



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:07 PM UTC

PDB ID : 8RGQ / pdb_00008rgq
EMDB ID : EMD-19146
Title : Open Complex I from murine liver
Authors : Vercellino, I.; Sazanov, L.A.
Deposited on : 2023-12-14
Resolution : 3.00 Å(reported)
Based on initial model : 6g2j

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

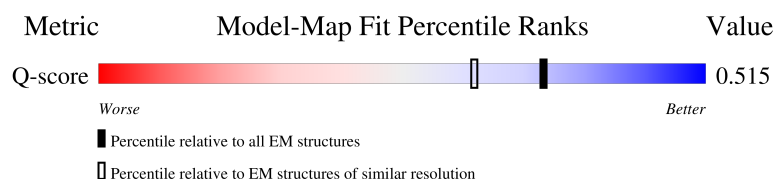
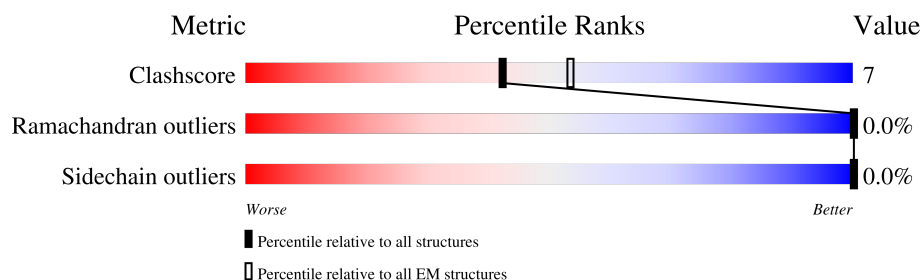
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	6	224	
2	C	263	
3	D	463	
4	2	248	

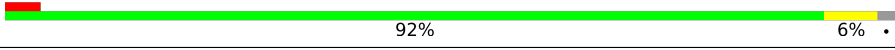
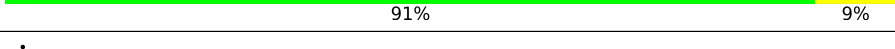
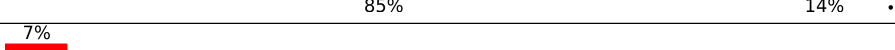
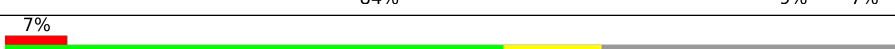
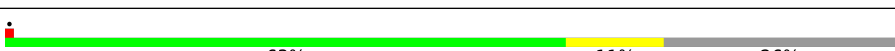
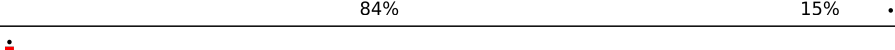
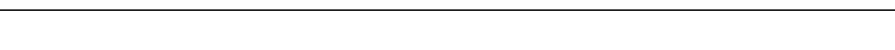
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Mol	Chain	Length	Quality of chain
5	1	464	
6	3	727	
7	9	212	
8	P	377	
9	Q	175	
10	7	116	
11	S	99	
12	T	156	
12	U	156	
13	V	116	
14	W	131	
15	q	145	
16	r	113	
17	s	104	
18	A	115	
19	H	318	
20	J	172	
21	K	98	
22	L	607	
23	M	459	
24	N	345	
25	O	355	
26	X	172	
27	Y	141	
28	Z	144	

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Mol	Chain	Length	Quality of chain
29	a	70	
30	b	84	
31	c	76	
32	d	120	
33	e	106	
34	f	57	
35	g	151	
36	h	189	
37	i	128	
38	j	105	
39	k	104	
40	l	186	
41	m	129	
42	n	179	
43	o	137	
44	p	176	

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 67118 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	6	157	Total	C	N	O	S	0	0
			1258	802	227	215	14		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	208	Total	C	N	O	S	0	0
			1730	1116	297	314	3		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	418	Total	C	N	O	S	0	0
			3371	2156	577	614	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	214	Total	C	N	O	S	0	0
			1660	1056	279	314	11		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1	430	Total	C	N	O	S	0	0
			3321	2092	596	611	22		

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3	690	Total	C	N	O	S	0	0
			5305	3326	921	1017	41		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	314	Total	C	N	O	S	0	0
			2513	1611	453	442	7		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	126	Total	C	N	O	S	0	0
			1022	646	180	192	4		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	7	96	Total	C	N	O	S	0	0
			758	470	141	144	3		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	84	Total	C	N	O	S	0	0
			671	421	127	120	3		

- Molecule 12 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	79	Total	C	N	O	S	0	0
			637	410	95	127	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	88	Total	C	N	O	S	0	0
			706	453	104	144	5		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	113	Total	C	N	O	S	0	0
			923	602	153	165	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	q	145	Total	C	N	O	S	0	0
			1209	777	215	212	5		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	r	97	Total	C	N	O	S	0	0
			781	493	146	139	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	s	42	Total	C	N	O	0	0
			351	219	62	70		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A	93	Total	C	N	O	S	0	0
			760	527	104	124	5		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	H	306	Total	C	N	O	S	0	0
			2452	1652	371	407	22		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	165	Total	C	N	O	S	0	0
			1246	837	178	216	15		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	345	Total	C	N	O	S	0	0
			2703	1795	417	454	37		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	70	Total	C	N	O	S	0	0
			572	370	101	97	4		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	82	Total	C	N	O	S	0	0
			643	422	104	113	4		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

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

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	139	Total	C	N	O	S	0	0
			1166	764	195	204	3		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	106	Total	C	N	O	S	0	0
			897	584	157	152	4		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	65	Total	C	N	O	S	0	0
			562	370	93	98	1		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	k	77	Total	C	N	O	S	0	0
			626	414	106	104	2		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	157	Total	C	N	O	S	0	0
			1323	855	220	237	11		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		

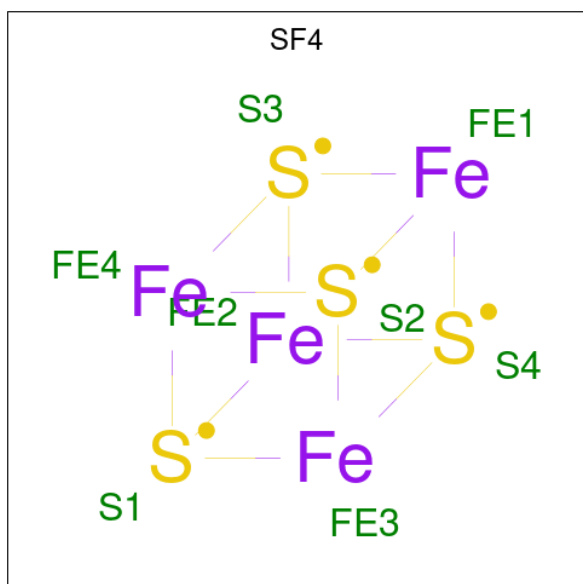
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	118	Total	C	N	O	S	0	0
			1014	639	190	177	8		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

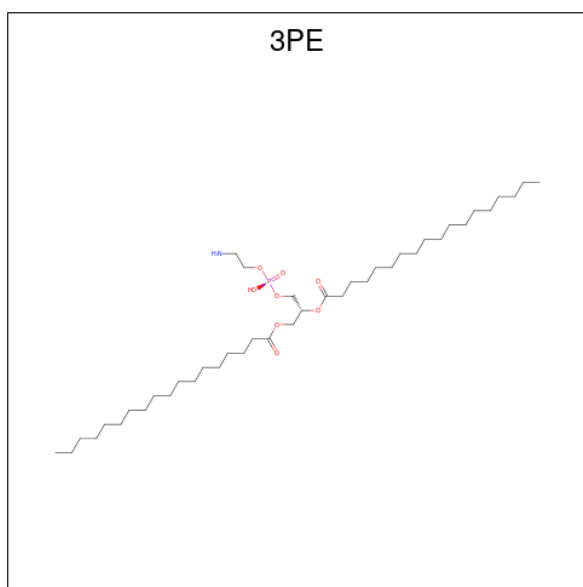
Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	169	Total	C	N	O	S	0	0
			1430	899	257	266	8		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
45	6	1	Total	Fe	S	0
			8	4	4	
45	1	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	9	1	Total	Fe	S	0
			8	4	4	
45	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $\text{C}_{41}\text{H}_{82}\text{NO}_8\text{P}$).



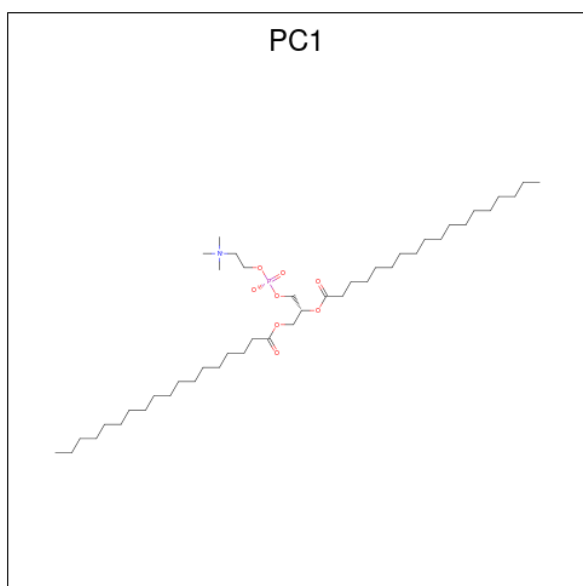
Mol	Chain	Residues	Atoms					AltConf
46	6	1	Total	C	N	O	P	0
			32	22	1	8	1	
46	r	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	K	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	M	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	N	1	Total	C	N	O	P	0
			38	28	1	8	1	
46	Y	1	Total	C	N	O	P	0
			28	18	1	8	1	
46	Y	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	d	1	Total	C	N	O	P	0
			31	21	1	8	1	

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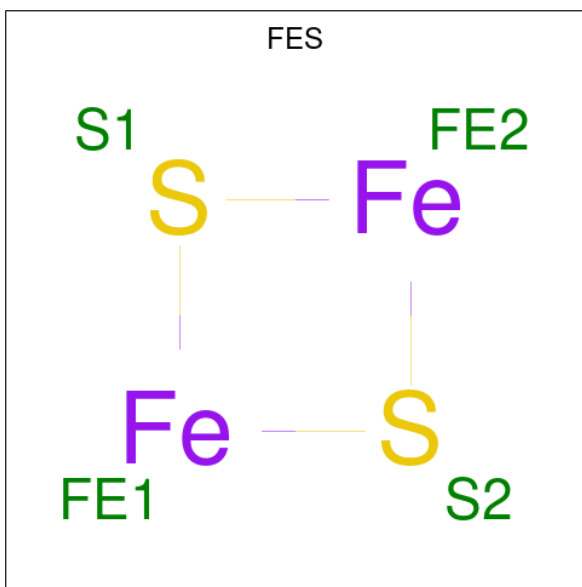
Mol	Chain	Residues	Atoms					AltConf
46	d	1	Total	C	N	O	P	0
			32	22	1	8	1	
46	i	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	m	1	Total	C	N	O	P	0
			30	20	1	8	1	

- Molecule 47 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



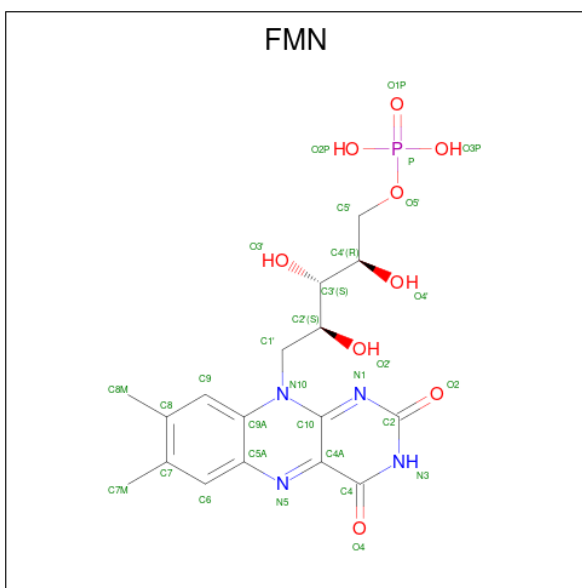
Mol	Chain	Residues	Atoms					AltConf
47	6	1	Total	C	N	O	P	0
			43	33	1	8	1	
47	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
47	9	1	Total	C	N	O	P	0
			47	37	1	8	1	
47	M	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
48	2	1	Total 4	Fe 2	S 2	0
48	3	1	Total 4	Fe 2	S 2	0

- Molecule 49 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

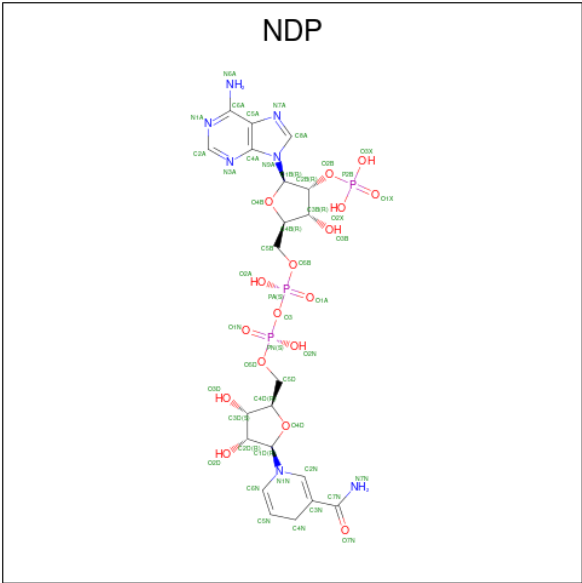


Mol	Chain	Residues	Atoms					AltConf
49	1	1	Total 31	C 17	N 4	O 9	P 1	0

- Molecule 50 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
50	3	1	Total	K	0
			1	1	

- Molecule 51 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

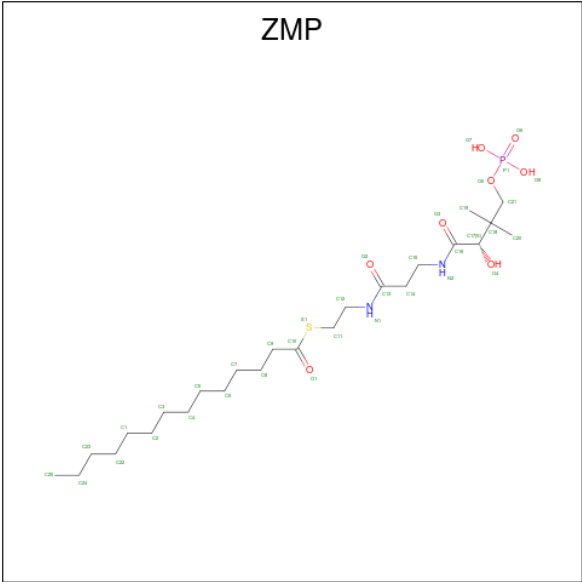


Mol	Chain	Residues	Atoms					AltConf
51	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

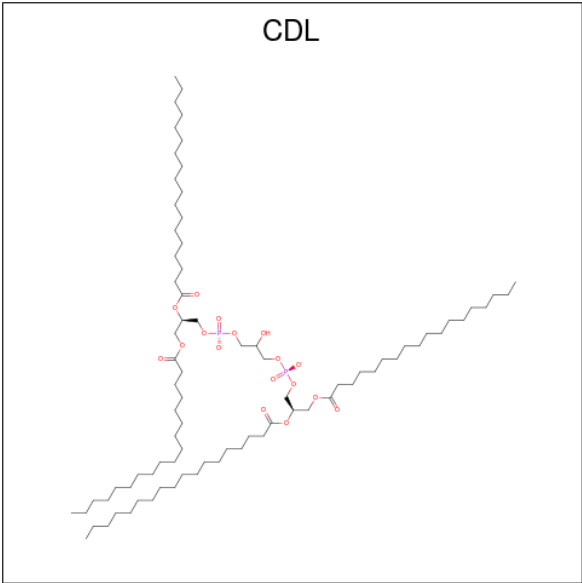
Mol	Chain	Residues	Atoms		AltConf
52	7	1	Total	Zn	0
			1	1	

- Molecule 53 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



Mol	Chain	Residues	Atoms						AltConf
53	W	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
53	n	1	Total	C	N	O	P	S	0
			32	21	2	7	1	1	

- Molecule 54 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



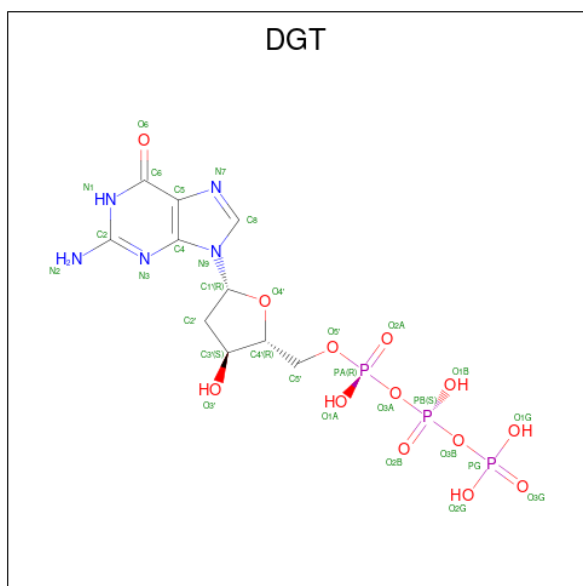
Mol	Chain	Residues	Atoms				AltConf
54	r	1	Total	C	O	P	0
			57	38	17	2	
54	L	1	Total	C	O	P	0
			78	59	17	2	

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Mol	Chain	Residues	Atoms				AltConf
54	N	1	Total	C	O	P	0
			90	71	17	2	
54	d	1	Total	C	O	P	0
			67	48	17	2	
54	h	1	Total	C	O	P	0
			70	51	17	2	
54	m	1	Total	C	O	P	0
			72	53	17	2	

- Molecule 55 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

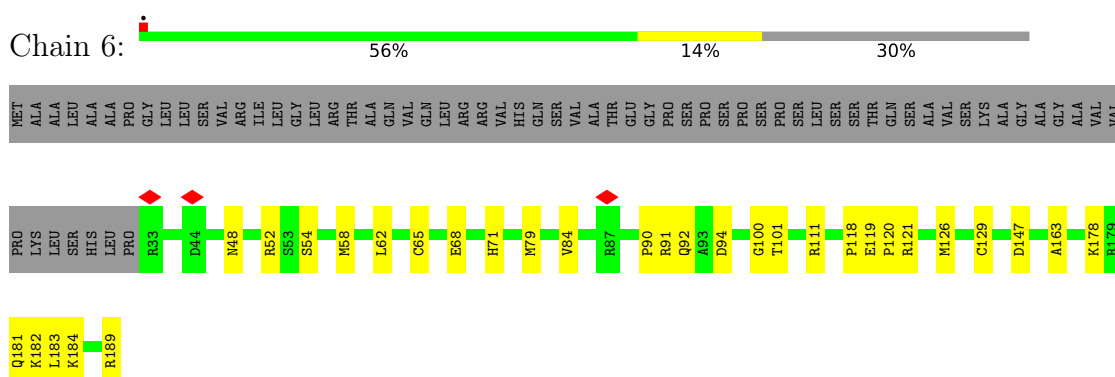
- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

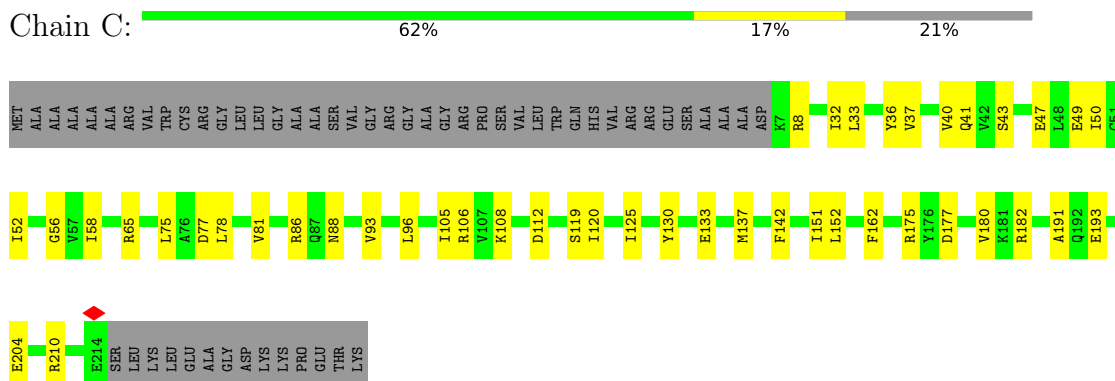
3 Residue-property plots [i](#)

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

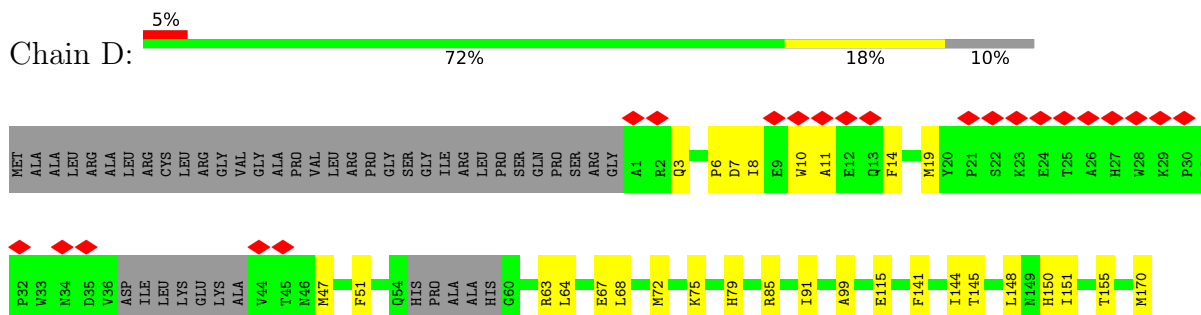
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

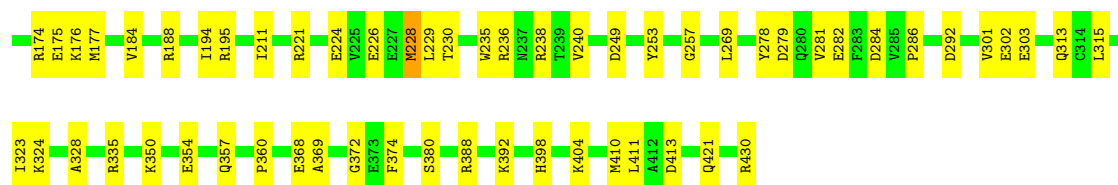


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



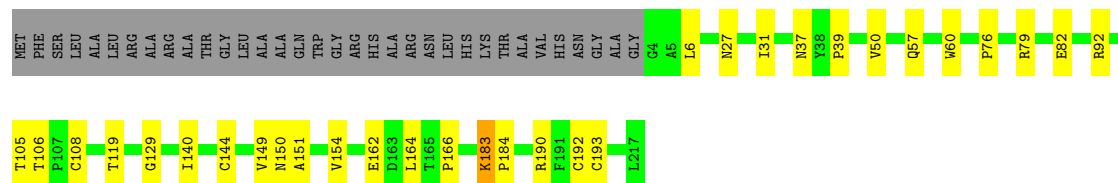
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial





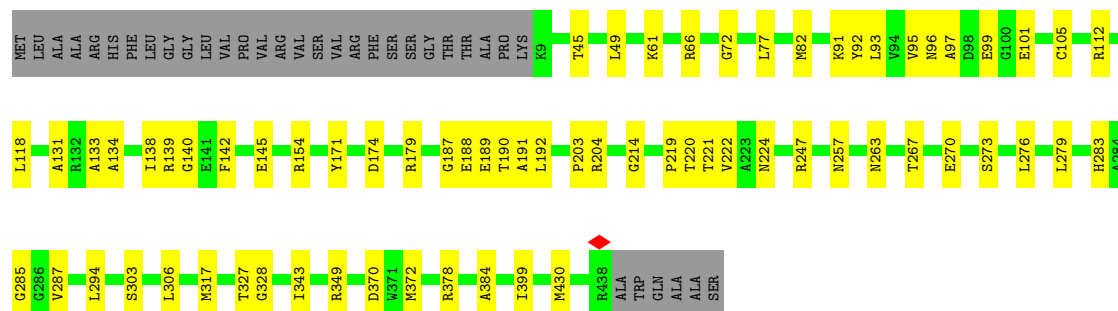
- Molecule 4: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 2: 74% 12% 14%



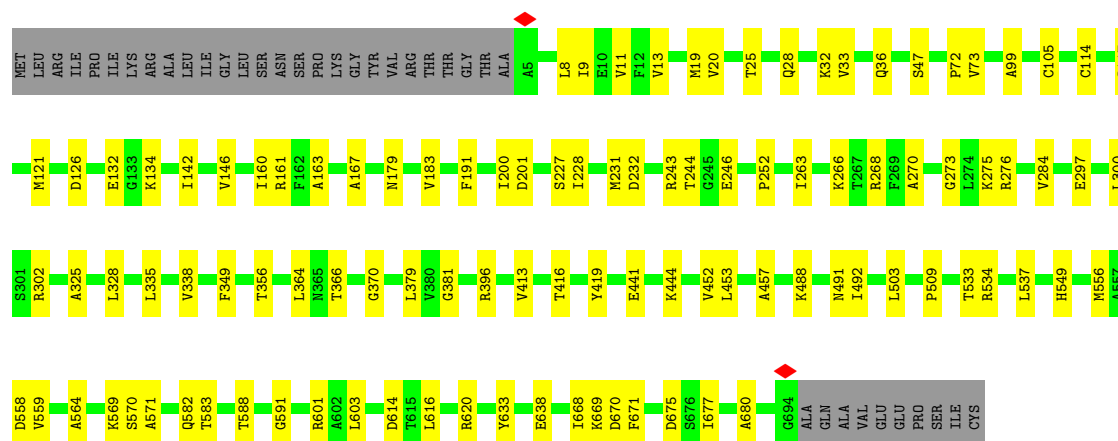
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1: 78% 15% 7%



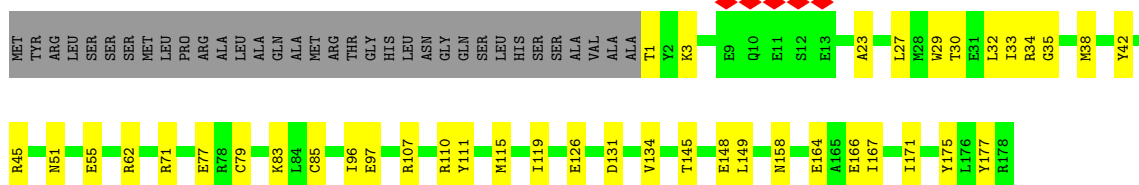
- Molecule 6: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 3: 80% 15% 5%



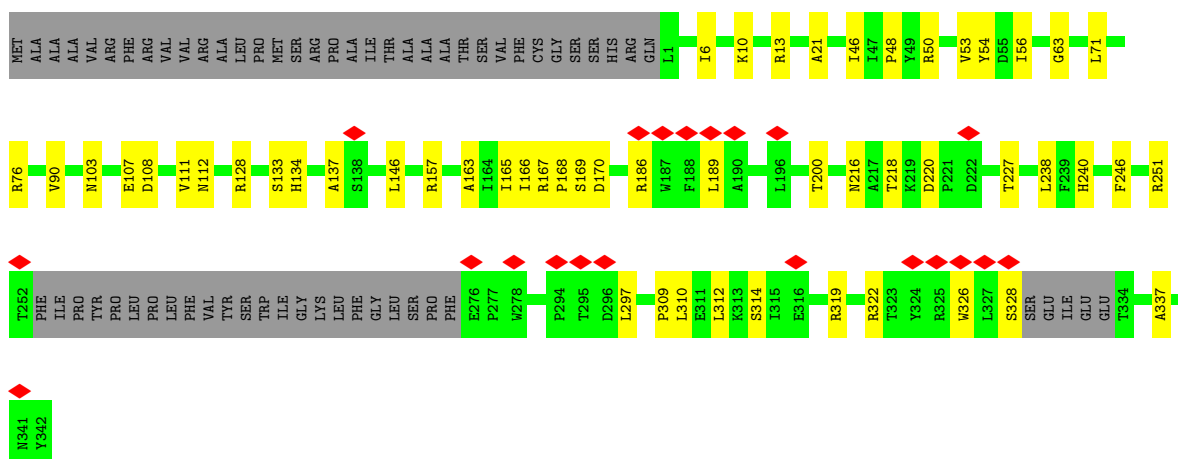
- Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 9: 



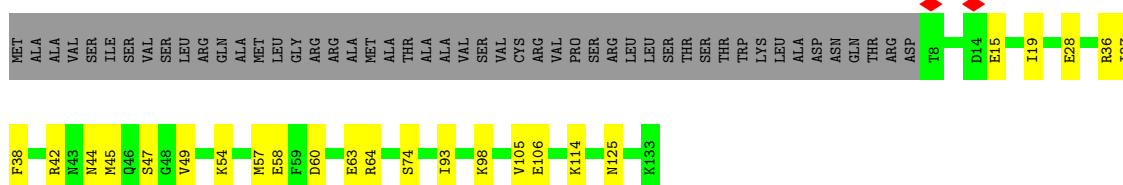
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 



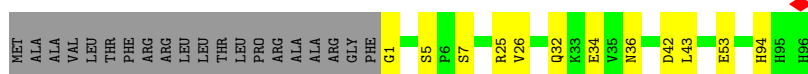
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q: 



- Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 7: 

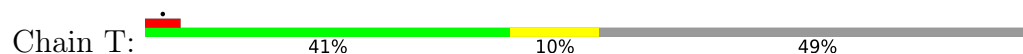


- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S: 



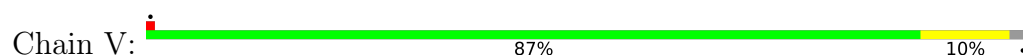
- Molecule 12: Acyl carrier protein, mitochondrial



- Molecule 12: Acyl carrier protein, mitochondrial



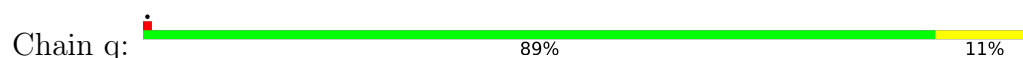
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

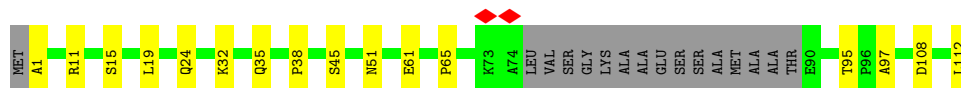


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

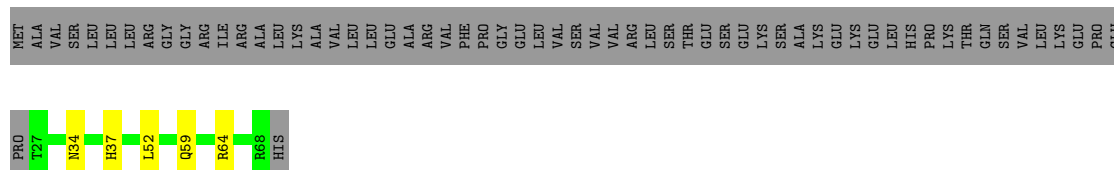


- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

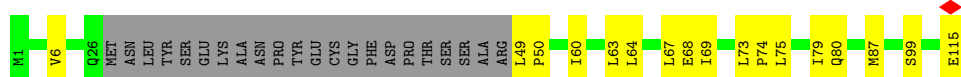




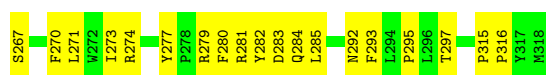
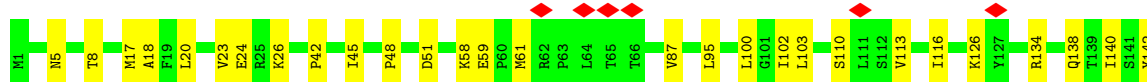
- Molecule 17: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



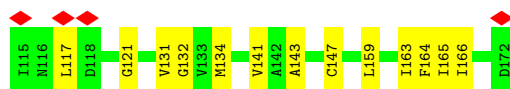
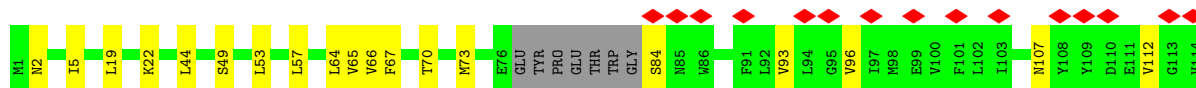
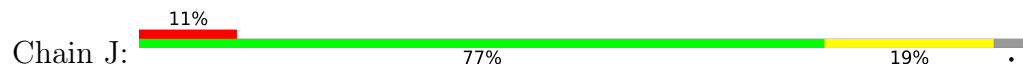
- Molecule 18: NADH-ubiquinone oxidoreductase chain 3



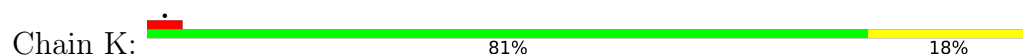
- Molecule 19: NADH-ubiquinone oxidoreductase chain 1

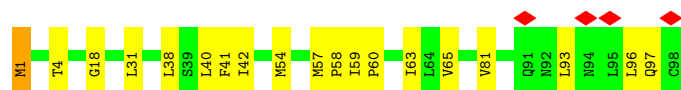


- Molecule 20: NADH-ubiquinone oxidoreductase chain 6

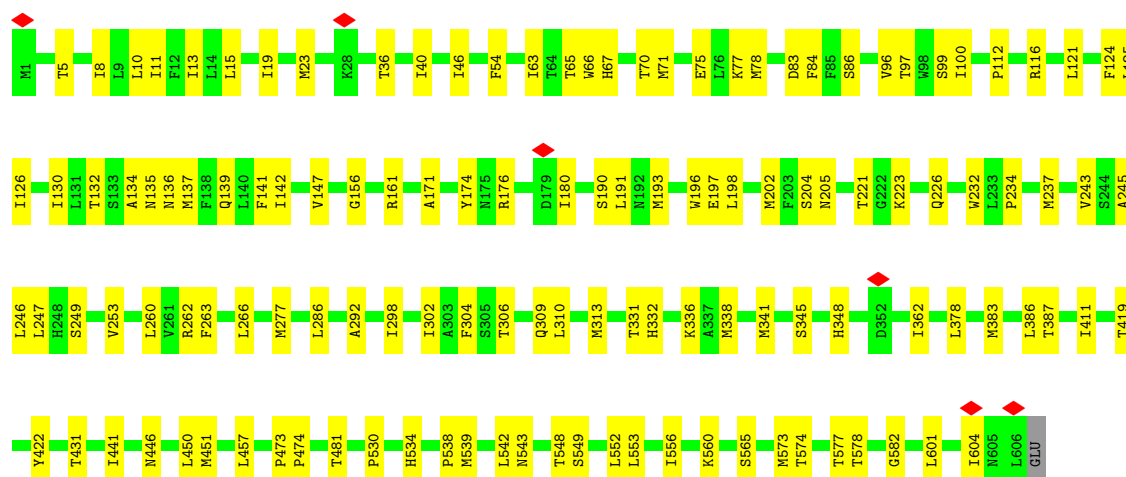
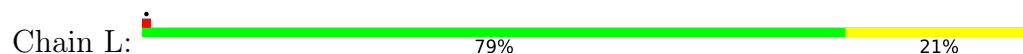


- Molecule 21: NADH-ubiquinone oxidoreductase chain 4L

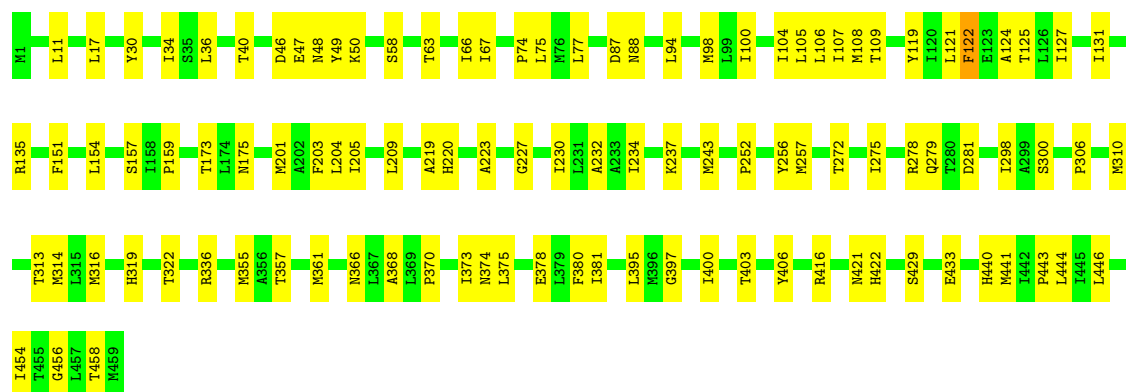
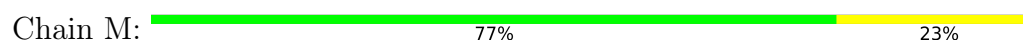




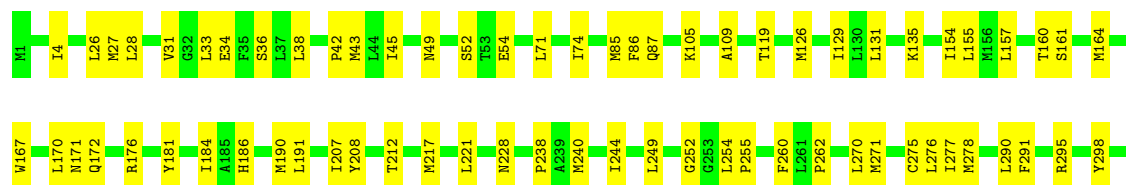
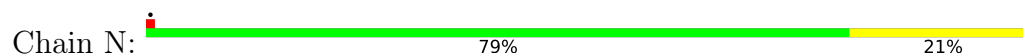
• Molecule 22: NADH-ubiquinone oxidoreductase chain 5

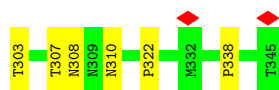


• Molecule 23: NADH-ubiquinone oxidoreductase chain 4



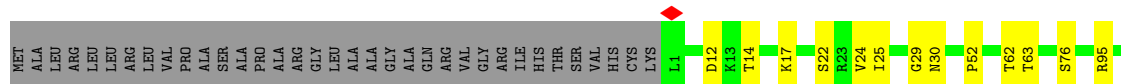
• Molecule 24: NADH-ubiquinone oxidoreductase chain 2





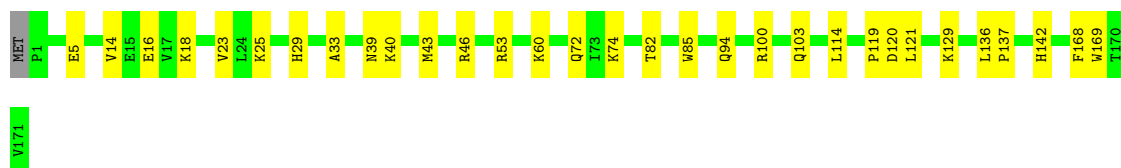
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 74% 16% 10%



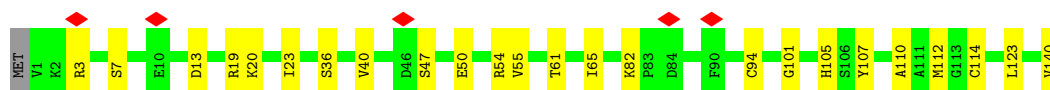
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X: 81% 18%



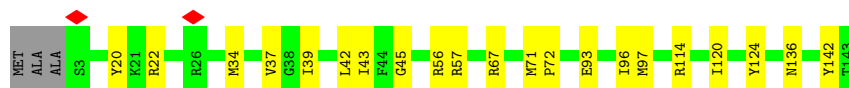
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y: 82% 17%



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z: 83% 15%

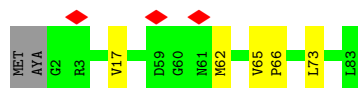


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

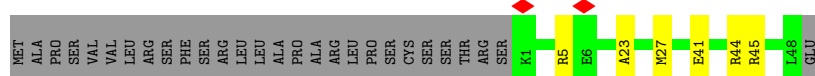
Chain a: 71% 29%



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



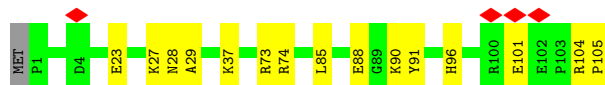
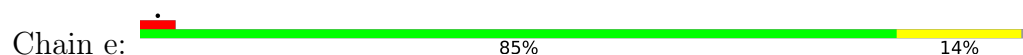
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



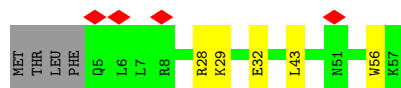
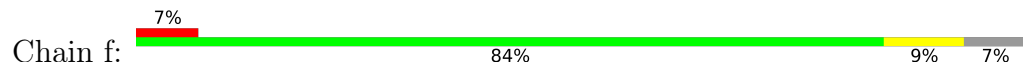
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 subunit C2



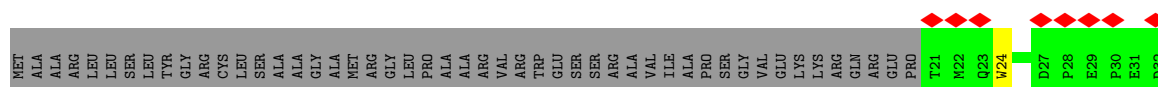
- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



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

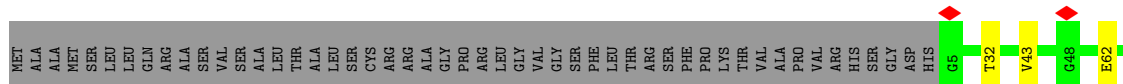


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

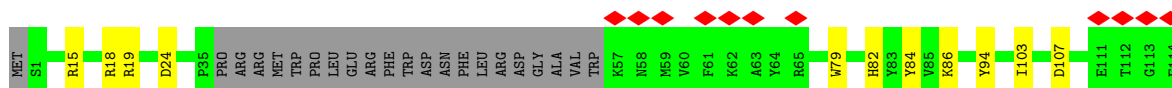
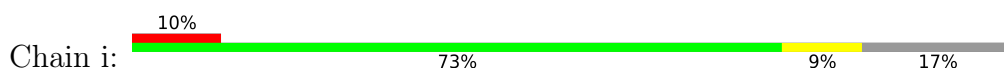




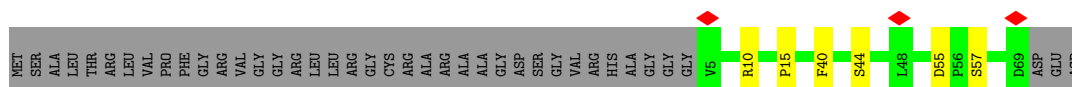
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



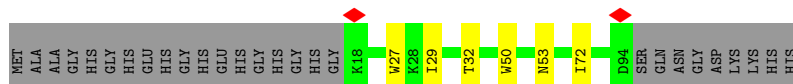
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



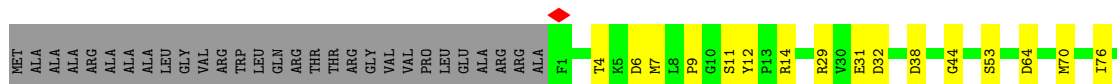
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

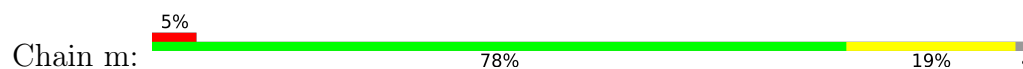


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

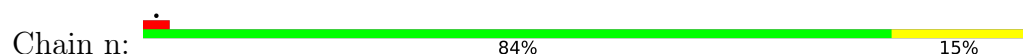




- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



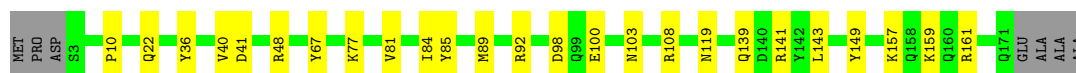
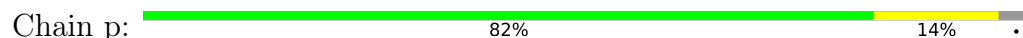
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	317317	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.122	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	232.13998, 207.76, 207.76	wwPDB
Map dimensions	219, 196, 196	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	6	0.21	0/1289	0.51	0/1744
2	C	0.16	0/1780	0.37	0/2424
3	D	0.19	0/3442	0.43	0/4659
4	2	0.18	0/1700	0.42	0/2316
5	1	0.19	0/3396	0.44	0/4586
6	3	0.17	0/5392	0.36	0/7305
7	9	0.19	0/1461	0.45	0/1974
8	P	0.16	0/2574	0.39	0/3483
9	Q	0.17	0/1045	0.34	0/1411
10	7	0.14	0/773	0.29	0/1041
11	S	0.17	0/682	0.50	0/920
12	T	0.22	0/646	0.59	0/869
12	U	0.17	0/718	0.41	0/970
13	V	0.17	0/945	0.36	0/1281
14	W	0.18	0/993	0.42	0/1335
15	q	0.16	0/1251	0.39	0/1702
16	r	0.15	0/791	0.31	0/1069
17	s	0.13	0/360	0.36	0/489
18	A	0.23	0/770	0.50	0/1052
19	H	0.26	0/2517	0.55	0/3441
20	J	0.24	0/1263	0.59	2/1715 (0.1%)
21	K	0.23	0/738	0.52	0/1002
22	L	0.23	0/4913	0.49	0/6686
23	M	0.23	0/3709	0.52	2/5052 (0.0%)
24	N	0.24	0/2755	0.53	0/3751
25	O	0.16	0/2674	0.42	0/3626
26	X	0.16	0/1434	0.39	0/1937
27	Y	0.22	0/1061	0.52	1/1439 (0.1%)
28	Z	0.17	0/1198	0.40	0/1616
29	a	0.25	0/585	0.45	0/788
30	b	0.16	0/666	0.40	0/914
31	c	0.13	0/409	0.33	0/555

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	d	0.15	0/1028	0.37	0/1387
33	e	0.13	0/900	0.31	0/1199
34	f	0.14	0/468	0.34	0/630
35	g	0.16	0/878	0.41	0/1196
36	h	0.18	0/1201	0.38	0/1626
37	i	0.17	0/917	0.39	0/1243
38	j	0.16	0/587	0.42	0/804
39	k	0.15	0/646	0.35	0/873
40	l	0.14	0/1379	0.38	0/1882
41	m	0.18	0/1079	0.43	0/1463
42	n	0.15	0/1596	0.40	0/2162
43	o	0.16	0/1039	0.42	0/1394
44	p	0.16	0/1463	0.35	0/1977
All	All	0.19	0/67111	0.44	5/90988 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	84	SER	CA-C-N	5.59	132.21	121.54
20	J	84	SER	C-N-CA	5.59	132.21	121.54
23	M	122	PHE	CA-C-N	-5.29	111.26	121.58
23	M	122	PHE	C-N-CA	-5.29	111.26	121.58
27	Y	82	LYS	CB-CA-C	5.09	116.99	110.98

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6	1258	0	1268	28	0
2	C	1730	0	1686	30	0
3	D	3371	0	3320	70	0
4	2	1660	0	1653	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1	3321	0	3278	43	0
6	3	5305	0	5330	63	0
7	9	1431	0	1383	41	0
8	P	2513	0	2536	35	0
9	Q	1022	0	1023	19	0
10	7	758	0	731	9	0
11	S	671	0	688	5	0
12	T	637	0	640	10	0
12	U	706	0	699	17	0
13	V	923	0	965	8	0
14	W	970	0	991	15	0
15	q	1209	0	1170	12	0
16	r	781	0	811	13	0
17	s	351	0	331	5	0
18	A	760	0	811	24	0
19	H	2452	0	2547	62	0
20	J	1246	0	1270	28	0
21	K	737	0	768	16	0
22	L	4800	0	4985	94	0
23	M	3632	0	3853	77	0
24	N	2703	0	2902	58	0
25	O	2607	0	2566	39	0
26	X	1396	0	1385	26	0
27	Y	1037	0	1025	15	0
28	Z	1167	0	1166	18	0
29	a	572	0	583	16	0
30	b	643	0	644	4	0
31	c	398	0	401	5	0
32	d	996	0	1001	10	0
33	e	877	0	871	13	0
34	f	456	0	452	4	0
35	g	850	0	783	14	0
36	h	1166	0	1166	16	0
37	i	897	0	902	13	0
38	j	562	0	515	4	0
39	k	626	0	620	5	0
40	l	1323	0	1216	23	0
41	m	1050	0	1061	19	0
42	n	1541	0	1473	22	0
43	o	1014	0	1002	12	0
44	p	1430	0	1400	22	0
45	1	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	3	16	0	0	0	0
45	6	8	0	0	0	0
45	9	16	0	0	1	0
46	6	32	0	38	2	0
46	A	43	0	60	3	0
46	H	51	0	82	2	0
46	K	41	0	59	0	0
46	L	102	0	164	5	0
46	M	138	0	210	5	0
46	N	38	0	50	2	0
46	Y	70	0	88	4	0
46	d	63	0	74	0	0
46	i	42	0	61	2	0
46	m	30	0	34	2	0
46	r	46	0	66	0	0
47	6	43	0	63	2	0
47	9	101	0	159	7	0
47	M	54	0	88	5	0
48	2	4	0	0	0	0
48	3	4	0	0	0	0
49	1	31	0	19	3	0
50	3	1	0	0	0	0
51	P	48	0	26	2	0
52	7	1	0	0	0	0
53	W	34	0	40	3	0
53	n	32	0	36	4	0
54	L	78	0	100	1	0
54	N	90	0	133	7	0
54	d	67	0	81	6	0
54	h	70	0	87	7	0
54	m	72	0	91	1	0
54	r	57	0	58	3	0
55	O	31	0	12	1	0
56	O	1	0	0	0	0
All	All	67118	0	67850	904	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 7.

All (904) 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)
18:A:49:LEU:CD1	19:H:126:LYS:HD3	1.78	1.14
18:A:49:LEU:HD13	19:H:126:LYS:HD3	1.09	1.09
3:D:228:MET:HA	3:D:228:MET:HE2	1.32	1.07
5:1:99:GLU:OE2	5:1:105:CYS:HA	1.67	0.95
18:A:49:LEU:HD13	19:H:126:LYS:CD	1.99	0.88
8:P:310:LEU:O	8:P:314:SER:HB2	1.73	0.86
3:D:228:MET:HA	3:D:228:MET:CE	2.06	0.86
22:L:245:ALA:O	22:L:249:SER:HB2	1.77	0.84
5:1:99:GLU:OE2	5:1:105:CYS:CA	2.29	0.80
3:D:170:MET:HE1	3:D:221:ARG:HB3	1.64	0.79
3:D:228:MET:HE1	7:9:35:GLY:HA3	1.65	0.77
8:P:216:ASN:O	8:P:220:ASP:HB2	1.86	0.76
3:D:47:MET:HB2	3:D:68:LEU:HB2	1.69	0.74
22:L:331:THR:HG23	22:L:387:THR:HG22	1.71	0.72
3:D:228:MET:HG2	7:9:38:MET:HE1	1.72	0.72
5:1:96:ASN:ND2	5:1:187:GLY:O	2.20	0.71
37:i:120:ARG:HB2	43:o:39:VAL:HG13	1.71	0.70
3:D:14:PHE:HA	3:D:19:MET:HE1	1.73	0.69
5:1:112:ARG:HB3	5:1:145:GLU:HG3	1.75	0.69
3:D:228:MET:HE1	7:9:35:GLY:CA	2.22	0.69
3:D:51:PHE:HB3	3:D:64:LEU:HB2	1.75	0.69
4:2:150:ASN:HB3	4:2:162:GLU:HB3	1.76	0.68
4:2:119:THR:HG21	4:2:166:PRO:HB3	1.74	0.68
18:A:49:LEU:HB3	18:A:50:PRO:HD2	1.76	0.68
35:g:81:TYR:O	35:g:84:GLN:NE2	2.27	0.68
3:D:410:MET:H	3:D:413:ASP:HB2	1.58	0.67
3:D:328:ALA:HB3	6:3:126:ASP:HB2	1.77	0.67
5:1:93:LEU:O	5:1:134:ALA:HA	1.95	0.67
7:9:71:ARG:NH2	10:7:36:ASN:OD1	2.29	0.66
23:M:232:ALA:O	23:M:237:LYS:NZ	2.30	0.65
2:C:77:ASP:HB3	3:D:392:LYS:HG3	1.80	0.64
24:N:172:GLN:HE22	24:N:181:TYR:HD2	1.46	0.64
22:L:578:THR:OG1	24:N:171:ASN:ND2	2.31	0.64
3:D:228:MET:CG	7:9:38:MET:HE1	2.28	0.64
16:r:112:LEU:HD23	28:Z:22:ARG:HH11	1.63	0.63
4:2:144:CYS:O	5:1:139:ARG:NH2	2.30	0.63
22:L:135:ASN:ND2	22:L:197:GLU:OE1	2.32	0.63
3:D:269:LEU:HB2	3:D:368:GLU:HB2	1.81	0.62
18:A:68:GLU:HG3	20:J:159:LEU:HD13	1.81	0.62
23:M:36:LEU:HB2	35:g:67:VAL:HG22	1.82	0.62
18:A:73:LEU:HD23	19:H:151:LEU:HD13	1.82	0.62
20:J:134:MET:O	33:e:28:ASN:ND2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:7:7:SER:HB2	10:7:25:ARG:HH12	1.65	0.61
8:P:128:ARG:NH1	8:P:220:ASP:O	2.33	0.61
22:L:221:THR:HG23	22:L:226:GLN:HB2	1.82	0.61
19:H:24:GLU:OE2	19:H:274:ARG:NH1	2.32	0.61
3:D:145:THR:HA	3:D:148:LEU:HD12	1.83	0.61
6:3:570:SER:HA	6:3:583:THR:O	2.00	0.61
1:6:92:GLN:NE2	19:H:215:TYR:O	2.34	0.61
18:A:49:LEU:HB3	18:A:50:PRO:CD	2.31	0.61
23:M:173:THR:HG23	23:M:175:ASN:H	1.65	0.61
12:U:48:VAL:HG12	12:U:52:MET:HE2	1.82	0.61
47:6:203:PC1:H342	47:6:203:PC1:H252	1.82	0.60
12:U:52:MET:HE1	42:n:23:LEU:HD12	1.82	0.60
22:L:234:PRO:HA	22:L:237:MET:HG2	1.83	0.60
9:Q:93:ILE:HD11	9:Q:105:VAL:HG21	1.83	0.60
22:L:362:ILE:HB	22:L:431:THR:HA	1.83	0.60
22:L:180:ILE:HD12	23:M:397:GLY:HA2	1.83	0.60
21:K:40:LEU:HD13	24:N:71:LEU:HD23	1.82	0.60
6:3:396:ARG:NH1	6:3:416:THR:O	2.33	0.60
8:P:186:ARG:HD2	8:P:246:PHE:HE2	1.67	0.60
18:A:75:LEU:HB3	19:H:155:LEU:HD21	1.83	0.60
19:H:110:SER:OG	19:H:143:GLU:OE2	2.18	0.60
5:1:224:ASN:ND2	49:1:501:FMN:O2	2.32	0.59
13:V:22:ARG:NH2	25:O:240:TYR:OH	2.34	0.59
27:Y:3:ARG:O	27:Y:7:SER:HB3	2.02	0.59
19:H:228:TYR:HA	19:H:231:ILE:HD12	1.84	0.59
37:i:79:TRP:HD1	44:p:40:VAL:HG13	1.67	0.59
19:H:26:LYS:HB3	29:a:5:ILE:HG12	1.85	0.59
37:i:86:LYS:NZ	44:p:41:ASP:OD1	2.31	0.59
19:H:175:LEU:O	19:H:179:TRP:HB3	2.02	0.59
7:9:33:ILE:HG13	47:9:204:PC1:H242	1.84	0.59
13:V:8:THR:HG21	13:V:13:LEU:HB3	1.83	0.59
20:J:19:LEU:HD11	21:K:31:LEU:HB3	1.84	0.59
21:K:59:ILE:HD12	24:N:27:MET:HG2	1.85	0.59
29:a:3:PHE:HA	29:a:6:LEU:HD23	1.84	0.59
1:6:62:LEU:HB2	1:6:100:GLY:HA3	1.84	0.59
22:L:75:GLU:OE1	22:L:77:LYS:NZ	2.33	0.58
23:M:300:SER:HB3	23:M:381:ILE:HG12	1.85	0.58
23:M:458:THR:O	44:p:149:TYR:OH	2.20	0.58
27:Y:94:CYS:HA	27:Y:114:CYS:HA	1.83	0.58
15:q:9:ARG:HH21	54:r:202:CDL:HA22	1.68	0.58
22:L:249:SER:HB3	22:L:336:LYS:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:ARG:NH1	13:V:110:GLN:O	2.36	0.58
5:1:99:GLU:HG2	5:1:99:GLU:O	2.02	0.58
6:3:620:ARG:NH1	6:3:633:TYR:OH	2.36	0.58
25:O:225:SER:O	25:O:228:ALA:C	2.46	0.58
7:9:55:GLU:OE2	15:q:34:ARG:NH2	2.36	0.58
22:L:565:SER:HB2	27:Y:112:MET:HE1	1.84	0.58
40:l:29:ARG:NH1	40:l:32:ASP:OD2	2.32	0.58
6:3:284:VAL:HG12	6:3:559:VAL:HG22	1.85	0.58
6:3:364:LEU:HD12	6:3:491:ASN:HB3	1.84	0.58
22:L:446:ASN:HA	22:L:451:MET:HE3	1.85	0.58
3:D:148:LEU:HG	3:D:177:MET:HE2	1.86	0.58
4:2:27:ASN:ND2	4:2:57:GLN:OE1	2.35	0.58
6:3:533:THR:O	6:3:537:LEU:HB2	2.03	0.58
22:L:139:GLN:HA	22:L:142:ILE:HD12	1.86	0.58
24:N:109:ALA:HB3	24:N:161:SER:HA	1.86	0.58
26:X:43:MET:HE3	28:Z:72:PRO:HA	1.86	0.58
26:X:129:LYS:HD3	30:b:65:VAL:HG13	1.85	0.58
7:9:97:GLU:HB2	7:9:110:ARG:HB3	1.85	0.58
11:S:78:LEU:HD12	11:S:86:VAL:HG22	1.86	0.58
20:J:2:ASN:HB3	20:J:121:GLY:HA3	1.86	0.58
25:O:62:THR:O	31:c:5:ARG:NH1	2.37	0.58
16:r:45:SER:O	16:r:51:ASN:ND2	2.36	0.57
24:N:42:PRO:HA	24:N:45:ILE:HG22	1.86	0.57
36:h:109:GLU:OE2	36:h:112:ARG:NH2	2.36	0.57
9:Q:37:ILE:HB	9:Q:105:VAL:HG22	1.85	0.57
21:K:60:PRO:HA	21:K:63:ILE:HG12	1.87	0.57
22:L:441:ILE:HG21	38:j:15:PRO:HB3	1.87	0.57
5:1:142:PHE:HB3	5:1:145:GLU:HB2	1.87	0.57
5:1:372:MET:HE2	5:1:399:ILE:HD13	1.87	0.57
13:V:8:THR:HG23	13:V:10:LEU:H	1.67	0.57
9:Q:15:GLU:OE2	14:W:76:THR:OG1	2.20	0.57
20:J:107:ASN:HD21	20:J:117:LEU:HB2	1.70	0.57
18:A:67:LEU:HD22	21:K:65:VAL:HA	1.86	0.57
24:N:87:GLN:NE2	36:h:126:PRO:O	2.37	0.57
27:Y:107:TYR:HB2	54:m:201:CDL:HB62	1.85	0.57
15:q:60:ARG:HH22	15:q:95:ASP:HA	1.70	0.57
22:L:161:ARG:NH1	42:n:90:PHE:O	2.33	0.57
7:9:30:THR:HB	47:9:204:PC1:H11	1.86	0.56
19:H:163:GLN:OE1	29:a:40:ARG:NH2	2.38	0.56
22:L:552:LEU:O	22:L:556:ILE:HB	2.04	0.56
43:o:38:MET:HE2	43:o:57:TYR:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:15:VAL:HG13	12:T:54:MET:HE1	1.88	0.56
18:A:73:LEU:O	19:H:160:TYR:OH	2.22	0.56
23:M:127:ILE:HD11	24:N:254:LEU:HB3	1.88	0.56
24:N:252:GLY:HA3	24:N:290:LEU:HD13	1.87	0.56
3:D:226:GLU:OE1	3:D:230:THR:OG1	2.15	0.56
12:T:25:ILE:HG12	12:T:40:LEU:HD12	1.86	0.56
22:L:161:ARG:NH2	42:n:87:GLY:O	2.39	0.56
4:2:76:PRO:HB2	4:2:79:ARG:HG2	1.87	0.56
22:L:243:VAL:O	22:L:247:LEU:HB2	2.05	0.56
6:3:533:THR:HA	6:3:556:MET:HE1	1.86	0.56
19:H:154:LEU:HA	19:H:157:ASN:HB3	1.87	0.56
26:X:72:GLN:HG2	26:X:114:LEU:HD21	1.88	0.56
35:g:65:SER:HA	36:h:32:THR:HG21	1.87	0.56
25:O:209:THR:HG22	25:O:213:LYS:HZ1	1.71	0.56
4:2:31:ILE:HG12	4:2:50:VAL:HG22	1.88	0.55
5:1:91:LYS:HG2	5:1:219:PRO:HG2	1.88	0.55
24:N:217:MET:HE2	46:N:402:3PE:H221	1.88	0.55
3:D:413:ASP:OD1	19:H:281:ARG:NH1	2.39	0.55
5:1:188:GLU:O	5:1:192:LEU:HB2	2.05	0.55
23:M:361:MET:HE2	23:M:441:MET:HE2	1.87	0.55
18:A:63:LEU:HG	20:J:66:VAL:HG21	1.88	0.55
23:M:204:LEU:HD22	23:M:209:LEU:HD13	1.89	0.55
24:N:43:MET:HB3	24:N:126:MET:SD	2.47	0.55
40:l:12:TYR:O	40:l:14:ARG:NH1	2.39	0.55
1:6:119:GLU:O	8:P:54:TYR:OH	2.22	0.55
22:L:539:MET:HG3	41:m:10:LEU:HD21	1.89	0.55
24:N:155:LEU:HB3	24:N:278:MET:HE2	1.88	0.55
9:Q:125:ASN:O	17:s:64:ARG:NH1	2.40	0.55
19:H:149:ILE:HG13	19:H:297:THR:HG23	1.87	0.55
32:d:108:THR:HA	44:p:77:LYS:HA	1.89	0.55
22:L:176:ARG:HD2	23:M:400:ILE:HG22	1.89	0.55
23:M:219:ALA:O	23:M:223:ALA:HB2	2.07	0.55
24:N:85:MET:HE3	24:N:86:PHE:H	1.72	0.55
6:3:534:ARG:NH2	6:3:558:ASP:OD1	2.40	0.55
9:Q:36:ARG:NH1	9:Q:106:GLU:OE2	2.40	0.55
1:6:52:ARG:HH22	46:6:202:3PE:H31	1.71	0.54
8:P:319:ARG:NH1	14:W:53:GLN:OE1	2.41	0.54
5:1:66:ARG:HB3	5:1:72:GLY:O	2.07	0.54
10:7:1:GLY:N	10:7:42:ASP:OD2	2.40	0.54
18:A:6:VAL:HG11	19:H:87:VAL:HG21	1.89	0.54
7:9:171:ILE:O	7:9:175:TYR:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:68:GLU:OE2	3:D:188:ARG:NH2	2.41	0.54
6:3:114:CYS:HB3	6:3:117:GLN:HB2	1.89	0.54
12:U:21:LEU:HD13	39:k:53:ASN:HA	1.89	0.54
1:6:94:ASP:O	1:6:121:ARG:HA	2.07	0.54
3:D:335:ARG:NH2	7:9:131:ASP:OD1	2.41	0.54
1:6:118:PRO:HB2	19:H:58:LYS:HE3	1.90	0.54
6:3:25:THR:HA	6:3:72:PRO:HA	1.89	0.54
25:O:133:VAL:HG13	25:O:205:ALA:HB3	1.90	0.54
2:C:137:MET:HB3	2:C:162:PHE:HB2	1.89	0.54
3:D:3:GLN:NE2	23:M:135:ARG:O	2.37	0.54
21:K:97:GLN:HB3	22:L:582:GLY:HA3	1.90	0.54
35:g:90:GLU:OE2	35:g:93:ARG:NH2	2.36	0.54
6:3:571:ALA:O	6:3:582:GLN:HA	2.08	0.54
7:9:42:TYR:HA	7:9:45:ARG:HD3	1.90	0.54
40:l:131:GLN:OE1	40:l:154:HIS:ND1	2.41	0.54
5:1:306:LEU:HD22	5:1:343:ILE:HD11	1.91	0.54
14:W:100:LYS:HG3	14:W:104:HIS:HB2	1.90	0.54
20:J:53:LEU:O	20:J:57:LEU:HB3	2.08	0.54
42:n:66:ALA:HB1	53:n:201:ZMP:H7	1.90	0.54
49:1:501:FMN:N1	49:1:501:FMN:O3'	2.39	0.53
11:S:17:GLU:HB3	11:S:67:ARG:HB3	1.90	0.53
12:T:11:ILE:HD12	12:T:80:ILE:HG23	1.91	0.53
40:l:70:MET:HE1	40:l:76:ILE:HA	1.90	0.53
8:P:53:VAL:HA	8:P:56:ILE:HG12	1.90	0.53
8:P:157:ARG:NH1	8:P:163:ALA:O	2.41	0.53
25:O:63:THR:HG22	31:c:5:ARG:HH22	1.73	0.53
33:e:29:ALA:HB2	36:h:138:LYS:HD3	1.90	0.53
33:e:96:HIS:HA	33:e:101:GLU:HB3	1.91	0.53
2:C:49:GLU:OE2	2:C:106:ARG:NH1	2.42	0.53
15:q:106:ARG:HB2	15:q:109:ILE:HG13	1.89	0.53
5:1:97:ALA:HB3	5:1:138:ILE:HA	1.89	0.53
25:O:25:ILE:HG12	25:O:168:ALA:HB3	1.90	0.53
26:X:5:GLU:O	26:X:53:ARG:NH1	2.41	0.53
19:H:138:GLN:HG3	19:H:285:LEU:HD21	1.91	0.53
26:X:29:HIS:HB3	26:X:119:PRO:HD2	1.90	0.53
3:D:257:GLY:HA3	3:D:372:GLY:HA2	1.90	0.53
25:O:104:ARG:NH2	55:O:401:DGT:N7	2.56	0.53
54:h:201:CDL:H152	46:i:201:3PE:H341	1.90	0.53
6:3:335:LEU:HA	6:3:338:VAL:HG22	1.91	0.53
46:A:201:3PE:H381	19:H:295:PRO:HB3	1.91	0.53
26:X:25:LYS:NZ	26:X:94:GLN:O	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:180:GLU:OE1	1:6:182:LYS:NZ	2.42	0.52
19:H:20:LEU:HA	19:H:23:VAL:HG12	1.91	0.52
22:L:338:MET:HB2	22:L:457:LEU:HB3	1.91	0.52
22:L:539:MET:O	22:L:543:ASN:HB2	2.09	0.52
12:U:51:ILE:HG21	12:U:67:ALA:HB1	1.91	0.52
28:Z:93:GLU:OE2	33:e:74:ARG:NH2	2.42	0.52
32:d:112:ILE:O	44:p:159:LYS:NZ	2.42	0.52
37:i:82:HIS:ND1	44:p:36:TYR:OH	2.38	0.52
3:D:228:MET:CE	3:D:228:MET:CA	2.86	0.52
22:L:8:ILE:HA	22:L:11:ILE:HD12	1.91	0.52
25:O:131:ASP:OD2	25:O:152:TYR:OH	2.25	0.52
2:C:78:LEU:HB3	2:C:130:TYR:HB3	1.91	0.52
19:H:134:ARG:HH21	19:H:282:TYR:HB2	1.73	0.52
22:L:574:THR:OG1	24:N:167:TRP:O	2.25	0.52
25:O:320:LYS:O	32:d:60:ARG:NH2	2.42	0.52
33:e:88:GLU:HG3	33:e:90:LYS:HG2	1.91	0.52
7:9:45:ARG:HE	16:r:19:LEU:HD13	1.74	0.52
23:M:74:PRO:HA	23:M:77:LEU:HD12	1.91	0.52
23:M:446:LEU:HB3	46:M:502:3PE:H342	1.92	0.52
40:l:29:ARG:NH2	40:l:31:GLU:OE2	2.43	0.52
7:9:79:CYS:O	7:9:107:ARG:NH1	2.42	0.52
19:H:316:PRO:HG3	28:Z:56:ARG:HB3	1.92	0.52
29:a:37:ARG:NH1	29:a:51:ASP:OD2	2.42	0.52
3:D:175:GLU:OE2	3:D:188:ARG:NH1	2.40	0.52
7:9:33:ILE:HD12	47:9:204:PC1:H3A2	1.91	0.52
21:K:54:MET:HA	21:K:57:MET:HE2	1.92	0.52
54:h:201:CDL:OB4	44:p:48:ARG:NH1	2.41	0.52
3:D:369:ALA:HB2	3:D:374:PHE:HB2	1.90	0.52
6:3:99:ALA:O	6:3:134:LYS:NZ	2.43	0.52
6:3:569:LYS:HG3	6:3:571:ALA:HB2	1.92	0.52
26:X:46:ARG:NH2	36:h:142:ASP:OD1	2.42	0.52
1:6:181:GLN:HB2	1:6:184:LYS:HB3	1.91	0.52
2:C:47:GLU:OE1	2:C:106:ARG:NH2	2.39	0.52
10:7:43:LEU:HD22	15:q:107:LYS:HE3	1.92	0.52
12:U:47:GLN:NE2	12:U:70:LEU:O	2.42	0.52
5:1:105:CYS:SG	5:1:267:THR:OG1	2.67	0.51
24:N:310:ASN:ND2	25:O:273:THR:O	2.39	0.51
5:1:276:LEU:HD13	5:1:317:MET:HE3	1.91	0.51
6:3:588:THR:HG21	9:Q:63:GLU:HA	1.91	0.51
8:P:319:ARG:HA	8:P:322:ARG:HD2	1.92	0.51
22:L:124:PHE:HE1	22:L:147:VAL:HG13	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:122:PHE:O	23:M:125:THR:OG1	2.26	0.51
23:M:456:GLY:O	35:g:82:ARG:NH1	2.41	0.51
25:O:76:SER:O	25:O:95:ARG:NH1	2.43	0.51
29:a:34:LYS:NZ	29:a:61:TYR:O	2.41	0.51
42:n:134:ARG:O	42:n:134:ARG:NH1	2.43	0.51
18:A:49:LEU:CD1	19:H:126:LYS:CD	2.69	0.51
23:M:313:THR:HA	23:M:316:MET:SD	2.49	0.51
32:d:120:ARG:O	41:m:108:ARG:NH2	2.42	0.51
5:1:61:LYS:HE2	5:1:77:LEU:HD23	1.91	0.51
22:L:190:SER:HB3	22:L:196:TRP:HE1	1.75	0.51
23:M:173:THR:HB	36:h:101:ALA:HB2	1.91	0.51
6:3:668:ILE:HA	6:3:671:PHE:HB3	1.93	0.51
8:P:166:ILE:HG22	8:P:168:PRO:HD3	1.91	0.51
17:s:34:ASN:O	17:s:37:HIS:ND1	2.39	0.51
20:J:132:GLY:HA2	28:Z:67:ARG:HH21	1.75	0.51
25:O:14:THR:HG21	25:O:116:LEU:HD22	1.92	0.51
6:3:349:PHE:H	6:3:509:PRO:HB2	1.76	0.51
40:l:133:PRO:HG3	43:o:38:MET:HE1	1.91	0.51
6:3:243:ARG:HG2	6:3:244:THR:HG23	1.92	0.51
6:3:366:THR:HG22	6:3:370:GLY:HA3	1.93	0.51
13:V:71:LEU:HD13	13:V:79:VAL:HG11	1.93	0.51
25:O:170:ILE:HD11	25:O:238:ILE:HD11	1.93	0.51
2:C:151:ILE:HG23	2:C:152:LEU:HG	1.93	0.51
8:P:328:SER:O	14:W:50:HIS:NE2	2.43	0.51
13:V:42:ALA:HA	13:V:45:LYS:HE2	1.92	0.51
19:H:87:VAL:HG23	19:H:95:LEU:HD23	1.92	0.51
22:L:75:GLU:OE2	35:g:88:ARG:NH1	2.36	0.51
46:L:703:3PE:H3C2	47:M:501:PC1:H3G2	1.93	0.51
1:6:58:MET:HE3	1:6:90:PRO:HG3	1.93	0.51
1:6:147:ASP:N	1:6:147:ASP:OD1	2.44	0.51
6:3:227:SER:OG	6:3:228:ILE:N	2.40	0.51
11:S:82:SER:N	11:S:85:GLU:OE1	2.43	0.51
22:L:132:THR:O	22:L:262:ARG:NH2	2.43	0.51
1:6:48:ASN:ND2	1:6:180:GLU:O	2.43	0.50
41:m:82:THR:OG1	41:m:85:ASN:ND2	2.44	0.50
8:P:108:ASP:OD1	8:P:112:ASN:ND2	2.44	0.50
42:n:169:ILE:O	42:n:172:ARG:NH1	2.43	0.50
3:D:68:LEU:HD21	3:D:411:LEU:HD21	1.93	0.50
4:2:79:ARG:NH1	4:2:82:GLU:OE2	2.44	0.50
6:3:276:ARG:NH1	6:3:680:ALA:O	2.44	0.50
19:H:17:MET:HE1	19:H:225:MET:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:66:ILE:HG23	23:M:107:ILE:HG12	1.94	0.50
22:L:253:VAL:HB	22:L:310:LEU:HD11	1.93	0.50
23:M:272:THR:HA	23:M:275:ILE:HD12	1.93	0.50
26:X:168:PHE:HE2	54:d:201:CDL:H542	1.77	0.50
2:C:93:VAL:HG22	2:C:108:LYS:HG2	1.93	0.50
3:D:224:GLU:OE1	7:9:42:TYR:OH	2.29	0.50
22:L:292:ALA:HB2	22:L:304:PHE:HB3	1.92	0.50
23:M:40:THR:HG1	36:h:80:TYR:HH	1.57	0.50
23:M:275:ILE:O	23:M:279:GLN:HB2	2.11	0.50
33:e:37:LYS:HG3	36:h:133:ILE:HG21	1.93	0.50
43:o:49:GLN:OE1	44:p:119:ASN:ND2	2.44	0.50
44:p:98:ASP:OD2	44:p:141:ARG:NH1	2.43	0.50
22:L:100:ILE:HG21	22:L:246:LEU:HB2	1.93	0.50
22:L:191:LEU:O	41:m:125:ASN:ND2	2.44	0.50
31:c:41:GLU:OE2	31:c:44:ARG:NH2	2.45	0.50
35:g:99:GLU:OE2	44:p:108:ARG:NH1	2.35	0.50
37:i:18:ARG:NH1	42:n:170:VAL:O	2.41	0.50
5:1:101:GLU:OE2	5:1:303:SER:N	2.45	0.50
7:9:51:ASN:O	7:9:55:GLU:N	2.44	0.50
28:Z:120:ILE:O	28:Z:124:TYR:HB2	2.12	0.50
14:W:37:LEU:HD21	14:W:88:GLY:HA3	1.94	0.50
22:L:136:ASN:HD21	54:h:201:CDL:H261	1.75	0.50
23:M:106:LEU:HD13	23:M:234:ILE:HG21	1.93	0.50
7:9:77:GLU:O	7:9:107:ARG:NH1	2.45	0.50
22:L:141:PHE:HE2	23:M:375:LEU:HD11	1.77	0.50
5:1:140:GLY:O	5:1:179:ARG:NH2	2.45	0.49
6:3:669:LYS:NZ	6:3:670:ASP:OD1	2.45	0.49
19:H:42:PRO:HD2	19:H:45:ILE:HG12	1.94	0.49
22:L:286:LEU:HD13	22:L:411:ILE:HB	1.93	0.49
25:O:156:LYS:HE2	25:O:160:LEU:HD22	1.94	0.49
47:9:204:PC1:H2C1	19:H:175:LEU:HD11	1.94	0.49
8:P:169:SER:OG	8:P:170:ASP:N	2.44	0.49
38:j:40:PHE:O	38:j:44:SER:OG	2.26	0.49
18:A:99:SER:HB2	46:A:201:3PE:H391	1.94	0.49
12:U:39:ASP:OD1	12:U:39:ASP:N	2.45	0.49
2:C:58:ILE:HD13	2:C:120:ILE:HG22	1.95	0.49
22:L:348:HIS:NE2	12:U:2:ASP:OD2	2.45	0.49
6:3:201:ASP:OD2	6:3:268:ARG:NH2	2.45	0.49
22:L:156:GLY:O	23:M:416:ARG:NH2	2.45	0.49
3:D:176:LYS:NZ	16:r:24:GLN:O	2.39	0.49
5:1:370:ASP:OD2	6:3:179:ASN:ND2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:488:LYS:HZ1	6:3:638:GLU:HB2	1.78	0.49
16:r:108:ASP:OD2	28:Z:20:TYR:OH	2.30	0.49
22:L:71:MET:HE1	23:M:380:PHE:CE2	2.48	0.49
22:L:137:MET:HB2	22:L:196:TRP:HB3	1.94	0.49
22:L:601:LEU:HA	22:L:604:ILE:HG12	1.94	0.49
27:Y:47:SER:N	27:Y:50:GLU:OE2	2.45	0.49
34:f:43:LEU:HD11	44:p:67:TYR:HB3	1.94	0.49
3:D:354:GLU:OE2	3:D:357:GLN:NE2	2.43	0.49
22:L:15:LEU:HB3	22:L:126:ILE:HG12	1.94	0.49
4:2:129:GLY:HA2	4:2:140:ILE:HG22	1.94	0.49
8:P:137:ALA:HB2	8:P:146:LEU:HD22	1.95	0.49
18:A:69:ILE:HD11	19:H:144:VAL:HG23	1.94	0.49
19:H:142:TYR:HA	19:H:145:THR:HG22	1.95	0.49
19:H:169:GLN:HB3	19:H:244:GLY:HA3	1.94	0.49
22:L:78:MET:HB2	54:h:201:CDL:H241	1.93	0.49
26:X:18:LYS:HB2	29:a:68:ASN:HB3	1.95	0.49
18:A:79:ILE:HA	18:A:87:MET:HE2	1.95	0.49
19:H:113:VAL:HA	19:H:116:ILE:HG22	1.95	0.49
22:L:67:HIS:NE2	22:L:70:THR:OG1	2.37	0.49
22:L:577:THR:HB	24:N:164:MET:HE1	1.94	0.49
2:C:175:ARG:NH2	2:C:177:ASP:OD2	2.44	0.49
37:i:107:ASP:OD2	43:o:70:ARG:NH1	2.41	0.49
22:L:10:LEU:HD23	22:L:46:ILE:HG21	1.94	0.48
35:g:112:ASP:HB3	35:g:115:LYS:HG2	1.94	0.48
6:3:381:GLY:HA3	6:3:457:ALA:HB2	1.95	0.48
20:J:112:VAL:HG13	33:e:73:ARG:HD2	1.94	0.48
8:P:186:ARG:NH2	8:P:189:LEU:O	2.46	0.48
23:M:98:MET:HE1	54:N:401:CDL:H822	1.95	0.48
36:h:81:ASP:OD2	36:h:85:LYS:NZ	2.37	0.48
4:2:6:LEU:O	4:2:92:ARG:NH2	2.46	0.48
23:M:105:LEU:O	23:M:109:THR:OG1	2.25	0.48
23:M:429:SER:O	35:g:36:TYR:OH	2.29	0.48
1:6:79:MET:HB2	1:6:84:VAL:HB	1.95	0.48
3:D:229:LEU:HD22	3:D:235:TRP:CD2	2.48	0.48
3:D:323:ILE:HG23	3:D:324:LYS:HG3	1.96	0.48
18:A:64:LEU:HD13	20:J:163:ILE:HG12	1.94	0.48
22:L:161:ARG:HH12	42:n:90:PHE:HB3	1.79	0.48
30:b:62:MET:HE3	30:b:65:VAL:HG11	1.96	0.48
3:D:398:HIS:O	3:D:421:GLN:NE2	2.47	0.48
22:L:538:PRO:HB2	40:l:88:VAL:HG22	1.95	0.48
40:l:64:ASP:OD1	41:m:43:LYS:NZ	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:o:71:ASP:OD2	44:p:22:GLN:NE2	2.47	0.48
3:D:279:ASP:OD1	3:D:279:ASP:N	2.46	0.48
3:D:286:PRO:HG2	3:D:303:GLU:HG3	1.96	0.48
5:1:279:LEU:HD12	5:1:283:HIS:HD2	1.79	0.48
7:9:158:ASN:ND2	10:7:34:GLU:OE1	2.42	0.48
14:W:25:ARG:N	14:W:29:GLU:OE2	2.44	0.48
24:N:208:TYR:O	24:N:212:THR:OG1	2.25	0.48
32:d:43:LEU:HG	32:d:53:VAL:HG12	1.96	0.48
51:P:501:NDP:N7N	51:P:501:NDP:O2N	2.47	0.48
12:T:73:PRO:HA	12:T:76:ILE:HD12	1.96	0.48
23:M:357:THR:O	23:M:361:MET:HG3	2.14	0.48
40:l:4:THR:OG1	40:l:6:ASP:OD1	2.24	0.48
2:C:119:SER:HB3	2:C:142:PHE:HB3	1.95	0.48
5:1:327:THR:HG22	5:1:328:GLY:H	1.78	0.48
6:3:591:GLY:HA2	8:P:6:ILE:HG21	1.95	0.48
19:H:273:ILE:HG23	19:H:277:TYR:HD2	1.78	0.48
40:l:137:LEU:HB3	40:l:140:GLU:HB2	1.96	0.48
3:D:8:ILE:HD11	35:g:24:TRP:HB3	1.96	0.48
19:H:5:ASN:HA	19:H:8:THR:HG22	1.96	0.48
19:H:24:GLU:HG3	19:H:271:LEU:HD22	1.96	0.48
24:N:119:THR:HG22	24:N:176:ARG:HB3	1.95	0.48
36:h:43:VAL:HG11	36:h:71:ILE:HD11	1.94	0.48
3:D:141:PHE:O	3:D:145:THR:OG1	2.32	0.47
3:D:350:LYS:HG3	6:3:121:MET:HG3	1.96	0.47
14:W:92:LEU:O	14:W:96:ILE:HG12	2.13	0.47
19:H:24:GLU:HA	19:H:271:LEU:HD13	1.96	0.47
19:H:169:GLN:NE2	19:H:241:ILE:O	2.47	0.47
22:L:560:LYS:HE3	46:Y:202:3PE:H221	1.94	0.47
23:M:403:THR:HA	23:M:406:TYR:CE2	2.49	0.47
8:P:76:ARG:NH2	8:P:103:ASN:O	2.47	0.47
22:L:5:THR:HG23	22:L:63:ILE:HG12	1.96	0.47
22:L:548:THR:O	22:L:552:LEU:HB3	2.14	0.47
23:M:314:MET:HG2	23:M:454:ILE:HG13	1.96	0.47
24:N:249:LEU:HD22	24:N:254:LEU:HD12	1.95	0.47
12:U:44:SER:HB2	42:n:16:LEU:HD11	1.95	0.47
3:D:184:VAL:O	7:9:62:ARG:NH1	2.45	0.47
3:D:228:MET:SD	7:9:38:MET:HE1	2.54	0.47
7:9:38:MET:HB2	16:r:15:SER:HA	1.94	0.47
8:P:10:LYS:NZ	9:Q:28:GLU:OE1	2.46	0.47
8:P:251:ARG:HA	8:P:326:TRP:HZ3	1.79	0.47
9:Q:36:ARG:O	9:Q:57:MET:HA	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:K:38:LEU:O	21:K:42:ILE:HG12	2.14	0.47
22:L:176:ARG:O	22:L:180:ILE:HG12	2.14	0.47
22:L:190:SER:HB3	22:L:196:TRP:NE1	2.29	0.47
40:l:44:GLY:HA3	41:m:78:ASN:HD22	1.80	0.47
40:l:93:THR:OG1	40:l:95:VAL:O	2.29	0.47
53:n:201:ZMP:H15	53:n:201:ZMP:H17	1.61	0.47
4:2:149:VAL:O	4:2:190:ARG:NH2	2.43	0.47
6:3:163:ALA:HA	6:3:167:ALA:HB3	1.96	0.47
6:3:601:ARG:NH2	6:3:614:ASP:OD1	2.38	0.47
23:M:30:TYR:O	23:M:34:ILE:HG12	2.15	0.47
23:M:67:ILE:HG22	46:M:502:3PE:H3D1	1.95	0.47
26:X:82:THR:HA	26:X:85:TRP:CD1	2.50	0.47
41:m:27:GLU:HA	41:m:30:ARG:HG2	1.96	0.47
5:1:257:ASN:ND2	5:1:267:THR:OG1	2.43	0.47
6:3:28:GLN:NE2	9:Q:114:LYS:O	2.42	0.47
23:M:203:PHE:HB2	23:M:243:MET:HG3	1.97	0.47
3:D:91:ILE:HG12	3:D:99:ALA:HB1	1.96	0.47
40:l:38:ASP:OD1	41:m:80:ARG:NH1	2.33	0.47
19:H:169:GLN:OE1	19:H:174:LEU:N	2.48	0.47
46:L:703:3PE:H3E1	47:M:501:PC1:H3H1	1.97	0.47
27:Y:36:SER:HB2	27:Y:55:VAL:HA	1.96	0.47
35:g:79:PRO:HG3	36:h:72:SER:HB3	1.96	0.47
2:C:8:ARG:NH1	16:r:61:GLU:OE2	2.39	0.47
19:H:162:LEU:HD23	19:H:165:LEU:HD12	1.97	0.47
23:M:46:ASP:OD2	23:M:48:ASN:ND2	2.48	0.47
47:M:501:PC1:H252	27:Y:123:LEU:HD13	1.96	0.47
25:O:30:ASN:O	25:O:126:ARG:NH2	2.47	0.47
39:k:29:ILE:O	39:k:32:THR:OG1	2.29	0.47
20:J:22:LYS:NZ	21:K:18:GLY:O	2.40	0.47
22:L:530:PRO:O	22:L:534:HIS:HB2	2.15	0.47
41:m:114:LEU:HB3	41:m:120:LEU:HB2	1.97	0.47
3:D:228:MET:CE	7:9:35:GLY:CA	2.91	0.47
3:D:249:ASP:OD2	3:D:404:LYS:NZ	2.45	0.47
22:L:97:THR:HG21	22:L:125:LEU:HD22	1.97	0.47
22:L:481:THR:OG1	43:o:91:HIS:ND1	2.35	0.47
12:U:17:TYR:OH	39:k:27:TRP:NE1	2.40	0.47
40:l:53:SER:HA	40:l:83:TYR:HB3	1.96	0.47
3:D:67:GLU:HB3	3:D:75:LYS:HB3	1.97	0.46
4:2:105:THR:HG22	4:2:106:THR:H	1.81	0.46
7:9:115:MET:HB2	7:9:149:LEU:HB3	1.95	0.46
20:J:164:PHE:HE2	24:N:4:ILE:HG22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:14:VAL:HB	26:X:60:LYS:HE3	1.97	0.46
5:1:214:GLY:HA3	5:1:220:THR:HG22	1.97	0.46
6:3:105:CYS:SG	6:3:117:GLN:NE2	2.88	0.46
22:L:260:LEU:HD13	22:L:277:MET:HE3	1.96	0.46
23:M:422:HIS:HB2	41:m:59:ILE:HD12	1.96	0.46
42:n:138:GLN:NE2	42:n:155:PRO:O	2.43	0.46
44:p:139:GLN:HG2	44:p:143:LEU:HD22	1.97	0.46
1:6:101:THR:HA	1:6:129:CYS:HB3	1.95	0.46
5:1:378:ARG:NH2	6:3:132:GLU:OE2	2.41	0.46
6:3:675:ASP:N	6:3:675:ASP:OD1	2.47	0.46
7:9:34:ARG:HB3	47:9:204:PC1:H31	1.97	0.46
15:q:1:MET:SD	15:q:3:LEU:N	2.86	0.46
22:L:298:ILE:O	22:L:302:ILE:HG12	2.15	0.46
54:d:201:CDL:OA4	34:f:29:LYS:NZ	2.49	0.46
16:r:32:LYS:O	16:r:35:GLN:NE2	2.43	0.46
19:H:179:TRP:HE1	28:Z:42:LEU:HG	1.79	0.46
12:U:49:GLU:HB3	39:k:50:TRP:HE1	1.81	0.46
27:Y:40:VAL:HG12	27:Y:54:ARG:HE	1.80	0.46
37:i:82:HIS:HD1	44:p:36:TYR:HH	1.49	0.46
2:C:133:GLU:OE2	3:D:430:ARG:NH1	2.45	0.46
10:7:53:GLU:OE2	10:7:94:HIS:ND1	2.40	0.46
19:H:199:ASP:OD1	19:H:200:LEU:N	2.47	0.46
20:J:143:ALA:O	20:J:147:CYS:N	2.43	0.46
23:M:11:LEU:HB3	23:M:100:ILE:HD13	1.97	0.46
24:N:181:TYR:HA	24:N:184:ILE:HD12	1.96	0.46
11:S:21:HIS:HA	11:S:55:ARG:O	2.16	0.46
14:W:34:VAL:HG21	53:W:201:ZMP:HN1	1.81	0.46
22:L:383:MET:HB3	22:L:386:LEU:HD12	1.97	0.46
23:M:104:ILE:O	23:M:108:MET:HG3	2.15	0.46
24:N:255:PRO:HG3	24:N:260:PHE:CG	2.50	0.46
3:D:151:ILE:HG23	3:D:170:MET:HB3	1.97	0.46
5:1:270:GLU:OE1	5:1:283:HIS:NE2	2.42	0.46
22:L:419:THR:HA	22:L:422:TYR:CE2	2.50	0.46
24:N:186:HIS:O	24:N:190:MET:HG3	2.16	0.46
40:l:81:ASP:OD1	40:l:81:ASP:N	2.48	0.46
4:2:39:PRO:HA	17:s:59:GLN:HB3	1.98	0.46
9:Q:60:ASP:OD1	9:Q:60:ASP:N	2.47	0.46
19:H:154:LEU:HD23	19:H:160:TYR:HA	1.97	0.46
20:J:131:VAL:HG23	29:a:43:TYR:HD1	1.81	0.46
23:M:46:ASP:OD1	23:M:47:GLU:N	2.49	0.46
25:O:247:PRO:HA	25:O:250:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:54:SER:OG	19:H:51:ASP:OD1	2.33	0.46
11:S:24:GLN:HE21	11:S:56:GLU:HG3	1.80	0.46
16:r:11:ARG:HB3	16:r:19:LEU:HD12	1.98	0.46
25:O:209:THR:HG22	25:O:213:LYS:NZ	2.29	0.46
12:U:2:ASP:OD1	12:U:2:ASP:N	2.47	0.46
33:e:23:GLU:OE2	33:e:27:LYS:NZ	2.48	0.46
37:i:24:ASP:OD2	42:n:124:TRP:NE1	2.42	0.46
1:6:91:ARG:NH2	19:H:61:MET:O	2.49	0.46
8:P:48:PRO:HA	8:P:71:LEU:O	2.16	0.46
24:N:338:PRO:HA	26:X:169:TRP:HZ2	1.81	0.46
12:U:11:ILE:HG22	12:U:77:VAL:HG22	1.98	0.46
34:f:56:TRP:NE1	36:h:88:GLU:OE1	2.38	0.46
10:7:32:GLN:HG2	15:q:122:GLU:HA	1.97	0.45
20:J:141:VAL:HA	21:K:58:PRO:HG3	1.97	0.45
24:N:221:LEU:HD12	24:N:221:LEU:HA	1.82	0.45
24:N:240:MET:HG2	24:N:244:ILE:HG12	1.98	0.45
25:O:138:MET:HB3	25:O:143:TYR:HB2	1.98	0.45
25:O:318:TRP:HE3	32:d:58:LEU:HD12	1.81	0.45
31:c:23:ALA:O	31:c:27:MET:HG3	2.16	0.45
5:1:190:THR:HB	5:1:204:ARG:HG2	1.99	0.45
6:3:441:GLU:HA	6:3:444:LYS:HE3	1.99	0.45
22:L:66:TRP:HB3	22:L:78:MET:HE2	1.99	0.45
22:L:223:LYS:HA	22:L:223:LYS:HD3	1.75	0.45
22:L:534:HIS:HB3	46:L:701:3PE:H2	1.99	0.45
23:M:58:SER:OG	23:M:63:THR:OG1	2.34	0.45
23:M:154:LEU:HD11	24:N:254:LEU:HD21	1.98	0.45
1:6:52:ARG:NH2	46:6:202:3PE:O32	2.50	0.45
3:D:72:MET:HG3	18:A:115:GLU:HB3	1.99	0.45
3:D:144:ILE:HG23	3:D:177:MET:HE3	1.97	0.45
22:L:83:ASP:H	22:L:86:SER:HB3	1.82	0.45
23:M:17:LEU:HD11	54:N:401:CDL:H141	1.99	0.45
25:O:265:ASP:OD2	25:O:267:THR:OG1	2.31	0.45
38:j:55:ASP:OD2	38:j:57:SER:OG	2.28	0.45
40:l:11:SER:OG	40:l:12:TYR:N	2.49	0.45
24:N:131:LEU:HA	24:N:135:LYS:HE2	1.99	0.45
46:M:502:3PE:H3A1	46:M:502:3PE:H372	1.77	0.45
35:g:64:PHE:HA	35:g:68:LEU:HB2	1.97	0.45
2:C:75:LEU:HA	2:C:96:LEU:HD23	1.99	0.45
3:D:226:GLU:OE2	3:D:301:VAL:HG11	2.16	0.45
6:3:8:LEU:HD13	6:3:19:MET:HB3	1.99	0.45
22:L:99:SER:HB3	22:L:341:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:91:ARG:HD2	1:6:91:ARG:HA	1.81	0.45
5:1:92:TYR:O	5:1:220:THR:HA	2.17	0.45
8:P:133:SER:OG	8:P:134:HIS:N	2.49	0.45
26:X:23:VAL:HG22	26:X:85:TRP:CD2	2.51	0.45
27:Y:140:VAL:O	36:h:123:TYR:OH	2.34	0.45
3:D:284:ASP:OD1	7:9:1:THR:OG1	2.35	0.45
5:1:287:VAL:HG21	5:1:294:LEU:HB2	1.99	0.45
6:3:36:GLN:NE2	9:Q:47:SER:O	2.47	0.45
19:H:172:MET:HE1	28:Z:45:GLY:HA2	1.99	0.45
22:L:345:SER:HB3	22:L:450:LEU:HD11	1.98	0.45
22:L:534:HIS:ND1	46:L:701:3PE:O12	2.46	0.45
23:M:50:LYS:HB2	23:M:58:SER:HB3	1.98	0.45
26:X:40:LYS:HA	26:X:40:LYS:HD3	1.75	0.45
40:l:6:ASP:OD1	40:l:6:ASP:N	2.50	0.45
6:3:297:GLU:HG3	14:W:125:TYR:CZ	2.52	0.45
19:H:196:ALA:HB3	19:H:274:ARG:HA	1.97	0.45
47:M:501:PC1:H251	24:N:277:ILE:HG23	1.99	0.45
24:N:254:LEU:HG	24:N:290:LEU:HD21	1.99	0.45
3:D:150:HIS:NE2	3:D:303:GLU:OE1	2.50	0.45
24:N:271:MET:HG2	24:N:276:LEU:HD23	1.99	0.45
2:C:37:VAL:HA	2:C:52:ILE:HG22	1.98	0.44
2:C:40:VAL:HG22	2:C:50:ILE:HG12	1.99	0.44
2:C:193:GLU:OE2	9:Q:64:ARG:NH1	2.49	0.44
6:3:300:LEU:HD22	6:3:603:LEU:HB2	1.98	0.44
9:Q:54:LYS:HA	9:Q:54:LYS:HD3	1.84	0.44
14:W:54:LEU:HB3	14:W:56:ILE:HG12	2.00	0.44
23:M:121:LEU:HA	23:M:124:ALA:HB3	1.99	0.44
23:M:252:PRO:HB3	32:d:117:HIS:CG	2.52	0.44
23:M:310:MET:HE2	23:M:310:MET:HB3	1.77	0.44
25:O:261:MET:HA	25:O:264:GLN:HG2	1.99	0.44
54:r:202:CDL:HB22	29:a:1:MET:HE2	1.99	0.44
46:A:201:3PE:H352	46:A:201:3PE:H382	1.82	0.44
46:H:401:3PE:N	28:Z:142:TYR:O	2.46	0.44
20:J:5:ILE:HG22	21:K:4:THR:HG21	1.99	0.44
20:J:93:VAL:HA	20:J:96:VAL:HG12	2.00	0.44
1:6:111:ARG:HD2	1:6:111:ARG:HA	1.80	0.44
3:D:11:ALA:O	24:N:228:ASN:ND2	2.41	0.44
6:3:325:ALA:HA	6:3:328:LEU:HD12	1.99	0.44
8:P:13:ARG:NH2	8:P:63:GLY:O	2.50	0.44
20:J:44:LEU:HD23	20:J:49:SER:HA	1.98	0.44
22:L:174:TYR:CD2	22:L:232:TRP:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:119:TYR:HE1	23:M:157:SER:HB2	1.82	0.44
24:N:298:TYR:O	24:N:303:THR:OG1	2.29	0.44
35:g:109:ASN:OD1	44:p:161:ARG:NH1	2.42	0.44
3:D:211:ILE:HG22	3:D:315:LEU:HD11	1.99	0.44
4:2:37:ASN:O	17:s:59:GLN:NE2	2.50	0.44
5:1:82:MET:SD	5:1:221:THR:OG1	2.71	0.44
22:L:306:THR:HA	22:L:332:HIS:CE1	2.52	0.44
8:P:167:ARG:HH21	8:P:297:LEU:HD11	1.83	0.44
15:q:1:MET:SD	15:q:2:GLU:N	2.91	0.44
28:Z:67:ARG:O	28:Z:71:MET:HG3	2.18	0.44
42:n:174:ARG:NH2	42:n:177:PRO:O	2.51	0.44
6:3:11:VAL:HG11	6:3:73:VAL:HB	2.00	0.44
6:3:160:ILE:HD11	6:3:183:VAL:HG13	1.99	0.44
7:9:45:ARG:HA	16:r:11:ARG:HH11	1.83	0.44
20:J:53:LEU:O	20:J:57:LEU:CB	2.65	0.44
24:N:207:ILE:HG21	24:N:262:PRO:HG3	2.00	0.44
12:U:26:ASP:OD1	12:U:26:ASP:N	2.45	0.44
1:6:65:CYS:HB3	1:6:126:MET:HE3	1.99	0.44
1:6:120:PRO:HD3	19:H:59:GLU:HG3	2.00	0.44
8:P:200:THR:HB	8:P:238:LEU:HB2	2.00	0.44
24:N:49:ASN:OD1	24:N:52:SER:N	2.43	0.44
24:N:160:THR:O	24:N:164:MET:HG2	2.18	0.44
26:X:136:LEU:HD12	26:X:137:PRO:HD2	2.00	0.44
5:1:154:ARG:HA	17:s:52:LEU:HD21	1.99	0.44
12:T:44:SER:OG	53:W:201:ZMP:O5	2.35	0.44
20:J:70:THR:HA	20:J:73:MET:HE3	1.99	0.44
25:O:17:LYS:HE2	25:O:17:LYS:HB3	1.78	0.44
44:p:81:VAL:HA	44:p:84:ILE:HB	2.00	0.44
3:D:63:ARG:HB3	3:D:79:HIS:HB2	2.00	0.43
3:D:195:ARG:NH1	7:9:126:GLU:OE2	2.41	0.43
23:M:159:PRO:HB3	47:M:501:PC1:H361	2.00	0.43
27:Y:19:ARG:O	27:Y:23:ILE:HG13	2.17	0.43
29:a:14:VAL:O	29:a:18:ILE:HD12	2.18	0.43
33:e:85:LEU:HB3	33:e:91:TYR:HB3	1.99	0.43
3:D:282:GLU:O	3:D:313:GLN:NE2	2.38	0.43
6:3:379:LEU:HD23	6:3:452:VAL:HB	2.00	0.43
21:K:1:FME:HE3	21:K:1:FME:HB2	1.79	0.43
21:K:96:LEU:N	24:N:54:GLU:OE2	2.50	0.43
23:M:49:TYR:O	36:h:86:ASN:ND2	2.44	0.43
23:M:319:HIS:HA	23:M:322:THR:HG22	2.00	0.43
43:o:82:GLU:HA	43:o:85:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:564:ALA:HB3	6:3:569:LYS:HD3	2.00	0.43
47:9:203:PC1:H332	19:H:280:PHE:HE2	1.83	0.43
8:P:21:ALA:HA	8:P:90:VAL:O	2.18	0.43
30:b:66:PRO:HB3	30:b:73:LEU:HB2	2.01	0.43
42:n:34:ASP:OD1	42:n:34:ASP:N	2.51	0.43
2:C:81:VAL:HG22	3:D:388:ARG:HG2	2.00	0.43
5:1:384:ALA:HB3	5:1:430:MET:HE3	1.99	0.43
22:L:142:ILE:HA	23:M:370:PRO:HB2	2.00	0.43
23:M:368:ALA:O	23:M:375:LEU:HD12	2.19	0.43
12:U:66:ASP:OD2	42:n:1:ALA:N	2.42	0.43
26:X:142:HIS:HB2	28:Z:114:ARG:HB3	1.99	0.43
35:g:24:TRP:H	35:g:24:TRP:CD1	2.35	0.43
41:m:18:ASP:HA	41:m:19:PRO:HD3	1.90	0.43
42:n:51:LYS:HG3	53:n:201:ZMP:H19B	2.00	0.43
2:C:88:ASN:HA	2:C:112:ASP:HB3	1.99	0.43
5:1:263:ASN:ND2	5:1:285:GLY:O	2.43	0.43
6:3:616:LEU:O	6:3:620:ARG:HG2	2.18	0.43
7:9:177:TYR:CZ	16:r:38:PRO:HG3	2.54	0.43
19:H:283:ASP:OD1	19:H:284:GLN:N	2.51	0.43
24:N:238:PRO:HG3	25:O:293:TYR:HE2	1.83	0.43
12:U:35:HIS:HB3	12:U:38:LYS:HB2	2.00	0.43
41:m:14:PRO:HG2	41:m:17:LEU:HD12	2.00	0.43
2:C:204:GLU:OE1	2:C:210:ARG:NH1	2.52	0.43
6:3:453:LEU:HB3	6:3:492:ILE:HD13	2.01	0.43
24:N:310:ASN:HB2	25:O:274:THR:HG22	2.01	0.43
28:Z:57:ARG:HA	28:Z:57:ARG:HD2	1.79	0.43
40:l:138:TYR:HD2	40:l:139:LEU:HD22	1.83	0.43
5:1:189:GLU:HG3	5:1:222:VAL:HB	1.99	0.43
6:3:9:ILE:HG13	6:3:20:VAL:HG23	2.00	0.43
7:9:164:GLU:HB3	15:q:109:ILE:HG12	2.01	0.43
19:H:293:PHE:O	19:H:297:THR:N	2.40	0.43
22:L:130:ILE:O	22:L:134:ALA:HB2	2.18	0.43
24:N:157:LEU:O	24:N:161:SER:OG	2.27	0.43
54:N:401:CDL:H861	54:d:201:CDL:H651	1.99	0.43
41:m:61:ASP:OD2	41:m:64:LEU:N	2.48	0.43
41:m:87:LEU:HB2	46:m:202:3PE:H332	2.00	0.43
43:o:17:ASP:OD2	43:o:20:LYS:NZ	2.52	0.43
3:D:7:ASP:OD1	3:D:7:ASP:N	2.44	0.43
7:9:166:GLU:HG3	15:q:88:ARG:HD3	2.01	0.43
23:M:151:PHE:HZ	24:N:291:PHE:HA	1.84	0.43
25:O:24:VAL:HB	25:O:166:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:n:146:ASP:HB3	42:n:148:ILE:HG22	2.01	0.43
44:p:85:TYR:O	44:p:89:MET:HG2	2.18	0.43
5:1:101:GLU:OE1	5:1:101:GLU:HA	2.19	0.43
12:T:54:MET:HE3	12:T:76:ILE:HD13	2.01	0.43
13:V:34:LEU:HD22	13:V:44:ARG:HA	2.01	0.43
22:L:573:MET:HE3	46:Y:202:3PE:H332	2.01	0.43
23:M:227:GLY:HA2	23:M:230:ILE:HG22	2.00	0.43
24:N:129:ILE:HD11	46:N:402:3PE:H322	2.00	0.43
24:N:154:ILE:HG23	24:N:191:LEU:HG	2.00	0.43
24:N:338:PRO:HD3	54:d:201:CDL:H572	1.99	0.43
2:C:180:VAL:HG23	2:C:182:ARG:HB2	2.01	0.43
3:D:302:GLU:HG2	7:9:3:LYS:HD2	2.01	0.43
6:3:266:LYS:O	6:3:270:ALA:CB	2.67	0.43
19:H:292:ASN:HA	30:b:17:VAL:HG11	2.00	0.43
22:L:19:ILE:HG22	22:L:23:MET:HE3	2.01	0.43
22:L:171:ALA:HA	22:L:232:TRP:HB2	2.00	0.43
23:M:47:GLU:OE2	44:p:92:ARG:NE	2.50	0.43
46:M:502:3PE:H2H2	54:h:201:CDL:H562	2.00	0.43
38:j:10:ARG:HG3	38:j:15:PRO:HA	2.01	0.43
41:m:47:LEU:HB3	42:n:165:LEU:HD13	2.01	0.43
9:Q:45:MET:HE3	9:Q:45:MET:HB3	1.87	0.42
18:A:60:ILE:HG21	20:J:166:ILE:HG13	2.01	0.42
24:N:221:LEU:HD22	24:N:240:MET:HE1	2.00	0.42
28:Z:34:MET:HA	28:Z:37:VAL:HG12	2.01	0.42
3:D:115:GLU:OE1	3:D:194:ILE:N	2.52	0.42
3:D:292:ASP:OD1	3:D:292:ASP:N	2.45	0.42
5:1:95:VAL:HG11	5:1:118:LEU:HD11	2.02	0.42
6:3:302:ARG:HE	6:3:302:ARG:HB2	1.63	0.42
46:H:401:3PE:H2A1	46:H:401:3PE:H2D2	1.88	0.42
23:M:201:MET:O	23:M:205:ILE:HG12	2.19	0.42
24:N:34:GLU:HB2	24:N:38:LEU:HD13	2.01	0.42
24:N:322:PRO:HG2	32:d:49:ARG:HD2	2.01	0.42
26:X:120:ASP:OD1	26:X:121:LEU:N	2.50	0.42
28:Z:39:ILE:O	28:Z:43:ILE:HG12	2.19	0.42
3:D:278:TYR:HA	3:D:281:VAL:HG22	2.00	0.42
4:2:192:CYS:SG	4:2:193:CYS:N	2.92	0.42
7:9:119:ILE:HG12	45:9:201:SF4:S3	2.60	0.42
22:L:473:PRO:HA	22:L:474:PRO:HD3	1.89	0.42
24:N:26:LEU:HB3	24:N:74:ILE:HG12	2.01	0.42
26:X:100:ARG:NH1	26:X:103:GLN:OE1	2.46	0.42
6:3:146:VAL:HG22	6:3:200:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:74:PRO:HG2	20:J:141:VAL:HG12	2.01	0.42
22:L:309:GLN:O	22:L:313:MET:HG3	2.19	0.42
23:M:87:ASP:OD1	23:M:88:ASN:N	2.53	0.42
25:O:126:ARG:HD3	25:O:134:PHE:HE2	1.84	0.42
26:X:33:ALA:HB2	26:X:119:PRO:HG3	2.01	0.42
26:X:39:ASN:HB3	28:Z:72:PRO:HG2	2.02	0.42
40:l:144:ASP:OD2	40:l:146:THR:OG1	2.33	0.42
1:6:71:HIS:HE1	3:D:174:ARG:HB3	1.84	0.42
2:C:43:SER:HA	16:r:65:PRO:HB3	2.01	0.42
8:P:90:VAL:HG11	8:P:218:THR:HG22	2.00	0.42
8:P:165:ILE:O	8:P:227:THR:HA	2.18	0.42
14:W:54:LEU:HD23	14:W:102:ARG:HG3	2.02	0.42
19:H:267:SER:O	19:H:271:LEU:HG	2.19	0.42
22:L:112:PRO:HG3	42:n:178:THR:HG21	2.01	0.42
22:L:542:LEU:HB3	23:M:278:ARG:HD3	2.02	0.42
23:M:366:ASN:HD21	23:M:406:TYR:HE1	1.67	0.42
25:O:12:ASP:OD1	25:O:17:LYS:NZ	2.44	0.42
25:O:221:LEU:HD23	25:O:221:LEU:HA	1.88	0.42
2:C:41:GLN:NE2	2:C:49:GLU:OE1	2.50	0.42
5:1:45:THR:O	5:1:49:LEU:HG	2.20	0.42
7:9:29:TRP:HB3	7:9:32:LEU:HD12	2.02	0.42
7:9:134:VAL:HG21	7:9:167:ILE:HG21	2.00	0.42
19:H:102:ILE:HD13	19:H:154:LEU:HD11	2.00	0.42
23:M:336:ARG:NH2	23:M:433:GLU:OE2	2.41	0.42
27:Y:101:GLY:HA3	27:Y:110:ALA:HB2	2.02	0.42
27:Y:105:HIS:HA	46:Y:201:3PE:H11	2.01	0.42
1:6:189:ARG:HA	8:P:50:ARG:HH12	1.85	0.42
2:C:191:ALA:O	9:Q:74:SER:OG	2.36	0.42
3:D:155:THR:HG21	3:D:170:MET:HB2	2.02	0.42
9:Q:19:ILE:HG12	9:Q:98:LYS:HG2	2.02	0.42
12:T:48:VAL:HG23	14:W:39:ARG:HH21	1.84	0.42
20:J:64:LEU:HA	20:J:67:PHE:HB2	2.01	0.42
22:L:96:VAL:O	22:L:100:ILE:HG12	2.20	0.42
24:N:221:LEU:HD11	24:N:322:PRO:HD3	2.01	0.42
25:O:311:GLU:HG2	25:O:312:VAL:HG13	2.01	0.42
1:6:101:THR:OG1	1:6:129:CYS:SG	2.69	0.42
9:Q:42:ARG:HD3	9:Q:49:VAL:HG12	2.01	0.42
12:T:47:GLN:NE2	12:T:67:ALA:O	2.53	0.42
22:L:198:LEU:O	22:L:202:MET:HG2	2.20	0.42
24:N:28:LEU:HA	24:N:31:VAL:HG22	2.01	0.42
25:O:209:THR:O	25:O:213:LYS:NZ	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:74:LYS:HB2	29:a:66:LEU:HD12	2.01	0.42
33:e:85:LEU:HA	33:e:88:GLU:HG2	2.02	0.42
43:o:25:PRO:HG2	43:o:28:LEU:HB2	2.02	0.42
3:D:236:ARG:O	3:D:240:VAL:HB	2.19	0.42
6:3:356:THR:HG21	6:3:503:LEU:HD22	2.02	0.42
20:J:166:ILE:HD13	20:J:166:ILE:HA	1.90	0.42
22:L:121:LEU:HD22	22:L:246:LEU:HD23	2.01	0.42
23:M:355:MET:HE2	23:M:355:MET:HB2	1.91	0.42
27:Y:112:MET:HE2	46:Y:202:3PE:H231	2.01	0.42
29:a:55:SER:HB2	29:a:62:VAL:HB	2.01	0.42
1:6:68:GLU:OE2	1:6:163:ALA:N	2.51	0.42
4:2:154:VAL:HG22	4:2:164:LEU:HD11	2.02	0.42
7:9:85:CYS:SG	7:9:111:TYR:OH	2.68	0.42
19:H:150:LEU:HA	19:H:153:VAL:HG12	2.01	0.42
22:L:78:MET:HE1	46:i:201:3PE:H361	2.02	0.42
31:c:45:ARG:NH2	32:d:16:ASP:OD1	2.53	0.42
36:h:62:GLU:O	36:h:65:GLU:HB2	2.20	0.42
41:m:87:LEU:HD13	46:m:202:3PE:H341	2.02	0.42
42:n:24:ARG:HD3	42:n:24:ARG:HA	1.88	0.42
42:n:30:CYS:O	42:n:32:HIS:N	2.52	0.42
2:C:125:ILE:HG21	3:D:253:TYR:CZ	2.54	0.41
7:9:23:ALA:O	7:9:27:LEU:HB2	2.19	0.41
14:W:91:GLU:OE1	14:W:100:LYS:NZ	2.47	0.41
19:H:173:TRP:NE1	19:H:244:GLY:O	2.53	0.41
22:L:205:ASN:HA	22:L:266:LEU:HD23	2.02	0.41
22:L:549:SER:O	22:L:553:LEU:HB2	2.20	0.41
23:M:230:ILE:HD12	23:M:230:ILE:HA	1.95	0.41
24:N:307:THR:OG1	24:N:308:ASN:N	2.52	0.41
8:P:309:PRO:HG2	8:P:312:LEU:HD13	2.02	0.41
22:L:36:THR:O	22:L:40:ILE:HG12	2.20	0.41
23:M:374:ASN:O	23:M:378:GLU:HG3	2.19	0.41
12:U:66:ASP:O	12:U:70:LEU:HG	2.20	0.41
29:a:6:LEU:HA	29:a:9:LEU:HB2	2.01	0.41
2:C:96:LEU:HB2	2:C:105:ILE:HG22	2.01	0.41
3:D:228:MET:HE2	3:D:228:MET:CA	2.21	0.41
6:3:47:SER:O	6:3:161:ARG:NH1	2.50	0.41
6:3:252:PRO:HB3	6:3:263:ILE:HG23	2.01	0.41
15:q:117:VAL:O	15:q:120:THR:OG1	2.28	0.41
20:J:165:ILE:HG23	24:N:42:PRO:HG3	2.01	0.41
23:M:256:TYR:HE1	23:M:257:MET:HE2	1.85	0.41
23:M:373:ILE:HD11	23:M:444:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:o:3:HIS:HA	43:o:6:ARG:HE	1.85	0.41
3:D:115:GLU:HB3	3:D:194:ILE:HB	2.01	0.41
5:1:247:ARG:HB2	5:1:273:SER:OG	2.19	0.41
5:1:349:ARG:HA	5:1:349:ARG:HD2	1.88	0.41
18:A:64:LEU:HD23	20:J:159:LEU:HD23	2.02	0.41
19:H:100:LEU:HD13	19:H:103:LEU:HD12	2.03	0.41
22:L:116:ARG:NH1	54:L:702:CDL:OB4	2.53	0.41
22:L:386:LEU:HD23	22:L:386:LEU:HA	1.90	0.41
24:N:338:PRO:O	26:X:169:TRP:NE1	2.52	0.41
25:O:52:PRO:O	25:O:107:GLN:NE2	2.45	0.41
26:X:74:LYS:NZ	29:a:69:ILE:O	2.41	0.41
27:Y:13:ASP:HA	27:Y:20:LYS:HE3	2.01	0.41
42:n:70:PHE:HA	53:n:201:ZMP:H2A	2.01	0.41
2:C:112:ASP:OD1	2:C:112:ASP:N	2.53	0.41
13:V:23:LEU:HD23	13:V:23:LEU:HA	1.94	0.41
40:l:7:MET:HE3	40:l:7:MET:HB2	1.93	0.41
40:l:135:ASN:HA	40:l:152:VAL:HB	2.02	0.41
42:n:135:GLU:HB2	42:n:164:PRO:HA	2.02	0.41
44:p:143:LEU:O	44:p:157:LYS:NZ	2.45	0.41
3:D:360:PRO:HA	3:D:380:SER:O	2.20	0.41
7:9:134:VAL:HG11	7:9:171:ILE:HD11	2.02	0.41
54:r:202:CDL:H182	29:a:7:PRO:HD3	2.03	0.41
19:H:140:ILE:HD11	20:J:65:VAL:HG11	2.02	0.41
22:L:13:ILE:HD13	22:L:13:ILE:HA	1.95	0.41
22:L:378:LEU:HD21	39:k:72:ILE:HD12	2.03	0.41
23:M:279:GLN:HG3	23:M:281:ASP:H	1.85	0.41
24:N:270:LEU:HB3	24:N:275:CYS:SG	2.61	0.41
25:O:225:SER:O	25:O:228:ALA:O	2.39	0.41
34:f:28:ARG:O	34:f:32:GLU:HG2	2.21	0.41
1:6:189:ARG:HD3	8:P:50:ARG:HH12	1.86	0.41
4:2:108:CYS:HA	4:2:151:ALA:HB1	2.02	0.41
4:2:183:LYS:HA	4:2:184:PRO:HD3	1.86	0.41
6:3:413:VAL:O	6:3:419:TYR:OH	2.32	0.41
14:W:73:ALA:HB1	53:W:201:ZMP:H17	2.02	0.41
16:r:95:THR:OG1	16:r:97:ALA:O	2.37	0.41
23:M:395:LEU:HD21	41:m:100:TRP:CE2	2.56	0.41
24:N:33:LEU:O	24:N:36:SER:OG	2.33	0.41
24:N:170:LEU:O	24:N:295:ARG:NH2	2.39	0.41
25:O:189:PRO:HA	25:O:192:MET:HE3	2.03	0.41
28:Z:136:ASN:HD22	28:Z:136:ASN:C	2.29	0.41
29:a:54:ILE:HD11	33:e:105:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:h:69:HIS:NE2	54:h:201:CDL:OA3	2.49	0.41
5:1:131:ALA:O	5:1:171:TYR:OH	2.32	0.41
5:1:133:ALA:HA	5:1:174:ASP:O	2.21	0.41
5:1:191:ALA:HB2	5:1:203:PRO:HG3	2.03	0.41
6:3:142:ILE:O	6:3:191:PHE:N	2.53	0.41
8:P:107:GLU:O	8:P:111:VAL:HB	2.21	0.41
9:Q:38:PHE:HE1	9:Q:58:GLU:HG2	1.86	0.41
15:q:32:ASP:OD2	15:q:58:ARG:NH2	2.54	0.41
22:L:54:PHE:CZ	22:L:84:PHE:HB2	2.56	0.41
22:L:65:THR:O	37:i:84:TYR:OH	2.35	0.41
23:M:306:PRO:HA	23:M:458:THR:HG21	2.03	0.41
40:l:9:PRO:HD3	41:m:66:ARG:HG2	2.02	0.41
4:2:60:TRP:H	4:2:60:TRP:CD1	2.39	0.41
6:3:13:VAL:HB	6:3:33:VAL:HG21	2.02	0.41
6:3:232:ASP:OD1	6:3:232:ASP:N	2.53	0.41
6:3:246:GLU:OE2	6:3:275:LYS:NZ	2.49	0.41
6:3:252:PRO:O	9:Q:44:ASN:ND2	2.53	0.41
7:9:33:ILE:HG21	47:9:204:PC1:H221	2.02	0.41
7:9:145:THR:OG1	7:9:148:GLU:OE2	2.37	0.41
8:P:46:ILE:HG12	10:7:26:VAL:HG21	2.03	0.41
8:P:134:HIS:HD2	51:P:501:NDP:H5N	1.86	0.41
12:T:16:LEU:O	12:T:20:LYS:HG2	2.21	0.41
12:T:45:LEU:HA	12:T:48:VAL:HG12	2.02	0.41
18:A:49:LEU:HD12	19:H:126:LYS:HD3	1.89	0.41
21:K:81:VAL:HG13	21:K:93:LEU:HD21	2.02	0.41
46:L:701:3PE:H222	40:l:87:ARG:HA	2.02	0.41
24:N:33:LEU:HD22	24:N:105:LYS:HE2	2.03	0.41
54:N:401:CDL:H342	54:N:401:CDL:H111	2.03	0.41
25:O:29:GLY:O	25:O:126:ARG:NH2	2.51	0.41
26:X:46:ARG:HD2	26:X:46:ARG:HA	1.87	0.41
26:X:94:GLN:HE22	29:a:37:ARG:NE	2.19	0.41
27:Y:61:THR:O	27:Y:65:ILE:HG12	2.20	0.41
28:Z:96:ILE:HG22	28:Z:97:MET:HG2	2.03	0.41
33:e:27:LYS:HA	33:e:27:LYS:HD3	1.93	0.41
37:i:82:HIS:CG	44:p:36:TYR:HH	2.37	0.41
44:p:100:GLU:HA	44:p:103:ASN:HD22	1.86	0.41
1:6:183:LEU:HD21	47:6:203:PC1:H331	2.02	0.41
3:D:238:ARG:NH1	19:H:279:ARG:O	2.54	0.41
8:P:157:ARG:NH2	8:P:227:THR:OG1	2.52	0.41
8:P:240:HIS:HB3	8:P:337:ALA:HB1	2.03	0.41
10:7:5:SER:OG	10:7:7:SER:OG	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:W:93:GLN:HE21	14:W:93:GLN:HB3	1.68	0.41
23:M:443:PRO:HB3	46:M:502:3PE:H3C1	2.03	0.41
54:N:401:CDL:H842	54:d:201:CDL:H671	2.02	0.41
26:X:16:GLU:OE2	33:e:104:ARG:NH2	2.54	0.41
32:d:54:MET:HE2	32:d:54:MET:HB3	1.84	0.41
37:i:103:ILE:HB	43:o:47:ASP:HB3	2.03	0.41
41:m:16:THR:O	41:m:22:TYR:OH	2.28	0.41
2:C:36:TYR:CG	2:C:56:GLY:HA3	2.56	0.40
49:1:501:FMN:H9	49:1:501:FMN:H1'1	1.82	0.40
6:3:273:GLY:O	6:3:549:HIS:NE2	2.42	0.40
22:L:193:MET:SD	22:L:204:SER:HB2	2.61	0.40
23:M:209:LEU:HD12	23:M:298:ILE:HD13	2.03	0.40
23:M:220:HIS:HE1	23:M:232:ALA:HB2	1.86	0.40
25:O:22:SER:OG	25:O:119:GLY:O	2.29	0.40
25:O:237:ASP:O	25:O:241:LEU:HB2	2.21	0.40
2:C:32:ILE:HG22	2:C:33:LEU:HG	2.03	0.40
2:C:65:ARG:HE	2:C:65:ARG:HB3	1.78	0.40
3:D:6:PRO:HB3	3:D:10:TRP:HB3	2.03	0.40
6:3:231:MET:HE1	6:3:677:ILE:HB	2.03	0.40
18:A:67:LEU:HB2	20:J:159:LEU:HD21	2.03	0.40
18:A:80:GLN:NE2	19:H:315:PRO:O	2.38	0.40
19:H:231:ILE:HG23	19:H:270:PHE:HD2	1.86	0.40
23:M:421:ASN:OD1	23:M:421:ASN:N	2.54	0.40
37:i:94:TYR:OH	44:p:10:PRO:O	2.35	0.40
1:6:48:ASN:HB3	1:6:178:LYS:HA	2.02	0.40
6:3:32:LYS:HE2	6:3:32:LYS:HB2	1.87	0.40
21:K:41:PHE:HA	21:K:63:ILE:HD11	2.03	0.40
21:K:57:MET:O	21:K:60:PRO:HD2	2.21	0.40
23:M:75:LEU:HD23	23:M:440:HIS:CE1	2.56	0.40
54:N:401:CDL:H652	54:d:201:CDL:H652	2.03	0.40
25:O:170:ILE:HG13	25:O:221:LEU:HB2	2.03	0.40
19:H:18:ALA:HB1	19:H:48:PRO:HB2	2.03	0.40
22:L:78:MET:HA	54:h:201:CDL:H262	2.02	0.40
23:M:94:LEU:O	23:M:98:MET:HG2	2.21	0.40
23:M:131:ILE:HD13	54:N:401:CDL:H781	2.02	0.40
23:M:220:HIS:CE1	23:M:232:ALA:HB2	2.55	0.40
24:N:254:LEU:HD23	24:N:254:LEU:HA	1.88	0.40
25:O:106:LEU:HD13	25:O:270:LEU:HD11	2.03	0.40
12:U:20:LYS:HG2	12:U:27:PRO:HB3	2.03	0.40
7:9:83:LYS:NZ	7:9:96:ILE:O	2.55	0.40
22:L:263:PHE:HD2	22:L:266:LEU:HD12	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:i:15:ARG:O	37:i:19:ARG:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6	155/224 (69%)	145 (94%)	10 (6%)	0	100	100
2	C	206/263 (78%)	198 (96%)	8 (4%)	0	100	100
3	D	411/463 (89%)	391 (95%)	20 (5%)	0	100	100
4	2	212/248 (86%)	202 (95%)	9 (4%)	1 (0%)	24	60
5	1	428/464 (92%)	409 (96%)	19 (4%)	0	100	100
6	3	688/727 (95%)	660 (96%)	28 (4%)	0	100	100
7	9	176/212 (83%)	173 (98%)	3 (2%)	0	100	100
8	P	308/377 (82%)	296 (96%)	12 (4%)	0	100	100
9	Q	124/175 (71%)	121 (98%)	3 (2%)	0	100	100
10	7	94/116 (81%)	91 (97%)	3 (3%)	0	100	100
11	S	82/99 (83%)	78 (95%)	4 (5%)	0	100	100
12	T	77/156 (49%)	75 (97%)	2 (3%)	0	100	100
12	U	86/156 (55%)	83 (96%)	3 (4%)	0	100	100
13	V	111/116 (96%)	109 (98%)	2 (2%)	0	100	100
14	W	112/131 (86%)	107 (96%)	5 (4%)	0	100	100
15	q	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
16	r	93/113 (82%)	91 (98%)	2 (2%)	0	100	100
17	s	40/104 (38%)	39 (98%)	1 (2%)	0	100	100
18	A	89/115 (77%)	86 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	H	302/318 (95%)	290 (96%)	12 (4%)	0	100	100
20	J	161/172 (94%)	151 (94%)	10 (6%)	0	100	100
21	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
22	L	604/607 (100%)	571 (94%)	33 (6%)	0	100	100
23	M	457/459 (100%)	443 (97%)	14 (3%)	0	100	100
24	N	343/345 (99%)	327 (95%)	16 (5%)	0	100	100
25	O	318/355 (90%)	305 (96%)	13 (4%)	0	100	100
26	X	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
27	Y	138/141 (98%)	138 (100%)	0	0	100	100
28	Z	139/144 (96%)	137 (99%)	2 (1%)	0	100	100
29	a	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
30	b	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
31	c	46/76 (60%)	46 (100%)	0	0	100	100
32	d	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
33	e	103/106 (97%)	99 (96%)	4 (4%)	0	100	100
34	f	51/57 (90%)	51 (100%)	0	0	100	100
35	g	99/151 (66%)	96 (97%)	3 (3%)	0	100	100
36	h	137/189 (72%)	133 (97%)	4 (3%)	0	100	100
37	i	102/128 (80%)	96 (94%)	6 (6%)	0	100	100
38	j	63/105 (60%)	59 (94%)	4 (6%)	0	100	100
39	k	75/104 (72%)	73 (97%)	2 (3%)	0	100	100
40	l	155/186 (83%)	151 (97%)	4 (3%)	0	100	100
41	m	124/129 (96%)	124 (100%)	0	0	100	100
42	n	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
43	o	116/137 (85%)	108 (93%)	8 (7%)	0	100	100
44	p	167/176 (95%)	165 (99%)	2 (1%)	0	100	100
All	All	8042/9212 (87%)	7742 (96%)	299 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	2	183	LYS

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	6	133/185 (72%)	133 (100%)	0	100	100
2	C	190/227 (84%)	190 (100%)	0	100	100
3	D	361/394 (92%)	360 (100%)	1 (0%)	86	91
4	2	184/206 (89%)	184 (100%)	0	100	100
5	1	345/370 (93%)	345 (100%)	0	100	100
6	3	580/610 (95%)	580 (100%)	0	100	100
7	9	152/178 (85%)	152 (100%)	0	100	100
8	P	273/325 (84%)	273 (100%)	0	100	100
9	Q	113/153 (74%)	113 (100%)	0	100	100
10	7	81/96 (84%)	81 (100%)	0	100	100
11	S	74/80 (92%)	74 (100%)	0	100	100
12	T	73/135 (54%)	73 (100%)	0	100	100
12	U	81/135 (60%)	81 (100%)	0	100	100
13	V	101/102 (99%)	101 (100%)	0	100	100
14	W	108/114 (95%)	108 (100%)	0	100	100
15	q	131/131 (100%)	131 (100%)	0	100	100
16	r	86/96 (90%)	86 (100%)	0	100	100
17	s	41/95 (43%)	41 (100%)	0	100	100
18	A	84/103 (82%)	84 (100%)	0	100	100
19	H	269/279 (96%)	269 (100%)	0	100	100
20	J	131/137 (96%)	131 (100%)	0	100	100
21	K	87/87 (100%)	87 (100%)	0	100	100
22	L	548/549 (100%)	548 (100%)	0	100	100
23	M	414/414 (100%)	414 (100%)	0	100	100
24	N	307/307 (100%)	307 (100%)	0	100	100
25	O	284/309 (92%)	284 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	X	153/154 (99%)	153 (100%)	0	100	100
27	Y	105/106 (99%)	105 (100%)	0	100	100
28	Z	122/123 (99%)	122 (100%)	0	100	100
29	a	60/60 (100%)	60 (100%)	0	100	100
30	b	72/73 (99%)	72 (100%)	0	100	100
31	c	42/67 (63%)	42 (100%)	0	100	100
32	d	107/107 (100%)	107 (100%)	0	100	100
33	e	93/94 (99%)	93 (100%)	0	100	100
34	f	49/53 (92%)	49 (100%)	0	100	100
35	g	92/129 (71%)	92 (100%)	0	100	100
36	h	123/162 (76%)	123 (100%)	0	100	100
37	i	99/119 (83%)	99 (100%)	0	100	100
38	j	61/87 (70%)	61 (100%)	0	100	100
39	k	60/78 (77%)	60 (100%)	0	100	100
40	l	142/161 (88%)	142 (100%)	0	100	100
41	m	112/114 (98%)	112 (100%)	0	100	100
42	n	163/164 (99%)	163 (100%)	0	100	100
43	o	109/121 (90%)	109 (100%)	0	100	100
44	p	154/158 (98%)	154 (100%)	0	100	100
All	All	7149/7947 (90%)	7148 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
3	D	228	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	6	174	GLN
3	D	280	GLN
4	2	9	HIS
4	2	37	ASN
4	2	42	HIS

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Mol	Chain	Res	Type
4	2	101	GLN
5	1	293	ASN
5	1	373	ASN
5	1	416	GLN
5	1	421	HIS
6	3	259	ASN
6	3	402	ASN
6	3	546	GLN
6	3	643	GLN
6	3	665	GLN
8	P	58	HIS
8	P	93	ASN
8	P	119	GLN
8	P	136	ASN
8	P	288	HIS
9	Q	44	ASN
11	S	47	HIS
11	S	72	GLN
11	S	79	ASN
11	S	80	ASN
12	T	33	ASN
12	T	74	GLN
13	V	40	HIS
13	V	109	ASN
14	W	101	GLN
15	q	123	GLN
16	r	109	GLN
17	s	49	ASN
20	J	107	ASN
21	K	50	ASN
22	L	29	HIS
22	L	205	ASN
22	L	209	ASN
22	L	269	ASN
22	L	296	ASN
22	L	309	GLN
22	L	328	HIS
22	L	332	HIS
22	L	505	ASN
23	M	48	ASN
23	M	81	GLN
23	M	138	ASN

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Mol	Chain	Res	Type
23	M	193	ASN
23	M	279	GLN
24	N	171	ASN
24	N	172	GLN
24	N	223	ASN
24	N	308	ASN
24	N	342	GLN
25	O	36	ASN
25	O	57	GLN
12	U	74	GLN
26	X	142	HIS
28	Z	75	GLN
32	d	3	ASN
32	d	88	HIS
33	e	81	GLN
33	e	96	HIS
36	h	143	ASN
37	i	25	GLN
40	l	54	GLN
40	l	86	ASN
40	l	136	ASN
41	m	78	ASN
41	m	85	ASN
41	m	125	ASN
42	n	140	GLN
43	o	75	ASN
44	p	54	GLN
44	p	90	GLN
44	p	103	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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
21	FME	K	1	21	8,9,10	0.94	0	8,9,11	1.88	2 (25%)
37	SAC	i	1	37	7,8,9	1.02	0	7,9,11	0.99	0
23	FME	M	1	23	8,9,10	1.01	0	8,9,11	0.76	0
24	FME	N	1	24	8,9,10	0.98	0	8,9,11	0.97	0
19	FME	H	1	19	8,9,10	0.98	0	8,9,11	0.88	0
20	FME	J	1	20	8,9,10	0.98	0	8,9,11	0.93	0
22	FME	L	1	22	8,9,10	0.96	0	8,9,11	0.91	0
16	AYA	r	1	16	6,7,8	1.27	1 (16%)	6,8,10	1.14	1 (16%)
18	FME	A	1	18	8,9,10	0.95	0	8,9,11	0.89	0
3	2MR	D	85	3	10,12,13	2.68	2 (20%)	5,13,15	3.04	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
21	FME	K	1	21	-	3/7/9/11	-
37	SAC	i	1	37	-	0/7/8/10	-
23	FME	M	1	23	-	1/7/9/11	-
24	FME	N	1	24	-	3/7/9/11	-
19	FME	H	1	19	-	3/7/9/11	-
20	FME	J	1	20	-	4/7/9/11	-
22	FME	L	1	22	-	3/7/9/11	-
16	AYA	r	1	16	-	0/5/6/8	-
18	FME	A	1	18	-	2/7/9/11	-
3	2MR	D	85	3	-	3/10/13/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	85	2MR	CZ-NE	5.97	1.47	1.34
3	D	85	2MR	CZ-NH2	5.43	1.44	1.33
16	r	1	AYA	CA-N	-2.40	1.44	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	85	2MR	CD-NE-CZ	5.73	134.13	123.36
21	K	1	FME	C-CA-N	4.49	118.17	109.50
3	D	85	2MR	NE-CZ-NH2	-3.45	116.32	119.48
16	r	1	AYA	CB-CA-N	2.53	112.53	109.68
21	K	1	FME	O-C-CA	-2.24	119.02	124.77

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	85	2MR	C-CA-CB-CG
18	A	1	FME	N-CA-CB-CG
19	H	1	FME	N-CA-CB-CG
19	H	1	FME	O-C-CA-CB
20	J	1	FME	CB-CA-N-CN
21	K	1	FME	O1-CN-N-CA
21	K	1	FME	N-CA-CB-CG
22	L	1	FME	N-CA-CB-CG
24	N	1	FME	N-CA-CB-CG
24	N	1	FME	C-CA-CB-CG
3	D	85	2MR	NE-CD-CG-CB
20	J	1	FME	CA-CB-CG-SD
20	J	1	FME	C-CA-CB-CG
23	M	1	FME	N-CA-CB-CG
3	D	85	2MR	CA-CB-CG-CD
21	K	1	FME	CA-CB-CG-SD
18	A	1	FME	C-CA-CB-CG
19	H	1	FME	C-CA-CB-CG
22	L	1	FME	C-CA-CB-CG
24	N	1	FME	CB-CG-SD-CE
20	J	1	FME	CB-CG-SD-CE
22	L	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	K	1	FME	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 43 ligands modelled in this entry, 3 are monoatomic - leaving 40 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	DGT	O	401	56	32,33,33	0.29	0	48,52,52	0.30	0
54	CDL	r	202	-	56,56,99	0.39	0	62,68,111	0.47	1 (1%)
46	3PE	A	201	-	42,42,50	0.33	0	45,47,55	0.33	0
47	PC1	6	203	-	42,42,53	0.34	0	48,50,61	0.50	1 (2%)
46	3PE	K	201	-	40,40,50	0.33	0	43,45,55	0.32	0
46	3PE	d	202	-	30,30,50	0.37	0	33,35,55	0.33	0
46	3PE	Y	202	-	41,41,50	0.33	0	44,46,55	0.32	0
49	FMN	1	501	-	33,33,33	0.28	0	48,50,50	0.37	0
46	3PE	6	202	-	31,31,50	0.37	0	34,36,55	0.31	0
45	SF4	1	502	5	0,12,12	-	-	-	-	-
53	ZMP	n	201	-	26,31,36	0.74	1 (3%)	30,38,45	0.92	1 (3%)
47	PC1	9	204	-	46,46,53	0.32	0	52,54,61	0.32	0
45	SF4	6	201	1	0,12,12	-	-	-	-	-
46	3PE	L	701	-	50,50,50	0.31	0	53,55,55	0.47	0
46	3PE	L	703	-	50,50,50	0.30	0	53,55,55	0.31	0
54	CDL	N	401	-	89,89,99	0.31	0	95,101,111	0.40	1 (1%)
54	CDL	L	702	-	77,77,99	0.34	0	83,89,111	0.31	0
46	3PE	M	504	-	35,35,50	0.35	0	38,40,55	0.31	0
45	SF4	9	202	7	0,12,12	-	-	-	-	-
45	SF4	3	802	6	0,12,12	-	-	-	-	-
51	NDP	P	501	-	51,52,52	0.33	0	71,80,80	0.41	0
46	3PE	Y	201	-	27,27,50	0.40	0	30,32,55	0.37	0
45	SF4	3	801	6	0,12,12	-	-	-	-	-
46	3PE	N	402	-	37,37,50	0.34	0	40,42,55	0.32	0
45	SF4	9	201	7	0,12,12	-	-	-	-	-
46	3PE	d	203	-	31,31,50	0.37	0	34,36,55	0.33	0
53	ZMP	W	201	-	28,33,36	0.62	1 (3%)	32,40,45	1.13	2 (6%)
46	3PE	M	502	-	50,50,50	0.30	0	53,55,55	0.30	0
46	3PE	r	201	-	45,45,50	0.31	0	48,50,55	0.29	0
46	3PE	H	401	-	50,50,50	0.31	0	53,55,55	0.48	1 (1%)
46	3PE	M	503	-	50,50,50	0.30	0	53,55,55	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	3PE	i	201	-	41,41,50	0.33	0	44,46,55	0.31	0
46	3PE	m	202	-	29,29,50	0.38	0	32,34,55	0.33	0
54	CDL	m	201	-	71,71,99	0.35	0	77,83,111	0.43	1 (1%)
54	CDL	h	201	-	69,69,99	0.35	0	75,81,111	0.43	1 (1%)
48	FES	2	301	4	0,4,4	-	-	-		
54	CDL	d	201	-	66,66,99	0.36	0	72,78,111	0.31	0
47	PC1	M	501	-	53,53,53	0.29	0	59,61,61	0.40	0
47	PC1	9	203	-	53,53,53	0.30	0	59,61,61	0.45	0
48	FES	3	803	6	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
55	DGT	O	401	56	-	9/22/34/34	0/3/3/3
54	CDL	r	202	-	-	13/67/67/110	-
46	3PE	A	201	-	-	8/46/46/54	-
47	PC1	6	203	-	-	10/46/46/57	-
46	3PE	K	201	-	-	10/44/44/54	-
46	3PE	d	202	-	-	9/34/34/54	-
46	3PE	Y	202	-	-	7/45/45/54	-
49	FMN	1	501	-	-	5/18/18/18	0/3/3/3
46	3PE	6	202	-	-	4/35/35/54	-
45	SF4	1	502	5	-	-	0/6/5/5
53	ZMP	n	201	-	-	13/36/38/43	-
47	PC1	9	204	-	-	10/50/50/57	-
46	3PE	L	701	-	-	8/54/54/54	-
46	3PE	L	703	-	-	9/54/54/54	-
45	SF4	6	201	1	-	-	0/6/5/5
54	CDL	N	401	-	-	15/100/100/110	-
54	CDL	L	702	-	-	15/88/88/110	-
46	3PE	M	504	-	-	9/39/39/54	-
51	NDP	P	501	-	-	5/34/77/77	0/5/5/5
45	SF4	3	802	6	-	-	0/6/5/5
45	SF4	9	202	7	-	-	0/6/5/5
46	3PE	Y	201	-	-	4/31/31/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	3	801	6	-	-	0/6/5/5
46	3PE	N	402	-	-	6/41/41/54	-
53	ZMP	W	201	-	-	9/38/40/43	-
46	3PE	d	203	-	-	6/35/35/54	-
45	SF4	9	201	7	-	-	0/6/5/5
46	3PE	M	502	-	-	13/54/54/54	-
46	3PE	H	401	-	-	11/54/54/54	-
46	3PE	r	201	-	-	7/49/49/54	-
46	3PE	M	503	-	-	12/54/54/54	-
46	3PE	i	201	-	-	7/45/45/54	-
46	3PE	m	202	-	-	11/33/33/54	-
54	CDL	m	201	-	-	20/82/82/110	-
54	CDL	h	201	-	-	20/80/80/110	-
48	FES	2	301	4	-	-	0/1/1/1
54	CDL	d	201	-	-	11/77/77/110	-
47	PC1	M	501	-	-	10/57/57/57	-
47	PC1	9	203	-	-	10/57/57/57	-
48	FES	3	803	6	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	n	201	ZMP	C9-C10	2.63	1.53	1.50
53	W	201	ZMP	C9-C10	2.11	1.53	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	W	201	ZMP	O1-C10-C9	-3.19	120.30	123.98
53	n	201	ZMP	O1-C10-C9	-2.54	121.05	123.98
53	W	201	ZMP	C15-C14-C13	-2.33	108.51	112.39
47	6	203	PC1	C2-O21-C21	2.15	122.94	117.80
46	H	401	3PE	C2-O21-C21	2.13	122.91	117.80
54	N	401	CDL	CB4-OB6-CB5	2.08	122.78	117.80
54	m	201	CDL	CA4-OA6-CA5	2.06	122.73	117.80
54	h	201	CDL	CB4-OB6-CB5	2.05	122.69	117.80
54	r	202	CDL	CA4-OA6-CA5	2.03	122.66	117.80

There are no chirality outliers.

All (316) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	6	202	3PE	C11-O13-P-O11
46	6	202	3PE	C11-O13-P-O14
46	6	202	3PE	O13-C11-C12-N
46	r	201	3PE	C1-O11-P-O12
46	r	201	3PE	C11-O13-P-O11
46	r	201	3PE	C11-O13-P-O12
46	r	201	3PE	O13-C11-C12-N
46	A	201	3PE	C11-O13-P-O11
46	A	201	3PE	C11-O13-P-O14
46	A	201	3PE	O13-C11-C12-N
46	H	401	3PE	C1-O11-P-O14
46	H	401	3PE	C11-O13-P-O11
46	H	401	3PE	C11-O13-P-O12
46	H	401	3PE	C11-O13-P-O14
46	K	201	3PE	C11-O13-P-O11
46	K	201	3PE	O13-C11-C12-N
46	L	701	3PE	C1-O11-P-O13
46	L	701	3PE	C1-O11-P-O14
46	L	703	3PE	C1-O11-P-O12
46	L	703	3PE	C1-O11-P-O13
46	L	703	3PE	O13-C11-C12-N
46	M	502	3PE	C1-O11-P-O12
46	M	502	3PE	C1-O11-P-O13
46	M	503	3PE	C1-O11-P-O13
46	M	503	3PE	C1-O11-P-O14
46	M	503	3PE	C11-O13-P-O11
46	M	503	3PE	C11-O13-P-O12
46	M	504	3PE	C1-O11-P-O13
46	M	504	3PE	C1-O11-P-O14
46	M	504	3PE	C11-O13-P-O11
46	M	504	3PE	C11-O13-P-O12
46	M	504	3PE	C11-O13-P-O14
46	N	402	3PE	C1-O11-P-O12
46	Y	201	3PE	C1-O11-P-O12
46	Y	201	3PE	C1-O11-P-O13
46	Y	201	3PE	C1-O11-P-O14
46	Y	201	3PE	O13-C11-C12-N
46	Y	202	3PE	C11-O13-P-O11
46	Y	202	3PE	O13-C11-C12-N
46	d	202	3PE	C1-O11-P-O12
46	d	202	3PE	C1-O11-P-O13
46	d	202	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
46	d	202	3PE	C11-O13-P-O11
46	d	202	3PE	C11-O13-P-O12
46	d	202	3PE	C11-O13-P-O14
46	d	202	3PE	O13-C11-C12-N
46	d	203	3PE	C1-O11-P-O12
46	d	203	3PE	C1-O11-P-O13
46	d	203	3PE	C1-O11-P-O14
46	d	203	3PE	C11-O13-P-O12
46	i	201	3PE	C1-O11-P-O12
46	i	201	3PE	C1-O11-P-O13
46	i	201	3PE	C1-O11-P-O14
46	i	201	3PE	C11-O13-P-O14
46	i	201	3PE	O13-C11-C12-N
46	m	202	3PE	C1-O11-P-O14
46	m	202	3PE	C11-O13-P-O11
46	m	202	3PE	C11-O13-P-O12
46	m	202	3PE	C11-O13-P-O14
46	m	202	3PE	O13-C11-C12-N
47	6	203	PC1	C1-O11-P-O12
47	6	203	PC1	C1-O11-P-O14
47	6	203	PC1	C1-O11-P-O13
47	9	204	PC1	C11-O13-P-O11
47	M	501	PC1	C11-O13-P-O12
47	M	501	PC1	C11-O13-P-O14
47	M	501	PC1	C11-O13-P-O11
49	1	501	FMN	N10-C1'-C2'-O2'
49	1	501	FMN	N10-C1'-C2'-C3'
49	1	501	FMN	C5'-O5'-P-O2P
49	1	501	FMN	C5'-O5'-P-O3P
53	W	201	ZMP	C19-C18-C21-O5
53	W	201	ZMP	C20-C18-C21-O5
53	W	201	ZMP	C17-C18-C21-O5
53	W	201	ZMP	S1-C11-C12-N1
53	W	201	ZMP	O1-C10-S1-C11
53	W	201	ZMP	C9-C10-S1-C11
53	n	201	ZMP	C16-C17-C18-C21
53	n	201	ZMP	C17-C16-N2-C15
54	r	202	CDL	CA2-OA2-PA1-OA3
54	r	202	CDL	CA2-OA2-PA1-OA4
54	r	202	CDL	CA2-OA2-PA1-OA5
54	r	202	CDL	CA3-OA5-PA1-OA3
54	r	202	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
54	r	202	CDL	CB2-OB2-PB2-OB3
54	r	202	CDL	CB3-OB5-PB2-OB2
54	L	702	CDL	CA2-OA2-PA1-OA3
54	L	702	CDL	CA2-OA2-PA1-OA4
54	L	702	CDL	CA2-OA2-PA1-OA5
54	L	702	CDL	CA3-OA5-PA1-OA2
54	L	702	CDL	CA3-OA5-PA1-OA3
54	L	702	CDL	CB2-OB2-PB2-OB3
54	L	702	CDL	CB2-OB2-PB2-OB5
54	N	401	CDL	OA6-CA4-CA6-OA8
54	N	401	CDL	CB2-OB2-PB2-OB3
54	N	401	CDL	CB2-OB2-PB2-OB5
54	d	201	CDL	CA3-OA5-PA1-OA2
54	d	201	CDL	CB2-OB2-PB2-OB3
54	d	201	CDL	CB2-OB2-PB2-OB5
54	h	201	CDL	CA2-OA2-PA1-OA3
54	h	201	CDL	CA2-OA2-PA1-OA5
54	h	201	CDL	CB2-OB2-PB2-OB4
54	h	201	CDL	CB2-OB2-PB2-OB5
54	h	201	CDL	CB3-OB5-PB2-OB2
54	h	201	CDL	CB3-OB5-PB2-OB3
54	h	201	CDL	CB3-OB5-PB2-OB4
54	m	201	CDL	CA2-OA2-PA1-OA3
54	m	201	CDL	CA2-OA2-PA1-OA5
54	m	201	CDL	CA3-OA5-PA1-OA2
54	m	201	CDL	CA3-OA5-PA1-OA3
54	m	201	CDL	CB2-OB2-PB2-OB3
54	m	201	CDL	CB2-OB2-PB2-OB4
54	m	201	CDL	CB2-OB2-PB2-OB5
54	m	201	CDL	CB3-OB5-PB2-OB2
54	m	201	CDL	CB3-OB5-PB2-OB3
54	m	201	CDL	CB3-OB5-PB2-OB4
54	m	201	CDL	OB5-CB3-CB4-OB6
55	O	401	DGT	PB-O3B-PG-O1G
55	O	401	DGT	C5'-O5'-PA-O1A
55	O	401	DGT	C5'-O5'-PA-O2A
53	n	201	ZMP	O3-C16-N2-C15
46	L	701	3PE	C21-C22-C23-C24
47	6	203	PC1	C11-C12-N-C14
47	9	204	PC1	C11-C12-N-C15
46	M	502	3PE	C21-C22-C23-C24
54	L	702	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
47	9	204	PC1	C11-C12-N-C13
53	n	201	ZMP	C6-C7-C8-C9
46	L	703	3PE	C38-C39-C3A-C3B
54	d	201	CDL	C63-C64-C65-C66
46	H	401	3PE	C21-C22-C23-C24
46	M	503	3PE	C26-C27-C28-C29
47	M	501	PC1	C37-C38-C39-C3A
54	N	401	CDL	C81-C82-C83-C84
47	6	203	PC1	C11-C12-N-C13
47	6	203	PC1	C11-C12-N-C15
47	9	204	PC1	C11-C12-N-C14
46	M	503	3PE	C22-C23-C24-C25
46	A	201	3PE	C39-C3A-C3B-C3C
46	L	703	3PE	C32-C33-C34-C35
54	d	201	CDL	C55-C56-C57-C58
54	d	201	CDL	OB5-CB3-CB4-OB6
46	N	402	3PE	O21-C2-C3-O31
47	9	204	PC1	C29-C2A-C2B-C2C
46	H	401	3PE	C31-C32-C33-C34
53	n	201	ZMP	O3-C16-C17-O4
46	M	502	3PE	O11-C1-C2-C3
54	m	201	CDL	OB5-CB3-CB4-CB6
46	A	201	3PE	C34-C35-C36-C37
46	N	402	3PE	C1-C2-C3-O31
46	Y	202	3PE	C1-C2-C3-O31
46	M	502	3PE	C22-C23-C24-C25
49	1	501	FMN	C5'-O5'-P-O1P
54	L	702	CDL	OB5-CB3-CB4-OB6
46	M	502	3PE	C36-C37-C38-C39
54	h	201	CDL	OB6-CB4-CB6-OB8
47	6	203	PC1	C35-C36-C37-C38
54	d	201	CDL	OB5-CB3-CB4-CB6
53	n	201	ZMP	N2-C16-C17-O4
54	m	201	CDL	CB3-CB4-CB6-OB8
46	M	502	3PE	O11-C1-C2-O21
46	M	504	3PE	C2-C1-O11-P
46	M	503	3PE	C34-C35-C36-C37
46	Y	202	3PE	O21-C2-C3-O31
47	6	203	PC1	O21-C2-C3-O31
46	N	402	3PE	C32-C33-C34-C35
47	M	501	PC1	C21-C22-C23-C24
47	9	204	PC1	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
53	n	201	ZMP	C13-C14-C15-N2
46	L	701	3PE	O11-C1-C2-C3
46	m	202	3PE	O11-C1-C2-C3
47	9	203	PC1	C28-C29-C2A-C2B
47	6	203	PC1	C33-C34-C35-C36
46	m	202	3PE	O11-C1-C2-O21
54	N	401	CDL	CA3-CA4-CA6-OA8
54	d	201	CDL	CA3-CA4-CA6-OA8
54	d	201	CDL	OA6-CA4-CA6-OA8
47	9	203	PC1	C35-C36-C37-C38
47	9	203	PC1	C11-C12-N-C13
47	9	203	PC1	C11-C12-N-C14
47	M	501	PC1	O13-C11-C12-N
51	P	501	NDP	PN-O3-PA-O2A
55	O	401	DGT	PB-O3A-PA-O1A
54	L	702	CDL	OB5-CB3-CB4-CB6
54	h	201	CDL	OB5-CB3-CB4-CB6
53	n	201	ZMP	C19-C18-C21-O5
54	h	201	CDL	C1-CA2-OA2-PA1
54	h	201	CDL	OB5-CB3-CB4-OB6
54	m	201	CDL	OB6-CB4-CB6-OB8
46	M	503	3PE	C1-C2-C3-O31
47	9	204	PC1	C35-C36-C37-C38
46	6	202	3PE	C1-O11-P-O14
46	r	201	3PE	C1-O11-P-O13
46	r	201	3PE	C1-O11-P-O14
46	K	201	3PE	C11-O13-P-O14
46	L	701	3PE	C1-O11-P-O12
46	M	503	3PE	C1-O11-P-O12
46	M	503	3PE	C11-O13-P-O14
46	M	504	3PE	C1-O11-P-O12
46	N	402	3PE	O13-C11-C12-N
46	Y	202	3PE	C11-O13-P-O14
46	d	203	3PE	C11-O13-P-O11
46	d	203	3PE	C11-O13-P-O14
46	i	201	3PE	C11-O13-P-O11
46	i	201	3PE	C11-O13-P-O12
54	r	202	CDL	CA3-OA5-PA1-OA2
54	r	202	CDL	CB3-OB5-PB2-OB3
54	L	702	CDL	CA3-OA5-PA1-OA4
54	N	401	CDL	CA2-OA2-PA1-OA3
54	N	401	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
54	N	401	CDL	CA2-OA2-PA1-OA5
54	N	401	CDL	CA3-OA5-PA1-OA3
54	N	401	CDL	CB2-OB2-PB2-OB4
54	d	201	CDL	CA3-OA5-PA1-OA3
54	h	201	CDL	CA2-OA2-PA1-OA4
55	O	401	DGT	C5'-O5'-PA-O3A
46	A	201	3PE	C2-C1-O11-P
46	K	201	3PE	C2-C1-O11-P
46	L	701	3PE	C2-C1-O11-P
54	h	201	CDL	CA4-CA3-OA5-PA1
46	M	502	3PE	C37-C38-C39-C3A
46	H	401	3PE	C33-C34-C35-C36
53	n	201	ZMP	C5-C6-C7-C8
46	A	201	3PE	C38-C39-C3A-C3B
46	L	703	3PE	C31-C32-C33-C34
47	9	203	PC1	C11-C12-N-C15
46	M	503	3PE	O21-C2-C3-O31
46	r	201	3PE	O31-C31-C32-C33
54	m	201	CDL	C72-C73-C74-C75
53	W	201	ZMP	C22-C1-C2-C3
46	L	703	3PE	C3D-C3E-C3F-C3G
46	M	502	3PE	C2-C1-O11-P
46	L	703	3PE	O21-C21-C22-C23
46	H	401	3PE	O31-C31-C32-C33
46	H	401	3PE	C3-C2-O21-C21
47	9	203	PC1	C3-C2-O21-C21
46	N	402	3PE	C2-C1-O11-P
46	M	502	3PE	C3D-C3E-C3F-C3G
54	N	401	CDL	OB6-CB4-CB6-OB8
51	P	501	NDP	O4D-C1D-N1N-C6N
51	P	501	NDP	C2N-C3N-C7N-N7N
47	M	501	PC1	C34-C35-C36-C37
51	P	501	NDP	C2B-O2B-P2B-O1X
54	d	201	CDL	C59-C60-C61-C62
54	m	201	CDL	C1-CB2-OB2-PB2
46	Y	202	3PE	O11-C1-C2-O21
46	H	401	3PE	C2A-C2B-C2C-C2D
47	9	204	PC1	O11-C1-C2-C3
46	M	502	3PE	O21-C21-C22-C23
54	N	401	CDL	CB4-CB3-OB5-PB2
54	L	702	CDL	O1-C1-CB2-OB2
55	O	401	DGT	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
54	r	202	CDL	C52-C51-CB5-OB6
46	L	701	3PE	C3-C2-O21-C21
54	h	201	CDL	CB6-CB4-OB6-CB5
55	O	401	DGT	PB-O3B-PG-O2G
54	h	201	CDL	CB3-CB4-CB6-OB8
47	M	501	PC1	C23-C24-C25-C26
53	n	201	ZMP	C16-C17-C18-C20
46	H	401	3PE	O11-C1-C2-C3
46	K	201	3PE	O31-C31-C32-C33
51	P	501	NDP	C2D-C1D-N1N-C6N
54	h	201	CDL	C12-C11-CA5-OA6
54	r	202	CDL	C1-CB2-OB2-PB2
55	O	401	DGT	PB-O3A-PA-O2A
53	n	201	ZMP	C3-C4-C5-C6
54	L	702	CDL	C11-C12-C13-C14
53	W	201	ZMP	C2-C1-C22-C23
46	M	504	3PE	O21-C21-C22-C23
54	m	201	CDL	C12-C11-CA5-OA6
47	9	204	PC1	O31-C31-C32-C33
46	K	201	3PE	O21-C21-C22-C23
54	h	201	CDL	C32-C31-CA7-OA8
46	M	502	3PE	O31-C31-C32-C33
46	m	202	3PE	O21-C21-C22-C23
47	M	501	PC1	O21-C2-C3-O31
46	d	202	3PE	O31-C31-C32-C33
54	h	201	CDL	C72-C71-CB7-OB8
47	9	203	PC1	C27-C28-C29-C2A
46	K	201	3PE	C2A-C2B-C2C-C2D
46	m	202	3PE	O31-C31-C32-C33
53	n	201	ZMP	C20-C18-C21-O5
54	N	401	CDL	C80-C81-C82-C83
47	6	203	PC1	C3-C2-O21-C21
54	r	202	CDL	CA3-CA4-OA6-CA5
54	N	401	CDL	CB6-CB4-OB6-CB5
54	m	201	CDL	CA6-CA4-OA6-CA5
47	M	501	PC1	C3B-C3C-C3D-C3E
55	O	401	DGT	C4'-C5'-O5'-PA
54	m	201	CDL	C12-C11-CA5-OA7
47	9	203	PC1	C2D-C2E-C2F-C2G
46	K	201	3PE	C25-C26-C27-C28
54	m	201	CDL	C52-C51-CB5-OB6
46	M	502	3PE	O32-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
46	M	503	3PE	O21-C21-C22-C23
54	h	201	CDL	C72-C71-CB7-OB9
47	9	203	PC1	C3D-C3E-C3F-C3G
46	K	201	3PE	O32-C31-C32-C33
46	K	201	3PE	O22-C21-C22-C23
46	d	202	3PE	O32-C31-C32-C33
54	h	201	CDL	C32-C31-CA7-OA9
53	W	201	ZMP	N2-C16-C17-O4
54	r	202	CDL	C1-CA2-OA2-PA1
54	L	702	CDL	C1-CA2-OA2-PA1
54	L	702	CDL	C52-C51-CB5-OB6
46	L	703	3PE	C39-C3A-C3B-C3C
53	n	201	ZMP	C17-C18-C21-O5
46	m	202	3PE	O32-C31-C32-C33
46	m	202	3PE	O22-C21-C22-C23
46	A	201	3PE	C33-C34-C35-C36
47	9	204	PC1	O32-C31-C32-C33
54	N	401	CDL	CA5-C11-C12-C13
46	L	701	3PE	O31-C31-C32-C33
47	9	203	PC1	O21-C21-C22-C23
46	M	504	3PE	O22-C21-C22-C23
46	Y	202	3PE	O31-C31-C32-C33

There are no ring outliers.

27 monomers are involved in 73 short contacts:

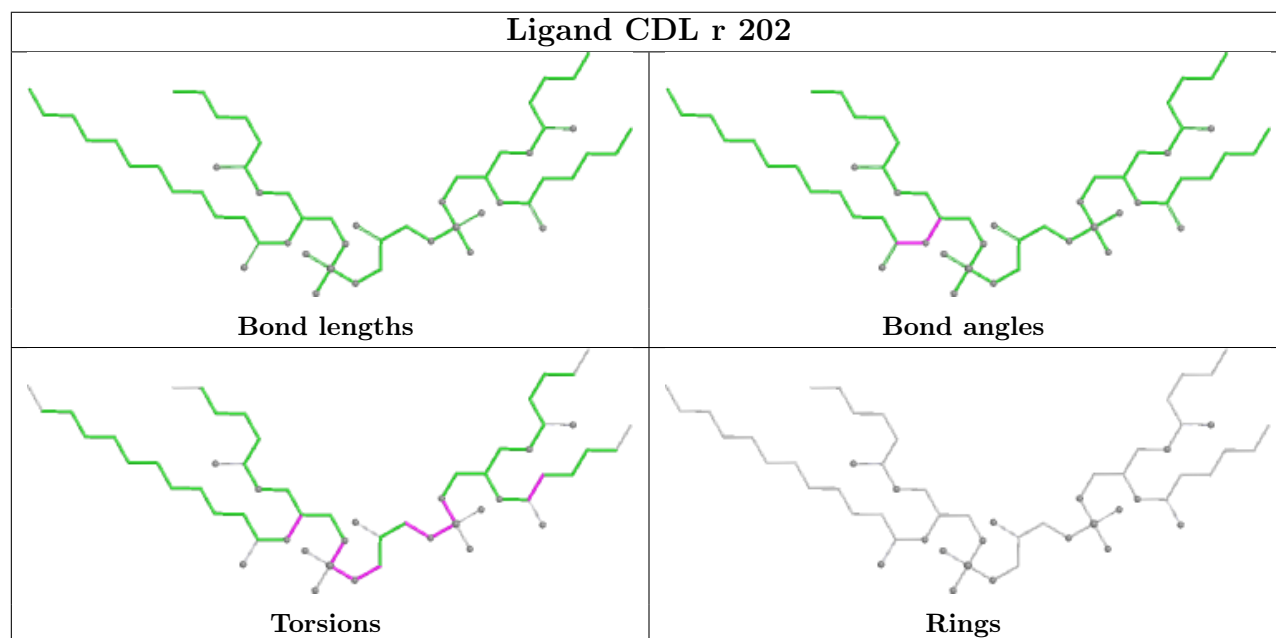
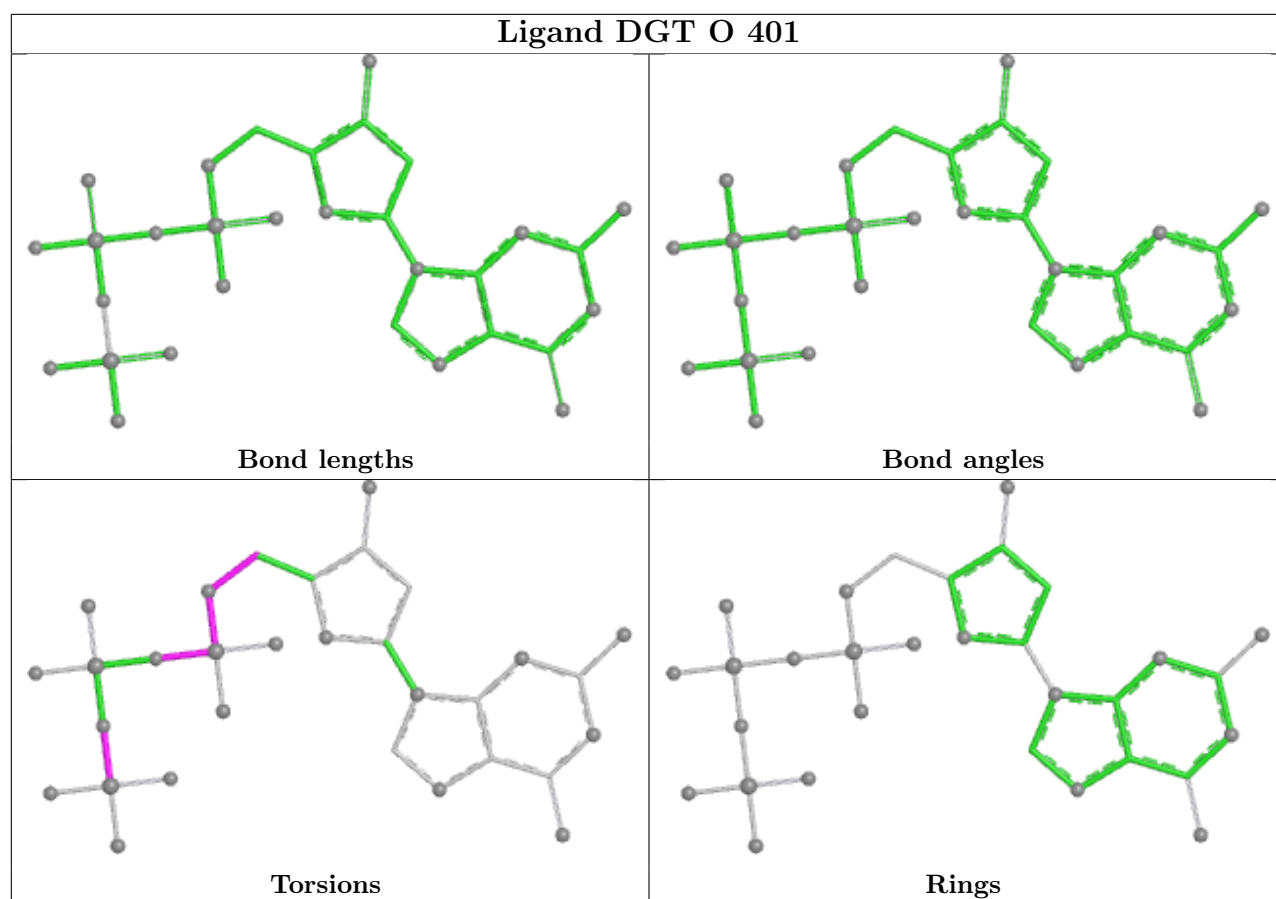
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	O	401	DGT	1	0
54	r	202	CDL	3	0
46	A	201	3PE	3	0
47	6	203	PC1	2	0
46	Y	202	3PE	3	0
49	1	501	FMN	3	0
46	6	202	3PE	2	0
53	n	201	ZMP	4	0
47	9	204	PC1	6	0
46	L	701	3PE	3	0
46	L	703	3PE	2	0
54	N	401	CDL	7	0
54	L	702	CDL	1	0
51	P	501	NDP	2	0
46	Y	201	3PE	1	0

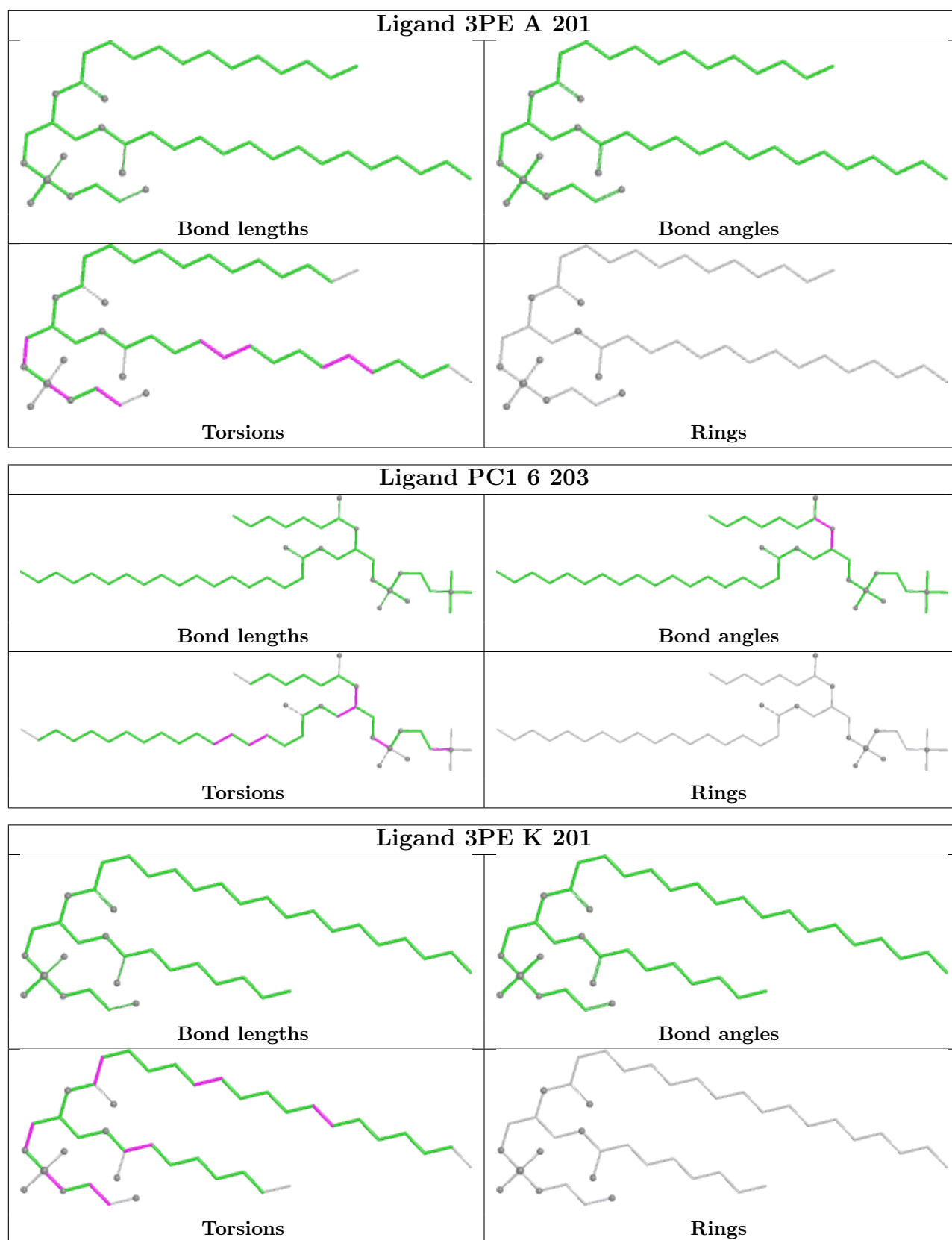
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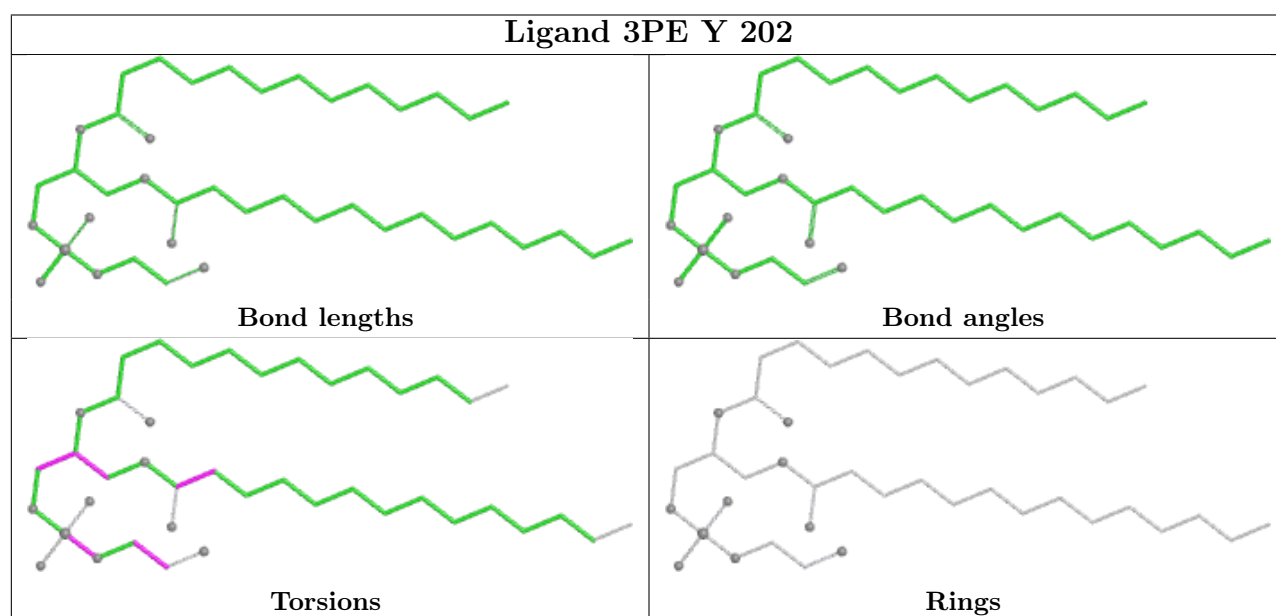
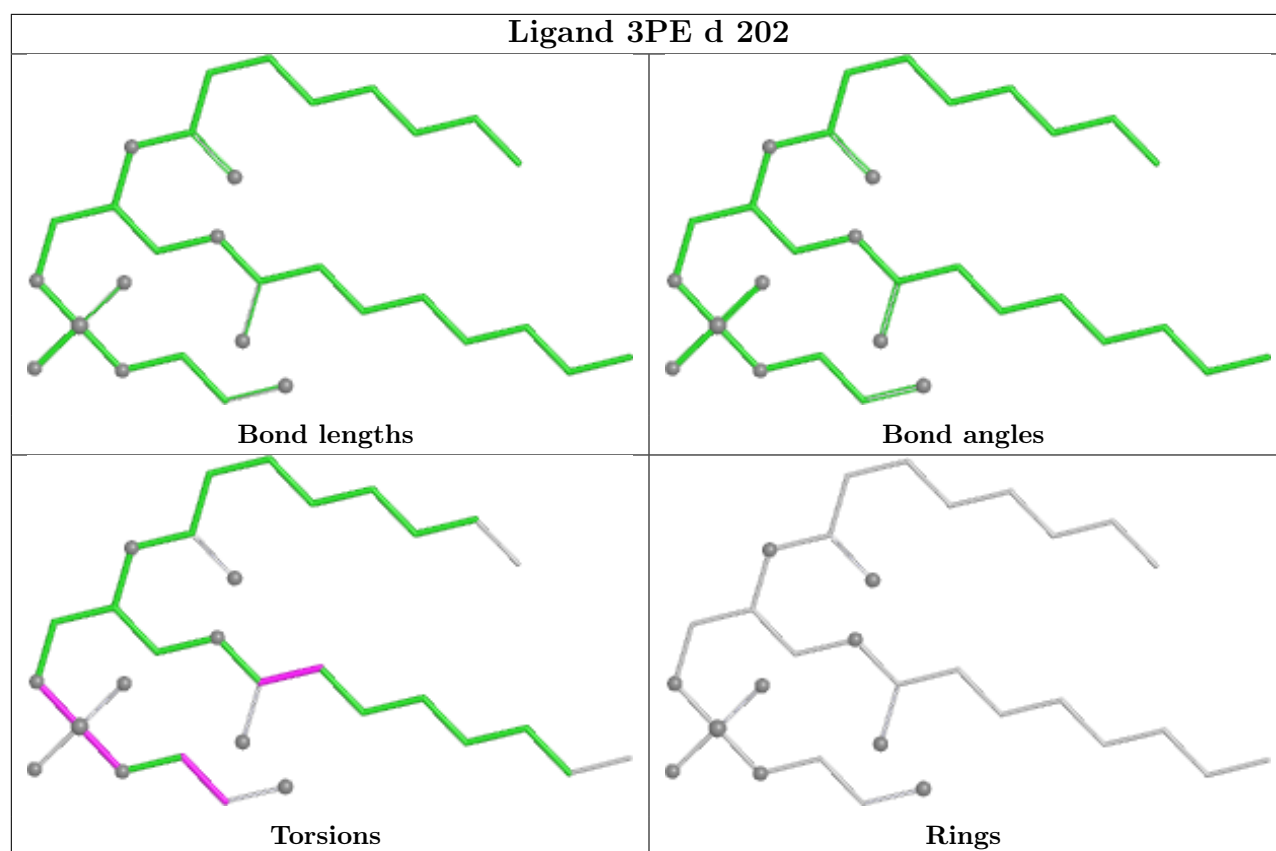
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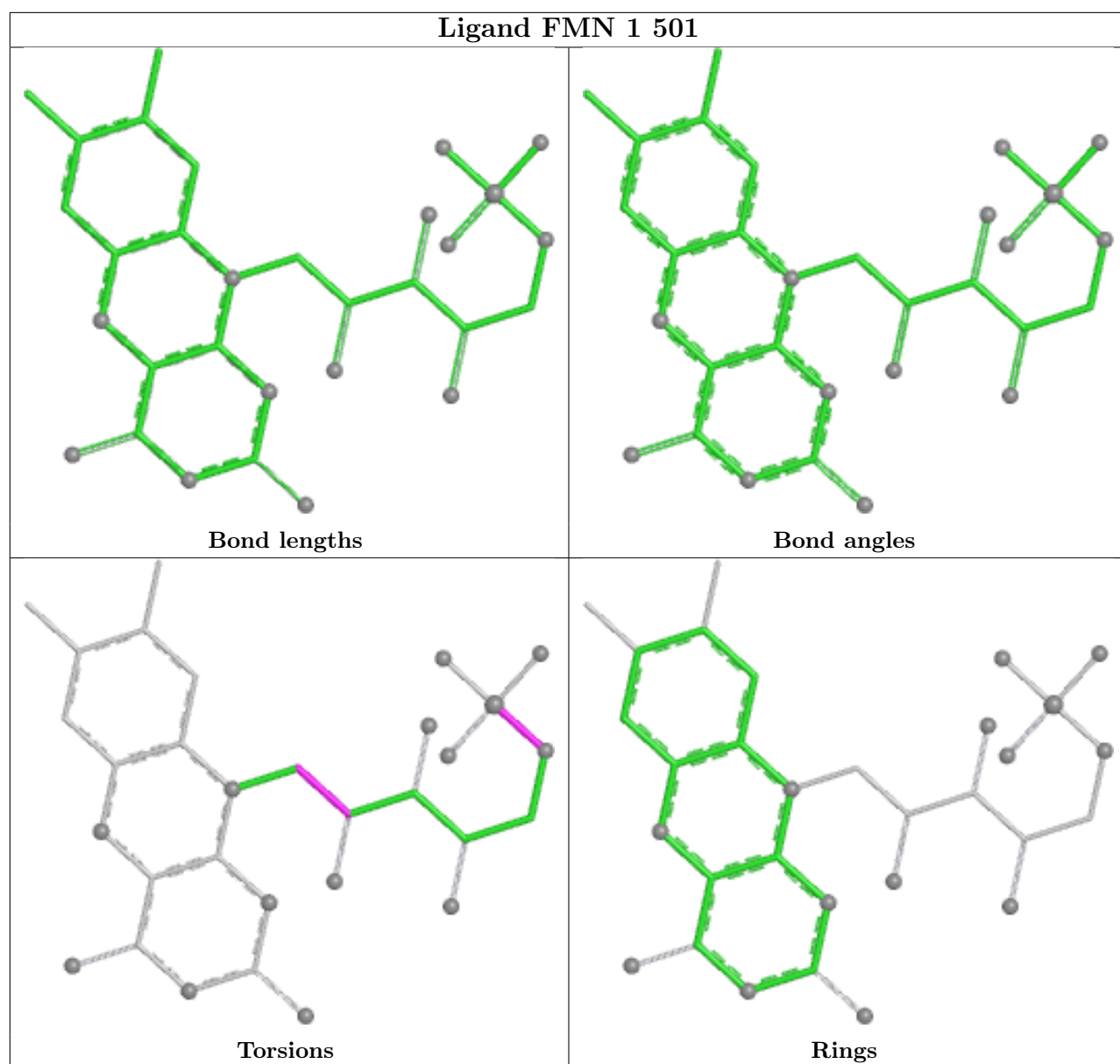
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	N	402	3PE	2	0
45	9	201	SF4	1	0
53	W	201	ZMP	3	0
46	M	502	3PE	5	0
46	H	401	3PE	2	0
46	i	201	3PE	2	0
46	m	202	3PE	2	0
54	m	201	CDL	1	0
54	h	201	CDL	7	0
54	d	201	CDL	6	0
47	M	501	PC1	5	0
47	9	203	PC1	1	0

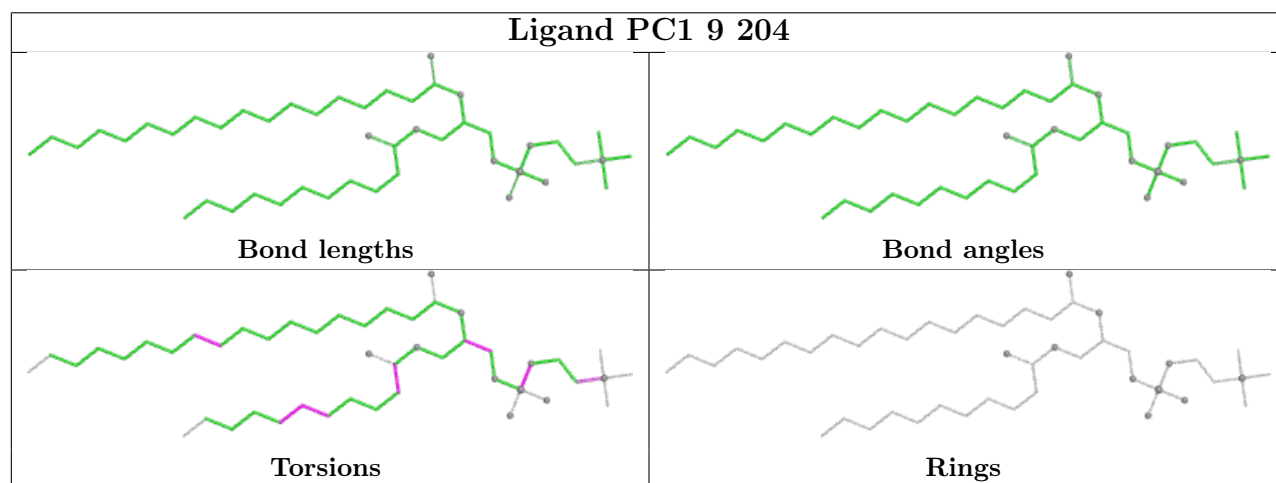
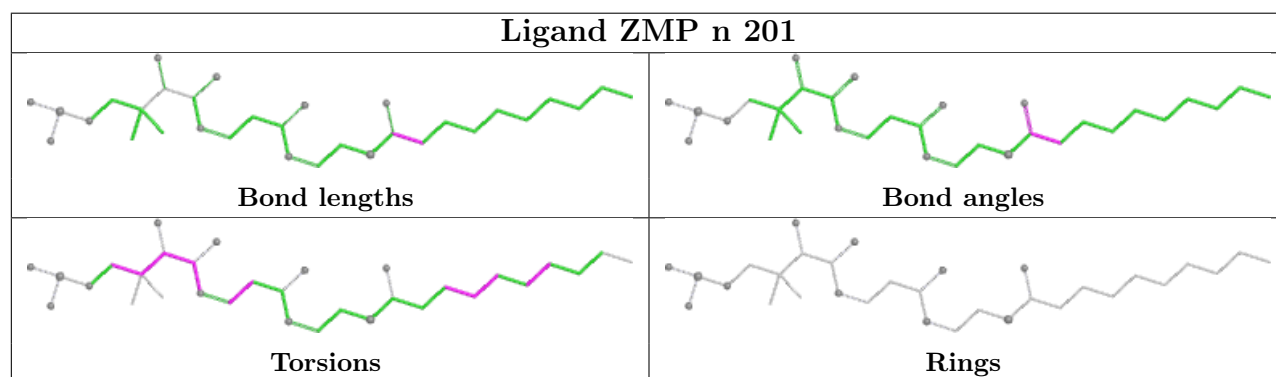
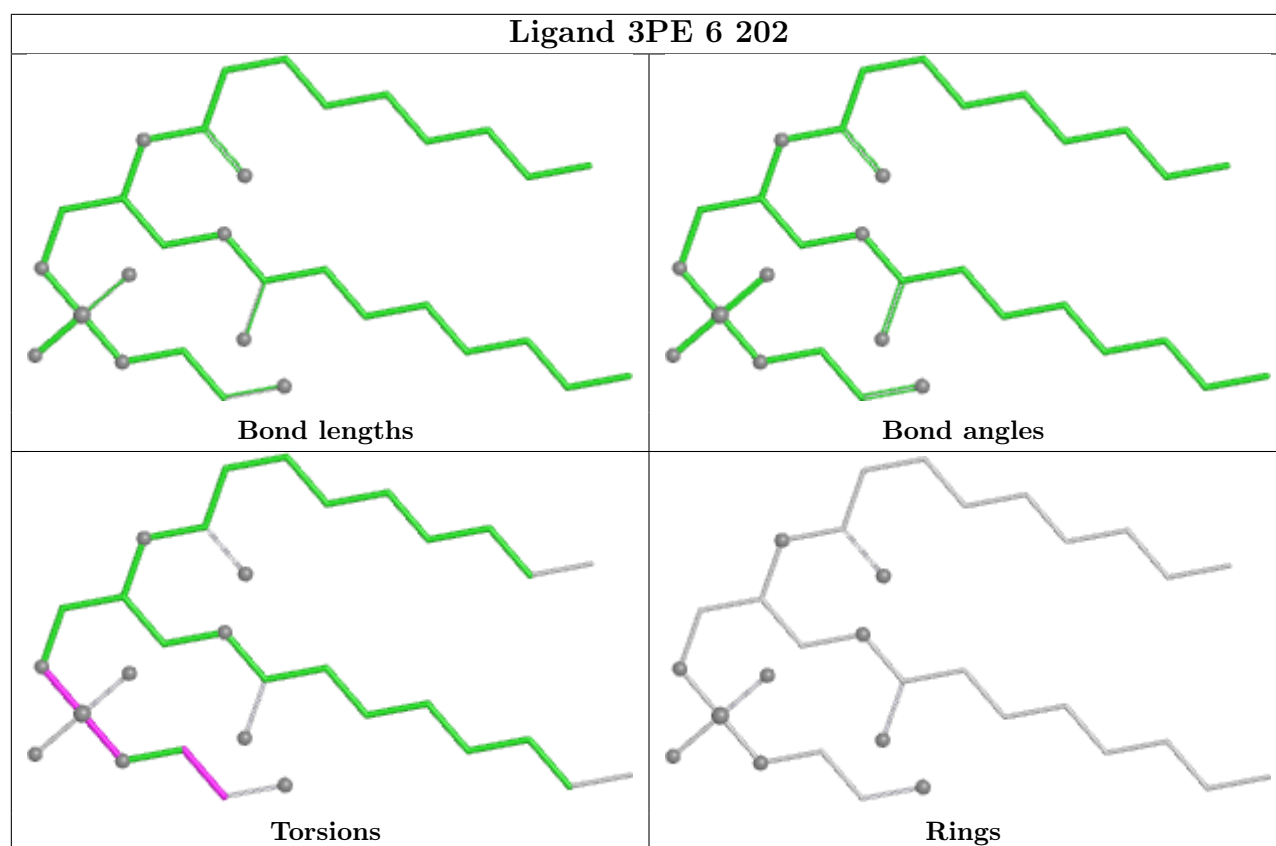
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

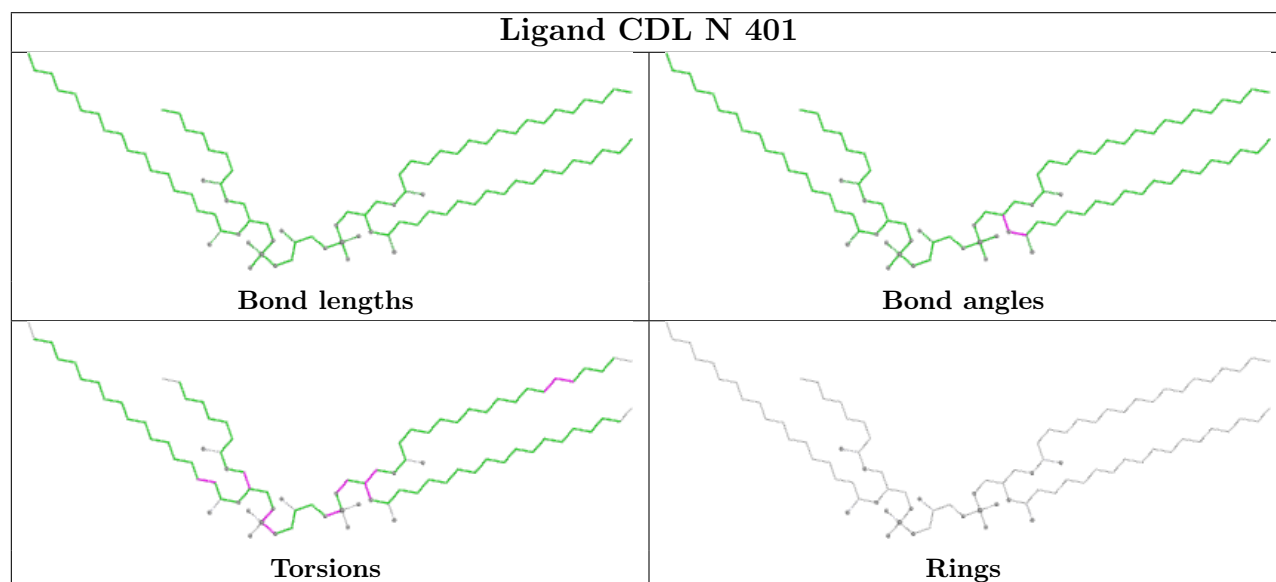
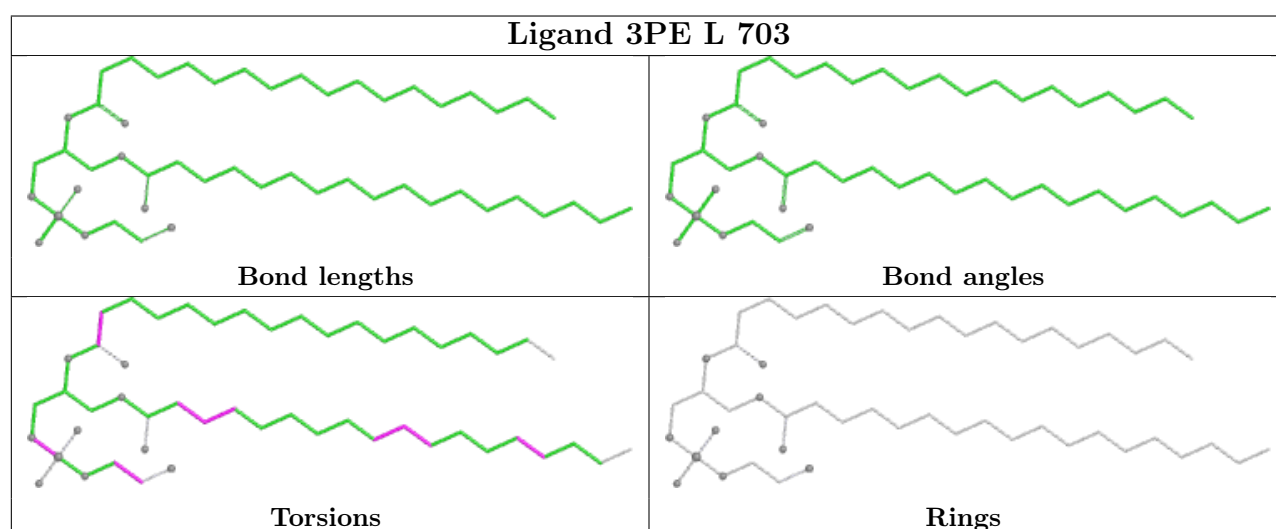
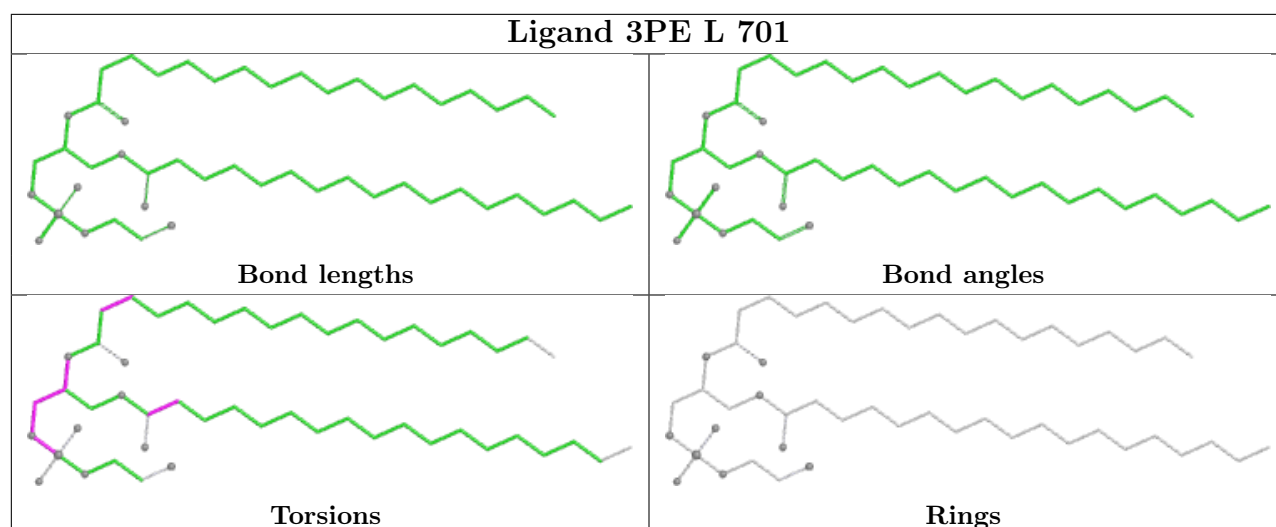


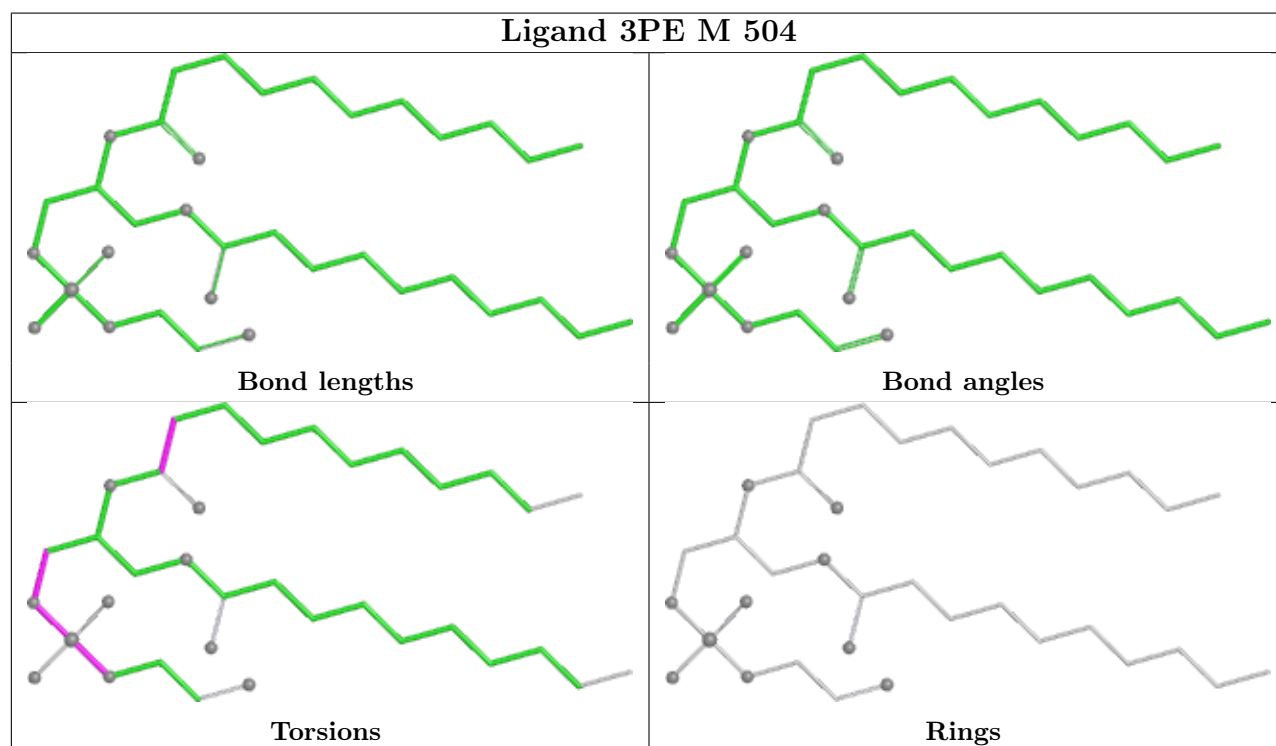
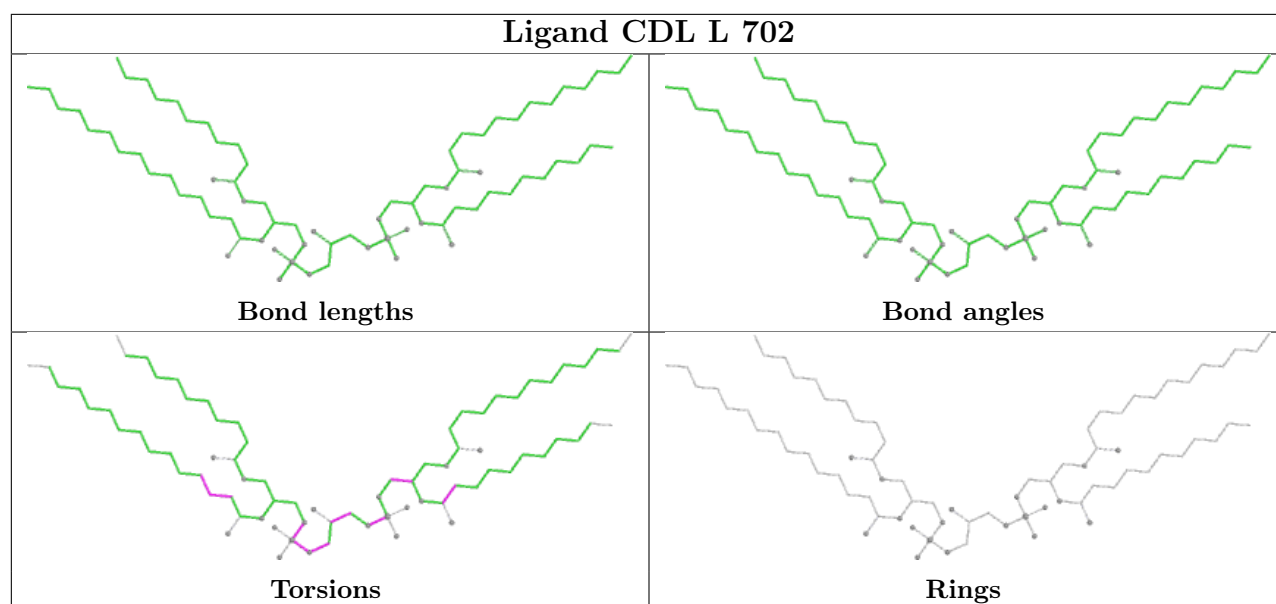


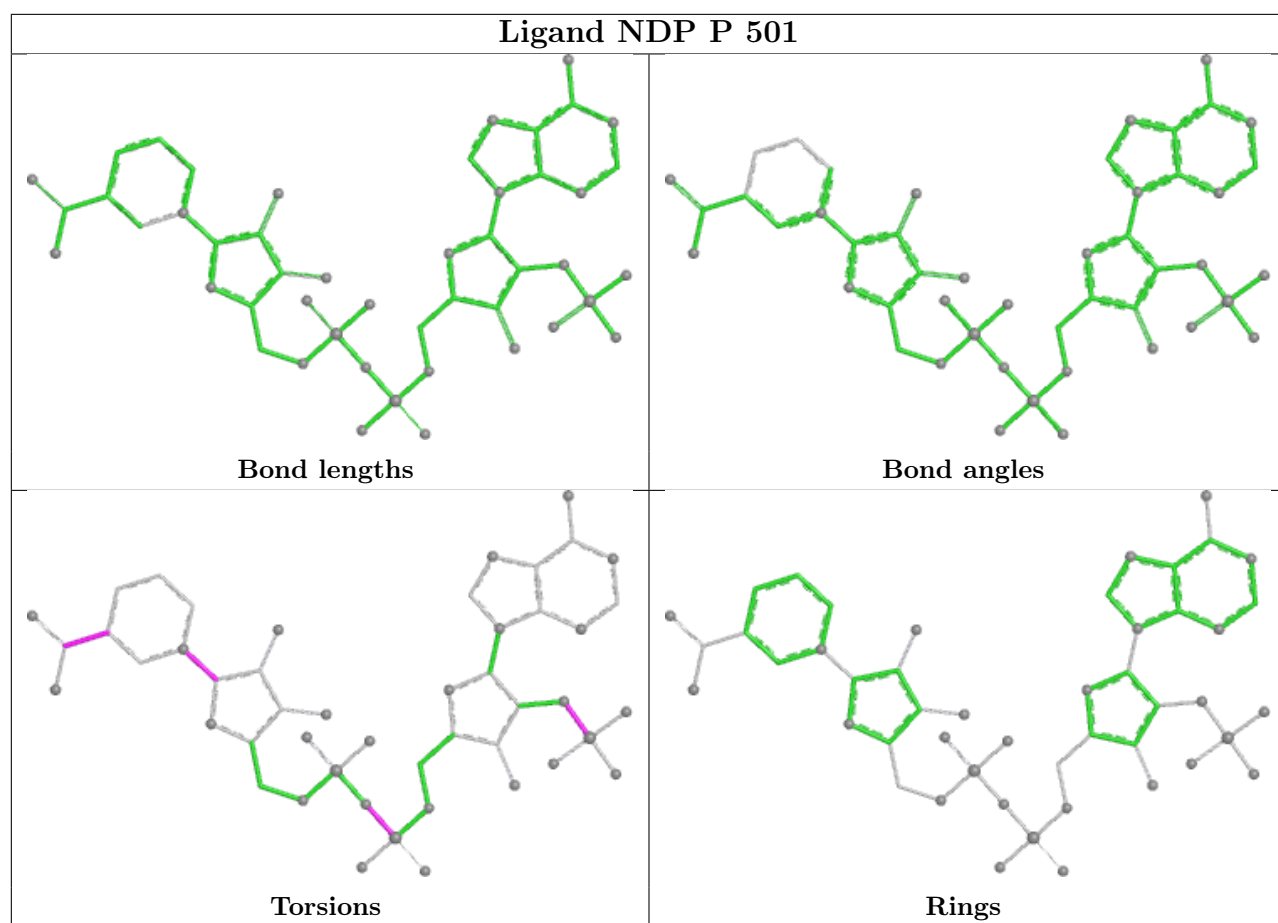


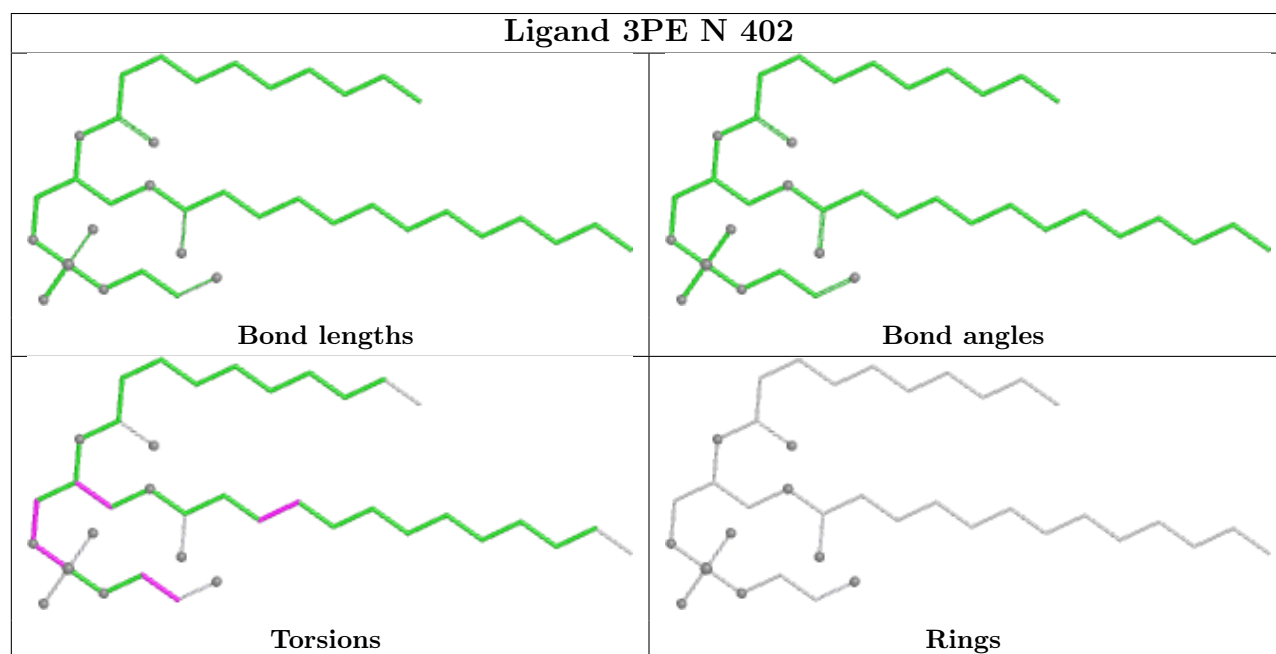
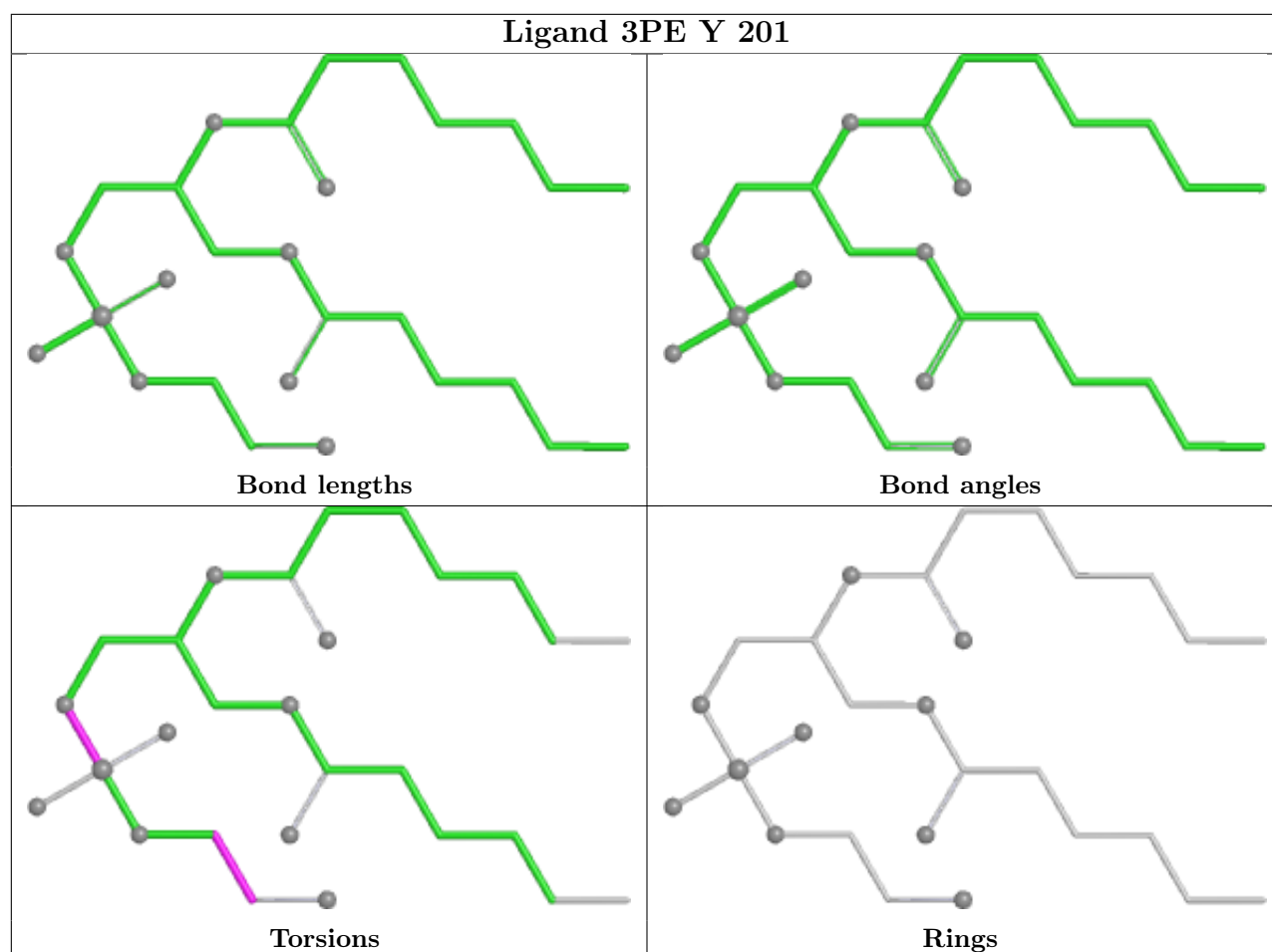


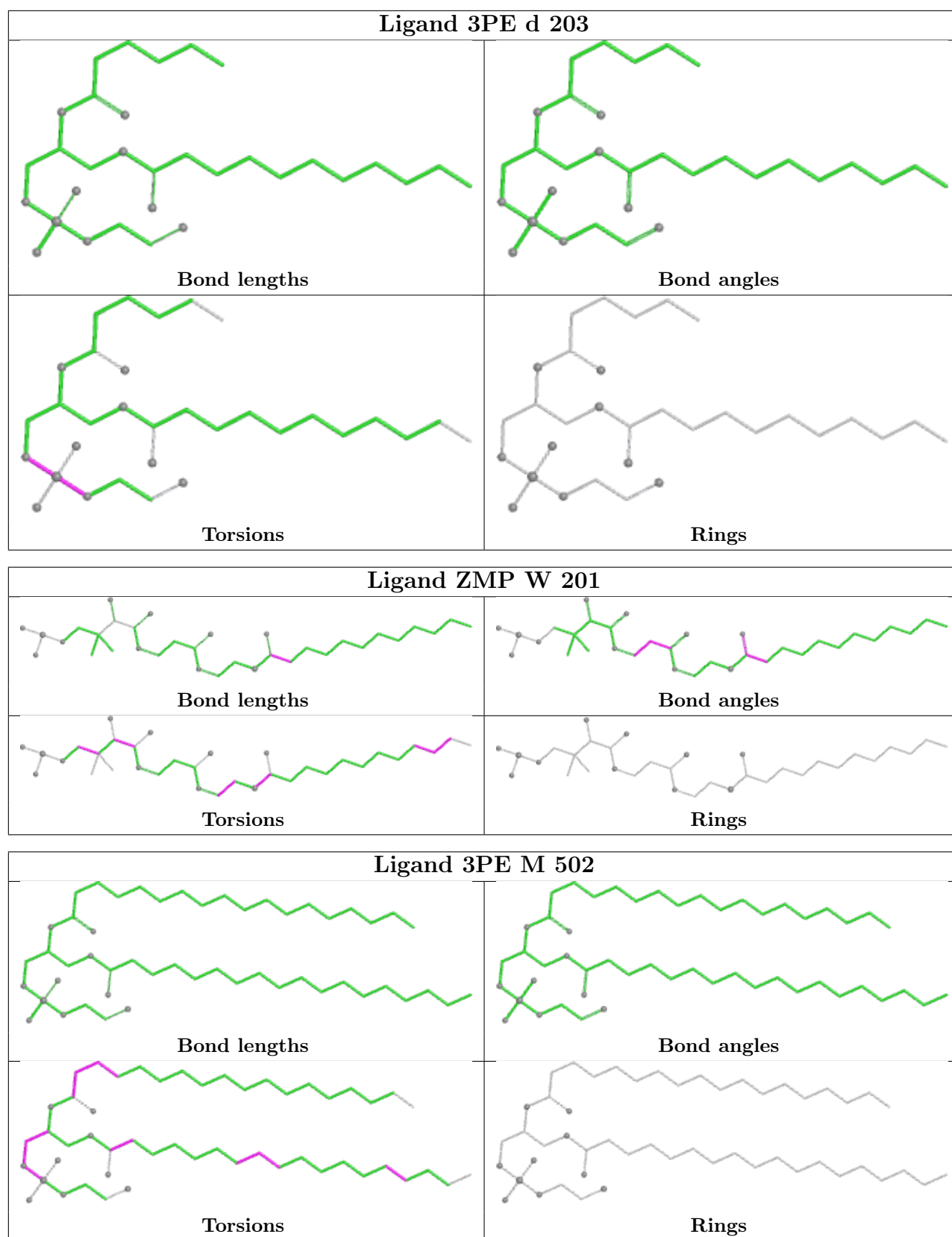


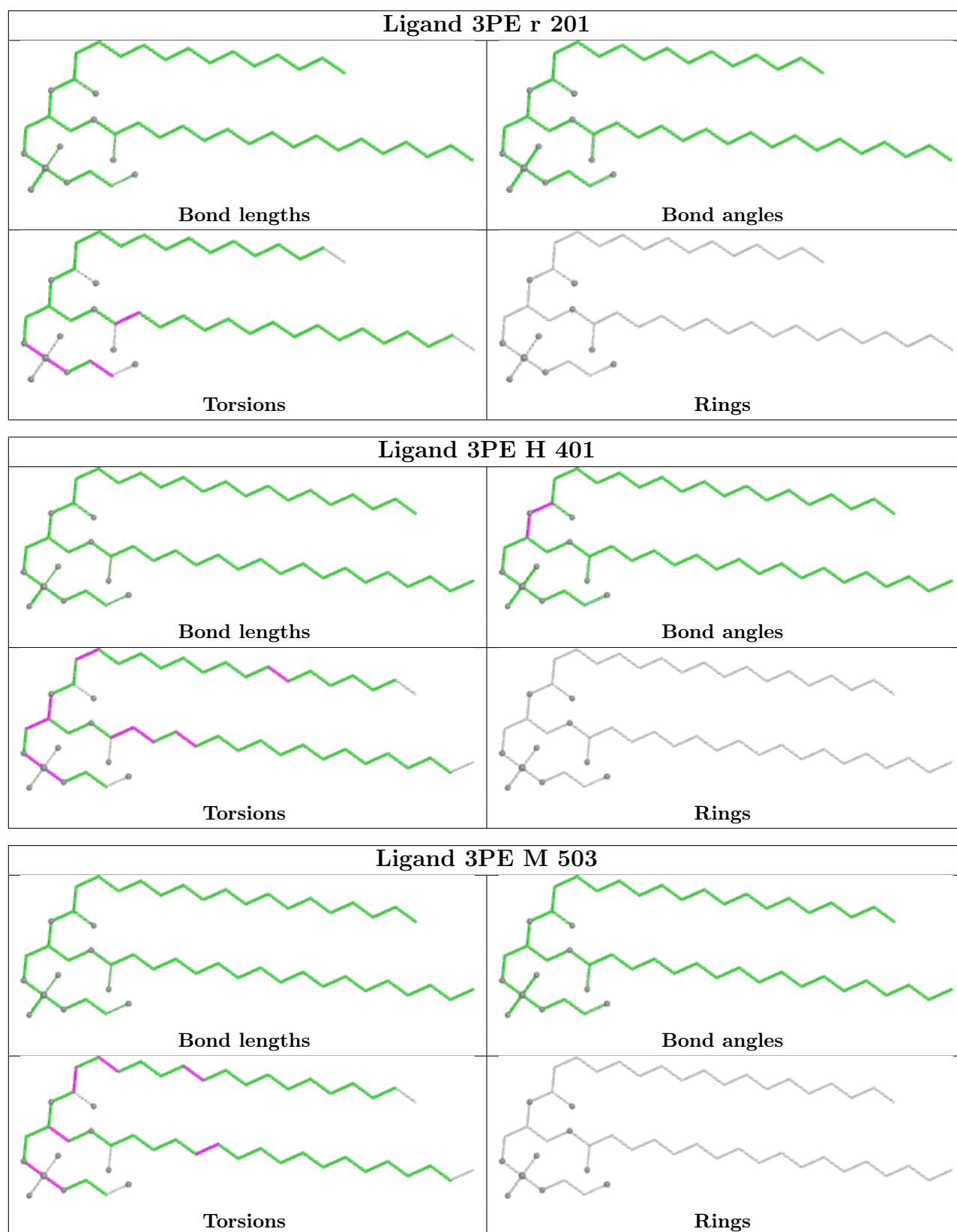


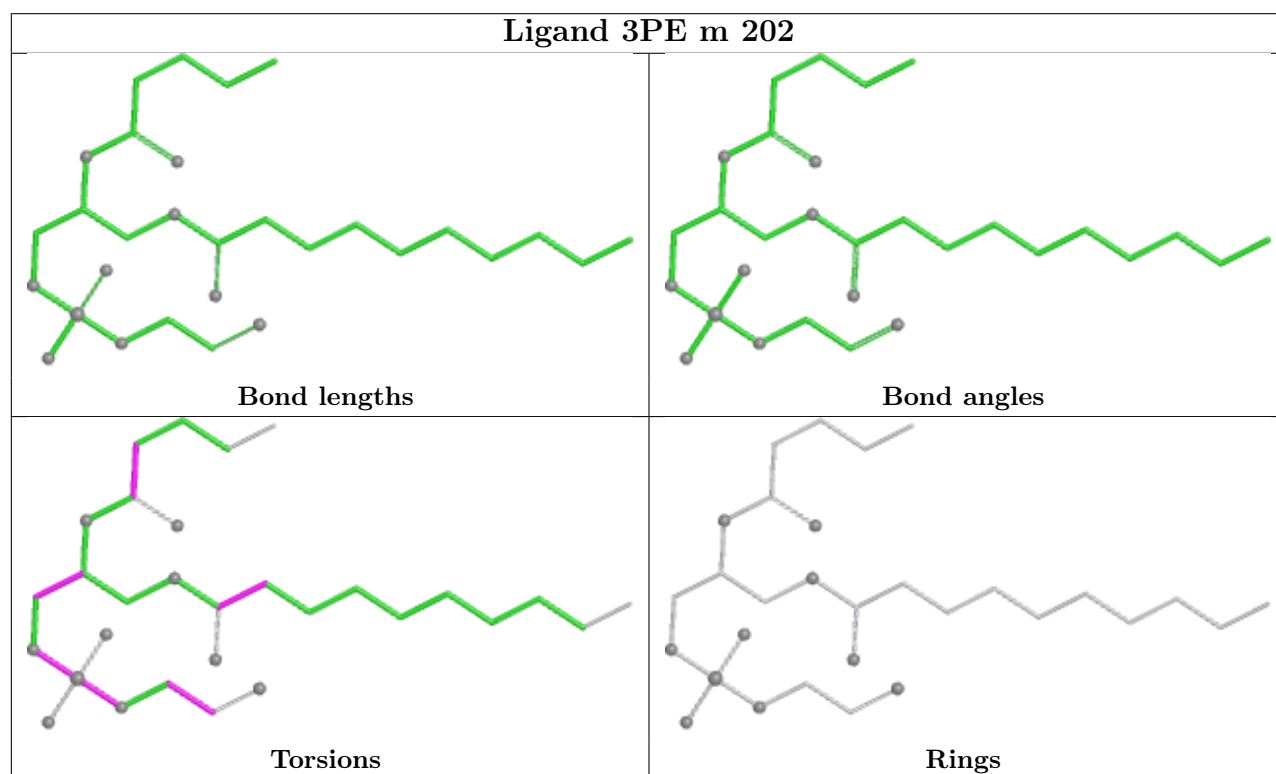
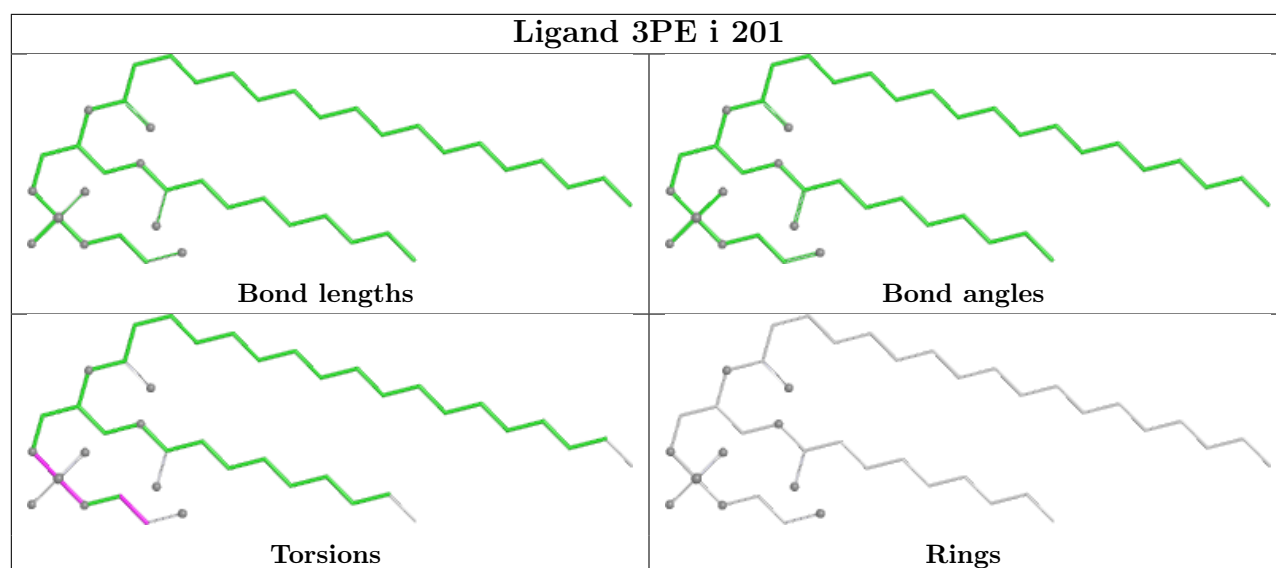


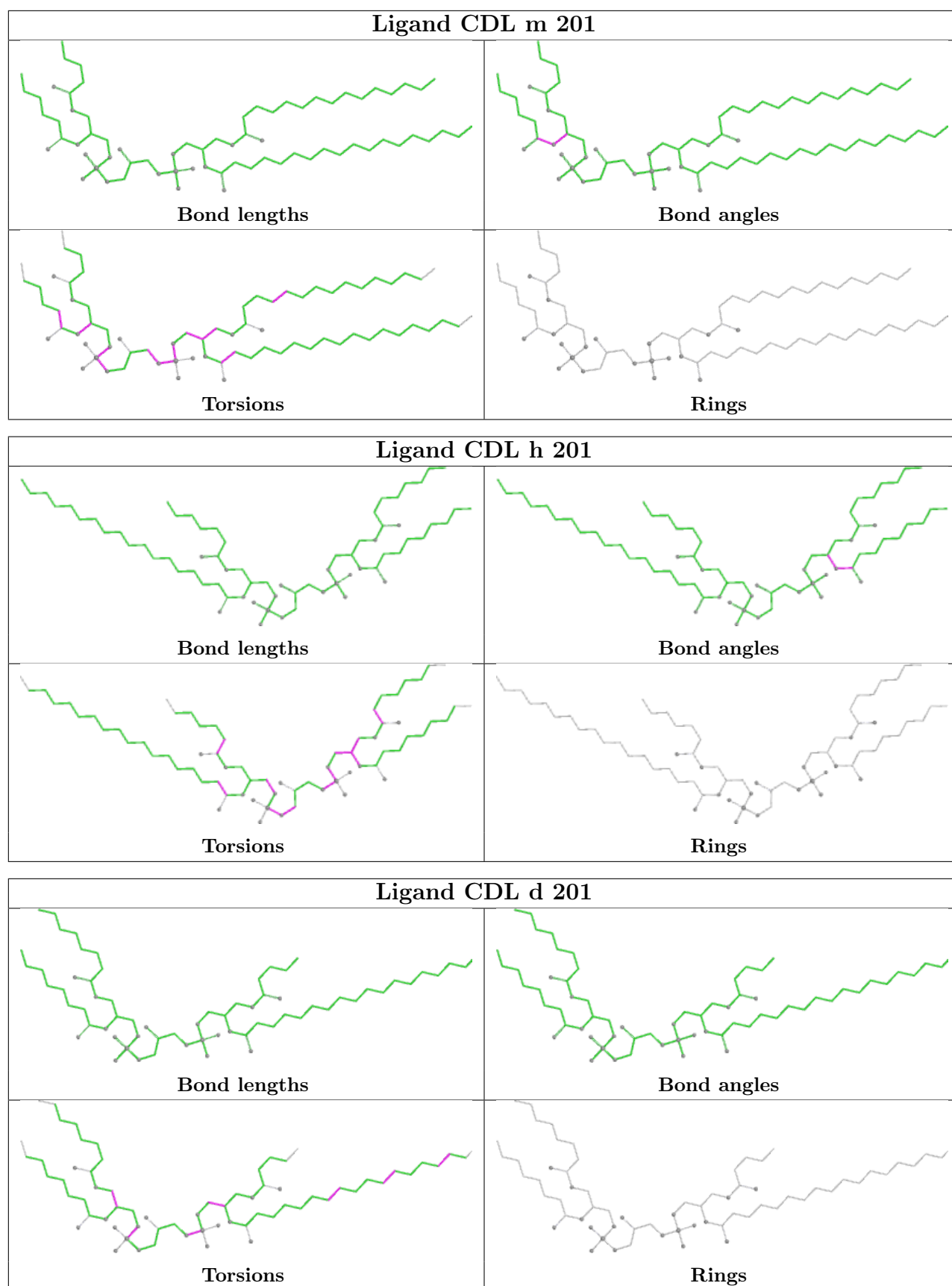


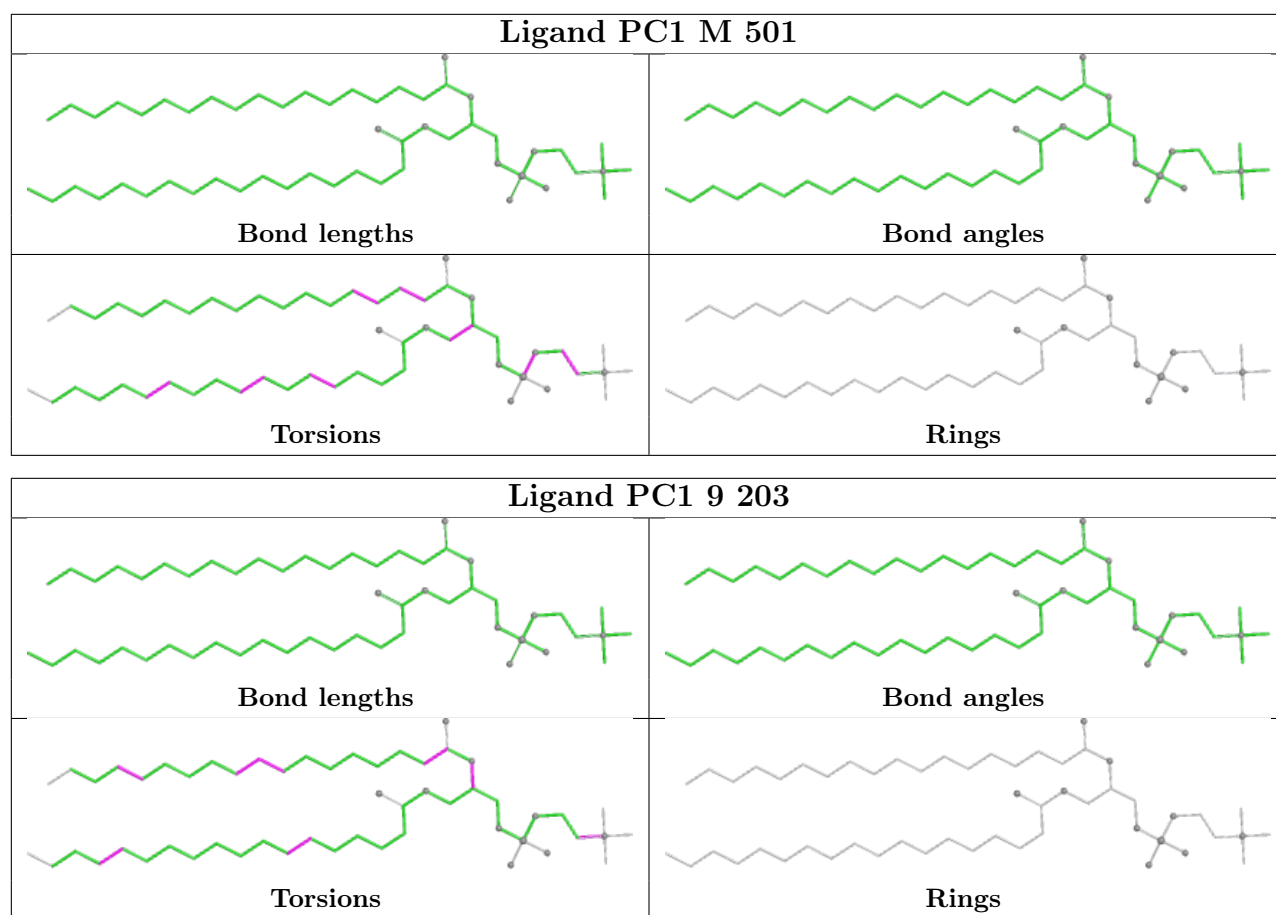












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

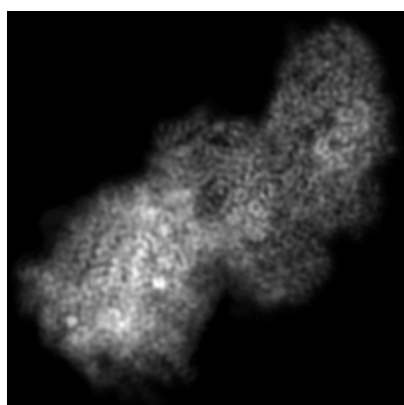
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19146. These allow visual inspection of the internal detail of the map and identification of artifacts.

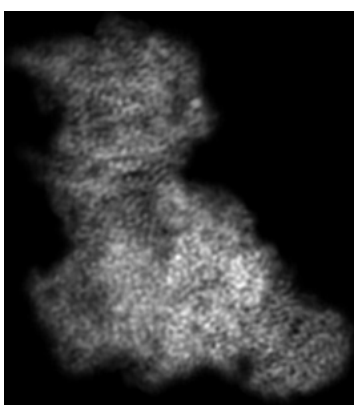
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

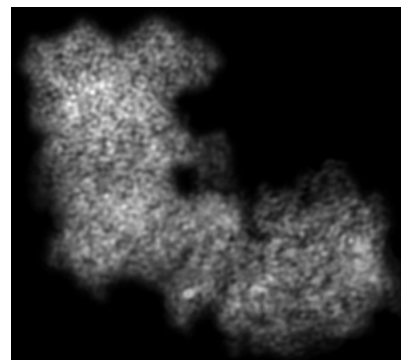
6.1.1 Primary map



X



Y

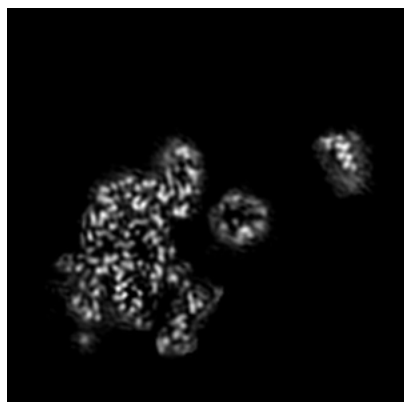


Z

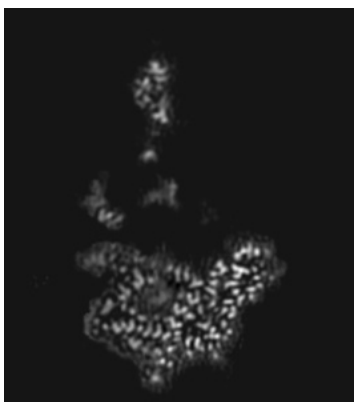
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

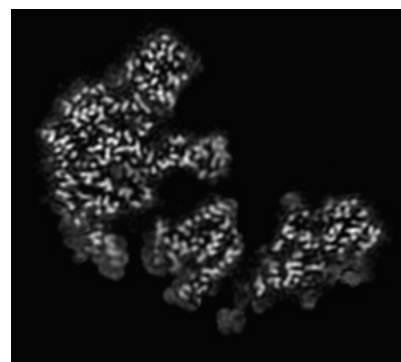
6.2.1 Primary map



X Index: 109



Y Index: 98

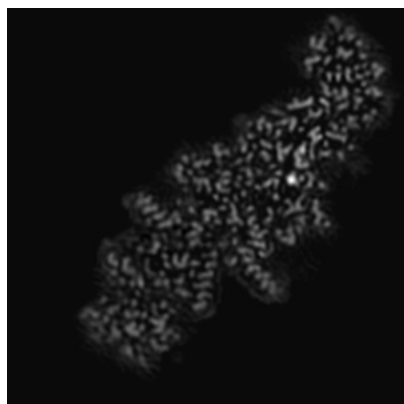


Z Index: 98

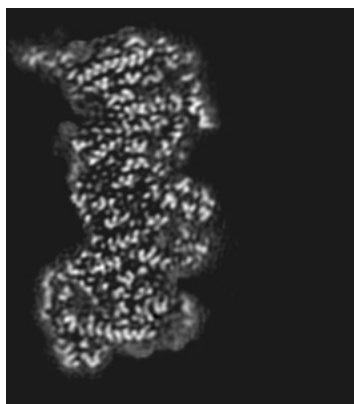
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

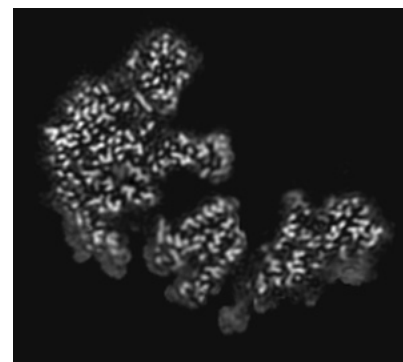
6.3.1 Primary map



X Index: 45



Y Index: 63



Z Index: 97

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

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

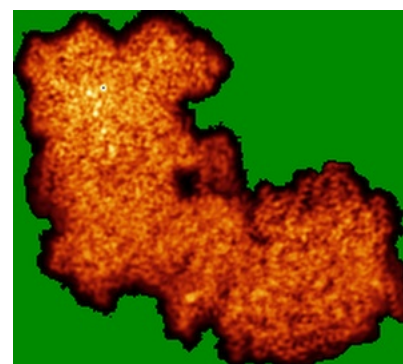
6.4.1 Primary map



X



Y

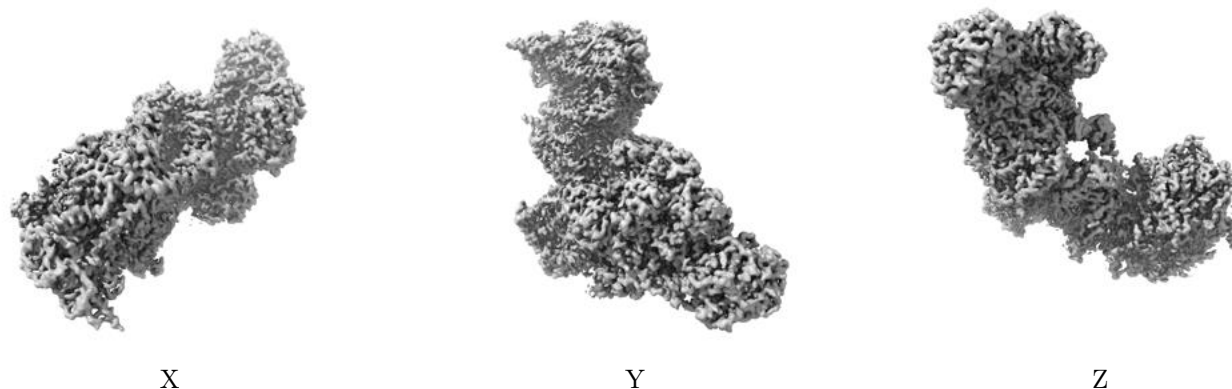


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

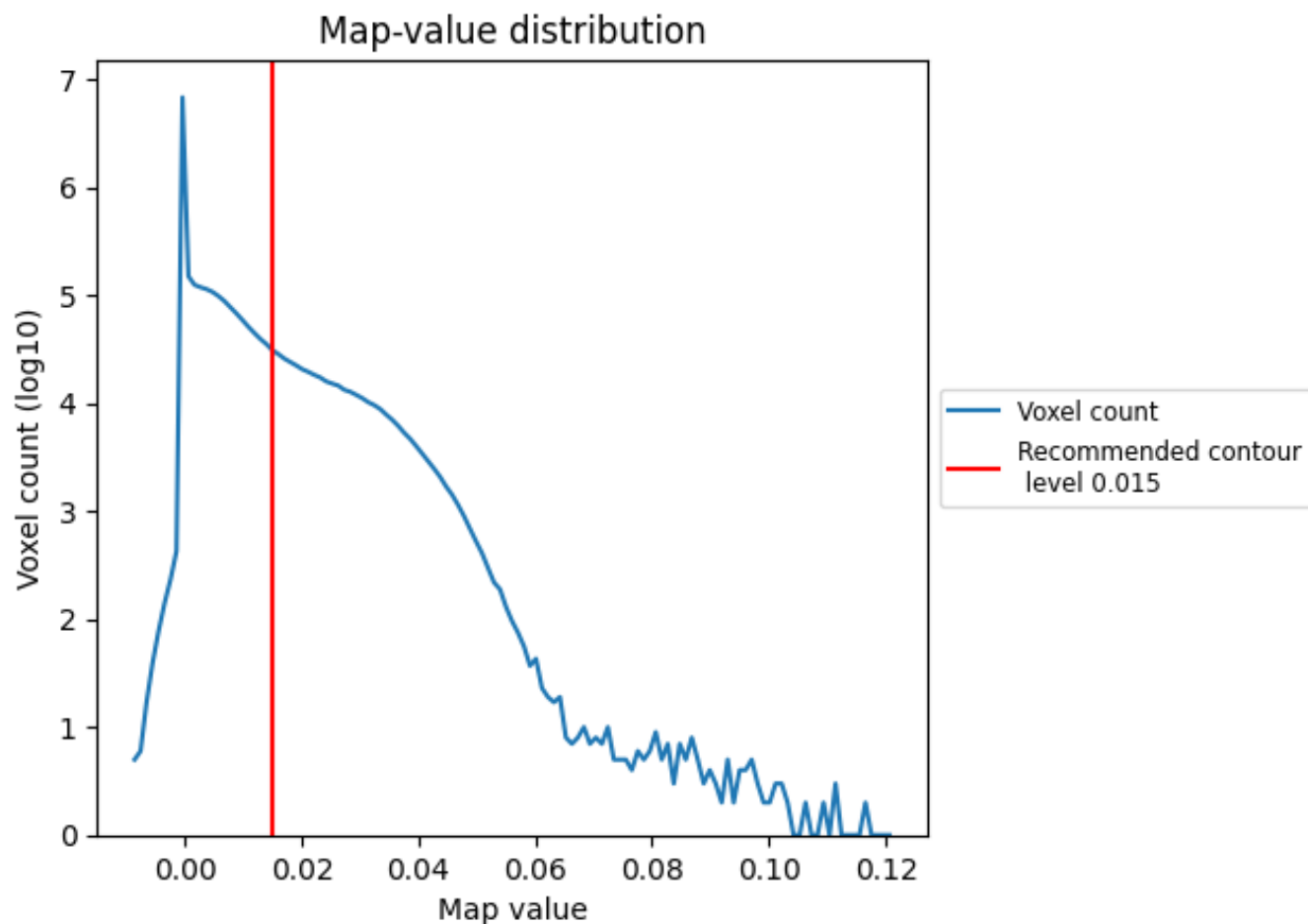
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

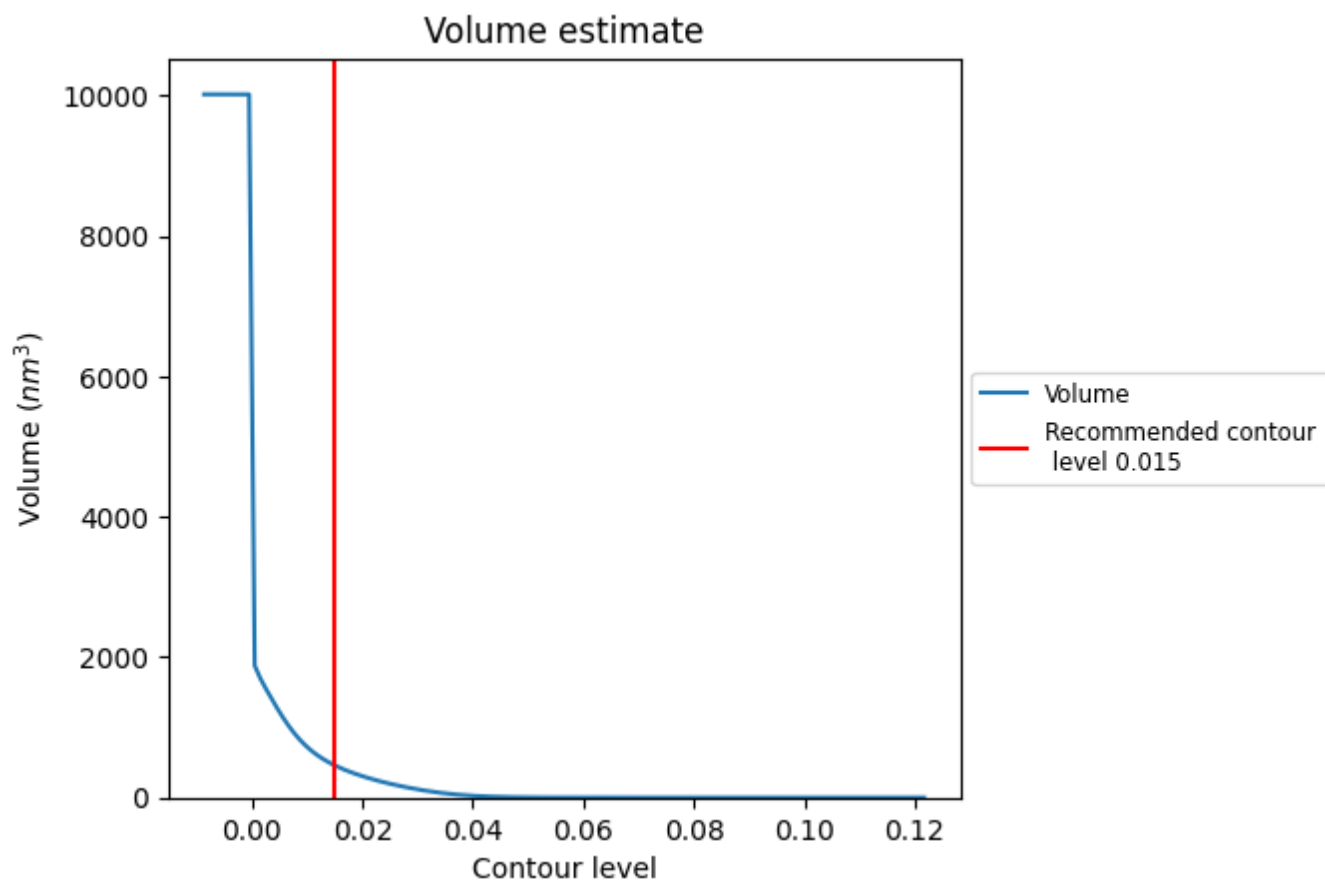
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 460 nm³; this corresponds to an approximate mass of 416 kDa.

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

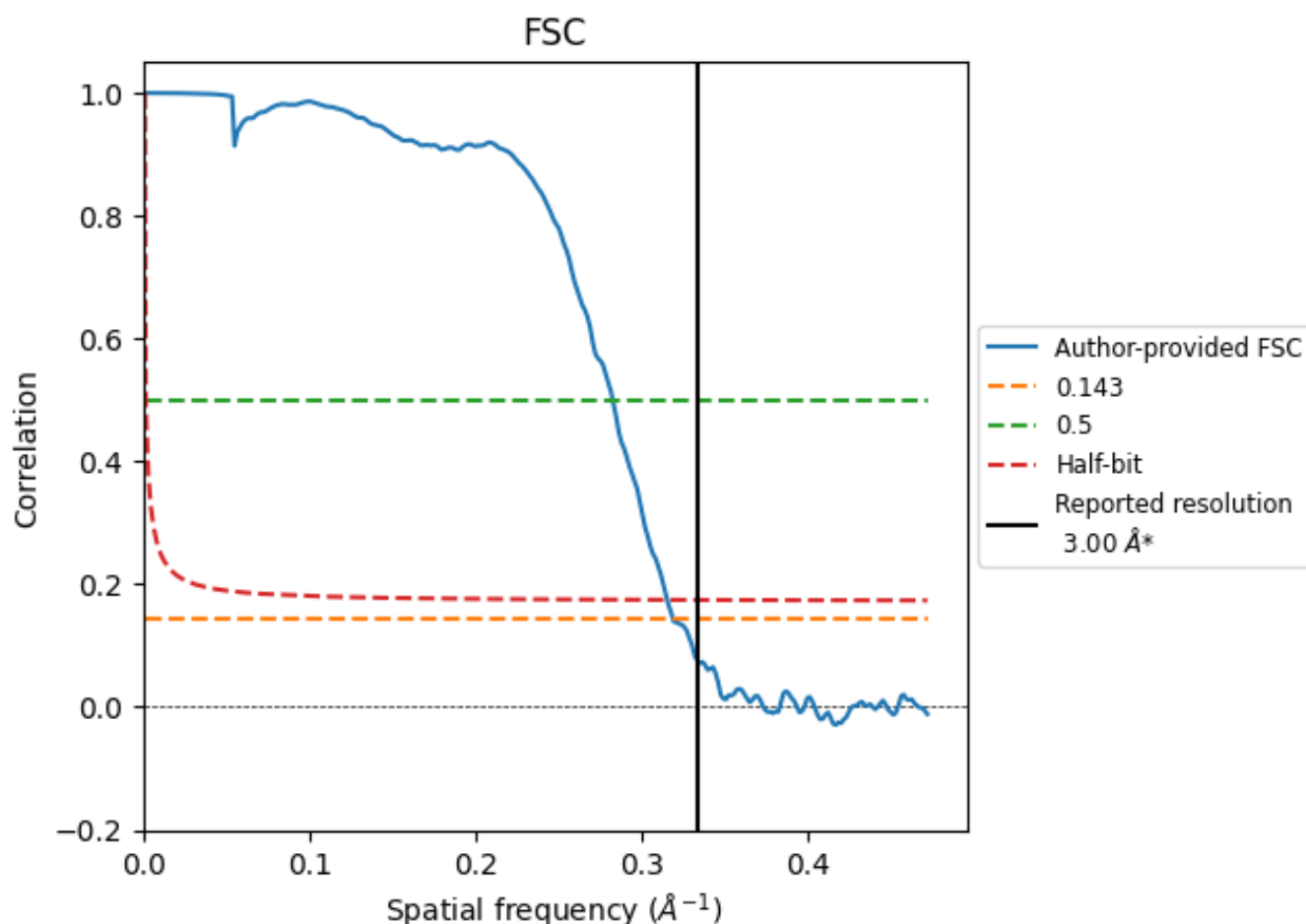
7.3 Rotationally averaged power spectrum [i](#)

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

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

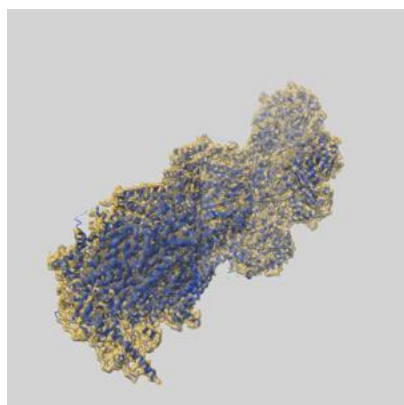
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.14	3.54	3.17
Unmasked-calculated*	-	-	-

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

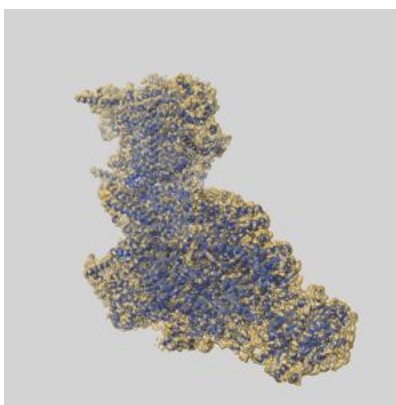
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19146 and PDB model 8RGQ. Per-residue inclusion information can be found in section [3](#) on page [19](#).

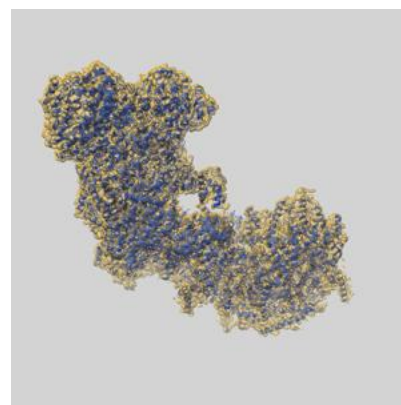
9.1 Map-model overlay [i](#)



X



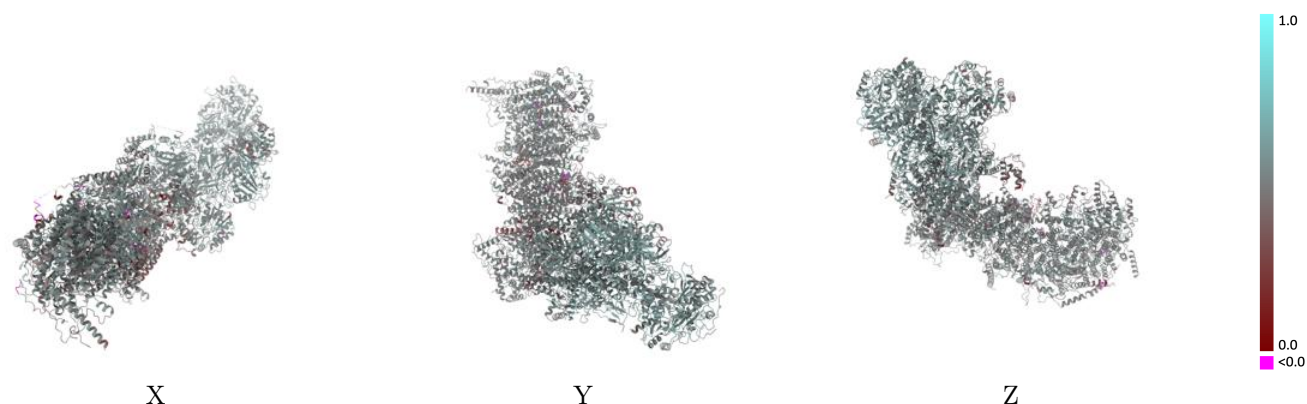
Y



Z

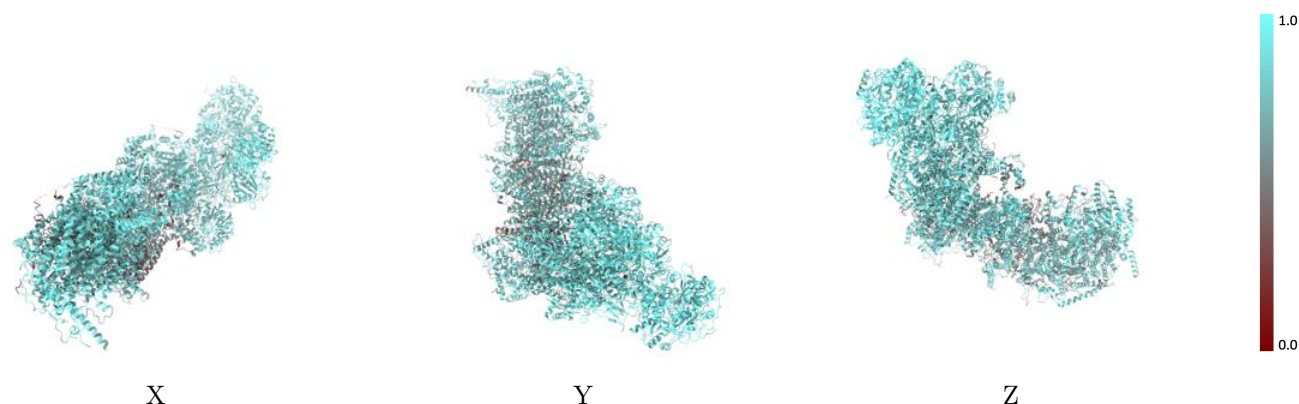
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



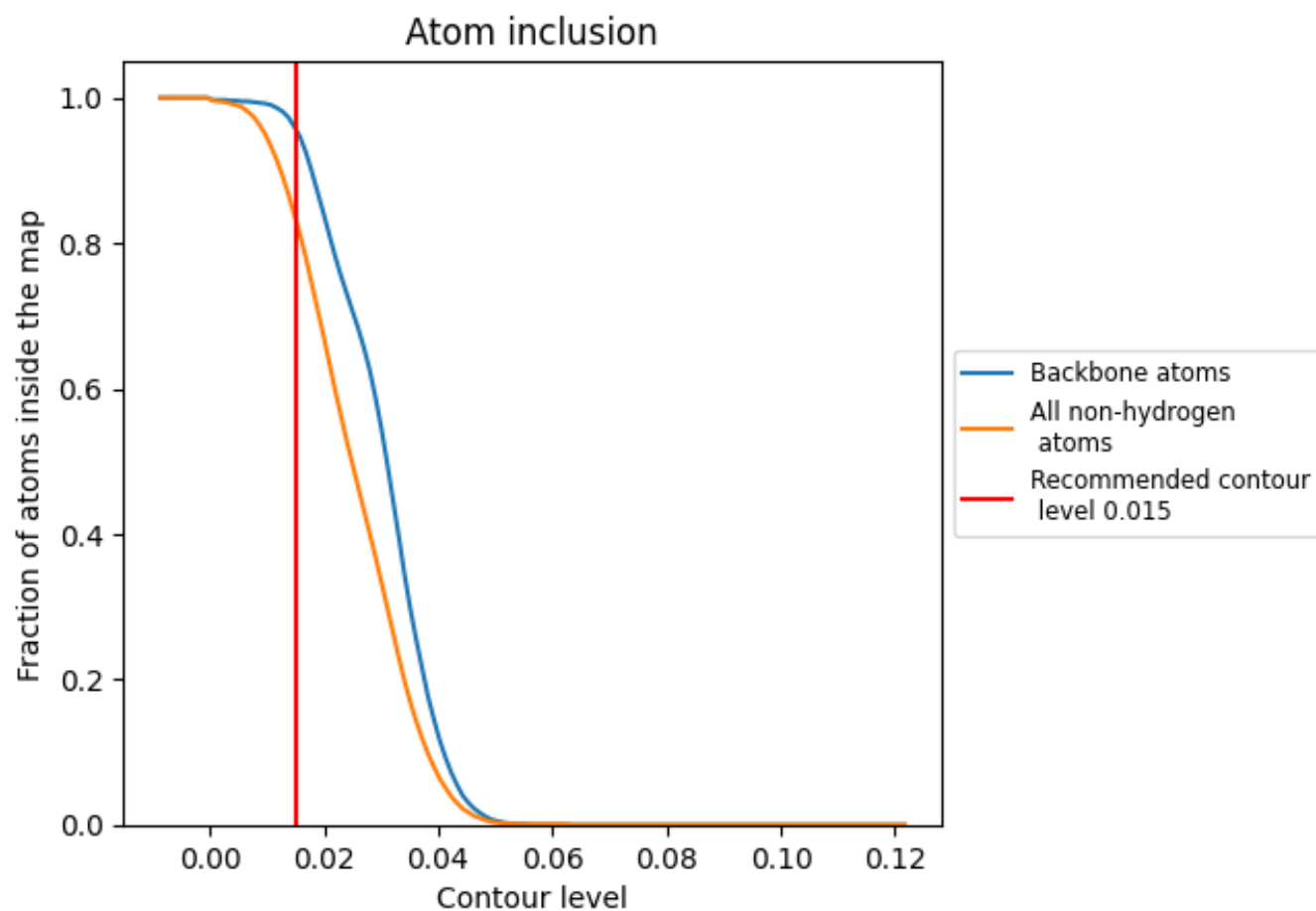
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 84% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8350	 0.5150
1	 0.9300	 0.5540
2	 0.9220	 0.5480
3	 0.9120	 0.5550
6	 0.8500	 0.5210
7	 0.9190	 0.5580
9	 0.8890	 0.5510
A	 0.7160	 0.4950
C	 0.9140	 0.5670
D	 0.8470	 0.5240
H	 0.7960	 0.4970
J	 0.6600	 0.4530
K	 0.7030	 0.4900
L	 0.7970	 0.5080
M	 0.7900	 0.5170
N	 0.7750	 0.5120
O	 0.8510	 0.5030
P	 0.8070	 0.5000
Q	 0.8800	 0.5670
S	 0.8790	 0.4970
T	 0.7180	 0.3940
U	 0.8400	 0.5000
V	 0.8740	 0.5270
W	 0.8870	 0.5350
X	 0.8630	 0.5020
Y	 0.7090	 0.4690
Z	 0.8650	 0.5080
a	 0.8450	 0.5090
b	 0.8310	 0.4760
c	 0.7930	 0.4890
d	 0.7680	 0.5080
e	 0.8120	 0.5070
f	 0.7700	 0.4850
g	 0.7820	 0.4840
h	 0.8430	 0.5010



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Chain	Atom inclusion	Q-score
i	 0.7480	 0.4570
j	 0.8360	 0.4780
k	 0.8410	 0.4970
l	 0.8500	 0.5170
m	 0.7190	 0.4480
n	 0.8550	 0.5090
o	 0.8330	 0.4820
p	 0.8710	 0.5110
q	 0.9170	 0.5540
r	 0.8510	 0.5470
s	 0.8920	 0.5290