



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:31 PM UTC

PDB ID : 7ZDH / pdb_00007zdh
EMDB ID : EMD-14648
Title : Complex I from Ovis aries at pH7.4, Closed state
Authors : Sazanov, L.; Petrova, O.
Deposited on : 2022-03-29
Resolution : 3.46 Å (reported)
Based on initial model : 6ZKC

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:

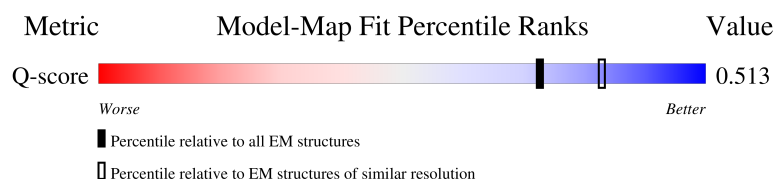
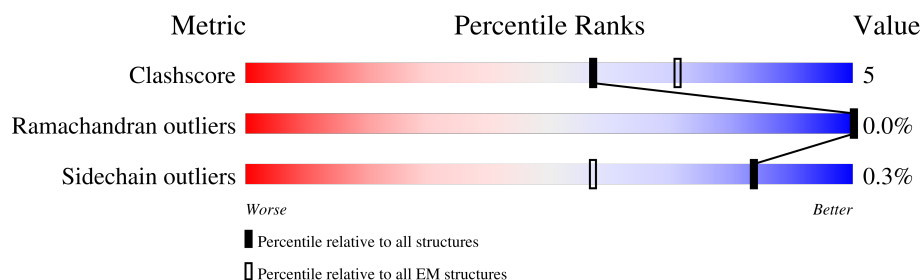
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.46 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.



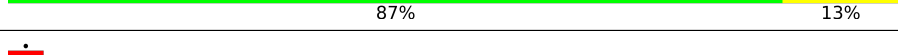
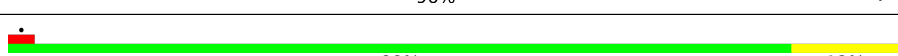
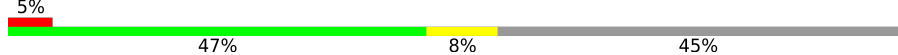
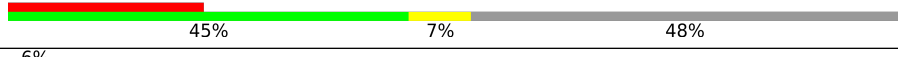
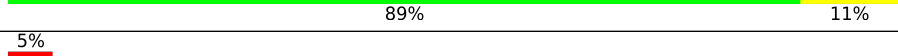
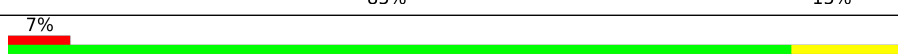
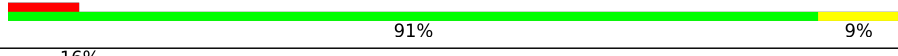
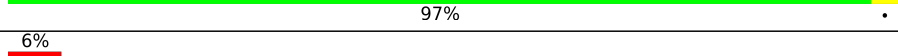
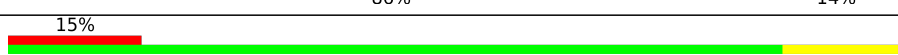
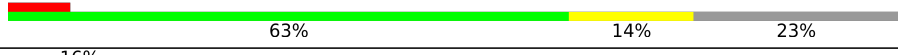
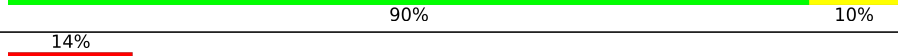
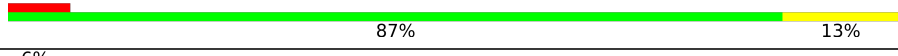
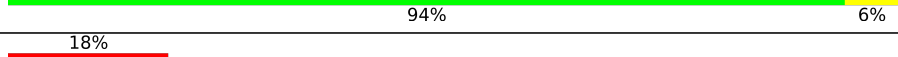
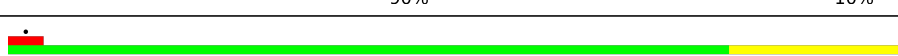
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13788 (2.96 - 3.96)

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

Mol	Chain	Length	Quality of chain
1	A	115	10% 88% 12%
2	H	318	84% 16%
3	J	175	82% 18%
4	K	98	74% 26%

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Mol	Chain	Length	Quality of chain
5	L	606	
6	M	459	
7	N	347	
8	V	140	
9	W	139	
10	X	157	
10	j	157	
11	Y	171	
12	Z	171	
13	k	320	
14	l	105	
15	m	80	
16	n	79	
17	o	120	
18	p	128	
19	q	139	
20	r	128	
21	s	122	
22	t	177	
23	u	65	
24	v	155	
25	w	101	
26	x	49	
27	y	50	
28	z	70	

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Mol	Chain	Length	Quality of chain
29	1	430	
30	2	213	
31	3	688	
32	4	430	
33	5	208	
34	6	156	
35	9	217	
36	a	44	
37	b	95	
38	c	126	
39	d	340	
40	e	86	
41	f	113	
42	g	114	
43	h	114	
44	i	145	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 67219 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	S	0	0
			922	621	133	161	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	318	Total	C	N	O	S	0	0
			2528	1704	384	421	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	175	Total	C	N	O	S	0	0
			1344	904	192	235	13		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	606	Total	C	N	O	S	0	0
			4807	3188	746	829	44		

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

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

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

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

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

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

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 10 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	87	Total	C	N	O	S	0	0
			701	451	103	142	5		
10	j	82	Total	C	N	O	S	0	0
			660	425	98	132	5		

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

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

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

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

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

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

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

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

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

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

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

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

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

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

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

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

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

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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

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

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

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

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

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

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

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

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

- Molecule 28 is a protein called Complex I-MWFE.

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

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1	430	Total	C	N	O	S	0	0
			3312	2086	593	613	20		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	2	213	Total	C	N	O	S	0	0
			1655	1058	278	309	10		

- Molecule 31 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	3	688	Total	C	N	O	S	0	0
			5275	3301	922	1011	41		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	4	430	Total	C	N	O	S	0	0
			3457	2207	594	631	25		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	5	208	Total	C	N	O	S	0	0
			1726	1112	296	315	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	6	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

- Molecule 35 is a protein called Complex I-23kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	a	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	b	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	c	126	Total	C	N	O	S	0	0
			1024	646	182	193	3		

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	d	340	Total	C	N	O	S	0	0
			2748	1775	489	478	6		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	e	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 41 is a protein called Mitochondrial complex I, B13 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	f	113	Total	C	N	O	S	0	0
			917	595	153	167	2		

- Molecule 42 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	g	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

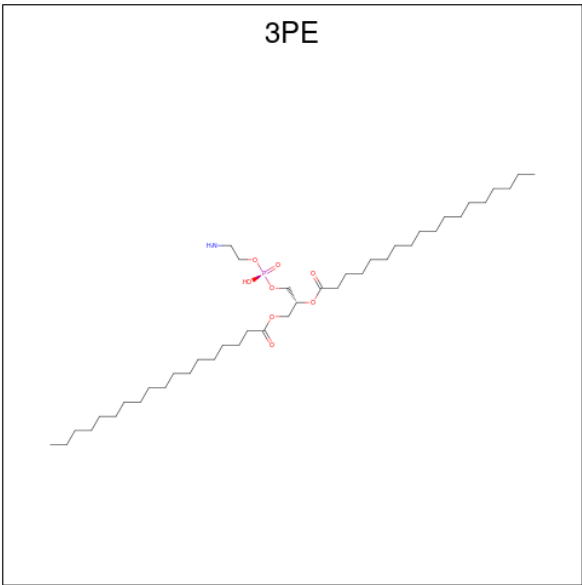
- Molecule 43 is a protein called Mitochondrial complex I, B14.5a subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	h	96	Total	C	N	O	S	0	0
			769	480	146	140	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	i	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

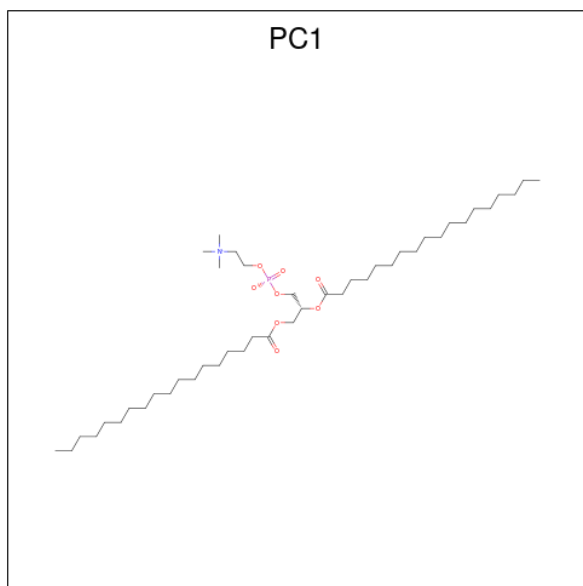
- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	J	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	J	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	N	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	V	1	Total	C	N	O	P	0
			37	27	1	8	1	
45	o	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	p	1	Total	C	O	P		0
			27	18	8	1		
45	6	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	i	1	Total	C	N	O	P	0
			51	41	1	8	1	

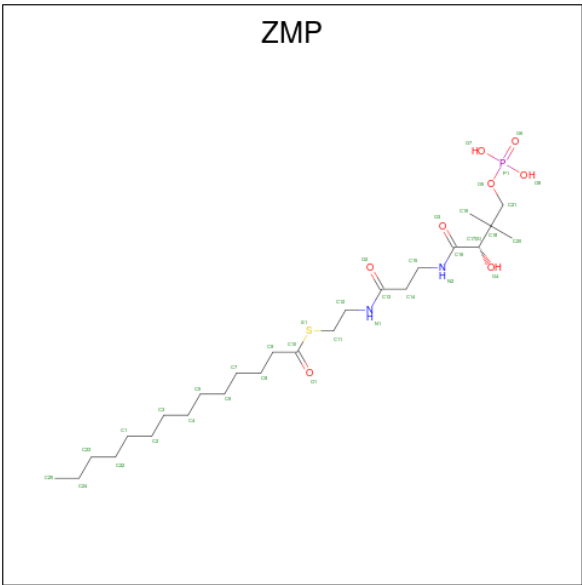
- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1)

(formula: $C_{44}H_{88}NO_8P$).



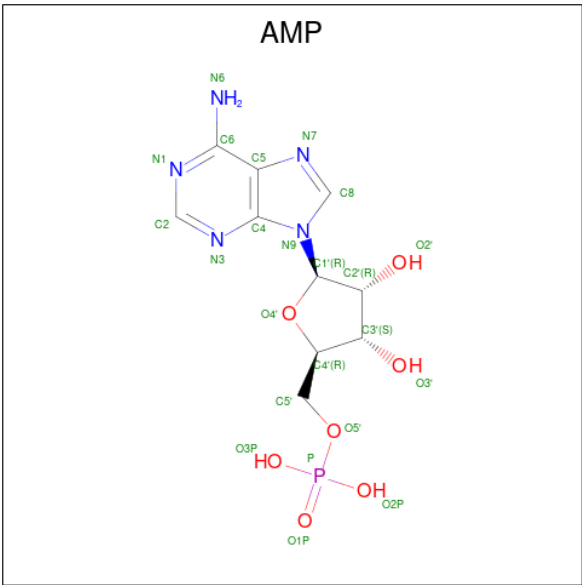
Mol	Chain	Residues	Atoms					AltConf
46	H	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	6	1	Total	C	N	O	P	0
			46	36	1	8	1	

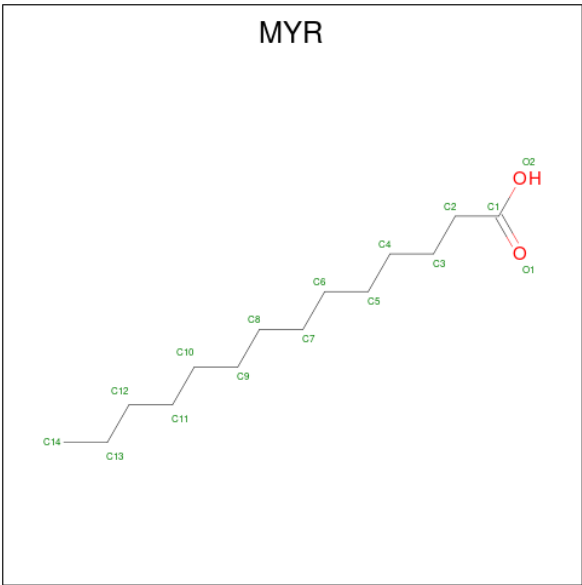
- Molecule 47 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



Mol	Chain	Residues	Atoms						AltConf
47	X	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	
47	j	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

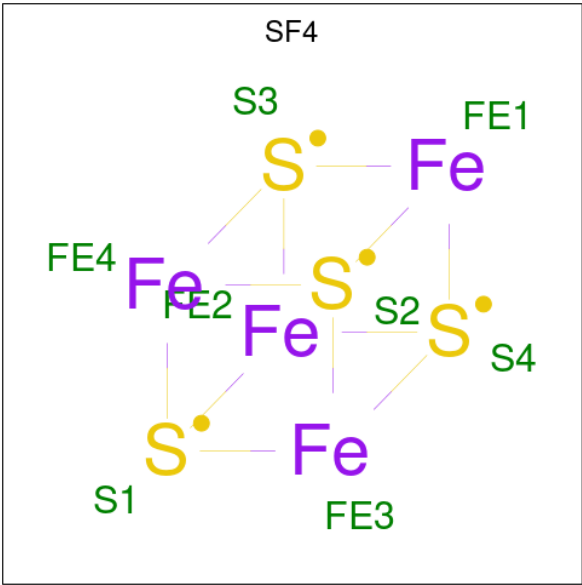
- Molecule 48 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).





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

- Molecule 50 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



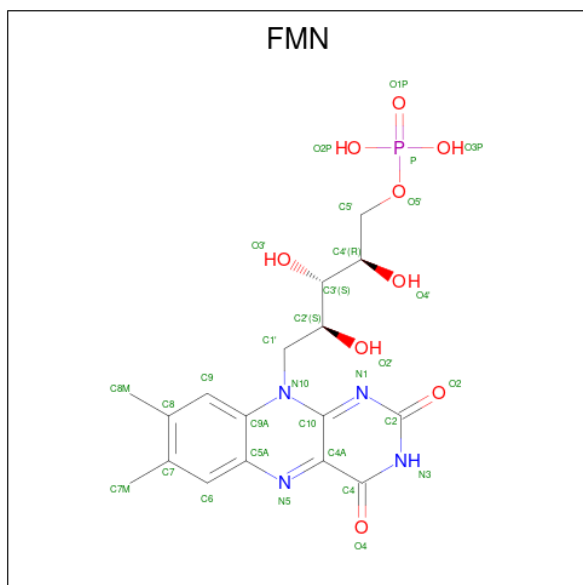
Mol	Chain	Residues	Atoms			AltConf
50	1	1	Total	Fe	S	0
			8	4	4	
50	3	1	Total	Fe	S	0
			8	4	4	
50	3	1	Total	Fe	S	0
			8	4	4	

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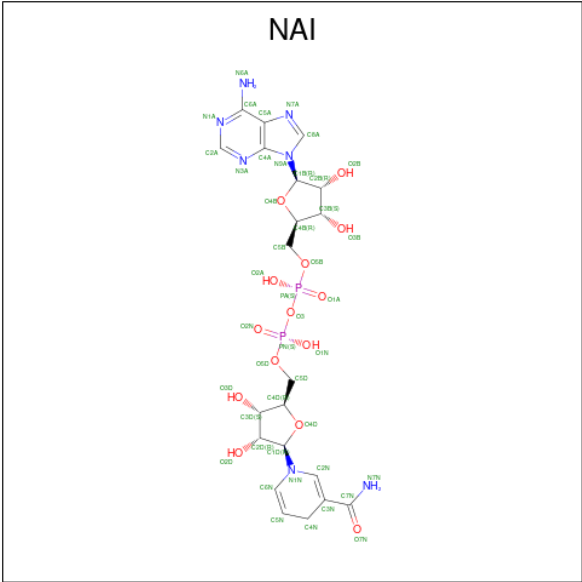
Mol	Chain	Residues	Atoms			AltConf
50	6	1	Total	Fe	S	0
			8	4	4	
50	9	1	Total	Fe	S	0
			8	4	4	
50	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 51 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



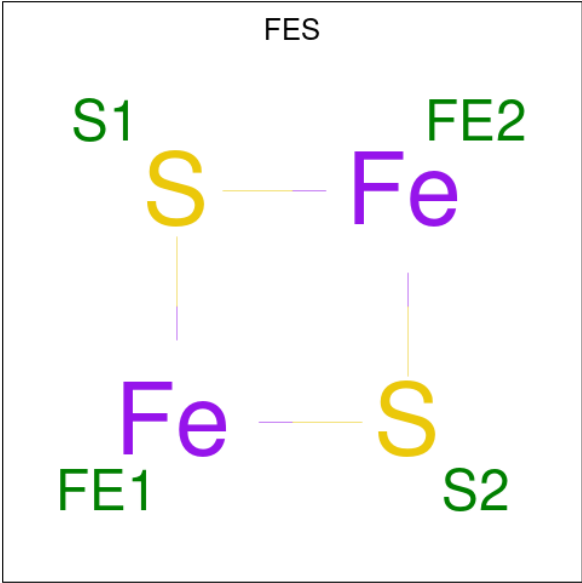
Mol	Chain	Residues	Atoms					AltConf
51	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 52 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
52	1	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 53 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
53	2	1	Total	Fe	S	0
			4	2	2	
53	3	1	Total	Fe	S	0
			4	2	2	

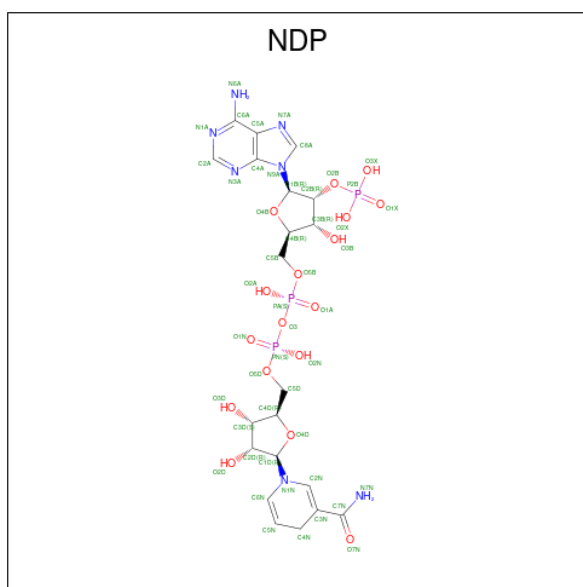
- Molecule 54 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
54	3	1	Total K 1 1	0

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

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

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).

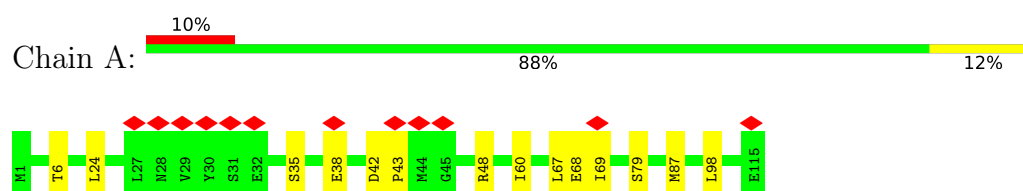


Mol	Chain	Residues	Atoms					AltConf
56	d	1	Total 48	C 21	N 7	O 17	P 3	0

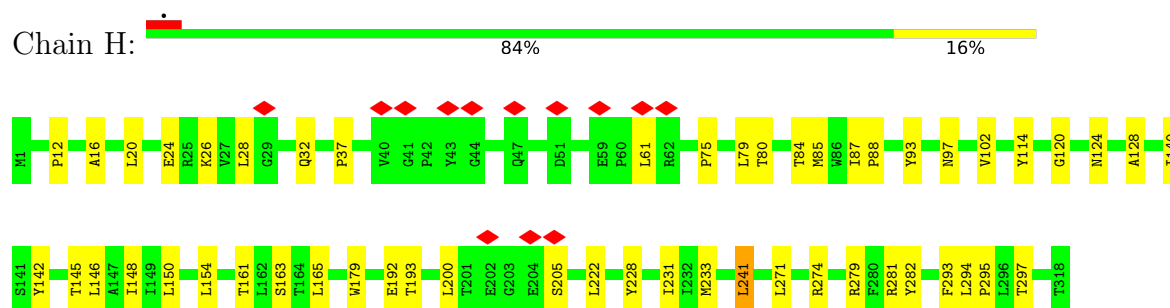
3 Residue-property plots [i](#)

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

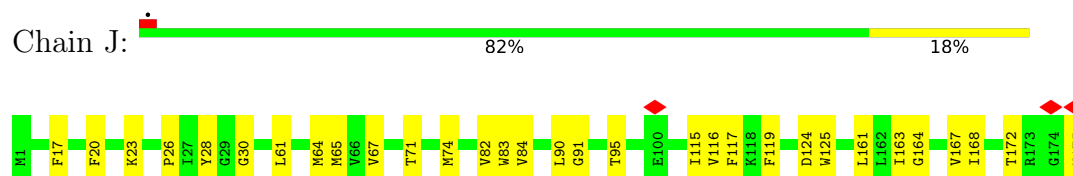
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



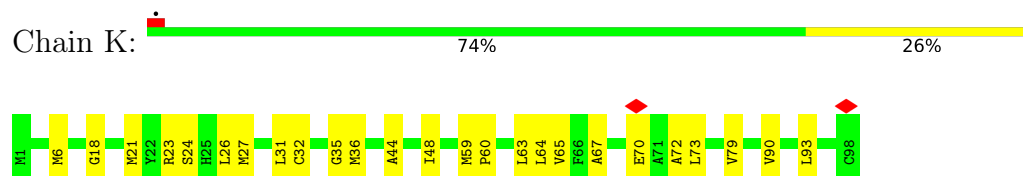
- Molecule 2: NADH-ubiquinone oxidoreductase chain 1



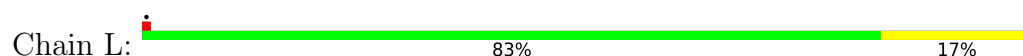
- Molecule 3: NADH-ubiquinone oxidoreductase chain 6

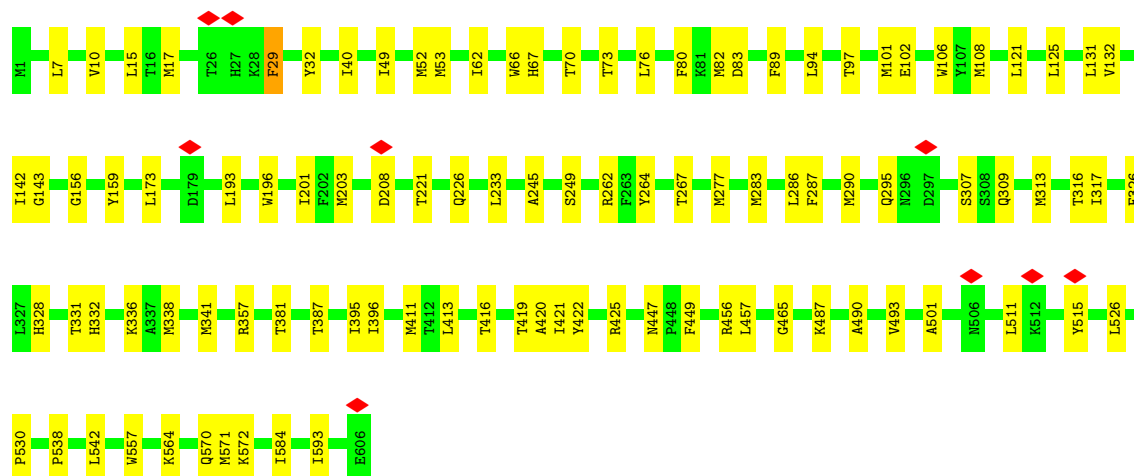


- Molecule 4: NADH-ubiquinone oxidoreductase chain 4L



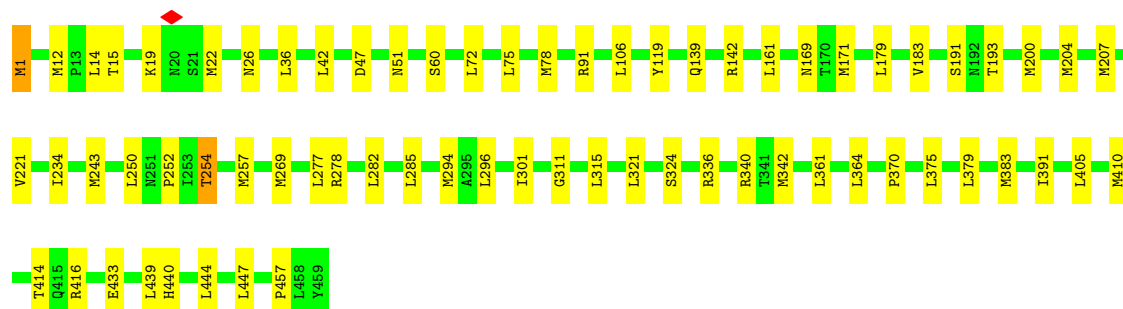
- Molecule 5: NADH-ubiquinone oxidoreductase chain 5





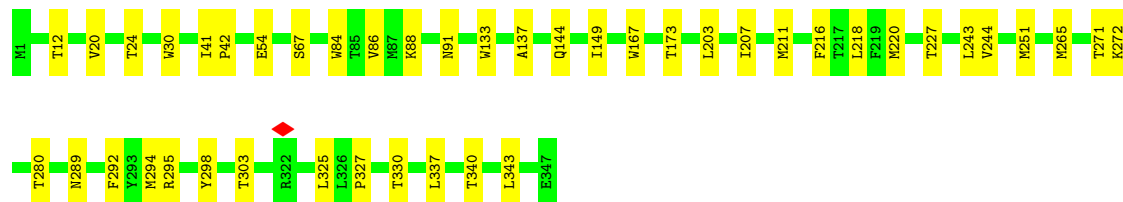
- Molecule 6: NADH-ubiquinone oxidoreductase chain 4

Chain M: 85% 15%



- Molecule 7: NADH-ubiquinone oxidoreductase chain 2

Chain N: 87% 13%



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

Chain V: 96%

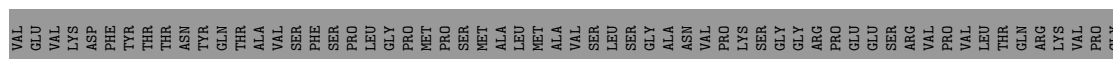


- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

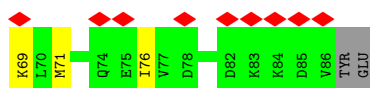
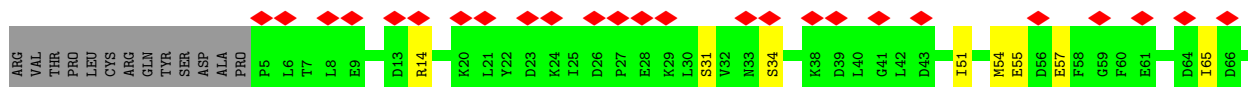
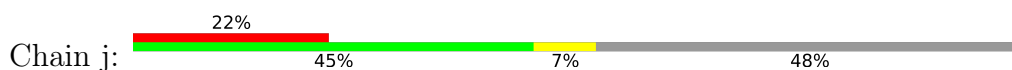
Chain W: 88% 12%



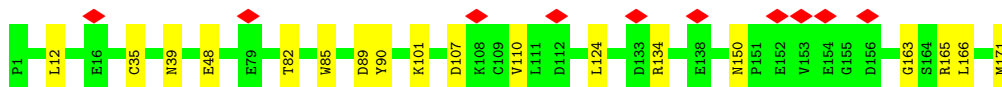
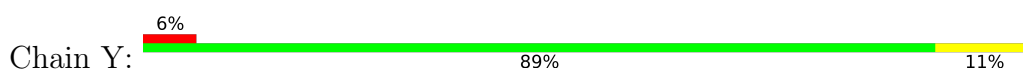
- Molecule 10: Acyl carrier protein



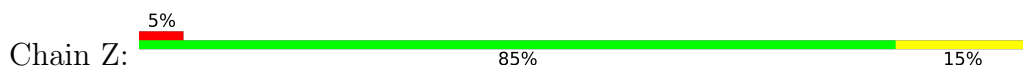
- Molecule 10: Acyl carrier protein



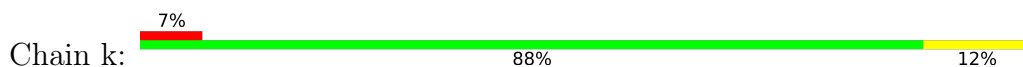
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

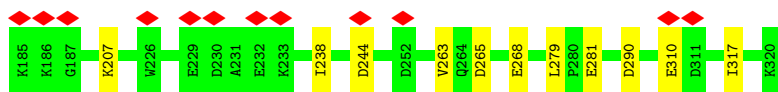


- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

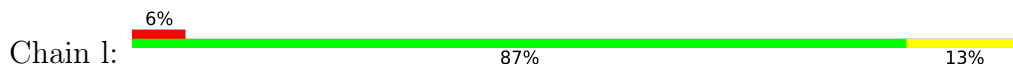


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

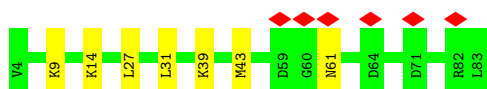




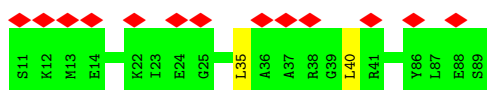
- Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



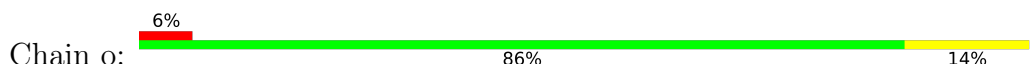
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



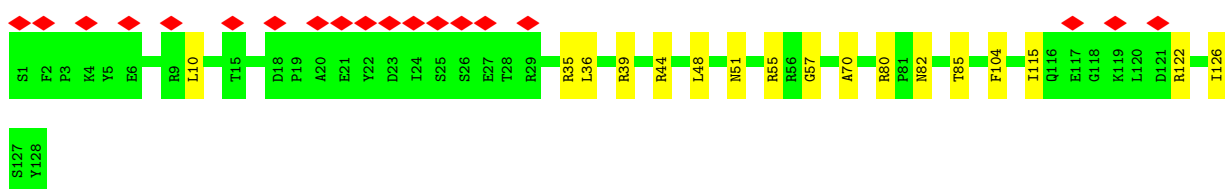
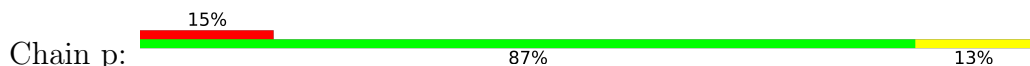
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



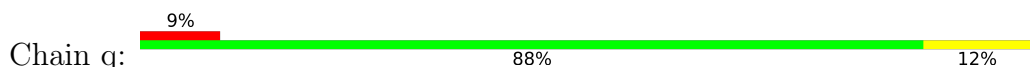
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 subunit C2



- Molecule 18: NADH:ubiquinone oxidoreductase subunit B4

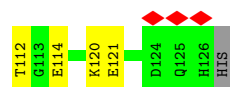
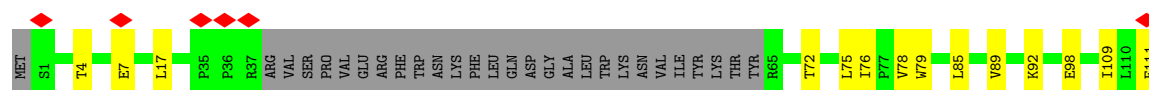


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

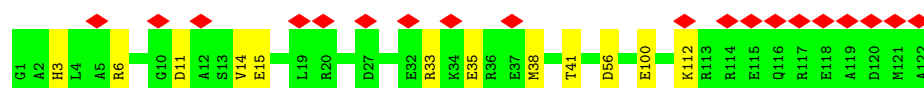
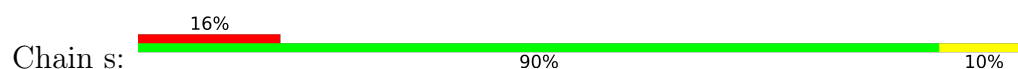




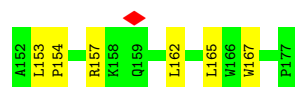
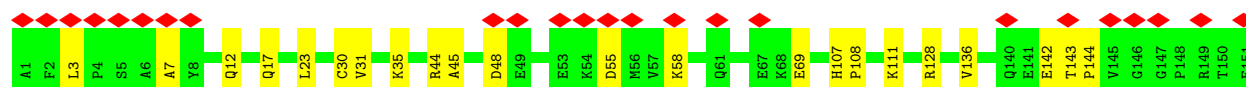
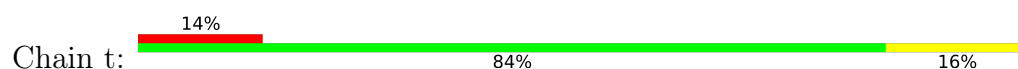
- Molecule 20: Mitochondrial complex I, B17 subunit



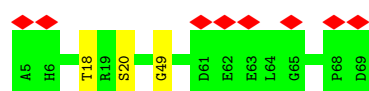
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



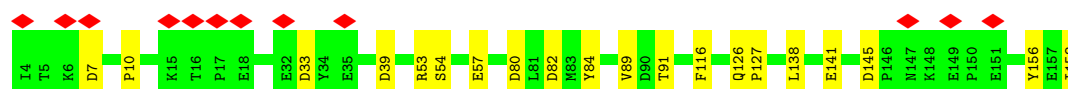
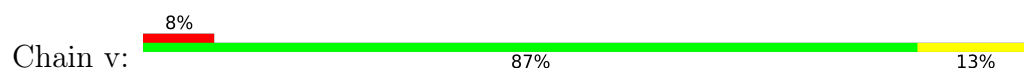
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



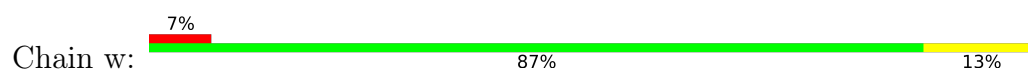
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



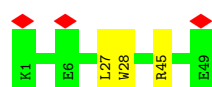
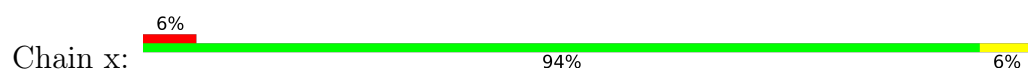
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



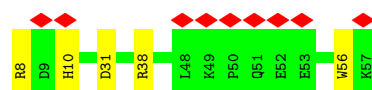
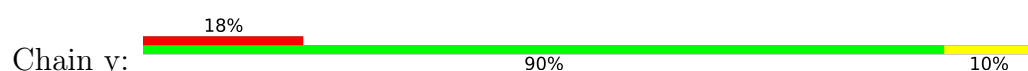
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



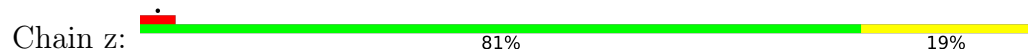
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



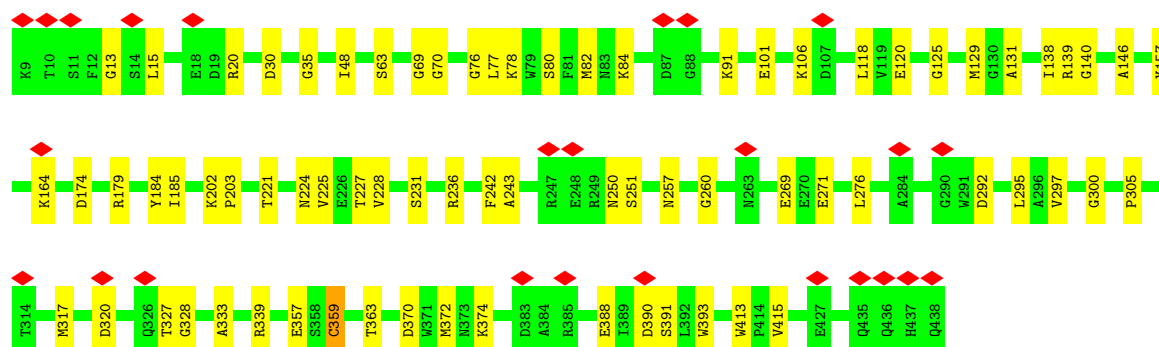
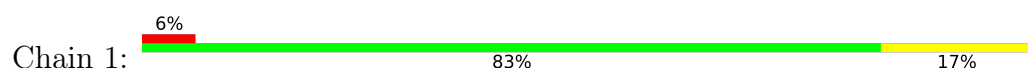
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



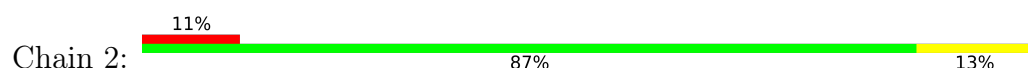
- Molecule 28: Complex I-MWFE

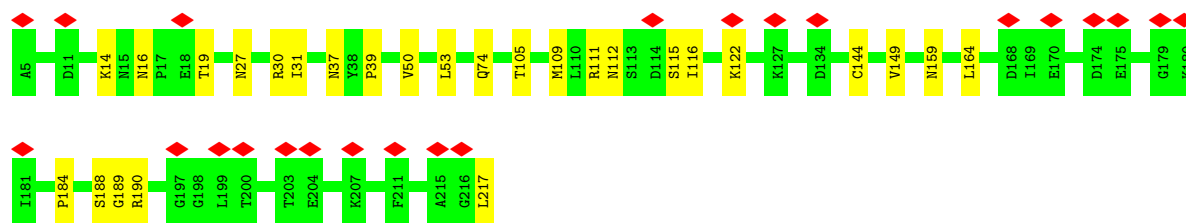


- Molecule 29: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

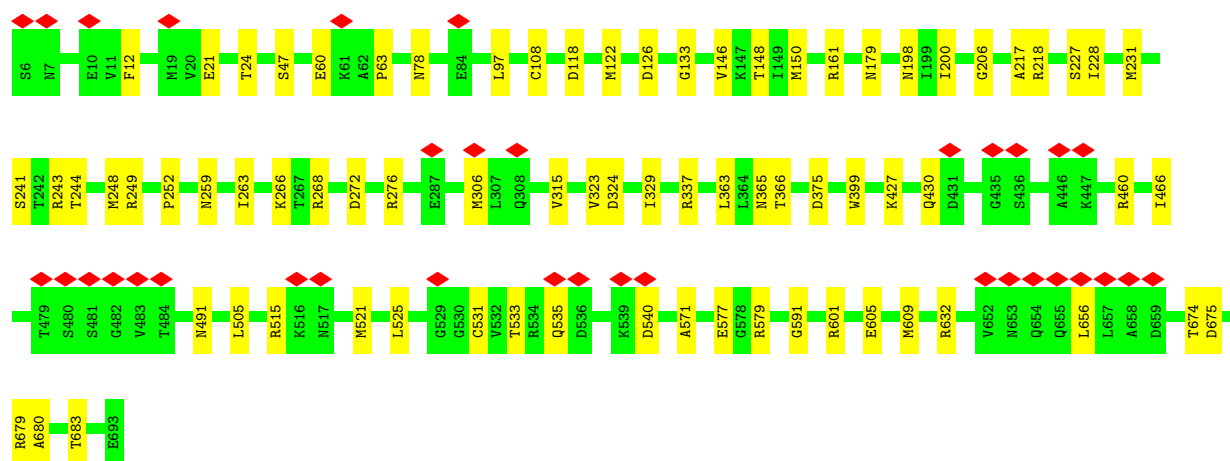
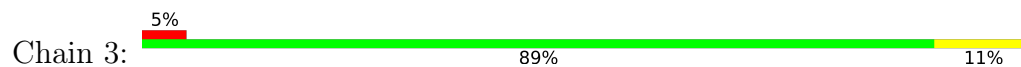


- Molecule 30: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

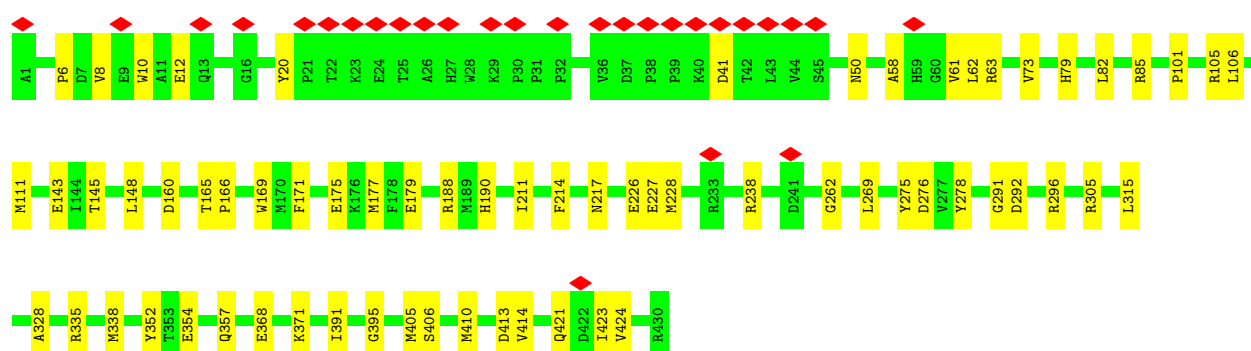
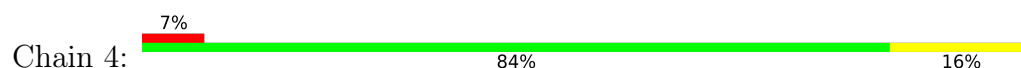




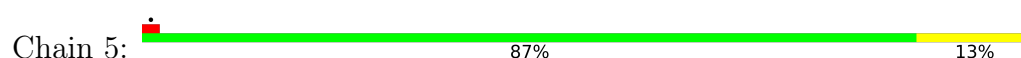
- Molecule 31: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



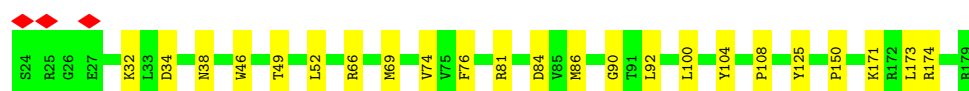
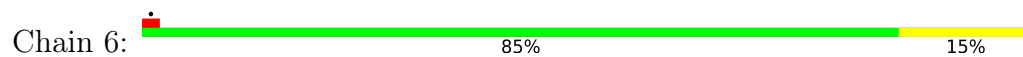
- Molecule 32: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



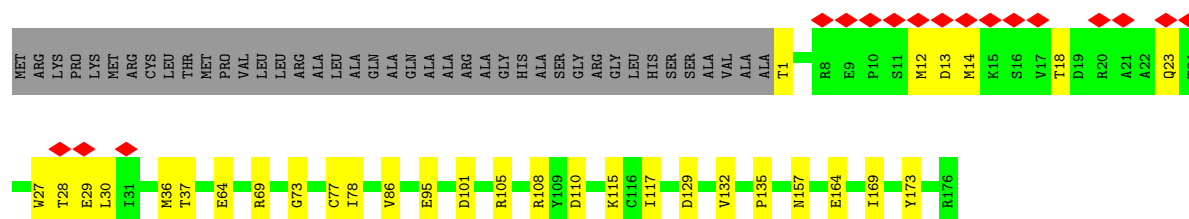
- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



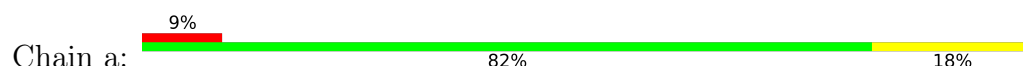
- Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



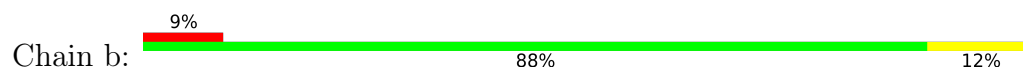
• Molecule 35: Complex I-23kD



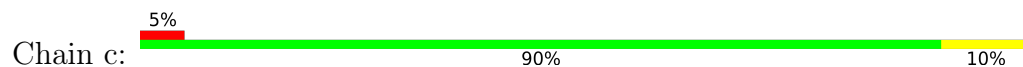
• Molecule 36: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



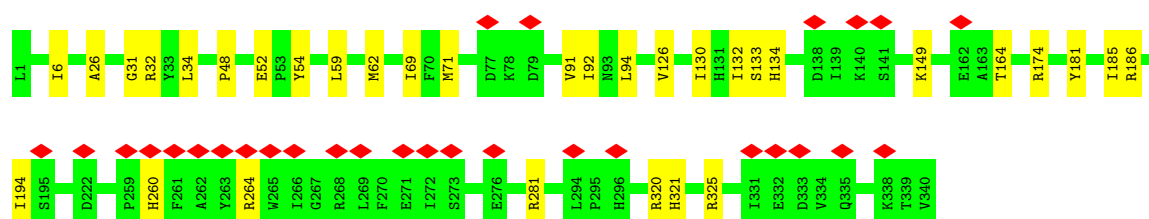
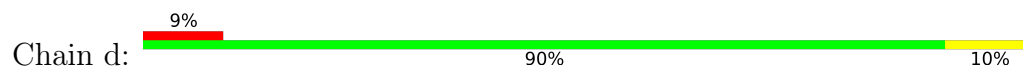
• Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



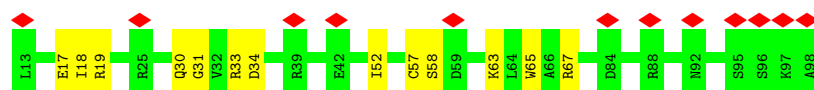
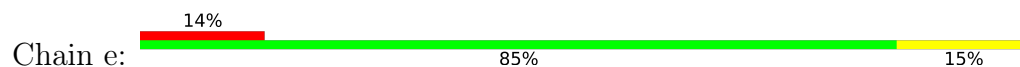
• Molecule 38: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



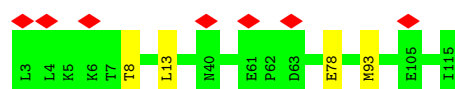
• Molecule 39: NADH:ubiquinone oxidoreductase subunit A9



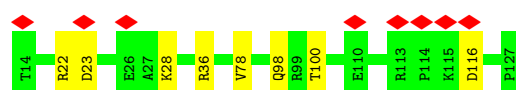
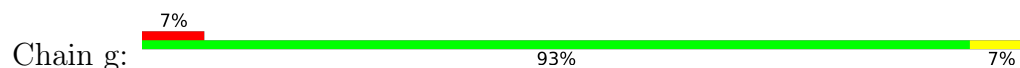
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



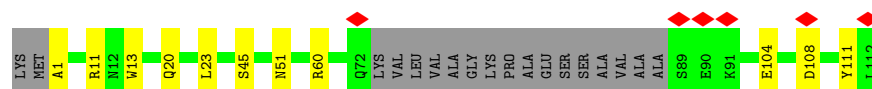
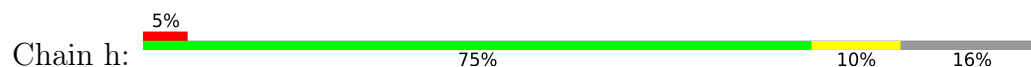
- Molecule 41: Mitochondrial complex I, B13 subunit



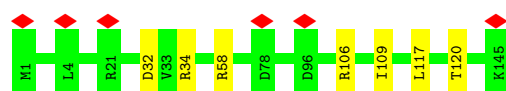
- Molecule 42: NADH:ubiquinone oxidoreductase subunit A6



- Molecule 43: Mitochondrial complex I, B14.5a subunit



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50789	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	90	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.532	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	172.02, 196.42, 286.7	wwPDB
Map dimensions	235, 161, 141	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AYA, SEP, SF4, K, FES, ZN, NDP, PC1, MYR, ZMP, FME, 2MR, AMP, 3PE, NAI, FMN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.21	0/947	0.43	0/1296
2	H	0.19	0/2603	0.46	0/3561
3	J	0.19	0/1378	0.43	0/1868
4	K	0.21	0/749	0.46	0/1014
5	L	0.19	0/4925	0.42	0/6700
6	M	0.20	0/3731	0.42	0/5085
7	N	0.20	0/2787	0.43	0/3795
8	V	0.15	0/1041	0.35	0/1412
9	W	0.15	0/1188	0.32	0/1607
10	X	0.16	0/713	0.38	0/963
10	j	0.18	0/670	0.42	0/902
11	Y	0.16	0/1440	0.36	0/1942
12	Z	0.15	0/1475	0.31	0/1989
13	k	0.13	0/2646	0.28	0/3579
14	l	0.16	0/896	0.36	0/1200
15	m	0.19	0/647	0.39	0/890
16	n	0.15	0/653	0.40	0/882
17	o	0.16	0/1035	0.32	0/1398
18	p	0.17	0/1085	0.40	0/1467
19	q	0.17	0/1171	0.33	0/1579
20	r	0.17	0/874	0.38	0/1188
21	s	0.14	0/1072	0.32	0/1436
22	t	0.14	0/1573	0.31	0/2130
23	u	0.15	0/590	0.38	0/810
24	v	0.14	0/1361	0.35	0/1861
25	w	0.15	0/872	0.39	0/1185
26	x	0.16	0/425	0.37	0/576
27	y	0.16	0/449	0.41	0/605
28	z	0.20	0/591	0.45	0/795
29	1	0.16	0/3386	0.38	0/4575
30	2	0.16	0/1695	0.40	0/2306
31	3	0.15	0/5362	0.39	3/7266 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	4	0.17	0/3535	0.36	0/4791
33	5	0.15	0/1776	0.36	0/2417
34	6	0.17	0/1278	0.36	0/1728
35	9	0.17	0/1445	0.37	0/1956
36	a	0.10	0/383	0.28	0/518
37	b	0.11	0/749	0.25	0/1009
38	c	0.14	0/1047	0.33	0/1415
39	d	0.14	0/2824	0.34	0/3830
40	e	0.17	0/702	0.44	0/945
41	f	0.16	0/937	0.31	0/1271
42	g	0.16	0/993	0.35	0/1336
43	h	0.14	0/779	0.35	0/1053
44	i	0.13	0/1250	0.32	0/1698
All	All	0.17	0/67728	0.38	3/91829 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	1
31	3	0	1
32	4	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	3	63	PRO	CA-N-CD	-9.98	98.03	112.00
31	3	366	THR	CA-C-N	5.27	131.60	121.54
31	3	366	THR	C-N-CA	5.27	131.60	121.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	3	259	ASN	Peptide
32	4	275	TYR	Peptide
3	J	115	ILE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	922	0	953	12	0
2	H	2528	0	2641	38	0
3	J	1344	0	1364	27	0
4	K	749	0	793	23	0
5	L	4807	0	4949	70	0
6	M	3647	0	3849	50	0
7	N	2723	0	2930	34	0
8	V	1028	0	1036	2	0
9	W	1155	0	1177	13	0
10	X	701	0	692	9	0
10	j	660	0	662	7	0
11	Y	1403	0	1392	13	0
12	Z	1441	0	1419	21	0
13	k	2596	0	2559	25	0
14	l	874	0	869	12	0
15	m	626	0	635	5	0
16	n	634	0	616	2	0
17	o	1004	0	995	13	0
18	p	1059	0	1062	16	0
19	q	1142	0	1137	14	0
20	r	846	0	864	15	0
21	s	1047	0	1013	9	0
22	t	1520	0	1477	23	0
23	u	563	0	509	2	0
24	v	1307	0	1207	18	0
25	w	846	0	792	10	0
26	x	412	0	411	3	0
27	y	436	0	437	4	0
28	z	576	0	570	9	0
29	1	3312	0	3266	48	0
30	2	1655	0	1668	20	0
31	3	5275	0	5300	47	0
32	4	3457	0	3397	43	0
33	5	1726	0	1676	19	0
34	6	1247	0	1256	17	0
35	9	1414	0	1371	23	0
36	a	371	0	344	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	b	737	0	710	8	0
38	c	1024	0	1023	10	0
39	d	2748	0	2763	20	0
40	e	691	0	706	8	0
41	f	917	0	958	2	0
42	g	969	0	980	8	0
43	h	769	0	780	8	0
44	i	1209	0	1182	5	0
45	6	51	0	82	2	0
45	A	51	0	82	1	0
45	J	91	0	136	3	0
45	L	82	0	118	0	0
45	M	44	0	65	0	0
45	N	91	0	136	4	0
45	V	37	0	48	1	0
45	i	51	0	82	1	0
45	o	31	0	36	0	0
45	p	27	0	27	0	0
46	6	46	0	69	1	0
46	H	54	0	88	0	0
46	L	108	0	176	3	0
46	M	54	0	88	2	0
47	X	31	0	34	1	0
47	j	34	0	40	1	0
48	k	23	0	12	3	0
49	s	15	0	27	0	0
50	1	8	0	0	0	0
50	3	16	0	0	1	0
50	6	8	0	0	0	0
50	9	16	0	0	0	0
51	1	31	0	19	1	0
52	1	44	0	27	5	0
53	2	4	0	0	1	0
53	3	4	0	0	0	0
54	3	1	0	0	0	0
55	b	1	0	0	0	0
56	d	48	0	26	0	0
All	All	67219	0	67808	645	0

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

All (645) 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)
16:n:40:LEU:HD21	22:t:45:ALA:HB2	1.64	0.78
15:m:27:LEU:O	15:m:31:LEU:HB2	1.93	0.68
32:4:269:LEU:HB2	32:4:368:GLU:HB2	1.76	0.68
5:L:203:MET:HB2	12:Z:113:GLN:HG3	1.77	0.67
1:A:68:GLU:HG3	3:J:161:LEU:HD13	1.77	0.66
16:n:35:LEU:HD12	16:n:40:LEU:HB2	1.77	0.66
34:6:171:LYS:HG2	34:6:174:ARG:HE	1.59	0.66
5:L:49:ILE:HA	5:L:52:MET:HE2	1.77	0.66
29:1:101:GLU:HB2	52:1:503:NAI:H42N	1.78	0.65
5:L:286:LEU:HD22	5:L:411:MET:HG2	1.78	0.65
5:L:387:THR:HG22	5:L:465:GLY:H	1.62	0.65
2:H:85:MET:HE3	2:H:233:MET:HE2	1.79	0.63
40:e:19:ARG:HB2	40:e:65:TRP:HB2	1.81	0.62
21:s:35:GLU:HA	24:v:156:TYR:HA	1.81	0.62
6:M:78:MET:HE1	6:M:439:LEU:HD12	1.82	0.62
45:J:201:3PE:H2F2	45:J:201:3PE:H371	1.81	0.62
45:A:201:3PE:H381	2:H:295:PRO:HB3	1.81	0.62
5:L:413:LEU:HD12	5:L:493:VAL:HG21	1.81	0.62
34:6:32:LYS:HE3	45:6:203:3PE:H3D2	1.81	0.62
13:k:126:ARG:HH12	48:k:501:AMP:H5'2	1.63	0.62
33:5:127:ALA:HA	33:5:130:TYR:HB2	1.81	0.61
5:L:221:THR:HG23	5:L:226:GLN:HB2	1.82	0.61
12:Z:159:LYS:NZ	17:o:112:VAL:O	2.34	0.61
5:L:106:TRP:HD1	5:L:447:ASN:HD22	1.50	0.60
6:M:193:THR:HG23	6:M:257:MET:HE1	1.82	0.60
13:k:147:GLN:HB3	13:k:279:LEU:HD11	1.84	0.60
42:g:36:ARG:NH2	10:j:55:GLU:OE1	2.34	0.60
13:k:310:GLU:HG3	13:k:317:ILE:HD12	1.83	0.60
1:A:42:ASP:OD1	42:g:98:GLN:NE2	2.34	0.59
11:Y:12:LEU:O	14:l:104:ARG:NH2	2.35	0.59
31:3:460:ARG:HH21	31:3:466:ILE:HD11	1.68	0.59
32:4:335:ARG:NH2	35:9:129:ASP:OD1	2.35	0.59
32:4:50:ASN:HD21	32:4:63:ARG:HH21	1.49	0.59
4:K:44:ALA:HB1	4:K:59:MET:HE1	1.83	0.58
31:3:118:ASP:OD2	38:c:46:GLN:NE2	2.37	0.58
29:1:30:ASP:HB3	29:1:35:GLY:HA3	1.84	0.58
31:3:126:ASP:HB2	32:4:328:ALA:HB3	1.86	0.58
13:k:104:ARG:NH2	48:k:501:AMP:N7	2.52	0.58
1:A:35:SER:O	34:6:81:ARG:NH2	2.37	0.58
34:6:46:TRP:H	34:6:84:ASP:HB2	1.69	0.58
34:6:49:THR:HG22	34:6:76:PHE:HB3	1.86	0.58
32:4:354:GLU:OE2	32:4:357:GLN:NE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:4:405:MET:SD	32:4:421:GLN:NE2	2.78	0.57
19:q:27:ARG:NH1	43:h:13:TRP:O	2.37	0.57
1:A:67:LEU:HD13	4:K:65:VAL:HA	1.87	0.57
3:J:84:VAL:HG12	3:J:90:LEU:HD13	1.87	0.57
29:1:300:GLY:HA2	29:1:333:ALA:H	1.70	0.57
1:A:60:ILE:HG23	4:K:72:ALA:HB1	1.86	0.57
32:4:145:THR:HA	32:4:148:LEU:HD12	1.87	0.57
40:e:31:GLY:O	40:e:34:ASP:HB3	2.05	0.57
5:L:73:THR:HG21	18:p:126:ILE:HD11	1.86	0.56
5:L:102:GLU:OE1	5:L:456:ARG:NH2	2.38	0.56
33:5:96:LEU:HB2	33:5:105:ILE:HG22	1.87	0.56
6:M:375:LEU:O	6:M:379:LEU:HB2	2.05	0.56
13:k:52:PRO:O	13:k:107:GLN:NE2	2.38	0.56
5:L:132:VAL:O	5:L:262:ARG:NH2	2.38	0.56
6:M:269:MET:HE1	6:M:296:LEU:HD13	1.88	0.56
30:2:37:ASN:OD1	36:a:62:ARG:NH1	2.38	0.56
31:3:324:ASP:HB3	31:3:571:ALA:HB1	1.87	0.56
32:4:276:ASP:OD1	32:4:276:ASP:N	2.38	0.56
33:5:151:ILE:HG23	33:5:152:LEU:HG	1.86	0.56
37:b:49:VAL:HG11	37:b:92:ARG:HH21	1.70	0.56
27:y:38:ARG:NH1	27:y:56:TRP:O	2.39	0.56
32:4:291:GLY:O	32:4:296:ARG:NH1	2.38	0.56
42:g:23:ASP:OD1	42:g:23:ASP:N	2.38	0.56
4:K:60:PRO:O	4:K:63:LEU:HB3	2.06	0.56
6:M:36:LEU:HB2	25:w:69:VAL:HG12	1.87	0.56
32:4:292:ASP:OD1	32:4:292:ASP:N	2.39	0.56
9:W:107:GLU:OE2	9:W:111:ARG:NH1	2.39	0.56
9:W:62:GLU:HB2	9:W:65:GLU:HG3	1.87	0.56
44:i:34:ARG:NH2	44:i:58:ARG:O	2.39	0.56
22:t:55:ASP:HB3	22:t:58:LYS:HB2	1.87	0.56
21:s:11:ASP:OD1	21:s:11:ASP:N	2.40	0.55
31:3:272:ASP:OD1	31:3:272:ASP:N	2.39	0.55
2:H:61:LEU:HD22	34:6:108:PRO:HG3	1.88	0.55
46:L:1003:PC1:O14	20:r:92:LYS:NZ	2.39	0.55
11:Y:89:ASP:OD2	28:z:34:ARG:NH1	2.38	0.55
13:k:173:ASP:OD2	13:k:207:LYS:NZ	2.37	0.55
29:1:292:ASP:OD1	29:1:292:ASP:N	2.35	0.55
4:K:24:SER:HA	4:K:90:VAL:HG22	1.88	0.55
5:L:156:GLY:O	6:M:416:ARG:NH1	2.40	0.55
5:L:196:TRP:HZ2	6:M:383:MET:HE2	1.72	0.55
11:Y:165:ARG:NH2	17:o:87:ASP:OD1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:140:GLY:O	29:1:179:ARG:NH2	2.39	0.55
28:z:3:PHE:O	28:z:6:LEU:HB2	2.07	0.55
31:3:577:GLU:OE2	31:3:579:ARG:NH1	2.40	0.55
32:4:371:LYS:HE2	32:4:424:VAL:HG22	1.88	0.55
39:d:59:LEU:HA	39:d:62:MET:HG3	1.89	0.55
10:X:65:ILE:HD13	22:t:3:LEU:HD22	1.89	0.54
11:Y:90:TYR:OH	28:z:28:ARG:NH1	2.39	0.54
29:1:164:LYS:HD3	36:a:63:MET:HE1	1.88	0.54
5:L:173:LEU:HD12	6:M:405:LEU:HD21	1.88	0.54
30:2:116:ILE:HD11	30:2:164:LEU:HB2	1.89	0.54
33:5:49:GLU:OE2	33:5:106:ARG:NH1	2.41	0.54
29:1:63:SER:HB2	29:1:242:PHE:HB3	1.90	0.54
32:4:175:GLU:OE2	32:4:188:ARG:NH2	2.41	0.54
6:M:277:LEU:HD21	6:M:405:LEU:HB3	1.89	0.54
21:s:6:ARG:NH1	21:s:15:GLU:OE2	2.40	0.53
2:H:293:PHE:O	2:H:297:THR:OG1	2.24	0.53
18:p:44:ARG:NH1	22:t:143:THR:OG1	2.41	0.53
31:3:540:ASP:OD1	31:3:540:ASP:N	2.37	0.53
2:H:20:LEU:HD21	2:H:231:ILE:HD11	1.90	0.53
12:Z:14:ARG:NH1	20:r:98:GLU:OE2	2.35	0.53
24:v:138:LEU:HB3	24:v:141:GLU:HB2	1.91	0.53
31:3:675:ASP:N	31:3:675:ASP:OD1	2.37	0.53
32:4:106:LEU:HD13	32:4:391:ILE:HG21	1.90	0.53
39:d:52:GLU:HG3	39:d:54:TYR:H	1.73	0.53
6:M:243:MET:HB3	6:M:301:ILE:HG21	1.89	0.53
22:t:142:GLU:OE2	22:t:157:ARG:NH2	2.41	0.53
24:v:145:ASP:OD1	24:v:145:ASP:N	2.41	0.53
30:2:74:GLN:O	36:a:74:ARG:NH2	2.41	0.53
1:A:48:ARG:NH1	2:H:124:ASN:OD1	2.41	0.53
12:Z:5:ASP:HB3	12:Z:8:VAL:HG12	1.90	0.53
30:2:159:ASN:HB3	30:2:184:PRO:HB3	1.90	0.53
3:J:30:GLY:HA2	3:J:64:MET:HE2	1.91	0.53
29:1:276:LEU:HD21	29:1:297:VAL:HG11	1.91	0.53
5:L:15:LEU:HD11	5:L:94:LEU:HD21	1.90	0.53
11:Y:48:GLU:OE1	11:Y:134:ARG:NH2	2.42	0.52
11:Y:124:LEU:HD13	19:q:69:ALA:HB2	1.90	0.52
18:p:55:ARG:NH1	18:p:57:GLY:O	2.41	0.52
29:1:363:THR:HG21	31:3:97:LEU:HG	1.90	0.52
33:5:165:ASP:OD1	33:5:165:ASP:N	2.42	0.52
35:9:13:ASP:N	35:9:13:ASP:OD1	2.38	0.52
37:b:10:LYS:NZ	37:b:37:GLU:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:82:MET:HE2	29:1:91:LYS:HB3	1.91	0.52
14:l:100:GLN:N	14:l:100:GLN:OE1	2.42	0.52
32:4:41:ASP:OD1	32:4:41:ASP:N	2.39	0.52
6:M:207:MET:HG3	6:M:294:MET:HB3	1.92	0.52
25:w:48:ASP:OD1	25:w:49:LYS:N	2.42	0.52
43:h:45:SER:O	43:h:51:ASN:ND2	2.41	0.52
18:p:35:ARG:NH1	24:v:33:ASP:OD2	2.42	0.52
31:3:363:LEU:O	31:3:365:ASN:ND2	2.43	0.52
2:H:24:GLU:OE2	2:H:274:ARG:NH1	2.43	0.52
2:H:281:ARG:NH1	32:4:413:ASP:OD1	2.43	0.52
29:1:139:ARG:NH2	30:2:144:CYS:O	2.41	0.52
6:M:171:MET:HE1	6:M:183:VAL:HA	1.91	0.52
6:M:191:SER:HB3	46:M:502:PC1:H31	1.92	0.52
29:1:305:PRO:HG3	29:1:413:TRP:HB3	1.92	0.52
1:A:69:ILE:HG22	1:A:98:LEU:HD11	1.90	0.52
5:L:396:ILE:HG21	5:L:490:ALA:HB2	1.91	0.52
29:1:185:ILE:HG12	29:1:359:CYS:HB3	1.91	0.52
32:4:177:MET:HE2	32:4:214:PHE:HZ	1.75	0.52
7:N:30:TRP:NE1	7:N:67:SER:OG	2.43	0.51
7:N:86:VAL:HG12	7:N:144:GLN:HG2	1.93	0.51
12:Z:8:VAL:HG11	25:w:94:GLU:HG2	1.92	0.51
29:1:250:ASN:ND2	29:1:320:ASP:OD2	2.40	0.51
32:4:217:ASN:ND2	43:h:23:LEU:O	2.43	0.51
35:9:108:ARG:NH1	35:9:110:ASP:OD2	2.41	0.51
2:H:75:PRO:HB2	2:H:222:LEU:HD12	1.91	0.51
29:1:69:GLY:O	52:1:503:NAI:N7N	2.37	0.51
30:2:16:ASN:OD1	30:2:19:THR:OG1	2.26	0.51
30:2:27:ASN:OD1	30:2:30:ARG:NH1	2.43	0.51
33:5:93:VAL:HG22	33:5:108:LYS:HG2	1.92	0.51
6:M:169:ASN:ND2	7:N:271:THR:OG1	2.44	0.51
9:W:125:TYR:HB2	14:l:48:SER:HB3	1.91	0.51
31:3:252:PRO:HG3	31:3:263:ILE:HG12	1.91	0.51
45:J:202:3PE:H222	4:K:21:MET:HB2	1.91	0.51
45:J:202:3PE:H11	4:K:23:ARG:HG2	1.92	0.51
3:J:125:TRP:HB2	19:q:136:THR:HG21	1.93	0.51
6:M:282:LEU:HD12	6:M:342:MET:HE2	1.93	0.51
10:X:64:ASP:OD2	22:t:17:GLN:NE2	2.43	0.51
40:e:18:ILE:HD12	40:e:52:ILE:HG12	1.90	0.51
40:e:57:CYS:SG	40:e:58:SER:N	2.84	0.51
6:M:336:ARG:NH2	6:M:433:GLU:OE1	2.43	0.51
31:3:148:THR:HG23	31:3:150:MET:HE2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:l:49:ILE:O	14:l:53:LYS:NZ	2.44	0.51
29:1:20:ARG:HH11	29:1:269:GLU:HG2	1.76	0.51
43:h:11:ARG:NH2	43:h:20:GLN:OE1	2.42	0.51
3:J:67:VAL:O	3:J:71:THR:HG23	2.11	0.51
5:L:76:LEU:HD21	5:L:196:TRP:HE3	1.76	0.51
24:v:7:ASP:OD1	24:v:7:ASP:N	2.44	0.51
35:9:77:CYS:O	35:9:105:ARG:NH1	2.44	0.51
39:d:264:ARG:HB3	39:d:281:ARG:HE	1.76	0.51
3:J:167:VAL:HG22	7:N:42:PRO:HG2	1.91	0.51
40:e:30:GLN:OE1	40:e:33:ARG:NH2	2.44	0.51
5:L:264:TYR:HA	5:L:267:THR:HG22	1.93	0.50
31:3:329:ILE:HD13	31:3:505:LEU:HD22	1.93	0.50
35:9:23:GLN:HG3	35:9:28:THR:HB	1.92	0.50
35:9:69:ARG:NH1	35:9:73:GLY:O	2.44	0.50
5:L:283:MET:HG2	24:v:116:PHE:HE2	1.76	0.50
45:N:402:3PE:H371	45:N:402:3PE:H292	1.93	0.50
12:Z:72:ASP:OD2	12:Z:74:THR:OG1	2.27	0.50
31:3:122:MET:O	43:h:60:ARG:NH2	2.44	0.50
33:5:192:GLN:OE1	35:9:115:LYS:NZ	2.42	0.50
37:b:31:ARG:HH22	39:d:69:ILE:HD12	1.77	0.50
42:g:78:VAL:HG23	47:j:101:ZMP:HN1	1.75	0.50
5:L:62:ILE:HG13	12:Z:114:GLN:HG3	1.92	0.50
10:X:55:GLU:HG2	10:X:61:GLU:HA	1.94	0.50
31:3:324:ASP:OD1	31:3:324:ASP:N	2.36	0.50
33:5:32:ILE:HG22	33:5:33:LEU:HG	1.93	0.50
41:f:8:THR:HG21	41:f:13:LEU:HB3	1.94	0.50
10:j:54:MET:HE3	10:j:76:ILE:HD13	1.93	0.50
3:J:74:MET:HE1	4:K:79:VAL:HG12	1.94	0.50
31:3:306:MET:HE3	31:3:521:MET:HB3	1.93	0.50
2:H:26:LYS:HG3	2:H:37:PRO:HD2	1.93	0.50
5:L:53:MET:HE2	12:Z:29:ILE:HG23	1.92	0.50
5:L:357:ARG:HG2	22:t:31:VAL:HG12	1.93	0.50
6:M:60:SER:HB3	6:M:457:PRO:HA	1.93	0.50
44:i:32:ASP:OD2	44:i:34:ARG:NH1	2.43	0.50
29:1:120:GLU:OE2	29:1:236:ARG:NH2	2.44	0.50
36:a:57:ASP:O	36:a:60:LYS:NZ	2.39	0.50
2:H:279:ARG:O	32:4:238:ARG:NH1	2.42	0.49
3:J:117:PHE:HE1	7:N:91:ASN:HD21	1.59	0.49
12:Z:158:GLN:O	12:Z:162:MET:HG3	2.12	0.49
11:Y:82:THR:HA	11:Y:85:TRP:CD1	2.47	0.49
30:2:149:VAL:O	30:2:190:ARG:NH2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:4:262:GLY:HA3	32:4:296:ARG:HG2	1.93	0.49
35:9:169:ILE:O	35:9:173:TYR:HB3	2.13	0.49
5:L:233:LEU:HD23	5:L:307:SER:HB3	1.95	0.49
5:L:295:GLN:O	5:L:425:ARG:NH2	2.45	0.49
13:k:97:GLN:NE2	13:k:131:ASP:OD2	2.45	0.49
17:o:66:THR:OG1	26:x:28:TRP:NE1	2.46	0.49
31:3:47:SER:O	31:3:161:ARG:NH1	2.42	0.49
31:3:674:THR:O	31:3:679:ARG:NH1	2.46	0.49
10:j:31:SER:O	10:j:34:SER:OG	2.30	0.49
3:J:163:ILE:HG21	7:N:12:THR:HG21	1.94	0.49
29:1:374:LYS:NZ	31:3:133:GLY:O	2.45	0.49
31:3:323:VAL:HG11	31:3:525:LEU:HD13	1.95	0.49
33:5:179:GLU:O	39:d:174:ARG:NH1	2.45	0.49
5:L:515:TYR:OH	22:t:69:GLU:OE2	2.30	0.49
24:v:54:SER:HA	24:v:84:TYR:HB3	1.95	0.49
29:1:84:LYS:O	29:1:91:LYS:NZ	2.42	0.49
31:3:60:GLU:HG2	31:3:78:ASN:HB3	1.94	0.49
31:3:365:ASN:N	31:3:491:ASN:OD1	2.46	0.49
6:M:250:LEU:O	6:M:254:THR:OG1	2.31	0.49
33:5:60:VAL:O	33:5:63:PHE:HB3	2.13	0.49
42:g:116:ASP:OD1	42:g:116:ASP:N	2.45	0.49
3:J:23:LYS:NZ	4:K:18:GLY:O	2.39	0.49
6:M:19:LYS:HB2	6:M:22:MET:HB2	1.95	0.49
6:M:139:GLN:O	6:M:142:ARG:NH1	2.44	0.49
7:N:298:TYR:O	7:N:303:THR:OG1	2.25	0.49
37:b:84:CYS:HB3	37:b:87:CYS:SG	2.53	0.49
5:L:570:GLN:OE1	7:N:167:TRP:NE1	2.41	0.49
31:3:399:TRP:O	38:c:127:ARG:NH1	2.46	0.49
31:3:601:ARG:NH1	31:3:605:GLU:OE1	2.38	0.49
2:H:102:VAL:HG21	2:H:154:LEU:HD11	1.93	0.48
18:p:70:ALA:HB2	24:v:10:PRO:HG2	1.95	0.48
33:5:129:TRP:O	33:5:132:ARG:HB3	2.12	0.48
30:2:188:SER:OG	30:2:189:GLY:N	2.45	0.48
4:K:70:GLU:O	4:K:73:LEU:HB3	2.13	0.48
13:k:31:ILE:HG23	48:k:501:AMP:H3'	1.95	0.48
31:3:272:ASP:OD2	31:3:683:THR:OG1	2.26	0.48
3:J:71:THR:HG22	4:K:27:MET:HG2	1.96	0.48
7:N:203:LEU:HD22	7:N:343:LEU:HD22	1.96	0.48
12:Z:40:VAL:HA	20:r:79:TRP:HE1	1.77	0.48
32:4:226:GLU:OE1	32:4:305:ARG:NH2	2.35	0.48
7:N:24:THR:HG22	14:l:2:PHE:HZ	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:107:ASP:HA	11:Y:110:VAL:HG12	1.95	0.48
31:3:108:CYS:O	31:3:218:ARG:NH1	2.46	0.48
32:4:6:PRO:HB3	32:4:10:TRP:HB3	1.95	0.48
6:M:42:LEU:HD13	25:w:80:LEU:HD11	1.96	0.48
29:1:138:ILE:HG21	29:1:146:ALA:HB2	1.96	0.48
44:i:106:ARG:HB2	44:i:109:ILE:HG13	1.96	0.48
5:L:97:THR:HG21	5:L:125:LEU:HD22	1.96	0.48
6:M:391:ILE:HB	18:p:104:PHE:HE1	1.79	0.48
18:p:82:ASN:OD1	18:p:82:ASN:N	2.47	0.48
32:4:211:ILE:HG22	32:4:315:LEU:HD11	1.96	0.48
3:J:91:GLY:O	3:J:95:THR:HG23	2.14	0.48
6:M:285:LEU:HD13	6:M:342:MET:HE1	1.95	0.48
11:Y:163:GLY:HA3	11:Y:171:MET:HA	1.95	0.48
32:4:228:MET:HE1	35:9:37:THR:HG23	1.95	0.48
38:c:60:ASP:N	38:c:60:ASP:OD1	2.44	0.48
2:H:61:LEU:HD23	34:6:81:ARG:HD3	1.96	0.47
45:6:203:3PE:H221	45:i:201:3PE:H332	1.95	0.47
5:L:142:ILE:HG12	6:M:370:PRO:HB2	1.96	0.47
45:V:400:3PE:H322	45:V:400:3PE:H261	1.96	0.47
29:1:157:TYR:OH	29:1:174:ASP:OD1	2.31	0.47
3:J:64:MET:HE1	4:K:31:LEU:HD22	1.96	0.47
5:L:593:ILE:HD12	8:V:41:ALA:HB2	1.96	0.47
18:p:80:ARG:NH2	24:v:39:ASP:O	2.48	0.47
5:L:542:LEU:HB3	6:M:278:ARG:HH11	1.80	0.47
12:Z:20:SER:O	12:Z:20:SER:OG	2.28	0.47
20:r:112:THR:HG23	20:r:114:GLU:HG2	1.96	0.47
5:L:421:ILE:HG12	5:L:501:ALA:HB2	1.96	0.47
8:V:39:SER:OG	8:V:54:ARG:NH2	2.48	0.47
13:k:53:GLU:OE2	13:k:126:ARG:NH1	2.47	0.47
29:1:184:TYR:HB3	29:1:357:GLU:HB3	1.96	0.47
29:1:390:ASP:O	29:1:393:TRP:HB3	2.15	0.47
31:3:231:MET:HE2	31:3:266:LYS:HD2	1.96	0.47
31:3:515:ARG:NH2	31:3:531:CYS:O	2.46	0.47
34:6:49:THR:O	34:6:49:THR:OG1	2.29	0.47
37:b:55:ARG:NH2	37:b:76:ASP:OD2	2.47	0.47
1:A:24:LEU:HD21	46:6:202:PC1:H3A1	1.95	0.47
2:H:12:PRO:HB2	28:z:19:PRO:HG3	1.97	0.47
5:L:10:VAL:HG21	20:r:78:VAL:HG23	1.96	0.47
5:L:67:HIS:NE2	5:L:70:THR:OG1	2.40	0.47
6:M:139:GLN:HG3	6:M:340:ARG:HH22	1.80	0.47
12:Z:144:ASP:OD2	18:p:122:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:p:48:LEU:HD11	22:t:136:VAL:HG23	1.96	0.47
34:6:92:LEU:HD13	34:6:100:LEU:HD13	1.95	0.47
10:X:2:ASP:N	10:X:2:ASP:OD1	2.48	0.47
32:4:395:GLY:HA2	32:4:423:ILE:HD12	1.96	0.47
35:9:132:VAL:HG11	35:9:169:ILE:HD11	1.97	0.47
5:L:245:ALA:O	5:L:249:SER:OG	2.32	0.47
32:4:73:VAL:HG11	32:4:414:VAL:HG21	1.97	0.47
33:5:182:ARG:HG2	42:g:100:THR:HG22	1.96	0.47
39:d:133:SER:OG	39:d:134:HIS:N	2.47	0.47
6:M:169:ASN:OD1	7:N:272:LYS:NZ	2.48	0.47
10:X:32:VAL:HG22	10:X:74:GLN:HG2	1.96	0.47
29:1:78:LYS:NZ	51:1:502:FMN:O3P	2.42	0.47
29:1:106:LYS:HG2	29:1:257:ASN:HD21	1.80	0.47
33:5:125:LYS:O	33:5:128:ASN:HB3	2.14	0.47
7:N:20:VAL:HG11	7:N:137:ALA:HB1	1.98	0.46
9:W:89:ARG:NH1	27:y:31:ASP:OD2	2.47	0.46
3:J:28:TYR:CZ	3:J:82:VAL:HG23	2.51	0.46
5:L:66:TRP:NE1	46:L:1004:PC1:O12	2.40	0.46
13:k:170:ILE:HD11	13:k:238:ILE:HD11	1.98	0.46
2:H:145:THR:HG22	2:H:294:LEU:HD13	1.97	0.46
5:L:80:PHE:HB3	5:L:82:MET:HE2	1.97	0.46
7:N:173:THR:O	7:N:227:THR:OG1	2.32	0.46
20:r:120:LYS:NZ	21:s:38:MET:O	2.48	0.46
29:1:224:ASN:HB3	29:1:227:THR:HG22	1.97	0.46
29:1:243:ALA:HA	29:1:251:SER:HB3	1.97	0.46
39:d:194:ILE:HD12	39:d:260:HIS:HA	1.97	0.46
7:N:295:ARG:NH2	32:4:20:TYR:OH	2.49	0.46
31:3:337:ARG:HG2	31:3:609:MET:HB3	1.98	0.46
13:k:94:TYR:OH	13:k:151:HIS:ND1	2.41	0.46
14:l:14:ASP:OD1	14:l:14:ASP:N	2.49	0.46
29:1:228:VAL:O	29:1:231:SER:OG	2.30	0.46
29:1:388:GLU:O	29:1:391:SER:HB3	2.16	0.46
31:3:198:ASN:OD1	31:3:268:ARG:NH2	2.46	0.46
39:d:325:ARG:O	39:d:325:ARG:NH1	2.45	0.46
6:M:1:FME:HE2	6:M:1:FME:HB2	1.78	0.46
47:X:101:ZMP:O6	22:t:12:GLN:NE2	2.42	0.46
11:Y:35:CYS:O	11:Y:39:ASN:ND2	2.49	0.46
13:k:157:LYS:HB3	13:k:157:LYS:HE3	1.77	0.46
15:m:14:LYS:HA	15:m:14:LYS:HD3	1.78	0.46
17:o:120:ARG:HD3	18:p:115:ILE:HD13	1.97	0.46
22:t:107:HIS:NE2	25:w:43:ASP:OD1	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:372:MET:HE3	29:1:415:VAL:HG21	1.98	0.46
32:4:101:PRO:O	32:4:105:ARG:NH1	2.48	0.46
32:4:406:SER:HB2	32:4:414:VAL:HG22	1.98	0.46
6:M:324:SER:OG	6:M:440:HIS:NE2	2.41	0.46
22:t:44:ARG:NE	22:t:48:ASP:OD2	2.49	0.46
30:2:112:ASN:O	30:2:115:SER:OG	2.33	0.46
29:1:15:LEU:O	29:1:20:ARG:NH2	2.49	0.46
30:2:16:ASN:OD1	30:2:16:ASN:N	2.48	0.46
5:L:101:MET:HE2	5:L:121:LEU:HB3	1.98	0.45
5:L:538:PRO:HB2	24:v:89:VAL:HG22	1.98	0.45
30:2:105:THR:O	30:2:109:MET:N	2.47	0.45
5:L:29:PHE:HB3	5:L:32:TYR:HB2	1.98	0.45
5:L:316:THR:HB	5:L:395:ILE:HG23	1.98	0.45
5:L:338:MET:HE2	5:L:338:MET:HB3	1.88	0.45
7:N:216:PHE:O	7:N:220:MET:HG2	2.16	0.45
9:W:138:LYS:HA	14:l:27:ARG:HB3	1.98	0.45
20:r:17:LEU:HD11	22:t:162:LEU:HD22	1.99	0.45
25:w:85:MET:HB2	25:w:88:TRP:HB3	1.98	0.45
39:d:181:TYR:O	39:d:185:ILE:HG13	2.16	0.45
6:M:75:LEU:HD11	6:M:439:LEU:HB3	1.98	0.45
7:N:327:PRO:HG3	17:o:45:ASP:HB2	1.98	0.45
29:1:327:THR:OG1	29:1:328:GLY:N	2.50	0.45
39:d:34:LEU:HD21	39:d:92:ILE:HD13	1.98	0.45
3:J:119:PHE:CG	4:K:6:MET:HB2	2.51	0.45
5:L:331:THR:HG23	5:L:387:THR:HB	1.98	0.45
10:X:70:LEU:HD22	10:X:75:GLU:HB3	1.99	0.45
35:9:23:GLN:NE2	35:9:29:GLU:OE1	2.46	0.45
37:b:60:ASP:OD1	37:b:60:ASP:N	2.47	0.45
38:c:133:LYS:HB3	38:c:133:LYS:HE2	1.77	0.45
21:s:33:ARG:HH21	24:v:158:ILE:HB	1.81	0.45
38:c:33:ARG:NH1	38:c:77:ASP:OD1	2.49	0.45
39:d:91:VAL:HG23	39:d:126:VAL:HG11	1.97	0.45
39:d:94:LEU:HD13	39:d:132:ILE:HG13	1.98	0.45
4:K:59:MET:HE2	7:N:84:TRP:HH2	1.82	0.45
5:L:557:TRP:HE1	18:p:85:THR:HG22	1.82	0.45
31:3:632:ARG:NH1	40:e:57:CYS:SG	2.89	0.45
1:A:69:ILE:HG21	2:H:148:ILE:HD11	1.98	0.45
31:3:533:THR:HG23	31:3:535:GLN:H	1.82	0.45
32:4:63:ARG:HB3	32:4:79:HIS:HB2	1.99	0.45
34:6:86:MET:HE1	34:6:104:TYR:HB2	1.99	0.45
5:L:277:MET:HE2	5:L:317:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:14:LEU:HD11	6:M:26:ASN:HB3	1.99	0.45
52:1:503:NAI:H2D	52:1:503:NAI:H6N	1.77	0.45
33:5:178:ASP:OD2	39:d:32:ARG:NH1	2.48	0.45
6:M:47:ASP:OD1	6:M:47:ASP:N	2.46	0.45
6:M:51:ASN:ND2	9:W:90:THR:OG1	2.44	0.45
9:W:48:GLY:O	12:Z:60:TYR:OH	2.34	0.45
17:o:2:MET:O	17:o:5:ARG:HB3	2.16	0.45
34:6:52:LEU:HB2	34:6:90:GLY:HA3	1.98	0.45
2:H:161:THR:HG22	2:H:163:SER:H	1.82	0.45
12:Z:167:LYS:O	12:Z:167:LYS:NZ	2.50	0.45
6:M:410:MET:O	6:M:414:THR:OG1	2.34	0.44
7:N:325:LEU:HD12	45:N:402:3PE:H271	1.99	0.44
12:Z:15:ARG:HB3	20:r:109:ILE:HD12	1.99	0.44
21:s:3:HIS:CE1	24:v:127:PRO:HD3	2.52	0.44
30:2:105:THR:OG1	53:2:300:FES:S2	2.65	0.44
39:d:134:HIS:HB2	39:d:149:LYS:HD2	2.00	0.44
5:L:108:MET:HE3	5:L:108:MET:HB3	1.82	0.44
5:L:338:MET:HB2	5:L:457:LEU:HB3	1.99	0.44
10:X:55:GLU:HG3	10:X:62:ILE:HD12	1.99	0.44
12:Z:27:ASN:OD1	12:Z:27:ASN:N	2.50	0.44
13:k:94:TYR:HB3	13:k:281:GLU:HG2	1.98	0.44
31:3:427:LYS:O	31:3:430:GLN:HB3	2.17	0.44
35:9:64:GLU:OE2	35:9:157:ASN:ND2	2.50	0.44
5:L:76:LEU:HD23	5:L:76:LEU:HA	1.89	0.44
13:k:132:PHE:O	13:k:135:LEU:HB3	2.17	0.44
19:q:6:LYS:HE3	19:q:6:LYS:HB3	1.68	0.44
37:b:84:CYS:CB	37:b:87:CYS:SG	3.06	0.44
43:h:108:ASP:OD1	43:h:108:ASP:N	2.49	0.44
2:H:114:TYR:OH	3:J:61:LEU:O	2.25	0.44
2:H:140:ILE:HG23	3:J:65:MET:HE1	2.00	0.44
2:H:150:LEU:HD12	2:H:150:LEU:HA	1.86	0.44
5:L:89:PHE:HB2	5:L:326:PHE:HZ	1.82	0.44
5:L:526:LEU:HD12	5:L:530:PRO:HG2	1.99	0.44
7:N:149:ILE:H	7:N:149:ILE:HD12	1.80	0.44
10:X:47:GLN:NE2	10:X:70:LEU:O	2.49	0.44
12:Z:26:PRO:HB2	12:Z:31:TYR:HE2	1.83	0.44
12:Z:167:LYS:HZ3	12:Z:170:LYS:HE2	1.82	0.44
13:k:91:GLY:HA3	13:k:281:GLU:HG3	1.98	0.44
2:H:228:TYR:HD1	2:H:228:TYR:HA	1.71	0.44
3:J:67:VAL:HG11	4:K:31:LEU:HD21	1.98	0.44
5:L:511:LEU:HD23	22:t:35:LYS:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:278:ARG:NH2	24:v:80:ASP:OD1	2.49	0.44
7:N:265:MET:HE1	11:Y:166:LEU:HD11	2.00	0.44
23:u:18:THR:HG22	23:u:20:SER:H	1.82	0.44
24:v:53:ARG:NH1	24:v:57:GLU:OE1	2.41	0.44
34:6:69:MET:HE3	34:6:74:VAL:HG12	1.99	0.44
2:H:24:GLU:O	2:H:28:LEU:HB2	2.18	0.44
4:K:32:CYS:O	4:K:36:MET:HG3	2.18	0.44
22:t:23:LEU:HD23	22:t:23:LEU:HA	1.85	0.44
31:3:146:VAL:HG22	31:3:200:ILE:HD11	1.99	0.44
3:J:124:ASP:N	3:J:124:ASP:OD1	2.51	0.44
10:X:15:VAL:HG23	10:X:54:MET:SD	2.58	0.44
39:d:48:PRO:HA	39:d:71:MET:O	2.18	0.44
19:q:22:ARG:NH2	43:h:111:TYR:OH	2.49	0.44
29:1:118:LEU:HD13	29:1:225:VAL:HG13	2.00	0.44
30:2:31:ILE:HG12	30:2:50:VAL:HG22	2.00	0.44
31:3:206:GLY:N	50:3:801:SF4:S2	2.85	0.44
31:3:243:ARG:HD2	31:3:244:THR:HG23	1.99	0.44
34:6:125:TYR:CE1	35:9:117:ILE:HD13	2.52	0.44
15:m:9:LYS:NZ	35:9:12:MET:SD	2.91	0.43
29:1:77:LEU:HD23	29:1:77:LEU:HA	1.87	0.43
31:3:126:ASP:OD1	31:3:126:ASP:N	2.51	0.43
32:4:8:VAL:O	32:4:12:GLU:HB2	2.18	0.43
39:d:186:ARG:HH21	39:d:321:HIS:HB3	1.81	0.43
10:j:71:MET:SD	10:j:71:MET:N	2.91	0.43
6:M:311:GLY:O	6:M:315:LEU:HB2	2.18	0.43
15:m:39:LYS:O	15:m:43:MET:HG3	2.18	0.43
18:p:39:ARG:NH2	22:t:3:LEU:O	2.51	0.43
20:r:4:THR:N	20:r:7:GLU:OE2	2.51	0.43
31:3:12:PHE:HB2	31:3:78:ASN:HA	1.99	0.43
33:5:56:GLY:HA2	33:5:59:PRO:HD2	2.00	0.43
35:9:95:GLU:HB2	35:9:108:ARG:HB3	1.99	0.43
35:9:101:ASP:OD1	35:9:101:ASP:N	2.36	0.43
6:M:171:MET:HE3	6:M:179:LEU:HD22	2.01	0.43
29:1:82:MET:SD	29:1:221:THR:OG1	2.72	0.43
33:5:33:LEU:HD21	41:f:93:MET:HE1	2.00	0.43
2:H:24:GLU:HA	2:H:271:LEU:HD13	2.00	0.43
2:H:97:ASN:H	19:q:143:THR:HG22	1.84	0.43
13:k:265:ASP:HB3	13:k:268:GLU:HB3	2.00	0.43
35:9:1:THR:N	43:h:104:GLU:O	2.39	0.43
10:j:14:ARG:NH2	10:j:57:GLU:OE2	2.51	0.43
2:H:165:LEU:HD21	2:H:241:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:221:VAL:O	6:M:340:ARG:NH1	2.50	0.43
13:k:244:ASP:OD1	13:k:244:ASP:N	2.50	0.43
28:z:59:ARG:HB2	28:z:62:VAL:HG23	2.00	0.43
29:1:260:GLY:O	30:2:111:ARG:NH1	2.52	0.43
31:3:244:THR:HB	38:c:73:ALA:HB2	2.01	0.43
5:L:249:SER:HB2	5:L:336:LYS:HG3	2.00	0.43
7:N:207:ILE:O	7:N:211:MET:HG3	2.18	0.43
19:q:34:MET:HE2	19:q:34:MET:HB3	1.91	0.43
32:4:58:ALA:HB1	32:4:62:LEU:HB3	2.01	0.43
33:5:49:GLU:HG2	33:5:108:LYS:HD2	2.00	0.43
34:6:34:ASP:OD2	34:6:173:LEU:N	2.50	0.43
21:s:56:ASP:OD1	21:s:56:ASP:N	2.45	0.43
25:w:80:LEU:HD23	25:w:80:LEU:HA	1.92	0.43
2:H:192:GLU:OE1	2:H:193:THR:OG1	2.31	0.43
3:J:17:PHE:HA	3:J:20:PHE:CE1	2.54	0.43
7:N:289:ASN:HA	7:N:292:PHE:CE2	2.54	0.43
29:1:48:ILE:HG12	30:2:217:LEU:HD11	2.01	0.43
3:J:172:THR:O	3:J:172:THR:OG1	2.36	0.43
6:M:91:ARG:NH2	13:k:290:ASP:OD2	2.52	0.43
14:l:103:LEU:HD12	14:l:103:LEU:HA	1.88	0.43
29:1:13:GLY:N	29:1:271:GLU:OE1	2.48	0.43
32:4:410:MET:H	32:4:413:ASP:HB2	1.84	0.43
13:k:1:LEU:HB3	13:k:2:GLN:H	1.61	0.43
13:k:51:PHE:HB3	13:k:107:GLN:HE21	1.84	0.43
33:5:33:LEU:HD13	33:5:60:VAL:HG22	2.00	0.43
35:9:135:PRO:HG3	35:9:164:GLU:HG2	2.01	0.43
2:H:16:ALA:HB2	28:z:15:CYS:HB3	2.00	0.42
2:H:142:TYR:HE2	2:H:146:LEU:HD22	1.84	0.42
5:L:7:LEU:HD23	5:L:7:LEU:HA	1.89	0.42
6:M:119:TYR:CZ	6:M:161:LEU:HB2	2.54	0.42
29:1:76:GLY:O	29:1:80:SER:OG	2.26	0.42
32:4:338:MET:HE3	32:4:338:MET:HB3	1.89	0.42
32:4:352:TYR:HD1	35:9:86:VAL:HG21	1.84	0.42
2:H:200:LEU:HD22	2:H:282:TYR:HB3	2.01	0.42
9:W:109:GLU:OE2	9:W:112:ARG:NH2	2.45	0.42
33:5:90:PHE:HZ	33:5:163:ARG:HE	1.66	0.42
35:9:105:ARG:NH2	37:b:86:TYR:O	2.48	0.42
46:M:502:PC1:H371	7:N:280:THR:HG21	2.01	0.42
20:r:72:THR:HA	20:r:76:ILE:HD12	2.01	0.42
24:v:82:ASP:OD1	24:v:82:ASP:N	2.51	0.42
29:1:164:LYS:NZ	36:a:63:MET:SD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:3:217:ALA:HB2	31:3:248:MET:HE2	2.01	0.42
10:j:65:ILE:O	10:j:69:LYS:NZ	2.52	0.42
2:H:32:GLN:HG2	32:4:165:THR:HG23	2.01	0.42
5:L:83:ASP:OD1	5:L:83:ASP:N	2.51	0.42
5:L:457:LEU:HD23	5:L:457:LEU:HA	1.89	0.42
7:N:133:TRP:HE3	45:N:402:3PE:H382	1.84	0.42
9:W:28:TYR:O	25:w:67:SER:OG	2.29	0.42
29:1:276:LEU:HD13	29:1:317:MET:HE2	2.01	0.42
3:J:175:ASN:OD1	3:J:175:ASN:N	2.53	0.42
5:L:131:LEU:HB2	5:L:143:GLY:HA3	2.00	0.42
29:1:370:ASP:OD2	31:3:179:ASN:ND2	2.43	0.42
38:c:45:MET:HE3	38:c:45:MET:HB3	1.94	0.42
44:i:32:ASP:OD2	44:i:58:ARG:NH2	2.52	0.42
5:L:419:THR:HA	5:L:422:TYR:CE2	2.55	0.42
7:N:251:MET:HE2	7:N:251:MET:HB3	1.81	0.42
20:r:75:LEU:HD12	20:r:75:LEU:HA	1.91	0.42
27:y:8:ARG:HG3	27:y:10:HIS:H	1.84	0.42
31:3:241:SER:HB2	31:3:249:ARG:HG2	2.01	0.42
32:4:190:HIS:CD2	34:6:150:PRO:HD3	2.54	0.42
35:9:27:TRP:HB3	35:9:30:LEU:HD12	2.01	0.42
3:J:164:GLY:O	3:J:168:ILE:HG12	2.20	0.42
7:N:218:LEU:HD13	7:N:244:VAL:HG12	2.02	0.42
13:k:112:LEU:HD23	13:k:112:LEU:HA	1.89	0.42
30:2:39:PRO:HA	36:a:65:GLN:HB3	2.01	0.42
3:J:82:VAL:HG13	3:J:83:TRP:H	1.84	0.42
5:L:487:LYS:HE3	23:u:49:GLY:HA2	2.02	0.42
6:M:106:LEU:HD13	6:M:234:ILE:HG21	2.01	0.42
7:N:337:LEU:O	7:N:340:THR:OG1	2.32	0.42
9:W:88:GLU:OE1	27:y:56:TRP:NE1	2.41	0.42
9:W:114:MET:HE2	9:W:120:GLY:HA3	2.02	0.42
13:k:67:LYS:HA	13:k:67:LYS:HD3	1.77	0.42
29:1:295:LEU:HD22	29:1:339:ARG:HA	2.02	0.42
32:4:143:GLU:OE2	32:4:278:TYR:OH	2.26	0.42
5:L:584:ILE:H	5:L:584:ILE:HG13	1.67	0.42
13:k:65:ASP:N	13:k:65:ASP:OD1	2.38	0.42
17:o:11:LEU:HD23	17:o:11:LEU:HA	1.94	0.42
17:o:46:ASN:HB3	17:o:53:VAL:HA	2.02	0.42
17:o:95:LYS:HB3	17:o:95:LYS:HE2	1.82	0.42
21:s:14:VAL:HG22	21:s:112:LYS:HD3	2.02	0.42
32:4:61:VAL:HB	32:4:82:LEU:HB2	2.02	0.42
2:H:87:ILE:HG13	2:H:88:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:106:TRP:HB2	5:L:449:PHE:HB2	2.02	0.42
5:L:287:PHE:HA	5:L:290:MET:HE3	2.01	0.42
7:N:243:LEU:HD22	7:N:330:THR:HG21	2.02	0.42
1:A:6:THR:HG21	2:H:87:ILE:HG21	2.02	0.41
5:L:572:LYS:HA	5:L:572:LYS:HD2	1.85	0.41
6:M:361:LEU:HD23	6:M:361:LEU:HA	1.91	0.41
12:Z:85:PHE:O	12:Z:89:MET:HG2	2.20	0.41
19:q:57:ARG:HD2	19:q:57:ARG:HA	1.78	0.41
38:c:9:GLN:HA	42:g:22:ARG:HH22	1.85	0.41
39:d:320:ARG:HH21	39:d:321:HIS:CE1	2.38	0.41
5:L:571:MET:HB2	5:L:571:MET:HE3	1.76	0.41
20:r:109:ILE:HG22	20:r:111:GLU:H	1.85	0.41
21:s:100:GLU:HG2	24:v:158:ILE:HG21	2.01	0.41
10:j:51:ILE:O	10:j:55:GLU:HG3	2.19	0.41
2:H:205:SER:OG	32:4:160:ASP:O	2.32	0.41
6:M:200:MET:O	6:M:204:MET:HG2	2.20	0.41
6:M:364:LEU:HD23	6:M:364:LEU:HA	1.85	0.41
7:N:41:ILE:HD13	7:N:41:ILE:HA	1.90	0.41
12:Z:42:ARG:HE	12:Z:42:ARG:HB3	1.64	0.41
28:z:52:ARG:NH1	28:z:58:ASN:OD1	2.45	0.41
29:1:202:LYS:HA	29:1:203:PRO:HD3	1.96	0.41
30:2:30:ARG:HD3	36:a:52:LEU:HB3	2.02	0.41
35:9:14:MET:O	35:9:18:THR:OG1	2.31	0.41
40:e:63:LYS:HB2	40:e:63:LYS:HE3	1.87	0.41
4:K:93:LEU:HD22	7:N:54:GLU:HG3	2.01	0.41
5:L:328:HIS:O	5:L:332:HIS:HB3	2.21	0.41
5:L:341:MET:HE3	5:L:341:MET:HB3	1.84	0.41
7:N:88:LYS:HE3	7:N:88:LYS:HB2	1.88	0.41
31:3:591:GLY:HA2	39:d:6:ILE:HG21	2.03	0.41
38:c:112:LYS:O	38:c:114:LYS:NZ	2.44	0.41
5:L:309:GLN:O	5:L:313:MET:HG2	2.20	0.41
45:N:402:3PE:H2G2	45:N:402:3PE:H2D2	1.95	0.41
18:p:51:ASN:HD22	22:t:165:LEU:HD22	1.85	0.41
24:v:126:GLN:HG3	24:v:127:PRO:HD2	2.03	0.41
29:1:91:LYS:HB2	29:1:131:ALA:HA	2.02	0.41
39:d:130:ILE:HG12	39:d:164:THR:HB	2.02	0.41
6:M:252:PRO:HG3	17:o:117:HIS:CD2	2.55	0.41
29:1:69:GLY:O	52:1:503:NAI:H2N	2.20	0.41
31:3:276:ARG:NH1	31:3:680:ALA:O	2.53	0.41
1:A:38:GLU:HB2	1:A:43:PRO:HG3	2.02	0.41
2:H:79:LEU:HD22	2:H:222:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:59:MET:HE2	7:N:84:TRP:CH2	2.56	0.41
11:Y:101:LYS:HE3	11:Y:101:LYS:HB3	1.98	0.41
18:p:10:LEU:HA	24:v:91:THR:HG22	2.01	0.41
19:q:120:MET:HE2	19:q:120:MET:HB2	1.97	0.41
22:t:153:LEU:HD13	22:t:154:PRO:HD2	2.02	0.41
30:2:14:LYS:HA	30:2:14:LYS:HD2	1.87	0.41
40:e:17:GLU:OE2	40:e:67:ARG:NE	2.40	0.41
5:L:159:TYR:HB2	6:M:416:ARG:HB3	2.02	0.41
15:m:31:LEU:HD12	15:m:31:LEU:HA	1.90	0.41
17:o:52:PRO:HG2	17:o:56:ALA:HB2	2.01	0.41
1:A:79:SER:HA	1:A:87:MET:HE2	2.03	0.41
2:H:120:GLY:HA2	2:H:128:ALA:HB1	2.02	0.41
3:J:23:LYS:O	4:K:23:ARG:NH1	2.54	0.41
3:J:26:PRO:HB2	3:J:71:THR:HG21	2.03	0.41
5:L:416:THR:O	5:L:419:THR:OG1	2.33	0.41
6:M:12:MET:HA	6:M:15:THR:HG22	2.02	0.41
18:p:36:LEU:HD22	22:t:7:ALA:HB2	2.03	0.41
25:w:97:VAL:HG13	25:w:107:LEU:HD11	2.02	0.41
30:2:53:LEU:HD12	36:a:52:LEU:HG	2.03	0.41
31:3:21:GLU:O	31:3:24:THR:OG1	2.38	0.41
32:4:179:GLU:OE2	34:6:66:ARG:NH1	2.43	0.41
42:g:28:LYS:HB3	42:g:28:LYS:HE2	1.87	0.41
4:K:26:LEU:HD23	4:K:26:LEU:HA	1.97	0.41
6:M:72:LEU:HD23	6:M:72:LEU:HA	1.91	0.41
14:l:82:ARG:HB2	19:q:96:ILE:HD13	2.02	0.41
2:H:93:TYR:OH	28:z:35:GLU:OE2	2.31	0.40
2:H:179:TRP:HE1	19:q:42:LEU:HG	1.85	0.40
46:L:1004:PC1:H3F1	6:M:447:LEU:HD11	2.02	0.40
19:q:89:ASN:ND2	19:q:123:LEU:O	2.44	0.40
22:t:128:ARG:HD2	22:t:167:TRP:CD2	2.56	0.40
25:w:114:ASP:HB3	25:w:117:LYS:HG2	2.03	0.40
29:1:70:GLY:O	52:1:503:NAI:O3D	2.36	0.40
29:1:125:GLY:O	29:1:129:MET:HG2	2.21	0.40
39:d:26:ALA:HA	39:d:31:GLY:HA3	2.03	0.40
3:J:20:PHE:HZ	4:K:35:GLY:HA3	1.86	0.40
5:L:381:THR:HG22	5:L:420:ALA:HA	2.02	0.40
9:W:95:GLN:HB2	12:Z:82:LEU:HD21	2.04	0.40
13:k:115:LEU:HD13	13:k:121:GLY:HA2	2.03	0.40
14:l:87:LYS:HB2	14:l:87:LYS:HE3	1.87	0.40
17:o:20:SER:OG	26:x:45:ARG:NH1	2.51	0.40
19:q:9:MET:HE3	19:q:9:MET:HB3	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:x:27:LEU:HD23	26:x:27:LEU:HA	1.94	0.40
5:L:208:ASP:OD1	5:L:208:ASP:N	2.44	0.40
5:L:564:LYS:HD3	5:L:564:LYS:HA	1.92	0.40
7:N:84:TRP:HB2	14:l:18:THR:HA	2.03	0.40
7:N:272:LYS:HD3	9:W:108:LEU:HD21	2.03	0.40
11:Y:150:ASN:OD1	14:l:50:ARG:NH1	2.54	0.40
19:q:19:ASP:OD1	19:q:19:ASP:N	2.54	0.40
20:r:17:LEU:HD23	20:r:17:LEU:HA	1.95	0.40
22:t:143:THR:HA	22:t:144:PRO:HD3	1.96	0.40
28:z:9:ILE:O	28:z:12:MET:HB2	2.22	0.40
32:4:166:PRO:HA	32:4:169:TRP:HB2	2.03	0.40
2:H:80:THR:O	2:H:84:THR:HG22	2.21	0.40
4:K:64:LEU:O	4:K:67:ALA:HB3	2.22	0.40
6:M:321:LEU:HD13	6:M:444:LEU:HB2	2.03	0.40
13:k:83:TYR:HD1	13:k:83:TYR:HA	1.79	0.40
22:t:30:CYS:HB3	22:t:35:LYS:HE2	2.02	0.40
22:t:108:PRO:HA	22:t:111:LYS:HB2	2.03	0.40
34:6:34:ASP:OD1	34:6:38:ASN:ND2	2.54	0.40
44:i:117:LEU:O	44:i:120:THR:OG1	2.34	0.40
4:K:48:ILE:HD11	4:K:59:MET:HE3	2.04	0.40
5:L:193:LEU:HD23	5:L:201:ILE:HA	2.04	0.40
17:o:110:ARG:HG3	17:o:111:GLU:HG3	2.02	0.40
20:r:85:LEU:HA	20:r:89:VAL:HB	2.04	0.40
20:r:121:GLU:OE1	20:r:121:GLU:N	2.52	0.40
31:3:227:SER:OG	31:3:228:ILE:N	2.54	0.40
31:3:375:ASP:N	31:3:375:ASP:OD1	2.55	0.40
32:4:111:MET:HE2	32:4:111:MET:HB2	1.95	0.40
32:4:227:GLU:HG2	35:9:36:MET:HE3	2.04	0.40
38:c:124:TRP:CD1	38:c:125:ASN:HD22	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
2	H	316/318 (99%)	305 (96%)	11 (4%)	0	100	100
3	J	173/175 (99%)	167 (96%)	5 (3%)	1 (1%)	21	53
4	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
5	L	604/606 (100%)	584 (97%)	20 (3%)	0	100	100
6	M	457/459 (100%)	449 (98%)	8 (2%)	0	100	100
7	N	345/347 (99%)	335 (97%)	10 (3%)	0	100	100
8	V	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
9	W	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
10	X	85/157 (54%)	80 (94%)	5 (6%)	0	100	100
10	j	80/157 (51%)	80 (100%)	0	0	100	100
11	Y	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
12	Z	169/171 (99%)	167 (99%)	2 (1%)	0	100	100
13	k	317/320 (99%)	307 (97%)	10 (3%)	0	100	100
14	l	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
15	m	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
16	n	77/79 (98%)	75 (97%)	2 (3%)	0	100	100
17	o	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
18	p	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
19	q	137/139 (99%)	135 (98%)	2 (2%)	0	100	100
20	r	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
21	s	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
22	t	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
23	u	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
24	v	153/155 (99%)	149 (97%)	4 (3%)	0	100	100
25	w	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
26	x	47/49 (96%)	47 (100%)	0	0	100	100
27	y	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
28	z	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
29	1	428/430 (100%)	415 (97%)	13 (3%)	0	100	100
30	2	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
31	3	686/688 (100%)	663 (97%)	23 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	4	427/430 (99%)	410 (96%)	17 (4%)	0	100	100
33	5	206/208 (99%)	197 (96%)	9 (4%)	0	100	100
34	6	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
35	9	174/217 (80%)	167 (96%)	7 (4%)	0	100	100
36	a	42/44 (96%)	42 (100%)	0	0	100	100
37	b	93/95 (98%)	91 (98%)	2 (2%)	0	100	100
38	c	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
39	d	338/340 (99%)	327 (97%)	11 (3%)	0	100	100
40	e	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
41	f	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
42	g	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
43	h	92/114 (81%)	89 (97%)	3 (3%)	0	100	100
44	i	143/145 (99%)	140 (98%)	3 (2%)	0	100	100
All	All	8131/8460 (96%)	7874 (97%)	256 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	116	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	103/103 (100%)	103 (100%)	0	100	100
2	H	278/278 (100%)	277 (100%)	1 (0%)	84	81
3	J	144/144 (100%)	144 (100%)	0	100	100
4	K	86/86 (100%)	86 (100%)	0	100	100
5	L	538/538 (100%)	535 (99%)	3 (1%)	78	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	M	411/411 (100%)	410 (100%)	1 (0%)	87	84
7	N	315/315 (100%)	314 (100%)	1 (0%)	86	83
8	V	101/101 (100%)	100 (99%)	1 (1%)	68	76
9	W	122/122 (100%)	122 (100%)	0	100	100
10	X	80/141 (57%)	80 (100%)	0	100	100
10	j	76/141 (54%)	76 (100%)	0	100	100
11	Y	154/154 (100%)	154 (100%)	0	100	100
12	Z	155/155 (100%)	155 (100%)	0	100	100
13	k	283/283 (100%)	282 (100%)	1 (0%)	84	81
14	l	94/94 (100%)	93 (99%)	1 (1%)	65	75
15	m	69/69 (100%)	68 (99%)	1 (1%)	59	72
16	n	61/61 (100%)	61 (100%)	0	100	100
17	o	107/107 (100%)	107 (100%)	0	100	100
18	p	114/114 (100%)	114 (100%)	0	100	100
19	q	119/119 (100%)	118 (99%)	1 (1%)	73	77
20	r	95/122 (78%)	95 (100%)	0	100	100
21	s	110/110 (100%)	109 (99%)	1 (1%)	70	76
22	t	159/159 (100%)	159 (100%)	0	100	100
23	u	59/59 (100%)	59 (100%)	0	100	100
24	v	140/140 (100%)	140 (100%)	0	100	100
25	w	92/92 (100%)	92 (100%)	0	100	100
26	x	44/44 (100%)	44 (100%)	0	100	100
27	y	46/46 (100%)	46 (100%)	0	100	100
28	z	59/59 (100%)	59 (100%)	0	100	100
29	1	344/344 (100%)	343 (100%)	1 (0%)	86	83
30	2	183/183 (100%)	182 (100%)	1 (0%)	81	81
31	3	578/578 (100%)	576 (100%)	2 (0%)	86	83
32	4	370/370 (100%)	369 (100%)	1 (0%)	86	83
33	5	189/189 (100%)	189 (100%)	0	100	100
34	6	132/132 (100%)	132 (100%)	0	100	100
35	9	151/179 (84%)	150 (99%)	1 (1%)	76	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	a	43/43 (100%)	42 (98%)	1 (2%)	44	65
37	b	79/79 (100%)	79 (100%)	0	100	100
38	c	113/113 (100%)	113 (100%)	0	100	100
39	d	294/294 (100%)	294 (100%)	0	100	100
40	e	76/76 (100%)	76 (100%)	0	100	100
41	f	101/101 (100%)	100 (99%)	1 (1%)	68	76
42	g	107/107 (100%)	107 (100%)	0	100	100
43	h	84/96 (88%)	84 (100%)	0	100	100
44	i	131/131 (100%)	131 (100%)	0	100	100
All	All	7189/7382 (97%)	7169 (100%)	20 (0%)	84	83

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	241	LEU
5	L	17	MET
5	L	29	PHE
5	L	40	ILE
6	M	254	THR
7	N	294	MET
8	V	84	ASP
13	k	263	VAL
14	l	17	MET
15	m	61	ASN
19	q	99	ASP
21	s	41	THR
29	1	359	CYS
30	2	122	LYS
31	3	315	VAL
31	3	656	LEU
32	4	171	PHE
35	9	78	ILE
36	a	58	LEU
41	f	78	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
2	H	194	ASN
2	H	304	HIS
5	L	135	ASN
5	L	199	GLN
5	L	210	ASN
5	L	270	ASN
5	L	434	GLN
5	L	479	GLN
5	L	603	ASN
6	M	399	ASN
7	N	222	ASN
8	V	78	GLN
10	X	35	HIS
11	Y	142	HIS
12	Z	54	GLN
12	Z	58	ASN
13	k	200	GLN
13	k	294	GLN
14	l	76	ASN
14	l	81	GLN
15	m	73	GLN
17	o	79	GLN
17	o	97	HIS
19	q	60	GLN
20	r	13	GLN
20	r	25	GLN
21	s	42	GLN
21	s	43	GLN
21	s	46	ASN
22	t	17	GLN
22	t	32	HIS
24	v	55	GLN
26	x	34	GLN
26	x	46	ASN
27	y	10	HIS
27	y	30	ASN
29	1	150	GLN
29	1	264	ASN
29	1	402	HIS
30	2	57	GLN
30	2	58	ASN
30	2	112	ASN

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Mol	Chain	Res	Type
30	2	150	ASN
31	3	36	GLN
31	3	237	ASN
31	3	255	HIS
31	3	475	GLN
31	3	581	GLN
31	3	621	ASN
32	4	280	GLN
36	a	75	HIS
37	b	16	GLN
39	d	67	GLN
39	d	103	ASN
39	d	148	ASN
39	d	184	ASN
39	d	234	ASN
10	j	33	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 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	$\# Z > 2$
43	AYA	h	1	43	6,7,8	1.29	1 (16%)	6,8,10	1.16	1 (16%)
32	2MR	4	85	32	10,12,13	2.50	2 (20%)	5,13,15	1.06	1 (20%)
5	FME	L	1	5	8,9,10	0.95	0	8,9,11	0.92	0
4	FME	K	1	4	8,9,10	0.94	0	8,9,11	0.97	0
8	AYA	V	1	8	6,7,8	1.24	1 (16%)	6,8,10	1.70	2 (33%)
6	FME	M	1	6	8,9,10	1.00	1 (12%)	8,9,11	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	SEP	k	36	13	8,9,10	1.61	1 (12%)	7,12,14	1.32	1 (14%)

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
43	AYA	h	1	43	-	0/5/6/8	-
32	2MR	4	85	32	-	2/10/13/15	-
5	FME	L	1	5	-	3/7/9/11	-
4	FME	K	1	4	-	3/7/9/11	-
8	AYA	V	1	8	-	3/5/6/8	-
6	FME	M	1	6	-	2/7/9/11	-
13	SEP	k	36	13	-	1/6/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	4	85	2MR	CZ-NH2	5.28	1.44	1.33
32	4	85	2MR	CZ-NE	5.24	1.45	1.34
13	k	36	SEP	P-O1P	3.52	1.61	1.50
43	h	1	AYA	CA-N	-2.45	1.43	1.46
8	V	1	AYA	CA-N	-2.23	1.44	1.46
6	M	1	FME	CA-N	-2.07	1.43	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	1	AYA	CB-CA-N	3.14	113.22	109.68
13	k	36	SEP	OG-CB-CA	2.88	110.94	108.14
43	h	1	AYA	CB-CA-N	2.57	112.58	109.68
8	V	1	AYA	CA-N-CT	2.24	124.39	121.50
32	4	85	2MR	CD-NE-CZ	2.11	127.32	123.36

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	1	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
4	K	1	FME	C-CA-CB-CG
4	K	1	FME	O-C-CA-CB
6	M	1	FME	C-CA-CB-CG
6	M	1	FME	O-C-CA-CB
8	V	1	AYA	O-C-CA-CB
32	4	85	2MR	C-CA-CB-CG
5	L	1	FME	CA-CB-CG-SD
8	V	1	AYA	OT-CT-N-CA
8	V	1	AYA	CM-CT-N-CA
5	L	1	FME	CB-CG-SD-CE
13	k	36	SEP	N-CA-CB-OG
32	4	85	2MR	CA-CB-CG-CD
5	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
6	M	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 2 are monoatomic - leaving 33 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	$\# Z > 2$
45	3PE	p	201	-	26,26,50	0.49	0	29,31,55	0.51	1 (3%)
50	SF4	3	802	31	0,12,12	-	-	-		
56	NDP	d	401	-	51,52,52	0.33	0	71,80,80	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	3PE	6	203	-	50,50,50	0.30	0	53,55,55	0.29	0
50	SF4	9	201	35	0,12,12	-	-	-		
46	PC1	L	1004	-	53,53,53	0.29	0	59,61,61	0.31	0
45	3PE	N	401	-	39,39,50	0.33	0	42,44,55	0.31	0
45	3PE	J	201	-	50,50,50	0.30	0	53,55,55	0.31	0
47	ZMP	X	101	10	25,30,36	0.74	1 (4%)	29,37,45	0.94	1 (3%)
45	3PE	V	400	-	36,36,50	0.34	0	39,41,55	0.33	0
50	SF4	1	501	29	0,12,12	-	-	-		
46	PC1	6	202	-	45,45,53	0.31	0	51,53,61	0.31	0
45	3PE	i	201	-	50,50,50	0.30	0	53,55,55	0.28	0
45	3PE	J	202	-	39,39,50	0.34	0	42,44,55	0.30	0
46	PC1	L	1003	-	53,53,53	0.30	0	59,61,61	0.56	2 (3%)
53	FES	2	300	30	0,4,4	-	-	-		
50	SF4	9	202	35	0,12,12	-	-	-		
45	3PE	M	501	-	43,43,50	0.32	0	46,48,55	0.35	0
46	PC1	H	401	-	53,53,53	0.29	0	59,61,61	0.45	0
45	3PE	L	1002	-	30,30,50	0.41	0	33,35,55	0.76	2 (6%)
45	3PE	o	501	-	30,30,50	0.38	0	33,35,55	0.36	0
46	PC1	M	502	-	53,53,53	0.29	0	59,61,61	0.33	0
49	MYR	s	201	21	13,14,15	0.15	0	12,13,15	0.15	0
51	FMN	1	502	-	33,33,33	1.05	2 (6%)	48,50,50	1.25	8 (16%)
52	NAI	1	503	-	47,48,48	0.41	1 (2%)	64,73,73	1.79	4 (6%)
48	AMP	k	501	-	25,25,25	1.40	4 (16%)	37,38,38	1.91	9 (24%)
47	ZMP	j	101	10	28,33,36	0.65	1 (3%)	32,40,45	1.05	1 (3%)
45	3PE	N	402	-	50,50,50	0.32	0	53,55,55	0.50	1 (1%)
53	FES	3	803	31	0,4,4	-	-	-		
50	SF4	6	201	34	0,12,12	-	-	-		
50	SF4	3	801	31	0,12,12	-	-	-		
45	3PE	A	201	-	50,50,50	0.30	0	53,55,55	0.29	0
45	3PE	L	1001	-	50,50,50	0.29	0	53,55,55	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	p	201	-	-	7/27/27/54	-
50	SF4	3	802	31	-	-	0/6/5/5
56	NDP	d	401	-	-	9/34/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	6	203	-	-	7/54/54/54	-
50	SF4	9	201	35	-	-	0/6/5/5
46	PC1	L	1004	-	-	10/57/57/57	-
45	3PE	N	401	-	-	9/43/43/54	-
45	3PE	J	201	-	-	12/54/54/54	-
47	ZMP	X	101	10	-	8/35/37/43	-
45	3PE	V	400	-	-	12/40/40/54	-
50	SF4	1	501	29	-	-	0/6/5/5
46	PC1	6	202	-	-	6/49/49/57	-
45	3PE	i	201	-	-	8/54/54/54	-
45	3PE	J	202	-	-	10/43/43/54	-
46	PC1	L	1003	-	-	18/57/57/57	-
53	FES	2	300	30	-	-	0/1/1/1
50	SF4	9	202	35	-	-	0/6/5/5
45	3PE	M	501	-	-	10/47/47/54	-
46	PC1	H	401	-	-	12/57/57/57	-
45	3PE	L	1002	-	-	8/34/34/54	-
45	3PE	o	501	-	-	5/34/34/54	-
46	PC1	M	502	-	-	16/57/57/57	-
49	MYR	s	201	21	-	0/12/12/13	-
51	FMN	1	502	-	-	9/18/18/18	0/3/3/3
52	NAI	1	503	-	-	6/29/72/72	0/5/5/5
48	AMP	k	501	-	-	2/10/26/26	0/3/3/3
47	ZMP	j	101	10	-	12/38/40/43	-
45	3PE	N	402	-	-	14/54/54/54	-
53	FES	3	803	31	-	-	0/1/1/1
50	SF4	6	201	34	-	-	0/6/5/5
50	SF4	3	801	31	-	-	0/6/5/5
45	3PE	A	201	-	-	16/54/54/54	-
45	3PE	L	1001	-	-	9/54/54/54	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	k	501	AMP	C5-C4	4.56	1.47	1.39
51	1	502	FMN	C4A-N5	3.24	1.37	1.30
48	k	501	AMP	C5-C6	2.67	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	X	101	ZMP	C9-C10	2.49	1.53	1.50
48	k	501	AMP	C8-N7	2.33	1.36	1.31
48	k	501	AMP	C5-N7	-2.30	1.34	1.39
51	1	502	FMN	C10-N1	2.27	1.37	1.33
47	j	101	ZMP	C9-C10	2.25	1.53	1.50
52	1	503	NAI	PA-O5B	2.12	1.67	1.59

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	1	503	NAI	O5B-PA-O1A	-9.57	70.99	108.94
52	1	503	NAI	O2A-PA-O1A	-8.31	73.79	112.44
48	k	501	AMP	C5-C4-N3	-5.76	118.78	126.72
52	1	503	NAI	O3-PA-O1A	-5.70	93.57	110.70
48	k	501	AMP	N3-C4-N9	4.62	135.03	127.17
48	k	501	AMP	C2-N3-C4	3.72	120.91	111.83
48	k	501	AMP	C4-C5-N7	-3.49	106.60	110.58
51	1	502	FMN	C4-N3-C2	-3.39	119.62	125.64
48	k	501	AMP	N3-C2-N1	-3.30	123.59	128.58
47	j	101	ZMP	O1-C10-C9	-3.03	120.48	123.98
48	k	501	AMP	C4-N9-C8	2.90	108.78	105.74
51	1	502	FMN	C4A-C10-N10	2.83	120.54	116.48
51	1	502	FMN	C4A-C4-N3	2.68	120.08	113.25
48	k	501	AMP	C5-N7-C8	2.63	107.58	103.45
47	X	101	ZMP	O1-C10-C9	-2.60	120.98	123.98
51	1	502	FMN	O4-C4-C4A	-2.54	119.82	126.53
52	1	503	NAI	O2A-PA-O5B	2.50	118.88	107.57
51	1	502	FMN	C10-C4A-N5	-2.30	120.10	124.81
46	L	1003	PC1	C2-O21-C21	2.27	123.23	117.80
45	L	1002	3PE	C2-O21-C21	2.19	123.03	117.80
48	k	501	AMP	C6-C5-N7	2.18	136.29	132.09
48	k	501	AMP	N9-C8-N7	-2.18	110.85	113.94
51	1	502	FMN	C5A-C9A-N10	2.17	119.93	117.97
45	p	201	3PE	O12-P-O14	2.12	119.10	110.83
45	L	1002	3PE	O21-C2-C1	2.12	115.93	108.34
51	1	502	FMN	C4A-C10-N1	-2.08	119.49	124.59
51	1	502	FMN	C9A-C5A-N5	-2.07	120.25	122.45
46	L	1003	PC1	O21-C2-C1	2.05	115.69	108.34
45	N	402	3PE	C2-O21-C21	2.04	122.69	117.80

There are no chirality outliers.

All (235) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C1-O11-P-O12
45	A	201	3PE	C1-O11-P-O13
45	A	201	3PE	C1-O11-P-O14
45	A	201	3PE	C11-O13-P-O14
45	A	201	3PE	O13-C11-C12-N
45	J	201	3PE	C1-O11-P-O12
45	J	201	3PE	C1-O11-P-O13
45	J	201	3PE	C11-O13-P-O11
45	J	202	3PE	C1-O11-P-O13
45	J	202	3PE	C1-O11-P-O14
45	J	202	3PE	O13-C11-C12-N
45	L	1001	3PE	C1-O11-P-O14
45	L	1001	3PE	C11-O13-P-O11
45	L	1001	3PE	C11-O13-P-O14
45	L	1001	3PE	O13-C11-C12-N
45	L	1002	3PE	C11-O13-P-O11
45	L	1002	3PE	C11-O13-P-O12
45	L	1002	3PE	O13-C11-C12-N
45	M	501	3PE	C1-O11-P-O13
45	M	501	3PE	C1-O11-P-O14
45	M	501	3PE	C11-O13-P-O11
45	M	501	3PE	C11-O13-P-O14
45	M	501	3PE	O13-C11-C12-N
45	N	401	3PE	C1-O11-P-O12
45	N	401	3PE	C1-O11-P-O13
45	N	401	3PE	C11-O13-P-O11
45	N	401	3PE	C11-O13-P-O12
45	N	401	3PE	C11-O13-P-O14
45	N	401	3PE	O13-C11-C12-N
45	N	402	3PE	C11-O13-P-O11
45	N	402	3PE	C11-O13-P-O12
45	N	402	3PE	C11-O13-P-O14
45	V	400	3PE	C11-O13-P-O11
45	V	400	3PE	O13-C11-C12-N
45	o	501	3PE	C11-O13-P-O14
45	p	201	3PE	C1-O11-P-O12
45	p	201	3PE	C1-O11-P-O13
45	p	201	3PE	C1-O11-P-O14
45	6	203	3PE	C1-O11-P-O12
45	6	203	3PE	C1-O11-P-O13
45	6	203	3PE	C1-O11-P-O14
45	6	203	3PE	C11-O13-P-O14
45	6	203	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
45	i	201	3PE	C1-O11-P-O12
45	i	201	3PE	C1-O11-P-O13
45	i	201	3PE	C1-O11-P-O14
46	H	401	PC1	C1-O11-P-O14
46	H	401	PC1	C1-O11-P-O13
46	L	1003	PC1	C11-O13-P-O14
46	L	1003	PC1	C11-O13-P-O11
46	L	1003	PC1	C1-O11-P-O12
46	L	1003	PC1	C1-O11-P-O14
46	L	1003	PC1	C1-O11-P-O13
46	L	1004	PC1	C11-O13-P-O12
46	L	1004	PC1	C11-O13-P-O14
46	L	1004	PC1	C11-O13-P-O11
46	M	502	PC1	C11-O13-P-O12
46	M	502	PC1	C11-O13-P-O14
46	M	502	PC1	C11-O13-P-O11
46	M	502	PC1	C1-O11-P-O12
46	6	202	PC1	C1-O11-P-O12
46	6	202	PC1	C1-O11-P-O13
47	X	101	ZMP	C16-C17-C18-C21
47	X	101	ZMP	O3-C16-C17-O4
47	X	101	ZMP	C17-C16-N2-C15
47	X	101	ZMP	C7-C8-C9-C10
47	j	101	ZMP	C13-C14-C15-N2
47	j	101	ZMP	S1-C11-C12-N1
47	j	101	ZMP	O1-C10-S1-C11
47	j	101	ZMP	C9-C10-S1-C11
51	1	502	FMN	N10-C1'-C2'-O2'
51	1	502	FMN	N10-C1'-C2'-C3'
51	1	502	FMN	C1'-C2'-C3'-C4'
51	1	502	FMN	C5'-O5'-P-O2P
51	1	502	FMN	C5'-O5'-P-O3P
52	1	503	NAI	C5B-O5B-PA-O1A
56	d	401	NDP	C5D-O5D-PN-O3
56	d	401	NDP	C5D-O5D-PN-O1N
56	d	401	NDP	C2N-C3N-C7N-N7N
47	X	101	ZMP	O3-C16-N2-C15
52	1	503	NAI	C2D-C1D-N1N-C6N
48	k	501	AMP	C3'-C4'-C5'-O5'
52	1	503	NAI	C2D-C1D-N1N-C2N
46	M	502	PC1	C11-C12-N-C14
46	L	1003	PC1	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
46	M	502	PC1	C11-C12-N-C15
46	6	202	PC1	C11-C12-N-C14
45	N	402	3PE	C37-C38-C39-C3A
45	J	202	3PE	C26-C27-C28-C29
45	i	201	3PE	C29-C2A-C2B-C2C
45	J	202	3PE	C31-C32-C33-C34
45	N	402	3PE	C29-C2A-C2B-C2C
51	1	502	FMN	O2'-C2'-C3'-O3'
45	J	202	3PE	C21-C22-C23-C24
45	A	201	3PE	C2D-C2E-C2F-C2G
46	L	1003	PC1	C38-C39-C3A-C3B
46	6	202	PC1	C11-C12-N-C13
51	1	502	FMN	O2'-C2'-C3'-C4'
45	6	203	3PE	C3C-C3D-C3E-C3F
46	L	1004	PC1	C11-C12-N-C14
46	L	1004	PC1	C11-C12-N-C15
46	M	502	PC1	C11-C12-N-C13
46	6	202	PC1	C11-C12-N-C15
45	N	402	3PE	C2C-C2D-C2E-C2F
46	L	1003	PC1	O11-C1-C2-C3
45	J	202	3PE	C25-C26-C27-C28
47	j	101	ZMP	C3-C4-C5-C6
46	L	1004	PC1	C11-C12-N-C13
51	1	502	FMN	C5'-O5'-P-O1P
46	M	502	PC1	C3A-C3B-C3C-C3D
46	L	1003	PC1	O11-C1-C2-O21
45	V	400	3PE	C2-C1-O11-P
45	J	201	3PE	O11-C1-C2-C3
45	J	202	3PE	C1-C2-C3-O31
46	L	1003	PC1	C2-C1-O11-P
45	J	202	3PE	O21-C2-C3-O31
48	k	501	AMP	O4'-C4'-C5'-O5'
45	p	201	3PE	C22-C23-C24-C25
47	X	101	ZMP	C6-C7-C8-C9
51	1	502	FMN	C1'-C2'-C3'-O3'
45	L	1001	3PE	C35-C36-C37-C38
45	M	501	3PE	C12-C11-O13-P
45	A	201	3PE	O21-C2-C3-O31
46	H	401	PC1	O13-C11-C12-N
46	L	1003	PC1	O13-C11-C12-N
46	H	401	PC1	C2C-C2D-C2E-C2F
47	j	101	ZMP	O3-C16-C17-O4

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Mol	Chain	Res	Type	Atoms
46	H	401	PC1	C3C-C3D-C3E-C3F
47	j	101	ZMP	C19-C18-C21-O5
46	M	502	PC1	C2-C1-O11-P
45	J	201	3PE	O11-C1-C2-O21
56	d	401	NDP	C2N-C3N-C7N-O7N
46	M	502	PC1	C25-C26-C27-C28
46	L	1003	PC1	C23-C24-C25-C26
45	A	201	3PE	C11-O13-P-O11
45	J	201	3PE	C1-O11-P-O14
45	J	201	3PE	C11-O13-P-O14
45	L	1002	3PE	C11-O13-P-O14
45	M	501	3PE	C1-O11-P-O12
45	N	401	3PE	C1-O11-P-O14
45	N	402	3PE	C1-O11-P-O12
45	N	402	3PE	C1-O11-P-O13
45	N	402	3PE	C1-O11-P-O14
45	V	400	3PE	C1-O11-P-O12
45	V	400	3PE	C1-O11-P-O13
45	V	400	3PE	C1-O11-P-O14
45	V	400	3PE	C11-O13-P-O14
45	o	501	3PE	C11-O13-P-O11
46	H	401	PC1	C1-O11-P-O12
46	L	1003	PC1	C11-O13-P-O12
46	M	502	PC1	C1-O11-P-O14
46	M	502	PC1	C1-O11-P-O13
56	d	401	NDP	C5D-O5D-PN-O2N
45	M	501	3PE	C2-C1-O11-P
45	M	501	3PE	C31-C32-C33-C34
46	H	401	PC1	C3-C2-O21-C21
52	1	503	NAI	O4D-C1D-N1N-C6N
46	H	401	PC1	C22-C23-C24-C25
46	M	502	PC1	O31-C31-C32-C33
45	A	201	3PE	C1-C2-C3-O31
56	d	401	NDP	C2B-O2B-P2B-O2X
45	V	400	3PE	O11-C1-C2-O21
46	H	401	PC1	C2B-C2C-C2D-C2E
46	L	1003	PC1	C29-C2A-C2B-C2C
45	N	402	3PE	C23-C24-C25-C26
45	L	1002	3PE	C1-C2-O21-C21
46	L	1003	PC1	C1-C2-O21-C21
46	M	502	PC1	C39-C3A-C3B-C3C
52	1	503	NAI	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
47	j	101	ZMP	C2-C3-C4-C5
45	V	400	3PE	O11-C1-C2-C3
52	1	503	NAI	C2N-C3N-C7N-N7N
56	d	401	NDP	O4D-C1D-N1N-C6N
56	d	401	NDP	C2B-O2B-P2B-O1X
45	A	201	3PE	C2-C1-O11-P
45	6	203	3PE	C33-C34-C35-C36
45	N	401	3PE	C21-C22-C23-C24
46	M	502	PC1	C36-C37-C38-C39
46	H	401	PC1	O11-C1-C2-C3
56	d	401	NDP	C2D-C1D-N1N-C6N
45	N	402	3PE	C24-C25-C26-C27
46	H	401	PC1	O22-C21-O21-C2
46	L	1003	PC1	C34-C35-C36-C37
45	J	201	3PE	C27-C28-C29-C2A
46	6	202	PC1	C3B-C3C-C3D-C3E
45	L	1001	3PE	O21-C21-C22-C23
46	L	1003	PC1	O31-C31-C32-C33
45	J	201	3PE	C33-C34-C35-C36
45	i	201	3PE	O31-C31-C32-C33
45	V	400	3PE	O31-C31-C32-C33
46	H	401	PC1	C22-C21-O21-C2
45	i	201	3PE	O21-C21-C22-C23
45	J	201	3PE	O21-C21-C22-C23
45	L	1002	3PE	O21-C21-C22-C23
46	L	1004	PC1	C26-C27-C28-C29
45	A	201	3PE	C38-C39-C3A-C3B
45	L	1001	3PE	C34-C35-C36-C37
47	X	101	ZMP	S1-C11-C12-N1
45	A	201	3PE	O31-C31-C32-C33
46	L	1004	PC1	O31-C31-C32-C33
45	o	501	3PE	O31-C31-C32-C33
47	j	101	ZMP	C16-C17-C18-C21
45	N	402	3PE	O21-C21-C22-C23
45	J	201	3PE	C3A-C3B-C3C-C3D
45	N	402	3PE	C3-C2-O21-C21
45	A	201	3PE	O21-C21-C22-C23
45	L	1001	3PE	C23-C24-C25-C26
45	J	202	3PE	C2-C1-O11-P
45	L	1002	3PE	C2-C1-O11-P
45	A	201	3PE	O32-C31-C32-C33
45	p	201	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
45	L	1001	3PE	O22-C21-C22-C23
45	A	201	3PE	C2A-C2B-C2C-C2D
45	J	201	3PE	O22-C21-C22-C23
45	i	201	3PE	O32-C31-C32-C33
45	i	201	3PE	O22-C21-C22-C23
46	L	1003	PC1	O21-C21-C22-C23
45	N	401	3PE	C32-C33-C34-C35
46	M	502	PC1	C3B-C3C-C3D-C3E
45	o	501	3PE	C25-C26-C27-C28
45	V	400	3PE	O32-C31-C32-C33
45	p	201	3PE	C21-C22-C23-C24
45	A	201	3PE	O22-C21-C22-C23
46	L	1004	PC1	C37-C38-C39-C3A
45	L	1002	3PE	O22-C21-C22-C23
47	X	101	ZMP	N2-C16-C17-O4
47	j	101	ZMP	N2-C16-C17-O4
45	N	402	3PE	O22-C21-C22-C23
45	M	501	3PE	O21-C21-C22-C23
45	o	501	3PE	O32-C31-C32-C33
46	L	1004	PC1	O32-C31-C32-C33
47	j	101	ZMP	C17-C18-C21-O5
45	V	400	3PE	O21-C21-C22-C23
45	p	201	3PE	O22-C21-C22-C23
47	j	101	ZMP	C22-C1-C2-C3

There are no ring outliers.

18 monomers are involved in 30 short contacts:

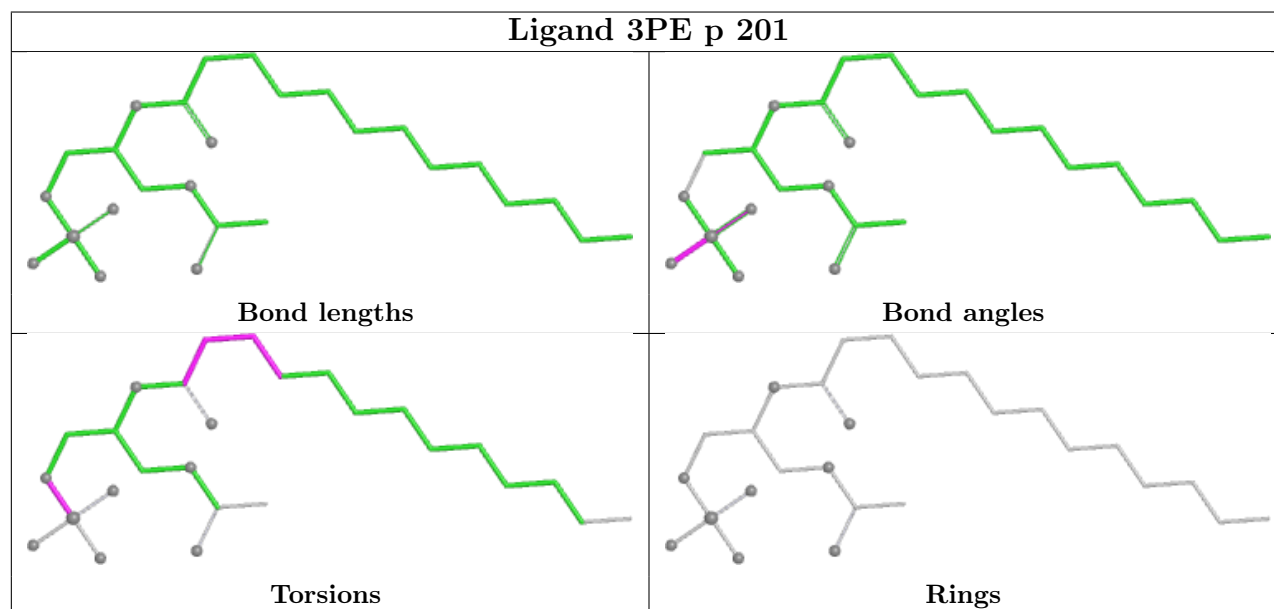
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	6	203	3PE	2	0
46	L	1004	PC1	2	0
45	J	201	3PE	1	0
47	X	101	ZMP	1	0
45	V	400	3PE	1	0
46	6	202	PC1	1	0
45	i	201	3PE	1	0
45	J	202	3PE	2	0
46	L	1003	PC1	1	0
53	2	300	FES	1	0
46	M	502	PC1	2	0
51	1	502	FMN	1	0
52	1	503	NAI	5	0

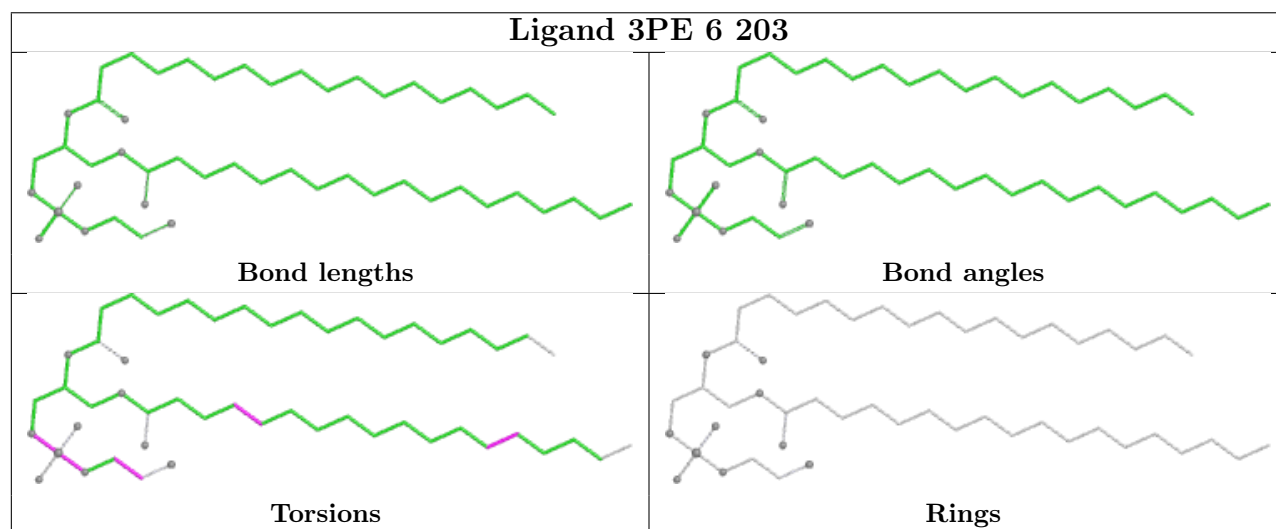
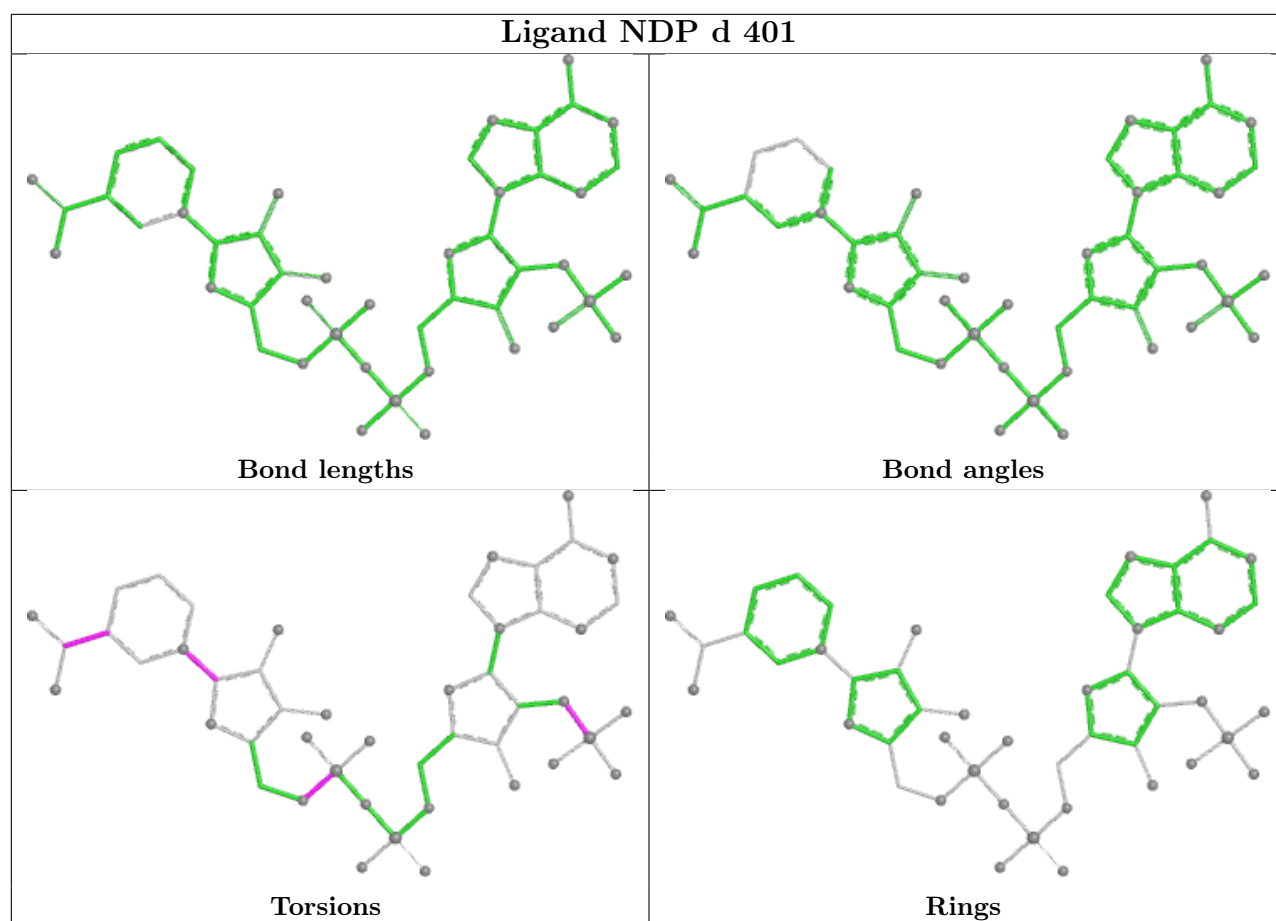
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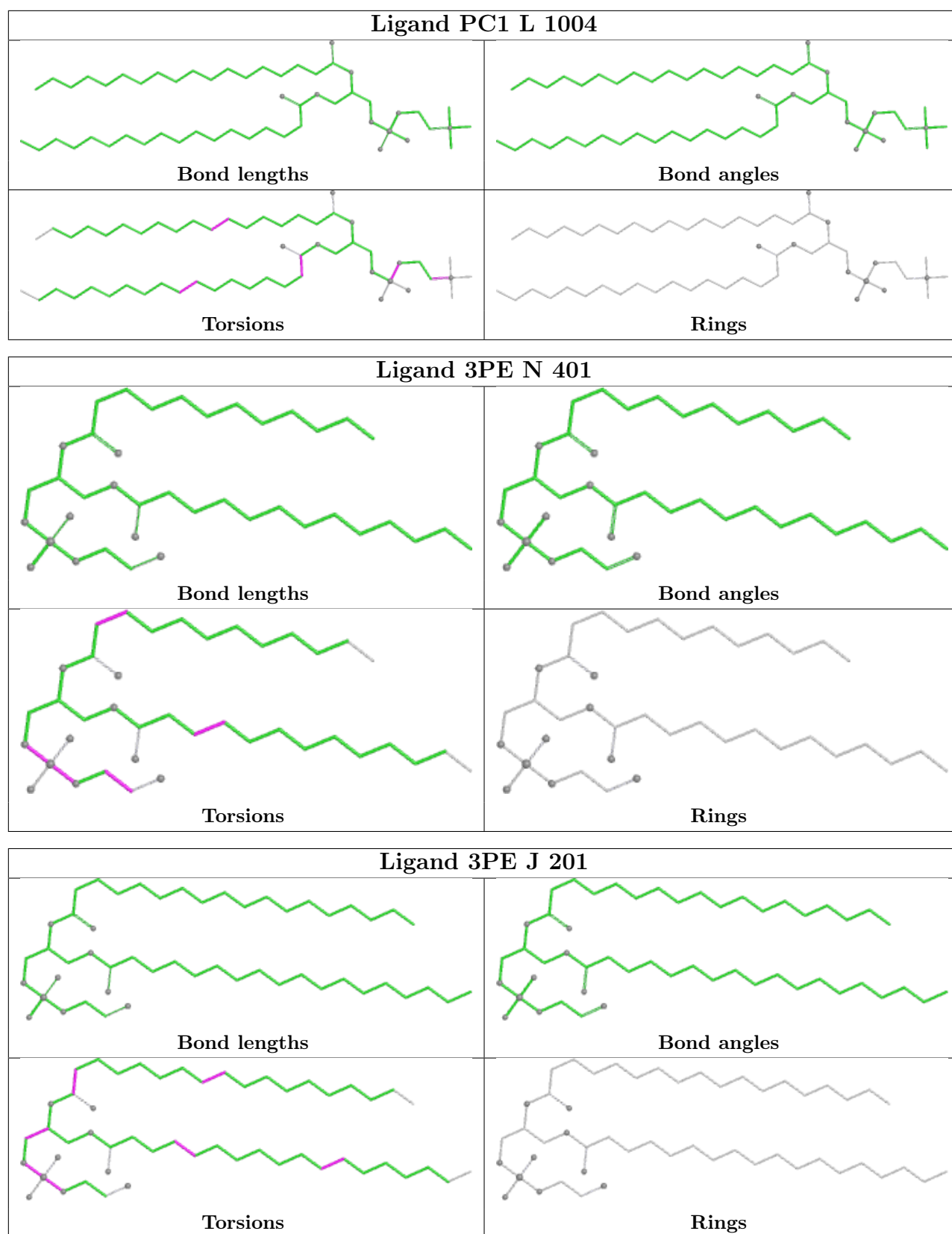
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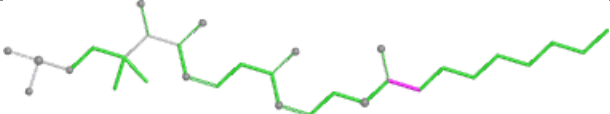
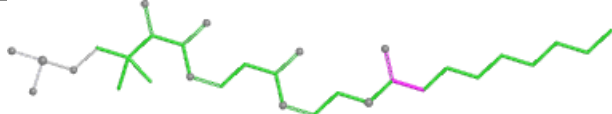
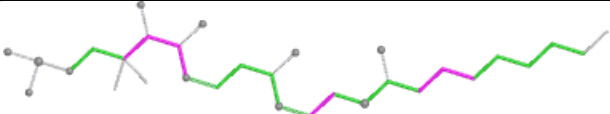
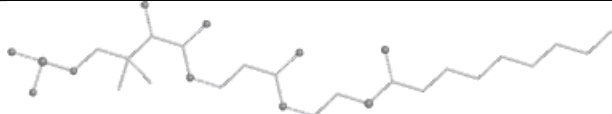
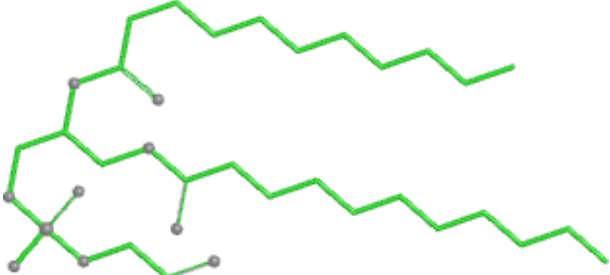
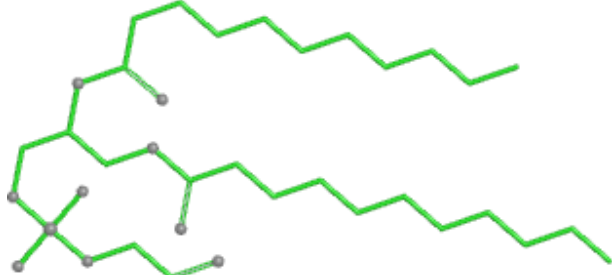
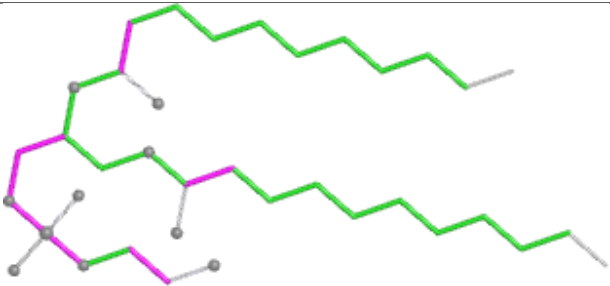
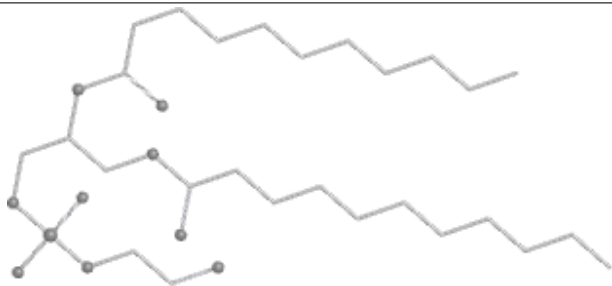
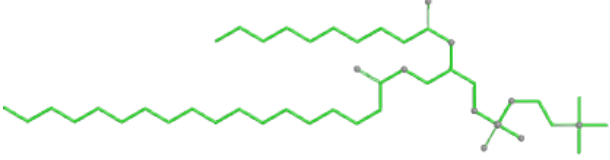
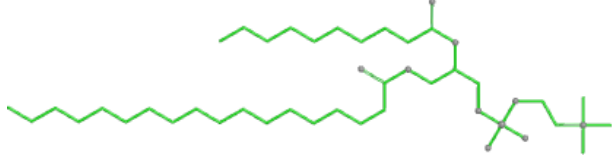
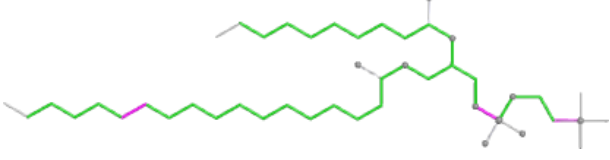
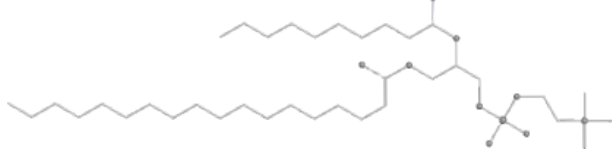
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	k	501	AMP	3	0
47	j	101	ZMP	1	0
45	N	402	3PE	4	0
50	3	801	SF4	1	0
45	A	201	3PE	1	0

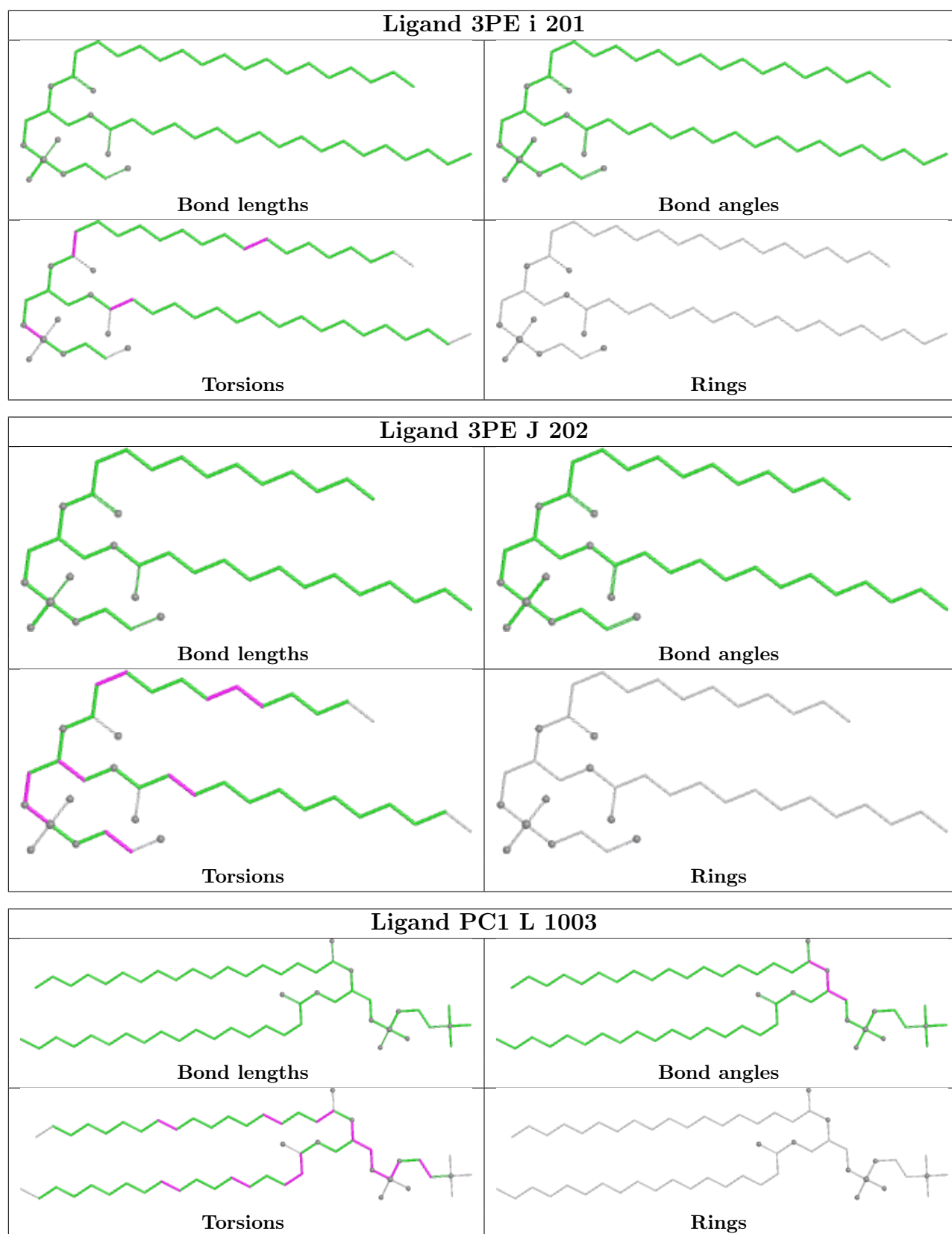
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

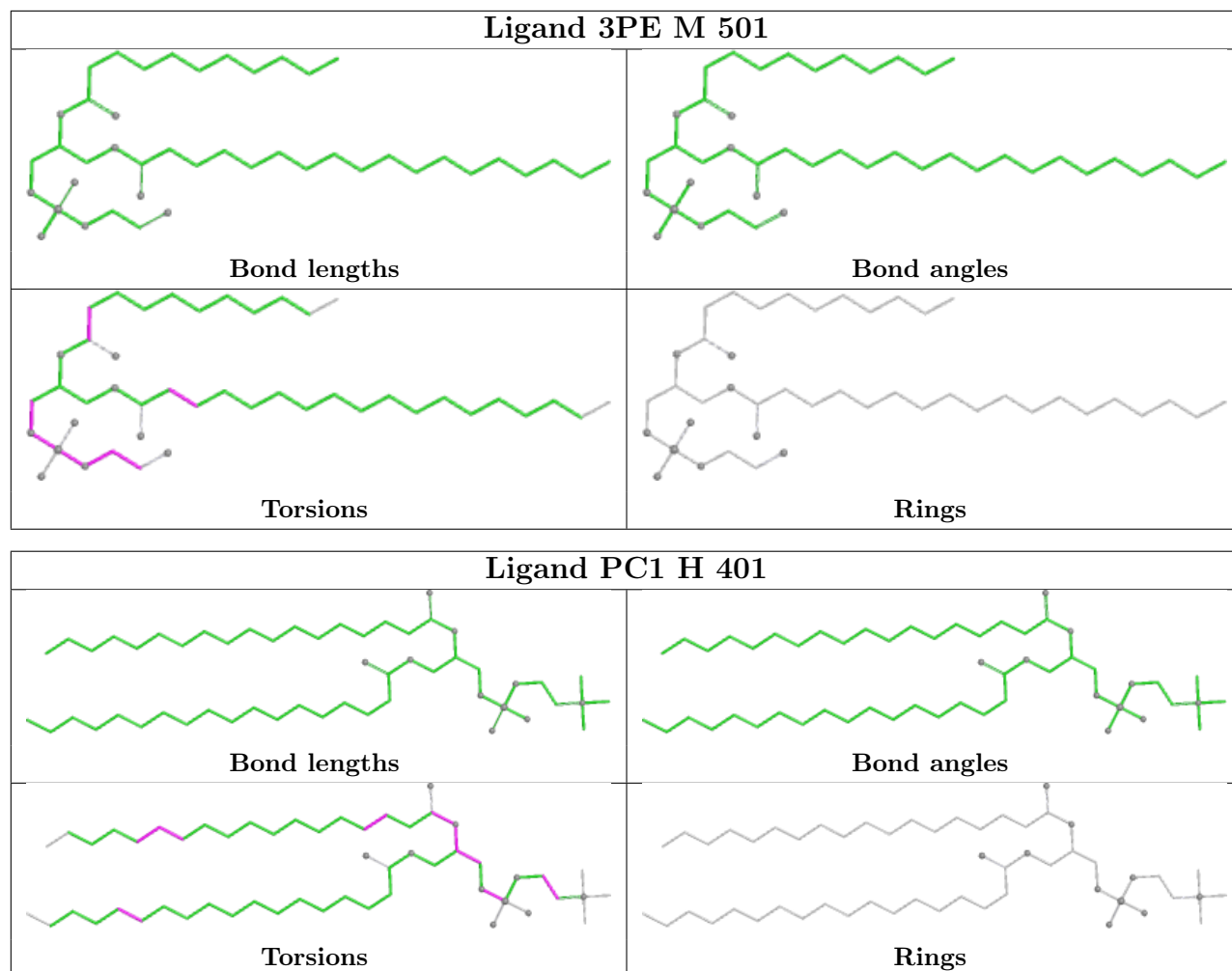


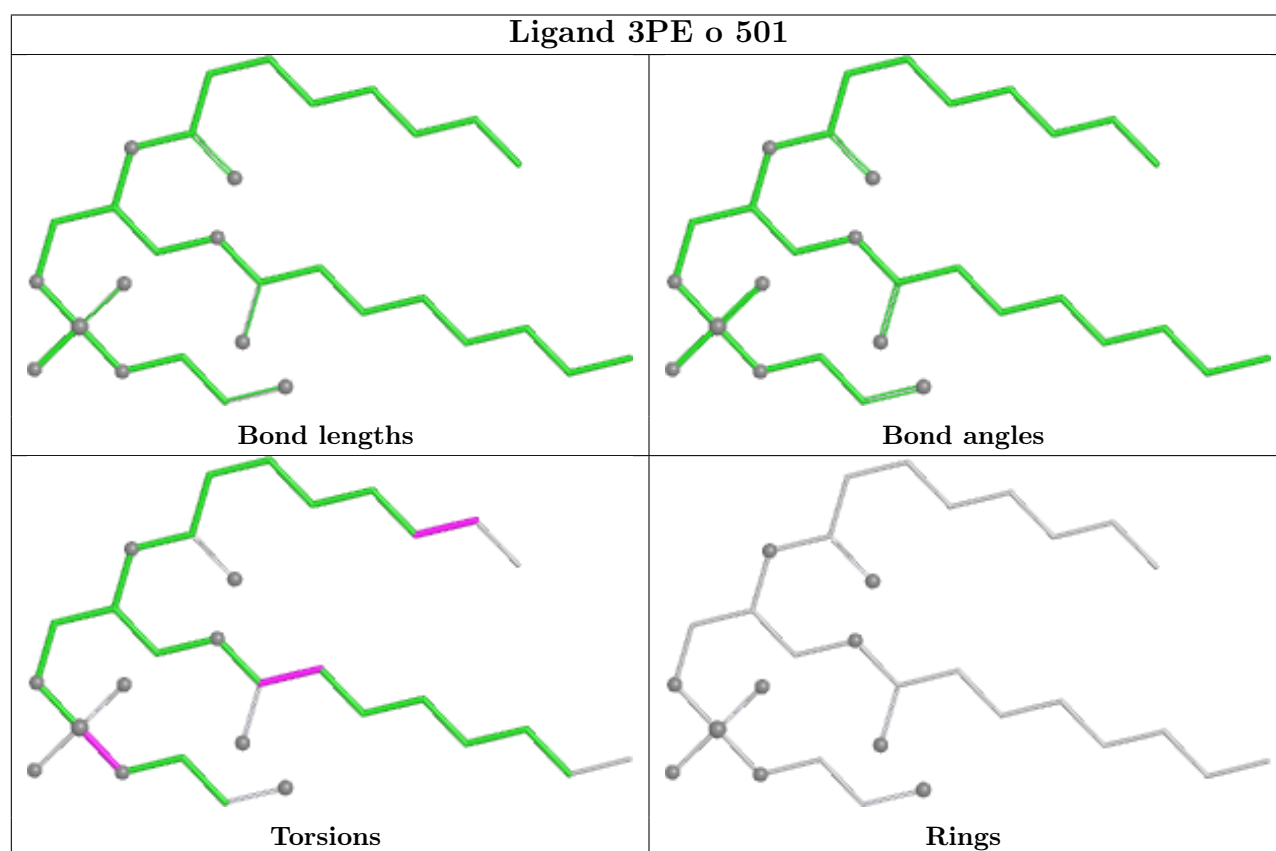
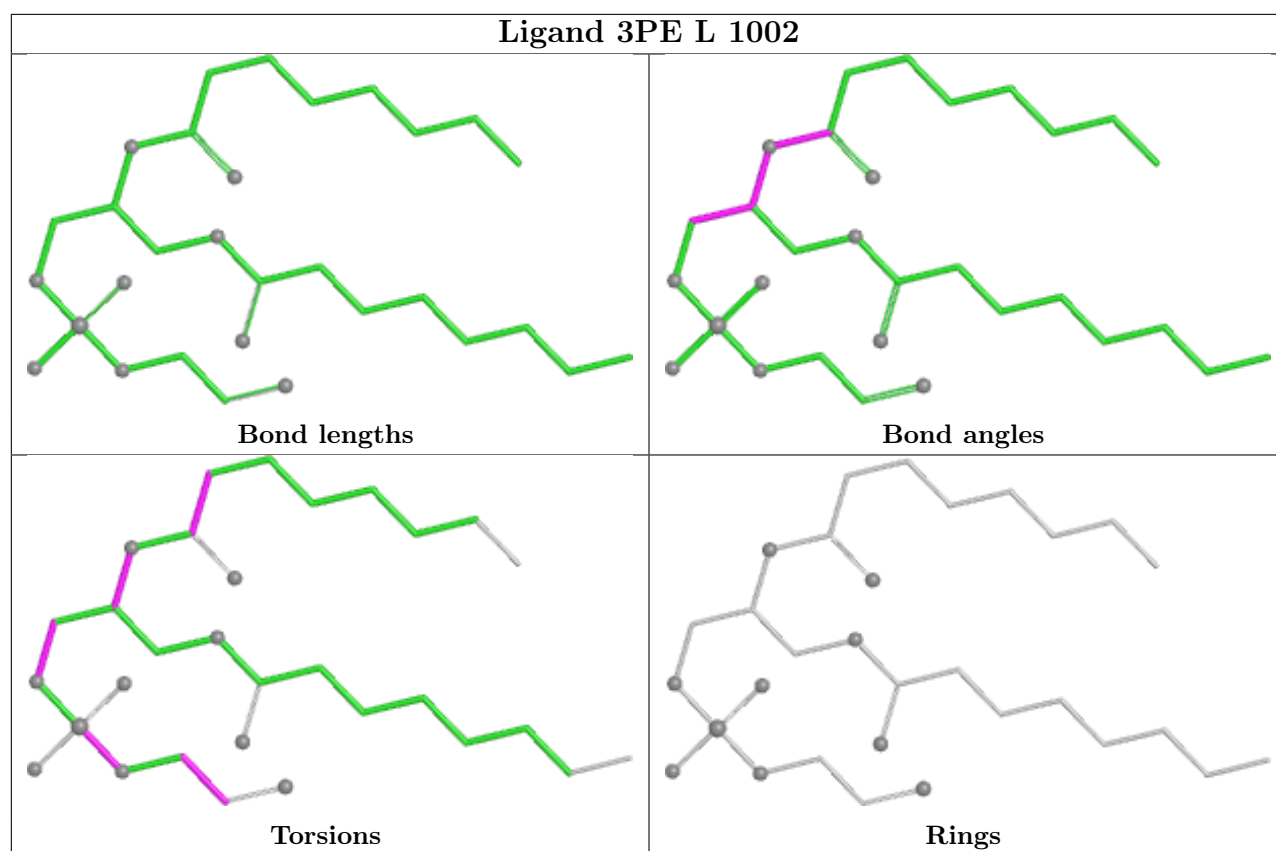


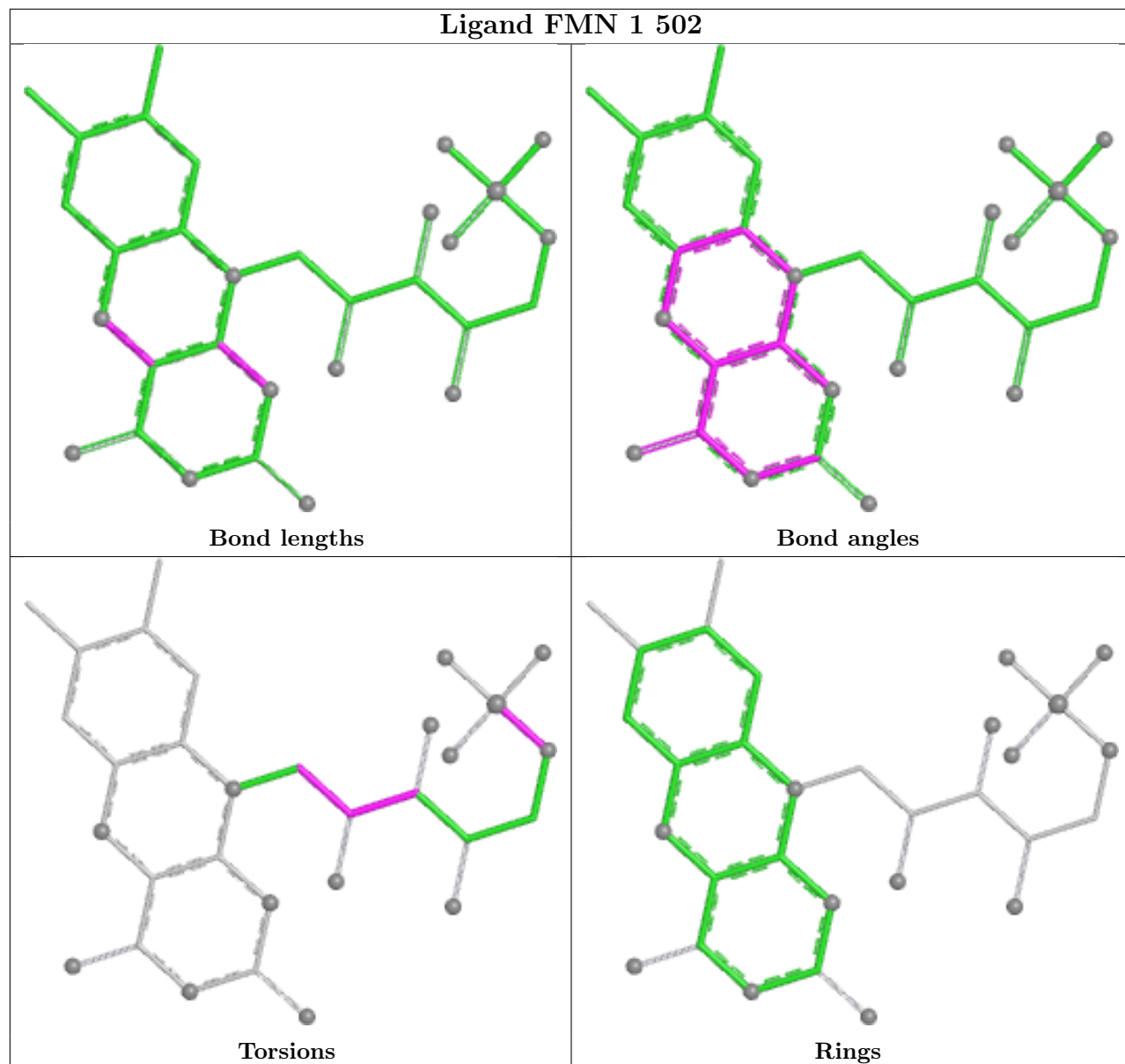
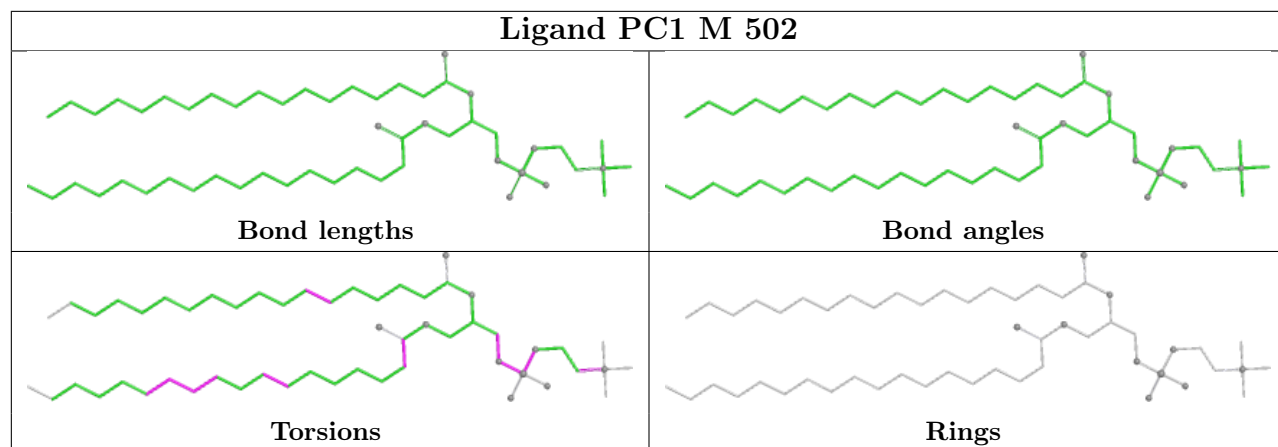


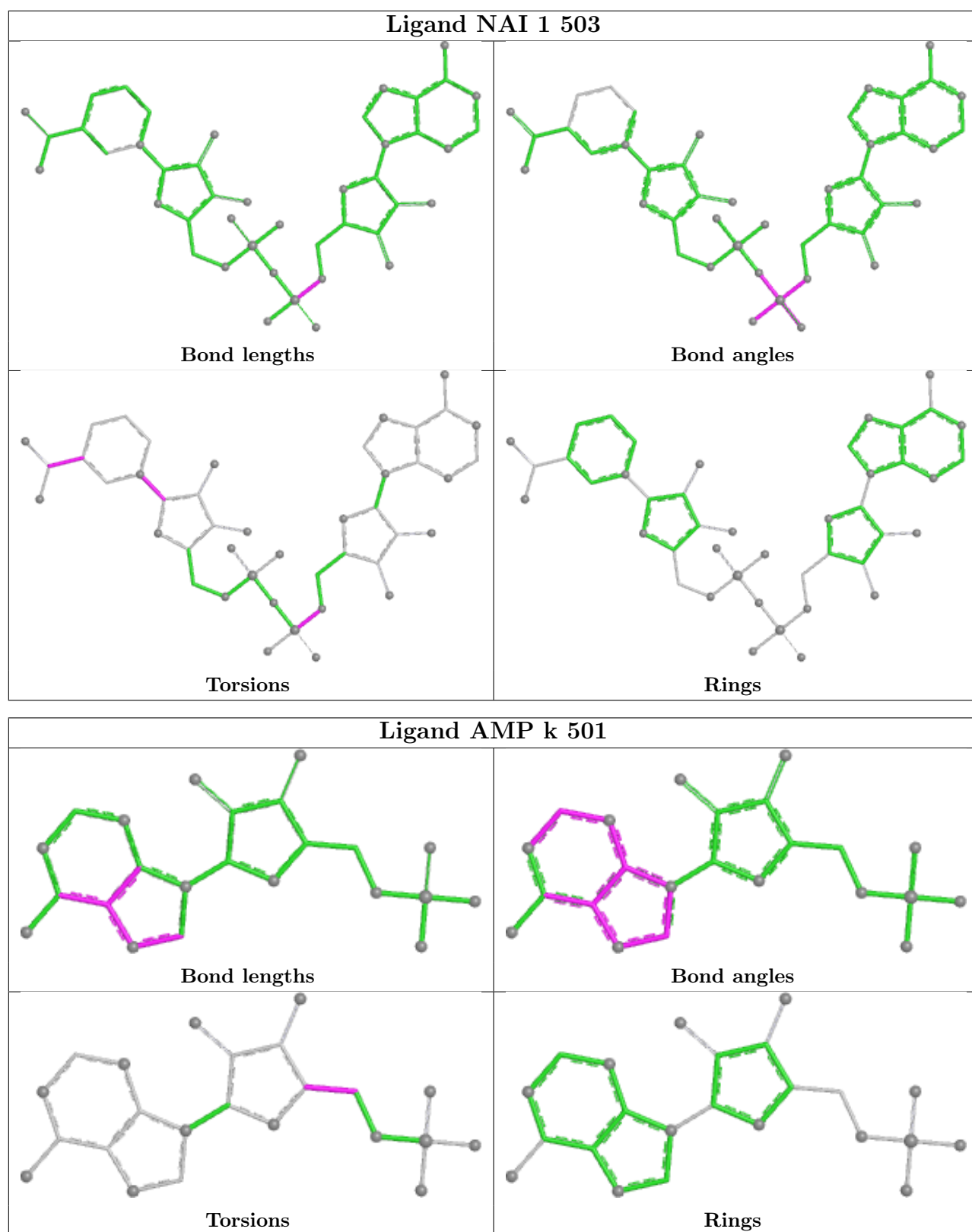
Ligand ZMP X 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand 3PE V 400	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 6 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

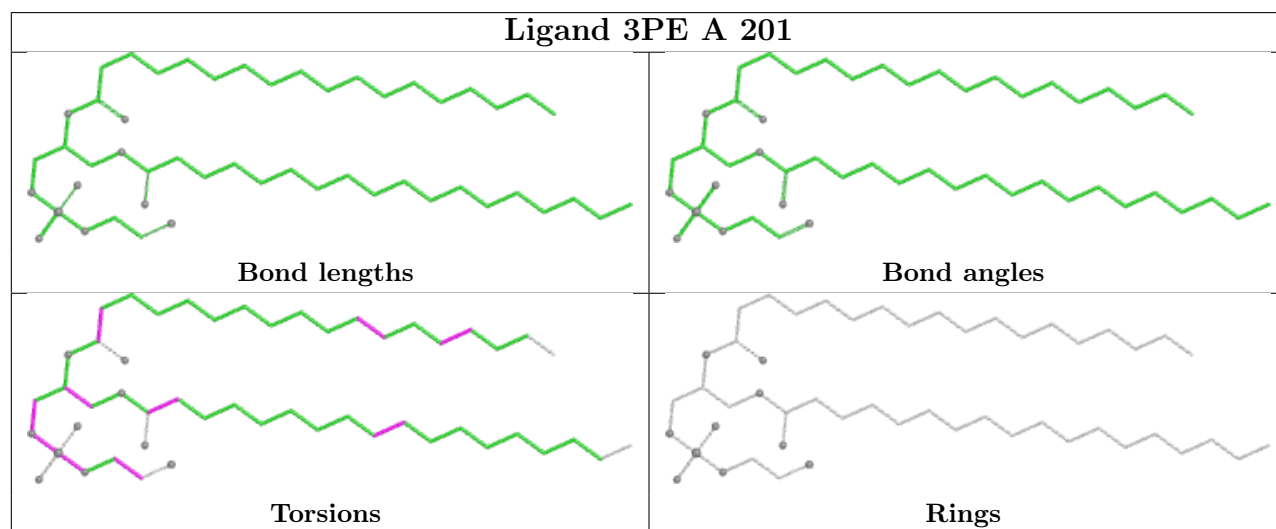
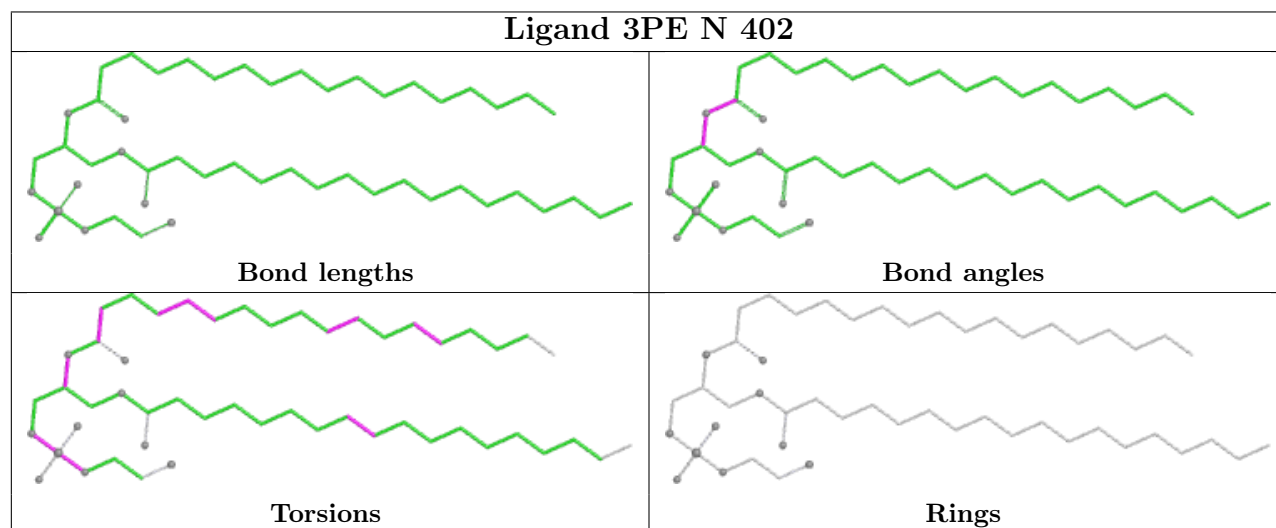
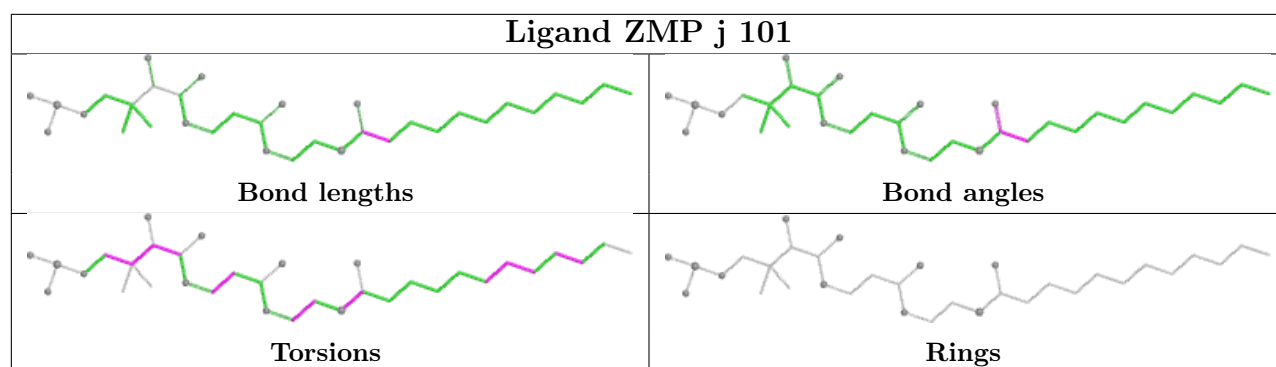


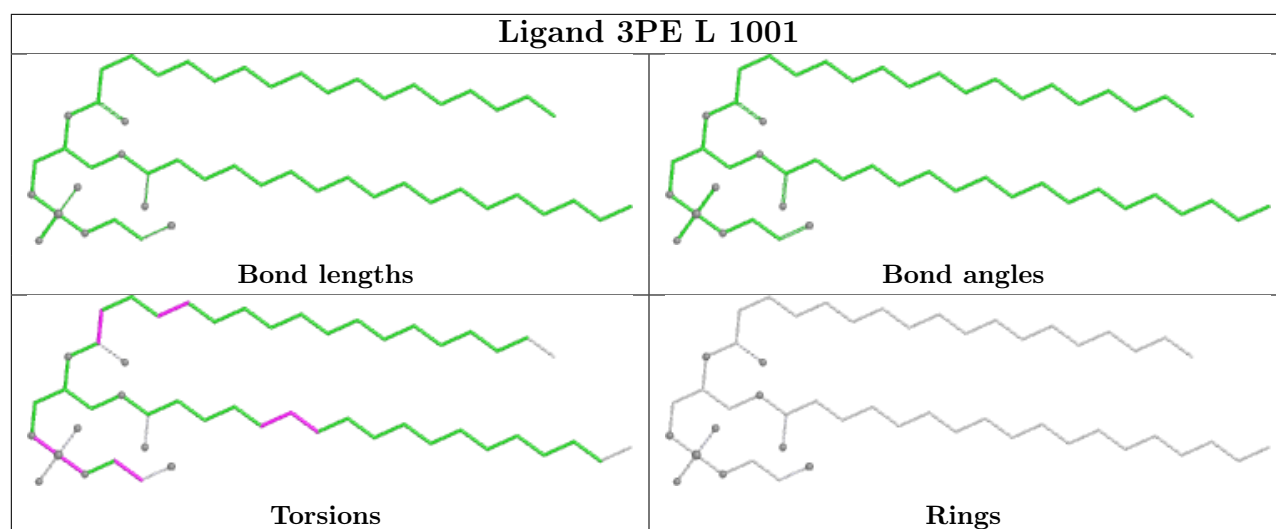












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

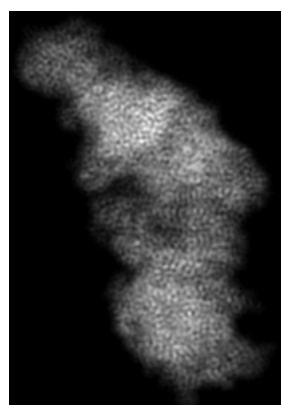
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14648. These allow visual inspection of the internal detail of the map and identification of artifacts.

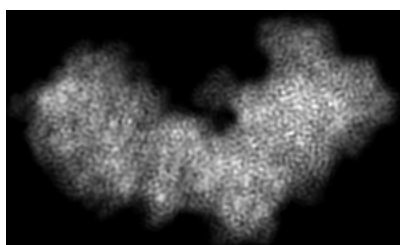
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

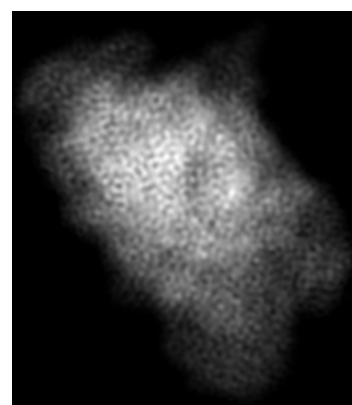
6.1.1 Primary map



X



Y

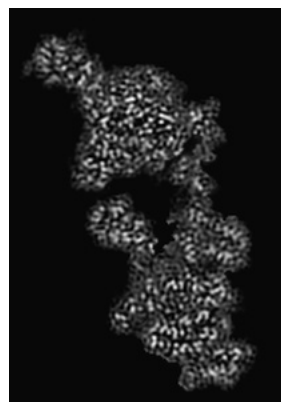


Z

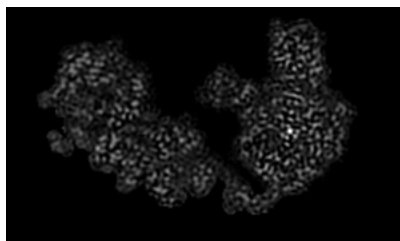
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

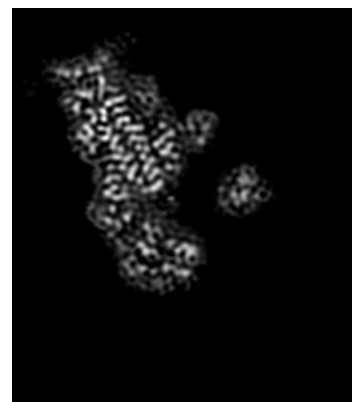
6.2.1 Primary map



X Index: 70



Y Index: 80

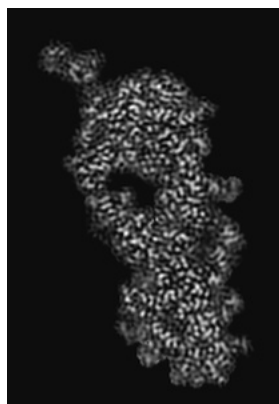


Z Index: 117

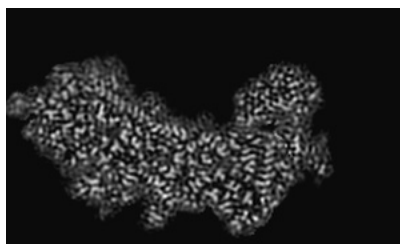
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

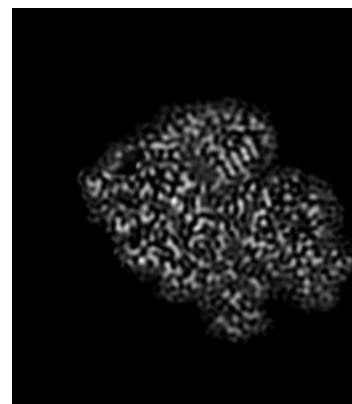
6.3.1 Primary map



X Index: 62



Y Index: 105

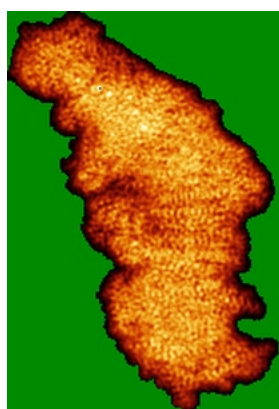


Z Index: 171

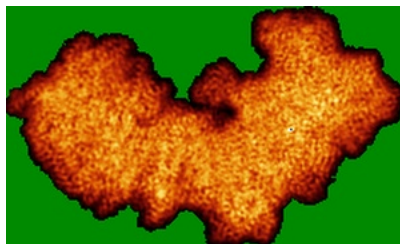
The images above show the largest variance slices of the map in three orthogonal directions.

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

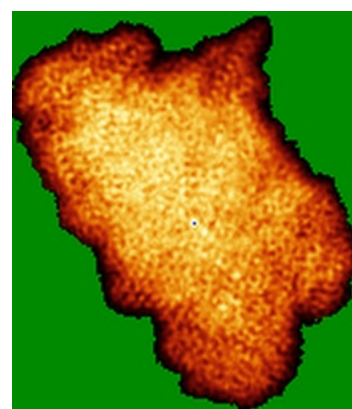
6.4.1 Primary map



X



Y

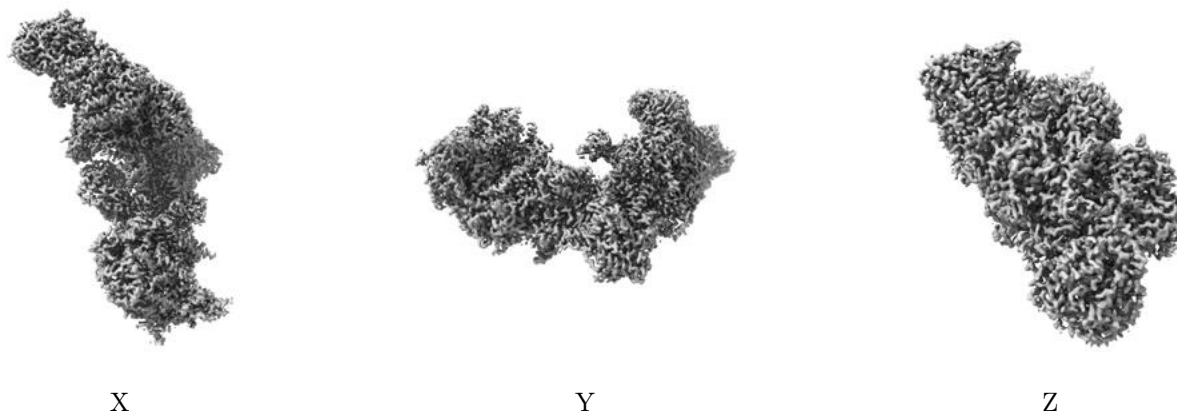


Z

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

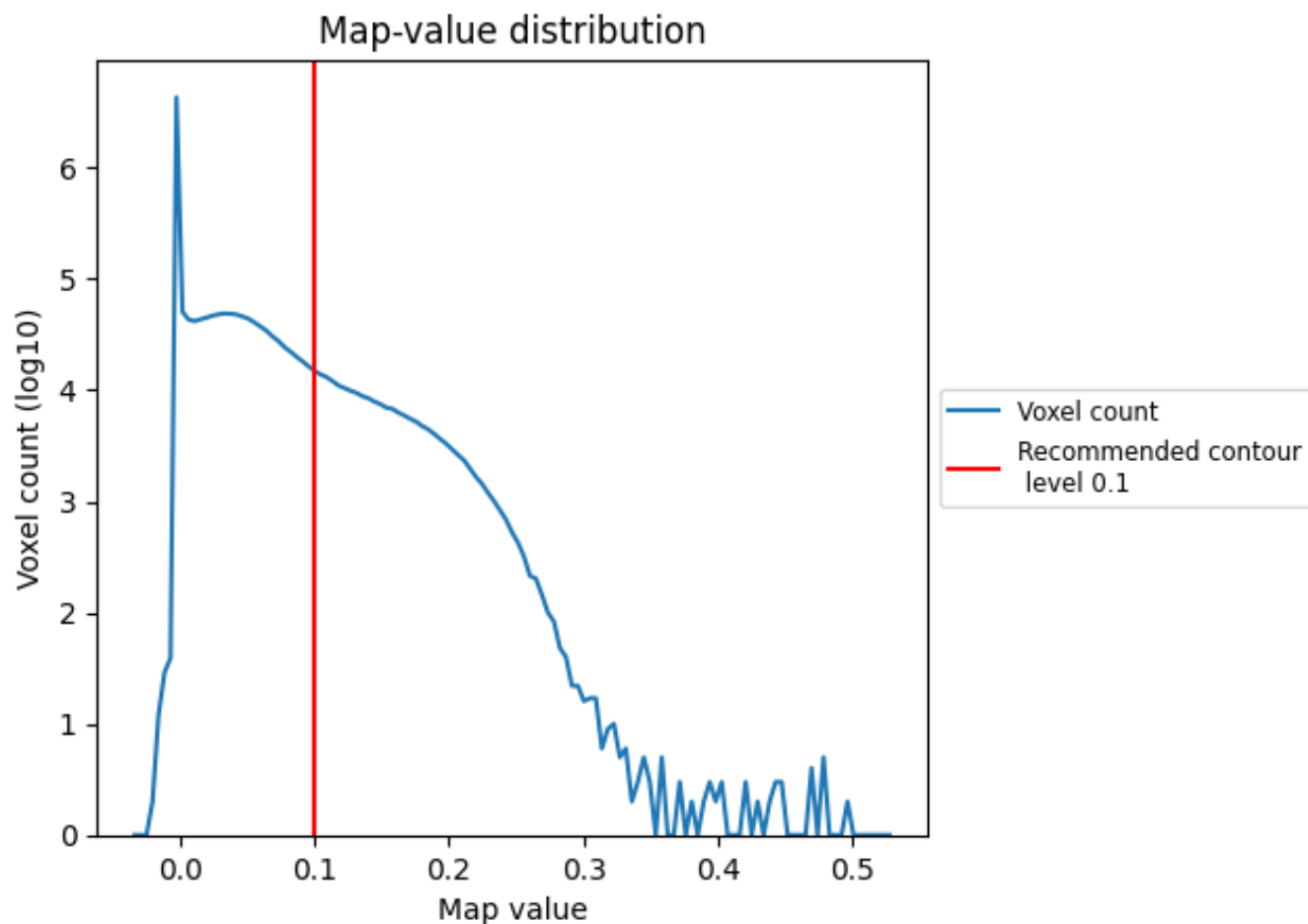
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

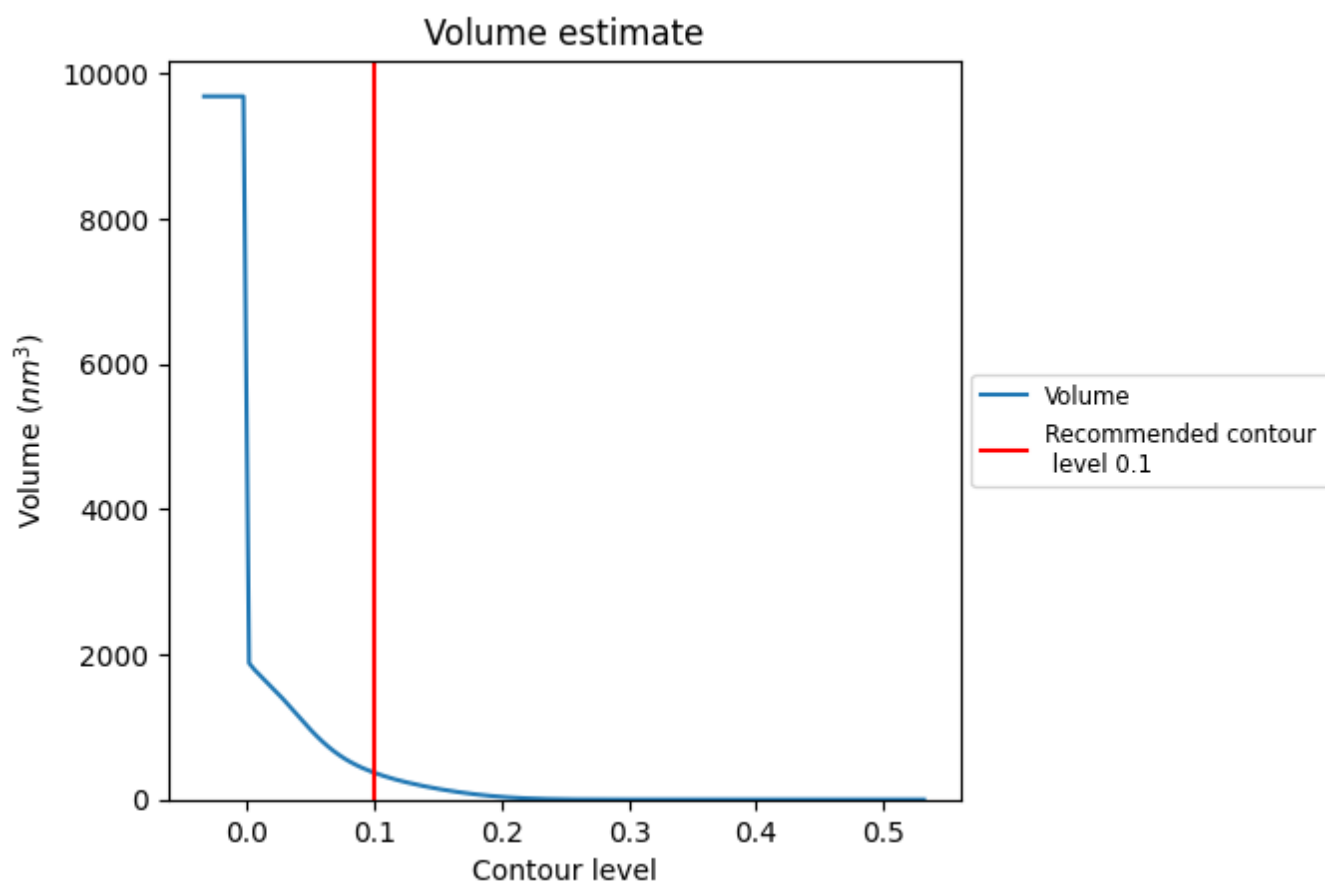
This section contains the results of statistical analysis of the map.

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 370 nm³; this corresponds to an approximate mass of 334 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.

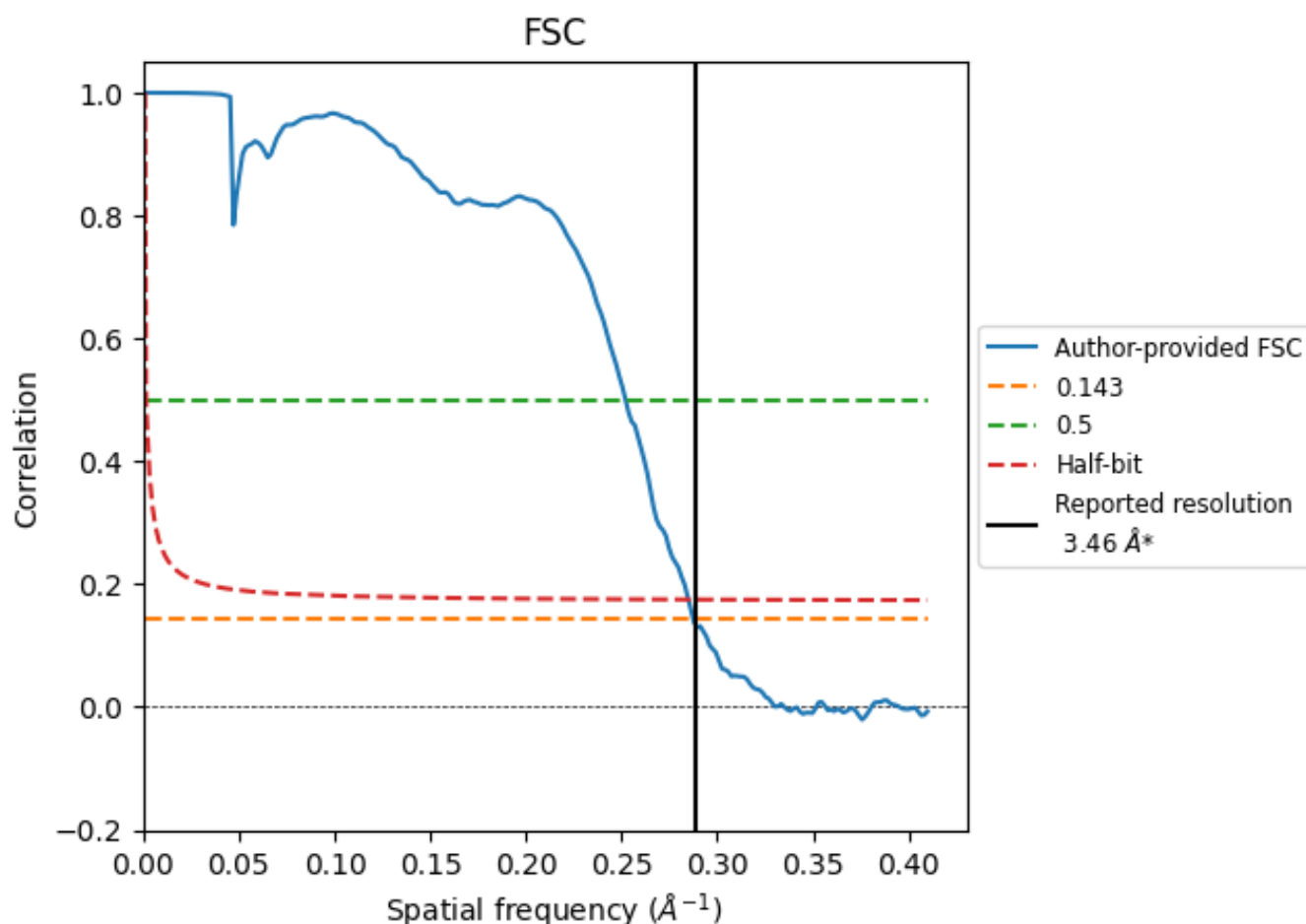
7.3 Rotationally averaged power spectrum [i](#)

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 0.289 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

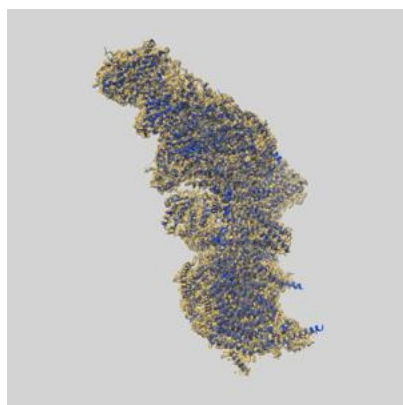
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	3.48	3.97	3.51
Unmasked-calculated*	-	-	-

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

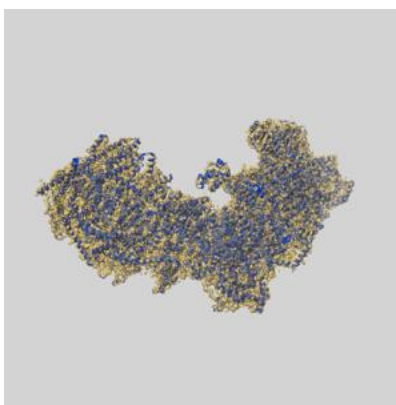
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14648 and PDB model 7ZDH. Per-residue inclusion information can be found in section 3 on page 19.

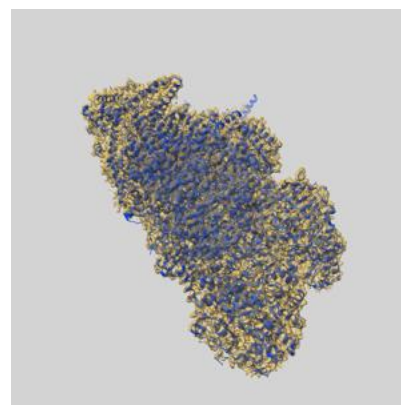
9.1 Map-model overlay [i](#)



X



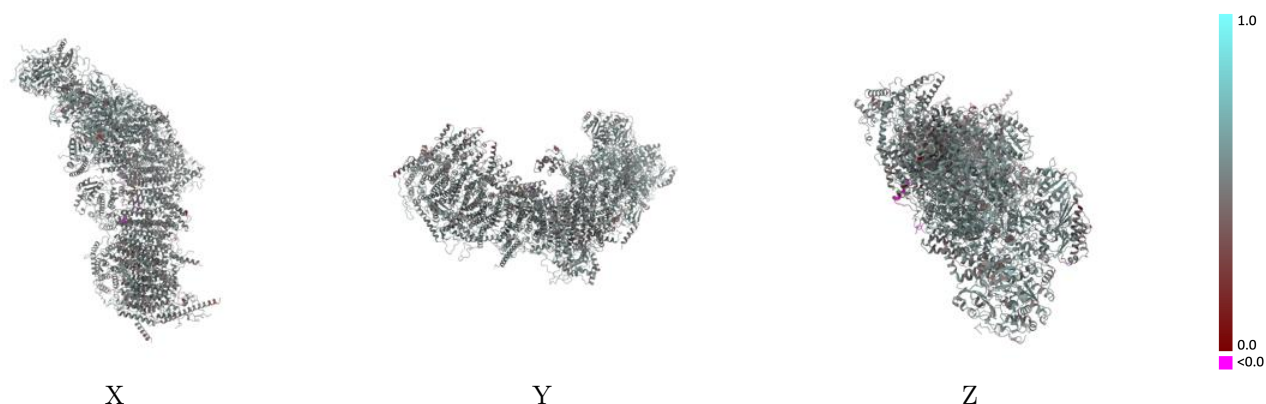
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

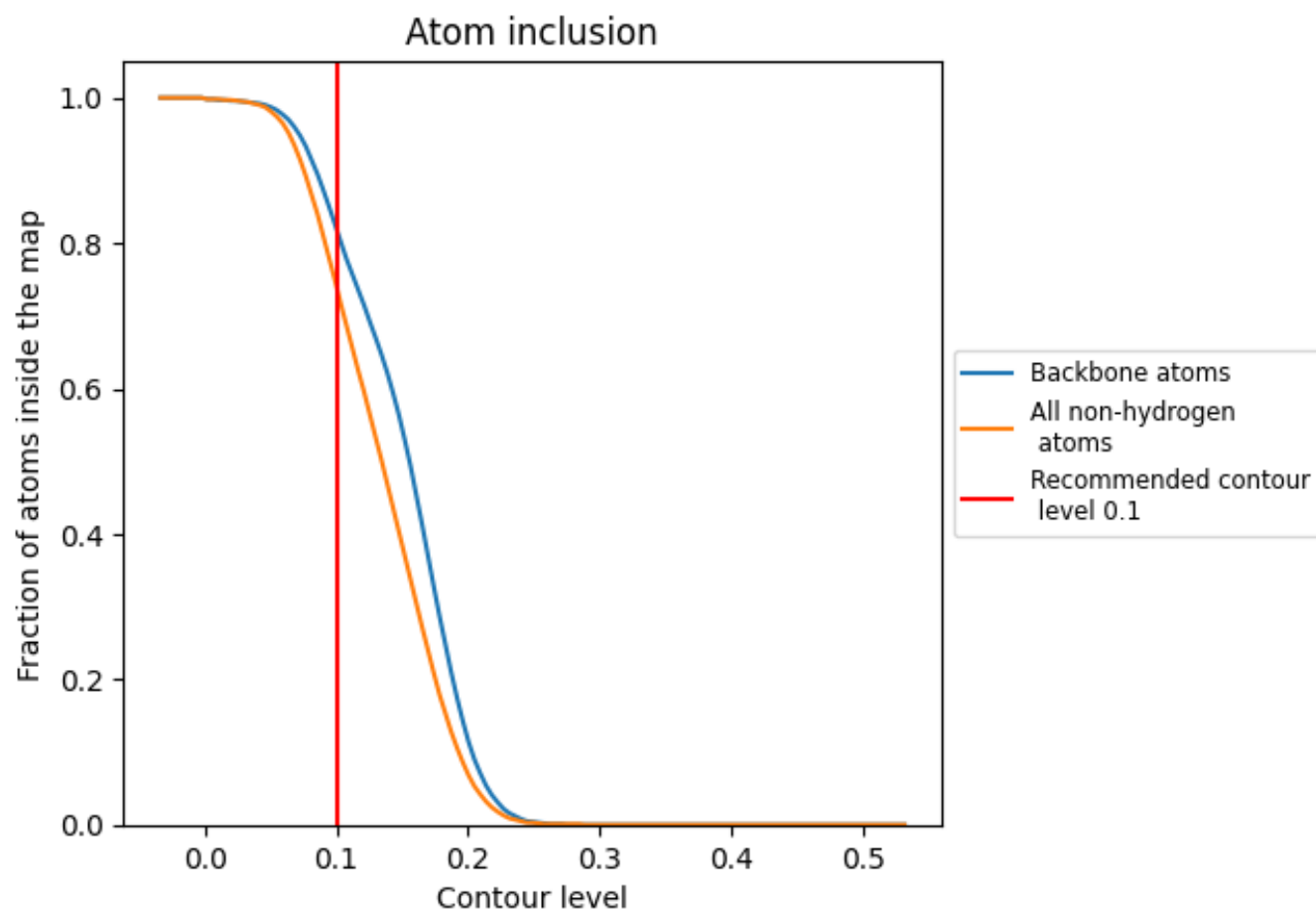


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 74% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7410	 0.5130
1	 0.7160	 0.5130
2	 0.6920	 0.5130
3	 0.7620	 0.5270
4	 0.7750	 0.5120
5	 0.7810	 0.5430
6	 0.8180	 0.5390
9	 0.7740	 0.5030
A	 0.6800	 0.4880
H	 0.7700	 0.5090
J	 0.7470	 0.5030
K	 0.7670	 0.5070
L	 0.7740	 0.5060
M	 0.8010	 0.5240
N	 0.7850	 0.5190
V	 0.6730	 0.4880
W	 0.8000	 0.5280
X	 0.6420	 0.4810
Y	 0.7480	 0.5200
Z	 0.7430	 0.5100
a	 0.6880	 0.5130
b	 0.7160	 0.5390
c	 0.7660	 0.5380
d	 0.7260	 0.5200
e	 0.6550	 0.4960
f	 0.6690	 0.5020
g	 0.7030	 0.5230
h	 0.6990	 0.5330
i	 0.7390	 0.5300
j	 0.4690	 0.4610
k	 0.7110	 0.5140
l	 0.7340	 0.5120
m	 0.7220	 0.5050
n	 0.6760	 0.4870
o	 0.7730	 0.5240



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Chain	Atom inclusion	Q-score
p	 0.6750	 0.4960
q	 0.7450	 0.5020
r	 0.7160	 0.5030
s	 0.6690	 0.4740
t	 0.7040	 0.5020
u	 0.7650	 0.4950
v	 0.7380	 0.5140
w	 0.7150	 0.5070
x	 0.7070	 0.4940
y	 0.6690	 0.5150
z	 0.7720	 0.5000