



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 10:40 PM UTC

PDB ID : 7O6Y / pdb_00007o6y
EMDB ID : EMD-12741
Title : Cryo-EM structure of respiratory complex I under turnover
Authors : Parey, K.; Vonck, J.
Deposited on : 2021-04-12
Resolution : 3.40 Å(reported)
Based on initial model : 6RFR

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:

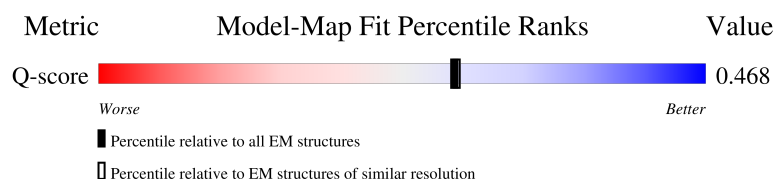
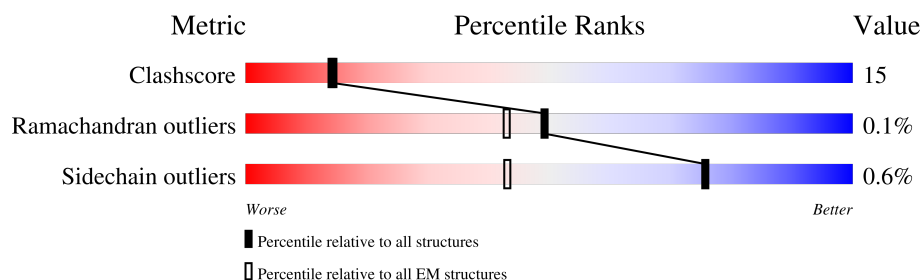
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	728	
2	B	488	
3	C	466	
4	G	281	

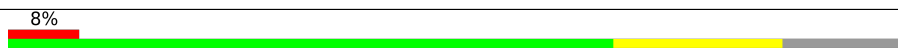
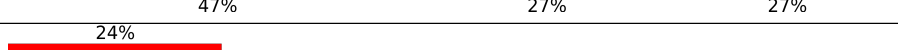
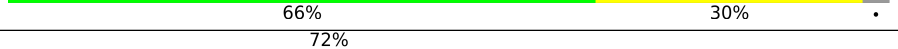
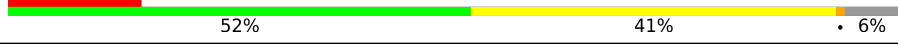
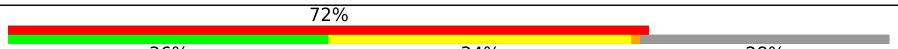
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Mol	Chain	Length	Quality of chain
5	H	243	
6	I	229	
7	K	210	
8	L	89	
9	S	249	
10	j	93	
11	1	341	
12	2	469	
13	3	128	
14	4	486	
15	5	655	
16	6	185	
17	g	78	
18	D	87	
19	E	375	
20	F	144	
21	J	198	
22	M	136	
23	O	109	
24	P	124	
25	Q	132	
26	R	109	
27	U	172	
28	W	123	
29	X	169	

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Mol	Chain	Length	Quality of chain
30	Y	161	
31	Z	182	
32	a	149	
33	b	74	
34	c	60	
35	d	92	
36	e	67	
37	f	87	
38	h	138	
39	i	90	
40	n	139	
41	8	99	
42	9	89	

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
44	FES	A	803	-	-	X	-

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 64866 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 Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	693	Total	C	N	O	S	0	0
			5269	3272	927	1041	29		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	457	Total	C	N	O	S	0	0
			3528	2230	619	655	24		

- Molecule 3 is a protein called NUCM protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	410	Total	C	N	O	S	0	0
			3247	2070	553	602	22		

- Molecule 4 is a protein called Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	239	Total	C	N	O	S	0	0
			1978	1272	336	366	4		

- Molecule 5 is a protein called Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	216	Total	C	N	O	S	0	0
			1688	1060	284	326	18		

- Molecule 6 is a protein called Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	190	Total	C	N	O	S	0	0
			1519	966	254	289	10		

- Molecule 7 is a protein called Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	177	Total	C	N	O	S	0	0
			1395	885	246	249	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	86	Total	C	N	O	S	0	0
			669	448	106	112	3		

- Molecule 9 is a protein called Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	182	Total	C	N	O	S	0	0
			1492	961	255	274	2		

- Molecule 10 is a protein called Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	90	Total	C	N	O	S	0	0
			724	465	132	127			

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1	340	Total	C	N	O	S	0	0
			2716	1850	393	466	7		

- Molecule 12 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2	469	Total	C	N	O	S	0	0
			3776	2558	550	656	12		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	117	Total	C	N	O	S	0	0
			930	642	129	156	3		

- Molecule 14 is a protein called Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	4	481	Total	C	N	O	S	0	0
			3815	2573	581	647	14		

- Molecule 15 is a protein called Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	5	648	Total	C	N	O	S	0	0
			5151	3453	775	895	28		

- Molecule 16 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	6	135	Total	C	N	O	S	0	0
			1078	740	150	180	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	1	FME	-	insertion	UNP S5U3X7

- Molecule 17 is a protein called subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
17	g	76	Total	C	N	O	0	0
			622	408	113	101		

- Molecule 18 is a protein called Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	D	86	Total	C	N	O	S	0	0
			681	432	127	119	3		

- Molecule 19 is a protein called Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	334	Total	C	N	O	S	0	0
			2673	1697	468	498	10		

- Molecule 20 is a protein called Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	F	120	Total	C	N	O	S	0	0
			981	624	164	191	2		

- Molecule 21 is a protein called Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	J	172	Total	C	N	O	S	0	0
			1274	811	228	230	5		

- Molecule 22 is a protein called Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	M	117	Total	C	N	O	S	0	0
			912	568	163	176	5		

- Molecule 23 is a protein called Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
23	O	71	Total	C	N	O	0	0
			543	344	83	116		

- Molecule 24 is a protein called Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	123	Total	C	N	O	S	0	0
			1036	667	182	185	2		

- Molecule 25 is a protein called Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	85	Total	C	N	O	S	0	0
			648	405	103	138	2		

- Molecule 26 is a protein called Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	106	Total	C	N	O	S	0	0
			884	562	168	151	3		

- Molecule 27 is a protein called Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	171	Total	C	N	O	S	0	0
			1345	847	236	252	10		

- Molecule 28 is a protein called Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	121	Total	C	N	O	S	0	0
			974	623	178	168	5		

- Molecule 29 is a protein called Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	164	Total	C	N	O	S	0	0
			1275	828	217	226	4		

- Molecule 30 is a protein called Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	125	Total	C	N	O	S	0	0
			1037	659	190	186	2		

- Molecule 31 is a protein called Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	181	Total	C	N	O	S	0	0
			1389	893	240	255	1		

- Molecule 32 is a protein called Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	124	Total	C	N	O	S	0	0
			1030	669	165	194	2		

- Molecule 33 is a protein called Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
33	b	64	Total	C	N	O	0	0
			490	326	83	81		

- Molecule 34 is a protein called Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
34	c	44	Total	C	N	O	0	0
			353	229	67	57		

- Molecule 35 is a protein called Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	89	Total	C	N	O	S	0	0
			751	467	136	145	3		

- Molecule 36 is a protein called Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	52	Total	C	N	O	S	0	0
			436	293	75	65	3		

- Molecule 37 is a protein called Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	82	Total	C	N	O	S	0	0
			642	403	121	117	1		

- Molecule 38 is a protein called Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	136	Total	C	N	O	S	0	0
			1130	727	193	208	2		

- Molecule 39 is a protein called Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	83	Total	C	N	O	S	0	0
			646	413	117	115	1		

- Molecule 40 is a protein called Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	114	Total	C	N	O	S	0	0
			913	587	154	171	1		

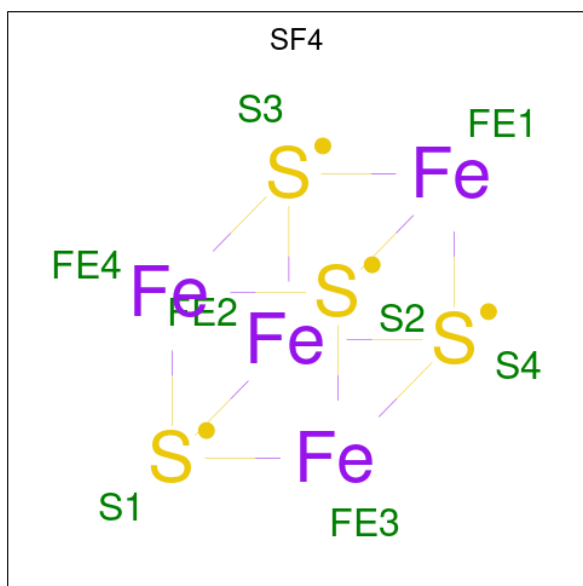
- Molecule 41 is a protein called Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
41	8	71	Total	C	N	O	S	0	0
			594	375	109	102	8		

- Molecule 42 is a protein called Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I).

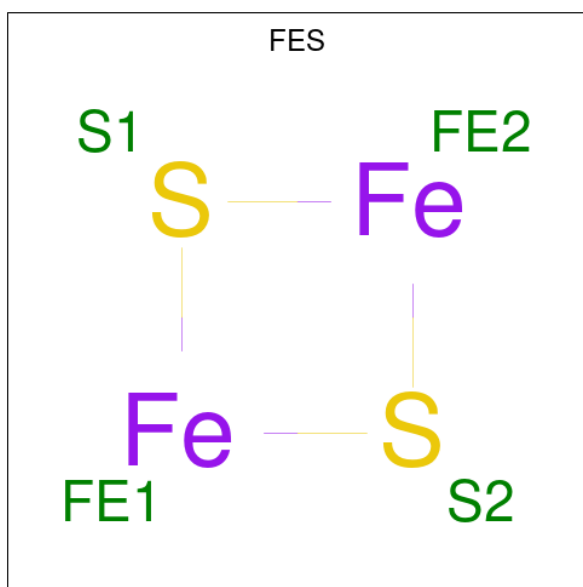
Mol	Chain	Residues	Atoms					AltConf	Trace
42	9	86	Total	C	N	O	S	0	0
			672	422	122	122	6		

- Molecule 43 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



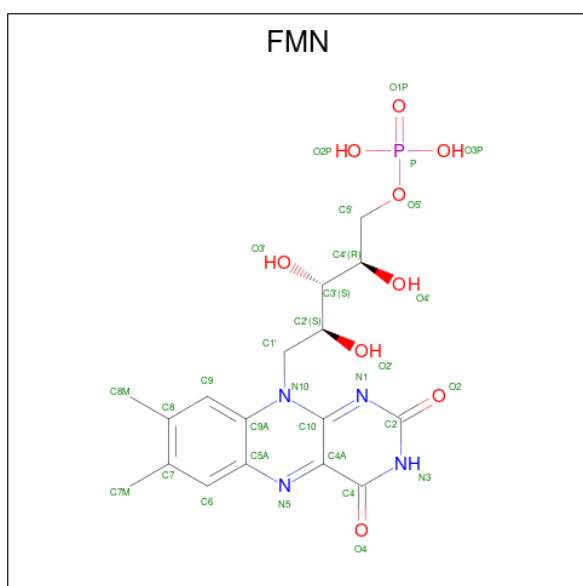
Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total	Fe	S	0
			8	4	4	
43	A	1	Total	Fe	S	0
			8	4	4	
43	B	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	
43	K	1	Total	Fe	S	0
			8	4	4	

- Molecule 44 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
44	A	1	Total	Fe	S	0
			4	2	2	
44	H	1	Total	Fe	S	0
			4	2	2	

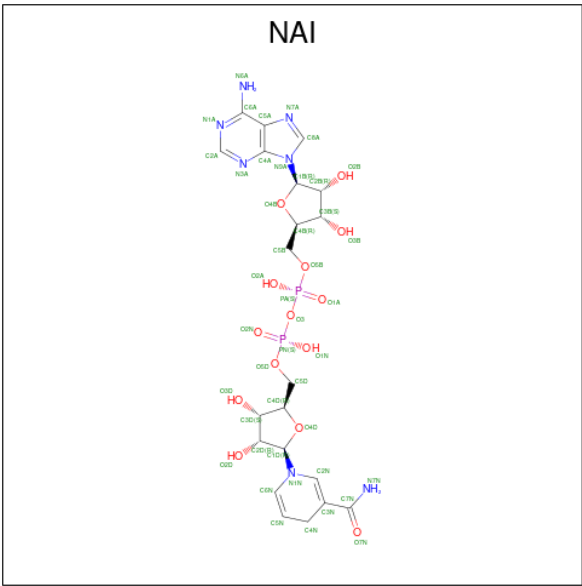
- Molecule 45 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

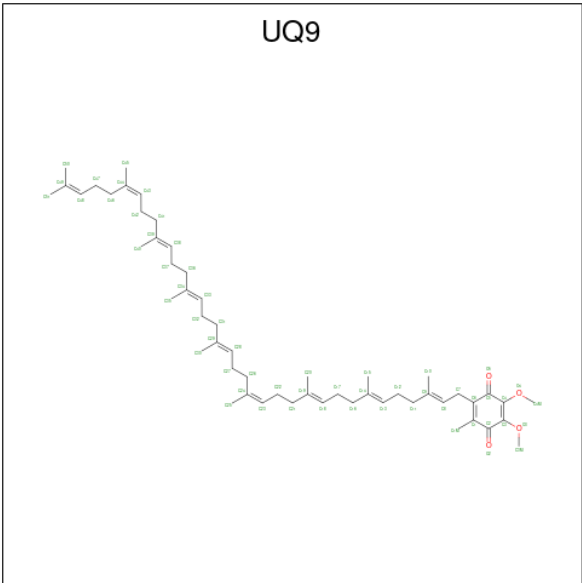
- Molecule 46 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID:

NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



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

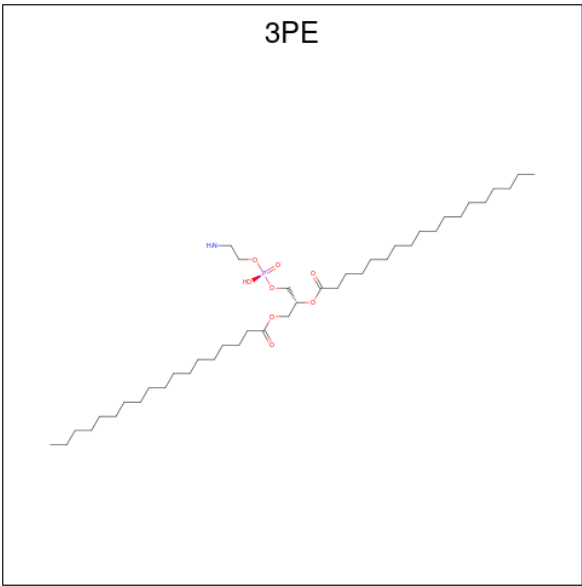
- Molecule 47 is Ubiquinone-9 (CCD ID: UQ9) (formula: C₅₄H₈₂O₄).



Mol	Chain	Residues	Atoms			AltConf
47	C	1	Total	C	O	0
			14	10	4	

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

C₄₁H₈₂NO₈P).



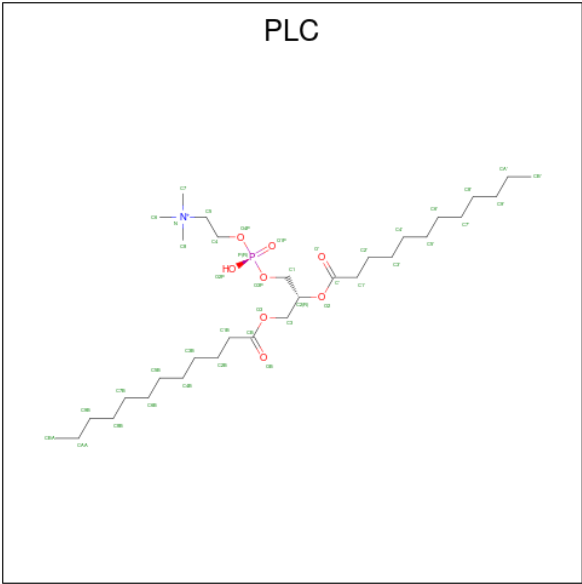
Mol	Chain	Residues	Atoms					AltConf
48	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	1	1	Total	C	N	O	P	0
			36	26	1	8	1	
48	1	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	2	1	Total	C	N	O	P	0
			42	32	1	8	1	
48	4	1	Total	C	N	O	P	0
			42	32	1	8	1	
48	4	1	Total	C	N	O	P	0
			43	33	1	8	1	
48	4	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
48	5	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	5	1	Total	C	N	O	P	0
			44	34	1	8	1	
48	6	1	Total	C	N	O	P	0
			36	26	1	8	1	
48	6	1	Total	C	N	O	P	0
			48	38	1	8	1	
48	g	1	Total	C	N	O	P	0
			43	33	1	8	1	

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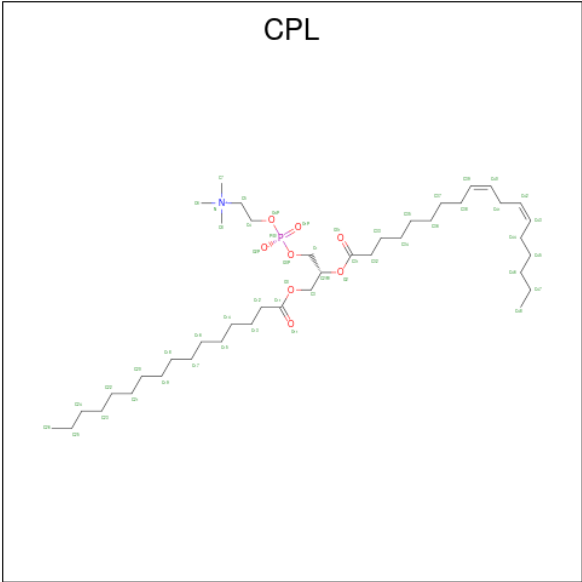
Mol	Chain	Residues	Atoms					AltConf
48	E	1	Total	C	N	O	P	0
			36	26	1	8	1	
48	J	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	b	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 49 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: C₃₂H₆₅NO₈P).



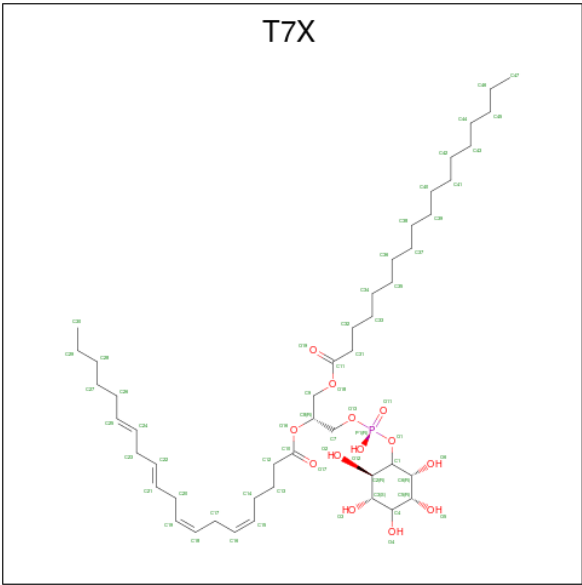
Mol	Chain	Residues	Atoms					AltConf
49	K	1	Total	C	N	O	P	0
			36	26	1	8	1	
49	1	1	Total	C	N	O	P	0
			35	25	1	8	1	
49	1	1	Total	C	N	O	P	0
			42	32	1	8	1	
49	4	1	Total	C	N	O	P	0
			35	25	1	8	1	
49	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
49	i	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 50 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: CPL) (formula: C₄₂H₈₀NO₈P).



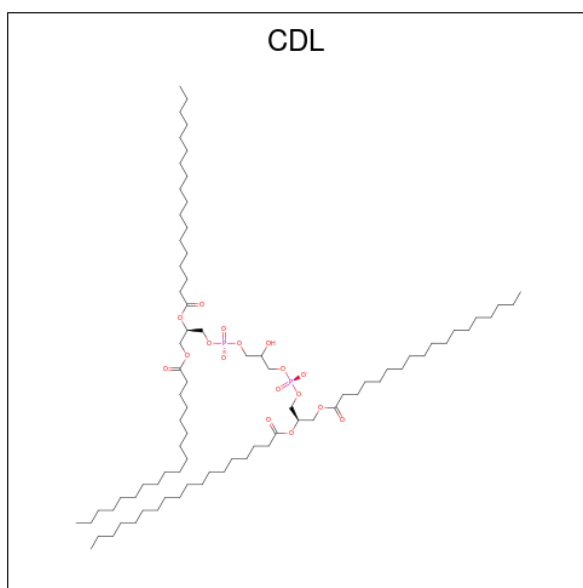
Mol	Chain	Residues	Atoms					AltConf
50	2	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 51 is Phosphatidylinositol (CCD ID: T7X) (formula: C₄₇H₈₃O₁₃P).



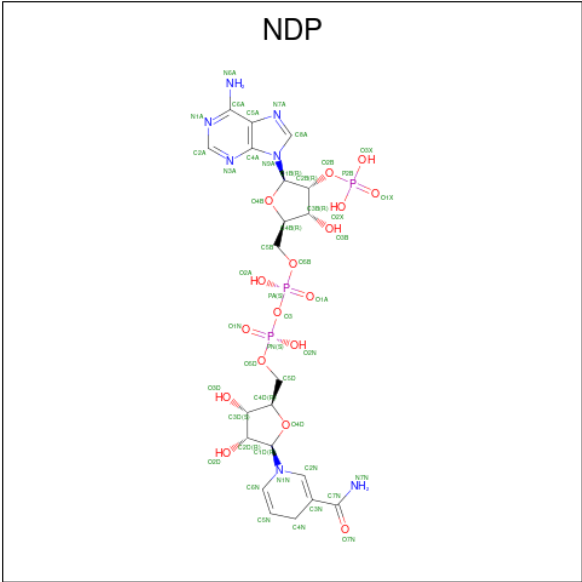
Mol	Chain	Residues	Atoms				AltConf
51	2	1	Total	C	O	P	0
			52	38	13	1	
51	3	1	Total	C	O	P	0
			44	30	13	1	
51	b	1	Total	C	O	P	0
			48	34	13	1	

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



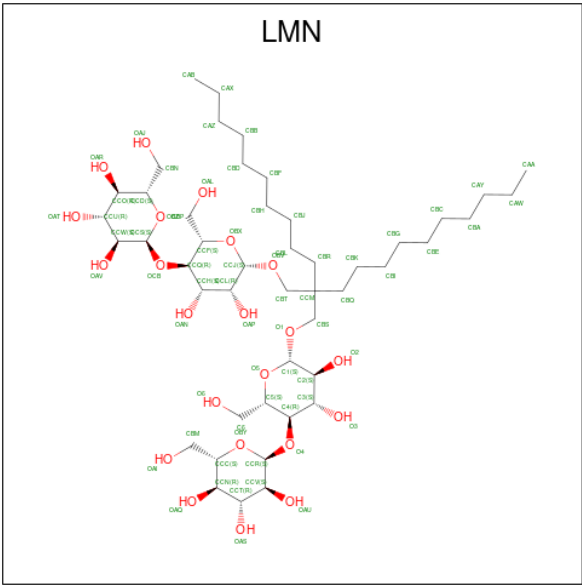
Mol	Chain	Residues	Atoms				AltConf
52	g	1	Total	C	O	P	0
			80	61	17	2	
52	E	1	Total	C	O	P	0
			72	53	17	2	
52	W	1	Total	C	O	P	0
			54	35	17	2	
52	X	1	Total	C	O	P	0
			86	67	17	2	
52	Z	1	Total	C	O	P	0
			76	57	17	2	
52	n	1	Total	C	O	P	0
			92	73	17	2	

- Molecule 53 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 54 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: $C_{47}H_{88}O_{22}$).

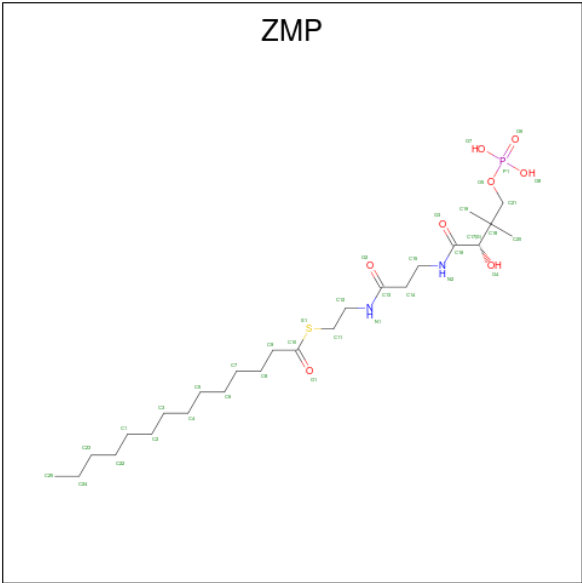


Mol	Chain	Residues	Atoms			AltConf
54	J	1	Total	C	O	0
			69	47	22	
54	a	1	Total	C	O	0
			65	43	22	

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

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

- Molecule 56 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).

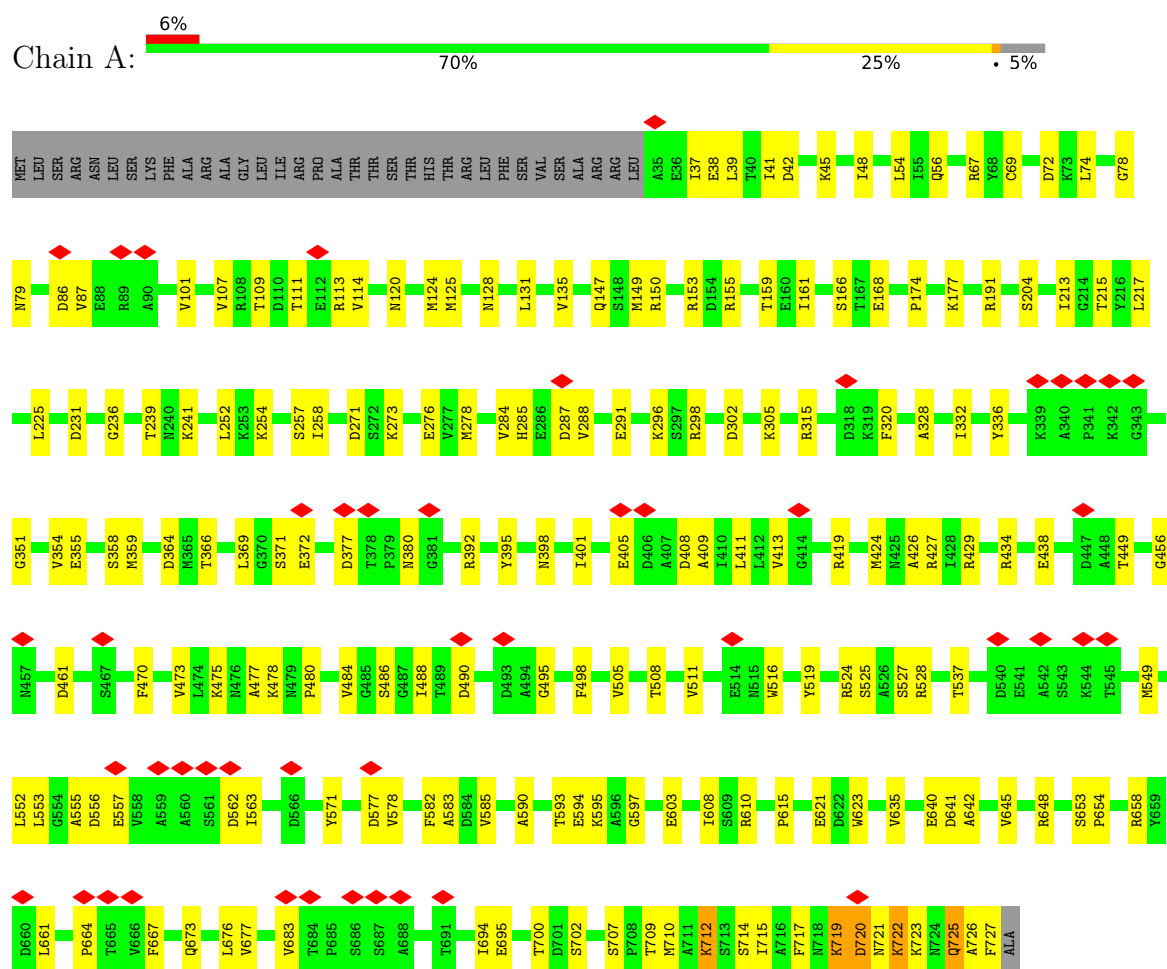


Mol	Chain	Residues	Atoms						AltConf
56	O	1	Total	C	N	O	P	S	0
			33	22	2	7	1	1	
56	Q	1	Total	C	N	O	P	S	0
			33	22	2	7	1	1	

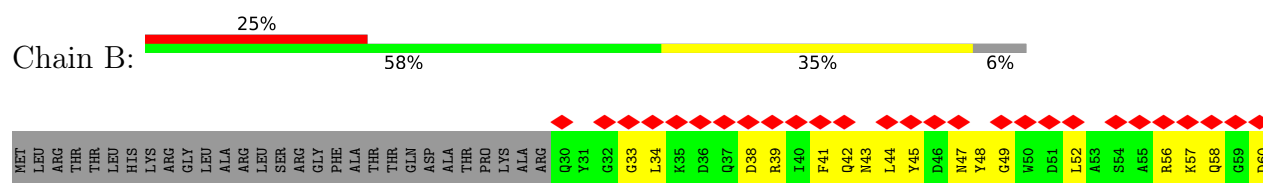
3 Residue-property plots

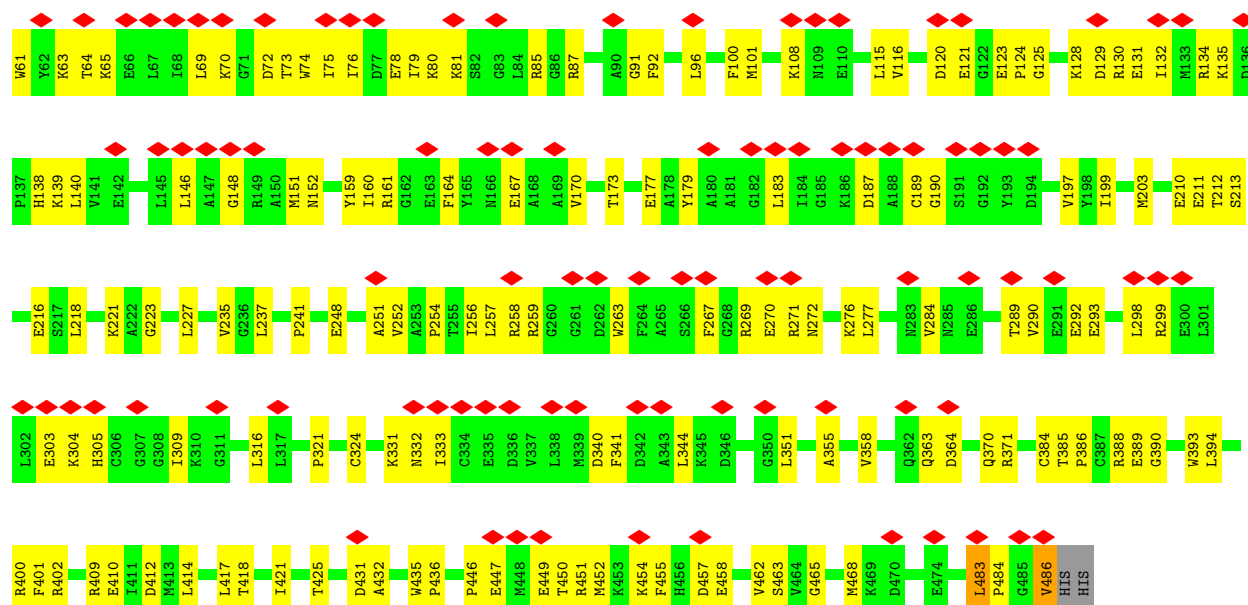
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

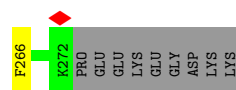
- Molecule 1: Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I)



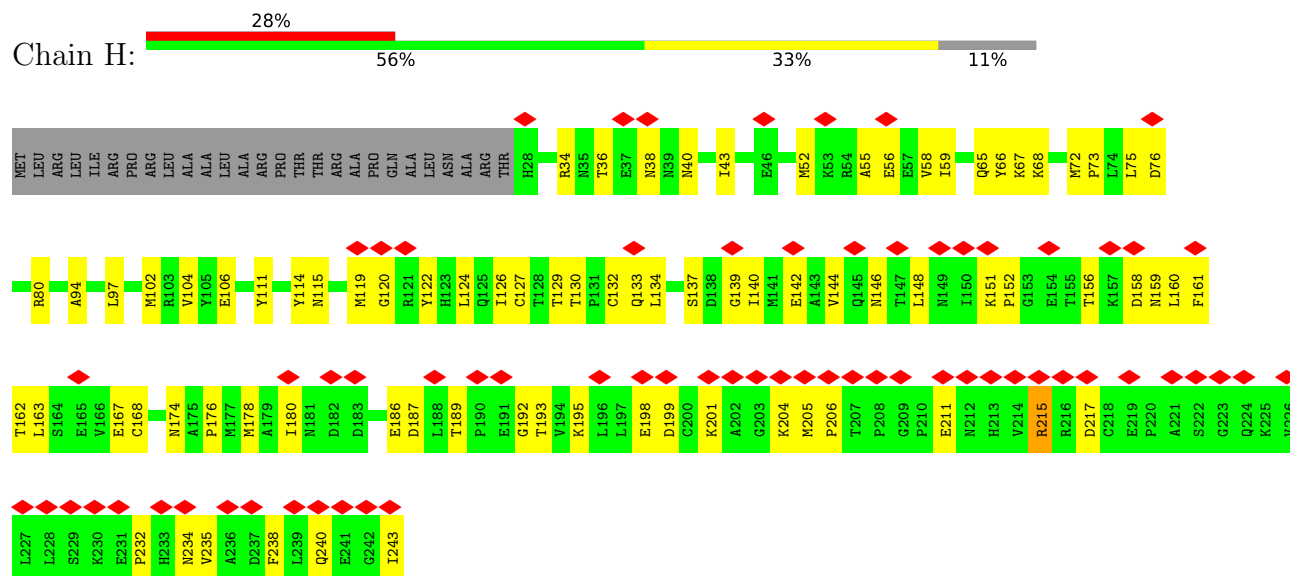
- Molecule 2: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



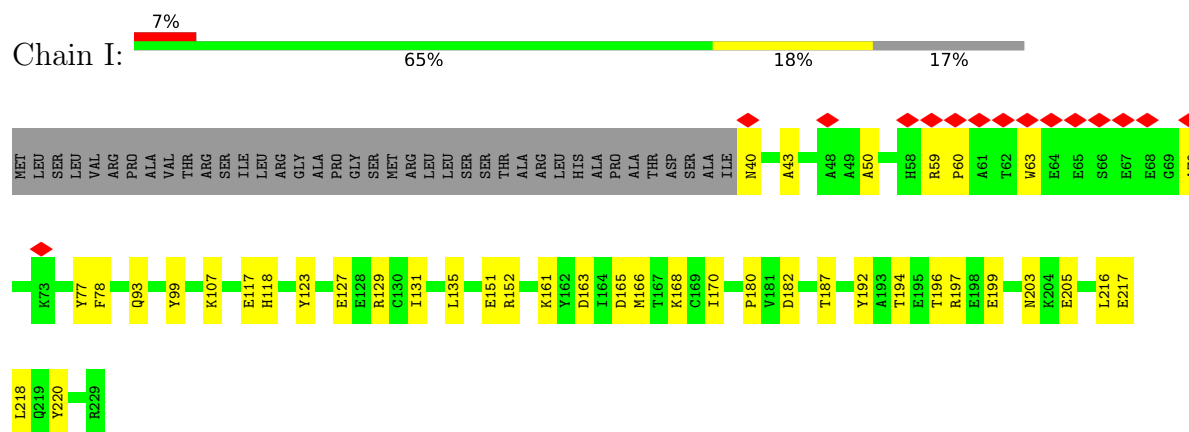




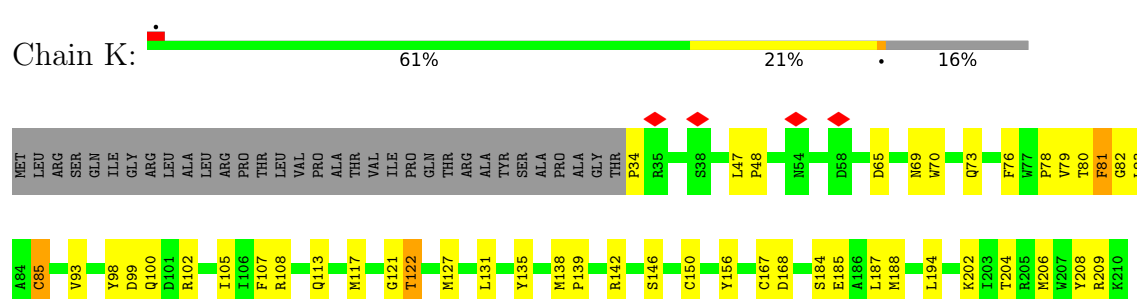
• Molecule 5: Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I)



• Molecule 6: Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I)

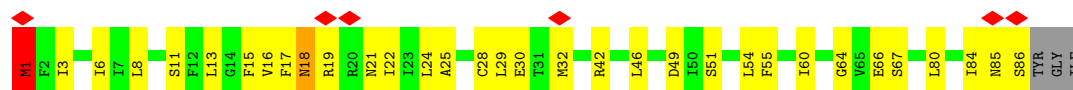


• Molecule 7: Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I)

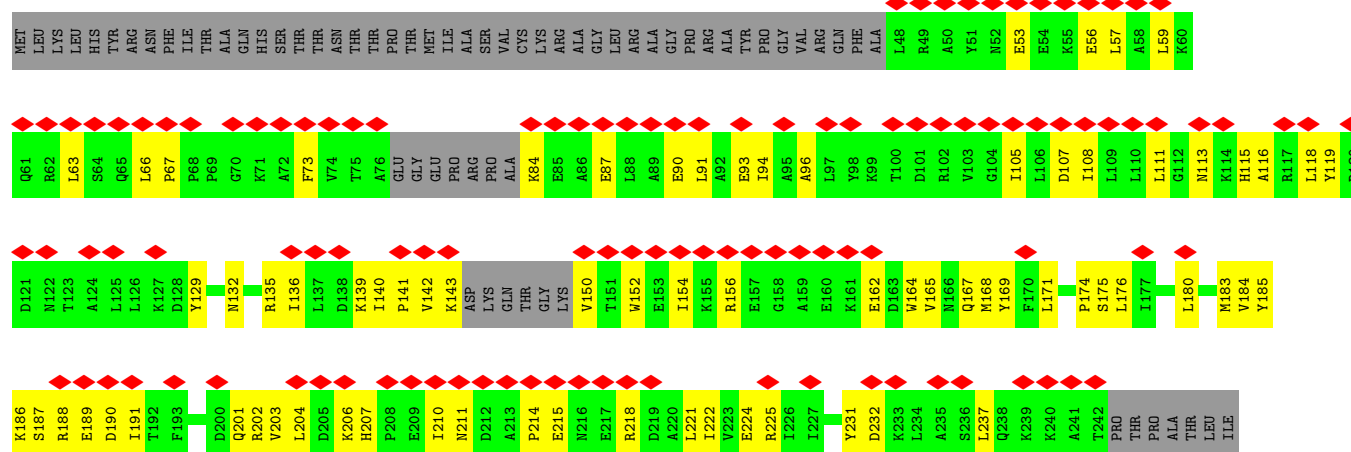


• Molecule 8: NADH-ubiquinone oxidoreductase chain 4L

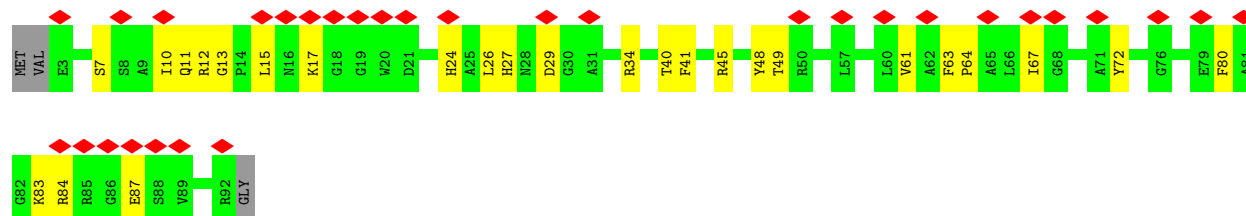




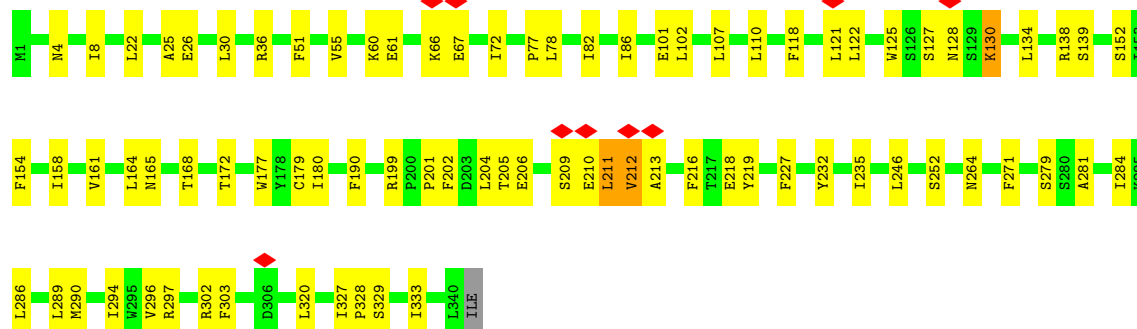
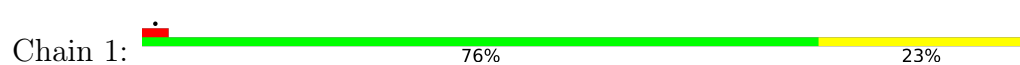
• Molecule 9: Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I)



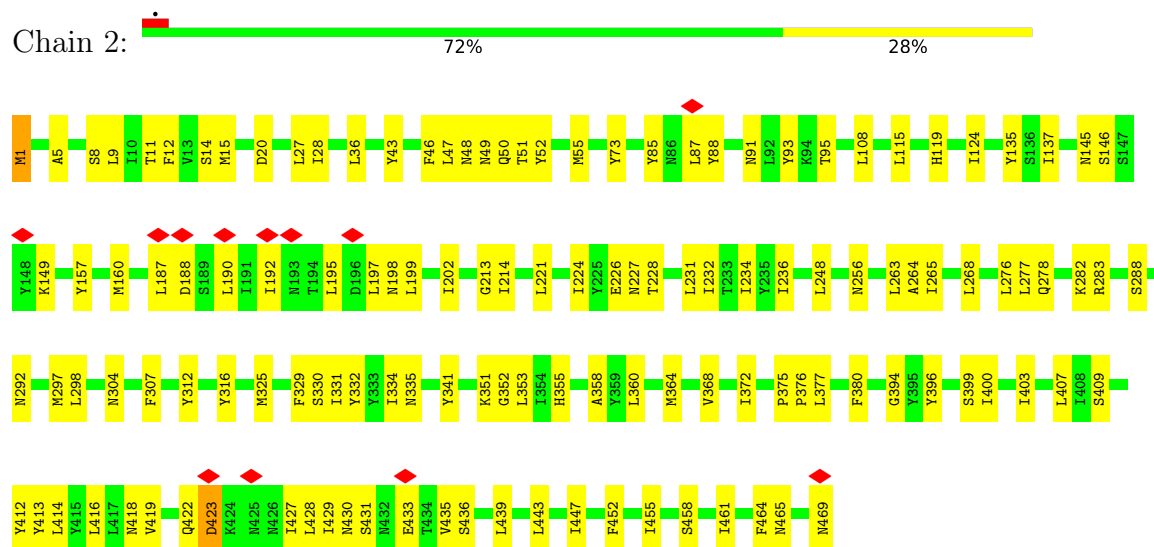
• Molecule 10: Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I)



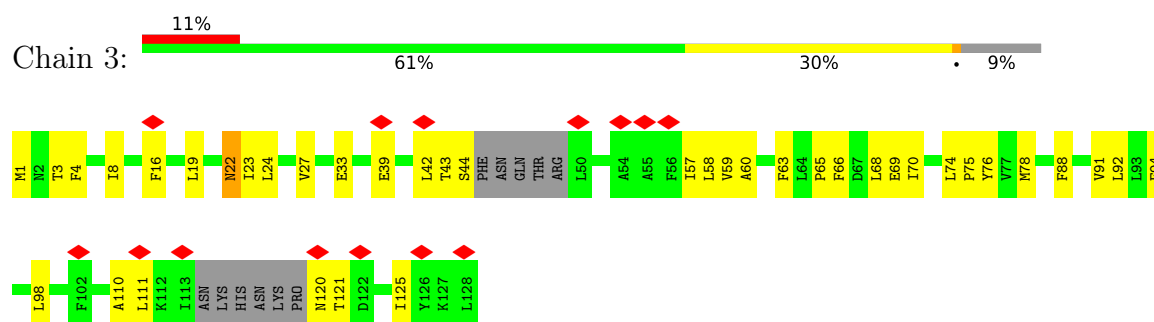
• Molecule 11: NADH-ubiquinone oxidoreductase chain 1



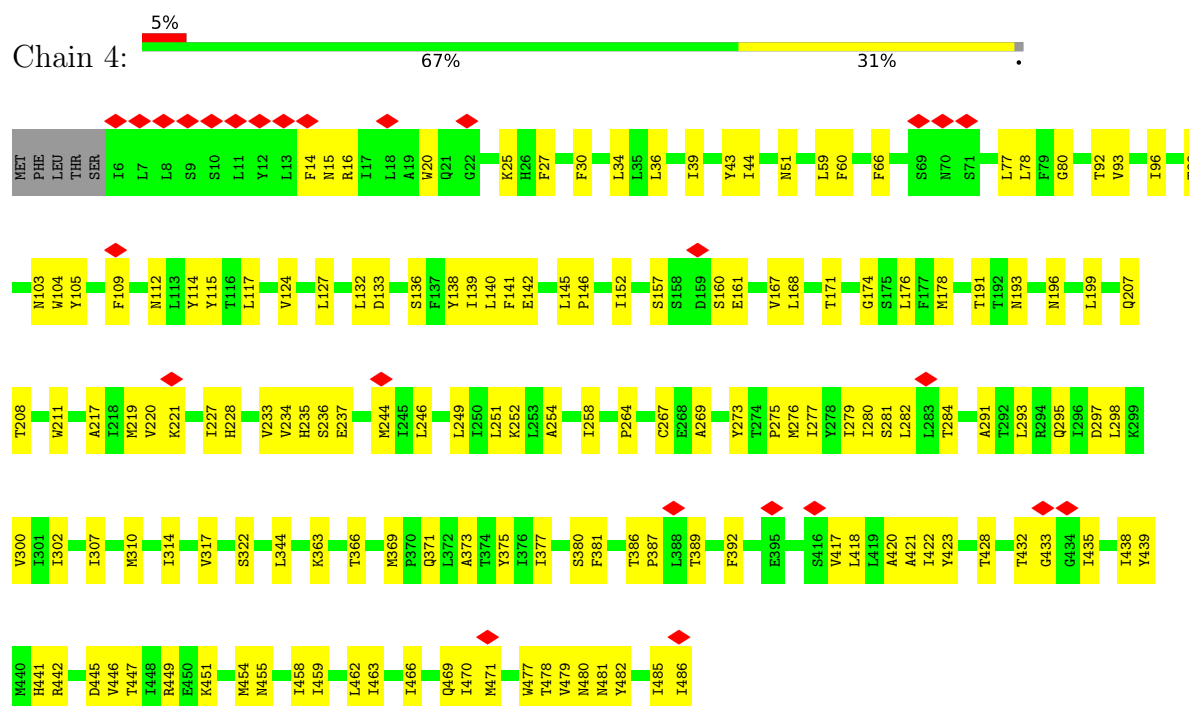
• Molecule 12: NADH dehydrogenase subunit 2



• Molecule 13: NADH-ubiquinone oxidoreductase chain 3

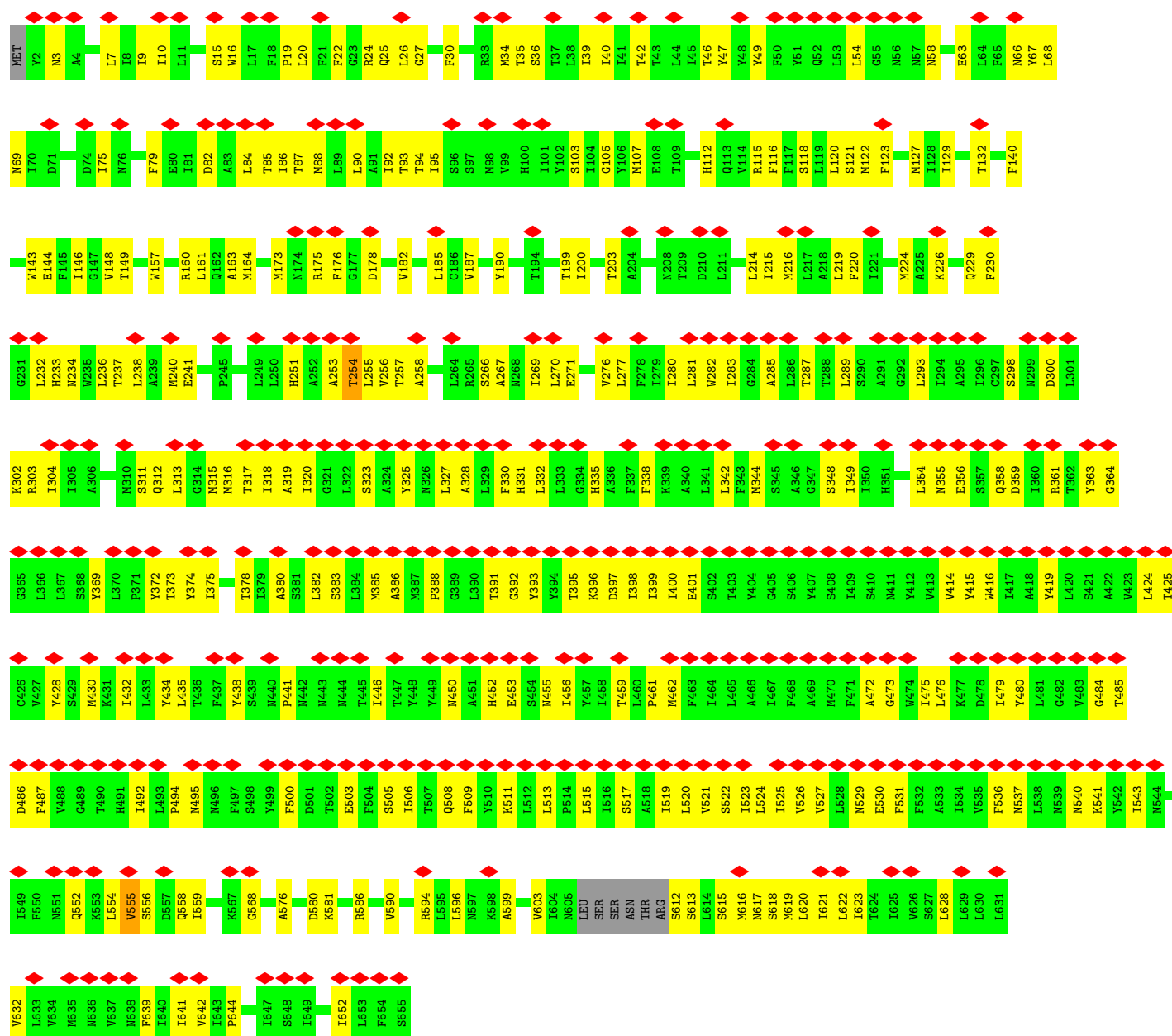


• Molecule 14: Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I)



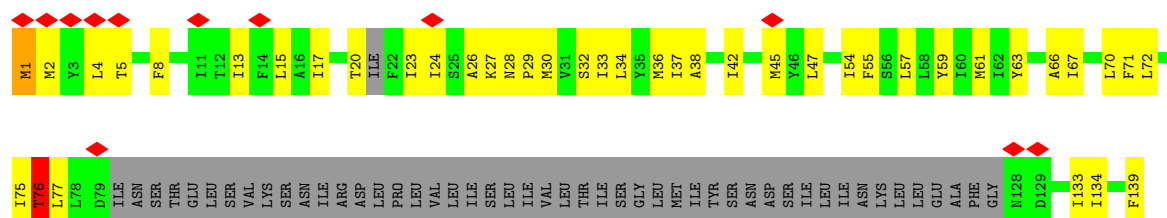
• Molecule 15: Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 5: 



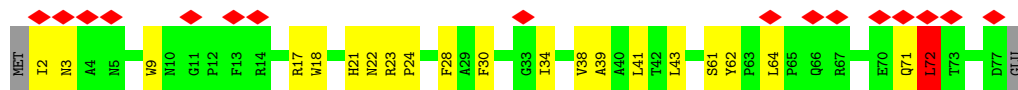
• Molecule 16: NADH-ubiquinone oxidoreductase chain 6

Chain 6: 

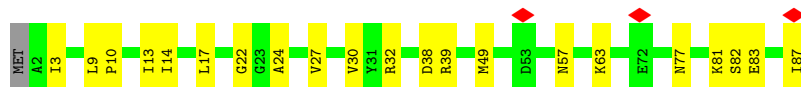




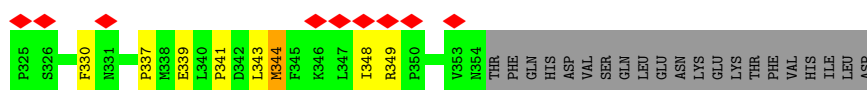
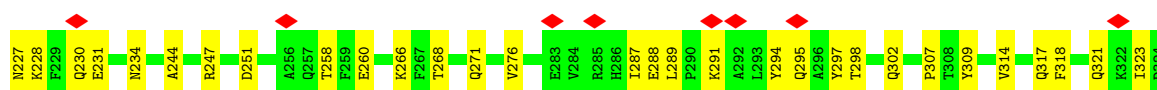
- Molecule 17: subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 18: Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 19: Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I)



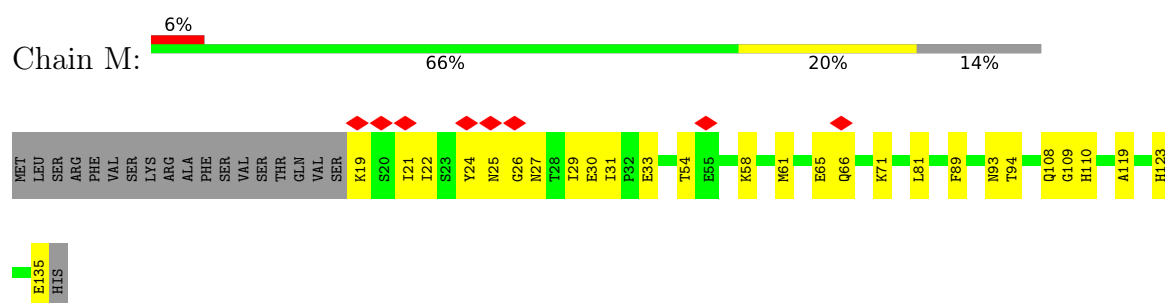
- Molecule 20: Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I)



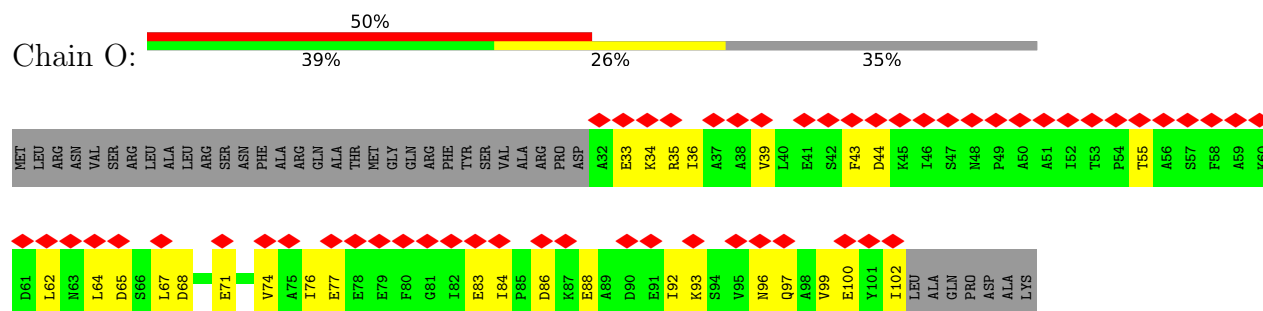
- Molecule 21: Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I)



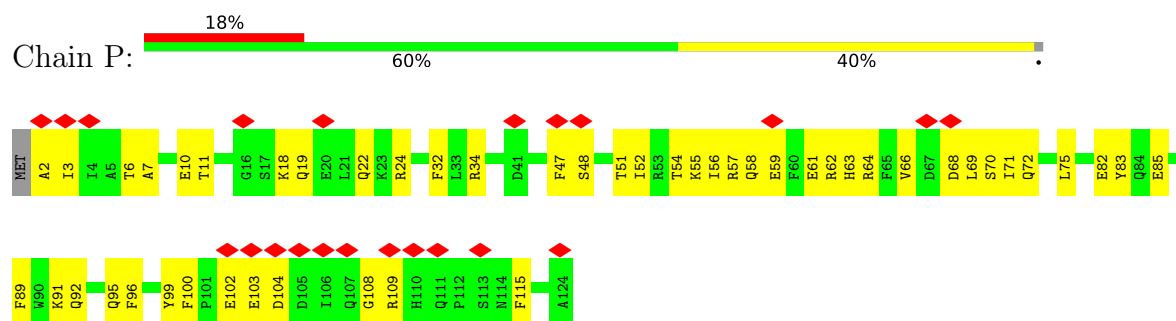
- Molecule 22: Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I)



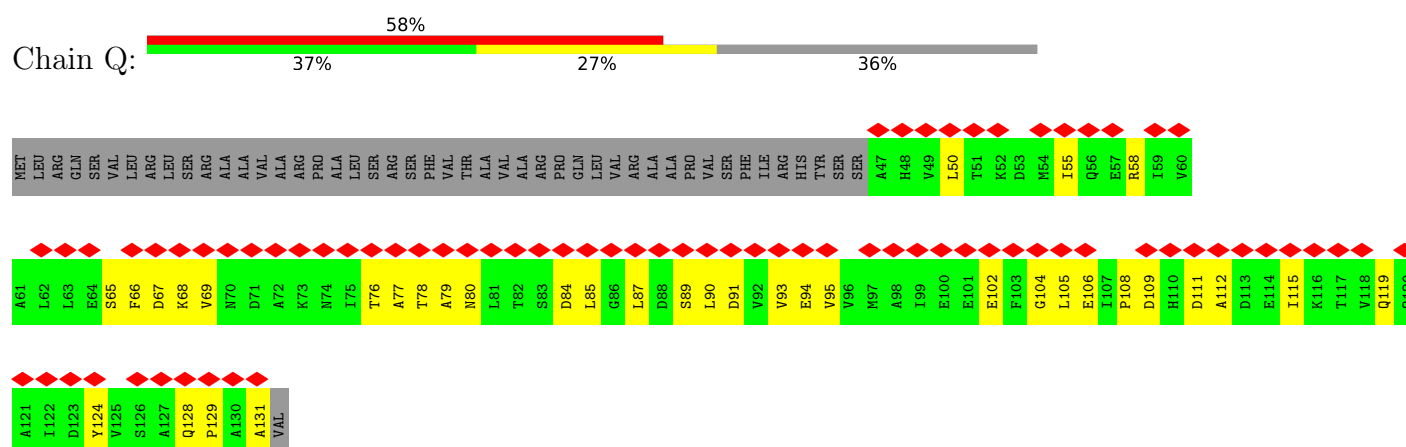
- Molecule 23: Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I)



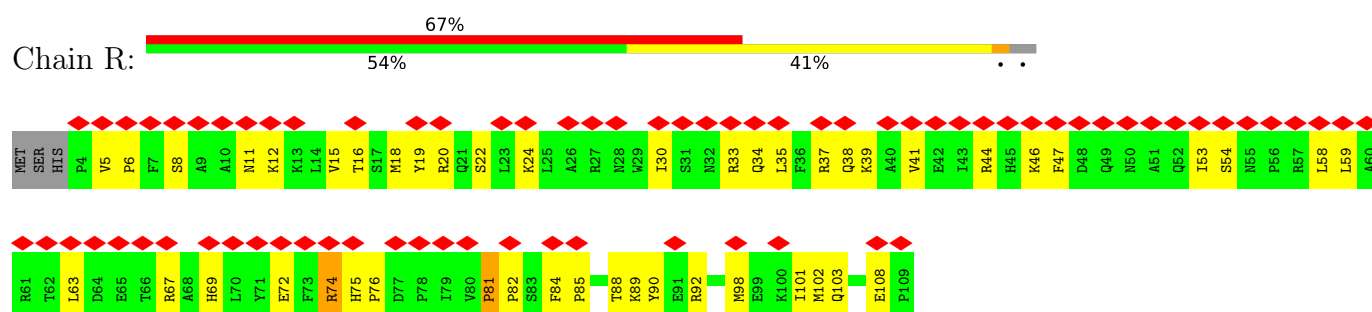
- Molecule 24: Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I)



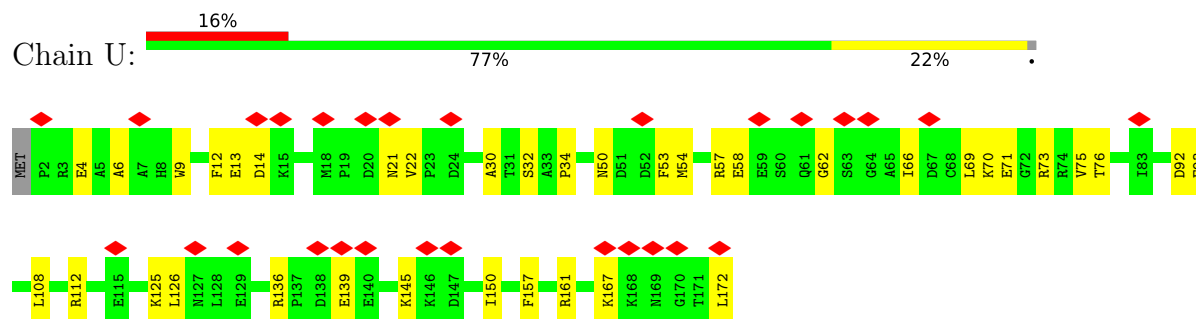
- Molecule 25: Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I)



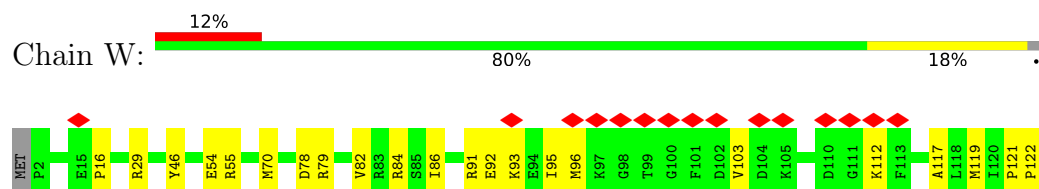
• Molecule 26: Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I)



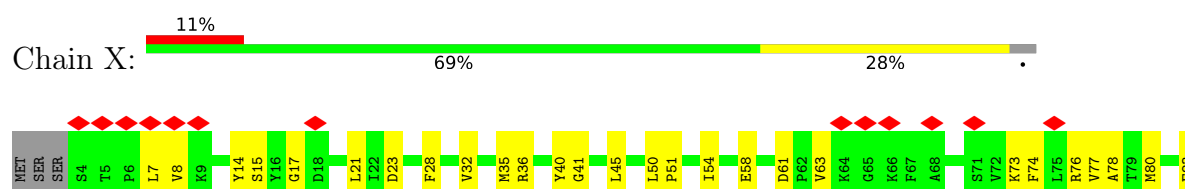
• Molecule 27: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)

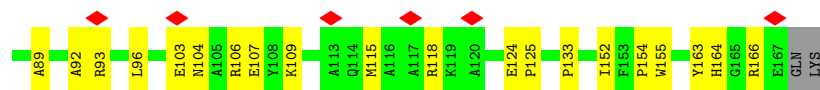


• Molecule 28: Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I)

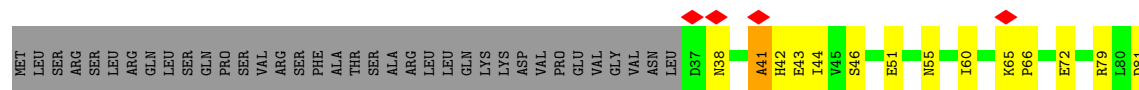


• Molecule 29: Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I)

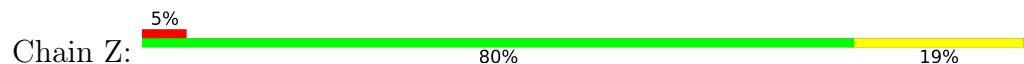




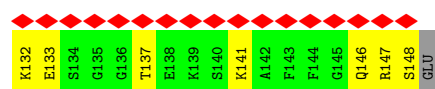
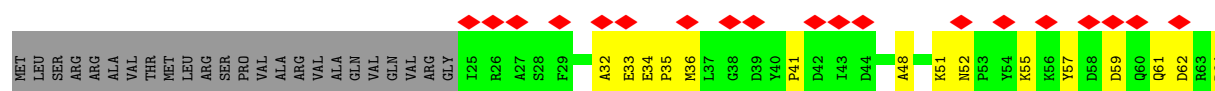
- Molecule 30: Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 31: Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I)



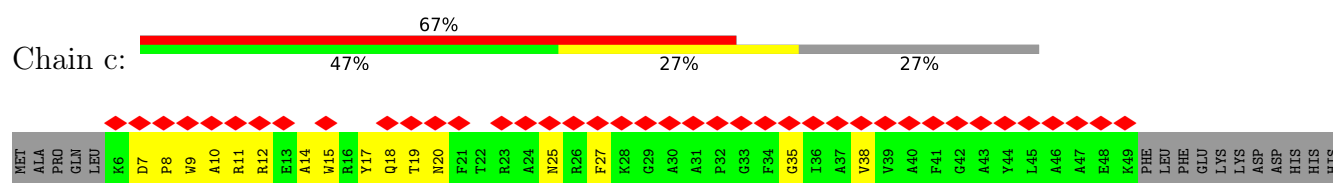
- Molecule 32: Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I)



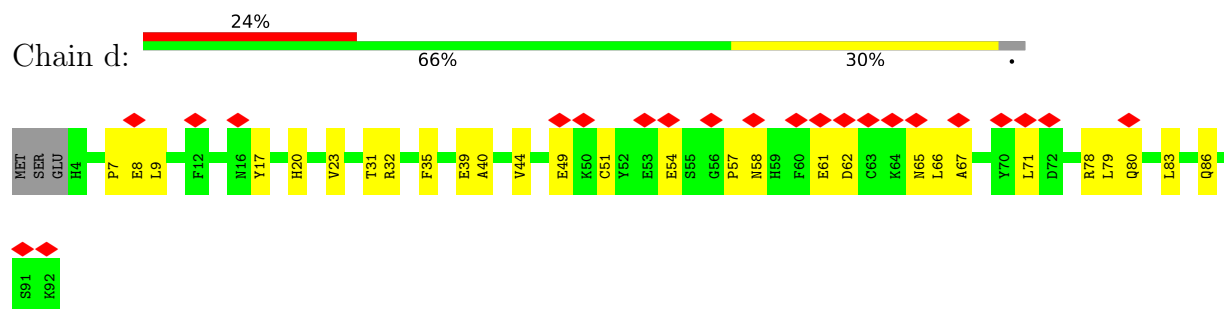
- Molecule 33: Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I)



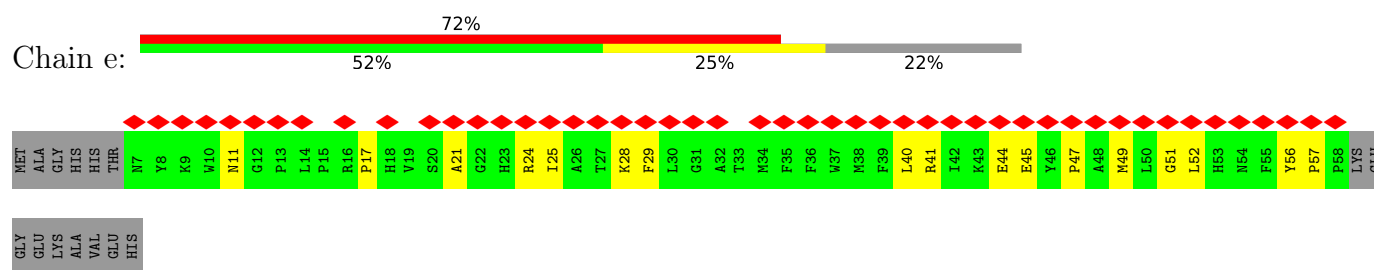
- Molecule 34: Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I)



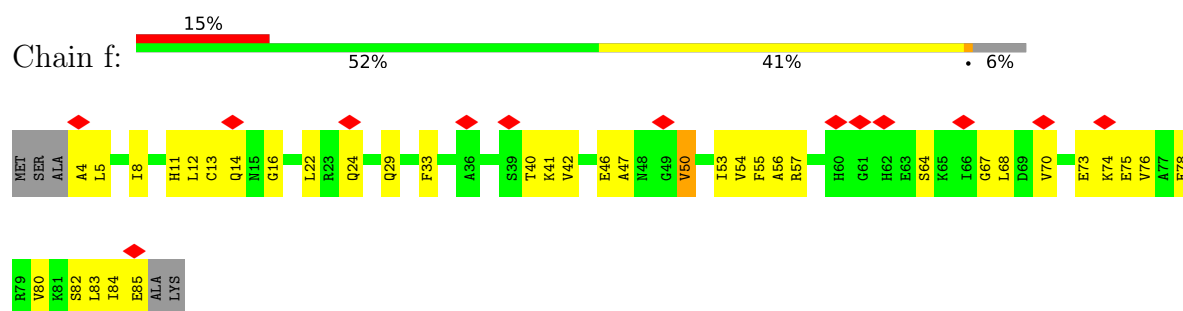
- Molecule 35: Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I)



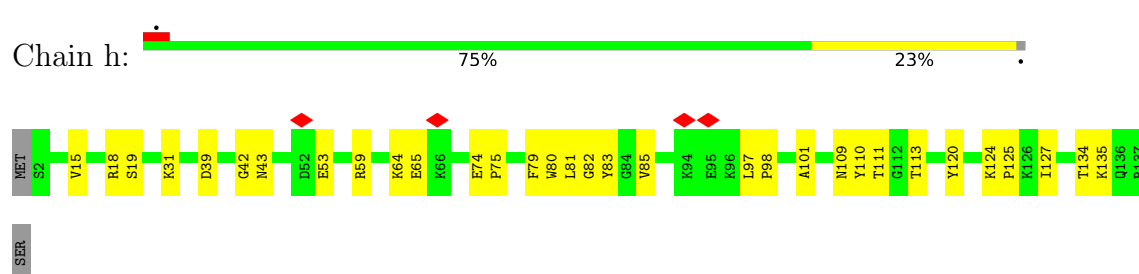
- Molecule 36: Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I)



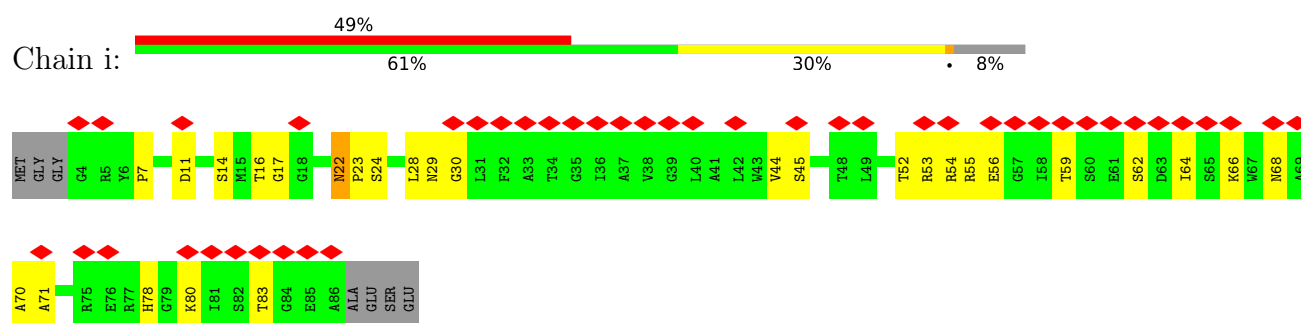
- Molecule 37: Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I)



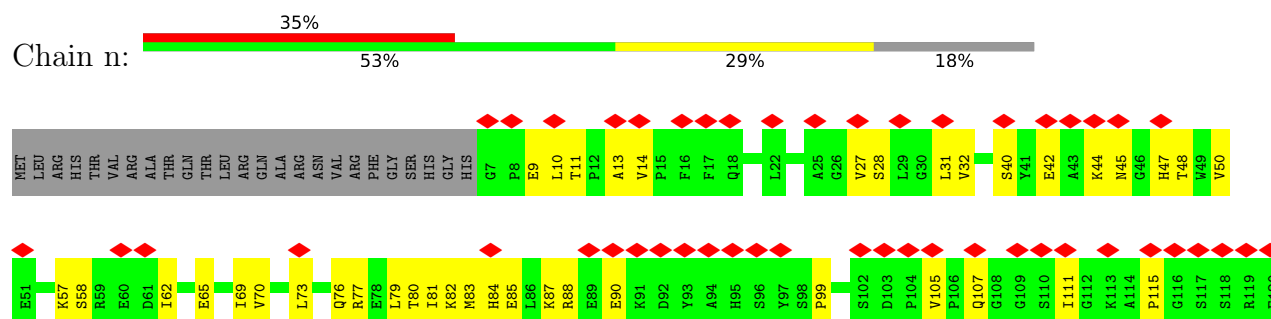
- Molecule 38: Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I)



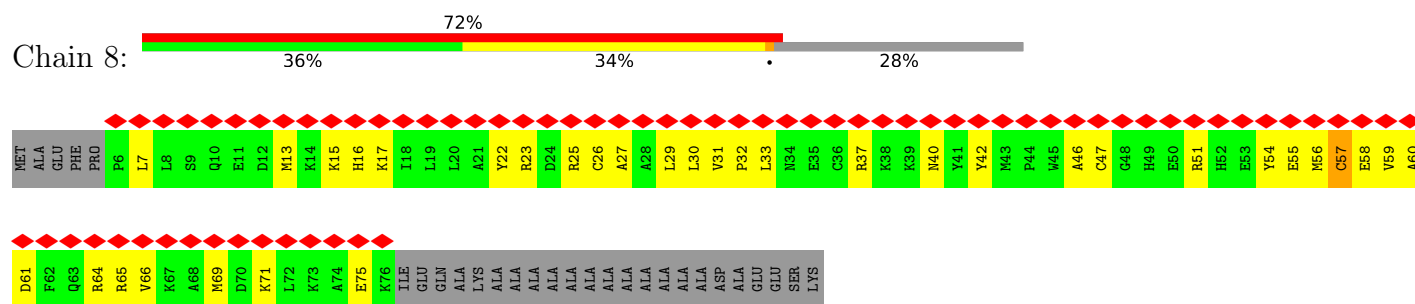
- Molecule 39: Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I)



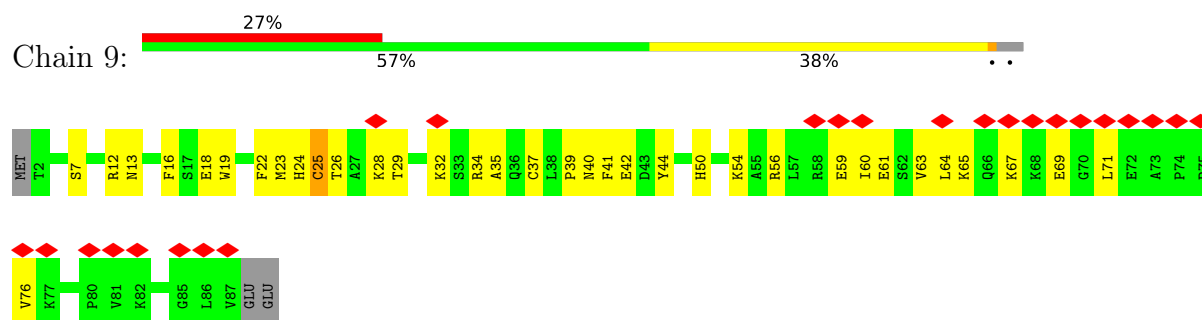
- Molecule 40: Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 41: Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 42: Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54863	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-3200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0115	Depositor
Map size (Å)	331.2, 331.2, 331.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FME, CPL, FMN, ZMP, NAI, CDL, LMN, ZN, T7X, 3PE, NDP, 2MR, FES, UQ9, SF4, PLC

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	0.38	0/5363	0.54	1/7278 (0.0%)
2	B	0.30	0/3605	0.52	0/4866
3	C	0.43	0/3307	0.54	0/4475
4	G	0.41	0/2040	0.52	0/2781
5	H	0.48	1/1725 (0.1%)	0.72	3/2343 (0.1%)
6	I	0.43	0/1557	0.51	0/2110
7	K	0.53	0/1434	0.72	0/1950
8	L	0.46	1/667 (0.1%)	0.73	3/903 (0.3%)
9	S	0.30	0/1517	0.62	0/2046
10	j	0.27	0/745	0.50	0/1006
11	1	0.43	0/2781	0.62	1/3798 (0.0%)
12	2	0.50	5/3846 (0.1%)	0.60	4/5242 (0.1%)
13	3	0.36	0/939	0.54	0/1280
14	4	0.32	0/3908	0.48	0/5337
15	5	0.31	0/5280	0.51	1/7208 (0.0%)
16	6	0.64	3/1088 (0.3%)	0.82	8/1483 (0.5%)
17	g	0.38	0/648	0.56	0/887
18	D	0.27	0/697	0.44	0/940
19	E	0.36	0/2732	0.52	0/3702
20	F	0.30	0/1002	0.49	0/1359
21	J	0.26	0/1304	0.46	0/1774
22	M	0.31	0/935	0.46	0/1268
23	O	0.21	0/549	0.47	0/746
24	P	0.30	0/1061	0.47	0/1427
25	Q	0.28	0/654	0.51	0/890
26	R	0.40	0/909	0.72	2/1229 (0.2%)
27	U	0.26	0/1374	0.48	0/1856
28	W	0.31	0/998	0.51	0/1346
29	X	0.28	0/1314	0.43	0/1783
30	Y	0.41	0/1067	0.62	3/1442 (0.2%)
31	Z	0.31	0/1430	0.50	0/1955
32	a	0.26	0/1064	0.49	0/1439

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.24	0/503	0.31	0/679
34	c	0.20	0/364	0.48	0/491
35	d	0.28	0/767	0.44	0/1031
36	e	0.20	0/456	0.46	0/619
37	f	0.35	0/652	0.71	2/874 (0.2%)
38	h	0.35	0/1168	0.45	0/1589
39	i	0.21	0/666	0.39	0/907
40	n	0.27	0/940	0.47	0/1273
41	8	0.33	0/606	0.68	1/808 (0.1%)
42	9	0.38	0/684	0.60	1/918 (0.1%)
All	All	0.37	10/64346 (0.0%)	0.55	30/87338 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	L	0	1
16	6	0	1
27	U	0	1
All	All	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	215	ARG	C-N	15.00	1.53	1.33
16	6	30	MET	C-N	-9.59	1.21	1.34
12	2	52	TYR	C-N	8.75	1.45	1.33
16	6	76	THR	C-N	-8.73	1.21	1.33
12	2	49	ASN	C-O	-8.45	1.11	1.23
12	2	43	TYR	C-N	-6.66	1.25	1.33
16	6	26	ALA	C-N	-6.51	1.25	1.33
8	L	18	ASN	C-N	-5.62	1.25	1.34
12	2	47	LEU	C-O	-5.42	1.17	1.23
12	2	51	THR	C-O	-5.22	1.17	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	215	ARG	O-C-N	11.61	135.85	123.42
5	H	215	ARG	CA-C-N	-11.51	106.06	122.06

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	215	ARG	C-N-CA	-11.51	106.06	122.06
8	L	18	ASN	O-C-N	9.92	135.45	122.96
8	L	18	ASN	CA-C-N	-7.83	109.06	122.14
8	L	18	ASN	C-N-CA	-7.83	109.06	122.14
16	6	30	MET	CA-C-N	-7.71	109.67	120.53
16	6	30	MET	C-N-CA	-7.71	109.67	120.53
37	f	50	VAL	CA-C-N	7.67	135.52	120.94
37	f	50	VAL	C-N-CA	7.67	135.52	120.94
16	6	30	MET	O-C-N	7.59	129.92	122.03
16	6	26	ALA	O-C-N	7.51	132.16	122.93
26	R	81	PRO	CA-N-CD	-7.25	101.85	112.00
16	6	26	ALA	CA-C-N	-6.62	111.83	120.44
16	6	26	ALA	C-N-CA	-6.62	111.83	120.44
42	9	25	CYS	CA-CB-SG	6.45	129.25	114.40
12	2	49	ASN	CB-CA-C	6.39	121.60	111.51
16	6	76	THR	CA-C-N	-6.28	110.84	122.09
16	6	76	THR	C-N-CA	-6.28	110.84	122.09
11	1	202	PHE	CB-CA-C	-6.28	103.02	111.88
15	5	254	THR	N-CA-C	6.27	120.52	112.12
41	8	57	CYS	CA-CB-SG	6.18	128.62	114.40
12	2	48	ASN	CB-CA-C	6.00	122.03	111.06
26	R	74	ARG	CG-CD-NE	-5.82	99.20	112.00
12	2	46	PHE	CB-CA-C	5.79	120.67	110.37
30	Y	96	ILE	N-CA-C	-5.75	107.53	113.10
30	Y	41	ALA	CA-C-N	5.39	132.23	123.93
30	Y	41	ALA	C-N-CA	5.39	132.23	123.93
12	2	49	ASN	CA-CB-CG	5.08	117.68	112.60
1	A	727	PHE	CB-CA-C	5.01	119.62	110.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	6	76	THR	Mainchain
8	L	1	FME	Mainchain
27	U	6	ALA	Peptide

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	5269	0	5168	148	0
2	B	3528	0	3488	156	0
3	C	3247	0	3195	87	0
4	G	1978	0	1908	46	0
5	H	1688	0	1660	76	0
6	I	1519	0	1460	38	0
7	K	1395	0	1375	48	0
8	L	669	0	730	33	0
9	S	1492	0	1536	74	0
10	j	724	0	706	49	0
11	1	2716	0	2812	77	0
12	2	3776	0	4004	133	0
13	3	930	0	994	36	0
14	4	3815	0	4010	142	0
15	5	5151	0	5305	264	0
16	6	1078	0	1161	57	0
17	g	622	0	602	20	0
18	D	681	0	671	19	0
19	E	2673	0	2658	82	0
20	F	981	0	969	25	0
21	J	1274	0	1256	50	0
22	M	912	0	869	27	0
23	O	543	0	537	20	0
24	P	1036	0	1018	56	0
25	Q	648	0	636	41	0
26	R	884	0	891	70	0
27	U	1345	0	1327	31	0
28	W	974	0	987	32	0
29	X	1275	0	1250	37	0
30	Y	1037	0	994	37	0
31	Z	1389	0	1395	28	0
32	a	1030	0	967	46	0
33	b	490	0	509	13	0
34	c	353	0	343	18	0
35	d	751	0	715	35	0
36	e	436	0	426	17	0
37	f	642	0	656	53	0
38	h	1130	0	1084	27	0
39	i	646	0	630	30	0
40	n	913	0	878	53	0
41	8	594	0	599	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	9	672	0	683	38	0
43	A	16	0	0	1	0
43	B	8	0	0	1	0
43	I	16	0	0	0	0
43	K	8	0	0	0	0
44	A	4	0	0	2	0
44	H	4	0	0	0	0
45	B	31	0	19	4	0
46	B	44	0	27	1	0
47	C	14	0	9	2	0
48	1	77	0	102	5	0
48	2	42	0	58	2	0
48	4	136	0	206	17	0
48	5	127	0	176	10	0
48	6	84	0	117	10	0
48	E	36	0	46	1	0
48	I	51	0	82	4	0
48	J	41	0	56	2	0
48	b	42	0	58	7	0
48	g	43	0	63	0	0
49	1	77	0	108	4	0
49	4	35	0	44	1	0
49	K	36	0	46	1	0
49	W	41	0	59	1	0
49	i	42	0	64	2	0
50	2	52	0	80	2	0
51	2	52	0	0	3	0
51	3	44	0	0	0	0
51	b	48	0	0	1	0
52	E	72	0	88	5	0
52	W	54	0	52	1	0
52	X	86	0	119	6	0
52	Z	76	0	96	3	0
52	g	80	0	110	7	0
52	n	92	0	137	10	0
53	E	48	0	26	2	0
54	J	69	0	88	12	0
54	a	65	0	77	2	0
55	M	1	0	0	0	0
56	O	33	0	38	6	0
56	Q	33	0	38	5	0
All	All	64866	0	65351	2003	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 15.

All (2003) 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)
10:j:48:TYR:CE2	15:5:586:ARG:NH1	1.89	1.38
37:f:12:LEU:HB3	37:f:22:LEU:CD2	1.56	1.36
10:j:48:TYR:HE2	15:5:586:ARG:NH1	1.22	1.31
37:f:24:GLN:HB3	37:f:73:GLU:OE2	1.24	1.29
4:G:36:TRP:CZ2	4:G:37:GLU:OE2	1.91	1.23
37:f:4:ALA:O	37:f:40:THR:HG21	1.33	1.22
37:f:12:LEU:CB	37:f:22:LEU:HD23	1.70	1.21
10:j:13:GLY:CA	12:2:429:ILE:HD11	1.71	1.20
4:G:227:GLU:OE2	19:E:72:LYS:HG2	1.47	1.14
37:f:4:ALA:O	37:f:40:THR:CG2	1.94	1.14
1:A:38:GLU:OE2	1:A:45:LYS:HE3	1.48	1.13
10:j:13:GLY:N	12:2:429:ILE:HG12	1.69	1.07
37:f:24:GLN:CB	37:f:73:GLU:OE2	2.01	1.07
37:f:12:LEU:HB3	37:f:22:LEU:HD23	1.14	1.07
10:j:13:GLY:HA3	12:2:429:ILE:HD11	1.36	1.03
11:1:121:LEU:HD21	16:6:72:LEU:HB2	1.41	1.02
37:f:12:LEU:HB3	37:f:22:LEU:HD21	1.43	1.00
4:G:36:TRP:CH2	4:G:37:GLU:OE2	2.14	1.00
10:j:13:GLY:N	12:2:429:ILE:CG1	2.24	0.99
15:5:24:ARG:HG3	39:i:17:GLY:HA2	1.42	0.98
10:j:48:TYR:CD2	15:5:586:ARG:NH1	2.30	0.98
14:4:193:ASN:HD22	40:n:73:LEU:HD13	1.27	0.97
4:G:227:GLU:OE2	19:E:72:LYS:CG	2.13	0.97
10:j:48:TYR:HE2	15:5:586:ARG:HH11	1.08	0.96
5:H:198:GLU:HA	5:H:201:LYS:HG3	1.46	0.95
2:B:63:LYS:HE2	5:H:243:ILE:HA	1.47	0.95
2:B:57:LYS:O	5:H:234:ASN:ND2	2.00	0.94
32:a:52:ASN:HB2	32:a:55:LYS:NZ	1.83	0.93
2:B:454:LYS:O	2:B:458:GLU:HB2	1.69	0.93
1:A:354:VAL:HG21	1:A:553:LEU:HD21	1.50	0.93
15:5:9:ILE:HG13	15:5:10:ILE:HG13	1.51	0.92
2:B:455:PHE:HE1	2:B:468:MET:HE1	1.33	0.92
11:1:26:GLU:HG3	11:1:294:ILE:HG12	1.52	0.92
12:2:9:LEU:HD21	12:2:28:ILE:HD11	1.53	0.89
10:j:13:GLY:HA3	12:2:429:ILE:CD1	2.02	0.89
14:4:219:MET:HB3	14:4:227:ILE:HD11	1.55	0.88
10:j:27:HIS:HE2	14:4:441:HIS:CD2	1.91	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:f:8:ILE:HD13	37:f:33:PHE:CE2	2.09	0.88
10:j:11:GLN:NE2	12:2:430:ASN:HB3	1.89	0.87
37:f:8:ILE:HD13	37:f:33:PHE:HE2	1.40	0.87
7:K:113:GLN:HE22	11:1:216:PHE:HD1	1.16	0.87
10:j:13:GLY:CA	12:2:429:ILE:CD1	2.52	0.86
23:O:36:ILE:HD13	23:O:76:ILE:HD12	1.57	0.86
17:g:64:LEU:HD21	40:n:115:PRO:HG3	1.57	0.86
41:8:13:MET:HG2	41:8:23:ARG:CZ	2.06	0.86
2:B:63:LYS:CE	5:H:243:ILE:HA	2.05	0.86
8:L:18:ASN:ND2	8:L:21:ASN:O	2.07	0.86
16:6:33:ILE:HD12	16:6:75:ILE:HD13	1.58	0.85
2:B:63:LYS:HZ1	5:H:243:ILE:HG23	1.41	0.85
15:5:327:LEU:HG	15:5:399:ILE:HG12	1.57	0.85
14:4:417:VAL:HG12	15:5:175:ARG:HD2	1.59	0.84
41:8:61:ASP:OD1	41:8:64:ARG:NH2	2.10	0.84
9:S:188:ARG:NH2	40:n:48:THR:HG21	1.92	0.84
3:C:61:ASP:OD1	12:2:283:ARG:NE	2.10	0.84
37:f:8:ILE:HD11	37:f:42:VAL:HG22	1.59	0.84
5:H:122:TYR:HE2	5:H:205:MET:HE1	1.42	0.84
8:L:16:VAL:HG13	8:L:17:PHE:CD2	2.13	0.84
37:f:12:LEU:HB2	37:f:22:LEU:HD23	1.60	0.83
4:G:199:ILE:HG23	4:G:200:MET:HG2	1.60	0.83
15:5:388:PRO:HD3	15:5:515:LEU:HD11	1.58	0.83
37:f:24:GLN:HB3	37:f:73:GLU:CD	2.03	0.82
19:E:247:ARG:HD3	24:P:109:ARG:HD2	1.61	0.82
29:X:35:MET:HE3	29:X:40:TYR:HE2	1.45	0.82
9:S:139:LYS:NZ	9:S:152:TRP:O	2.10	0.82
11:1:121:LEU:HD21	16:6:72:LEU:CB	2.07	0.82
15:5:342:LEU:HD22	15:5:380:ALA:HB1	1.60	0.82
15:5:568:GLY:HA3	48:5:702:3PE:H292	1.62	0.82
3:C:209:GLU:OE2	3:C:250:TRP:NE1	2.11	0.82
15:5:344:MET:HE1	15:5:461:PRO:HB2	1.61	0.81
7:K:93:VAL:HG21	7:K:187:LEU:HD23	1.61	0.81
1:A:241:LYS:NZ	6:I:151:GLU:OE2	2.12	0.81
15:5:240:MET:HB3	15:5:302:LYS:HE3	1.62	0.81
42:9:25:CYS:SG	42:9:40:ASN:ND2	2.53	0.81
32:a:33:GLU:HA	32:a:36:MET:HE2	1.60	0.81
12:2:160:MET:HE3	15:5:617:ASN:HB3	1.62	0.81
23:O:34:LYS:H	23:O:34:LYS:HD2	1.45	0.81
37:f:75:GLU:HA	37:f:78:GLU:OE2	1.79	0.81
10:j:13:GLY:N	12:2:429:ILE:CD1	2.44	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:29:LEU:HA	8:L:32:MET:HE3	1.62	0.80
5:H:187:ASP:HB2	5:H:211:GLU:HG2	1.62	0.80
7:K:113:GLN:NE2	11:1:216:PHE:HD1	1.78	0.80
1:A:615:PRO:HD2	30:Y:86:ASP:OD2	1.81	0.80
15:5:161:LEU:HB2	32:a:61:GLN:HE21	1.47	0.80
10:j:11:GLN:HE21	12:2:430:ASN:HB3	1.47	0.80
7:K:117:MET:HE1	7:K:135:TYR:HB2	1.63	0.79
9:S:93:GLU:HG3	9:S:150:VAL:HB	1.62	0.79
10:j:13:GLY:H	12:2:429:ILE:HG12	1.46	0.79
37:f:12:LEU:CB	37:f:22:LEU:CD2	2.41	0.79
2:B:41:PHE:HZ	2:B:277:LEU:HD11	1.46	0.79
25:Q:66:PHE:HD2	25:Q:69:VAL:HG13	1.47	0.79
21:J:89:ARG:HH21	21:J:91:ARG:NH2	1.80	0.78
15:5:220:PHE:HZ	15:5:283:ILE:HG21	1.48	0.78
1:A:405:GLU:OE1	1:A:434:ARG:NH2	2.16	0.78
1:A:438:GLU:OE1	1:A:473:VAL:HG11	1.84	0.78
49:1:404:PLC:H2'2	49:1:404:PLC:H1A1	1.64	0.78
11:1:199:ARG:HD3	11:1:235:ILE:HD11	1.66	0.78
30:Y:119:ILE:HD11	30:Y:131:ILE:HD11	1.66	0.78
15:5:256:VAL:HB	15:5:313:LEU:HD11	1.66	0.77
7:K:80:THR:HG22	7:K:107:PHE:HB3	1.66	0.77
7:K:99:ASP:OD2	7:K:102:ARG:HB3	1.84	0.77
10:j:13:GLY:N	12:2:429:ILE:HD11	1.99	0.77
37:f:75:GLU:HA	37:f:78:GLU:CD	2.09	0.77
12:2:430:ASN:OD1	12:2:431:SER:N	2.17	0.77
19:E:173:ILE:O	19:E:181:HIS:ND1	2.17	0.77
21:J:161:GLN:NE2	21:J:167:VAL:HG13	2.00	0.76
4:G:36:TRP:CE2	4:G:37:GLU:OE2	2.38	0.76
13:3:42:LEU:HB2	24:P:92:GLN:HE22	1.49	0.76
40:n:80:THR:HG22	40:n:84:HIS:HE1	1.51	0.76
10:j:13:GLY:H	12:2:429:ILE:CD1	1.98	0.76
32:a:52:ASN:HB2	32:a:55:LYS:HZ3	1.48	0.76
10:j:12:ARG:HD2	12:2:428:LEU:HA	1.66	0.76
9:S:188:ARG:HH22	40:n:48:THR:HG21	1.51	0.76
14:4:442:ARG:HH22	39:i:11:ASP:HB2	1.51	0.76
25:Q:77:ALA:HB1	25:Q:119:GLN:NE2	2.00	0.76
15:5:271:GLU:OE2	15:5:492:ILE:HA	1.86	0.75
9:S:210:ILE:HG22	9:S:221:LEU:HD13	1.69	0.75
11:1:216:PHE:HA	11:1:219:TYR:HD2	1.52	0.75
14:4:369:MET:HG2	14:4:445:ASP:HA	1.68	0.75
8:L:19:ARG:NH1	21:J:49:SER:O	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:d:83:LEU:HD23	35:d:86:GLN:HE21	1.52	0.74
1:A:408:ASP:OD1	1:A:477:ALA:HB1	1.85	0.74
11:1:177:TRP:CD2	48:1:403:3PE:H322	2.22	0.74
9:S:185:TYR:CD2	40:n:50:VAL:HG11	2.22	0.74
14:4:276:MET:HA	14:4:279:ILE:HD12	1.69	0.74
5:H:126:ILE:HD13	5:H:178:MET:HG3	1.68	0.74
15:5:157:TRP:CE3	26:R:92:ARG:HD2	2.22	0.74
2:B:44:LEU:O	2:B:135:LYS:NZ	2.20	0.74
4:G:194:PRO:HA	24:P:11:THR:HG22	1.70	0.74
2:B:179:TYR:OH	2:B:197:VAL:O	2.06	0.74
1:A:419:ARG:HB3	1:A:694:ILE:HD11	1.71	0.73
9:S:162:GLU:OE1	9:S:164:TRP:NE1	2.21	0.73
2:B:132:ILE:HG22	2:B:140:LEU:HD21	1.70	0.73
4:G:228:LYS:HZ1	24:P:104:ASP:HB2	1.51	0.73
12:2:195:LEU:HD22	12:2:197:LEU:HG	1.70	0.73
15:5:164:MET:HE1	32:a:80:TRP:CH2	2.22	0.73
37:f:4:ALA:HB2	37:f:56:ALA:HB1	1.68	0.73
19:E:213:PHE:HD2	19:E:214:LEU:H	1.35	0.73
25:Q:105:LEU:HD11	25:Q:131:ALA:HA	1.70	0.73
14:4:466:ILE:HD11	49:i:1101:PLC:H6'2	1.70	0.73
15:5:391:THR:HG22	15:5:473:GLY:H	1.53	0.73
36:e:25:ILE:HG23	36:e:28:LYS:HE2	1.69	0.73
2:B:269:ARG:HD2	2:B:270:GLU:HG3	1.70	0.73
5:H:115:ASN:HB3	5:H:119:MET:HE1	1.71	0.73
38:h:42:GLY:HA3	38:h:64:LYS:HD2	1.69	0.73
40:n:42:GLU:OE1	40:n:48:THR:N	2.21	0.73
3:C:144:TYR:HB2	7:K:85:CYS:HB3	1.70	0.73
4:G:227:GLU:OE2	19:E:72:LYS:NZ	2.21	0.73
15:5:164:MET:HE1	32:a:80:TRP:HH2	1.51	0.73
12:2:288:SER:HG	12:2:413:TYR:HH	1.33	0.73
18:D:38:ASP:OD1	18:D:39:ARG:N	2.22	0.73
15:5:530:GLU:HG3	15:5:531:PHE:HD1	1.52	0.72
3:C:155:SER:O	3:C:159:GLU:HG3	1.88	0.72
18:D:57:ASN:ND2	18:D:63:LYS:O	2.23	0.72
12:2:11:THR:HG22	12:2:15:MET:HE2	1.69	0.72
13:3:120:ASN:OD1	20:F:26:ARG:NH1	2.23	0.72
16:6:133:ILE:HG12	28:W:119:MET:CE	2.19	0.72
5:H:156:THR:HG22	5:H:158:ASP:H	1.54	0.72
15:5:163:ALA:HA	15:5:241:GLU:HG2	1.72	0.72
2:B:34:LEU:HD23	2:B:39:ARG:HD3	1.72	0.72
2:B:455:PHE:CE1	2:B:468:MET:HE1	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:237:THR:HA	15:5:240:MET:HE1	1.72	0.71
8:L:49:ASP:OD2	8:L:51:SER:OG	2.08	0.71
10:j:15:LEU:HD12	12:2:427:ILE:HG21	1.71	0.71
15:5:484:GLY:HA2	41:8:22:TYR:CE2	2.25	0.71
40:n:80:THR:O	40:n:84:HIS:ND1	2.20	0.71
3:C:103:GLU:OE1	3:C:111:ARG:NH1	2.22	0.71
12:2:376:PRO:HG3	48:4:503:3PE:H3G1	1.72	0.71
54:J:202:LMN:HCS	54:J:202:LMN:HBP	1.71	0.71
22:M:22:ILE:HD11	22:M:26:GLY:O	1.91	0.71
15:5:356:GLU:HG3	26:R:89:LYS:HZ1	1.56	0.71
5:H:65:GLN:HG2	5:H:66:TYR:CD2	2.25	0.71
2:B:272:ASN:HD21	2:B:341:PHE:HB2	1.56	0.70
12:2:5:ALA:O	12:2:9:LEU:HD23	1.91	0.70
15:5:63:GLU:OE2	39:i:53:ARG:NE	2.24	0.70
2:B:60:ASP:OD1	2:B:139:LYS:NZ	2.24	0.70
9:S:191:ILE:HG12	35:d:35:PHE:HD1	1.56	0.70
15:5:230:PHE:H	15:5:287:THR:HG22	1.55	0.70
29:X:35:MET:HE3	29:X:40:TYR:CE2	2.27	0.70
14:4:420:ALA:HA	14:4:423:TYR:CE1	2.25	0.70
21:J:27:GLY:O	21:J:31:GLN:NE2	2.25	0.70
24:P:47:PHE:HE2	24:P:52:ILE:HG13	1.56	0.70
32:a:52:ASN:HB2	32:a:55:LYS:HZ1	1.53	0.70
15:5:401:GLU:OE1	15:5:511:LYS:HA	1.91	0.70
15:5:281:LEU:HD21	15:5:414:VAL:HG21	1.74	0.69
32:a:100:PHE:HD2	32:a:101:LEU:HD22	1.56	0.69
8:L:8:LEU:HD12	8:L:32:MET:HG2	1.73	0.69
15:5:36:SER:O	15:5:40:ILE:HG12	1.91	0.69
25:Q:87:LEU:HD12	25:Q:91:ASP:HB3	1.74	0.69
29:X:14:TYR:CE1	40:n:99:PRO:HB3	2.27	0.69
2:B:390:GLY:HA3	2:B:421:ILE:HD11	1.73	0.69
3:C:434:HIS:HB3	3:C:457:MET:HE3	1.75	0.69
9:S:141:PRO:HG3	9:S:152:TRP:CZ3	2.27	0.69
12:2:85:TYR:HB2	12:2:439:LEU:HD11	1.75	0.69
12:2:360:LEU:HD13	33:b:24:ILE:HD11	1.74	0.69
1:A:525:SER:HB2	1:A:528:ARG:HG2	1.73	0.69
9:S:169:TYR:OH	52:n:201:CDL:OB3	2.06	0.69
11:1:110:LEU:HB2	16:6:61:MET:HE1	1.75	0.69
15:5:552:GLN:HE22	32:a:87:HIS:CB	2.06	0.69
40:n:80:THR:HG22	40:n:84:HIS:CE1	2.28	0.69
12:2:414:LEU:HD11	14:4:168:LEU:HD22	1.73	0.69
15:5:425:THR:HA	15:5:428:TYR:CE1	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:136:ASN:HA	4:G:160:THR:HG22	1.75	0.69
9:S:167:GLN:HE22	14:4:30:PHE:HB2	1.57	0.69
17:g:22:ASN:O	17:g:23:ARG:NH1	2.26	0.69
5:H:140:ILE:HG23	5:H:193:THR:HG21	1.73	0.69
10:j:13:GLY:C	12:2:429:ILE:HD11	2.17	0.69
26:R:81:PRO:HG2	26:R:84:PHE:CD2	2.26	0.69
12:2:325:MET:HB3	12:2:443:LEU:HD13	1.73	0.69
15:5:348:SER:HB3	15:5:462:MET:HE1	1.74	0.69
30:Y:65:LYS:HE2	30:Y:72:GLU:CB	2.23	0.69
1:A:408:ASP:OD2	1:A:478:LYS:N	2.24	0.68
1:A:429:ARG:NH1	1:A:449:THR:O	2.26	0.68
7:K:146:SER:OG	7:K:167:CYS:SG	2.50	0.68
37:f:5:LEU:C	37:f:40:THR:HG22	2.17	0.68
9:S:141:PRO:HG3	9:S:152:TRP:CH2	2.28	0.68
25:Q:65:SER:HB3	34:c:12:ARG:HD3	1.75	0.68
12:2:256:ASN:O	51:2:502:T7X:O6	2.11	0.68
13:3:65:PRO:O	13:3:69:GLU:HG3	1.92	0.68
19:E:172:GLU:HG3	19:E:175:SER:HB2	1.76	0.68
21:J:89:ARG:NE	21:J:91:ARG:HD2	2.09	0.68
24:P:47:PHE:HD2	24:P:51:THR:OG1	1.76	0.68
14:4:418:LEU:HD12	15:5:176:PHE:HA	1.75	0.68
15:5:276:VAL:O	15:5:280:ILE:HG13	1.93	0.68
1:A:38:GLU:OE2	1:A:45:LYS:CE	2.34	0.68
10:j:12:ARG:C	12:2:429:ILE:HG12	2.17	0.68
16:6:45:MET:HG3	48:6:201:3PE:H371	1.75	0.68
14:4:254:ALA:O	14:4:258:ILE:HD12	1.92	0.68
14:4:449:ARG:NH2	26:R:108:GLU:OE1	2.27	0.68
15:5:283:ILE:O	15:5:287:THR:HG23	1.94	0.68
19:E:228:LYS:HD2	19:E:288:GLU:OE2	1.94	0.68
29:X:73:LYS:O	29:X:77:VAL:HG23	1.94	0.68
14:4:178:MET:HB2	14:4:217:ALA:HB2	1.76	0.68
29:X:7:LEU:N	29:X:163:TYR:OH	2.26	0.68
1:A:177:LYS:HB2	1:A:241:LYS:HD3	1.75	0.67
1:A:86:ASP:OD1	1:A:113:ARG:NH2	2.24	0.67
14:4:174:GLY:HA3	14:4:220:VAL:HG21	1.76	0.67
3:C:439:ASP:HB3	24:P:3:ILE:HD12	1.75	0.67
11:1:67:GLU:HB2	11:1:128:ASN:HD22	1.59	0.67
13:3:22:ASN:C	13:3:22:ASN:HD22	2.02	0.67
31:Z:90:ASP:OD1	31:Z:91:GLN:N	2.26	0.67
37:f:24:GLN:CG	37:f:73:GLU:OE2	2.41	0.67
41:8:15:LYS:HZ1	41:8:16:HIS:CE1	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:LYS:HE3	30:Y:159:ARG:O	1.94	0.67
15:5:358:GLN:NE2	26:R:88:THR:HG21	2.10	0.67
38:h:110:TYR:O	38:h:113:THR:OG1	2.12	0.67
7:K:65:ASP:OD1	7:K:204:THR:OG1	2.12	0.67
14:4:386:THR:O	14:4:389:THR:OG1	2.10	0.67
56:Q:201:ZMP:H4	26:R:22:SER:HB2	1.75	0.67
37:f:12:LEU:HD22	37:f:22:LEU:HG	1.76	0.67
9:S:176:LEU:HB3	52:n:201:CDL:H582	1.76	0.67
2:B:344:LEU:HD12	2:B:351:LEU:HD23	1.74	0.67
2:B:309:ILE:HG12	2:B:316:LEU:HD12	1.76	0.67
20:F:47:ILE:O	20:F:51:GLU:HG2	1.94	0.67
2:B:258:ARG:O	5:H:240:GLN:HB2	1.94	0.67
11:1:206:GLU:OE1	11:1:216:PHE:CE2	2.48	0.67
2:B:370:GLN:OE1	2:B:402:ARG:HD2	1.94	0.66
6:I:118:HIS:ND1	6:I:166:MET:HE1	2.10	0.66
10:j:34:ARG:HH22	32:a:41:PRO:HD3	1.60	0.66
16:6:133:ILE:HG12	28:W:119:MET:HE3	1.77	0.66
19:E:268:THR:HB	19:E:271:GLN:HG3	1.75	0.66
5:H:174:ASN:ND2	5:H:186:GLU:OE1	2.24	0.66
35:d:65:ASN:HB3	39:i:71:ALA:HB3	1.76	0.66
42:9:18:GLU:HG3	42:9:44:TYR:HA	1.76	0.66
1:A:72:ASP:OD2	30:Y:137:ARG:NH1	2.28	0.66
5:H:76:ASP:OD1	5:H:80:ARG:HD3	1.95	0.66
8:L:16:VAL:HG11	15:5:622:LEU:HD22	1.76	0.66
4:G:223:ARG:HE	4:G:234:GLU:CD	2.03	0.66
22:M:21:ILE:HG23	22:M:29:ILE:HB	1.76	0.66
25:Q:77:ALA:C	25:Q:119:GLN:HE21	2.03	0.66
37:f:4:ALA:O	37:f:40:THR:HG22	1.92	0.66
11:1:177:TRP:CG	48:1:403:3PE:H322	2.30	0.66
15:5:187:VAL:HG21	15:5:214:LEU:HD22	1.78	0.66
26:R:34:GLN:HE21	34:c:17:TYR:HE2	1.43	0.66
9:S:185:TYR:CG	40:n:50:VAL:HG11	2.31	0.66
12:2:435:VAL:HG12	33:b:25:ARG:HG2	1.78	0.66
2:B:42:GLN:HB3	2:B:48:TYR:CE2	2.31	0.66
3:C:210:ARG:O	3:C:214:MET:HG3	1.96	0.66
15:5:229:GLN:NE2	15:5:317:THR:OG1	2.28	0.66
15:5:47:TYR:OH	15:5:94:THR:HG22	1.96	0.66
15:5:95:ILE:HD12	15:5:253:ALA:HB2	1.78	0.66
15:5:90:LEU:O	15:5:94:THR:HG23	1.96	0.65
21:J:89:ARG:HH12	21:J:95:TRP:CD1	2.14	0.65
2:B:447:GLU:OE1	2:B:447:GLU:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Z:100:LEU:HD13	31:Z:118:LEU:HD23	1.77	0.65
9:S:237:LEU:HD21	35:d:9:LEU:HB3	1.78	0.65
14:4:439:TYR:OH	32:a:64:ARG:NH1	2.29	0.65
19:E:121:HIS:NE2	22:M:65:GLU:OE2	2.23	0.65
1:A:582:PHE:HE1	38:h:135:LYS:HD2	1.61	0.65
31:Z:68:ASP:OD2	31:Z:70:ALA:N	2.19	0.65
10:j:27:HIS:NE2	14:4:441:HIS:CD2	2.63	0.65
25:Q:78:THR:HG22	25:Q:119:GLN:HG3	1.78	0.65
5:H:148:LEU:HD11	5:H:161:PHE:HD2	1.61	0.65
10:j:67:ILE:HD13	14:4:282:LEU:HD23	1.77	0.65
15:5:639:PHE:O	15:5:642:VAL:HG12	1.97	0.65
14:4:446:VAL:O	14:4:451:LYS:NZ	2.29	0.65
1:A:593:THR:OG1	1:A:594:GLU:OE1	2.14	0.65
2:B:63:LYS:NZ	5:H:243:ILE:HG23	2.10	0.65
8:L:60:ILE:HD11	16:6:59:TYR:HE2	1.62	0.65
23:O:97:GLN:HA	23:O:100:GLU:HG3	1.77	0.65
3:C:95:HIS:ND1	47:C:601:UQ9:O4	2.29	0.65
3:C:262:GLU:OE1	3:C:341:ARG:NH2	2.18	0.65
28:W:96:MET:HE1	42:9:63:VAL:HB	1.79	0.65
30:Y:43:GLU:OE1	30:Y:43:GLU:N	2.29	0.65
1:A:296:LYS:NZ	1:A:700:THR:OG1	2.27	0.64
1:A:552:LEU:HB3	1:A:555:ALA:HB3	1.79	0.64
1:A:354:VAL:CG2	1:A:553:LEU:HD21	2.25	0.64
2:B:41:PHE:CZ	2:B:277:LEU:HD11	2.31	0.64
2:B:385:THR:HG22	2:B:388:ARG:HH12	1.62	0.64
12:2:213:GLY:HA3	12:2:221:LEU:HD12	1.79	0.64
33:b:18:LYS:HE3	33:b:35:GLY:HA3	1.79	0.64
12:2:213:GLY:CA	12:2:221:LEU:HD12	2.27	0.64
19:E:127:ASN:ND2	19:E:127:ASN:O	2.30	0.64
1:A:302:ASP:OD2	1:A:709:THR:OG1	2.12	0.64
15:5:187:VAL:HG13	15:5:215:ILE:HG12	1.77	0.64
20:F:67:TYR:CZ	20:F:117:MET:HG3	2.32	0.64
15:5:495:ASN:HB2	32:a:146:GLN:HE22	1.63	0.64
1:A:429:ARG:HD2	1:A:449:THR:HB	1.79	0.64
32:a:124:GLU:HG2	41:8:65:ARG:NH1	2.13	0.64
48:4:502:3PE:H322	48:b:502:3PE:H242	1.80	0.64
15:5:485:THR:HG23	41:8:42:TYR:HE2	1.61	0.64
25:Q:66:PHE:CE2	25:Q:68:LYS:HB2	2.32	0.64
1:A:147:GLN:NE2	4:G:252:TRP:CH2	2.65	0.64
2:B:173:THR:O	2:B:177:GLU:HG2	1.98	0.64
9:S:116:ALA:HA	14:4:20:TRP:CZ3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:430:MET:HG3	15:5:522:SER:HA	1.80	0.64
6:I:170:ILE:HG21	7:K:156:TYR:CD1	2.33	0.63
41:8:13:MET:HG2	41:8:23:ARG:NH2	2.13	0.63
1:A:654:PRO:HD3	37:f:11:HIS:ND1	2.13	0.63
3:C:113:ASP:OD2	3:C:115:HIS:NE2	2.29	0.63
17:g:41:LEU:HG	52:X:201:CDL:H152	1.79	0.63
30:Y:65:LYS:HE2	30:Y:72:GLU:HB3	1.81	0.63
2:B:218:LEU:HD22	2:B:237:LEU:HD11	1.80	0.63
18:D:3:ILE:HD13	52:Z:201:CDL:HA4	1.79	0.63
26:R:85:PRO:HA	26:R:90:TYR:CD1	2.32	0.63
37:f:8:ILE:CD1	37:f:42:VAL:HG22	2.27	0.63
37:f:8:ILE:CD1	37:f:33:PHE:CE2	2.80	0.63
22:M:21:ILE:HD12	22:M:54:THR:HG23	1.80	0.63
1:A:87:VAL:HG22	1:A:107:VAL:HG22	1.80	0.63
26:R:18:MET:HE3	26:R:67:ARG:HD3	1.79	0.63
15:5:26:LEU:HD23	15:5:30:PHE:CD1	2.34	0.63
23:O:84:ILE:HB	23:O:88:GLU:OE2	1.98	0.63
32:a:118:LYS:HG3	41:8:69:MET:HE1	1.81	0.63
34:c:14:ALA:HB1	34:c:18:GLN:HE21	1.64	0.63
3:C:205:TRP:CZ2	6:I:93:GLN:HG3	2.33	0.63
38:h:31:LYS:HE3	38:h:53:GLU:OE1	1.98	0.63
2:B:269:ARG:HD2	2:B:270:GLU:N	2.14	0.63
5:H:148:LEU:HD11	5:H:161:PHE:CD2	2.34	0.63
42:9:19:TRP:O	42:9:23:MET:HG2	1.99	0.63
3:C:378:MET:HE3	3:C:382:ILE:HG13	1.81	0.62
15:5:270:LEU:HB3	15:5:277:LEU:HD11	1.81	0.62
36:e:45:GLU:HB2	36:e:49:MET:HE3	1.81	0.62
37:f:76:VAL:O	37:f:80:VAL:HG23	1.99	0.62
5:H:122:TYR:CE2	5:H:205:MET:HE1	2.31	0.62
15:5:87:THR:OG1	15:5:480:TYR:OH	2.06	0.62
19:E:59:PHE:HB2	19:E:127:ASN:HA	1.80	0.62
29:X:14:TYR:CD1	40:n:99:PRO:HB3	2.33	0.62
6:I:63:TRP:HH2	17:g:17:ARG:HE	1.44	0.62
20:F:54:LEU:O	20:F:58:GLN:HG3	2.00	0.62
1:A:351:GLY:HA3	1:A:555:ALA:H	1.64	0.62
12:2:443:LEU:O	12:2:447:ILE:HG12	1.99	0.62
2:B:269:ARG:HD2	2:B:270:GLU:H	1.64	0.62
56:O:201:ZMP:H15	24:P:63:HIS:O	1.99	0.62
5:H:120:GLY:HA3	5:H:159:ASN:O	2.00	0.62
16:6:33:ILE:HD12	16:6:75:ILE:CD1	2.29	0.62
21:J:25:THR:HG23	21:J:83:CYS:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:n:9:GLU:CD	40:n:10:LEU:H	2.07	0.62
9:S:206:LYS:HE2	9:S:207:HIS:CE1	2.35	0.62
13:3:57:ILE:HD11	16:6:77:LEU:HD22	1.80	0.62
14:4:77:LEU:HD22	14:4:136:SER:HB3	1.81	0.62
14:4:196:ASN:HB2	14:4:199:LEU:HD12	1.81	0.62
15:5:311:SER:OG	15:5:312:GLN:NE2	2.32	0.62
15:5:495:ASN:OD1	32:a:147:ARG:NH2	2.33	0.62
1:A:408:ASP:CG	1:A:477:ALA:HB1	2.24	0.62
8:L:1:FME:H	8:L:42:ARG:HD3	1.65	0.62
15:5:46:THR:HG21	15:5:93:THR:HG21	1.80	0.62
24:P:100:PHE:HB3	24:P:103:GLU:OE2	1.98	0.62
5:H:59:ILE:HD11	5:H:67:LYS:HD2	1.80	0.62
11:1:134:LEU:HD23	11:1:211:LEU:HD11	1.82	0.62
12:2:160:MET:HE3	15:5:617:ASN:CB	2.29	0.62
24:P:68:ASP:HB3	24:P:71:ILE:HD13	1.81	0.62
41:8:40:ASN:ND2	41:8:47:CYS:SG	2.73	0.61
1:A:434:ARG:HH12	30:Y:140:ARG:CZ	2.14	0.61
15:5:652:ILE:HD11	21:J:71:PHE:HE1	1.65	0.61
2:B:34:LEU:HD13	2:B:293:GLU:HG2	1.82	0.61
2:B:63:LYS:H	2:B:258:ARG:HH12	1.47	0.61
12:2:55:MET:HE3	16:6:160:PHE:HB2	1.82	0.61
15:5:123:PHE:HD1	15:5:149:THR:HG1	1.47	0.61
15:5:484:GLY:H	41:8:37:ARG:HH12	1.47	0.61
42:9:22:PHE:CE1	42:9:41:PHE:HB2	2.36	0.61
42:9:37:CYS:HA	42:9:39:PRO:HD2	1.82	0.61
2:B:160:ILE:HD13	2:B:199:ILE:HG23	1.81	0.61
2:B:210:GLU:OE1	45:B:502:FMN:HM82	2.00	0.61
2:B:455:PHE:HE1	2:B:468:MET:CE	2.10	0.61
12:2:187:LEU:HD13	12:2:192:ILE:HD11	1.83	0.61
14:4:124:VAL:HG22	48:4:503:3PE:H2I3	1.83	0.61
49:4:504:PLC:H7A2	48:J:201:3PE:H3G1	1.82	0.61
16:6:134:ILE:HB	18:D:81:LYS:HB2	1.83	0.61
41:8:30:LEU:HD21	41:8:54:TYR:CZ	2.36	0.61
1:A:328:ALA:O	1:A:332:ILE:HD12	1.99	0.61
5:H:192:GLY:O	5:H:195:LYS:HG2	2.01	0.61
11:1:72:ILE:HG13	11:1:125:TRP:HZ3	1.66	0.61
27:U:92:ASP:OD1	27:U:93:GLU:N	2.33	0.61
1:A:124:MET:HE1	2:B:390:GLY:HA2	1.82	0.61
4:G:202:ASP:OD1	4:G:203:TYR:N	2.34	0.61
7:K:69:ASN:O	7:K:73:GLN:HG3	2.00	0.61
35:d:58:ASN:HD21	41:8:23:ARG:NH2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:191:ILE:HG12	35:d:35:PHE:CD1	2.36	0.61
12:2:190:LEU:HD12	42:9:35:ALA:HA	1.82	0.60
35:d:83:LEU:HD23	35:d:86:GLN:NE2	2.15	0.60
14:4:220:VAL:HG12	14:4:227:ILE:HD12	1.83	0.60
16:6:33:ILE:HD13	16:6:71:PHE:HB3	1.82	0.60
6:I:196:THR:OG1	6:I:199:GLU:OE1	2.13	0.60
14:4:420:ALA:HA	14:4:423:TYR:CZ	2.36	0.60
27:U:76:THR:HG21	28:W:79:ARG:HH12	1.65	0.60
40:n:57:LYS:HB2	40:n:62:ILE:HD11	1.82	0.60
25:Q:109:ASP:HA	26:R:20:ARG:HH12	1.66	0.60
11:1:279:SER:OG	18:D:22:GLY:HA3	2.00	0.60
12:2:50:GLN:NE2	40:n:99:PRO:HG3	2.16	0.60
15:5:3:ASN:HD21	39:i:52:THR:HG21	1.65	0.60
2:B:284:VAL:HG13	2:B:358:VAL:HG11	1.84	0.60
12:2:119:HIS:CD2	29:X:152:ILE:HD11	2.36	0.60
21:J:155:VAL:HG11	21:J:161:GLN:OE1	2.02	0.60
22:M:22:ILE:HD12	22:M:27:ASN:O	2.01	0.60
15:5:92:ILE:HD13	15:5:127:MET:HG3	1.83	0.60
28:W:82:VAL:O	28:W:86:ILE:HG12	2.02	0.60
2:B:34:LEU:HD11	2:B:267:PHE:CE1	2.36	0.60
8:L:55:PHE:CD2	12:2:124:ILE:HG22	2.37	0.60
11:1:206:GLU:OE1	11:1:216:PHE:HE2	1.84	0.60
15:5:20:LEU:HB3	48:5:701:3PE:H351	1.83	0.60
15:5:293:LEU:HD23	15:5:424:LEU:HD21	1.83	0.60
24:P:47:PHE:CE2	24:P:52:ILE:HG13	2.36	0.60
32:a:133:GLU:CD	41:8:23:ARG:HE	2.09	0.60
10:j:13:GLY:CA	12:2:429:ILE:CG1	2.78	0.60
15:5:590:VAL:O	15:5:594:ARG:HG2	2.01	0.60
19:E:343:LEU:O	19:E:344:MET:C	2.43	0.60
21:J:134:TRP:CE2	54:J:202:LMN:HBDA	2.37	0.60
28:W:92:GLU:OE1	42:9:60:ILE:HD13	2.00	0.60
2:B:85:ARG:NE	2:B:91:GLY:O	2.31	0.60
12:2:188:ASP:OD2	42:9:34:ARG:HG2	2.00	0.60
19:E:25:GLU:HB3	24:P:108:GLY:HA3	1.83	0.60
25:Q:109:ASP:HA	26:R:20:ARG:NH1	2.17	0.60
3:C:144:TYR:CB	7:K:85:CYS:HB3	2.32	0.59
48:4:501:3PE:H251	48:b:502:3PE:H352	1.84	0.59
19:E:131:ARG:NH1	53:E:401:NDP:O2X	2.34	0.59
37:f:8:ILE:HD11	37:f:42:VAL:CG2	2.30	0.59
40:n:107:GLN:C	42:9:12:ARG:HH12	2.09	0.59
14:4:433:GLY:HA3	15:5:164:MET:SD	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:J:168:HIS:HB3	35:d:17:TYR:HD2	1.67	0.59
23:O:34:LYS:HD2	23:O:34:LYS:N	2.14	0.59
2:B:216:GLU:OE2	2:B:221:LYS:HD2	2.01	0.59
29:X:50:LEU:HD22	29:X:78:ALA:HA	1.82	0.59
31:Z:99:GLU:O	31:Z:107:ARG:NH1	2.35	0.59
32:a:120:ALA:C	41:8:69:MET:HE3	2.27	0.59
1:A:654:PRO:HD3	37:f:11:HIS:CE1	2.38	0.59
4:G:253:GLU:OE2	4:G:256:GLY:N	2.30	0.59
5:H:176:PRO:HG2	5:H:187:ASP:HA	1.84	0.59
15:5:552:GLN:HE22	32:a:87:HIS:CG	2.21	0.59
25:Q:67:ASP:HB2	34:c:11:ARG:NH1	2.17	0.59
16:6:42:ILE:HD11	48:6:202:3PE:H3E2	1.85	0.59
20:F:61:HIS:O	20:F:68:ARG:NH1	2.32	0.59
21:J:168:HIS:HB3	35:d:17:TYR:CD2	2.37	0.59
36:e:25:ILE:HA	36:e:28:LYS:HG2	1.85	0.59
9:S:175:SER:HB3	14:4:36:LEU:HD22	1.85	0.59
12:2:9:LEU:HD21	12:2:28:ILE:CD1	2.30	0.59
14:4:267:CYS:SG	35:d:83:LEU:HD13	2.43	0.59
5:H:80:ARG:N	5:H:80:ARG:HD2	2.17	0.59
8:L:11:SER:OG	8:L:28:CYS:HA	2.03	0.59
11:1:30:LEU:HD11	11:1:297:ARG:HD3	1.84	0.59
24:P:48:SER:O	24:P:51:THR:OG1	2.20	0.59
14:4:39:ILE:HG13	14:4:93:VAL:HG11	1.82	0.59
7:K:48:PRO:HD3	7:K:209:ARG:CZ	2.32	0.59
9:S:186:LYS:HD2	9:S:189:GLU:OE2	2.03	0.59
15:5:240:MET:HG2	15:5:302:LYS:HB3	1.85	0.59
36:e:21:ALA:HA	36:e:24:ARG:NH1	2.17	0.59
2:B:61:TRP:HA	2:B:64:THR:HG23	1.85	0.59
12:2:149:LYS:HB3	12:2:227:ASN:HB3	1.85	0.59
25:Q:89:SER:OG	26:R:12:LYS:NZ	2.35	0.58
31:Z:14:THR:HG21	31:Z:37:GLY:H	1.68	0.58
1:A:590:ALA:HB3	1:A:595:LYS:HD3	1.85	0.58
2:B:371:ARG:HH22	5:H:167:GLU:CD	2.10	0.58
9:S:143:LYS:C	9:S:150:VAL:HA	2.28	0.58
12:2:400:ILE:HG21	21:J:131:LEU:HD21	1.84	0.58
9:S:186:LYS:NZ	14:4:44:ILE:O	2.37	0.58
10:j:48:TYR:HD2	15:5:586:ARG:HH12	1.44	0.58
25:Q:77:ALA:HB1	25:Q:119:GLN:HE22	1.67	0.58
32:a:128:GLU:HB2	32:a:131:TRP:CD1	2.38	0.58
3:C:407:LYS:HD3	3:C:458:ASP:O	2.03	0.58
29:X:115:MET:SD	29:X:125:PRO:HB3	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:LYS:HZ1	5:H:243:ILE:CG2	2.15	0.58
21:J:89:ARG:HH21	21:J:91:ARG:HH21	1.50	0.58
41:8:40:ASN:HD22	41:8:46:ALA:HB3	1.67	0.58
2:B:299:ARG:O	2:B:303:GLU:HG3	2.03	0.58
6:I:217:GLU:HG3	38:h:79:PHE:HB2	1.84	0.58
9:S:119:TYR:HD2	14:4:20:TRP:HE3	1.51	0.58
13:3:69:GLU:HB3	13:3:98:LEU:HD13	1.83	0.58
5:H:40:ASN:H	5:H:43:ILE:HD12	1.69	0.58
26:R:53:ILE:HD11	26:R:58:LEU:HD23	1.85	0.58
2:B:61:TRP:HE1	2:B:138:HIS:HB3	1.68	0.58
26:R:19:TYR:OH	26:R:44:ARG:HA	2.04	0.58
2:B:87:ARG:HB2	2:B:248:GLU:OE2	2.04	0.58
12:2:368:VAL:O	12:2:372:ILE:HG13	2.04	0.58
14:4:251:LEU:HB3	14:4:310:MET:HE3	1.86	0.58
39:i:24:SER:OG	40:n:13:ALA:HB2	2.03	0.58
1:A:254:LYS:HE2	4:G:247:ALA:HB1	1.86	0.57
1:A:641:ASP:O	1:A:645:VAL:HG23	2.04	0.57
2:B:146:LEU:HD13	2:B:257:LEU:HD12	1.86	0.57
2:B:401:PHE:CE2	2:B:414:LEU:HD22	2.38	0.57
9:S:183:MET:HG2	14:4:43:TYR:HE2	1.68	0.57
14:4:25:LYS:HG3	14:4:104:TRP:CH2	2.38	0.57
12:2:353:LEU:HD21	12:2:360:LEU:HD23	1.84	0.57
14:4:236:SER:OG	14:4:237:GLU:OE2	2.22	0.57
16:6:54:ILE:HD11	16:6:147:LEU:HD22	1.86	0.57
22:M:21:ILE:HD11	22:M:58:LYS:HB2	1.85	0.57
42:9:56:ARG:HD2	42:9:60:ILE:HD11	1.85	0.57
8:L:64:GLY:HA3	13:3:68:LEU:HD11	1.86	0.57
16:6:55:PHE:HE1	16:6:146:LEU:HD21	1.69	0.57
40:n:42:GLU:HB2	40:n:48:THR:HG22	1.86	0.57
40:n:76:GLN:O	40:n:80:THR:OG1	2.19	0.57
3:C:191:CYS:HB3	3:C:203:PHE:HA	1.85	0.57
19:E:21:MET:HE2	30:Y:51:GLU:OE2	2.03	0.57
37:f:64:SER:OG	37:f:83:LEU:HD11	2.04	0.57
9:S:190:ASP:OD1	9:S:191:ILE:N	2.37	0.57
10:j:17:LYS:HE3	14:4:109:PHE:CB	2.34	0.57
10:j:27:HIS:NE2	14:4:441:HIS:NE2	2.50	0.57
11:1:67:GLU:CB	11:1:128:ASN:HD22	2.18	0.57
17:g:30:PHE:CE2	17:g:34:ILE:HG13	2.40	0.57
56:O:201:ZMP:H14	24:P:66:VAL:HG23	1.86	0.57
40:n:84:HIS:HB3	40:n:88:ARG:NH2	2.19	0.57
15:5:511:LYS:HD3	36:e:51:GLY:HA3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:LYS:NZ	5:H:243:ILE:HA	2.18	0.57
10:j:13:GLY:H	12:2:429:ILE:CG1	2.00	0.57
15:5:479:ILE:O	15:5:485:THR:HG21	2.05	0.57
5:H:139:GLY:O	5:H:142:GLU:HG3	2.05	0.57
12:2:8:SER:HB3	12:2:12:PHE:HE2	1.70	0.57
14:4:103:ASN:ND2	14:4:114:TYR:OH	2.38	0.57
48:4:502:3PE:H32	48:b:502:3PE:H272	1.86	0.57
15:5:173:MET:HE1	15:5:234:ASN:HB2	1.86	0.57
26:R:46:LYS:HE2	26:R:46:LYS:HA	1.87	0.57
2:B:33:GLY:N	2:B:292:GLU:OE2	2.38	0.57
3:C:39:GLN:NE2	12:2:277:LEU:HD12	2.20	0.57
5:H:36:THR:OG1	5:H:38:ASN:O	2.17	0.57
14:4:78:LEU:HD11	40:n:73:LEU:HD11	1.87	0.57
28:W:95:ILE:HD13	42:9:64:LEU:HD12	1.85	0.57
39:i:22:ASN:O	40:n:11:THR:N	2.37	0.57
14:4:140:LEU:HD11	48:4:503:3PE:H3E2	1.87	0.56
2:B:76:ILE:O	2:B:80:LYS:HG2	2.04	0.56
5:H:152:PRO:HA	5:H:163:LEU:HD23	1.87	0.56
7:K:80:THR:O	7:K:82:GLY:N	2.38	0.56
9:S:214:PRO:O	9:S:218:ARG:HG3	2.04	0.56
30:Y:133:GLU:OE1	30:Y:134:PRO:HD2	2.05	0.56
1:A:37:ILE:HD11	1:A:101:VAL:HG23	1.87	0.56
1:A:159:THR:O	2:B:465:GLY:HA3	2.05	0.56
3:C:453:ILE:O	3:C:457:MET:HG2	2.05	0.56
15:5:66:ASN:ND2	15:5:75:ILE:O	2.39	0.56
15:5:313:LEU:HA	15:5:316:MET:HE2	1.86	0.56
4:G:227:GLU:CD	19:E:72:LYS:HZ2	2.13	0.56
5:H:132:CYS:HB3	5:H:137:SER:OG	2.05	0.56
15:5:644:PRO:HG3	21:J:78:TYR:HB3	1.86	0.56
23:O:68:ASP:OD1	24:P:57:ARG:NH1	2.38	0.56
42:9:39:PRO:HA	42:9:42:GLU:OE1	2.05	0.56
1:A:553:LEU:HD23	1:A:553:LEU:C	2.31	0.56
19:E:61:ALA:HB3	19:E:82:VAL:HG13	1.88	0.56
12:2:11:THR:O	12:2:14:SER:OG	2.15	0.56
2:B:449:GLU:HA	2:B:452:MET:HE3	1.87	0.56
26:R:35:LEU:HD12	26:R:39:LYS:NZ	2.20	0.56
22:M:25:ASN:ND2	22:M:27:ASN:OD1	2.38	0.56
27:U:53:PHE:HA	27:U:71:GLU:HG3	1.88	0.56
31:Z:15:VAL:HG22	31:Z:38:ASN:HB2	1.87	0.56
1:A:315:ARG:NH2	1:A:583:ALA:O	2.39	0.56
13:3:39:GLU:OE2	13:3:44:SER:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLN:NE2	30:Y:140:ARG:O	2.35	0.56
2:B:259:ARG:HD2	2:B:263:TRP:CZ3	2.41	0.56
12:2:55:MET:HE1	29:X:155:TRP:CH2	2.41	0.56
15:5:349:ILE:HG13	15:5:373:THR:HG21	1.87	0.56
29:X:7:LEU:HD11	29:X:133:PRO:HB2	1.88	0.56
5:H:94:ALA:HB2	5:H:104:VAL:HG21	1.88	0.55
9:S:207:HIS:CE1	9:S:225:ARG:NH1	2.74	0.55
15:5:236:LEU:HD12	15:5:251:HIS:HE1	1.71	0.55
40:n:82:LYS:HE3	40:n:83:MET:HE3	1.88	0.55
8:L:13:LEU:HA	8:L:16:VAL:HG12	1.88	0.55
14:4:146:PRO:HB2	48:4:502:3PE:H2D1	1.89	0.55
25:Q:108:PRO:HG2	25:Q:111:ASP:HB3	1.87	0.55
41:8:30:LEU:HD21	41:8:54:TYR:CE2	2.40	0.55
15:5:220:PHE:CZ	15:5:283:ILE:HG21	2.35	0.55
39:i:44:VAL:HG13	49:i:1101:PLC:H6A1	1.88	0.55
1:A:39:LEU:C	1:A:39:LEU:HD12	2.31	0.55
19:E:105:LEU:HD11	22:M:66:GLN:HG3	1.89	0.55
39:i:55:ARG:HG2	39:i:56:GLU:CD	2.31	0.55
8:L:42:ARG:NH1	18:D:87:ILE:O	2.38	0.55
15:5:330:PHE:CE2	15:5:395:THR:HG22	2.42	0.55
19:E:291:LYS:HZ2	19:E:295:GLN:CG	2.19	0.55
1:A:398:ASN:ND2	1:A:519:TYR:O	2.38	0.55
3:C:202:PRO:HB3	3:C:261:ILE:HD12	1.88	0.55
15:5:509:PHE:HE1	15:5:513:LEU:HD13	1.70	0.55
1:A:67:ARG:H	1:A:147:GLN:HE22	1.53	0.55
7:K:80:THR:HG22	7:K:107:PHE:HD1	1.70	0.55
21:J:89:ARG:HE	21:J:91:ARG:HD2	1.72	0.55
42:9:28:LYS:HG3	42:9:29:THR:HG23	1.88	0.55
2:B:87:ARG:HD2	2:B:276:LYS:HD2	1.88	0.55
3:C:269:ARG:NH2	48:I:501:3PE:O32	2.40	0.55
15:5:3:ASN:ND2	39:i:52:THR:HG21	2.20	0.55
21:J:32:SER:HB3	21:J:79:VAL:HG11	1.89	0.55
31:Z:174:LYS:N	31:Z:174:LYS:HD2	2.22	0.55
13:3:60:ALA:HB1	16:6:70:LEU:HD21	1.88	0.55
19:E:121:HIS:HB3	22:M:61:MET:HE3	1.88	0.55
1:A:673:GLN:HA	1:A:677:VAL:HG22	1.89	0.55
14:4:469:GLN:OE1	15:5:68:LEU:HD12	2.07	0.55
19:E:227:ASN:HB3	19:E:231:GLU:OE2	2.07	0.55
27:U:66:ILE:HG22	28:W:82:VAL:HG12	1.89	0.55
2:B:101:MET:HG2	2:B:151:MET:HB3	1.89	0.54
6:I:165:ASP:OD2	6:I:168:LYS:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:6:ILE:HG21	16:6:17:ILE:HG12	1.87	0.54
26:R:34:GLN:O	26:R:38:GLN:NE2	2.39	0.54
27:U:50:ASN:O	27:U:54:MET:HG2	2.07	0.54
1:A:174:PRO:HD2	1:A:717:PHE:CZ	2.42	0.54
12:2:55:MET:CE	16:6:160:PHE:HB2	2.37	0.54
27:U:58:GLU:OE2	40:n:115:PRO:HA	2.07	0.54
31:Z:114:GLY:O	31:Z:118:LEU:HG	2.07	0.54
6:I:70:ALA:HB2	17:g:21:HIS:CD2	2.42	0.54
36:e:47:PRO:HA	36:e:52:LEU:HD13	1.88	0.54
17:g:9:TRP:CD1	52:g:201:CDL:HA31	2.42	0.54
3:C:197:VAL:HG21	3:C:271:TRP:HZ3	1.72	0.54
4:G:118:THR:HB	4:G:120:TYR:CE2	2.43	0.54
13:3:60:ALA:HB1	16:6:70:LEU:CD2	2.37	0.54
14:4:441:HIS:HB3	26:R:102:MET:HE1	1.89	0.54
42:9:18:GLU:OE1	42:9:18:GLU:N	2.30	0.54
1:A:484:VAL:HG11	1:A:498:PHE:HE2	1.73	0.54
14:4:211:TRP:HZ2	14:4:277:ILE:HD11	1.71	0.54
23:O:99:VAL:O	23:O:102:ILE:HG22	2.08	0.54
30:Y:41:ALA:O	30:Y:42:HIS:ND1	2.41	0.54
40:n:27:VAL:O	40:n:31:LEU:HD23	2.07	0.54
2:B:272:ASN:CG	2:B:340:ASP:HB2	2.32	0.54
3:C:338:ALA:HB1	31:Z:171:ILE:HD13	1.90	0.54
6:I:43:ALA:O	20:F:78:ARG:NH1	2.41	0.54
12:2:358:ALA:HB1	48:4:502:3PE:H232	1.89	0.54
15:5:335:HIS:HA	15:5:338:PHE:CZ	2.42	0.54
9:S:168:MET:HE2	9:S:168:MET:HA	1.90	0.54
14:4:251:LEU:HD23	14:4:310:MET:HG3	1.89	0.54
28:W:93:LYS:C	28:W:93:LYS:HD3	2.33	0.54
38:h:97:LEU:HD12	38:h:98:PRO:HD2	1.89	0.54
2:B:483:LEU:HD22	2:B:486:VAL:HG13	1.90	0.54
6:I:194:THR:HA	38:h:111:THR:HG21	1.90	0.54
14:4:235:HIS:NE2	14:4:246:LEU:HD22	2.23	0.54
14:4:469:GLN:OE1	15:5:68:LEU:HA	2.07	0.54
22:M:19:LYS:HD3	22:M:33:GLU:HB2	1.90	0.54
22:M:21:ILE:HD12	22:M:54:THR:CG2	2.38	0.54
7:K:80:THR:HG22	7:K:107:PHE:CD1	2.43	0.53
12:2:91:ASN:O	12:2:95:THR:HG23	2.08	0.53
14:4:30:PHE:O	14:4:34:LEU:HD23	2.08	0.53
17:g:34:ILE:O	17:g:38:VAL:HG12	2.08	0.53
56:Q:201:ZMP:O5	26:R:12:LYS:NZ	2.41	0.53
1:A:315:ARG:NH1	38:h:134:THR:HB	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:218:ARG:O	9:S:222:ILE:HD12	2.07	0.53
12:2:224:ILE:O	12:2:228:THR:HG23	2.08	0.53
24:P:71:ILE:O	24:P:75:LEU:HG	2.08	0.53
35:d:58:ASN:HB2	41:8:17:LYS:HZ3	1.72	0.53
2:B:227:LEU:HB2	30:Y:144:TYR:CE2	2.43	0.53
2:B:364:ASP:CG	2:B:451:ARG:HH22	2.17	0.53
8:L:55:PHE:HD2	12:2:124:ILE:HG22	1.72	0.53
9:S:56:GLU:HB3	9:S:118:LEU:CD2	2.38	0.53
10:j:40:THR:O	15:5:581:LYS:NZ	2.42	0.53
15:5:123:PHE:HD1	15:5:149:THR:OG1	1.92	0.53
15:5:157:TRP:CD2	26:R:92:ARG:HD2	2.43	0.53
15:5:374:TYR:OH	15:5:438:TYR:OH	2.26	0.53
15:5:452:HIS:ND1	15:5:453:GLU:N	2.55	0.53
15:5:522:SER:O	15:5:526:VAL:HG23	2.08	0.53
19:E:216:ARG:O	19:E:220:SER:OG	2.13	0.53
35:d:35:PHE:CE2	35:d:79:LEU:HD11	2.42	0.53
35:d:57:PRO:HG2	41:8:17:LYS:HD2	1.90	0.53
1:A:285:HIS:HD2	30:Y:135:HIS:NE2	2.06	0.53
9:S:59:LEU:O	9:S:63:LEU:HD23	2.07	0.53
16:6:23:ILE:HD11	16:6:36:MET:HA	1.89	0.53
48:E:402:3PE:H271	48:E:402:3PE:H3A1	1.91	0.53
1:A:621:GLU:OE1	1:A:623:TRP:NE1	2.40	0.53
5:H:195:LYS:HA	5:H:198:GLU:CD	2.34	0.53
30:Y:38:ASN:OD1	30:Y:126:GLY:HA2	2.08	0.53
32:a:131:TRP:CH2	32:a:141:LYS:HE2	2.43	0.53
1:A:285:HIS:HD2	30:Y:135:HIS:CD2	2.26	0.53
2:B:170:VAL:O	2:B:173:THR:OG1	2.25	0.53
2:B:393:TRP:CE2	2:B:417:LEU:HD21	2.44	0.53
2:B:454:LYS:HA	2:B:458:GLU:OE1	2.08	0.53
7:K:202:LYS:HB2	7:K:206:MET:HG2	1.90	0.53
9:S:66:LEU:HD11	9:S:94:ILE:HD12	1.89	0.53
14:4:387:PRO:HD3	15:5:144:GLU:OE1	2.08	0.53
32:a:33:GLU:HA	32:a:36:MET:CE	2.37	0.53
37:f:80:VAL:O	37:f:84:ILE:HG12	2.09	0.53
1:A:653:SER:HA	37:f:11:HIS:HE1	1.73	0.53
2:B:432:ALA:O	2:B:436:PRO:HD3	2.08	0.53
3:C:258:LEU:HD11	3:C:340:PHE:HB3	1.90	0.53
4:G:79:MET:SD	31:Z:91:GLN:HG2	2.48	0.53
5:H:36:THR:O	5:H:40:ASN:HB2	2.08	0.53
7:K:81:PHE:HE2	7:K:131:LEU:HD12	1.74	0.53
15:5:79:PHE:HB3	15:5:132:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:300:ASP:O	15:5:304:ILE:HG12	2.08	0.53
15:5:434:TYR:HD1	15:5:435:LEU:HD22	1.73	0.53
20:F:60:LYS:HE2	20:F:118:SER:HB3	1.90	0.53
41:8:29:LEU:HD12	41:8:57:CYS:SG	2.48	0.53
1:A:135:VAL:CG1	6:I:131:ILE:HD12	2.39	0.53
2:B:58:GLN:O	5:H:235:VAL:HG23	2.08	0.53
3:C:448:PRO:HG3	11:1:210:GLU:HG2	1.91	0.53
10:j:17:LYS:HE3	14:4:109:PHE:HB2	1.91	0.53
12:2:469:ASN:ND2	40:n:87:LYS:HB2	2.24	0.53
52:g:201:CDL:H371	52:g:201:CDL:H192	1.91	0.53
27:U:12:PHE:CE1	28:W:119:MET:HE1	2.43	0.53
42:9:67:LYS:HD2	42:9:69:GLU:OE2	2.09	0.53
2:B:213:SER:OG	2:B:223:GLY:O	2.26	0.53
8:L:66:GLU:HB2	12:2:135:TYR:OH	2.09	0.53
29:X:76:ARG:NE	29:X:80:MET:HE2	2.24	0.53
32:a:118:LYS:HE3	32:a:122:PRO:HD3	1.90	0.53
35:d:54:GLU:OE2	39:i:59:THR:OG1	2.23	0.53
4:G:185:MET:HB3	4:G:210:LEU:HD12	1.91	0.53
14:4:478:THR:HG23	14:4:482:TYR:HE2	1.73	0.53
26:R:20:ARG:O	26:R:24:LYS:HE2	2.09	0.53
28:W:91:ARG:NH2	28:W:91:ARG:HB2	2.23	0.53
1:A:39:LEU:CD1	1:A:41:ILE:HG13	2.38	0.52
1:A:354:VAL:HG22	1:A:355:GLU:N	2.24	0.52
4:G:80:ALA:O	4:G:83:PRO:HD3	2.09	0.52
4:G:203:TYR:HD1	24:P:85:GLU:OE1	1.92	0.52
5:H:127:CYS:SG	5:H:168:CYS:HA	2.50	0.52
7:K:139:PRO:HG2	11:1:60:LYS:NZ	2.24	0.52
15:5:525:ILE:O	15:5:529:ASN:ND2	2.32	0.52
17:g:18:TRP:CD1	17:g:22:ASN:HD22	2.26	0.52
22:M:21:ILE:CD1	22:M:58:LYS:HB2	2.40	0.52
56:Q:201:ZMP:P1	26:R:12:LYS:NZ	2.82	0.52
14:4:141:PHE:CZ	14:4:221:LYS:HD3	2.44	0.52
15:5:494:PRO:HB3	32:a:125:PHE:CZ	2.44	0.52
19:E:206:PHE:HB2	19:E:214:LEU:HD12	1.90	0.52
1:A:610:ARG:NH1	30:Y:81:ASP:OD1	2.39	0.52
3:C:332:ARG:HH21	3:C:456:THR:HG21	1.73	0.52
7:K:76:PHE:HZ	7:K:194:LEU:HD23	1.74	0.52
10:j:13:GLY:HA3	12:2:429:ILE:CG1	2.39	0.52
15:5:500:PHE:CD1	41:8:58:GLU:HG2	2.45	0.52
15:5:537:ASN:HB3	26:R:30:ILE:HD12	1.91	0.52
39:i:24:SER:CB	40:n:10:LEU:HD21	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:n:58:SER:O	40:n:62:ILE:HG12	2.09	0.52
40:n:107:GLN:O	42:9:12:ARG:NH1	2.41	0.52
42:9:56:ARG:O	42:9:60:ILE:HG13	2.08	0.52
3:C:82:ALA:HB1	3:C:103:GLU:HB3	1.91	0.52
11:1:118:PHE:CE2	16:6:37:ILE:HD13	2.45	0.52
11:1:180:ILE:HD11	48:1:403:3PE:H361	1.90	0.52
15:5:16:TRP:CE2	15:5:122:MET:HG3	2.44	0.52
21:J:136:GLY:HA2	54:J:202:LMN:H3	1.89	0.52
28:W:93:LYS:HA	28:W:103:VAL:HG21	1.91	0.52
29:X:50:LEU:HD22	29:X:78:ALA:CA	2.39	0.52
38:h:109:ASN:OD1	38:h:111:THR:HG23	2.09	0.52
1:A:332:ILE:HD11	1:A:585:VAL:HG11	1.90	0.52
9:S:207:HIS:CE1	9:S:225:ARG:CZ	2.92	0.52
11:1:25:ALA:HB2	18:D:10:PRO:HB2	1.90	0.52
13:3:59:VAL:HG22	13:3:111:LEU:HD22	1.91	0.52
15:5:434:TYR:HA	15:5:438:TYR:HB2	1.90	0.52
15:5:559:ILE:HG13	32:a:97:PHE:CD1	2.45	0.52
24:P:18:LYS:HG2	24:P:69:LEU:HD13	1.91	0.52
1:A:380:ASN:ND2	1:A:490:ASP:O	2.43	0.52
3:C:440:HIS:HD1	24:P:2:ALA:N	2.08	0.52
11:1:82:ILE:O	11:1:86:ILE:HG12	2.10	0.52
14:4:477:TRP:HZ3	35:d:31:THR:OG1	1.92	0.52
15:5:115:ARG:HB2	39:i:16:THR:HG21	1.90	0.52
26:R:37:ARG:HA	26:R:37:ARG:NH2	2.24	0.52
34:c:20:ASN:HA	34:c:25:ASN:HD22	1.74	0.52
1:A:411:LEU:HB2	1:A:470:PHE:HE1	1.75	0.52
4:G:72:HIS:HB3	4:G:266:PHE:CE1	2.45	0.52
14:4:485:ILE:HB	35:d:80:GLN:HB3	1.92	0.52
21:J:115:VAL:HG11	54:a:201:LMN:HBHA	1.92	0.52
40:n:40:SER:C	40:n:44:LYS:HZ2	2.17	0.52
41:8:27:ALA:HA	41:8:30:LEU:HD12	1.90	0.52
1:A:358:SER:OG	1:A:553:LEU:HD11	2.10	0.52
1:A:722:LYS:HA	1:A:725:GLN:NE2	2.25	0.52
4:G:161:GLU:HG3	4:G:162:VAL:HG13	1.92	0.52
4:G:223:ARG:NE	4:G:234:GLU:OE2	2.36	0.52
6:I:129:ARG:NH1	22:M:108:GLN:O	2.43	0.52
7:K:79:VAL:HG12	7:K:117:MET:HA	1.92	0.52
15:5:54:LEU:HD23	15:5:487:PHE:CE1	2.45	0.52
12:2:330:SER:HB2	12:2:353:LEU:HD11	1.90	0.52
15:5:331:HIS:HB2	15:5:399:ILE:HD11	1.91	0.52
15:5:517:SER:HA	15:5:520:LEU:HG	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:d:51:CYS:HA	39:i:64:ILE:HD12	1.92	0.52
40:n:81:ILE:O	40:n:85:GLU:HG2	2.10	0.52
6:I:163:ASP:OD1	6:I:203:ASN:HA	2.10	0.52
15:5:615:SER:O	15:5:619:MET:HG3	2.10	0.52
19:E:216:ARG:HG3	52:E:403:CDL:HA21	1.92	0.52
26:R:33:ARG:O	26:R:33:ARG:HD3	2.10	0.52
12:2:88:TYR:OH	12:2:332:TYR:CD2	2.61	0.51
12:2:399:SER:O	12:2:403:ILE:HG12	2.09	0.51
13:3:24:LEU:HD21	52:E:403:CDL:H731	1.93	0.51
15:5:358:GLN:HA	15:5:363:TYR:OH	2.10	0.51
15:5:419:TYR:OH	15:5:517:SER:OG	2.05	0.51
21:J:48:ASN:ND2	21:J:60:THR:HB	2.25	0.51
2:B:401:PHE:HE2	2:B:414:LEU:HD22	1.73	0.51
2:B:454:LYS:O	2:B:458:GLU:OE1	2.29	0.51
15:5:216:MET:HE3	15:5:219:LEU:HB2	1.90	0.51
17:g:41:LEU:HD11	52:X:201:CDL:H201	1.91	0.51
21:J:161:GLN:OE1	21:J:161:GLN:HA	2.10	0.51
24:P:61:GLU:OE1	24:P:64:ARG:HG3	2.10	0.51
25:Q:111:ASP:OD2	25:Q:124:TYR:CZ	2.64	0.51
3:C:37:LEU:HB2	3:C:39:GLN:OE1	2.10	0.51
5:H:115:ASN:CB	5:H:119:MET:HE1	2.38	0.51
8:L:3:ILE:HB	16:6:13:ILE:HG12	1.92	0.51
15:5:419:TYR:CZ	15:5:513:LEU:HG	2.46	0.51
19:E:330:PHE:CD2	19:E:337:PRO:HG3	2.45	0.51
6:I:127:GLU:OE1	6:I:152:ARG:NH1	2.27	0.51
15:5:455:ASN:O	15:5:459:THR:HG23	2.09	0.51
27:U:167:LYS:HD3	27:U:172:LEU:HD22	1.92	0.51
2:B:130:ARG:HG2	2:B:134:ARG:NH2	2.26	0.51
2:B:449:GLU:HA	2:B:452:MET:CE	2.41	0.51
9:S:162:GLU:O	9:S:165:VAL:HG22	2.10	0.51
24:P:47:PHE:CD2	24:P:51:THR:OG1	2.61	0.51
25:Q:94:GLU:HB3	34:c:9:TRP:HZ2	1.75	0.51
8:L:54:LEU:HD11	16:6:154:LEU:HD13	1.93	0.51
13:3:88:PHE:CE1	13:3:92:LEU:HD11	2.46	0.51
15:5:505:SER:O	36:e:56:TYR:OH	2.28	0.51
21:J:162:THR:HG1	21:J:165:GLU:CD	2.18	0.51
1:A:359:MET:CE	1:A:527:SER:HB2	2.41	0.51
48:1:402:3PE:H371	52:E:403:CDL:H741	1.92	0.51
18:D:82:SER:OG	28:W:119:MET:SD	2.63	0.51
40:n:44:LYS:HG3	40:n:45:ASN:OD1	2.11	0.51
1:A:372:GLU:OE2	37:f:57:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:ARG:O	2:B:451:ARG:HD3	2.11	0.51
7:K:76:PHE:O	7:K:105:ILE:HA	2.09	0.51
19:E:73:LEU:O	19:E:78:THR:HG22	2.11	0.51
25:Q:93:VAL:HG13	26:R:20:ARG:HG3	1.93	0.51
33:b:25:ARG:NH1	51:b:501:T7X:O12	2.43	0.51
36:e:45:GLU:O	36:e:49:MET:HG2	2.11	0.51
2:B:130:ARG:HG2	2:B:134:ARG:HH22	1.76	0.51
3:C:61:ASP:OD1	12:2:278:GLN:NE2	2.44	0.51
16:6:20:THR:O	16:6:24:ILE:HD12	2.10	0.51
24:P:18:LYS:HB3	24:P:22:GLN:HE22	1.76	0.51
40:n:42:GLU:OE1	40:n:48:THR:HG23	2.11	0.51
2:B:38:ASP:HB3	2:B:267:PHE:HE1	1.76	0.51
2:B:61:TRP:CE3	2:B:183:LEU:HD23	2.46	0.51
3:C:98:LEU:HD13	3:C:461:PHE:HE1	1.76	0.51
3:C:208:GLU:HG2	6:I:99:TYR:CE2	2.46	0.51
12:2:436:SER:HB2	29:X:61:ASP:OD2	2.10	0.51
14:4:386:THR:HA	15:5:144:GLU:OE2	2.11	0.51
16:6:45:MET:HG3	48:6:201:3PE:C37	2.39	0.51
19:E:205:MET:HE3	53:E:401:NDP:C3N	2.41	0.51
34:c:12:ARG:NH1	36:e:11:ASN:HB3	2.26	0.51
40:n:105:VAL:HG11	42:9:24:HIS:NE2	2.26	0.51
41:8:71:LYS:O	41:8:75:GLU:HG2	2.11	0.51
1:A:42:ASP:OD2	1:A:109:THR:OG1	2.26	0.50
3:C:179:GLU:HA	3:C:179:GLU:OE1	2.12	0.50
7:K:70:TRP:HD1	49:K:302:PLC:H42	1.76	0.50
9:S:203:VAL:HA	9:S:231:TYR:CE2	2.46	0.50
13:3:78:MET:HG3	16:6:147:LEU:HD23	1.92	0.50
15:5:558:GLN:OE1	32:a:85:PHE:HB2	2.11	0.50
27:U:108:LEU:O	27:U:112:ARG:NH2	2.44	0.50
33:b:21:SER:O	33:b:25:ARG:HG3	2.11	0.50
39:i:62:SER:HB2	39:i:66:LYS:NZ	2.26	0.50
42:9:63:VAL:O	42:9:67:LYS:HG3	2.12	0.50
1:A:215:THR:OG1	1:A:217:LEU:O	2.22	0.50
2:B:400:ARG:HH22	2:B:410:GLU:CD	2.19	0.50
3:C:203:PHE:HD1	3:C:204:LEU:HD22	1.76	0.50
15:5:419:TYR:OH	15:5:513:LEU:HG	2.11	0.50
19:E:251:ASP:OD2	24:P:109:ARG:NH2	2.44	0.50
40:n:84:HIS:HB3	40:n:88:ARG:HH21	1.76	0.50
1:A:707:SER:HB2	1:A:710:MET:HG2	1.94	0.50
4:G:51:ASP:OD1	4:G:52:GLU:N	2.44	0.50
12:2:11:THR:HG22	12:2:15:MET:CE	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:121:THR:OG1	20:F:27:GLU:OE2	2.24	0.50
14:4:233:VAL:O	14:4:237:GLU:OE1	2.28	0.50
21:J:83:CYS:O	21:J:87:ASN:ND2	2.45	0.50
3:C:257:ARG:NH1	3:C:260:GLU:OE1	2.42	0.50
39:i:23:PRO:HB3	40:n:14:VAL:HG22	1.92	0.50
41:8:60:ALA:O	41:8:64:ARG:HG3	2.11	0.50
42:9:12:ARG:HD3	42:9:16:PHE:CD2	2.46	0.50
3:C:439:ASP:OD2	24:P:3:ILE:HA	2.11	0.50
6:I:161:LYS:HE2	6:I:163:ASP:OD2	2.11	0.50
9:S:53:GLU:HA	9:S:56:GLU:OE1	2.12	0.50
9:S:113:ASN:OD1	14:4:16:ARG:NH2	2.45	0.50
9:S:224:GLU:OE2	39:i:70:ALA:HB2	2.11	0.50
20:F:25:MET:HG3	20:F:40:PRO:HD3	1.94	0.50
23:O:43:PHE:HE2	23:O:71:GLU:HG2	1.77	0.50
32:a:32:ALA:O	32:a:36:MET:HE1	2.11	0.50
1:A:74:LEU:O	30:Y:142:LYS:NZ	2.31	0.50
3:C:98:LEU:HD22	3:C:461:PHE:HZ	1.76	0.50
19:E:165:HIS:HB3	19:E:199:ILE:HD13	1.93	0.50
1:A:285:HIS:CD2	30:Y:135:HIS:CD2	2.99	0.50
1:A:438:GLU:OE1	1:A:473:VAL:CG1	2.58	0.50
4:G:228:LYS:NZ	24:P:104:ASP:HB2	2.24	0.50
8:L:16:VAL:CG1	8:L:17:PHE:CD2	2.90	0.50
12:2:226:GLU:OE1	12:2:283:ARG:NH1	2.36	0.50
14:4:145:LEU:HD21	14:4:171:THR:HG21	1.94	0.50
15:5:160:ARG:NE	15:5:241:GLU:OE1	2.45	0.50
26:R:59:LEU:O	26:R:63:LEU:HD23	2.11	0.50
32:a:97:PHE:O	32:a:101:LEU:HD23	2.12	0.50
34:c:7:ASP:HB3	34:c:10:ALA:HB2	1.93	0.50
2:B:120:ASP:HB2	2:B:159:TYR:HD1	1.77	0.50
3:C:95:HIS:HD1	47:C:601:UQ9:C4	2.25	0.50
9:S:191:ILE:HG21	35:d:35:PHE:CE1	2.47	0.50
11:1:26:GLU:OE2	11:1:232:TYR:OH	2.20	0.50
14:4:237:GLU:OE1	14:4:237:GLU:N	2.45	0.50
16:6:15:LEU:HD23	48:6:202:3PE:C3F	2.42	0.50
28:W:95:ILE:HG12	42:9:71:LEU:HD22	1.94	0.50
3:C:184:LEU:HD23	3:C:210:ARG:HG2	1.94	0.50
3:C:197:VAL:HG21	3:C:271:TRP:CZ3	2.47	0.50
9:S:53:GLU:O	9:S:57:LEU:HG	2.12	0.50
14:4:199:LEU:HD21	35:d:23:VAL:HG11	1.93	0.50
56:O:201:ZMP:H14	24:P:66:VAL:CG2	2.42	0.50
25:Q:112:ALA:HB3	26:R:20:ARG:NH1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:215:ILE:O	15:5:219:LEU:HG	2.12	0.49
15:5:315:MET:SD	15:5:399:ILE:HG21	2.52	0.49
15:5:652:ILE:HD11	21:J:71:PHE:CE1	2.47	0.49
20:F:68:ARG:NE	20:F:72:GLU:OE1	2.39	0.49
21:J:155:VAL:HG22	21:J:167:VAL:HG12	1.93	0.49
56:O:201:ZMP:H17	24:P:64:ARG:HD2	1.94	0.49
27:U:76:THR:HG21	28:W:79:ARG:NH1	2.26	0.49
35:d:7:PRO:HG2	35:d:32:ARG:CZ	2.42	0.49
1:A:664:PRO:O	37:f:14:GLN:NE2	2.44	0.49
8:L:30:GLU:OE2	8:L:67:SER:OG	2.30	0.49
11:1:107:LEU:HG	16:6:57:LEU:HB3	1.94	0.49
12:2:231:LEU:O	12:2:234:ILE:HG22	2.11	0.49
12:2:307:PHE:HB2	12:2:464:PHE:CZ	2.48	0.49
14:4:363:LYS:NZ	14:4:435:ILE:O	2.38	0.49
16:6:54:ILE:CD1	16:6:147:LEU:HB2	2.42	0.49
19:E:215:ASP:OD1	19:E:216:ARG:N	2.45	0.49
21:J:64:SER:OG	21:J:67:VAL:HG22	2.12	0.49
28:W:96:MET:HE2	28:W:96:MET:HA	1.92	0.49
32:a:62:ASP:HA	32:a:79:MET:HG3	1.94	0.49
38:h:74:GLU:HG2	38:h:75:PRO:O	2.12	0.49
11:1:66:LYS:HG3	11:1:67:GLU:HG3	1.94	0.49
14:4:228:HIS:HB2	14:4:307:ILE:HD13	1.94	0.49
15:5:236:LEU:CD1	15:5:251:HIS:CE1	2.95	0.49
16:6:55:PHE:CE1	16:6:146:LEU:HD21	2.47	0.49
24:P:91:LYS:HD3	24:P:96:PHE:HA	1.94	0.49
26:R:35:LEU:HA	26:R:38:GLN:OE1	2.13	0.49
42:9:22:PHE:O	42:9:25:CYS:HB2	2.12	0.49
2:B:115:LEU:HD23	2:B:116:VAL:N	2.27	0.49
2:B:148:GLY:O	2:B:152:ASN:N	2.45	0.49
12:2:400:ILE:HD11	54:J:202:LMN:HAZ	1.94	0.49
31:Z:15:VAL:HG23	31:Z:16:GLY:H	1.78	0.49
41:8:56:MET:HE2	41:8:56:MET:HA	1.93	0.49
14:4:421:ALA:CB	15:5:175:ARG:HG2	2.42	0.49
23:O:92:ILE:C	23:O:93:LYS:HD3	2.38	0.49
31:Z:15:VAL:HG23	31:Z:16:GLY:N	2.27	0.49
41:8:7:LEU:HD13	41:8:25:ARG:HA	1.94	0.49
2:B:210:GLU:OE1	45:B:502:FMN:C8M	2.60	0.49
9:S:108:ILE:HA	14:4:20:TRP:NE1	2.27	0.49
48:4:503:3PE:H3H2	48:4:503:3PE:H2I1	1.95	0.49
15:5:10:ILE:HD13	39:i:44:VAL:HG11	1.94	0.49
26:R:37:ARG:HA	26:R:37:ARG:HH21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:THR:HG22	1:A:371:SER:HB3	1.95	0.49
1:A:377:ASP:HB3	1:A:528:ARG:HH12	1.77	0.49
5:H:199:ASP:HB3	5:H:206:PRO:HD3	1.94	0.49
9:S:67:PRO:O	9:S:129:TYR:OH	2.26	0.49
13:3:4:PHE:O	13:3:8:ILE:HG12	2.13	0.49
23:O:67:LEU:HB2	24:P:57:ARG:NH1	2.27	0.49
8:L:24:LEU:HD11	16:6:24:ILE:HG23	1.95	0.49
11:1:216:PHE:HA	11:1:219:TYR:CD2	2.41	0.49
12:2:137:ILE:HD11	12:2:236:ILE:HG22	1.94	0.49
12:2:264:ALA:HB1	12:2:298:LEU:HD12	1.95	0.49
14:4:441:HIS:HB3	26:R:102:MET:CE	2.42	0.49
15:5:396:LYS:O	15:5:400:ILE:HG12	2.12	0.49
29:X:15:SER:OG	29:X:17:GLY:O	2.30	0.49
35:d:20:HIS:CD2	40:n:70:VAL:HG21	2.47	0.49
1:A:369:LEU:HD12	1:A:635:VAL:HG11	1.95	0.49
2:B:121:GLU:HB3	2:B:129:ASP:OD1	2.13	0.49
4:G:39:ILE:HD13	31:Z:10:PHE:O	2.12	0.49
15:5:112:HIS:CE1	48:5:701:3PE:H112	2.48	0.49
15:5:527:VAL:HA	15:5:530:GLU:HG2	1.94	0.49
18:D:9:LEU:O	18:D:13:ILE:HG12	2.13	0.49
20:F:43:ARG:HB2	20:F:44:PRO:HD3	1.94	0.49
20:F:57:LEU:HD11	20:F:71:ILE:HG22	1.95	0.49
21:J:66:GLY:O	21:J:69:THR:OG1	2.22	0.49
31:Z:139:VAL:HA	31:Z:143:GLU:OE1	2.13	0.49
3:C:200:LEU:HD23	3:C:200:LEU:H	1.78	0.49
3:C:385:PHE:CE2	6:I:135:LEU:HD11	2.48	0.49
5:H:176:PRO:O	5:H:187:ASP:N	2.46	0.49
5:H:189:THR:O	5:H:193:THR:N	2.45	0.49
7:K:93:VAL:HG12	7:K:100:GLN:HB3	1.94	0.49
15:5:364:GLY:HA3	15:5:441:PRO:HA	1.93	0.49
30:Y:51:GLU:HG2	30:Y:55:ASN:OD1	2.13	0.49
3:C:90:GLN:NE2	7:K:79:VAL:HG22	2.27	0.48
6:I:170:ILE:CG2	7:K:156:TYR:HB2	2.43	0.48
10:j:80:PHE:HB2	15:5:190:TYR:CE2	2.47	0.48
12:2:88:TYR:CZ	12:2:332:TYR:CD2	3.01	0.48
12:2:403:ILE:O	12:2:407:LEU:HG	2.13	0.48
14:4:469:GLN:CD	15:5:69:ASN:H	2.21	0.48
15:5:24:ARG:HD3	39:i:14:SER:O	2.13	0.48
15:5:26:LEU:HD12	15:5:26:LEU:N	2.28	0.48
27:U:125:LYS:O	27:U:126:LEU:HD23	2.12	0.48
36:e:40:LEU:O	36:e:44:GLU:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:90:GLU:HA	9:S:93:GLU:OE1	2.13	0.48
9:S:201:GLN:HA	9:S:201:GLN:OE1	2.12	0.48
11:1:201:PRO:O	11:1:302:ARG:HA	2.13	0.48
12:2:288:SER:OG	12:2:413:TYR:OH	2.03	0.48
22:M:81:LEU:HD23	38:h:101:ALA:HB3	1.95	0.48
28:W:92:GLU:OE1	42:9:60:ILE:HG21	2.13	0.48
49:W:401:PLC:HTA1	52:Z:201:CDL:H592	1.95	0.48
35:d:66:LEU:CD1	39:i:68:ASN:HA	2.43	0.48
36:e:28:LYS:HG3	36:e:29:PHE:N	2.28	0.48
2:B:400:ARG:HG2	2:B:484:PRO:HG2	1.95	0.48
5:H:122:TYR:HE2	5:H:205:MET:CE	2.21	0.48
7:K:113:GLN:NE2	11:1:216:PHE:CD1	2.63	0.48
16:6:29:PRO:O	16:6:32:SER:HB3	2.13	0.48
52:g:201:CDL:H411	29:X:83:PHE:CG	2.49	0.48
1:A:284:VAL:HG12	1:A:291:GLU:HB3	1.95	0.48
1:A:640:GLU:HB2	24:P:115:PHE:CD1	2.47	0.48
2:B:269:ARG:NH1	2:B:340:ASP:OD2	2.46	0.48
2:B:309:ILE:HD12	2:B:309:ILE:H	1.78	0.48
5:H:130:THR:O	5:H:133:GLN:HG2	2.13	0.48
10:j:72:TYR:CE1	14:4:275:PRO:HB2	2.48	0.48
14:4:117:LEU:HD23	48:b:502:3PE:H2B1	1.96	0.48
15:5:35:THR:O	15:5:39:ILE:HG12	2.13	0.48
48:5:701:3PE:H111	48:5:701:3PE:H11	1.96	0.48
19:E:24:PHE:CZ	19:E:46:GLY:HA2	2.48	0.48
54:J:202:LMN:HBC	54:J:202:LMN:HBI	1.46	0.48
22:M:89:PHE:CD1	22:M:135:GLU:HG3	2.49	0.48
42:9:56:ARG:O	42:9:59:GLU:HG3	2.13	0.48
14:4:447:THR:OG1	26:R:108:GLU:OE2	2.18	0.48
15:5:30:PHE:CE1	39:i:30:GLY:HA2	2.48	0.48
15:5:240:MET:HE3	15:5:303:ARG:HA	1.96	0.48
15:5:644:PRO:HG3	21:J:78:TYR:CD2	2.48	0.48
40:n:79:LEU:O	40:n:83:MET:HG2	2.13	0.48
41:8:40:ASN:HD22	41:8:46:ALA:CB	2.27	0.48
42:9:56:ARG:HD2	42:9:60:ILE:CD1	2.43	0.48
1:A:411:LEU:HB2	1:A:470:PHE:CE1	2.48	0.48
1:A:486:SER:OG	1:A:524:ARG:HG2	2.13	0.48
10:j:63:PHE:CZ	10:j:67:ILE:HD11	2.49	0.48
12:2:452:PHE:CE1	48:2:503:3PE:H3E2	2.49	0.48
15:5:355:ASN:O	26:R:82:PRO:HG2	2.13	0.48
27:U:14:ASP:OD1	42:9:76:VAL:HG22	2.13	0.48
29:X:36:ARG:HE	29:X:106:ARG:HH12	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:f:74:LYS:O	37:f:78:GLU:OE1	2.32	0.48
1:A:149:MET:HE1	3:C:365:LYS:HA	1.95	0.48
1:A:577:ASP:CG	1:A:578:VAL:H	2.21	0.48
3:C:87:PHE:HB3	3:C:100:LEU:HB3	1.95	0.48
12:2:1:FME:N	12:2:1:FME:SD	2.87	0.48
12:2:20:ASP:HB3	29:X:74:PHE:HZ	1.78	0.48
13:3:42:LEU:HB2	24:P:92:GLN:NE2	2.25	0.48
15:5:226:LYS:HG2	15:5:258:ALA:HB3	1.96	0.48
15:5:383:SER:O	15:5:392:GLY:HA3	2.12	0.48
33:b:32:TYR:CE2	33:b:34:LEU:HB3	2.48	0.48
5:H:151:LYS:HB3	5:H:152:PRO:HD2	1.95	0.48
8:L:11:SER:OG	8:L:28:CYS:CA	2.62	0.48
10:j:49:THR:HB	54:a:201:LMN:H5	1.95	0.48
12:2:8:SER:O	12:2:12:PHE:HD2	1.96	0.48
14:4:207:GLN:HB3	14:4:269:ALA:HB2	1.95	0.48
14:4:459:ILE:HD12	52:n:201:CDL:H551	1.95	0.48
15:5:84:LEU:O	15:5:88:MET:HG2	2.13	0.48
1:A:557:GLU:OE1	1:A:557:GLU:N	2.46	0.48
2:B:211:GLU:OE1	45:B:502:FMN:O2'	2.16	0.48
9:S:184:VAL:O	9:S:187:SER:OG	2.25	0.48
12:2:355:HIS:CD2	12:2:423:ASP:HA	2.49	0.48
15:5:105:GLY:CA	15:5:455:ASN:HD21	2.27	0.48
15:5:552:GLN:HE21	26:R:76:PRO:HB3	1.78	0.48
29:X:51:PRO:HA	29:X:54:ILE:HG22	1.94	0.48
41:8:37:ARG:HA	41:8:40:ASN:OD1	2.14	0.48
1:A:475:LYS:HD3	1:A:508:THR:HG23	1.96	0.48
1:A:505:VAL:HG22	1:A:511:VAL:HG11	1.95	0.48
2:B:316:LEU:O	2:B:331:LYS:HD3	2.14	0.48
9:S:183:MET:HB3	14:4:470:ILE:HG12	1.96	0.48
12:2:352:GLY:HA2	12:2:422:GLN:O	2.14	0.48
13:3:58:LEU:HD21	13:3:110:ALA:HB1	1.96	0.48
15:5:224:MET:HE3	15:5:283:ILE:HG12	1.96	0.48
31:Z:95:THR:O	31:Z:98:LEU:N	2.47	0.48
37:f:82:SER:O	37:f:85:GLU:HG3	2.14	0.48
12:2:146:SER:HB2	12:2:341:TYR:OH	2.14	0.47
13:3:88:PHE:O	13:3:91:VAL:HG12	2.14	0.47
14:4:14:PHE:HD1	14:4:27:PHE:CD1	2.32	0.47
15:5:216:MET:SD	15:5:270:LEU:HD23	2.54	0.47
15:5:618:SER:O	15:5:621:ILE:HG22	2.14	0.47
40:n:90:GLU:N	40:n:90:GLU:OE2	2.45	0.47
1:A:72:ASP:HB2	30:Y:137:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:GLU:OE2	2:B:304:LYS:HG2	2.13	0.47
14:4:99:THR:HA	14:4:244:MET:CE	2.44	0.47
15:5:520:LEU:O	15:5:524:LEU:HD13	2.14	0.47
21:J:80:PHE:O	21:J:84:SER:OG	2.27	0.47
1:A:537:THR:O	37:f:41:LYS:NZ	2.48	0.47
2:B:167:GLU:OE1	2:B:167:GLU:N	2.37	0.47
4:G:162:VAL:HB	24:P:70:SER:HB3	1.96	0.47
5:H:72:MET:HB2	5:H:73:PRO:HD3	1.96	0.47
15:5:236:LEU:HD11	15:5:251:HIS:CE1	2.50	0.47
1:A:120:ASN:O	1:A:124:MET:HG2	2.13	0.47
1:A:231:ASP:OD2	1:A:298:ARG:NH2	2.47	0.47
15:5:354:LEU:HD21	15:5:450:ASN:HB2	1.96	0.47
35:d:83:LEU:CD2	35:d:86:GLN:HE21	2.24	0.47
12:2:73:TYR:HE2	12:2:115:LEU:HD11	1.79	0.47
12:2:304:ASN:OD1	40:n:87:LYS:HE3	2.14	0.47
14:4:471:MET:HE1	52:n:201:CDL:H671	1.96	0.47
15:5:319:ALA:HB3	15:5:328:ALA:HB2	1.95	0.47
15:5:520:LEU:HD12	15:5:521:VAL:N	2.30	0.47
29:X:41:GLY:O	29:X:45:LEU:HG	2.13	0.47
1:A:401:ILE:HB	1:A:603:GLU:OE2	2.14	0.47
1:A:556:ASP:OD2	1:A:702:SER:HB3	2.15	0.47
15:5:24:ARG:O	40:n:14:VAL:HG21	2.14	0.47
15:5:391:THR:CG2	15:5:473:GLY:H	2.24	0.47
16:6:133:ILE:HD12	28:W:117:ALA:HA	1.95	0.47
24:P:68:ASP:O	24:P:72:GLN:HG3	2.14	0.47
26:R:84:PHE:HB3	26:R:85:PRO:HD2	1.95	0.47
36:e:41:ARG:NH1	36:e:44:GLU:OE1	2.48	0.47
38:h:31:LYS:HB3	38:h:31:LYS:HE2	1.75	0.47
38:h:39:ASP:OD1	38:h:43:ASN:HB2	2.14	0.47
1:A:413:VAL:HG12	1:A:488:ILE:CD1	2.45	0.47
2:B:134:ARG:HH11	2:B:135:LYS:HE3	1.80	0.47
3:C:143:ASP:HB2	3:C:463:GLU:HG3	1.97	0.47
3:C:424:LYS:HZ3	3:C:426:LYS:HB2	1.79	0.47
4:G:84:LYS:HA	20:F:126:LEU:HA	1.96	0.47
4:G:116:THR:N	20:F:110:GLU:OE1	2.47	0.47
15:5:267:ALA:HA	15:5:270:LEU:HD12	1.97	0.47
48:5:702:3PE:O22	32:a:82:PRO:HG3	2.14	0.47
48:6:202:3PE:H3D1	48:6:202:3PE:H3G2	1.54	0.47
54:J:202:LMN:HBKA	54:J:202:LMN:HBR	1.42	0.47
25:Q:94:GLU:CB	34:c:9:TRP:HZ2	2.27	0.47
29:X:23:ASP:CG	29:X:164:HIS:HD1	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:89:ALA:O	29:X:93:ARG:HG3	2.15	0.47
29:X:106:ARG:NH1	29:X:107:GLU:OE2	2.47	0.47
40:n:28:SER:O	40:n:32:VAL:HG23	2.14	0.47
1:A:302:ASP:OD1	1:A:707:SER:HB3	2.15	0.47
1:A:480:PRO:O	1:A:516:TRP:NE1	2.32	0.47
3:C:152:GLN:O	3:C:156:LEU:HG	2.14	0.47
8:L:11:SER:OG	8:L:28:CYS:O	2.32	0.47
11:1:26:GLU:OE1	11:1:199:ARG:NH1	2.45	0.47
11:1:78:LEU:HD11	13:3:16:PHE:CD1	2.50	0.47
13:3:63:PHE:HE2	16:6:66:ALA:HA	1.80	0.47
14:4:133:ASP:OD1	14:4:136:SER:OG	2.31	0.47
26:R:5:VAL:HG11	26:R:8:SER:HB3	1.97	0.47
42:9:61:GLU:HG3	42:9:65:LYS:HE3	1.97	0.47
48:I:501:3PE:H242	11:1:303:PHE:HZ	1.80	0.47
11:1:152:SER:HB2	11:1:320:LEU:HD13	1.97	0.47
16:6:163:LEU:HD13	52:X:201:CDL:H421	1.97	0.47
24:P:92:GLN:HB2	24:P:95:GLN:OE1	2.14	0.47
52:X:201:CDL:HB4	52:X:201:CDL:H512	1.75	0.47
52:n:201:CDL:H342	52:n:201:CDL:H111	1.97	0.47
1:A:168:GLU:OE2	5:H:34:ARG:NH2	2.47	0.47
2:B:409:ARG:NH2	2:B:412:ASP:OD2	2.48	0.47
3:C:61:ASP:CG	12:2:278:GLN:HE22	2.23	0.47
3:C:123:THR:HG23	3:C:138:TYR:CD1	2.49	0.47
11:1:281:ALA:O	11:1:284:ILE:HG22	2.14	0.47
14:4:152:ILE:HD12	14:4:167:VAL:HG11	1.97	0.47
15:5:372:TYR:O	15:5:375:ILE:HG22	2.15	0.47
20:F:121:LYS:HG2	20:F:123:TRP:CZ2	2.50	0.47
2:B:252:VAL:O	2:B:256:ILE:HG13	2.15	0.46
3:C:194:ALA:HB1	3:C:199:ALA:HB3	1.96	0.46
4:G:224:TRP:NE1	4:G:226:GLU:OE2	2.35	0.46
9:S:73:PHE:CZ	9:S:91:LEU:HD23	2.50	0.46
9:S:165:VAL:O	9:S:169:TYR:HB2	2.14	0.46
10:j:11:GLN:NE2	12:2:430:ASN:CB	2.69	0.46
11:1:118:PHE:CE2	16:6:37:ILE:CD1	2.98	0.46
11:1:190:PHE:HE2	11:1:296:VAL:HG21	1.80	0.46
49:1:404:PLC:H1'1	49:1:404:PLC:H2	1.47	0.46
12:2:316:TYR:CD2	12:2:316:TYR:C	2.93	0.46
12:2:418:ASN:ND2	14:4:161:GLU:OE2	2.35	0.46
12:2:465:ASN:O	12:2:469:ASN:HB2	2.15	0.46
15:5:58:ASN:HB3	39:i:54:ARG:NH2	2.30	0.46
15:5:123:PHE:HE2	15:5:254:THR:HG21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:6:27:LYS:HD2	16:6:28:ASN:HB2	1.96	0.46
17:g:9:TRP:NE1	52:g:201:CDL:HA31	2.29	0.46
19:E:276:VAL:HG23	19:E:344:MET:HE1	1.96	0.46
26:R:38:GLN:HA	26:R:41:VAL:HG22	1.97	0.46
52:X:201:CDL:H511	52:X:201:CDL:H142	1.96	0.46
2:B:341:PHE:CE1	2:B:351:LEU:HB2	2.50	0.46
3:C:325:MET:HE2	3:C:325:MET:HB3	1.81	0.46
11:1:122:LEU:HD21	16:6:34:LEU:HD21	1.97	0.46
12:2:292:ASN:OD1	12:2:312:TYR:OH	2.33	0.46
14:4:139:ILE:HG22	14:4:140:LEU:HD12	1.97	0.46
15:5:42:THR:O	15:5:46:THR:HG23	2.15	0.46
15:5:123:PHE:HE2	15:5:254:THR:CG2	2.28	0.46
15:5:395:THR:OG1	15:5:396:LYS:N	2.48	0.46
15:5:476:LEU:HA	15:5:479:ILE:HD13	1.98	0.46
19:E:149:ARG:HG3	19:E:193:ILE:HD11	1.97	0.46
23:O:97:GLN:HA	23:O:100:GLU:CG	2.44	0.46
38:h:124:LYS:HB2	38:h:125:PRO:HD2	1.96	0.46
42:9:32:LYS:HB2	42:9:32:LYS:HE3	1.75	0.46
42:9:56:ARG:CD	42:9:60:ILE:HD11	2.45	0.46
3:C:371:ARG:NH2	6:I:182:ASP:OD1	2.48	0.46
6:I:70:ALA:HB2	17:g:21:HIS:NE2	2.29	0.46
6:I:107:LYS:HB3	38:h:81:LEU:HD23	1.97	0.46
7:K:208:TYR:HA	19:E:136:LYS:NZ	2.30	0.46
12:2:8:SER:O	12:2:12:PHE:CD2	2.68	0.46
12:2:396:TYR:O	12:2:399:SER:OG	2.26	0.46
14:4:387:PRO:HD3	15:5:144:GLU:CD	2.40	0.46
15:5:316:MET:CG	15:5:331:HIS:HD2	2.28	0.46
19:E:210:ASP:OD2	19:E:213:PHE:HB3	2.15	0.46
19:E:291:LYS:HZ2	19:E:295:GLN:HG3	1.80	0.46
35:d:8:GLU:OE1	35:d:8:GLU:HA	2.14	0.46
1:A:562:ASP:OD1	1:A:563:ILE:HG12	2.15	0.46
8:L:19:ARG:CZ	15:5:619:MET:HE1	2.45	0.46
19:E:208:ARG:HB3	19:E:209:GLU:OE1	2.15	0.46
36:e:21:ALA:HA	36:e:24:ARG:HH12	1.79	0.46
6:I:187:THR:HG22	6:I:218:LEU:HD21	1.97	0.46
6:I:205:GLU:HG3	38:h:120:TYR:OH	2.15	0.46
11:1:72:ILE:HG13	11:1:125:TRP:CZ3	2.48	0.46
11:1:320:LEU:HD23	11:1:320:LEU:HA	1.72	0.46
19:E:127:ASN:HD21	19:E:165:HIS:HA	1.81	0.46
21:J:195:GLU:OE1	21:J:195:GLU:HA	2.16	0.46
26:R:101:ILE:O	26:R:101:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:123:ARG:HA	41:8:65:ARG:HE	1.80	0.46
33:b:3:LEU:O	33:b:7:LEU:HG	2.15	0.46
36:e:51:GLY:C	36:e:52:LEU:HD12	2.40	0.46
1:A:667:PHE:CE2	37:f:46:GLU:OE2	2.68	0.46
2:B:128:LYS:HG3	2:B:129:ASP:N	2.30	0.46
3:C:113:ASP:O	3:C:115:HIS:HD2	1.98	0.46
14:4:103:ASN:O	14:4:115:TYR:OH	2.32	0.46
15:5:19:PRO:HB2	15:5:118:SER:HB3	1.97	0.46
15:5:103:SER:O	15:5:107:MET:HB2	2.16	0.46
15:5:105:GLY:HA2	15:5:455:ASN:HD21	1.80	0.46
15:5:164:MET:HB2	15:5:164:MET:HE3	1.45	0.46
19:E:133:TYR:CE2	19:E:307:PRO:HB3	2.51	0.46
19:E:260:GLU:HG2	19:E:323:ILE:HG23	1.97	0.46
25:Q:65:SER:HB3	34:c:12:ARG:CD	2.45	0.46
38:h:65:GLU:N	38:h:65:GLU:OE2	2.48	0.46
1:A:408:ASP:OD2	1:A:477:ALA:HB1	2.15	0.46
3:C:168:LEU:HD12	3:C:168:LEU:HA	1.67	0.46
5:H:160:LEU:HD23	5:H:161:PHE:CE1	2.50	0.46
25:Q:115:ILE:HG13	25:Q:115:ILE:O	2.15	0.46
29:X:51:PRO:O	29:X:54:ILE:HG22	2.15	0.46
29:X:58:GLU:OE1	29:X:63:VAL:HG23	2.15	0.46
1:A:111:THR:OG1	1:A:114:VAL:HG23	2.15	0.46
1:A:285:HIS:CE1	1:A:288:VAL:HG23	2.51	0.46
1:A:359:MET:HE1	1:A:527:SER:HB2	1.98	0.46
2:B:61:TRP:CD2	2:B:183:LEU:HD23	2.51	0.46
48:I:501:3PE:H2A2	48:I:501:3PE:H272	1.40	0.46
7:K:139:PRO:HG2	11:1:60:LYS:HZ2	1.81	0.46
13:3:33:GLU:OE2	19:E:208:ARG:NH1	2.45	0.46
48:6:202:3PE:H381	48:6:202:3PE:H351	1.59	0.46
24:P:19:GLN:HA	24:P:22:GLN:OE1	2.16	0.46
26:R:89:LYS:HD2	26:R:92:ARG:NH1	2.31	0.46
27:U:157:PHE:O	27:U:161:ARG:HG3	2.16	0.46
31:Z:97:LEU:HD23	31:Z:97:LEU:HA	1.80	0.46
2:B:52:LEU:O	2:B:56:ARG:HG2	2.16	0.46
2:B:270:GLU:C	2:B:272:ASN:H	2.24	0.46
2:B:344:LEU:HA	2:B:344:LEU:HD23	1.62	0.46
5:H:59:ILE:HD11	5:H:67:LYS:CD	2.46	0.46
7:K:34:PRO:HD2	19:E:181:HIS:HB2	1.98	0.46
7:K:47:LEU:HG	19:E:111:ASN:HD22	1.81	0.46
15:5:16:TRP:CD1	15:5:122:MET:HB2	2.51	0.46
15:5:127:MET:HG2	15:5:254:THR:OG1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:g:71:GLN:O	17:g:72:LEU:HB2	2.16	0.46
19:E:170:ASN:HD21	19:E:321:GLN:HA	1.81	0.46
21:J:27:GLY:C	21:J:31:GLN:HE22	2.24	0.46
35:d:39:GLU:OE2	35:d:39:GLU:HA	2.15	0.46
37:f:53:ILE:HD13	37:f:67:GLY:HA2	1.97	0.46
2:B:48:TYR:CD1	5:H:232:PRO:HD3	2.51	0.46
7:K:80:THR:O	7:K:81:PHE:C	2.59	0.46
11:1:139:SER:HB3	11:1:205:THR:HG23	1.98	0.46
12:2:377:LEU:HD11	48:4:502:3PE:H2F2	1.98	0.46
15:5:22:PHE:HB3	15:5:26:LEU:CD1	2.45	0.46
15:5:266:SER:O	15:5:270:LEU:HG	2.16	0.46
15:5:397:ASP:O	15:5:401:GLU:HG2	2.16	0.46
15:5:500:PHE:HZ	41:8:54:TYR:CE2	2.34	0.46
23:O:86:ASP:OD1	23:O:86:ASP:N	2.49	0.46
1:A:69:CYS:O	1:A:191:ARG:NH2	2.36	0.45
1:A:305:LYS:HA	38:h:127:ILE:HD12	1.97	0.45
2:B:47:ASN:OD1	2:B:48:TYR:N	2.49	0.45
3:C:427:ILE:HB	3:C:466:ARG:HD2	1.98	0.45
6:I:170:ILE:HG21	7:K:156:TYR:HB2	1.98	0.45
7:K:99:ASP:OD1	11:1:36:ARG:HD2	2.16	0.45
7:K:138:MET:HE3	7:K:142:ARG:HB2	1.98	0.45
12:2:469:ASN:HD21	40:n:87:LYS:HB2	1.81	0.45
14:4:469:GLN:HG2	15:5:67:TYR:O	2.16	0.45
20:F:79:LYS:HA	20:F:82:VAL:HG12	1.98	0.45
27:U:71:GLU:O	27:U:75:VAL:HG23	2.15	0.45
32:a:132:LYS:HA	32:a:132:LYS:HE3	1.98	0.45
52:n:201:CDL:H631	52:n:201:CDL:H602	1.57	0.45
1:A:654:PRO:HB3	37:f:50:VAL:HG11	1.98	0.45
2:B:123:GLU:HB2	46:B:503:NAI:H42N	1.99	0.45
2:B:303:GLU:CD	2:B:304:LYS:HG2	2.40	0.45
11:1:168:THR:O	11:1:172:THR:HG23	2.17	0.45
11:1:327:ILE:HB	11:1:328:PRO:HD3	1.97	0.45
14:4:141:PHE:HD2	14:4:142:GLU:OE1	1.98	0.45
17:g:61:SER:HB3	40:n:111:ILE:O	2.16	0.45
19:E:38:LYS:HG3	22:M:24:TYR:HB3	1.97	0.45
22:M:30:GLU:HG2	22:M:30:GLU:O	2.16	0.45
26:R:6:PRO:HB3	26:R:54:SER:HA	1.98	0.45
32:a:34:GLU:CG	32:a:35:PRO:HD3	2.45	0.45
32:a:124:GLU:HB2	32:a:148:SER:C	2.41	0.45
3:C:305:ILE:HB	3:C:404:GLU:HB2	1.99	0.45
3:C:318:ASP:O	3:C:349:GLN:NE2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:76:PHE:HB3	7:K:105:ILE:HG12	1.99	0.45
9:S:142:VAL:HG12	9:S:143:LYS:N	2.32	0.45
11:1:101:GLU:OE1	11:1:165:ASN:ND2	2.28	0.45
11:1:206:GLU:HB2	11:1:216:PHE:HE2	1.81	0.45
14:4:25:LYS:HD2	14:4:104:TRP:CZ3	2.52	0.45
14:4:80:GLY:HA3	14:4:132:LEU:HD11	1.97	0.45
14:4:233:VAL:O	14:4:236:SER:N	2.49	0.45
15:5:327:LEU:HD11	15:5:398:ILE:HG23	1.97	0.45
15:5:385:MET:SD	15:5:430:MET:HE3	2.56	0.45
16:6:70:LEU:HD23	16:6:70:LEU:HA	1.61	0.45
19:E:213:PHE:CD2	19:E:214:LEU:N	2.82	0.45
24:P:24:ARG:HH11	24:P:24:ARG:HG2	1.79	0.45
31:Z:146:THR:HG23	31:Z:148:ASN:H	1.82	0.45
34:c:20:ASN:HA	34:c:25:ASN:ND2	2.31	0.45
41:8:61:ASP:HA	41:8:64:ARG:HE	1.81	0.45
1:A:405:GLU:OE2	1:A:427:ARG:HD2	2.17	0.45
2:B:96:LEU:HG	2:B:100:PHE:CZ	2.51	0.45
7:K:184:SER:O	7:K:188:MET:HG3	2.16	0.45
9:S:66:LEU:HD22	9:S:91:LEU:HD11	1.99	0.45
10:j:7:SER:O	10:j:10:ILE:HG22	2.17	0.45
11:1:161:VAL:HG13	11:1:172:THR:HG21	1.99	0.45
13:3:66:PHE:O	13:3:70:ILE:HG12	2.17	0.45
48:4:502:3PE:H2H1	48:4:502:3PE:H2E2	1.53	0.45
19:E:131:ARG:HG3	19:E:133:TYR:H	1.81	0.45
21:J:61:PHE:HA	21:J:64:SER:HB2	1.98	0.45
30:Y:65:LYS:HD3	30:Y:66:PRO:HD2	1.98	0.45
38:h:15:VAL:HG22	38:h:19:SER:HB3	1.98	0.45
2:B:43:ASN:HD21	2:B:49:GLY:C	2.24	0.45
2:B:131:GLU:HG3	2:B:289:THR:HG21	1.98	0.45
3:C:447:LEU:HB3	3:C:448:PRO:HD3	1.97	0.45
5:H:55:ALA:HA	5:H:58:VAL:HG12	1.99	0.45
5:H:144:VAL:HG11	5:H:163:LEU:HD13	1.99	0.45
13:3:74:LEU:HB3	13:3:75:PRO:HD3	1.98	0.45
14:4:92:THR:HA	14:4:249:LEU:HD21	1.97	0.45
16:6:1:FME:H	16:6:1:FME:HG2	1.52	0.45
24:P:52:ILE:O	24:P:56:ILE:HG13	2.15	0.45
56:Q:201:ZMP:H3	26:R:69:HIS:CE1	2.52	0.45
34:c:8:PRO:O	34:c:11:ARG:NH1	2.48	0.45
1:A:128:ASN:ND2	2:B:389:GLU:OE1	2.50	0.45
2:B:290:VAL:HG21	2:B:305:HIS:CD2	2.51	0.45
11:1:329:SER:O	11:1:333:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:219:MET:HE2	14:4:280:ILE:HD13	1.99	0.45
21:J:89:ARG:NH2	21:J:91:ARG:HH21	2.14	0.45
25:Q:106:GLU:H	26:R:84:PHE:HE2	1.65	0.45
29:X:35:MET:CE	29:X:40:TYR:HE2	2.24	0.45
35:d:58:ASN:HB2	41:8:17:LYS:NZ	2.32	0.45
37:f:78:GLU:OE1	37:f:78:GLU:N	2.46	0.45
45:B:502:FMN:H9	45:B:502:FMN:H1'1	1.75	0.45
3:C:170:GLY:O	3:C:174:ARG:HG3	2.17	0.45
3:C:182:ARG:HG2	3:C:186:HIS:CE1	2.51	0.45
11:1:77:PRO:HB3	11:1:227:PHE:CE2	2.52	0.45
49:1:404:PLC:H1'2	28:W:46:TYR:HA	1.98	0.45
12:2:226:GLU:OE1	12:2:283:ARG:HD2	2.17	0.45
14:4:291:ALA:O	14:4:295:GLN:NE2	2.31	0.45
15:5:316:MET:HE3	15:5:316:MET:HB2	1.82	0.45
15:5:616:MET:HE1	21:J:50:LEU:HA	1.99	0.45
18:D:77:ASN:HA	27:U:13:GLU:OE2	2.17	0.45
25:Q:78:THR:HA	25:Q:119:GLN:HG2	1.98	0.45
30:Y:41:ALA:O	30:Y:42:HIS:CG	2.70	0.45
41:8:61:ASP:HA	41:8:64:ARG:NE	2.32	0.45
3:C:295:MET:HE3	3:C:295:MET:HB3	1.90	0.45
11:1:211:LEU:O	11:1:212:VAL:C	2.59	0.45
12:2:329:PHE:C	12:2:331:ILE:H	2.24	0.45
12:2:403:ILE:HG23	14:4:176:LEU:HB3	1.98	0.45
14:4:105:TYR:HD2	14:4:449:ARG:NH2	2.15	0.45
15:5:517:SER:O	15:5:521:VAL:HG12	2.17	0.45
19:E:224:VAL:HA	19:E:287:ILE:O	2.17	0.45
33:b:21:SER:O	33:b:24:ILE:HG22	2.17	0.45
37:f:54:VAL:HG12	37:f:68:LEU:HD11	1.97	0.45
1:A:125:MET:HE3	1:A:125:MET:HB2	1.72	0.45
2:B:187:ASP:OD2	2:B:190:GLY:HA2	2.17	0.45
3:C:142:LEU:HA	3:C:142:LEU:HD23	1.70	0.45
15:5:116:PHE:O	15:5:120:LEU:HD23	2.17	0.45
15:5:298:SER:HB2	15:5:304:ILE:CD1	2.46	0.45
19:E:244:ALA:HB2	19:E:330:PHE:HE1	1.82	0.45
19:E:309:TYR:HE2	19:E:314:VAL:HG22	1.82	0.45
22:M:21:ILE:HD11	22:M:58:LYS:HD2	1.98	0.45
56:O:201:ZMP:HN2	24:P:64:ARG:HA	1.82	0.45
24:P:32:PHE:CZ	24:P:83:TYR:HB2	2.52	0.45
24:P:89:PHE:CD2	24:P:89:PHE:O	2.70	0.45
32:a:121:ILE:HG23	41:8:65:ARG:HD2	1.99	0.45
40:n:9:GLU:CD	40:n:10:LEU:N	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:291:LEU:O	3:C:296:LEU:HD12	2.16	0.45
5:H:65:GLN:CG	5:H:66:TYR:CD2	2.96	0.45
9:S:202:ARG:NH1	9:S:232:ASP:HA	2.32	0.45
11:1:252:SER:HB3	11:1:281:ALA:HB2	1.98	0.45
48:4:503:3PE:H2A2	48:4:503:3PE:H271	1.60	0.45
15:5:472:ALA:HA	15:5:475:ILE:HG22	1.99	0.45
15:5:541:LYS:HE2	26:R:72:GLU:O	2.16	0.45
17:g:2:ILE:HG22	17:g:3:ASN:N	2.32	0.45
18:D:24:ALA:HA	18:D:27:VAL:HG12	1.98	0.45
19:E:227:ASN:HB2	19:E:318:PHE:CE1	2.52	0.45
19:E:309:TYR:CE2	19:E:314:VAL:HG22	2.52	0.45
19:E:314:VAL:O	19:E:317:GLN:HB2	2.17	0.45
23:O:83:GLU:OE1	24:P:34:ARG:NH1	2.50	0.45
5:H:195:LYS:HA	5:H:198:GLU:OE1	2.18	0.44
11:1:72:ILE:HD11	48:6:202:3PE:H31	1.98	0.44
12:2:375:PRO:HB3	12:2:380:PHE:CD2	2.52	0.44
12:2:394:GLY:HA2	12:2:396:TYR:CE1	2.53	0.44
17:g:62:TYR:HB2	28:W:70:MET:HE1	1.99	0.44
19:E:155:VAL:HG13	19:E:160:ILE:HB	1.99	0.44
22:M:93:ASN:OD1	22:M:94:THR:HG23	2.18	0.44
37:f:5:LEU:O	37:f:40:THR:HG22	2.16	0.44
3:C:137:PRO:HB2	7:K:156:TYR:OH	2.18	0.44
7:K:80:THR:CG2	7:K:107:PHE:HB3	2.41	0.44
12:2:214:ILE:HG21	12:2:297:MET:HE2	2.00	0.44
15:5:335:HIS:HA	15:5:338:PHE:CE2	2.53	0.44
15:5:415:TYR:HD1	15:5:416:TRP:HD1	1.64	0.44
15:5:519:ILE:O	15:5:523:ILE:HG12	2.17	0.44
2:B:72:ASP:HA	2:B:75:ILE:HD13	2.00	0.44
2:B:276:LYS:HE3	2:B:276:LYS:HB3	1.84	0.44
9:S:87:GLU:HA	9:S:90:GLU:OE1	2.18	0.44
9:S:154:ILE:O	9:S:156:ARG:N	2.51	0.44
13:3:33:GLU:CD	19:E:208:ARG:HH12	2.24	0.44
14:4:233:VAL:O	14:4:234:VAL:C	2.59	0.44
15:5:425:THR:HG23	15:5:428:TYR:CZ	2.52	0.44
15:5:438:TYR:HB3	34:c:27:PHE:HE2	1.81	0.44
15:5:530:GLU:HG3	15:5:531:PHE:CD1	2.42	0.44
15:5:540:ASN:HB3	15:5:543:ILE:HD12	1.99	0.44
21:J:31:GLN:O	21:J:35:VAL:HG23	2.17	0.44
26:R:74:ARG:HH12	32:a:87:HIS:HA	1.82	0.44
1:A:582:PHE:CE1	38:h:135:LYS:HD2	2.45	0.44
2:B:75:ILE:O	2:B:79:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:78:PHE:O	48:I:501:3PE:H382	2.17	0.44
8:L:46:LEU:HD23	8:L:46:LEU:HA	1.81	0.44
9:S:119:TYR:HD2	14:4:20:TRP:CE3	2.32	0.44
48:4:501:3PE:H3C2	48:4:501:3PE:H391	1.76	0.44
15:5:129:ILE:HD13	15:5:129:ILE:HA	1.85	0.44
15:5:486:ASP:OD1	41:8:42:TYR:OH	2.34	0.44
22:M:19:LYS:HA	22:M:31:ILE:O	2.18	0.44
23:O:35:ARG:O	23:O:39:VAL:HG23	2.17	0.44
26:R:81:PRO:HD2	26:R:81:PRO:O	2.17	0.44
26:R:92:ARG:HH21	26:R:92:ARG:HG2	1.83	0.44
35:d:61:GLU:HG3	35:d:62:ASP:N	2.32	0.44
36:e:21:ALA:HA	36:e:24:ARG:CZ	2.48	0.44
1:A:166:SER:OG	22:M:94:THR:HG22	2.17	0.44
4:G:229:ARG:HD3	4:G:229:ARG:HA	1.76	0.44
11:1:22:LEU:HD13	11:1:290:MET:CE	2.48	0.44
12:2:27:LEU:HD11	29:X:50:LEU:HD21	2.00	0.44
12:2:409:SER:HA	12:2:412:TYR:CE1	2.52	0.44
14:4:178:MET:HB2	14:4:217:ALA:CB	2.46	0.44
14:4:297:ASP:HB3	14:4:300:VAL:HB	1.99	0.44
48:4:502:3PE:H341	48:4:502:3PE:H372	1.82	0.44
15:5:369:TYR:CE2	36:e:17:PRO:HG3	2.53	0.44
37:f:11:HIS:CD2	37:f:55:PHE:CE1	3.05	0.44
1:A:401:ILE:HG12	1:A:424:MET:HE3	2.00	0.44
11:1:264:ASN:O	27:U:161:ARG:NH2	2.49	0.44
14:4:138:TYR:O	14:4:142:GLU:HG2	2.18	0.44
15:5:289:LEU:O	15:5:293:LEU:HG	2.18	0.44
15:5:327:LEU:HD21	15:5:399:ILE:HA	2.00	0.44
19:E:228:LYS:HB2	19:E:230:GLN:HG3	1.99	0.44
27:U:150:ILE:HD11	28:W:55:ARG:HG2	1.99	0.44
29:X:8:VAL:HG12	29:X:163:TYR:CZ	2.53	0.44
29:X:92:ALA:O	29:X:96:LEU:HD23	2.17	0.44
48:b:502:3PE:H322	48:b:502:3PE:H221	2.00	0.44
1:A:359:MET:HE1	1:A:527:SER:O	2.18	0.44
2:B:257:LEU:O	5:H:240:GLN:OE1	2.36	0.44
3:C:90:GLN:OE1	7:K:81:PHE:HD1	2.01	0.44
3:C:150:ASN:O	3:C:153:VAL:HG12	2.17	0.44
48:4:501:3PE:N	48:b:502:3PE:H112	2.33	0.44
15:5:344:MET:C	15:5:462:MET:HE2	2.41	0.44
15:5:374:TYR:O	15:5:378:THR:OG1	2.32	0.44
15:5:456:ILE:HD12	15:5:459:THR:OG1	2.17	0.44
19:E:173:ILE:HG23	19:E:185:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:J:93:ASP:HA	54:J:202:LMN:H6	2.00	0.44
25:Q:91:ASP:O	25:Q:95:VAL:HG23	2.17	0.44
26:R:35:LEU:O	26:R:39:LYS:HD3	2.18	0.44
29:X:103:GLU:OE1	29:X:104:ASN:N	2.51	0.44
33:b:37:VAL:O	33:b:41:VAL:HG23	2.17	0.44
1:A:236:GLY:O	1:A:239:THR:HG23	2.17	0.44
3:C:258:LEU:HD21	3:C:340:PHE:CG	2.53	0.44
10:j:17:LYS:HD2	10:j:17:LYS:HA	1.38	0.44
11:1:86:ILE:HD12	13:3:8:ILE:HD13	1.99	0.44
12:2:264:ALA:O	12:2:268:LEU:HD23	2.18	0.44
16:6:42:ILE:HD11	48:6:202:3PE:C3E	2.47	0.44
19:E:339:GLU:HB3	19:E:341:PRO:HD2	2.00	0.44
25:Q:85:LEU:HB3	25:Q:87:LEU:CD2	2.48	0.44
26:R:12:LYS:HE2	26:R:12:LYS:HB2	1.72	0.44
30:Y:79:ARG:HD2	30:Y:111:LYS:HZ2	1.83	0.44
30:Y:90:ARG:HA	30:Y:100:SER:O	2.18	0.44
33:b:29:ALA:HB2	48:b:502:3PE:O14	2.18	0.44
1:A:712:LYS:HE2	1:A:712:LYS:HB2	1.67	0.44
10:j:83:LYS:HD3	10:j:83:LYS:HA	1.76	0.44
12:2:436:SER:OG	12:2:439:LEU:HD13	2.17	0.44
15:5:20:LEU:HD13	48:5:701:3PE:H352	1.98	0.44
15:5:282:TRP:CZ3	32:a:108:SER:HB3	2.52	0.44
15:5:323:SER:HA	15:5:325:TYR:CE2	2.53	0.44
16:6:139:PHE:HA	28:W:70:MET:SD	2.58	0.44
25:Q:66:PHE:CE2	25:Q:87:LEU:HD11	2.53	0.44
25:Q:77:ALA:O	25:Q:119:GLN:HG2	2.18	0.44
27:U:30:ALA:HB1	27:U:34:PRO:HB2	2.00	0.44
27:U:57:ARG:NH1	28:W:78:ASP:OD1	2.51	0.44
1:A:408:ASP:OD1	1:A:409:ALA:N	2.51	0.43
2:B:43:ASN:ND2	2:B:49:GLY:O	2.51	0.43
2:B:61:TRP:HE3	2:B:64:THR:HG21	1.83	0.43
7:K:98:TYR:CE1	7:K:185:GLU:HG3	2.53	0.43
8:L:15:PHE:CE2	15:5:618:SER:HB3	2.53	0.43
14:4:66:PHE:CD1	33:b:9:GLY:HA3	2.53	0.43
14:4:191:THR:HG23	40:n:77:ARG:HD2	2.00	0.43
15:5:143:TRP:CD1	15:5:178:ASP:OD1	2.71	0.43
15:5:232:LEU:HD21	48:5:702:3PE:H391	2.00	0.43
15:5:285:ALA:HA	15:5:318:ILE:HD11	1.98	0.43
42:9:25:CYS:O	42:9:28:LYS:N	2.51	0.43
8:L:16:VAL:HG13	8:L:17:PHE:N	2.32	0.43
14:4:252:LYS:N	14:4:252:LYS:HD2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:418:LEU:HA	15:5:175:ARG:HG3	2.00	0.43
14:4:459:ILE:O	14:4:463:ILE:HG13	2.19	0.43
15:5:388:PRO:HA	15:5:393:TYR:CD1	2.53	0.43
15:5:599:ALA:O	15:5:603:VAL:HG13	2.18	0.43
21:J:32:SER:CB	21:J:79:VAL:HG11	2.49	0.43
25:Q:66:PHE:CD2	25:Q:69:VAL:HG13	2.39	0.43
35:d:40:ALA:O	35:d:44:VAL:HG23	2.18	0.43
39:i:62:SER:HB2	39:i:66:LYS:HZ1	1.82	0.43
42:9:7:SER:HB3	42:9:13:ASN:HA	1.99	0.43
4:G:179:GLU:HG2	4:G:190:PHE:CD2	2.53	0.43
5:H:160:LEU:HD23	5:H:161:PHE:CD1	2.53	0.43
9:S:96:ALA:HB2	9:S:141:PRO:O	2.17	0.43
11:1:130:LYS:HD3	11:1:130:LYS:HA	1.48	0.43
13:3:94:PHE:CD1	16:6:166:ALA:HB2	2.53	0.43
14:4:381:PHE:CE1	15:5:148:VAL:HG22	2.53	0.43
16:6:72:LEU:O	16:6:76:THR:HG23	2.19	0.43
29:X:36:ARG:HE	29:X:106:ARG:NH1	2.17	0.43
41:8:31:VAL:HB	41:8:32:PRO:HD3	1.99	0.43
2:B:431:ASP:HB3	2:B:435:TRP:CZ2	2.53	0.43
3:C:375:LYS:HE2	22:M:109:GLY:O	2.17	0.43
10:j:24:HIS:NE2	10:j:26:LEU:O	2.51	0.43
13:3:39:GLU:HG3	13:3:42:LEU:O	2.17	0.43
14:4:314:ILE:HA	14:4:317:VAL:HG12	2.00	0.43
15:5:230:PHE:H	15:5:287:THR:CG2	2.28	0.43
15:5:425:THR:HG23	15:5:428:TYR:OH	2.18	0.43
25:Q:76:THR:H	25:Q:79:ALA:HB2	1.84	0.43
32:a:118:LYS:CG	41:8:69:MET:HE1	2.47	0.43
34:c:19:THR:HG23	34:c:20:ASN:N	2.34	0.43
37:f:29:GLN:OE1	37:f:29:GLN:N	2.51	0.43
40:n:42:GLU:OE1	40:n:47:HIS:C	2.59	0.43
41:8:30:LEU:HA	41:8:30:LEU:HD23	1.83	0.43
5:H:178:MET:HE3	5:H:180:ILE:HD11	2.00	0.43
11:1:290:MET:HE1	18:D:14:ILE:HD13	1.99	0.43
12:2:265:ILE:HD12	21:J:139:PHE:HD1	1.82	0.43
12:2:364:MET:O	12:2:368:VAL:HG23	2.19	0.43
12:2:427:ILE:O	12:2:428:LEU:C	2.61	0.43
12:2:458:SER:HA	12:2:461:ILE:HG22	2.01	0.43
13:3:60:ALA:C	16:6:70:LEU:HD21	2.43	0.43
15:5:620:LEU:HA	15:5:620:LEU:HD23	1.68	0.43
19:E:127:ASN:C	19:E:127:ASN:HD22	2.14	0.43
19:E:222:CYS:HB2	19:E:287:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:P:10:GLU:OE2	24:P:24:ARG:NH1	2.49	0.43
7:K:79:VAL:C	7:K:80:THR:HG23	2.43	0.43
12:2:1:FME:O1	29:X:154:PRO:HD3	2.19	0.43
15:5:304:ILE:HG13	15:5:432:ILE:HD11	1.99	0.43
18:D:83:GLU:HG2	27:U:9:TRP:HB3	2.01	0.43
19:E:294:TYR:HD2	19:E:314:VAL:HG11	1.84	0.43
23:O:74:VAL:HA	23:O:77:GLU:OE1	2.19	0.43
26:R:12:LYS:O	26:R:16:THR:HG23	2.18	0.43
37:f:4:ALA:N	37:f:8:ILE:CG2	2.82	0.43
38:h:79:PHE:CD2	38:h:85:VAL:HG13	2.53	0.43
38:h:82:GLY:C	38:h:83:TYR:HD2	2.26	0.43
42:9:19:TRP:HB2	42:9:44:TYR:CE1	2.53	0.43
1:A:257:SER:OG	1:A:258:ILE:N	2.40	0.43
2:B:121:GLU:CD	2:B:129:ASP:HB2	2.42	0.43
2:B:446:PRO:O	2:B:450:THR:HG23	2.19	0.43
4:G:81:ALA:HA	20:F:66:VAL:HG13	2.01	0.43
9:S:87:GLU:O	9:S:91:LEU:HD13	2.19	0.43
12:2:375:PRO:HG2	14:4:142:GLU:HB2	2.01	0.43
14:4:293:LEU:HD21	14:4:422:ILE:HG22	2.00	0.43
14:4:298:LEU:O	14:4:302:ILE:HG12	2.19	0.43
26:R:33:ARG:HD3	26:R:33:ARG:C	2.43	0.43
30:Y:120:LYS:HB3	30:Y:120:LYS:HE2	1.80	0.43
32:a:57:TYR:HA	32:a:65:ASN:OD1	2.18	0.43
40:n:65:GLU:OE1	40:n:65:GLU:HA	2.18	0.43
1:A:377:ASP:HB3	1:A:528:ARG:NH1	2.34	0.43
1:A:392:ARG:HD2	1:A:395:TYR:OH	2.18	0.43
1:A:641:ASP:OD1	1:A:642:ALA:N	2.52	0.43
3:C:445:HIS:HB3	3:C:449:ASP:HB2	2.00	0.43
12:2:137:ILE:HG23	12:2:157:TYR:CE2	2.53	0.43
14:4:174:GLY:HA3	14:4:220:VAL:CG2	2.47	0.43
15:5:203:THR:HG22	35:d:67:ALA:HB1	2.00	0.43
26:R:85:PRO:HA	26:R:90:TYR:CE1	2.53	0.43
29:X:118:ARG:NE	29:X:124:GLU:O	2.52	0.43
52:n:201:CDL:H422	52:n:201:CDL:H452	1.73	0.43
42:9:37:CYS:O	42:9:37:CYS:SG	2.77	0.43
1:A:150:ARG:HD3	4:G:254:PRO:HA	2.01	0.43
1:A:215:THR:C	1:A:217:LEU:H	2.27	0.43
8:L:16:VAL:CG2	15:5:619:MET:HA	2.48	0.43
10:j:87:GLU:OE1	10:j:87:GLU:HA	2.19	0.43
14:4:112:ASN:HB3	48:4:502:3PE:H11	2.01	0.43
15:5:327:LEU:HG	15:5:399:ILE:CG1	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:555:VAL:O	15:5:559:ILE:HG12	2.19	0.43
24:P:102:GLU:OE1	24:P:102:GLU:N	2.52	0.43
30:Y:119:ILE:CD1	30:Y:131:ILE:HD11	2.44	0.43
52:Z:201:CDL:H561	52:Z:201:CDL:H591	1.75	0.43
1:A:225:LEU:HD11	1:A:426:ALA:HB2	2.00	0.43
1:A:597:GLY:O	1:A:608:ILE:HD12	2.18	0.43
2:B:298:LEU:HD23	2:B:298:LEU:HA	1.67	0.43
3:C:426:LYS:HD2	4:G:127:THR:HB	2.01	0.43
5:H:66:TYR:HH	30:Y:151:SER:H	1.59	0.43
5:H:204:LYS:NZ	5:H:206:PRO:HA	2.34	0.43
6:I:50:ALA:HB2	20:F:96:GLY:HA2	2.00	0.43
7:K:122:THR:HA	7:K:150:CYS:HB3	2.00	0.43
9:S:84:LYS:O	9:S:87:GLU:HG3	2.18	0.43
9:S:215:GLU:HA	9:S:218:ARG:HD2	2.00	0.43
13:3:43:THR:O	24:P:89:PHE:CE2	2.72	0.43
14:4:92:THR:O	14:4:96:ILE:HG13	2.18	0.43
14:4:366:THR:OG1	14:4:432:THR:O	2.21	0.43
15:5:479:ILE:HG22	15:5:480:TYR:CD1	2.54	0.43
19:E:131:ARG:HD2	19:E:133:TYR:CE2	2.54	0.43
21:J:26:LEU:HD12	21:J:27:GLY:N	2.33	0.43
21:J:26:LEU:O	21:J:30:THR:HG23	2.19	0.43
23:O:33:GLU:O	23:O:36:ILE:HB	2.19	0.43
24:P:89:PHE:O	24:P:89:PHE:CG	2.72	0.43
30:Y:110:MET:HE2	30:Y:110:MET:HB3	1.94	0.43
37:f:67:GLY:C	37:f:68:LEU:HD12	2.44	0.43
1:A:213:ILE:HG13	43:A:802:SF4:S1	2.59	0.42
2:B:124:PRO:HD2	2:B:324:CYS:SG	2.59	0.42
2:B:290:VAL:HG21	2:B:305:HIS:CG	2.54	0.42
11:1:107:LEU:HB2	11:1:164:LEU:HD23	2.01	0.42
11:1:286:LEU:HD23	11:1:286:LEU:HA	1.91	0.42
14:4:237:GLU:N	14:4:237:GLU:CD	2.77	0.42
16:6:157:ASN:O	16:6:158:ASN:ND2	2.52	0.42
19:E:38:LYS:HE3	19:E:38:LYS:HB2	1.83	0.42
19:E:90:LYS:HD3	19:E:104:PHE:CE1	2.54	0.42
19:E:224:VAL:HG13	19:E:289:LEU:HD13	2.01	0.42
21:J:162:THR:HA	54:J:202:LMN:OAT	2.18	0.42
31:Z:117:ALA:HA	31:Z:120:ASN:OD1	2.19	0.42
37:f:13:CYS:SG	37:f:14:GLN:N	2.91	0.42
38:h:82:GLY:C	38:h:83:TYR:CD2	2.97	0.42
1:A:364:ASP:OD2	1:A:648:ARG:NH1	2.52	0.42
2:B:92:PHE:HE2	2:B:100:PHE:HE2	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:256:ASP:O	3:C:260:GLU:HG3	2.19	0.42
7:K:83:LEU:HB2	7:K:121:GLY:HA3	2.00	0.42
9:S:56:GLU:HB3	9:S:118:LEU:HD21	2.00	0.42
14:4:380:SER:OG	14:4:428:THR:HG21	2.19	0.42
19:E:297:TYR:CD2	52:E:403:CDL:H341	2.54	0.42
21:J:174:LEU:HA	21:J:177:GLU:HG2	2.01	0.42
27:U:4:GLU:CD	27:U:4:GLU:H	2.26	0.42
30:Y:60:ILE:HB	30:Y:131:ILE:HD13	2.00	0.42
36:e:57:PRO:HD3	41:8:66:VAL:HG11	2.01	0.42
40:n:82:LYS:HE3	40:n:83:MET:CE	2.49	0.42
2:B:72:ASP:OD1	2:B:73:THR:N	2.51	0.42
2:B:120:ASP:HB2	2:B:159:TYR:CD1	2.54	0.42
2:B:259:ARG:NH1	5:H:238:PHE:HD2	2.16	0.42
2:B:321:PRO:HB2	2:B:344:LEU:HD11	2.01	0.42
5:H:124:LEU:N	5:H:162:THR:O	2.50	0.42
5:H:174:ASN:HD22	5:H:186:GLU:CD	2.24	0.42
6:I:117:GLU:HB2	6:I:192:TYR:CE1	2.54	0.42
11:1:67:GLU:OE2	11:1:128:ASN:ND2	2.52	0.42
54:J:202:LMN:HCS	54:J:202:LMN:CBP	2.43	0.42
25:Q:94:GLU:OE2	26:R:19:TYR:HE2	2.01	0.42
27:U:62:GLY:HA3	28:W:112:LYS:HD2	2.01	0.42
30:Y:119:ILE:HD11	30:Y:131:ILE:CD1	2.44	0.42
32:a:131:TRP:CZ3	32:a:132:LYS:HD2	2.54	0.42
3:C:104:LEU:HD23	3:C:109:ILE:HA	2.02	0.42
4:G:120:TYR:HB3	4:G:144:PHE:HB3	2.02	0.42
12:2:452:PHE:O	12:2:455:ILE:HG12	2.19	0.42
14:4:371:GLN:HB2	14:4:445:ASP:OD2	2.19	0.42
15:5:479:ILE:HG13	41:8:42:TYR:HB3	2.01	0.42
20:F:126:LEU:HD22	31:Z:91:GLN:OE1	2.20	0.42
21:J:163:PHE:HB2	54:J:202:LMN:HCW	2.01	0.42
24:P:82:GLU:HG3	24:P:99:TYR:OH	2.20	0.42
26:R:35:LEU:HD12	26:R:39:LYS:HZ3	1.83	0.42
29:X:109:LYS:HD2	29:X:109:LYS:O	2.19	0.42
37:f:24:GLN:HG3	37:f:73:GLU:OE2	2.18	0.42
41:8:13:MET:SD	41:8:23:ARG:HB3	2.59	0.42
2:B:61:TRP:HA	2:B:64:THR:CG2	2.48	0.42
3:C:429:ALA:HB1	3:C:463:GLU:HB3	2.02	0.42
5:H:215:ARG:HG3	5:H:217:ASP:H	1.84	0.42
8:L:22:ILE:O	8:L:25:ALA:HB3	2.20	0.42
10:j:61:VAL:C	10:j:64:PRO:HD2	2.45	0.42
12:2:232:ILE:HD13	12:2:232:ILE:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:369:MET:HE3	14:4:369:MET:HB2	1.89	0.42
15:5:146:ILE:HD12	15:5:255:LEU:HD12	2.02	0.42
15:5:386:ALA:HB1	15:5:393:TYR:HA	2.00	0.42
15:5:446:ILE:HB	25:Q:58:ARG:NH1	2.34	0.42
15:5:628:LEU:O	15:5:632:VAL:HG23	2.19	0.42
24:P:58:GLN:O	24:P:62:ARG:HG3	2.19	0.42
26:R:34:GLN:NE2	34:c:17:TYR:HE2	2.15	0.42
35:d:35:PHE:HE2	35:d:79:LEU:HD11	1.84	0.42
1:A:252:LEU:HD13	1:A:271:ASP:HB3	2.02	0.42
2:B:70:LYS:HZ2	2:B:74:TRP:CG	2.38	0.42
2:B:203:MET:O	5:H:111:TYR:HB3	2.20	0.42
2:B:363:GLN:HG3	5:H:134:LEU:HD22	2.02	0.42
3:C:424:LYS:NZ	3:C:426:LYS:HB2	2.35	0.42
5:H:102:MET:O	5:H:106:GLU:HG3	2.20	0.42
6:I:216:LEU:HD11	6:I:220:TYR:CZ	2.54	0.42
13:3:125:ILE:HD13	20:F:22:LEU:HA	2.01	0.42
14:4:51:ASN:HD21	14:4:481:ASN:ND2	2.17	0.42
14:4:264:PRO:HG3	14:4:482:TYR:CE1	2.55	0.42
14:4:373:ALA:O	14:4:377:ILE:HG12	2.20	0.42
15:5:530:GLU:OE1	34:c:27:PHE:CE1	2.73	0.42
16:6:38:ALA:O	16:6:42:ILE:HG12	2.20	0.42
19:E:167:SER:O	19:E:202:PRO:HD2	2.20	0.42
27:U:14:ASP:OD2	28:W:84:ARG:NE	2.47	0.42
32:a:48:ALA:HA	32:a:51:LYS:HG3	2.01	0.42
37:f:13:CYS:SG	37:f:16:GLY:N	2.90	0.42
1:A:654:PRO:CB	37:f:50:VAL:HG11	2.48	0.42
2:B:269:ARG:CD	2:B:270:GLU:HG3	2.43	0.42
8:L:66:GLU:HB2	12:2:135:TYR:CZ	2.55	0.42
11:1:4:ASN:OD1	18:D:32:ARG:NH2	2.53	0.42
11:1:102:LEU:HD22	48:6:201:3PE:H2	2.01	0.42
11:1:127:SER:HB3	11:1:218:GLU:HG3	2.00	0.42
11:1:271:PHE:CD2	18:D:30:VAL:HG11	2.54	0.42
12:2:455:ILE:HG22	14:4:60:PHE:CE1	2.55	0.42
15:5:216:MET:CE	15:5:219:LEU:HB2	2.49	0.42
52:g:201:CDL:H241	52:X:201:CDL:H672	2.02	0.42
20:F:73:ASN:HD22	31:Z:149:GLY:C	2.28	0.42
24:P:34:ARG:HE	24:P:34:ARG:HB2	1.68	0.42
25:Q:80:ASN:N	25:Q:84:ASP:OD2	2.36	0.42
41:8:17:LYS:HD3	41:8:17:LYS:HA	1.91	0.42
1:A:273:LYS:HG2	1:A:278:MET:HE3	2.01	0.42
1:A:354:VAL:HG13	1:A:359:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:106:ILE:HB	4:G:107:PRO:HD3	2.02	0.42
4:G:262:ARG:HE	4:G:262:ARG:HB2	1.64	0.42
5:H:198:GLU:CA	5:H:201:LYS:HG3	2.34	0.42
6:I:123:TYR:OH	22:M:110:HIS:HB3	2.19	0.42
6:I:197:ARG:NH2	7:K:168:ASP:OD1	2.52	0.42
8:L:80:LEU:HD11	12:2:145:ASN:O	2.20	0.42
14:4:281:SER:O	14:4:284:THR:HG22	2.19	0.42
15:5:200:ILE:HG22	15:5:269:ILE:HD11	2.02	0.42
15:5:395:THR:O	15:5:399:ILE:HG13	2.20	0.42
19:E:217:MET:HG2	19:E:223:LEU:HD11	2.01	0.42
20:F:46:LEU:HD21	20:F:103:VAL:HG12	2.01	0.42
23:O:65:ASP:N	23:O:68:ASP:HB2	2.35	0.42
25:Q:104:GLY:C	25:Q:105:LEU:HD12	2.44	0.42
35:d:35:PHE:HE2	35:d:79:LEU:HD21	1.85	0.42
35:d:71:LEU:HD23	35:d:71:LEU:HA	1.88	0.42
37:f:75:GLU:OE1	37:f:78:GLU:OE2	2.37	0.42
39:i:24:SER:HB2	40:n:10:LEU:HD21	2.00	0.42
52:n:201:CDL:H741	52:n:201:CDL:H772	1.86	0.42
1:A:498:PHE:HB3	1:A:676:LEU:HD12	2.02	0.42
2:B:284:VAL:HG13	2:B:358:VAL:CG1	2.50	0.42
2:B:414:LEU:O	2:B:418:THR:HG23	2.20	0.42
8:L:16:VAL:HG23	15:5:619:MET:HA	2.01	0.42
9:S:180:LEU:O	9:S:184:VAL:HG23	2.20	0.42
10:j:34:ARG:HH22	32:a:41:PRO:CD	2.29	0.42
15:5:7:LEU:HD21	39:i:45:SER:HB3	2.02	0.42
19:E:213:PHE:HD2	19:E:214:LEU:N	2.11	0.42
25:Q:89:SER:HB3	26:R:12:LYS:HD2	2.02	0.42
27:U:145:LYS:NZ	28:W:54:GLU:OE2	2.32	0.42
52:n:201:CDL:H531	52:n:201:CDL:H561	1.82	0.42
1:A:571:TYR:HB2	1:A:583:ALA:HB2	2.01	0.42
3:C:91:HIS:HE1	11:1:209:SER:O	2.03	0.42
3:C:256:ASP:CG	31:Z:12:LYS:HZ2	2.27	0.42
4:G:65:LEU:HD23	4:G:65:LEU:HA	1.91	0.42
5:H:52:MET:O	5:H:55:ALA:N	2.52	0.42
5:H:56:GLU:O	5:H:59:ILE:HG22	2.19	0.42
5:H:68:LYS:HA	5:H:97:LEU:HD13	2.02	0.42
5:H:75:LEU:HB3	5:H:114:TYR:CE1	2.55	0.42
9:S:135:ARG:HD2	26:R:103:GLN:HG3	2.02	0.42
11:1:213:ALA:HB1	11:1:216:PHE:CE1	2.54	0.42
12:2:108:LEU:HD23	12:2:108:LEU:HA	1.73	0.42
48:4:503:3PE:H3F1	48:4:503:3PE:H3C1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:34:MET:HE3	15:5:34:MET:HB3	1.87	0.42
15:5:382:LEU:HA	15:5:385:MET:HE3	2.01	0.42
22:M:22:ILE:HD11	22:M:26:GLY:C	2.43	0.42
24:P:32:PHE:HB3	24:P:56:ILE:HG21	2.01	0.42
25:Q:50:LEU:HD13	25:Q:55:ILE:HD11	2.01	0.42
41:8:55:GLU:O	41:8:59:VAL:HG23	2.20	0.42
1:A:78:GLY:HA2	44:A:803:FES:S1	2.59	0.41
1:A:241:LYS:NZ	6:I:151:GLU:CD	2.76	0.41
2:B:78:GLU:HA	2:B:81:LYS:NZ	2.35	0.41
5:H:76:ASP:O	5:H:80:ARG:HG2	2.20	0.41
9:S:53:GLU:HA	9:S:53:GLU:OE1	2.20	0.41
9:S:207:HIS:ND1	9:S:231:TYR:OH	2.49	0.41
11:1:138:ARG:NH1	11:1:204:LEU:HD11	2.34	0.41
12:2:28:ILE:HD13	12:2:28:ILE:HA	1.77	0.41
14:4:15:ASN:C	14:4:15:ASN:HD22	2.28	0.41
14:4:458:ILE:O	14:4:462:LEU:HD23	2.20	0.41
15:5:123:PHE:HZ	15:5:255:LEU:HB2	1.85	0.41
15:5:236:LEU:CD1	15:5:251:HIS:HE1	2.30	0.41
15:5:576:ALA:O	15:5:580:ASP:HB2	2.20	0.41
19:E:234:ASN:N	19:E:321:GLN:OE1	2.37	0.41
26:R:98:MET:HE3	39:i:7:PRO:HB2	2.02	0.41
28:W:29:ARG:HH12	52:W:402:CDL:H711	1.85	0.41
34:c:35:GLY:O	34:c:38:VAL:HG22	2.20	0.41
39:i:78:HIS:HB3	39:i:80:LYS:NZ	2.35	0.41
1:A:276:GLU:HG3	1:A:278:MET:HE2	2.02	0.41
1:A:495:GLY:HA3	1:A:683:VAL:HG21	2.02	0.41
2:B:332:ASN:OD1	2:B:333:ILE:HG12	2.19	0.41
6:I:59:ARG:HG3	6:I:60:PRO:HD2	2.01	0.41
9:S:132:ASN:O	9:S:136:ILE:HG22	2.20	0.41
9:S:171:LEU:C	9:S:174:PRO:HD2	2.46	0.41
11:1:110:LEU:CB	16:6:61:MET:HE1	2.47	0.41
12:2:198:ASN:O	12:2:202:ILE:HG12	2.20	0.41
12:2:199:LEU:HD13	51:2:502:T7X:C31	2.50	0.41
15:5:529:ASN:ND2	15:5:536:PHE:HE1	2.18	0.41
26:R:11:ASN:O	26:R:15:VAL:HG22	2.20	0.41
26:R:20:ARG:HB3	26:R:24:LYS:HZ1	1.85	0.41
27:U:150:ILE:CD1	28:W:55:ARG:HG2	2.50	0.41
30:Y:90:ARG:HE	30:Y:90:ARG:HB2	1.65	0.41
32:a:34:GLU:HG2	32:a:35:PRO:HD3	2.02	0.41
37:f:8:ILE:CG1	37:f:42:VAL:HG22	2.49	0.41
2:B:385:THR:OG1	2:B:386:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:454:LYS:HA	2:B:458:GLU:CD	2.46	0.41
3:C:365:LYS:HD2	31:Z:74:TYR:CZ	2.54	0.41
9:S:211:ASN:HA	9:S:218:ARG:HH12	1.86	0.41
48:1:403:3PE:H332	48:1:403:3PE:H251	2.03	0.41
14:4:211:TRP:CZ3	14:4:273:TYR:CD1	3.08	0.41
15:5:257:THR:HB	15:5:332:LEU:HD11	2.02	0.41
15:5:434:TYR:CZ	15:5:529:ASN:HB3	2.56	0.41
18:D:17:LEU:HD23	18:D:17:LEU:HA	1.79	0.41
19:E:59:PHE:CD1	19:E:107:MET:HE2	2.55	0.41
19:E:70:THR:HG23	19:E:80:VAL:HG11	2.03	0.41
19:E:266:LYS:HB2	19:E:266:LYS:HE3	1.87	0.41
19:E:298:THR:O	19:E:302:GLN:HG2	2.20	0.41
21:J:48:ASN:HD22	21:J:60:THR:HB	1.85	0.41
48:J:201:3PE:H3A1	48:J:201:3PE:H372	1.82	0.41
25:Q:90:LEU:HD21	26:R:47:PHE:CD2	2.55	0.41
31:Z:7:VAL:HG23	31:Z:12:LYS:HE2	2.02	0.41
31:Z:95:THR:O	31:Z:99:GLU:OE1	2.38	0.41
32:a:108:SER:O	32:a:112:THR:HG23	2.20	0.41
38:h:18:ARG:N	38:h:18:ARG:HD2	2.35	0.41
42:9:50:HIS:O	42:9:54:LYS:HG3	2.20	0.41
1:A:67:ARG:HB2	44:A:803:FES:S2	2.61	0.41
1:A:204:SER:O	5:H:106:GLU:HG2	2.20	0.41
1:A:658:ARG:HB3	1:A:661:LEU:HD12	2.03	0.41
2:B:61:TRP:CE3	2:B:64:THR:HG21	2.56	0.41
2:B:65:LYS:HD3	2:B:189:CYS:O	2.20	0.41
2:B:121:GLU:O	2:B:161:ARG:HD2	2.21	0.41
2:B:211:GLU:HG2	2:B:212:THR:N	2.35	0.41
2:B:425:THR:HB	43:B:501:SF4:S3	2.60	0.41
7:K:78:PRO:HG2	7:K:107:PHE:CE2	2.55	0.41
50:2:501:CPL:HC51	33:b:53:VAL:HG21	2.01	0.41
14:4:127:LEU:HG	14:4:140:LEU:HD21	2.02	0.41
14:4:322:SER:OG	14:4:479:VAL:HB	2.20	0.41
14:4:438:ILE:HD13	32:a:59:ASP:HB2	2.02	0.41
15:5:240:MET:N	15:5:240:MET:SD	2.93	0.41
15:5:316:MET:HG3	15:5:331:HIS:HD2	1.85	0.41
16:6:47:LEU:HD23	16:6:47:LEU:HA	1.94	0.41
19:E:24:PHE:CE1	19:E:52:THR:HG22	2.54	0.41
21:J:27:GLY:C	21:J:31:GLN:NE2	2.78	0.41
24:P:54:THR:O	24:P:58:GLN:HG2	2.20	0.41
28:W:119:MET:HE2	28:W:119:MET:HB3	1.82	0.41
37:f:13:CYS:HA	37:f:47:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:h:59:ARG:HD3	38:h:80:TRP:CZ2	2.56	0.41
2:B:65:LYS:HZ2	2:B:69:LEU:HD21	1.84	0.41
2:B:235:VAL:HG11	30:Y:148:PHE:HB2	2.02	0.41
4:G:80:ALA:C	20:F:66:VAL:HG11	2.45	0.41
6:I:77:TYR:CE2	17:g:24:PRO:HG2	2.55	0.41
11:1:51:PHE:O	11:1:55:VAL:HG23	2.20	0.41
11:1:61:GLU:HG3	13:3:27:VAL:O	2.20	0.41
12:2:188:ASP:O	12:2:192:ILE:HG12	2.21	0.41
12:2:351:LYS:HA	12:2:419:VAL:O	2.21	0.41
13:3:76:TYR:HD1	16:6:155:LEU:CD1	2.33	0.41
14:4:157:SER:O	14:4:160:SER:HB3	2.21	0.41
14:4:375:TYR:CE2	14:4:451:LYS:HG2	2.55	0.41
14:4:455:ASN:O	14:4:459:ILE:HG12	2.20	0.41
15:5:359:ASP:OD1	15:5:361:ARG:HB2	2.21	0.41
15:5:509:PHE:CE1	15:5:513:LEU:HD13	2.54	0.41
15:5:641:ILE:O	15:5:644:PRO:HD2	2.21	0.41
16:6:63:TYR:HA	16:6:67:ILE:HD12	2.03	0.41
19:E:213:PHE:O	19:E:216:ARG:N	2.54	0.41
21:J:75:SER:O	21:J:79:VAL:HG12	2.21	0.41
23:O:43:PHE:HD1	23:O:44:ASP:O	2.03	0.41
24:P:82:GLU:OE1	24:P:99:TYR:CE2	2.74	0.41
25:Q:94:GLU:OE2	26:R:19:TYR:CE2	2.74	0.41
26:R:33:ARG:O	26:R:37:ARG:HG2	2.20	0.41
28:W:121:PRO:HA	28:W:122:PRO:HD3	1.88	0.41
31:Z:135:SER:OG	31:Z:139:VAL:HG13	2.20	0.41
2:B:101:MET:SD	2:B:241:PRO:HB2	2.61	0.41
2:B:457:ASP:HB2	2:B:458:GLU:OE1	2.20	0.41
3:C:98:LEU:HB2	3:C:461:PHE:CZ	2.56	0.41
3:C:385:PHE:O	3:C:389:THR:OG1	2.34	0.41
5:H:127:CYS:HB3	5:H:132:CYS:SG	2.61	0.41
15:5:49:TYR:CD1	15:5:86:ILE:HD13	2.56	0.41
15:5:182:VAL:HA	15:5:185:LEU:HD12	2.02	0.41
15:5:354:LEU:HD21	15:5:450:ASN:CB	2.50	0.41
18:D:24:ALA:O	18:D:27:VAL:HG12	2.20	0.41
21:J:89:ARG:HH12	21:J:95:TRP:CG	2.36	0.41
56:O:201:ZMP:H6	24:P:59:GLU:HB3	2.03	0.41
1:A:135:VAL:HG13	6:I:131:ILE:HD12	2.02	0.41
2:B:125:GLY:C	2:B:355:ALA:HB1	2.46	0.41
3:C:119:LEU:HD23	3:C:461:PHE:O	2.20	0.41
3:C:453:ILE:O	3:C:456:THR:HG22	2.20	0.41
9:S:206:LYS:HD3	9:S:207:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1:134:LEU:O	11:1:138:ARG:HG3	2.21	0.41
13:3:69:GLU:OE2	13:3:98:LEU:HB3	2.21	0.41
14:4:16:ARG:CZ	14:4:16:ARG:HA	2.51	0.41
15:5:456:ILE:HD12	15:5:456:ILE:HA	1.93	0.41
48:5:702:3PE:H241	48:5:702:3PE:H272	1.81	0.41
16:6:4:LEU:HA	16:6:4:LEU:HD12	1.77	0.41
16:6:155:LEU:HD23	16:6:162:LEU:HD22	2.03	0.41
19:E:297:TYR:CZ	52:E:403:CDL:H312	2.56	0.41
25:Q:66:PHE:CZ	25:Q:68:LYS:HB2	2.55	0.41
27:U:69:LEU:O	27:U:73:ARG:HG3	2.21	0.41
27:U:70:LYS:HA	27:U:73:ARG:CZ	2.50	0.41
29:X:28:PHE:O	29:X:32:VAL:HG12	2.20	0.41
1:A:48:ILE:HD11	30:Y:139:PHE:CE1	2.55	0.41
1:A:155:ARG:HE	1:A:155:ARG:HB3	1.64	0.41
1:A:719:LYS:HD3	1:A:720:ASP:OD2	2.21	0.41
4:G:128:ALA:HB3	4:G:186:TYR:CD2	2.55	0.41
4:G:227:GLU:CD	19:E:72:LYS:NZ	2.76	0.41
10:j:41:PHE:O	10:j:45:ARG:NH1	2.54	0.41
11:1:118:PHE:HE2	16:6:37:ILE:CD1	2.33	0.41
12:2:416:LEU:HA	12:2:416:LEU:HD23	1.83	0.41
56:Q:201:ZMP:H19	26:R:15:VAL:HG21	2.01	0.41
26:R:74:ARG:H	26:R:74:ARG:HG2	1.65	0.41
31:Z:14:THR:HA	31:Z:38:ASN:O	2.21	0.41
37:f:70:VAL:CG1	37:f:75:GLU:HB3	2.51	0.41
39:i:28:LEU:HD12	39:i:29:ASN:N	2.36	0.41
1:A:79:ASN:O	2:B:384:CYS:HA	2.20	0.41
1:A:159:THR:O	1:A:159:THR:OG1	2.33	0.41
1:A:320:PHE:CE2	38:h:134:THR:HG22	2.56	0.41
1:A:577:ASP:OD2	1:A:578:VAL:HG12	2.20	0.41
1:A:640:GLU:HB2	24:P:115:PHE:HD1	1.86	0.41
2:B:44:LEU:HD22	2:B:45:TYR:CE2	2.56	0.41
2:B:108:LYS:HD2	2:B:108:LYS:HA	1.77	0.41
2:B:270:GLU:OE1	2:B:271:ARG:HB2	2.19	0.41
2:B:462:VAL:HG22	2:B:463:SER:O	2.21	0.41
3:C:288:ASN:OD1	4:G:172:TYR:HA	2.21	0.41
3:C:293:GLY:HA3	3:C:408:GLY:HA2	2.02	0.41
3:C:374:MET:HE1	6:I:180:PRO:HA	2.03	0.41
5:H:142:GLU:OE1	5:H:146:ASN:ND2	2.54	0.41
7:K:127:MET:HG3	7:K:127:MET:O	2.21	0.41
9:S:105:ILE:HA	9:S:108:ILE:HG12	2.02	0.41
9:S:143:LYS:O	9:S:150:VAL:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:167:GLN:NE2	14:4:30:PHE:HB2	2.32	0.41
9:S:204:LEU:HD22	9:S:211:ASN:ND2	2.35	0.41
10:j:17:LYS:HE3	14:4:109:PHE:CG	2.56	0.41
11:1:289:LEU:HD23	11:1:289:LEU:HA	1.79	0.41
12:2:263:LEU:HD23	12:2:263:LEU:HA	1.80	0.41
12:2:360:LEU:CD1	33:b:24:ILE:HD11	2.47	0.41
14:4:344:LEU:HD23	14:4:454:MET:HG3	2.03	0.41
14:4:480:ASN:HD22	35:d:31:THR:HG22	1.85	0.41
15:5:15:SER:OG	15:5:121:SER:HB2	2.21	0.41
15:5:230:PHE:O	15:5:233:HIS:ND1	2.52	0.41
15:5:238:LEU:HD13	48:5:702:3PE:H122	2.03	0.41
15:5:503:GLU:O	15:5:506:ILE:HG22	2.20	0.41
15:5:623:ILE:CD1	21:J:50:LEU:HD11	2.51	0.41
52:g:201:CDL:H121	52:g:201:CDL:H152	1.68	0.41
19:E:201:ARG:HH12	19:E:258:THR:HG21	1.84	0.41
22:M:30:GLU:OE1	22:M:30:GLU:N	2.52	0.41
22:M:71:LYS:HD2	38:h:110:TYR:CZ	2.55	0.41
24:P:6:THR:OG1	24:P:7:ALA:N	2.53	0.41
25:Q:77:ALA:CB	25:Q:119:GLN:NE2	2.79	0.41
26:R:19:TYR:OH	26:R:44:ARG:HD2	2.21	0.41
26:R:33:ARG:HD2	26:R:37:ARG:HD3	2.02	0.41
27:U:21:ASN:OD1	27:U:22:VAL:HG23	2.21	0.41
30:Y:44:ILE:HG22	30:Y:46:SER:H	1.85	0.41
30:Y:106:GLN:H	30:Y:106:GLN:HG3	1.74	0.41
40:n:65:GLU:O	40:n:69:ILE:HG12	2.21	0.41
42:9:18:GLU:HG2	42:9:19:TRP:N	2.35	0.41
42:9:22:PHE:O	42:9:26:THR:HG23	2.21	0.41
1:A:336:TYR:HA	1:A:549:MET:SD	2.61	0.41
1:A:456:GLY:HA3	1:A:461:ASP:CG	2.46	0.41
4:G:83:PRO:O	20:F:126:LEU:HB3	2.21	0.41
11:1:8:ILE:HD11	13:3:3:THR:HA	2.02	0.41
12:2:36:LEU:HD21	50:2:501:CPL:H42	2.03	0.41
51:2:502:T7X:C9	15:5:632:VAL:HG11	2.51	0.41
15:5:230:PHE:N	15:5:287:THR:HG22	2.28	0.41
16:6:27:LYS:HD2	16:6:28:ASN:N	2.36	0.41
17:g:17:ARG:O	17:g:21:HIS:HD2	2.04	0.41
31:Z:130:GLN:HB3	31:Z:134:LYS:NZ	2.35	0.41
40:n:42:GLU:OE1	40:n:47:HIS:HA	2.21	0.41
41:8:33:LEU:HD11	41:8:51:ARG:HA	2.02	0.41
1:A:54:LEU:HD11	1:A:107:VAL:HG21	2.04	0.40
3:C:348:GLU:OE2	28:W:16:PRO:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:124:LEU:HD12	5:H:178:MET:SD	2.60	0.40
9:S:140:ILE:HA	9:S:141:PRO:HD3	1.96	0.40
10:j:84:ARG:NH1	39:i:83:THR:HA	2.36	0.40
11:1:154:PHE:O	11:1:158:ILE:HG12	2.21	0.40
12:2:87:LEU:HB2	12:2:93:TYR:CD2	2.56	0.40
12:2:146:SER:CB	12:2:341:TYR:OH	2.68	0.40
14:4:486:ILE:HD13	14:4:486:ILE:HA	1.91	0.40
15:5:25:GLN:HA	40:n:14:VAL:CG2	2.50	0.40
15:5:82:ASP:H	15:5:85:THR:HB	1.87	0.40
15:5:86:ILE:O	15:5:90:LEU:HG	2.21	0.40
20:F:57:LEU:HD11	20:F:71:ILE:CG2	2.51	0.40
23:O:55:THR:HA	23:O:96:ASN:HB2	2.02	0.40
24:P:64:ARG:HG3	24:P:64:ARG:HH11	1.86	0.40
26:R:81:PRO:HA	26:R:82:PRO:HD3	1.94	0.40
1:A:131:LEU:HA	3:C:378:MET:SD	2.61	0.40
4:G:259:ARG:O	31:Z:84:PRO:HA	2.21	0.40
14:4:392:PHE:CE1	15:5:140:PHE:HE2	2.39	0.40
14:4:469:GLN:CD	15:5:68:LEU:HA	2.46	0.40
16:6:42:ILE:HD11	48:6:202:3PE:H3C1	2.03	0.40
52:g:201:CDL:H122	52:g:201:CDL:H321	2.03	0.40
18:D:49:MET:HE3	27:U:32:SER:HB2	2.03	0.40
21:J:163:PHE:CZ	54:J:202:LMN:HBK	2.56	0.40
26:R:75:HIS:CG	26:R:76:PRO:HD2	2.55	0.40
26:R:92:ARG:HG2	26:R:92:ARG:NH2	2.37	0.40
27:U:136:ARG:CG	27:U:139:GLU:HG2	2.52	0.40
29:X:21:LEU:HD22	29:X:166:ARG:HD2	2.02	0.40
1:A:695:GLU:H	1:A:695:GLU:CD	2.28	0.40
5:H:129:THR:HG22	5:H:130:THR:N	2.35	0.40
6:I:170:ILE:HD13	7:K:156:TYR:CE1	2.56	0.40
9:S:107:ASP:HB3	9:S:111:LEU:HD12	2.02	0.40
9:S:207:HIS:ND1	9:S:225:ARG:CZ	2.84	0.40
11:1:179:CYS:HA	11:1:246:LEU:HD12	2.03	0.40
12:2:228:THR:O	12:2:282:LYS:NZ	2.54	0.40
15:5:27:GLY:HA3	39:i:23:PRO:HD2	2.02	0.40
15:5:163:ALA:HA	15:5:241:GLU:CG	2.47	0.40
18:D:9:LEU:HA	18:D:9:LEU:HD23	1.87	0.40
23:O:62:LEU:HB3	23:O:64:LEU:HG	2.03	0.40
24:P:55:LYS:O	24:P:59:GLU:HG2	2.21	0.40
29:X:36:ARG:HG2	29:X:106:ARG:NH1	2.37	0.40
32:a:131:TRP:HZ3	32:a:137:THR:C	2.30	0.40
2:B:73:THR:HA	2:B:76:ILE:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:ARG:O	2:B:164:PHE:HB2	2.21	0.40
2:B:371:ARG:HA	2:B:371:ARG:HD2	1.69	0.40
2:B:390:GLY:O	2:B:394:LEU:HG	2.21	0.40
10:j:29:ASP:CG	32:a:64:ARG:HH22	2.29	0.40
10:j:48:TYR:HE2	15:5:586:ARG:CZ	2.14	0.40
49:1:404:PLC:H42	49:1:404:PLC:H72	1.90	0.40
48:2:503:3PE:H341	14:4:59:LEU:HD11	2.03	0.40
14:4:208:THR:HG23	14:4:273:TYR:CE2	2.57	0.40
15:5:122:MET:HE1	48:5:701:3PE:H291	2.03	0.40
15:5:229:GLN:HB3	15:5:287:THR:HG21	2.03	0.40
17:g:24:PRO:O	17:g:28:PHE:HD1	2.04	0.40
19:E:222:CYS:HB2	19:E:287:ILE:CD1	2.51	0.40
21:J:134:TRP:CD1	54:J:202:LMN:HBH	2.56	0.40
22:M:119:ALA:HB3	22:M:123:HIS:NE2	2.36	0.40
27:U:12:PHE:CZ	28:W:119:MET:HE1	2.56	0.40
30:Y:91:TRP:CE2	30:Y:100:SER:HB2	2.56	0.40
35:d:78:ARG:H	35:d:78:ARG:HG2	1.70	0.40
52:n:201:CDL:H311	52:n:201:CDL:HA62	1.82	0.40
41:8:26:CYS:O	41:8:26:CYS:SG	2.79	0.40
42:9:61:GLU:O	42:9:65:LYS:HG2	2.21	0.40
1:A:161:ILE:HG12	2:B:483:LEU:HD12	2.04	0.40
1:A:285:HIS:CE1	1:A:287:ASP:HB2	2.57	0.40
2:B:63:LYS:HG2	2:B:63:LYS:O	2.21	0.40
2:B:251:ALA:O	2:B:254:PRO:HD2	2.21	0.40
3:C:98:LEU:HD13	3:C:461:PHE:CE1	2.53	0.40
6:I:197:ARG:NH2	19:E:99:LEU:HD11	2.36	0.40
12:2:248:LEU:HA	12:2:248:LEU:HD23	1.92	0.40
12:2:276:LEU:HD13	15:5:596:LEU:HB3	2.03	0.40
12:2:332:TYR:OH	12:2:433:GLU:HB2	2.22	0.40
13:3:19:LEU:O	13:3:23:ILE:HG12	2.22	0.40
14:4:30:PHE:CE1	14:4:34:LEU:HD21	2.56	0.40
14:4:78:LEU:HB3	14:4:132:LEU:HB2	2.04	0.40
15:5:199:THR:HG23	35:d:49:GLU:HG2	2.04	0.40
15:5:316:MET:O	15:5:320:ILE:HG12	2.22	0.40
17:g:39:ALA:O	17:g:43:LEU:HB2	2.22	0.40
25:Q:102:GLU:HA	25:Q:102:GLU:OE1	2.22	0.40
25:Q:128:GLN:HA	25:Q:129:PRO:HD3	1.94	0.40
26:R:46:LYS:HA	26:R:46:LYS:CE	2.50	0.40
34:c:15:TRP:CD1	34:c:15:TRP:H	2.40	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	691/728 (95%)	667 (96%)	23 (3%)	1 (0%)	48	78
2	B	455/488 (93%)	441 (97%)	14 (3%)	0	100	100
3	C	403/466 (86%)	386 (96%)	16 (4%)	1 (0%)	43	71
4	G	237/281 (84%)	231 (98%)	5 (2%)	1 (0%)	30	59
5	H	214/243 (88%)	192 (90%)	22 (10%)	0	100	100
6	I	188/229 (82%)	182 (97%)	6 (3%)	0	100	100
7	K	175/210 (83%)	168 (96%)	6 (3%)	1 (1%)	21	50
8	L	84/89 (94%)	84 (100%)	0	0	100	100
9	S	176/249 (71%)	166 (94%)	10 (6%)	0	100	100
10	j	88/93 (95%)	83 (94%)	5 (6%)	0	100	100
11	1	338/341 (99%)	323 (96%)	15 (4%)	0	100	100
12	2	467/469 (100%)	463 (99%)	4 (1%)	0	100	100
13	3	111/128 (87%)	108 (97%)	3 (3%)	0	100	100
14	4	479/486 (99%)	464 (97%)	15 (3%)	0	100	100
15	5	644/655 (98%)	622 (97%)	21 (3%)	1 (0%)	43	71
16	6	129/185 (70%)	125 (97%)	4 (3%)	0	100	100
17	g	74/78 (95%)	63 (85%)	10 (14%)	1 (1%)	9	31
18	D	84/87 (97%)	80 (95%)	4 (5%)	0	100	100
19	E	332/375 (88%)	317 (96%)	14 (4%)	1 (0%)	36	65
20	F	118/144 (82%)	111 (94%)	7 (6%)	0	100	100
21	J	168/198 (85%)	164 (98%)	4 (2%)	0	100	100
22	M	115/136 (85%)	114 (99%)	1 (1%)	0	100	100
23	O	69/109 (63%)	65 (94%)	4 (6%)	0	100	100
24	P	121/124 (98%)	121 (100%)	0	0	100	100
25	Q	83/132 (63%)	80 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	R	104/109 (95%)	103 (99%)	1 (1%)	0	100	100
27	U	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
28	W	119/123 (97%)	117 (98%)	2 (2%)	0	100	100
29	X	162/169 (96%)	158 (98%)	4 (2%)	0	100	100
30	Y	123/161 (76%)	119 (97%)	4 (3%)	0	100	100
31	Z	179/182 (98%)	171 (96%)	8 (4%)	0	100	100
32	a	122/149 (82%)	116 (95%)	6 (5%)	0	100	100
33	b	62/74 (84%)	62 (100%)	0	0	100	100
34	c	42/60 (70%)	40 (95%)	2 (5%)	0	100	100
35	d	87/92 (95%)	84 (97%)	3 (3%)	0	100	100
36	e	50/67 (75%)	47 (94%)	3 (6%)	0	100	100
37	f	80/87 (92%)	77 (96%)	3 (4%)	0	100	100
38	h	134/138 (97%)	130 (97%)	4 (3%)	0	100	100
39	i	81/90 (90%)	79 (98%)	2 (2%)	0	100	100
40	n	111/139 (80%)	107 (96%)	4 (4%)	0	100	100
41	8	69/99 (70%)	66 (96%)	3 (4%)	0	100	100
42	9	84/89 (94%)	80 (95%)	4 (5%)	0	100	100
All	All	7821/8723 (90%)	7542 (96%)	272 (4%)	7 (0%)	49	78

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	K	81	PHE
1	A	726	ALA
17	g	72	LEU
4	G	93	LYS
19	E	344	MET
15	5	555	VAL
3	C	310	PRO

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	566/595 (95%)	556 (98%)	10 (2%)	51	67
2	B	364/389 (94%)	362 (100%)	2 (0%)	81	81
3	C	346/393 (88%)	346 (100%)	0	100	100
4	G	216/245 (88%)	216 (100%)	0	100	100
5	H	191/212 (90%)	191 (100%)	0	100	100
6	I	156/187 (83%)	155 (99%)	1 (1%)	78	80
7	K	154/180 (86%)	151 (98%)	3 (2%)	50	66
8	L	74/76 (97%)	71 (96%)	3 (4%)	27	52
9	S	157/211 (74%)	156 (99%)	1 (1%)	78	80
10	j	71/73 (97%)	71 (100%)	0	100	100
11	1	300/301 (100%)	297 (99%)	3 (1%)	68	75
12	2	432/432 (100%)	429 (99%)	3 (1%)	76	78
13	3	102/113 (90%)	101 (99%)	1 (1%)	68	75
14	4	429/434 (99%)	429 (100%)	0	100	100
15	5	573/580 (99%)	568 (99%)	5 (1%)	70	76
16	6	119/166 (72%)	116 (98%)	3 (2%)	42	62
17	g	63/65 (97%)	62 (98%)	1 (2%)	55	68
18	D	68/69 (99%)	68 (100%)	0	100	100
19	E	290/329 (88%)	287 (99%)	3 (1%)	68	75
20	F	108/129 (84%)	108 (100%)	0	100	100
21	J	124/147 (84%)	124 (100%)	0	100	100
22	M	97/115 (84%)	97 (100%)	0	100	100
23	O	60/91 (66%)	60 (100%)	0	100	100
24	P	109/110 (99%)	109 (100%)	0	100	100
25	Q	72/111 (65%)	72 (100%)	0	100	100
26	R	97/100 (97%)	97 (100%)	0	100	100
27	U	147/148 (99%)	147 (100%)	0	100	100
28	W	100/102 (98%)	100 (100%)	0	100	100
29	X	128/133 (96%)	128 (100%)	0	100	100
30	Y	107/140 (76%)	104 (97%)	3 (3%)	38	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	Z	147/148 (99%)	146 (99%)	1 (1%)	76	78
32	a	108/129 (84%)	108 (100%)	0	100	100
33	b	50/59 (85%)	50 (100%)	0	100	100
34	c	30/45 (67%)	30 (100%)	0	100	100
35	d	82/85 (96%)	82 (100%)	0	100	100
36	e	44/55 (80%)	44 (100%)	0	100	100
37	f	70/73 (96%)	70 (100%)	0	100	100
38	h	121/123 (98%)	121 (100%)	0	100	100
39	i	64/68 (94%)	63 (98%)	1 (2%)	55	68
40	n	98/119 (82%)	98 (100%)	0	100	100
41	8	63/76 (83%)	63 (100%)	0	100	100
42	9	73/76 (96%)	73 (100%)	0	100	100
All	All	6770/7432 (91%)	6726 (99%)	44 (1%)	76	80

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	ARG
1	A	712	LYS
1	A	714	SER
1	A	715	ILE
1	A	719	LYS
1	A	720	ASP
1	A	721	ASN
1	A	722	LYS
1	A	723	LYS
1	A	725	GLN
2	B	483	LEU
2	B	486	VAL
6	I	40	ASN
7	K	85	CYS
7	K	108	ARG
7	K	122	THR
8	L	84	ILE
8	L	85	ASN
8	L	86	SER
9	S	115	HIS
11	1	130	LYS

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Mol	Chain	Res	Type
11	1	211	LEU
11	1	212	VAL
12	2	334	ILE
12	2	335	ASN
12	2	423	ASP
13	3	22	ASN
15	5	508	GLN
15	5	554	LEU
15	5	556	SER
15	5	612	SER
15	5	613	SER
16	6	2	MET
16	6	5	THR
16	6	8	PHE
17	g	72	LEU
19	E	127	ASN
19	E	348	ILE
19	E	349	ARG
30	Y	90	ARG
30	Y	95	LEU
30	Y	100	SER
31	Z	67	ASN
39	i	22	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	285	HIS
1	A	416	ASN
1	A	425	ASN
1	A	479	ASN
1	A	499	ASN
1	A	607	GLN
1	A	721	ASN
1	A	724	ASN
1	A	725	GLN
2	B	37	GLN
2	B	43	ASN
2	B	152	ASN
2	B	272	ASN
3	C	186	HIS

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Mol	Chain	Res	Type
3	C	308	ASN
4	G	67	HIS
4	G	87	GLN
5	H	145	GLN
5	H	224	GLN
7	K	200	ASN
9	S	167	GLN
10	j	37	HIS
11	1	49	GLN
11	1	128	ASN
12	2	29	ASN
12	2	119	HIS
12	2	180	ASN
12	2	292	ASN
13	3	53	ASN
14	4	15	ASN
14	4	45	ASN
14	4	51	ASN
14	4	56	ASN
14	4	103	ASN
14	4	193	ASN
14	4	355	HIS
14	4	400	GLN
14	4	480	ASN
15	5	229	GLN
15	5	251	HIS
15	5	299	ASN
15	5	358	GLN
15	5	455	ASN
15	5	552	GLN
15	5	636	ASN
17	g	21	HIS
17	g	71	GLN
19	E	144	HIS
19	E	158	HIS
19	E	354	ASN
20	F	61	HIS
20	F	69	GLN
21	J	31	GLN
21	J	87	ASN
22	M	25	ASN
22	M	27	ASN

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Mol	Chain	Res	Type
24	P	80	HIS
24	P	84	GLN
24	P	92	GLN
24	P	110	HIS
25	Q	119	GLN
30	Y	69	GLN
30	Y	93	ASN
30	Y	99	GLN
30	Y	132	GLN
31	Z	79	HIS
32	a	60	GLN
32	a	90	ASN
32	a	146	GLN
34	c	25	ASN
35	d	58	ASN
37	f	11	HIS
40	n	18	GLN
40	n	47	HIS
40	n	74	ASN
40	n	95	HIS
41	8	16	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	$\# Z > 2$
11	FME	1	1	11	8,9,10	0.98	0	8,9,11	0.72	0
12	FME	2	1	12	8,9,10	1.01	1 (12%)	8,9,11	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	FME	3	1	13	8,9,10	0.91	0	8,9,11	1.40	1 (12%)
8	FME	L	1	8	8,9,10	1.02	1 (12%)	8,9,11	0.96	0
16	FME	6	1	16	8,9,10	0.53	0	8,9,11	0.93	1 (12%)
3	2MR	C	121	3	10,12,13	1.92	1 (10%)	5,13,15	2.62	2 (40%)

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
11	FME	1	1	11	-	0/7/9/11	-
12	FME	2	1	12	-	5/7/9/11	-
13	FME	3	1	13	-	2/7/9/11	-
8	FME	L	1	8	-	3/7/9/11	-
16	FME	6	1	16	-	6/7/9/11	-
3	2MR	C	121	3	-	2/10/13/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	121	2MR	CZ-NE	5.22	1.45	1.34
12	2	1	FME	CA-N	-2.14	1.43	1.46
8	L	1	FME	CA-N	-2.02	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	121	2MR	CD-NE-CZ	4.15	131.15	123.36
3	C	121	2MR	NE-CZ-NH2	3.95	123.10	119.48
13	3	1	FME	C-CA-N	2.88	115.07	109.50
16	6	1	FME	O-C-CA	-2.47	118.41	124.77

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	121	2MR	C-CA-CB-CG
8	L	1	FME	O1-CN-N-CA

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Mol	Chain	Res	Type	Atoms
12	2	1	FME	C-CA-CB-CG
12	2	1	FME	O-C-CA-CB
16	6	1	FME	O1-CN-N-CA
16	6	1	FME	N-CA-CB-CG
16	6	1	FME	C-CA-CB-CG
16	6	1	FME	CA-CB-CG-SD
13	3	1	FME	CA-CB-CG-SD
8	L	1	FME	N-CA-CB-CG
12	2	1	FME	CB-CG-SD-CE
16	6	1	FME	CB-CG-SD-CE
13	3	1	FME	CB-CG-SD-CE
12	2	1	FME	N-CA-CB-CG
12	2	1	FME	CA-CB-CG-SD
8	L	1	FME	CB-CG-SD-CE
3	C	121	2MR	CA-CB-CG-CD
16	6	1	FME	CB-CA-N-CN

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	2	1	FME	2	0
8	L	1	FME	1	0
16	6	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 1 is monoatomic - leaving 48 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
54	LMN	a	201	-	68,68,72	1.66	13 (19%)	88,94,98	0.99	3 (3%)
48	3PE	5	701	-	41,41,50	0.96	4 (9%)	44,46,55	1.00	2 (4%)
49	PLC	W	401	-	40,40,41	1.23	3 (7%)	46,48,49	1.18	4 (8%)
49	PLC	K	302	-	35,35,41	0.32	0	41,43,49	0.35	0
54	LMN	J	202	-	72,72,72	1.54	12 (16%)	92,98,98	1.31	11 (11%)
51	T7X	2	502	-	52,52,61	0.92	5 (9%)	61,64,73	1.41	8 (13%)
44	FES	A	803	1	0,4,4	-	-	-	-	-
51	T7X	3	201	-	44,44,61	1.02	4 (9%)	53,56,73	1.08	5 (9%)
45	FMN	B	502	-	33,33,33	1.13	2 (6%)	48,50,50	1.29	6 (12%)
52	CDL	E	403	-	71,71,99	1.06	7 (9%)	77,83,111	1.08	6 (7%)
43	SF4	A	801	1	0,12,12	-	-	-	-	-
48	3PE	1	402	-	35,35,50	1.02	4 (11%)	38,40,55	1.01	2 (5%)
47	UQ9	C	601	-	14,14,58	2.67	6 (42%)	20,20,73	1.01	0
43	SF4	B	501	2	0,12,12	-	-	-	-	-
49	PLC	4	504	-	34,34,41	1.34	5 (14%)	40,42,49	1.22	3 (7%)
48	3PE	5	703	-	43,43,50	0.29	0	46,48,55	0.33	0
52	CDL	n	201	-	91,91,99	0.95	7 (7%)	97,103,111	0.98	5 (5%)
48	3PE	6	202	-	46,46,50	0.90	4 (8%)	49,51,55	0.91	2 (4%)
43	SF4	A	802	1	0,12,12	-	-	-	-	-
48	3PE	5	702	-	40,40,50	0.96	4 (10%)	43,45,55	1.09	3 (6%)
49	PLC	i	1101	-	41,41,41	1.25	5 (12%)	47,49,49	1.14	3 (6%)
56	ZMP	Q	201	25	27,32,36	1.64	4 (14%)	31,39,45	1.47	3 (9%)
48	3PE	6	201	-	35,35,50	1.03	4 (11%)	38,40,55	1.15	2 (5%)
52	CDL	X	201	-	85,85,99	0.98	6 (7%)	91,97,111	1.01	4 (4%)
49	PLC	1	404	-	41,41,41	1.27	5 (12%)	47,49,49	1.21	5 (10%)
50	CPL	2	501	-	51,51,51	1.16	3 (5%)	57,59,59	1.25	6 (10%)
51	T7X	b	501	-	48,48,61	0.95	4 (8%)	57,60,73	1.20	4 (7%)
52	CDL	Z	201	-	75,75,99	1.06	7 (9%)	81,87,111	1.01	4 (4%)
56	ZMP	O	201	23	27,32,36	1.74	5 (18%)	31,39,45	1.98	8 (25%)
48	3PE	4	503	-	50,50,50	0.87	3 (6%)	53,55,55	0.94	3 (5%)
52	CDL	W	402	-	53,53,99	1.25	7 (13%)	59,65,111	1.18	4 (6%)
48	3PE	J	201	-	40,40,50	0.97	3 (7%)	43,45,55	0.99	3 (6%)
48	3PE	b	502	-	41,41,50	0.95	4 (9%)	44,46,55	0.87	2 (4%)
48	3PE	E	402	-	35,35,50	1.02	3 (8%)	38,40,55	1.15	3 (7%)
48	3PE	I	501	-	50,50,50	0.86	3 (6%)	53,55,55	0.99	4 (7%)
48	3PE	4	501	-	41,41,50	0.95	4 (9%)	44,46,55	0.97	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	3PE	1	403	-	40,40,50	0.93	3 (7%)	43,45,55	0.81	1 (2%)
43	SF4	K	301	7	0,12,12	-	-	-		
46	NAI	B	503	-	47,48,48	0.51	0	64,73,73	0.65	1 (1%)
52	CDL	g	201	-	79,79,99	1.02	7 (8%)	85,91,111	1.10	6 (7%)
43	SF4	I	502	6	0,12,12	-	-	-		
48	3PE	4	502	-	42,42,50	0.95	4 (9%)	45,47,55	1.03	3 (6%)
48	3PE	g	202	-	42,42,50	0.95	4 (9%)	45,47,55	0.89	2 (4%)
49	PLC	1	401	-	34,34,41	1.33	4 (11%)	40,42,49	1.29	4 (10%)
48	3PE	2	503	-	41,41,50	0.95	4 (9%)	44,46,55	0.91	2 (4%)
53	NDP	E	401	-	51,52,52	2.28	7 (13%)	71,80,80	1.64	17 (23%)
43	SF4	I	503	6	0,12,12	-	-	-		
44	FES	H	301	5	0,4,4	-	-	-		

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
54	LMN	a	201	-	-	22/46/126/130	0/4/4/4
48	3PE	5	701	-	-	18/45/45/54	-
49	PLC	W	401	-	-	17/44/44/45	-
49	PLC	K	302	-	-	7/39/39/45	-
54	LMN	J	202	-	-	40/50/130/130	0/4/4/4
51	T7X	2	502	-	-	21/47/71/80	0/1/1/1
51	T7X	3	201	-	-	12/39/63/80	0/1/1/1
52	CDL	E	403	-	-	35/82/82/110	-
45	FMN	B	502	-	-	7/18/18/18	0/3/3/3
44	FES	A	803	1	-	-	0/1/1/1
43	SF4	A	801	1	-	-	0/6/5/5
48	3PE	1	402	-	-	20/39/39/54	-
47	UQ9	C	601	-	-	1/4/28/81	0/1/1/1
43	SF4	B	501	2	-	-	0/6/5/5
49	PLC	4	504	-	-	22/38/38/45	-
48	3PE	5	703	-	-	26/47/47/54	-
52	CDL	n	201	-	-	55/102/102/110	-
48	3PE	6	202	-	-	20/50/50/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	3PE	5	702	-	-	21/44/44/54	-
56	ZMP	Q	201	25	-	11/37/39/43	-
49	PLC	i	1101	-	-	25/45/45/45	-
43	SF4	A	802	1	-	-	0/6/5/5
48	3PE	6	201	-	-	20/39/39/54	-
52	CDL	X	201	-	-	40/96/96/110	-
49	PLC	1	404	-	-	20/45/45/45	-
50	CPL	2	501	-	-	22/55/55/55	-
51	T7X	b	501	-	-	18/43/67/80	0/1/1/1
52	CDL	Z	201	-	-	38/86/86/110	-
56	ZMP	O	201	23	-	19/37/39/43	-
48	3PE	4	503	-	-	26/54/54/54	-
52	CDL	W	402	-	-	32/64/64/110	-
48	3PE	J	201	-	-	19/44/44/54	-
48	3PE	b	502	-	-	24/45/45/54	-
48	3PE	E	402	-	-	16/39/39/54	-
48	3PE	I	501	-	-	28/54/54/54	-
48	3PE	4	501	-	-	22/45/45/54	-
48	3PE	1	403	-	-	15/44/44/54	-
43	SF4	K	301	7	-	-	0/6/5/5
46	NAI	B	503	-	-	8/29/72/72	0/5/5/5
52	CDL	g	201	-	-	35/90/90/110	-
43	SF4	I	502	6	-	-	0/6/5/5
48	3PE	4	502	-	-	24/46/46/54	-
48	3PE	g	202	-	-	22/46/46/54	-
49	PLC	1	401	-	-	16/38/38/45	-
48	3PE	2	503	-	-	21/45/45/54	-
53	NDP	E	401	-	-	6/34/77/77	0/5/5/5
43	SF4	I	503	6	-	-	0/6/5/5
44	FES	H	301	5	-	-	0/1/1/1

All (183) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	E	401	NDP	P2B-O2B	12.86	1.82	1.59
47	C	601	UQ9	O4-C4	-5.60	1.23	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	C	601	UQ9	O3-C3	-5.38	1.23	1.36
56	O	201	ZMP	C16-N2	5.30	1.46	1.33
56	Q	201	ZMP	C16-N2	5.15	1.45	1.33
56	O	201	ZMP	C13-N1	5.11	1.45	1.33
56	Q	201	ZMP	C13-N1	4.79	1.44	1.33
54	a	201	LMN	O5-C5	4.24	1.54	1.44
54	J	202	LMN	O5-C5	4.16	1.54	1.44
54	a	201	LMN	CBQ-CCM	4.06	1.61	1.54
54	a	201	LMN	CBT-CCM	3.77	1.62	1.53
54	a	201	LMN	CBR-CCM	3.72	1.60	1.54
54	J	202	LMN	CBR-CCM	3.71	1.60	1.54
54	J	202	LMN	CBT-CCM	3.59	1.61	1.53
47	C	601	UQ9	C4-C5	-3.42	1.39	1.48
53	E	401	NDP	O2B-C2B	-3.40	1.32	1.44
54	a	201	LMN	OBY-CCR	3.40	1.50	1.41
54	J	202	LMN	CBQ-CCM	3.40	1.60	1.54
53	E	401	NDP	PN-O5D	3.29	1.72	1.59
54	a	201	LMN	CBS-CCM	3.24	1.60	1.53
50	2	501	CPL	O3-C11	3.17	1.42	1.33
53	E	401	NDP	PA-O3	3.14	1.62	1.59
48	E	402	3PE	O21-C2	-3.13	1.39	1.46
49	1	401	PLC	O3-CB	3.10	1.42	1.33
54	J	202	LMN	OBY-CCR	3.09	1.49	1.41
47	C	601	UQ9	C3-C2	-3.08	1.39	1.48
49	W	401	PLC	O2-C'	3.08	1.43	1.34
49	1	404	PLC	O2-C2	-3.07	1.39	1.46
49	4	504	PLC	O2-C'	3.04	1.42	1.34
52	W	402	CDL	OB6-CB5	3.04	1.42	1.34
54	J	202	LMN	CBS-CCM	3.02	1.60	1.53
49	i	1101	PLC	O3-CB	3.00	1.42	1.33
49	4	504	PLC	O3-CB	3.00	1.42	1.33
49	W	401	PLC	O3-CB	2.98	1.42	1.33
48	I	501	3PE	O21-C2	-2.95	1.39	1.46
49	1	404	PLC	O3-CB	2.95	1.41	1.33
48	J	201	3PE	O21-C2	-2.95	1.39	1.46
45	B	502	FMN	C4A-N5	2.94	1.37	1.30
54	a	201	LMN	OBX-CCJ	2.92	1.49	1.41
48	4	503	3PE	O21-C2	-2.91	1.39	1.46
51	3	201	T7X	O16-C8	-2.91	1.39	1.46
48	5	702	3PE	O21-C2	-2.91	1.39	1.46
50	2	501	CPL	O2-C31	2.91	1.42	1.34
49	i	1101	PLC	O2-C'	2.86	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	1	401	PLC	O2-C'	2.85	1.42	1.34
48	4	502	3PE	O21-C2	-2.84	1.39	1.46
48	b	502	3PE	O21-C2	-2.84	1.39	1.46
50	2	501	CPL	O2-C2	-2.83	1.39	1.46
52	g	201	CDL	OA6-CA4	-2.83	1.39	1.46
53	E	401	NDP	O4B-C4B	-2.81	1.38	1.45
48	2	503	3PE	O21-C2	-2.81	1.40	1.46
52	X	201	CDL	OB6-CB5	2.80	1.42	1.34
52	Z	201	CDL	OB6-CB4	-2.80	1.40	1.46
48	g	202	3PE	O21-C2	-2.79	1.40	1.46
52	Z	201	CDL	OA6-CA4	-2.78	1.40	1.46
52	n	201	CDL	OB6-CB5	2.77	1.42	1.34
48	4	501	3PE	O21-C2	-2.76	1.40	1.46
48	5	701	3PE	O21-C2	-2.75	1.40	1.46
48	6	202	3PE	O21-C2	-2.74	1.40	1.46
49	1	401	PLC	O2-C2	-2.74	1.40	1.46
52	W	402	CDL	OA6-CA4	-2.73	1.40	1.46
49	i	1101	PLC	O2-C2	-2.73	1.40	1.46
52	E	403	CDL	OA6-CA4	-2.71	1.40	1.46
48	6	201	3PE	O21-C2	-2.70	1.40	1.46
49	1	404	PLC	O2-C'	2.69	1.41	1.34
49	4	504	PLC	O2-C2	-2.69	1.40	1.46
52	E	403	CDL	OB6-CB4	-2.68	1.40	1.46
52	n	201	CDL	OA6-CA4	-2.67	1.40	1.46
52	g	201	CDL	OB6-CB5	2.66	1.41	1.34
48	1	402	3PE	O21-C2	-2.65	1.40	1.46
49	W	401	PLC	O2-C2	-2.65	1.40	1.46
52	X	201	CDL	OA8-CA6	-2.65	1.39	1.45
52	W	402	CDL	OB8-CB7	2.64	1.41	1.33
52	Z	201	CDL	OA8-CA6	-2.62	1.39	1.45
52	X	201	CDL	OB6-CB4	-2.60	1.40	1.46
54	J	202	LMN	C6-C5	-2.59	1.43	1.51
52	W	402	CDL	OA8-CA6	-2.55	1.39	1.45
48	1	403	3PE	O31-C31	2.55	1.40	1.33
54	a	201	LMN	C6-C5	-2.55	1.43	1.51
45	B	502	FMN	C10-N1	2.54	1.38	1.33
52	n	201	CDL	OA8-CA6	-2.53	1.39	1.45
52	Z	201	CDL	OB6-CB5	2.52	1.41	1.34
56	O	201	ZMP	O2-C13	-2.52	1.18	1.23
52	g	201	CDL	OB6-CB4	-2.51	1.40	1.46
52	E	403	CDL	OB6-CB5	2.51	1.41	1.34
51	2	502	T7X	O16-C8	-2.49	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	Z	201	CDL	OB8-CB6	-2.49	1.39	1.45
52	g	201	CDL	OB8-CB7	2.48	1.40	1.33
48	5	702	3PE	O31-C3	-2.47	1.39	1.45
47	C	601	UQ9	C6-C5	-2.47	1.38	1.47
52	n	201	CDL	OB6-CB4	-2.44	1.40	1.46
54	J	202	LMN	C3-C2	-2.43	1.46	1.52
52	X	201	CDL	OB8-CB7	2.43	1.40	1.33
48	4	502	3PE	O31-C31	2.42	1.40	1.33
52	g	201	CDL	OA8-CA6	-2.42	1.39	1.45
48	6	202	3PE	O31-C31	2.41	1.40	1.33
53	E	401	NDP	C7N-C3N	-2.41	1.43	1.48
48	4	501	3PE	O31-C31	2.41	1.40	1.33
52	E	403	CDL	OA8-CA6	-2.41	1.39	1.45
48	5	701	3PE	O31-C3	-2.40	1.39	1.45
48	1	403	3PE	O21-C2	-2.40	1.41	1.46
52	n	201	CDL	OB8-CB6	-2.39	1.39	1.45
54	J	202	LMN	OBX-CCJ	2.39	1.48	1.41
52	E	403	CDL	OB8-CB6	-2.39	1.39	1.45
48	g	202	3PE	O31-C31	2.37	1.40	1.33
48	2	503	3PE	O31-C31	2.36	1.40	1.33
51	b	501	T7X	O16-C10	2.36	1.40	1.34
54	a	201	LMN	OBZ-CCS	2.35	1.47	1.41
51	b	501	T7X	O18-C11	2.34	1.40	1.33
48	1	402	3PE	O31-C31	2.34	1.40	1.33
56	O	201	ZMP	C10-S1	2.34	1.81	1.76
48	6	201	3PE	O31-C3	-2.34	1.39	1.45
48	4	503	3PE	O31-C31	2.34	1.40	1.33
54	a	201	LMN	C3-C2	-2.33	1.46	1.52
48	b	502	3PE	O31-C31	2.33	1.40	1.33
51	3	201	T7X	O18-C11	2.33	1.40	1.33
51	2	502	T7X	P1-O1	2.32	1.66	1.59
54	a	201	LMN	CBR-CBL	2.32	1.60	1.52
52	X	201	CDL	OB8-CB6	-2.32	1.40	1.45
48	I	501	3PE	O31-C31	2.31	1.40	1.33
48	g	202	3PE	O31-C3	-2.31	1.40	1.45
48	J	201	3PE	O31-C3	-2.31	1.40	1.45
52	X	201	CDL	OA6-CA4	-2.31	1.41	1.46
51	b	501	T7X	O16-C8	-2.30	1.41	1.46
51	2	502	T7X	O18-C11	2.30	1.40	1.33
48	I	501	3PE	O31-C3	-2.29	1.40	1.45
47	C	601	UQ9	C1-C2	-2.29	1.39	1.47
54	J	202	LMN	CBR-CBL	2.28	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	1	403	3PE	O21-C21	2.28	1.40	1.34
48	J	201	3PE	O31-C31	2.27	1.40	1.33
52	Z	201	CDL	OA8-CA7	2.26	1.39	1.33
48	b	502	3PE	O31-C3	-2.26	1.40	1.45
56	Q	201	ZMP	O2-C13	-2.25	1.18	1.23
49	4	504	PLC	P-O3P	2.25	1.68	1.59
52	Z	201	CDL	OB8-CB7	2.25	1.39	1.33
48	5	701	3PE	O21-C21	2.24	1.40	1.34
56	Q	201	ZMP	C10-S1	2.24	1.81	1.76
51	2	502	T7X	O18-C9	-2.23	1.40	1.45
52	E	403	CDL	OB8-CB7	2.23	1.39	1.33
48	E	402	3PE	O31-C31	2.23	1.39	1.33
52	n	201	CDL	OB8-CB7	2.22	1.39	1.33
56	O	201	ZMP	O3-C16	-2.22	1.19	1.23
48	4	503	3PE	O31-C3	-2.22	1.40	1.45
52	g	201	CDL	OB8-CB6	-2.21	1.40	1.45
48	1	402	3PE	O31-C3	-2.21	1.40	1.45
48	2	503	3PE	O31-C3	-2.21	1.40	1.45
48	5	701	3PE	O31-C31	2.20	1.39	1.33
52	g	201	CDL	OA8-CA7	2.20	1.39	1.33
48	6	201	3PE	O31-C31	2.20	1.39	1.33
48	g	202	3PE	O21-C21	2.18	1.40	1.34
51	b	501	T7X	O18-C9	-2.18	1.40	1.45
48	E	402	3PE	O31-C3	-2.18	1.40	1.45
48	4	502	3PE	O31-C3	-2.17	1.40	1.45
51	3	201	T7X	O18-C9	-2.17	1.40	1.45
48	6	202	3PE	O31-C3	-2.17	1.40	1.45
48	1	402	3PE	O21-C21	2.17	1.40	1.34
48	6	201	3PE	O21-C21	2.16	1.40	1.34
48	4	501	3PE	O21-C21	2.15	1.40	1.34
51	2	502	T7X	O16-C10	2.15	1.40	1.34
48	4	502	3PE	O21-C21	2.14	1.40	1.34
54	J	202	LMN	O2-C2	2.14	1.48	1.43
53	E	401	NDP	O5D-C5D	-2.13	1.36	1.44
49	4	504	PLC	P-O4P	2.13	1.67	1.59
54	a	201	LMN	O1-C1	2.13	1.43	1.40
48	5	702	3PE	O31-C31	2.13	1.39	1.33
52	W	402	CDL	OA8-CA7	2.13	1.39	1.33
48	b	502	3PE	O21-C21	2.13	1.40	1.34
54	J	202	LMN	OBZ-CCS	2.11	1.47	1.41
49	i	1101	PLC	P-O3P	2.11	1.67	1.59
52	n	201	CDL	OA8-CA7	2.11	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	a	201	LMN	O2-C2	2.10	1.48	1.43
48	6	202	3PE	O21-C21	2.10	1.40	1.34
49	1	401	PLC	P-O3P	2.09	1.67	1.59
52	E	403	CDL	OA8-CA7	2.09	1.39	1.33
48	4	501	3PE	O31-C3	-2.07	1.40	1.45
52	W	402	CDL	OB8-CB6	-2.07	1.40	1.45
49	i	1101	PLC	P-O4P	2.07	1.67	1.59
48	2	503	3PE	O21-C21	2.06	1.40	1.34
49	1	404	PLC	P-O4P	2.05	1.67	1.59
51	3	201	T7X	P1-O1	2.04	1.65	1.59
52	W	402	CDL	OB6-CB4	-2.04	1.41	1.46
48	5	702	3PE	O21-C21	2.02	1.40	1.34
49	1	404	PLC	C1'-C'	2.02	1.56	1.50

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	O	201	ZMP	C9-C10-S1	6.86	121.58	113.40
51	2	502	T7X	C6-C1-C2	5.68	118.75	110.86
56	Q	201	ZMP	C9-C10-S1	5.17	119.57	113.40
50	2	501	CPL	C37-C38-C39	-4.85	85.46	112.60
52	g	201	CDL	OA6-CA5-C11	4.59	121.41	111.48
52	W	402	CDL	OB6-CB5-C51	4.57	121.38	111.48
51	b	501	T7X	C6-C1-C2	4.52	117.13	110.86
48	E	402	3PE	O21-C21-C22	4.48	121.16	111.48
52	X	201	CDL	OB6-CB5-C51	4.46	121.13	111.48
53	E	401	NDP	P2B-O2B-C2B	-4.43	111.60	123.43
49	1	401	PLC	C7-N-C6	4.41	120.55	108.98
50	2	501	CPL	O2-C31-C32	4.39	120.98	111.48
49	1	404	PLC	O2-C'-C1'	4.34	120.86	111.48
52	g	201	CDL	OB6-CB5-C51	4.32	120.82	111.48
51	b	501	T7X	O16-C10-C12	4.30	120.78	111.48
52	n	201	CDL	OB6-CB5-C51	4.28	120.75	111.48
48	6	201	3PE	O21-C21-C22	4.26	120.70	111.48
49	4	504	PLC	O2-C'-C1'	4.17	120.50	111.48
48	5	702	3PE	O21-C21-C22	4.17	120.50	111.48
52	W	402	CDL	OA6-CA5-C11	4.14	120.44	111.48
52	E	403	CDL	OA6-CA5-C11	4.13	120.42	111.48
51	2	502	T7X	O16-C10-C12	4.12	120.40	111.48
52	Z	201	CDL	OA6-CA5-C11	4.11	120.37	111.48
48	4	503	3PE	O21-C21-C22	4.11	120.36	111.48
48	5	701	3PE	O21-C21-C22	4.11	120.36	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	1	401	PLC	O2-C'-C1'	4.09	120.32	111.48
48	6	202	3PE	O21-C21-C22	4.05	120.25	111.48
52	X	201	CDL	OA6-CA5-C11	4.03	120.21	111.48
52	n	201	CDL	OA6-CA5-C11	4.02	120.18	111.48
49	i	1101	PLC	O2-C'-C1'	4.00	120.13	111.48
51	3	201	T7X	O16-C10-C12	3.99	120.12	111.48
48	4	502	3PE	O21-C21-C22	3.99	120.11	111.48
48	I	501	3PE	O21-C21-C22	3.98	120.09	111.48
56	O	201	ZMP	O1-C10-C9	-3.93	119.44	123.98
49	W	401	PLC	C7-N-C6	3.91	119.25	108.98
52	E	403	CDL	OB6-CB5-C51	3.90	119.92	111.48
48	4	501	3PE	O21-C21-C22	3.86	119.83	111.48
48	1	402	3PE	O21-C21-C22	3.83	119.76	111.48
49	4	504	PLC	C7-N-C6	3.82	119.01	108.98
49	i	1101	PLC	C7-N-C6	3.82	119.00	108.98
48	J	201	3PE	O21-C21-C22	3.77	119.64	111.48
49	1	404	PLC	C7-N-C6	3.74	118.79	108.98
48	2	503	3PE	O21-C21-C22	3.72	119.53	111.48
53	E	401	NDP	O2B-P2B-O1X	-3.70	96.15	109.33
48	g	202	3PE	O21-C21-C22	3.63	119.33	111.48
45	B	502	FMN	C4-N3-C2	-3.61	119.22	125.64
52	Z	201	CDL	OB6-CB5-C51	3.60	119.28	111.48
48	b	502	3PE	O21-C21-C22	3.55	119.16	111.48
48	1	403	3PE	O21-C21-C22	3.54	119.14	111.48
54	J	202	LMN	OBY-CCC-CCN	3.43	115.88	109.70
49	W	401	PLC	O2-C'-C1'	3.40	118.83	111.48
54	J	202	LMN	CCT-CCN-CCC	3.39	116.38	110.23
56	O	201	ZMP	C14-C13-N1	3.34	122.42	116.34
53	E	401	NDP	PN-O5D-C5D	-3.32	102.33	121.35
53	E	401	NDP	PA-O5B-C5B	-3.31	102.37	121.35
53	E	401	NDP	O3-PA-O1A	-3.29	100.82	110.70
54	J	202	LMN	CCL-CCH-CCQ	3.24	117.04	109.68
51	2	502	T7X	C5-C6-C1	3.19	116.92	109.68
51	2	502	T7X	C3-C2-C1	3.16	116.86	109.68
52	g	201	CDL	OB8-CB7-C71	3.16	121.46	111.83
51	b	501	T7X	C5-C6-C1	3.10	116.72	109.68
54	J	202	LMN	OCB-CCS-CCW	3.08	115.66	108.09
51	3	201	T7X	O18-C11-C31	3.07	121.19	111.83
56	Q	201	ZMP	O1-C10-C9	-3.06	120.45	123.98
52	n	201	CDL	OB8-CB7-C71	3.03	121.07	111.83
48	I	501	3PE	O31-C31-C32	3.02	121.03	111.83
52	W	402	CDL	OB8-CB7-C71	2.95	120.84	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	2	502	T7X	O18-C11-C31	2.95	120.83	111.83
45	B	502	FMN	O4-C4-C4A	-2.95	118.75	126.53
48	4	502	3PE	O31-C31-C32	2.94	120.81	111.83
56	O	201	ZMP	O1-C10-S1	-2.92	118.97	122.68
52	Z	201	CDL	OB8-CB7-C71	2.90	120.67	111.83
54	J	202	LMN	CCS-OBZ-CCD	-2.88	108.09	113.72
52	E	403	CDL	OA8-CA7-C31	2.87	120.59	111.83
45	B	502	FMN	C4A-C4-N3	2.86	120.55	113.25
53	E	401	NDP	O2N-PN-O3	2.83	114.93	107.27
54	a	201	LMN	CCR-O4-C4	-2.83	111.28	117.98
48	6	201	3PE	O31-C31-C32	2.81	120.40	111.83
49	4	504	PLC	O3-CB-C1B	2.81	120.40	111.83
52	g	201	CDL	OA8-CA7-C31	2.81	120.39	111.83
52	X	201	CDL	OB8-CB7-C71	2.77	120.28	111.83
48	4	501	3PE	O31-C31-C32	2.75	120.23	111.83
53	E	401	NDP	O5D-PN-O1N	-2.75	98.03	108.94
49	1	404	PLC	O3-CB-C1B	2.75	120.22	111.83
56	O	201	ZMP	C19-C18-C17	2.75	113.45	108.77
48	J	201	3PE	O31-C31-C32	2.74	120.17	111.83
52	Z	201	CDL	OA8-CA7-C31	2.73	120.17	111.83
52	E	403	CDL	OB8-CB7-C71	2.73	120.16	111.83
49	W	401	PLC	O3-CB-C1B	2.72	120.12	111.83
49	W	401	PLC	C3-C2-C1	-2.71	105.46	111.78
49	i	1101	PLC	O3-CB-C1B	2.71	120.11	111.83
51	b	501	T7X	O18-C11-C31	2.70	120.06	111.83
49	1	401	PLC	O3-CB-C1B	2.69	120.03	111.83
54	J	202	LMN	O3-C3-C2	-2.68	104.06	110.38
48	E	402	3PE	C2-O21-C21	-2.68	111.39	117.80
50	2	501	CPL	O3-C11-C12	2.65	119.92	111.83
56	O	201	ZMP	C15-C14-C13	2.64	116.80	112.39
52	X	201	CDL	OA8-CA7-C31	2.64	119.87	111.83
48	5	702	3PE	O31-C31-C32	2.60	119.77	111.83
54	J	202	LMN	CCJ-CCL-CCH	2.60	115.48	110.01
53	E	401	NDP	C2A-N1A-C6A	-2.60	114.46	118.73
53	E	401	NDP	O2N-PN-O1N	2.60	124.53	112.44
53	E	401	NDP	O3X-P2B-O2X	2.57	117.45	107.80
52	E	403	CDL	CB4-OB6-CB5	-2.57	111.65	117.80
48	1	402	3PE	O31-C31-C32	2.56	119.65	111.83
54	J	202	LMN	CBK-CBQ-CCM	-2.56	109.42	117.19
52	g	201	CDL	CA4-OA6-CA5	-2.55	111.70	117.80
48	6	202	3PE	O31-C31-C32	2.54	119.58	111.83
48	E	402	3PE	O31-C31-C32	2.53	119.54	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	b	502	3PE	O31-C31-C32	2.52	119.53	111.83
48	g	202	3PE	O31-C31-C32	2.48	119.38	111.83
48	2	503	3PE	O31-C31-C32	2.47	119.38	111.83
54	J	202	LMN	OCB-CCQ-CCH	-2.46	100.97	107.23
48	4	503	3PE	O31-C31-C32	2.44	119.27	111.83
45	B	502	FMN	C4A-C10-N1	-2.42	118.66	124.59
56	O	201	ZMP	C12-N1-C13	-2.42	118.32	122.82
52	n	201	CDL	OA8-CA7-C31	2.41	119.17	111.83
48	5	701	3PE	O31-C31-C32	2.37	119.07	111.83
51	2	502	T7X	O12-P1-O1	2.37	116.33	106.70
52	W	402	CDL	OA8-CA7-C31	2.37	119.05	111.83
53	E	401	NDP	C4B-O4B-C1B	-2.36	104.25	109.47
49	1	404	PLC	C2-O2-C'	-2.36	112.16	117.80
54	J	202	LMN	OCB-CCQ-CCF	2.35	115.63	109.48
49	1	401	PLC	C4-C5-N	-2.34	108.32	115.82
54	a	201	LMN	CCS-OCB-CCQ	-2.32	112.47	117.98
56	O	201	ZMP	O2-C13-C14	-2.30	117.85	122.02
48	J	201	3PE	C2-O21-C21	-2.29	112.32	117.80
53	E	401	NDP	C3N-C2N-N1N	-2.26	119.88	123.20
51	3	201	T7X	O1-C1-C2	2.25	113.50	108.73
51	3	201	T7X	O1-C1-C6	2.24	113.47	108.73
48	4	503	3PE	C2-O21-C21	-2.23	112.45	117.80
52	E	403	CDL	CA4-OA6-CA5	-2.23	112.47	117.80
54	J	202	LMN	O4-C4-C5	-2.22	103.65	109.48
53	E	401	NDP	N3A-C4A-N9A	2.22	130.94	127.17
49	1	404	PLC	O2-C'-O'	-2.22	118.53	123.70
51	3	201	T7X	C8-O16-C10	-2.22	112.49	117.80
50	2	501	CPL	C6-N-C5	2.19	118.62	109.91
46	B	503	NAI	C3D-C2D-C1D	2.18	105.59	101.46
48	4	502	3PE	C2-O21-C21	-2.17	112.59	117.80
45	B	502	FMN	C4A-C10-N10	2.15	119.56	116.48
53	E	401	NDP	C5B-C4B-C3B	-2.15	107.47	115.21
56	Q	201	ZMP	O1-C10-S1	-2.12	119.99	122.68
54	a	201	LMN	C1-O5-C5	-2.12	109.58	113.72
51	2	502	T7X	O1-C1-C6	2.11	113.21	108.73
50	2	501	CPL	C4-C5-N	-2.11	109.05	115.82
48	I	501	3PE	C2-O21-C21	-2.11	112.75	117.80
52	g	201	CDL	CB4-OB6-CB5	-2.11	112.75	117.80
48	5	702	3PE	C2-O21-C21	-2.11	112.75	117.80
45	B	502	FMN	C4-C4A-C10	2.11	120.54	116.93
53	E	401	NDP	O3X-P2B-O2B	-2.07	97.77	105.85
51	2	502	T7X	C9-C8-C7	-2.03	107.05	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	n	201	CDL	CA4-OA6-CA5	-2.03	112.94	117.80
53	E	401	NDP	C5D-C4D-C3D	-2.03	107.92	115.21
50	2	501	CPL	C2-O2-C31	-2.01	112.97	117.80
53	E	401	NDP	C5A-C4A-N3A	-2.01	123.95	126.72
48	4	501	3PE	C3-C2-C1	-2.01	107.11	111.78
48	I	501	3PE	O21-C21-O22	-2.00	119.02	123.70

There are no chirality outliers.

All (871) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	B	502	FMN	C3'-C4'-C5'-O5'
45	B	502	FMN	O4'-C4'-C5'-O5'
45	B	502	FMN	C5'-O5'-P-O1P
45	B	502	FMN	C5'-O5'-P-O2P
45	B	502	FMN	C5'-O5'-P-O3P
48	I	501	3PE	C1-O11-P-O13
48	I	501	3PE	C1-O11-P-O14
48	I	501	3PE	C11-O13-P-O11
48	1	402	3PE	C1-O11-P-O12
48	1	402	3PE	C1-O11-P-O13
48	1	402	3PE	C1-O11-P-O14
48	1	402	3PE	O13-C11-C12-N
48	1	402	3PE	C22-C21-O21-C2
48	1	403	3PE	O32-C31-O31-C3
48	1	403	3PE	C32-C31-O31-C3
48	2	503	3PE	C1-O11-P-O12
48	2	503	3PE	C1-O11-P-O13
48	4	501	3PE	C1-O11-P-O12
48	4	501	3PE	C1-O11-P-O14
48	4	501	3PE	C11-O13-P-O11
48	4	501	3PE	C11-O13-P-O12
48	4	501	3PE	C11-O13-P-O14
48	4	501	3PE	O13-C11-C12-N
48	4	502	3PE	C11-O13-P-O11
48	4	502	3PE	C11-O13-P-O14
48	4	503	3PE	C1-O11-P-O13
48	4	503	3PE	C1-O11-P-O14
48	5	701	3PE	O13-C11-C12-N
48	5	701	3PE	C22-C21-O21-C2
48	5	702	3PE	O13-C11-C12-N
48	5	703	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
48	5	703	3PE	C1-O11-P-O14
48	5	703	3PE	C11-O13-P-O11
48	5	703	3PE	C11-O13-P-O12
48	5	703	3PE	C11-O13-P-O14
48	5	703	3PE	O13-C11-C12-N
48	6	201	3PE	C1-O11-P-O12
48	6	201	3PE	C1-O11-P-O13
48	6	201	3PE	C1-O11-P-O14
48	6	201	3PE	C11-O13-P-O14
48	6	202	3PE	C1-O11-P-O13
48	6	202	3PE	C1-O11-P-O14
48	g	202	3PE	C11-O13-P-O11
48	g	202	3PE	C11-O13-P-O12
48	g	202	3PE	O13-C11-C12-N
48	g	202	3PE	C22-C21-O21-C2
48	E	402	3PE	C1-O11-P-O12
48	E	402	3PE	C1-O11-P-O13
48	E	402	3PE	C1-O11-P-O14
48	E	402	3PE	C11-O13-P-O11
48	E	402	3PE	C11-O13-P-O12
48	E	402	3PE	C11-O13-P-O14
48	E	402	3PE	O13-C11-C12-N
48	J	201	3PE	C11-O13-P-O11
48	J	201	3PE	C11-O13-P-O12
48	J	201	3PE	O13-C11-C12-N
48	J	201	3PE	O22-C21-O21-C2
48	J	201	3PE	C22-C21-O21-C2
48	b	502	3PE	C1-O11-P-O13
48	b	502	3PE	C1-O11-P-O14
49	K	302	PLC	C1'-C'-O2-C2
49	K	302	PLC	O'-C'-O2-C2
49	1	401	PLC	O4P-C4-C5-N
49	1	401	PLC	O'-C'-O2-C2
49	1	401	PLC	C1-O3P-P-O1P
49	1	401	PLC	C1-O3P-P-O4P
49	1	404	PLC	O4P-C4-C5-N
49	1	404	PLC	C1'-C'-O2-C2
49	1	404	PLC	O'-C'-O2-C2
49	1	404	PLC	C1-O3P-P-O2P
49	1	404	PLC	C1-O3P-P-O4P
49	1	404	PLC	C4-O4P-P-O2P
49	1	404	PLC	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
49	4	504	PLC	C4-O4P-P-O1P
49	4	504	PLC	C4-O4P-P-O2P
49	W	401	PLC	C4-O4P-P-O2P
49	W	401	PLC	C4-O4P-P-O3P
49	i	1101	PLC	C1-O3P-P-O2P
49	i	1101	PLC	C1-O3P-P-O4P
49	i	1101	PLC	C4-O4P-P-O1P
49	i	1101	PLC	C4-O4P-P-O2P
49	i	1101	PLC	C4-O4P-P-O3P
50	2	501	CPL	C1-O3P-P-O1P
50	2	501	CPL	C1-O3P-P-O2P
50	2	501	CPL	C1-O3P-P-O4P
51	2	502	T7X	C6-C1-O1-P1
51	2	502	T7X	C1-O1-P1-O12
51	2	502	T7X	C1-O1-P1-O13
51	2	502	T7X	C12-C10-O16-C8
51	2	502	T7X	O19-C11-O18-C9
51	2	502	T7X	C31-C11-O18-C9
51	2	502	T7X	C19-C20-C21-C22
51	3	201	T7X	C2-C1-O1-P1
51	3	201	T7X	C6-C1-O1-P1
51	3	201	T7X	C31-C11-O18-C9
51	b	501	T7X	C12-C10-O16-C8
52	g	201	CDL	CB2-C1-CA2-OA2
52	E	403	CDL	CA2-OA2-PA1-OA5
52	E	403	CDL	CB3-OB5-PB2-OB2
52	E	403	CDL	CB3-OB5-PB2-OB3
52	E	403	CDL	CB3-OB5-PB2-OB4
52	W	402	CDL	CA3-OA5-PA1-OA2
52	W	402	CDL	CA3-OA5-PA1-OA3
52	X	201	CDL	CB2-OB2-PB2-OB3
52	X	201	CDL	OB7-CB5-OB6-CB4
52	X	201	CDL	C51-CB5-OB6-CB4
52	Z	201	CDL	CA3-OA5-PA1-OA2
52	Z	201	CDL	CA3-OA5-PA1-OA4
52	Z	201	CDL	C11-CA5-OA6-CA4
52	Z	201	CDL	CB3-OB5-PB2-OB4
52	n	201	CDL	C1-CA2-OA2-PA1
52	n	201	CDL	CA2-OA2-PA1-OA4
52	n	201	CDL	CA2-OA2-PA1-OA5
52	n	201	CDL	CA3-OA5-PA1-OA2
52	n	201	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
52	n	201	CDL	C11-CA5-OA6-CA4
52	n	201	CDL	CB2-OB2-PB2-OB4
52	n	201	CDL	CB2-OB2-PB2-OB5
52	n	201	CDL	CB3-OB5-PB2-OB2
52	n	201	CDL	CB3-OB5-PB2-OB3
52	n	201	CDL	CB3-OB5-PB2-OB4
52	n	201	CDL	OB7-CB5-OB6-CB4
53	E	401	NDP	O4D-C4D-C5D-O5D
54	J	202	LMN	C2-C1-O1-CBS
54	J	202	LMN	CBK-CBQ-CCM-CBS
54	J	202	LMN	CBL-CBR-CCM-CBQ
54	J	202	LMN	CBL-CBR-CCM-CBS
54	J	202	LMN	CBL-CBR-CCM-CBT
54	J	202	LMN	O1-CBS-CCM-CBQ
54	J	202	LMN	O1-CBS-CCM-CBR
54	J	202	LMN	OBV-CBT-CCM-CBR
54	J	202	LMN	OBX-CCJ-OBV-CBT
54	a	201	LMN	OBY-CCR-O4-C4
54	a	201	LMN	CBK-CBQ-CCM-CBR
54	a	201	LMN	CBK-CBQ-CCM-CBT
54	a	201	LMN	OBX-CCJ-OBV-CBT
56	O	201	ZMP	O4-C17-C18-C21
56	O	201	ZMP	C16-C17-C18-C21
56	O	201	ZMP	O4-C17-C18-C19
56	O	201	ZMP	C16-C17-C18-C19
56	O	201	ZMP	O4-C17-C18-C20
56	O	201	ZMP	C16-C17-C18-C20
56	O	201	ZMP	C12-C11-S1-C10
56	O	201	ZMP	O1-C10-S1-C11
56	O	201	ZMP	C9-C10-S1-C11
56	O	201	ZMP	C7-C8-C9-C10
56	Q	201	ZMP	C19-C18-C21-O5
56	Q	201	ZMP	C20-C18-C21-O5
56	Q	201	ZMP	C17-C18-C21-O5
56	Q	201	ZMP	C12-C11-S1-C10
56	Q	201	ZMP	C7-C8-C9-C10
48	1	402	3PE	O32-C31-O31-C3
48	4	501	3PE	O32-C31-O31-C3
48	4	502	3PE	O32-C31-O31-C3
51	3	201	T7X	O19-C11-O18-C9
52	n	201	CDL	OA9-CA7-OA8-CA6
48	1	402	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
48	4	501	3PE	C32-C31-O31-C3
48	4	502	3PE	C32-C31-O31-C3
52	n	201	CDL	C31-CA7-OA8-CA6
52	Z	201	CDL	OA9-CA7-OA8-CA6
52	n	201	CDL	OB9-CB7-OB8-CB6
48	1	402	3PE	O22-C21-O21-C2
48	5	701	3PE	O22-C21-O21-C2
48	g	202	3PE	O22-C21-O21-C2
51	b	501	T7X	O17-C10-O16-C8
52	n	201	CDL	OA7-CA5-OA6-CA4
49	1	401	PLC	C1'-C'-O2-C2
52	E	403	CDL	C11-CA5-OA6-CA4
52	n	201	CDL	C51-CB5-OB6-CB4
49	1	404	PLC	OB-CB-O3-C3
52	Z	201	CDL	OB9-CB7-OB8-CB6
52	Z	201	CDL	C31-CA7-OA8-CA6
52	n	201	CDL	C71-CB7-OB8-CB6
49	i	1101	PLC	OB-CB-O3-C3
51	2	502	T7X	O17-C10-O16-C8
52	E	403	CDL	OA7-CA5-OA6-CA4
52	Z	201	CDL	OA7-CA5-OA6-CA4
56	O	201	ZMP	C14-C15-N2-C16
52	E	403	CDL	O1-C1-CA2-OA2
52	W	402	CDL	O1-C1-CA2-OA2
52	Z	201	CDL	O1-C1-CB2-OB2
49	1	404	PLC	C1B-CB-O3-C3
49	i	1101	PLC	C1B-CB-O3-C3
54	J	202	LMN	OAL-CBP-CCF-OBX
54	a	201	LMN	OAI-CBM-CCC-OBX
48	I	501	3PE	C22-C21-O21-C2
48	4	502	3PE	C22-C21-O21-C2
48	4	503	3PE	C22-C21-O21-C2
48	b	502	3PE	C22-C21-O21-C2
51	3	201	T7X	C12-C10-O16-C8
52	X	201	CDL	C11-CA5-OA6-CA4
46	B	503	NAI	O4B-C4B-C5B-O5B
46	B	503	NAI	C3B-C4B-C5B-O5B
52	Z	201	CDL	C71-CB7-OB8-CB6
48	b	502	3PE	O22-C21-O21-C2
52	X	201	CDL	OA7-CA5-OA6-CA4
54	J	202	LMN	OAI-CBM-CCC-CCN
54	J	202	LMN	O5-C1-O1-CBS

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Mol	Chain	Res	Type	Atoms
54	a	201	LMN	O5-C1-O1-CBS
49	K	302	PLC	C1B-CB-O3-C3
49	K	302	PLC	OB-CB-O3-C3
52	X	201	CDL	C54-C55-C56-C57
48	5	702	3PE	C22-C21-O21-C2
48	4	502	3PE	O22-C21-O21-C2
48	4	503	3PE	O22-C21-O21-C2
52	E	403	CDL	CB2-C1-CA2-OA2
48	4	503	3PE	C32-C31-O31-C3
48	4	503	3PE	C3C-C3D-C3E-C3F
50	2	501	CPL	C35-C36-C37-C38
49	W	401	PLC	C4-C5-N-C8
52	X	201	CDL	C71-C72-C73-C74
54	J	202	LMN	CCW-CCS-OCB-CCQ
54	a	201	LMN	C2-C1-O1-CBS
54	a	201	LMN	CCL-CCJ-OBV-CBT
48	I	501	3PE	C27-C28-C29-C2A
52	g	201	CDL	O1-C1-CA2-OA2
52	E	403	CDL	O1-C1-CB2-OB2
54	J	202	LMN	OAL-CBP-CCF-CCQ
54	a	201	LMN	OAI-CBM-CCC-CCN
48	4	503	3PE	O32-C31-O31-C3
48	I	501	3PE	O22-C21-O21-C2
51	3	201	T7X	O17-C10-O16-C8
48	1	403	3PE	C22-C21-O21-C2
52	W	402	CDL	C11-CA5-OA6-CA4
49	1	401	PLC	C'-C1'-C2'-C3'
48	6	202	3PE	C3D-C3E-C3F-C3G
54	J	202	LMN	OAJ-CBN-CCD-OBZ
54	J	202	LMN	CBC-CBE-CBG-CBI
54	J	202	LMN	OBZ-CCS-OCB-CCQ
48	5	702	3PE	C21-C22-C23-C24
48	4	502	3PE	C2E-C2F-C2G-C2H
48	1	403	3PE	O22-C21-O21-C2
52	Z	201	CDL	C72-C73-C74-C75
48	5	701	3PE	C21-C22-C23-C24
48	J	201	3PE	C31-C32-C33-C34
51	b	501	T7X	C10-C12-C13-C14
54	J	202	LMN	OAI-CBM-CCC-OBY
48	1	402	3PE	C31-C32-C33-C34
48	5	701	3PE	C31-C32-C33-C34
49	1	401	PLC	CB-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
49	1	404	PLC	CB-C1B-C2B-C3B
49	4	504	PLC	CB-C1B-C2B-C3B
52	Z	201	CDL	C17-C18-C19-C20
52	n	201	CDL	C60-C61-C62-C63
48	b	502	3PE	C24-C25-C26-C27
52	n	201	CDL	C53-C54-C55-C56
48	4	503	3PE	C27-C28-C29-C2A
48	5	702	3PE	O22-C21-O21-C2
52	W	402	CDL	CA5-C11-C12-C13
48	4	503	3PE	C29-C2A-C2B-C2C
52	g	201	CDL	C11-CA5-OA6-CA4
49	i	1101	PLC	C6B-C7B-C8B-C9B
51	2	502	T7X	C10-C12-C13-C14
52	W	402	CDL	OA7-CA5-OA6-CA4
52	W	402	CDL	CB2-C1-CA2-OA2
52	E	403	CDL	C31-CA7-OA8-CA6
52	W	402	CDL	C31-CA7-OA8-CA6
49	W	401	PLC	C4-C5-N-C6
49	W	401	PLC	C4-C5-N-C7
48	6	202	3PE	C35-C36-C37-C38
52	g	201	CDL	C12-C13-C14-C15
54	a	201	LMN	CCH-CCQ-OCB-CCS
53	E	401	NDP	C3D-C4D-C5D-O5D
49	4	504	PLC	C1'-C'-O2-C2
52	W	402	CDL	C51-CB5-OB6-CB4
49	4	504	PLC	O'-C'-O2-C2
52	g	201	CDL	OA7-CA5-OA6-CA4
52	W	402	CDL	OB7-CB5-OB6-CB4
48	2	503	3PE	C21-C22-C23-C24
51	2	502	T7X	C9-C8-O16-C10
54	J	202	LMN	CBJ-CBL-CBR-CCM
49	4	504	PLC	C6B-C7B-C8B-C9B
52	X	201	CDL	C17-C18-C19-C20
52	Z	201	CDL	C54-C55-C56-C57
48	5	703	3PE	O21-C2-C3-O31
48	4	502	3PE	C29-C2A-C2B-C2C
51	b	501	T7X	C32-C33-C34-C35
52	Z	201	CDL	C32-C33-C34-C35
50	2	501	CPL	C20-C21-C22-C23
56	Q	201	ZMP	C3-C4-C5-C6
48	2	503	3PE	C36-C37-C38-C39
52	Z	201	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
52	n	201	CDL	C51-C52-C53-C54
54	a	201	LMN	CCF-CCQ-OCB-CCS
49	1	404	PLC	C2B-C3B-C4B-C5B
49	W	401	PLC	C2'-C3'-C4'-C5'
48	5	703	3PE	C26-C27-C28-C29
48	E	402	3PE	C32-C33-C34-C35
48	4	502	3PE	C26-C27-C28-C29
48	4	503	3PE	C33-C34-C35-C36
48	6	202	3PE	C37-C38-C39-C3A
49	i	1101	PLC	C3'-C4'-C5'-C6'
54	J	202	LMN	CBA-CBC-CBE-CBG
54	J	202	LMN	C5-C4-O4-CCR
48	6	201	3PE	C21-C22-C23-C24
48	E	402	3PE	C31-C32-C33-C34
52	n	201	CDL	CB5-C51-C52-C53
48	I	501	3PE	C38-C39-C3A-C3B
48	g	202	3PE	C2C-C2D-C2E-C2F
52	g	201	CDL	C72-C73-C74-C75
52	n	201	CDL	C41-C42-C43-C44
52	n	201	CDL	C54-C55-C56-C57
52	E	403	CDL	OA9-CA7-OA8-CA6
52	W	402	CDL	OA9-CA7-OA8-CA6
54	J	202	LMN	C3-C4-O4-CCR
48	2	503	3PE	C32-C33-C34-C35
52	X	201	CDL	C51-C52-C53-C54
48	6	201	3PE	C35-C36-C37-C38
48	4	502	3PE	C2D-C2E-C2F-C2G
52	Z	201	CDL	CB3-CB4-CB6-OB8
54	J	202	LMN	OBY-CCR-O4-C4
48	1	402	3PE	C24-C25-C26-C27
49	1	404	PLC	C1B-C2B-C3B-C4B
50	2	501	CPL	C21-C22-C23-C24
52	Z	201	CDL	C56-C57-C58-C59
48	4	502	3PE	C21-C22-C23-C24
49	i	1101	PLC	C'-C1'-C2'-C3'
48	4	503	3PE	C36-C37-C38-C39
48	5	701	3PE	C32-C33-C34-C35
48	5	701	3PE	C36-C37-C38-C39
48	5	702	3PE	C26-C27-C28-C29
48	6	201	3PE	C28-C29-C2A-C2B
48	6	202	3PE	C32-C33-C34-C35
48	b	502	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
49	i	1101	PLC	C5B-C6B-C7B-C8B
51	2	502	T7X	C31-C32-C33-C34
51	2	502	T7X	C34-C35-C36-C37
50	2	501	CPL	C32-C33-C34-C35
52	n	201	CDL	C14-C15-C16-C17
48	6	202	3PE	C3E-C3F-C3G-C3H
52	g	201	CDL	C15-C16-C17-C18
52	g	201	CDL	C51-C52-C53-C54
48	I	501	3PE	C2D-C2E-C2F-C2G
48	2	503	3PE	C3B-C3C-C3D-C3E
49	i	1101	PLC	C1'-C2'-C3'-C4'
49	i	1101	PLC	C4B-C5B-C6B-C7B
52	g	201	CDL	C74-C75-C76-C77
51	b	501	T7X	C11-C31-C32-C33
48	5	703	3PE	C3B-C3C-C3D-C3E
48	I	501	3PE	C3B-C3C-C3D-C3E
48	5	703	3PE	C23-C24-C25-C26
48	5	703	3PE	C29-C2A-C2B-C2C
49	i	1101	PLC	C6'-C7'-C8'-C9'
52	Z	201	CDL	C14-C15-C16-C17
54	J	202	LMN	CAX-CAZ-CBB-CBD
52	n	201	CDL	C33-C34-C35-C36
51	3	201	T7X	C10-C12-C13-C14
50	2	501	CPL	C12-C11-O3-C3
48	I	501	3PE	C26-C27-C28-C29
52	E	403	CDL	C33-C34-C35-C36
52	X	201	CDL	C11-C12-C13-C14
48	4	501	3PE	C33-C34-C35-C36
48	b	502	3PE	C2A-C2B-C2C-C2D
52	n	201	CDL	C34-C35-C36-C37
48	5	701	3PE	C37-C38-C39-C3A
49	1	401	PLC	C2B-C3B-C4B-C5B
48	2	503	3PE	C33-C34-C35-C36
51	2	502	T7X	C36-C37-C38-C39
48	I	501	3PE	C22-C23-C24-C25
48	6	201	3PE	C32-C33-C34-C35
52	X	201	CDL	C14-C15-C16-C17
52	n	201	CDL	C59-C60-C61-C62
54	J	202	LMN	CBD-CBF-CBH-CBJ
52	n	201	CDL	O1-C1-CA2-OA2
48	1	403	3PE	C29-C2A-C2B-C2C
51	3	201	T7X	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
52	g	201	CDL	C33-C34-C35-C36
56	O	201	ZMP	C13-C14-C15-N2
48	2	503	3PE	C31-C32-C33-C34
52	g	201	CDL	CA7-C31-C32-C33
54	a	201	LMN	OAL-CBP-CCF-CCQ
48	g	202	3PE	C21-C22-C23-C24
48	4	503	3PE	C37-C38-C39-C3A
48	5	703	3PE	C38-C39-C3A-C3B
49	1	401	PLC	C3'-C4'-C5'-C6'
52	g	201	CDL	C22-C23-C24-C25
54	J	202	LMN	CBB-CBD-CBF-CBH
54	J	202	LMN	CBK-CBQ-CCM-CBT
54	a	201	LMN	CBK-CBQ-CCM-CBS
48	5	703	3PE	C2B-C2C-C2D-C2E
48	5	701	3PE	C28-C29-C2A-C2B
48	E	402	3PE	C37-C38-C39-C3A
52	g	201	CDL	C14-C15-C16-C17
52	X	201	CDL	C57-C58-C59-C60
52	X	201	CDL	CA7-C31-C32-C33
48	g	202	3PE	C29-C2A-C2B-C2C
49	i	1101	PLC	O3P-C1-C2-O2
52	g	201	CDL	OA5-CA3-CA4-OA6
48	4	501	3PE	C3D-C3E-C3F-C3G
48	5	703	3PE	C37-C38-C39-C3A
49	i	1101	PLC	C5'-C6'-C7'-C8'
56	O	201	ZMP	C2-C3-C4-C5
48	b	502	3PE	C23-C24-C25-C26
52	Z	201	CDL	CA5-C11-C12-C13
48	2	503	3PE	O21-C2-C3-O31
48	b	502	3PE	C32-C31-O31-C3
48	5	701	3PE	C35-C36-C37-C38
49	1	401	PLC	C1'-C2'-C3'-C4'
53	E	401	NDP	O4D-C1D-N1N-C6N
48	I	501	3PE	C28-C29-C2A-C2B
54	a	201	LMN	CAY-CBA-CBC-CBE
54	a	201	LMN	CBJ-CBL-CBR-CCM
48	I	501	3PE	C2A-C2B-C2C-C2D
48	5	701	3PE	C33-C34-C35-C36
48	b	502	3PE	C25-C26-C27-C28
49	4	504	PLC	C3B-C4B-C5B-C6B
52	E	403	CDL	C72-C73-C74-C75
48	6	202	3PE	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
52	n	201	CDL	C74-C75-C76-C77
54	J	202	LMN	O1-CBS-CCM-CBT
52	X	201	CDL	C31-C32-C33-C34
48	I	501	3PE	C2E-C2F-C2G-C2H
48	5	701	3PE	C26-C27-C28-C29
52	E	403	CDL	C31-C32-C33-C34
48	2	503	3PE	C22-C23-C24-C25
51	3	201	T7X	C36-C37-C38-C39
52	E	403	CDL	C59-C60-C61-C62
54	J	202	LMN	CAY-CBA-CBC-CBE
48	I	501	3PE	C32-C31-O31-C3
49	i	1101	PLC	C4'-C5'-C6'-C7'
52	g	201	CDL	C42-C43-C44-C45
48	5	703	3PE	O11-C1-C2-C3
52	Z	201	CDL	OA5-CA3-CA4-CA6
48	5	703	3PE	C21-C22-C23-C24
52	g	201	CDL	CA5-C11-C12-C13
49	i	1101	PLC	C7'-C8'-C9'-CA'
52	X	201	CDL	C56-C57-C58-C59
48	I	501	3PE	C3C-C3D-C3E-C3F
48	1	402	3PE	C23-C24-C25-C26
52	E	403	CDL	C55-C56-C57-C58
52	n	201	CDL	C11-C12-C13-C14
50	2	501	CPL	O11-C11-O3-C3
48	6	202	3PE	C33-C34-C35-C36
49	4	504	PLC	C2B-C3B-C4B-C5B
50	2	501	CPL	C18-C19-C20-C21
48	4	503	3PE	C1-C2-C3-O31
48	5	701	3PE	C1-C2-C3-O31
48	5	702	3PE	C1-C2-C3-O31
48	5	703	3PE	C1-C2-C3-O31
48	6	201	3PE	C1-C2-C3-O31
48	E	402	3PE	C1-C2-C3-O31
49	1	404	PLC	C1-C2-C3-O3
49	4	504	PLC	C1-C2-C3-O3
52	E	403	CDL	CA3-CA4-CA6-OA8
52	E	403	CDL	CB3-CB4-CB6-OB8
52	W	402	CDL	CA3-CA4-CA6-OA8
52	W	402	CDL	CB3-CB4-CB6-OB8
52	X	201	CDL	CA3-CA4-CA6-OA8
52	Z	201	CDL	C57-C58-C59-C60
51	2	502	T7X	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
54	J	202	LMN	CCH-CCQ-OCB-CCS
52	E	403	CDL	C71-CB7-OB8-CB6
52	X	201	CDL	C13-C14-C15-C16
54	J	202	LMN	OAJ-CBN-CCD-CCO
48	g	202	3PE	C2B-C2C-C2D-C2E
48	5	703	3PE	C31-C32-C33-C34
48	b	502	3PE	O32-C31-O31-C3
48	5	702	3PE	C32-C33-C34-C35
48	5	703	3PE	C34-C35-C36-C37
48	b	502	3PE	C2C-C2D-C2E-C2F
48	5	702	3PE	C27-C28-C29-C2A
52	n	201	CDL	C57-C58-C59-C60
49	i	1101	PLC	C3B-C4B-C5B-C6B
48	b	502	3PE	C29-C2A-C2B-C2C
52	n	201	CDL	C35-C36-C37-C38
48	4	501	3PE	C21-C22-C23-C24
52	g	201	CDL	CB7-C71-C72-C73
48	b	502	3PE	C27-C28-C29-C2A
48	2	503	3PE	O11-C1-C2-O21
52	n	201	CDL	OA5-CA3-CA4-OA6
48	I	501	3PE	C3A-C3B-C3C-C3D
49	W	401	PLC	C6'-C7'-C8'-C9'
48	4	502	3PE	C23-C24-C25-C26
50	2	501	CPL	C44-C45-C46-C47
48	4	501	3PE	C26-C27-C28-C29
50	2	501	CPL	C12-C13-C14-C15
48	4	501	3PE	C3A-C3B-C3C-C3D
49	1	404	PLC	C1'-C2'-C3'-C4'
52	g	201	CDL	C19-C20-C21-C22
48	2	503	3PE	C27-C28-C29-C2A
48	1	402	3PE	C35-C36-C37-C38
49	4	504	PLC	C1'-C2'-C3'-C4'
48	4	503	3PE	O21-C2-C3-O31
48	6	201	3PE	O21-C2-C3-O31
52	g	201	CDL	O1-C1-CB2-OB2
51	2	502	T7X	C32-C33-C34-C35
54	J	202	LMN	CCF-CCQ-OCB-CCS
54	J	202	LMN	CBK-CBQ-CCM-CBR
48	6	201	3PE	C26-C27-C28-C29
49	1	404	PLC	C4'-C5'-C6'-C7'
48	g	202	3PE	C2F-C2G-C2H-C2I
52	E	403	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
48	I	501	3PE	O32-C31-O31-C3
48	4	502	3PE	C24-C25-C26-C27
48	4	503	3PE	C26-C27-C28-C29
52	g	201	CDL	C72-C71-CB7-OB8
54	a	201	LMN	O5-C5-C6-O6
52	g	201	CDL	C31-C32-C33-C34
52	X	201	CDL	C35-C36-C37-C38
48	1	402	3PE	C34-C35-C36-C37
48	4	503	3PE	C2F-C2G-C2H-C2I
52	Z	201	CDL	C13-C14-C15-C16
52	W	402	CDL	C12-C13-C14-C15
48	g	202	3PE	C27-C28-C29-C2A
48	6	201	3PE	O21-C21-C22-C23
48	6	202	3PE	C36-C37-C38-C39
52	Z	201	CDL	C33-C34-C35-C36
48	b	502	3PE	C37-C38-C39-C3A
51	3	201	T7X	C32-C33-C34-C35
48	5	702	3PE	O11-C1-C2-C3
50	2	501	CPL	O3P-C1-C2-C3
52	g	201	CDL	OA5-CA3-CA4-CA6
52	n	201	CDL	OA5-CA3-CA4-CA6
48	4	503	3PE	C39-C3A-C3B-C3C
48	1	402	3PE	C28-C29-C2A-C2B
52	X	201	CDL	C32-C33-C34-C35
48	I	501	3PE	C39-C3A-C3B-C3C
48	4	501	3PE	C36-C37-C38-C39
56	Q	201	ZMP	C5-C6-C7-C8
52	E	403	CDL	OB9-CB7-OB8-CB6
52	W	402	CDL	C54-C55-C56-C57
48	b	502	3PE	C38-C39-C3A-C3B
48	4	501	3PE	C3B-C3C-C3D-C3E
56	O	201	ZMP	C1-C2-C3-C4
48	5	703	3PE	C35-C36-C37-C38
48	6	202	3PE	C3B-C3C-C3D-C3E
52	Z	201	CDL	C19-C20-C21-C22
54	a	201	LMN	C4-C5-C6-O6
52	Z	201	CDL	CA2-C1-CB2-OB2
52	n	201	CDL	CB2-C1-CA2-OA2
52	E	403	CDL	C16-C17-C18-C19
48	5	702	3PE	C32-C31-O31-C3
48	2	503	3PE	C1-C2-C3-O31
48	g	202	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
52	X	201	CDL	CB5-C51-C52-C53
48	g	202	3PE	C25-C26-C27-C28
52	g	201	CDL	C37-C38-C39-C40
48	1	403	3PE	C34-C35-C36-C37
48	5	702	3PE	C33-C34-C35-C36
52	n	201	CDL	C72-C73-C74-C75
48	4	502	3PE	O11-C1-C2-O21
48	5	703	3PE	O11-C1-C2-O21
49	4	504	PLC	O3P-C1-C2-O2
52	X	201	CDL	OA5-CA3-CA4-OA6
52	Z	201	CDL	OB5-CB3-CB4-OB6
48	4	501	3PE	C32-C33-C34-C35
45	B	502	FMN	C4'-C5'-O5'-P
49	i	1101	PLC	C1B-C2B-C3B-C4B
52	E	403	CDL	C57-C58-C59-C60
52	X	201	CDL	C60-C61-C62-C63
48	1	402	3PE	O21-C2-C3-O31
48	6	202	3PE	O21-C2-C3-O31
48	g	202	3PE	O21-C2-C3-O31
49	W	401	PLC	C8B-C9B-CAA-CBA
51	3	201	T7X	C15-C16-C17-C18
51	b	501	T7X	C16-C17-C18-C19
51	b	501	T7X	C22-C23-C24-C25
48	I	501	3PE	C2F-C2G-C2H-C2I
46	B	503	NAI	C2D-C1D-N1N-C2N
49	W	401	PLC	C'-C1'-C2'-C3'
48	6	202	3PE	C24-C25-C26-C27
48	E	402	3PE	C33-C34-C35-C36
49	K	302	PLC	C2B-C3B-C4B-C5B
54	a	201	LMN	OAL-CBP-CCF-OBX
48	1	403	3PE	C2B-C2C-C2D-C2E
48	b	502	3PE	C32-C33-C34-C35
52	n	201	CDL	CA5-C11-C12-C13
52	n	201	CDL	C37-C38-C39-C40
48	5	703	3PE	C2A-C2B-C2C-C2D
54	J	202	LMN	CAA-CAW-CAY-CBA
48	5	703	3PE	C24-C25-C26-C27
48	1	402	3PE	C25-C26-C27-C28
49	4	504	PLC	C2'-C3'-C4'-C5'
48	b	502	3PE	C35-C36-C37-C38
52	X	201	CDL	C53-C54-C55-C56
48	5	702	3PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
52	n	201	CDL	C22-C23-C24-C25
51	b	501	T7X	C34-C35-C36-C37
48	1	402	3PE	C21-C22-C23-C24
49	W	401	PLC	C1B-C2B-C3B-C4B
48	I	501	3PE	C32-C33-C34-C35
52	n	201	CDL	C16-C17-C18-C19
48	2	503	3PE	O11-C1-C2-C3
48	6	201	3PE	O11-C1-C2-C3
48	g	202	3PE	O11-C1-C2-C3
52	Z	201	CDL	OB5-CB3-CB4-CB6
48	6	201	3PE	C25-C26-C27-C28
48	5	702	3PE	C2C-C2D-C2E-C2F
48	J	201	3PE	C22-C23-C24-C25
49	1	404	PLC	C5B-C6B-C7B-C8B
50	2	501	CPL	C33-C34-C35-C36
48	5	702	3PE	O32-C31-O31-C3
52	X	201	CDL	C71-CB7-OB8-CB6
51	b	501	T7X	C7-C8-O16-C10
52	X	201	CDL	CA6-CA4-OA6-CA5
48	J	201	3PE	C24-C25-C26-C27
48	5	702	3PE	O11-C1-C2-O21
48	6	201	3PE	O11-C1-C2-O21
50	2	501	CPL	O3P-C1-C2-O2
51	2	502	T7X	O13-C7-C8-O16
52	Z	201	CDL	OA5-CA3-CA4-OA6
48	6	202	3PE	C1-C2-C3-O31
48	b	502	3PE	C2D-C2E-C2F-C2G
49	1	404	PLC	C2'-C3'-C4'-C5'
49	4	504	PLC	C5-C4-O4P-P
48	J	201	3PE	C39-C3A-C3B-C3C
52	n	201	CDL	C42-C43-C44-C45
48	4	502	3PE	C28-C29-C2A-C2B
48	5	701	3PE	O21-C2-C3-O31
48	5	702	3PE	O21-C2-C3-O31
48	E	402	3PE	O21-C2-C3-O31
49	4	504	PLC	O2-C2-C3-O3
52	E	403	CDL	OA6-CA4-CA6-OA8
52	W	402	CDL	OA6-CA4-CA6-OA8
52	Z	201	CDL	OA6-CA4-CA6-OA8
52	g	201	CDL	C38-C39-C40-C41
52	E	403	CDL	C56-C57-C58-C59
48	5	701	3PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
52	W	402	CDL	C51-C52-C53-C54
49	W	401	PLC	O2-C'-C1'-C2'
46	B	503	NAI	PN-O3-PA-O2A
49	K	302	PLC	O4P-C4-C5-N
49	i	1101	PLC	O4P-C4-C5-N
52	E	403	CDL	CA2-C1-CB2-OB2
52	X	201	CDL	OB9-CB7-OB8-CB6
48	1	403	3PE	C38-C39-C3A-C3B
48	5	702	3PE	C34-C35-C36-C37
48	6	202	3PE	C39-C3A-C3B-C3C
54	J	202	LMN	OBV-CBT-CCM-CBQ
49	W	401	PLC	C5B-C6B-C7B-C8B
48	I	501	3PE	C3D-C3E-C3F-C3G
54	J	202	LMN	OBV-CBT-CCM-CBS
52	n	201	CDL	C64-C65-C66-C67
48	4	502	3PE	C25-C26-C27-C28
56	O	201	ZMP	O3-C16-C17-O4
52	n	201	CDL	C43-C44-C45-C46
46	B	503	NAI	C2D-C1D-N1N-C6N
49	4	504	PLC	O3P-C1-C2-C3
49	i	1101	PLC	O3P-C1-C2-C3
52	E	403	CDL	OA5-CA3-CA4-CA6
48	4	502	3PE	C36-C37-C38-C39
53	E	401	NDP	O4B-C4B-C5B-O5B
52	g	201	CDL	C1-CB2-OB2-PB2
48	g	202	3PE	O11-C1-C2-O21
52	E	403	CDL	OA5-CA3-CA4-OA6
52	W	402	CDL	OA5-CA3-CA4-OA6
48	1	403	3PE	C24-C25-C26-C27
52	E	403	CDL	C36-C37-C38-C39
48	2	503	3PE	C35-C36-C37-C38
48	I	501	3PE	C36-C37-C38-C39
51	2	502	T7X	C11-C31-C32-C33
49	W	401	PLC	C7B-C8B-C9B-CAA
48	4	502	3PE	O21-C2-C3-O31
49	1	401	PLC	O2-C2-C3-O3
51	b	501	T7X	O16-C8-C9-O18
52	E	403	CDL	OB6-CB4-CB6-OB8
52	X	201	CDL	OA6-CA4-CA6-OA8
52	Z	201	CDL	OB6-CB4-CB6-OB8
48	I	501	3PE	C1-C2-C3-O31
48	1	402	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
48	4	502	3PE	C1-C2-C3-O31
51	3	201	T7X	C7-C8-C9-O18
52	Z	201	CDL	CA3-CA4-CA6-OA8
48	4	503	3PE	O31-C31-C32-C33
51	2	502	T7X	C33-C34-C35-C36
52	Z	201	CDL	C31-C32-C33-C34
52	Z	201	CDL	C59-C60-C61-C62
52	n	201	CDL	C20-C21-C22-C23
47	C	601	UQ9	C5-C4-O4-C4M
48	1	403	3PE	C36-C37-C38-C39
52	n	201	CDL	C39-C40-C41-C42
48	1	403	3PE	C1-O11-P-O12
48	2	503	3PE	O13-C11-C12-N
48	4	501	3PE	C1-O11-P-O13
48	4	503	3PE	C1-O11-P-O12
48	5	703	3PE	C1-O11-P-O13
48	6	202	3PE	O13-C11-C12-N
48	g	202	3PE	C1-O11-P-O12
48	g	202	3PE	C1-O11-P-O13
48	g	202	3PE	C1-O11-P-O14
48	g	202	3PE	C11-O13-P-O14
48	J	201	3PE	C1-O11-P-O12
48	J	201	3PE	C1-O11-P-O13
48	J	201	3PE	C1-O11-P-O14
48	J	201	3PE	C11-O13-P-O14
49	1	401	PLC	C1-O3P-P-O2P
49	1	404	PLC	C1-O3P-P-O1P
49	4	504	PLC	C1-O3P-P-O1P
49	4	504	PLC	C4-O4P-P-O3P
49	W	401	PLC	C4-O4P-P-O1P
49	i	1101	PLC	C1-O3P-P-O1P
51	b	501	T7X	C7-O13-P1-O1
51	b	501	T7X	C7-O13-P1-O11
52	E	403	CDL	CA2-OA2-PA1-OA3
52	W	402	CDL	CB3-OB5-PB2-OB2
52	W	402	CDL	CB3-OB5-PB2-OB3
52	W	402	CDL	CB3-OB5-PB2-OB4
52	X	201	CDL	CA2-OA2-PA1-OA4
52	X	201	CDL	CB2-OB2-PB2-OB4
52	X	201	CDL	CB2-OB2-PB2-OB5
52	Z	201	CDL	CB3-OB5-PB2-OB2
52	Z	201	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
48	6	201	3PE	C27-C28-C29-C2A
48	1	402	3PE	C2-C1-O11-P
52	X	201	CDL	CA4-CA3-OA5-PA1
52	g	201	CDL	C76-C77-C78-C79
48	E	402	3PE	C21-C22-C23-C24
52	n	201	CDL	C76-C77-C78-C79
49	i	1101	PLC	CB-C1B-C2B-C3B
48	1	403	3PE	C3-C2-O21-C21
54	J	202	LMN	CBF-CBH-CBJ-CBL
52	Z	201	CDL	C11-C12-C13-C14
49	4	504	PLC	C4-C5-N-C7
48	4	502	3PE	O11-C1-C2-C3
51	2	502	T7X	O13-C7-C8-C9
49	1	401	PLC	C3B-C4B-C5B-C6B
49	i	1101	PLC	C8'-C9'-CA'-CB'
52	W	402	CDL	CA7-C31-C32-C33
48	2	503	3PE	C37-C38-C39-C3A
48	6	202	3PE	O21-C21-C22-C23
48	4	502	3PE	C22-C23-C24-C25
48	4	503	3PE	C3E-C3F-C3G-C3H
48	1	403	3PE	C22-C23-C24-C25
49	W	401	PLC	C3'-C4'-C5'-C6'
48	I	501	3PE	O21-C2-C3-O31
49	1	404	PLC	O2-C2-C3-O3
52	W	402	CDL	OB6-CB4-CB6-OB8
48	4	502	3PE	C34-C35-C36-C37
48	E	402	3PE	C38-C39-C3A-C3B
48	4	503	3PE	C3D-C3E-C3F-C3G
49	1	401	PLC	C1-C2-C3-O3
51	b	501	T7X	C33-C34-C35-C36
48	g	202	3PE	C26-C27-C28-C29
52	X	201	CDL	C64-C65-C66-C67
53	E	401	NDP	C2B-O2B-P2B-O3X
52	g	201	CDL	CB5-C51-C52-C53
49	W	401	PLC	C6B-C7B-C8B-C9B
48	5	702	3PE	C2A-C2B-C2C-C2D
52	g	201	CDL	C13-C14-C15-C16
52	g	201	CDL	C41-C42-C43-C44
46	B	503	NAI	O4D-C1D-N1N-C2N
48	5	702	3PE	C35-C36-C37-C38
49	1	401	PLC	O3P-C1-C2-O2
52	g	201	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
54	J	202	LMN	CAZ-CBB-CBD-CBF
54	J	202	LMN	CAW-CAY-CBA-CBC
48	5	702	3PE	C22-C23-C24-C25
48	4	501	3PE	C39-C3A-C3B-C3C
52	W	402	CDL	C1-CA2-OA2-PA1
48	4	502	3PE	C37-C38-C39-C3A
56	O	201	ZMP	C11-C12-N1-C13
48	J	201	3PE	C26-C27-C28-C29
54	a	201	LMN	CBC-CBE-CBG-CBI
48	1	402	3PE	C36-C37-C38-C39
52	W	402	CDL	CA6-CA4-OA6-CA5
48	g	202	3PE	C36-C37-C38-C39
52	W	402	CDL	C32-C31-CA7-OA8
52	g	201	CDL	C72-C71-CB7-OB9
52	Z	201	CDL	CA4-CA3-OA5-PA1
52	n	201	CDL	C1-CB2-OB2-PB2
52	E	403	CDL	C53-C54-C55-C56
52	W	402	CDL	OA5-CA3-CA4-CA6
52	X	201	CDL	OA5-CA3-CA4-CA6
50	2	501	CPL	C39-C40-C41-C42
50	2	501	CPL	C40-C41-C42-C43
51	b	501	T7X	C15-C16-C17-C18
50	2	501	CPL	C45-C46-C47-C48
53	E	401	NDP	C2B-O2B-P2B-O1X
54	a	201	LMN	CAW-CAY-CBA-CBC
52	n	201	CDL	C19-C20-C21-C22
56	Q	201	ZMP	C1-C2-C3-C4
54	a	201	LMN	CBA-CBC-CBE-CBG
49	4	504	PLC	C2-C1-O3P-P
52	W	402	CDL	C32-C33-C34-C35
48	b	502	3PE	C34-C35-C36-C37
48	6	201	3PE	O22-C21-C22-C23
56	O	201	ZMP	O2-C13-C14-C15
48	5	701	3PE	C25-C26-C27-C28
48	E	402	3PE	C39-C3A-C3B-C3C
52	E	403	CDL	C51-C52-C53-C54
52	X	201	CDL	C12-C13-C14-C15
52	g	201	CDL	CA2-C1-CB2-OB2
49	4	504	PLC	C4-C5-N-C8
48	J	201	3PE	O31-C31-C32-C33
48	I	501	3PE	C35-C36-C37-C38
48	4	502	3PE	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
52	n	201	CDL	C58-C59-C60-C61
52	g	201	CDL	C44-C45-C46-C47
48	b	502	3PE	C26-C27-C28-C29
49	K	302	PLC	CB-C1B-C2B-C3B
50	2	501	CPL	C42-C43-C44-C45
48	J	201	3PE	C23-C24-C25-C26
52	n	201	CDL	C56-C57-C58-C59
48	I	501	3PE	C24-C25-C26-C27
54	a	201	LMN	CBG-CBI-CBK-CBQ
48	b	502	3PE	O11-C1-C2-O21
48	5	703	3PE	C2C-C2D-C2E-C2F
56	O	201	ZMP	N1-C13-C14-C15
52	n	201	CDL	C31-C32-C33-C34
48	6	202	3PE	C3F-C3G-C3H-C3I
49	4	504	PLC	C4B-C5B-C6B-C7B
48	4	503	3PE	C2C-C2D-C2E-C2F
51	2	502	T7X	C13-C14-C15-C16
51	b	501	T7X	C13-C14-C15-C16
56	Q	201	ZMP	C16-C17-C18-C20
48	4	501	3PE	C22-C23-C24-C25
48	6	201	3PE	C24-C25-C26-C27
48	2	503	3PE	O21-C21-C22-C23
54	J	202	LMN	CCV-CCR-O4-C4
48	5	703	3PE	C39-C3A-C3B-C3C
50	2	501	CPL	C22-C23-C24-C25
45	B	502	FMN	O3'-C3'-C4'-C5'
48	J	201	3PE	O21-C21-C22-C23
52	X	201	CDL	C40-C41-C42-C43
51	2	502	T7X	C1-O1-P1-O11
52	X	201	CDL	C72-C71-CB7-OB8
50	2	501	CPL	O31-C31-O2-C2
48	4	501	3PE	C3C-C3D-C3E-C3F
48	1	403	3PE	C26-C27-C28-C29
51	b	501	T7X	O16-C10-C12-C13
52	Z	201	CDL	C73-C74-C75-C76
52	n	201	CDL	C44-C45-C46-C47
48	b	502	3PE	O21-C21-C22-C23
51	b	501	T7X	C31-C32-C33-C34
52	E	403	CDL	OB5-CB3-CB4-OB6
52	g	201	CDL	C32-C31-CA7-OA8
52	X	201	CDL	C62-C63-C64-C65
48	4	503	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
52	W	402	CDL	C72-C71-CB7-OB8
48	2	503	3PE	O31-C31-C32-C33
52	W	402	CDL	CB7-C71-C72-C73
48	5	701	3PE	C2A-C2B-C2C-C2D
48	1	403	3PE	O31-C31-C32-C33
48	6	201	3PE	O31-C31-C32-C33
48	4	501	3PE	C24-C25-C26-C27
52	W	402	CDL	CA3-CA4-OA6-CA5
48	4	501	3PE	C34-C35-C36-C37
52	X	201	CDL	C38-C39-C40-C41
48	4	503	3PE	C38-C39-C3A-C3B
46	B	503	NAI	O4D-C1D-N1N-C6N
56	Q	201	ZMP	C6-C7-C8-C9
49	W	401	PLC	O'-C'-C1'-C2'
48	2	503	3PE	O32-C31-C32-C33
48	4	503	3PE	O22-C21-C22-C23
52	n	201	CDL	C32-C33-C34-C35
52	E	403	CDL	C71-C72-C73-C74
51	b	501	T7X	O17-C10-C12-C13
48	6	202	3PE	C3A-C3B-C3C-C3D
52	n	201	CDL	C61-C62-C63-C64
48	J	201	3PE	O22-C21-C22-C23
52	W	402	CDL	C31-C32-C33-C34
48	5	702	3PE	C24-C25-C26-C27
48	2	503	3PE	O22-C21-C22-C23
52	X	201	CDL	C72-C71-CB7-OB9
56	O	201	ZMP	N2-C16-C17-O4
56	Q	201	ZMP	N2-C16-C17-O4
48	b	502	3PE	O22-C21-C22-C23
49	4	504	PLC	C4-C5-N-C6
52	g	201	CDL	C32-C31-CA7-OA9
48	6	202	3PE	O31-C31-C32-C33
48	I	501	3PE	C37-C38-C39-C3A
48	J	201	3PE	C37-C38-C39-C3A
49	1	401	PLC	O3P-C1-C2-C3
48	5	701	3PE	O21-C21-C22-C23
50	2	501	CPL	C32-C31-O2-C2
46	B	503	NAI	PN-O3-PA-O1A
48	4	503	3PE	C35-C36-C37-C38
49	1	404	PLC	C2B-C1B-CB-O3
48	6	201	3PE	O32-C31-C32-C33
52	X	201	CDL	C61-C62-C63-C64

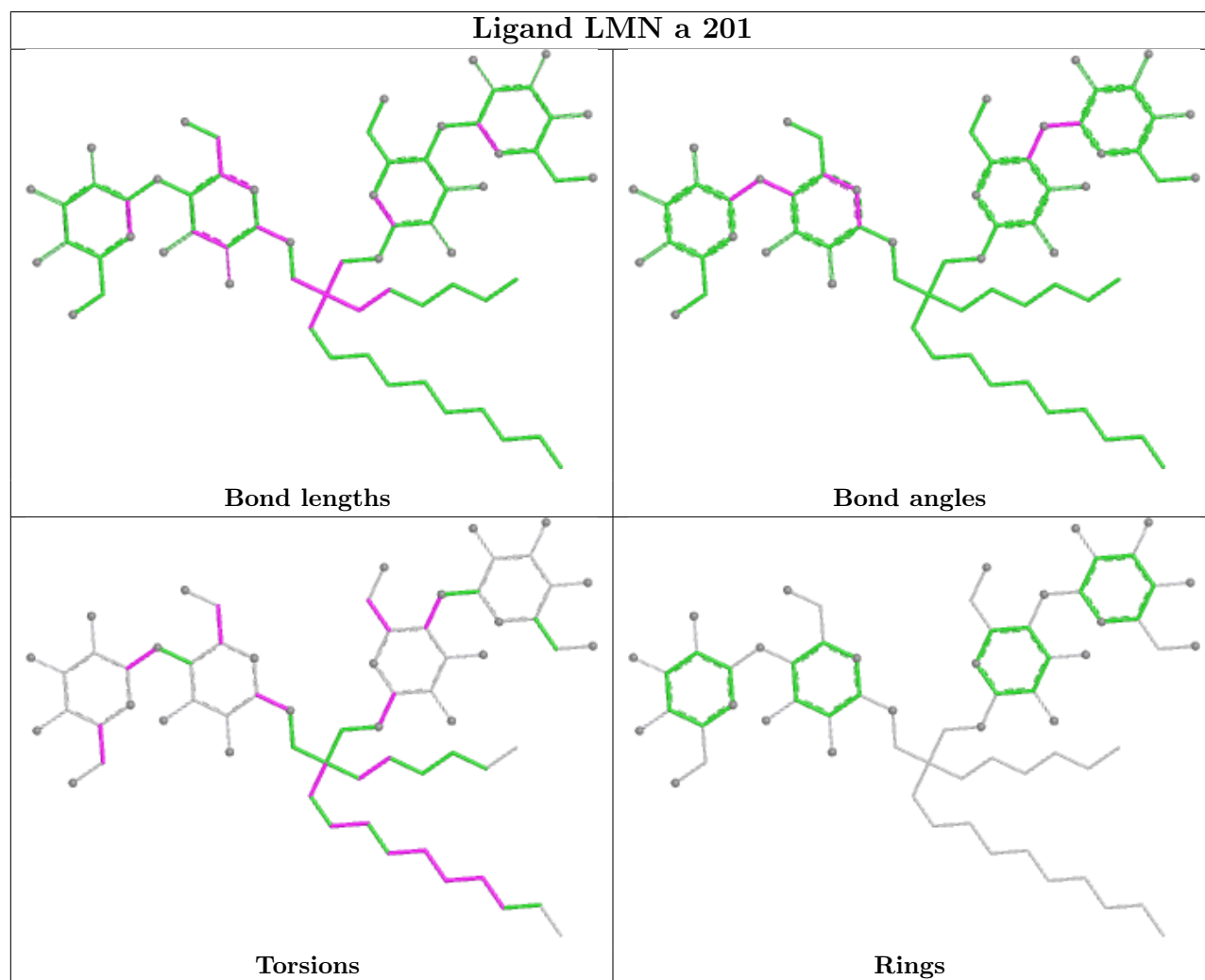
There are no ring outliers.

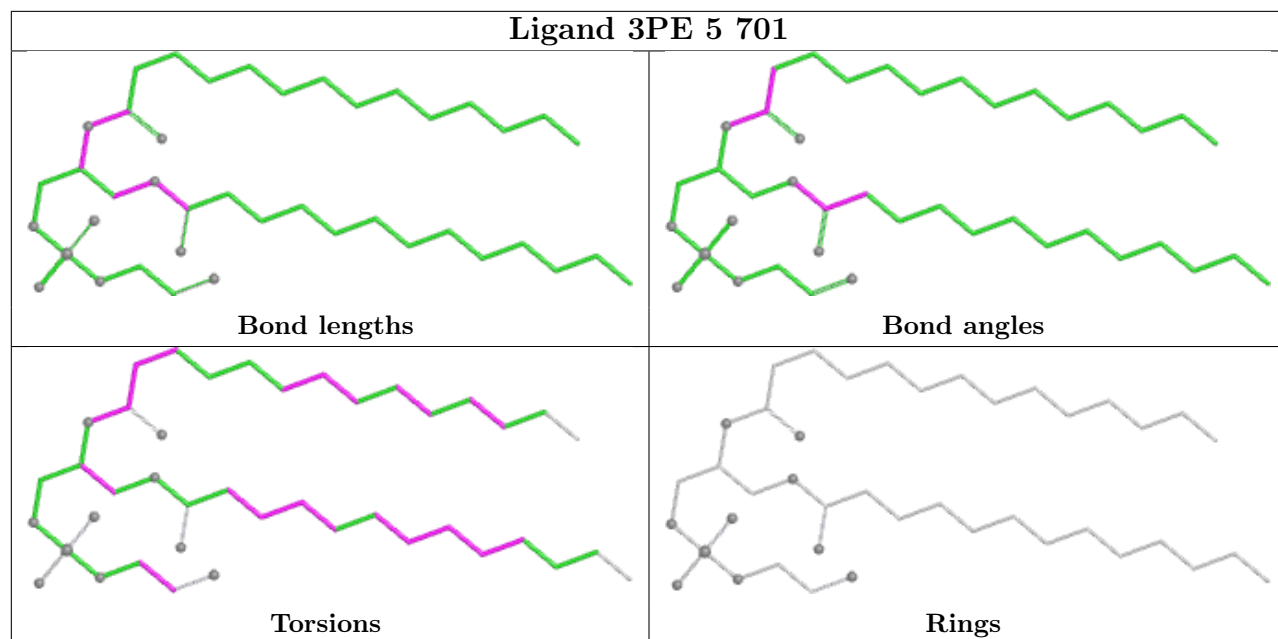
39 monomers are involved in 135 short contacts:

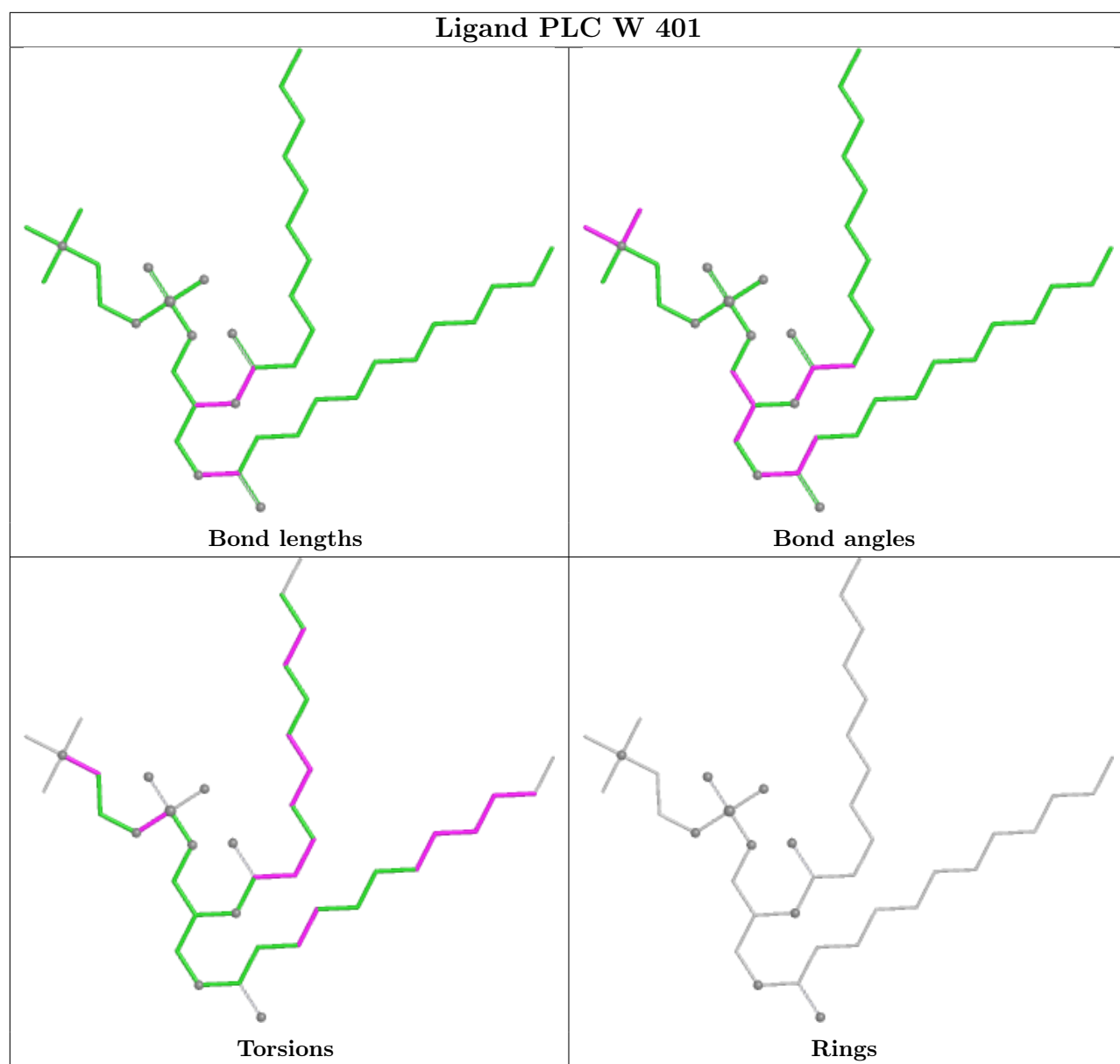
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	a	201	LMN	2	0
48	5	701	3PE	5	0
49	W	401	PLC	1	0
49	K	302	PLC	1	0
54	J	202	LMN	12	0
51	2	502	T7X	3	0
44	A	803	FES	2	0
45	B	502	FMN	4	0
52	E	403	CDL	5	0
48	1	402	3PE	1	0
47	C	601	UQ9	2	0
43	B	501	SF4	1	0
49	4	504	PLC	1	0
52	n	201	CDL	10	0
48	6	202	3PE	7	0
43	A	802	SF4	1	0
48	5	702	3PE	5	0
49	i	1101	PLC	2	0
56	Q	201	ZMP	5	0
48	6	201	3PE	3	0
52	X	201	CDL	6	0
49	1	404	PLC	4	0
50	2	501	CPL	2	0
51	b	501	T7X	1	0
52	Z	201	CDL	3	0
56	O	201	ZMP	6	0
48	4	503	3PE	6	0
52	W	402	CDL	1	0
48	J	201	3PE	2	0
48	b	502	3PE	7	0
48	E	402	3PE	1	0
48	I	501	3PE	4	0
48	4	501	3PE	3	0
48	1	403	3PE	4	0
46	B	503	NAI	1	0
52	g	201	CDL	7	0
48	4	502	3PE	8	0
48	2	503	3PE	2	0
53	E	401	NDP	2	0

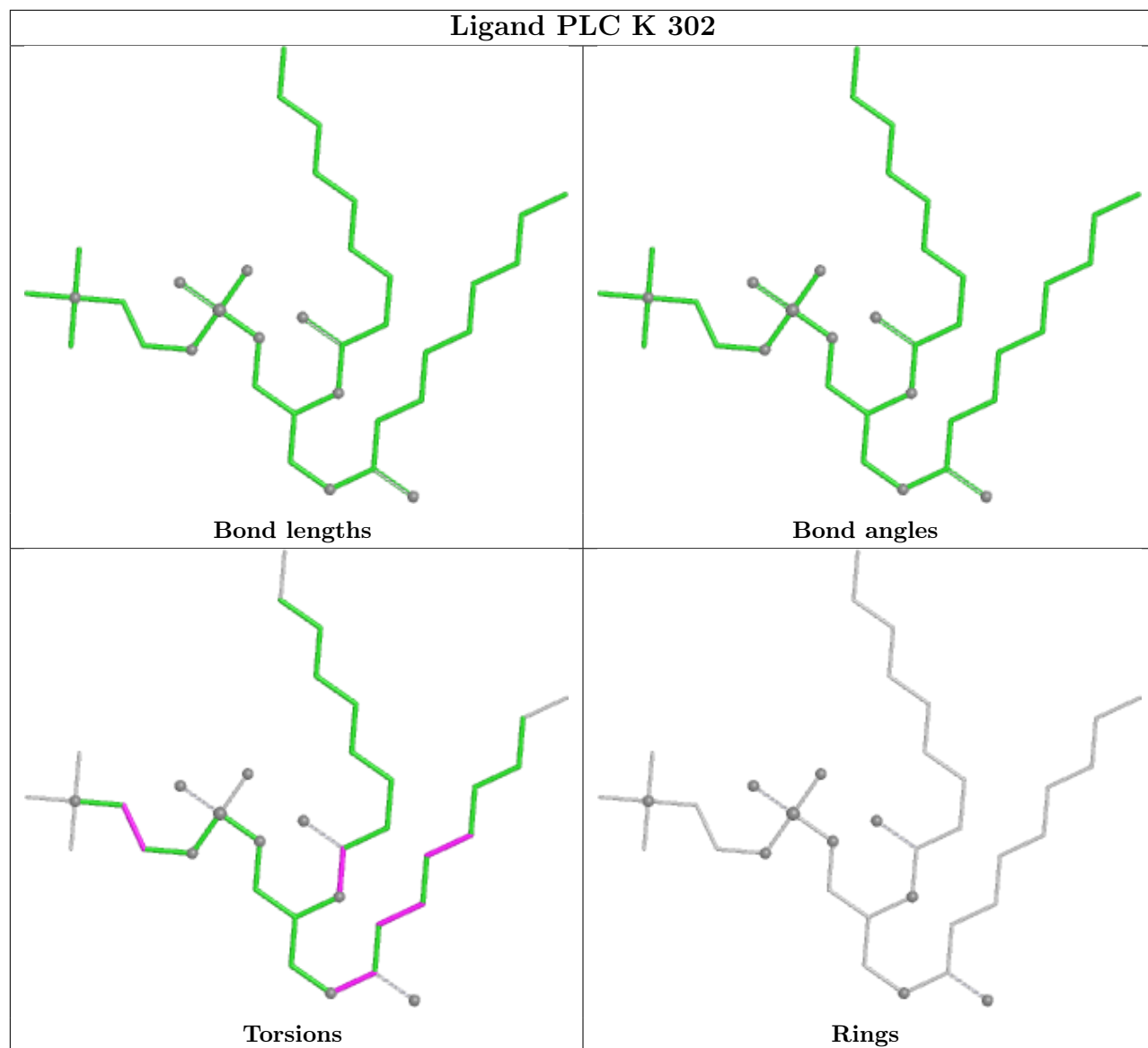
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

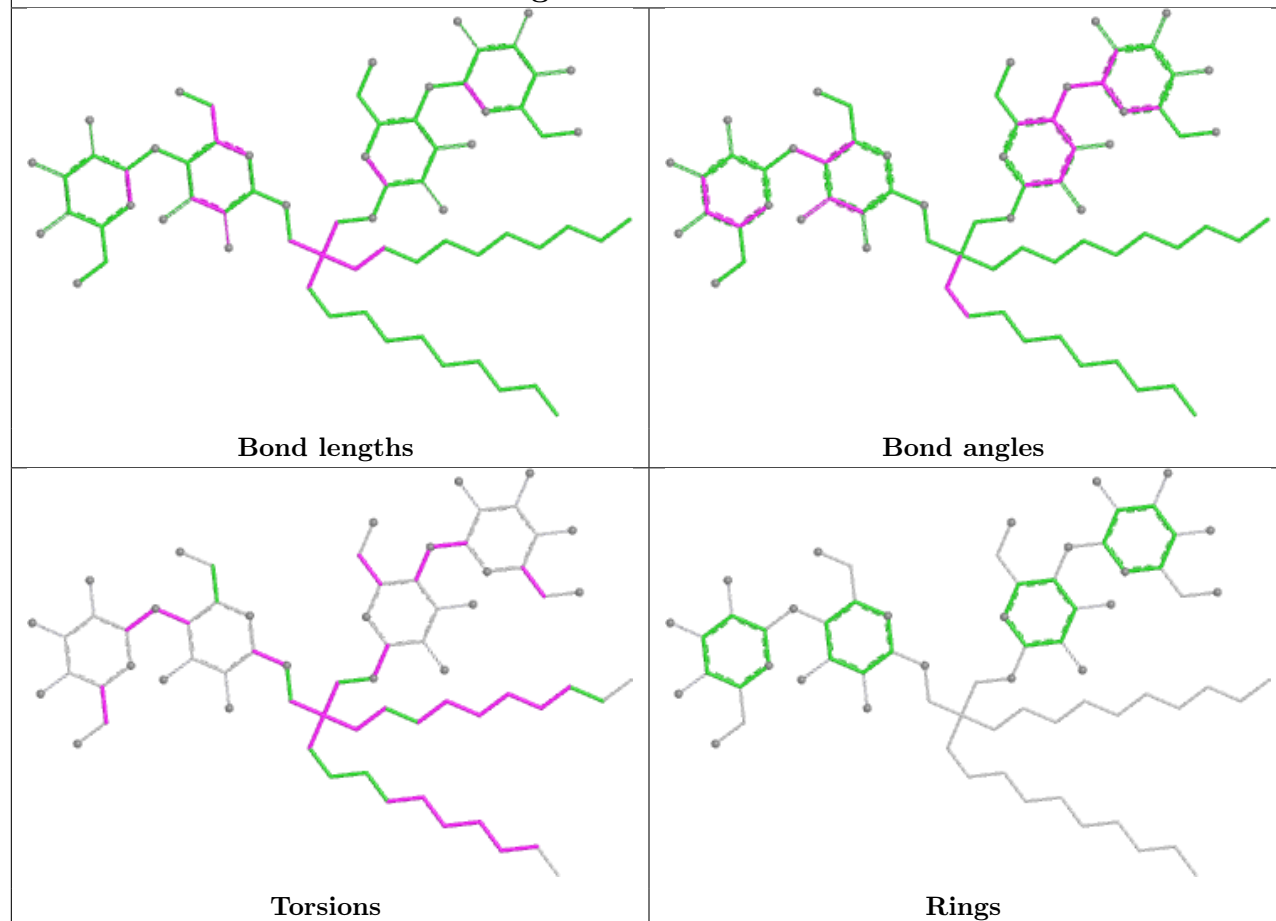




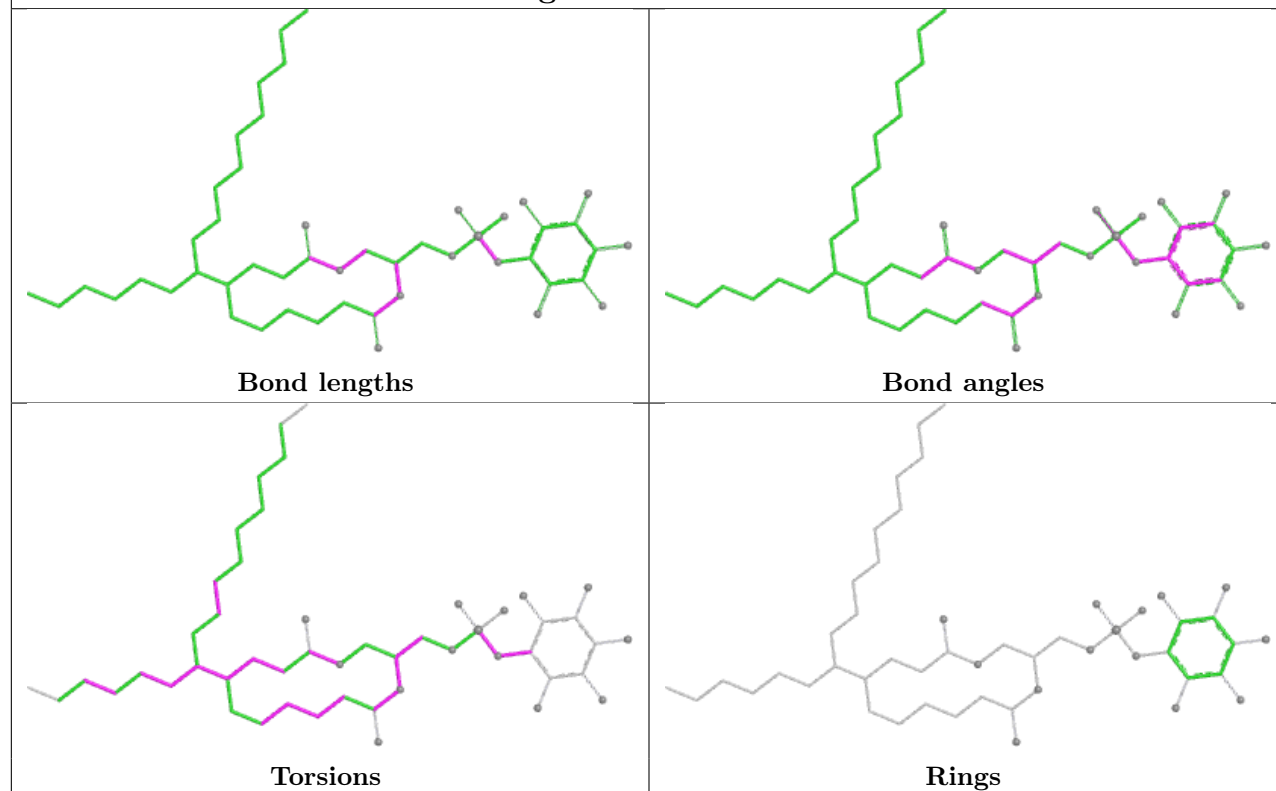


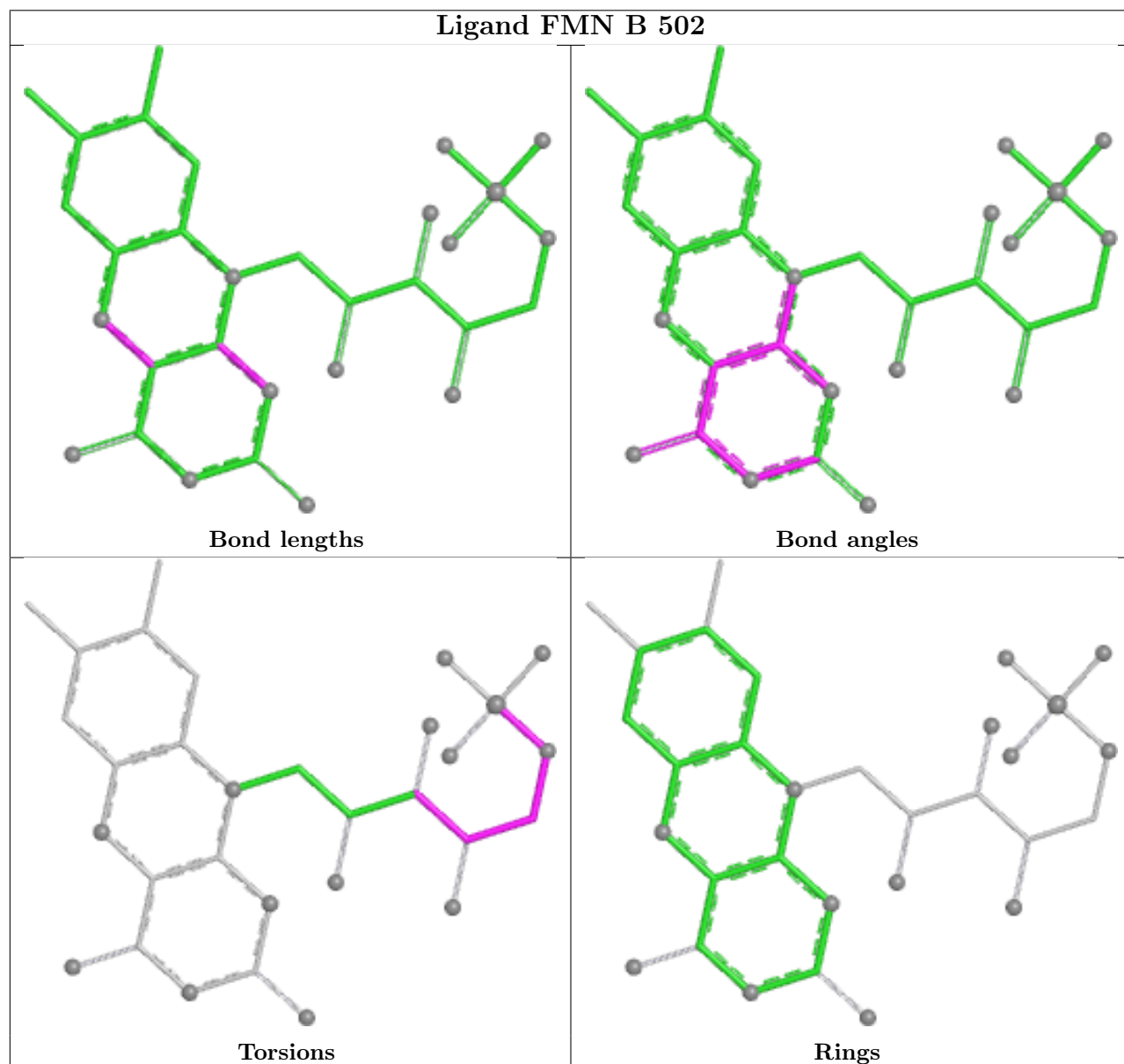
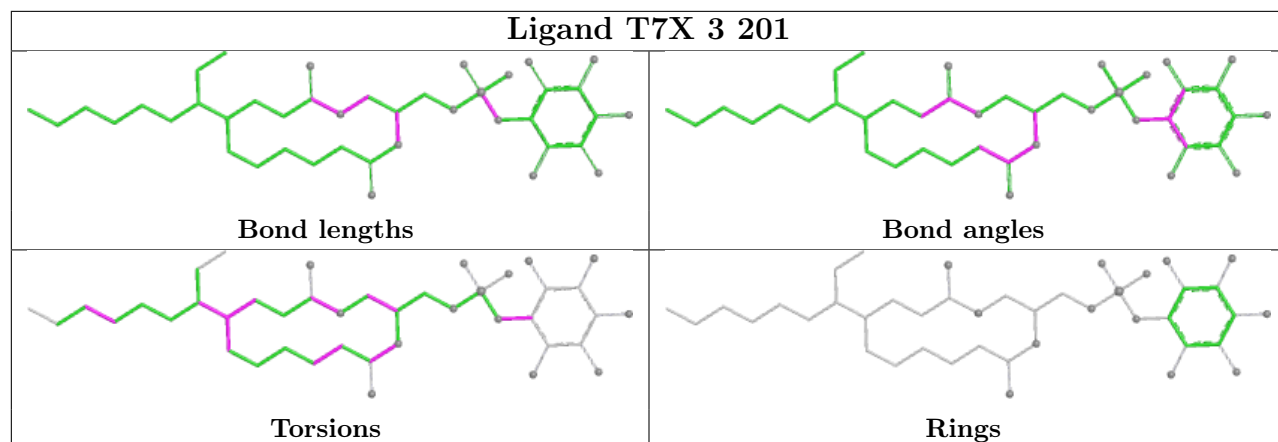


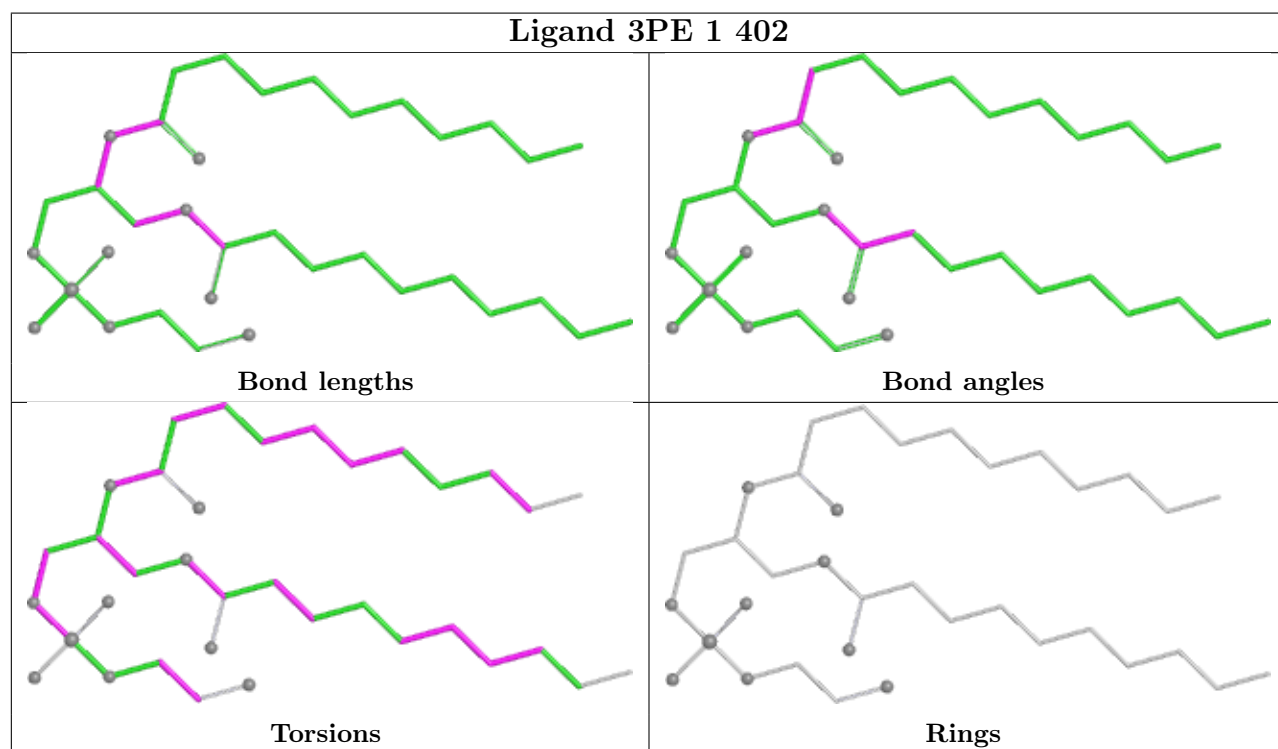
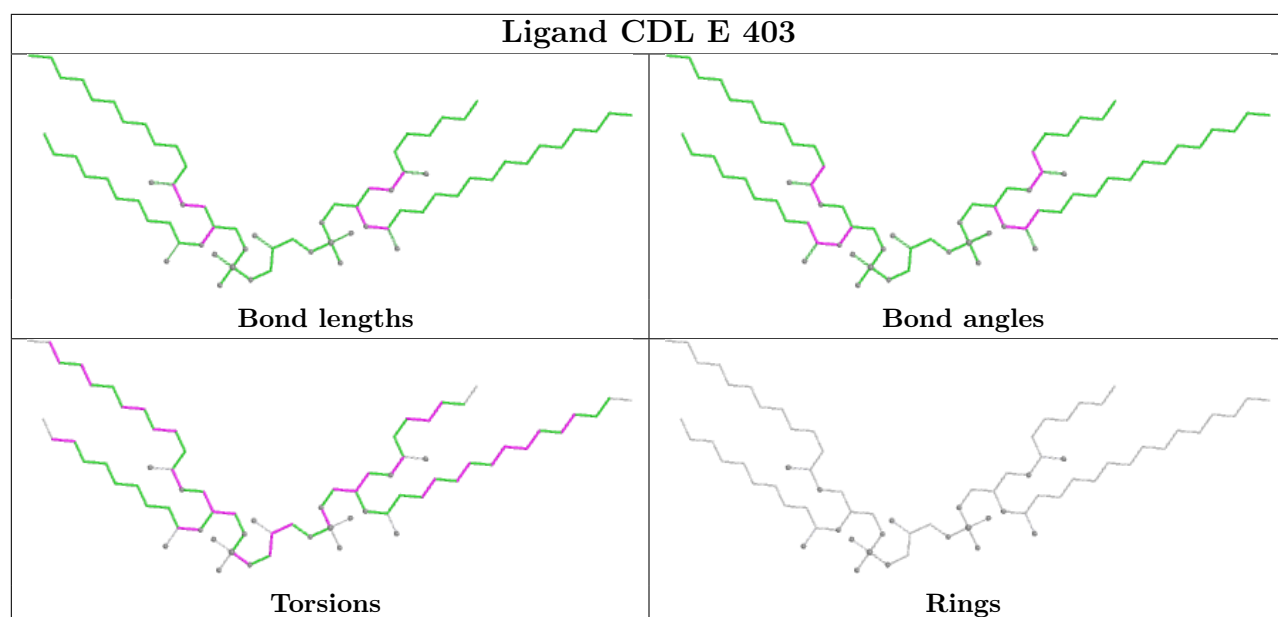
Ligand LMN J 202

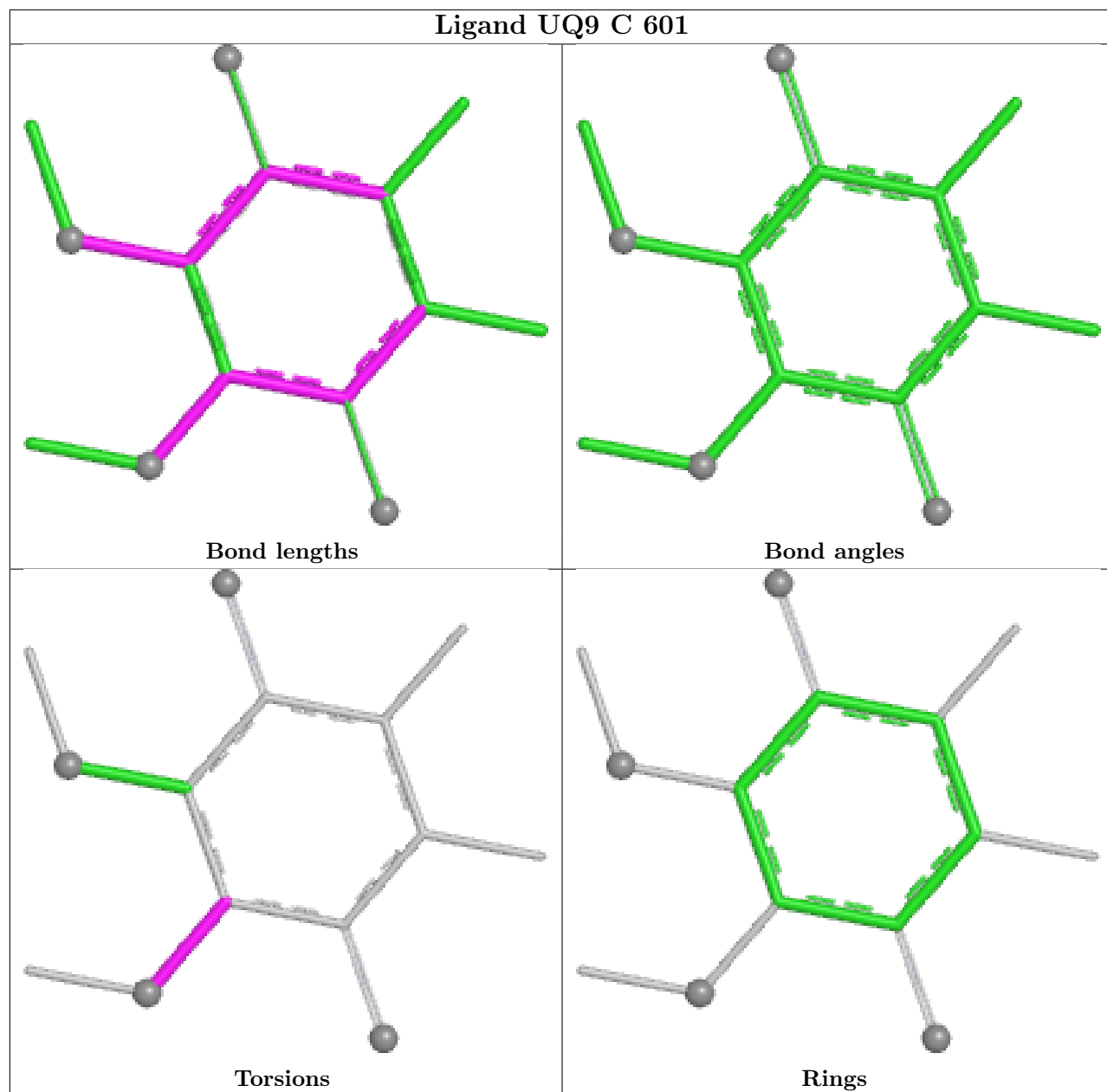


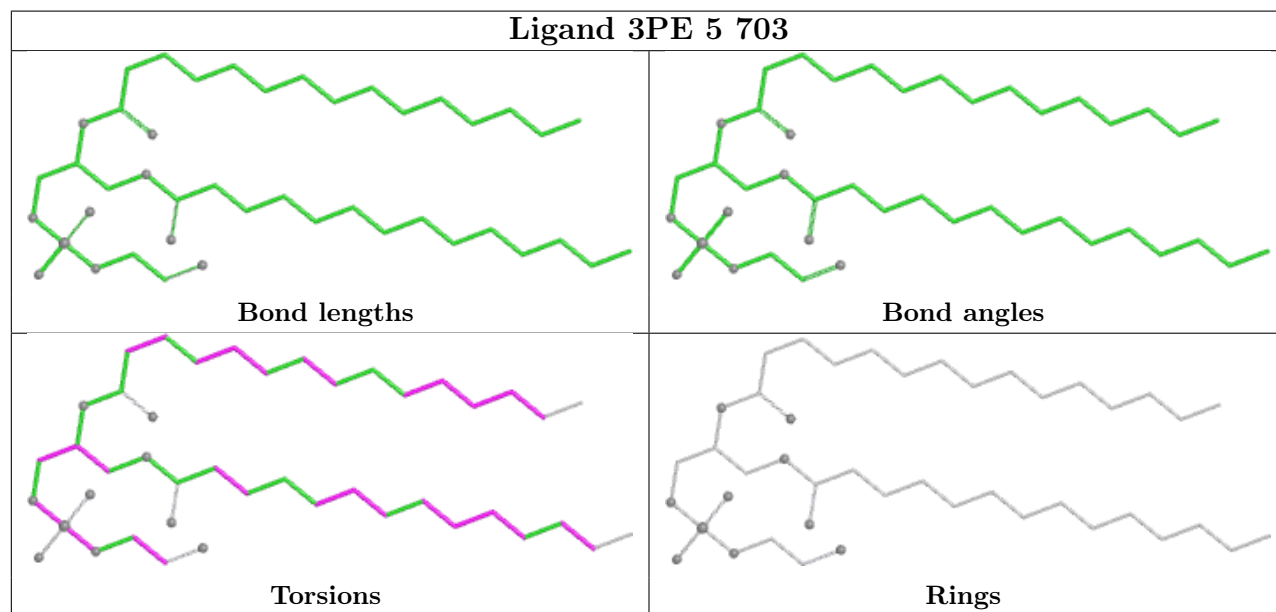
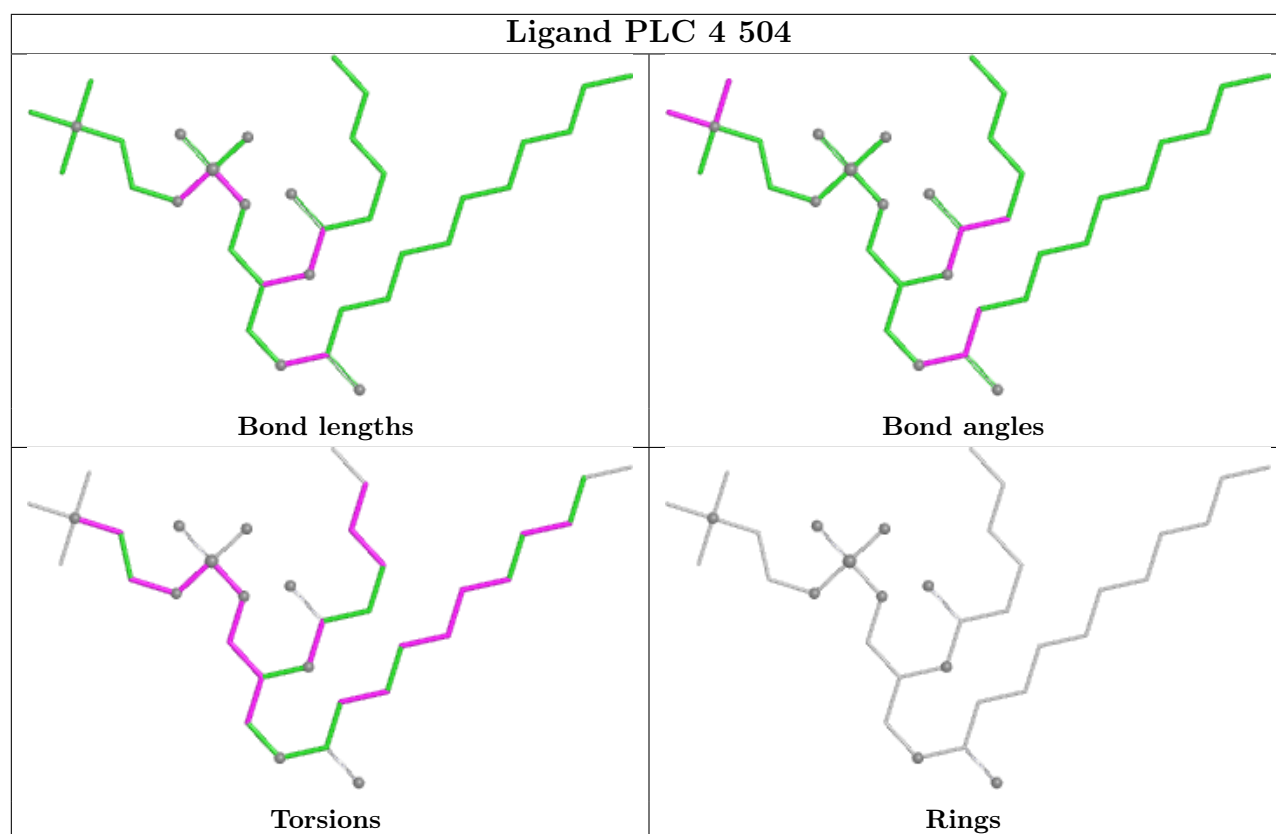
Ligand T7X 2 502

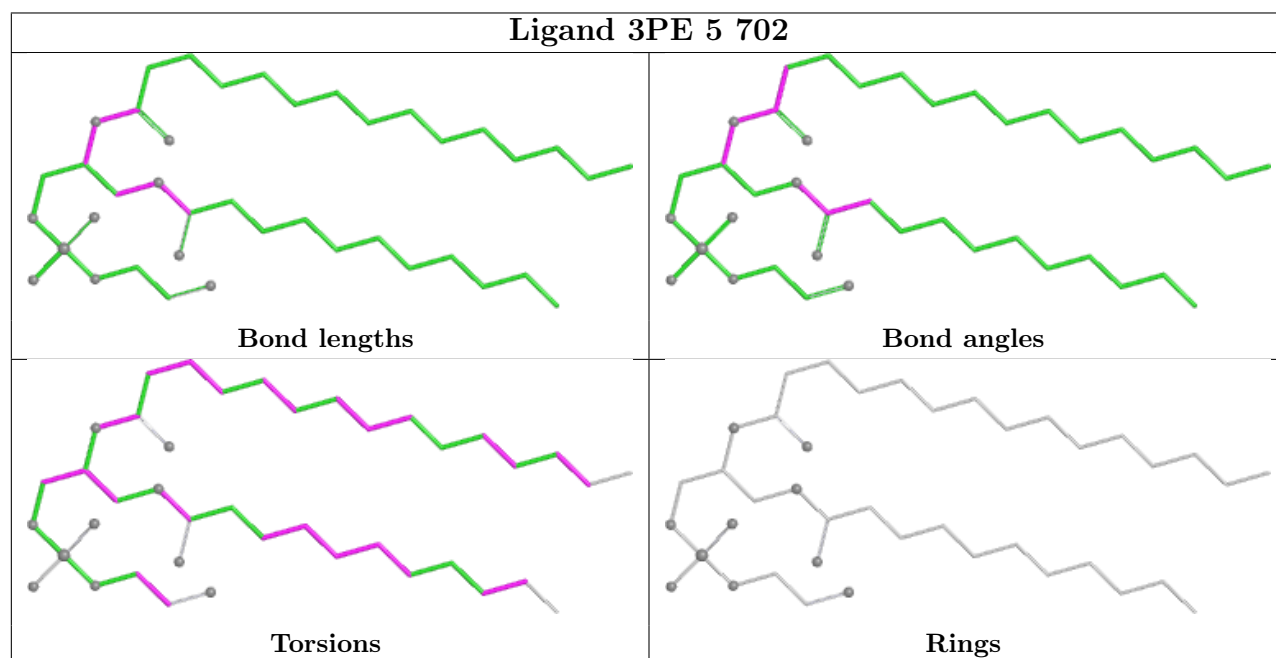
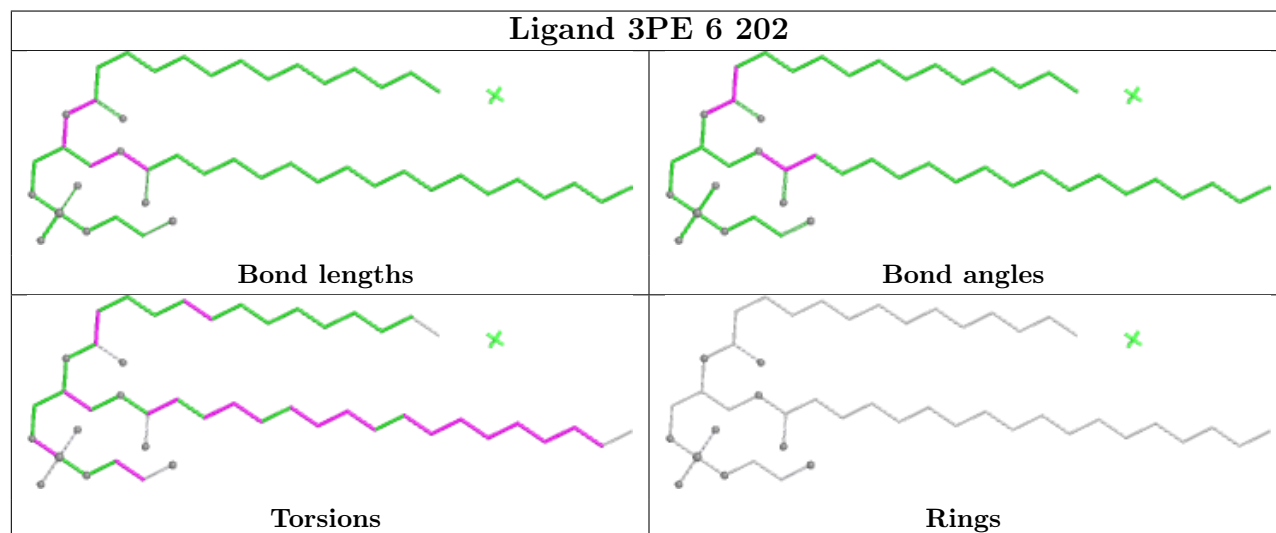
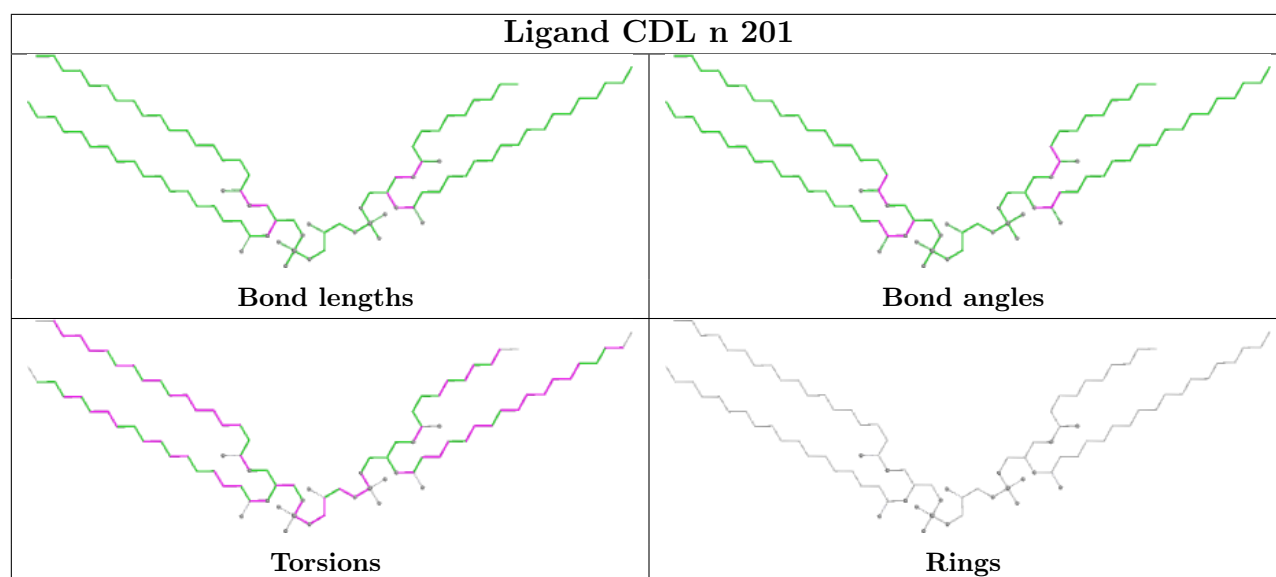


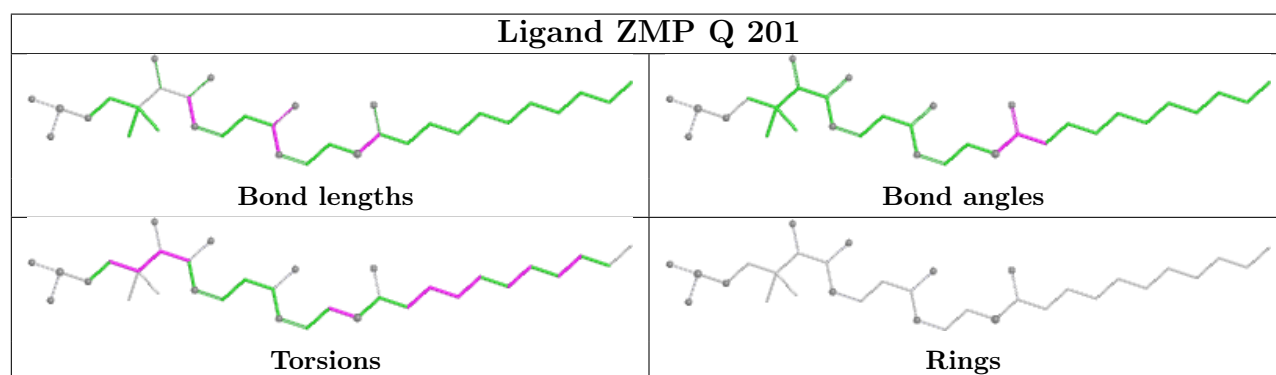
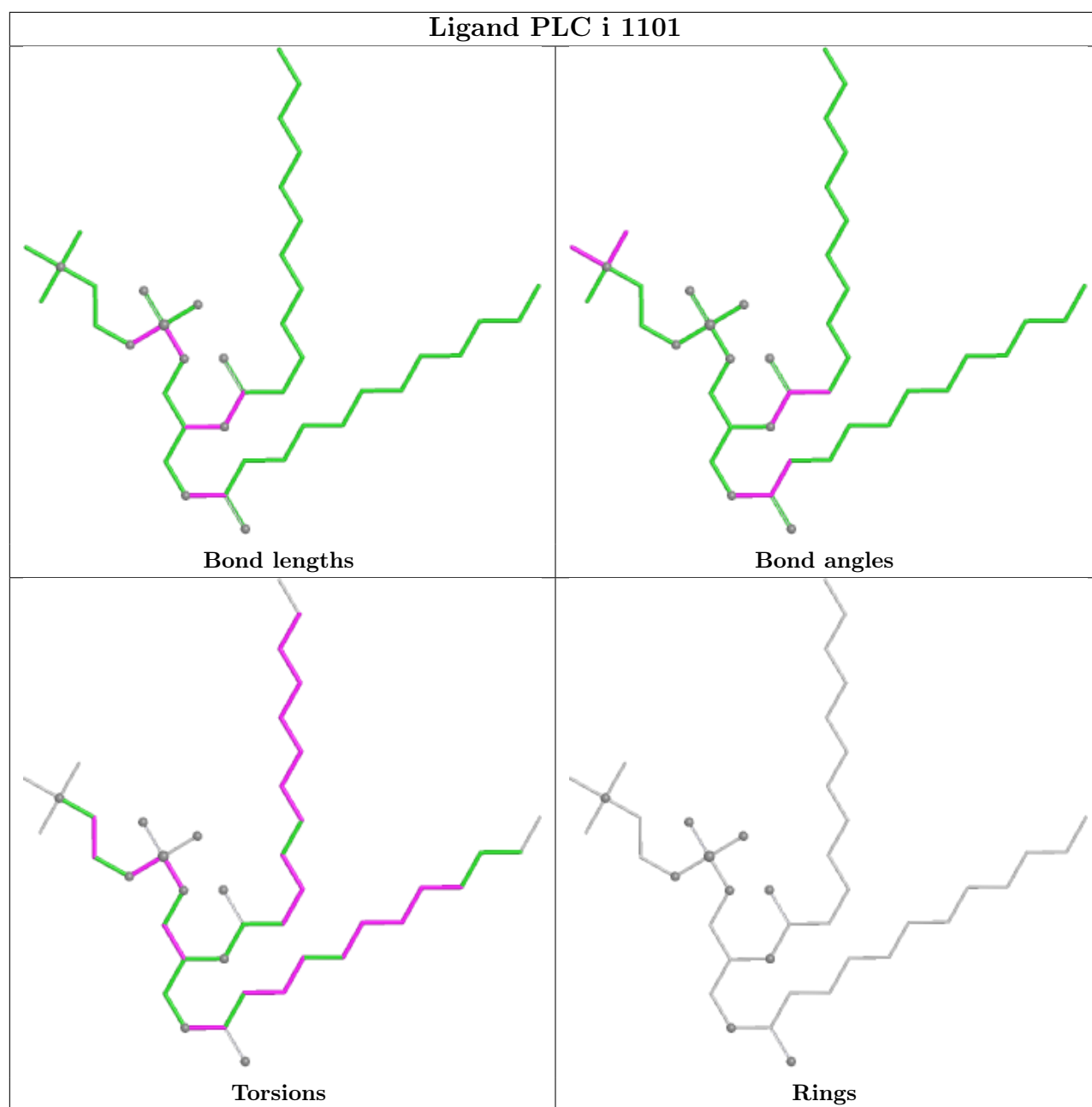


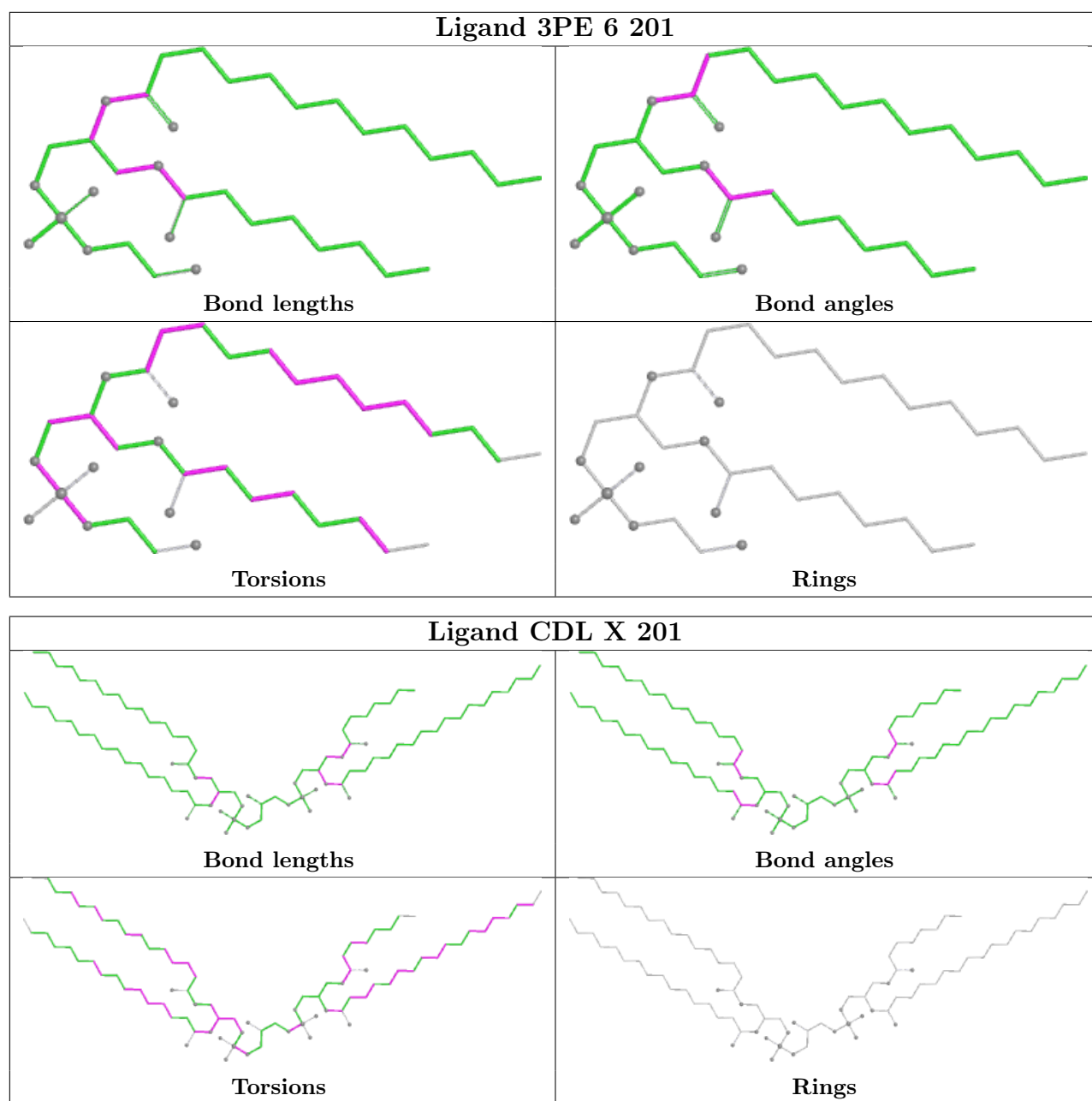


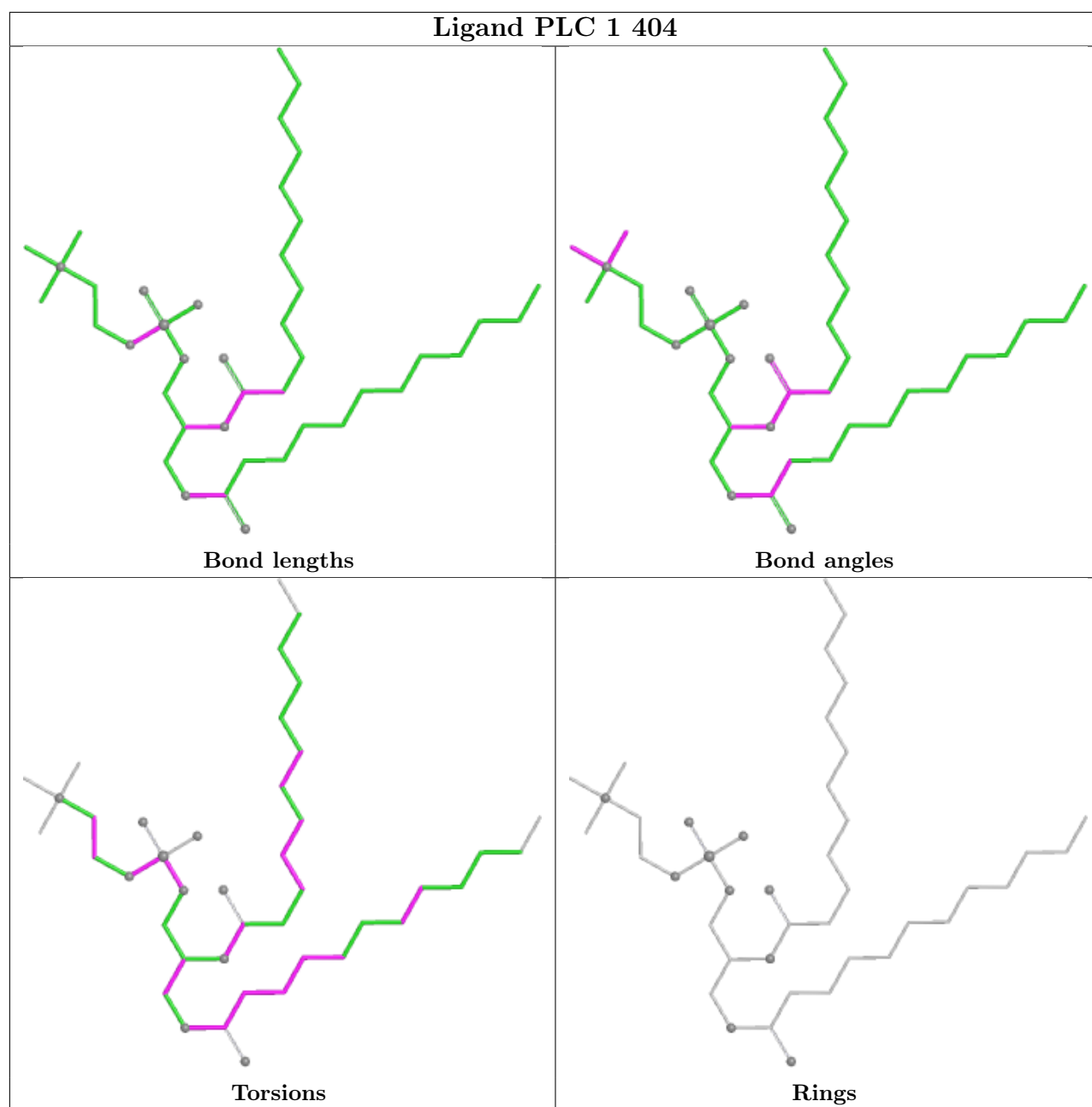


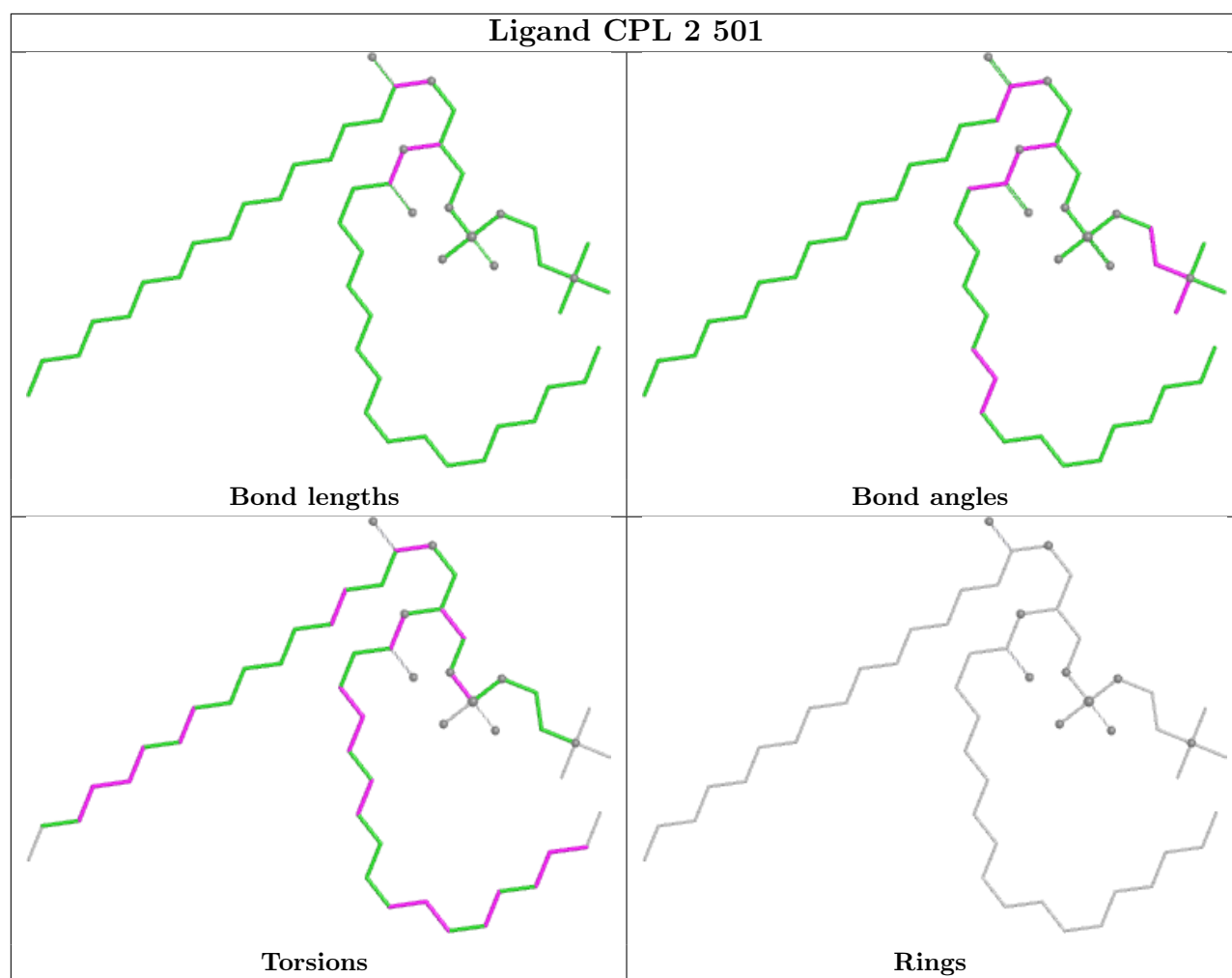


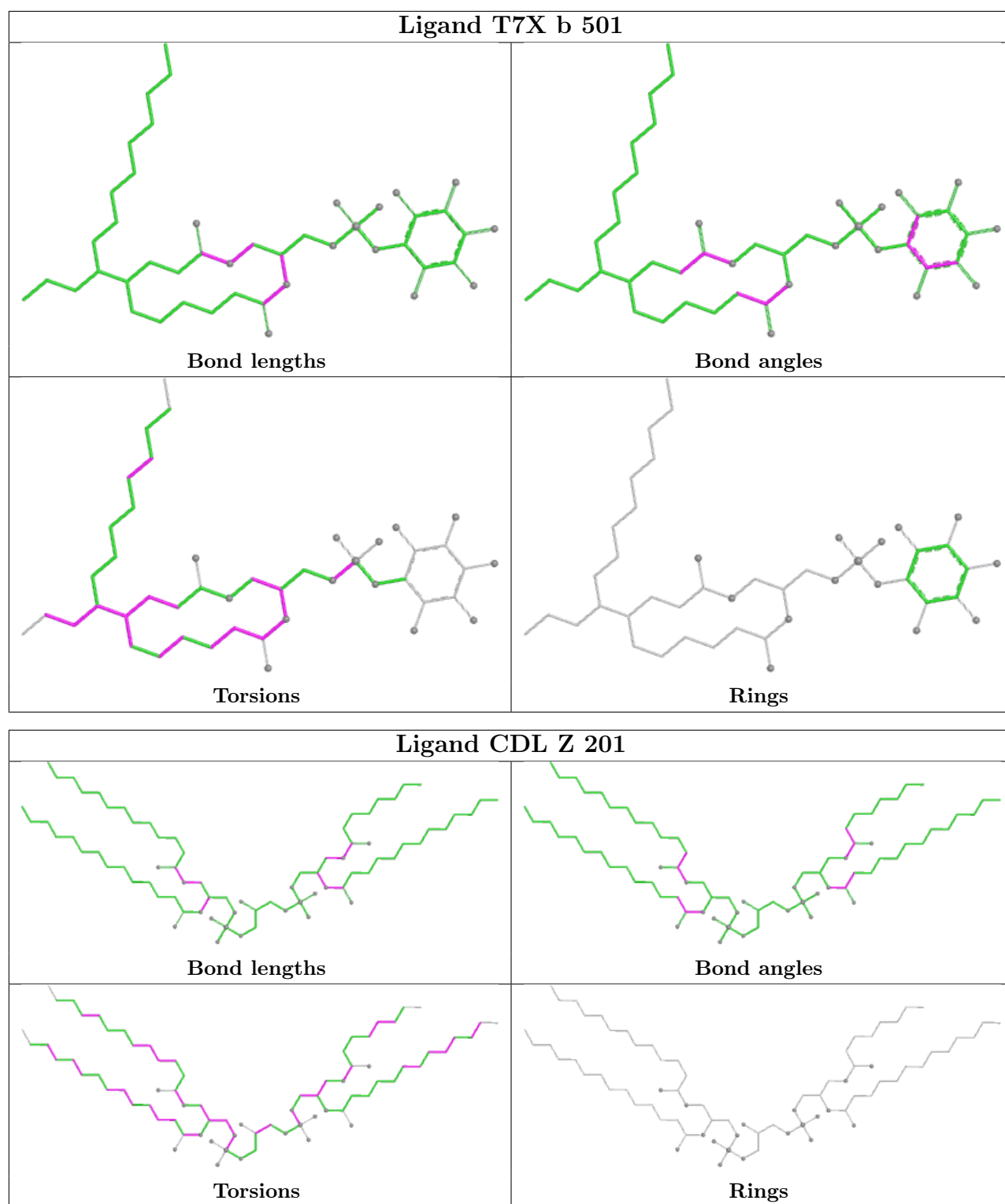


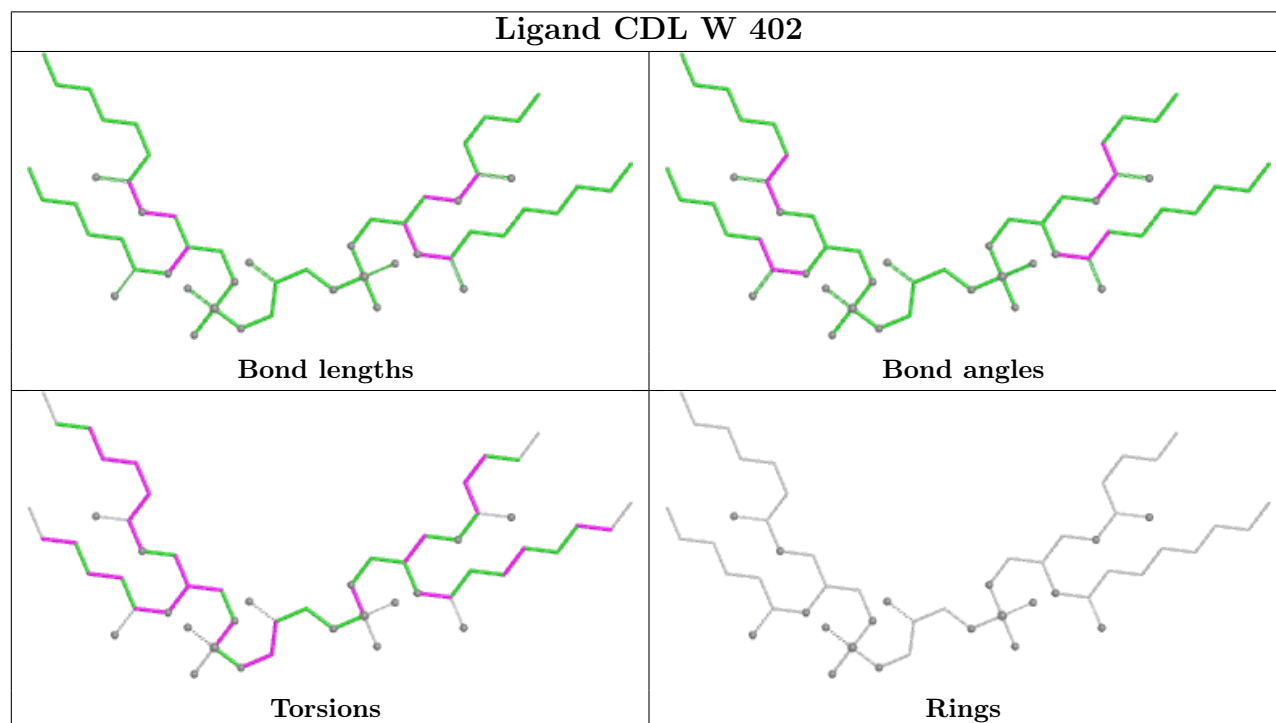
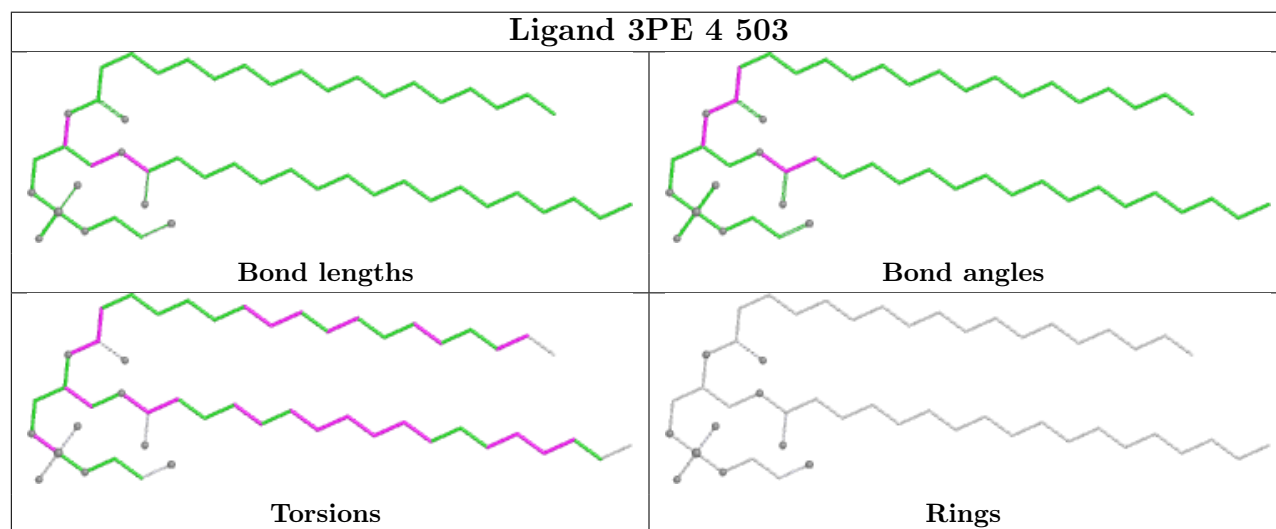
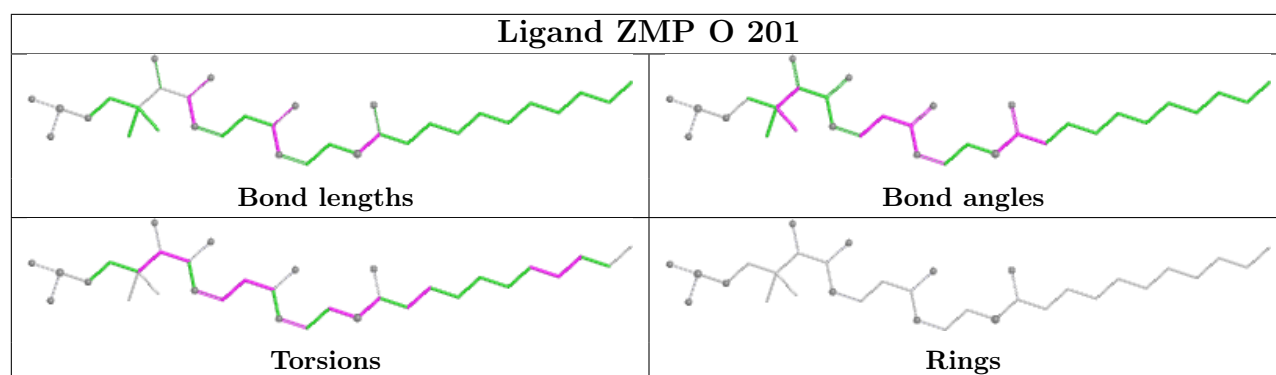


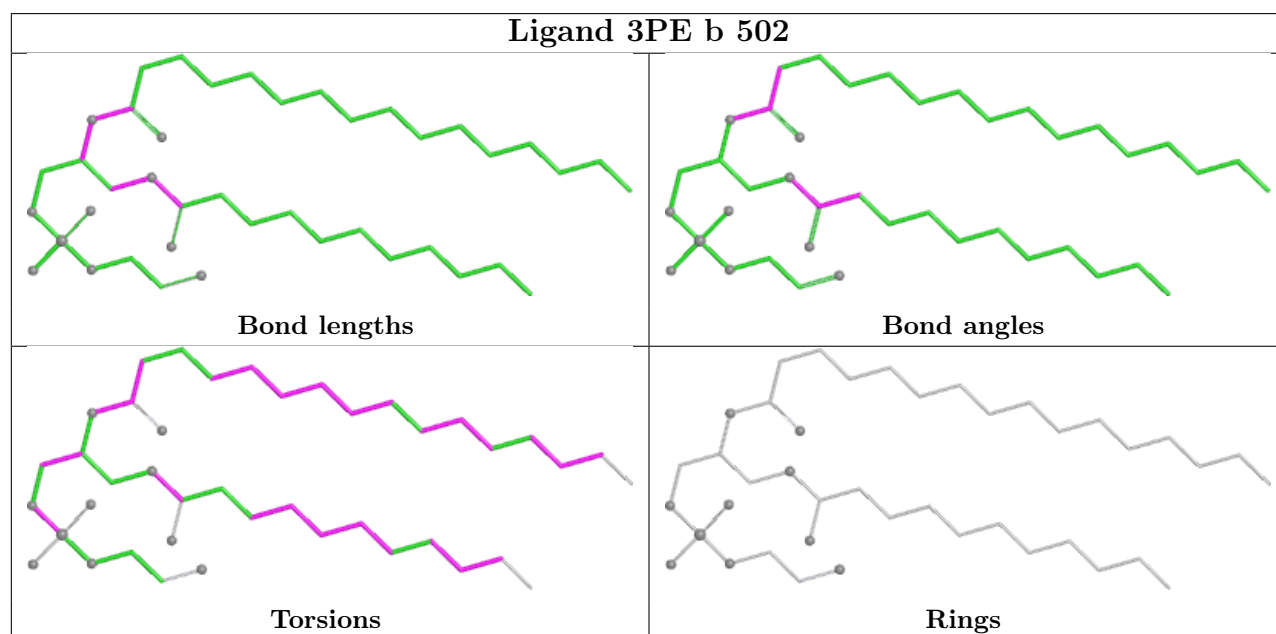
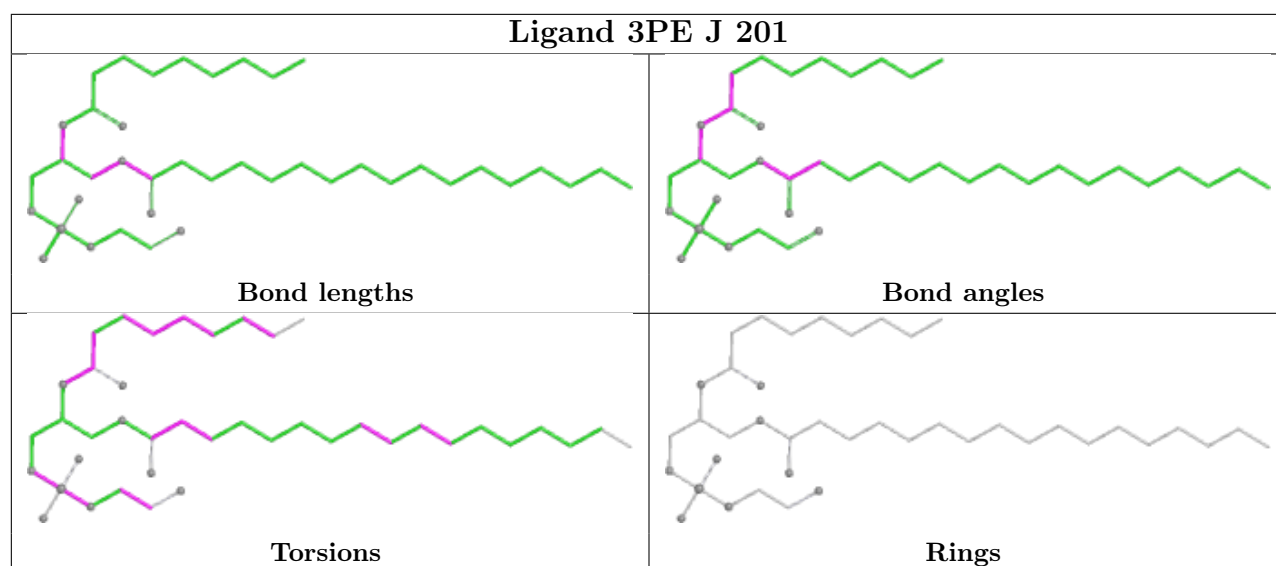


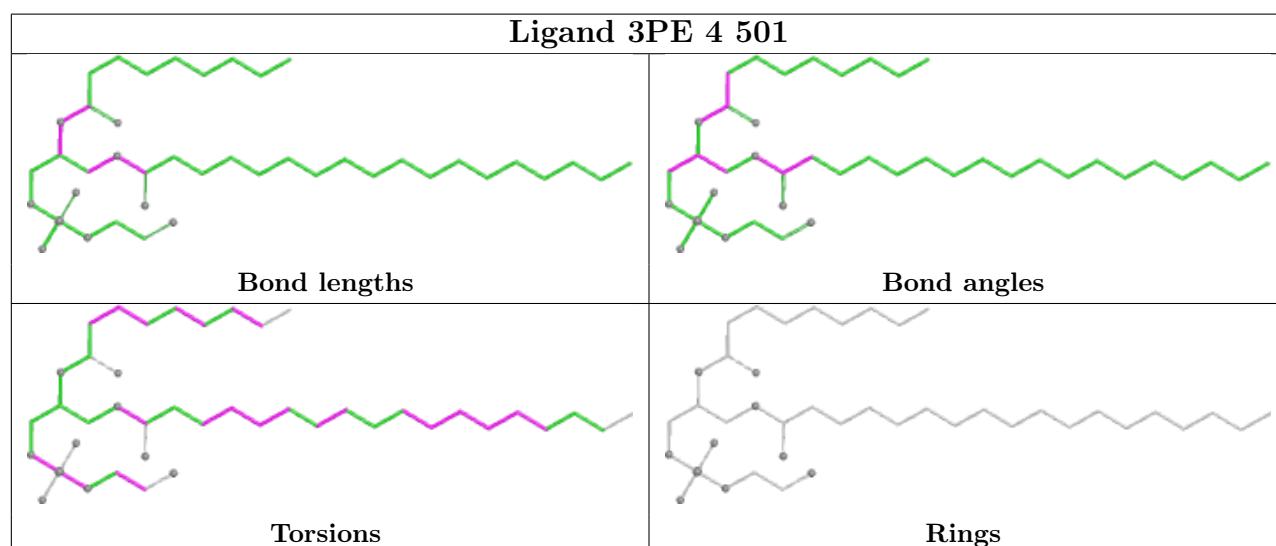
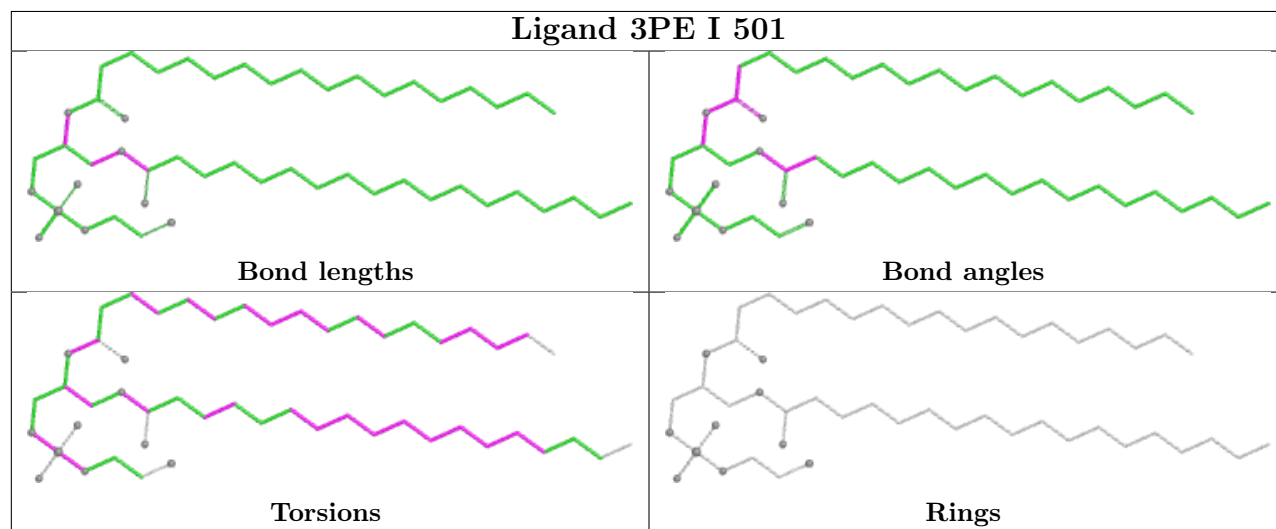
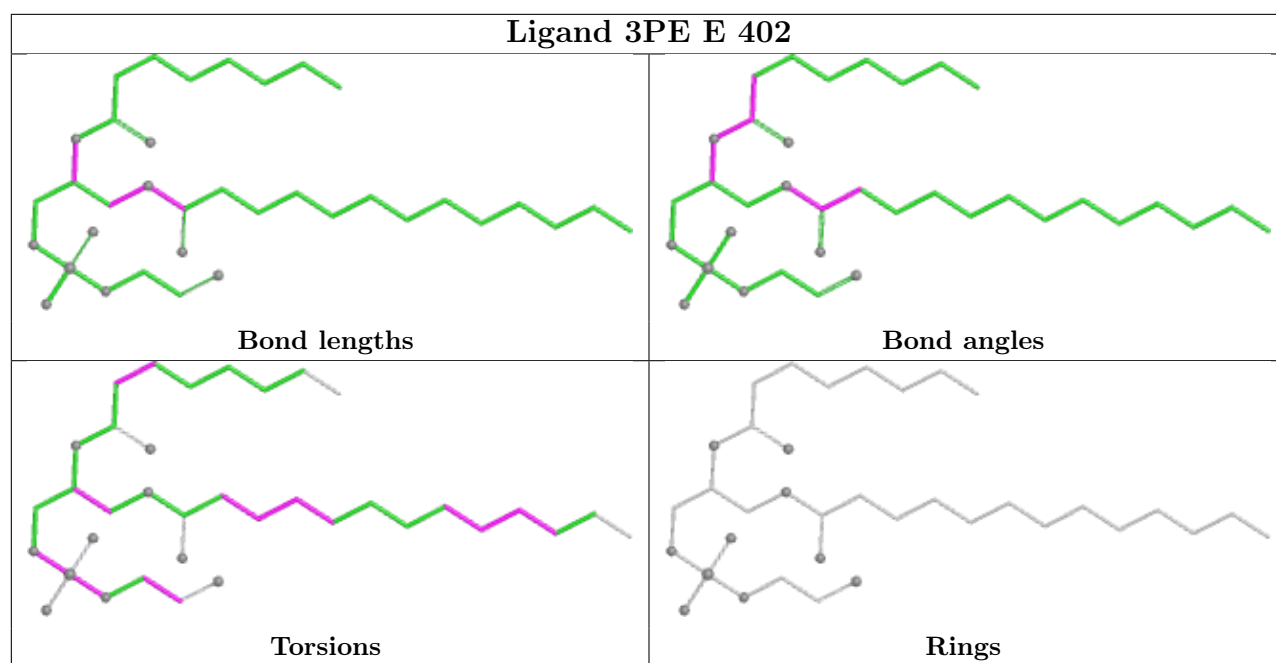


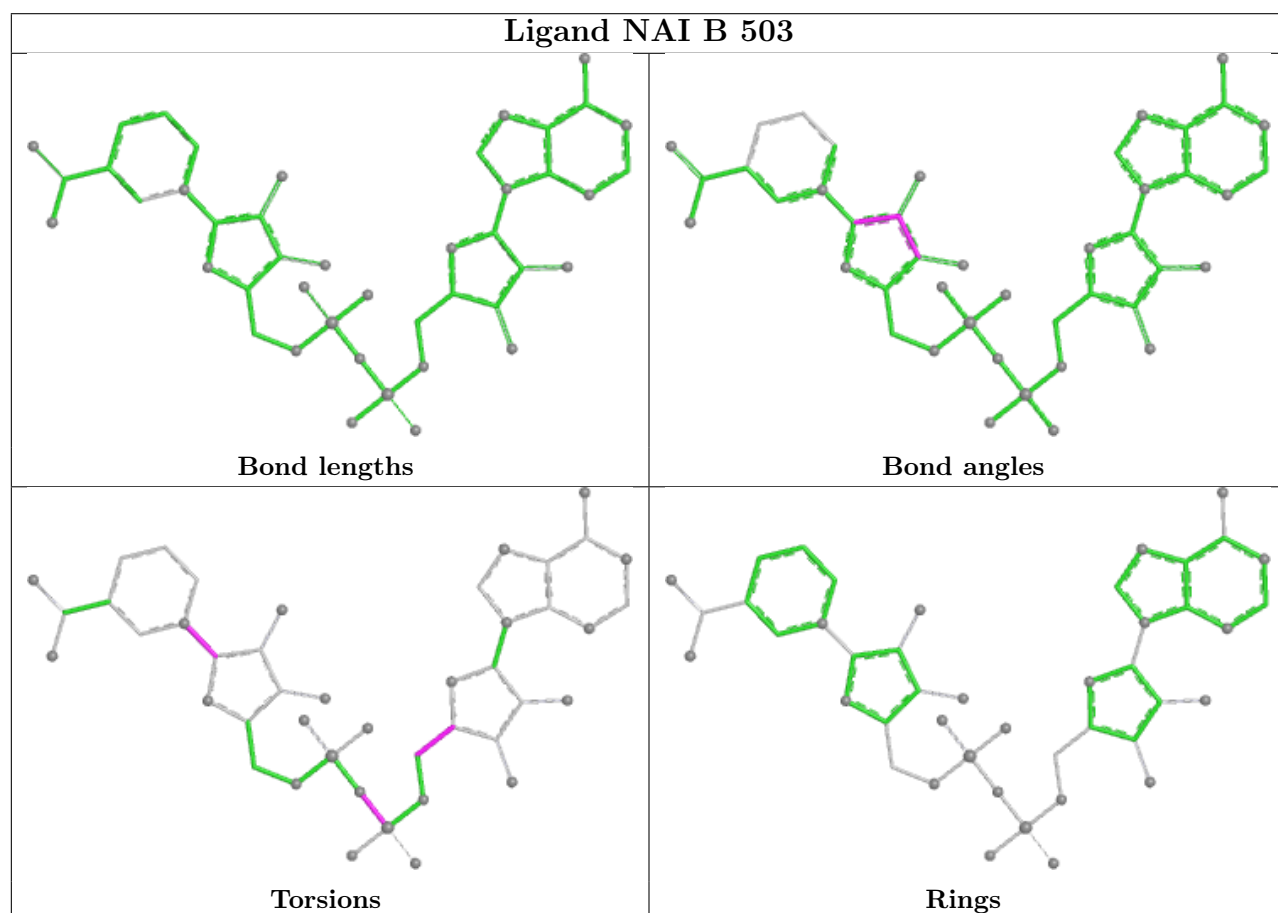
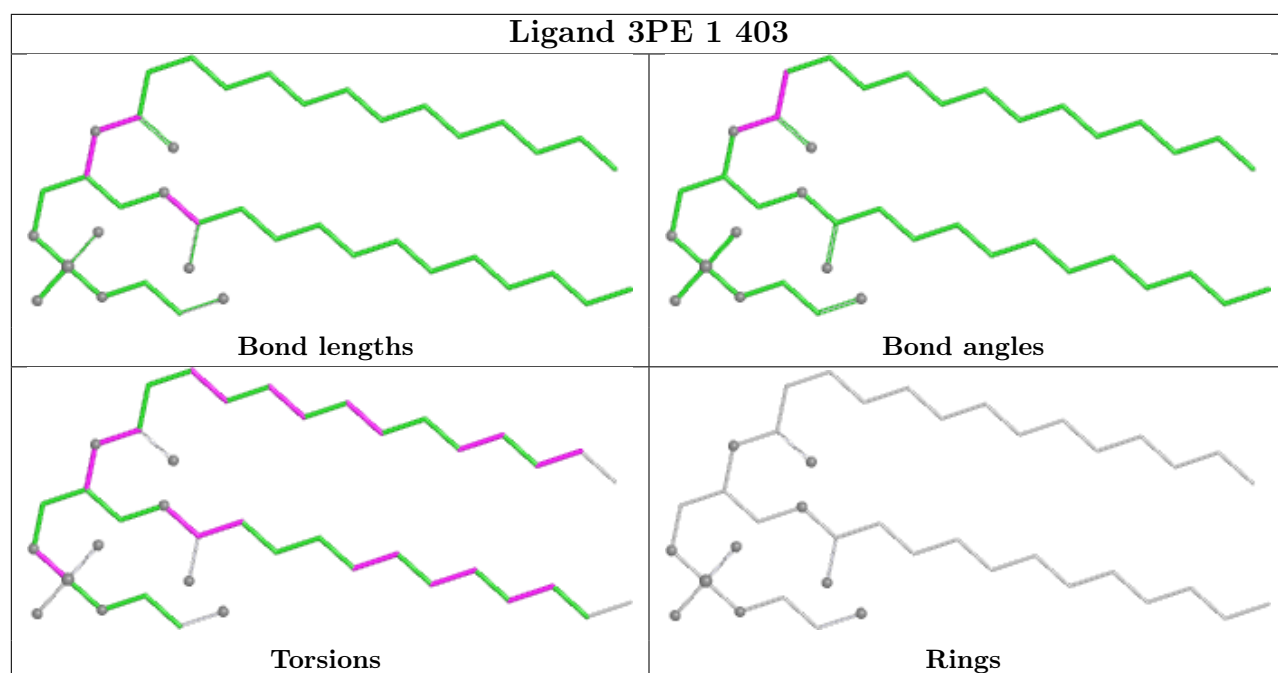


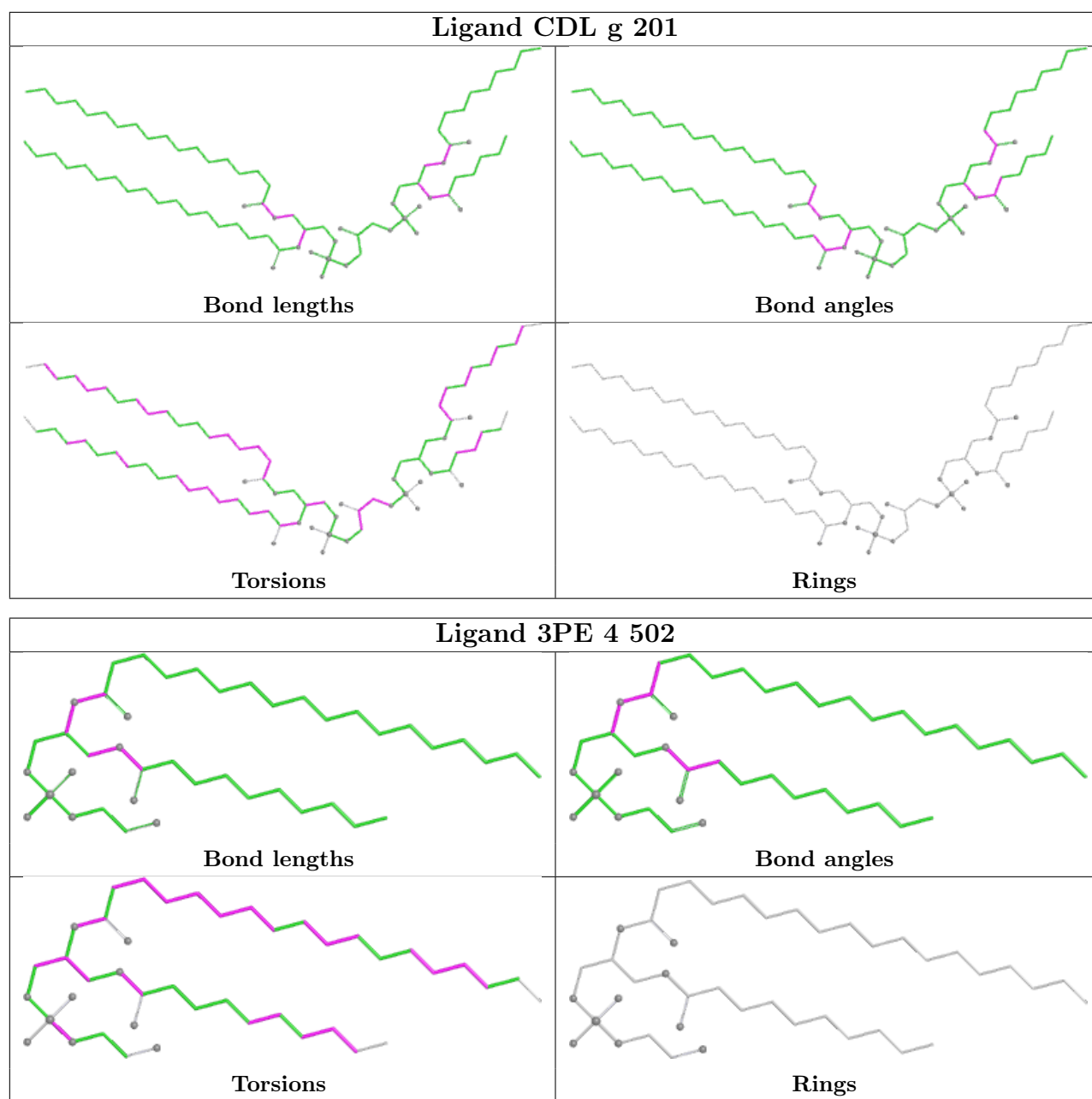


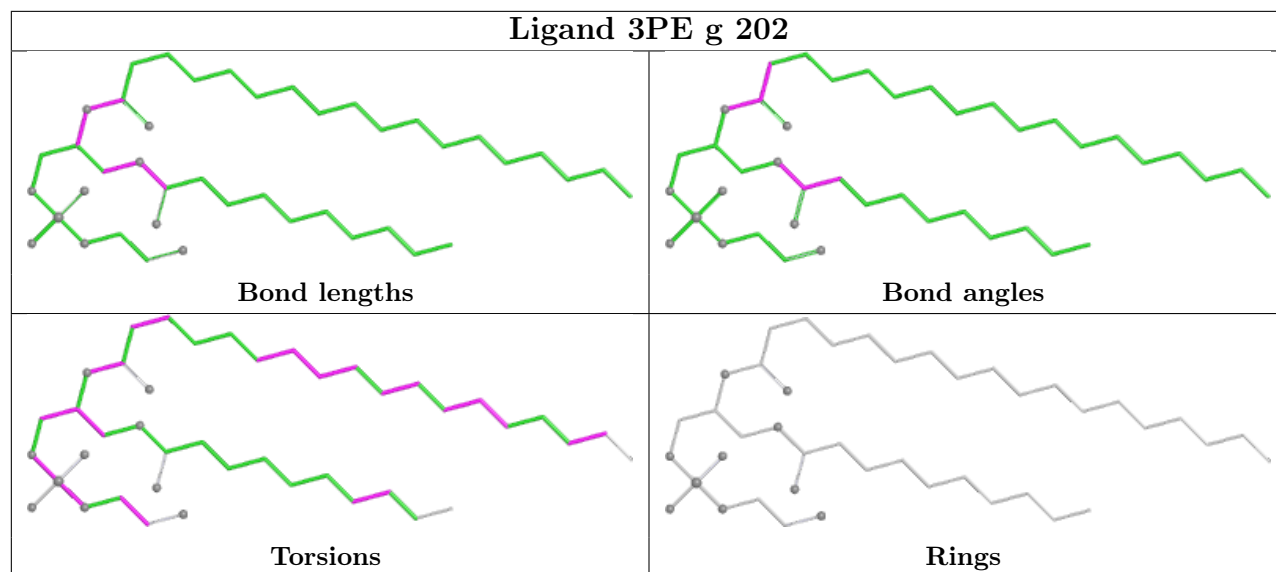


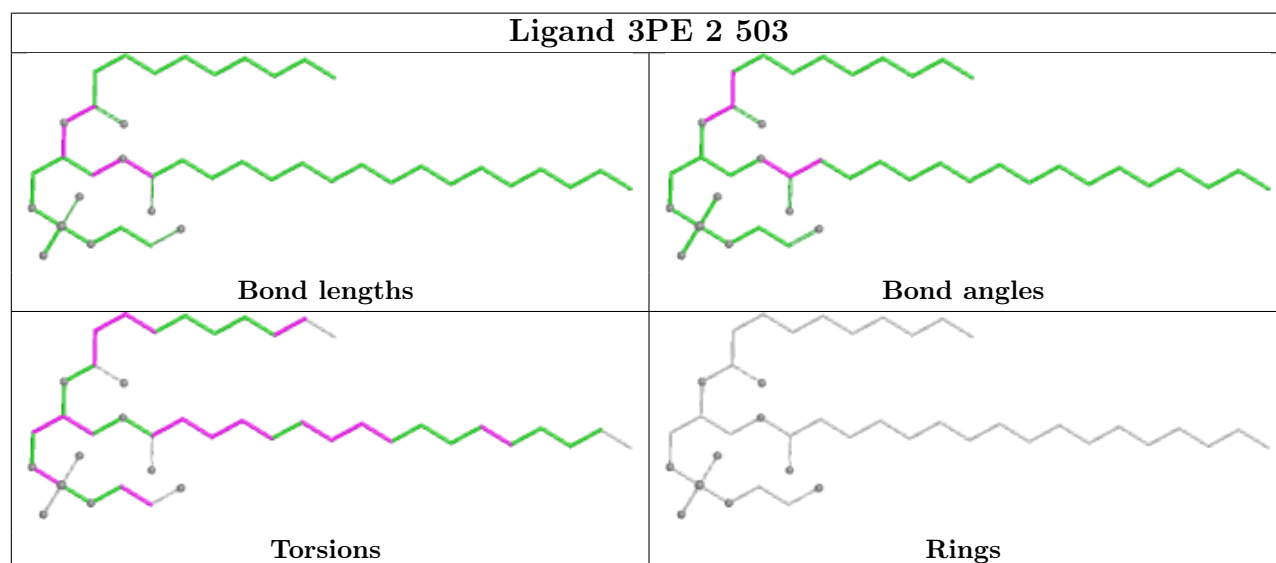
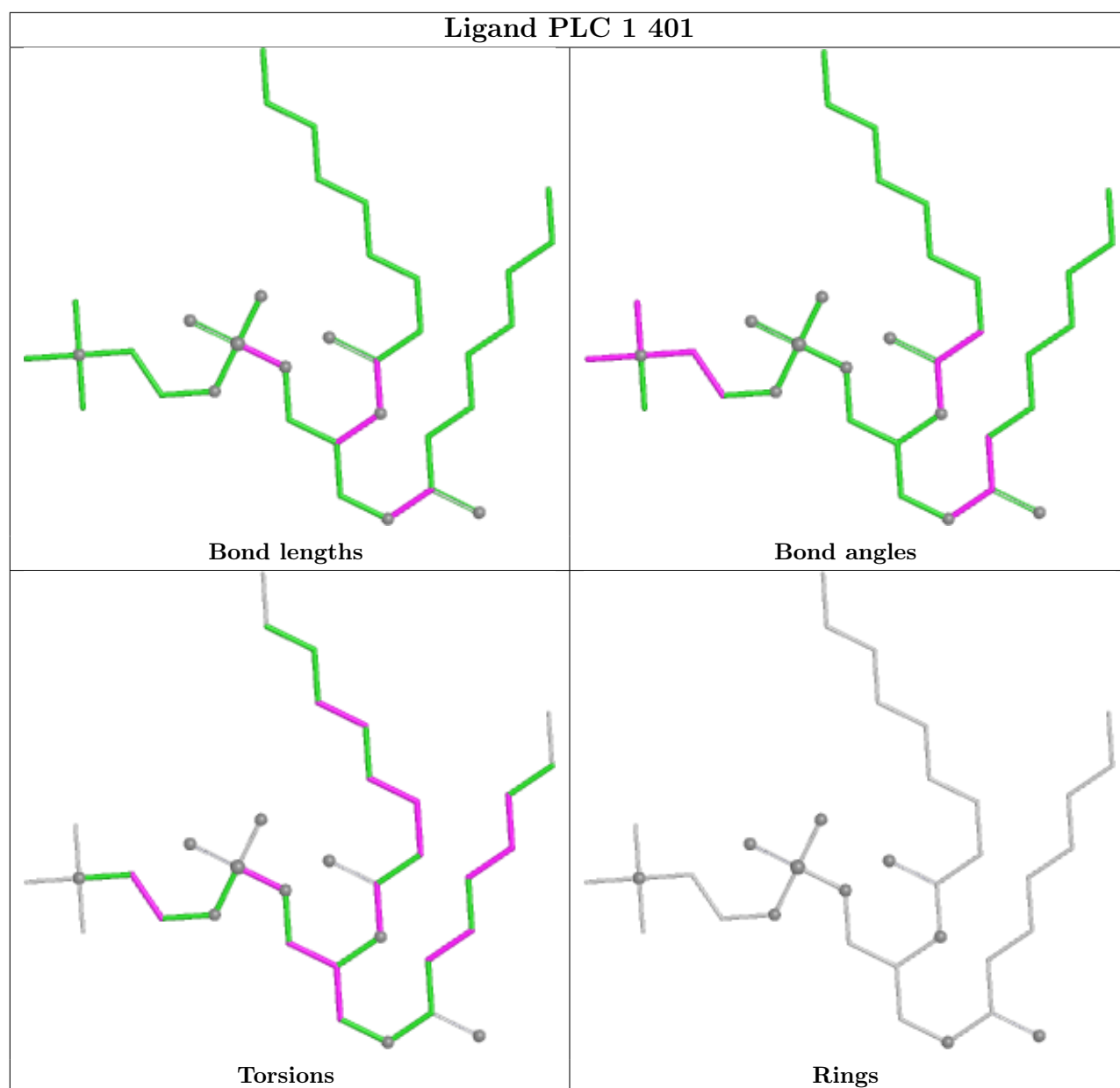


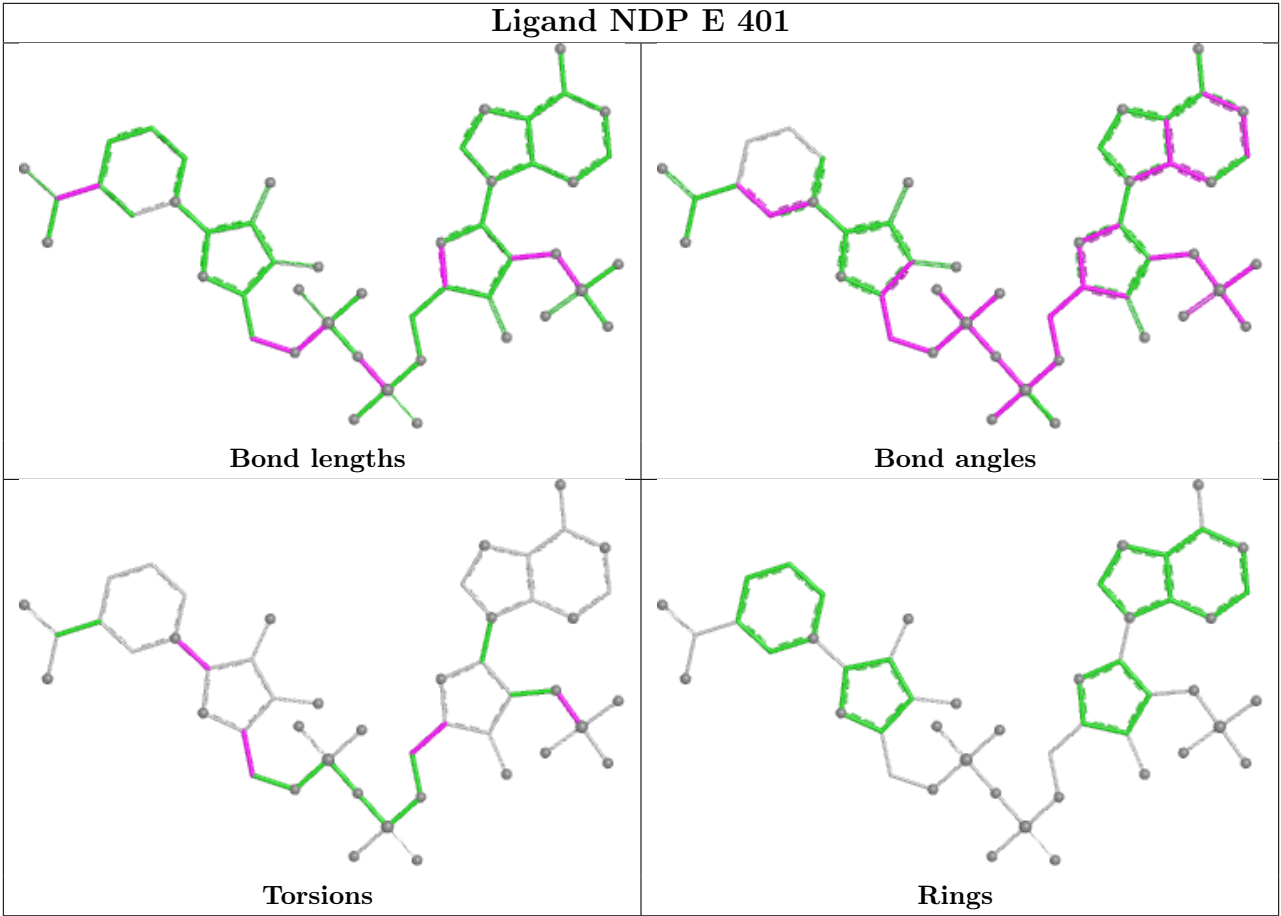












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
40	n	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	n	119:ARG	C	120:GLU	N	3.11

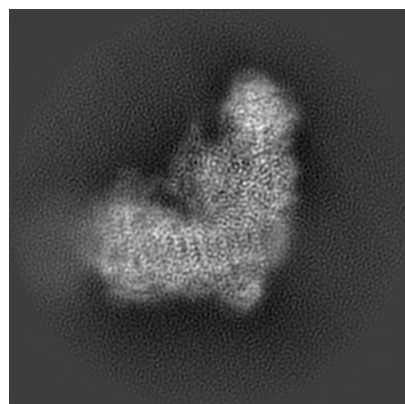
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12741. These allow visual inspection of the internal detail of the map and identification of artifacts.

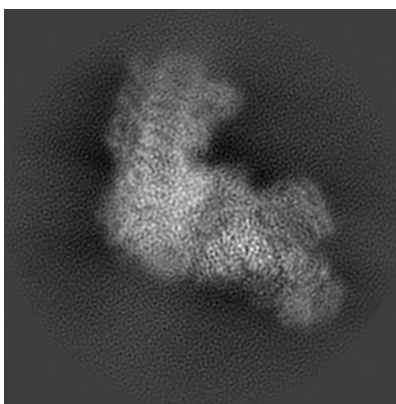
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

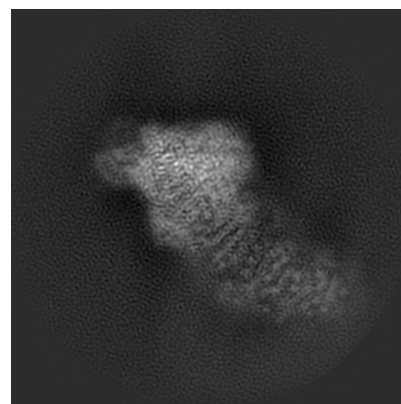
6.1.1 Primary map



X

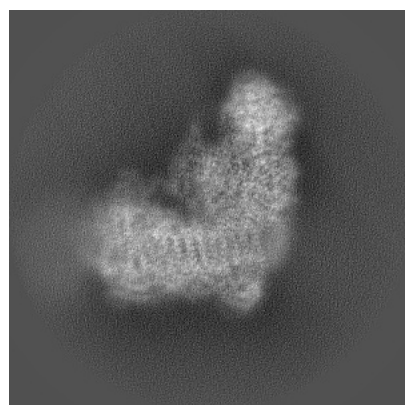


Y

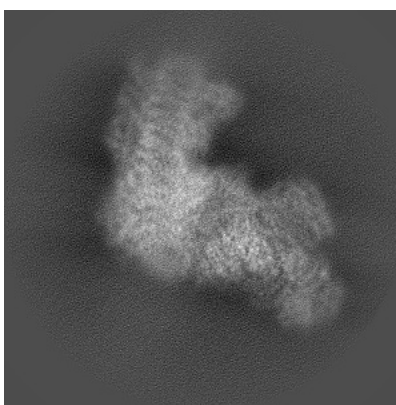


Z

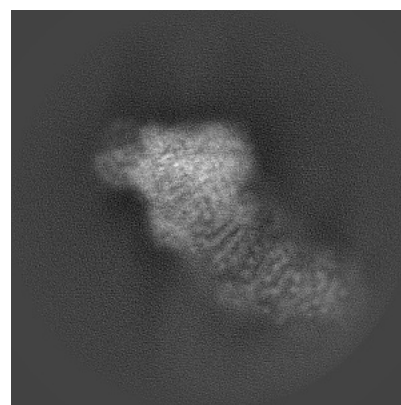
6.1.2 Raw map



X



Y

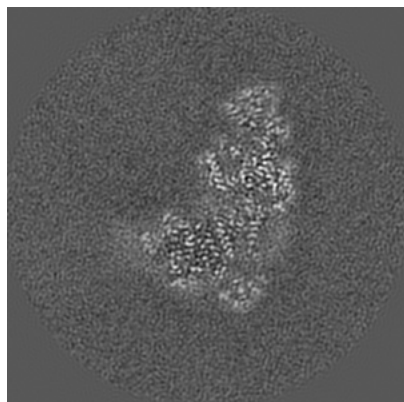


Z

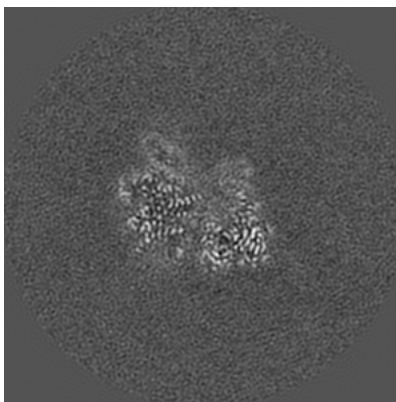
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

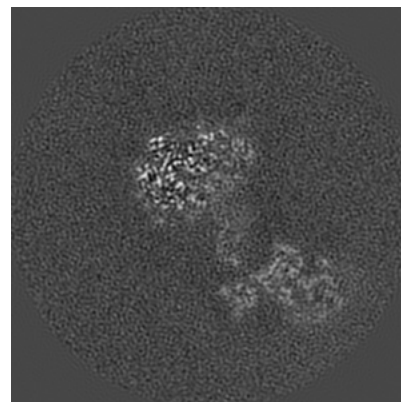
6.2.1 Primary map



X Index: 200

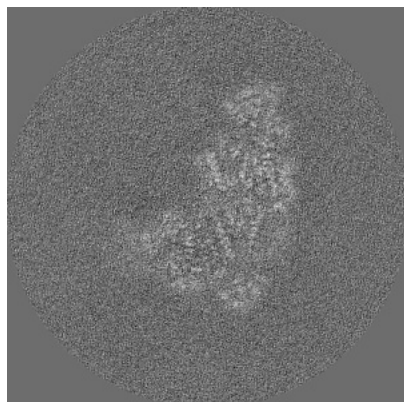


Y Index: 200

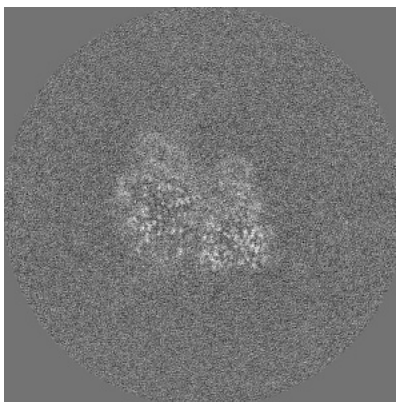


Z Index: 200

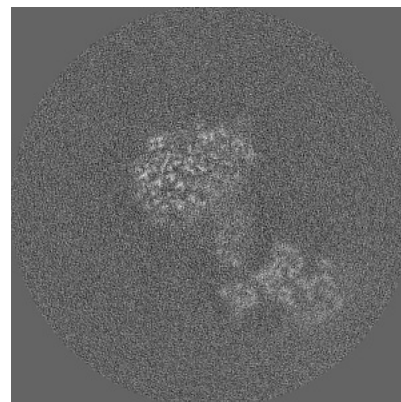
6.2.2 Raw map



X Index: 200



Y Index: 200

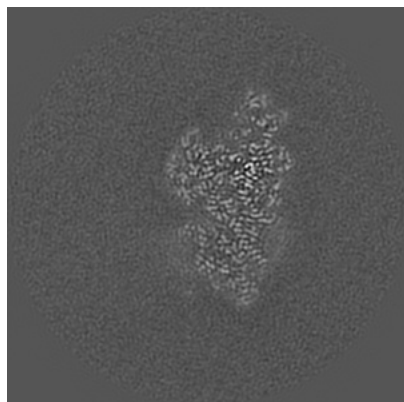


Z Index: 200

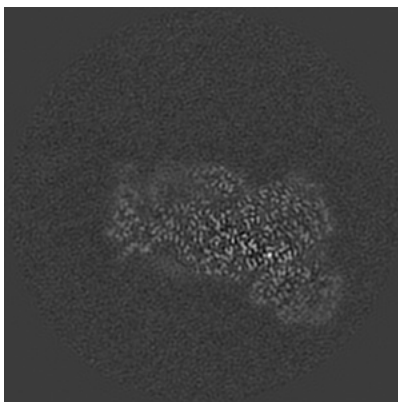
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

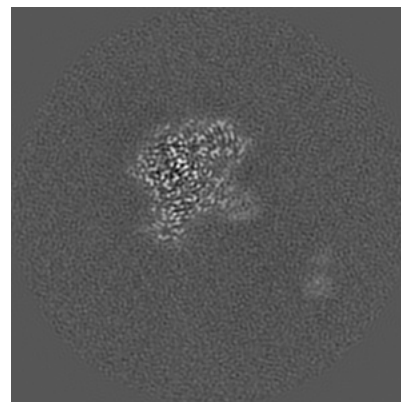
6.3.1 Primary map



X Index: 166

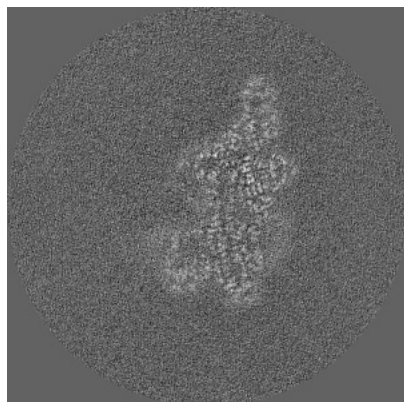


Y Index: 248

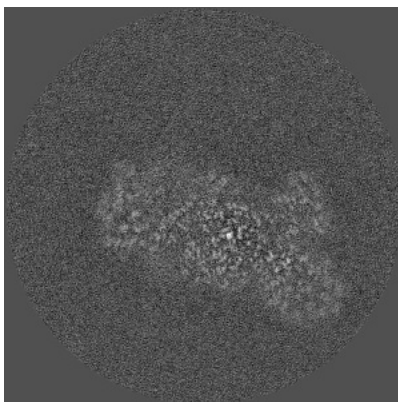


Z Index: 233

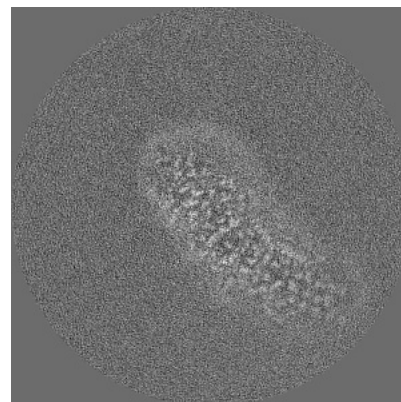
6.3.2 Raw map



X Index: 179



Y Index: 236

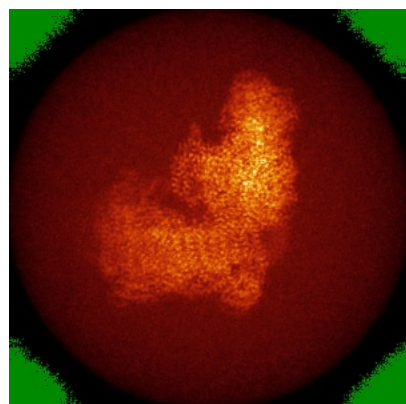


Z Index: 175

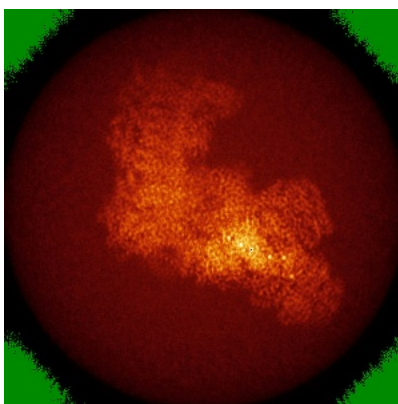
The images above show the largest variance slices of the map in three orthogonal directions.

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

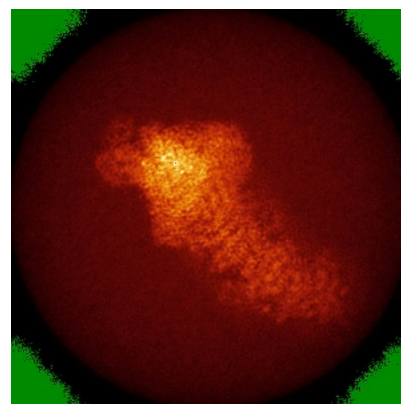
6.4.1 Primary map



X

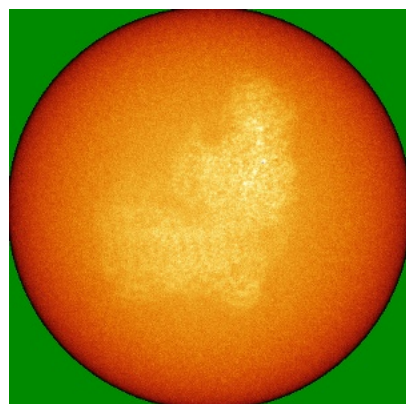


Y

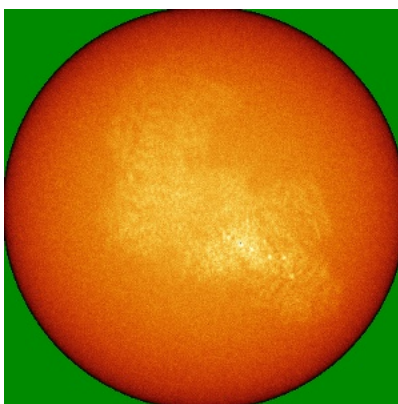


Z

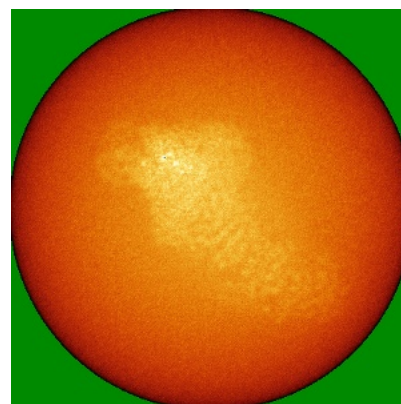
6.4.2 Raw map



X



Y

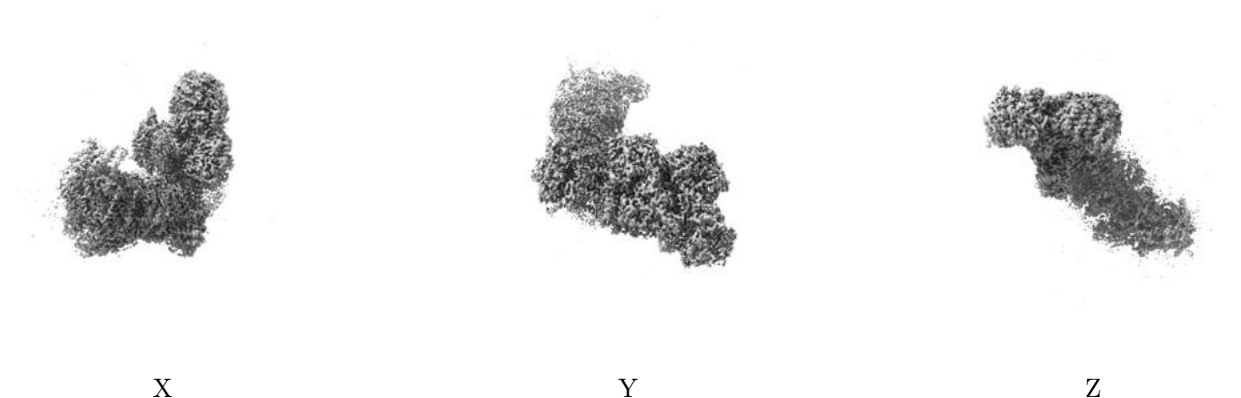


Z

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

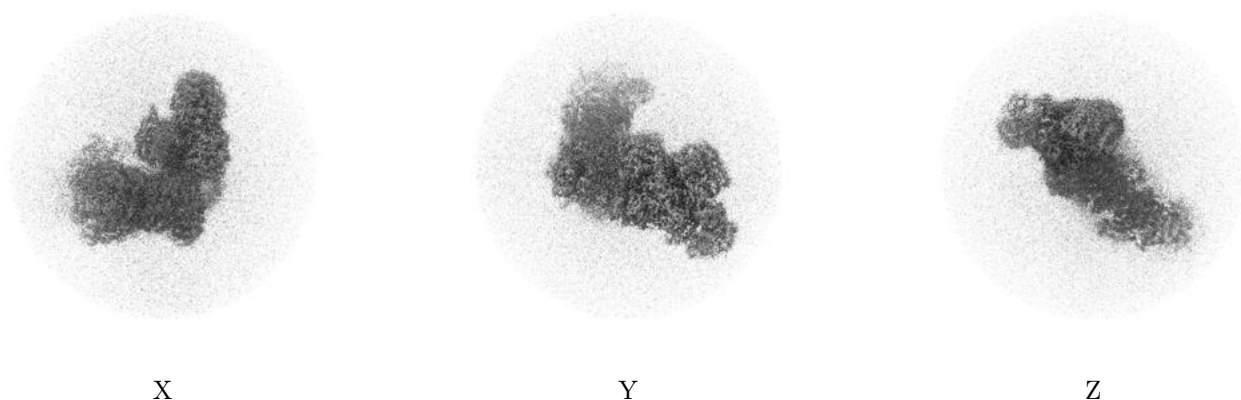
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0115. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

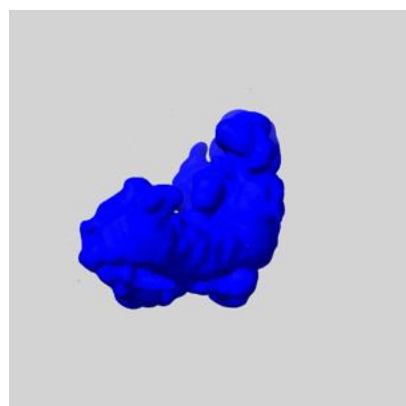
6.6 Mask visualisation [i](#)

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

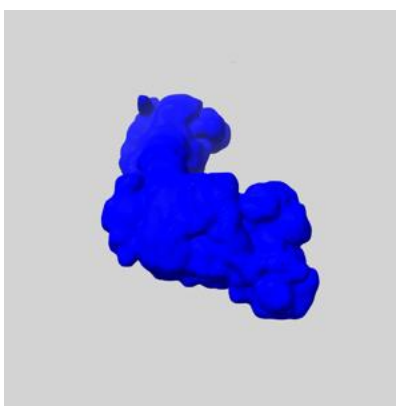
A mask typically either:

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

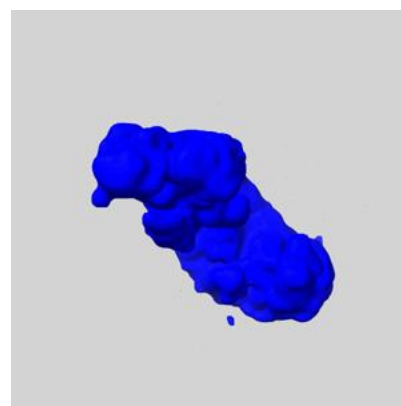
6.6.1 emd_12741_msk_1.map [i](#)



X



Y

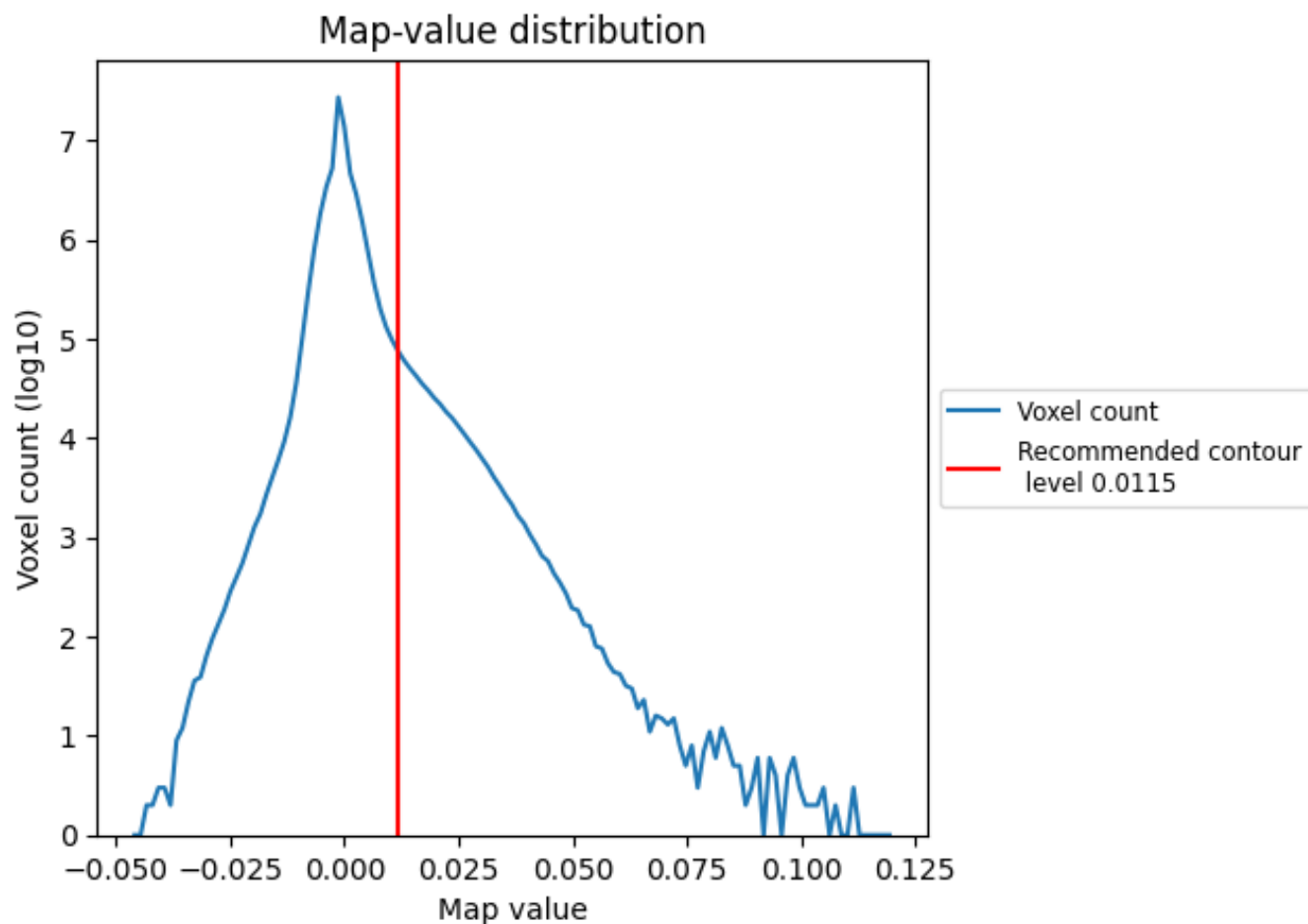


Z

7 Map analysis [i](#)

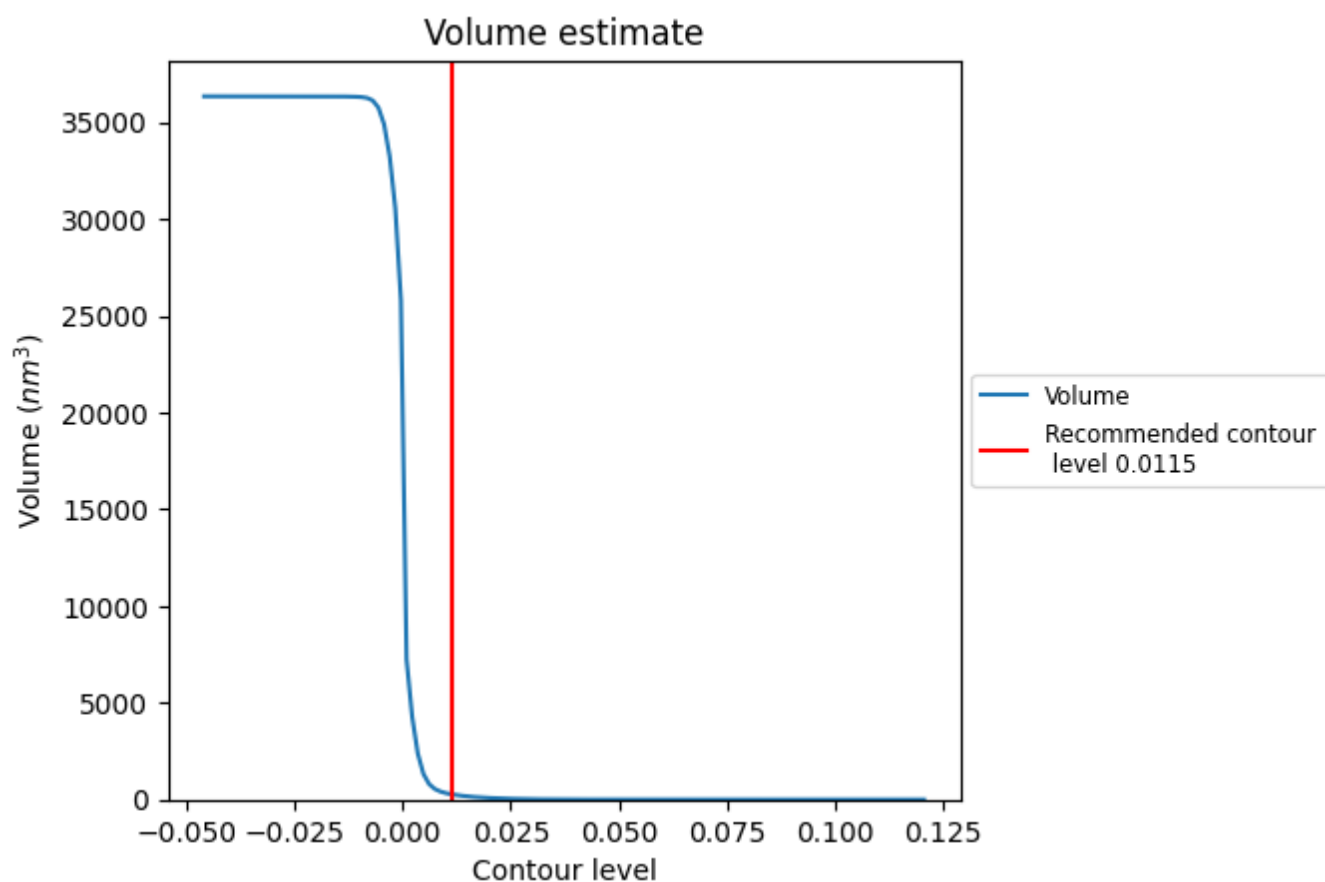
This section contains the results of statistical analysis of the map.

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.

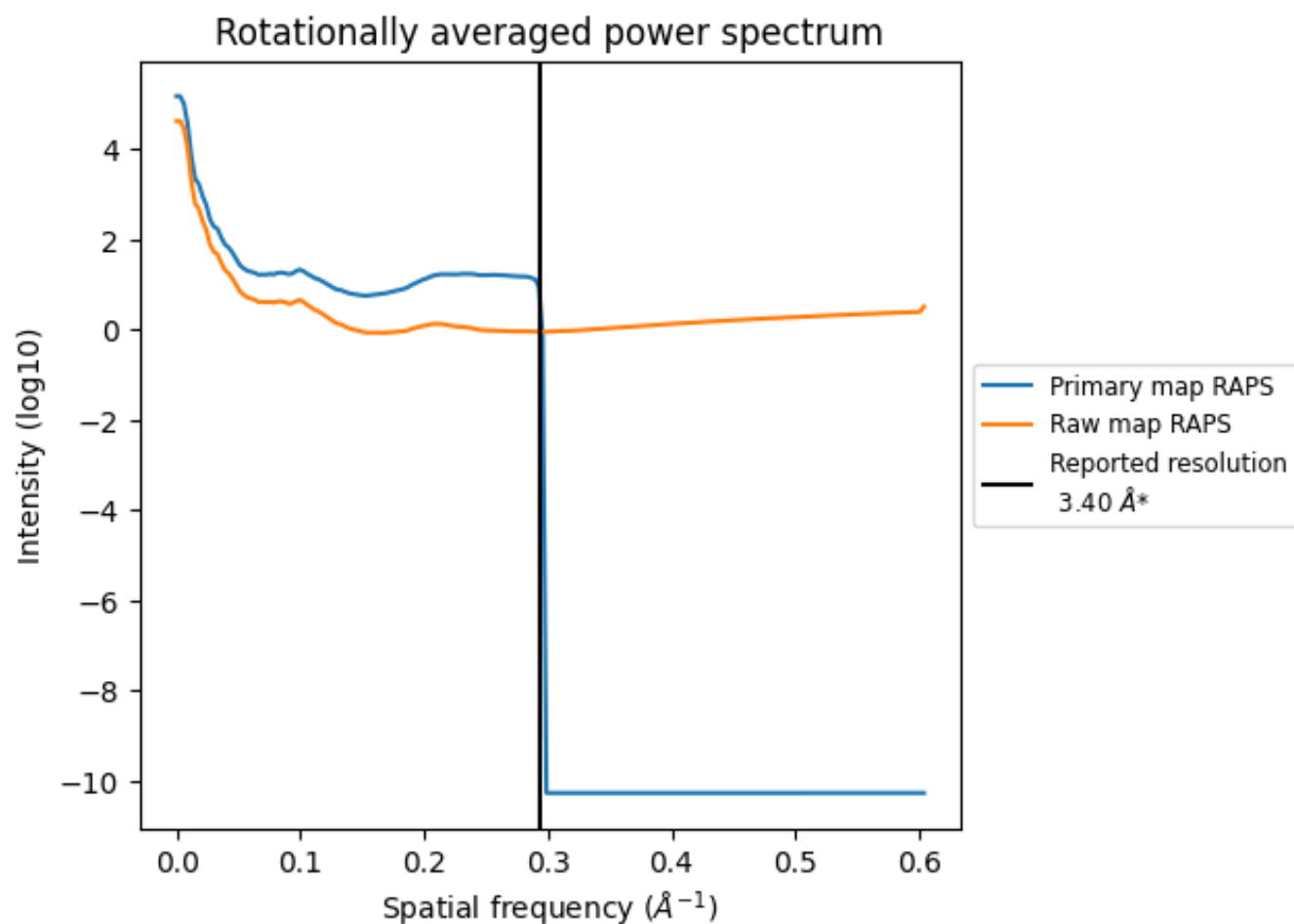
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 266 nm^3 ; this corresponds to an approximate mass of 240 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 ⓘ

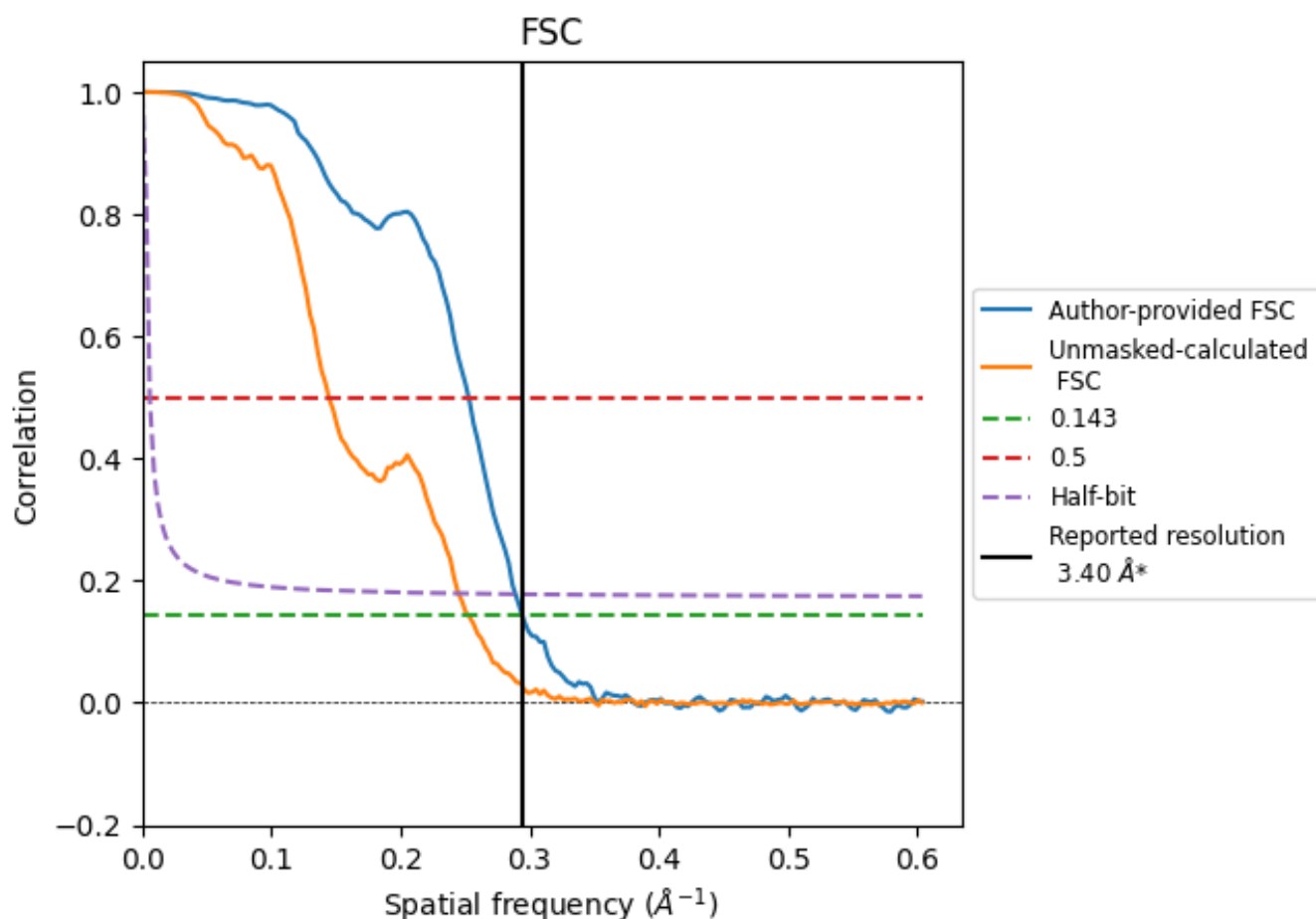


*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

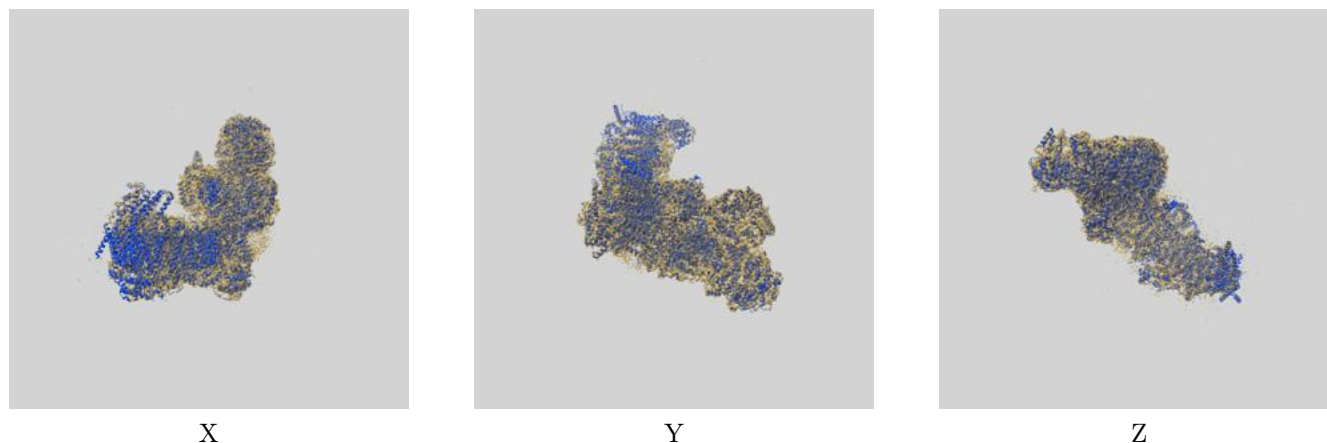
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.96	3.46
Unmasked-calculated*	3.96	6.92	4.08

*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 3.96 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

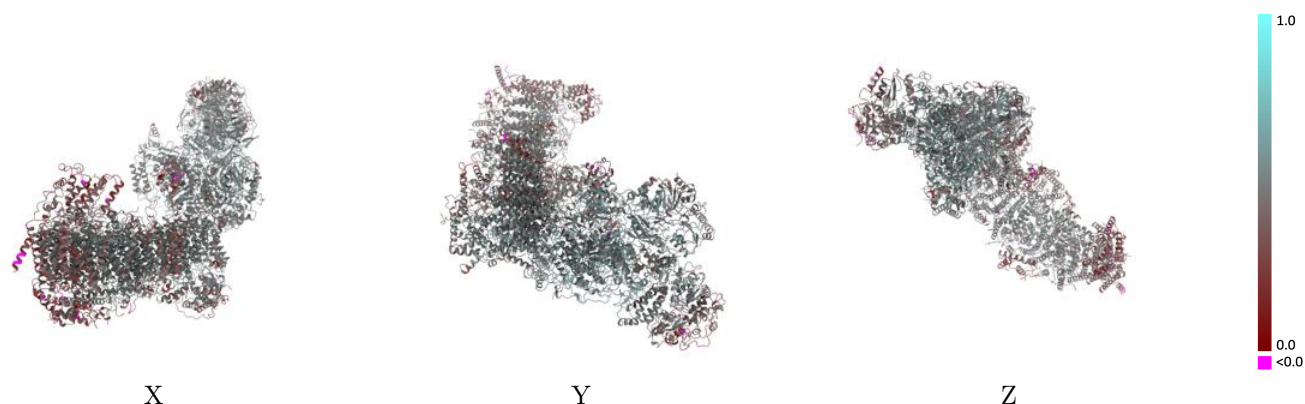
This section contains information regarding the fit between EMDB map EMD-12741 and PDB model 7O6Y. Per-residue inclusion information can be found in [section 3](#) on [page 21](#).

9.1 Map-model overlay [i](#)



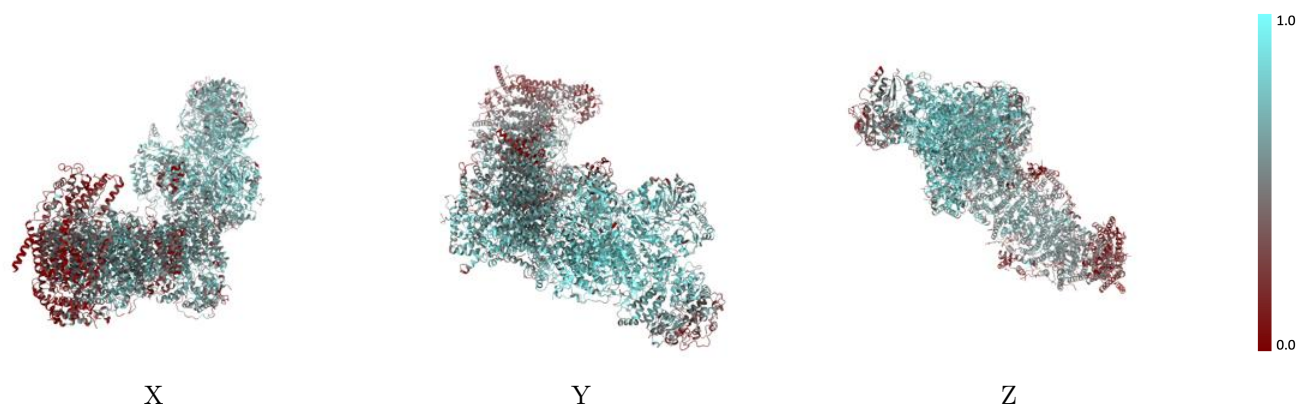
The images above show the 3D surface view of the map at the recommended contour level 0.0115 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



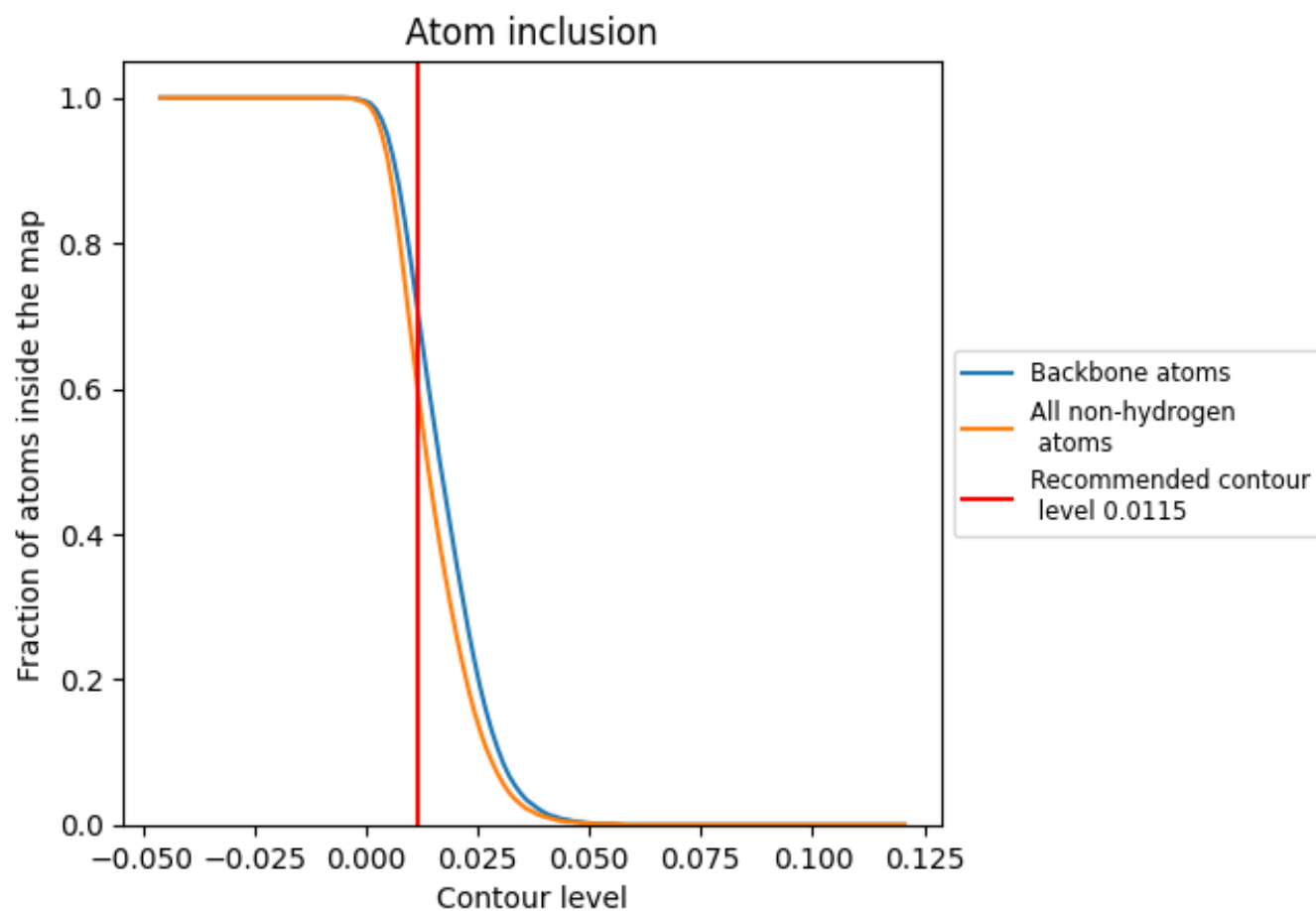
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0115).

9.4 Atom inclusion ⓘ



At the recommended contour level, 71% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0115) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6050	 0.4680
1	 0.7030	 0.5090
2	 0.7170	 0.5060
3	 0.6410	 0.4750
4	 0.6330	 0.5010
5	 0.4040	 0.4330
6	 0.6080	 0.4630
8	 0.1110	 0.2870
9	 0.5170	 0.4090
A	 0.7220	 0.5040
B	 0.5710	 0.4530
C	 0.7650	 0.5240
D	 0.7130	 0.5050
E	 0.6860	 0.4930
F	 0.7080	 0.5010
G	 0.8110	 0.5390
H	 0.5190	 0.3980
I	 0.8100	 0.5410
J	 0.3760	 0.3910
K	 0.8030	 0.5410
L	 0.6410	 0.4780
M	 0.7560	 0.5150
O	 0.2710	 0.2780
P	 0.6500	 0.4550
Q	 0.1560	 0.2720
R	 0.3270	 0.3570
S	 0.3500	 0.3580
U	 0.6180	 0.4590
W	 0.6670	 0.4770
X	 0.6670	 0.4760
Y	 0.7650	 0.5240
Z	 0.7320	 0.5110
a	 0.3010	 0.3720
b	 0.5440	 0.4440
c	 0.1710	 0.3080



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Chain	Atom inclusion	Q-score
d	 0.5240	 0.4490
e	 0.1080	 0.3150
f	 0.5980	 0.4370
g	 0.5340	 0.4480
h	 0.8060	 0.5400
i	 0.3790	 0.4050
j	 0.5150	 0.4520
n	 0.4280	 0.4110