



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 01:19 PM UTC

PDB ID : 8CA3 / pdb_00008ca3
EMDB ID : EMD-16516
Title : Cryo-EM structure NDUFS4 knockout complex I from Mus musculus heart (Class 2).
Authors : Yin, Z.; Bridges, H.R.; Agip, A.N.A.; Hirst, J.
Deposited on : 2023-01-24
Resolution : 3.20 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:

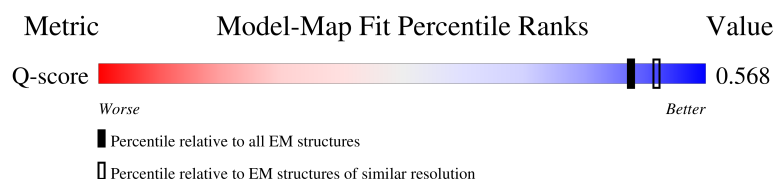
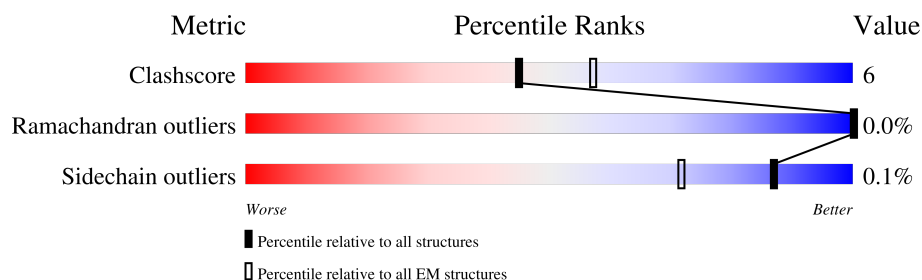
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	A	115	 90% 10%
2	B	224	 56% 14% 30%
3	C	263	 69% 10% 21%
4	D	463	 77% 16% 7%

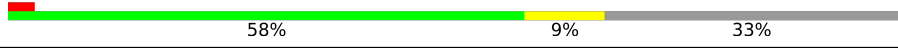
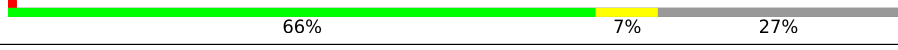
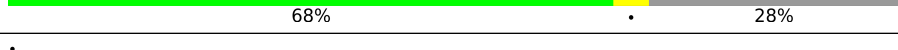
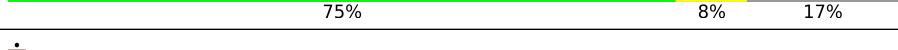
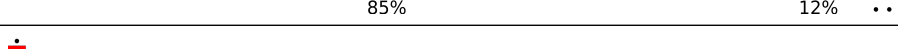
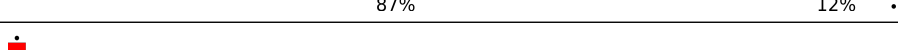
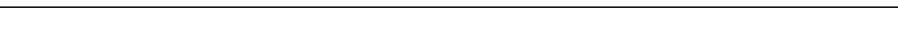
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Mol	Chain	Length	Quality of chain
5	E	245	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	172	
11	K	98	
12	L	607	
13	M	459	
14	N	345	
15	O	355	
16	P	377	
17	R	116	
18	S	99	
19	T	156	
19	U	156	
20	V	116	
21	W	131	
22	X	172	
23	Y	143	
24	Z	144	
25	a	70	
26	b	84	
27	c	76	
28	d	120	

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Mol	Chain	Length	Quality of chain
29	e	106	
30	f	57	
31	g	151	
32	h	189	
33	i	127	
34	j	105	
35	k	104	
36	l	186	
37	m	129	
38	n	179	
39	o	137	
40	p	176	
41	r	113	
42	s	104	

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
43	SF4	I	201	-	-	X	-
46	FMN	F	502	-	X	-	-

2 Entry composition [i](#)

There are 54 unique types of molecules in this entry. The entry contains 63712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	S	0	0
			933	633	133	160	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	156	Total	C	N	O	S	0	0
			1247	796	223	214	14		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	430	Total	C	N	O	S	0	0
			3463	2215	595	629	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	210	Total	C	N	O	S	0	0
			1639	1043	275	310	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	428	Total	C	N	O	S	0	0
			3300	2080	589	609	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	688	Total	C	N	O	S	0	0
			5248	3294	910	1003	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2540	1706	384	428	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	171	Total	C	N	O	S	0	0
			1300	874	185	226	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			737	477	112	137	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4800	3182	746	827	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3632	2408	567	617	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	344	Total	C	N	O	S	0	0
			2696	1791	416	452	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2607	1674	431	492	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	325	Total	C	N	O	S	0	0
			2626	1702	456	461	7		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	55	Total	C	N	O	S	0	0
			413	258	74	78	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	82	Total	C	N	O	S	0	0
			594	374	108	110	2		

- Molecule 19 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	76	Total	C	N	O	S	0	0
			611	392	90	124	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	86	Total	C	N	O	S	0	0
			692	446	102	139	5		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	112	Total	C	N	O	S	0	0
			915	596	152	164	3		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	109	Total	C	N	O	S	0	0
			935	598	175	156	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	171	Total	C	N	O	S	0	0
			1396	889	250	247	10		

- Molecule 23 is a protein called MCG5603.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	140	Total	C	N	O	S	0	0
			1037	662	175	192	8		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	141	Total	C	N	O	S	0	0
			1167	750	207	202	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	68	Total	C	N	O	S	0	0
			556	360	99	93	4		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	80	Total	C	N	O	S	0	0
			628	414	99	111	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	48	Total	C	N	O	S	0	0
			398	261	69	67	1		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	53	Total	C	N	O	S	0	0
			456	295	82	77	2		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	101	Total	C	N	O	S	0	0
			850	549	136	161	4		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	138	Total	C	N	O	S	0	0
			1162	762	194	203	3		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	94	Total	C	N	O	S	0	0
			787	515	134	135	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	62	Total	C	N	O	S	0	0
			537	355	88	93	1		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	k	75	Total	C	N	O	S	0	0
			609	404	103	100	2		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	l	154	Total	C	N	O	S	0	0
			1294	834	215	234	11		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	m	126	Total	C	N	O		0	0
			1050	676	189	185			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	n	177	Total	C	N	O	S	0	0
			1534	981	275	267	11		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	o	113	Total	C	N	O	S	0	0
			979	617	184	170	8		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	p	168	Total	C	N	O	S	0	0
			1424	896	256	264	8		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	61	Total	C	N	O	S	0	0
			487	311	87	86	3		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

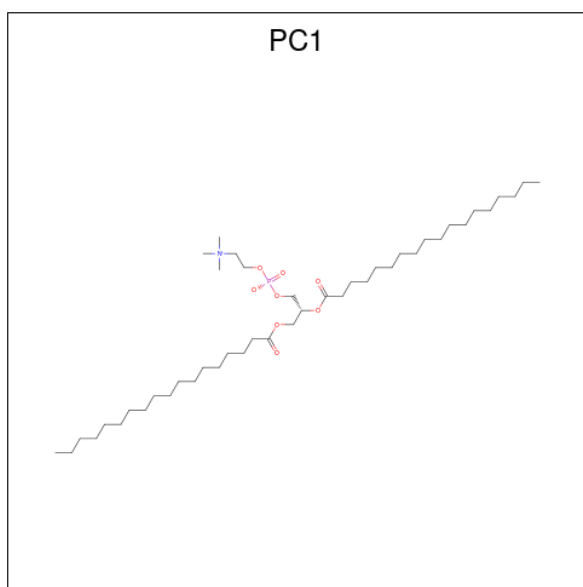
Mol	Chain	Residues	Atoms				AltConf	Trace
42	s	31	Total	C	N	O	0	0
			269	174	45	50		

- Molecule 43 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



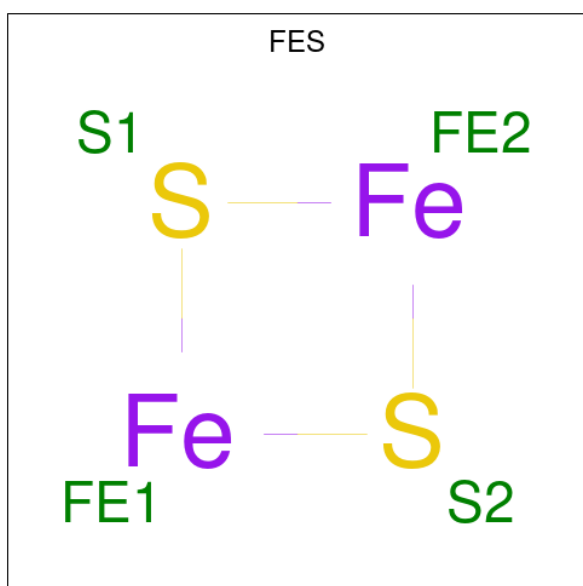
Mol	Chain	Residues	Atoms			AltConf
43	B	1	Total	Fe	S	0
			8	4	4	
43	F	1	Total	Fe	S	0
			8	4	4	
43	G	1	Total	Fe	S	0
			8	4	4	
43	G	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	

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



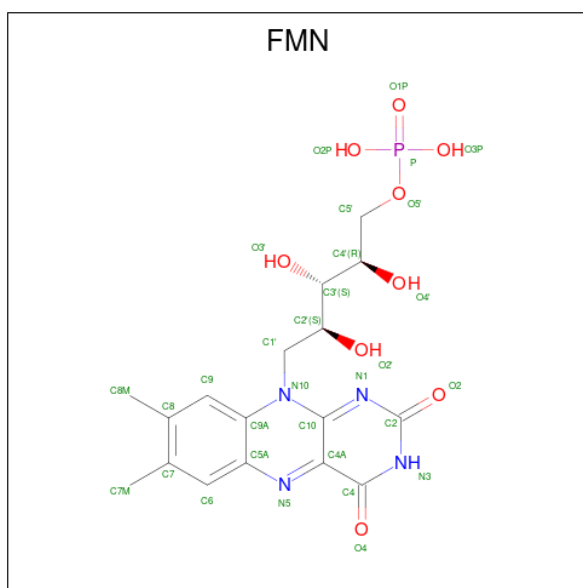
Mol	Chain	Residues	Atoms					AltConf
44	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
44	H	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 45 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



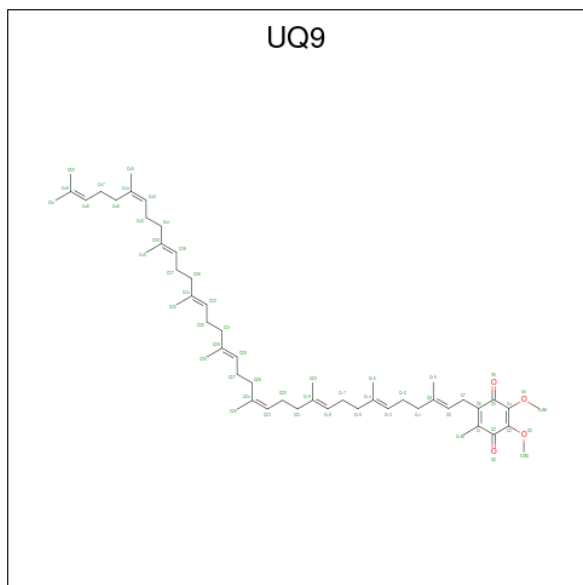
Mol	Chain	Residues	Atoms			AltConf
45	E	1	Total	Fe	S	0
			4	2	2	
45	G	1	Total	Fe	S	0
			4	2	2	

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



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

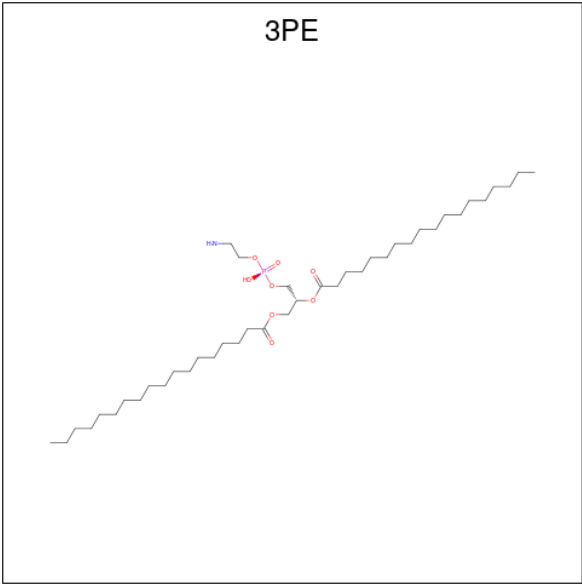
- Molecule 47 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$).



Mol	Chain	Residues	Atoms		AltConf
47	H	1	Total	C	0
			45	45	

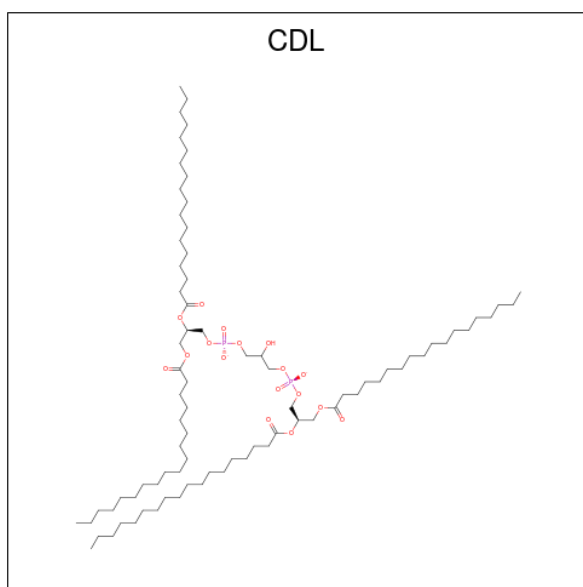
- Molecule 48 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:

C₄₁H₈₂NO₈P).



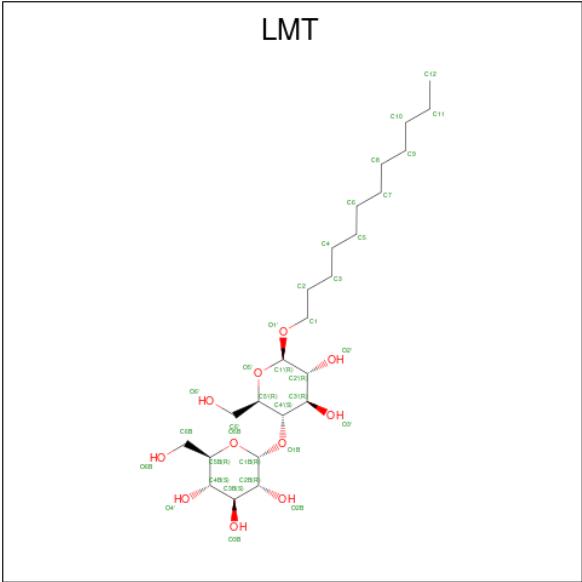
Mol	Chain	Residues	Atoms					AltConf
48	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	J	1	Total	C	N	O	P	0
			33	23	1	8	1	
48	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
48	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
48	Y	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	Z	1	Total	C	N	O	P	0
			44	34	1	8	1	
48	i	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 49 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



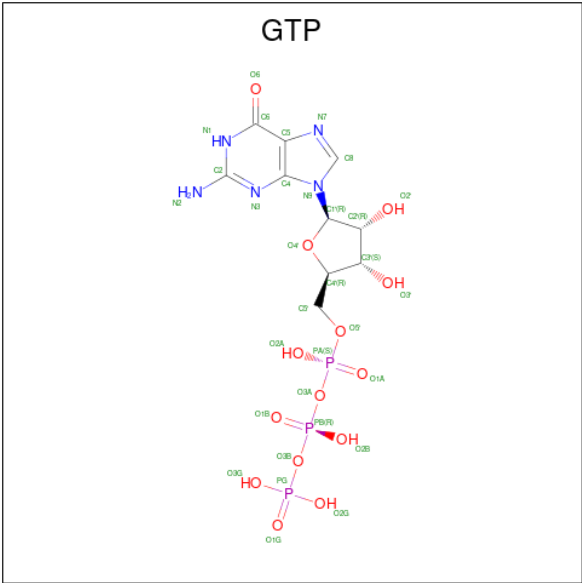
Mol	Chain	Residues	Atoms				AltConf
49	L	1	Total	C	O	P	0
			74	55	17	2	
49	M	1	Total	C	O	P	0
			59	41	16	2	
49	N	1	Total	C	O	P	0
			65	46	17	2	
49	N	1	Total	C	O	P	0
			63	44	17	2	
49	d	1	Total	C	O	P	0
			67	48	17	2	
49	h	1	Total	C	O	P	0
			70	51	17	2	

- Molecule 50 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
50	L	1	Total	C	O	0
			35	24	11	
50	L	1	Total	C	O	0
			35	24	11	

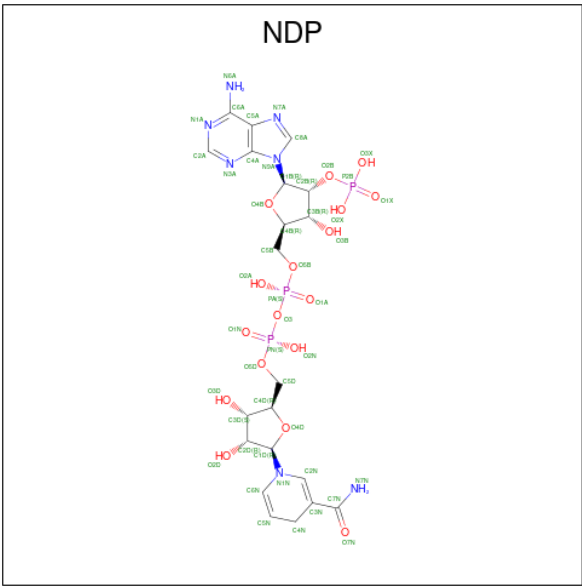
- Molecule 51 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

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

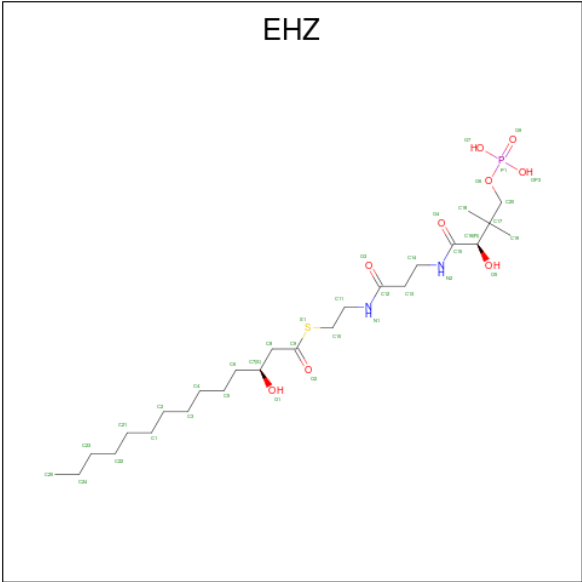


Mol	Chain	Residues	Atoms					AltConf
52	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

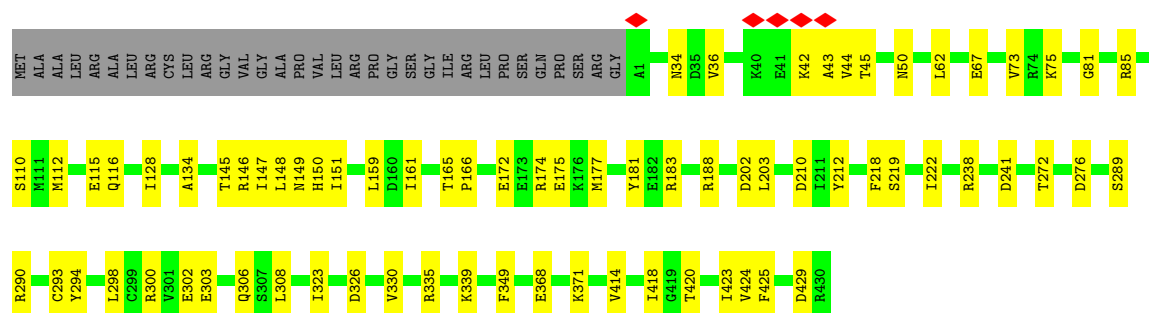
- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	R	1	Total	Zn	0
			1	1	

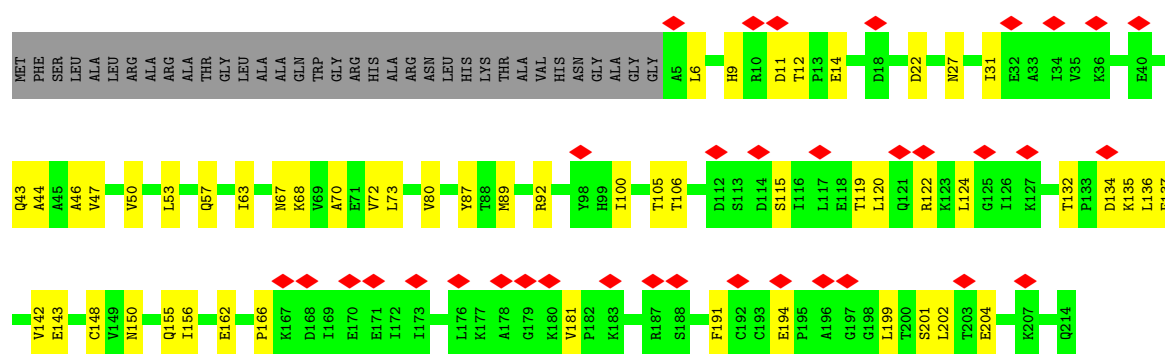
- Molecule 54 is {S}-[2-[3-[[2 {R}]-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



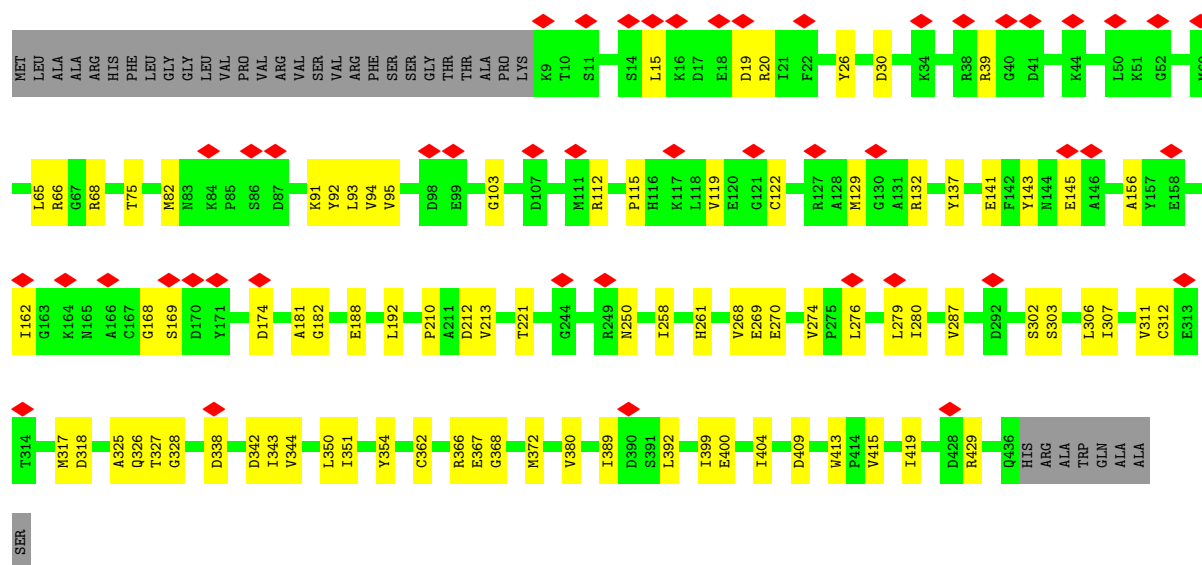
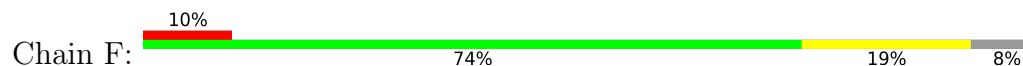
Mol	Chain	Residues	Atoms						AltConf
54	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
54	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	



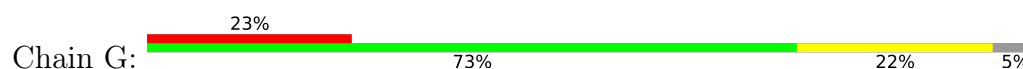
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

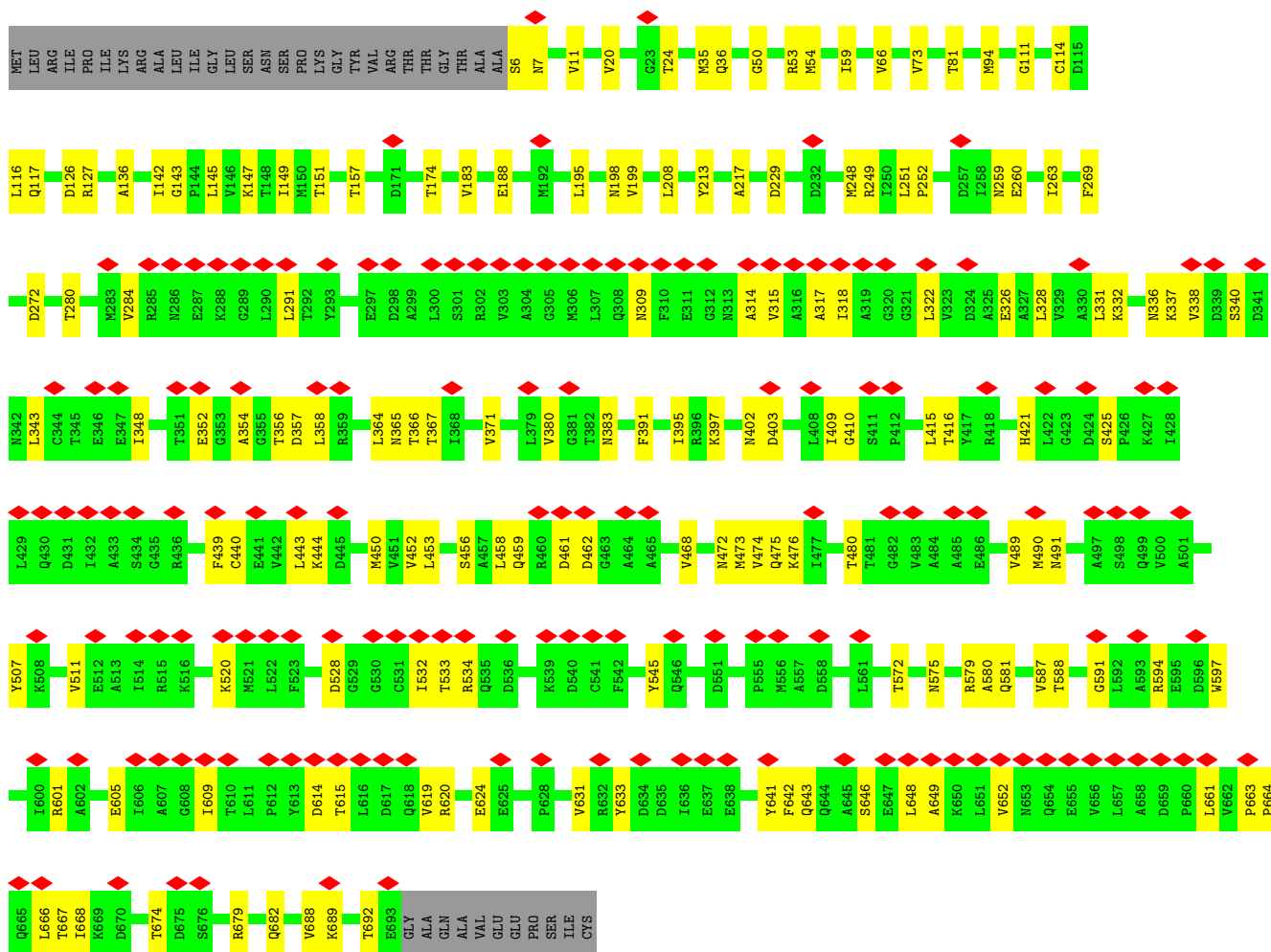


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

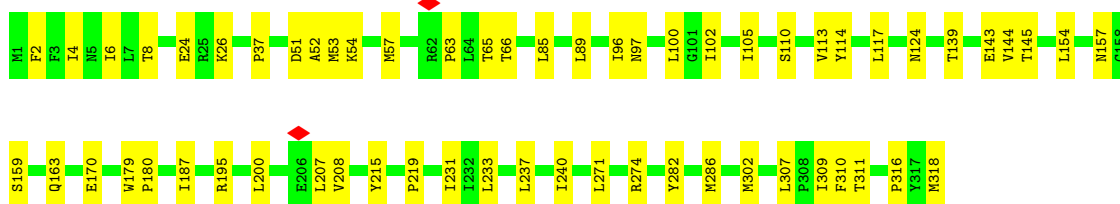
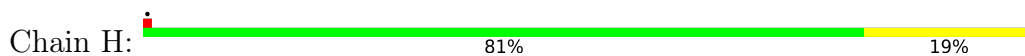


- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

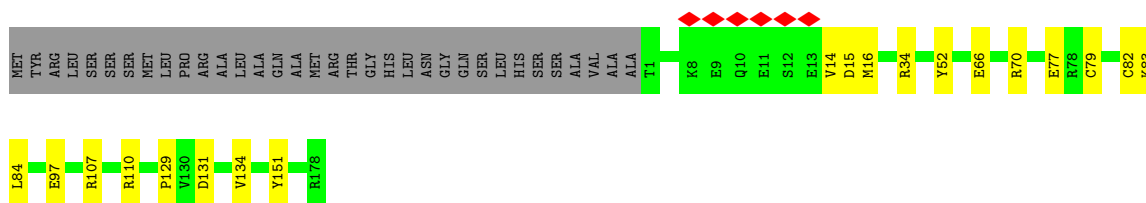
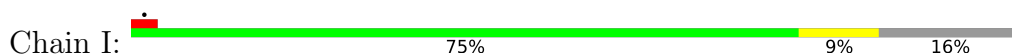




• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

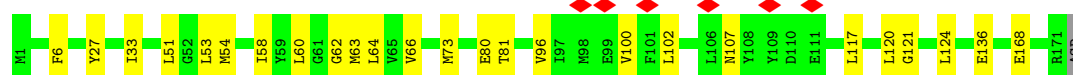


• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  85% 15%



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  84% 16%



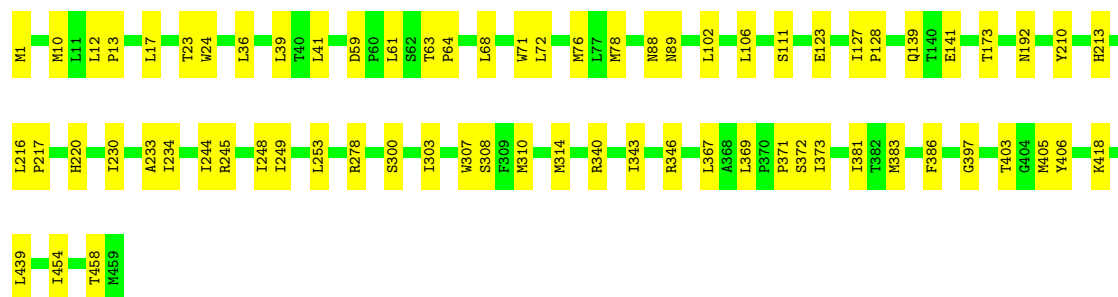
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  84% 16%



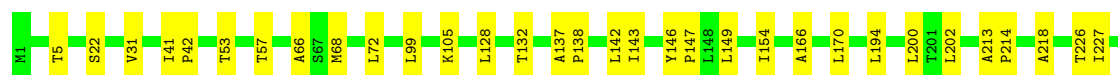
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  85% 15%



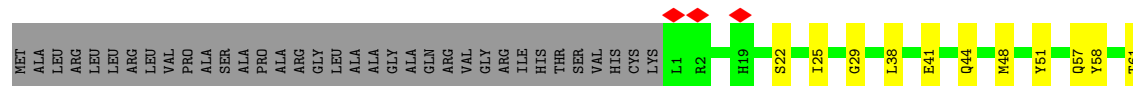
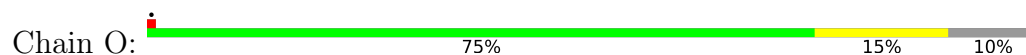
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:  83% 17%

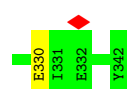
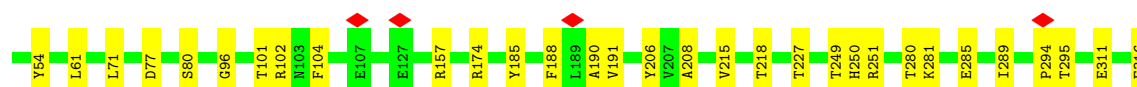
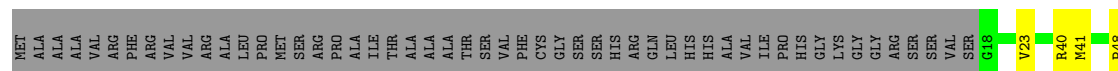
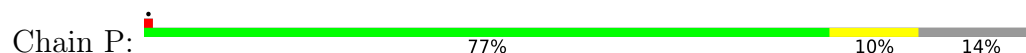




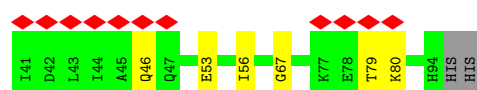
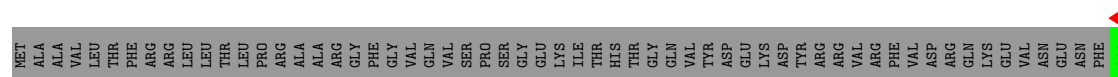
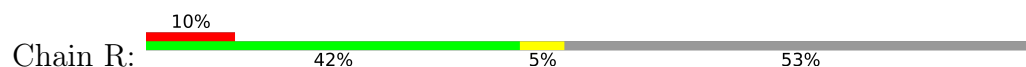
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



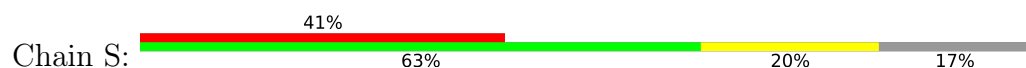
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

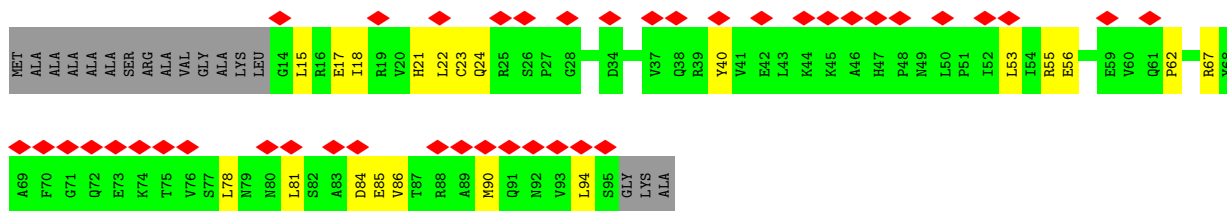


- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

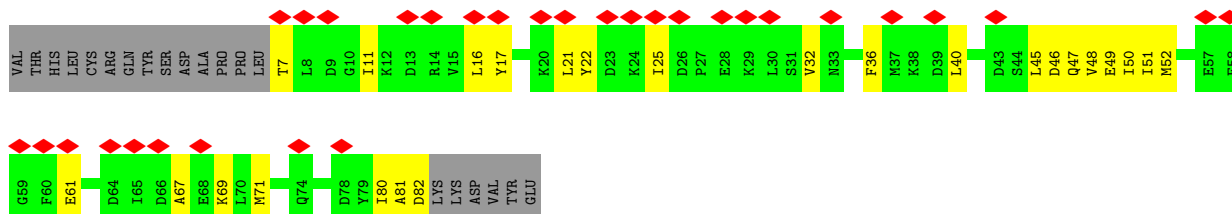
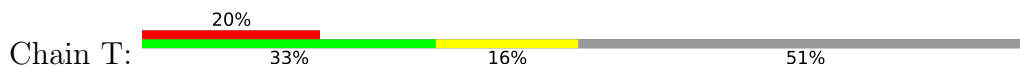


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

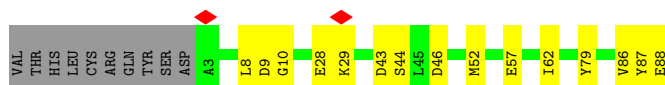




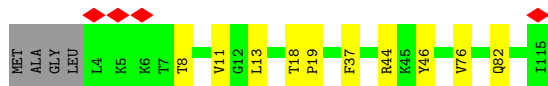
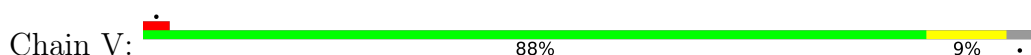
• Molecule 19: Acyl carrier protein, mitochondrial



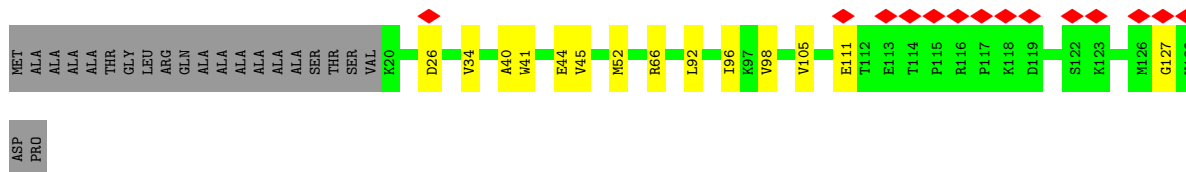
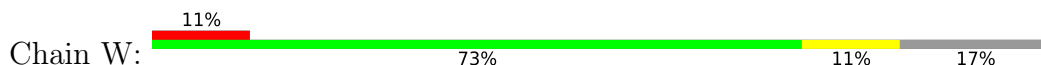
• Molecule 19: Acyl carrier protein, mitochondrial



• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

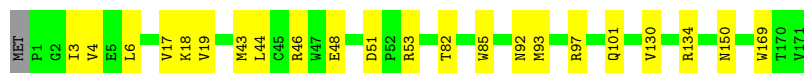


• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



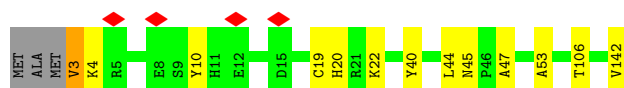
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:  87% 13% .



- Molecule 23: MCG5603

Chain Y:  89% 8% ..



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:  83% 15% .



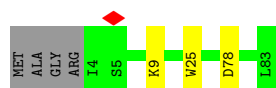
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:  87% 10% .



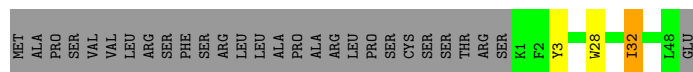
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:  92% 5% .



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

Chain c:  59% .. 37%



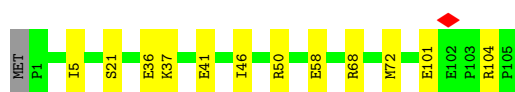
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:  89% 11%



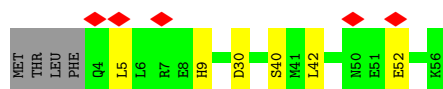
- Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e: 



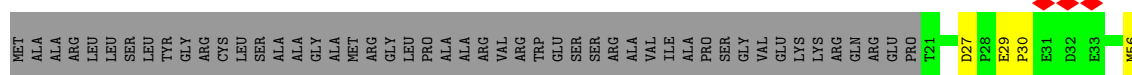
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f: 



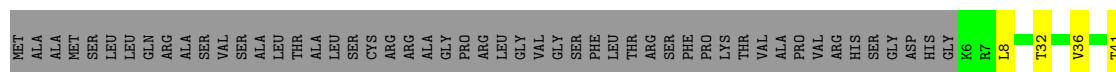
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g: 



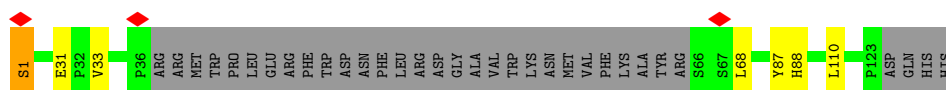
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h: 

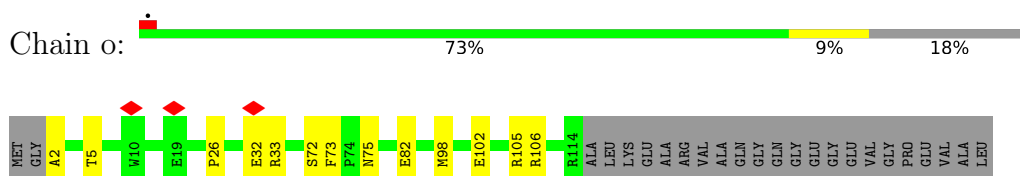


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i: 



- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



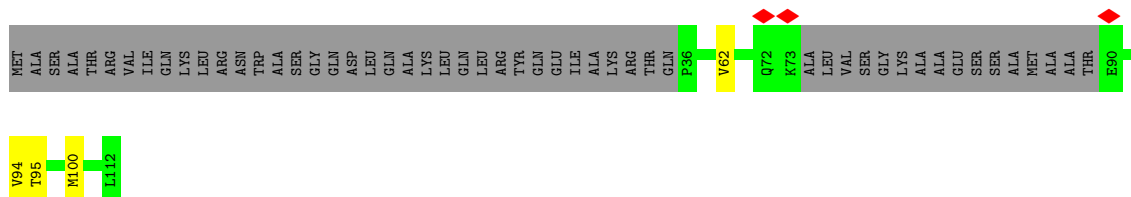
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:  79% 16% 5%



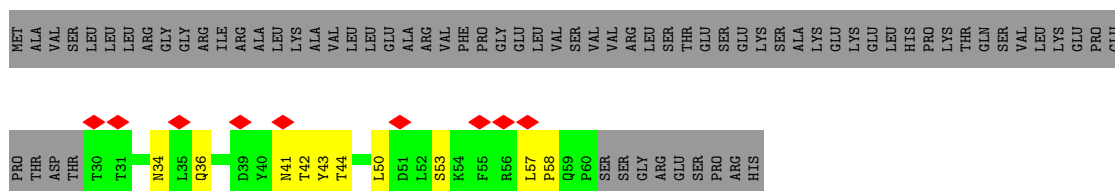
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:  50% 46%



- Molecule 42: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:  9% 20% 10% 70%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10005	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	13.939	Depositor
Minimum map value	-4.972	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.422	Depositor
Recommended contour level	1.9	Depositor
Map size (Å)	608.4, 608.4, 608.4	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.352, 1.352, 1.352	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 3PE, CDL, LMT, GTP, FES, SAC, EHZ, FMN, 2MR, NDP, UQ9, SF4, FME, PC1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.16	0/949	0.30	0/1297
2	B	0.20	0/1278	0.39	0/1730
3	C	0.17	0/1771	0.30	0/2412
4	D	0.18	0/3539	0.30	0/4793
5	E	0.12	0/1679	0.31	0/2288
6	F	0.13	0/3374	0.29	0/4557
7	G	0.14	0/5335	0.30	0/7236
8	H	0.18	0/2607	0.33	0/3564
9	I	0.18	0/1461	0.30	0/1974
10	J	0.18	0/1322	0.33	0/1799
11	K	0.16	0/738	0.27	0/1002
12	L	0.17	0/4913	0.32	0/6686
13	M	0.18	0/3709	0.31	0/5052
14	N	0.18	0/2748	0.34	0/3741
15	O	0.16	0/2674	0.29	0/3626
16	P	0.14	0/2697	0.27	0/3658
17	R	0.17	0/420	0.30	0/566
18	S	0.10	0/604	0.27	0/827
19	T	0.13	0/620	0.33	0/836
19	U	0.16	0/704	0.36	0/951
20	V	0.15	0/937	0.25	0/1270
21	W	0.15	0/957	0.29	0/1284
22	X	0.16	0/1434	0.30	0/1937
23	Y	0.14	0/1061	0.26	0/1439
24	Z	0.18	0/1198	0.33	0/1616
25	a	0.18	0/569	0.29	0/766
26	b	0.23	0/651	0.31	0/895
27	c	0.17	0/409	0.26	0/555
28	d	0.17	0/1028	0.28	0/1387
29	e	0.15	0/900	0.27	0/1199
30	f	0.13	0/468	0.30	0/630
31	g	0.16	0/878	0.30	0/1196

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	h	0.16	0/1197	0.28	0/1621
33	i	0.15	0/804	0.32	0/1094
34	j	0.14	0/561	0.27	0/768
35	k	0.14	0/629	0.26	0/851
36	l	0.15	0/1348	0.27	0/1840
37	m	0.18	0/1079	0.31	0/1463
38	n	0.17	0/1589	0.30	0/2152
39	o	0.14	0/1004	0.26	0/1348
40	p	0.16	0/1457	0.30	0/1969
41	r	0.13	0/502	0.27	0/680
42	s	0.09	0/277	0.23	0/377
All	All	0.16	0/64079	0.30	0/86932

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

Mol	Chain	#Chirality outliers	#Planarity outliers
37	m	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
37	m	29	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	933	0	969	9	0
2	B	1247	0	1255	22	0
3	C	1721	0	1680	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	3463	0	3416	51	0
5	E	1639	0	1631	41	0
6	F	3300	0	3258	65	0
7	G	5248	0	5236	113	0
8	H	2540	0	2626	43	0
9	I	1431	0	1383	19	0
10	J	1300	0	1315	19	0
11	K	737	0	768	12	0
12	L	4800	0	4985	67	0
13	M	3632	0	3853	51	0
14	N	2696	0	2895	45	0
15	O	2607	0	2566	37	0
16	P	2626	0	2642	22	0
17	R	413	0	403	5	0
18	S	594	0	543	17	0
19	T	611	0	602	16	0
19	U	692	0	686	13	0
20	V	915	0	954	8	0
21	W	935	0	959	12	0
22	X	1396	0	1383	18	0
23	Y	1037	0	1024	9	0
24	Z	1167	0	1166	19	0
25	a	556	0	568	5	0
26	b	628	0	628	7	0
27	c	398	0	401	2	0
28	d	996	0	1001	14	0
29	e	877	0	871	9	0
30	f	456	0	452	6	0
31	g	850	0	783	14	0
32	h	1162	0	1163	14	0
33	i	787	0	797	6	0
34	j	537	0	495	9	0
35	k	609	0	603	3	0
36	l	1294	0	1186	13	0
37	m	1050	0	1061	14	0
38	n	1534	0	1466	20	0
39	o	979	0	963	12	0
40	p	1424	0	1393	24	0
41	r	487	0	502	3	0
42	s	269	0	256	8	0
43	B	8	0	0	0	0
43	F	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	G	16	0	0	1	0
43	I	16	0	0	3	0
44	B	41	0	59	0	0
44	H	42	0	58	0	0
45	E	4	0	0	0	0
45	G	4	0	0	1	0
46	F	31	0	18	1	0
47	H	45	0	71	3	0
48	H	51	0	82	1	0
48	J	33	0	40	0	0
48	L	91	0	136	1	0
48	Y	41	0	56	0	0
48	Z	44	0	65	1	0
48	i	42	0	61	0	0
49	L	74	0	92	0	0
49	M	59	0	68	0	0
49	N	128	0	147	0	0
49	d	67	0	81	0	0
49	h	70	0	87	0	0
50	L	70	0	90	1	0
51	O	31	0	10	2	0
52	P	48	0	26	1	0
53	R	1	0	0	0	0
54	T	37	0	0	2	0
54	U	37	0	0	1	0
All	All	63712	0	64034	803	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 (803) 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)
40:p:131:PHE:O	40:p:135:THR:OG1	1.81	0.98
22:X:19:VAL:O	25:a:50:ARG:NH2	2.07	0.88
14:N:170:LEU:HD11	14:N:288:LEU:HD12	1.56	0.87
4:D:146:ARG:NH2	4:D:368:GLU:O	2.09	0.86
16:P:215:VAL:O	16:P:218:THR:OG1	1.93	0.86
16:P:249:THR:O	16:P:251:ARG:N	2.10	0.84
15:O:22:SER:OG	15:O:119:GLY:O	1.94	0.84
15:O:104:ARG:NE	15:O:131:ASP:OD1	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:318:ILE:HD11	7:G:511:VAL:HG23	1.60	0.81
7:G:260:GLU:OE2	7:G:397:LYS:NZ	2.13	0.81
3:C:47:GLU:OE1	3:C:106:ARG:NH2	2.13	0.81
15:O:90:ASP:O	15:O:95:ARG:NH2	2.13	0.81
13:M:346:ARG:NE	36:l:67:GLU:OE2	2.13	0.80
4:D:159:LEU:HD11	47:H:401:UQ9:H20	1.63	0.79
5:E:6:LEU:O	5:E:92:ARG:NH2	2.16	0.79
39:o:26:PRO:O	39:o:33:ARG:NH1	2.15	0.78
7:G:410:GLY:O	7:G:421:HIS:NE2	2.18	0.77
3:C:119:SER:OG	3:C:131:GLU:OE1	2.03	0.76
8:H:110:SER:OG	8:H:143:GLU:OE2	2.01	0.76
6:F:66:ARG:O	6:F:68:ARG:NH1	2.19	0.75
6:F:82:MET:SD	6:F:221:THR:OG1	2.43	0.75
7:G:439:PHE:CE2	7:G:443:LEU:HD21	2.22	0.74
12:L:594:ASN:OD1	23:Y:40:TYR:OH	2.03	0.74
14:N:332:MET:HA	14:N:332:MET:HE2	1.68	0.74
25:a:31:ASN:OD1	25:a:60:TYR:OH	2.01	0.74
7:G:111:GLY:O	7:G:117:GLN:NE2	2.20	0.74
12:L:227:PHE:O	12:L:230:HIS:ND1	2.21	0.73
8:H:97:ASN:ND2	8:H:163:GLN:OE1	2.21	0.73
4:D:145:THR:HG1	4:D:181:TYR:HH	1.30	0.72
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.71	0.72
34:j:39:ARG:NH1	34:j:43:ASP:OD2	2.22	0.72
5:E:12:THR:OG1	5:E:14:GLU:O	2.08	0.72
7:G:352:GLU:OE1	7:G:352:GLU:N	2.23	0.72
14:N:332:MET:HE1	28:d:37:LEU:HD13	1.72	0.71
13:M:139:GLN:OE1	13:M:340:ARG:NH1	2.23	0.71
6:F:258:ILE:HD11	6:F:279:LEU:HD11	1.73	0.71
40:p:11:GLU:OE1	40:p:115:ARG:NH1	2.24	0.71
9:I:34:ARG:NH2	24:Z:25:PRO:O	2.23	0.71
12:L:248:HIS:O	12:L:249:SER:OG	2.08	0.71
4:D:45:THR:HG23	4:D:45:THR:O	1.90	0.70
6:F:342:ASP:OD1	6:F:429:ARG:NH2	2.23	0.70
16:P:285:GLU:O	16:P:289:ILE:HG23	1.90	0.70
15:O:170:ILE:HD11	15:O:238:ILE:HD11	1.72	0.70
40:p:102:MET:HE1	40:p:134:VAL:HG12	1.72	0.70
6:F:132:ARG:NH2	42:s:58:PRO:O	2.24	0.70
7:G:317:ALA:CB	7:G:331:LEU:HD21	2.22	0.69
37:m:24:VAL:HG13	37:m:29:ARG:NH1	2.07	0.69
2:B:50:ALA:HB2	8:H:53:MET:HE2	1.74	0.69
40:p:98:ASP:OD2	40:p:142:TYR:OH	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:101:GLN:OE1	22:X:101:GLN:N	2.24	0.69
2:B:132:GLY:O	2:B:145:GLY:N	2.25	0.69
19:T:51:ILE:HD13	19:T:67:ALA:HB1	1.74	0.69
16:P:330:GLU:N	16:P:330:GLU:OE1	2.26	0.69
6:F:93:LEU:HD13	6:F:129:MET:HE1	1.75	0.69
7:G:476:LYS:O	7:G:480:THR:HG23	1.93	0.68
7:G:415:LEU:O	7:G:416:THR:OG1	2.11	0.68
15:O:281:GLU:N	15:O:281:GLU:OE1	2.26	0.68
2:B:44:ASP:OD1	2:B:45:ASP:N	2.27	0.68
7:G:468:VAL:HG23	7:G:649:ALA:HB1	1.76	0.68
22:X:46:ARG:NH1	24:Z:79:ASP:OD2	2.27	0.68
7:G:620:ARG:NE	7:G:633:TYR:OH	2.27	0.68
17:R:53:GLU:N	17:R:53:GLU:OE1	2.27	0.68
7:G:688:VAL:O	7:G:692:THR:HG23	1.94	0.68
11:K:12:PHE:CE1	14:N:72:LEU:HD22	2.29	0.68
28:d:108:THR:OG1	28:d:111:GLU:OE2	2.11	0.67
4:D:202:ASP:OD1	4:D:203:LEU:N	2.27	0.67
10:J:27:TYR:CE2	10:J:81:THR:HG22	2.29	0.67
16:P:185:TYR:HD2	16:P:191:VAL:HG13	1.59	0.67
2:B:76:ARG:NH2	4:D:172:GLU:OE2	2.27	0.66
7:G:528:ASP:OD2	7:G:545:TYR:OH	2.12	0.66
5:E:204:GLU:N	5:E:204:GLU:OE1	2.28	0.66
38:n:88:THR:O	38:n:89:SER:OG	2.13	0.66
3:C:182:ARG:NH1	21:W:111:GLU:OE1	2.29	0.66
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.29	0.66
7:G:371:VAL:HG22	7:G:450:MET:HE1	1.77	0.66
6:F:303:SER:OG	6:F:354:TYR:OH	1.94	0.65
8:H:200:LEU:HD23	8:H:282:TYR:HB3	1.78	0.65
34:j:60:THR:HG23	34:j:63:GLU:H	1.59	0.65
5:E:22:ASP:OD1	5:E:68:LYS:NZ	2.19	0.65
14:N:218:ALA:CB	14:N:244:ILE:HD11	2.25	0.65
15:O:191:GLU:O	15:O:194:VAL:HG12	1.97	0.65
5:E:27:ASN:ND2	5:E:57:GLN:OE1	2.30	0.65
32:h:87:TYR:OH	40:p:86:GLU:OE1	2.11	0.65
4:D:339:LYS:NZ	17:R:67:GLY:O	2.29	0.65
7:G:322:LEU:HD23	7:G:322:LEU:H	1.61	0.65
7:G:453:LEU:HD21	7:G:458:LEU:HD21	1.78	0.64
13:M:210:TYR:O	13:M:213:HIS:ND1	2.30	0.64
4:D:73:VAL:HG21	4:D:414:VAL:HG21	1.78	0.64
5:E:119:THR:HG21	5:E:166:PRO:HB3	1.78	0.64
12:L:187:VAL:HG12	13:M:383:MET:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:15:LEU:HD21	18:S:18:ILE:HD11	1.79	0.64
12:L:156:GLY:HA2	12:L:164:ALA:HB1	1.80	0.64
13:M:141:GLU:N	13:M:141:GLU:OE1	2.28	0.64
48:Z:401:3PE:O14	48:Z:401:3PE:N	2.23	0.64
5:E:202:LEU:HD12	5:E:202:LEU:O	1.98	0.63
8:H:302:MET:HE1	26:b:25:TRP:CD1	2.34	0.63
39:o:2:ALA:N	39:o:5:THR:HG1	1.95	0.63
8:H:195:ARG:HD3	8:H:231:ILE:HD11	1.80	0.63
31:g:90:GLU:OE1	40:p:64:HIS:NE2	2.29	0.63
42:s:50:LEU:O	42:s:53:SER:OG	2.10	0.63
2:B:54:SER:OG	8:H:51:ASP:OD1	2.11	0.63
4:D:42:LYS:NZ	4:D:43:ALA:O	2.31	0.63
42:s:36:GLN:OE1	42:s:36:GLN:N	2.30	0.63
5:E:50:VAL:HG21	5:E:73:LEU:HD21	1.79	0.63
6:F:82:MET:HE1	6:F:92:TYR:O	1.98	0.63
6:F:327:THR:OG1	6:F:328:GLY:N	2.30	0.63
16:P:157:ARG:NH2	16:P:227:THR:OG1	2.32	0.63
9:I:82:CYS:N	43:I:201:SF4:S1	2.72	0.63
27:c:28:TRP:O	27:c:32:ILE:HD12	1.98	0.63
37:m:128:TYR:OH	40:p:145:LEU:O	2.12	0.63
13:M:369:LEU:O	13:M:372:SER:OG	2.12	0.62
14:N:218:ALA:HB1	14:N:244:ILE:HD11	1.81	0.62
13:M:78:MET:HE1	13:M:439:LEU:HD12	1.81	0.62
7:G:20:VAL:HB	7:G:24:THR:HG21	1.82	0.62
19:T:47:GLN:NE2	19:T:51:ILE:HD11	2.15	0.62
8:H:157:ASN:ND2	8:H:159:SER:O	2.33	0.62
13:M:244:ILE:O	40:p:148:TYR:OH	2.17	0.62
14:N:128:LEU:O	14:N:132:THR:OG1	2.17	0.62
21:W:52:MET:HE1	21:W:105:VAL:HG21	1.81	0.62
31:g:98:ARG:NH1	31:g:105:ILE:O	2.30	0.62
22:X:150:ASN:OD1	29:e:50:ARG:NH1	2.33	0.62
33:i:110:LEU:HD11	40:p:18:ALA:HA	1.82	0.62
5:E:31:ILE:HD11	5:E:53:LEU:HD23	1.82	0.61
32:h:81:ASP:OD1	32:h:85:LYS:NZ	2.31	0.61
4:D:81:GLY:N	4:D:429:ASP:OD1	2.32	0.61
5:E:31:ILE:HD12	5:E:50:VAL:HG22	1.83	0.61
31:g:73:THR:HG21	32:h:36:VAL:HG11	1.81	0.61
2:B:148:ARG:NH1	3:C:174:LEU:O	2.32	0.61
18:S:24:GLN:NE2	18:S:56:GLU:OE1	2.34	0.61
12:L:202:MET:HA	12:L:202:MET:HE2	1.83	0.61
4:D:293:CYS:SG	4:D:420:THR:HG21	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:22:TYR:CD2	19:T:50:ILE:HD11	2.36	0.60
7:G:199:VAL:HG11	7:G:208:LEU:HD11	1.82	0.60
5:E:119:THR:HG22	5:E:122:ARG:HH21	1.67	0.60
12:L:513:MET:HE1	38:n:30:CYS:SG	2.41	0.60
7:G:366:THR:O	7:G:367:THR:OG1	2.12	0.60
7:G:472:ASN:OD1	7:G:473:MET:N	2.35	0.60
7:G:474:VAL:HG13	7:G:489:VAL:HG23	1.82	0.60
16:P:174:ARG:NH2	16:P:316:GLU:OE1	2.35	0.60
18:S:15:LEU:HD23	18:S:15:LEU:O	2.01	0.60
12:L:427:ILE:O	12:L:431:THR:OG1	2.10	0.60
13:M:88:ASN:OD1	13:M:89:ASN:N	2.34	0.60
36:l:76:ILE:HG23	36:l:80:LEU:HD22	1.84	0.59
15:O:25:ILE:HD12	15:O:48:MET:HE1	1.84	0.59
6:F:168:GLY:O	6:F:169:SER:OG	2.17	0.59
12:L:315:VAL:HG11	12:L:399:ILE:HD11	1.84	0.59
18:S:78:LEU:HD22	18:S:86:VAL:HG22	1.82	0.59
7:G:674:THR:O	7:G:679:ARG:NH1	2.35	0.59
15:O:194:VAL:HG21	15:O:199:LEU:HD21	1.84	0.59
7:G:474:VAL:HG13	7:G:489:VAL:CG2	2.32	0.59
12:L:96:VAL:HG12	12:L:100:ILE:HD12	1.86	0.58
6:F:389:ILE:HG23	6:F:419:ILE:HD12	1.85	0.58
13:M:1:FME:HE2	13:M:111:SER:HB3	1.85	0.58
4:D:212:TYR:CE1	24:Z:18:ILE:HD11	2.38	0.58
5:E:14:GLU:N	5:E:14:GLU:OE1	2.36	0.58
24:Z:97:MET:HE3	24:Z:100:VAL:HG21	1.86	0.58
8:H:170:GLU:OE1	22:X:97:ARG:NH2	2.35	0.58
9:I:79:CYS:HA	43:I:201:SF4:S2	2.44	0.58
7:G:11:VAL:HG11	7:G:73:VAL:CG2	2.34	0.58
6:F:368:GLY:HA3	6:F:399:ILE:HD11	1.86	0.58
29:e:101:GLU:N	29:e:101:GLU:OE1	2.37	0.58
6:F:276:LEU:HD23	6:F:312:CYS:HB2	1.86	0.57
22:X:51:ASP:OD2	22:X:53:ARG:NH2	2.37	0.57
36:l:67:GLU:OE1	36:l:67:GLU:N	2.30	0.57
9:I:66:GLU:OE2	9:I:151:TYR:OH	2.16	0.57
33:i:31:GLU:O	33:i:33:VAL:N	2.36	0.57
13:M:343:ILE:O	13:M:346:ARG:NH1	2.34	0.57
3:C:61:LEU:HD12	3:C:120:ILE:HG21	1.87	0.57
4:D:151:ILE:HD12	4:D:177:MET:HE1	1.87	0.57
12:L:486:LEU:O	12:L:489:THR:HG22	2.05	0.57
37:m:23:ASP:OD2	37:m:28:THR:HG21	2.05	0.57
12:L:430:VAL:O	12:L:430:VAL:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:251:THR:O	12:L:254:VAL:HG22	2.04	0.57
24:Z:23:ASN:O	24:Z:23:ASN:OD1	2.22	0.57
26:b:78:ASP:OD1	26:b:78:ASP:N	2.36	0.57
40:p:143:LEU:O	40:p:157:LYS:NZ	2.29	0.57
3:C:61:LEU:CD1	3:C:120:ILE:HD13	2.35	0.57
7:G:365:ASN:ND2	7:G:490:MET:O	2.34	0.57
19:U:86:VAL:HG23	19:U:87:TYR:N	2.19	0.56
38:n:131:SER:HB2	38:n:162:LEU:HD23	1.87	0.56
31:g:69:VAL:O	31:g:73:THR:HG23	2.05	0.56
21:W:52:MET:HE1	21:W:105:VAL:CG2	2.35	0.56
3:C:50:ILE:HD12	3:C:105:ILE:HD11	1.88	0.56
7:G:661:LEU:HD12	7:G:661:LEU:H	1.71	0.56
4:D:161:ILE:HG23	4:D:238:ARG:HG2	1.87	0.56
5:E:72:VAL:HG13	5:E:73:LEU:HD22	1.88	0.56
5:E:181:VAL:O	5:E:181:VAL:HG13	2.06	0.56
38:n:170:VAL:O	38:n:171:THR:OG1	2.23	0.56
7:G:126:ASP:OD2	7:G:127:ARG:NH2	2.39	0.56
7:G:597:TRP:CE3	7:G:619:VAL:HG21	2.41	0.56
40:p:105:ILE:HD13	40:p:134:VAL:HG21	1.88	0.56
4:D:148:LEU:HD23	4:D:174:ARG:HG2	1.88	0.56
12:L:293:LEU:O	12:L:294:THR:OG1	2.18	0.56
54:U:201:EHZ:O7	54:U:201:EHZ:O5	2.24	0.56
39:o:72:SER:OG	39:o:75:ASN:O	2.23	0.55
6:F:93:LEU:HD12	6:F:94:VAL:H	1.72	0.55
8:H:102:ILE:HD13	8:H:154:LEU:HD11	1.88	0.55
22:X:44:LEU:HD22	22:X:130:VAL:HG13	1.89	0.55
22:X:6:LEU:O	24:Z:87:ARG:NH2	2.40	0.55
7:G:356:THR:O	18:S:55:ARG:NH2	2.39	0.55
15:O:51:TYR:HB2	15:O:124:LEU:HD23	1.89	0.55
7:G:575:ASN:OD1	7:G:579:ARG:N	2.40	0.55
23:Y:19:CYS:SG	23:Y:20:HIS:N	2.79	0.55
32:h:142:ASP:O	32:h:143:ASN:ND2	2.39	0.55
3:C:179:GLU:OE1	16:P:40:ARG:NH2	2.38	0.55
12:L:407:TRP:CZ3	12:L:410:LEU:HD23	2.42	0.55
19:T:36:PHE:HD1	19:T:40:LEU:HD12	1.72	0.55
2:B:119:GLU:OE2	16:P:54:TYR:OH	2.14	0.55
5:E:63:ILE:O	5:E:67:ASN:ND2	2.38	0.55
13:M:216:LEU:HD11	13:M:220:HIS:CE1	2.42	0.55
1:A:58:VAL:HG11	8:H:286:MET:SD	2.47	0.55
7:G:391:PHE:CE2	7:G:395:ILE:HD11	2.42	0.55
12:L:97:THR:HG21	12:L:125:LEU:HD22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:335:ARG:NH2	9:I:131:ASP:OD1	2.40	0.54
7:G:199:VAL:CG1	7:G:208:LEU:HD11	2.37	0.54
13:M:36:LEU:HB2	31:g:67:VAL:HG22	1.89	0.54
18:S:81:LEU:O	18:S:86:VAL:HG23	2.07	0.54
2:B:101:THR:HA	2:B:129:CYS:HB3	1.89	0.54
7:G:11:VAL:HG11	7:G:73:VAL:HG22	1.89	0.54
7:G:35:MET:SD	7:G:36:GLN:N	2.80	0.54
15:O:73:PHE:CE2	15:O:299:LEU:HD11	2.41	0.54
14:N:68:MET:HA	14:N:68:MET:HE3	1.89	0.54
6:F:112:ARG:O	42:s:34:ASN:ND2	2.41	0.54
14:N:249:LEU:HD22	14:N:254:LEU:HD12	1.88	0.54
6:F:141:GLU:OE1	6:F:141:GLU:N	2.38	0.54
7:G:601:ARG:NH2	7:G:614:ASP:OD1	2.39	0.54
28:d:119:VAL:HG12	40:p:144:ASP:O	2.06	0.54
2:B:47:ILE:HD12	8:H:57:MET:SD	2.48	0.54
13:M:373:ILE:HG21	13:M:454:ILE:HD11	1.89	0.54
6:F:145:GLU:OE1	6:F:145:GLU:N	2.39	0.54
10:J:80:GLU:OE2	11:K:23:ARG:NH2	2.40	0.54
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.90	0.54
28:d:112:ILE:O	40:p:159:LYS:NZ	2.32	0.53
22:X:44:LEU:HD22	22:X:130:VAL:CG1	2.37	0.53
5:E:9:HIS:NE2	5:E:11:ASP:OD1	2.38	0.53
17:R:46:GLN:CG	17:R:46:GLN:O	2.56	0.53
28:d:119:VAL:HG11	40:p:146:GLY:HA2	1.90	0.53
3:C:66:ASP:O	20:V:82:GLN:NE2	2.40	0.53
6:F:400:GLU:OE2	6:F:413:TRP:NE1	2.41	0.53
13:M:106:LEU:HD13	13:M:234:ILE:HG21	1.89	0.53
15:O:104:ARG:NH2	51:O:401:GTP:O6	2.41	0.53
6:F:372:MET:HE2	6:F:399:ILE:CD1	2.39	0.53
20:V:8:THR:OG1	20:V:13:LEU:O	2.25	0.53
2:B:44:ASP:OD1	2:B:44:ASP:C	2.52	0.53
6:F:115:PRO:O	6:F:119:VAL:HG23	2.09	0.53
12:L:22:SER:HA	12:L:27:ILE:HD12	1.91	0.53
5:E:134:ASP:OD2	5:E:136:LEU:HD12	2.09	0.52
7:G:642:PHE:O	7:G:646:SER:OG	2.26	0.52
11:K:57:MET:N	11:K:58:PRO:CD	2.72	0.52
31:g:121:ASP:O	40:p:166:ARG:NH2	2.41	0.52
10:J:168:GLU:CG	14:N:5:THR:HG21	2.39	0.52
36:l:53:SER:OG	36:l:55:HIS:ND1	2.32	0.52
38:n:140:GLN:O	38:n:143:THR:HG22	2.09	0.52
7:G:461:ASP:OD1	7:G:462:ASP:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:307:LEU:O	8:H:311:THR:OG1	2.20	0.52
15:O:41:GLU:OE1	15:O:44:GLN:NE2	2.42	0.52
5:E:31:ILE:CD1	5:E:53:LEU:HD23	2.39	0.52
7:G:605:GLU:C	7:G:605:GLU:OE1	2.53	0.52
12:L:362:ILE:HA	12:L:365:ILE:HG22	1.92	0.52
18:S:22:LEU:HD12	18:S:23:CYS:N	2.25	0.52
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.45	0.52
7:G:24:THR:HG23	7:G:73:VAL:HG12	1.92	0.52
36:l:33:TYR:OH	36:l:45:ASP:OD1	2.25	0.52
5:E:191:PHE:N	5:E:194:GLU:OE2	2.43	0.52
6:F:344:VAL:HG23	6:F:380:VAL:HG22	1.91	0.52
6:F:366:ARG:NH1	6:F:367:GLU:OE2	2.43	0.52
12:L:400:ASN:OD1	12:L:489:THR:HG21	2.10	0.52
5:E:100:ILE:HG12	5:E:156:ILE:HD12	1.91	0.52
10:J:33:ILE:HD11	10:J:63:MET:HB2	1.92	0.52
19:U:86:VAL:HG23	19:U:87:TYR:H	1.75	0.52
9:I:70:ARG:HD2	9:I:134:VAL:HG11	1.92	0.51
19:T:16:LEU:HD21	19:T:32:VAL:HG22	1.91	0.51
29:e:68:ARG:O	29:e:72:MET:HG3	2.10	0.51
28:d:119:VAL:HG13	28:d:119:VAL:O	2.11	0.51
7:G:35:MET:HE3	7:G:81:THR:HB	1.93	0.51
7:G:366:THR:HG21	7:G:450:MET:SD	2.51	0.51
14:N:243:MET:HG3	28:d:44:MET:HE2	1.91	0.51
7:G:188:GLU:OE1	7:G:188:GLU:N	2.42	0.51
10:J:73:MET:HE1	11:K:79:VAL:HG22	1.91	0.51
19:U:88:GLU:OE1	32:h:8:LEU:HD11	2.10	0.51
6:F:212:ASP:OD2	6:F:212:ASP:C	2.53	0.51
13:M:405:MET:HE2	13:M:405:MET:HA	1.90	0.51
2:B:102:LEU:HD13	2:B:110:LEU:HD13	1.93	0.51
5:E:70:ALA:HB2	5:E:80:VAL:HG21	1.92	0.51
5:E:155:GLN:C	5:E:156:ILE:HD13	2.36	0.51
12:L:89:PHE:CE2	12:L:132:THR:HG21	2.44	0.51
20:V:19:PRO:HB2	20:V:76:VAL:HG21	1.92	0.51
7:G:511:VAL:HG21	7:G:532:ILE:HG13	1.93	0.51
7:G:572:THR:HG23	7:G:633:TYR:HE1	1.76	0.51
15:O:211:LEU:O	15:O:215:SER:OG	2.27	0.51
35:k:29:ILE:HD11	35:k:52:ARG:HG3	1.93	0.51
6:F:30:ASP:O	6:F:39:ARG:NH1	2.43	0.51
7:G:648:LEU:HD11	18:S:40:TYR:HE1	1.75	0.51
19:U:28:GLU:O	19:U:29:LYS:HG2	2.11	0.51
7:G:53:ARG:N	45:G:803:FES:S1	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:110:SER:O	8:H:113:VAL:HG12	2.11	0.51
12:L:205:ASN:OD1	12:L:206:ASN:N	2.44	0.51
14:N:243:MET:SD	14:N:330:ALA:HB1	2.51	0.51
31:g:83:MET:HE1	40:p:93:ARG:HG2	1.91	0.50
50:L:705:LMT:O3'	50:L:705:LMT:O2B	2.24	0.50
14:N:53:THR:O	14:N:57:THR:HG23	2.11	0.50
39:o:102:GLU:OE2	39:o:105:ARG:NH2	2.44	0.50
5:E:105:THR:HG22	5:E:106:THR:H	1.76	0.50
13:M:72:LEU:HD11	13:M:233:ALA:HB1	1.94	0.50
16:P:294:PRO:O	16:P:295:THR:OG1	2.27	0.50
1:A:88:MET:CE	8:H:309:ILE:HG21	2.42	0.50
7:G:136:ALA:HB3	17:R:56:ILE:HD13	1.94	0.50
28:d:107:LYS:O	28:d:112:ILE:HD11	2.11	0.50
5:E:46:ALA:O	5:E:50:VAL:HG23	2.11	0.50
5:E:201:SER:OG	6:F:20:ARG:NE	2.45	0.50
7:G:439:PHE:CD2	7:G:443:LEU:HD21	2.47	0.50
10:J:96:VAL:O	10:J:100:VAL:HG23	2.11	0.50
21:W:44:GLU:CD	21:W:96:ILE:HD13	2.37	0.50
29:e:58:GLU:N	29:e:58:GLU:OE1	2.43	0.50
12:L:513:MET:HE3	12:L:514:ASN:H	1.76	0.50
13:M:307:TRP:CZ2	37:m:127:SER:HB3	2.46	0.50
14:N:255:PRO:HA	14:N:260:PHE:CG	2.47	0.50
40:p:118:GLU:OE2	40:p:118:GLU:O	2.30	0.50
8:H:65:THR:O	8:H:124:ASN:ND2	2.41	0.50
37:m:27:GLU:OE1	37:m:27:GLU:C	2.55	0.50
7:G:157:THR:N	43:G:802:SF4:S4	2.82	0.50
7:G:511:VAL:HG21	7:G:532:ILE:CG1	2.42	0.50
14:N:296:LEU:O	14:N:300:THR:HG22	2.12	0.50
7:G:145:LEU:HD22	7:G:269:PHE:CD2	2.47	0.50
12:L:399:ILE:HD13	12:L:412:THR:HG21	1.93	0.49
8:H:179:TRP:N	8:H:180:PRO:CD	2.75	0.49
8:H:207:LEU:O	8:H:208:VAL:C	2.56	0.49
15:O:170:ILE:CD1	15:O:238:ILE:HD11	2.41	0.49
5:E:194:GLU:HA	6:F:26:TYR:CE1	2.47	0.49
6:F:302:SER:OG	6:F:350:LEU:HD22	2.12	0.49
9:I:16:MET:HG3	24:Z:32:TYR:OH	2.12	0.49
12:L:71:MET:SD	13:M:310:MET:SD	3.10	0.49
15:O:138:MET:HE2	51:O:401:GTP:HN21	1.76	0.49
15:O:84:ASP:OD1	15:O:193:LYS:NZ	2.27	0.49
4:D:147:ILE:HG22	4:D:177:MET:HE1	1.94	0.49
7:G:252:PRO:HB3	7:G:263:ILE:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:146:TYR:N	14:N:147:PRO:CD	2.76	0.49
14:N:166:ALA:HB1	14:N:288:LEU:HB2	1.95	0.49
22:X:46:ARG:NH2	32:h:142:ASP:OD1	2.46	0.49
39:o:2:ALA:O	39:o:5:THR:OG1	2.31	0.49
5:E:100:ILE:HG21	5:E:120:LEU:HD11	1.93	0.49
7:G:142:ILE:HG22	7:G:143:GLY:N	2.27	0.49
7:G:664:PRO:O	7:G:666:LEU:N	2.45	0.49
31:g:62:PHE:O	31:g:67:VAL:HG23	2.11	0.49
12:L:261:VAL:HG22	12:L:317:LEU:HD21	1.95	0.49
13:M:278:ARG:O	37:m:71:ARG:NH2	2.45	0.49
16:P:61:LEU:C	16:P:61:LEU:HD12	2.38	0.49
33:i:87:TYR:O	33:i:88:HIS:ND1	2.45	0.49
36:l:33:TYR:OH	36:l:45:ASP:O	2.30	0.49
4:D:148:LEU:HD21	4:D:177:MET:HB2	1.94	0.49
7:G:272:ASP:OD2	7:G:682:GLN:N	2.43	0.49
7:G:315:VAL:O	7:G:340:SER:OG	2.20	0.49
7:G:587:VAL:HG12	7:G:588:THR:N	2.28	0.49
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.48	0.49
12:L:349:SER:HB2	12:L:366:MET:HE1	1.94	0.49
14:N:273:ASN:OD1	23:Y:142:VAL:N	2.39	0.49
3:C:78:LEU:HB3	3:C:130:TYR:HB3	1.95	0.48
7:G:309:ASN:OD1	7:G:309:ASN:C	2.56	0.48
12:L:187:VAL:HG12	13:M:383:MET:CG	2.43	0.48
8:H:187:ILE:HD12	48:H:403:3PE:H261	1.95	0.48
12:L:285:THR:HG22	12:L:415:ALA:HB1	1.95	0.48
34:j:66:ILE:HD11	39:o:106:ARG:HB2	1.95	0.48
8:H:113:VAL:HG21	8:H:139:THR:OG1	2.13	0.48
12:L:383:MET:HE2	12:L:383:MET:HA	1.96	0.48
12:L:451:MET:HE3	34:j:24:GLN:OE1	2.13	0.48
3:C:204:GLU:OE2	3:C:210:ARG:NH2	2.43	0.48
7:G:54:MET:HE2	7:G:94:MET:HE2	1.95	0.48
13:M:36:LEU:HD12	13:M:39:LEU:HD12	1.94	0.48
13:M:403:THR:HA	13:M:406:TYR:CE2	2.48	0.48
6:F:250:ASN:CB	6:F:318:ASP:OD2	2.62	0.48
19:T:45:LEU:O	19:T:49:GLU:HG3	2.14	0.48
24:Z:97:MET:CE	24:Z:100:VAL:HG21	2.43	0.48
29:e:21:SER:N	29:e:36:GLU:OE1	2.42	0.48
8:H:200:LEU:HD23	8:H:282:TYR:CB	2.43	0.48
13:M:173:THR:HB	32:h:101:ALA:HB2	1.95	0.48
14:N:149:LEU:HD13	14:N:154:ILE:HD11	1.95	0.48
7:G:594:ARG:NH1	21:W:127:GLY:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:26:LEU:HD23	11:K:78:LEU:HD12	1.95	0.48
16:P:188:PHE:O	16:P:190:ALA:N	2.46	0.48
30:f:5:LEU:HD12	30:f:5:LEU:O	2.14	0.48
37:m:110:ARG:O	37:m:114:LEU:HD23	2.14	0.48
42:s:41:ASN:OD1	42:s:43:TYR:N	2.43	0.48
12:L:161:ARG:NH1	12:L:238:GLU:OE1	2.47	0.48
12:L:230:HIS:N	12:L:231:PRO:CD	2.77	0.48
12:L:399:ILE:CD1	12:L:412:THR:HG21	2.44	0.48
12:L:503:GLU:OE1	12:L:503:GLU:HA	2.13	0.48
2:B:180:GLU:O	2:B:181:GLN:HG2	2.14	0.48
13:M:41:LEU:HB3	13:M:63:THR:HG22	1.96	0.48
14:N:267:ILE:HD11	14:N:283:ALA:HB2	1.96	0.48
8:H:144:VAL:HG13	8:H:145:THR:HG23	1.96	0.47
15:O:240:TYR:OH	20:V:18:THR:OG1	2.18	0.47
14:N:213:ALA:HB3	14:N:214:PRO:HD3	1.96	0.47
19:T:25:ILE:HD12	19:T:25:ILE:C	2.39	0.47
13:M:17:LEU:HD21	28:d:54:MET:SD	2.54	0.47
14:N:300:THR:HG23	14:N:301:SER:N	2.30	0.47
7:G:338:VAL:O	7:G:338:VAL:HG12	2.14	0.47
7:G:358:LEU:HD23	7:G:641:TYR:HB2	1.96	0.47
9:I:15:ASP:N	26:b:9:LYS:NZ	2.63	0.47
19:T:11:ILE:HG23	19:T:80:ILE:HG21	1.95	0.47
2:B:73:ALA:HA	2:B:79:MET:HG2	1.96	0.47
9:I:77:GLU:O	9:I:107:ARG:NH1	2.47	0.47
7:G:456:SER:OG	7:G:663:PRO:O	2.18	0.47
15:O:51:TYR:CB	15:O:124:LEU:HD23	2.45	0.47
19:U:8:LEU:HD12	19:U:87:TYR:CD1	2.50	0.47
4:D:45:THR:O	4:D:45:THR:CG2	2.60	0.47
4:D:218:PHE:HD2	4:D:308:LEU:HD11	1.80	0.47
10:J:51:LEU:HD11	11:K:57:MET:HE2	1.97	0.47
12:L:529:PHE:HB3	12:L:530:PRO:HD3	1.96	0.47
13:M:63:THR:OG1	13:M:64:PRO:HD3	2.13	0.47
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.95	0.47
15:O:221:LEU:HD11	15:O:241:LEU:HD11	1.97	0.47
19:T:61:GLU:OE2	19:T:61:GLU:N	2.36	0.47
19:U:43:ASP:OD2	19:U:44:SER:N	2.48	0.47
31:g:29:GLU:OE1	31:g:30:PRO:HD2	2.15	0.47
39:o:72:SER:O	39:o:73:PHE:C	2.57	0.47
7:G:317:ALA:HB3	7:G:331:LEU:HD21	1.97	0.47
9:I:129:PRO:HD2	43:I:201:SF4:S3	2.54	0.47
14:N:314:MET:HE1	15:O:267:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:106:THR:HG22	23:Y:106:THR:O	2.13	0.47
1:A:65:PHE:CE2	1:A:98:LEU:HD21	2.50	0.47
5:E:72:VAL:HG13	5:E:73:LEU:CD2	2.44	0.47
12:L:180:ILE:HD12	13:M:397:GLY:HA2	1.97	0.47
15:O:58:TYR:CZ	15:O:62:THR:HG21	2.50	0.47
4:D:326:ASP:OD1	7:G:127:ARG:NH1	2.48	0.47
6:F:306:LEU:CD2	6:F:343:ILE:HD11	2.45	0.47
10:J:33:ILE:HD12	10:J:60:LEU:HD23	1.97	0.47
28:d:101:PHE:CZ	32:h:110:VAL:HG22	2.50	0.47
7:G:667:THR:HG22	7:G:668:ILE:H	1.79	0.46
12:L:554:ASP:OD2	13:M:213:HIS:NE2	2.45	0.46
15:O:214:MET:HE3	15:O:218:CYS:SG	2.54	0.46
19:T:7:THR:O	19:T:7:THR:OG1	2.33	0.46
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.96	0.46
13:M:10:MET:HE2	13:M:10:MET:HA	1.96	0.46
3:C:57:VAL:HG13	3:C:58:ILE:N	2.30	0.46
5:E:119:THR:HG22	5:E:122:ARG:NH2	2.30	0.46
14:N:289:ASN:HA	14:N:292:PHE:CE2	2.50	0.46
40:p:76:CYS:SG	40:p:77:LYS:N	2.87	0.46
40:p:102:MET:HA	40:p:102:MET:HE2	1.97	0.46
4:D:165:THR:HG23	4:D:166:PRO:HD3	1.96	0.46
6:F:362:CYS:HB3	6:F:404:ILE:HD12	1.96	0.46
7:G:533:THR:OG1	7:G:534:ARG:N	2.49	0.46
8:H:85:LEU:HD13	8:H:233:LEU:CD2	2.45	0.46
13:M:23:THR:HG23	13:M:24:TRP:N	2.31	0.46
16:P:101:THR:HG22	16:P:102:ARG:N	2.30	0.46
16:P:280:THR:HG22	16:P:281:LYS:N	2.31	0.46
19:T:81:ALA:O	19:T:82:ASP:C	2.59	0.46
7:G:452:VAL:HG12	7:G:491:ASN:OD1	2.16	0.46
7:G:475:GLN:NE2	7:G:643:GLN:OE1	2.49	0.46
9:I:16:MET:HE1	26:b:9:LYS:HG3	1.98	0.46
15:O:57:GLN:O	15:O:61:THR:HG23	2.15	0.46
4:D:300:ARG:NH2	4:D:420:THR:O	2.42	0.46
8:H:24:GLU:OE2	8:H:274:ARG:NH1	2.48	0.46
13:M:59:ASP:OD2	13:M:245:ARG:NH2	2.41	0.46
13:M:216:LEU:HB3	13:M:217:PRO:HD3	1.98	0.46
13:M:367:LEU:C	13:M:367:LEU:HD12	2.40	0.46
37:m:24:VAL:HG12	37:m:24:VAL:O	2.16	0.46
1:A:70:ALA:HB2	10:J:58:ILE:HD11	1.97	0.46
5:E:120:LEU:HD23	5:E:124:LEU:HD13	1.97	0.46
6:F:143:TYR:OH	42:s:42:THR:O	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:156:ALA:HB1	6:F:162:ILE:HD12	1.98	0.46
6:F:188:GLU:OE1	46:F:502:FMN:HM83	2.16	0.46
7:G:315:VAL:HG21	7:G:338:VAL:HG11	1.98	0.46
8:H:63:PRO:HB2	8:H:66:THR:HG23	1.96	0.46
10:J:121:GLY:HA2	10:J:124:LEU:HD13	1.98	0.46
11:K:92:ASN:O	11:K:94:ASN:N	2.49	0.46
12:L:241:THR:HG21	12:L:344:GLY:HA3	1.96	0.46
16:P:311:GLU:OE1	16:P:311:GLU:N	2.45	0.46
2:B:43:LEU:O	2:B:47:ILE:HG12	2.15	0.46
15:O:29:GLY:O	15:O:126:ARG:NH1	2.49	0.46
16:P:206:TYR:CE2	16:P:208:ALA:HB3	2.51	0.46
31:g:69:VAL:HG11	32:h:32:THR:HG22	1.98	0.46
4:D:165:THR:N	4:D:166:PRO:HD2	2.31	0.46
8:H:24:GLU:CA	8:H:271:LEU:HD13	2.45	0.46
14:N:142:LEU:HB3	14:N:194:LEU:HD21	1.97	0.46
18:S:40:TYR:CD1	18:S:40:TYR:C	2.93	0.46
23:Y:19:CYS:O	23:Y:20:HIS:C	2.59	0.46
24:Z:104:LYS:HB2	24:Z:107:GLU:HB2	1.98	0.46
36:l:57:ARG:NH2	36:l:74:GLU:OE2	2.47	0.46
6:F:302:SER:CB	6:F:350:LEU:HD22	2.47	0.45
7:G:337:LYS:HD3	7:G:609:ILE:HG23	1.98	0.45
7:G:402:ASN:O	7:G:403:ASP:C	2.60	0.45
14:N:277:ILE:HD12	14:N:277:ILE:H	1.80	0.45
18:S:21:HIS:O	18:S:62:PRO:HA	2.16	0.45
20:V:37:PHE:O	20:V:44:ARG:NH1	2.49	0.45
24:Z:142:TYR:O	24:Z:143:THR:C	2.58	0.45
30:f:52:GLU:OE2	30:f:52:GLU:N	2.45	0.45
37:m:23:ASP:CG	37:m:25:SER:HG	2.25	0.45
38:n:162:LEU:N	38:n:162:LEU:HD22	2.31	0.45
6:F:15:LEU:HD11	6:F:19:ASP:HB3	1.98	0.45
7:G:217:ALA:HB2	7:G:248:MET:HE2	1.99	0.45
7:G:511:VAL:O	7:G:511:VAL:HG22	2.16	0.45
12:L:191:LEU:HD12	13:M:386:PHE:HD2	1.82	0.45
11:K:39:SER:O	11:K:43:MET:HG3	2.15	0.45
14:N:313:MET:HE1	15:O:102:ALA:HB3	1.98	0.45
14:N:319:LYS:HD3	15:O:267:THR:HG21	1.96	0.45
15:O:291:ARG:NE	31:g:27:ASP:OD2	2.37	0.45
35:k:29:ILE:HD12	35:k:29:ILE:N	2.31	0.45
35:k:68:PHE:CE1	35:k:72:ILE:HD11	2.52	0.45
7:G:136:ALA:HA	7:G:151:THR:HG23	1.98	0.45
7:G:195:LEU:O	7:G:198:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:315:VAL:CG1	12:L:399:ILE:HD11	2.46	0.45
13:M:192:ASN:HB3	13:M:253:LEU:HD11	1.98	0.45
15:O:198:TYR:CE2	15:O:202:ILE:HD11	2.51	0.45
25:a:6:LEU:N	25:a:7:PRO:CD	2.79	0.45
6:F:15:LEU:O	6:F:20:ARG:NH1	2.50	0.45
6:F:137:TYR:CB	6:F:192:LEU:HD21	2.46	0.45
6:F:268:VAL:HG22	6:F:269:GLU:N	2.31	0.45
36:l:98:ASP:OD1	36:l:99:VAL:N	2.50	0.45
19:U:57:GLU:OE2	34:j:11:TYR:OH	2.28	0.45
33:i:1:SAC:HB3	33:i:1:SAC:H2A1	1.98	0.45
34:j:54:PRO:HD2	39:o:98:MET:HE1	1.99	0.45
54:T:201:EHZ:O2	54:T:201:EHZ:O1	2.31	0.45
19:U:46:ASP:OD1	38:n:44:ARG:NH2	2.49	0.45
6:F:409:ASP:OD1	6:F:409:ASP:N	2.49	0.45
7:G:213:TYR:O	7:G:213:TYR:CG	2.70	0.45
7:G:440:CYS:O	7:G:444:LYS:HG2	2.17	0.45
12:L:350:LEU:O	12:L:352:ASP:N	2.43	0.45
22:X:17:VAL:HG23	22:X:18:LYS:N	2.31	0.45
33:i:1:SAC:H2A1	33:i:1:SAC:CB	2.46	0.45
7:G:354:ALA:HB2	7:G:648:LEU:HD12	1.99	0.45
12:L:264:HIS:N	12:L:265:PRO:HD2	2.32	0.45
37:m:33:VAL:HG12	38:n:148:ILE:HD12	1.99	0.45
39:o:82:GLU:OE1	39:o:82:GLU:N	2.48	0.45
4:D:73:VAL:HG21	4:D:414:VAL:CG2	2.45	0.44
5:E:142:VAL:HG12	5:E:143:GLU:N	2.32	0.44
7:G:6:SER:OG	7:G:7:ASN:N	2.49	0.44
7:G:648:LEU:O	7:G:652:VAL:HG23	2.17	0.44
12:L:378:LEU:CD1	34:j:32:MET:HE1	2.47	0.44
38:n:170:VAL:HG12	38:n:171:THR:N	2.32	0.44
12:L:352:ASP:CG	12:L:352:ASP:O	2.60	0.44
19:U:52:MET:HE1	38:n:23:LEU:HD13	1.99	0.44
30:f:5:LEU:HD13	30:f:9:HIS:CD2	2.52	0.44
7:G:624:GLU:HB2	7:G:631:VAL:HG21	1.99	0.44
12:L:305:SER:OG	12:L:336:LYS:NZ	2.50	0.44
41:r:94:VAL:HG22	41:r:95:THR:N	2.31	0.44
4:D:371:LYS:HE2	4:D:424:VAL:HG13	1.98	0.44
6:F:91:LYS:O	6:F:132:ARG:N	2.41	0.44
11:K:66:PHE:CZ	14:N:31:VAL:HG13	2.52	0.44
37:m:111:LYS:O	37:m:115:ILE:HG13	2.17	0.44
2:B:106:MET:HE3	2:B:109:ALA:HB3	2.00	0.44
5:E:115:SER:O	5:E:119:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:174:THR:HG22	7:G:183:VAL:HG22	1.99	0.44
8:H:26:LYS:NZ	8:H:37:PRO:O	2.44	0.44
12:L:15:LEU:CD1	12:L:129:LEU:HD12	2.48	0.44
32:h:32:THR:HG22	32:h:32:THR:O	2.17	0.44
12:L:378:LEU:HD12	34:j:32:MET:HE1	2.00	0.44
13:M:61:LEU:HD22	13:M:244:ILE:HG21	2.00	0.44
38:n:139:LEU:HD11	38:n:165:LEU:HG	2.00	0.44
7:G:284:VAL:O	7:G:291:LEU:HD12	2.18	0.44
7:G:689:LYS:O	7:G:692:THR:OG1	2.25	0.44
8:H:100:LEU:HD12	10:J:53:LEU:HD12	2.00	0.44
23:Y:47:ALA:HB3	23:Y:53:ALA:HB2	2.00	0.44
6:F:65:LEU:O	6:F:75:THR:OG1	2.30	0.44
7:G:667:THR:HG22	7:G:668:ILE:N	2.32	0.44
12:L:203:PHE:CZ	40:p:109:LEU:HD11	2.51	0.44
12:L:309:GLN:O	12:L:313:MET:HG3	2.18	0.44
14:N:200:LEU:HD11	14:N:269:GLU:HG3	1.99	0.44
15:O:306:PRO:O	27:c:3:TYR:CZ	2.71	0.44
21:W:40:ALA:HB1	21:W:92:LEU:HD21	1.99	0.44
6:F:93:LEU:HD12	6:F:94:VAL:N	2.33	0.44
6:F:268:VAL:HG22	6:F:269:GLU:H	1.82	0.44
11:K:91:GLN:OE1	11:K:91:GLN:N	2.47	0.44
2:B:94:ASP:OD1	8:H:54:LYS:HD2	2.18	0.43
4:D:34:ASN:O	4:D:36:VAL:N	2.51	0.43
7:G:114:CYS:SG	7:G:116:LEU:HB3	2.58	0.43
7:G:332:LYS:HA	7:G:343:LEU:HD13	2.00	0.43
9:I:97:GLU:HB2	9:I:110:ARG:HG2	2.00	0.43
48:L:703:3PE:H3E2	13:M:68:LEU:HD13	2.00	0.43
15:O:38:LEU:CD2	15:O:172:ILE:HD11	2.48	0.43
16:P:101:THR:N	16:P:104:PHE:O	2.51	0.43
36:l:81:ASP:OD1	36:l:81:ASP:N	2.50	0.43
3:C:71:GLN:O	3:C:73:LYS:N	2.51	0.43
5:E:44:ALA:O	5:E:47:VAL:HG23	2.18	0.43
8:H:215:TYR:HD1	8:H:219:PRO:HB2	1.82	0.43
14:N:314:MET:HE1	15:O:267:THR:CG2	2.48	0.43
19:T:69:LYS:O	19:T:71:MET:N	2.51	0.43
5:E:199:LEU:N	5:E:199:LEU:HD22	2.33	0.43
6:F:95:VAL:HG21	6:F:122:CYS:SG	2.57	0.43
7:G:663:PRO:N	7:G:664:PRO:HA	2.33	0.43
12:L:223:LYS:HG2	12:L:255:ALA:HB3	2.01	0.43
15:O:145:ARG:NH1	15:O:147:GLN:OE1	2.51	0.43
29:e:37:LYS:NZ	29:e:41:GLU:OE1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:m:127:SER:O	37:m:128:TYR:C	2.60	0.43
40:p:166:ARG:O	40:p:170:ARG:HD2	2.18	0.43
7:G:615:THR:O	7:G:619:VAL:HG23	2.19	0.43
4:D:145:THR:OG1	4:D:181:TYR:OH	2.08	0.43
13:M:12:LEU:HB2	13:M:13:PRO:HD3	2.00	0.43
4:D:112:MET:HA	4:D:115:GLU:HG2	2.00	0.43
4:D:149:ASN:OD1	4:D:149:ASN:C	2.60	0.43
4:D:294:TYR:CE2	4:D:298:LEU:HD11	2.53	0.43
6:F:270:GLU:HG2	6:F:274:VAL:HG21	1.99	0.43
8:H:114:TYR:OH	10:J:60:LEU:O	2.34	0.43
16:P:96:GLY:O	52:P:501:NDP:H8A	2.19	0.43
31:g:120:GLU:OE2	31:g:120:GLU:HA	2.19	0.43
2:B:96:MET:CE	2:B:113:VAL:HG23	2.48	0.43
4:D:241:ASP:OD1	4:D:290:ARG:NH2	2.52	0.43
5:E:132:THR:HG23	5:E:135:LYS:H	1.84	0.43
6:F:192:LEU:HD23	6:F:192:LEU:O	2.19	0.43
8:H:316:PRO:HG3	24:Z:56:ARG:HB3	2.00	0.43
11:K:23:ARG:O	11:K:24:SER:OG	2.31	0.43
12:L:111:ASP:OD1	12:L:112:PRO:O	2.37	0.43
14:N:338:PRO:O	22:X:169:TRP:NE1	2.49	0.43
19:U:62:ILE:HD12	19:U:79:TYR:CE1	2.54	0.43
23:Y:44:LEU:O	23:Y:45:ASN:CB	2.66	0.43
4:D:151:ILE:HD12	4:D:177:MET:CE	2.48	0.43
12:L:295:GLN:O	12:L:301:ILE:HD11	2.18	0.43
15:O:97:GLN:NE2	15:O:131:ASP:OD2	2.51	0.43
16:P:23:VAL:O	16:P:48:PRO:HD2	2.19	0.43
4:D:272:THR:HG22	41:r:100:MET:HE1	2.00	0.43
13:M:123:GLU:HB3	14:N:255:PRO:CG	2.49	0.43
14:N:292:PHE:CD1	14:N:292:PHE:C	2.96	0.43
22:X:4:VAL:HG23	22:X:4:VAL:O	2.17	0.43
37:m:36:LEU:HD22	38:n:7:ALA:N	2.34	0.43
2:B:57:PRO:HA	2:B:95:VAL:O	2.18	0.43
2:B:167:LEU:HD23	9:I:52:TYR:CD2	2.53	0.43
3:C:209:TYR:OH	41:r:62:VAL:HG12	2.19	0.43
4:D:134:ALA:HB2	4:D:323:ILE:O	2.19	0.43
7:G:474:VAL:HG21	7:G:490:MET:HB2	2.00	0.43
12:L:352:ASP:O	12:L:352:ASP:OD1	2.36	0.43
13:M:303:ILE:HD11	13:M:308:SER:OG	2.19	0.43
13:M:310:MET:HE3	13:M:314:MET:HE1	2.00	0.43
13:M:418:LYS:NZ	38:n:94:GLU:OE1	2.50	0.43
30:f:5:LEU:HD12	30:f:5:LEU:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:N	1:A:74:PRO:CD	2.82	0.42
2:B:96:MET:HE2	2:B:113:VAL:HG23	2.00	0.42
3:C:117:ILE:HG22	3:C:118:ASP:N	2.33	0.42
4:D:302:GLU:OE2	4:D:306:GLN:NE2	2.46	0.42
6:F:30:ASP:O	6:F:39:ARG:NH2	2.52	0.42
6:F:137:TYR:HB2	6:F:192:LEU:HD21	2.00	0.42
14:N:41:ILE:N	14:N:42:PRO:HD2	2.34	0.42
14:N:242:THR:HG23	14:N:243:MET:N	2.35	0.42
16:P:41:MET:HE2	16:P:215:VAL:HG13	2.00	0.42
19:T:49:GLU:OE1	21:W:66:ARG:NH2	2.52	0.42
6:F:302:SER:HB2	6:F:350:LEU:HD22	2.02	0.42
7:G:35:MET:HG2	7:G:81:THR:HG21	2.01	0.42
8:H:52:ALA:HB2	47:H:401:UQ9:H42A	2.01	0.42
8:H:310:PHE:CD1	8:H:310:PHE:C	2.98	0.42
12:L:131:LEU:HD23	12:L:131:LEU:C	2.44	0.42
22:X:92:ASN:OD1	22:X:93:MET:N	2.53	0.42
6:F:276:LEU:HD13	6:F:317:MET:SD	2.59	0.42
7:G:580:ALA:O	7:G:581:GLN:NE2	2.45	0.42
9:I:15:ASP:N	26:b:9:LYS:HZ1	2.17	0.42
18:S:15:LEU:HD21	18:S:18:ILE:CD1	2.47	0.42
18:S:17:GLU:OE2	18:S:67:ARG:NH2	2.52	0.42
32:h:8:LEU:N	32:h:8:LEU:HD12	2.35	0.42
38:n:6:PRO:HG2	38:n:8:TYR:O	2.20	0.42
3:C:17:VAL:HG23	3:C:18:THR:N	2.34	0.42
6:F:261:HIS:ND1	6:F:338:ASP:OD1	2.53	0.42
6:F:351:ILE:HD11	6:F:415:VAL:HG23	2.01	0.42
6:F:392:LEU:HD23	6:F:419:ILE:HD11	2.01	0.42
7:G:348:ILE:N	7:G:459:GLN:OE1	2.49	0.42
9:I:16:MET:CE	26:b:9:LYS:HG3	2.49	0.42
12:L:221:THR:HG23	12:L:226:GLN:HB2	2.01	0.42
15:O:80:GLU:OE1	15:O:80:GLU:N	2.48	0.42
16:P:77:ASP:O	16:P:80:SER:OG	2.38	0.42
18:S:78:LEU:HD23	18:S:81:LEU:HD22	2.01	0.42
31:g:105:ILE:HG21	40:p:105:ILE:HD11	2.01	0.42
39:o:2:ALA:N	39:o:5:THR:OG1	2.51	0.42
40:p:27:ASN:OD1	40:p:30:THR:HG23	2.19	0.42
6:F:404:ILE:HD11	7:G:50:GLY:O	2.20	0.42
7:G:249:ARG:NE	7:G:251:LEU:HD11	2.33	0.42
15:O:252:ASP:OD1	15:O:255:THR:OG1	2.30	0.42
36:l:67:GLU:H	36:l:67:GLU:CD	2.25	0.42
4:D:110:SER:HA	4:D:145:THR:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:349:PHE:CE2	9:I:84:LEU:HD11	2.55	0.42
10:J:54:MET:O	10:J:58:ILE:HG12	2.19	0.42
13:M:458:THR:O	40:p:149:TYR:OH	2.37	0.42
19:U:9:ASP:OD1	19:U:10:GLY:N	2.53	0.42
22:X:82:THR:HA	22:X:85:TRP:CD1	2.55	0.42
25:a:1:MET:SD	25:a:1:MET:N	2.93	0.42
13:M:127:ILE:HB	13:M:128:PRO:HD3	2.01	0.42
13:M:406:TYR:CD1	13:M:406:TYR:C	2.98	0.42
19:T:17:TYR:O	19:T:21:LEU:HD23	2.20	0.42
23:Y:10:TYR:O	23:Y:22:LYS:NZ	2.53	0.42
24:Z:143:THR:HB	25:a:48:MET:HE1	2.02	0.42
32:h:41:THR:HG22	32:h:45:ILE:HD12	2.02	0.42
10:J:6:PHE:CG	10:J:120:LEU:HD21	2.55	0.42
10:J:62:GLY:O	10:J:66:VAL:HG23	2.19	0.42
14:N:335:MET:O	28:d:33:TYR:OH	2.29	0.42
16:P:48:PRO:HA	16:P:71:LEU:O	2.20	0.42
23:Y:3:VAL:HG12	23:Y:4:LYS:H	1.84	0.42
28:d:105:GLU:N	28:d:105:GLU:OE1	2.53	0.42
38:n:88:THR:O	38:n:89:SER:CB	2.67	0.42
38:n:127:LEU:HD11	38:n:162:LEU:HD21	2.01	0.42
4:D:128:ILE:HD13	4:D:330:VAL:HG11	2.02	0.42
4:D:150:HIS:NE2	4:D:303:GLU:OE1	2.53	0.42
6:F:325:ALA:O	6:F:326:GLN:HB2	2.20	0.42
7:G:336:ASN:OD1	18:S:67:ARG:CZ	2.67	0.42
47:H:401:UQ9:H12	47:H:401:UQ9:H15	1.76	0.42
19:T:48:VAL:HG12	19:T:52:MET:HE2	2.01	0.42
19:U:52:MET:HE1	38:n:23:LEU:CD1	2.50	0.42
22:X:43:MET:HE3	24:Z:72:PRO:HA	2.01	0.42
29:e:46:ILE:HG22	29:e:50:ARG:NH1	2.35	0.42
1:A:38:GLU:HG2	4:D:50:ASN:HB2	2.02	0.41
4:D:44:VAL:O	4:D:44:VAL:HG13	2.20	0.41
7:G:147:LYS:HD2	7:G:149:ILE:HD11	2.02	0.41
7:G:357:ASP:HA	18:S:53:LEU:HD23	2.01	0.41
10:J:102:LEU:HD21	11:K:6:PHE:HZ	1.84	0.41
4:D:62:LEU:HB2	4:D:425:PHE:CZ	2.55	0.41
4:D:202:ASP:N	4:D:323:ILE:HD13	2.35	0.41
7:G:380:VAL:HG12	7:G:409:ILE:HD12	2.00	0.41
8:H:307:LEU:HD21	24:Z:46:TYR:CD1	2.56	0.41
12:L:233:LEU:HB3	12:L:234:PRO:HD3	2.02	0.41
18:S:84:ASP:OD1	18:S:85:GLU:N	2.53	0.41
30:f:40:SER:OG	30:f:42:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:219:SER:HA	4:D:222:ILE:HG22	2.03	0.41
7:G:24:THR:HG23	7:G:73:VAL:CG1	2.50	0.41
12:L:428:TYR:OH	12:L:509:MET:HE2	2.21	0.41
54:T:201:EHZ:S1	21:W:34:VAL:HG13	2.60	0.41
22:X:3:ILE:N	22:X:3:ILE:HD12	2.35	0.41
5:E:43:GLN:O	5:E:73:LEU:HD12	2.21	0.41
5:E:87:TYR:HB3	6:F:181:ALA:HB3	2.02	0.41
17:R:79:THR:HG23	17:R:80:LYS:N	2.35	0.41
19:U:8:LEU:HD12	19:U:87:TYR:CE1	2.55	0.41
34:j:59:TRP:O	39:o:106:ARG:NH2	2.46	0.41
36:l:80:LEU:O	36:l:84:ILE:HG23	2.20	0.41
39:o:32:GLU:O	39:o:32:GLU:CG	2.68	0.41
7:G:59:ILE:HD11	7:G:66:VAL:HG21	2.01	0.41
7:G:425:SER:C	7:G:661:LEU:HD11	2.44	0.41
9:I:14:VAL:HB	26:b:9:LYS:HZ3	1.85	0.41
13:M:76:MET:SD	13:M:230:ILE:HB	2.61	0.41
14:N:143:ILE:HD13	14:N:202:LEU:HD21	2.02	0.41
24:Z:23:ASN:OD1	24:Z:23:ASN:C	2.62	0.41
24:Z:84:GLN:OE1	29:e:104:ARG:NH1	2.51	0.41
38:n:167:TRP:O	38:n:170:VAL:O	2.39	0.41
7:G:364:LEU:HA	7:G:491:ASN:HB2	2.03	0.41
7:G:383:ASN:HB2	7:G:663:PRO:HB3	2.02	0.41
8:H:117:LEU:CD2	10:J:64:LEU:HD12	2.50	0.41
20:V:18:THR:OG1	20:V:18:THR:O	2.34	0.41
24:Z:119:LEU:HD23	24:Z:119:LEU:H	1.85	0.41
6:F:372:MET:HE2	6:F:399:ILE:HD13	2.01	0.41
7:G:326:GLU:OE1	7:G:326:GLU:N	2.50	0.41
7:G:328:LEU:O	7:G:507:TYR:OH	2.29	0.41
9:I:14:VAL:HG23	9:I:14:VAL:O	2.21	0.41
12:L:49:LEU:HB3	12:L:50:PRO:HD3	2.02	0.41
12:L:230:HIS:H	12:L:231:PRO:HD3	1.86	0.41
38:n:65:GLU:C	38:n:65:GLU:OE1	2.64	0.41
4:D:289:SER:O	20:V:11:VAL:HG22	2.20	0.41
5:E:150:ASN:HB3	5:E:162:GLU:HB3	2.02	0.41
7:G:314:ALA:O	7:G:520:LYS:N	2.54	0.41
14:N:22:SER:HB3	29:e:5:ILE:HD12	2.02	0.41
15:O:311:GLU:HG2	15:O:312:VAL:HG13	2.03	0.41
33:i:68:LEU:O	33:i:68:LEU:HD23	2.20	0.41
6:F:210:PRO:HA	6:F:213:VAL:O	2.21	0.41
6:F:280:ILE:HG21	6:F:287:VAL:HG12	2.03	0.41
6:F:344:VAL:HG22	6:F:429:ARG:HH22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:259:ASN:O	7:G:260:GLU:CB	2.69	0.41
7:G:332:LYS:O	7:G:336:ASN:ND2	2.47	0.41
8:H:89:LEU:HD22	8:H:240:ILE:CD1	2.51	0.41
8:H:105:ILE:HG21	8:H:237:LEU:HD11	2.03	0.41
12:L:245:ALA:HB2	12:L:340:PHE:HB3	2.02	0.41
13:M:300:SER:HB3	13:M:381:ILE:HG23	2.03	0.41
14:N:66:ALA:HB1	14:N:105:LYS:HG3	2.03	0.41
18:S:90:MET:O	18:S:94:LEU:HD13	2.21	0.41
24:Z:121:GLY:HA2	24:Z:132:MET:HE1	2.03	0.41
36:l:132:TYR:O	36:l:154:HIS:NE2	2.53	0.41
1:A:44:THR:HG22	21:W:98:VAL:HB	2.03	0.41
2:B:147:ASP:HA	2:B:150:VAL:O	2.21	0.41
5:E:148:CYS:SG	6:F:103:GLY:N	2.94	0.41
7:G:452:VAL:O	7:G:452:VAL:HG23	2.21	0.41
14:N:99:LEU:HD21	14:N:154:ILE:HG13	2.03	0.41
19:T:46:ASP:OD1	21:W:66:ARG:NH1	2.54	0.41
28:d:5:ARG:HD2	28:d:89:ASP:OD2	2.21	0.41
36:l:76:ILE:CG2	36:l:80:LEU:HD22	2.51	0.41
42:s:41:ASN:ND2	42:s:44:THR:OG1	2.54	0.41
1:A:2:ASN:O	8:H:96:ILE:HD11	2.20	0.40
5:E:89:MET:HG3	6:F:182:GLY:N	2.36	0.40
9:I:82:CYS:SG	9:I:83:LYS:N	2.94	0.40
21:W:26:ASP:OD2	21:W:26:ASP:N	2.53	0.40
21:W:41:TRP:O	21:W:45:VAL:HG23	2.21	0.40
24:Z:128:THR:HG23	24:Z:131:GLU:H	1.86	0.40
30:f:30:ASP:OD2	32:h:85:LYS:NZ	2.52	0.40
31:g:56:MET:SD	31:g:56:MET:C	3.04	0.40
3:C:31:GLU:OE2	20:V:46:TYR:OH	2.28	0.40
6:F:174:ASP:OD2	42:s:57:LEU:HB2	2.22	0.40
12:L:316:THR:O	12:L:319:MET:O	2.39	0.40
12:L:574:THR:HG23	12:L:575:THR:N	2.37	0.40
12:L:601:LEU:C	12:L:601:LEU:HD23	2.46	0.40
32:h:110:VAL:CG1	32:h:114:MET:HE3	2.51	0.40
37:m:121:ASP:C	37:m:121:ASP:OD1	2.63	0.40
1:A:77:TRP:NE1	10:J:136:GLU:OE2	2.54	0.40
2:B:99:ALA:CB	2:B:126:MET:HE3	2.52	0.40
4:D:175:GLU:OE2	4:D:188:ARG:NH2	2.48	0.40
4:D:183:ARG:NH2	4:D:210:ASP:OD2	2.54	0.40
6:F:307:ILE:HG23	6:F:311:VAL:HB	2.03	0.40
7:G:280:THR:HG23	7:G:591:GLY:HA3	2.04	0.40
7:G:472:ASN:OD1	7:G:472:ASN:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:318:MET:HE3	8:H:318:MET:HB3	1.99	0.40
12:L:281:GLY:O	12:L:285:THR:OG1	2.38	0.40
14:N:214:PRO:HB2	14:N:247:MET:SD	2.62	0.40
4:D:418:ILE:HG23	4:D:423:ILE:HD11	2.03	0.40
5:E:132:THR:HG22	5:E:137:PHE:H	1.86	0.40
8:H:4:ILE:O	8:H:8:THR:HG23	2.22	0.40
10:J:107:ASN:ND2	10:J:117:LEU:HD12	2.35	0.40
13:M:71:TRP:CH2	13:M:439:LEU:HD22	2.56	0.40
13:M:248:ILE:HG23	13:M:249:ILE:HG23	2.03	0.40
14:N:226:THR:HG22	14:N:227:ILE:N	2.36	0.40
22:X:48:GLU:OE1	22:X:134:ARG:NH1	2.49	0.40
4:D:67:GLU:HB2	4:D:75:LYS:HB3	2.03	0.40
12:L:2:ASN:OD1	12:L:2:ASN:N	2.50	0.40
12:L:142:ILE:HD11	13:M:371:PRO:HB3	2.03	0.40
14:N:332:MET:CE	28:d:37:LEU:HD13	2.45	0.40
38:n:143:THR:O	38:n:143:THR:HG23	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
2	B	154/224 (69%)	147 (96%)	7 (4%)	0	100	100
3	C	205/263 (78%)	196 (96%)	9 (4%)	0	100	100
4	D	427/463 (92%)	407 (95%)	20 (5%)	0	100	100
5	E	208/245 (85%)	193 (93%)	15 (7%)	0	100	100
6	F	426/464 (92%)	391 (92%)	35 (8%)	0	100	100
7	G	686/727 (94%)	631 (92%)	55 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	316/318 (99%)	300 (95%)	16 (5%)	0	100	100
9	I	176/212 (83%)	169 (96%)	7 (4%)	0	100	100
10	J	169/172 (98%)	155 (92%)	14 (8%)	0	100	100
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/607 (100%)	572 (95%)	30 (5%)	2 (0%)	36	68
13	M	457/459 (100%)	448 (98%)	9 (2%)	0	100	100
14	N	342/345 (99%)	330 (96%)	12 (4%)	0	100	100
15	O	318/355 (90%)	308 (97%)	10 (3%)	0	100	100
16	P	323/377 (86%)	301 (93%)	21 (6%)	1 (0%)	36	68
17	R	53/116 (46%)	52 (98%)	1 (2%)	0	100	100
18	S	80/99 (81%)	75 (94%)	5 (6%)	0	100	100
19	T	74/156 (47%)	70 (95%)	4 (5%)	0	100	100
19	U	84/156 (54%)	81 (96%)	3 (4%)	0	100	100
20	V	110/116 (95%)	108 (98%)	2 (2%)	0	100	100
21	W	107/131 (82%)	101 (94%)	6 (6%)	0	100	100
22	X	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
23	Y	138/143 (96%)	128 (93%)	10 (7%)	0	100	100
24	Z	139/144 (96%)	134 (96%)	5 (4%)	0	100	100
25	a	66/70 (94%)	65 (98%)	1 (2%)	0	100	100
26	b	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
27	c	46/76 (60%)	44 (96%)	2 (4%)	0	100	100
28	d	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
29	e	103/106 (97%)	102 (99%)	1 (1%)	0	100	100
30	f	51/57 (90%)	47 (92%)	4 (8%)	0	100	100
31	g	99/151 (66%)	96 (97%)	3 (3%)	0	100	100
32	h	136/189 (72%)	132 (97%)	4 (3%)	0	100	100
33	i	90/127 (71%)	84 (93%)	6 (7%)	0	100	100
34	j	60/105 (57%)	60 (100%)	0	0	100	100
35	k	73/104 (70%)	72 (99%)	1 (1%)	0	100	100
36	l	152/186 (82%)	147 (97%)	5 (3%)	0	100	100
37	m	124/129 (96%)	119 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	n	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
39	o	111/137 (81%)	107 (96%)	4 (4%)	0	100	100
40	p	166/176 (94%)	158 (95%)	8 (5%)	0	100	100
41	r	57/113 (50%)	55 (96%)	2 (4%)	0	100	100
42	s	29/104 (28%)	28 (97%)	1 (3%)	0	100	100
All	All	7708/8890 (87%)	7332 (95%)	373 (5%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	P	250	HIS
12	L	249	SER
12	L	562	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	103/103 (100%)	103 (100%)	0	100	100
2	B	132/185 (71%)	132 (100%)	0	100	100
3	C	189/227 (83%)	189 (100%)	0	100	100
4	D	370/394 (94%)	370 (100%)	0	100	100
5	E	183/205 (89%)	183 (100%)	0	100	100
6	F	343/370 (93%)	343 (100%)	0	100	100
7	G	567/610 (93%)	566 (100%)	1 (0%)	87	89
8	H	279/279 (100%)	279 (100%)	0	100	100
9	I	152/178 (85%)	152 (100%)	0	100	100
10	J	136/137 (99%)	136 (100%)	0	100	100
11	K	87/87 (100%)	87 (100%)	0	100	100
12	L	548/549 (100%)	548 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	414/414 (100%)	413 (100%)	1 (0%)	87	89
14	N	306/307 (100%)	306 (100%)	0	100	100
15	O	284/309 (92%)	284 (100%)	0	100	100
16	P	286/325 (88%)	286 (100%)	0	100	100
17	R	43/96 (45%)	43 (100%)	0	100	100
18	S	56/80 (70%)	56 (100%)	0	100	100
19	T	70/135 (52%)	70 (100%)	0	100	100
19	U	79/135 (58%)	79 (100%)	0	100	100
20	V	100/102 (98%)	100 (100%)	0	100	100
21	W	103/114 (90%)	103 (100%)	0	100	100
22	X	153/154 (99%)	153 (100%)	0	100	100
23	Y	105/107 (98%)	104 (99%)	1 (1%)	68	80
24	Z	122/123 (99%)	122 (100%)	0	100	100
25	a	58/60 (97%)	58 (100%)	0	100	100
26	b	71/73 (97%)	71 (100%)	0	100	100
27	c	42/67 (63%)	41 (98%)	1 (2%)	43	70
28	d	107/107 (100%)	107 (100%)	0	100	100
29	e	93/94 (99%)	93 (100%)	0	100	100
30	f	49/53 (92%)	49 (100%)	0	100	100
31	g	92/129 (71%)	92 (100%)	0	100	100
32	h	123/162 (76%)	123 (100%)	0	100	100
33	i	88/118 (75%)	88 (100%)	0	100	100
34	j	58/87 (67%)	58 (100%)	0	100	100
35	k	58/78 (74%)	58 (100%)	0	100	100
36	l	139/161 (86%)	139 (100%)	0	100	100
37	m	112/114 (98%)	112 (100%)	0	100	100
38	n	162/164 (99%)	162 (100%)	0	100	100
39	o	106/121 (88%)	106 (100%)	0	100	100
40	p	153/158 (97%)	153 (100%)	0	100	100
41	r	57/96 (59%)	57 (100%)	0	100	100
42	s	31/95 (33%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	6809/7662 (89%)	6805 (100%)	4 (0%)	87	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	229	ASP
13	M	102	LEU
23	Y	3	VAL
27	c	32	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	137	HIS
3	C	124	HIS
3	C	160	HIS
3	C	192	GLN
4	D	149	ASN
4	D	237	ASN
5	E	150	ASN
6	F	373	ASN
7	G	392	ASN
7	G	430	GLN
7	G	475	GLN
7	G	618	GLN
7	G	653	ASN
7	G	665	GLN
8	H	194	ASN
10	J	107	ASN
11	K	25	HIS
12	L	25	ASN
12	L	56	HIS
12	L	175	ASN
12	L	248	HIS
12	L	270	ASN
12	L	296	ASN
13	M	48	ASN
13	M	144	ASN
13	M	170	HIS
13	M	220	HIS
13	M	427	GLN

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Mol	Chain	Res	Type
14	N	63	GLN
14	N	308	ASN
14	N	317	GLN
15	O	114	HIS
15	O	141	GLN
15	O	288	GLN
16	P	44	GLN
16	P	67	GLN
16	P	87	HIS
16	P	103	ASN
16	P	181	HIS
16	P	184	ASN
16	P	288	HIS
17	R	94	HIS
18	S	30	GLN
19	T	47	GLN
26	b	82	ASN
29	e	96	HIS
30	f	9	HIS
31	g	34	ASN
31	g	84	GLN
31	g	109	ASN
32	h	78	ASN
32	h	95	GLN
33	i	25	GLN
36	l	71	ASN
37	m	116	GLN
37	m	125	ASN
38	n	13	GLN
40	p	171	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	A	1	1	8,9,10	0.98	0	8,9,11	0.81	0
13	FME	M	1	13	8,9,10	0.97	0	8,9,11	0.76	0
14	FME	N	1	14	8,9,10	0.96	0	8,9,11	0.91	0
12	FME	L	1	12	8,9,10	0.98	0	8,9,11	0.91	0
8	FME	H	1	8	8,9,10	0.95	0	8,9,11	1.31	0
11	FME	K	1	11	8,9,10	1.00	0	8,9,11	1.20	1 (12%)
33	SAC	i	1	33	7,8,9	1.02	0	7,9,11	1.54	1 (14%)
10	FME	J	1	10	8,9,10	0.98	0	8,9,11	0.89	0
4	2MR	D	85	4	10,12,13	1.84	1 (10%)	5,13,15	2.74	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	2/7/9/11	-
13	FME	M	1	13	-	0/7/9/11	-
14	FME	N	1	14	-	1/7/9/11	-
12	FME	L	1	12	-	1/7/9/11	-
8	FME	H	1	8	-	4/7/9/11	-
11	FME	K	1	11	-	2/7/9/11	-
33	SAC	i	1	33	-	6/7/8/10	-
10	FME	J	1	10	-	5/7/9/11	-
4	2MR	D	85	4	-	5/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NE	5.16	1.45	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	85	2MR	NE-CZ-NH2	5.77	124.77	119.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	i	1	SAC	C2A-C1A-N	2.70	120.60	116.12
11	K	1	FME	C-CA-N	2.59	114.49	109.50

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	85	2MR	N-CA-CB-CG
4	D	85	2MR	C-CA-CB-CG
8	H	1	FME	O1-CN-N-CA
8	H	1	FME	CB-CA-N-CN
10	J	1	FME	O1-CN-N-CA
10	J	1	FME	C-CA-CB-CG
10	J	1	FME	O-C-CA-CB
11	K	1	FME	N-CA-CB-CG
11	K	1	FME	C-CA-CB-CG
33	i	1	SAC	CB-CA-N-C1A
33	i	1	SAC	N-CA-CB-OG
33	i	1	SAC	C-CA-CB-OG
4	D	85	2MR	NE-CD-CG-CB
33	i	1	SAC	C2A-C1A-N-CA
33	i	1	SAC	OAC-C1A-N-CA
4	D	85	2MR	CG-CD-NE-CZ
12	L	1	FME	N-CA-CB-CG
1	A	1	FME	CB-CG-SD-CE
8	H	1	FME	CB-CG-SD-CE
33	i	1	SAC	C-CA-N-C1A
4	D	85	2MR	CA-CB-CG-CD
1	A	1	FME	N-CA-CB-CG
14	N	1	FME	CA-CB-CG-SD
10	J	1	FME	N-CA-CB-CG
8	H	1	FME	C-CA-CB-CG
10	J	1	FME	CB-CA-N-CN

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1	FME	1	0
33	i	1	SAC	2	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 1 is monoatomic - leaving 31 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$
48	3PE	i	201	-	41,41,50	0.96	4 (9%)	44,46,55	1.08	2 (4%)
43	SF4	F	501	6	0,12,12	-	-	-		
44	PC1	H	402	-	41,41,53	1.45	6 (14%)	47,49,61	1.13	3 (6%)
43	SF4	G	802	7	0,12,12	-	-	-		
48	3PE	H	403	-	50,50,50	0.87	4 (8%)	53,55,55	1.09	2 (3%)
49	CDL	h	201	-	69,69,99	1.08	7 (10%)	75,81,111	1.18	5 (6%)
49	CDL	N	402	-	62,62,99	1.14	7 (11%)	68,74,111	1.16	4 (5%)
43	SF4	B	201	2	0,12,12	-	-	-		
49	CDL	d	201	-	66,66,99	1.11	7 (10%)	72,78,111	1.18	4 (5%)
48	3PE	J	201	-	32,32,50	1.07	4 (12%)	35,37,55	1.15	2 (5%)
48	3PE	Y	401	-	40,40,50	0.97	4 (10%)	43,45,55	1.04	2 (4%)
44	PC1	B	202	-	40,40,53	1.45	6 (15%)	46,48,61	1.08	2 (4%)
43	SF4	G	801	7	0,12,12	-	-	-		
52	NDP	P	501	-	51,52,52	2.35	7 (13%)	71,80,80	1.51	15 (21%)
51	GTP	O	401	-	32,33,34	3.05	16 (50%)	48,52,54	1.52	9 (18%)
43	SF4	I	201	9	0,12,12	-	-	-		
48	3PE	L	703	-	41,41,50	0.96	4 (9%)	44,46,55	1.09	2 (4%)
54	EHZ	U	201	19	31,36,37	1.79	5 (16%)	36,44,47	1.72	9 (25%)
46	FMN	F	502	-	33,33,33	4.74	20 (60%)	48,50,50	4.97	22 (45%)
50	LMT	L	705	-	36,36,36	1.14	5 (13%)	47,47,47	0.96	1 (2%)
45	FES	G	803	7	0,4,4	-	-	-		
54	EHZ	T	201	19	31,36,37	1.78	5 (16%)	36,44,47	1.49	4 (11%)
49	CDL	N	401	-	64,64,99	1.12	7 (10%)	70,76,111	1.17	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	3PE	L	701	-	48,48,50	0.90	2 (4%)	51,53,55	1.04	2 (3%)
45	FES	E	301	5	0,4,4	-	-	-	-	-
48	3PE	Z	401	-	43,43,50	0.93	4 (9%)	46,48,55	1.12	2 (4%)
49	CDL	L	702	-	73,73,99	1.05	7 (9%)	79,85,111	1.14	4 (5%)
47	UQ9	H	401	-	44,44,58	0.83	0	51,52,73	1.96	16 (31%)
50	LMT	L	704	-	36,36,36	1.12	6 (16%)	47,47,47	1.03	3 (6%)
49	CDL	M	501	-	58,58,99	1.08	5 (8%)	63,69,111	1.08	3 (4%)
43	SF4	I	202	9	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
48	3PE	i	201	-	-	15/45/45/54	-
43	SF4	F	501	6	-	-	0/6/5/5
44	PC1	H	402	-	-	17/45/45/57	-
43	SF4	G	802	7	-	-	0/6/5/5
48	3PE	H	403	-	-	22/54/54/54	-
49	CDL	h	201	-	-	38/80/80/110	-
49	CDL	N	402	-	-	32/73/73/110	-
49	CDL	d	201	-	-	29/77/77/110	-
43	SF4	B	201	2	-	-	0/6/5/5
48	3PE	J	201	-	-	10/36/36/54	-
48	3PE	Y	401	-	-	11/44/44/54	-
44	PC1	B	202	-	-	18/44/44/57	-
43	SF4	G	801	7	-	-	0/6/5/5
52	NDP	P	501	-	-	9/34/77/77	0/5/5/5
51	GTP	O	401	-	-	4/22/34/38	0/3/3/3
43	SF4	I	201	9	-	-	0/6/5/5
48	3PE	L	703	-	-	17/45/45/54	-
54	EHZ	U	201	19	-	19/42/44/45	-
46	FMN	F	502	-	-	6/18/18/18	0/3/3/3
50	LMT	L	705	-	-	10/21/61/61	0/2/2/2
45	FES	G	803	7	-	-	0/1/1/1
54	EHZ	T	201	19	-	13/42/44/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	CDL	N	401	-	-	41/75/75/110	-
48	3PE	L	701	-	-	14/52/52/54	-
45	FES	E	301	5	-	-	0/1/1/1
48	3PE	Z	401	-	-	16/47/47/54	-
49	CDL	L	702	-	-	32/84/84/110	-
47	UQ9	H	401	-	-	15/50/50/81	-
50	LMT	L	704	-	-	13/21/61/61	0/2/2/2
49	CDL	M	501	-	-	41/67/67/110	-
43	SF4	I	202	9	-	-	0/6/5/5

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	P2B-O2B	13.14	1.82	1.59
46	F	502	FMN	C6-C5A	11.94	1.58	1.40
46	F	502	FMN	C9A-C5A	10.74	1.58	1.41
46	F	502	FMN	C9-C8	-10.68	1.25	1.39
51	O	401	GTP	O6-C6	8.70	1.40	1.23
46	F	502	FMN	O4-C4	8.50	1.39	1.23
46	F	502	FMN	O2-C2	8.04	1.40	1.24
46	F	502	FMN	C8-C7	-7.07	1.23	1.40
46	F	502	FMN	C4A-C4	6.11	1.67	1.44
46	F	502	FMN	C2-N3	-5.74	1.26	1.39
54	U	201	EHZ	C15-N2	5.73	1.47	1.33
54	T	201	EHZ	C12-N1	5.57	1.46	1.33
54	U	201	EHZ	C12-N1	5.57	1.46	1.33
54	T	201	EHZ	C15-N2	5.50	1.46	1.33
52	P	501	NDP	PA-O3	5.24	1.65	1.59
51	O	401	GTP	PB-O3A	5.03	1.64	1.59
51	O	401	GTP	PA-O3A	5.00	1.64	1.59
51	O	401	GTP	PB-O3B	4.93	1.64	1.59
51	O	401	GTP	C2-N2	4.75	1.45	1.34
51	O	401	GTP	C2-N1	4.53	1.48	1.37
51	O	401	GTP	C5-N7	4.40	1.47	1.39
46	F	502	FMN	C4A-N5	4.35	1.40	1.30
51	O	401	GTP	C2-N3	4.04	1.43	1.33
52	P	501	NDP	PN-O5D	3.99	1.75	1.59
44	B	202	PC1	O31-C31	3.75	1.44	1.33
44	H	402	PC1	O31-C31	3.71	1.44	1.33
46	F	502	FMN	C8M-C8	3.63	1.57	1.51
44	H	402	PC1	O21-C21	3.49	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	B	202	PC1	O21-C21	3.46	1.44	1.34
46	F	502	FMN	C4A-C10	3.36	1.54	1.44
52	P	501	NDP	O2B-C2B	-3.22	1.33	1.44
46	F	502	FMN	C9A-N10	3.01	1.46	1.41
48	L	701	3PE	O21-C2	-2.91	1.39	1.46
49	h	201	CDL	OA6-CA4	-2.89	1.39	1.46
54	U	201	EHZ	C9-S1	2.82	1.82	1.76
54	T	201	EHZ	C9-S1	2.78	1.82	1.76
44	B	202	PC1	O21-C2	-2.76	1.40	1.46
48	H	403	3PE	O21-C2	-2.76	1.40	1.46
49	L	702	CDL	OB8-CB7	2.74	1.41	1.33
49	N	401	CDL	OA6-CA4	-2.74	1.40	1.46
49	d	201	CDL	OB8-CB7	2.73	1.41	1.33
46	F	502	FMN	C5A-N5	2.71	1.44	1.39
49	L	702	CDL	OB6-CB4	-2.69	1.40	1.46
50	L	705	LMT	O3'-C3'	-2.67	1.36	1.43
49	N	402	CDL	OB8-CB7	2.67	1.41	1.33
48	i	201	3PE	O21-C2	-2.65	1.40	1.46
48	J	201	3PE	O21-C2	-2.65	1.40	1.46
49	M	501	CDL	OB8-CB7	2.65	1.41	1.33
49	h	201	CDL	OB8-CB7	2.64	1.41	1.33
49	N	401	CDL	OB8-CB7	2.64	1.41	1.33
49	d	201	CDL	OA6-CA4	-2.62	1.40	1.46
48	Y	401	3PE	O21-C2	-2.62	1.40	1.46
48	L	703	3PE	O21-C2	-2.62	1.40	1.46
44	H	402	PC1	O21-C2	-2.61	1.40	1.46
51	O	401	GTP	O4'-C1'	2.61	1.48	1.42
49	N	402	CDL	OB6-CB4	-2.60	1.40	1.46
50	L	704	LMT	O3'-C3'	-2.58	1.36	1.43
49	N	401	CDL	OB6-CB4	-2.58	1.40	1.46
49	M	501	CDL	OB6-CB5	2.58	1.41	1.34
51	O	401	GTP	C8-N9	-2.56	1.31	1.37
46	F	502	FMN	P-O2P	-2.56	1.45	1.54
49	d	201	CDL	OB6-CB5	2.52	1.41	1.34
49	M	501	CDL	OA8-CA7	2.50	1.40	1.33
49	N	402	CDL	OB6-CB5	2.50	1.41	1.34
49	N	402	CDL	OA8-CA7	2.49	1.40	1.33
49	h	201	CDL	OB6-CB5	2.49	1.41	1.34
49	h	201	CDL	OB6-CB4	-2.49	1.40	1.46
49	N	401	CDL	OA8-CA7	2.48	1.40	1.33
48	L	701	3PE	O31-C31	2.48	1.40	1.33
46	F	502	FMN	C10-N1	2.48	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	U	201	EHZ	O4-C15	-2.48	1.18	1.23
49	N	402	CDL	OA6-CA4	-2.47	1.40	1.46
54	T	201	EHZ	O4-C15	-2.47	1.18	1.23
49	d	201	CDL	OB6-CB4	-2.47	1.40	1.46
46	F	502	FMN	P-O3P	-2.47	1.45	1.54
51	O	401	GTP	C2'-C3'	-2.47	1.46	1.52
49	N	401	CDL	OB6-CB5	2.43	1.41	1.34
46	F	502	FMN	C1'-C2'	2.43	1.56	1.52
48	Z	401	3PE	O31-C31	2.43	1.40	1.33
50	L	705	LMT	O2'-C2'	-2.43	1.36	1.43
49	L	702	CDL	OA6-CA4	-2.42	1.40	1.46
49	h	201	CDL	OA8-CA7	2.42	1.40	1.33
48	H	403	3PE	O31-C3	-2.41	1.39	1.45
48	L	703	3PE	O31-C31	2.39	1.40	1.33
51	O	401	GTP	C1'-N9	-2.39	1.42	1.48
46	F	502	FMN	C7M-C7	2.38	1.55	1.51
48	Z	401	3PE	O21-C2	-2.37	1.41	1.46
49	L	702	CDL	OB6-CB5	2.37	1.41	1.34
49	d	201	CDL	OA8-CA6	-2.37	1.39	1.45
49	d	201	CDL	OA8-CA7	2.36	1.40	1.33
48	J	201	3PE	O31-C31	2.35	1.40	1.33
48	i	201	3PE	O31-C31	2.34	1.40	1.33
48	Y	401	3PE	O31-C31	2.34	1.40	1.33
49	L	702	CDL	OA8-CA7	2.33	1.40	1.33
49	L	702	CDL	OA8-CA6	-2.32	1.40	1.45
44	H	402	PC1	P-O11	2.32	1.68	1.59
51	O	401	GTP	PG-O2G	-2.30	1.46	1.54
50	L	704	LMT	O2'-C2'	-2.30	1.37	1.43
44	B	202	PC1	C22-C21	2.29	1.57	1.50
51	O	401	GTP	PG-O3G	-2.27	1.46	1.54
54	T	201	EHZ	O3-C12	-2.27	1.18	1.23
52	P	501	NDP	C5A-C4A	2.26	1.43	1.39
50	L	704	LMT	O3B-C3B	-2.24	1.37	1.43
49	h	201	CDL	OA8-CA6	-2.24	1.40	1.45
48	Y	401	3PE	O31-C3	-2.23	1.40	1.45
46	F	502	FMN	O4'-C4'	-2.22	1.38	1.43
48	Z	401	3PE	O31-C3	-2.22	1.40	1.45
44	H	402	PC1	C22-C21	2.22	1.57	1.50
44	B	202	PC1	P-O11	2.21	1.68	1.59
50	L	704	LMT	O2B-C2B	-2.21	1.37	1.43
54	U	201	EHZ	O3-C12	-2.20	1.18	1.23
48	i	201	3PE	O21-C21	2.20	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	L	702	CDL	OA6-CA5	2.20	1.40	1.34
50	L	705	LMT	O3B-C3B	-2.20	1.37	1.43
51	O	401	GTP	C4-N3	2.18	1.39	1.34
50	L	705	LMT	O1'-C1'	-2.18	1.36	1.40
48	Y	401	3PE	O21-C21	2.18	1.40	1.34
48	Z	401	3PE	O21-C21	2.17	1.40	1.34
49	d	201	CDL	OA6-CA5	2.17	1.40	1.34
48	L	703	3PE	O31-C3	-2.16	1.40	1.45
51	O	401	GTP	C4-N9	-2.16	1.32	1.38
48	J	201	3PE	O31-C3	-2.16	1.40	1.45
44	H	402	PC1	P-O13	2.15	1.67	1.59
48	i	201	3PE	O31-C3	-2.15	1.40	1.45
49	N	402	CDL	OA6-CA5	2.14	1.40	1.34
49	N	401	CDL	OA6-CA5	2.14	1.40	1.34
49	M	501	CDL	OB6-CB4	-2.14	1.41	1.46
48	L	703	3PE	O21-C21	2.14	1.40	1.34
48	J	201	3PE	O21-C21	2.13	1.40	1.34
48	H	403	3PE	O31-C31	2.13	1.39	1.33
49	N	402	CDL	OA8-CA6	-2.12	1.40	1.45
50	L	705	LMT	O2B-C2B	-2.11	1.37	1.43
52	P	501	NDP	C2A-N1A	2.09	1.37	1.33
44	B	202	PC1	P-O13	2.09	1.67	1.59
48	H	403	3PE	O21-C21	2.06	1.40	1.34
49	N	401	CDL	OA8-CA6	-2.06	1.40	1.45
50	L	704	LMT	O1'-C1'	-2.06	1.36	1.40
52	P	501	NDP	O5D-C5D	-2.05	1.36	1.44
49	h	201	CDL	OA6-CA5	2.02	1.40	1.34
49	M	501	CDL	OA8-CA6	-2.01	1.40	1.45
46	F	502	FMN	C2-N1	-2.01	1.32	1.36
50	L	704	LMT	O4'-C4B	-2.01	1.38	1.43

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	F	502	FMN	C6-C5A-N5	16.13	145.22	118.44
46	F	502	FMN	C4-C4A-N5	15.79	140.02	118.21
46	F	502	FMN	C6-C5A-C9A	-12.56	101.79	119.05
46	F	502	FMN	C5A-N5-C4A	9.98	134.24	118.09
46	F	502	FMN	C9A-C5A-N5	-8.92	112.99	122.45
46	F	502	FMN	C9A-N10-C10	8.00	132.95	120.75
46	F	502	FMN	C5A-C9A-N10	-7.43	111.25	117.97
46	F	502	FMN	C10-C4A-N5	-6.35	111.84	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	F	502	FMN	C10-N1-C2	6.31	130.51	116.85
54	U	201	EHZ	C8-C9-S1	5.69	120.75	113.56
46	F	502	FMN	C4-C4A-C10	-5.13	108.14	116.93
47	H	401	UQ9	C40-C39-C41	4.82	123.60	115.23
54	T	201	EHZ	C8-C9-S1	4.78	119.59	113.56
47	H	401	UQ9	C35-C34-C36	4.74	123.45	115.23
49	d	201	CDL	OA6-CA5-C11	4.72	121.69	111.48
44	H	402	PC1	O21-C21-C22	4.71	121.67	111.48
48	i	201	3PE	O21-C21-C22	4.52	121.27	111.48
52	P	501	NDP	P2B-O2B-C2B	-4.52	111.37	123.43
51	O	401	GTP	C8-N9-C4	4.45	114.36	106.03
49	M	501	CDL	OB6-CB5-C51	4.35	120.90	111.48
49	L	702	CDL	OA6-CA5-C11	4.23	120.62	111.48
44	B	202	PC1	O21-C21-C22	4.09	120.33	111.48
48	J	201	3PE	O21-C21-C22	4.03	120.20	111.48
47	H	401	UQ9	C20-C19-C21	4.01	122.19	115.23
49	N	401	CDL	OB6-CB5-C51	3.98	120.09	111.48
49	N	402	CDL	OA6-CA5-C11	3.97	120.06	111.48
49	h	201	CDL	OB6-CB5-C51	3.95	120.02	111.48
48	Z	401	3PE	O21-C21-C22	3.94	120.00	111.48
48	H	403	3PE	O21-C21-C22	3.90	119.91	111.48
48	L	703	3PE	O21-C21-C22	3.89	119.89	111.48
49	h	201	CDL	OA6-CA5-C11	3.87	119.84	111.48
49	N	401	CDL	OA6-CA5-C11	3.86	119.84	111.48
46	F	502	FMN	C9-C9A-N10	3.83	127.00	121.85
48	Y	401	3PE	O21-C21-C22	3.76	119.62	111.48
49	d	201	CDL	OB6-CB5-C51	3.68	119.45	111.48
49	N	402	CDL	OB6-CB5-C51	3.65	119.38	111.48
49	L	702	CDL	OB6-CB5-C51	3.63	119.34	111.48
52	P	501	NDP	O2B-P2B-O1X	-3.59	96.52	109.33
52	P	501	NDP	O3-PA-O1A	-3.51	100.13	110.70
48	Z	401	3PE	O31-C31-C32	3.43	122.28	111.83
48	L	701	3PE	O21-C21-C22	3.39	118.82	111.48
47	H	401	UQ9	C45-C44-C46	3.37	121.08	115.23
47	H	401	UQ9	C25-C24-C26	3.35	121.05	115.23
51	O	401	GTP	C2-N1-C6	-3.22	119.28	125.11
52	P	501	NDP	PA-O5B-C5B	-3.16	103.24	121.35
49	N	402	CDL	OB8-CB7-C71	3.11	121.31	111.83
46	F	502	FMN	C9A-C9-C8	3.09	125.43	119.22
47	H	401	UQ9	C20-C19-C18	-3.04	115.82	123.63
47	H	401	UQ9	C35-C34-C33	-3.03	115.85	123.63
48	L	701	3PE	O31-C31-C32	3.00	120.98	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	F	502	FMN	O3P-P-O5'	2.97	114.42	106.67
49	h	201	CDL	OB8-CB7-C71	2.95	120.82	111.83
49	L	702	CDL	OB8-CB7-C71	2.93	120.78	111.83
47	H	401	UQ9	C42-C43-C44	-2.93	120.91	127.62
47	H	401	UQ9	C37-C38-C39	-2.93	120.92	127.62
49	h	201	CDL	OA8-CA7-C31	2.91	120.71	111.83
47	H	401	UQ9	C30-C29-C31	2.89	120.24	115.23
49	N	401	CDL	OA8-CA7-C31	2.88	120.63	111.83
49	M	501	CDL	OB8-CB7-C71	2.88	120.62	111.83
54	T	201	EHZ	C10-S1-C9	2.88	110.35	101.84
48	Y	401	3PE	O31-C31-C32	2.88	120.61	111.83
54	U	201	EHZ	C16-C15-N2	2.87	121.93	116.48
49	N	402	CDL	OA8-CA7-C31	2.86	120.57	111.83
46	F	502	FMN	O2P-P-O5'	2.85	114.09	106.67
48	J	201	3PE	O31-C31-C32	2.82	120.44	111.83
49	d	201	CDL	OA8-CA7-C31	2.82	120.43	111.83
51	O	401	GTP	O2G-PG-O3B	2.81	114.05	104.64
51	O	401	GTP	O3G-PG-O3B	2.79	114.00	104.64
49	d	201	CDL	OB8-CB7-C71	2.79	120.35	111.83
48	H	403	3PE	O31-C31-C32	2.75	120.23	111.83
50	L	704	LMT	C1'-O5'-C5'	-2.74	108.37	113.72
49	N	401	CDL	OB8-CB7-C71	2.71	120.11	111.83
52	P	501	NDP	PN-O5D-C5D	-2.71	105.85	121.35
46	F	502	FMN	C4A-C10-N1	-2.70	117.98	124.59
54	U	201	EHZ	C10-S1-C9	2.69	109.79	101.84
49	M	501	CDL	OA8-CA7-C31	2.69	120.03	111.83
50	L	705	LMT	C3'-C4'-C5'	-2.68	104.99	110.93
48	L	703	3PE	O31-C31-C32	2.65	119.91	111.83
46	F	502	FMN	O5'-P-O1P	2.64	113.57	106.44
47	H	401	UQ9	C10-C9-C11	2.64	119.81	115.23
54	U	201	EHZ	O2-C9-C8	-2.58	119.69	123.74
52	P	501	NDP	O3X-P2B-O2X	2.55	117.36	107.80
54	U	201	EHZ	C14-C13-C12	-2.52	108.19	112.39
46	F	502	FMN	C5A-C6-C7	2.48	125.42	120.83
47	H	401	UQ9	C7-C8-C9	-2.48	120.80	126.44
52	P	501	NDP	C2A-N1A-C6A	-2.47	114.67	118.73
52	P	501	NDP	O2N-PN-O3	2.47	113.94	107.27
54	U	201	EHZ	O2-C9-S1	-2.45	119.56	122.68
44	B	202	PC1	O31-C31-C32	2.43	119.25	111.83
49	L	702	CDL	OA8-CA7-C31	2.43	119.25	111.83
51	O	401	GTP	O2A-PA-O1A	-2.43	101.13	112.44
51	O	401	GTP	C5-C6-N1	2.43	119.44	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	H	401	UQ9	C12-C13-C14	-2.41	122.10	127.62
44	H	402	PC1	O31-C31-C32	2.40	119.15	111.83
51	O	401	GTP	O2B-PB-O1B	-2.40	101.28	112.44
48	i	201	3PE	O31-C31-C32	2.40	119.14	111.83
54	U	201	EHZ	C7-C8-C9	-2.39	108.51	113.86
47	H	401	UQ9	C22-C23-C24	-2.39	122.16	127.62
52	P	501	NDP	N3A-C4A-N9A	2.38	131.21	127.17
49	h	201	CDL	CA4-OA6-CA5	-2.36	112.14	117.80
51	O	401	GTP	O6-C6-C5	-2.36	120.30	126.53
46	F	502	FMN	N10-C10-N1	2.30	125.29	118.51
46	F	502	FMN	C4-N3-C2	2.30	129.73	125.64
46	F	502	FMN	C1'-N10-C9A	-2.30	116.17	120.63
51	O	401	GTP	C1'-N9-C8	-2.28	122.80	127.91
54	T	201	EHZ	O2-C9-C8	-2.27	120.17	123.74
52	P	501	NDP	O2N-PN-O1N	2.25	122.90	112.44
52	P	501	NDP	C5B-C4B-C3B	-2.22	107.23	115.21
52	P	501	NDP	C5A-C4A-N3A	-2.22	123.66	126.72
46	F	502	FMN	C9-C8-C7	2.20	122.91	119.69
54	U	201	EHZ	C13-C12-N1	2.18	120.31	116.34
52	P	501	NDP	O4B-C4B-C3B	2.13	109.38	105.15
44	H	402	PC1	C2-O21-C21	-2.13	112.70	117.80
50	L	704	LMT	O5B-C5B-C4B	2.12	113.51	109.70
47	H	401	UQ9	C32-C33-C34	-2.09	122.83	127.62
54	T	201	EHZ	C13-C12-N1	2.08	120.13	116.34
50	L	704	LMT	O5B-C5B-C6B	2.05	111.53	106.44
47	H	401	UQ9	C27-C28-C29	-2.05	122.94	127.62
46	F	502	FMN	C6-C7-C8	2.04	122.69	119.69
52	P	501	NDP	C3N-C2N-N1N	-2.03	120.22	123.20
54	U	201	EHZ	C19-C17-C16	2.02	112.21	108.77
52	P	501	NDP	O3X-P2B-O2B	-2.02	97.98	105.85

There are no chirality outliers.

All (442) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	B	202	PC1	C1-O11-P-O14
44	B	202	PC1	C12-C11-O13-P
44	B	202	PC1	O13-C11-C12-N
44	B	202	PC1	O11-C1-C2-O21
44	B	202	PC1	O22-C21-O21-C2
44	B	202	PC1	C22-C21-O21-C2
44	H	402	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
46	F	502	FMN	N10-C1'-C2'-O2'
46	F	502	FMN	C1'-C2'-C3'-O3'
46	F	502	FMN	C1'-C2'-C3'-C4'
47	H	401	UQ9	C29-C31-C32-C33
48	H	403	3PE	C1-O11-P-O13
48	H	403	3PE	C1-O11-P-O14
48	H	403	3PE	C11-O13-P-O11
48	H	403	3PE	C11-O13-P-O14
48	L	703	3PE	C11-O13-P-O14
48	L	703	3PE	O11-C1-C2-O21
48	L	703	3PE	C22-C21-O21-C2
48	Y	401	3PE	C1-O11-P-O13
48	Y	401	3PE	C1-O11-P-O14
48	Z	401	3PE	C11-O13-P-O14
48	Z	401	3PE	C22-C21-O21-C2
48	i	201	3PE	C1-O11-P-O13
48	i	201	3PE	C1-O11-P-O14
48	i	201	3PE	C22-C21-O21-C2
49	L	702	CDL	CA2-OA2-PA1-OA4
49	L	702	CDL	CA2-OA2-PA1-OA5
49	L	702	CDL	CB2-OB2-PB2-OB3
49	L	702	CDL	CB2-OB2-PB2-OB4
49	L	702	CDL	CB2-OB2-PB2-OB5
49	L	702	CDL	C51-CB5-OB6-CB4
49	M	501	CDL	O1-C1-CB2-OB2
49	M	501	CDL	CA2-OA2-PA1-OA3
49	M	501	CDL	CA2-OA2-PA1-OA4
49	M	501	CDL	CA2-OA2-PA1-OA5
49	M	501	CDL	CA3-OA5-PA1-OA2
49	M	501	CDL	CA3-OA5-PA1-OA3
49	M	501	CDL	CB2-OB2-PB2-OB3
49	M	501	CDL	CB2-OB2-PB2-OB5
49	N	401	CDL	O1-C1-CB2-OB2
49	N	401	CDL	C1-CA2-OA2-PA1
49	N	401	CDL	CA2-OA2-PA1-OA3
49	N	401	CDL	CA2-OA2-PA1-OA4
49	N	401	CDL	CA2-OA2-PA1-OA5
49	N	401	CDL	CA3-OA5-PA1-OA2
49	N	401	CDL	CA3-OA5-PA1-OA3
49	N	401	CDL	CA3-OA5-PA1-OA4
49	N	401	CDL	CB2-OB2-PB2-OB5
49	N	401	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
49	N	402	CDL	C1-CA2-OA2-PA1
49	N	402	CDL	CA3-OA5-PA1-OA3
49	N	402	CDL	CB2-OB2-PB2-OB3
49	N	402	CDL	CB2-OB2-PB2-OB4
49	N	402	CDL	CB2-OB2-PB2-OB5
49	d	201	CDL	CB2-OB2-PB2-OB3
49	d	201	CDL	CB2-OB2-PB2-OB4
49	d	201	CDL	CB2-OB2-PB2-OB5
49	d	201	CDL	CB3-OB5-PB2-OB2
49	d	201	CDL	CB3-OB5-PB2-OB4
49	d	201	CDL	C51-CB5-OB6-CB4
49	h	201	CDL	CA2-OA2-PA1-OA3
49	h	201	CDL	CA2-OA2-PA1-OA5
49	h	201	CDL	CA3-OA5-PA1-OA2
49	h	201	CDL	CA3-OA5-PA1-OA3
49	h	201	CDL	CA3-OA5-PA1-OA4
49	h	201	CDL	CB2-OB2-PB2-OB3
49	h	201	CDL	CB2-OB2-PB2-OB4
49	h	201	CDL	CB2-OB2-PB2-OB5
49	h	201	CDL	C51-CB5-OB6-CB4
50	L	704	LMT	O5'-C1'-O1'-C1
50	L	705	LMT	C2'-C1'-O1'-C1
50	L	705	LMT	O5'-C1'-O1'-C1
51	O	401	GTP	C5'-O5'-PA-O1A
51	O	401	GTP	C5'-O5'-PA-O2A
52	P	501	NDP	O4B-C4B-C5B-O5B
54	T	201	EHZ	C6-C7-C8-C9
54	T	201	EHZ	S1-C10-C11-N1
54	T	201	EHZ	C16-C17-C20-O6
54	T	201	EHZ	C18-C17-C20-O6
54	T	201	EHZ	C19-C17-C20-O6
54	T	201	EHZ	O2-C9-S1-C10
54	T	201	EHZ	C8-C9-S1-C10
54	U	201	EHZ	C5-C6-C7-O1
54	U	201	EHZ	C5-C6-C7-C8
54	U	201	EHZ	S1-C10-C11-N1
54	U	201	EHZ	C12-C13-C14-N2
54	U	201	EHZ	C16-C15-N2-C14
54	U	201	EHZ	C15-C16-C17-C18
54	U	201	EHZ	C15-C16-C17-C19
54	U	201	EHZ	C15-C16-C17-C20
54	U	201	EHZ	O5-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
54	U	201	EHZ	O5-C16-C17-C19
54	U	201	EHZ	O5-C16-C17-C20
54	U	201	EHZ	O2-C9-S1-C10
54	U	201	EHZ	C8-C9-S1-C10
48	Z	401	3PE	O32-C31-O31-C3
48	Z	401	3PE	C32-C31-O31-C3
49	L	702	CDL	C71-CB7-OB8-CB6
49	h	201	CDL	C31-CA7-OA8-CA6
48	Y	401	3PE	O32-C31-O31-C3
49	L	702	CDL	OB9-CB7-OB8-CB6
49	N	401	CDL	OB9-CB7-OB8-CB6
49	N	402	CDL	OA9-CA7-OA8-CA6
49	h	201	CDL	OA9-CA7-OA8-CA6
48	L	703	3PE	O22-C21-O21-C2
48	Z	401	3PE	O22-C21-O21-C2
48	i	201	3PE	O22-C21-O21-C2
49	L	702	CDL	OB7-CB5-OB6-CB4
49	N	401	CDL	OA7-CA5-OA6-CA4
49	N	401	CDL	OB7-CB5-OB6-CB4
49	d	201	CDL	OB7-CB5-OB6-CB4
49	h	201	CDL	OB7-CB5-OB6-CB4
49	N	401	CDL	C71-CB7-OB8-CB6
49	N	402	CDL	C31-CA7-OA8-CA6
49	N	401	CDL	C11-CA5-OA6-CA4
47	H	401	UQ9	C40-C39-C41-C42
47	H	401	UQ9	C35-C34-C36-C37
47	H	401	UQ9	C38-C39-C41-C42
48	H	403	3PE	C32-C31-O31-C3
48	Y	401	3PE	C32-C31-O31-C3
49	d	201	CDL	C31-CA7-OA8-CA6
48	H	403	3PE	O32-C31-O31-C3
49	M	501	CDL	OB9-CB7-OB8-CB6
49	d	201	CDL	OA9-CA7-OA8-CA6
50	L	704	LMT	O5B-C1B-O1B-C4'
49	N	401	CDL	O1-C1-CA2-OA2
48	J	201	3PE	C32-C31-O31-C3
49	d	201	CDL	C71-CB7-OB8-CB6
54	U	201	EHZ	O4-C15-N2-C14
50	L	704	LMT	C4'-C5'-C6'-O6'
49	h	201	CDL	C11-CA5-OA6-CA4
52	P	501	NDP	C3B-C4B-C5B-O5B
49	M	501	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
47	H	401	UQ9	C20-C19-C21-C22
47	H	401	UQ9	C18-C19-C21-C22
49	d	201	CDL	OB9-CB7-OB8-CB6
50	L	704	LMT	O5'-C5'-C6'-O6'
47	H	401	UQ9	C44-C46-C47-C48
49	N	401	CDL	CA4-CA3-OA5-PA1
48	J	201	3PE	O32-C31-O31-C3
44	B	202	PC1	C32-C31-O31-C3
44	H	402	PC1	C32-C31-O31-C3
49	N	402	CDL	C71-CB7-OB8-CB6
44	H	402	PC1	O32-C31-O31-C3
49	h	201	CDL	OA7-CA5-OA6-CA4
49	M	501	CDL	CB2-C1-CA2-OA2
49	M	501	CDL	CA2-C1-CB2-OB2
49	N	401	CDL	CA2-C1-CB2-OB2
47	H	401	UQ9	C33-C34-C36-C37
49	N	402	CDL	C78-C79-C80-C81
50	L	704	LMT	C2'-C1'-O1'-C1
49	M	501	CDL	O1-C1-CA2-OA2
49	N	401	CDL	C71-C72-C73-C74
54	T	201	EHZ	C5-C6-C7-O1
48	H	403	3PE	C22-C21-O21-C2
49	M	501	CDL	C51-CB5-OB6-CB4
46	F	502	FMN	O2'-C2'-C3'-C4'
50	L	705	LMT	C2B-C1B-O1B-C4'
50	L	705	LMT	O5B-C1B-O1B-C4'
44	B	202	PC1	O32-C31-O31-C3
48	H	403	3PE	C21-C22-C23-C24
49	M	501	CDL	CB5-C51-C52-C53
48	L	701	3PE	C2-C3-O31-C31
49	N	402	CDL	O1-C1-CA2-OA2
49	N	402	CDL	OB9-CB7-OB8-CB6
49	N	401	CDL	CA7-C31-C32-C33
49	d	201	CDL	CB5-C51-C52-C53
49	M	501	CDL	OB7-CB5-OB6-CB4
46	F	502	FMN	O2'-C2'-C3'-O3'
50	L	704	LMT	C3'-C4'-O1B-C1B
48	L	701	3PE	C32-C31-O31-C3
48	H	403	3PE	O22-C21-O21-C2
50	L	704	LMT	C5'-C4'-O1B-C1B
49	N	402	CDL	CB2-C1-CA2-OA2
49	h	201	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
49	N	402	CDL	C11-CA5-OA6-CA4
49	N	402	CDL	OA7-CA5-OA6-CA4
47	H	401	UQ9	C24-C26-C27-C28
49	h	201	CDL	O1-C1-CA2-OA2
49	L	702	CDL	C11-CA5-OA6-CA4
50	L	705	LMT	O5'-C5'-C6'-O6'
49	M	501	CDL	C53-C54-C55-C56
48	i	201	3PE	C25-C26-C27-C28
49	N	402	CDL	C75-C76-C77-C78
49	h	201	CDL	C20-C21-C22-C23
48	L	701	3PE	O32-C31-O31-C3
49	N	401	CDL	C75-C76-C77-C78
49	L	702	CDL	OA7-CA5-OA6-CA4
48	Z	401	3PE	C34-C35-C36-C37
49	N	402	CDL	C72-C73-C74-C75
48	L	703	3PE	C3B-C3C-C3D-C3E
49	N	402	CDL	CA5-C11-C12-C13
48	H	403	3PE	C2D-C2E-C2F-C2G
49	h	201	CDL	OB9-CB7-OB8-CB6
49	N	401	CDL	C51-C52-C53-C54
49	L	702	CDL	C52-C53-C54-C55
44	B	202	PC1	C37-C38-C39-C3A
48	H	403	3PE	C25-C26-C27-C28
44	B	202	PC1	C35-C36-C37-C38
49	d	201	CDL	C31-C32-C33-C34
44	H	402	PC1	C27-C28-C29-C2A
48	H	403	3PE	C3C-C3D-C3E-C3F
49	N	401	CDL	C83-C84-C85-C86
49	N	402	CDL	C51-CB5-OB6-CB4
48	Y	401	3PE	C31-C32-C33-C34
49	N	402	CDL	C51-C52-C53-C54
48	H	403	3PE	C37-C38-C39-C3A
48	L	703	3PE	C35-C36-C37-C38
50	L	704	LMT	C11-C10-C9-C8
48	L	703	3PE	C3A-C3B-C3C-C3D
49	h	201	CDL	CA5-C11-C12-C13
48	H	403	3PE	C3A-C3B-C3C-C3D
50	L	704	LMT	C1-C2-C3-C4
49	d	201	CDL	C57-C58-C59-C60
48	Y	401	3PE	O21-C2-C3-O31
49	L	702	CDL	OB6-CB4-CB6-OB8
49	N	401	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
49	L	702	CDL	C77-C78-C79-C80
44	H	402	PC1	C24-C25-C26-C27
49	M	501	CDL	OA5-CA3-CA4-CA6
49	M	501	CDL	OA5-CA3-CA4-OA6
49	N	402	CDL	C71-C72-C73-C74
48	L	701	3PE	O11-C1-C2-C3
48	L	703	3PE	O11-C1-C2-C3
49	N	402	CDL	OB7-CB5-OB6-CB4
54	T	201	EHZ	C5-C6-C7-C8
49	M	501	CDL	C55-C56-C57-C58
52	P	501	NDP	O4D-C4D-C5D-O5D
49	N	401	CDL	CB5-C51-C52-C53
44	H	402	PC1	C33-C34-C35-C36
49	N	401	CDL	CA5-C11-C12-C13
49	N	401	CDL	CA3-CA4-CA6-OA8
49	N	401	CDL	CB3-CB4-CB6-OB8
48	i	201	3PE	C33-C34-C35-C36
48	i	201	3PE	C24-C25-C26-C27
49	N	401	CDL	C76-C77-C78-C79
49	M	501	CDL	C75-C76-C77-C78
48	Z	401	3PE	C3-C2-O21-C21
49	M	501	CDL	CB6-CB4-OB6-CB5
49	d	201	CDL	CB3-CB4-OB6-CB5
49	M	501	CDL	C31-C32-C33-C34
49	d	201	CDL	C55-C56-C57-C58
49	L	702	CDL	CB5-C51-C52-C53
52	P	501	NDP	C3D-C4D-C5D-O5D
48	Z	401	3PE	C32-C33-C34-C35
49	N	401	CDL	C78-C79-C80-C81
49	M	501	CDL	C31-CA7-OA8-CA6
48	L	701	3PE	C27-C28-C29-C2A
49	h	201	CDL	C51-C52-C53-C54
48	L	701	3PE	C22-C23-C24-C25
49	L	702	CDL	C14-C15-C16-C17
50	L	705	LMT	C6-C7-C8-C9
49	M	501	CDL	OA6-CA4-CA6-OA8
48	i	201	3PE	C22-C23-C24-C25
49	N	401	CDL	C53-C54-C55-C56
49	N	402	CDL	C76-C77-C78-C79
49	L	702	CDL	C75-C76-C77-C78
50	L	704	LMT	C5-C6-C7-C8
48	H	403	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
48	J	201	3PE	O11-C1-C2-C3
54	T	201	EHZ	C2-C3-C4-C5
49	L	702	CDL	C55-C56-C57-C58
48	Z	401	3PE	C36-C37-C38-C39
49	N	401	CDL	CB2-C1-CA2-OA2
48	Y	401	3PE	C1-C2-C3-O31
49	L	702	CDL	CB3-CB4-CB6-OB8
54	U	201	EHZ	C2-C3-C4-C5
48	L	703	3PE	C37-C38-C39-C3A
48	J	201	3PE	O11-C1-C2-O21
48	L	701	3PE	O11-C1-C2-O21
49	L	702	CDL	OB5-CB3-CB4-OB6
49	d	201	CDL	OA5-CA3-CA4-OA6
49	h	201	CDL	C73-C74-C75-C76
48	Y	401	3PE	C33-C34-C35-C36
54	T	201	EHZ	O1-C7-C8-C9
49	L	702	CDL	C13-C14-C15-C16
49	M	501	CDL	CA3-CA4-CA6-OA8
52	P	501	NDP	PN-O3-PA-O5B
49	M	501	CDL	C52-C51-CB5-OB6
49	N	401	CDL	C84-C85-C86-C87
49	M	501	CDL	OA9-CA7-OA8-CA6
44	B	202	PC1	O11-C1-C2-C3
49	L	702	CDL	OB5-CB3-CB4-CB6
49	M	501	CDL	C51-C52-C53-C54
49	L	702	CDL	CA6-CA4-OA6-CA5
49	N	402	CDL	CA6-CA4-OA6-CA5
50	L	705	LMT	C5-C6-C7-C8
48	L	701	3PE	C32-C33-C34-C35
48	L	701	3PE	C26-C27-C28-C29
48	H	403	3PE	O11-C1-C2-O21
49	M	501	CDL	CB3-CB4-CB6-OB8
49	h	201	CDL	CB5-C51-C52-C53
48	H	403	3PE	C12-C11-O13-P
48	Z	401	3PE	C12-C11-O13-P
48	H	403	3PE	O21-C2-C3-O31
49	N	402	CDL	OB6-CB4-CB6-OB8
48	L	703	3PE	C3D-C3E-C3F-C3G
49	h	201	CDL	C72-C73-C74-C75
44	H	402	PC1	O13-C11-C12-N
49	d	201	CDL	O1-C1-CA2-OA2
44	B	202	PC1	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
50	L	705	LMT	C9-C10-C11-C12
49	M	501	CDL	CA4-CA6-OA8-CA7
49	N	401	CDL	C79-C80-C81-C82
48	L	703	3PE	C22-C23-C24-C25
44	H	402	PC1	C34-C35-C36-C37
49	L	702	CDL	C73-C74-C75-C76
49	N	402	CDL	C74-C75-C76-C77
49	d	201	CDL	C1-CA2-OA2-PA1
44	B	202	PC1	C3F-C3G-C3H-C3I
54	U	201	EHZ	C11-C10-S1-C9
54	U	201	EHZ	C22-C23-C24-C25
44	H	402	PC1	O11-C1-C2-O21
48	H	403	3PE	C35-C36-C37-C38
44	B	202	PC1	O21-C2-C3-O31
44	B	202	PC1	C3B-C3C-C3D-C3E
48	L	701	3PE	C36-C37-C38-C39
48	Y	401	3PE	C34-C35-C36-C37
48	L	703	3PE	C32-C31-O31-C3
49	d	201	CDL	C51-C52-C53-C54
44	B	202	PC1	C1-O11-P-O13
48	J	201	3PE	C1-O11-P-O12
48	J	201	3PE	C1-O11-P-O13
48	L	703	3PE	C1-O11-P-O12
48	L	703	3PE	C1-O11-P-O13
48	L	703	3PE	C1-O11-P-O14
48	Z	401	3PE	C1-O11-P-O14
48	Z	401	3PE	C11-O13-P-O11
48	Z	401	3PE	C11-O13-P-O12
48	i	201	3PE	C1-O11-P-O12
49	L	702	CDL	CA2-OA2-PA1-OA3
49	M	501	CDL	CA3-OA5-PA1-OA4
49	M	501	CDL	CB2-OB2-PB2-OB4
49	N	401	CDL	CB2-OB2-PB2-OB3
49	d	201	CDL	CA3-OA5-PA1-OA3
49	h	201	CDL	CA2-OA2-PA1-OA4
49	h	201	CDL	CB3-OB5-PB2-OB2
49	h	201	CDL	CB3-OB5-PB2-OB3
49	h	201	CDL	CB3-OB5-PB2-OB4
51	O	401	GTP	C5'-O5'-PA-O3A
52	P	501	NDP	C5B-O5B-PA-O3
47	H	401	UQ9	C25-C24-C26-C27
49	L	702	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
49	d	201	CDL	C62-C63-C64-C65
48	H	403	3PE	C34-C35-C36-C37
50	L	704	LMT	C4-C5-C6-C7
48	L	703	3PE	O32-C31-O31-C3
44	H	402	PC1	C39-C3A-C3B-C3C
48	i	201	3PE	C3-C2-O21-C21
49	L	702	CDL	C71-C72-C73-C74
48	i	201	3PE	O21-C21-C22-C23
49	M	501	CDL	OB5-CB3-CB4-CB6
49	N	401	CDL	OB5-CB3-CB4-CB6
44	H	402	PC1	C31-C32-C33-C34
49	d	201	CDL	C54-C55-C56-C57
49	M	501	CDL	OB6-CB4-CB6-OB8
49	N	401	CDL	OB6-CB4-CB6-OB8
49	M	501	CDL	C58-C59-C60-C61
49	N	401	CDL	C81-C82-C83-C84
48	L	701	3PE	C34-C35-C36-C37
44	H	402	PC1	C37-C38-C39-C3A
48	L	703	3PE	C32-C33-C34-C35
49	M	501	CDL	C54-C55-C56-C57
48	J	201	3PE	C25-C26-C27-C28
49	M	501	CDL	C73-C74-C75-C76
49	N	402	CDL	CB5-C51-C52-C53
52	P	501	NDP	O4D-C1D-N1N-C6N
49	M	501	CDL	C1-CB2-OB2-PB2
54	T	201	EHZ	C3-C4-C5-C6
50	L	705	LMT	O5B-C5B-C6B-O6B
54	T	201	EHZ	C21-C22-C23-C24
49	N	402	CDL	C32-C33-C34-C35
49	h	201	CDL	CB3-CB4-OB6-CB5
48	L	701	3PE	C24-C25-C26-C27
48	Z	401	3PE	C27-C28-C29-C2A
54	U	201	EHZ	O4-C15-C16-O5
44	H	402	PC1	O21-C2-C3-O31
44	H	402	PC1	C35-C36-C37-C38
49	L	702	CDL	C56-C57-C58-C59
48	H	403	3PE	C32-C33-C34-C35
49	N	402	CDL	CA2-C1-CB2-OB2
52	P	501	NDP	PN-O3-PA-O1A
49	L	702	CDL	CA7-C31-C32-C33
48	i	201	3PE	C1-C2-C3-O31
49	N	402	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
49	h	201	CDL	O1-C1-CB2-OB2
48	Z	401	3PE	O11-C1-C2-O21
47	H	401	UQ9	C45-C44-C46-C47
48	L	701	3PE	O21-C21-C22-C23
44	H	402	PC1	O11-C1-C2-C3
49	d	201	CDL	OA5-CA3-CA4-CA6
49	h	201	CDL	OA6-CA4-CA6-OA8
48	J	201	3PE	O31-C31-C32-C33
48	H	403	3PE	C3F-C3G-C3H-C3I
48	Y	401	3PE	C35-C36-C37-C38
49	d	201	CDL	C52-C53-C54-C55
48	i	201	3PE	C23-C24-C25-C26
49	d	201	CDL	CA5-C11-C12-C13
48	i	201	3PE	C21-C22-C23-C24
49	h	201	CDL	C17-C18-C19-C20
44	B	202	PC1	C38-C39-C3A-C3B
47	H	401	UQ9	C23-C24-C26-C27
48	L	701	3PE	C28-C29-C2A-C2B
49	L	702	CDL	C78-C79-C80-C81
52	P	501	NDP	C2D-C1D-N1N-C6N
44	B	202	PC1	C1-C2-C3-O31
47	H	401	UQ9	C39-C41-C42-C43
49	h	201	CDL	CA3-CA4-CA6-OA8
49	L	702	CDL	C74-C75-C76-C77
48	i	201	3PE	C12-C11-O13-P
49	M	501	CDL	C52-C51-CB5-OB7
49	N	401	CDL	C12-C11-CA5-OA6
49	h	201	CDL	C12-C11-CA5-OA6
49	M	501	CDL	C76-C77-C78-C79
48	Z	401	3PE	C38-C39-C3A-C3B
49	h	201	CDL	C21-C22-C23-C24
44	H	402	PC1	O22-C21-O21-C2
44	H	402	PC1	C22-C21-O21-C2
49	N	402	CDL	OB5-CB3-CB4-OB6
47	H	401	UQ9	C15-C14-C16-C17
50	L	705	LMT	C3-C4-C5-C6
51	O	401	GTP	O4'-C4'-C5'-O5'
47	H	401	UQ9	C36-C37-C38-C39
49	d	201	CDL	C52-C51-CB5-OB6
46	F	502	FMN	N10-C1'-C2'-C3'
49	h	201	CDL	CB6-CB4-OB6-CB5
49	d	201	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
48	Y	401	3PE	O31-C31-C32-C33
49	N	401	CDL	C12-C11-CA5-OA7
49	N	402	CDL	O1-C1-CB2-OB2
49	h	201	CDL	C12-C11-CA5-OA7
49	L	702	CDL	C36-C37-C38-C39
54	U	201	EHZ	N2-C15-C16-O5
49	N	401	CDL	C1-CB2-OB2-PB2
48	J	201	3PE	O21-C21-C22-C23
49	h	201	CDL	C19-C20-C21-C22
50	L	704	LMT	C2-C3-C4-C5
50	L	704	LMT	C9-C10-C11-C12
49	N	402	CDL	C12-C11-CA5-OA6
48	J	201	3PE	O22-C21-C22-C23
49	d	201	CDL	C32-C31-CA7-OA9
49	h	201	CDL	C32-C31-CA7-OA9

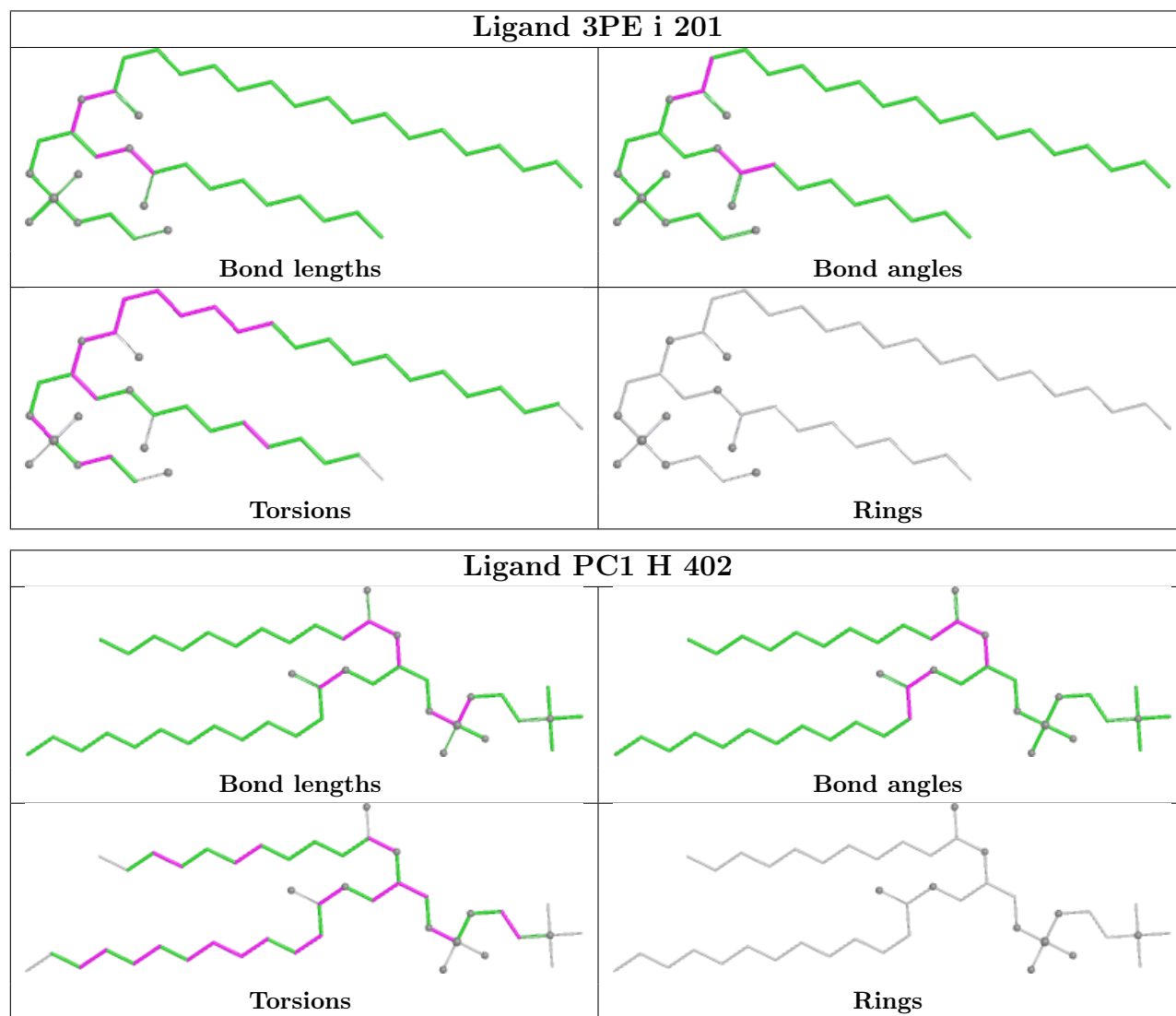
There are no ring outliers.

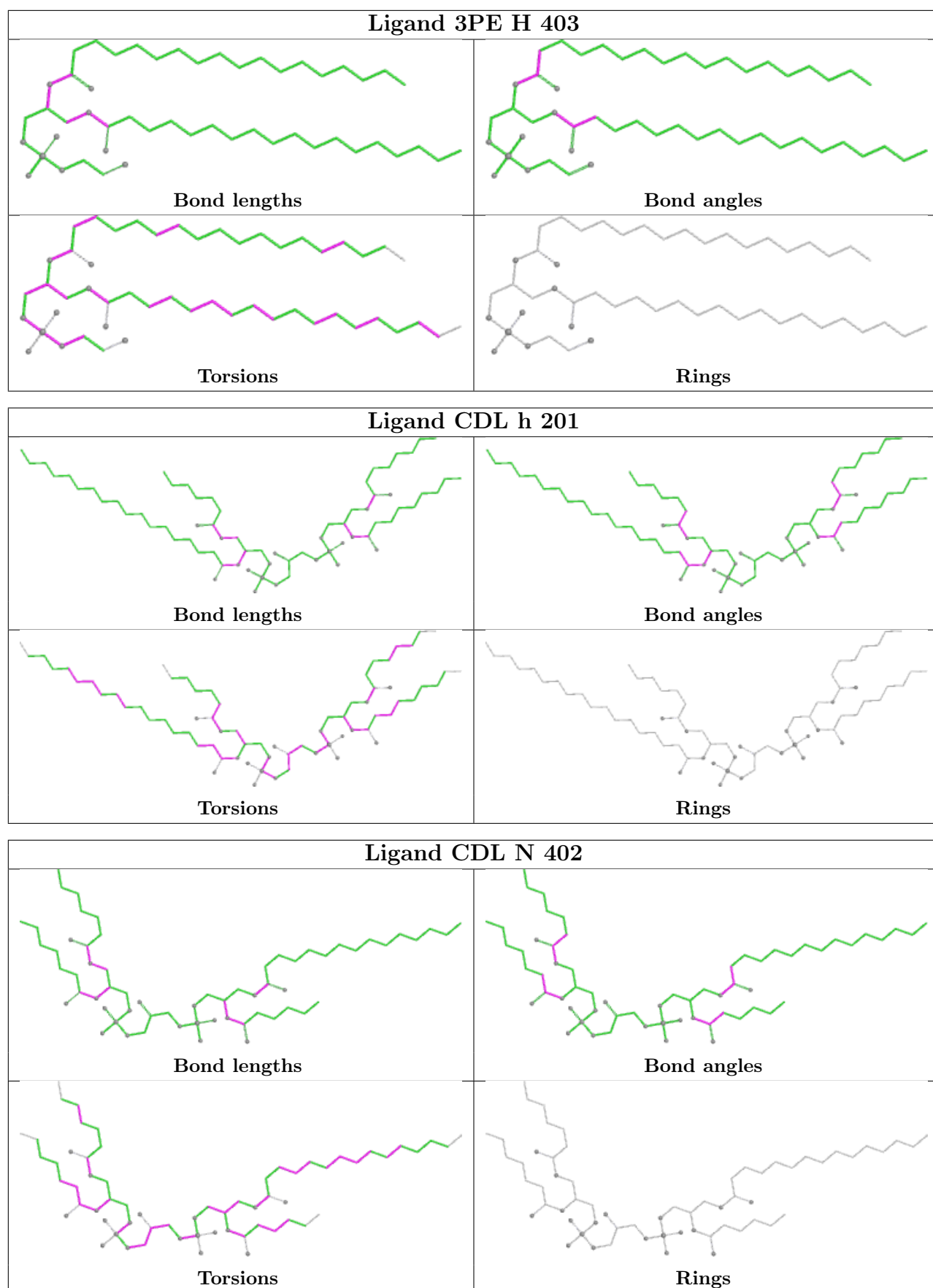
13 monomers are involved in 19 short contacts:

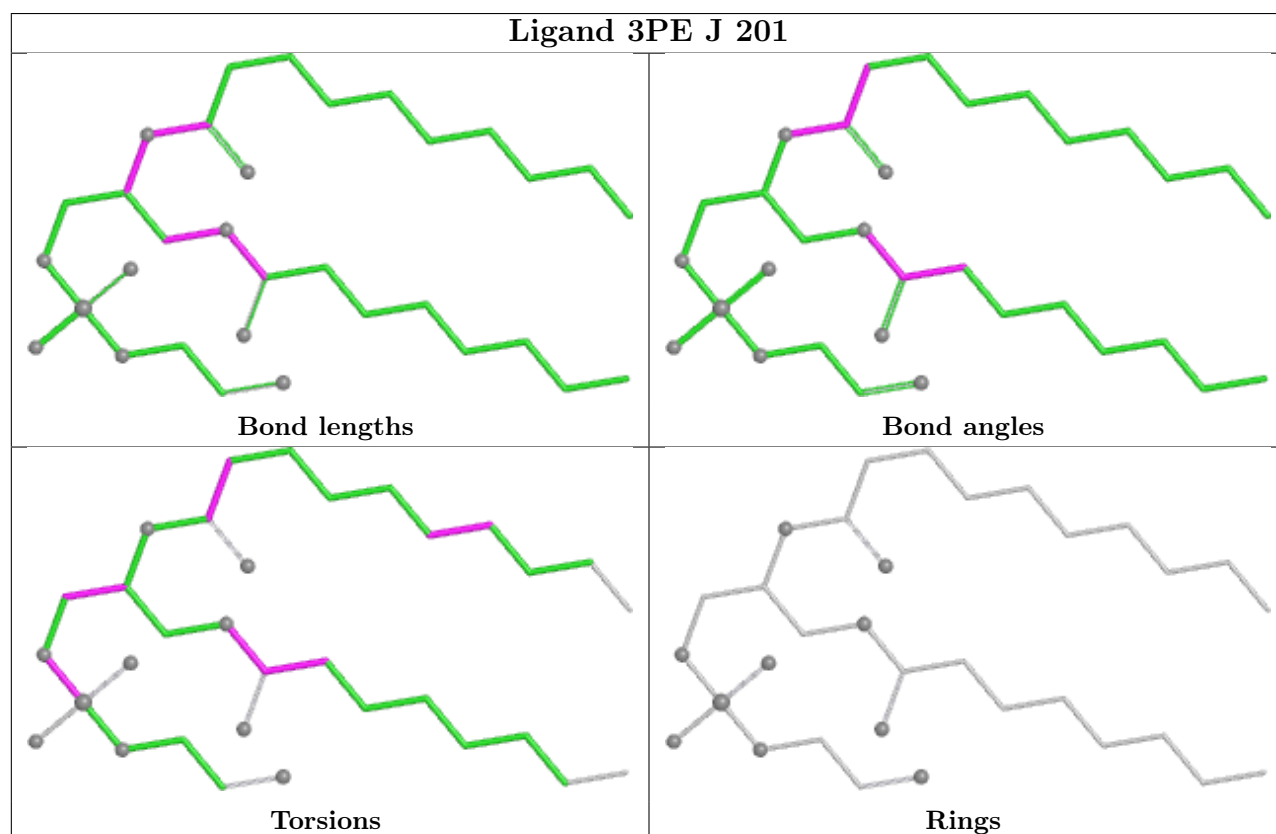
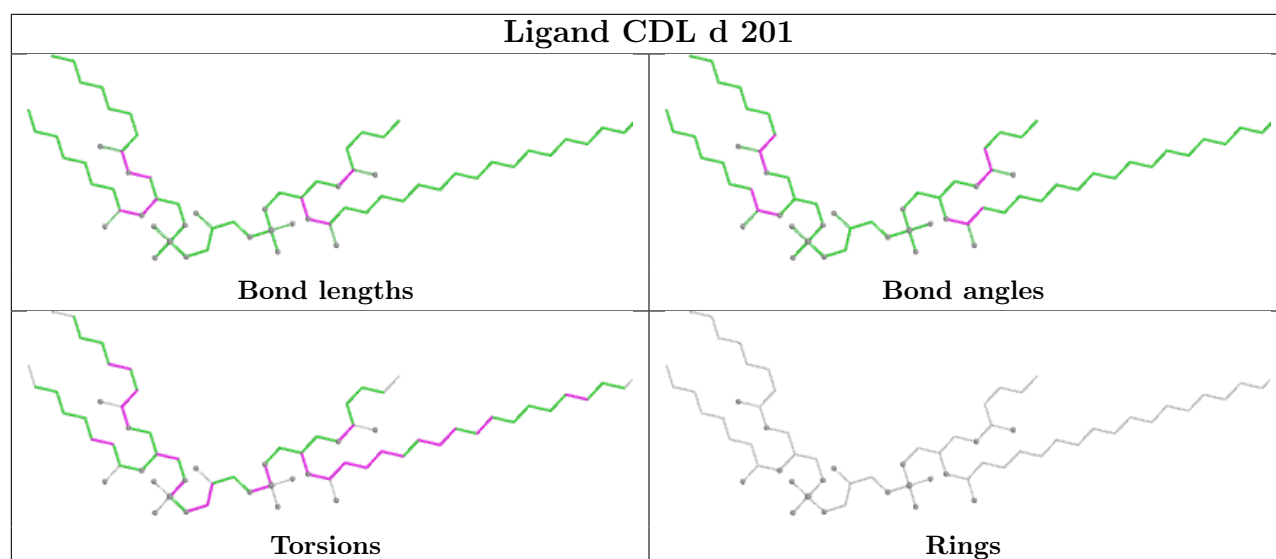
Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	G	802	SF4	1	0
48	H	403	3PE	1	0
52	P	501	NDP	1	0
51	O	401	GTP	2	0
43	I	201	SF4	3	0
48	L	703	3PE	1	0
54	U	201	EHZ	1	0
46	F	502	FMN	1	0
50	L	705	LMT	1	0
45	G	803	FES	1	0
54	T	201	EHZ	2	0
48	Z	401	3PE	1	0
47	H	401	UQ9	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

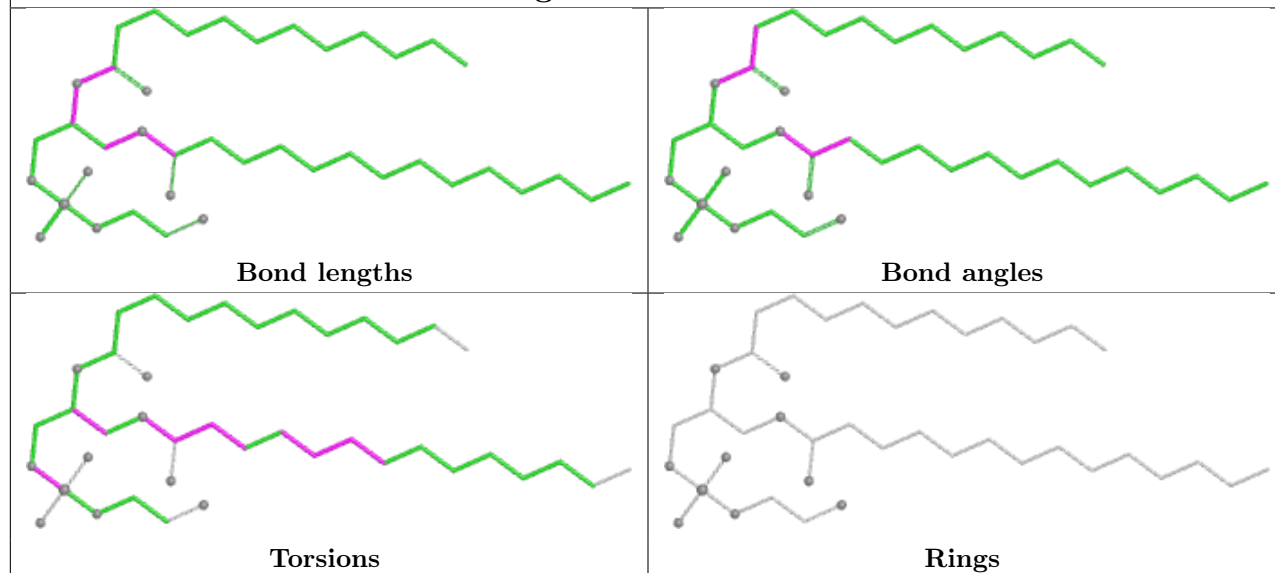
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



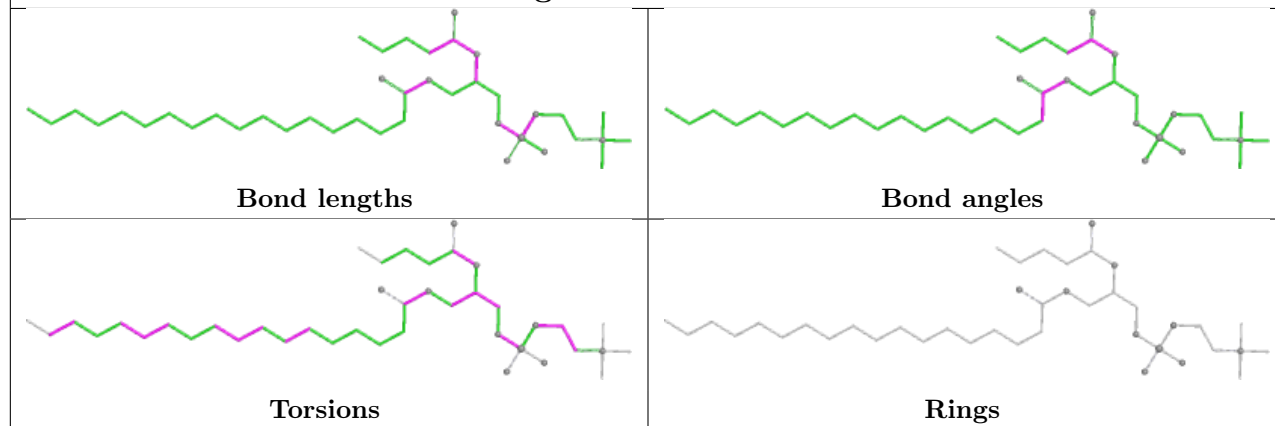


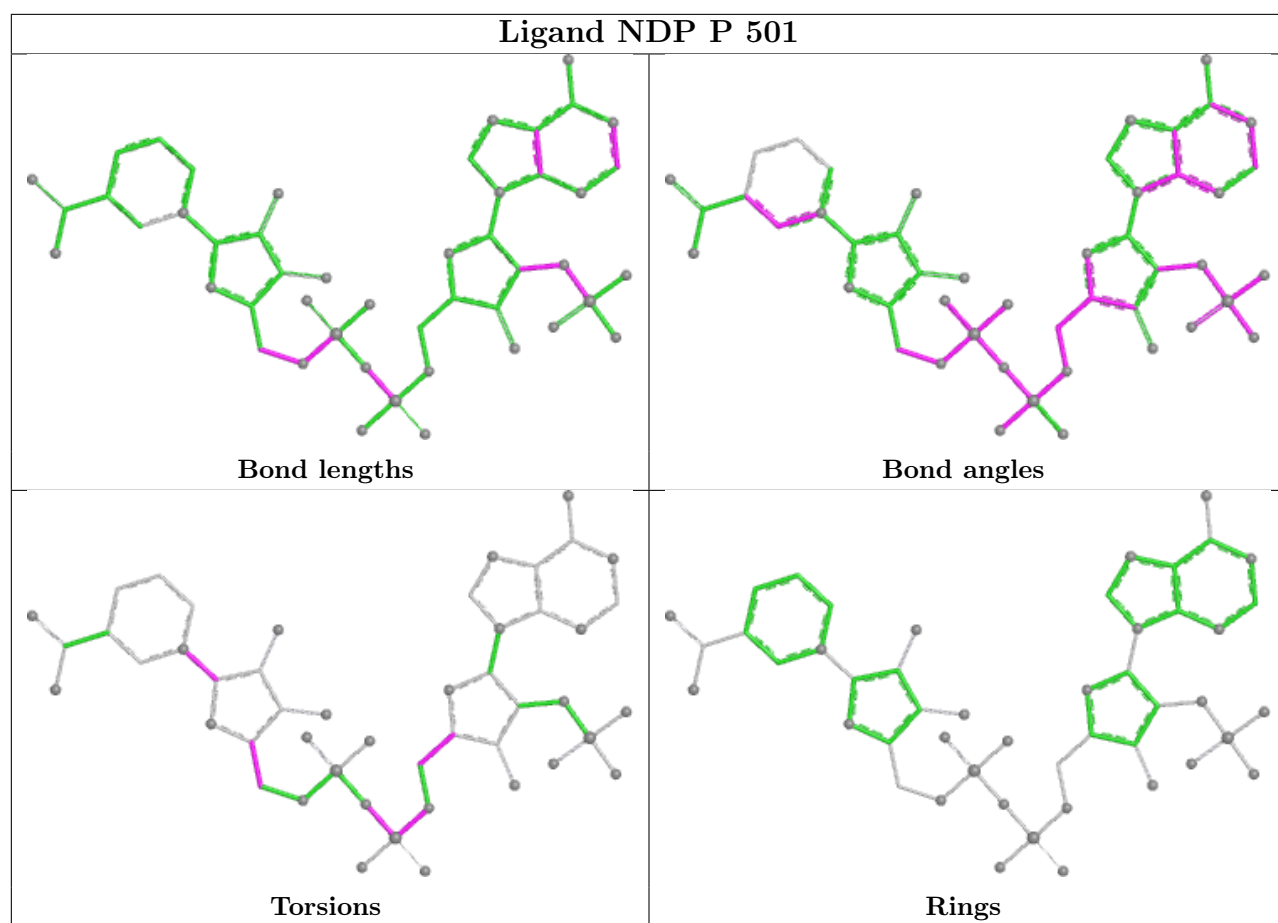


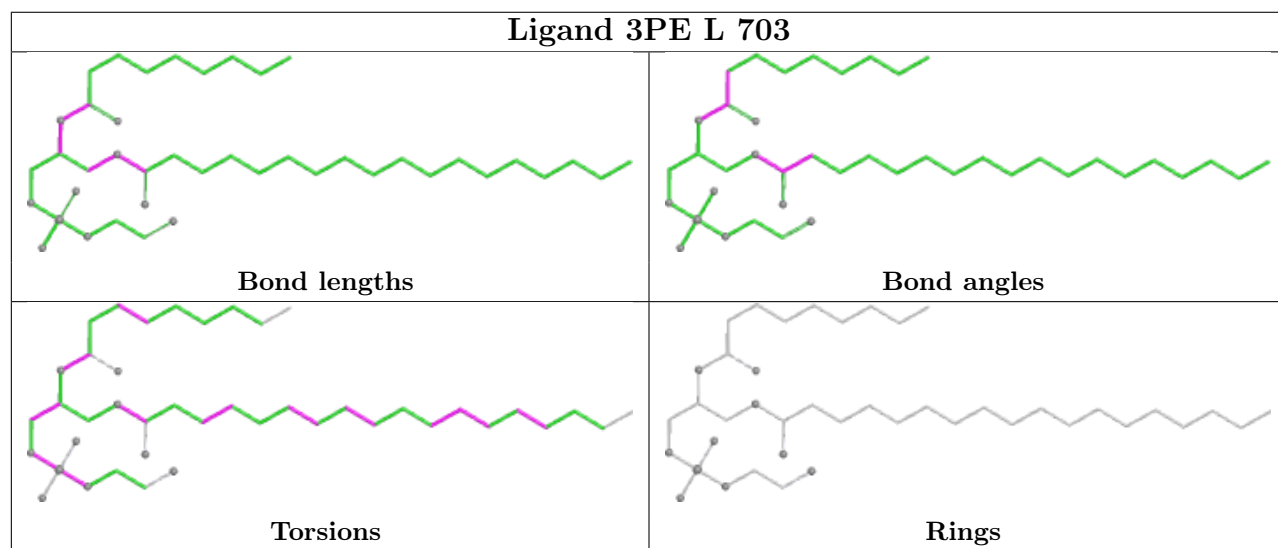
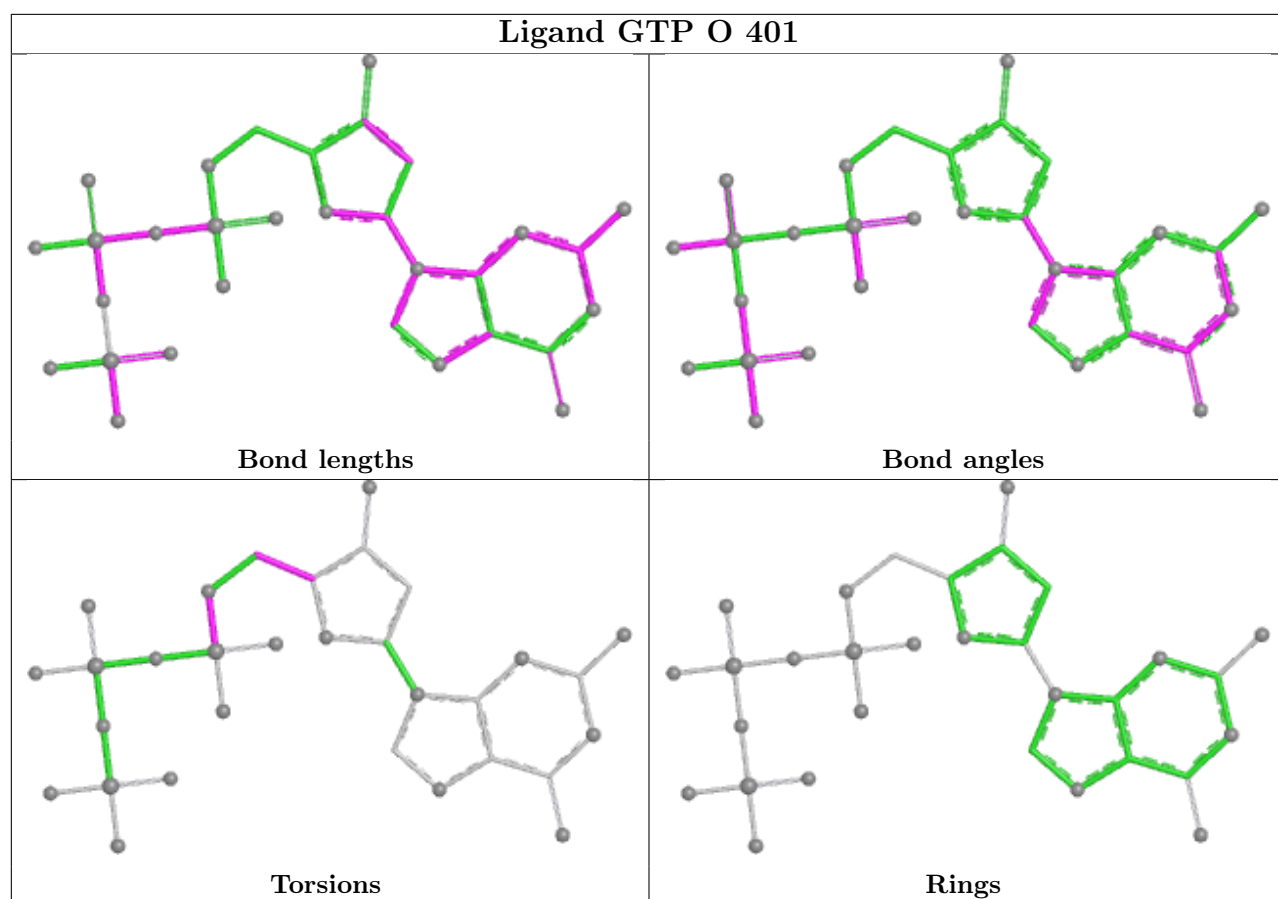
Ligand 3PE Y 401

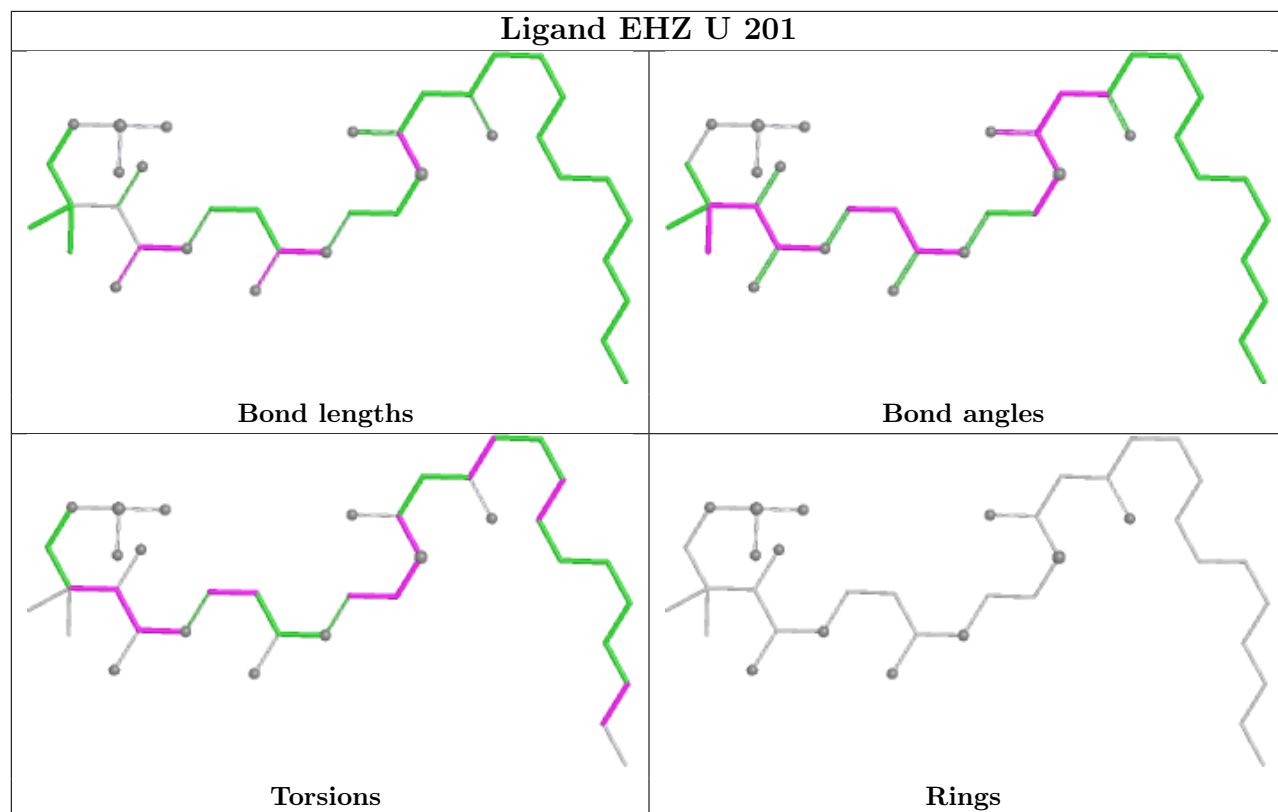


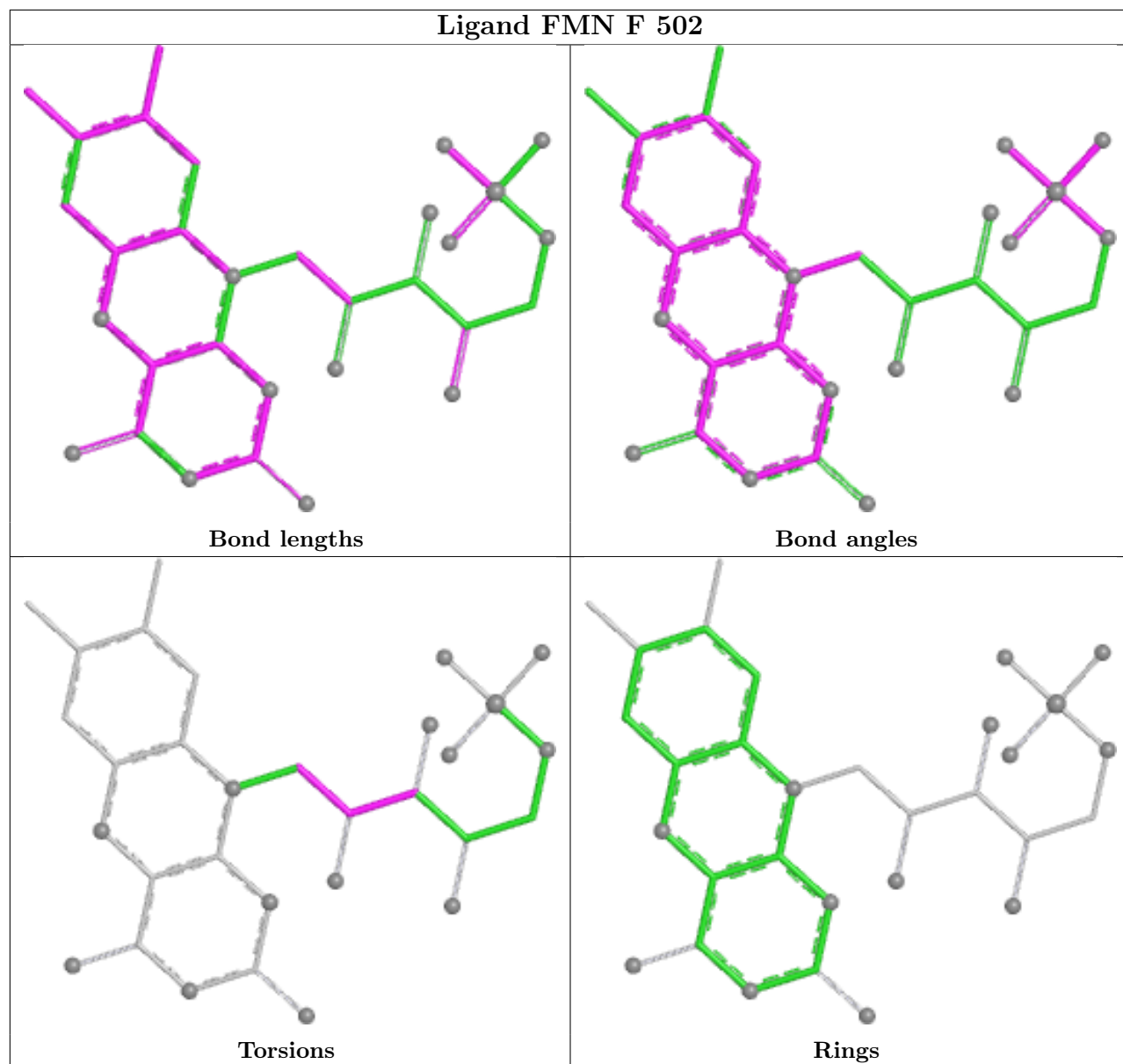
Ligand PC1 B 202

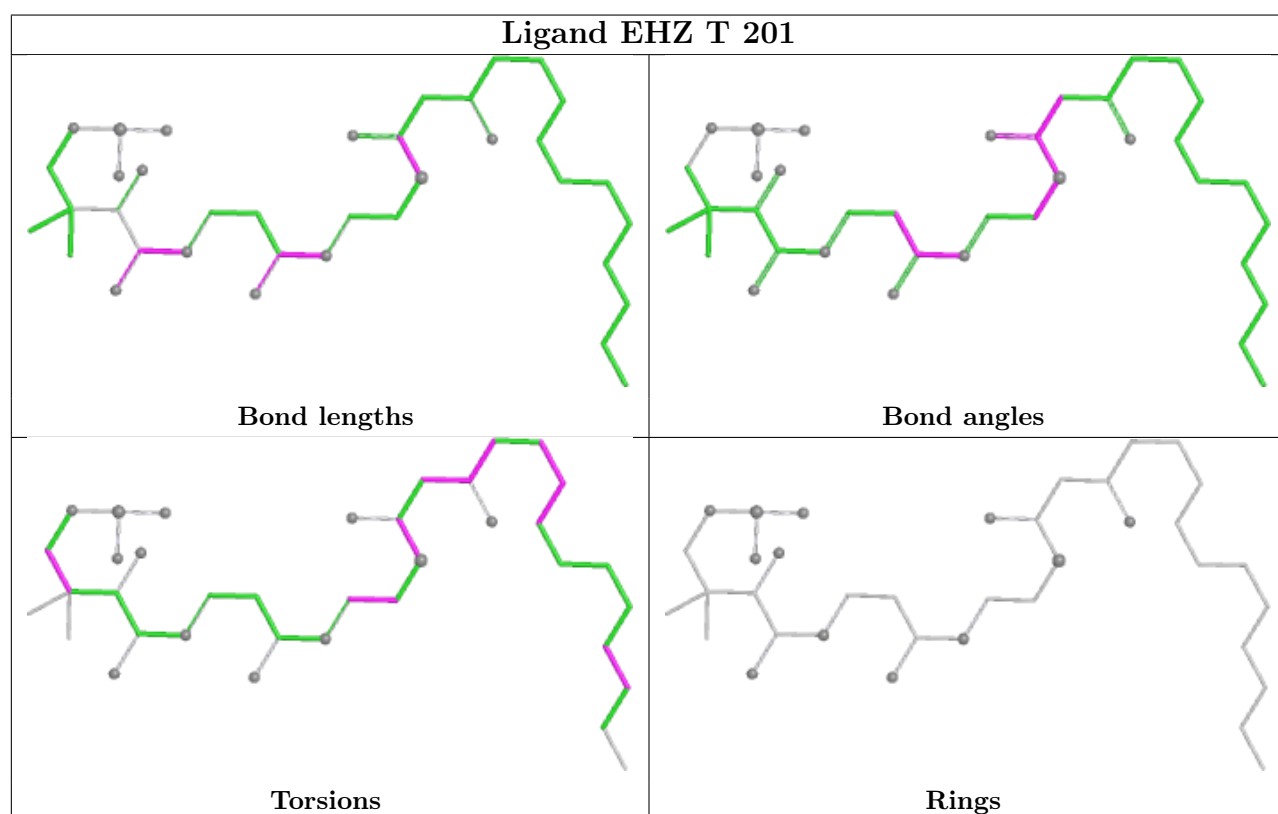
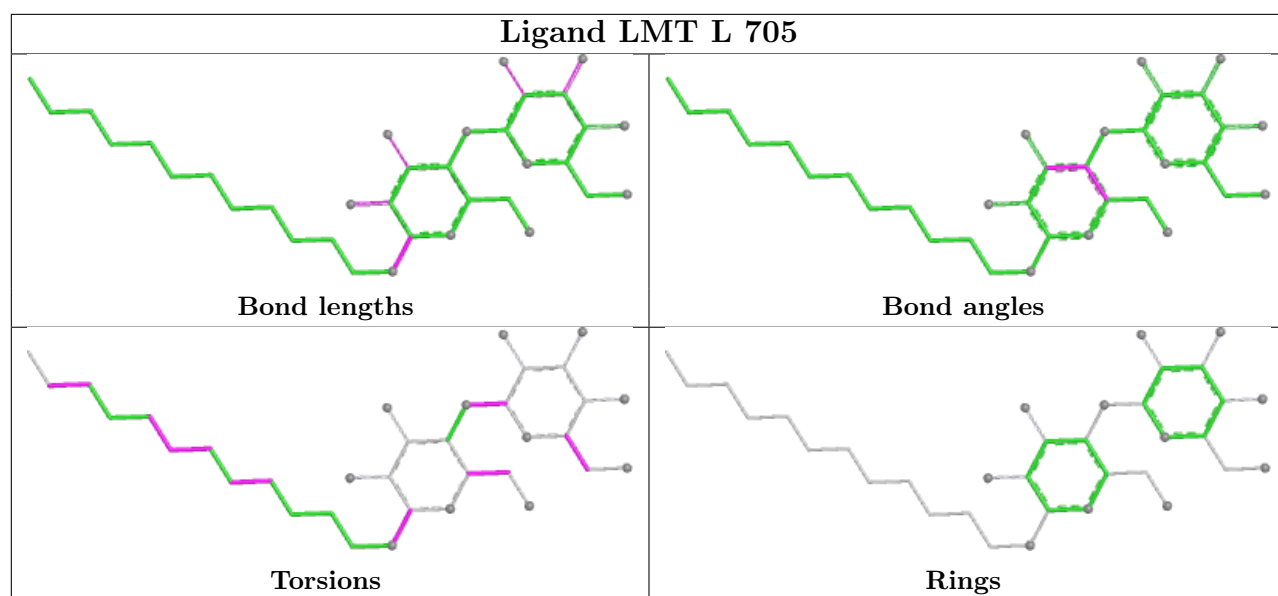


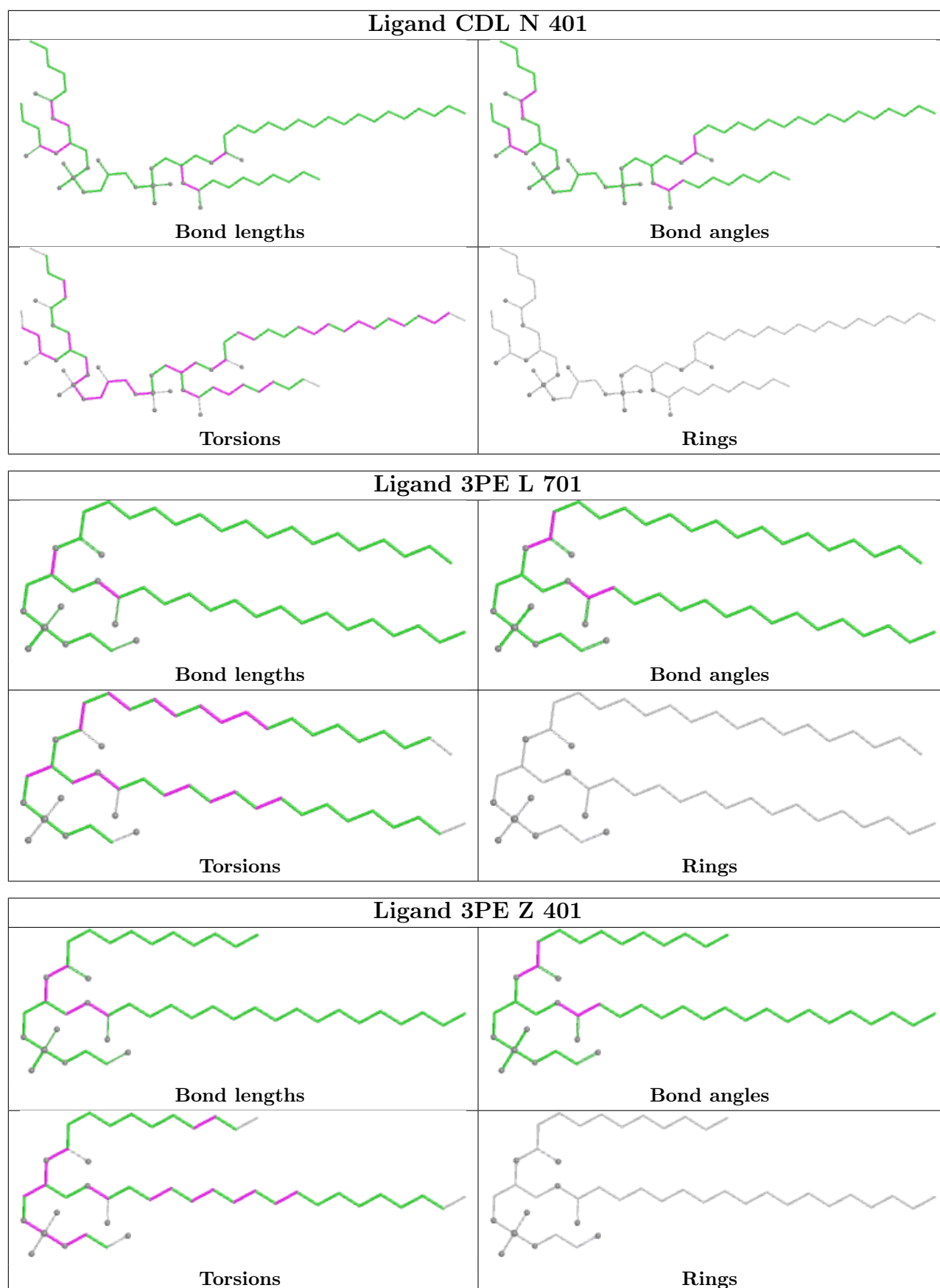


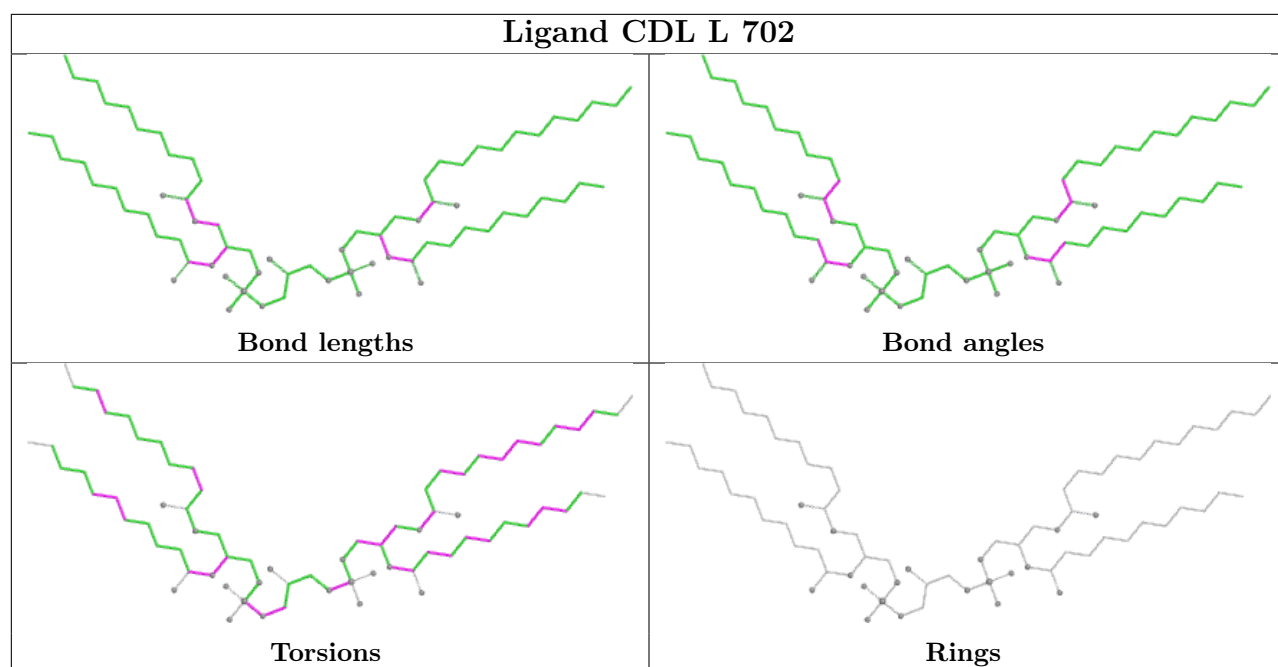


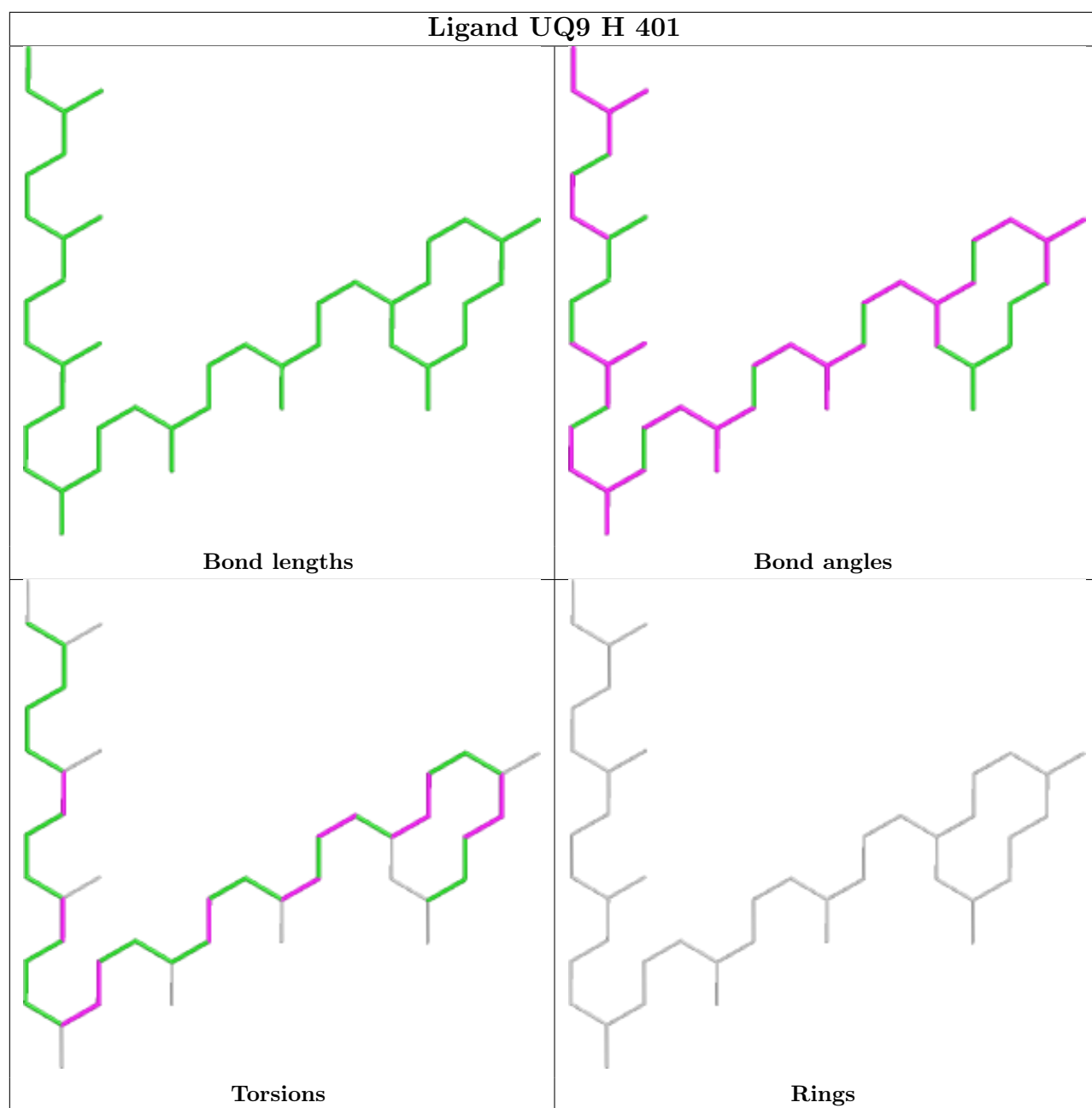


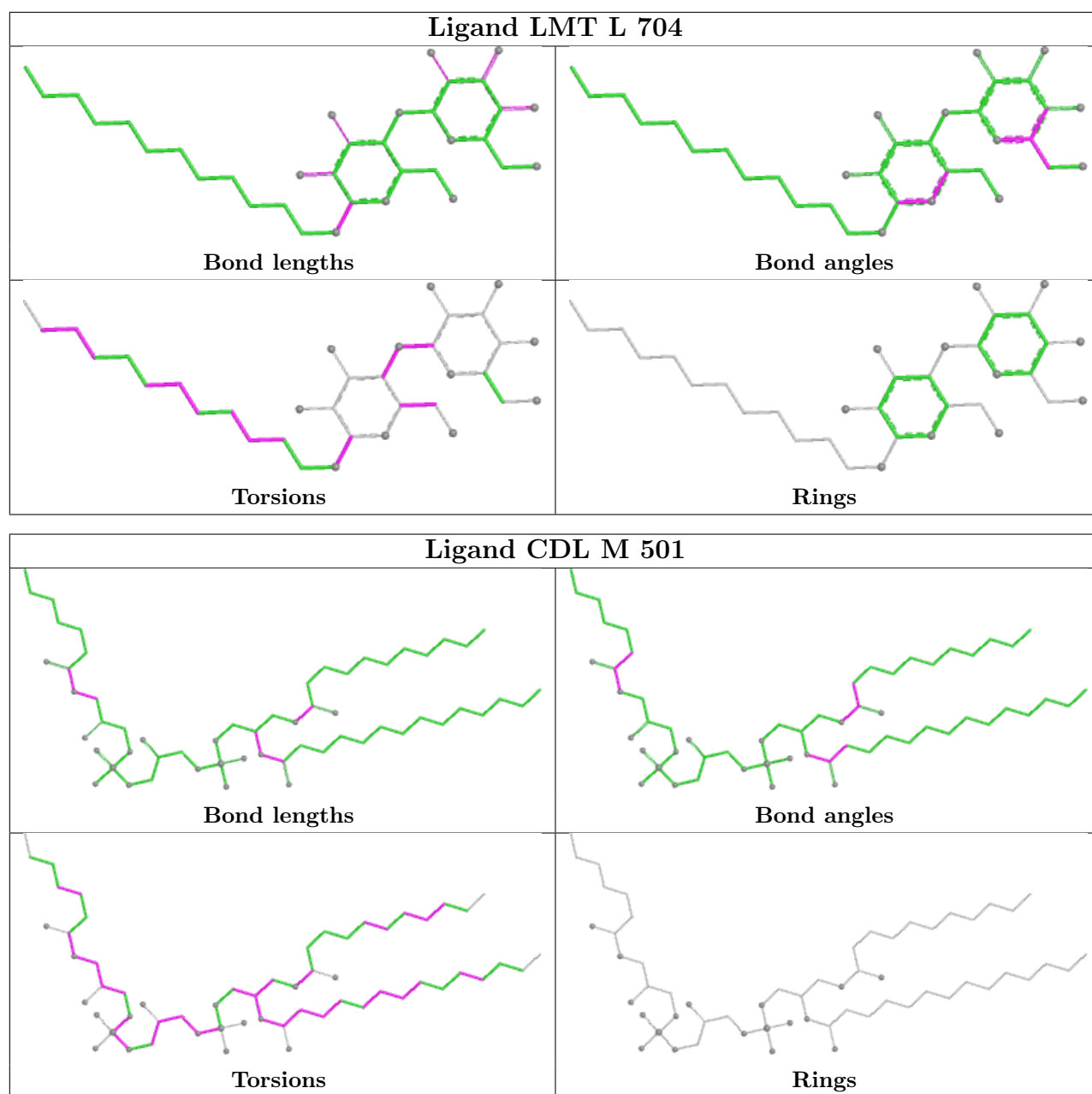












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

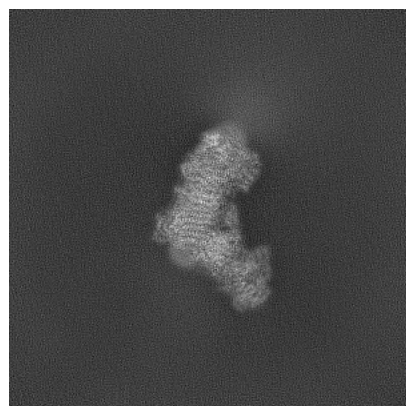
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16516. These allow visual inspection of the internal detail of the map and identification of artifacts.

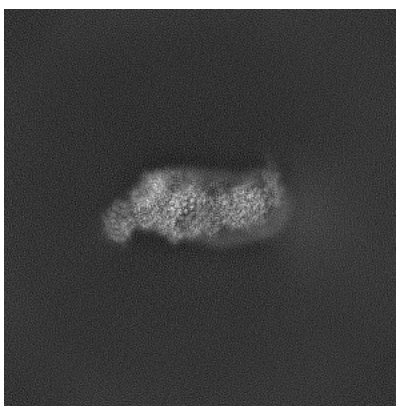
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

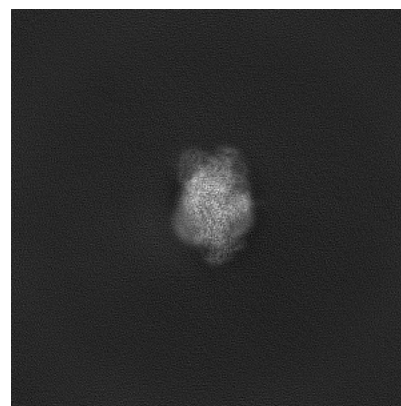
6.1.1 Primary map



X

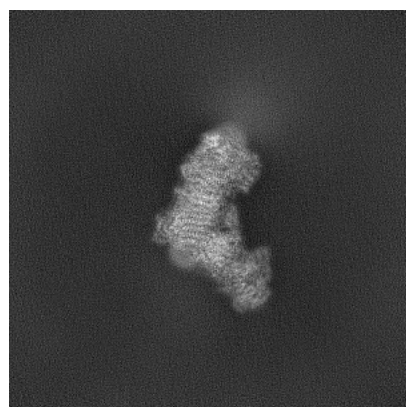


Y

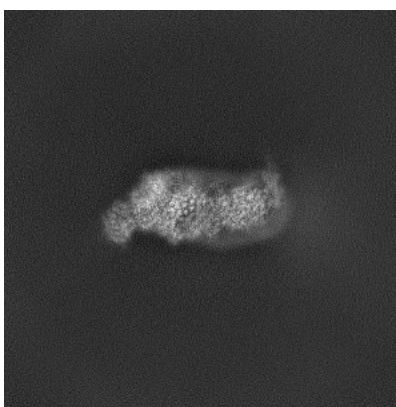


Z

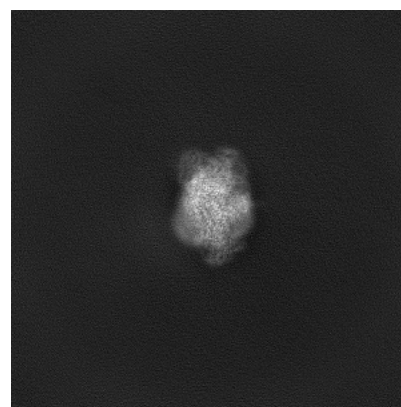
6.1.2 Raw map



X



Y

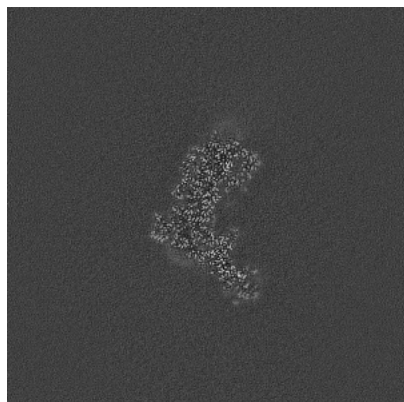


Z

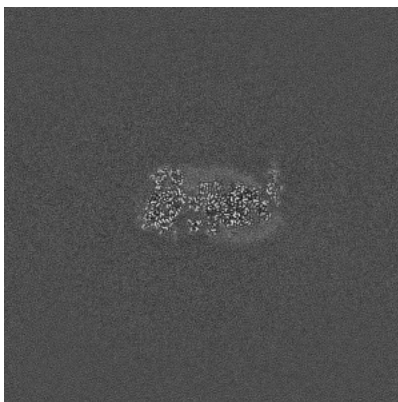
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

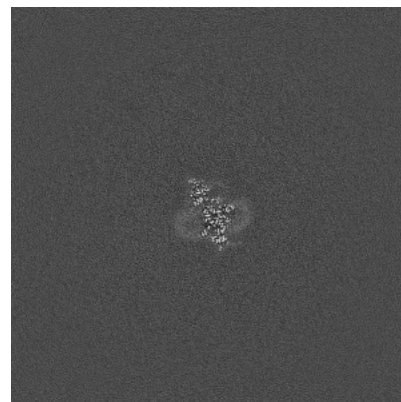
6.2.1 Primary map



X Index: 225

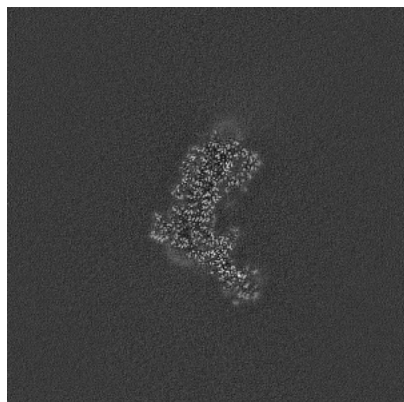


Y Index: 225

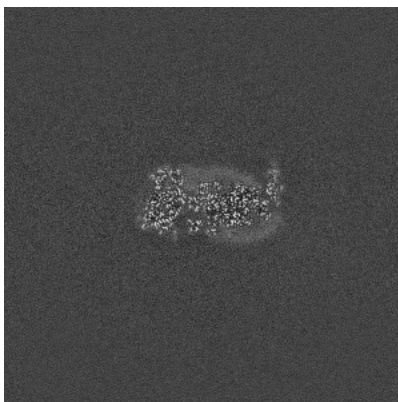


Z Index: 225

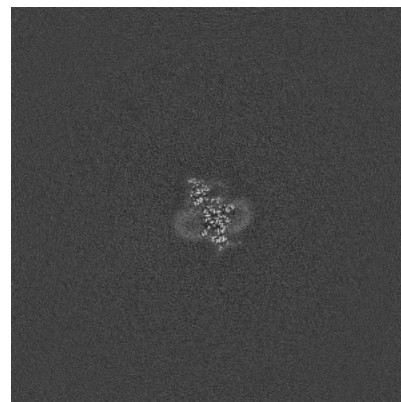
6.2.2 Raw map



X Index: 225



Y Index: 225

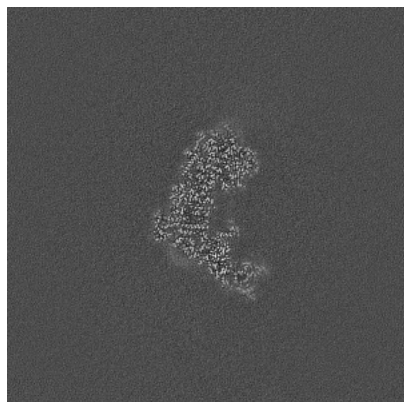


Z Index: 225

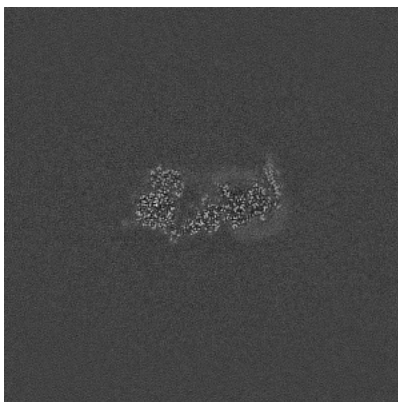
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 230

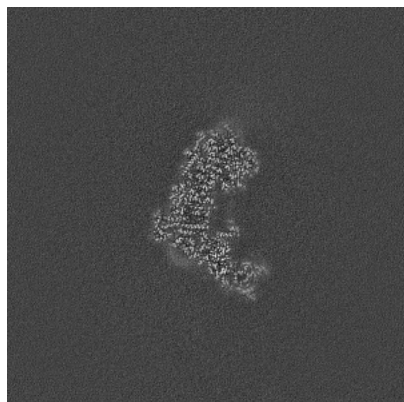


Y Index: 234



Z Index: 189

6.3.2 Raw map



X Index: 230



Y Index: 234

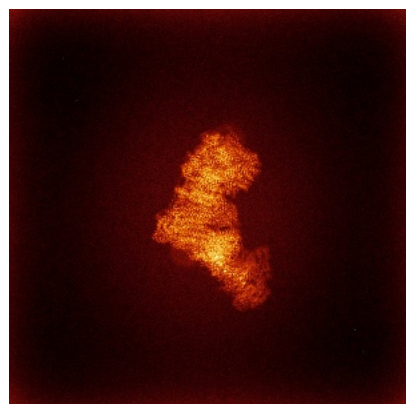


Z Index: 189

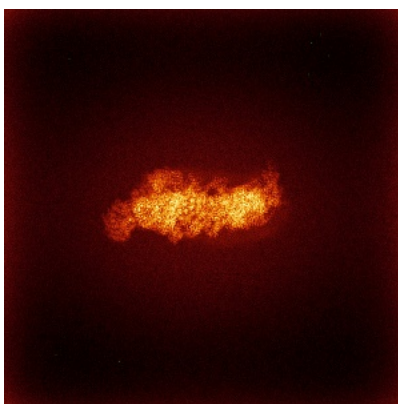
The images above show the largest variance slices of the map in three orthogonal directions.

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

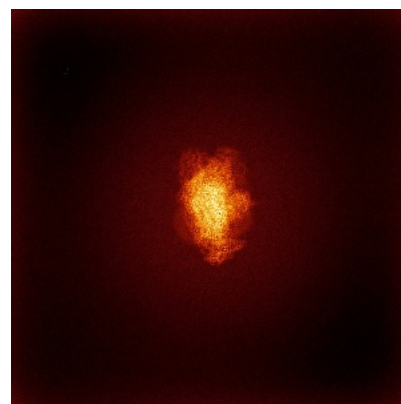
6.4.1 Primary map



X

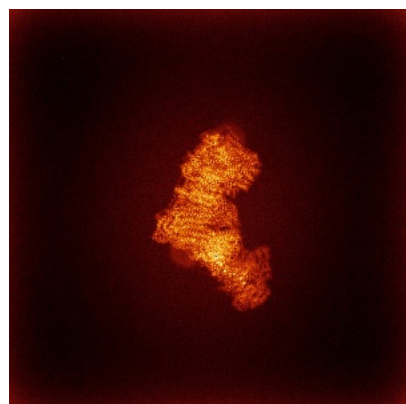


Y

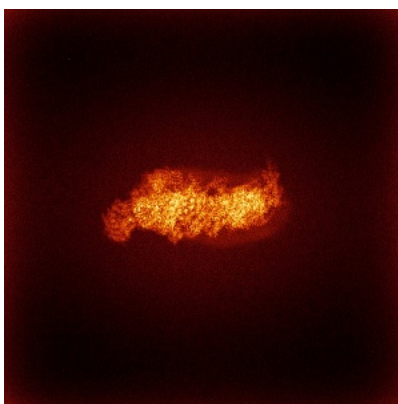


Z

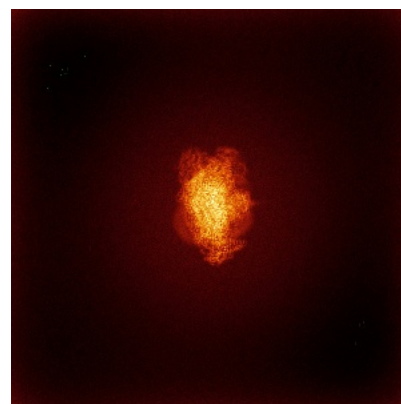
6.4.2 Raw map



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



X



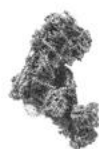
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.9. 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



X



Y



Z

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.

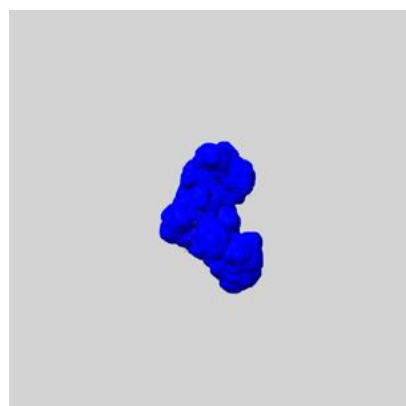
6.6 Mask visualisation [i](#)

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

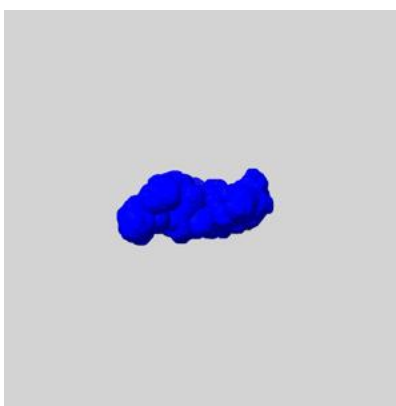
A mask typically either:

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

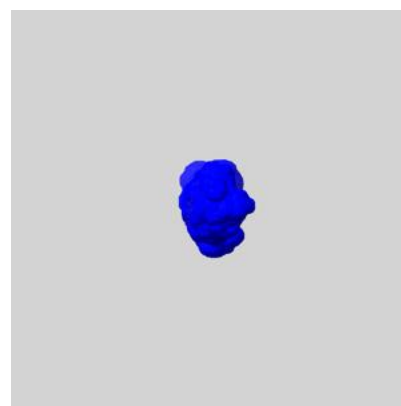
6.6.1 emd_16516_msk_1.map [i](#)



X



Y

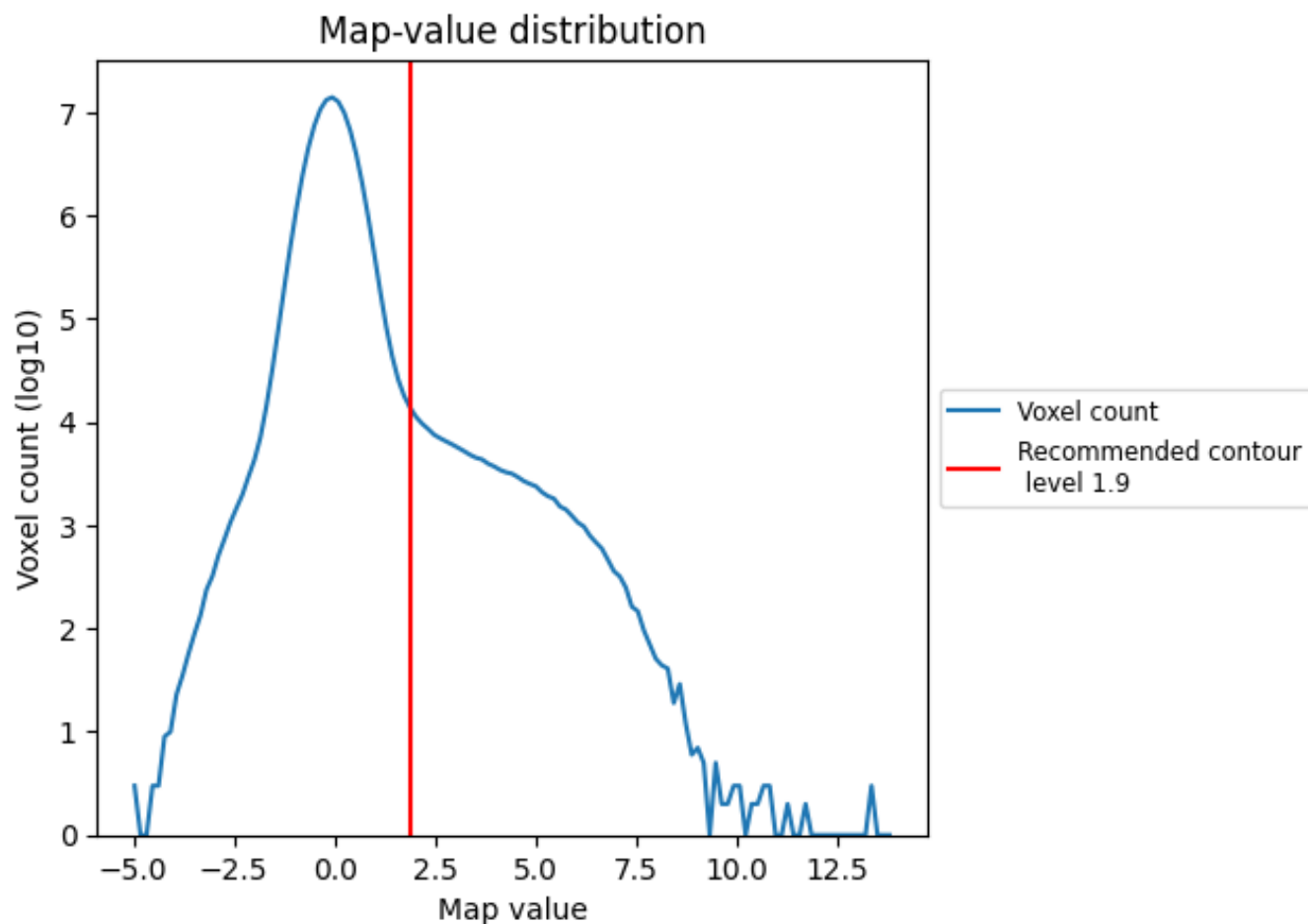


Z

7 Map analysis [i](#)

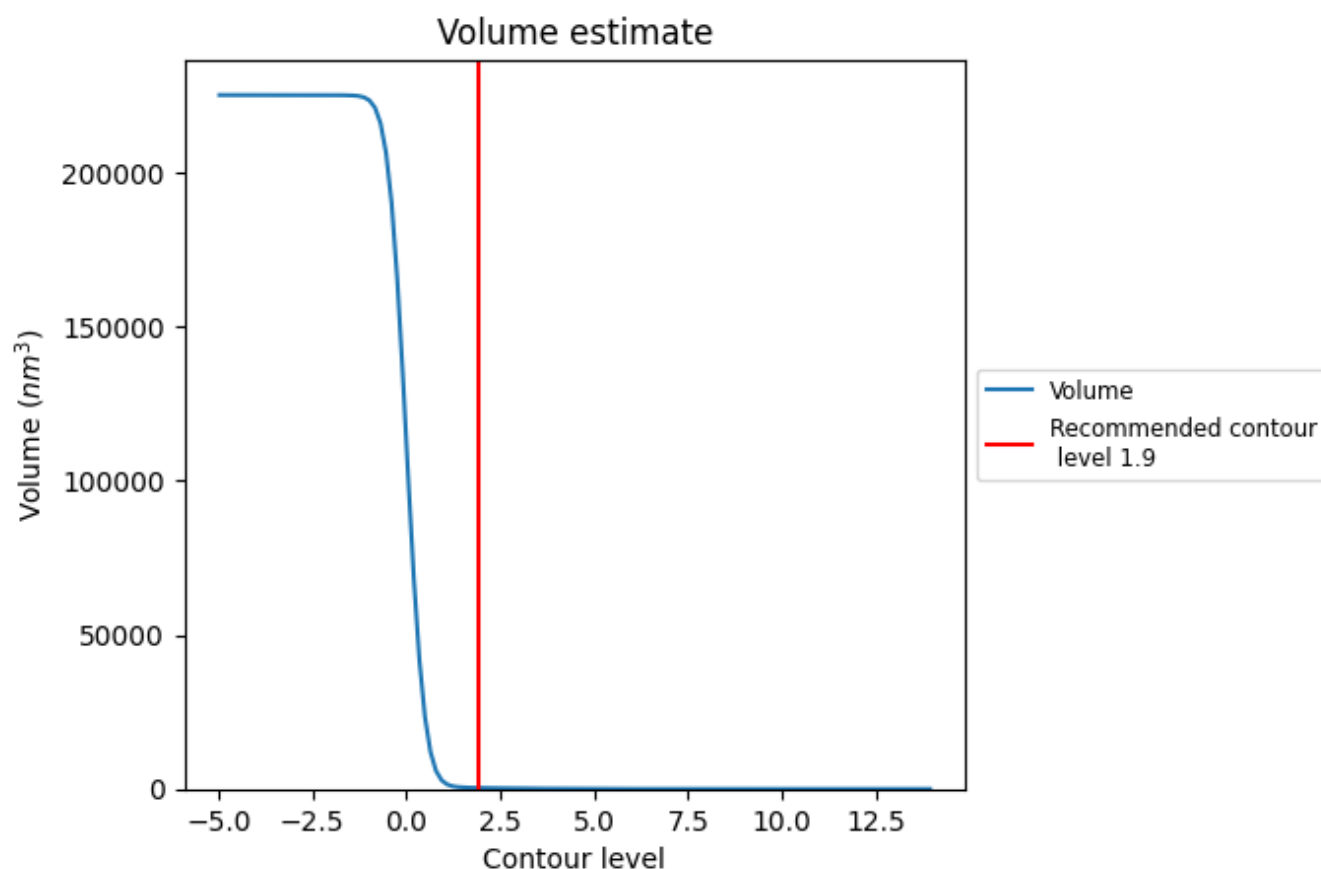
This section contains the results of statistical analysis of the map.

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.

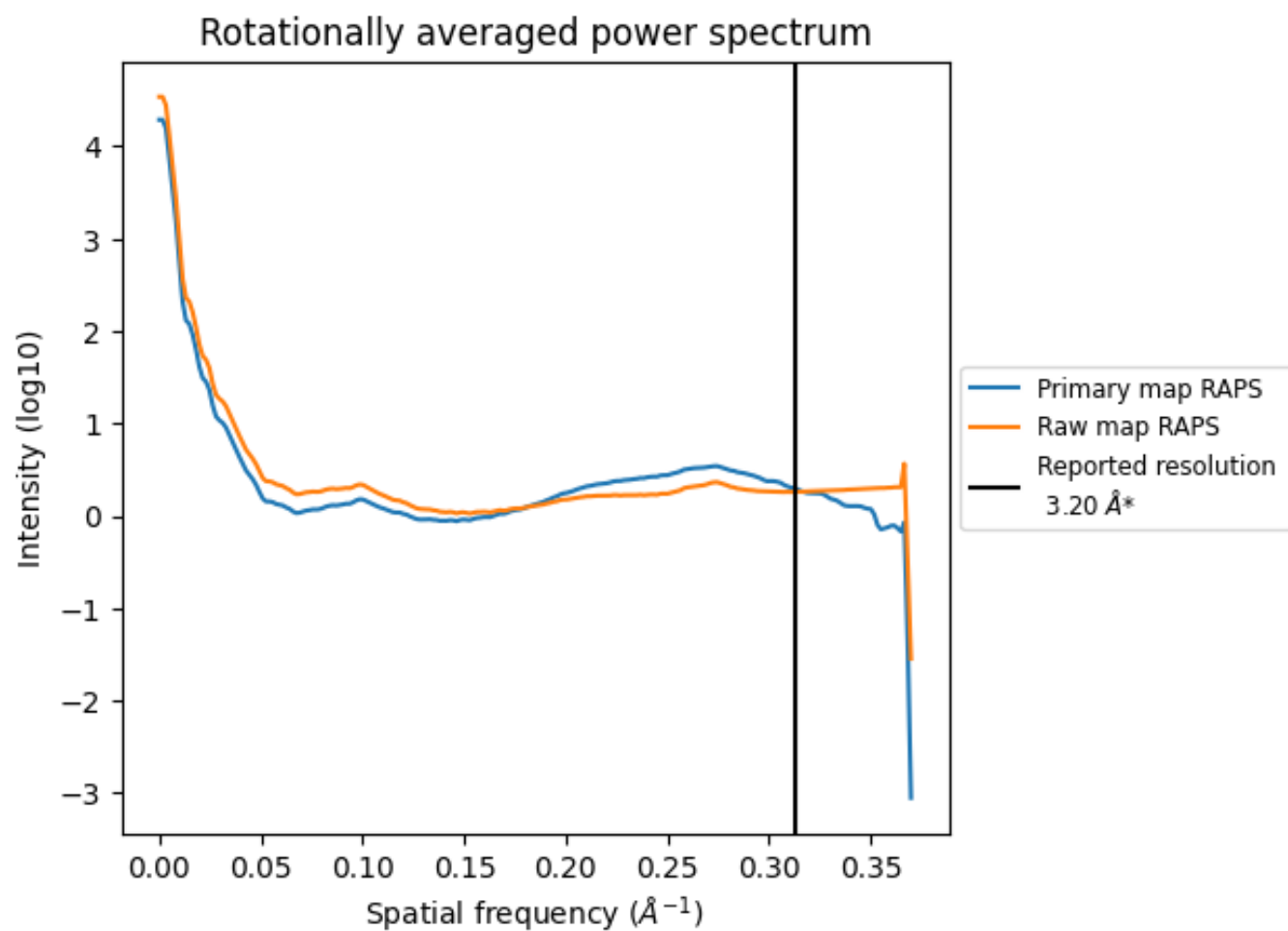
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 339 nm^3 ; this corresponds to an approximate mass of 306 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 ⓘ

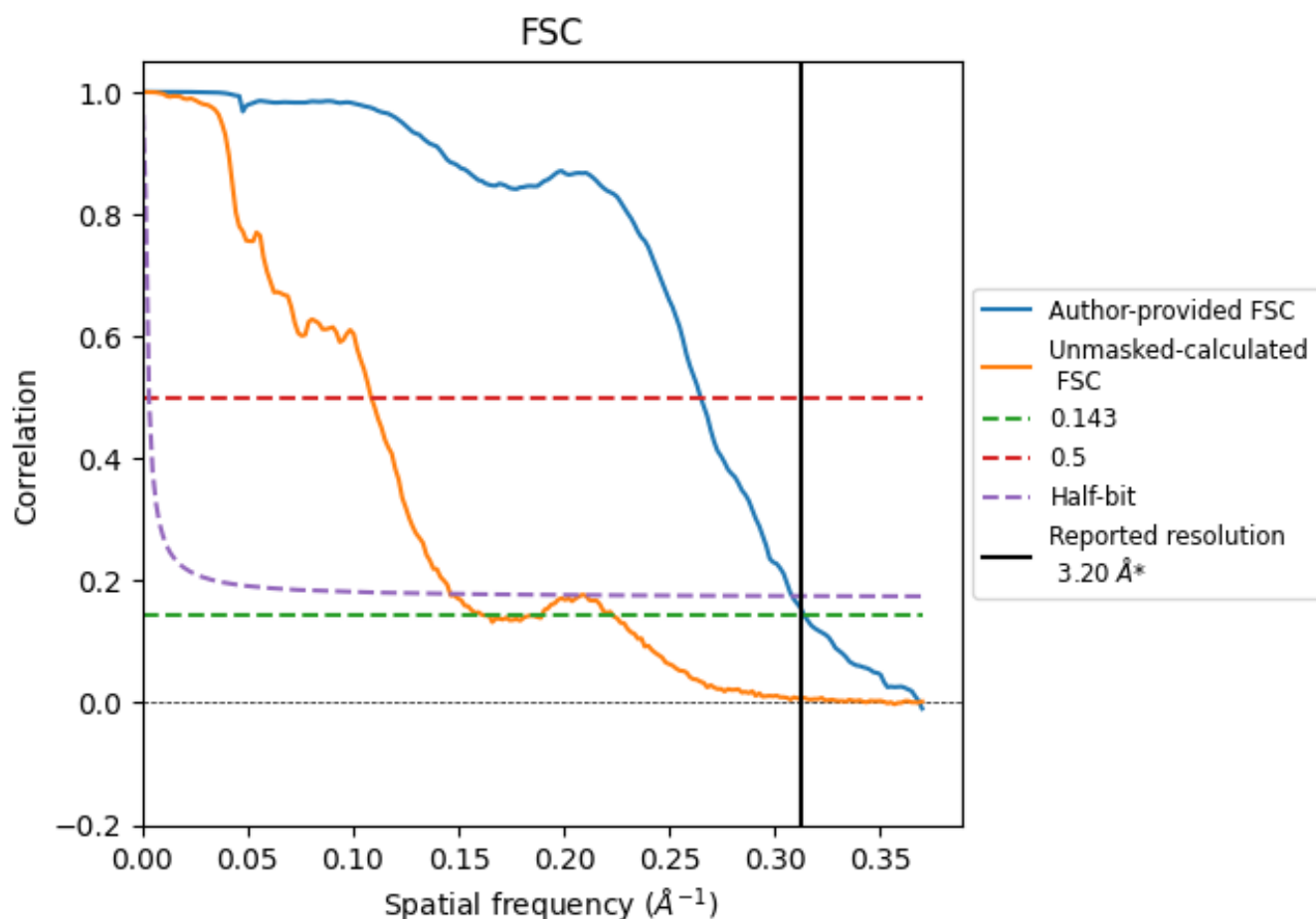


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

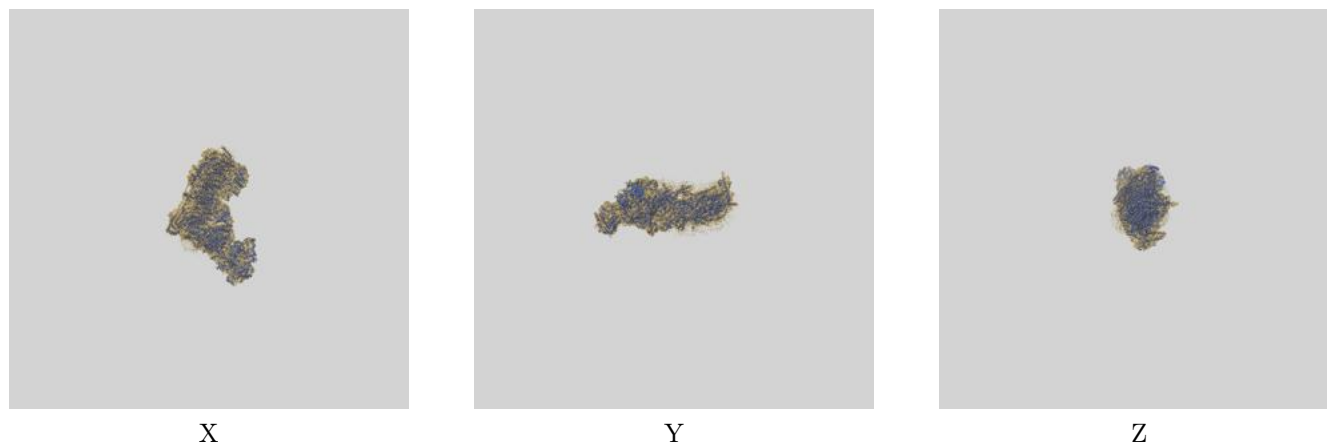
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.78	3.25
Unmasked-calculated*	6.17	9.22	6.85

*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 6.17 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

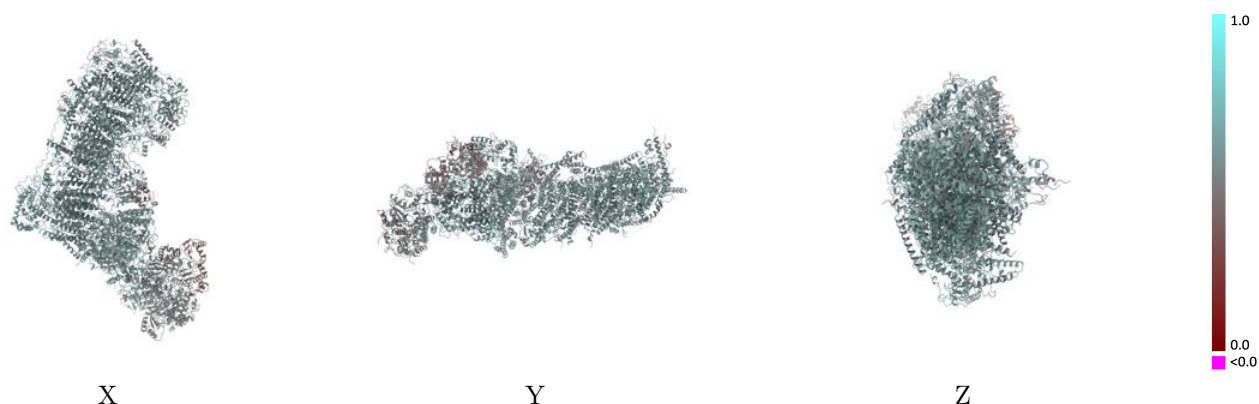
This section contains information regarding the fit between EMDB map EMD-16516 and PDB model 8CA3. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



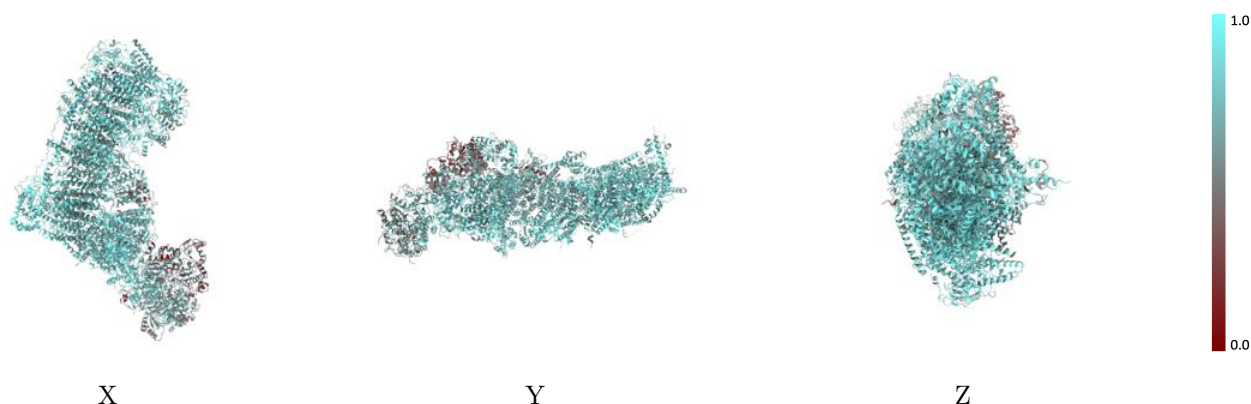
The images above show the 3D surface view of the map at the recommended contour level 1.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



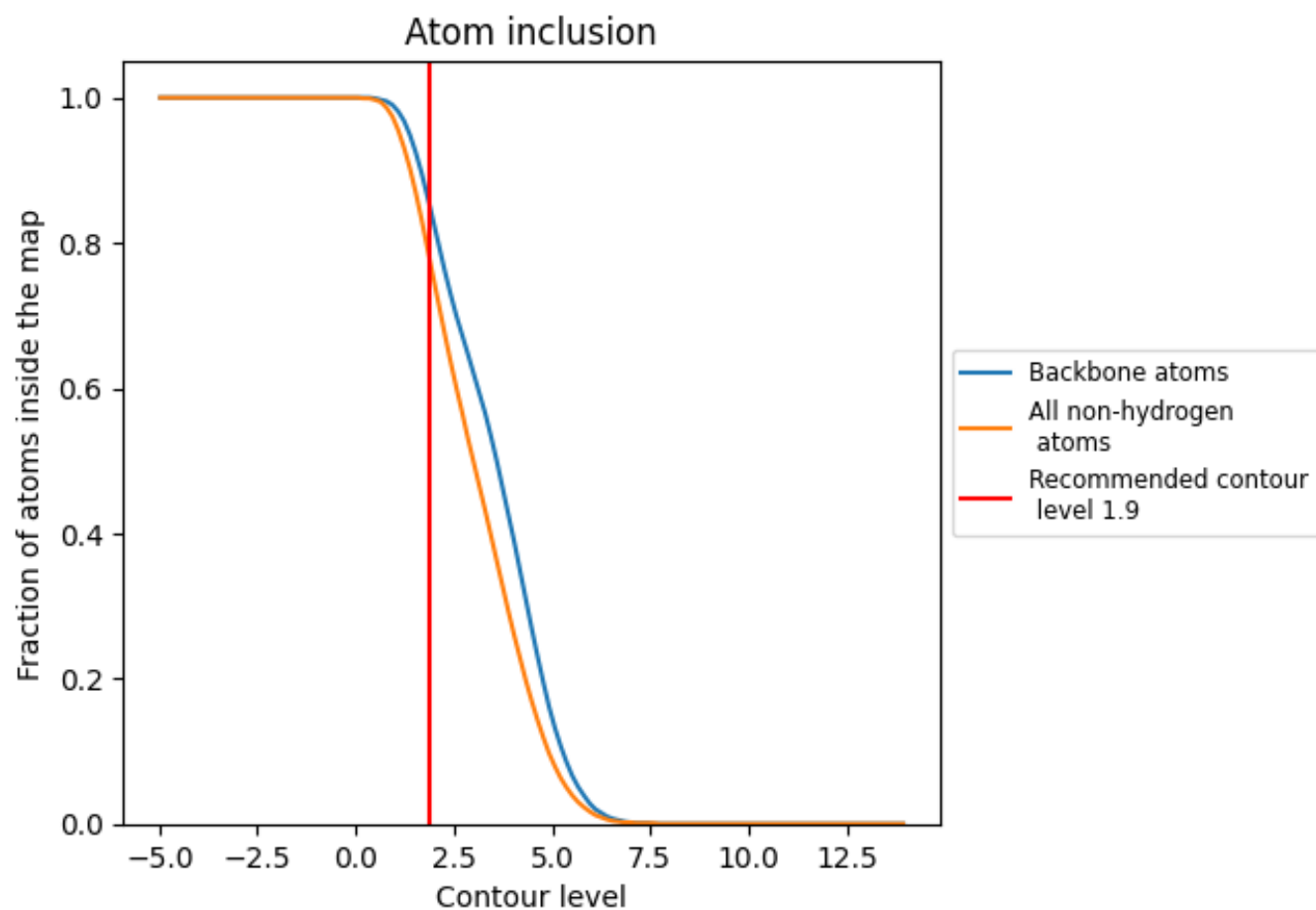
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.9).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 77% 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 (1.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7730	 0.5680
A	 0.8020	 0.5870
B	 0.8710	 0.6010
C	 0.8420	 0.6030
D	 0.8530	 0.6010
E	 0.6070	 0.5000
F	 0.6360	 0.5160
G	 0.5940	 0.5110
H	 0.8160	 0.5850
I	 0.8400	 0.5830
J	 0.7710	 0.5720
K	 0.8210	 0.5880
L	 0.8090	 0.5820
M	 0.8610	 0.5990
N	 0.8350	 0.5950
O	 0.8380	 0.5860
P	 0.7820	 0.5780
R	 0.6150	 0.5580
S	 0.4410	 0.4350
T	 0.4950	 0.4590
U	 0.7570	 0.5510
V	 0.7960	 0.5760
W	 0.7100	 0.5620
X	 0.8320	 0.5800
Y	 0.7610	 0.5640
Z	 0.8000	 0.5770
a	 0.8660	 0.5990
b	 0.8090	 0.5720
c	 0.7670	 0.5620
d	 0.8380	 0.5920
e	 0.8480	 0.5910
f	 0.7340	 0.5520
g	 0.8050	 0.5800
h	 0.8360	 0.5910
i	 0.7640	 0.5670



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Chain	Atom inclusion	Q-score
j	 0.7870	 0.5670
k	 0.7570	 0.5510
l	 0.8320	 0.5810
m	 0.8100	 0.5760
n	 0.8140	 0.5770
o	 0.7610	 0.5530
p	 0.8080	 0.5730
r	 0.7730	 0.5880
s	 0.5040	 0.4750