:GLY:O	34:S1:444:HIS:NE2	2.31	0.59
32:N5:419:THR:HA	32:N5:422:TYR:CE2	2.38	0.59
19:B5:163:ARG:NH1	27:CB:102:ASP:OD2	2.28	0.59
34:S1:251:ILE:HD13	34:S1:604:GLN:HB2	1.85	0.59
41:S8:205:ILE:O	41:S8:209:TYR:HB3	2.02	0.59
2:A1:52:ARG:NH1	2:A1:58:ASN:OD1	2.36	0.58
1:4L:2:PRO:HG3	33:N6:127:ILE:HD13	1.85	0.58
24:BK:114:GLN:HG3	32:N5:203:MET:HG2	1.84	0.58
36:S3:187:ILE:HG23	36:S3:188:LEU:HG	1.84	0.58
35:S2:412:GLU:OE2	36:S3:140:ARG:NH2	2.37	0.58
29:N2:142:LEU:HB3	29:N2:194:LEU:HD21	1.85	0.58
1:4L:16:LEU:HD23	45:4L:201:CDL:H862	1.85	0.58
31:N4:168:GLN:HB2	31:N4:174:LEU:HG	1.84	0.58
29:N2:289:ASN:HA	29:N2:292:PHE:CE2	2.39	0.58
13:AM:106:ARG:HB2	13:AM:109:ILE:HG13	1.86	0.57
9:A9:163:LYS:NZ	9:A9:253:ILE:O	2.31	0.57
28:N1:69:SER:HA	45:N1:401:CDL:H141	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:N4:1:MET:HE2	31:N4:111:THR:HG21	1.85	0.57
37:S4:109:ASN:ND2	37:S4:111:LEU:O	2.37	0.57
15:B1:57:TRP:NE1	19:B5:134:GLU:OE1	2.21	0.57
28:N1:102:VAL:HG11	28:N1:154:LEU:HD11	1.85	0.57
34:S1:144:MET:HG3	35:S2:389:LYS:HG3	1.86	0.57
34:S1:428:LYS:HE2	34:S1:465:ILE:HD13	1.86	0.57
10:AC:114:ASP:OD1	23:B9:87:ARG:NH2	2.37	0.57
34:S1:340:ALA:HB3	34:S1:366:LEU:HD23	1.87	0.57
12:AL:35:ILE:HD12	45:AL:201:CDL:H811	1.86	0.57
31:N4:41:LEU:O	31:N4:44:GLN:NE2	2.37	0.57
32:N5:97:THR:HG21	32:N5:125:LEU:HD22	1.85	0.57
45:4L:201:CDL:H181	32:N5:589:LEU:HD11	1.85	0.57
10:AB:93:ILE:HD12	10:AB:108:LEU:HD13	1.85	0.57
3:A2:89:ARG:O	3:A2:93:ASN:ND2	2.37	0.57
14:AN:49:SER:HB2	28:N1:172:ILE:HD13	1.86	0.57
6:A6:81:SER:OG	9:A9:367:GLU:OE2	2.22	0.56
12:AL:67:GLY:HA2	45:AL:201:CDL:H221	1.87	0.56
16:B2:101:PRO:HD2	21:B7:99:MET:HE1	1.87	0.56
28:N1:180:PRO:HB3	47:N1:404:PEE:H21	1.88	0.56
45:N1:401:CDL:H331	45:N1:401:CDL:H181	1.86	0.56
30:N3:70:ALA:HB2	33:N6:59:ILE:HD11	1.87	0.56
31:N4:447:LEU:HD11	50:N4:503:PLX:H381	1.87	0.56
32:N5:375:ILE:HD12	32:N5:458:LEU:HD11	1.87	0.56
43:V2:93:LEU:HD12	43:V2:122:TYR:HB3	1.87	0.56
28:N1:139:THR:HA	28:N1:142:TYR:CE2	2.40	0.56
35:S2:464:PHE:HA	35:S2:467:VAL:HB	1.87	0.56
9:A9:180:TYR:OH	46:A9:401:NDP:O2D	2.24	0.56
11:AK:213:VAL:HG12	11:AK:217:GLN:HE21	1.70	0.56
31:N4:369:LEU:HD23	45:N5:703:CDL:H362	1.87	0.56
25:BL:95:PHE:O	25:BL:99:LEU:HB2	2.06	0.56
28:N1:187:ILE:HD12	47:N1:404:PEE:H52	1.88	0.56
45:B4:202:CDL:H372	31:N4:197:LEU:HD13	1.88	0.56
40:S7:62:LEU:O	40:S7:91:VAL:HA	2.06	0.56
13:AM:117:VAL:O	13:AM:120:THR:OG1	2.23	0.56
25:BL:150:PRO:HG3	27:CB:115:LEU:HD22	1.88	0.56
47:N4:501:PEE:H53	47:N4:501:PEE:H24	1.88	0.56
23:B9:218:GLU:HG2	23:B9:219:ARG:HG2	1.88	0.55
7:A7:34:ARG:NH2	41:S8:93:LEU:O	2.38	0.55
9:A9:61:ALA:HB3	9:A9:82:VAL:HG13	1.87	0.55
32:N5:3:PRO:HB2	32:N5:53:MET:HE1	1.89	0.55
8:A8:107:HIS:HB3	8:A8:197:PRO:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:S7:51:ASP:HB3	40:S7:190:LEU:HB2	1.88	0.55
13:AM:88:ARG:HD3	41:S8:200:GLU:HG3	1.87	0.55
16:B2:108:ASP:OD1	21:B7:107:ARG:NH1	2.40	0.55
9:A9:204:SER:HB2	9:A9:266:VAL:HG12	1.88	0.55
35:S2:190:ILE:HD11	35:S2:257:PHE:HZ	1.72	0.55
35:S2:469:ARG:NH2	36:S3:169:GLU:OE2	2.40	0.55
11:AK:127:ASP:O	11:AK:132:ARG:NH1	2.40	0.55
20:B6:85:ASP:OD2	23:B9:167:TRP:NE1	2.30	0.55
25:BL:89:VAL:HG21	31:N4:25:ILE:HG23	1.89	0.55
35:S2:300:ARG:NH2	35:S2:407:GLU:OE2	2.39	0.55
42:V1:109:ARG:NH1	42:V1:237:GLY:O	2.39	0.55
42:V1:112:TYR:CD1	42:V1:153:ALA:HB3	2.41	0.55
31:N4:392:THR:O	31:N4:396:MET:HG2	2.06	0.54
42:V1:364:VAL:HG12	42:V1:400:VAL:HG12	1.90	0.54
9:A9:198:ALA:O	9:A9:260:GLY:CA	2.53	0.54
28:N1:24:GLU:OE1	28:N1:228:TYR:OH	2.17	0.54
29:N2:131:LEU:O	29:N2:135:LYS:HG2	2.08	0.54
31:N4:383:THR:HG21	32:N5:190:LEU:HD22	1.90	0.54
35:S2:162:GLU:OE2	35:S2:177:ARG:NH2	2.39	0.54
35:S2:391:TYR:HD1	41:S8:122:VAL:HG21	1.72	0.54
31:N4:122:PHE:HE2	31:N4:206:LYS:HG3	1.72	0.54
32:N5:562:LEU:HB3	32:N5:563:PRO:HD3	1.89	0.54
35:S2:90:PHE:HB3	35:S2:103:LEU:HB3	1.90	0.54
42:V1:112:TYR:HD1	42:V1:153:ALA:HB3	1.73	0.54
3:A2:65:LEU:HD11	3:A2:91:LEU:HD13	1.90	0.54
16:B2:90:ASP:OD1	16:B2:90:ASP:N	2.41	0.54
29:N2:235:ASN:O	29:N2:315:TRP:NE1	2.41	0.54
36:S3:132:LEU:HB2	36:S3:141:ILE:HG22	1.90	0.54
9:A9:344:PRO:HG2	9:A9:347:LEU:HD13	1.88	0.54
26:CA:68:GLU:OE2	26:CA:71:ARG:NH2	2.41	0.54
35:S2:145:LEU:HD13	35:S2:430:ILE:HG21	1.90	0.54
47:N5:701:PEE:H36	45:N5:703:CDL:H231	1.90	0.53
20:B6:165:PHE:O	20:B6:168:ASP:HB2	2.08	0.53
31:N4:133:ILE:HD11	31:N4:231:LEU:HD11	1.90	0.53
2:A1:28:LYS:NZ	8:A8:168:TYR:OH	2.34	0.53
25:BL:77:ASP:OD1	25:BL:78:LYS:N	2.41	0.53
35:S2:299:LEU:HD22	35:S2:304:ILE:HD12	1.89	0.53
35:S2:393:GLU:OE2	35:S2:396:GLN:NE2	2.40	0.53
9:A9:357:ARG:NH1	9:A9:364:SER:OG	2.41	0.53
11:AK:134:GLN:HE22	49:AK:401:ADP:HN62	1.57	0.53
20:B6:143:HIS:HD2	24:BK:45:VAL:HG21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:N1:24:GLU:HG3	28:N1:271:LEU:HD22	1.91	0.53
28:N1:113:VAL:HG13	28:N1:139:THR:HG21	1.90	0.53
28:N1:174:MET:HB2	28:N1:242:PHE:HA	1.91	0.53
32:N5:2:ASN:ND2	32:N5:59:GLN:OE1	2.42	0.53
42:V1:302:LYS:HE3	42:V1:303:HIS:CE1	2.44	0.53
34:S1:347:ASP:OD1	34:S1:347:ASP:N	2.41	0.53
35:S2:180:PHE:HZ	35:S2:223:VAL:HG11	1.74	0.53
35:S2:257:PHE:HD2	35:S2:347:LEU:HD11	1.73	0.53
9:A9:212:ARG:NH1	9:A9:311:GLU:OE2	2.41	0.53
10:AC:94:ASP:HB3	10:AC:97:LYS:HG2	1.90	0.53
45:N1:401:CDL:H112	47:N1:403:PEE:H7	1.91	0.53
29:N2:298:TYR:O	29:N2:303:THR:OG1	2.25	0.53
34:S1:611:THR:HG21	37:S4:105:GLU:HA	1.90	0.53
36:S3:147:THR:HB	36:S3:153:ILE:HD11	1.90	0.53
28:N1:100:LEU:HD23	28:N1:160:TYR:HD2	1.73	0.53
33:N6:82:VAL:HG12	33:N6:85:SER:HB2	1.89	0.53
1:4L:56:ALA:HA	38:S5:18:MET:HE3	1.91	0.53
9:A9:50:SER:OG	36:S3:225:GLU:OE2	2.27	0.53
12:AL:140:LYS:H	29:N2:273:ASN:ND2	2.07	0.53
30:N3:38:GLU:HB3	30:N3:41:PHE:O	2.09	0.53
34:S1:556:THR:OG1	34:S1:557:ARG:N	2.41	0.53
36:S3:128:ILE:HB	36:S3:145:THR:HG23	1.91	0.53
24:BK:65:HIS:CD2	25:BL:124:ARG:HH12	2.27	0.52
28:N1:99:ASN:N	53:N6:401:6F6:O12	2.38	0.52
30:N3:56:PHE:O	33:N6:70:TYR:OH	2.27	0.52
35:S2:418:VAL:HB	35:S2:427:ARG:HB3	1.91	0.52
5:A5:44:TYR:O	5:A5:48:THR:HG22	2.08	0.52
8:A8:201:GLU:HA	8:A8:204:LYS:HD3	1.91	0.52
34:S1:387:LEU:HD12	34:S1:514:ASN:HB3	1.91	0.52
11:AK:66:GLY:O	11:AK:163:ARG:NH2	2.42	0.52
14:AN:119:PRO:HB3	14:AN:123:GLU:HB2	1.91	0.52
34:S1:591:GLU:HG2	34:S1:610:VAL:HG23	1.91	0.52
14:AN:98:MET:HE3	14:AN:101:VAL:HG21	1.91	0.52
24:BK:33:LEU:HD13	32:N5:49:VAL:HG13	1.91	0.52
43:V2:85:LEU:HD13	44:V3:400:LEU:HD22	1.91	0.52
42:V1:338:ASP:OD1	42:V1:339:PHE:N	2.42	0.52
8:A8:174:PHE:O	8:A8:178:ARG:NH1	2.42	0.52
45:AL:201:CDL:H532	32:N5:577:VAL:HA	1.92	0.52
35:S2:105:MET:HE1	35:S2:450:LEU:HD13	1.92	0.52
42:V1:102:MET:HE2	42:V1:111:LYS:HE3	1.92	0.52
50:AM:201:PLX:H171	28:N1:45:LEU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:N5:15:LEU:HD11	32:N5:94:LEU:HD21	1.92	0.52
36:S3:83:GLU:OE1	36:S3:142:ARG:NH2	2.35	0.52
1:4L:73:LEU:HD21	29:N2:41:ILE:HG13	1.91	0.52
8:A8:160:THR:HA	8:A8:163:TRP:CD1	2.43	0.52
17:B3:47:ARG:HA	17:B3:50:ALA:HB3	1.92	0.52
21:B7:12:ASP:OD1	21:B7:14:SER:OG	2.25	0.52
27:CB:19:GLU:OE2	27:CB:83:TYR:OH	2.27	0.52
4:A3:95:LYS:NZ	41:S8:50:MET:SD	2.77	0.52
29:N2:26:TRP:HB3	29:N2:74:ILE:HD13	1.92	0.52
32:N5:399:VAL:HG12	32:N5:409:LEU:HD13	1.91	0.52
34:S1:534:VAL:HG22	34:S1:537:ILE:HB	1.92	0.52
35:S2:188:ASN:OD1	35:S2:410:LYS:NZ	2.37	0.52
7:A7:52:ASN:OD1	7:A7:57:ARG:NE	2.43	0.51
9:A9:217:PHE:HA	9:A9:220:MET:HE2	1.92	0.51
42:V1:214:GLU:OE2	42:V1:224:ARG:NE	2.26	0.51
42:V1:281:HIS:ND1	42:V1:358:ASP:OD1	2.43	0.51
42:V1:326:LEU:HD22	42:V1:363:ILE:HD11	1.91	0.51
21:B7:15:LYS:HG2	21:B7:113:LYS:HG3	1.93	0.51
27:CB:56:VAL:HG21	31:N4:17:MET:HE1	1.92	0.51
29:N2:211:MET:HG2	29:N2:333:SER:HB2	1.92	0.51
31:N4:318:ALA:HB2	31:N4:373:ILE:HG13	1.92	0.51
34:S1:422:TRP:HA	34:S1:427:LEU:HB3	1.93	0.51
16:B2:65:THR:HB	16:B2:68:GLN:HG2	1.92	0.51
13:AM:44:TYR:OH	13:AM:113:HIS:N	2.36	0.51
34:S1:104:THR:O	34:S1:113:ARG:NH2	2.44	0.51
34:S1:338:VAL:HB	34:S1:363:SER:HB2	1.93	0.51
41:S8:100:GLU:O	41:S8:170:GLY:N	2.39	0.51
28:N1:133:LEU:HD11	33:N6:72:THR:HG21	1.93	0.51
2:A1:50:ARG:NH2	8:A8:95:VAL:O	2.43	0.51
3:A2:18:GLU:HG2	3:A2:68:ARG:HB3	1.92	0.51
6:A6:90:ARG:HE	6:A6:94:MET:HE2	1.75	0.51
29:N2:112:HIS:O	29:N2:116:PRO:HD2	2.11	0.51
34:S1:666:GLN:NE2	34:S1:670:GLU:OE2	2.43	0.51
35:S2:140:PRO:HB2	40:S7:142:TYR:CE2	2.46	0.51
10:AC:85:TYR:OH	17:B3:22:TRP:NE1	2.32	0.51
29:N2:2:ASN:HD22	29:N2:4:ILE:H	1.59	0.51
29:N2:95:MET:HE2	29:N2:149:ILE:HA	1.92	0.51
32:N5:253:VAL:HG23	32:N5:310:LEU:HD21	1.93	0.51
51:N5:706:3PE:H2B2	51:N5:706:3PE:H381	1.93	0.51
10:AC:112:SER:HB3	23:B9:59:LEU:HD11	1.93	0.51
42:V1:162:PHE:HB3	42:V1:165:GLU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:225:ASN:HB3	11:AK:228:GLU:HG2	1.93	0.51
29:N2:182:SER:OG	29:N2:293:TYR:OH	2.25	0.51
42:V1:288:VAL:HG21	42:V1:303:HIS:CD2	2.46	0.51
8:A8:196:ARG:NH2	14:AN:63:GLU:OE2	2.43	0.50
40:S7:108:THR:HA	40:S7:136:CYS:HB3	1.92	0.50
50:AM:201:PLX:H91	50:S7:302:PLX:H72	1.92	0.50
32:N5:208:CYS:HB2	32:N5:266:LEU:HD22	1.93	0.50
32:N5:290:LEU:O	32:N5:523:SER:OG	2.29	0.50
32:N5:536:LEU:HB3	32:N5:537:PRO:HD3	1.94	0.50
8:A8:202:LEU:HD13	14:AN:70:ALA:HB2	1.92	0.50
6:A6:92:MET:HB2	48:AB:201:ZMP:H4A	1.93	0.50
29:N2:100:MET:HE1	32:N5:595:ILE:HG23	1.93	0.50
32:N5:102:GLU:OE1	32:N5:456:ARG:NH2	2.38	0.50
32:N5:249:SER:HA	32:N5:306:THR:HG21	1.92	0.50
34:S1:389:THR:HG21	34:S1:473:MET:HE2	1.93	0.50
42:V1:112:TYR:O	42:V1:240:THR:HA	2.12	0.50
42:V1:311:TRP:NE1	42:V1:333:GLU:OE1	2.38	0.50
31:N4:216:LEU:HB3	31:N4:217:PRO:HD3	1.93	0.50
31:N4:368:ALA:HB1	31:N4:375:LEU:HD12	1.94	0.50
32:N5:400:ASN:HB3	32:N5:486:MET:HE3	1.93	0.50
34:S1:208:THR:HG21	34:S1:212:LYS:HB3	1.94	0.50
35:S2:448:HIS:HB3	35:S2:452:ASP:HB2	1.93	0.50
28:N1:24:GLU:HA	28:N1:271:LEU:HD13	1.93	0.50
28:N1:58:LYS:HG2	28:N1:217:ALA:HB2	1.92	0.50
30:N3:35:SER:O	40:S7:98:ARG:NH2	2.45	0.50
37:S4:84:ARG:NH1	37:S4:88:GLN:O	2.44	0.50
28:N1:31:MET:HG2	41:S8:77:LEU:HB2	1.93	0.50
20:B6:89:SER:HB2	20:B6:92:GLU:HB2	1.93	0.50
28:N1:120:GLY:HA2	28:N1:128:ALA:HB1	1.94	0.50
35:S2:228:MET:SD	40:S7:167:PRO:HG3	2.52	0.50
13:AM:55:PHE:CZ	13:AM:58:ARG:HG3	2.47	0.50
21:B7:107:ARG:HA	21:B7:110:GLN:HG2	1.93	0.50
31:N4:408:LEU:HD12	32:N5:172:ILE:HG21	1.94	0.50
6:A6:78:LEU:HD22	6:A6:130:MET:HE3	1.93	0.49
34:S1:70:SER:O	34:S1:184:ARG:NH1	2.45	0.49
34:S1:476:LEU:HD21	34:S1:481:LEU:HD21	1.93	0.49
35:S2:180:PHE:CZ	35:S2:223:VAL:HG11	2.47	0.49
8:A8:115:LYS:HB3	8:A8:116:PRO:HD3	1.94	0.49
9:A9:220:MET:HG2	47:A9:402:PEE:H17	1.94	0.49
32:N5:241:THR:HG21	32:N5:344:GLY:HA3	1.93	0.49
5:A5:9:THR:HG23	5:A5:16:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A8:86:THR:OG1	8:A8:88:GLU:OE1	2.26	0.49
32:N5:103:PHE:HB2	32:N5:341:MET:HE3	1.94	0.49
32:N5:126:ILE:HG21	45:N5:703:CDL:H621	1.93	0.49
28:N1:281:ARG:NE	28:N1:283:ASP:OD2	2.43	0.49
36:S3:190:ASP:OD1	36:S3:191:TYR:N	2.46	0.49
42:V1:357:MET:HB3	42:V1:361:THR:HG21	1.92	0.49
1:4L:32:CYS:HA	33:N6:20:PHE:HE1	1.77	0.49
30:N3:68:GLU:HG3	30:N3:98:LEU:HD13	1.93	0.49
30:N3:79:SER:HA	30:N3:87:MET:HE2	1.94	0.49
34:S1:191:GLY:HA3	34:S1:439:THR:HB	1.95	0.49
35:S2:190:ILE:HG23	35:S2:209:MET:HB3	1.95	0.49
42:V1:138:LEU:HD13	42:V1:245:VAL:HG13	1.94	0.49
45:B4:202:CDL:H412	47:N4:501:PEE:H43	1.93	0.49
34:S1:389:THR:OG1	34:S1:511:LYS:O	2.30	0.49
37:S4:112:MET:O	41:S8:144:ARG:NH1	2.40	0.49
42:V1:296:LEU:HD21	42:V1:317:VAL:HG11	1.94	0.49
18:B4:15:PRO:HG2	18:B4:18:LEU:HB2	1.95	0.49
28:N1:213:VAL:HG13	28:N1:214:GLU:HG2	1.93	0.49
33:N6:17:PHE:HA	33:N6:20:PHE:CE2	2.48	0.49
37:S4:112:MET:HG3	41:S8:184:LEU:HD23	1.94	0.49
21:B7:103:GLU:O	21:B7:107:ARG:HG2	2.13	0.49
29:N2:182:SER:HG	29:N2:293:TYR:HH	1.55	0.49
30:N3:66:ASP:O	30:N3:69:ILE:HG13	2.13	0.49
35:S2:194:THR:HG21	35:S2:209:MET:HB2	1.94	0.49
16:B2:92:ASP:HB3	16:B2:97:HIS:HB2	1.95	0.49
31:N4:394:ILE:HG12	51:N5:706:3PE:H362	1.95	0.49
34:S1:592:LYS:NZ	34:S1:619:ASP:OD2	2.40	0.49
45:4L:201:CDL:H262	45:4L:201:CDL:H371	1.94	0.49
34:S1:161:GLU:OE2	43:V2:42:ARG:NH1	2.44	0.49
13:AM:127:TYR:OH	39:S6:61:GLU:O	2.21	0.48
21:B7:22:MET:HE1	21:B7:102:PHE:CD2	2.48	0.48
34:S1:251:ILE:HD11	34:S1:596:TYR:HB2	1.93	0.48
34:S1:408:ARG:HD2	34:S1:439:THR:HG23	1.95	0.48
1:4L:35:GLY:HA3	33:N6:20:PHE:HZ	1.78	0.48
19:B5:83:ALA:HA	45:B5:202:CDL:H162	1.94	0.48
28:N1:103:LEU:HD13	33:N6:55:MET:HE3	1.95	0.48
34:S1:347:ASP:HB3	34:S1:594:ALA:HB1	1.94	0.48
23:B9:143:GLU:O	23:B9:164:ARG:NH2	2.47	0.48
32:N5:292:ALA:HB2	32:N5:304:PHE:HB3	1.95	0.48
11:AK:97:ASP:N	11:AK:97:ASP:OD1	2.45	0.48
11:AK:241:ASN:HB3	11:AK:245:LYS:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B9:212:ILE:O	23:B9:215:ARG:NH1	2.45	0.48
36:S3:89:HIS:CG	36:S3:90:PRO:HD2	2.49	0.48
23:B9:52:LEU:O	23:B9:57:LYS:NZ	2.43	0.48
28:N1:169:GLN:HB3	28:N1:244:GLY:HA3	1.94	0.48
29:N2:25:HIS:HB2	38:S5:15:ASP:HB2	1.94	0.48
32:N5:248:HIS:O	32:N5:253:VAL:HG22	2.13	0.48
32:N5:559:GLU:O	32:N5:564:LYS:HB2	2.13	0.48
34:S1:624:ARG:NH2	34:S1:637:ASP:OD1	2.43	0.48
35:S2:430:ILE:HB	35:S2:469:ARG:HD2	1.94	0.48
7:A7:39:PRO:HG3	41:S8:211:TYR:CZ	2.49	0.48
32:N5:359:MET:O	32:N5:436:ARG:NH2	2.47	0.48
14:AN:21:TYR:CE2	35:S2:348:ARG:HD2	2.49	0.48
47:N2:402:PEE:H38	31:N4:155:ALA:HB3	1.95	0.48
31:N4:76:MET:SD	31:N4:230:VAL:HB	2.54	0.48
31:N4:361:VAL:HG13	45:N5:703:CDL:H332	1.94	0.48
32:N5:213:LEU:HB3	32:N5:273:VAL:HG11	1.96	0.48
34:S1:82:ILE:HB	34:S1:85:ALA:HB3	1.95	0.48
12:AL:110:ILE:HG12	47:N5:702:PEE:H14	1.96	0.48
28:N1:162:LEU:HD23	28:N1:165:LEU:HD12	1.94	0.48
35:S2:187:LEU:HD23	35:S2:213:ARG:HG2	1.95	0.48
28:N1:123:SER:HB3	28:N1:214:GLU:HG3	1.96	0.48
32:N5:383:MET:O	32:N5:389:PHE:HB2	2.14	0.48
35:S2:296:GLY:HA2	35:S2:300:ARG:HH21	1.79	0.48
14:AN:95:ALA:HA	14:AN:106:VAL:HG11	1.95	0.48
24:BK:60:ARG:NH1	24:BK:62:TYR:OH	2.47	0.48
34:S1:259:SER:HB3	34:S1:282:ASN:HD22	1.78	0.48
42:V1:203:ALA:HB3	42:V1:206:CYS:HB2	1.96	0.48
43:V2:99:ASN:OD1	43:V2:113:TYR:OH	2.26	0.48
8:A8:95:VAL:HG12	8:A8:97:VAL:HG22	1.96	0.47
34:S1:43:VAL:HG12	34:S1:55:LYS:HD2	1.96	0.47
35:S2:194:THR:HB	35:S2:206:PHE:HA	1.96	0.47
10:AB:104:PHE:HD1	10:AB:108:LEU:HD12	1.79	0.47
6:A6:94:MET:HE2	10:AB:113:LEU:HD12	1.95	0.47
11:AK:120:TYR:OH	49:AK:401:ADP:O2'	2.12	0.47
14:AN:43:LEU:HG	28:N1:179:TRP:HE1	1.79	0.47
14:AN:82:ARG:HA	38:S5:105:ARG:HD3	1.96	0.47
29:N2:190:MET:HE1	29:N2:205:LEU:HB2	1.96	0.47
31:N4:73:LEU:HA	31:N4:76:MET:HE2	1.96	0.47
31:N4:382:ILE:HG12	31:N4:396:MET:HG3	1.96	0.47
32:N5:566:THR:O	32:N5:570:GLN:HG2	2.13	0.47
42:V1:131:ILE:HD13	42:V1:158:ILE:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4L:65:VAL:HA	30:N3:67:LEU:HD22	1.95	0.47
9:A9:303:ARG:HB2	9:A9:316:ARG:HD3	1.96	0.47
11:AK:109:GLN:OE1	11:AK:328:ARG:NH1	2.45	0.47
12:AL:124:LEU:HD11	47:N4:501:PEE:H70	1.96	0.47
21:B7:29:TYR:OH	21:B7:111:ARG:NH2	2.47	0.47
31:N4:364:LEU:HD22	31:N4:369:LEU:HD22	1.95	0.47
36:S3:145:THR:OG1	36:S3:146:TYR:N	2.47	0.47
28:N1:195:ARG:HD3	28:N1:231:ILE:HD11	1.97	0.47
50:N4:502:PLX:H281	50:N4:502:PLX:H332	1.96	0.47
35:S2:101:LEU:HB2	35:S2:464:PHE:CZ	2.49	0.47
35:S2:190:ILE:HD11	35:S2:257:PHE:CZ	2.49	0.47
42:V1:55:GLY:O	42:V1:58:SER:OG	2.28	0.47
8:A8:228:ASN:OD1	38:S5:51:ARG:NH1	2.44	0.47
28:N1:273:ILE:HD13	47:N1:404:PEE:H59	1.97	0.47
31:N4:16:TRP:CE2	45:N4:504:CDL:H272	2.50	0.47
34:S1:541:PRO:HB3	34:S1:561:PRO:HD3	1.97	0.47
35:S2:214:GLU:OE2	35:S2:227:ARG:NH2	2.48	0.47
42:V1:118:ASP:HB3	42:V1:207:GLY:HA2	1.97	0.47
1:4L:17:ALA:HB2	45:4L:201:CDL:H821	1.96	0.47
1:4L:35:GLY:HA3	33:N6:20:PHE:CZ	2.49	0.47
45:4L:201:CDL:H231	12:AL:41:ILE:HD12	1.97	0.47
9:A9:231:LEU:HD13	9:A9:292:PRO:HG3	1.95	0.47
12:AL:81:ARG:HH11	12:AL:89:ASN:HD21	1.61	0.47
13:AM:60:ARG:HH22	13:AM:95:ASP:HA	1.80	0.47
14:AN:26:PRO:O	41:S8:68:ARG:NH2	2.39	0.47
31:N4:82:SER:HB2	31:N4:432:ARG:NH1	2.29	0.47
34:S1:130:ILE:HG23	41:S8:114:ILE:HD12	1.96	0.47
5:A5:48:THR:HA	5:A5:51:ILE:HG12	1.96	0.47
35:S2:321:GLU:O	35:S2:352:GLN:NE2	2.48	0.47
28:N1:200:LEU:HD21	28:N1:280:PHE:O	2.15	0.47
29:N2:36:ASN:OD1	29:N2:134:GLN:NE2	2.33	0.47
6:A6:42:SER:HB3	37:S4:52:LEU:HB3	1.97	0.47
35:S2:149:SER:HB2	35:S2:152:CYS:HB2	1.97	0.47
42:V1:86:ARG:O	42:V1:88:ARG:NH1	2.48	0.47
6:A6:62:TYR:OH	10:AB:117:GLU:OE2	2.32	0.46
14:AN:93:GLU:HG3	38:S5:98:HIS:CD2	2.50	0.46
16:B2:79:MET:SD	32:N5:375:ILE:HG12	2.55	0.46
18:B4:14:LEU:HD12	18:B4:15:PRO:HD2	1.96	0.46
29:N2:42:PRO:HG3	33:N6:167:VAL:HG13	1.96	0.46
31:N4:79:ALA:O	31:N4:82:SER:HB3	2.15	0.46
34:S1:224:ASP:OD2	34:S1:291:ARG:NH2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A7:25:GLN:O	35:S2:215:LYS:NZ	2.37	0.46
9:A9:64:PHE:O	9:A9:67:ARG:HG2	2.16	0.46
28:N1:288:LEU:HD11	47:N1:404:PEE:H8	1.96	0.46
29:N2:24:SER:OG	38:S5:15:ASP:OD1	2.34	0.46
11:AK:340:LYS:O	27:CB:52:ARG:NH2	2.49	0.46
34:S1:576:GLY:O	34:S1:580:ALA:HB2	2.14	0.46
50:AM:201:PLX:H372	50:S7:302:PLX:H171	1.97	0.46
16:B2:90:ASP:O	32:N5:385:TYR:OH	2.22	0.46
24:BK:74:ILE:HG23	24:BK:156:LEU:HD22	1.97	0.46
28:N1:197:PRO:HB3	28:N1:278:PRO:O	2.15	0.46
42:V1:118:ASP:HA	42:V1:159:ARG:HB3	1.98	0.46
8:A8:157:GLU:HB2	8:A8:158:PRO:HD3	1.98	0.46
20:B6:143:HIS:CD2	24:BK:45:VAL:HG21	2.50	0.46
31:N4:445:LEU:HD22	45:N5:703:CDL:H401	1.97	0.46
34:S1:575:VAL:C	34:S1:578:PRO:HD2	2.40	0.46
35:S2:363:LYS:HD3	35:S2:370:SER:HB2	1.98	0.46
39:S6:74:GLN:HG3	41:S8:108:SER:HB2	1.98	0.46
41:S8:150:THR:HG21	41:S8:180:HIS:CD2	2.50	0.46
30:N3:33:LYS:O	40:S7:98:ARG:NH1	2.42	0.46
45:N4:504:CDL:H832	45:N4:504:CDL:H231	1.96	0.46
10:AB:138:LEU:HD23	10:AB:144:ILE:HD13	1.98	0.46
15:B1:28:ASP:OD2	31:N4:3:LYS:NZ	2.37	0.46
47:BL:201:PEE:H23	47:BL:201:PEE:H29	1.68	0.46
28:N1:128:ALA:HA	28:N1:211:PHE:HA	1.97	0.46
34:S1:405:THR:HB	34:S1:477:GLY:HA3	1.97	0.46
43:V2:59:ASN:ND2	43:V2:89:GLN:OE1	2.48	0.46
8:A8:219:TYR:OH	19:B5:189:ASN:ND2	2.37	0.46
45:A8:301:CDL:H381	29:N2:256:PRO:HB2	1.96	0.46
45:A8:301:CDL:HB61	27:CB:29:THR:HB	1.97	0.46
9:A9:223:PHE:HB3	47:A9:402:PEE:H28	1.97	0.46
25:BL:85:TRP:CD1	47:BL:201:PEE:H7	2.51	0.46
28:N1:114:TYR:OH	33:N6:61:LEU:O	2.25	0.46
45:N4:504:CDL:H812	45:N4:504:CDL:H422	1.98	0.46
9:A9:328:THR:HG22	9:A9:330:PRO:HD3	1.96	0.46
10:AC:115:GLN:NE2	10:AC:138:LEU:O	2.44	0.46
15:B1:30:ARG:O	15:B1:33:GLU:HG2	2.16	0.46
18:B4:48:LEU:HB3	23:B9:208:LEU:HD13	1.98	0.46
51:CA:101:3PE:H2E2	29:N2:332:LEU:HD11	1.96	0.46
28:N1:138:GLN:HG3	28:N1:285:LEU:HD21	1.98	0.46
29:N2:173:THR:HG22	35:S2:58:MET:HG2	1.98	0.46
32:N5:174:TYR:CD2	32:N5:232:TRP:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:N5:297:ASP:O	32:N5:301:ILE:HG13	2.16	0.46
51:S7:303:3PE:H342	51:S7:303:3PE:H281	1.98	0.46
42:V1:384:PRO:HB2	42:V1:423:THR:HG22	1.98	0.46
50:AM:201:PLX:H291	50:AM:201:PLX:H322	1.69	0.46
50:CB:201:PLX:H362	29:N2:339:MET:HB2	1.98	0.46
28:N1:100:LEU:HD22	28:N1:103:LEU:HD12	1.98	0.46
33:N6:82:VAL:HG22	33:N6:83:TRP:H	1.81	0.46
34:S1:307:ILE:HG23	34:S1:317:THR:HG21	1.97	0.46
34:S1:385:TYR:OH	34:S1:527:ASP:OD1	2.20	0.46
35:S2:382:GLU:OE1	35:S2:382:GLU:N	2.44	0.46
36:S3:157:VAL:HG21	36:S3:182:PRO:HD3	1.96	0.46
41:S8:63:TRP:HB3	41:S8:66:LEU:HD12	1.96	0.46
7:A7:42:PRO:HG3	14:AN:6:VAL:HG11	1.98	0.45
28:N1:169:GLN:NE2	28:N1:240:ILE:O	2.39	0.45
29:N2:342:ALA:O	29:N2:345:SER:OG	2.28	0.45
34:S1:51:GLN:NE2	37:S4:156:LYS:O	2.48	0.45
35:S2:90:PHE:HB2	35:S2:105:MET:HE2	1.97	0.45
47:N5:705:PEE:H71	47:N5:705:PEE:H76	1.77	0.45
43:V2:224:SER:OG	43:V2:226:GLU:OE1	2.23	0.45
21:B7:22:MET:HE2	21:B7:105:GLU:HG2	1.98	0.45
22:B8:150:TYR:CE1	51:B8:201:3PE:H221	2.52	0.45
50:CB:201:PLX:H302	50:CB:201:PLX:H271	1.62	0.45
32:N5:228:GLY:H	32:N5:230:HIS:HD2	1.65	0.45
43:V2:215:LYS:O	43:V2:219:ARG:NH1	2.42	0.45
8:A8:124:ARG:NE	14:AN:80:ASP:OD2	2.44	0.45
9:A9:170:LEU:HA	9:A9:202:LYS:HB3	1.99	0.45
9:A9:293:LEU:HD12	9:A9:294:PRO:HD2	1.98	0.45
29:N2:130:LEU:HD12	29:N2:134:GLN:HG3	1.99	0.45
29:N2:249:LEU:HD22	29:N2:254:LEU:HD12	1.98	0.45
47:N3:201:PEE:H27	47:N3:201:PEE:H22	1.69	0.45
34:S1:152:ARG:NH1	42:V1:414:GLU:OE1	2.49	0.45
8:A8:175:ARG:NH1	28:N1:170:GLU:OE1	2.49	0.45
45:B5:202:CDL:H211	45:B5:202:CDL:H251	1.99	0.45
20:B6:159:GLU:HG3	32:N5:61:MET:HG2	1.98	0.45
8:A8:160:THR:HA	8:A8:163:TRP:NE1	2.32	0.45
29:N2:137:ALA:HB3	29:N2:138:PRO:HD3	1.99	0.45
34:S1:401:LEU:HD11	34:S1:432:ILE:HG13	1.98	0.45
34:S1:484:SER:HB2	34:S1:680:LEU:HD11	1.97	0.45
18:B4:25:ILE:HG21	18:B4:30:ARG:CZ	2.47	0.45
20:B6:186:GLN:HG3	21:B7:89:TYR:HE2	1.81	0.45
28:N1:160:TYR:OH	30:N3:73:LEU:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:N5:49:VAL:HB	32:N5:50:PRO:HD3	1.99	0.45
34:S1:185:PHE:CZ	34:S1:221:ASN:HB2	2.50	0.45
36:S3:211:ARG:NH2	36:S3:213:ASP:OD1	2.49	0.45
23:B9:87:ARG:NH1	23:B9:91:ASP:OD2	2.49	0.45
27:CB:13:LEU:HD22	50:CB:201:PLX:H81	1.99	0.45
27:CB:13:LEU:HD21	38:S5:4:PHE:HB3	1.98	0.45
32:N5:295:GLN:HB2	32:N5:301:ILE:HG12	1.99	0.45
41:S8:153:ILE:HG12	54:S8:302:SF4:S1	2.57	0.45
42:V1:210:THR:HB	42:V1:224:ARG:H	1.82	0.45
1:4L:36:MET:HE3	29:N2:68:MET:HG3	1.99	0.45
20:B6:140:TRP:HD1	24:BK:41:VAL:HG13	1.82	0.45
50:N3:202:PLX:H182	50:N3:202:PLX:H212	1.81	0.45
45:N5:704:CDL:H622	45:N5:704:CDL:H581	1.99	0.45
35:S2:145:LEU:HD11	35:S2:430:ILE:HD13	1.99	0.45
41:S8:75:SER:O	41:S8:79:ARG:HG3	2.17	0.45
29:N2:167:TRP:O	32:N5:574:SER:OG	2.21	0.45
34:S1:339:ALA:HA	34:S1:365:SER:HB2	1.99	0.45
42:V1:174:ARG:HA	44:V3:406:LEU:HD21	1.98	0.45
1:4L:4:VAL:O	1:4L:8:ILE:HG12	2.17	0.44
1:4L:62:ILE:HG21	29:N2:31:ILE:HD11	1.99	0.44
4:A3:144:ASP:HB3	8:A8:209:LYS:HD2	2.00	0.44
11:AK:59:SER:OG	11:AK:156:GLY:O	2.22	0.44
29:N2:170:LEU:HD11	29:N2:288:LEU:HD22	1.97	0.44
31:N4:201:MET:HE1	31:N4:212:LEU:HD11	1.98	0.44
33:N6:24:PRO:HG2	33:N6:28:TYR:HB2	1.99	0.44
36:S3:148:ASP:OD1	36:S3:148:ASP:N	2.50	0.44
11:AK:51:THR:HG21	11:AK:153:LEU:HD22	1.99	0.44
29:N2:112:HIS:HB2	29:N2:184:ILE:HD13	2.00	0.44
19:B5:147:ALA:HB2	31:N4:173:SER:HB2	2.00	0.44
29:N2:43:VAL:HG11	29:N2:129:LEU:HD23	1.98	0.44
8:A8:117:ASN:HB3	14:AN:73:PRO:HG2	2.00	0.44
9:A9:64:PHE:HZ	9:A9:208:GLY:HA3	1.83	0.44
47:N2:402:PEE:H36	32:N5:562:LEU:HG	1.99	0.44
41:S8:168:VAL:HG21	41:S8:201:ILE:HG21	1.99	0.44
47:A9:402:PEE:H49	47:A9:402:PEE:H54	1.75	0.44
10:AB:139:MET:N	10:AB:143:GLU:OE1	2.51	0.44
31:N4:398:MET:O	31:N4:402:ILE:HG13	2.18	0.44
33:N6:28:TYR:HB3	33:N6:83:TRP:CH2	2.53	0.44
34:S1:124:HIS:CG	34:S1:125:PRO:HD2	2.53	0.44
35:S2:160:ALA:HA	35:S2:404:THR:HG21	1.99	0.44
42:V1:244:ASN:OD1	42:V1:245:VAL:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A7:112:TYR:HE2	41:S8:43:MET:HE2	1.82	0.44
50:CB:201:PLX:H101	50:CB:201:PLX:H131	1.83	0.44
31:N4:211:GLY:H	31:N4:213:HIS:CD2	2.35	0.44
34:S1:593:SER:HA	34:S1:606:THR:O	2.17	0.44
43:V2:242:GLY:HA2	43:V2:245:VAL:HG23	1.99	0.44
6:A6:78:LEU:HD11	6:A6:129:ILE:HG21	1.99	0.44
13:AM:139:PRO:HG3	34:S1:306:MET:HE1	2.00	0.44
21:B7:95:TYR:HD2	21:B7:99:MET:HE2	1.82	0.44
28:N1:28:LEU:HD21	28:N1:274:ARG:HE	1.83	0.44
29:N2:83:GLN:HE22	38:S5:20:ILE:HG22	1.83	0.44
31:N4:106:LEU:HD13	31:N4:234:VAL:HG11	2.00	0.44
32:N5:96:VAL:O	32:N5:100:ILE:HG12	2.18	0.44
35:S2:218:GLU:OE2	40:S7:83:ARG:NH2	2.49	0.44
44:V3:386:TYR:CZ	44:V3:388:ASN:HB3	2.52	0.44
6:A6:78:LEU:HD23	6:A6:126:ARG:HD3	2.00	0.44
11:AK:37:ARG:C	11:AK:39:GLN:H	2.26	0.44
11:AK:88:PHE:HB2	11:AK:161:LEU:HD23	1.99	0.44
28:N1:2:PHE:HD2	30:N3:5:LEU:HD23	1.82	0.44
35:S2:203:MET:O	35:S2:206:PHE:HB3	2.18	0.44
43:V2:137:THR:HG22	43:V2:138:THR:H	1.83	0.44
50:N4:502:PLX:H91	50:N4:502:PLX:H351	2.00	0.44
42:V1:263:ALA:HA	42:V1:271:SER:HB3	2.00	0.44
45:4L:201:CDL:H261	45:4L:201:CDL:H221	2.00	0.43
9:A9:359:TYR:HB2	28:N1:65:THR:HA	2.00	0.43
20:B6:132:VAL:O	20:B6:136:LEU:CB	2.64	0.43
23:B9:77:ASP:OD1	23:B9:77:ASP:N	2.51	0.43
28:N1:18:ALA:HB1	28:N1:48:PRO:HB3	2.00	0.43
50:AM:201:PLX:H352	50:AM:201:PLX:H201	2.00	0.43
28:N1:25:ARG:HD3	28:N1:37:PRO:HG2	2.00	0.43
31:N4:225:ILE:HD13	31:N4:331:ASN:HB2	2.00	0.43
35:S2:151:MET:HE2	35:S2:232:TYR:HB3	2.00	0.43
42:V1:347:THR:HG22	42:V1:348:GLY:H	1.83	0.43
1:4L:55:LEU:H	38:S5:25:GLN:HE22	1.65	0.43
11:AK:317:PRO:HB3	25:BL:54:ARG:HA	2.00	0.43
14:AN:94:GLU:OE2	38:S5:75:ARG:NH2	2.51	0.43
45:B4:201:CDL:H1	45:B4:201:CDL:H512	1.99	0.43
29:N2:245:MET:HE1	45:N4:504:CDL:H172	1.99	0.43
32:N5:172:ILE:O	32:N5:176:ARG:HG2	2.18	0.43
33:N6:122:LEU:HG	33:N6:123:GLY:H	1.83	0.43
34:S1:534:VAL:HG23	34:S1:537:ILE:HD12	2.00	0.43
35:S2:137:GLN:O	40:S7:142:TYR:OH	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:S7:88:ARG:HD2	41:S8:83:THR:HG21	2.00	0.43
6:A6:88:LYS:HD2	6:A6:88:LYS:HA	1.67	0.43
10:AC:90:TYR:CE1	17:B3:44:PRO:HB2	2.54	0.43
17:B3:18:ASP:O	17:B3:21:GLN:HG2	2.19	0.43
32:N5:66:TRP:CD1	47:N5:701:PEE:H16	2.53	0.43
9:A9:201:ILE:HG22	9:A9:203:PRO:HD3	2.00	0.43
28:N1:90:PRO:HB3	28:N1:94:PRO:HD3	2.01	0.43
32:N5:152:PHE:CD1	32:N5:168:ALA:HB1	2.54	0.43
32:N5:264:TYR:CD2	32:N5:265:PRO:HD3	2.53	0.43
42:V1:62:TRP:CD2	42:V1:181:LEU:HD13	2.54	0.43
43:V2:237:PRO:HA	43:V2:238:PRO:HD3	1.94	0.43
10:AC:105:MET:HE3	10:AC:139:MET:HE1	1.99	0.43
31:N4:267:TRP:O	31:N4:271:MET:HG2	2.18	0.43
32:N5:327:LEU:O	32:N5:331:MET:HG2	2.18	0.43
18:B4:71:ALA:HB2	22:B8:38:PRO:HG2	2.00	0.43
28:N1:212:ASN:O	40:S7:99:GLN:NE2	2.52	0.43
29:N2:313:MET:HE3	29:N2:313:MET:HB2	1.91	0.43
31:N4:210:TYR:CG	31:N4:268:GLY:HA3	2.54	0.43
32:N5:264:TYR:CG	32:N5:265:PRO:HD3	2.53	0.43
32:N5:331:MET:HB3	32:N5:387:THR:HG22	2.01	0.43
42:V1:119:GLU:HA	58:V1:502:FMN:HM71	2.00	0.43
11:AK:67:ASN:ND2	11:AK:68:ILE:H	2.17	0.43
26:CA:47:THR:HG23	27:CB:65:LEU:HD22	2.01	0.43
29:N2:186:HIS:O	29:N2:190:MET:HG3	2.18	0.43
34:S1:338:VAL:HB	34:S1:363:SER:CB	2.48	0.43
6:A6:88:LYS:NZ	6:A6:133:PHE:HA	2.33	0.43
7:A7:27:ARG:HD2	7:A7:31:ILE:HG21	2.01	0.43
47:N2:402:PEE:H50	32:N5:570:GLN:HB2	2.01	0.43
31:N4:82:SER:HB2	31:N4:432:ARG:CZ	2.49	0.43
32:N5:290:LEU:HD11	45:N5:704:CDL:H731	2.01	0.43
35:S2:142:PHE:HZ	35:S2:428:CYS:SG	2.41	0.43
42:V1:65:THR:O	42:V1:69:LEU:HG	2.19	0.43
42:V1:113:LEU:O	42:V1:154:ALA:HA	2.18	0.43
6:A6:46:ILE:HG12	36:S3:152:PRO:HG3	2.01	0.43
28:N1:179:TRP:CG	28:N1:180:PRO:HD3	2.54	0.43
32:N5:435:PRO:HB3	32:N5:437:PHE:CZ	2.54	0.43
33:N6:17:PHE:HA	33:N6:20:PHE:CD2	2.54	0.43
34:S1:169:VAL:HG22	34:S1:223:ILE:HD11	1.99	0.43
35:S2:150:MET:SD	35:S2:228:MET:HB2	2.58	0.43
41:S8:49:ASP:OD1	41:S8:49:ASP:N	2.52	0.43
42:V1:192:ASP:HB3	44:V3:411:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:352:LYS:HE2	11:AK:352:LYS:HB2	1.84	0.42
50:AM:201:PLX:H101	50:AM:201:PLX:H301	2.01	0.42
14:AN:85:GLN:OE1	38:S5:105:ARG:NH1	2.39	0.42
19:B5:96:ALA:HB2	24:BK:61:TYR:CE2	2.54	0.42
51:CA:101:3PE:H292	51:CA:101:3PE:H2D2	2.01	0.42
45:N1:401:CDL:H752	45:N1:401:CDL:H782	1.75	0.42
42:V1:300:ILE:HG22	42:V1:306:GLY:HA2	2.01	0.42
22:B8:149:ILE:HG13	22:B8:150:TYR:CD2	2.53	0.42
28:N1:142:TYR:CE2	28:N1:192:GLU:HA	2.54	0.42
31:N4:12:LEU:HB2	31:N4:13:PRO:HD3	2.01	0.42
34:S1:419:ARG:NH1	34:S1:439:THR:O	2.52	0.42
35:S2:61:THR:H	35:S2:64:THR:HG1	1.61	0.42
15:B1:42:SER:O	15:B1:46:LYS:HB2	2.20	0.42
31:N4:266:MET:HB3	31:N4:395:LEU:HD13	2.00	0.42
32:N5:504:LEU:HD11	45:N5:704:CDL:H311	2.01	0.42
34:S1:180:THR:N	54:S1:802:SF4:S4	2.87	0.42
9:A9:167:ILE:HD13	9:A9:201:ILE:HB	2.00	0.42
31:N4:324:SER:HG	31:N4:440:HIS:CD2	2.33	0.42
32:N5:14:ILE:HD11	32:N5:43:ALA:HA	1.99	0.42
35:S2:410:LYS:HE2	35:S2:463:VAL:HG23	2.01	0.42
10:AC:119:ILE:HG21	10:AC:135:ALA:HB1	2.00	0.42
22:B8:162:PRO:HB2	22:B8:163:TYR:CD2	2.54	0.42
29:N2:168:GLY:O	29:N2:172:GLN:HG2	2.18	0.42
47:N2:402:PEE:H71	47:N2:402:PEE:H76	1.75	0.42
35:S2:219:PHE:O	35:S2:223:VAL:HG22	2.20	0.42
40:S7:131:VAL:HG22	40:S7:161:ILE:HB	2.01	0.42
9:A9:76:MET:HE2	9:A9:76:MET:HB3	1.96	0.42
9:A9:126:VAL:HG23	9:A9:161:VAL:HG11	2.02	0.42
11:AK:355:TRP:H	11:AK:355:TRP:CD1	2.36	0.42
17:B3:52:ARG:HD3	32:N5:435:PRO:O	2.20	0.42
28:N1:59:GLU:HG3	30:N3:27:LEU:HD13	2.01	0.42
29:N2:14:MET:HA	29:N2:133:TRP:HE1	1.85	0.42
50:N4:503:PLX:H192	45:N5:703:CDL:H631	2.01	0.42
42:V1:396:MET:O	42:V1:400:VAL:HG13	2.19	0.42
9:A9:219:SER:HB3	47:A9:402:PEE:H1	2.01	0.42
11:AK:82:LYS:HZ1	11:AK:268:ALA:HB3	1.85	0.42
11:AK:131:TYR:CD1	11:AK:185:CYS:HB3	2.55	0.42
45:AL:201:CDL:H322	45:AL:201:CDL:H352	1.89	0.42
19:B5:110:TRP:O	19:B5:119:ARG:HG2	2.20	0.42
29:N2:295:ARG:HD3	35:S2:53:PHE:HE1	1.83	0.42
35:S2:98:HIS:HB2	35:S2:464:PHE:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:114:LYS:HE3	35:S2:114:LYS:HB2	1.92	0.42
41:S8:131:GLU:HB2	41:S8:144:ARG:HB3	2.00	0.42
1:4L:37:MET:HG2	1:4L:67:ALA:CB	2.41	0.42
1:4L:55:LEU:HD13	38:S5:17:TRP:HE3	1.84	0.42
11:AK:328:ARG:HH21	25:BL:58:ASP:CG	2.27	0.42
32:N5:298:ILE:O	32:N5:302:VAL:HG23	2.20	0.42
34:S1:267:THR:HB	37:S4:115:SER:HB2	2.02	0.42
34:S1:281:ILE:HD11	34:S1:602:ARG:HD2	2.00	0.42
34:S1:449:PRO:HB2	34:S1:679:LEU:HD13	2.02	0.42
1:4L:90:VAL:HB	32:N5:584:ILE:HD11	2.02	0.42
2:A1:68:ASN:ND2	8:A8:96:LYS:HB3	2.35	0.42
9:A9:127:ILE:HD11	9:A9:253:ILE:HD11	2.02	0.42
27:CB:106:LYS:NZ	27:CB:107:ASP:OD1	2.36	0.42
28:N1:273:ILE:HG23	28:N1:277:TYR:CD2	2.55	0.42
31:N4:94:LEU:HD21	45:N4:504:CDL:H312	2.01	0.42
47:N4:501:PEE:H47	47:N4:501:PEE:H40	1.68	0.42
35:S2:147:TYR:CB	40:S7:71:CYS:HB3	2.50	0.42
36:S3:119:VAL:HG12	36:S3:121:THR:HG22	2.02	0.42
45:4L:201:CDL:H192	32:N5:593:ILE:HD11	2.02	0.42
9:A9:168:SER:HA	9:A9:184:LYS:NZ	2.35	0.42
10:AB:78:ALA:HA	10:AB:81:ASP:OD2	2.20	0.42
11:AK:260:TYR:HB3	11:AK:264:GLU:HB2	2.01	0.42
13:AM:12:GLN:O	13:AM:16:GLY:N	2.53	0.42
34:S1:36:VAL:HG11	34:S1:56:VAL:HG21	2.01	0.42
34:S1:306:MET:HB2	34:S1:583:ILE:HB	2.01	0.42
34:S1:488:ALA:HB2	34:S1:677:GLN:HG3	2.00	0.42
43:V2:48:ASN:OD1	43:V2:51:THR:OG1	2.30	0.42
1:4L:41:PHE:O	1:4L:45:THR:HG22	2.19	0.41
3:A2:23:LEU:HD12	3:A2:34:ARG:HG2	2.02	0.41
8:A8:222:ARG:NH1	38:S5:58:ILE:HD12	2.35	0.41
45:A8:301:CDL:HA21	15:B1:34:LYS:NZ	2.35	0.41
20:B6:148:TYR:CE1	24:BK:49:ARG:HG2	2.55	0.41
23:B9:119:PRO:HB3	32:N5:525:MET:HE2	2.02	0.41
28:N1:32:GLN:OE1	28:N1:34:ARG:NH2	2.51	0.41
29:N2:276:ILE:C	29:N2:279:PRO:HD2	2.44	0.41
31:N4:433:GLU:O	31:N4:437:MET:HG2	2.20	0.41
34:S1:219:SER:O	34:S1:222:ILE:HG12	2.20	0.41
40:S7:101:ASP:N	40:S7:101:ASP:OD1	2.52	0.41
42:V1:128:ARG:HD2	42:V1:162:PHE:CZ	2.55	0.41
42:V1:168:ASN:ND2	44:V3:388:ASN:HD21	2.18	0.41
42:V1:276:PHE:CD1	42:V1:352:ALA:HB1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:V2:185:MET:HE2	43:V2:185:MET:HB2	1.99	0.41
24:BK:164:LEU:HD23	25:BL:149:LEU:HD13	2.01	0.41
27:CB:15:PHE:O	27:CB:80:ARG:NH1	2.51	0.41
31:N4:366:ASN:ND2	31:N4:407:SER:OG	2.52	0.41
32:N5:233:LEU:HB3	32:N5:234:PRO:HD3	2.01	0.41
32:N5:294:THR:O	32:N5:294:THR:OG1	2.36	0.41
34:S1:53:CYS:HA	34:S1:56:VAL:HG22	2.02	0.41
42:V1:141:GLY:HA3	42:V1:248:VAL:O	2.19	0.41
11:AK:284:PRO:O	11:AK:288:GLN:HG2	2.20	0.41
23:B9:150:HIS:CD2	23:B9:151:PRO:HD2	2.55	0.41
29:N2:2:ASN:ND2	29:N2:4:ILE:H	2.18	0.41
33:N6:2:THR:HG22	33:N6:4:TYR:H	1.84	0.41
33:N6:24:PRO:HG3	33:N6:83:TRP:CE2	2.55	0.41
34:S1:198:THR:HG21	34:S1:209:TYR:HB2	2.01	0.41
35:S2:149:SER:HA	35:S2:184:THR:HG22	2.01	0.41
40:S7:161:ILE:HG13	40:S7:180:LEU:HB2	2.02	0.41
41:S8:168:VAL:HG11	41:S8:205:ILE:HD11	2.02	0.41
44:V3:383:ASN:O	44:V3:383:ASN:ND2	2.53	0.41
1:4L:55:LEU:HD23	1:4L:55:LEU:HA	1.92	0.41
45:B5:202:CDL:H752	25:BL:103:SER:HB2	2.02	0.41
23:B9:156:MET:HE2	23:B9:156:MET:HB3	1.93	0.41
28:N1:233:MET:HE3	28:N1:233:MET:HB3	1.81	0.41
29:N2:140:SER:HB3	38:S5:2:PRO:HA	2.02	0.41
29:N2:190:MET:HB3	29:N2:190:MET:HE2	1.66	0.41
31:N4:119:TYR:CZ	31:N4:161:LEU:HB2	2.56	0.41
31:N4:282:LEU:HD11	31:N4:410:MET:HG3	2.02	0.41
33:N6:135:PHE:HD1	33:N6:135:PHE:HA	1.74	0.41
34:S1:432:ILE:HG12	34:S1:445:LEU:HB2	2.01	0.41
3:A2:69:TYR:CE2	3:A2:75:LYS:HD3	2.55	0.41
27:CB:107:ASP:OD1	27:CB:107:ASP:N	2.54	0.41
31:N4:207:MET:HE2	31:N4:298:ILE:HG13	2.02	0.41
34:S1:279:GLU:CD	37:S4:154:LYS:H	2.28	0.41
34:S1:308:ARG:NH1	34:S1:312:GLY:O	2.52	0.41
4:A3:135:PRO:HB2	14:AN:69:ILE:HD11	2.03	0.41
9:A9:65:LEU:HG	9:A9:129:LEU:HD22	2.02	0.41
24:BK:163:MET:HE2	25:BL:149:LEU:HD11	2.01	0.41
29:N2:9:LEU:HD13	29:N2:42:PRO:HB2	2.01	0.41
31:N4:75:LEU:HD13	31:N4:440:HIS:CE1	2.56	0.41
33:N6:59:ILE:HD13	33:N6:59:ILE:HA	1.92	0.41
1:4L:97:GLN:O	29:N2:177:LYS:NZ	2.52	0.41
45:B5:202:CDL:H821	45:N5:703:CDL:H473	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:S1:632:MET:HE2	34:S1:632:MET:HB3	1.96	0.41
40:S7:193:TRP:CG	51:S7:303:3PE:H32	2.55	0.41
45:4L:201:CDL:H252	12:AL:38:ALA:HB2	2.02	0.41
14:AN:19:ILE:HD12	35:S2:351:SER:HB2	2.02	0.41
21:B7:17:PRO:HB3	21:B7:105:GLU:HG2	2.03	0.41
28:N1:81:LEU:O	28:N1:85:MET:HG2	2.20	0.41
31:N4:322:THR:HG21	31:N4:366:ASN:HA	2.03	0.41
4:A3:110:ILE:HD11	47:N1:404:PEE:H36	2.02	0.41
10:AC:120:MET:HE1	23:B9:66:LEU:HB3	2.03	0.41
13:AM:144:TYR:OH	34:S1:581:ASP:OD1	2.27	0.41
26:CA:31:ILE:HG23	26:CA:32:ARG:HG3	2.03	0.41
26:CA:70:LYS:HD3	26:CA:76:GLU:HB2	2.02	0.41
28:N1:70:MET:HB3	28:N1:122:ALA:HB2	2.02	0.41
28:N1:142:TYR:CD1	28:N1:142:TYR:C	2.98	0.41
47:N3:201:PEE:H72	47:N3:201:PEE:H67	1.85	0.41
31:N4:16:TRP:HB3	45:N4:504:CDL:H511	2.03	0.41
31:N4:210:TYR:HA	31:N4:213:HIS:HD2	1.85	0.41
31:N4:211:GLY:H	31:N4:213:HIS:HD2	1.69	0.41
31:N4:232:ALA:O	31:N4:237:LYS:NZ	2.54	0.41
32:N5:176:ARG:HA	32:N5:176:ARG:HD2	1.86	0.41
34:S1:69:LEU:O	37:S4:158:LYS:NZ	2.36	0.41
39:S6:67:ALA:HB2	41:S8:111:GLU:HG3	2.03	0.41
12:AL:4:THR:HG22	12:AL:8:LYS:HE3	2.03	0.41
29:N2:139:LEU:HD13	29:N2:190:MET:HE1	2.03	0.41
34:S1:354:LEU:HD22	34:S1:548:LEU:HD22	2.02	0.41
15:B1:30:ARG:NH1	15:B1:33:GLU:OE2	2.54	0.40
17:B3:24:ILE:O	17:B3:30:GLU:HB3	2.20	0.40
18:B4:26:SER:OG	18:B4:28:GLU:OE1	2.39	0.40
23:B9:120:GLN:HB2	32:N5:524:ASN:HD21	1.85	0.40
29:N2:280:THR:HG21	47:N4:501:PEE:H19	2.02	0.40
32:N5:293:ILE:HD11	45:N5:704:CDL:H721	2.03	0.40
34:S1:522:GLN:O	34:S1:526:LEU:HG	2.21	0.40
40:S7:190:LEU:HD22	51:S7:303:3PE:H332	2.03	0.40
42:V1:116:ASN:O	42:V1:245:VAL:HG23	2.21	0.40
42:V1:204:TYR:HB3	42:V1:377:GLU:HB3	2.04	0.40
48:AC:201:ZMP:H25B	48:AC:201:ZMP:H22	1.49	0.40
11:AK:232:THR:HG23	11:AK:235:TYR:H	1.86	0.40
15:B1:32:ASP:OD1	19:B5:135:LYS:NZ	2.53	0.40
19:B5:80:ILE:HB	19:B5:81:PRO:HD3	2.04	0.40
24:BK:142:ARG:NH1	24:BK:143:TYR:OH	2.54	0.40
28:N1:202:GLU:HA	28:N1:210:GLY:HA3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:N1:273:ILE:HD11	47:N1:404:PEE:H65	2.03	0.40
29:N2:5:ILE:O	29:N2:8:THR:HG22	2.20	0.40
32:N5:208:CYS:HA	32:N5:209:PRO:HD3	1.81	0.40
32:N5:346:ILE:HD11	32:N5:431:PHE:CZ	2.57	0.40
32:N5:485:TYR:CE2	32:N5:486:MET:HG3	2.57	0.40
9:A9:211:ASP:O	9:A9:215:ASN:ND2	2.54	0.40
10:AC:133:ILE:HG13	23:B9:46:SER:HB2	2.03	0.40
11:AK:283:GLY:O	11:AK:286:PRO:HD2	2.20	0.40
21:B7:95:TYR:CZ	22:B8:156:VAL:HG11	2.55	0.40
31:N4:243:MET:HB3	31:N4:301:ILE:HG21	2.02	0.40
45:N4:504:CDL:H722	45:N4:504:CDL:H751	1.94	0.40
33:N6:129:ASP:HB2	38:S5:32:ARG:NH1	2.36	0.40
35:S2:204:THR:HB	35:S2:208:TRP:CZ2	2.57	0.40
50:S7:302:PLX:H1A2	50:S7:302:PLX:H21	1.63	0.40
42:V1:99:TRP:N	42:V1:99:TRP:CD1	2.90	0.40
1:4L:98:CYS:HB3	32:N5:580:GLN:HB2	2.03	0.40
4:A3:139:PRO:HD3	14:AN:69:ILE:HD13	2.02	0.40
5:A5:38:ILE:O	5:A5:45:ARG:NH1	2.55	0.40
11:AK:316:LEU:HB2	11:AK:319:ILE:HG12	2.03	0.40
45:AL:201:CDL:H552	29:N2:112:HIS:HE1	1.86	0.40
15:B1:27:LEU:HD12	31:N4:6:ILE:HD11	2.02	0.40
18:B4:2:SER:OG	18:B4:3:PHE:N	2.53	0.40
28:N1:9:LEU:O	28:N1:13:ILE:HG12	2.21	0.40
28:N1:185:TRP:NE1	28:N1:238:THR:OG1	2.39	0.40
29:N2:111:PHE:HA	32:N5:591:PHE:CE1	2.57	0.40
31:N4:108:MET:HB3	31:N4:121:LEU:HD13	2.03	0.40
32:N5:295:GLN:O	32:N5:425:ARG:NH1	2.54	0.40
35:S2:112:VAL:HG21	35:S2:453:VAL:HG21	2.04	0.40
35:S2:272:ARG:NE	41:S8:65:GLU:OE2	2.47	0.40
6:A6:127:THR:O	6:A6:131:ARG:HG3	2.21	0.40
6:A6:131:ARG:NH2	36:S3:210:LEU:HD21	2.36	0.40
10:AC:140:CYS:HB3	10:AC:143:GLU:HG3	2.04	0.40
10:AC:155:TYR:CD2	10:AC:156:GLU:HG3	2.56	0.40
12:AL:36:VAL:HG22	45:AL:201:CDL:H742	2.04	0.40
17:B3:32:VAL:HG21	23:B9:77:ASP:HB2	2.04	0.40
24:BK:144:SER:HB3	24:BK:158:LYS:NZ	2.37	0.40
28:N1:273:ILE:HG23	28:N1:277:TYR:HD2	1.86	0.40
29:N2:167:TRP:HB3	32:N5:574:SER:HA	2.04	0.40
47:N2:402:PEE:H22	47:N2:402:PEE:H16	1.75	0.40
47:N2:402:PEE:H30	47:N2:402:PEE:H23	1.82	0.40
32:N5:407:TRP:O	32:N5:411:MET:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:S1:466:LEU:HD13	34:S1:500:ILE:HD11	2.03	0.40
35:S2:46:ASP:OD1	35:S2:46:ASP:N	2.53	0.40
42:V1:295:PRO:HG2	42:V1:298:GLU:HB2	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	4L	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
2	A1	68/70 (97%)	68 (100%)	0	0	100	100
3	A2	83/85 (98%)	82 (99%)	1 (1%)	0	100	100
4	A3	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
5	A5	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
6	A6	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
7	A7	93/112 (83%)	91 (98%)	2 (2%)	0	100	100
8	A8	169/171 (99%)	164 (97%)	5 (3%)	0	100	100
9	A9	339/341 (99%)	327 (96%)	12 (4%)	0	100	100
10	AB	75/87 (86%)	74 (99%)	1 (1%)	0	100	100
10	AC	85/87 (98%)	85 (100%)	0	0	100	100
11	AK	319/321 (99%)	310 (97%)	9 (3%)	0	100	100
12	AL	138/140 (99%)	138 (100%)	0	0	100	100
13	AM	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	AN	140/142 (99%)	130 (93%)	10 (7%)	0	100	100
15	B1	54/56 (96%)	54 (100%)	0	0	100	100
16	B2	65/67 (97%)	64 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	B3	78/80 (98%)	77 (99%)	1 (1%)	0	100	100
18	B4	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
19	B5	136/138 (99%)	135 (99%)	1 (1%)	0	100	100
20	B6	99/126 (79%)	94 (95%)	5 (5%)	0	100	100
21	B7	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
22	B8	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
23	B9	176/178 (99%)	176 (100%)	0	0	100	100
24	BK	172/176 (98%)	171 (99%)	1 (1%)	0	100	100
25	BL	97/102 (95%)	89 (92%)	8 (8%)	0	100	100
26	CA	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
27	CB	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
28	N1	316/318 (99%)	307 (97%)	9 (3%)	0	100	100
29	N2	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
30	N3	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
31	N4	457/459 (100%)	453 (99%)	4 (1%)	0	100	100
32	N5	601/603 (100%)	575 (96%)	26 (4%)	0	100	100
33	N6	172/174 (99%)	162 (94%)	10 (6%)	0	100	100
34	S1	687/689 (100%)	660 (96%)	27 (4%)	0	100	100
35	S2	427/430 (99%)	412 (96%)	15 (4%)	0	100	100
36	S3	206/208 (99%)	199 (97%)	7 (3%)	0	100	100
37	S4	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
38	S5	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
39	S6	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
40	S7	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
41	S8	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
42	V1	429/431 (100%)	410 (96%)	19 (4%)	0	100	100
43	V2	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
44	V3	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
All	All	8151/8299 (98%)	7914 (97%)	237 (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	4L	85/85 (100%)	85 (100%)	0	100	100
2	A1	58/58 (100%)	58 (100%)	0	100	100
3	A2	76/76 (100%)	76 (100%)	0	100	100
4	A3	69/69 (100%)	69 (100%)	0	100	100
5	A5	99/99 (100%)	99 (100%)	0	100	100
6	A6	107/107 (100%)	107 (100%)	0	100	100
7	A7	87/97 (90%)	85 (98%)	2 (2%)	44	66
8	A8	153/153 (100%)	153 (100%)	0	100	100
9	A9	295/295 (100%)	294 (100%)	1 (0%)	86	85
10	AB	71/80 (89%)	71 (100%)	0	100	100
10	AC	80/80 (100%)	79 (99%)	1 (1%)	61	73
11	AK	284/284 (100%)	282 (99%)	2 (1%)	76	79
12	AL	101/101 (100%)	100 (99%)	1 (1%)	68	76
13	AM	130/130 (100%)	129 (99%)	1 (1%)	73	78
14	AN	123/123 (100%)	123 (100%)	0	100	100
15	B1	53/53 (100%)	53 (100%)	0	100	100
16	B2	62/62 (100%)	62 (100%)	0	100	100
17	B3	62/62 (100%)	62 (100%)	0	100	100
18	B4	113/113 (100%)	113 (100%)	0	100	100
19	B5	121/121 (100%)	121 (100%)	0	100	100
20	B6	98/119 (82%)	98 (100%)	0	100	100
21	B7	112/112 (100%)	112 (100%)	0	100	100
22	B8	141/141 (100%)	141 (100%)	0	100	100
23	B9	159/159 (100%)	159 (100%)	0	100	100
24	BK	155/156 (99%)	155 (100%)	0	100	100
25	BL	91/94 (97%)	91 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	CA	45/45 (100%)	45 (100%)	0	100	100
27	CB	108/108 (100%)	108 (100%)	0	100	100
28	N1	275/275 (100%)	267 (97%)	8 (3%)	37	61
29	N2	311/311 (100%)	311 (100%)	0	100	100
30	N3	100/100 (100%)	100 (100%)	0	100	100
31	N4	410/410 (100%)	407 (99%)	3 (1%)	76	79
32	N5	537/537 (100%)	535 (100%)	2 (0%)	84	84
33	N6	140/140 (100%)	139 (99%)	1 (1%)	76	79
34	S1	579/579 (100%)	576 (100%)	3 (0%)	81	82
35	S2	370/370 (100%)	368 (100%)	2 (0%)	81	82
36	S3	190/190 (100%)	189 (100%)	1 (0%)	81	82
37	S4	112/112 (100%)	111 (99%)	1 (1%)	70	77
38	S5	93/93 (100%)	92 (99%)	1 (1%)	65	75
39	S6	79/79 (100%)	79 (100%)	0	100	100
40	S7	132/132 (100%)	128 (97%)	4 (3%)	36	61
41	S8	151/151 (100%)	150 (99%)	1 (1%)	76	79
42	V1	344/344 (100%)	341 (99%)	3 (1%)	70	77
43	V2	183/183 (100%)	180 (98%)	3 (2%)	55	71
44	V3	41/41 (100%)	41 (100%)	0	100	100
All	All	7185/7229 (99%)	7144 (99%)	41 (1%)	76	80

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	A7	31	ILE
7	A7	43	VAL
9	A9	129	LEU
10	AC	112	SER
11	AK	97	ASP
11	AK	255	CYS
12	AL	115	CYS
13	AM	144	TYR
28	N1	21	THR
28	N1	133	LEU
28	N1	155	LEU

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Mol	Chain	Res	Type
28	N1	156	MET
28	N1	175	ILE
28	N1	224	PHE
28	N1	251	THR
28	N1	282	TYR
31	N4	81	GLN
31	N4	122	PHE
31	N4	375	LEU
32	N5	21	MET
32	N5	340	PHE
33	N6	169	MET
34	S1	100	TRP
34	S1	253	VAL
34	S1	690	THR
35	S2	148	VAL
35	S2	204	THR
36	S3	145	THR
37	S4	86	ASN
38	S5	15	ASP
40	S7	71	CYS
40	S7	91	VAL
40	S7	101	ASP
40	S7	142	TYR
41	S8	98	ARG
42	V1	347	THR
42	V1	379	CYS
42	V1	457	HIS
43	V2	137	THR
43	V2	213	ILE
43	V2	249	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	4L	7	ASN
1	4L	57	ASN
3	A2	25	GLN
3	A2	73	GLN
3	A2	86	GLN
5	A5	71	GLN
5	A5	86	ASN
6	A6	84	GLN

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Mol	Chain	Res	Type
7	A7	9	GLN
7	A7	21	GLN
8	A8	107	HIS
8	A8	112	GLN
8	A8	141	ASN
8	A8	142	GLN
9	A9	37	HIS
9	A9	72	HIS
9	A9	79	GLN
9	A9	122	HIS
9	A9	138	ASN
9	A9	269	ASN
11	AK	67	ASN
11	AK	134	GLN
11	AK	151	HIS
11	AK	217	GLN
11	AK	221	GLN
12	AL	79	GLN
12	AL	89	ASN
13	AM	17	HIS
13	AM	112	ASN
14	AN	61	GLN
14	AN	90	ASN
15	B1	3	ASN
15	B1	6	GLN
16	B2	63	GLN
16	B2	68	GLN
16	B2	71	GLN
17	B3	21	GLN
17	B3	33	GLN
18	B4	50	GLN
19	B5	181	HIS
20	B6	127	HIS
21	B7	76	ASN
21	B7	85	HIS
21	B7	110	GLN
22	B8	56	ASN
22	B8	100	ASN
22	B8	127	ASN
22	B8	164	ASN
23	B9	104	GLN
23	B9	108	GLN

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Mol	Chain	Res	Type
23	B9	117	GLN
24	BK	107	GLN
24	BK	149	HIS
28	N1	138	GLN
28	N1	304	HIS
29	N2	2	ASN
29	N2	49	ASN
29	N2	83	GLN
29	N2	112	HIS
29	N2	186	HIS
29	N2	273	ASN
29	N2	316	GLN
29	N2	322	GLN
30	N3	26	GLN
31	N4	175	ASN
31	N4	192	ASN
31	N4	213	HIS
31	N4	251	ASN
31	N4	279	GLN
31	N4	304	GLN
31	N4	366	ASN
32	N5	2	ASN
32	N5	59	GLN
32	N5	136	ASN
32	N5	139	GLN
32	N5	159	HIS
32	N5	230	HIS
32	N5	248	HIS
32	N5	471	ASN
32	N5	518	GLN
32	N5	524	ASN
32	N5	580	GLN
34	S1	39	GLN
34	S1	282	ASN
34	S1	304	GLN
34	S1	331	GLN
34	S1	336	ASN
34	S1	498	GLN
34	S1	604	GLN
34	S1	652	ASN
34	S1	688	GLN
35	S2	93	GLN

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Mol	Chain	Res	Type
35	S2	166	ASN
36	S3	74	GLN
36	S3	77	GLN
36	S3	82	ASN
36	S3	123	GLN
36	S3	196	HIS
37	S4	123	ASN
37	S4	163	ASN
38	S5	25	GLN
38	S5	45	HIS
39	S6	74	GLN
39	S6	117	GLN
40	S7	144	HIS
41	S8	85	ASN
42	V1	133	HIS
42	V1	220	GLN
42	V1	270	ASN
42	V1	303	HIS
42	V1	344	GLN
42	V1	376	HIS
42	V1	381	GLN
42	V1	393	ASN
42	V1	456	GLN
43	V2	74	HIS
43	V2	133	GLN
43	V2	153	GLN
43	V2	187	GLN
43	V2	246	GLN
44	V3	388	ASN
44	V3	419	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	2MR	S2	124	35	10,12,13	2.50	2 (20%)	5,13,15	1.00	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
35	2MR	S2	124	35	-	2/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S2	124	2MR	CZ-NH2	5.34	1.44	1.33
35	S2	124	2MR	CZ-NE	5.15	1.45	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	S2	124	2MR	NE-CD-CG-CB
35	S2	124	2MR	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	S2	124	2MR	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 53 ligands modelled in this entry, 2 are monoatomic - leaving 51 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$
55	FES	S1	803	34	0,4,4	-	-	-		
45	CDL	N2	401	-	67,67,99	0.35	0	73,79,111	0.37	0
45	CDL	B4	202	-	61,61,99	0.37	0	67,73,111	0.36	0
51	3PE	B8	201	-	31,31,50	0.37	0	34,36,55	0.38	0
45	CDL	AL	201	-	93,93,99	0.31	0	99,105,111	0.32	0
53	6F6	N3	203	-	53,53,53	0.28	0	59,61,61	0.30	0
45	CDL	4L	201	-	91,91,99	0.32	0	97,103,111	0.35	0
51	3PE	CB	202	-	45,45,50	0.31	0	48,50,55	0.29	0
47	PEE	N5	705	-	50,50,50	1.34	5 (10%)	53,55,55	1.18	6 (11%)
48	ZMP	AC	201	10	30,35,36	0.73	1 (3%)	34,42,45	0.79	1 (2%)
53	6F6	N6	401	-	47,47,53	0.30	0	53,55,61	0.30	0
45	CDL	B4	201	-	79,79,99	0.32	0	85,91,111	0.30	0
45	CDL	A8	301	-	82,82,99	0.32	0	88,94,111	0.33	0
46	NDP	A9	401	-	51,52,52	0.31	0	71,80,80	0.33	0
47	PEE	N1	403	-	30,30,50	1.30	3 (10%)	33,35,55	1.15	2 (6%)
47	PEE	N5	702	-	39,39,50	1.51	5 (12%)	42,44,55	1.29	5 (11%)
54	SF4	S1	802	34	0,12,12	-	-	-		
47	PEE	N1	404	-	50,50,50	1.34	5 (10%)	53,55,55	1.26	4 (7%)
48	ZMP	AB	201	10	30,35,36	0.67	1 (3%)	34,42,45	0.70	0
45	CDL	B5	202	-	99,99,99	0.30	0	105,111,111	0.34	0
51	3PE	CA	101	-	50,50,50	0.30	0	53,55,55	0.29	0
51	3PE	N5	706	-	45,45,50	0.32	0	48,50,55	0.30	0
51	3PE	S7	303	-	50,50,50	0.31	0	53,55,55	0.48	0
52	XEW	N1	402	-	14,17,17	5.00	14 (100%)	17,22,22	1.91	2 (11%)
47	PEE	N2	402	-	47,47,50	1.37	5 (10%)	50,52,55	1.21	4 (8%)
47	PEE	N3	201	-	50,50,50	1.34	5 (10%)	53,55,55	1.20	6 (11%)
45	CDL	A7	201	-	50,50,99	0.40	0	56,62,111	0.33	0
45	CDL	N1	401	-	77,77,99	0.33	0	83,89,111	0.30	0
54	SF4	S1	801	34	0,12,12	-	-	-		
50	PLX	B5	201	-	51,51,51	1.14	3 (5%)	53,59,59	0.89	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	PEE	A9	402	-	38,38,50	1.51	5 (13%)	41,43,55	1.24	5 (12%)
47	PEE	BL	201	-	50,50,50	1.34	5 (10%)	53,55,55	1.16	4 (7%)
47	PEE	N4	501	-	48,48,50	1.36	5 (10%)	51,53,55	1.22	6 (11%)
50	PLX	CB	201	-	51,51,51	1.14	3 (5%)	53,59,59	0.92	1 (1%)
55	FES	V2	301	43	0,4,4	-	-	-	-	-
45	CDL	N4	504	-	99,99,99	0.29	0	105,111,111	0.29	0
50	PLX	N4	503	-	48,48,51	1.18	5 (10%)	50,56,59	0.91	1 (2%)
58	FMN	V1	502	-	33,33,33	0.23	0	48,50,50	0.34	0
45	CDL	N5	703	-	88,88,99	0.31	0	94,100,111	0.31	0
54	SF4	S8	302	41	0,12,12	-	-	-	-	-
50	PLX	N4	502	-	46,46,51	1.20	5 (10%)	48,54,59	0.89	1 (2%)
50	PLX	AM	201	-	51,51,51	1.14	5 (9%)	53,59,59	0.92	1 (1%)
47	PEE	N5	701	-	45,45,50	1.41	5 (11%)	48,50,55	1.21	6 (12%)
45	CDL	N5	704	-	99,99,99	0.30	0	105,111,111	0.28	0
52	XEW	S2	501	-	14,17,17	5.07	14 (100%)	17,22,22	2.09	3 (17%)
54	SF4	S8	301	41	0,12,12	-	-	-	-	-
50	PLX	S7	302	-	51,51,51	1.14	4 (7%)	53,59,59	0.90	1 (1%)
50	PLX	N3	202	-	51,51,51	1.14	5 (9%)	53,59,59	0.88	1 (1%)
54	SF4	S7	301	40	0,12,12	-	-	-	-	-
49	ADP	AK	401	-	28,29,29	1.41	4 (14%)	43,45,45	1.82	9 (20%)
54	SF4	V1	501	42	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	FES	S1	803	34	-	-	0/1/1/1
45	CDL	N2	401	-	-	14/78/78/110	-
45	CDL	B4	202	-	-	24/72/72/110	-
51	3PE	B8	201	-	-	3/35/35/54	-
45	CDL	AL	201	-	-	23/104/104/110	-
53	6F6	N3	203	-	-	14/57/57/57	-
45	CDL	4L	201	-	-	16/102/102/110	-
51	3PE	CB	202	-	-	9/49/49/54	-
47	PEE	N5	705	-	-	22/54/54/54	-
48	ZMP	AC	201	10	-	18/40/42/43	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	6F6	N6	401	-	-	14/51/51/57	-
45	CDL	B4	201	-	-	20/90/90/110	-
45	CDL	A8	301	-	-	24/93/93/110	-
46	NDP	A9	401	-	-	6/34/77/77	0/5/5/5
47	PEE	N1	403	-	-	24/34/34/54	-
47	PEE	N5	702	-	-	24/43/43/54	-
54	SF4	S1	802	34	-	-	0/6/5/5
47	PEE	N1	404	-	-	25/54/54/54	-
48	ZMP	AB	201	10	-	13/40/42/43	-
45	CDL	B5	202	-	-	25/110/110/110	-
51	3PE	CA	101	-	-	10/54/54/54	-
51	3PE	N5	706	-	-	11/49/49/54	-
51	3PE	S7	303	-	-	14/54/54/54	-
52	XEW	N1	402	-	-	6/12/12/12	0/1/1/1
47	PEE	N2	402	-	-	26/51/51/54	-
47	PEE	N3	201	-	-	21/54/54/54	-
45	CDL	A7	201	-	-	11/61/61/110	-
45	CDL	N1	401	-	-	16/88/88/110	-
54	SF4	S1	801	34	-	-	0/6/5/5
50	PLX	B5	201	-	-	20/55/55/55	-
47	PEE	A9	402	-	-	24/42/42/54	-
47	PEE	BL	201	-	-	28/54/54/54	-
47	PEE	N4	501	-	-	25/52/52/54	-
50	PLX	CB	201	-	-	19/55/55/55	-
55	FES	V2	301	43	-	-	0/1/1/1
45	CDL	N4	504	-	-	25/110/110/110	-
50	PLX	N4	503	-	-	20/52/52/55	-
58	FMN	V1	502	-	-	0/18/18/18	0/3/3/3
45	CDL	N5	703	-	-	24/99/99/110	-
54	SF4	S8	302	41	-	-	0/6/5/5
50	PLX	N4	502	-	-	19/50/50/55	-
50	PLX	AM	201	-	-	22/55/55/55	-
47	PEE	N5	701	-	-	23/49/49/54	-
45	CDL	N5	704	-	-	15/110/110/110	-
52	XEW	S2	501	-	-	9/12/12/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	SF4	S8	301	41	-	-	0/6/5/5
50	PLX	S7	302	-	-	13/55/55/55	-
50	PLX	N3	202	-	-	13/55/55/55	-
54	SF4	S7	301	40	-	-	0/6/5/5
49	ADP	AK	401	-	-	4/16/32/32	0/3/3/3
54	SF4	V1	501	42	-	-	0/6/5/5

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	S2	501	XEW	C5-N2	7.86	1.53	1.34
52	N1	402	XEW	C5-N2	7.57	1.52	1.34
52	S2	501	XEW	C5-N1	7.19	1.52	1.36
52	N1	402	XEW	C4-N1	7.17	1.52	1.36
52	S2	501	XEW	C4-N1	7.15	1.52	1.36
52	N1	402	XEW	C5-N1	7.11	1.52	1.36
52	N1	402	XEW	C-CL	5.76	1.87	1.74
52	S2	501	XEW	C-CL	5.73	1.87	1.74
52	N1	402	XEW	C3-N	5.72	1.53	1.41
52	S2	501	XEW	C3-N	5.54	1.52	1.41
49	AK	401	ADP	C5-C4	4.63	1.47	1.39
52	S2	501	XEW	C9-C10	4.42	1.46	1.38
52	S2	501	XEW	C1-C2	4.30	1.45	1.38
52	N1	402	XEW	C9-C10	4.29	1.45	1.38
52	S2	501	XEW	C10-C	4.27	1.45	1.38
52	N1	402	XEW	C1-C2	4.26	1.45	1.38
52	S2	501	XEW	C1-C	4.25	1.45	1.38
52	N1	402	XEW	C1-C	4.24	1.45	1.38
47	N5	705	PEE	C18-C19	4.14	1.55	1.31
47	N5	702	PEE	C18-C19	4.14	1.55	1.31
47	BL	201	PEE	C18-C19	4.14	1.55	1.31
47	N5	701	PEE	C18-C19	4.14	1.55	1.31
47	N1	404	PEE	C18-C19	4.13	1.55	1.31
47	N2	402	PEE	C18-C19	4.12	1.55	1.31
47	N3	201	PEE	C18-C19	4.11	1.55	1.31
47	A9	402	PEE	C18-C19	4.11	1.55	1.31
52	N1	402	XEW	C10-C	4.10	1.45	1.38
47	N4	501	PEE	C18-C19	4.09	1.54	1.31
47	BL	201	PEE	C39-C38	4.04	1.54	1.31
47	N5	702	PEE	C39-C38	4.04	1.54	1.31
47	N4	501	PEE	C39-C38	4.04	1.54	1.31
47	N1	404	PEE	C39-C38	4.03	1.54	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	N5	701	PEE	C39-C38	4.03	1.54	1.31
47	N2	402	PEE	C39-C38	4.02	1.54	1.31
47	N3	201	PEE	C39-C38	4.02	1.54	1.31
47	N5	705	PEE	C39-C38	4.01	1.54	1.31
47	A9	402	PEE	C39-C38	3.96	1.54	1.29
52	N1	402	XEW	C9-C3	3.94	1.45	1.39
52	S2	501	XEW	C9-C3	3.89	1.45	1.39
52	S2	501	XEW	C2-C3	3.85	1.45	1.39
52	N1	402	XEW	C2-C3	3.65	1.45	1.39
47	N5	701	PEE	O3-C30	3.26	1.42	1.33
47	N1	403	PEE	O3-C30	3.26	1.42	1.33
47	N3	201	PEE	O3-C30	3.25	1.42	1.33
47	A9	402	PEE	O3-C30	3.23	1.42	1.33
47	BL	201	PEE	O3-C30	3.22	1.42	1.33
47	N5	702	PEE	O3-C30	3.22	1.42	1.33
47	N5	705	PEE	O3-C30	3.21	1.42	1.33
47	N2	402	PEE	O3-C30	3.21	1.42	1.33
47	N1	404	PEE	O3-C30	3.18	1.42	1.33
52	S2	501	XEW	C6-N2	3.14	1.53	1.47
50	CB	201	PLX	O6-C4	-3.13	1.40	1.44
47	N4	501	PEE	O3-C30	3.11	1.42	1.33
50	S7	302	PLX	O6-C4	-3.10	1.40	1.44
50	N4	503	PLX	O6-C4	-3.09	1.40	1.44
50	N4	502	PLX	O6-C4	-3.06	1.40	1.44
50	AM	201	PLX	O6-C4	-3.04	1.40	1.44
50	B5	201	PLX	O6-C4	-2.99	1.40	1.44
50	N3	202	PLX	O6-C4	-2.93	1.40	1.44
52	S2	501	XEW	C8-C6	2.93	1.60	1.51
52	S2	501	XEW	C7-C6	2.91	1.60	1.51
52	N1	402	XEW	C7-C6	2.85	1.60	1.51
52	N1	402	XEW	C8-C6	2.84	1.60	1.51
52	N1	402	XEW	C6-N2	2.80	1.52	1.47
47	N4	501	PEE	O2-C2	-2.76	1.40	1.46
48	AC	201	ZMP	C9-C10	-2.76	1.48	1.50
47	N1	404	PEE	O2-C10	2.72	1.42	1.34
47	BL	201	PEE	O2-C10	2.72	1.42	1.34
49	AK	401	ADP	C5-C6	2.72	1.48	1.41
47	N5	705	PEE	O2-C2	-2.71	1.40	1.46
47	N2	402	PEE	O2-C2	-2.69	1.40	1.46
47	A9	402	PEE	O2-C2	-2.67	1.40	1.46
47	N5	701	PEE	O2-C10	2.65	1.41	1.34
47	N3	201	PEE	O2-C2	-2.65	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	N5	702	PEE	O2-C2	-2.64	1.40	1.46
47	N1	403	PEE	O2-C10	2.63	1.41	1.34
47	N5	702	PEE	O2-C10	2.63	1.41	1.34
47	N1	403	PEE	O2-C2	-2.62	1.40	1.46
47	N3	201	PEE	O2-C10	2.62	1.41	1.34
47	N5	701	PEE	O2-C2	-2.61	1.40	1.46
47	A9	402	PEE	O2-C10	2.59	1.41	1.34
47	N2	402	PEE	O2-C10	2.59	1.41	1.34
47	N5	705	PEE	O2-C10	2.58	1.41	1.34
47	N1	404	PEE	O2-C2	-2.54	1.40	1.46
47	N4	501	PEE	O2-C10	2.50	1.41	1.34
48	AB	201	ZMP	C9-C10	-2.49	1.48	1.50
47	BL	201	PEE	O2-C2	-2.41	1.40	1.46
49	AK	401	ADP	C8-N7	2.30	1.36	1.31
49	AK	401	ADP	C5-N7	-2.26	1.35	1.39
50	N4	503	PLX	C1B-N1	-2.21	1.43	1.50
50	N4	502	PLX	C1B-N1	-2.19	1.43	1.50
50	S7	302	PLX	C1B-N1	-2.18	1.43	1.50
50	B5	201	PLX	C1B-N1	-2.17	1.43	1.50
50	N3	202	PLX	C1B-N1	-2.16	1.43	1.50
50	CB	201	PLX	C1B-N1	-2.13	1.43	1.50
50	AM	201	PLX	C1B-N1	-2.10	1.43	1.50
50	CB	201	PLX	C1C-N1	-2.10	1.43	1.50
50	N3	202	PLX	P1-O4	2.09	1.67	1.59
50	S7	302	PLX	C1C-N1	-2.08	1.44	1.50
50	AM	201	PLX	P1-O4	2.07	1.67	1.59
50	N4	503	PLX	P1-O4	2.07	1.67	1.59
50	N4	502	PLX	C1C-N1	-2.06	1.44	1.50
50	B5	201	PLX	P1-O4	2.04	1.67	1.59
50	N4	503	PLX	C1C-N1	-2.04	1.44	1.50
50	N4	502	PLX	P1-O4	2.03	1.67	1.59
50	N3	202	PLX	C1C-N1	-2.03	1.44	1.50
50	S7	302	PLX	C7-C6	2.03	1.55	1.50
50	N4	502	PLX	C7-C6	2.02	1.55	1.50
50	N4	503	PLX	C7-C6	2.02	1.55	1.50
50	N3	202	PLX	C7-C6	2.01	1.54	1.50
50	AM	201	PLX	C1C-N1	-2.00	1.44	1.50
50	AM	201	PLX	C7-C6	2.00	1.54	1.50

All (70) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	501	XEW	C6-N2-C5	7.48	138.91	124.06
52	N1	402	XEW	C6-N2-C5	6.13	136.24	124.06
49	AK	401	ADP	C5-C4-N3	-5.77	118.77	126.72
47	N1	404	PEE	O2-C10-C11	4.71	121.67	111.48
49	AK	401	ADP	N3-C4-N9	4.61	135.00	127.17
52	N1	402	XEW	N2-C5-N3	-4.20	110.57	120.15
47	N5	702	PEE	O2-C10-C11	4.10	120.36	111.48
47	N4	501	PEE	O2-C10-C11	4.06	120.26	111.48
47	N2	402	PEE	O2-C10-C11	4.04	120.23	111.48
47	N3	201	PEE	O2-C10-C11	4.03	120.21	111.48
47	N5	701	PEE	O2-C10-C11	4.02	120.18	111.48
47	N5	705	PEE	O2-C10-C11	3.92	119.95	111.48
47	N1	403	PEE	O2-C10-C11	3.89	119.89	111.48
47	BL	201	PEE	O2-C10-C11	3.89	119.89	111.48
47	A9	402	PEE	O2-C10-C11	3.77	119.64	111.48
49	AK	401	ADP	C2-N3-C4	3.68	120.82	111.83
49	AK	401	ADP	C4-C5-N7	-3.45	106.64	110.58
49	AK	401	ADP	N3-C2-N1	-3.21	123.73	128.58
52	S2	501	XEW	N2-C5-N3	-2.88	113.58	120.15
47	N2	402	PEE	O3-C30-C31	2.82	120.42	111.83
49	AK	401	ADP	C4-N9-C8	2.78	108.66	105.74
47	N5	702	PEE	C20-C19-C18	-2.76	109.83	126.42
47	N1	404	PEE	O3-C30-C31	2.75	120.23	111.83
47	N5	705	PEE	O3-C30-C31	2.74	120.18	111.83
47	N4	501	PEE	O3-C30-C31	2.70	120.06	111.83
47	A9	402	PEE	O3-C30-C31	2.68	120.01	111.83
47	BL	201	PEE	O3-C30-C31	2.68	120.01	111.83
47	N5	701	PEE	O3-C30-C31	2.68	120.00	111.83
47	N1	403	PEE	O3-C30-C31	2.67	119.98	111.83
47	N3	201	PEE	O3-C30-C31	2.63	119.86	111.83
47	N5	702	PEE	O3-C30-C31	2.61	119.79	111.83
49	AK	401	ADP	C5-N7-C8	2.54	107.44	103.45
52	S2	501	XEW	C3-N-C4	-2.44	120.08	126.73
50	B5	201	PLX	O3-P1-O2	-2.41	101.22	112.44
50	N3	202	PLX	O3-P1-O2	-2.40	101.29	112.44
50	AM	201	PLX	O3-P1-O2	-2.38	101.35	112.44
50	N4	502	PLX	O3-P1-O2	-2.36	101.46	112.44
50	N4	503	PLX	O3-P1-O2	-2.35	101.50	112.44
47	A9	402	PEE	C37-C38-C39	-2.35	109.53	126.65
50	CB	201	PLX	O3-P1-O2	-2.32	101.65	112.44
50	S7	302	PLX	O3-P1-O2	-2.31	101.69	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	N1	404	PEE	C17-C18-C19	-2.14	108.78	124.83
47	N4	501	PEE	C20-C19-C18	-2.12	108.91	124.83
47	N2	402	PEE	C37-C38-C39	-2.12	108.93	124.83
47	N3	201	PEE	C37-C38-C39	-2.11	109.00	124.83
47	A9	402	PEE	C17-C18-C19	-2.11	109.01	124.83
47	N4	501	PEE	C17-C18-C19	-2.10	109.10	124.83
49	AK	401	ADP	C6-C5-N7	2.10	136.13	132.09
47	A9	402	PEE	C20-C19-C18	-2.09	109.18	124.83
47	BL	201	PEE	C40-C39-C38	-2.09	109.18	124.83
48	AC	201	ZMP	O1-C10-C9	-2.09	121.57	123.98
47	N5	705	PEE	C37-C38-C39	-2.08	109.25	124.83
47	N5	701	PEE	C37-C38-C39	-2.07	109.29	124.83
47	N3	201	PEE	C17-C18-C19	-2.06	109.38	124.83
47	N4	501	PEE	C37-C38-C39	-2.06	109.38	124.83
47	N5	705	PEE	C40-C39-C38	-2.06	109.39	124.83
47	N5	701	PEE	C20-C19-C18	-2.06	109.40	124.83
47	N3	201	PEE	C40-C39-C38	-2.06	109.40	124.83
47	BL	201	PEE	C37-C38-C39	-2.05	109.45	124.83
47	N5	701	PEE	C40-C39-C38	-2.05	109.45	124.83
47	N1	404	PEE	C37-C38-C39	-2.05	109.46	124.83
47	N5	705	PEE	C17-C18-C19	-2.05	109.48	124.83
49	AK	401	ADP	N9-C8-N7	-2.05	111.03	113.94
47	N4	501	PEE	C40-C39-C38	-2.04	109.52	124.83
47	N3	201	PEE	C20-C19-C18	-2.04	109.57	124.83
47	N5	701	PEE	C17-C18-C19	-2.03	109.66	124.83
47	N5	702	PEE	C37-C38-C39	-2.02	109.70	124.83
47	N2	402	PEE	C17-C18-C19	-2.02	109.71	124.83
47	N5	705	PEE	C20-C19-C18	-2.01	109.76	124.83
47	N5	702	PEE	C17-C18-C19	-2.00	109.84	124.83

There are no chirality outliers.

All (736) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	4L	201	CDL	CA2-OA2-PA1-OA5
45	4L	201	CDL	CA3-OA5-PA1-OA2
45	4L	201	CDL	CA3-OA5-PA1-OA3
45	4L	201	CDL	CA3-OA5-PA1-OA4
45	4L	201	CDL	CB2-OB2-PB2-OB4
45	4L	201	CDL	CB2-OB2-PB2-OB5
45	A7	201	CDL	CB2-C1-CA2-OA2
45	A7	201	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
45	A7	201	CDL	CB3-OB5-PB2-OB2
45	A7	201	CDL	CB3-OB5-PB2-OB3
45	A7	201	CDL	CB3-OB5-PB2-OB4
45	A8	301	CDL	CA2-OA2-PA1-OA3
45	A8	301	CDL	CA2-OA2-PA1-OA4
45	A8	301	CDL	CA2-OA2-PA1-OA5
45	A8	301	CDL	CB2-OB2-PB2-OB3
45	A8	301	CDL	CB2-OB2-PB2-OB5
45	A8	301	CDL	CB3-OB5-PB2-OB2
45	A8	301	CDL	CB3-OB5-PB2-OB4
45	AL	201	CDL	CA2-OA2-PA1-OA3
45	AL	201	CDL	CA2-OA2-PA1-OA5
45	AL	201	CDL	CB2-OB2-PB2-OB4
45	AL	201	CDL	CB2-OB2-PB2-OB5
45	AL	201	CDL	CB3-OB5-PB2-OB2
45	AL	201	CDL	CB3-OB5-PB2-OB3
45	AL	201	CDL	CB3-OB5-PB2-OB4
45	B4	201	CDL	CA2-OA2-PA1-OA3
45	B4	201	CDL	CA2-OA2-PA1-OA4
45	B4	201	CDL	CA2-OA2-PA1-OA5
45	B4	201	CDL	CA3-OA5-PA1-OA2
45	B4	201	CDL	CA3-OA5-PA1-OA3
45	B4	201	CDL	CA3-OA5-PA1-OA4
45	B4	201	CDL	CB2-OB2-PB2-OB3
45	B4	201	CDL	CB2-OB2-PB2-OB5
45	B4	202	CDL	CA2-OA2-PA1-OA3
45	B4	202	CDL	CA2-OA2-PA1-OA5
45	B4	202	CDL	CA3-OA5-PA1-OA4
45	B4	202	CDL	CB2-OB2-PB2-OB5
45	B5	202	CDL	CA2-OA2-PA1-OA3
45	B5	202	CDL	CA2-OA2-PA1-OA5
45	B5	202	CDL	CB3-OB5-PB2-OB2
45	B5	202	CDL	CB3-OB5-PB2-OB3
45	N1	401	CDL	CA3-OA5-PA1-OA2
45	N1	401	CDL	CA3-OA5-PA1-OA4
45	N1	401	CDL	CB2-OB2-PB2-OB3
45	N1	401	CDL	CB2-OB2-PB2-OB4
45	N1	401	CDL	CB2-OB2-PB2-OB5
45	N2	401	CDL	CA2-OA2-PA1-OA4
45	N2	401	CDL	CA3-OA5-PA1-OA2
45	N2	401	CDL	CA3-OA5-PA1-OA3
45	N2	401	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
45	N2	401	CDL	CB2-OB2-PB2-OB3
45	N2	401	CDL	CB2-OB2-PB2-OB4
45	N2	401	CDL	CB2-OB2-PB2-OB5
45	N4	504	CDL	CA2-OA2-PA1-OA3
45	N4	504	CDL	CA2-OA2-PA1-OA5
45	N4	504	CDL	CA3-OA5-PA1-OA2
45	N4	504	CDL	CA3-OA5-PA1-OA4
45	N4	504	CDL	CB3-OB5-PB2-OB2
45	N5	703	CDL	CA2-OA2-PA1-OA3
45	N5	703	CDL	CA2-OA2-PA1-OA4
45	N5	703	CDL	CA2-OA2-PA1-OA5
45	N5	703	CDL	CA3-OA5-PA1-OA2
45	N5	703	CDL	CA3-OA5-PA1-OA3
45	N5	703	CDL	CA3-OA5-PA1-OA4
45	N5	703	CDL	CB2-OB2-PB2-OB4
45	N5	703	CDL	CB2-OB2-PB2-OB5
45	N5	703	CDL	CB3-OB5-PB2-OB2
45	N5	703	CDL	CB3-OB5-PB2-OB3
45	N5	703	CDL	CB3-OB5-PB2-OB4
47	A9	402	PEE	C11-C10-O2-C2
47	A9	402	PEE	C1-O3P-P-O2P
47	A9	402	PEE	C1-O3P-P-O4P
47	A9	402	PEE	C4-O4P-P-O3P
47	A9	402	PEE	C4-O4P-P-O2P
47	A9	402	PEE	C4-O4P-P-O1P
47	BL	201	PEE	C1-O3P-P-O1P
47	BL	201	PEE	C1-O3P-P-O4P
47	BL	201	PEE	C4-O4P-P-O3P
47	N1	403	PEE	C1-O3P-P-O2P
47	N1	403	PEE	C1-O3P-P-O1P
47	N1	403	PEE	C1-O3P-P-O4P
47	N1	404	PEE	C11-C10-O2-C2
47	N1	404	PEE	O4-C10-O2-C2
47	N1	404	PEE	O3P-C1-C2-O2
47	N1	404	PEE	C1-O3P-P-O2P
47	N1	404	PEE	C1-O3P-P-O4P
47	N2	402	PEE	C11-C10-O2-C2
47	N2	402	PEE	O4-C10-O2-C2
47	N2	402	PEE	C1-O3P-P-O2P
47	N2	402	PEE	C1-O3P-P-O1P
47	N2	402	PEE	C1-O3P-P-O4P
47	N2	402	PEE	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
47	N2	402	PEE	C4-O4P-P-O1P
47	N3	201	PEE	C1-O3P-P-O1P
47	N3	201	PEE	C1-O3P-P-O4P
47	N4	501	PEE	C1-O3P-P-O2P
47	N4	501	PEE	C1-O3P-P-O4P
47	N4	501	PEE	O4P-C4-C5-N
47	N5	701	PEE	C4-O4P-P-O3P
47	N5	701	PEE	C4-O4P-P-O2P
47	N5	702	PEE	C11-C10-O2-C2
47	N5	702	PEE	O4-C10-O2-C2
47	N5	702	PEE	C1-O3P-P-O2P
47	N5	702	PEE	C1-O3P-P-O1P
47	N5	702	PEE	C1-O3P-P-O4P
47	N5	702	PEE	C4-O4P-P-O1P
47	N5	702	PEE	O5-C30-O3-C3
47	N5	705	PEE	C1-O3P-P-O2P
47	N5	705	PEE	C1-O3P-P-O1P
47	N5	705	PEE	C1-O3P-P-O4P
48	AC	201	ZMP	C20-C18-C21-O5
48	AC	201	ZMP	C17-C18-C21-O5
48	AC	201	ZMP	S1-C11-C12-N1
48	AC	201	ZMP	O1-C10-S1-C11
48	AC	201	ZMP	C9-C10-S1-C11
48	AC	201	ZMP	C7-C8-C9-C10
49	AK	401	ADP	PB-O3A-PA-O5'
49	AK	401	ADP	C5'-O5'-PA-O2A
49	AK	401	ADP	C5'-O5'-PA-O3A
50	AM	201	PLX	C3-O4-P1-O1
50	AM	201	PLX	C3-O4-P1-O2
50	AM	201	PLX	C3-O4-P1-O3
50	B5	201	PLX	O7-C6-O6-C4
50	B5	201	PLX	C3-O4-P1-O3
50	B5	201	PLX	N1-C1-C2-O1
50	B5	201	PLX	C25-C24-O8-C5
50	CB	201	PLX	C3-O4-P1-O1
50	CB	201	PLX	C3-O4-P1-O2
50	CB	201	PLX	C3-O4-P1-O3
50	CB	201	PLX	O9-C24-O8-C5
50	N3	202	PLX	O7-C6-O6-C4
50	N3	202	PLX	C3-O4-P1-O3
50	N3	202	PLX	O9-C24-C25-C26
50	N4	502	PLX	C7-C6-O6-C4

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Mol	Chain	Res	Type	Atoms
50	N4	502	PLX	O7-C6-O6-C4
50	N4	502	PLX	O6-C4-C5-O8
50	N4	503	PLX	O7-C6-O6-C4
50	N4	503	PLX	C3-O4-P1-O1
50	N4	503	PLX	C3-O4-P1-O2
50	N4	503	PLX	C3-O4-P1-O3
50	N4	503	PLX	O9-C24-O8-C5
50	S7	302	PLX	O7-C6-C7-C8
50	S7	302	PLX	O6-C6-C7-C8
50	S7	302	PLX	O9-C24-C25-C26
51	B8	201	3PE	C11-O13-P-O11
51	B8	201	3PE	C11-O13-P-O12
51	B8	201	3PE	C11-O13-P-O14
51	CA	101	3PE	C1-O11-P-O13
51	CA	101	3PE	C11-O13-P-O11
51	CB	202	3PE	C1-O11-P-O12
51	CB	202	3PE	C1-O11-P-O13
51	CB	202	3PE	C11-O13-P-O11
51	CB	202	3PE	C11-O13-P-O12
51	CB	202	3PE	C11-O13-P-O14
51	N5	706	3PE	C1-O11-P-O12
51	N5	706	3PE	C1-O11-P-O13
51	N5	706	3PE	C1-O11-P-O14
51	N5	706	3PE	C11-O13-P-O11
51	N5	706	3PE	C11-O13-P-O14
51	S7	303	3PE	C1-O11-P-O13
51	S7	303	3PE	C2-C1-O11-P
51	S7	303	3PE	O13-C11-C12-N
52	N1	402	XEW	N-C4-N1-C5
52	N1	402	XEW	N4-C4-N1-C5
52	N1	402	XEW	N1-C5-N2-C6
52	N1	402	XEW	N3-C5-N2-C6
52	S2	501	XEW	N1-C4-N-C3
52	S2	501	XEW	N4-C4-N1-C5
52	S2	501	XEW	N1-C5-N2-C6
52	S2	501	XEW	N3-C5-N2-C6
52	S2	501	XEW	C8-C6-N2-C5
53	N3	203	6F6	C1-O11-P-O12
53	N3	203	6F6	C1-O11-P-O14
53	N6	401	6F6	C11-O13-P-O14
53	N6	401	6F6	C11-O13-P-O11
53	N6	401	6F6	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
53	N6	401	6F6	C1-O11-P-O14
53	N6	401	6F6	C1-O11-P-O13
47	N4	501	PEE	C31-C30-O3-C3
47	N1	403	PEE	O5-C30-O3-C3
47	N4	501	PEE	O5-C30-O3-C3
47	A9	402	PEE	O4-C10-O2-C2
47	BL	201	PEE	O4-C10-O2-C2
47	N5	702	PEE	C31-C30-O3-C3
47	BL	201	PEE	C11-C10-O2-C2
47	N1	403	PEE	C31-C30-O3-C3
47	BL	201	PEE	C17-C18-C19-C20
47	N3	201	PEE	C17-C18-C19-C20
47	N4	501	PEE	C17-C18-C19-C20
47	N4	501	PEE	C37-C38-C39-C40
47	N5	705	PEE	C37-C38-C39-C40
45	A7	201	CDL	O1-C1-CA2-OA2
45	N5	703	CDL	O1-C1-CB2-OB2
47	N2	402	PEE	C31-C30-O3-C3
47	BL	201	PEE	C37-C38-C39-C40
47	N5	702	PEE	C37-C38-C39-C40
47	N5	705	PEE	C11-C10-O2-C2
45	N1	401	CDL	CA2-C1-CB2-OB2
47	BL	201	PEE	C31-C30-O3-C3
47	N3	201	PEE	C31-C30-O3-C3
47	N2	402	PEE	C12-C13-C14-C15
45	N1	401	CDL	O1-C1-CB2-OB2
47	BL	201	PEE	O5-C30-O3-C3
47	N3	201	PEE	O5-C30-O3-C3
47	BL	201	PEE	C30-C31-C32-C33
47	N3	201	PEE	C10-C11-C12-C13
45	A8	301	CDL	OB6-CB4-CB6-OB8
47	A9	402	PEE	C17-C18-C19-C20
47	N5	701	PEE	C37-C38-C39-C40
45	B4	202	CDL	CA7-C31-C32-C33
47	N1	403	PEE	C10-C11-C12-C13
53	N3	203	6F6	C11-C12-N-C15
47	N2	402	PEE	O5-C30-O3-C3
45	AL	201	CDL	C1-CA2-OA2-PA1
47	BL	201	PEE	C10-C11-C12-C13
47	N1	403	PEE	C33-C34-C35-C36
45	A8	301	CDL	O1-C1-CB2-OB2
47	N1	404	PEE	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
53	N3	203	6F6	C21-C22-C23-C24
47	N5	702	PEE	C30-C31-C32-C33
47	N5	705	PEE	O4-C10-O2-C2
45	A8	301	CDL	CA2-C1-CB2-OB2
50	B5	201	PLX	C2-C1-N1-C1C
50	B5	201	PLX	C2-C1-N1-C1A
47	A9	402	PEE	C31-C30-O3-C3
47	N5	705	PEE	C33-C34-C35-C36
50	S7	302	PLX	O8-C24-C25-C26
48	AC	201	ZMP	C14-C15-N2-C16
50	B5	201	PLX	C2-C1-N1-C1B
53	N3	203	6F6	C11-C12-N-C13
47	A9	402	PEE	C12-C13-C14-C15
47	N1	403	PEE	C12-C13-C14-C15
47	N5	702	PEE	C10-C11-C12-C13
47	N5	702	PEE	C11-C12-C13-C14
50	B5	201	PLX	O9-C24-C25-C26
50	N4	502	PLX	O9-C24-C25-C26
45	N4	504	CDL	C78-C79-C80-C81
50	AM	201	PLX	C14-C15-C16-C17
50	N4	502	PLX	C29-C30-C31-C32
53	N3	203	6F6	C2C-C2D-C2E-C2F
50	S7	302	PLX	C32-C33-C34-C35
52	S2	501	XEW	N4-C4-N-C3
45	N4	504	CDL	C32-C33-C34-C35
50	AM	201	PLX	C34-C35-C36-C37
45	N5	703	CDL	CB5-C51-C52-C53
51	CA	101	3PE	C23-C24-C25-C26
47	N5	702	PEE	C14-C15-C16-C17
47	A9	402	PEE	C30-C31-C32-C33
47	N5	701	PEE	C32-C33-C34-C35
47	N5	701	PEE	C14-C15-C16-C17
48	AB	201	ZMP	C6-C7-C8-C9
47	A9	402	PEE	O5-C30-O3-C3
45	N1	401	CDL	C76-C77-C78-C79
50	N4	502	PLX	C7-C8-C9-C10
50	N4	503	PLX	C9-C10-C11-C12
48	AC	201	ZMP	C1-C22-C23-C24
47	BL	201	PEE	C33-C34-C35-C36
47	N1	404	PEE	C11-C12-C13-C14
47	N3	201	PEE	C22-C23-C24-C25
47	N3	201	PEE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
48	AB	201	ZMP	C2-C3-C4-C5
47	N1	403	PEE	C11-C12-C13-C14
47	N2	402	PEE	C19-C20-C21-C22
48	AC	201	ZMP	C6-C7-C8-C9
50	AM	201	PLX	C9-C10-C11-C12
47	N5	705	PEE	C21-C22-C23-C24
47	N2	402	PEE	C40-C41-C42-C43
47	N5	702	PEE	C12-C13-C14-C15
50	N4	503	PLX	C31-C32-C33-C34
50	S7	302	PLX	C11-C10-C9-C8
45	N5	704	CDL	C72-C73-C74-C75
50	N4	502	PLX	C11-C10-C9-C8
45	AL	201	CDL	C52-C53-C54-C55
47	N1	404	PEE	C33-C34-C35-C36
47	N4	501	PEE	C23-C24-C25-C26
50	N4	503	PLX	C33-C34-C35-C36
45	4L	201	CDL	C39-C40-C41-C42
47	N4	501	PEE	C11-C12-C13-C14
47	N5	701	PEE	C31-C32-C33-C34
50	N3	202	PLX	C34-C35-C36-C37
47	N5	702	PEE	C18-C19-C20-C21
50	N3	202	PLX	C26-C27-C28-C29
50	N4	503	PLX	C34-C35-C36-C37
47	N4	501	PEE	C11-C10-O2-C2
47	N5	701	PEE	C11-C10-O2-C2
50	N4	503	PLX	C12-C13-C14-C15
47	N4	501	PEE	C39-C40-C41-C42
50	S7	302	PLX	C7-C8-C9-C10
47	BL	201	PEE	C11-C12-C13-C14
53	N3	203	6F6	C11-C12-N-C14
53	N6	401	6F6	C11-C12-N-C15
47	N2	402	PEE	C10-C11-C12-C13
47	N2	402	PEE	C16-C17-C18-C19
51	CB	202	3PE	C21-C22-C23-C24
45	AL	201	CDL	C33-C34-C35-C36
47	N4	501	PEE	O4-C10-O2-C2
47	N5	701	PEE	O4-C10-O2-C2
45	4L	201	CDL	CA5-C11-C12-C13
51	S7	303	3PE	C21-C22-C23-C24
50	N4	502	PLX	C28-C29-C30-C31
45	B4	202	CDL	C37-C38-C39-C40
45	N5	703	CDL	C59-C60-C61-C62

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Mol	Chain	Res	Type	Atoms
47	N1	404	PEE	C22-C23-C24-C25
50	N4	502	PLX	C30-C31-C32-C33
47	BL	201	PEE	C16-C17-C18-C19
47	N2	402	PEE	C18-C19-C20-C21
45	B5	202	CDL	CB2-C1-CA2-OA2
45	N5	703	CDL	CA2-C1-CB2-OB2
45	N4	504	CDL	C61-C62-C63-C64
48	AB	201	ZMP	C3-C4-C5-C6
50	CB	201	PLX	C31-C32-C33-C34
48	AB	201	ZMP	O3-C16-C17-O4
47	A9	402	PEE	C35-C36-C37-C38
47	N3	201	PEE	C43-C44-C45-C46
47	N5	701	PEE	C11-C12-C13-C14
45	B5	202	CDL	OB5-CB3-CB4-CB6
47	N4	501	PEE	O3P-C1-C2-C3
45	B4	201	CDL	C79-C80-C81-C82
47	N4	501	PEE	C10-C11-C12-C13
50	N4	502	PLX	C33-C34-C35-C36
50	N3	202	PLX	O8-C24-C25-C26
48	AC	201	ZMP	C22-C23-C24-C25
47	N5	701	PEE	C33-C34-C35-C36
45	B4	201	CDL	C32-C33-C34-C35
45	N1	401	CDL	C32-C33-C34-C35
45	N4	504	CDL	CB3-CB4-CB6-OB8
47	N1	403	PEE	C1-C2-C3-O3
47	N3	201	PEE	C1-C2-C3-O3
47	N4	501	PEE	C1-C2-C3-O3
47	N5	701	PEE	C1-C2-C3-O3
50	N4	503	PLX	C3-C4-C5-O8
47	N3	201	PEE	C13-C14-C15-C16
48	AC	201	ZMP	C2-C3-C4-C5
47	N1	404	PEE	C35-C36-C37-C38
47	N4	501	PEE	C35-C36-C37-C38
47	N5	701	PEE	C21-C22-C23-C24
48	AC	201	ZMP	C3-C4-C5-C6
50	N3	202	PLX	C35-C36-C37-C38
48	AC	201	ZMP	C1-C2-C3-C4
51	CB	202	3PE	C39-C3A-C3B-C3C
45	N4	504	CDL	C38-C39-C40-C41
47	N2	402	PEE	C33-C34-C35-C36
53	N6	401	6F6	C11-C12-N-C14
45	N4	504	CDL	C63-C64-C65-C66

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Mol	Chain	Res	Type	Atoms
47	N4	501	PEE	C24-C25-C26-C27
53	N6	401	6F6	C31-C32-C33-C34
47	N2	402	PEE	C14-C15-C16-C17
47	N3	201	PEE	C31-C32-C33-C34
47	N5	701	PEE	C12-C13-C14-C15
47	BL	201	PEE	C3-C2-O2-C10
47	N1	404	PEE	C3-C2-O2-C10
50	N4	502	PLX	C14-C15-C16-C17
47	A9	402	PEE	C15-C16-C17-C18
47	N2	402	PEE	C35-C36-C37-C38
47	N3	201	PEE	C35-C36-C37-C38
47	N3	201	PEE	C39-C40-C41-C42
47	N5	701	PEE	C35-C36-C37-C38
47	N5	705	PEE	C19-C20-C21-C22
47	N5	705	PEE	C35-C36-C37-C38
45	N1	401	CDL	C75-C76-C77-C78
45	N4	504	CDL	C33-C34-C35-C36
45	B4	201	CDL	C73-C74-C75-C76
47	N2	402	PEE	C11-C12-C13-C14
47	N3	201	PEE	C32-C33-C34-C35
47	N4	501	PEE	C22-C23-C24-C25
45	4L	201	CDL	C15-C16-C17-C18
45	N5	704	CDL	C22-C23-C24-C25
50	CB	201	PLX	C7-C8-C9-C10
50	N4	503	PLX	C13-C14-C15-C16
47	A9	402	PEE	O2-C2-C3-O3
47	N3	201	PEE	O2-C2-C3-O3
50	AM	201	PLX	O6-C4-C5-O8
50	S7	302	PLX	C27-C28-C29-C30
47	N1	404	PEE	C14-C15-C16-C17
47	N1	404	PEE	C30-C31-C32-C33
48	AB	201	ZMP	O3-C16-C17-C18
45	B5	202	CDL	C17-C18-C19-C20
50	N4	502	PLX	O7-C6-C7-C8
50	AM	201	PLX	C28-C29-C30-C31
47	N2	402	PEE	C38-C39-C40-C41
45	N5	704	CDL	CA4-CA3-OA5-PA1
47	A9	402	PEE	C33-C34-C35-C36
47	N4	501	PEE	C12-C13-C14-C15
47	N1	403	PEE	C31-C32-C33-C34
47	N1	404	PEE	O3P-C1-C2-C3
51	S7	303	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
51	CA	101	3PE	C35-C36-C37-C38
48	AB	201	ZMP	N2-C16-C17-C18
47	N1	404	PEE	C21-C22-C23-C24
47	N1	403	PEE	C13-C14-C15-C16
47	N3	201	PEE	C44-C45-C46-C47
47	N5	701	PEE	C22-C23-C24-C25
45	A8	301	CDL	CB3-CB4-CB6-OB8
47	BL	201	PEE	C1-C2-C3-O3
47	N5	705	PEE	C1-C2-C3-O3
51	S7	303	3PE	C1-C2-C3-O31
47	N5	705	PEE	C14-C15-C16-C17
45	N4	504	CDL	OA5-CA3-CA4-OA6
47	BL	201	PEE	O3P-C1-C2-O2
47	N5	702	PEE	O3P-C1-C2-O2
45	N5	703	CDL	C1-CB2-OB2-PB2
45	N5	703	CDL	CA7-C31-C32-C33
45	B4	202	CDL	C13-C14-C15-C16
47	N1	404	PEE	C42-C43-C44-C45
47	BL	201	PEE	O2-C2-C3-O3
47	N4	501	PEE	O2-C2-C3-O3
47	N5	705	PEE	O2-C2-C3-O3
51	S7	303	3PE	O21-C2-C3-O31
46	A9	401	NDP	C2D-C1D-N1N-C6N
45	A8	301	CDL	C17-C18-C19-C20
48	AB	201	ZMP	C22-C23-C24-C25
48	AC	201	ZMP	O1-C10-C9-C8
47	N5	705	PEE	C10-C11-C12-C13
45	A8	301	CDL	C11-C12-C13-C14
47	N2	402	PEE	C20-C21-C22-C23
45	N5	704	CDL	C59-C60-C61-C62
53	N6	401	6F6	C11-C12-N-C13
47	BL	201	PEE	C18-C19-C20-C21
45	N5	704	CDL	C17-C18-C19-C20
45	N4	504	CDL	C21-C22-C23-C24
45	A8	301	CDL	OB5-CB3-CB4-CB6
45	AL	201	CDL	OB5-CB3-CB4-CB6
45	B4	202	CDL	OB5-CB3-CB4-CB6
45	N2	401	CDL	OA5-CA3-CA4-CA6
47	A9	402	PEE	O3P-C1-C2-C3
45	B4	202	CDL	CB4-CB3-OB5-PB2
47	N5	705	PEE	C11-C12-C13-C14
50	S7	302	PLX	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
46	A9	401	NDP	C2D-C1D-N1N-C2N
45	4L	201	CDL	C79-C80-C81-C82
50	N4	503	PLX	C10-C11-C12-C13
50	B5	201	PLX	C14-C15-C16-C17
50	N4	503	PLX	C15-C16-C17-C18
47	N5	702	PEE	C32-C33-C34-C35
47	A9	402	PEE	C11-C12-C13-C14
48	AC	201	ZMP	C22-C1-C2-C3
45	N4	504	CDL	CB5-C51-C52-C53
47	N5	702	PEE	C33-C34-C35-C36
50	S7	302	PLX	C25-C26-C27-C28
47	A9	402	PEE	O3P-C1-C2-O2
47	N1	403	PEE	O3P-C1-C2-O2
47	N4	501	PEE	O3P-C1-C2-O2
50	N3	202	PLX	O4-C3-C4-O6
50	CB	201	PLX	C3-C4-C5-O8
47	BL	201	PEE	C14-C15-C16-C17
47	N1	403	PEE	C5-C4-O4P-P
53	N6	401	6F6	C12-C11-O13-P
50	B5	201	PLX	C11-C12-C13-C14
53	N3	203	6F6	O21-C2-C3-O31
45	N4	504	CDL	C81-C82-C83-C84
47	N1	404	PEE	C41-C42-C43-C44
45	N4	504	CDL	C12-C13-C14-C15
45	B4	202	CDL	C1-CA2-OA2-PA1
45	N2	401	CDL	C1-CA2-OA2-PA1
53	N6	401	6F6	C2-C1-O11-P
45	B4	201	CDL	C78-C79-C80-C81
50	AM	201	PLX	N1-C1-C2-O1
50	N3	202	PLX	N1-C1-C2-O1
50	N4	503	PLX	N1-C1-C2-O1
45	B5	202	CDL	O1-C1-CA2-OA2
47	N1	404	PEE	C13-C14-C15-C16
45	N2	401	CDL	C53-C54-C55-C56
47	N1	404	PEE	C34-C35-C36-C37
53	N3	203	6F6	C36-C37-C38-C39
48	AC	201	ZMP	O3-C16-C17-O4
50	N4	502	PLX	C25-C24-O8-C5
50	S7	302	PLX	C25-C24-O8-C5
45	N4	504	CDL	OA5-CA3-CA4-CA6
45	N5	703	CDL	OB5-CB3-CB4-CB6
47	N1	403	PEE	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
47	N5	701	PEE	O3P-C1-C2-C3
50	S7	302	PLX	C14-C15-C16-C17
48	AB	201	ZMP	C19-C18-C21-O5
48	AC	201	ZMP	C19-C18-C21-O5
52	N1	402	XEW	N4-C4-N-C3
50	CB	201	PLX	C11-C10-C9-C8
47	N5	705	PEE	C12-C13-C14-C15
47	N1	404	PEE	C17-C18-C19-C20
47	N4	501	PEE	C33-C34-C35-C36
45	A8	301	CDL	OB5-CB3-CB4-OB6
45	AL	201	CDL	OB5-CB3-CB4-OB6
45	B4	202	CDL	OB5-CB3-CB4-OB6
45	B5	202	CDL	OB5-CB3-CB4-OB6
45	N2	401	CDL	OA5-CA3-CA4-OA6
47	N5	701	PEE	O3P-C1-C2-O2
51	S7	303	3PE	O11-C1-C2-O21
50	N4	503	PLX	C7-C8-C9-C10
52	S2	501	XEW	N-C4-N1-C5
52	S2	501	XEW	N2-C5-N1-C4
47	A9	402	PEE	C18-C19-C20-C21
45	N4	504	CDL	OB6-CB4-CB6-OB8
47	N1	403	PEE	O2-C2-C3-O3
47	N1	404	PEE	O2-C2-C3-O3
50	CB	201	PLX	O6-C4-C5-O8
50	B5	201	PLX	C3-C4-C5-O8
50	N4	502	PLX	C3-C4-C5-O8
53	N3	203	6F6	C1-C2-C3-O31
45	N4	504	CDL	C77-C78-C79-C80
45	N1	401	CDL	C13-C14-C15-C16
47	N5	701	PEE	C30-C31-C32-C33
47	N2	402	PEE	C21-C22-C23-C24
45	4L	201	CDL	CA2-OA2-PA1-OA3
45	A7	201	CDL	CA2-OA2-PA1-OA3
45	A7	201	CDL	CB2-OB2-PB2-OB5
45	AL	201	CDL	CA2-OA2-PA1-OA4
45	B4	201	CDL	CB2-OB2-PB2-OB4
45	B4	202	CDL	CA2-OA2-PA1-OA4
45	B4	202	CDL	CA3-OA5-PA1-OA2
45	B4	202	CDL	CA3-OA5-PA1-OA3
45	B4	202	CDL	CB2-OB2-PB2-OB3
45	B4	202	CDL	CB3-OB5-PB2-OB3
45	B5	202	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
45	B5	202	CDL	CA3-OA5-PA1-OA2
45	B5	202	CDL	CA3-OA5-PA1-OA3
45	B5	202	CDL	CA3-OA5-PA1-OA4
45	N1	401	CDL	CA2-OA2-PA1-OA3
45	N1	401	CDL	CA3-OA5-PA1-OA3
45	N1	401	CDL	CB3-OB5-PB2-OB3
45	N2	401	CDL	CA2-OA2-PA1-OA3
45	N2	401	CDL	CA2-OA2-PA1-OA5
45	N4	504	CDL	CA2-OA2-PA1-OA4
45	N4	504	CDL	CB2-OB2-PB2-OB3
45	N4	504	CDL	CB3-OB5-PB2-OB3
45	N5	703	CDL	CB2-OB2-PB2-OB3
47	BL	201	PEE	C1-O3P-P-O2P
47	BL	201	PEE	C4-O4P-P-O1P
47	N1	403	PEE	C4-O4P-P-O3P
47	N1	403	PEE	C4-O4P-P-O2P
47	N1	403	PEE	C4-O4P-P-O1P
47	N1	404	PEE	O4P-C4-C5-N
47	N2	402	PEE	C4-O4P-P-O3P
47	N3	201	PEE	C1-O3P-P-O2P
47	N3	201	PEE	C4-O4P-P-O1P
47	N4	501	PEE	C1-O3P-P-O1P
50	B5	201	PLX	C3-C4-O6-C6
50	B5	201	PLX	C5-C4-O6-C6
50	B5	201	PLX	C3-O4-P1-O1
50	B5	201	PLX	C3-O4-P1-O2
50	B5	201	PLX	C2-O1-P1-O2
50	CB	201	PLX	C3-C4-O6-C6
50	CB	201	PLX	C5-C4-O6-C6
50	N3	202	PLX	C3-O4-P1-O1
50	N4	502	PLX	C3-O4-P1-O1
50	N4	502	PLX	C3-O4-P1-O2
51	CA	101	3PE	C11-O13-P-O14
51	CB	202	3PE	C1-O11-P-O14
51	N5	706	3PE	C11-O13-P-O12
51	S7	303	3PE	C1-O11-P-O14
53	N3	203	6F6	C11-O13-P-O12
53	N3	203	6F6	C1-O11-P-O13
53	N6	401	6F6	C11-O13-P-O12
50	AM	201	PLX	C35-C36-C37-C38
45	B4	202	CDL	C72-C71-CB7-OB8
45	A8	301	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
45	B5	202	CDL	CB4-CB3-OB5-PB2
50	N4	503	PLX	C4-C3-O4-P1
45	N5	703	CDL	C60-C61-C62-C63
46	A9	401	NDP	O4D-C1D-N1N-C2N
45	A8	301	CDL	C38-C39-C40-C41
45	B5	202	CDL	C21-C22-C23-C24
45	N5	704	CDL	O1-C1-CA2-OA2
50	S7	302	PLX	C26-C27-C28-C29
51	S7	303	3PE	C1-C2-O21-C21
45	B4	202	CDL	C72-C71-CB7-OB9
47	BL	201	PEE	O3P-C1-C2-C3
50	N3	202	PLX	O4-C3-C4-C5
47	BL	201	PEE	C36-C37-C38-C39
45	B4	201	CDL	OB5-CB3-CB4-OB6
45	N5	703	CDL	OB5-CB3-CB4-OB6
47	N2	402	PEE	C42-C43-C44-C45
46	A9	401	NDP	O4D-C1D-N1N-C6N
45	B5	202	CDL	OB6-CB4-CB6-OB8
45	N5	704	CDL	OB6-CB4-CB6-OB8
47	N5	701	PEE	O2-C2-C3-O3
50	N4	503	PLX	O6-C4-C5-O8
47	N1	404	PEE	C15-C16-C17-C18
45	AL	201	CDL	C52-C51-CB5-OB6
47	A9	402	PEE	C1-C2-C3-O3
47	N1	404	PEE	C1-C2-C3-O3
50	AM	201	PLX	C3-C4-C5-O8
45	AL	201	CDL	C36-C37-C38-C39
50	AM	201	PLX	O6-C6-C7-C8
45	AL	201	CDL	CB4-CB3-OB5-PB2
45	N1	401	CDL	C73-C74-C75-C76
45	N4	504	CDL	OB5-CB3-CB4-OB6
50	CB	201	PLX	O4-C3-C4-O6
47	N5	702	PEE	C36-C37-C38-C39
45	N5	703	CDL	C61-C62-C63-C64
50	CB	201	PLX	C15-C16-C17-C18
53	N6	401	6F6	C36-C37-C38-C39
47	N1	404	PEE	C36-C37-C38-C39
47	N5	705	PEE	C18-C19-C20-C21
50	AM	201	PLX	C33-C34-C35-C36
51	CA	101	3PE	C2B-C2C-C2D-C2E
45	A7	201	CDL	C1-CA2-OA2-PA1
49	AK	401	ADP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
45	B4	202	CDL	CA3-CA4-CA6-OA8
45	N5	704	CDL	CB3-CB4-CB6-OB8
48	AB	201	ZMP	N2-C16-C17-O4
48	AC	201	ZMP	N2-C16-C17-O4
50	N3	202	PLX	C3-C4-C5-O8
45	N5	704	CDL	CB5-C51-C52-C53
45	4L	201	CDL	CA6-CA4-OA6-CA5
45	N5	704	CDL	C12-C11-CA5-OA6
50	B5	201	PLX	C25-C26-C27-C28
45	N5	704	CDL	C11-C12-C13-C14
45	B4	202	CDL	CA4-CA3-OA5-PA1
50	AM	201	PLX	C4-C3-O4-P1
47	N5	702	PEE	C13-C14-C15-C16
47	N5	702	PEE	C34-C35-C36-C37
51	CA	101	3PE	C2A-C2B-C2C-C2D
45	AL	201	CDL	OB6-CB4-CB6-OB8
50	B5	201	PLX	O6-C4-C5-O8
47	BL	201	PEE	C42-C43-C44-C45
50	CB	201	PLX	C27-C28-C29-C30
47	A9	402	PEE	C31-C32-C33-C34
50	CB	201	PLX	O8-C24-C25-C26
46	A9	401	NDP	PN-O3-PA-O1A
48	AB	201	ZMP	C1-C22-C23-C24
50	AM	201	PLX	C29-C30-C31-C32
51	CA	101	3PE	C29-C2A-C2B-C2C
50	N4	503	PLX	C16-C17-C18-C19
47	N2	402	PEE	C2-C1-O3P-P
50	B5	201	PLX	C18-C19-C20-C21
52	S2	501	XEW	N3-C5-N1-C4
50	AM	201	PLX	O7-C6-C7-C8
50	AM	201	PLX	O4-C3-C4-O6
45	B5	202	CDL	C80-C81-C82-C83
50	CB	201	PLX	C11-C12-C13-C14
53	N3	203	6F6	C28-C29-C2A-C2B
45	N5	704	CDL	C53-C54-C55-C56
45	N4	504	CDL	C72-C71-CB7-OB8
47	N5	701	PEE	C17-C18-C19-C20
45	B5	202	CDL	CA2-C1-CB2-OB2
50	AM	201	PLX	C31-C32-C33-C34
45	A8	301	CDL	OA5-CA3-CA4-CA6
51	N5	706	3PE	O21-C2-C3-O31
47	N5	705	PEE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
47	N5	705	PEE	C42-C43-C44-C45
45	N1	401	CDL	C11-C12-C13-C14
50	N4	502	PLX	C13-C14-C15-C16
45	N5	704	CDL	C15-C16-C17-C18
53	N6	401	6F6	C34-C35-C36-C37
50	AM	201	PLX	C36-C37-C38-C39
45	AL	201	CDL	CA6-CA4-OA6-CA5
45	B4	202	CDL	CB3-CB4-OB6-CB5
45	B5	202	CDL	CB3-CB4-OB6-CB5
45	N2	401	CDL	CA6-CA4-OA6-CA5
47	BL	201	PEE	C21-C22-C23-C24
47	N2	402	PEE	C32-C33-C34-C35
47	BL	201	PEE	C32-C33-C34-C35
45	A8	301	CDL	OA5-CA3-CA4-OA6
45	A8	301	CDL	C22-C23-C24-C25
45	4L	201	CDL	C23-C24-C25-C26
51	N5	706	3PE	C1-C2-C3-O31
45	B5	202	CDL	C33-C34-C35-C36
48	AB	201	ZMP	C4-C5-C6-C7
50	B5	201	PLX	C1-C2-O1-P1
47	N4	501	PEE	C32-C33-C34-C35
50	CB	201	PLX	C32-C33-C34-C35
45	A7	201	CDL	C72-C71-CB7-OB8
47	N5	705	PEE	O3-C30-C31-C32
47	N1	403	PEE	C14-C15-C16-C17
47	BL	201	PEE	C20-C21-C22-C23
45	N5	704	CDL	OB5-CB3-CB4-CB6
47	N5	702	PEE	O3P-C1-C2-C3
50	AM	201	PLX	O4-C3-C4-C5
51	S7	303	3PE	C3B-C3C-C3D-C3E
45	A8	301	CDL	C33-C34-C35-C36
47	N5	705	PEE	C40-C41-C42-C43
45	B4	201	CDL	C12-C11-CA5-OA6
51	N5	706	3PE	C23-C24-C25-C26
45	B4	201	CDL	C37-C38-C39-C40
45	B5	202	CDL	O1-C1-CB2-OB2
47	N1	403	PEE	O2-C10-C11-C12
51	N5	706	3PE	O21-C21-C22-C23
47	N3	201	PEE	O2-C10-C11-C12
45	AL	201	CDL	C59-C60-C61-C62
45	N5	704	CDL	C42-C43-C44-C45
45	AL	201	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
51	CA	101	3PE	C36-C37-C38-C39
50	N4	502	PLX	C36-C37-C38-C39
45	N5	703	CDL	C12-C11-CA5-OA6
51	S7	303	3PE	O31-C31-C32-C33
45	B4	201	CDL	C80-C81-C82-C83
46	A9	401	NDP	O4B-C4B-C5B-O5B
45	B4	202	CDL	CA5-C11-C12-C13
47	A9	402	PEE	C34-C35-C36-C37
45	A8	301	CDL	C32-C31-CA7-OA8
47	N5	701	PEE	O2-C10-C11-C12
48	AB	201	ZMP	C20-C18-C21-O5
45	B4	201	CDL	C72-C73-C74-C75
45	AL	201	CDL	CA3-CA4-OA6-CA5
45	B4	202	CDL	CB6-CB4-OB6-CB5
47	N5	702	PEE	C1-C2-O2-C10
47	N5	702	PEE	C3-C2-O2-C10
50	CB	201	PLX	C2-C1-N1-C1A
45	4L	201	CDL	C17-C18-C19-C20
45	B5	202	CDL	C59-C60-C61-C62
48	AB	201	ZMP	C1-C2-C3-C4
45	B5	202	CDL	C1-CA2-OA2-PA1
47	A9	402	PEE	C2-C1-O3P-P
50	N4	503	PLX	C24-C25-C26-C27
51	CA	101	3PE	C24-C25-C26-C27
45	B4	201	CDL	C12-C11-CA5-OA7
51	CB	202	3PE	O31-C31-C32-C33
45	AL	201	CDL	C12-C11-CA5-OA7
50	CB	201	PLX	C2-C1-N1-C1C
45	A8	301	CDL	C32-C31-CA7-OA9
45	A7	201	CDL	C72-C71-CB7-OB9
51	N5	706	3PE	O22-C21-C22-C23
45	B4	201	CDL	C32-C31-CA7-OA8
50	AM	201	PLX	O9-C24-O8-C5
47	N5	701	PEE	O4-C10-C11-C12
52	N1	402	XEW	C2-C3-N-C4
45	4L	201	CDL	C11-C12-C13-C14
47	N1	403	PEE	O3-C30-C31-C32
47	N5	705	PEE	O5-C30-C31-C32
45	A8	301	CDL	C54-C55-C56-C57
50	N4	502	PLX	C4-C5-O8-C24
45	B4	202	CDL	OA6-CA4-CA6-OA8
51	S7	303	3PE	O32-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
47	N4	501	PEE	O2-C10-C11-C12
45	AL	201	CDL	C32-C33-C34-C35
50	N3	202	PLX	C32-C33-C34-C35
53	N3	203	6F6	C4-C5-C6-C7
47	N3	201	PEE	O4-C10-C11-C12
45	4L	201	CDL	C12-C11-CA5-OA6
45	N5	703	CDL	C12-C11-CA5-OA7
47	N1	403	PEE	O4-C10-C11-C12
45	B5	202	CDL	C81-C82-C83-C84
45	B5	202	CDL	C12-C11-CA5-OA6
51	S7	303	3PE	C34-C35-C36-C37
47	N1	403	PEE	O5-C30-C31-C32
47	N5	701	PEE	C16-C17-C18-C19
50	AM	201	PLX	C11-C10-C9-C8

There are no ring outliers.

38 monomers are involved in 123 short contacts:

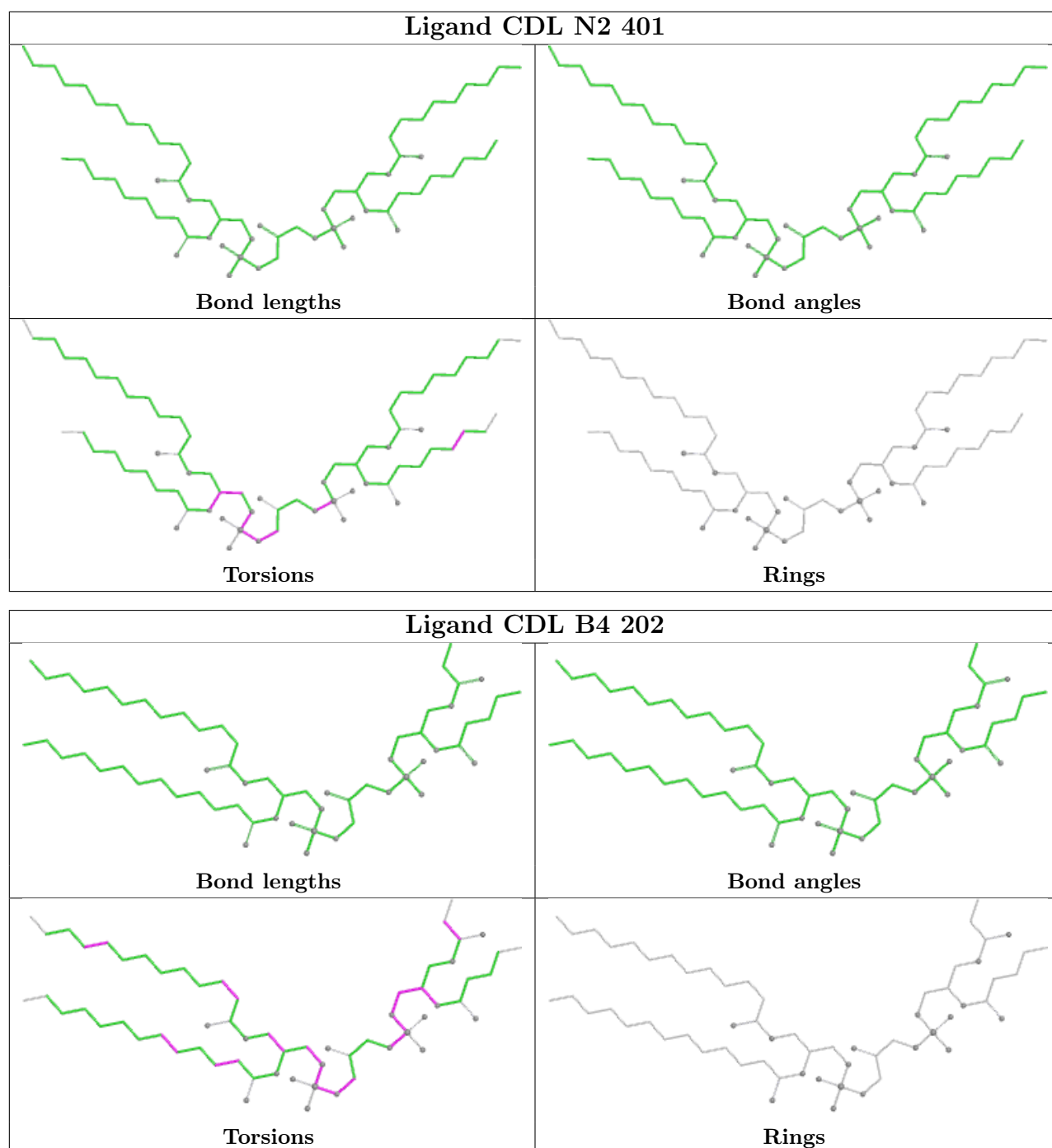
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	B4	202	CDL	2	0
51	B8	201	3PE	1	0
45	AL	201	CDL	6	0
45	4L	201	CDL	10	0
47	N5	705	PEE	1	0
48	AC	201	ZMP	2	0
53	N6	401	6F6	1	0
45	B4	201	CDL	1	0
45	A8	301	CDL	6	0
46	A9	401	NDP	1	0
47	N1	403	PEE	1	0
47	N5	702	PEE	1	0
54	S1	802	SF4	1	0
47	N1	404	PEE	7	0
48	AB	201	ZMP	2	0
45	B5	202	CDL	4	0
51	CA	101	3PE	2	0
51	N5	706	3PE	2	0
51	S7	303	3PE	3	0
47	N2	402	PEE	7	0
47	N3	201	PEE	2	0
45	N1	401	CDL	5	0
47	A9	402	PEE	4	0

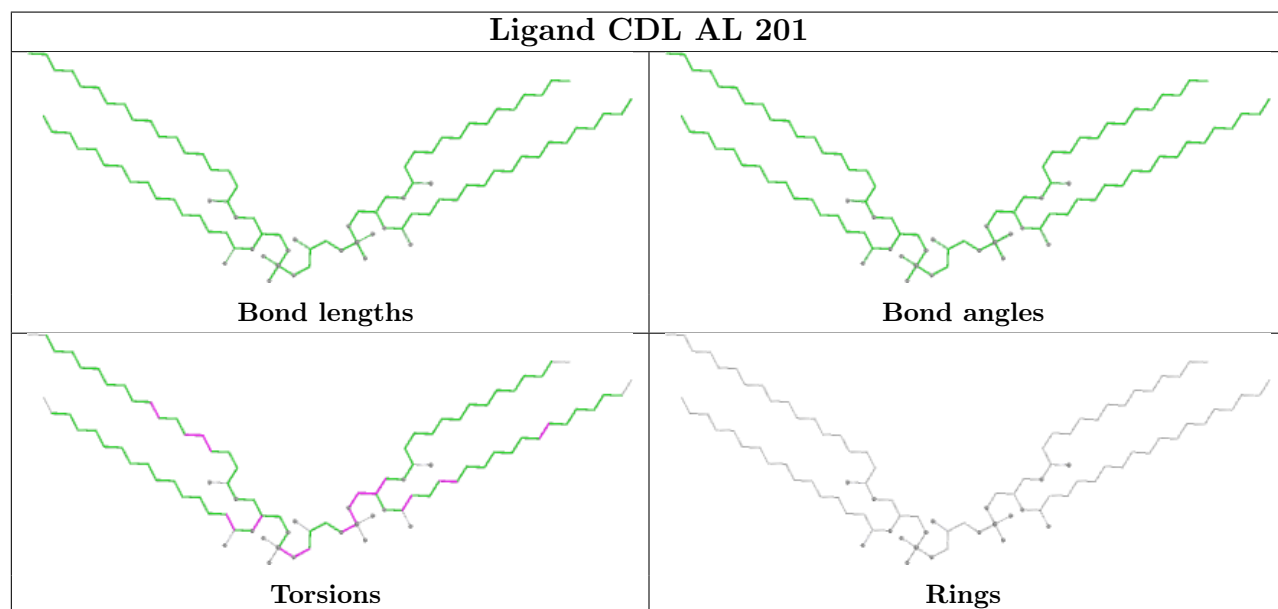
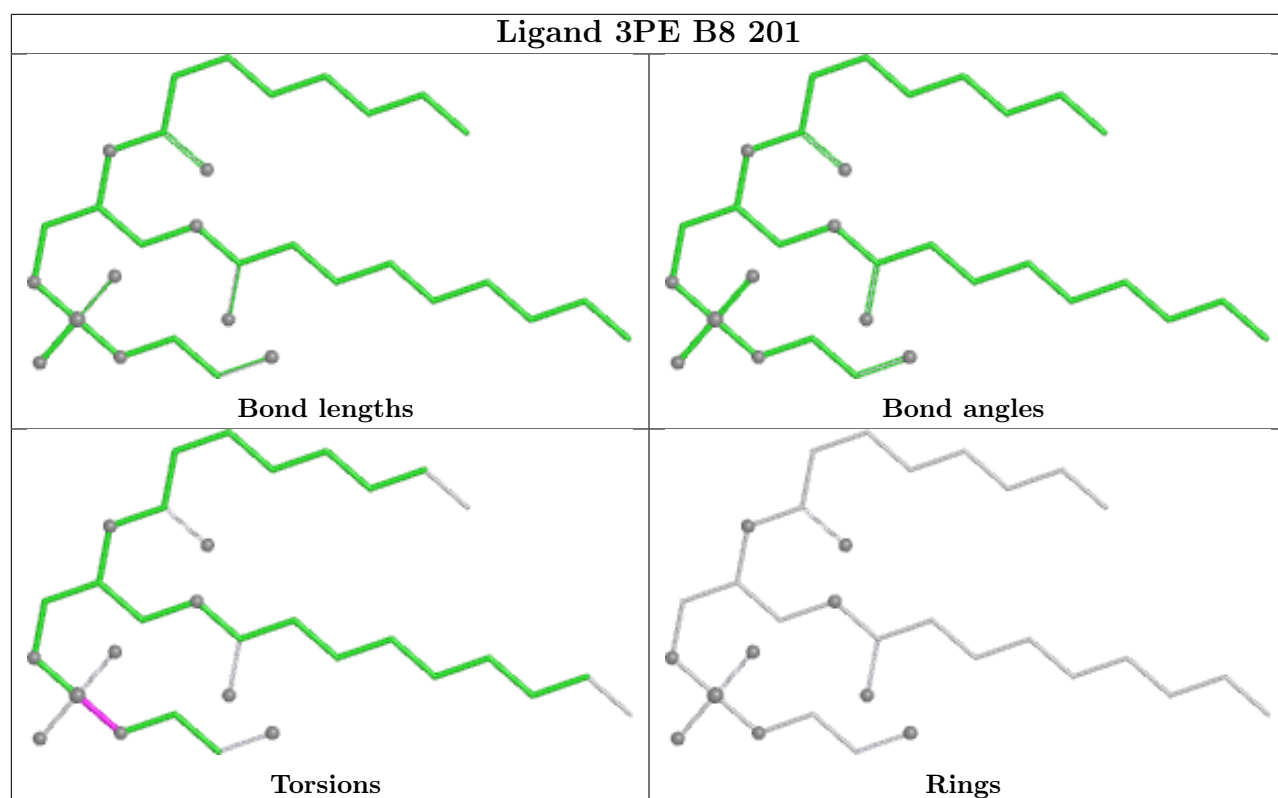
Continued on next page...

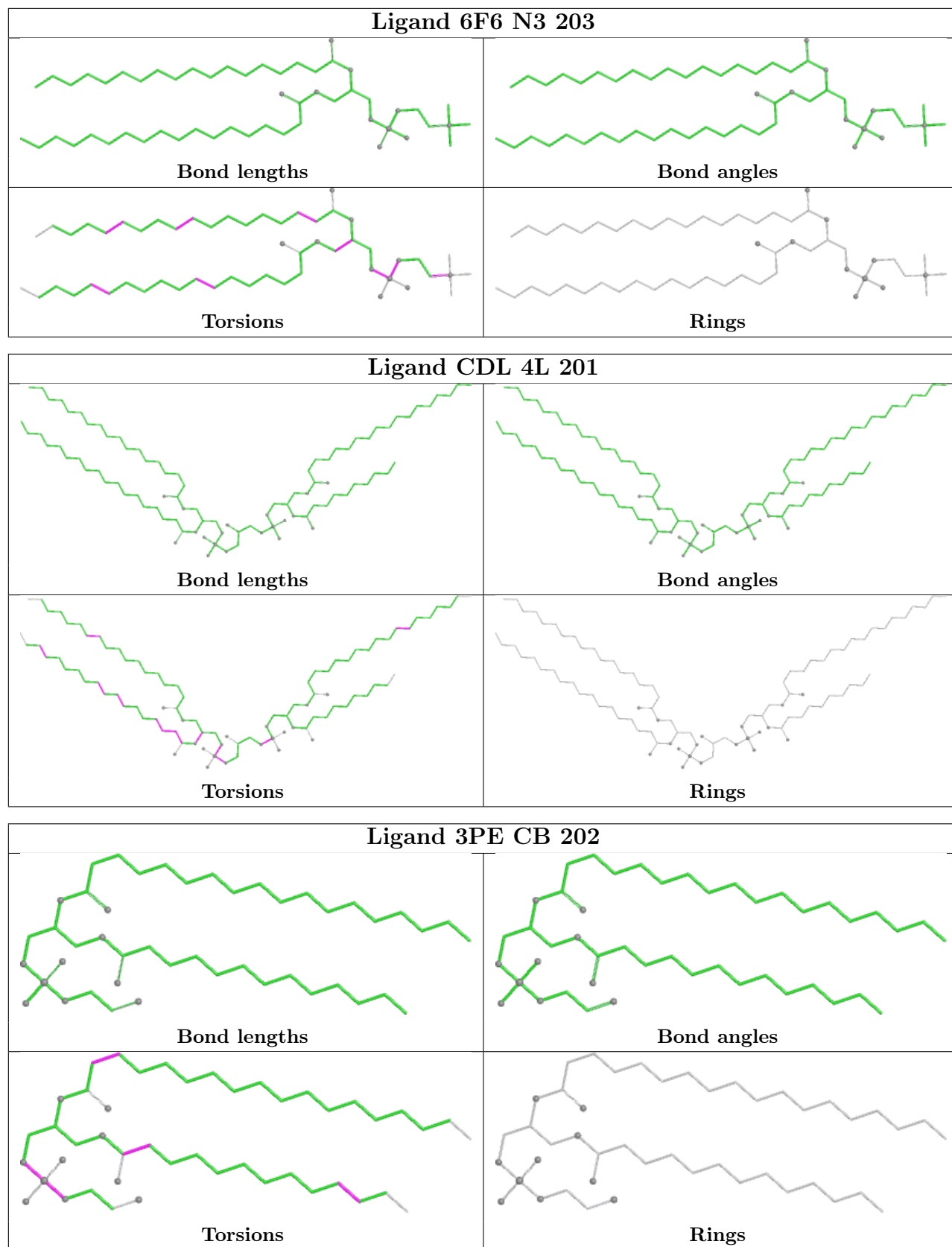
Continued from previous page...

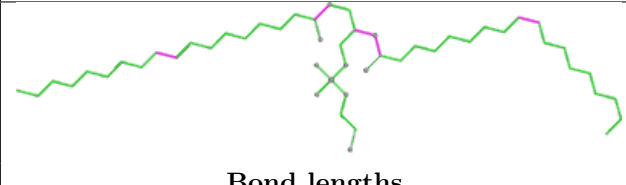
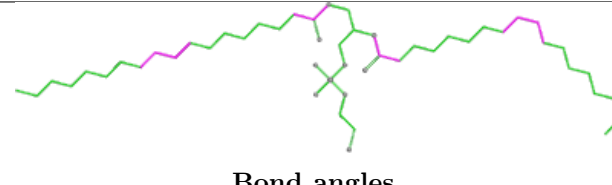
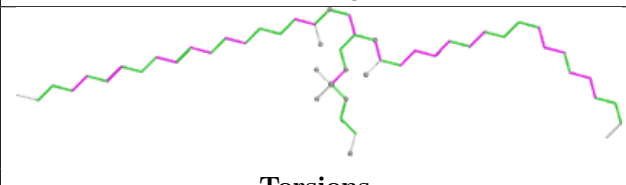
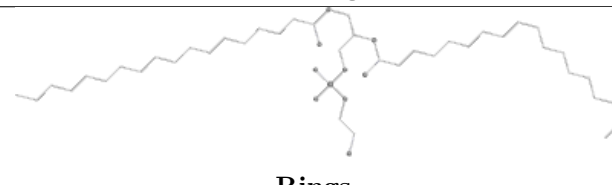
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	BL	201	PEE	2	0
47	N4	501	PEE	6	0
50	CB	201	PLX	4	0
45	N4	504	CDL	8	0
50	N4	503	PLX	2	0
58	V1	502	FMN	1	0
45	N5	703	CDL	11	0
54	S8	302	SF4	1	0
50	N4	502	PLX	2	0
50	AM	201	PLX	6	0
47	N5	701	PEE	2	0
45	N5	704	CDL	5	0
50	S7	302	PLX	4	0
50	N3	202	PLX	1	0
49	AK	401	ADP	4	0

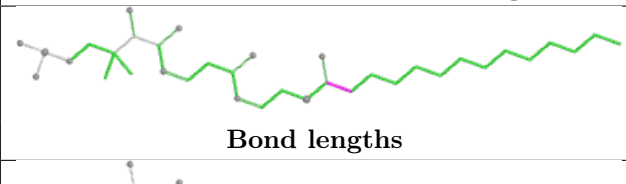
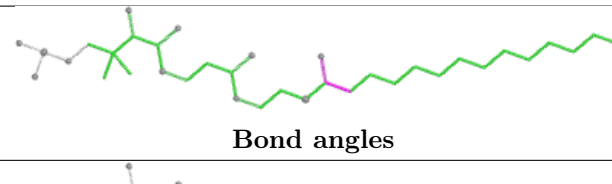
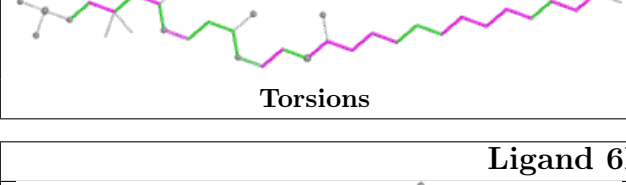
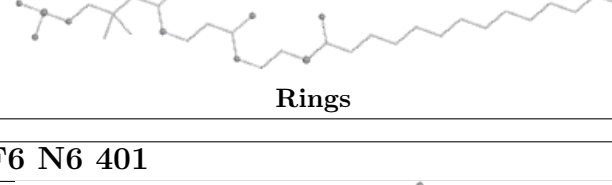
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

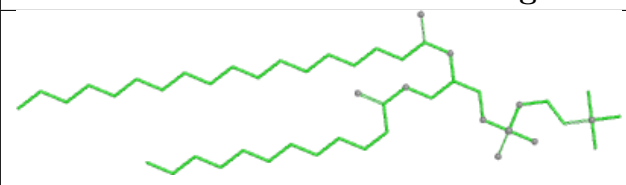
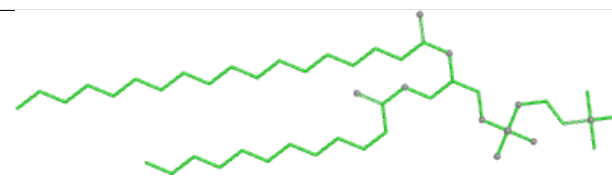
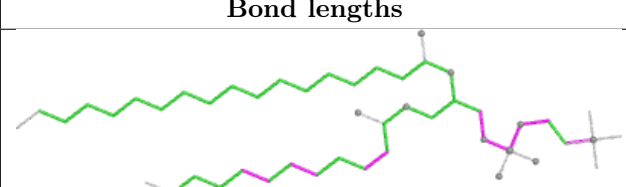
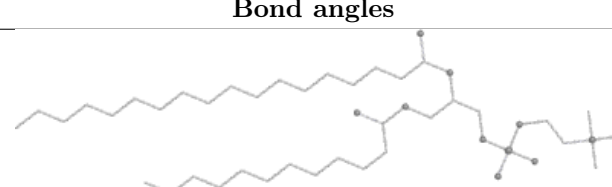


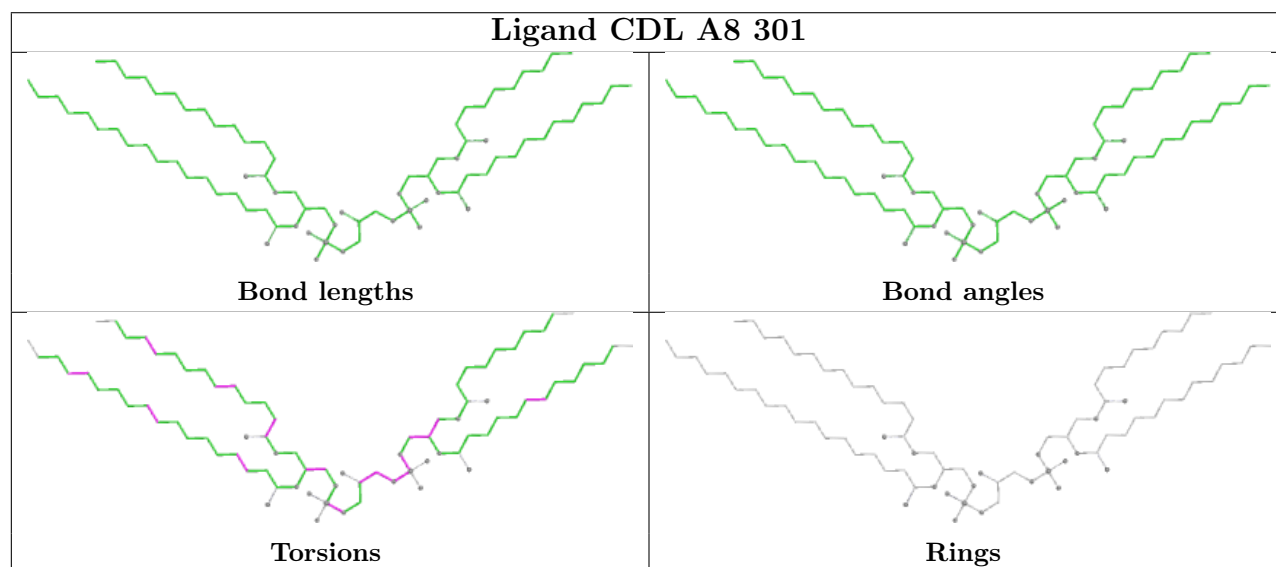
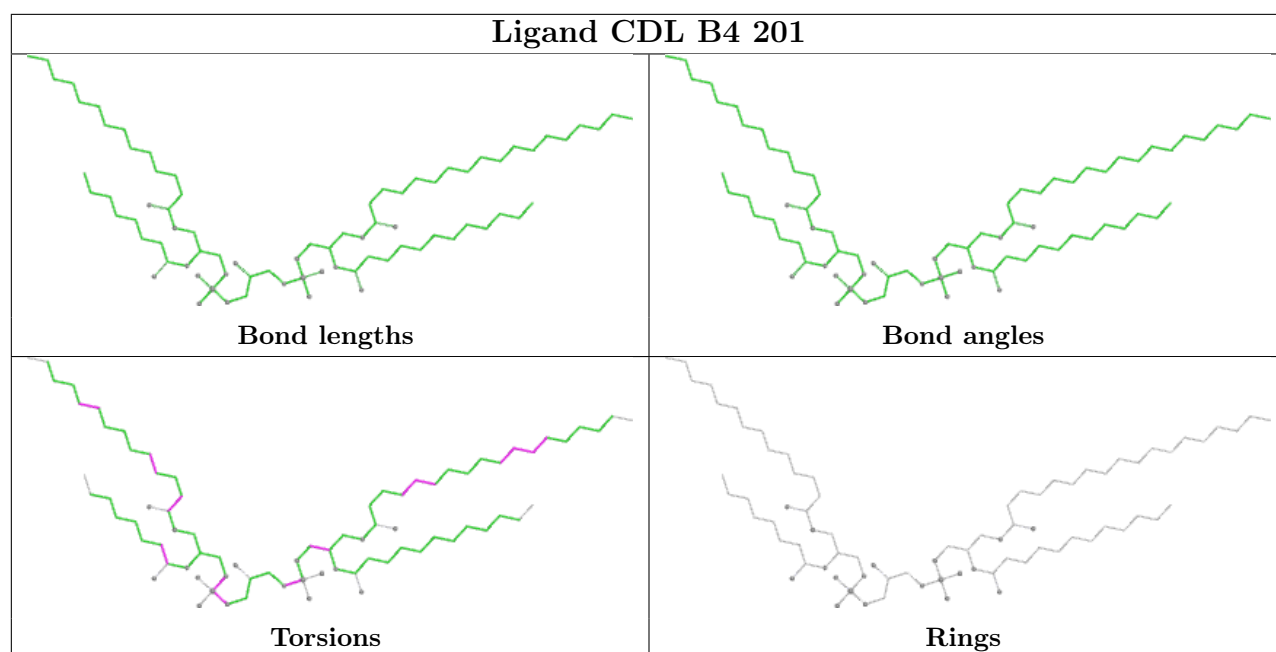




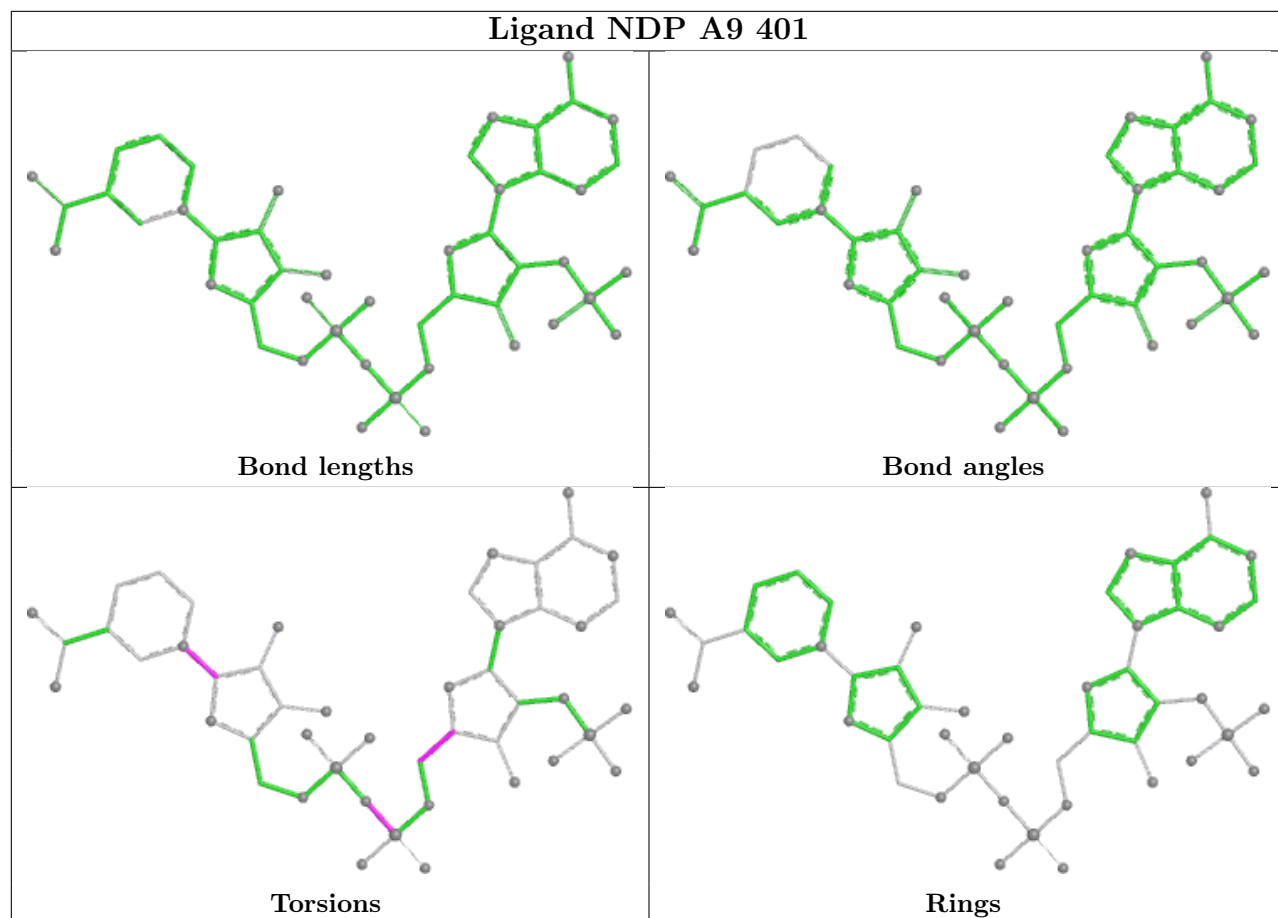
Ligand PEE N5 705	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ZMP AC 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

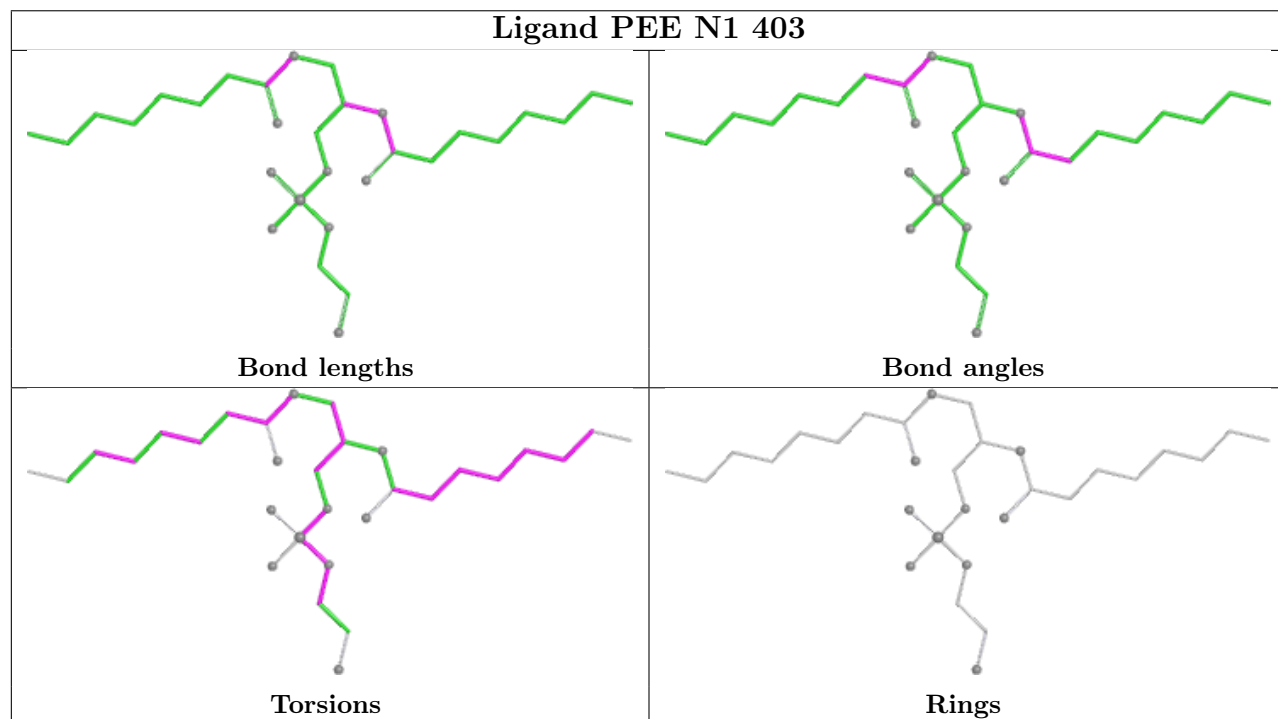
Ligand 6F6 N6 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

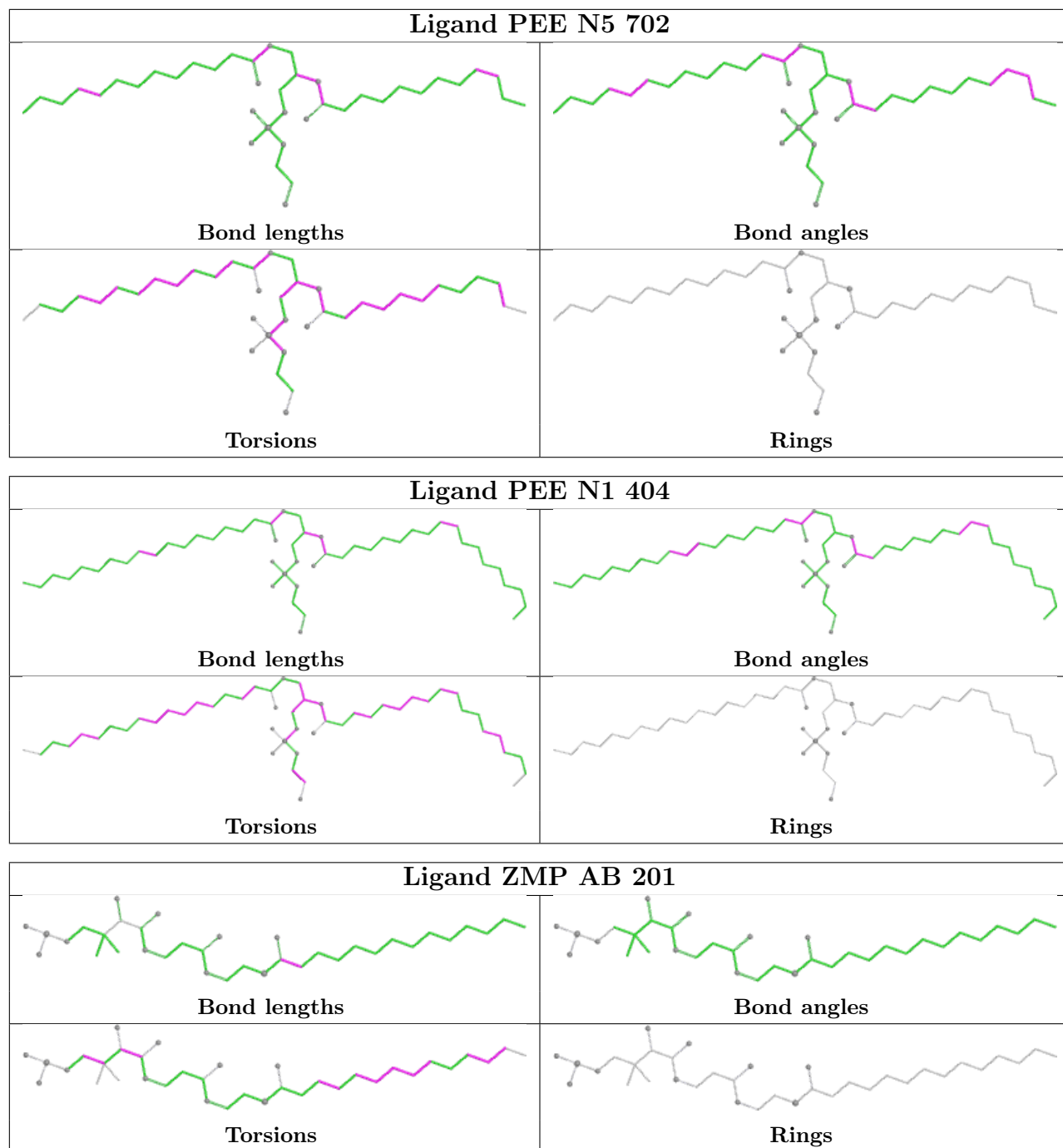


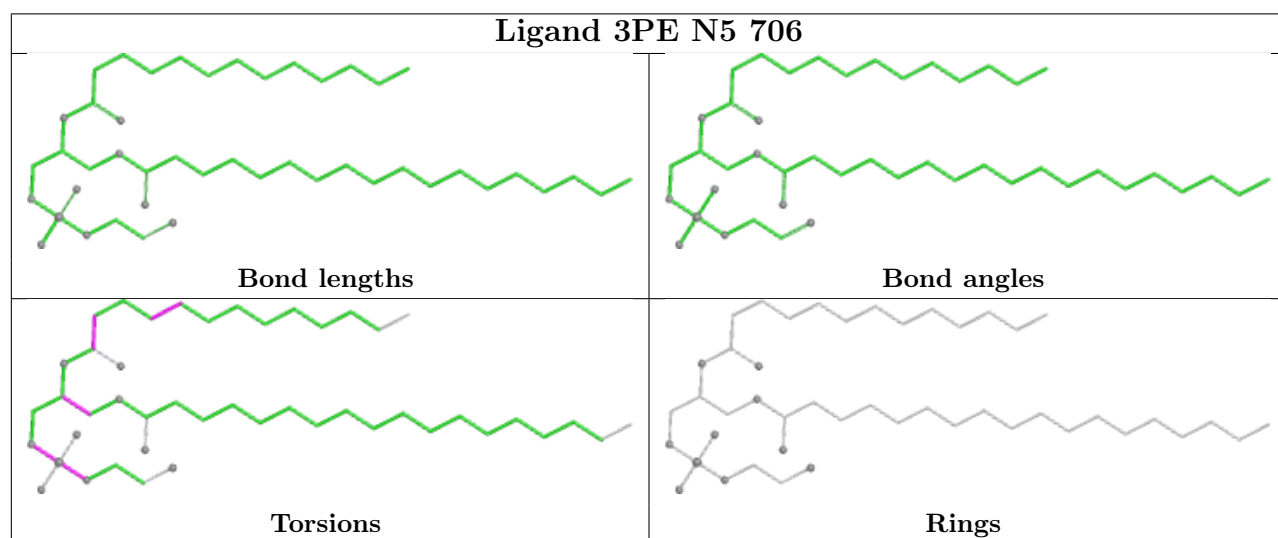
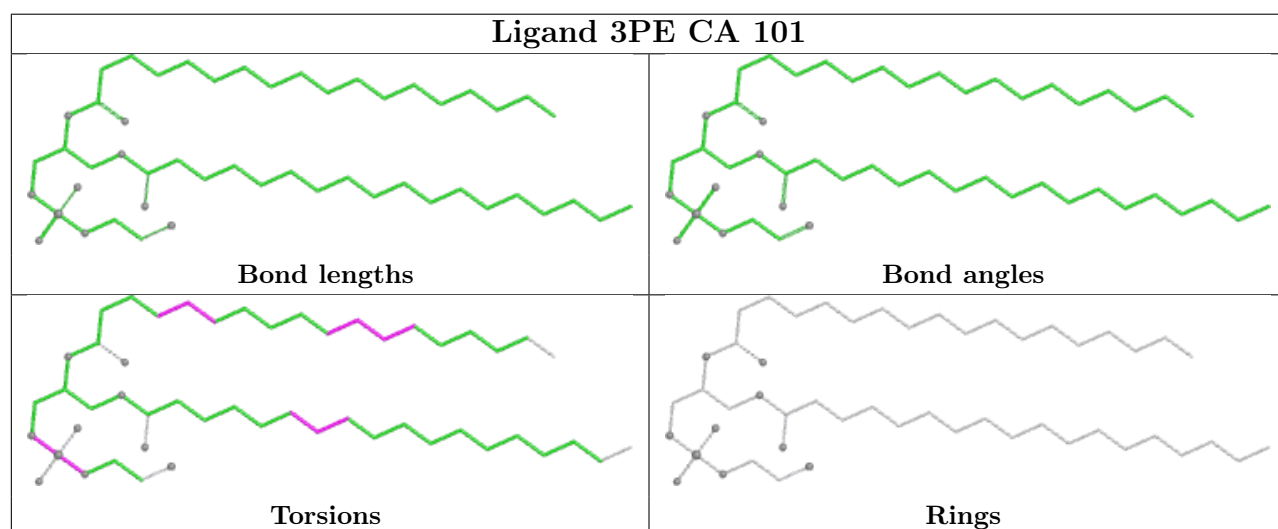
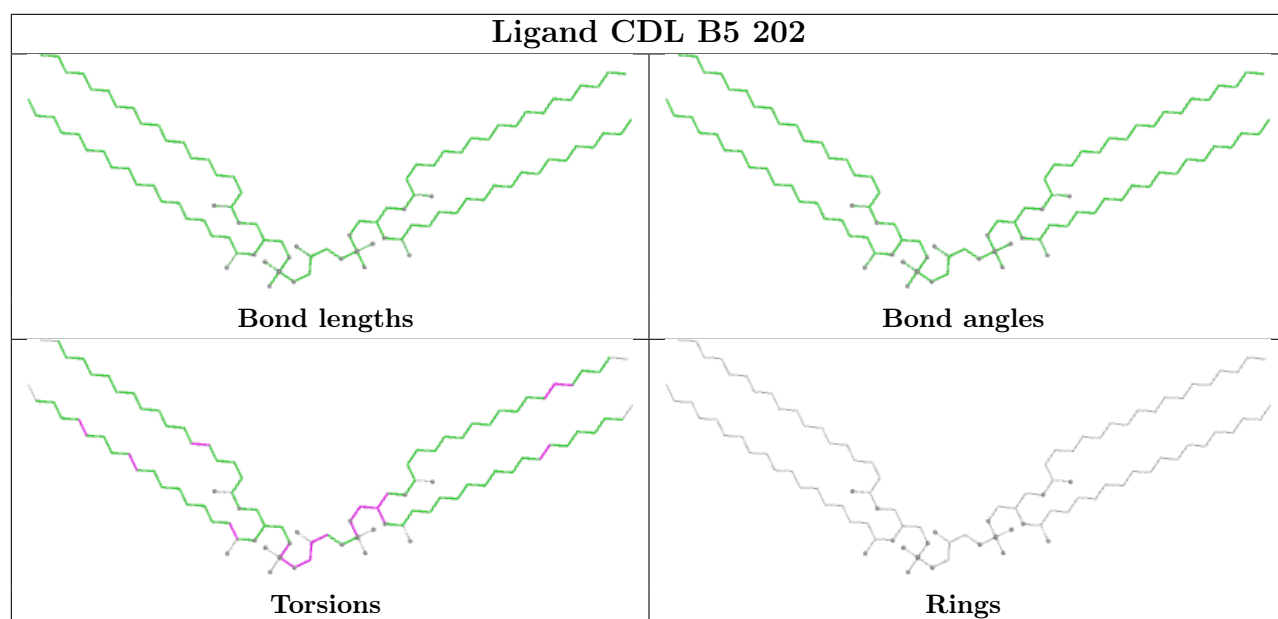
Ligand NDP A9 401

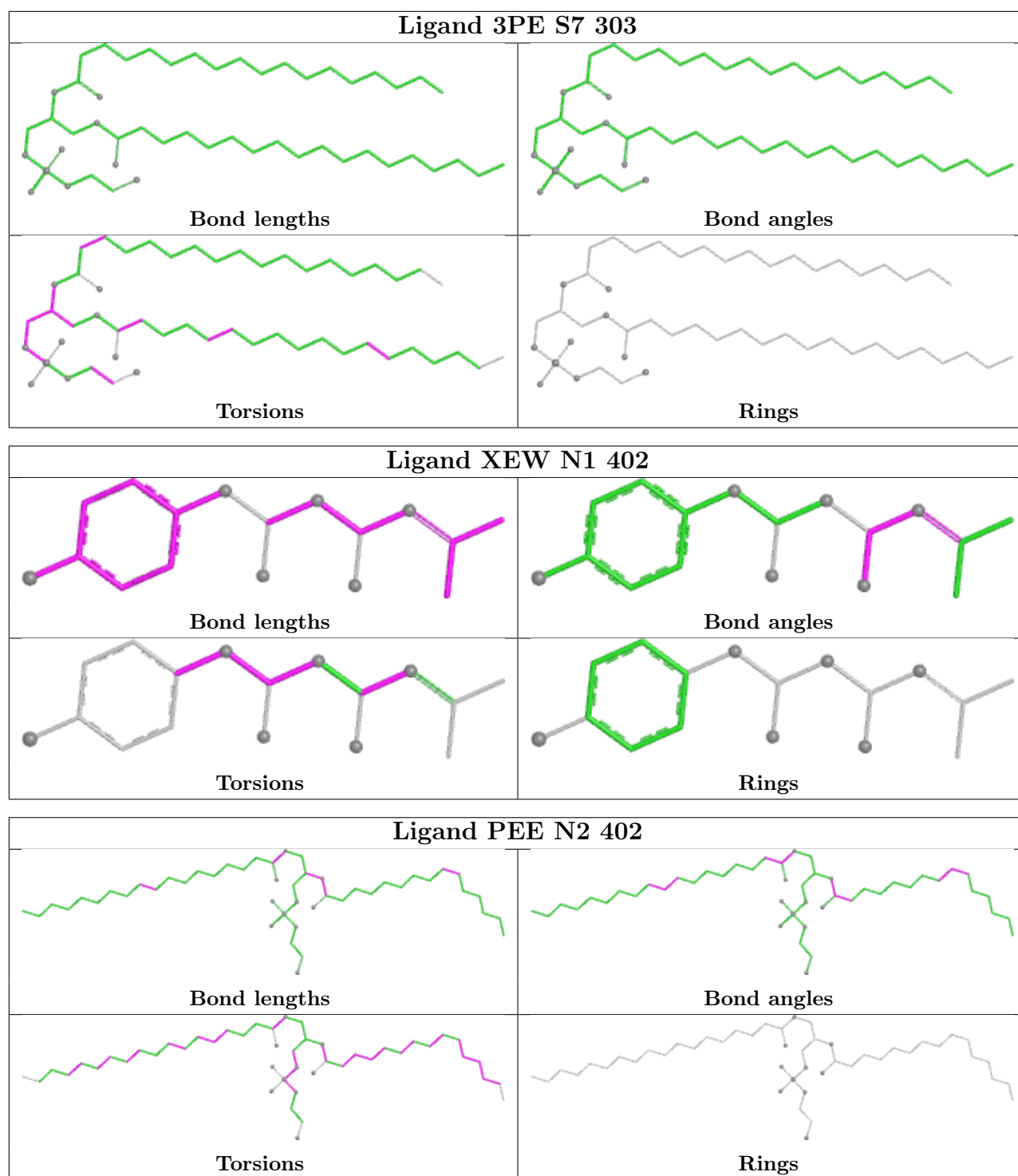


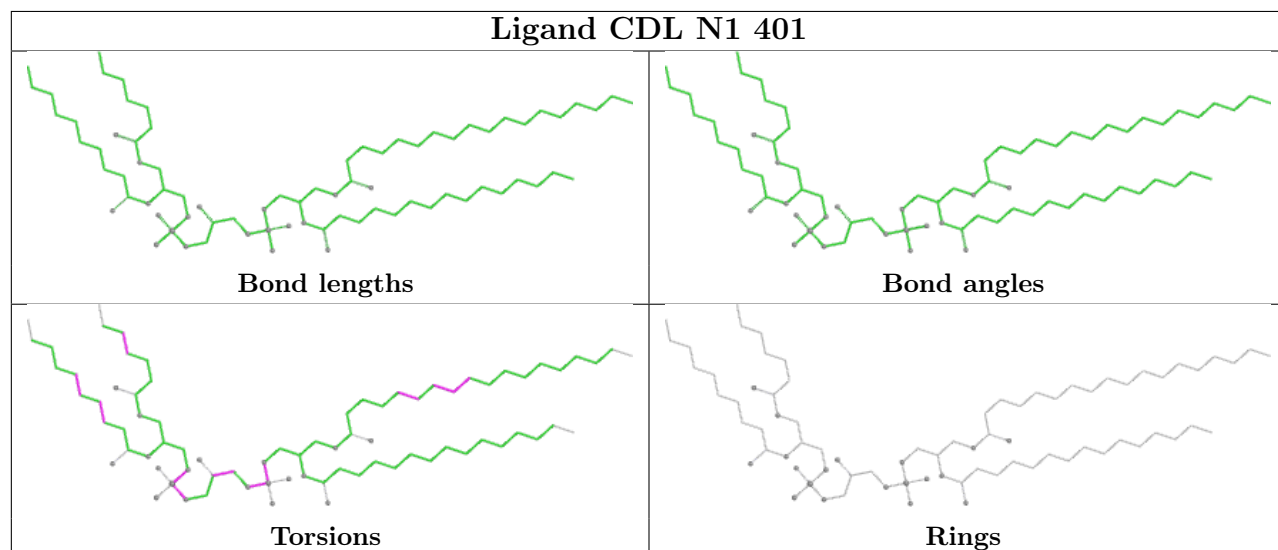
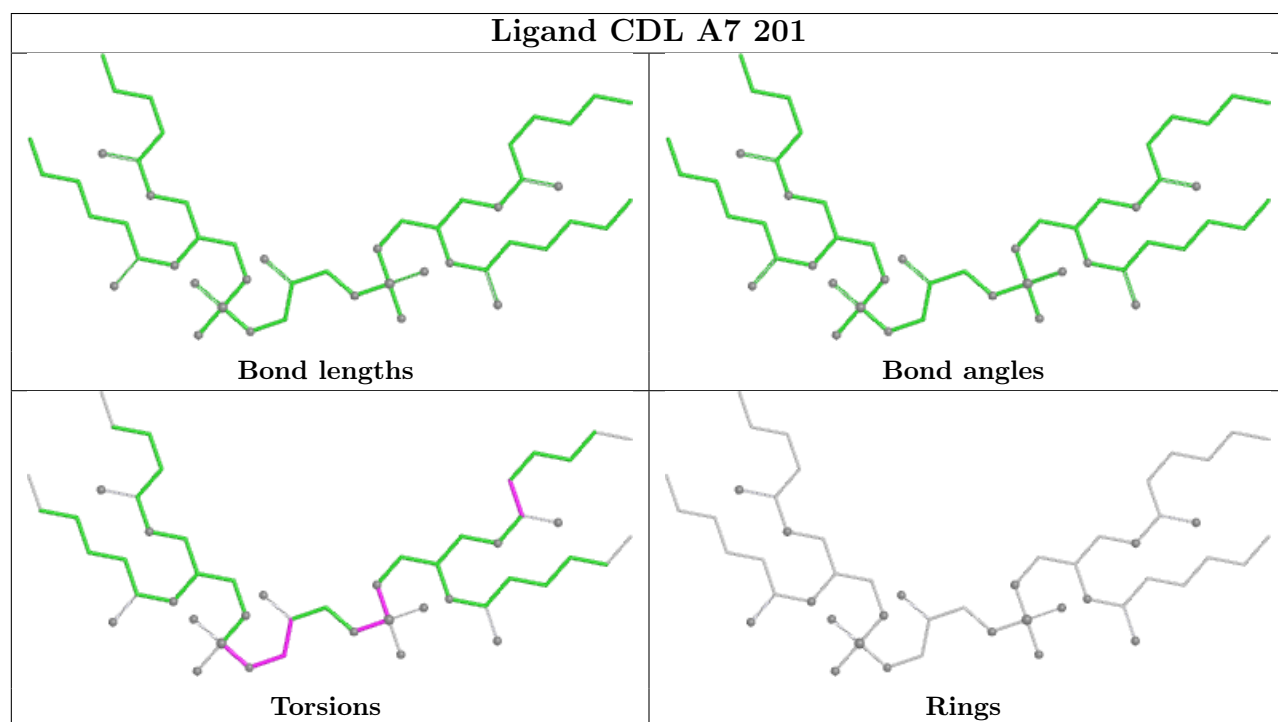
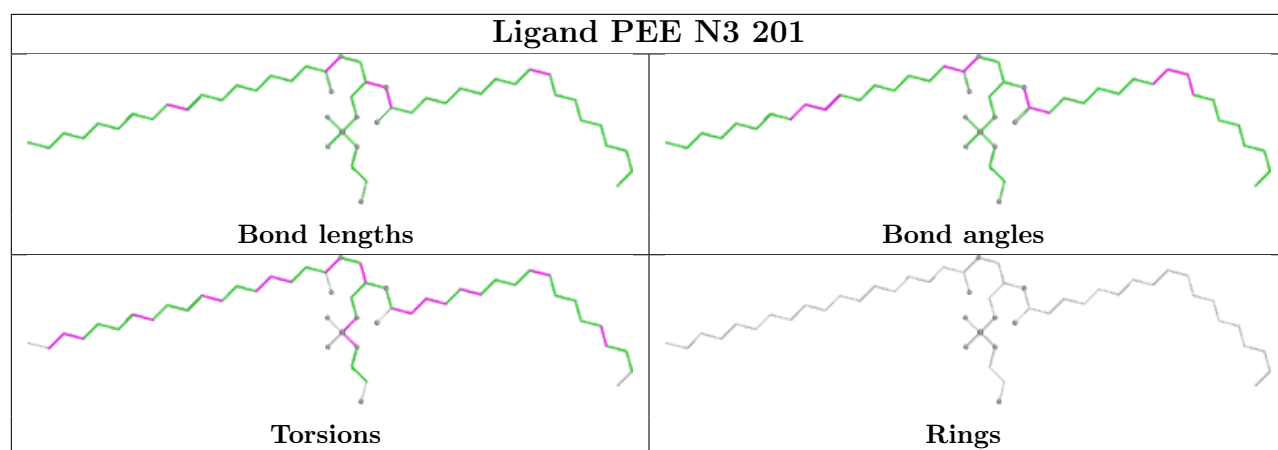
Ligand PEE N1 403

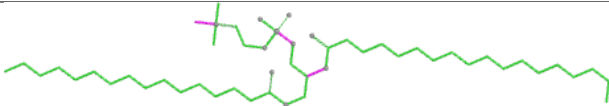
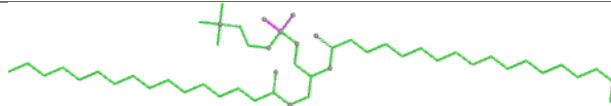
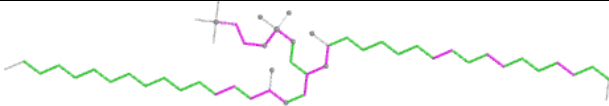
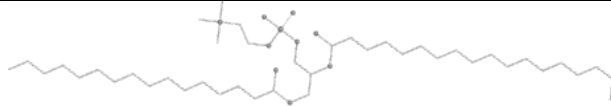


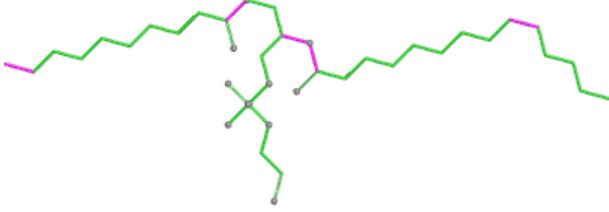
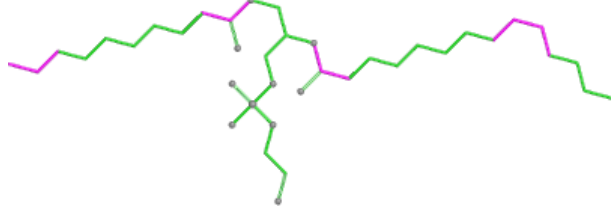
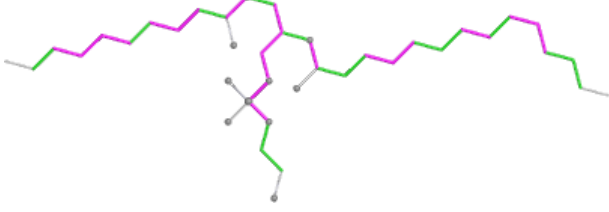
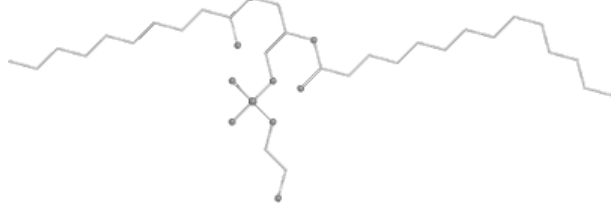


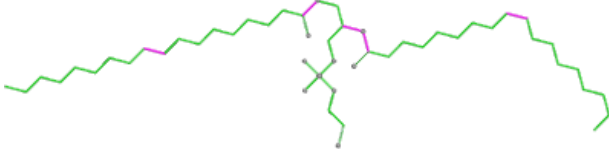
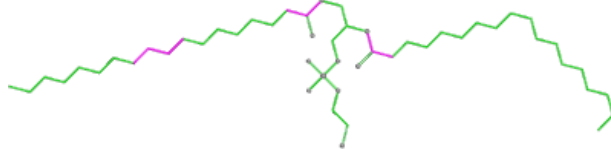
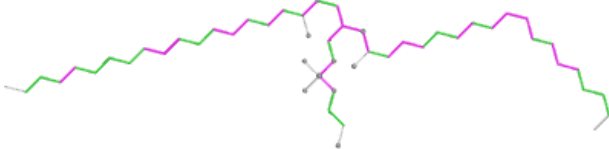
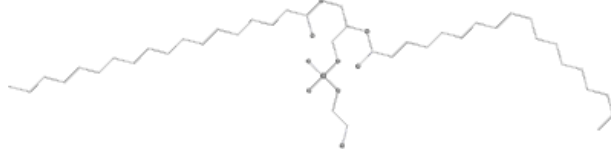


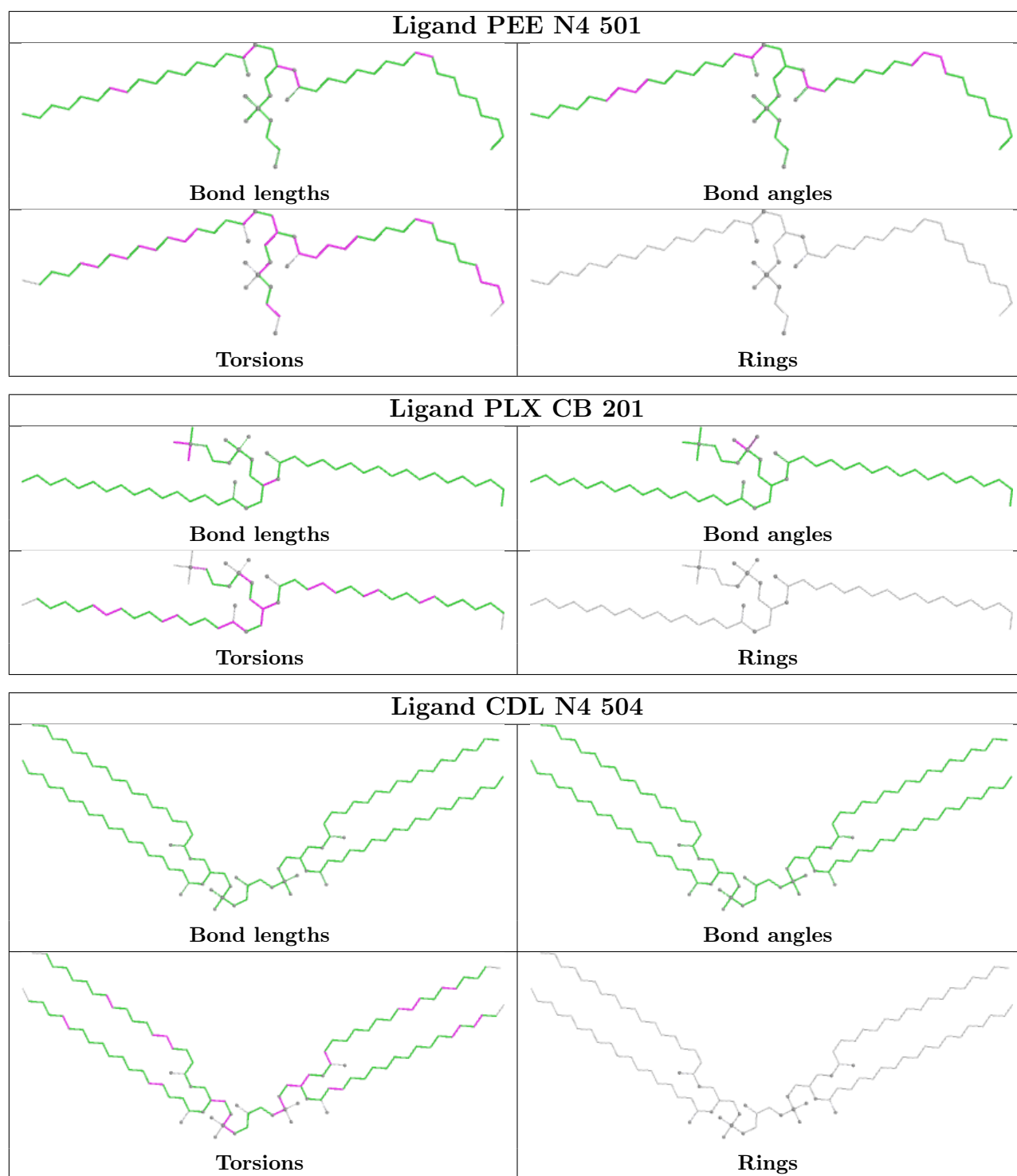


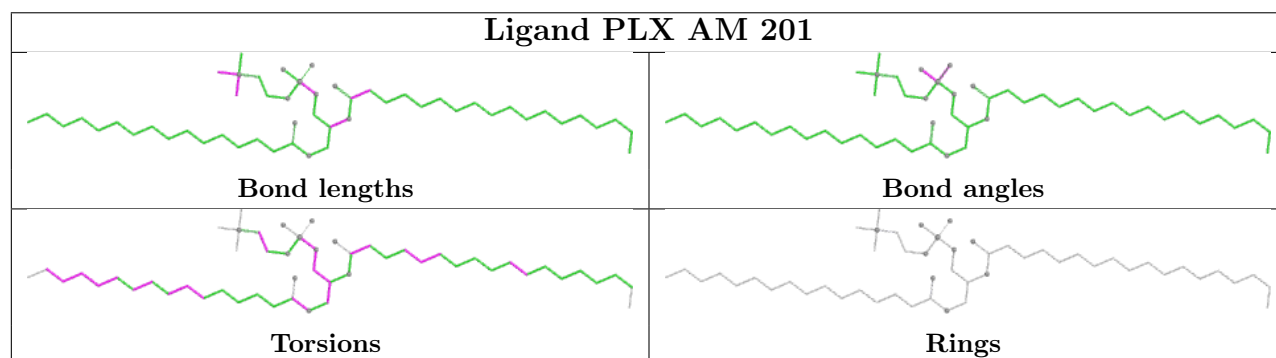
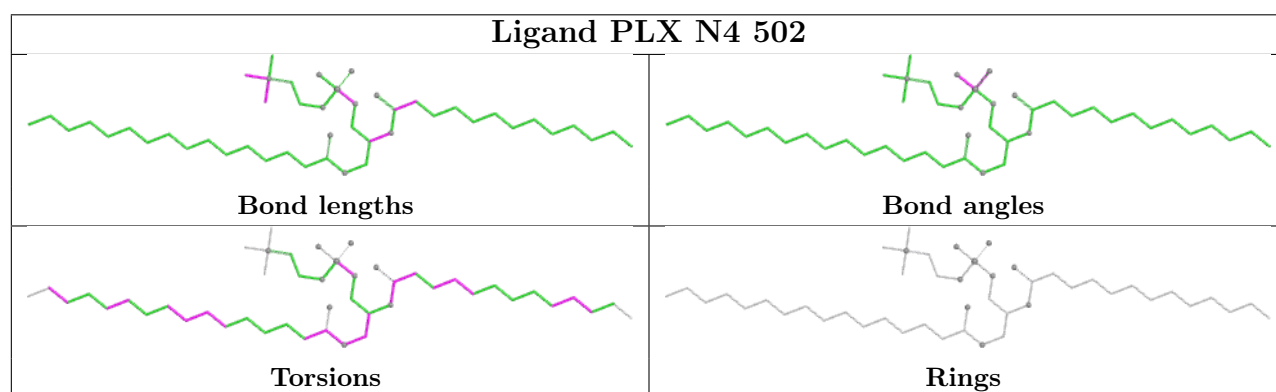
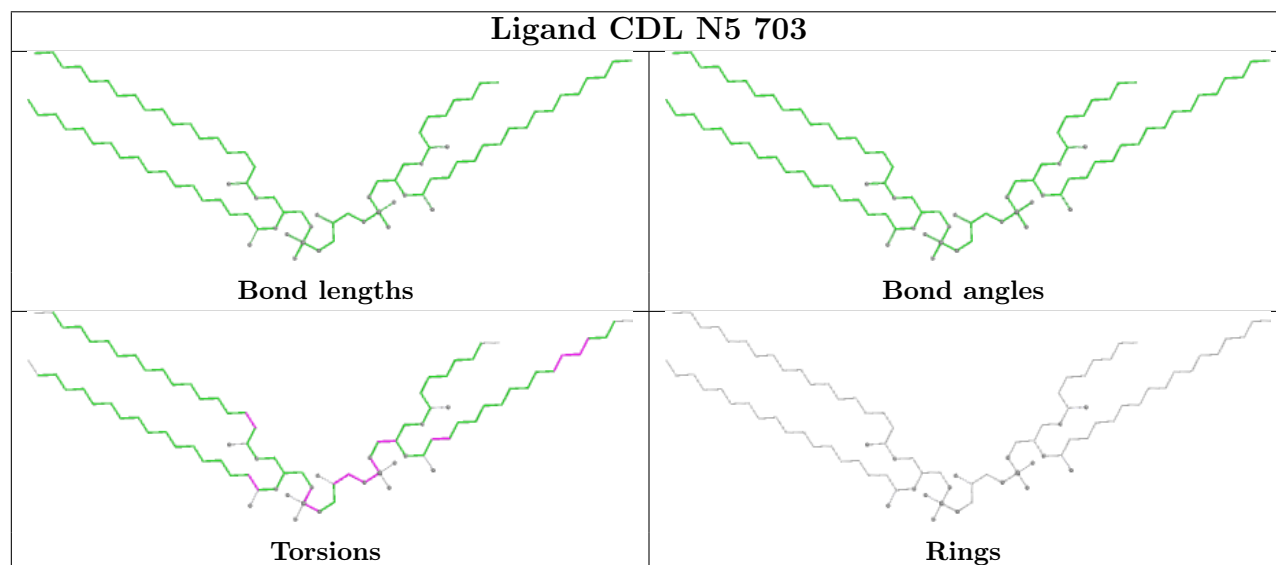
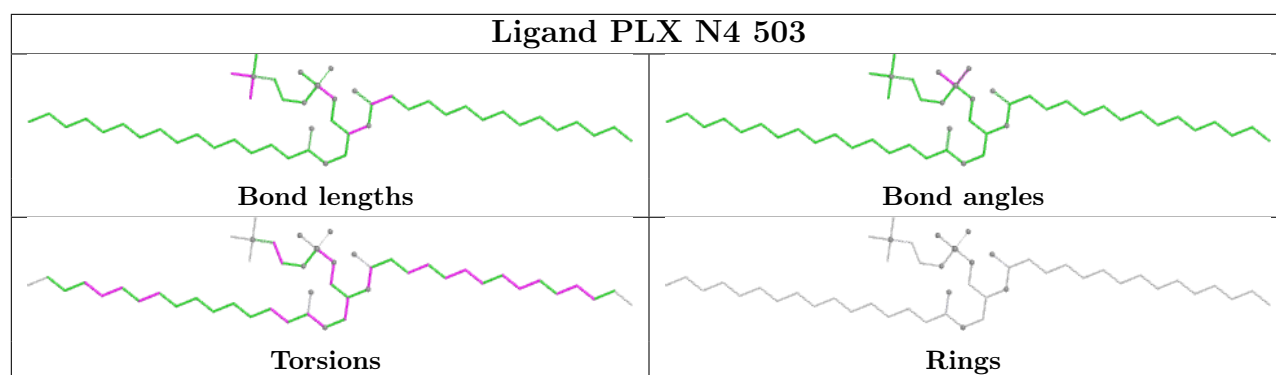


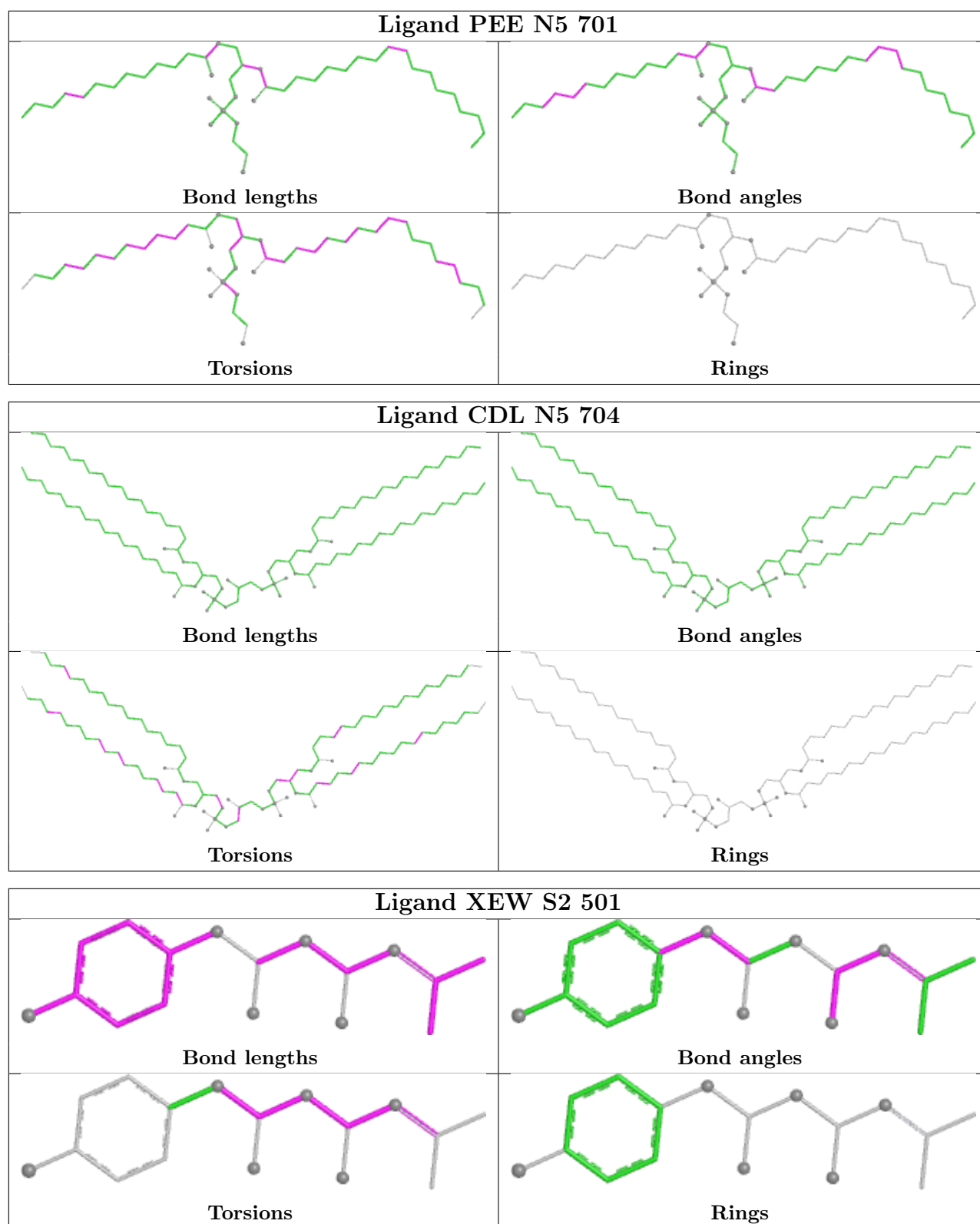
Ligand PLX B5 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

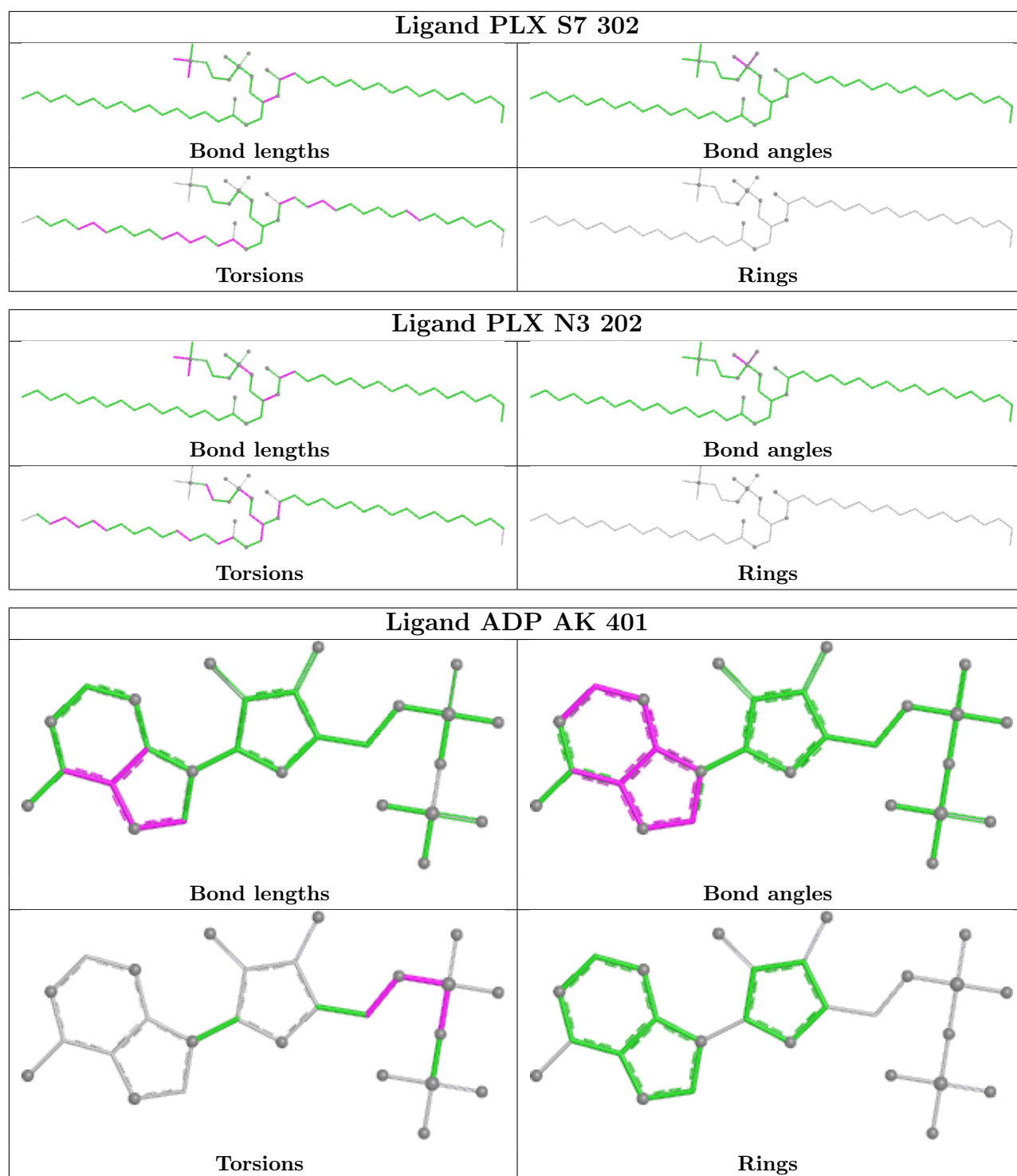
Ligand PEE A9 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEE BL 201	
	
Bond lengths	Bond angles
	
Torsions	Rings









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.

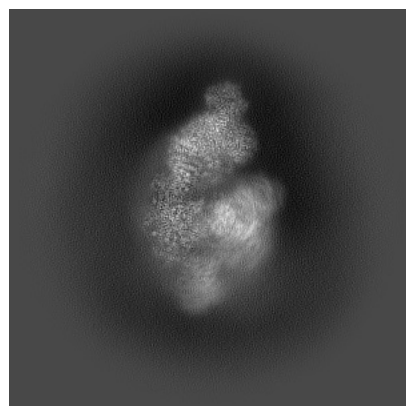
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60550. These allow visual inspection of the internal detail of the map and identification of artifacts.

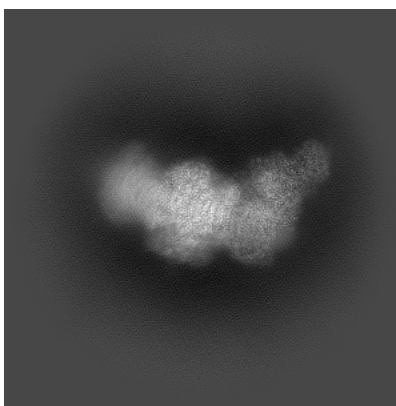
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

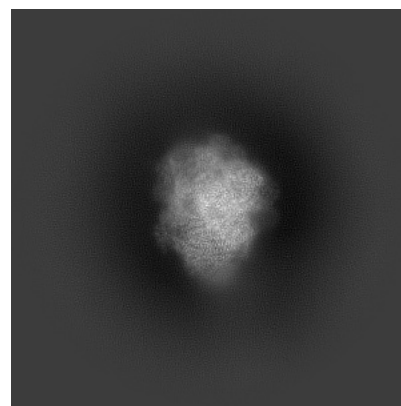
6.1.1 Primary map



X

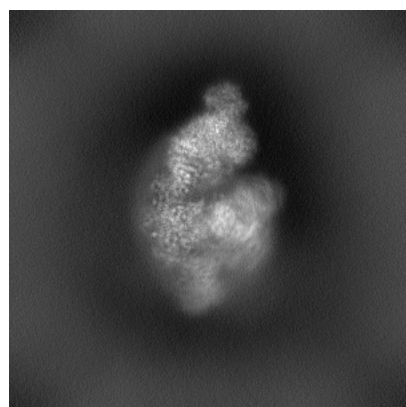


Y

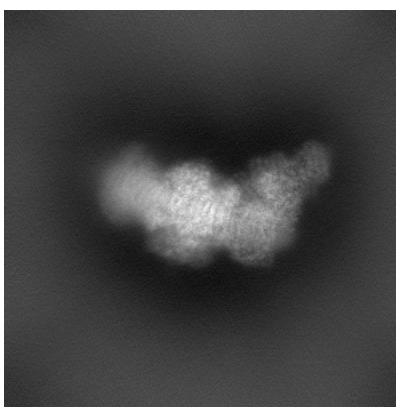


Z

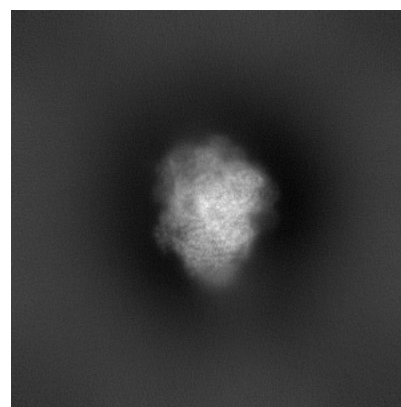
6.1.2 Raw map



X



Y

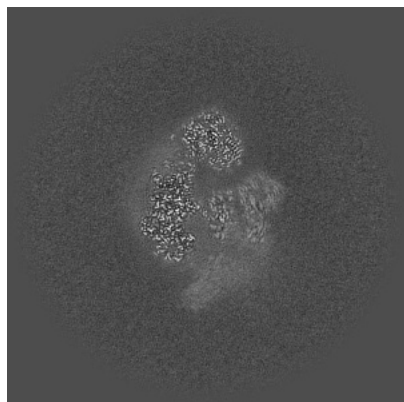


Z

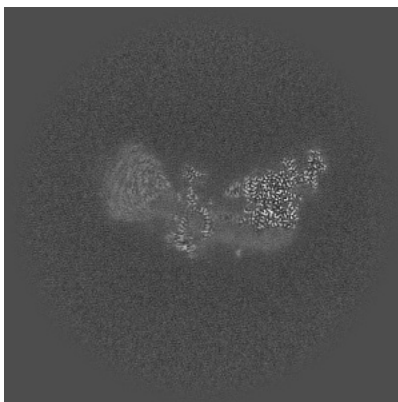
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

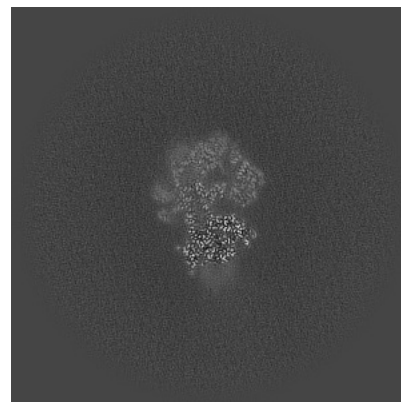
6.2.1 Primary map



X Index: 240

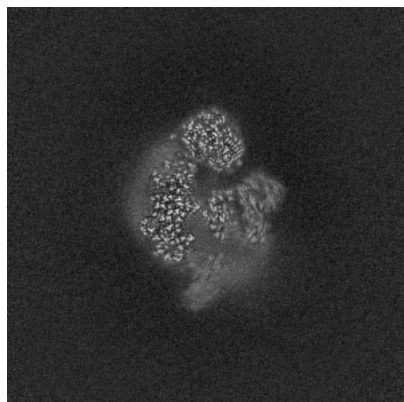


Y Index: 240

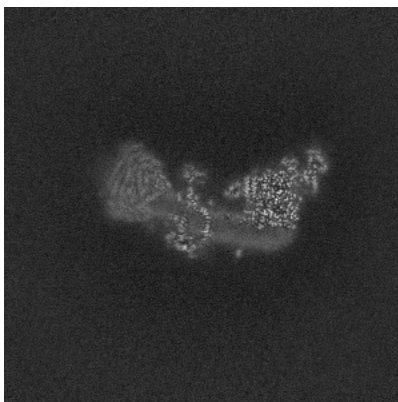


Z Index: 240

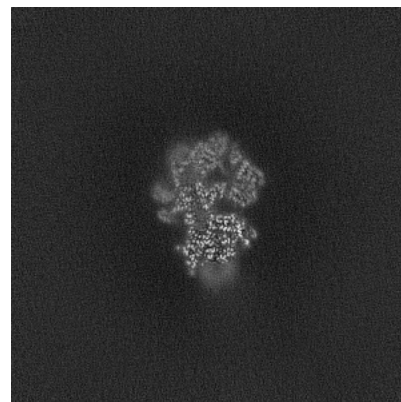
6.2.2 Raw map



X Index: 240



Y Index: 240

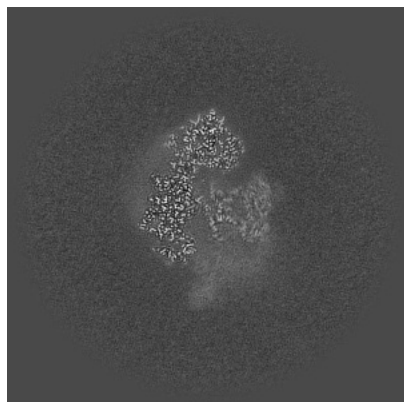


Z Index: 240

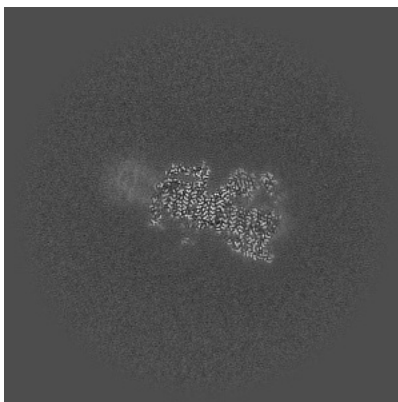
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

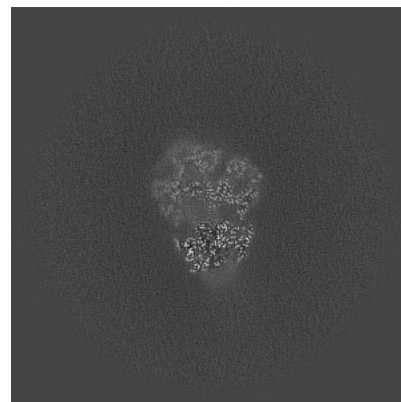
6.3.1 Primary map



X Index: 235

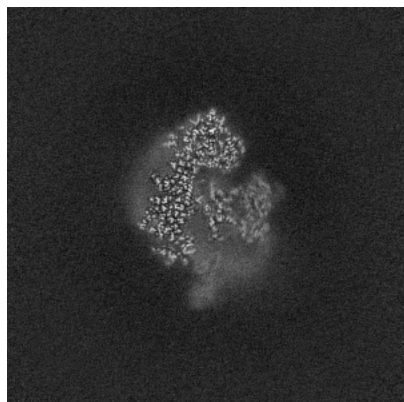


Y Index: 204

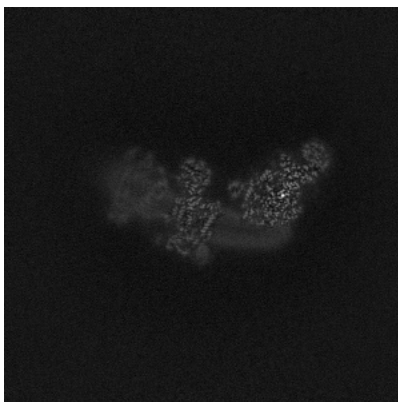


Z Index: 228

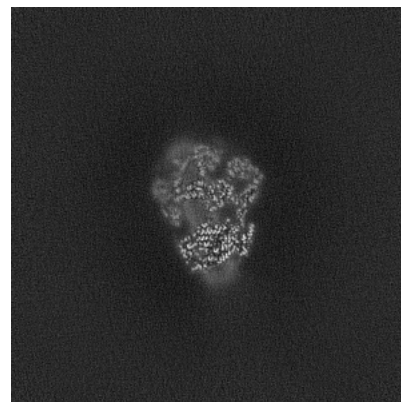
6.3.2 Raw map



X Index: 235



Y Index: 249

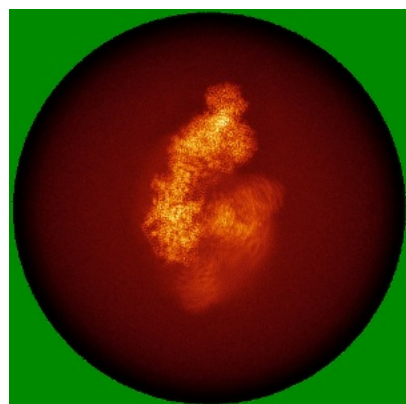


Z Index: 231

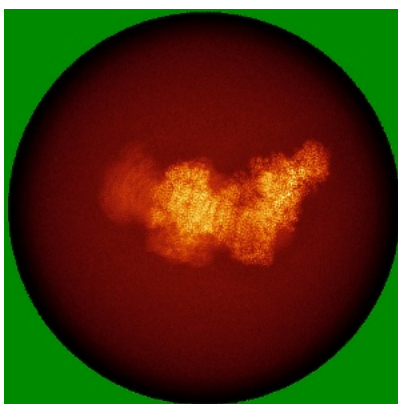
The images above show the largest variance slices of the map in three orthogonal directions.

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

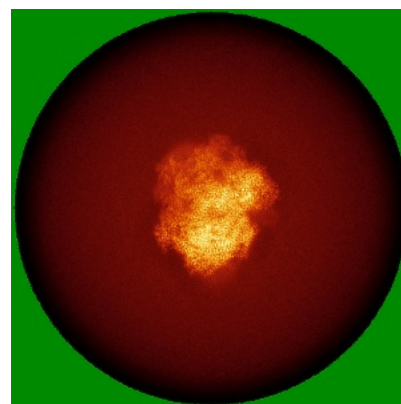
6.4.1 Primary map



X

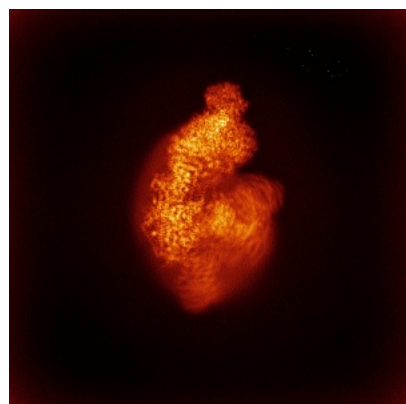


Y

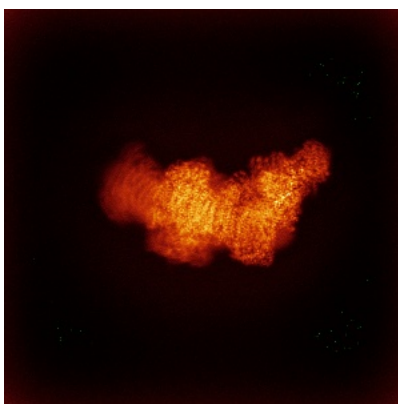


Z

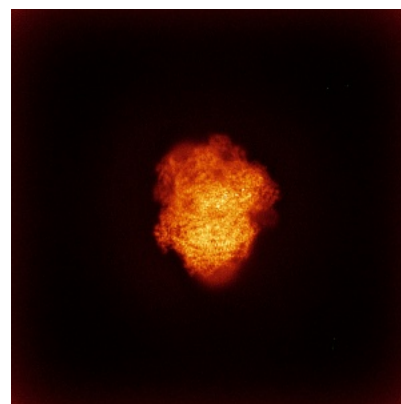
6.4.2 Raw map



X



Y

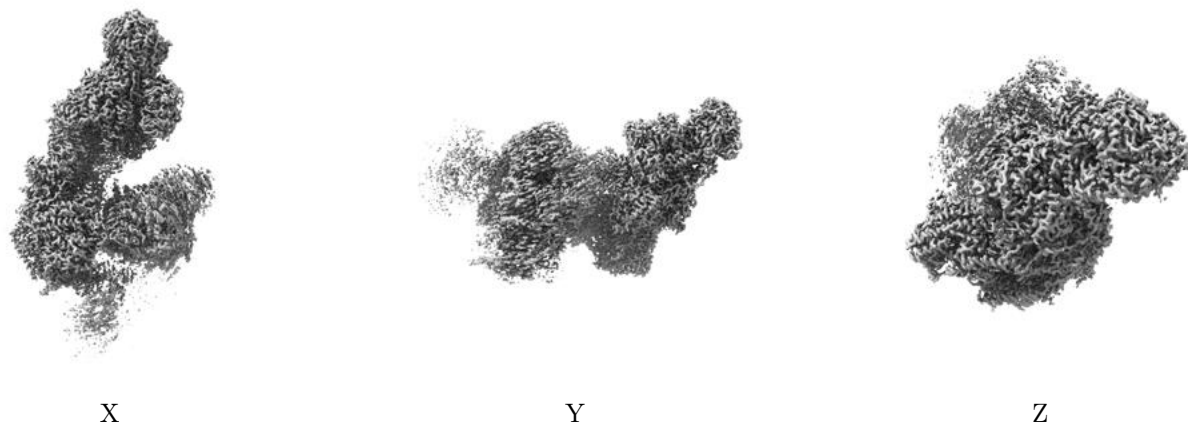


Z

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

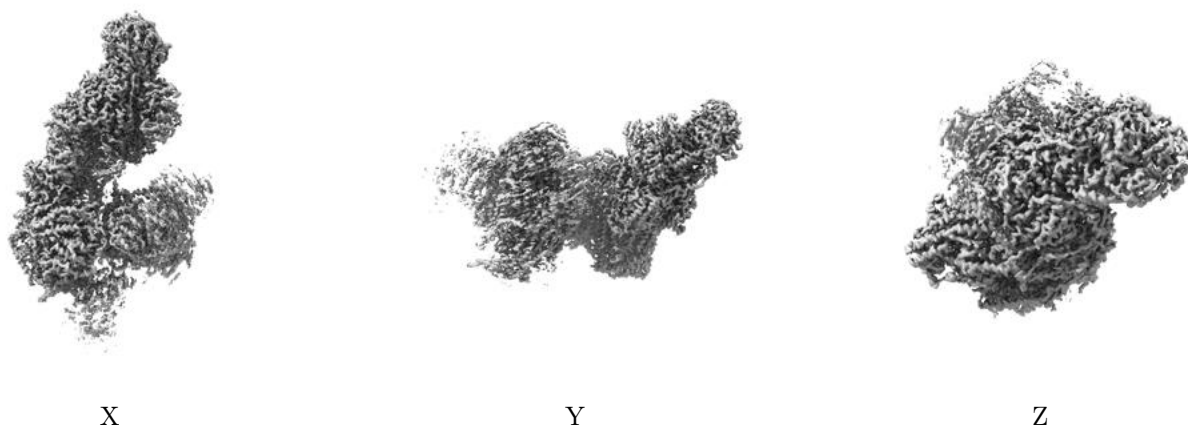
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 7.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

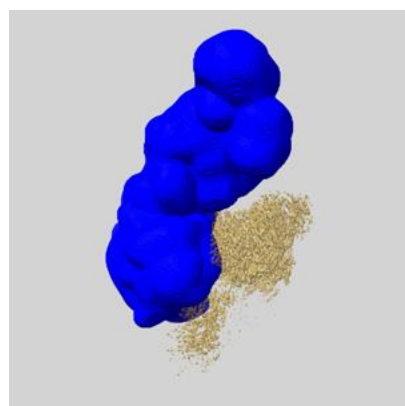
6.6 Mask visualisation [i](#)

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

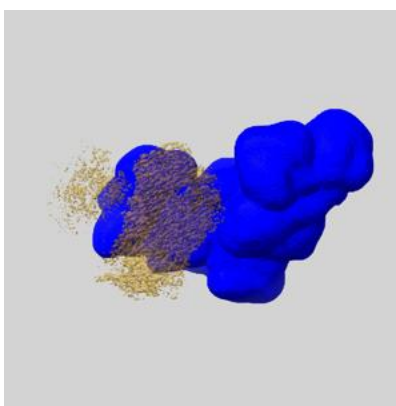
A mask typically either:

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

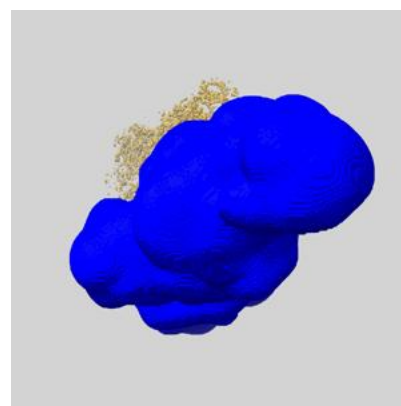
6.6.1 emd_60550_msk_1.map [i](#)



X



Y

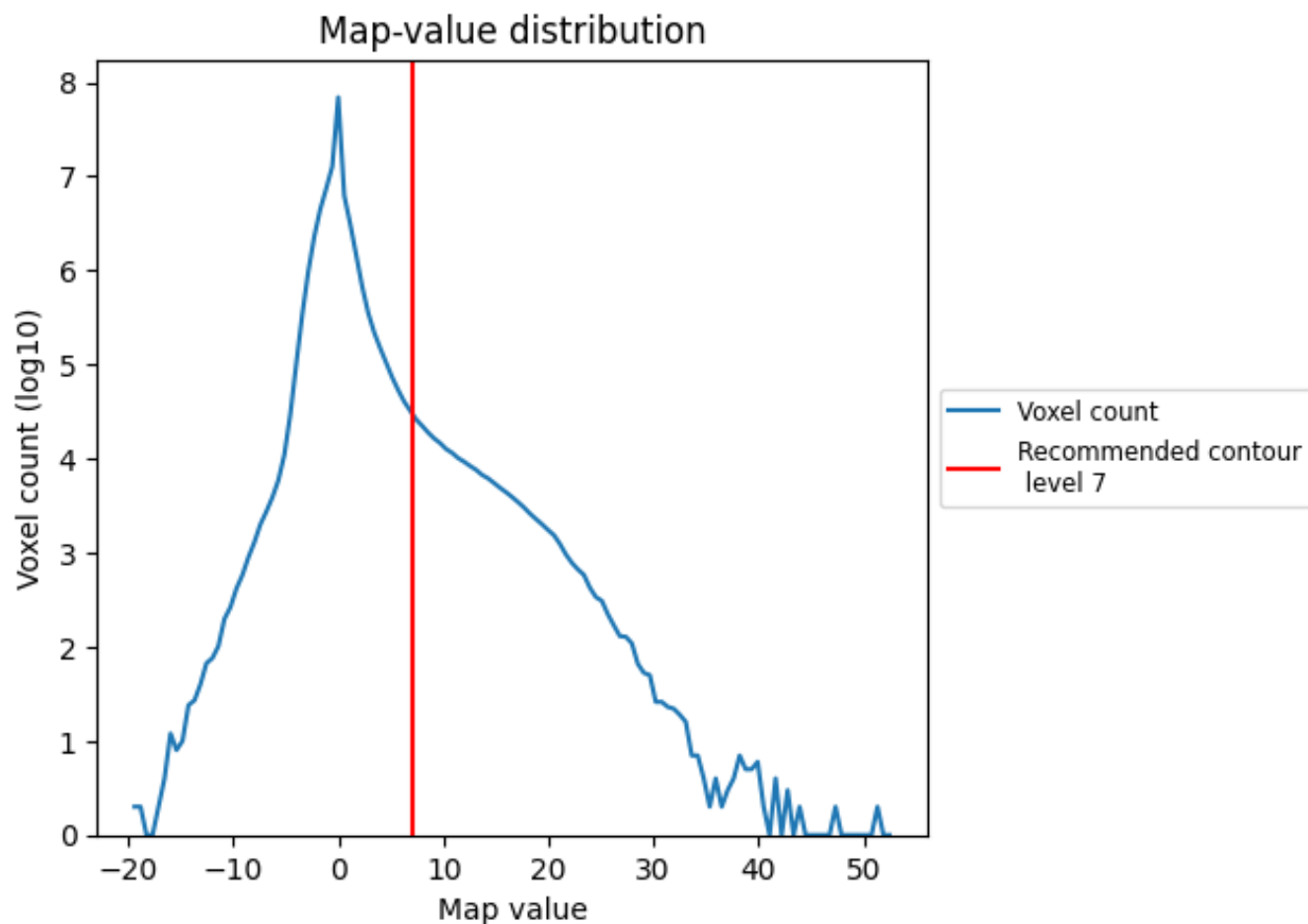


Z

7 Map analysis [i](#)

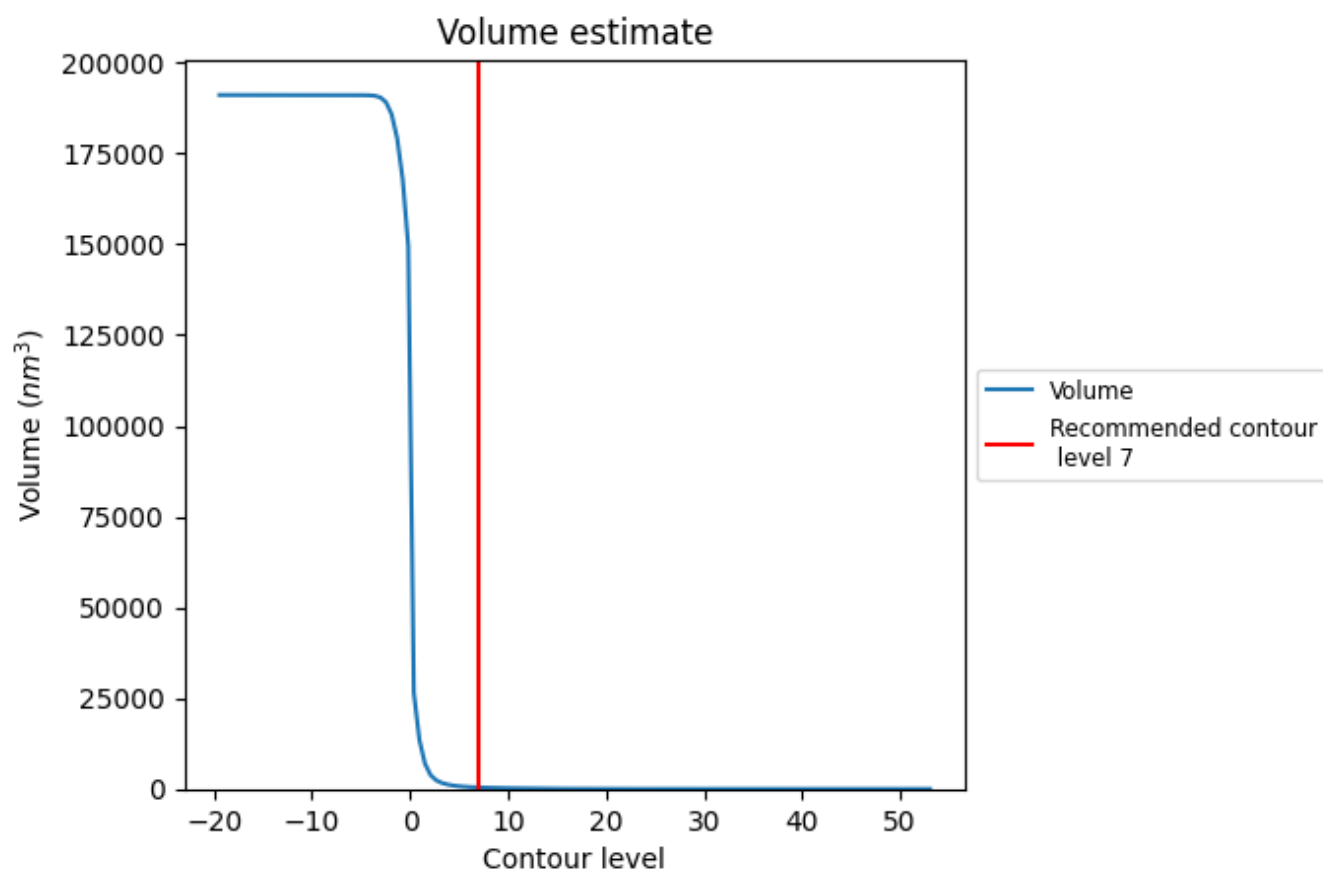
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

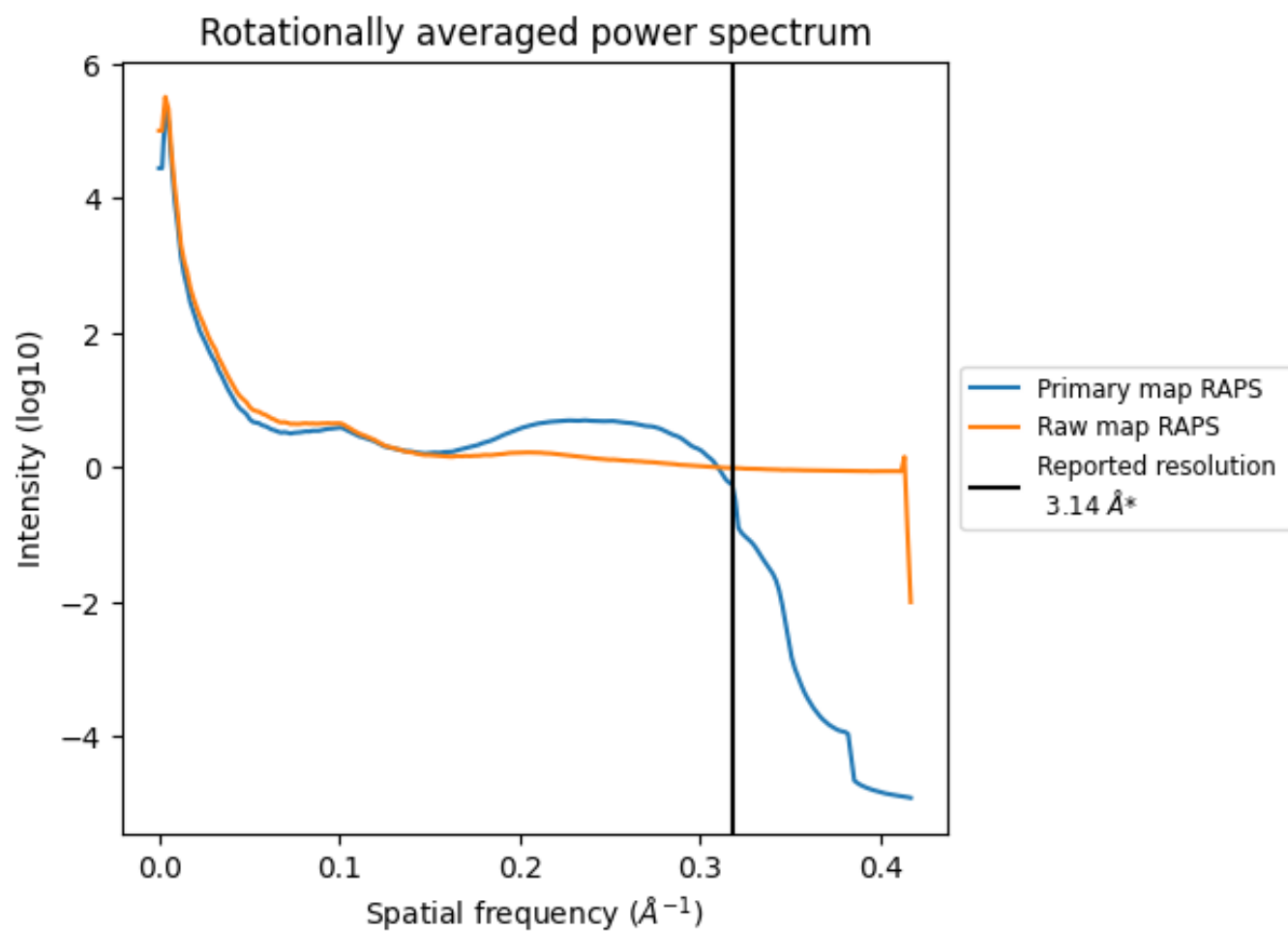
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 406 nm³; this corresponds to an approximate mass of 367 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

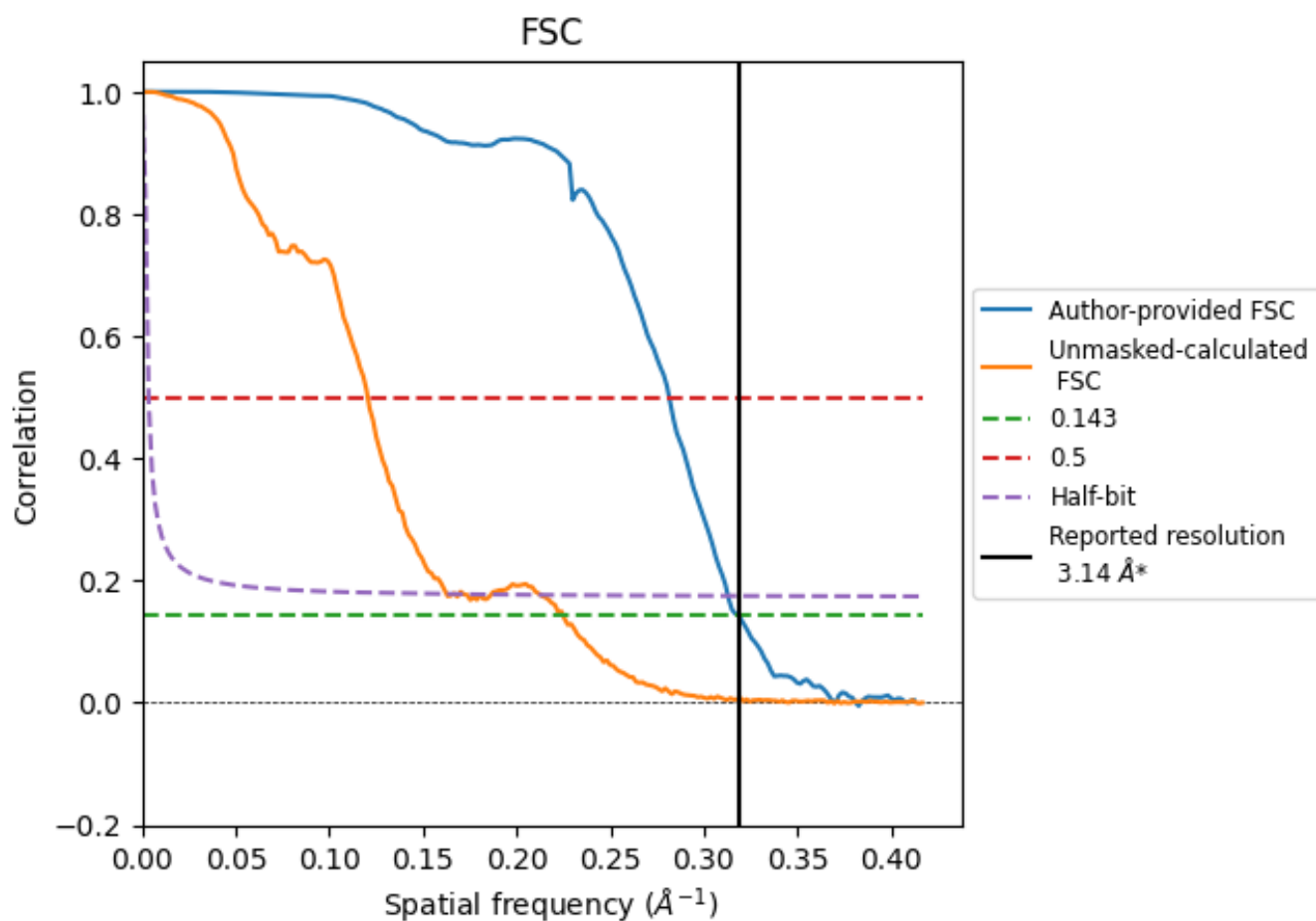


*Reported resolution corresponds to spatial frequency of $0.318 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.318 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

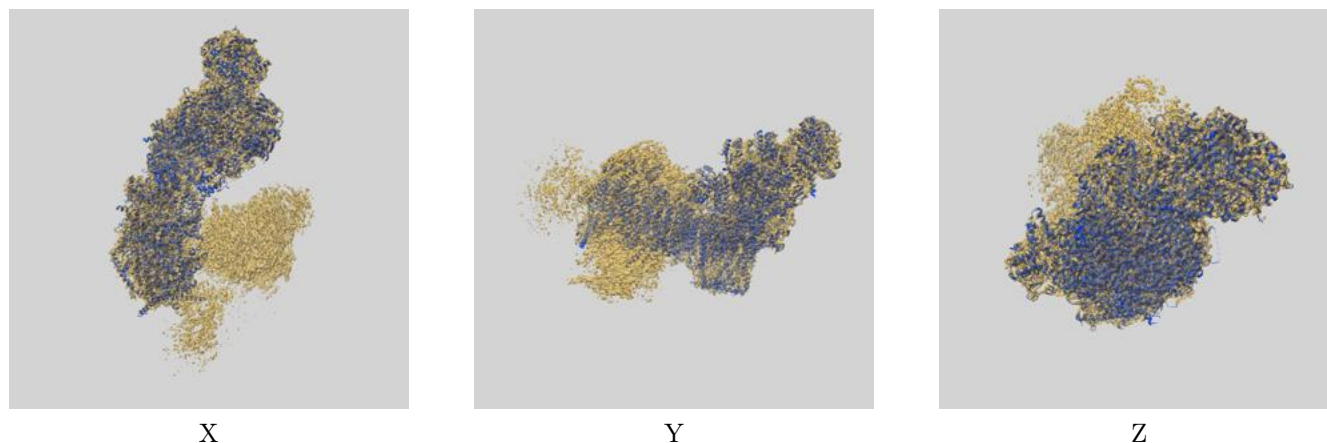
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.14	3.55	3.19
Unmasked-calculated*	4.45	8.30	6.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.45 differs from the reported value 3.14 by more than 10 %

9 Map-model fit [i](#)

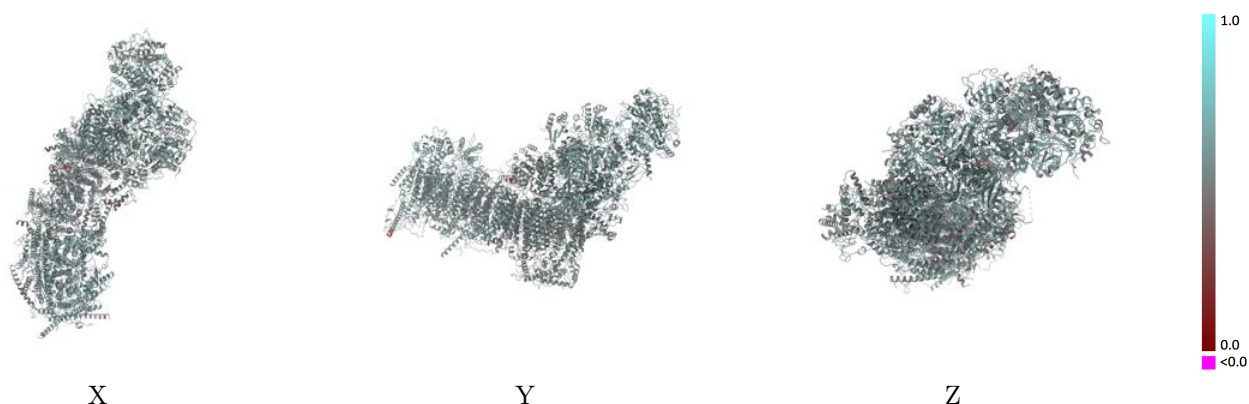
This section contains information regarding the fit between EMDB map EMD-60550 and PDB model 8ZXZ. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



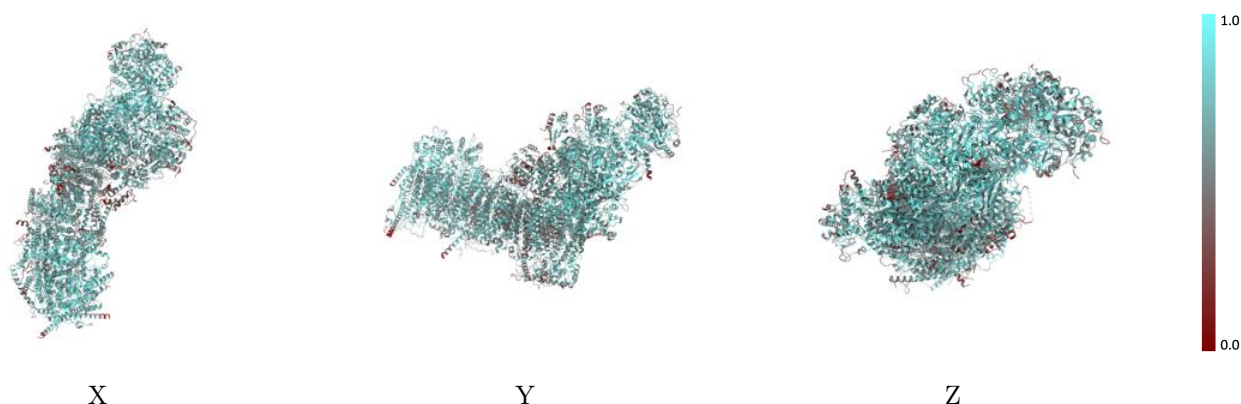
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



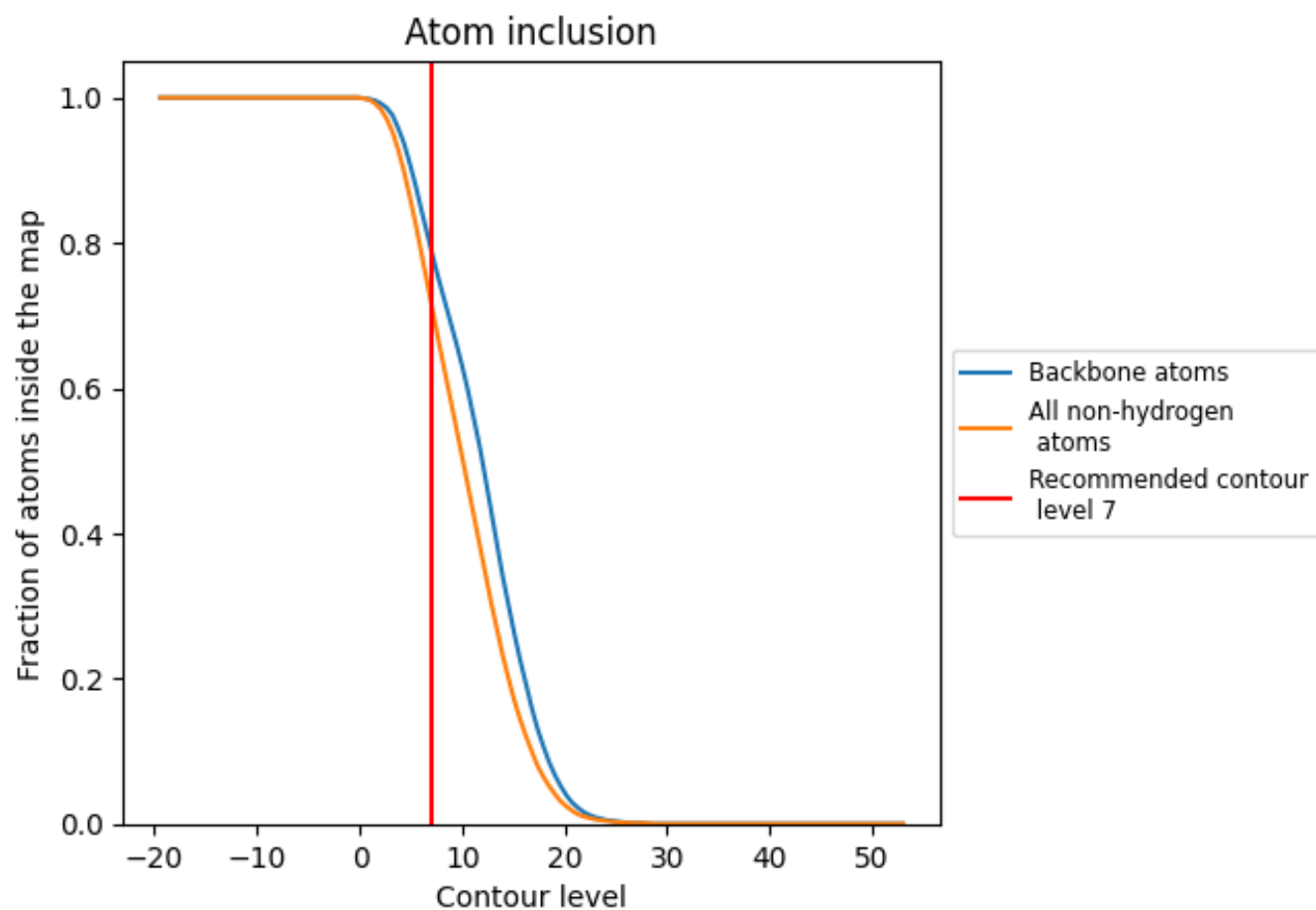
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7).

9.4 Atom inclusion ⓘ



At the recommended contour level, 79% of all backbone atoms, 72% 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 (7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7160	 0.5580
4L	 0.6500	 0.5520
A1	 0.7400	 0.5580
A2	 0.5730	 0.5310
A3	 0.6330	 0.5350
A5	 0.6160	 0.5460
A6	 0.6400	 0.5380
A7	 0.6040	 0.5340
A8	 0.6420	 0.5430
A9	 0.6960	 0.5550
AB	 0.3590	 0.4530
AC	 0.7400	 0.5710
AK	 0.5930	 0.5150
AL	 0.6380	 0.5420
AM	 0.6800	 0.5550
AN	 0.6740	 0.5350
B1	 0.6490	 0.5390
B2	 0.7210	 0.5560
B3	 0.6670	 0.5400
B4	 0.6960	 0.5620
B5	 0.7420	 0.5700
B6	 0.6610	 0.5320
B7	 0.6820	 0.5360
B8	 0.7650	 0.5770
B9	 0.7860	 0.5780
BK	 0.7110	 0.5550
BL	 0.6840	 0.5550
CA	 0.5670	 0.5390
CB	 0.7340	 0.5670
N1	 0.7620	 0.5600
N2	 0.7790	 0.5700
N3	 0.6530	 0.5530
N4	 0.8210	 0.5790
N5	 0.7820	 0.5770
N6	 0.6240	 0.5160



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Chain	Atom inclusion	Q-score
S1	 0.7320	 0.5670
S2	 0.7970	 0.5730
S3	 0.7970	 0.5850
S4	 0.7040	 0.5650
S5	 0.5970	 0.5220
S6	 0.6700	 0.5560
S7	 0.8220	 0.5770
S8	 0.8460	 0.5830
V1	 0.6990	 0.5590
V2	 0.6720	 0.5490
V3	 0.6370	 0.5530