



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 07:56 AM UTC

PDB ID : 7ZDM / pdb_00007zdm
EMDB ID : EMD-14658
Title : Complex I from *Ovis aries* at pH5.5, Closed state
Authors : Sazanov, L.; Petrova, O.
Deposited on : 2022-03-29
Resolution : 3.44 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:

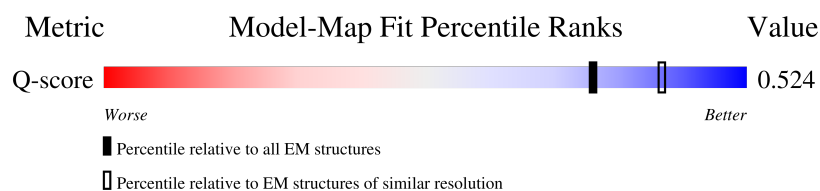
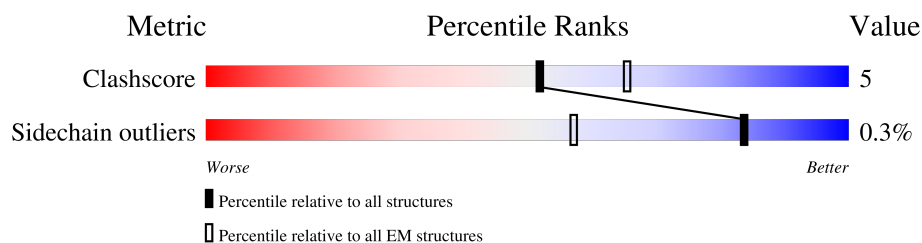
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.44 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13877 (2.94 - 3.94)

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	1	464	
2	2	246	
3	3	727	
4	4	463	
5	5	266	

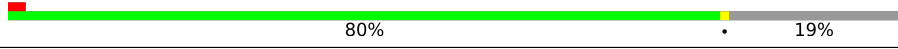
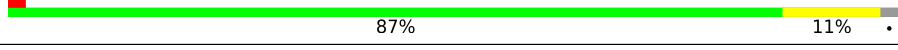
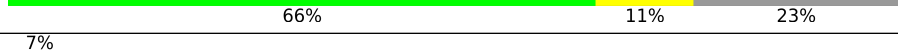
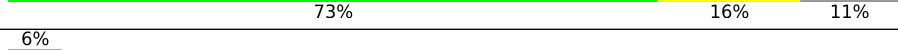
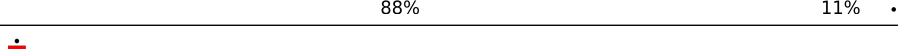
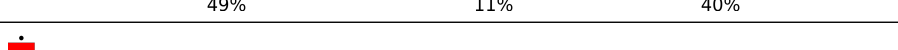
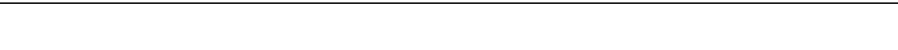
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Mol	Chain	Length	Quality of chain
6	6	223	
7	9	217	
8	a	109	
9	b	124	
10	c	170	
11	d	380	
12	e	99	
13	f	116	
14	g	140	
15	h	114	
16	i	145	
17	X	157	
17	j	157	
18	A	115	
19	H	318	
20	J	175	
21	K	98	
22	L	606	
23	M	459	
24	N	347	
25	V	141	
26	W	189	
27	Y	171	
28	Z	175	
29	k	355	

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Mol	Chain	Length	Quality of chain
30	l	106	
31	m	84	
32	n	98	
33	o	122	
34	p	130	
35	q	144	
36	r	128	
37	s	137	
38	t	179	
39	u	108	
40	v	186	
41	w	154	
42	x	76	
43	y	58	
44	z	70	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 67086 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called Mitochondrial complex I, 24 kDa subunit.

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

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

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

- Molecule 4 is a protein called Complex I-49kD.

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

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

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

- Molecule 6 is a protein called Complex I-20kD.

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

- Molecule 7 is a protein called Complex I-23kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 8 is a protein called Complex I-9kD.

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

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 11 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

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

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 13 is a protein called Mitochondrial complex I, B13 subunit.

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

- Molecule 14 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

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

- Molecule 15 is a protein called Mitochondrial complex I, B14.5a subunit.

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

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

- Molecule 17 is a protein called Acyl carrier protein.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

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

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 34 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

- Molecule 36 is a protein called Mitochondrial complex I, B17 subunit.

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

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

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

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

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

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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

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

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

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

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

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

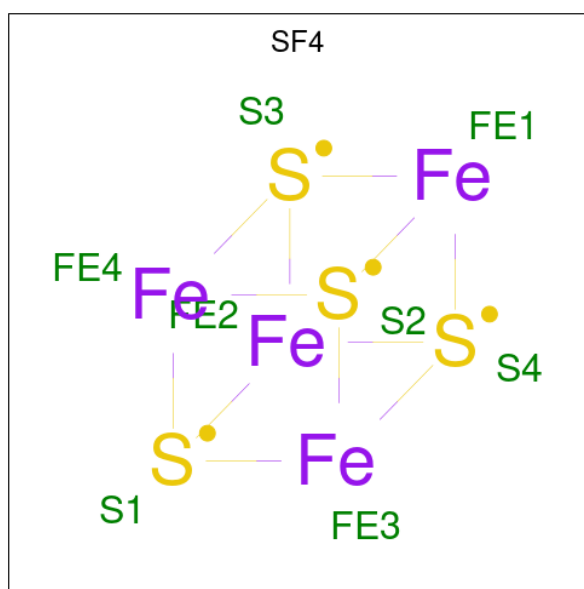
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

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

- Molecule 44 is a protein called Complex I-MWFE.

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

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



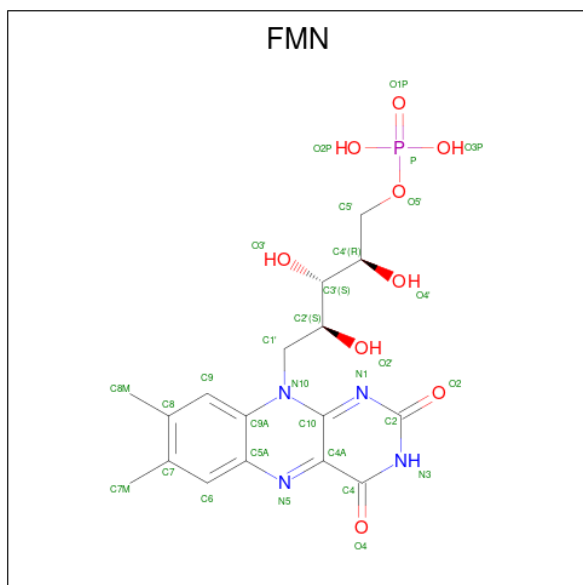
Mol	Chain	Residues	Atoms			AltConf
45	1	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	

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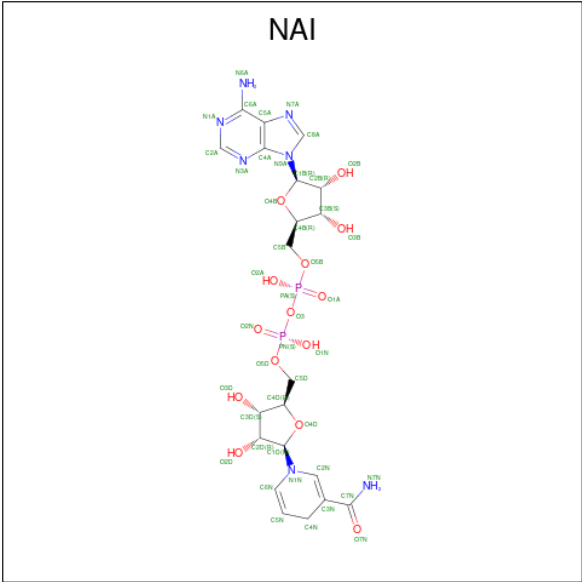
Mol	Chain	Residues	Atoms			AltConf
45	6	1	Total	Fe	S	0
			8	4	4	
45	9	1	Total	Fe	S	0
			8	4	4	
45	9	1	Total	Fe	S	0
			8	4	4	

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



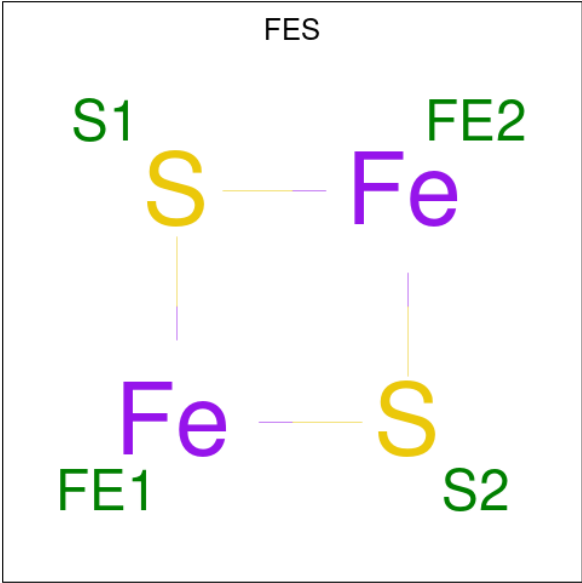
Mol	Chain	Residues	Atoms					AltConf
46	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
47	1	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

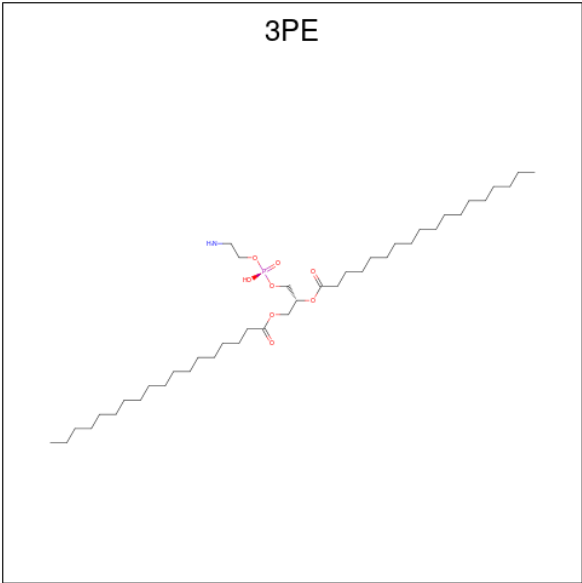


Mol	Chain	Residues	Atoms			AltConf
48	2	1	Total	Fe	S	0
			4	2	2	
48	3	1	Total	Fe	S	0
			4	2	2	

- Molecule 49 is POTASSIUM ION (CCD ID: K) (formula: K).

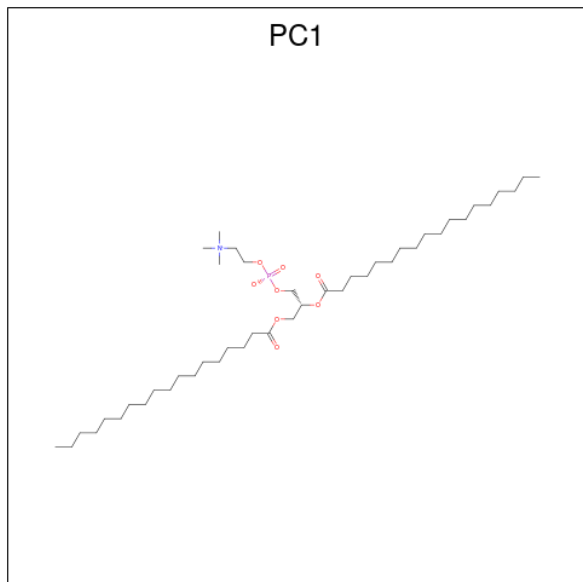
Mol	Chain	Residues	Atoms		AltConf
49	3	1	Total	K	0
			1	1	

- Molecule 50 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
50	4	1	Total	C	N	O	P	0
			40	30	1	8	1	
50	6	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	J	1	Total	C	N	O	P	0
			40	30	1	8	1	
50	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
50	V	1	Total	C	O	P		0
			27	18	8	1		
50	V	1	Total	C	N	O	P	0
			37	27	1	8	1	
50	o	1	Total	C	N	O	P	0
			31	21	1	8	1	

- Molecule 51 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).

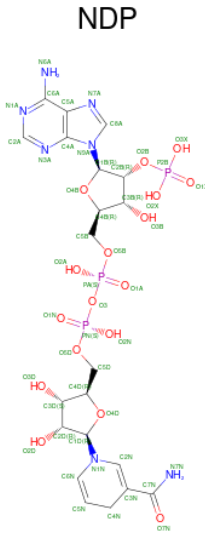


Mol	Chain	Residues	Atoms					AltConf
51	6	1	Total	C	N	O	P	0
			46	36	1	8	1	
51	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
51	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
51	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
51	M	1	Total	C	N	O	P	0
			54	44	1	8	1	

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

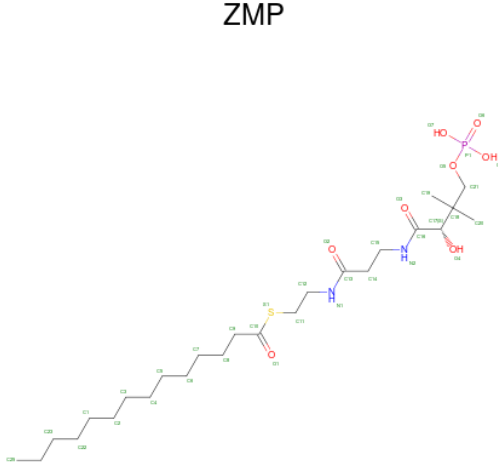
Mol	Chain	Residues	Atoms		AltConf
52	b	1	Total	Zn	0
			1	1	

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



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

- Molecule 54 is S-[2-($\{N-[(2S)-2\text{-hydroxy-}3,3\text{-dimethyl-}4\text{-(phosphonooxy)butanoyl}]\text{-beta-alanyl}\}$ amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



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

- # AMP
-
- The diagram illustrates the chemical structure of Adenosine Monophosphate (AMP). It features an adenine base (a purine ring system with atoms N1, N3, N6, N7, N9 and C2, C4, C5, C6, C8) linked to a ribose sugar (a five-membered ring with atoms C1', C2', C3', C4', C5' and O4'). The ribose is further linked to a phosphate group (a phosphorus atom P bonded to O1P, O2P, O3P, and O5'). Stereochemistry is indicated by wedge and dash bonds at C1' and C4'.
- Nc1ncnc2n(cnc12)[C@H]3O[C@@H](COP(=O)(O)O)[C@H](O)[C@H]3O

MYR

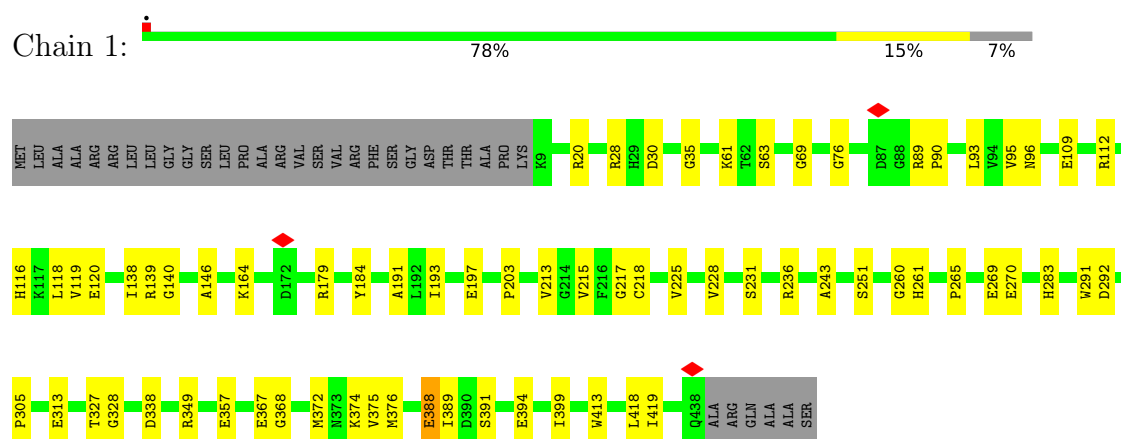
The diagram shows the chemical structure of Myristic acid (MYR), a saturated fatty acid. It consists of a long hydrocarbon chain with 14 carbon atoms, labeled C1 through C14. The chain is shown in a zigzag conformation. The carboxyl group is at the right end, with C1 being the carbonyl carbon, double-bonded to an oxygen atom (O1) and single-bonded to a hydroxyl group (O2 and H). The hydroxyl group is shown in red. The remaining carbons (C2 to C14) are part of the alkyl chain, with C14 being the terminal methyl group.



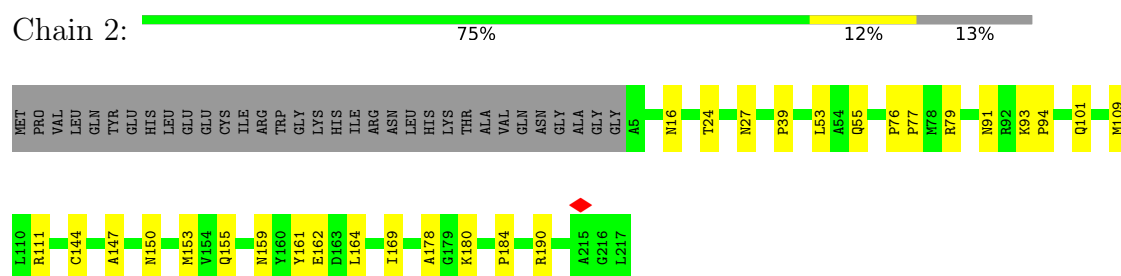
3 Residue-property plots

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

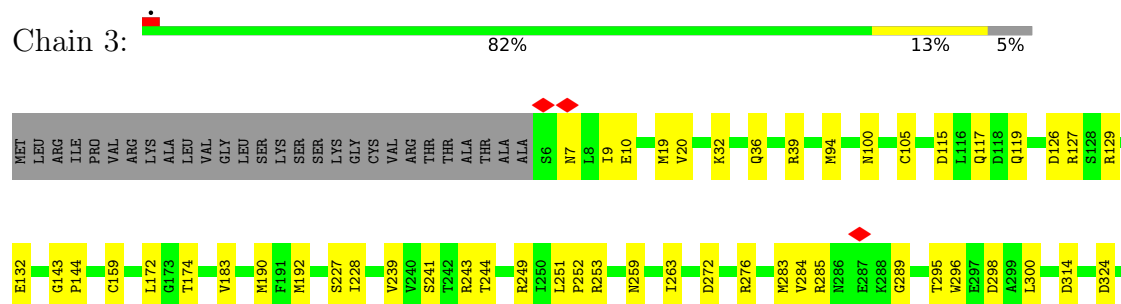
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

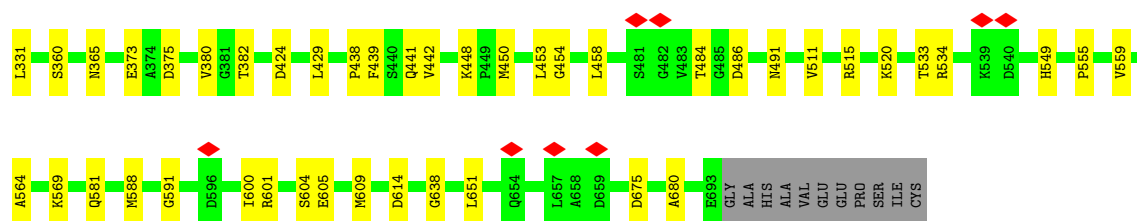


- Molecule 2: Mitochondrial complex I, 24 kDa subunit

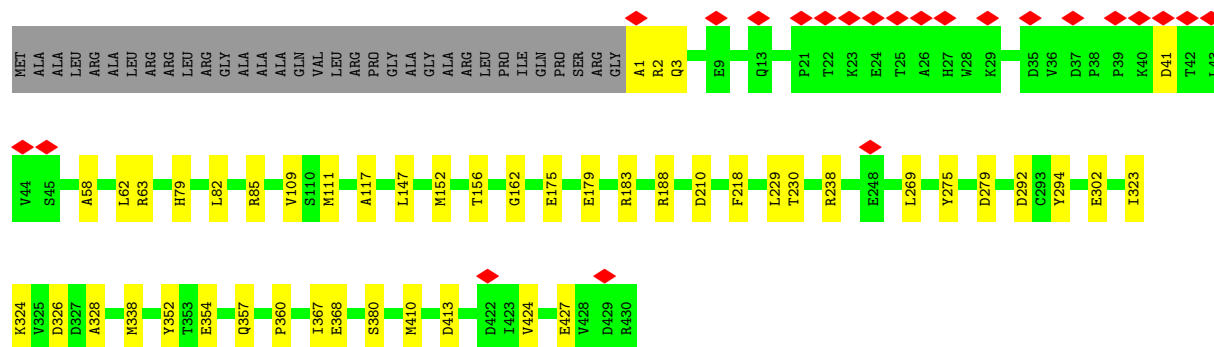
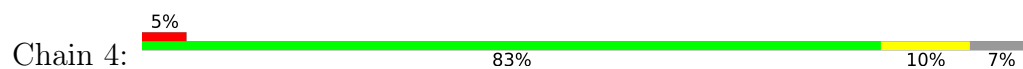


- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

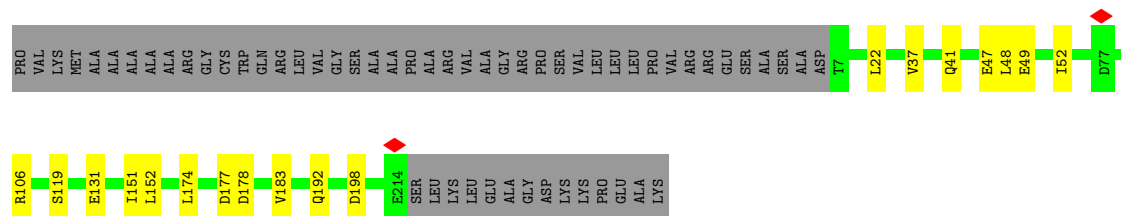




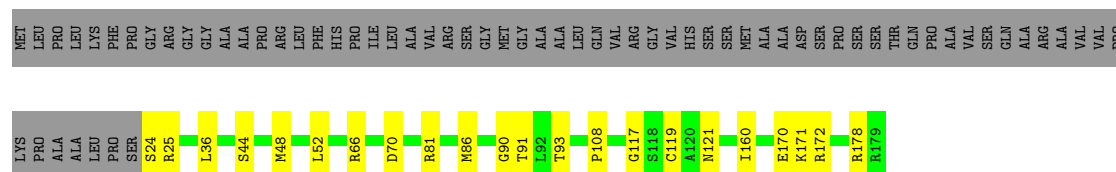
• Molecule 4: Complex I-49kD



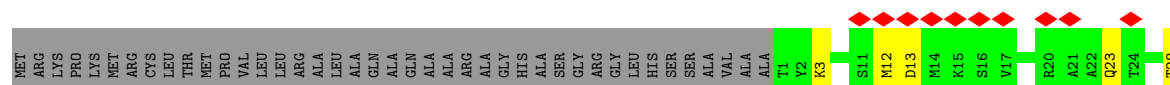
• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3



• Molecule 6: Complex I-20kD

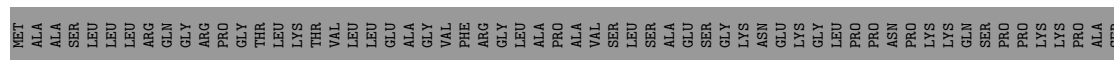
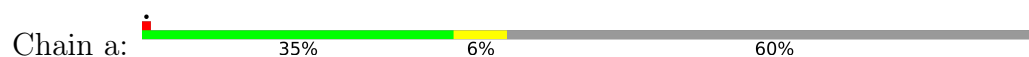


• Molecule 7: Complex I-23kD

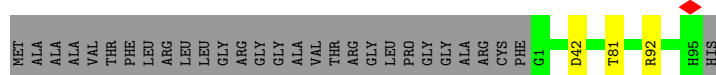
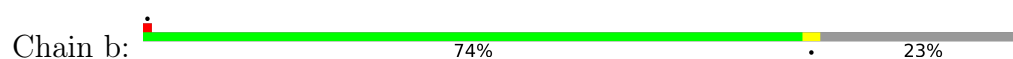




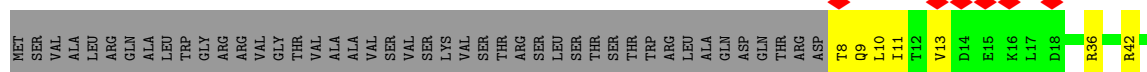
• Molecule 8: Complex I-9kD



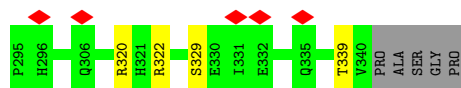
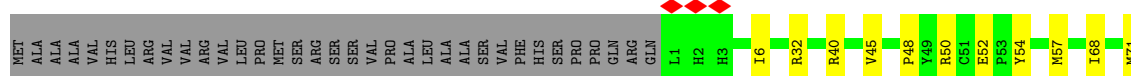
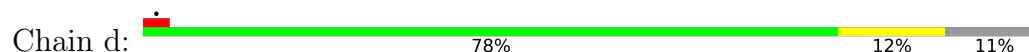
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



• Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

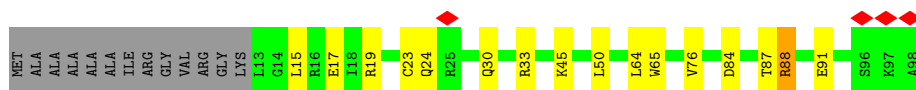


• Molecule 11: NADH:ubiquinone oxidoreductase subunit A9

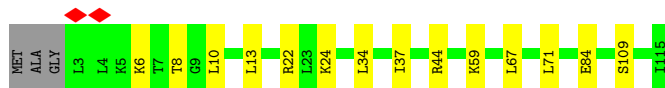
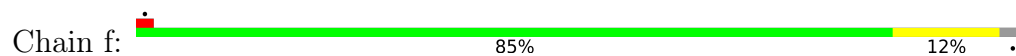


• Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2





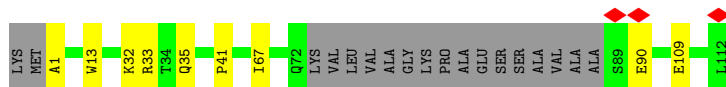
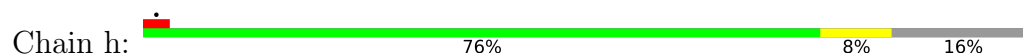
- Molecule 13: Mitochondrial complex I, B13 subunit



- Molecule 14: NADH:ubiquinone oxidoreductase subunit A6



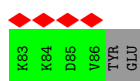
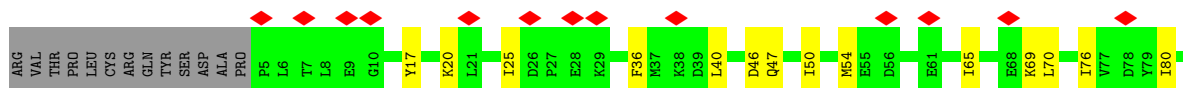
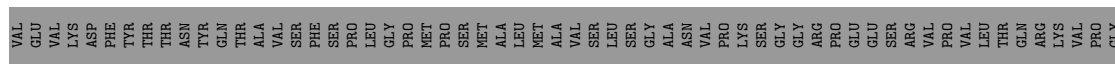
- Molecule 15: Mitochondrial complex I, B14.5a subunit



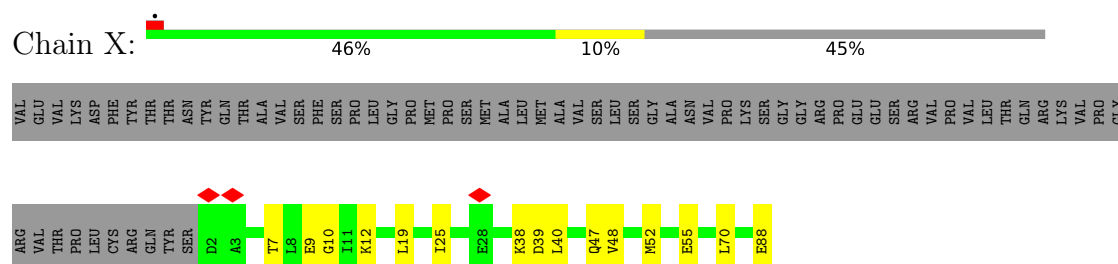
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



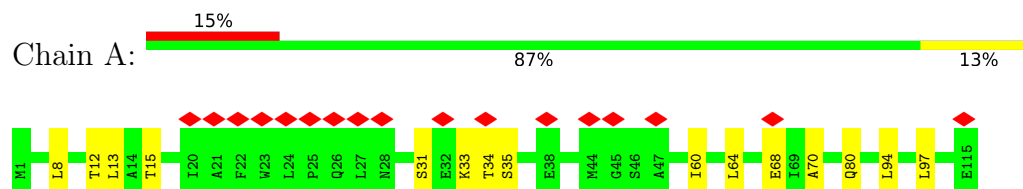
- Molecule 17: Acyl carrier protein



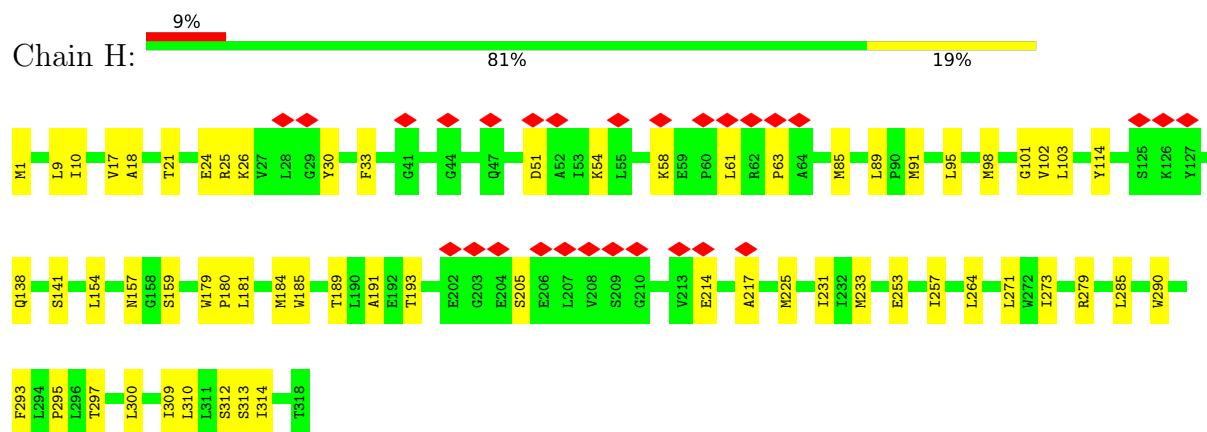
- Molecule 17: Acyl carrier protein



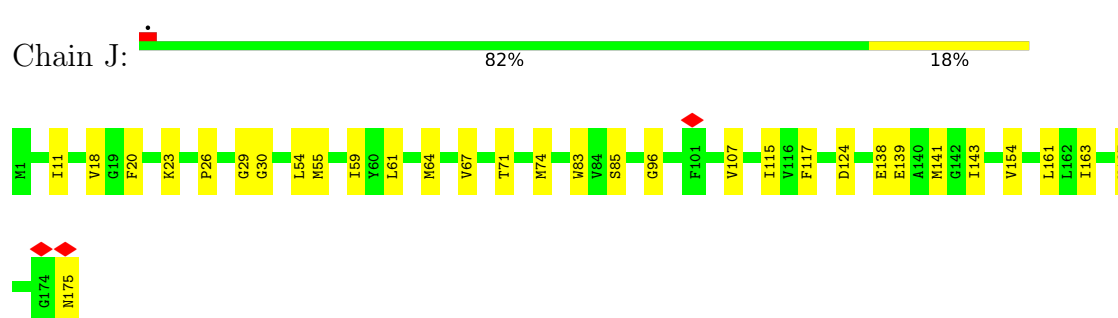
- Molecule 18: NADH-ubiquinone oxidoreductase chain 3



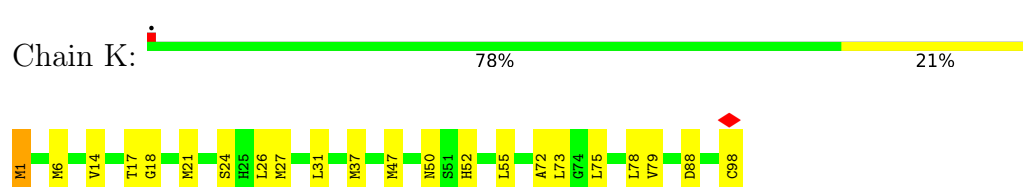
- Molecule 19: NADH-ubiquinone oxidoreductase chain 1



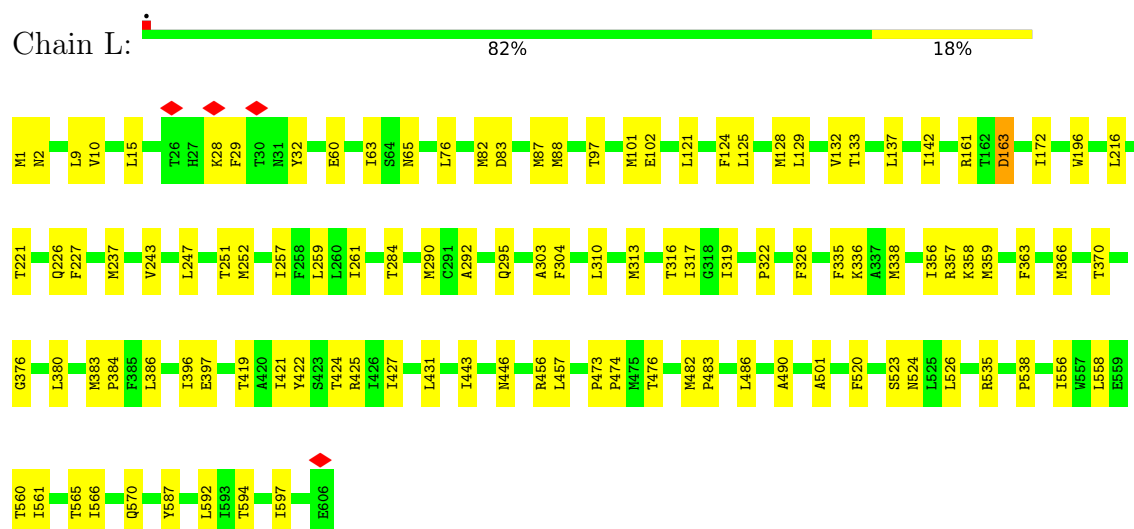
- Molecule 20: NADH-ubiquinone oxidoreductase chain 6



- Molecule 21: NADH-ubiquinone oxidoreductase chain 4L



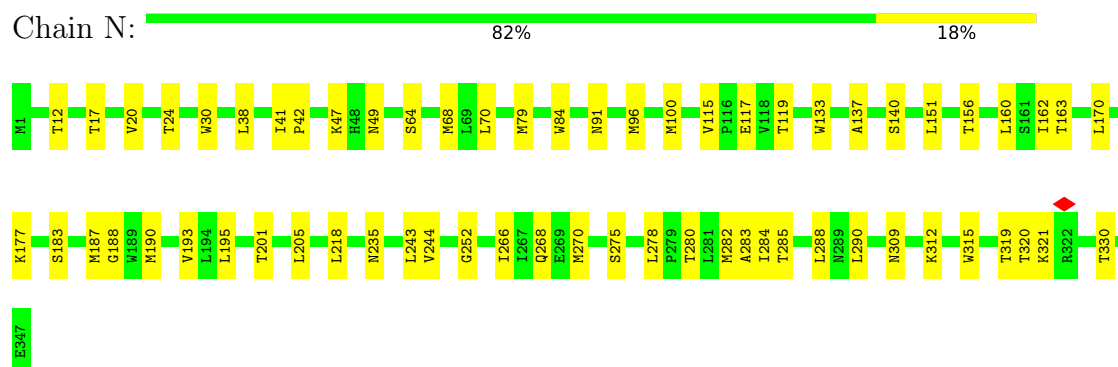
- Molecule 22: NADH-ubiquinone oxidoreductase chain 5



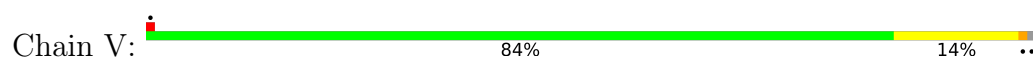
- Molecule 23: NADH-ubiquinone oxidoreductase chain 4

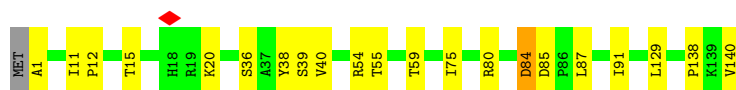


- Molecule 24: NADH-ubiquinone oxidoreductase chain 2

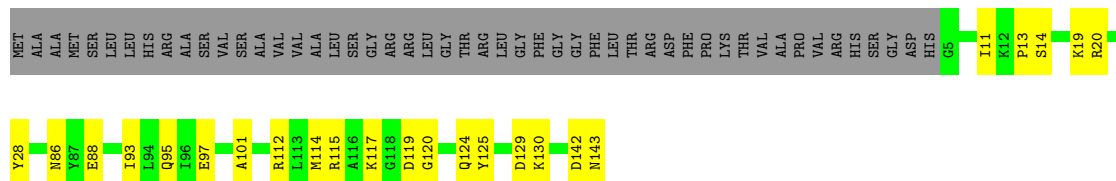


- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

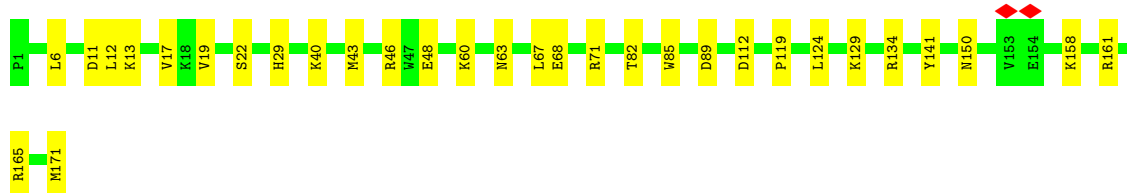
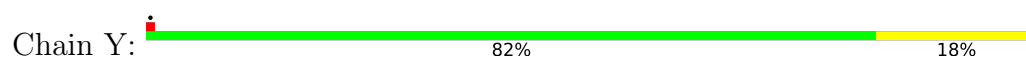




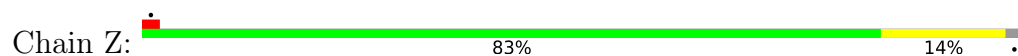
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



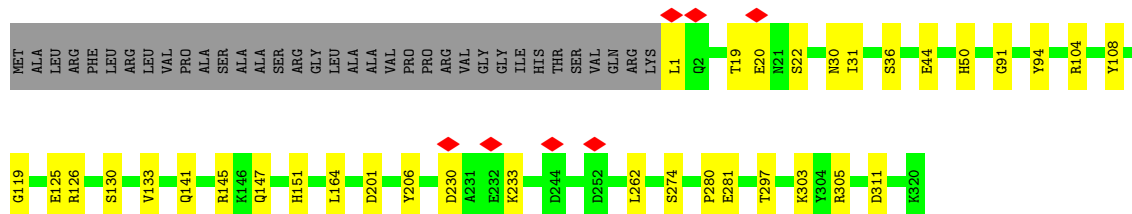
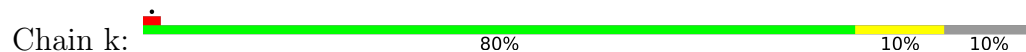
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



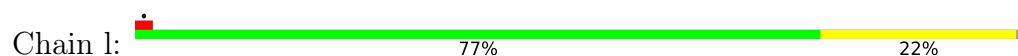
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

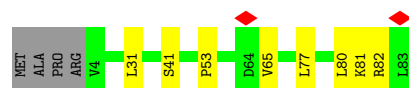
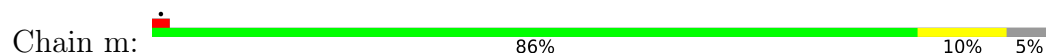


- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

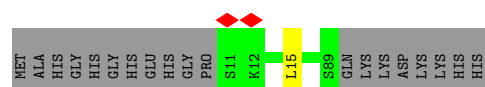
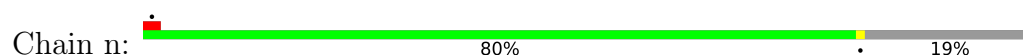




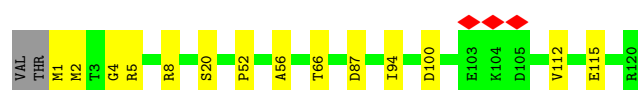
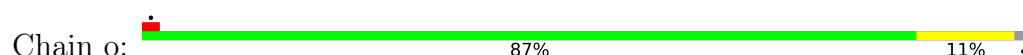
- Molecule 31: NADH:ubiquinone oxidoreductase subunit A3



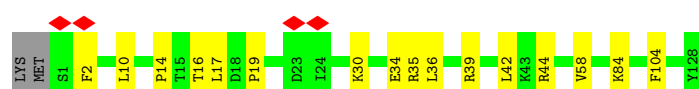
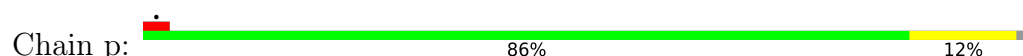
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



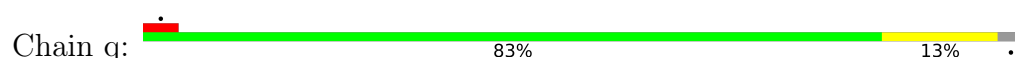
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2



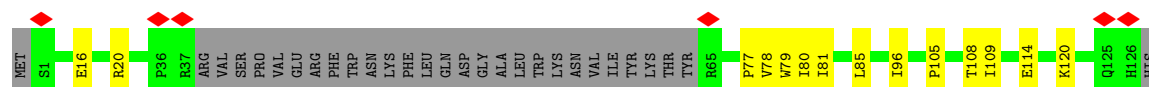
- Molecule 34: NADH:ubiquinone oxidoreductase subunit B4



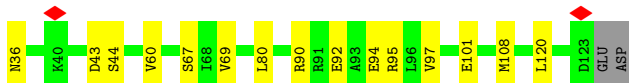
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



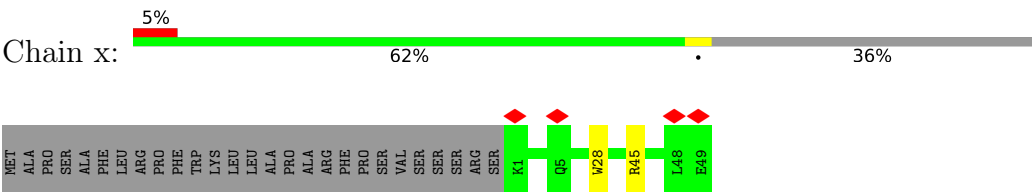
- Molecule 36: Mitochondrial complex I, B17 subunit



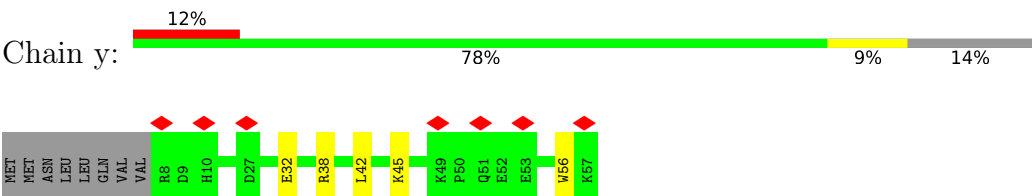
- Molecule 37: NADH:ubiquinone oxidoreductase subunit B7



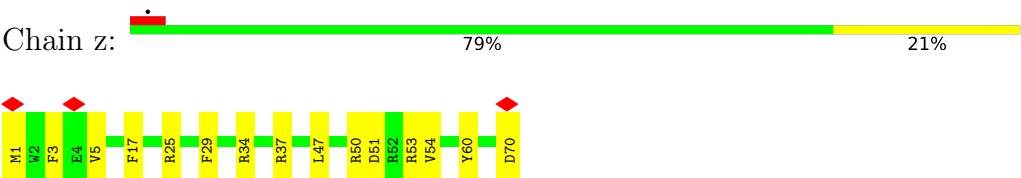
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



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



- Molecule 44: Complex I-MWFE



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32982	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	0.561	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	173.24, 197.64, 285.48	wwPDB
Map dimensions	162, 142, 234	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: SEP, FES, MYR, PC1, ZMP, SF4, K, FME, AMP, NDP, ZN, FMN, AYA, 3PE, 2MR, NAI

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	1	0.21	0/3386	0.40	0/4575
2	2	0.19	0/1695	0.42	0/2306
3	3	0.19	0/5362	0.37	0/7266
4	4	0.22	0/3535	0.39	0/4791
5	5	0.21	0/1776	0.40	0/2417
6	6	0.22	0/1278	0.38	0/1728
7	9	0.22	0/1445	0.39	0/1956
8	a	0.17	0/383	0.34	0/518
9	b	0.17	0/749	0.29	0/1009
10	c	0.21	0/1047	0.42	0/1415
11	d	0.18	0/2824	0.37	0/3830
12	e	0.24	0/702	0.52	1/945 (0.1%)
13	f	0.21	0/937	0.36	0/1271
14	g	0.22	0/993	0.40	0/1336
15	h	0.18	0/779	0.38	0/1053
16	i	0.20	0/1250	0.38	0/1698
17	X	0.23	0/713	0.45	0/963
17	j	0.24	0/670	0.52	0/902
18	A	0.23	0/947	0.46	0/1296
19	H	0.25	0/2603	0.49	0/3561
20	J	0.27	0/1378	0.56	0/1868
21	K	0.29	0/749	0.52	0/1014
22	L	0.26	0/4925	0.49	0/6700
23	M	0.28	0/3731	0.49	0/5085
24	N	0.28	0/2787	0.49	0/3795
25	V	0.20	0/1041	0.38	0/1412
26	W	0.22	0/1188	0.37	0/1607
27	Y	0.20	0/1440	0.38	0/1942
28	Z	0.22	0/1475	0.37	0/1989
29	k	0.20	0/2646	0.33	0/3579
30	l	0.22	0/896	0.46	0/1200
31	m	0.20	0/647	0.47	0/890

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	n	0.18	0/653	0.34	0/882
33	o	0.22	0/1035	0.33	0/1398
34	p	0.21	0/1085	0.36	0/1467
35	q	0.21	0/1171	0.35	0/1579
36	r	0.22	0/874	0.40	0/1188
37	s	0.22	0/1072	0.50	1/1436 (0.1%)
38	t	0.21	0/1573	0.37	0/2130
39	u	0.20	0/590	0.43	0/810
40	v	0.21	0/1361	0.42	0/1861
41	w	0.23	0/872	0.48	0/1185
42	x	0.18	0/425	0.34	0/576
43	y	0.18	0/449	0.33	0/605
44	z	0.24	0/591	0.51	0/795
All	All	0.22	0/67728	0.42	2/91829 (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	3	0	1
4	4	0	1
20	J	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	s	117	ARG	CB-CG-CD	5.55	124.07	111.30
12	e	88	ARG	CA-CB-CG	5.03	124.16	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	259	ASN	Peptide
4	4	275	TYR	Peptide
20	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	1	3312	0	3266	42	0
2	2	1655	0	1668	20	0
3	3	5275	0	5300	61	0
4	4	3457	0	3398	33	0
5	5	1726	0	1676	14	0
6	6	1247	0	1256	22	0
7	9	1414	0	1371	25	0
8	a	371	0	344	5	0
9	b	737	0	710	1	0
10	c	1024	0	1023	19	0
11	d	2748	0	2763	28	0
12	e	691	0	706	11	0
13	f	917	0	958	9	0
14	g	969	0	980	15	0
15	h	769	0	780	7	0
16	i	1209	0	1182	5	0
17	X	701	0	692	10	0
17	j	660	0	662	10	0
18	A	922	0	953	16	0
19	H	2528	0	2641	46	0
20	J	1344	0	1364	25	0
21	K	749	0	793	22	0
22	L	4807	0	4949	79	0
23	M	3647	0	3849	65	0
24	N	2723	0	2930	44	0
25	V	1028	0	1036	13	0
26	W	1155	0	1177	23	0
27	Y	1403	0	1392	25	0
28	Z	1441	0	1419	21	0
29	k	2596	0	2559	21	0
30	l	874	0	869	22	0
31	m	626	0	635	8	0
32	n	634	0	616	0	0
33	o	1004	0	995	11	0
34	p	1059	0	1062	14	0
35	q	1142	0	1137	17	0
36	r	846	0	864	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	s	1047	0	1013	16	0
38	t	1520	0	1477	16	0
39	u	563	0	509	8	0
40	v	1307	0	1207	15	0
41	w	846	0	792	16	0
42	x	412	0	411	2	0
43	y	436	0	437	3	0
44	z	576	0	570	13	0
45	1	8	0	0	0	0
45	3	16	0	0	0	0
45	6	8	0	0	0	0
45	9	16	0	0	0	0
46	1	31	0	19	0	0
47	1	44	0	27	3	0
48	2	4	0	0	0	0
48	3	4	0	0	0	0
49	3	1	0	0	0	0
50	4	40	0	54	0	0
50	6	51	0	82	1	0
50	A	51	0	82	1	0
50	H	51	0	82	1	0
50	J	40	0	54	2	0
50	L	51	0	82	1	0
50	M	44	0	65	0	0
50	V	64	0	75	2	0
50	o	31	0	36	0	0
51	6	46	0	69	0	0
51	9	54	0	88	0	0
51	L	108	0	176	3	0
51	M	54	0	88	4	0
52	b	1	0	0	0	0
53	d	48	0	26	3	0
54	X	31	0	34	0	0
54	j	34	0	40	1	0
55	k	23	0	12	3	0
56	s	15	0	26	0	0
All	All	67086	0	67608	730	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 (730) 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)
29:k:94:TYR:HH	29:k:151:HIS:HD1	1.31	0.77
2:2:79:ARG:HE	10:c:131:SER:HB3	1.58	0.68
22:L:356:ILE:HA	22:L:359:MET:HE2	1.75	0.68
3:3:36:GLN:HE22	10:c:49:VAL:H	1.39	0.67
3:3:126:ASP:HB2	4:4:328:ALA:HB3	1.77	0.67
20:J:30:GLY:HA2	20:J:64:MET:HE2	1.77	0.66
22:L:558:LEU:HD13	23:M:211:GLY:HA2	1.79	0.64
23:M:375:LEU:O	23:M:379:LEU:HB2	1.97	0.64
23:M:61:LEU:HB2	23:M:457:PRO:HG3	1.80	0.64
3:3:373:GLU:OE2	3:3:448:LYS:NZ	2.31	0.63
1:1:69:GLY:O	47:1:503:NAI:N7N	2.30	0.63
1:1:118:LEU:HD13	1:1:225:VAL:HG13	1.80	0.63
4:4:183:ARG:NH1	4:4:210:ASP:OD2	2.31	0.63
17:j:17:TYR:HA	17:j:20:LYS:HE2	1.81	0.62
22:L:216:LEU:HD22	22:L:259:LEU:HD21	1.81	0.62
5:5:174:LEU:HD12	5:5:183:VAL:HG12	1.82	0.62
23:M:36:LEU:HB2	41:w:69:VAL:HG12	1.80	0.62
11:d:200:THR:HA	11:d:290:THR:HG22	1.82	0.61
21:K:26:LEU:HD23	21:K:78:LEU:HD13	1.81	0.61
19:H:205:SER:HB3	19:H:279:ARG:HH21	1.64	0.61
50:A:201:3PE:H381	19:H:295:PRO:HB3	1.82	0.61
1:1:389:ILE:HG23	1:1:419:ILE:HD12	1.82	0.61
30:l:105:PRO:HG2	44:z:53:ARG:HH11	1.66	0.60
1:1:261:HIS:ND1	1:1:338:ASP:OD1	2.34	0.60
24:N:319:THR:O	29:k:305:ARG:NH2	2.34	0.60
26:W:114:MET:HE2	26:W:120:GLY:HA3	1.83	0.60
27:Y:48:GLU:OE1	27:Y:134:ARG:NH2	2.34	0.60
50:J:201:3PE:H292	21:K:14:VAL:HG22	1.82	0.60
22:L:396:ILE:HG21	22:L:490:ALA:HB2	1.83	0.60
10:c:42:ARG:NH1	10:c:46:GLN:O	2.35	0.60
22:L:221:THR:HG23	22:L:226:GLN:HB2	1.82	0.60
14:g:23:ASP:OD1	14:g:23:ASP:N	2.35	0.60
17:j:50:ILE:HG22	17:j:54:MET:HE2	1.84	0.60
1:1:376:MET:HE1	1:1:418:LEU:HD23	1.84	0.59
14:g:78:VAL:HA	14:g:81:LEU:HD12	1.83	0.59
23:M:165:ILE:HG21	24:N:268:GLN:HA	1.84	0.59
27:Y:89:ASP:OD2	44:z:34:ARG:NH1	2.36	0.59
4:4:354:GLU:OE2	4:4:357:GLN:NE2	2.34	0.59
1:1:368:GLY:HA3	1:1:399:ILE:HD11	1.85	0.59
5:5:41:GLN:HB3	15:h:67:ILE:HD13	1.85	0.59
7:9:13:ASP:N	7:9:13:ASP:OD1	2.35	0.59
29:k:108:TYR:OH	29:k:164:LEU:O	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:49:GLU:OE2	5:5:106:ARG:NH1	2.36	0.59
7:9:44:GLU:HA	44:z:1:MET:HE1	1.83	0.59
17:j:65:ILE:O	17:j:69:LYS:NZ	2.36	0.59
33:o:4:GLY:O	33:o:8:ARG:NH2	2.36	0.59
2:2:150:ASN:HB3	2:2:162:GLU:HB3	1.84	0.58
19:H:312:SER:HA	31:m:41:SER:HB2	1.83	0.58
21:K:78:LEU:HD11	21:K:88:ASP:HB2	1.84	0.58
37:s:11:ASP:OD1	37:s:11:ASP:N	2.36	0.58
40:v:55:GLN:NE2	40:v:69:LEU:O	2.34	0.58
4:4:269:LEU:HB2	4:4:368:GLU:HB2	1.86	0.58
11:d:134:HIS:HB2	11:d:149:LYS:HD3	1.86	0.58
13:f:24:LYS:HD3	13:f:59:LYS:HD3	1.85	0.58
22:L:446:ASN:ND2	39:u:21:GLN:OE1	2.34	0.58
22:L:561:ILE:O	22:L:565:THR:OG1	2.21	0.58
2:2:159:ASN:HB3	2:2:184:PRO:HB3	1.86	0.58
14:g:34:LEU:HD13	14:g:86:LYS:HG2	1.86	0.58
19:H:293:PHE:O	19:H:297:THR:OG1	2.22	0.58
3:3:144:PRO:HD2	3:3:192:MET:HE3	1.86	0.57
16:i:1:MET:HE3	16:i:3:LEU:H	1.69	0.57
29:k:311:ASP:N	29:k:311:ASP:OD1	2.37	0.57
40:v:138:LEU:HB3	40:v:141:GLU:HB2	1.86	0.57
2:2:101:GLN:NE2	2:2:155:GLN:OE1	2.36	0.57
5:5:37:VAL:HA	5:5:52:ILE:HG22	1.86	0.57
6:6:81:ARG:NH2	18:A:35:SER:O	2.36	0.57
22:L:290:MET:O	22:L:523:SER:OG	2.23	0.57
51:L:1002:PC1:H121	51:L:1003:PC1:H112	1.86	0.57
2:2:164:LEU:HD13	2:2:169:ILE:HD12	1.86	0.57
12:e:30:GLN:OE1	12:e:33:ARG:NH1	2.34	0.57
24:N:140:SER:HA	30:l:1:PRO:HD2	1.85	0.57
3:3:511:VAL:HG23	3:3:515:ARG:HH21	1.69	0.57
5:5:192:GLN:OE1	7:9:115:LYS:NZ	2.38	0.57
25:V:39:SER:OG	25:V:54:ARG:NH2	2.36	0.57
41:w:92:GLU:OE1	41:w:95:ARG:NH1	2.37	0.57
19:H:102:VAL:HG21	19:H:154:LEU:HD11	1.84	0.57
7:9:95:GLU:HB2	7:9:108:ARG:HB3	1.87	0.57
12:e:17:GLU:OE2	12:e:19:ARG:NH1	2.37	0.57
23:M:270:ILE:HD11	23:M:398:LEU:HB3	1.87	0.57
26:W:95:GLN:HG3	28:Z:82:LEU:HD11	1.87	0.57
21:K:1:FME:HB2	30:l:67:LEU:HD12	1.87	0.57
5:5:22:LEU:HD12	5:5:48:LEU:HB2	1.87	0.56
8:a:72:SER:OG	8:a:75:HIS:ND1	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:d:169:ALA:HB2	11:d:231:VAL:HG12	1.86	0.56
12:e:19:ARG:HB2	12:e:65:TRP:HB2	1.87	0.56
22:L:338:MET:HB2	22:L:457:LEU:HB3	1.87	0.56
29:k:141:GLN:NE2	29:k:201:ASP:OD2	2.39	0.56
4:4:111:MET:SD	4:4:111:MET:N	2.73	0.56
19:H:114:TYR:OH	20:J:61:LEU:O	2.21	0.56
1:1:243:ALA:HA	1:1:251:SER:HB2	1.86	0.56
4:4:175:GLU:OE2	4:4:188:ARG:NH2	2.38	0.56
6:6:81:ARG:NH1	18:A:33:LYS:O	2.37	0.56
19:H:18:ALA:O	19:H:21:THR:OG1	2.24	0.56
22:L:520:PHE:O	22:L:524:ASN:HB2	2.05	0.56
20:J:18:VAL:HG21	20:J:96:GLY:HA3	1.87	0.56
29:k:104:ARG:NH2	55:k:501:AMP:N7	2.54	0.56
11:d:98:GLU:OE1	11:d:286:ARG:NH2	2.32	0.56
11:d:97:ARG:HH21	53:d:401:NDP:H2B	1.71	0.56
1:1:270:GLU:OE1	1:1:283:HIS:NE2	2.39	0.55
1:1:388:GLU:HA	1:1:391:SER:HB3	1.88	0.55
24:N:243:LEU:HD22	24:N:330:THR:HG21	1.87	0.55
37:s:21:MET:HE1	40:v:129:GLY:HA2	1.88	0.55
33:o:5:ARG:O	33:o:8:ARG:NH1	2.38	0.55
1:1:139:ARG:NH2	2:2:144:CYS:O	2.39	0.55
23:M:158:LEU:HD13	24:N:283:ALA:HB1	1.88	0.55
26:W:124:GLN:HB2	33:o:4:GLY:HA3	1.87	0.55
13:f:8:THR:HG23	13:f:10:LEU:H	1.71	0.55
50:V:202:3PE:H322	50:V:202:3PE:H261	1.88	0.55
1:1:265:PRO:O	2:2:190:ARG:NH2	2.39	0.55
18:A:12:THR:HA	18:A:15:THR:HG22	1.88	0.55
34:p:36:LEU:HD22	38:t:7:ALA:HB2	1.89	0.55
31:m:80:LEU:O	35:q:58:ARG:NH1	2.39	0.55
2:2:53:LEU:HD12	8:a:52:LEU:HD13	1.89	0.55
21:K:37:MET:HG2	24:N:68:MET:HE1	1.87	0.55
27:Y:165:ARG:NH2	33:o:87:ASP:OD1	2.39	0.55
5:5:177:ASP:OD1	11:d:40:ARG:NH2	2.40	0.55
11:d:48:PRO:HA	11:d:71:MET:O	2.08	0.54
19:H:9:LEU:HD22	19:H:95:LEU:HD22	1.90	0.54
27:Y:29:HIS:HB3	27:Y:119:PRO:HD2	1.89	0.54
3:3:252:PRO:HG3	3:3:263:ILE:HG12	1.88	0.54
38:t:175:GLU:HG2	38:t:176:ARG:HG2	1.88	0.54
40:v:62:TYR:HE2	40:v:72:ASN:HD21	1.56	0.54
3:3:601:ARG:NH1	3:3:605:GLU:OE1	2.35	0.54
11:d:320:ARG:HB3	18:A:31:SER:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:j:101:ZMP:N2	54:j:101:ZMP:O2	2.38	0.54
23:M:25:ILE:HG23	41:w:60:VAL:HG21	1.89	0.54
26:W:88:GLU:OE1	43:y:56:TRP:NE1	2.31	0.54
34:p:84:LYS:HE3	40:v:40:ASP:HB2	1.88	0.54
23:M:305:THR:OG1	23:M:384:SER:OG	2.23	0.54
11:d:50:ARG:NH2	53:d:401:NDP:O3X	2.40	0.54
23:M:59:ASP:OD2	23:M:245:ARG:NH2	2.36	0.54
31:m:77:LEU:HD13	31:m:80:LEU:HD23	1.90	0.54
35:q:85:MET:HE2	35:q:123:LEU:HD22	1.89	0.54
1:l:61:LYS:HG3	1:l:76:GLY:HA3	1.89	0.54
18:A:13:LEU:HD22	19:H:10:ILE:HD12	1.90	0.54
19:H:89:LEU:HD11	19:H:233:MET:HE2	1.90	0.54
23:M:255:ASP:OD1	23:M:255:ASP:N	2.37	0.54
41:w:34:ASP:OD1	41:w:34:ASP:N	2.37	0.54
23:M:368:ALA:HB1	23:M:375:LEU:HB2	1.89	0.53
36:r:120:LYS:HB3	37:s:39:VAL:HG13	1.90	0.53
12:e:84:ASP:O	12:e:88:ARG:NH1	2.41	0.53
20:J:23:LYS:NZ	21:K:18:GLY:O	2.39	0.53
17:X:38:LYS:NZ	17:X:39:ASP:OD1	2.42	0.53
28:Z:78:GLU:HG2	28:Z:79:LYS:HG3	1.91	0.53
33:o:20:SER:OG	42:x:45:ARG:NH1	2.41	0.53
3:3:276:ARG:NH1	3:3:680:ALA:O	2.42	0.53
24:N:49:ASN:OD1	24:N:49:ASN:N	2.41	0.53
3:3:174:THR:HG22	3:3:183:VAL:HG22	1.90	0.53
3:3:272:ASP:OD1	3:3:272:ASP:N	2.40	0.53
37:s:6:ARG:NH1	37:s:15:GLU:OE1	2.41	0.53
40:v:30:ARG:NH1	40:v:33:ASP:OD2	2.40	0.53
19:H:17:VAL:HG11	19:H:225:MET:HB3	1.91	0.53
11:d:271:GLU:OE2	11:d:281:ARG:NH2	2.42	0.53
19:H:85:MET:HG3	19:H:233:MET:HE3	1.90	0.53
23:M:130:LEU:HD13	23:M:150:LEU:HD13	1.91	0.53
34:p:2:PHE:HE2	38:t:69:GLU:HG2	1.73	0.53
1:l:109:GLU:OE2	1:l:112:ARG:NH2	2.42	0.53
19:H:26:LYS:HE3	44:z:5:VAL:HA	1.90	0.53
26:W:13:PRO:HD3	38:t:98:VAL:HG11	1.91	0.53
6:6:36:LEU:HD13	50:6:203:3PE:H392	1.91	0.52
38:t:55:ASP:HB3	38:t:58:LYS:HB2	1.91	0.52
5:5:178:ASP:OD2	11:d:32:ARG:NH2	2.42	0.52
21:K:98:CYS:O	24:N:177:LYS:NZ	2.42	0.52
20:J:67:VAL:O	20:J:71:THR:HG23	2.10	0.52
22:L:128:MET:HG2	22:L:251:THR:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:339:SER:HB3	23:M:344:LEU:HD22	1.91	0.52
1:1:228:VAL:O	1:1:231:SER:OG	2.27	0.52
9:b:81:THR:HG22	9:b:92:ARG:HB2	1.91	0.52
17:j:47:GLN:NE2	17:j:70:LEU:O	2.43	0.52
20:J:26:PRO:HB2	20:J:71:THR:HG21	1.92	0.52
40:v:40:ASP:OD1	40:v:40:ASP:N	2.38	0.52
1:1:260:GLY:O	2:2:111:ARG:NH1	2.41	0.52
4:4:410:MET:H	4:4:413:ASP:HB2	1.74	0.52
11:d:101:THR:OG1	11:d:102:LYS:N	2.43	0.52
22:L:366:MET:HE2	22:L:443:ILE:HG23	1.91	0.52
24:N:252:GLY:HA3	24:N:290:LEU:HD13	1.91	0.52
39:u:10:ARG:NH1	39:u:14:PHE:O	2.38	0.52
1:1:28:ARG:NH1	8:a:35:ASN:O	2.38	0.52
3:3:285:ARG:NH2	3:3:555:PRO:O	2.42	0.52
6:6:170:GLU:OE1	6:6:172:ARG:NH2	2.42	0.52
7:9:23:GLN:HG3	7:9:28:THR:HB	1.92	0.52
23:M:60:SER:HB3	23:M:457:PRO:HA	1.92	0.52
24:N:30:TRP:HD1	24:N:70:LEU:HD23	1.74	0.52
1:1:120:GLU:OE2	1:1:236:ARG:NH1	2.43	0.52
13:f:8:THR:HG21	13:f:13:LEU:HB3	1.92	0.52
17:X:47:GLN:NE2	17:X:70:LEU:O	2.43	0.52
34:p:14:PRO:HG2	34:p:17:LEU:HD12	1.91	0.52
4:4:179:GLU:OE2	6:6:66:ARG:NH1	2.43	0.52
30:l:14:ASP:OD1	30:l:14:ASP:N	2.43	0.52
7:9:53:GLU:OE2	16:i:34:ARG:NH2	2.40	0.52
24:N:163:THR:HA	24:N:285:THR:HG21	1.92	0.52
4:4:238:ARG:NH1	19:H:279:ARG:O	2.43	0.52
7:9:57:LEU:O	15:h:33:ARG:NH2	2.42	0.52
24:N:84:TRP:HB2	30:l:18:THR:HA	1.92	0.51
29:k:126:ARG:HH12	55:k:501:AMP:H5'2	1.75	0.51
34:p:35:ARG:NH2	40:v:33:ASP:OD2	2.43	0.51
3:3:105:CYS:SG	3:3:117:GLN:NE2	2.78	0.51
6:6:178:ARG:O	11:d:103:ASN:ND2	2.40	0.51
20:J:141:MET:HE1	30:l:26:HIS:CE1	2.45	0.51
36:r:105:PRO:O	37:s:67:LYS:NZ	2.44	0.51
3:3:36:GLN:OE1	3:3:39:ARG:NH2	2.44	0.51
3:3:601:ARG:NH2	3:3:614:ASP:OD1	2.42	0.51
6:6:81:ARG:NH2	19:H:214:GLU:OE1	2.43	0.51
10:c:36:ARG:NE	10:c:106:GLU:OE2	2.43	0.51
19:H:141:SER:HA	19:H:290:TRP:HE1	1.74	0.51
3:3:10:GLU:HB2	3:3:19:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:K:50:ASN:O	30:l:31:ARG:NH1	2.43	0.51
3:3:127:ARG:NH2	4:4:326:ASP:O	2.43	0.51
11:d:54:TYR:HA	11:d:57:MET:HG2	1.91	0.51
24:N:235:ASN:O	24:N:315:TRP:NE1	2.41	0.51
29:k:274:SER:O	29:k:274:SER:OG	2.25	0.51
10:c:8:THR:OG1	10:c:9:GLN:N	2.43	0.51
18:A:68:GLU:HG2	20:J:161:LEU:HD23	1.93	0.51
24:N:64:SER:O	24:N:68:MET:HG2	2.11	0.51
43:y:32:GLU:OE2	43:y:38:ARG:NH2	2.37	0.51
2:2:147:ALA:HB3	2:2:153:MET:HE3	1.92	0.51
4:4:63:ARG:HB3	4:4:79:HIS:HB2	1.92	0.51
22:L:88:MET:HB3	22:L:326:PHE:HE2	1.76	0.51
1:1:140:GLY:O	1:1:179:ARG:NH2	2.43	0.51
11:d:97:ARG:NH2	53:d:401:NDP:O3X	2.44	0.51
22:L:535:ARG:NH1	34:p:10:LEU:O	2.44	0.51
24:N:190:MET:HB3	24:N:201:THR:HG23	1.92	0.51
3:3:453:LEU:HD21	3:3:458:LEU:HD21	1.93	0.50
24:N:320:THR:HB	29:k:1:LEU:HD21	1.93	0.50
26:W:142:ASP:OD1	27:Y:46:ARG:NH1	2.35	0.50
33:o:66:THR:OG1	42:x:28:TRP:NE1	2.44	0.50
2:2:178:ALA:O	2:2:180:LYS:NZ	2.43	0.50
21:K:73:LEU:HD21	24:N:41:ILE:HG13	1.93	0.50
34:p:19:PRO:HA	38:t:64:ARG:HH12	1.77	0.50
3:3:484:THR:OG1	3:3:486:ASP:OD1	2.29	0.50
5:5:151:ILE:HG23	5:5:152:LEU:HG	1.93	0.50
18:A:60:ILE:HG23	21:K:72:ALA:HB1	1.93	0.50
19:H:138:GLN:NE2	19:H:191:ALA:O	2.44	0.50
22:L:129:LEU:HA	22:L:132:VAL:HG22	1.94	0.50
23:M:359:TRP:HZ3	23:M:410:MET:HE3	1.76	0.50
3:3:243:ARG:HD2	3:3:244:THR:HG23	1.94	0.50
4:4:175:GLU:HG2	6:6:66:ARG:HD2	1.94	0.50
7:9:108:ARG:NH1	7:9:110:ASP:OD1	2.44	0.50
20:J:167:VAL:HG22	24:N:42:PRO:HG2	1.93	0.50
23:M:126:LEU:HD22	23:M:150:LEU:HD12	1.91	0.50
25:V:140:VAL:HG12	26:W:112:ARG:HB2	1.93	0.50
27:Y:129:LYS:HD3	31:m:65:VAL:HG13	1.93	0.50
4:4:292:ASP:OD1	4:4:292:ASP:N	2.34	0.50
7:9:132:VAL:HG21	7:9:165:ILE:HG21	1.93	0.50
23:M:310:MET:HE3	23:M:458:LEU:HD12	1.93	0.50
23:M:310:MET:HE2	23:M:459:TYR:HA	1.94	0.50
27:Y:43:MET:HE3	35:q:72:PRO:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:l:64:GLU:HG3	30:l:70:LYS:HE3	1.93	0.50
3:3:424:ASP:OD1	3:3:424:ASP:N	2.39	0.50
8:a:71:GLU:OE1	8:a:75:HIS:ND1	2.44	0.50
1:1:20:ARG:NH1	1:1:269:GLU:O	2.42	0.50
3:3:382:THR:HB	3:3:454:GLY:HA3	1.94	0.50
12:e:23:CYS:SG	12:e:24:GLN:N	2.83	0.50
51:L:1002:PC1:H3B1	36:r:80:ILE:HD12	1.94	0.50
23:M:38:SER:HB2	23:M:70:MET:HE2	1.92	0.50
28:Z:20:SER:O	28:Z:20:SER:OG	2.30	0.50
28:Z:25:LEU:HD12	37:s:75:ASN:HB2	1.92	0.50
17:X:55:GLU:OE1	38:t:24:ARG:NH2	2.42	0.50
33:o:52:PRO:HG2	33:o:56:ALA:HB2	1.93	0.50
1:1:197:GLU:OE1	10:c:129:ARG:NH2	2.42	0.50
10:c:10:LEU:HB3	14:g:15:SER:HB3	1.94	0.50
22:L:227:PHE:N	22:L:284:THR:OG1	2.45	0.49
25:V:11:ILE:HB	25:V:20:LYS:HD3	1.94	0.49
27:Y:6:LEU:HD21	35:q:86:LEU:HB3	1.93	0.49
36:r:16:GLU:OE2	36:r:20:ARG:NH1	2.44	0.49
6:6:117:GLY:O	6:6:121:ASN:ND2	2.46	0.49
4:4:3:GLN:NE2	23:M:135:ARG:O	2.45	0.49
22:L:10:VAL:HG21	36:r:78:VAL:HG23	1.95	0.49
23:M:328:CYS:HB3	23:M:437:MET:HE1	1.95	0.49
3:3:94:MET:HE1	3:3:119:GLN:HG3	1.94	0.49
7:9:40:TYR:HE2	19:H:33:PHE:HB2	1.78	0.49
29:k:130:SER:O	29:k:130:SER:OG	2.26	0.49
1:1:367:GLU:OE1	3:3:100:ASN:ND2	2.44	0.49
3:3:450:MET:HG3	3:3:491:ASN:HD22	1.78	0.49
3:3:651:LEU:HD11	12:e:45:LYS:HZ2	1.77	0.49
11:d:91:VAL:HG23	11:d:126:VAL:HG11	1.93	0.49
11:d:268:ARG:NH1	11:d:271:GLU:OE2	2.45	0.49
11:d:322:ARG:NH1	11:d:329:SER:OG	2.45	0.49
19:H:181:LEU:HG	19:H:300:LEU:HD13	1.95	0.49
13:f:22:ARG:NH2	13:f:84:GLU:OE2	2.45	0.49
19:H:253:GLU:OE2	44:z:25:ARG:NH1	2.46	0.49
24:N:17:THR:OG1	24:N:133:TRP:NE1	2.45	0.49
26:W:119:ASP:O	27:Y:150:ASN:ND2	2.46	0.49
31:m:53:PRO:HD3	35:q:68:ILE:HD13	1.94	0.49
3:3:159:CYS:HB3	3:3:172:LEU:HD13	1.95	0.49
23:M:391:ILE:HG23	23:M:394:ILE:HD12	1.95	0.49
39:u:10:ARG:HD2	39:u:15:PRO:HA	1.94	0.49
1:1:372:MET:HA	1:1:375:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:j:54:MET:HE3	17:j:76:ILE:HD12	1.95	0.49
3:3:675:ASP:OD1	3:3:675:ASP:N	2.46	0.49
43:y:42:LEU:HA	43:y:45:LYS:HE3	1.95	0.49
22:L:10:VAL:HB	36:r:81:ILE:HD11	1.95	0.49
22:L:570:GLN:HG3	24:N:288:LEU:HD21	1.94	0.49
29:k:145:ARG:NH1	29:k:147:GLN:OE1	2.45	0.49
6:6:108:PRO:HA	18:A:33:LYS:HE2	1.95	0.48
50:J:201:3PE:H222	21:K:21:MET:HB2	1.95	0.48
1:1:291:TRP:NE1	1:1:313:GLU:OE1	2.44	0.48
15:h:13:TRP:O	35:q:27:ARG:NH1	2.42	0.48
1:1:95:VAL:HG11	1:1:118:LEU:HD11	1.96	0.48
24:N:24:THR:HG22	30:l:2:PHE:HZ	1.76	0.48
28:Z:138:TYR:HB2	41:w:108:MET:HE1	1.94	0.48
1:1:305:PRO:HG3	1:1:413:TRP:HB3	1.95	0.48
29:k:19:THR:OG1	29:k:20:GLU:N	2.46	0.48
20:J:175:ASN:OD1	20:J:175:ASN:N	2.46	0.48
36:r:77:PRO:O	36:r:81:ILE:HG12	2.14	0.48
37:s:8:TYR:OH	40:v:123:PRO:O	2.29	0.48
3:3:324:ASP:OD1	3:3:324:ASP:N	2.37	0.48
3:3:365:ASN:N	3:3:491:ASN:OD1	2.46	0.48
6:6:44:SER:HB3	19:H:54:LYS:HE2	1.96	0.48
23:M:379:LEU:O	23:M:383:MET:HG2	2.14	0.48
26:W:28:TYR:O	41:w:67:SER:OG	2.23	0.48
28:Z:122:GLN:NE2	37:s:46:ASN:OD1	2.40	0.48
27:Y:12:LEU:O	30:l:104:ARG:NH1	2.46	0.48
27:Y:82:THR:HA	27:Y:85:TRP:CD1	2.49	0.48
29:k:31:ILE:HG23	55:k:501:AMP:H3'	1.96	0.48
2:2:24:THR:OG1	2:2:27:ASN:ND2	2.45	0.48
26:W:20:ARG:NH2	41:w:44:SER:O	2.45	0.48
4:4:162:GLY:HA3	19:H:279:ARG:HG3	1.96	0.48
1:1:116:HIS:HA	1:1:119:VAL:HG22	1.96	0.47
13:f:37:ILE:O	13:f:44:ARG:NH1	2.47	0.47
51:L:1003:PC1:H3F1	23:M:447:LEU:HD11	1.96	0.47
23:M:390:ASN:O	23:M:393:ILE:HG22	2.14	0.47
1:1:184:TYR:HB3	1:1:357:GLU:HB3	1.95	0.47
4:4:41:ASP:OD1	4:4:41:ASP:N	2.41	0.47
17:j:46:ASP:O	17:j:50:ILE:HG13	2.14	0.47
20:J:11:ILE:HD12	20:J:11:ILE:HA	1.75	0.47
26:W:117:LYS:NZ	33:o:100:ASP:OD2	2.46	0.47
38:t:108:PRO:HA	38:t:111:LYS:HB2	1.95	0.47
3:3:533:THR:OG1	3:3:534:ARG:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:3:LYS:NZ	15:h:109:GLU:OE1	2.42	0.47
11:d:240:ASP:OD1	11:d:240:ASP:N	2.38	0.47
28:Z:159:LYS:NZ	33:o:112:VAL:O	2.44	0.47
22:L:97:THR:O	22:L:101:MET:HB2	2.15	0.47
22:L:295:GLN:HE21	22:L:526:LEU:HD11	1.78	0.47
24:N:162:ILE:HG13	24:N:188:GLY:HA3	1.96	0.47
4:4:352:TYR:HD1	7:9:86:VAL:HG21	1.79	0.47
19:H:185:TRP:O	19:H:189:THR:HG23	2.14	0.47
22:L:132:VAL:HG23	22:L:133:THR:HG23	1.95	0.47
22:L:316:THR:HA	22:L:319:ILE:HG12	1.95	0.47
3:3:360:SER:O	3:3:365:ASN:ND2	2.36	0.47
19:H:157:ASN:ND2	19:H:159:SER:O	2.47	0.47
35:q:68:ILE:HA	35:q:71:MET:HG3	1.97	0.47
1:1:193:ILE:HD12	1:1:215:VAL:HB	1.96	0.47
11:d:157:ARG:HH12	11:d:225:GLY:HA2	1.79	0.47
19:H:193:THR:HB	19:H:231:ILE:HG22	1.97	0.47
22:L:102:GLU:OE1	22:L:456:ARG:NH1	2.47	0.47
7:9:135:PRO:HG3	7:9:164:GLU:HG2	1.96	0.47
22:L:63:ILE:HG23	36:r:96:ILE:HG13	1.96	0.47
23:M:173:SER:HB2	26:W:101:ALA:HB2	1.96	0.47
25:V:87:LEU:O	25:V:91:ILE:HG13	2.15	0.47
29:k:133:VAL:HG11	29:k:206:TYR:CZ	2.50	0.47
30:l:91:TYR:OH	35:q:92:GLU:OE1	2.31	0.47
3:3:228:ILE:HG13	3:3:581:GLN:HB3	1.97	0.47
3:3:604:SER:OG	3:3:609:MET:O	2.32	0.47
14:g:114:PRO:HB3	14:g:119:SER:HB2	1.95	0.47
19:H:179:TRP:HE1	35:q:42:LEU:HG	1.79	0.47
21:K:52:HIS:HB2	30:l:31:ARG:HG2	1.97	0.47
22:L:292:ALA:HB2	22:L:304:PHE:HB3	1.97	0.47
24:N:190:MET:HE3	24:N:205:LEU:HB2	1.97	0.47
33:o:5:ARG:HA	33:o:8:ARG:HH22	1.78	0.47
7:9:64:GLU:OE1	7:9:136:ASN:ND2	2.47	0.47
11:d:196:LEU:HD22	11:d:257:PRO:HB3	1.97	0.47
39:u:27:PHE:O	39:u:31:THR:HG23	2.15	0.47
33:o:1:MET:HE2	33:o:2:MET:HE2	1.97	0.46
41:w:97:VAL:O	41:w:101:GLU:HB2	2.15	0.46
1:1:89:ARG:NH1	1:1:217:GLY:O	2.48	0.46
23:M:312:ALA:O	23:M:316:MET:HG3	2.16	0.46
22:L:243:VAL:O	22:L:247:LEU:HB2	2.14	0.46
29:k:297:THR:HG23	29:k:303:LYS:HG3	1.97	0.46
3:3:588:MET:HG3	10:c:63:GLU:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:40:LYS:HA	27:Y:40:LYS:HD3	1.71	0.46
2:2:55:GLN:NE2	2:2:91:ASN:OD1	2.49	0.46
19:H:313:SER:HB2	35:q:50:MET:HA	1.97	0.46
22:L:60:GLU:HB2	22:L:83:ASP:HA	1.97	0.46
40:v:82:ASP:N	40:v:82:ASP:OD1	2.48	0.46
19:H:180:PRO:O	19:H:184:MET:HG3	2.15	0.46
22:L:295:GLN:O	22:L:425:ARG:NH1	2.49	0.46
44:z:70:ASP:OD1	44:z:70:ASP:N	2.39	0.46
4:4:117:ALA:HB2	4:4:367:ILE:HG12	1.98	0.46
18:A:70:ALA:HB2	20:J:59:ILE:HD11	1.98	0.46
24:N:309:ASN:OD1	24:N:312:LYS:NZ	2.48	0.46
27:Y:11:ASP:O	27:Y:60:LYS:NZ	2.42	0.46
3:3:439:PHE:HA	3:3:442:VAL:HB	1.98	0.46
4:4:302:GLU:HG2	7:9:3:LYS:HD2	1.97	0.46
25:V:138:PRO:HB2	26:W:115:ARG:HE	1.81	0.46
29:k:230:ASP:OD2	29:k:233:LYS:NZ	2.37	0.46
1:1:327:THR:OG1	1:1:328:GLY:N	2.49	0.46
7:9:34:LEU:HD21	19:H:273:ILE:HD13	1.97	0.46
13:f:109:SER:O	13:f:109:SER:OG	2.33	0.46
22:L:538:PRO:HB2	40:v:89:VAL:HG22	1.97	0.46
3:3:296:TRP:O	3:3:300:LEU:HB2	2.16	0.46
5:5:183:VAL:O	14:g:100:THR:OG1	2.27	0.46
6:6:70:ASP:OD1	19:H:25:ARG:NH2	2.49	0.46
14:g:61:LYS:NZ	14:g:105:PHE:O	2.44	0.46
24:N:47:LYS:HA	24:N:47:LYS:HD3	1.71	0.46
28:Z:3:SER:OG	28:Z:4:TRP:N	2.49	0.46
44:z:1:MET:HB2	44:z:3:PHE:CZ	2.51	0.46
2:2:39:PRO:HA	8:a:65:GLN:HB3	1.98	0.45
15:h:41:PRO:HB3	35:q:5:VAL:HG11	1.97	0.45
25:V:36:SER:O	25:V:40:VAL:HG22	2.16	0.45
1:1:374:LYS:HB3	3:3:132:GLU:HG2	1.98	0.45
14:g:38:TRP:O	14:g:42:VAL:HG23	2.17	0.45
14:g:91:GLU:HG2	14:g:97:LYS:HG3	1.99	0.45
50:H:401:3PE:H3A1	50:H:401:3PE:H2F2	1.98	0.45
20:J:167:VAL:HG13	24:N:42:PRO:HG3	1.98	0.45
24:N:170:LEU:HD11	24:N:288:LEU:HD22	1.98	0.45
24:N:183:SER:O	24:N:187:MET:HG2	2.16	0.45
2:2:161:TYR:HB3	2:2:164:LEU:HD21	1.98	0.45
3:3:638:GLY:O	12:e:24:GLN:NE2	2.48	0.45
6:6:24:SER:OG	6:6:25:ARG:N	2.49	0.45
20:J:107:VAL:HG21	21:K:6:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:49:SER:O	23:M:51:ASN:ND2	2.50	0.45
1:1:191:ALA:HB2	1:1:203:PRO:HG3	1.98	0.45
18:A:80:GLN:OE1	35:q:57:ARG:NH1	2.44	0.45
22:L:15:LEU:HA	22:L:15:LEU:HD23	1.74	0.45
27:Y:124:LEU:HD13	35:q:69:ALA:HB2	1.99	0.45
1:1:394:GLU:OE1	3:3:129:ARG:NH1	2.50	0.45
3:3:331:LEU:HD13	3:3:600:ILE:HD12	1.99	0.45
4:4:1:ALA:N	41:w:31:GLU:OE1	2.41	0.45
25:V:80:ARG:NH2	25:V:85:ASP:OD2	2.49	0.45
17:X:88:GLU:H	17:X:88:GLU:CD	2.24	0.45
30:l:104:ARG:HH21	35:q:84:GLN:HG3	1.82	0.45
7:9:94:ILE:HG12	7:9:109:TYR:HD2	1.82	0.45
13:f:6:LYS:HA	13:f:6:LYS:HD3	1.80	0.45
17:j:76:ILE:O	17:j:80:ILE:HG22	2.17	0.45
22:L:237:MET:HE3	22:L:303:ALA:HB2	1.98	0.45
14:g:67:LYS:HE2	14:g:67:LYS:HB2	1.76	0.45
22:L:257:ILE:O	22:L:261:ILE:HG13	2.16	0.45
24:N:156:THR:O	24:N:160:LEU:HB2	2.17	0.45
28:Z:15:ARG:HB3	36:r:109:ILE:HD12	1.98	0.45
19:H:103:LEU:HB2	20:J:54:LEU:HD13	1.99	0.45
21:K:75:LEU:O	21:K:79:VAL:HG23	2.17	0.45
23:M:50:LEU:HA	26:W:86:ASN:HD21	1.81	0.45
17:X:9:GLU:HA	17:X:12:LYS:HE3	1.97	0.45
5:5:41:GLN:HG3	5:5:49:GLU:HB2	1.98	0.45
12:e:64:LEU:HB3	12:e:76:VAL:HB	1.99	0.45
20:J:163:ILE:HD13	24:N:12:THR:HG21	1.98	0.45
4:4:82:LEU:O	6:6:93:THR:OG1	2.33	0.44
14:g:74:ASP:HB3	14:g:77:VAL:HG12	1.97	0.44
22:L:28:LYS:NZ	22:L:29:PHE:O	2.41	0.44
22:L:97:THR:HG21	22:L:125:LEU:HD13	1.98	0.44
22:L:594:THR:OG1	25:V:38:TYR:OH	2.28	0.44
23:M:74:PRO:O	23:M:78:MET:HG3	2.17	0.44
30:l:38:GLU:HG3	35:q:114:ARG:HH12	1.81	0.44
30:l:87:LYS:HB3	30:l:87:LYS:HE3	1.68	0.44
19:H:58:LYS:HB3	19:H:217:ALA:HB3	1.99	0.44
22:L:383:MET:HG2	22:L:384:PRO:HD2	1.99	0.44
23:M:94:LEU:O	23:M:98:MET:HG2	2.17	0.44
22:L:363:PHE:HA	22:L:370:THR:HG21	1.98	0.44
23:M:263:MET:SD	23:M:263:MET:N	2.90	0.44
27:Y:129:LYS:NZ	31:m:65:VAL:O	2.46	0.44
28:Z:143:HIS:O	28:Z:157:LYS:NZ	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:N:278:LEU:O	24:N:282:MET:HG3	2.18	0.44
26:W:95:GLN:HB2	28:Z:82:LEU:HD21	1.98	0.44
30:l:78:ILE:HA	35:q:97:MET:HE2	1.98	0.44
13:f:67:LEU:O	13:f:71:LEU:HB2	2.17	0.44
22:L:338:MET:HE1	22:L:376:GLY:HA3	1.99	0.44
23:M:419:HIS:ND1	23:M:420:THR:O	2.51	0.44
17:X:7:THR:HG23	17:X:10:GLY:H	1.82	0.44
1:l:292:ASP:OD1	1:l:292:ASP:N	2.50	0.44
11:d:160:PHE:HB3	11:d:163:ALA:HB2	2.00	0.44
14:g:116:ASP:N	14:g:116:ASP:OD1	2.46	0.44
22:L:313:MET:HA	22:L:316:THR:HG22	1.99	0.44
23:M:68:LEU:O	23:M:72:LEU:HB2	2.17	0.44
26:W:14:SER:OG	38:t:110:GLU:OE2	2.35	0.44
28:Z:18:ALA:N	36:r:108:THR:O	2.49	0.44
3:3:115:ASP:O	3:3:119:GLN:HG2	2.18	0.44
19:H:309:ILE:HD13	19:H:314:ILE:HD11	1.99	0.44
22:L:101:MET:SD	22:L:121:LEU:HD23	2.57	0.44
22:L:421:ILE:HG12	22:L:501:ALA:HB2	1.99	0.44
22:L:587:TYR:OH	24:N:117:GLU:OE2	2.28	0.44
23:M:47:ASP:OD2	28:Z:93:ARG:NH1	2.50	0.44
23:M:77:LEU:HD23	23:M:77:LEU:HA	1.87	0.44
29:k:280:PRO:HB3	41:w:25:ARG:HA	1.99	0.44
4:4:338:MET:HB3	4:4:338:MET:HE3	1.81	0.44
6:6:81:ARG:NH1	19:H:61:LEU:HD21	2.33	0.44
7:9:79:ALA:HB2	7:9:106:THR:HG22	1.99	0.44
20:J:64:MET:HE1	21:K:31:LEU:HD22	2.00	0.44
22:L:76:LEU:HD21	22:L:196:TRP:HE3	1.83	0.44
3:3:239:VAL:HG23	3:3:253:ARG:HG3	2.00	0.44
4:4:323:ILE:HD12	4:4:324:LYS:HG3	2.00	0.44
13:f:34:LEU:HD23	13:f:37:ILE:HD12	1.99	0.44
18:A:34:THR:HB	19:H:63:PRO:HA	1.98	0.44
22:L:161:ARG:HA	38:t:91:GLU:HG3	2.00	0.44
23:M:263:MET:HE1	34:p:104:PHE:CD2	2.53	0.44
34:p:30:LYS:O	34:p:34:GLU:HG3	2.18	0.44
3:3:283:MET:HE3	3:3:283:MET:HB2	1.85	0.43
4:4:109:VAL:HG11	4:4:152:MET:SD	2.58	0.43
7:9:148:LEU:HD23	10:c:70:MET:HG3	1.99	0.43
16:i:84:PRO:HA	16:i:87:HIS:HB3	2.00	0.43
18:A:94:LEU:HD23	18:A:94:LEU:HA	1.91	0.43
22:L:366:MET:O	22:L:370:THR:HG23	2.18	0.43
23:M:1:FME:HE2	23:M:1:FME:HB2	1.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:130:LEU:O	23:M:134:THR:OG1	2.32	0.43
23:M:181:TYR:HB3	28:Z:84:MET:HE3	2.00	0.43
23:M:243:MET:HB3	23:M:301:ILE:HG21	1.99	0.43
24:N:20:VAL:HG11	24:N:137:ALA:HB1	2.00	0.43
24:N:270:MET:O	24:N:275:SER:OG	2.35	0.43
26:W:11:ILE:HG23	38:t:103:LEU:HD21	1.99	0.43
17:X:25:ILE:HD12	17:X:40:LEU:HD13	2.00	0.43
37:s:64:ARG:HG2	37:s:82:GLU:HG2	1.99	0.43
3:3:241:SER:OG	3:3:249:ARG:HG2	2.18	0.43
3:3:375:ASP:OD1	3:3:375:ASP:N	2.50	0.43
10:c:128:THR:O	10:c:128:THR:OG1	2.36	0.43
21:K:47:MET:HE2	24:N:79:MET:HA	2.00	0.43
23:M:59:ASP:OD1	23:M:59:ASP:N	2.41	0.43
23:M:123:GLU:OE1	23:M:157:SER:OG	2.21	0.43
28:Z:128:LEU:HD12	28:Z:128:LEU:HA	1.87	0.43
34:p:16:THR:O	34:p:16:THR:OG1	2.36	0.43
12:e:87:THR:O	12:e:91:GLU:HG2	2.19	0.43
19:H:91:MET:HE3	19:H:91:MET:HB2	1.94	0.43
20:J:139:GLU:O	20:J:143:ILE:HG13	2.18	0.43
22:L:63:ILE:HG22	22:L:65:ASN:HB3	2.00	0.43
22:L:566:ILE:HD13	51:M:502:PC1:H2I3	2.00	0.43
24:N:218:LEU:HD13	24:N:244:VAL:HG12	2.01	0.43
6:6:160:ILE:HD13	6:6:160:ILE:HA	1.88	0.43
19:H:257:ILE:HB	44:z:17:PHE:HE1	1.82	0.43
10:c:70:MET:HE3	10:c:70:MET:HB3	1.77	0.43
15:h:33:ARG:HA	15:h:33:ARG:HD2	1.87	0.43
20:J:71:THR:HG22	21:K:27:MET:HE3	2.01	0.43
23:M:283:LYS:HG3	23:M:327:PHE:HE1	1.83	0.43
23:M:403:THR:HA	23:M:406:TYR:CE2	2.54	0.43
17:X:48:VAL:O	17:X:52:MET:HG3	2.18	0.43
29:k:91:GLY:HA3	29:k:281:GLU:HG3	2.01	0.43
38:t:107:HIS:NE2	41:w:43:ASP:OD1	2.36	0.43
19:H:24:GLU:HA	19:H:271:LEU:HD13	2.01	0.43
23:M:133:ILE:HD11	23:M:231:LEU:HD11	2.01	0.43
51:M:502:PC1:H272	50:V:202:3PE:H392	2.01	0.43
1:1:69:GLY:O	47:1:503:NAI:H2N	2.18	0.43
3:3:284:VAL:HG12	3:3:559:VAL:HG22	2.01	0.43
4:4:360:PRO:HA	4:4:380:SER:O	2.18	0.43
22:L:386:LEU:HD23	22:L:386:LEU:HA	1.85	0.43
22:L:397:GLU:HB3	22:L:482:MET:HE1	2.01	0.43
23:M:1:FME:HG2	23:M:111:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:c:115:SER:O	10:c:115:SER:OG	2.33	0.43
11:d:280:THR:HG23	11:d:283:LYS:H	1.84	0.43
19:H:25:ARG:HE	19:H:25:ARG:HB3	1.72	0.43
21:K:73:LEU:HD11	24:N:41:ILE:HG21	2.01	0.43
22:L:29:PHE:HB3	22:L:32:TYR:HB2	2.01	0.43
23:M:31:SER:HB2	23:M:74:PRO:HG3	2.00	0.43
25:V:55:THR:O	25:V:59:THR:HG22	2.19	0.43
27:Y:17:VAL:HG22	27:Y:67:LEU:HD13	2.00	0.43
1:1:138:ILE:HG21	1:1:146:ALA:HB2	2.01	0.43
6:6:171:LYS:N	11:d:52:GLU:OE1	2.50	0.43
18:A:8:LEU:O	18:A:12:THR:HG23	2.19	0.43
20:J:55:MET:HA	20:J:55:MET:HE3	2.01	0.43
20:J:124:ASP:OD1	20:J:124:ASP:N	2.44	0.43
22:L:597:ILE:HD13	22:L:597:ILE:HA	1.89	0.43
4:4:152:MET:O	4:4:156:THR:OG1	2.28	0.42
22:L:257:ILE:HG23	22:L:317:ILE:HD11	2.01	0.42
23:M:135:ARG:HA	23:M:135:ARG:HD2	1.88	0.42
24:N:115:VAL:O	24:N:119:THR:OG1	2.32	0.42
31:m:81:LYS:HG3	31:m:82:ARG:HH11	1.83	0.42
6:6:91:THR:HA	6:6:119:CYS:HB3	2.01	0.42
28:Z:162:MET:HB3	41:w:120:LEU:HD21	2.00	0.42
37:s:17:GLU:HA	37:s:18:PRO:HD3	1.92	0.42
39:u:44:SER:O	39:u:44:SER:OG	2.32	0.42
3:3:276:ARG:O	3:3:549:HIS:NE2	2.52	0.42
6:6:44:SER:OG	19:H:51:ASP:OD1	2.26	0.42
11:d:153:GLU:HG2	11:d:165:ILE:HD13	2.01	0.42
23:M:27:THR:O	23:M:31:SER:OG	2.30	0.42
27:Y:158:LYS:HE2	27:Y:158:LYS:HB3	1.80	0.42
27:Y:161:ARG:HD2	27:Y:161:ARG:HA	1.75	0.42
29:k:50:HIS:NE2	29:k:125:GLU:OE2	2.38	0.42
20:J:117:PHE:HE1	24:N:91:ASN:HD21	1.67	0.42
21:K:24:SER:O	21:K:24:SER:OG	2.31	0.42
22:L:9:LEU:HD12	36:r:85:LEU:HD11	2.01	0.42
2:2:109:MET:HE2	2:2:109:MET:HB3	1.93	0.42
3:3:9:ILE:HG13	3:3:20:VAL:HG23	2.02	0.42
17:j:36:PHE:HD1	17:j:40:LEU:HD12	1.83	0.42
22:L:538:PRO:HG3	50:L:1001:3PE:H321	2.00	0.42
27:Y:13:LYS:HA	30:l:104:ARG:HH12	1.85	0.42
4:4:2:ARG:HD3	41:w:32:PRO:HD2	2.01	0.42
22:L:310:LEU:HD22	22:L:313:MET:HE3	2.02	0.42
44:z:37:ARG:HG3	44:z:60:TYR:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:164:LYS:HE2	1:1:164:LYS:HB3	1.86	0.42
3:3:314:ASP:HB3	3:3:520:LYS:HE2	2.02	0.42
10:c:91:ASP:OD1	10:c:91:ASP:N	2.53	0.42
15:h:32:LYS:O	15:h:35:GLN:NE2	2.50	0.42
18:A:64:LEU:HD23	18:A:64:LEU:HA	1.88	0.42
19:H:310:LEU:HD11	31:m:31:LEU:HB3	2.02	0.42
21:K:55:LEU:HD12	21:K:55:LEU:HA	1.88	0.42
27:Y:63:ASN:HD22	35:q:80:ARG:NH2	2.18	0.42
7:9:143:THR:HB	7:9:146:GLU:HG3	2.00	0.42
17:j:25:ILE:HD13	17:j:40:LEU:HB3	2.02	0.42
22:L:83:ASP:O	22:L:87:MET:HG2	2.20	0.42
22:L:424:THR:HA	22:L:427:ILE:HG22	2.01	0.42
23:M:369:LEU:HD12	23:M:370:PRO:HD2	2.01	0.42
23:M:423:ILE:HG12	34:p:58:VAL:HG22	2.02	0.42
27:Y:68:GLU:OE1	27:Y:71:ARG:NH2	2.53	0.42
28:Z:42:ARG:HE	28:Z:42:ARG:HB3	1.67	0.42
39:u:39:ARG:NH1	39:u:43:ASP:OD1	2.53	0.42
2:2:76:PRO:HA	2:2:77:PRO:HD3	1.95	0.42
2:2:180:LYS:HA	2:2:180:LYS:HD3	1.86	0.42
3:3:7:ASN:N	3:3:7:ASN:OD1	2.52	0.42
3:3:295:THR:OG1	3:3:296:TRP:N	2.53	0.42
4:4:424:VAL:HG23	4:4:427:GLU:HG2	2.01	0.42
30:l:85:LEU:HD12	30:l:85:LEU:HA	1.93	0.42
5:5:47:GLU:OE1	5:5:106:ARG:NH2	2.43	0.42
22:L:82:MET:HE2	22:L:82:MET:HB2	1.96	0.42
27:Y:19:VAL:O	44:z:50:ARG:NH1	2.52	0.42
34:p:44:ARG:HH12	38:t:143:THR:HG21	1.85	0.42
1:1:63:SER:O	1:1:251:SER:OG	2.33	0.41
3:3:249:ARG:HH21	3:3:251:LEU:HD11	1.85	0.41
24:N:151:LEU:HD12	24:N:195:LEU:HD12	2.02	0.41
25:V:84:ASP:HB3	25:V:129:LEU:HD21	2.02	0.41
3:3:143:GLY:HA2	3:3:190:MET:HG2	2.02	0.41
7:9:12:MET:SD	7:9:12:MET:N	2.94	0.41
10:c:116:LYS:HA	10:c:116:LYS:HD3	1.82	0.41
12:e:87:THR:HG23	12:e:88:ARG:NH1	2.35	0.41
14:g:108:GLU:H	14:g:108:GLU:HG2	1.66	0.41
51:M:502:PC1:H381	51:M:502:PC1:H281	2.02	0.41
3:3:295:THR:HG23	3:3:298:ASP:H	1.85	0.41
10:c:69:LEU:HG	10:c:70:MET:HG2	2.02	0.41
18:A:97:LEU:HD23	18:A:97:LEU:HA	1.92	0.41
25:V:12:PRO:O	25:V:15:THR:OG1	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:16:ASN:OD1	2:2:16:ASN:N	2.53	0.41
3:3:591:GLY:HA2	11:d:6:ILE:HG21	2.01	0.41
5:5:119:SER:OG	5:5:131:GLU:OE2	2.34	0.41
6:6:81:ARG:HH11	19:H:61:LEU:HD21	1.85	0.41
11:d:236:TYR:HE1	11:d:339:THR:HG22	1.85	0.41
19:H:98:MET:HE2	19:H:101:GLY:HA2	2.03	0.41
21:K:17:THR:HG22	22:L:592:LEU:HD11	2.01	0.41
22:L:556:ILE:O	22:L:560:THR:OG1	2.30	0.41
1:1:349:ARG:HA	1:1:349:ARG:HD2	1.91	0.41
47:1:503:NAI:H2D	47:1:503:NAI:H6N	1.85	0.41
2:2:93:LYS:HG2	2:2:94:PRO:HD2	2.02	0.41
3:3:438:PRO:HA	3:3:441:GLN:NE2	2.36	0.41
6:6:48:MET:HE3	6:6:86:MET:HG3	2.02	0.41
6:6:52:LEU:HB2	6:6:90:GLY:HA3	2.01	0.41
11:d:45:VAL:O	11:d:68:ILE:HA	2.20	0.41
19:H:1:MET:HE1	44:z:29:PHE:HE2	1.85	0.41
22:L:357:ARG:HG2	38:t:31:VAL:HG13	2.02	0.41
22:L:457:LEU:HD23	22:L:457:LEU:HA	1.88	0.41
28:Z:98:ASP:O	28:Z:102:VAL:HG23	2.21	0.41
4:4:58:ALA:HB1	4:4:62:LEU:HB3	2.02	0.41
4:4:279:ASP:OD1	4:4:279:ASP:N	2.42	0.41
22:L:261:ILE:HG23	22:L:322:PRO:HB2	2.01	0.41
23:M:207:MET:HG2	23:M:298:ILE:HG13	2.02	0.41
27:Y:22:SER:OG	27:Y:89:ASP:OD1	2.30	0.41
44:z:47:LEU:HD23	44:z:47:LEU:HA	1.91	0.41
44:z:51:ASP:HA	44:z:54:VAL:HG12	2.02	0.41
1:1:213:VAL:HG13	1:1:217:GLY:HA2	2.02	0.41
10:c:11:ILE:HD11	14:g:22:ARG:HD2	2.03	0.41
10:c:13:VAL:O	14:g:14:THR:OG1	2.30	0.41
10:c:60:ASP:N	10:c:60:ASP:OD1	2.51	0.41
22:L:137:LEU:HD23	22:L:137:LEU:HA	1.94	0.41
22:L:335:PHE:HE1	22:L:380:LEU:HD13	1.86	0.41
22:L:419:THR:HA	22:L:422:TYR:CE2	2.55	0.41
22:L:476:THR:HA	37:s:53:GLN:HE22	1.85	0.41
23:M:311:GLY:O	23:M:315:LEU:HB2	2.20	0.41
23:M:379:LEU:HD12	23:M:379:LEU:HA	1.81	0.41
24:N:193:VAL:HG11	24:N:266:ILE:HD12	2.02	0.41
17:X:19:LEU:HD23	17:X:19:LEU:HA	1.86	0.41
30:l:50:ARG:NE	30:l:54:GLU:OE2	2.41	0.41
4:4:229:LEU:HD23	4:4:229:LEU:HA	1.89	0.41
10:c:64:ARG:HG3	10:c:75:THR:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:e:15:LEU:HD23	12:e:50:LEU:HD21	2.03	0.41
16:i:84:PRO:HD3	16:i:113:HIS:CD2	2.56	0.41
17:j:70:LEU:HG	17:j:76:ILE:HG22	2.03	0.41
23:M:282:LEU:HD21	23:M:359:TRP:HH2	1.86	0.41
17:X:12:LYS:HE3	17:X:12:LYS:HB3	1.86	0.41
37:s:28:TYR:O	37:s:103:ARG:NH2	2.54	0.41
40:v:148:LYS:HE2	40:v:148:LYS:HB2	1.86	0.41
1:1:90:PRO:O	1:1:218:CYS:HB3	2.21	0.41
3:3:380:VAL:HG11	3:3:429:LEU:HD11	2.02	0.41
4:4:230:THR:O	4:4:294:TYR:OH	2.38	0.41
5:5:198:ASP:OD1	5:5:198:ASP:N	2.54	0.41
7:9:41:LEU:HD12	19:H:30:TYR:HD1	1.86	0.41
16:i:60:ARG:HH22	16:i:95:ASP:HA	1.86	0.41
20:J:20:PHE:HB2	20:J:29:GLY:HA2	2.02	0.41
21:K:55:LEU:HD13	30:l:25:PRO:HD3	2.03	0.41
22:L:370:THR:HA	22:L:431:LEU:HD11	2.02	0.41
22:L:386:LEU:HD11	39:u:32:MET:HE3	2.03	0.41
22:L:483:PRO:HD2	22:L:486:LEU:HD12	2.02	0.41
23:M:164:LEU:HD23	23:M:164:LEU:HA	1.90	0.41
51:M:502:PC1:H352	51:M:502:PC1:H382	1.93	0.41
24:N:280:THR:O	24:N:284:ILE:HG12	2.21	0.41
25:V:75:ILE:HD13	25:V:75:ILE:HA	1.86	0.41
26:W:125:TYR:HB2	30:l:48:SER:HB3	2.03	0.41
26:W:129:ASP:OD1	26:W:130:LYS:N	2.53	0.41
28:Z:163:LEU:HD22	41:w:120:LEU:HD23	2.02	0.41
34:p:42:LEU:HD23	34:p:42:LEU:HA	1.92	0.41
37:s:24:PHE:HE2	37:s:111:LYS:HE2	1.86	0.41
37:s:107:LEU:HD23	37:s:107:LEU:HA	1.86	0.41
3:3:564:ALA:HB3	3:3:569:LYS:HD3	2.02	0.41
22:L:163:ASP:OD1	22:L:163:ASP:N	2.52	0.41
22:L:336:LYS:HD2	22:L:336:LYS:HA	1.92	0.41
26:W:19:LYS:HB3	26:W:19:LYS:HE2	1.82	0.41
20:J:83:TRP:C	20:J:85:SER:H	2.29	0.40
22:L:124:PHE:CE1	22:L:252:MET:HB2	2.55	0.40
29:k:22:SER:OG	29:k:119:GLY:O	2.28	0.40
30:l:5:VAL:HG13	30:l:9:LEU:HD13	2.03	0.40
37:s:3:HIS:CE1	40:v:127:PRO:HD3	2.56	0.40
40:v:82:ASP:O	40:v:88:ARG:NE	2.51	0.40
3:3:32:LYS:HE3	3:3:32:LYS:HB3	1.91	0.40
4:4:147:LEU:HD22	4:4:218:PHE:HE2	1.85	0.40
7:9:132:VAL:HG11	7:9:169:ILE:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:94:LEU:HG	20:J:154:VAL:HG13	2.03	0.40
23:M:178:ILE:HD11	26:W:97:GLU:HB2	2.02	0.40
23:M:209:LEU:HB3	23:M:212:LEU:HD12	2.03	0.40
28:Z:5:ASP:HB3	28:Z:8:VAL:HG22	2.04	0.40
28:Z:40:VAL:HA	36:r:79:TRP:HE1	1.87	0.40
38:t:56:MET:HE2	38:t:56:MET:HA	2.03	0.40
1:1:30:ASP:HB3	1:1:35:GLY:HA3	2.03	0.40
3:3:227:SER:OG	3:3:228:ILE:N	2.50	0.40
7:9:114:THR:HG21	7:9:144:HIS:CD2	2.57	0.40
22:L:172:ILE:HD13	22:L:172:ILE:HA	1.96	0.40
23:M:106:LEU:HD13	23:M:234:ILE:HG21	2.03	0.40
23:M:282:LEU:HD12	23:M:282:LEU:HA	1.97	0.40
26:W:143:ASN:O	27:Y:141:TYR:OH	2.35	0.40
27:Y:171:MET:HE3	27:Y:171:MET:HB3	1.91	0.40
37:s:33:ARG:HG2	40:v:156:TYR:HB3	2.04	0.40
39:u:55:ASP:HA	39:u:56:PRO:HD2	1.96	0.40
3:3:285:ARG:NH1	3:3:289:GLY:O	2.48	0.40
19:H:154:LEU:HD23	19:H:154:LEU:HA	1.94	0.40
22:L:2:ASN:OD1	22:L:2:ASN:N	2.50	0.40
22:L:358:LYS:HA	22:L:358:LYS:HD3	1.78	0.40
23:M:311:GLY:HA2	23:M:377:GLY:HA2	2.04	0.40
29:k:30:ASN:O	29:k:126:ARG:NH2	2.52	0.40
34:p:39:ARG:NH2	38:t:3:LEU:O	2.54	0.40
7:9:65:HIS:HD2	7:9:113:MET:HE1	1.86	0.40
22:L:142:ILE:HD11	23:M:371:PRO:HB3	2.03	0.40
22:L:473:PRO:HA	22:L:474:PRO:HD3	1.98	0.40
23:M:54:LEU:HD23	26:W:93:ILE:HG12	2.04	0.40
24:N:96:MET:HE3	24:N:100:MET:SD	2.62	0.40
24:N:321:LYS:HE3	24:N:321:LYS:HB3	1.84	0.40
25:V:129:LEU:HD23	25:V:129:LEU:HA	1.90	0.40
41:w:80:LEU:HD23	41:w:80:LEU:HA	1.97	0.40
41:w:90:ARG:O	41:w:94:GLU:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

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	1	344/368 (94%)	341 (99%)	3 (1%)	70	76
2	2	183/210 (87%)	183 (100%)	0	100	100
3	3	578/608 (95%)	578 (100%)	0	100	100
4	4	370/391 (95%)	370 (100%)	0	100	100
5	5	189/230 (82%)	189 (100%)	0	100	100
6	6	132/181 (73%)	132 (100%)	0	100	100
7	9	151/179 (84%)	150 (99%)	1 (1%)	76	78
8	a	43/93 (46%)	43 (100%)	0	100	100
9	b	79/97 (81%)	78 (99%)	1 (1%)	61	72
10	c	113/150 (75%)	113 (100%)	0	100	100
11	d	294/326 (90%)	293 (100%)	1 (0%)	86	84
12	e	76/82 (93%)	76 (100%)	0	100	100
13	f	101/102 (99%)	101 (100%)	0	100	100
14	g	107/124 (86%)	107 (100%)	0	100	100
15	h	84/96 (88%)	83 (99%)	1 (1%)	63	73
16	i	131/131 (100%)	130 (99%)	1 (1%)	73	77
17	X	80/141 (57%)	80 (100%)	0	100	100
17	j	76/141 (54%)	76 (100%)	0	100	100
18	A	103/103 (100%)	103 (100%)	0	100	100
19	H	278/278 (100%)	276 (99%)	2 (1%)	76	78
20	J	144/144 (100%)	142 (99%)	2 (1%)	59	71
21	K	86/86 (100%)	86 (100%)	0	100	100
22	L	538/538 (100%)	537 (100%)	1 (0%)	87	85
23	M	411/411 (100%)	411 (100%)	0	100	100
24	N	315/315 (100%)	314 (100%)	1 (0%)	86	84
25	V	101/102 (99%)	100 (99%)	1 (1%)	68	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	W	122/160 (76%)	122 (100%)	0	100	100
27	Y	154/154 (100%)	153 (99%)	1 (1%)	78	80
28	Z	155/157 (99%)	155 (100%)	0	100	100
29	k	283/309 (92%)	281 (99%)	2 (1%)	76	78
30	l	94/95 (99%)	93 (99%)	1 (1%)	65	74
31	m	69/72 (96%)	69 (100%)	0	100	100
32	n	61/76 (80%)	60 (98%)	1 (2%)	55	70
33	o	107/109 (98%)	105 (98%)	2 (2%)	50	67
34	p	114/116 (98%)	114 (100%)	0	100	100
35	q	119/122 (98%)	118 (99%)	1 (1%)	73	77
36	r	95/122 (78%)	94 (99%)	1 (1%)	65	74
37	s	110/120 (92%)	110 (100%)	0	100	100
38	t	159/161 (99%)	159 (100%)	0	100	100
39	u	59/84 (70%)	59 (100%)	0	100	100
40	v	140/160 (88%)	140 (100%)	0	100	100
41	w	92/130 (71%)	91 (99%)	1 (1%)	65	74
42	x	44/67 (66%)	44 (100%)	0	100	100
43	y	46/54 (85%)	46 (100%)	0	100	100
44	z	59/59 (100%)	59 (100%)	0	100	100
All	All	7189/7954 (90%)	7164 (100%)	25 (0%)	84	84

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	93	LEU
1	1	96	ASN
1	1	388	GLU
7	9	84	GLU
9	b	42	ASP
11	d	185	ILE
15	h	90	GLU
16	i	7	LEU
19	H	264	LEU
19	H	285	LEU
20	J	74	MET

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Mol	Chain	Res	Type
20	J	138	GLU
22	L	163	ASP
24	N	38	LEU
25	V	84	ASP
27	Y	112	ASP
29	k	44	GLU
29	k	262	LEU
30	l	76	ASN
32	n	15	LEU
33	o	94	ILE
33	o	115	GLU
35	q	77	GLU
36	r	114	GLU
41	w	36	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	116	HIS
1	1	150	GLN
1	1	324	GLN
1	1	361	GLN
2	2	27	ASN
2	2	67	ASN
2	2	74	GLN
2	2	101	GLN
2	2	214	GLN
3	3	277	GLN
3	3	437	HIS
4	4	79	HIS
5	5	95	ASN
5	5	144	ASN
5	5	145	HIS
11	d	148	ASN
11	d	184	ASN
12	e	47	ASN
12	e	85	GLN
14	g	71	HIS
15	h	46	HIS
16	i	52	ASN
16	i	69	ASN
19	H	138	GLN

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Mol	Chain	Res	Type
19	H	157	ASN
19	H	230	ASN
20	J	120	ASN
22	L	23	ASN
22	L	175	ASN
22	L	194	ASN
22	L	210	ASN
22	L	270	ASN
22	L	295	GLN
22	L	296	ASN
23	M	83	HIS
23	M	338	HIS
23	M	366	ASN
26	W	124	GLN
27	Y	63	ASN
27	Y	64	GLN
28	Z	22	GLN
28	Z	55	HIS
28	Z	77	HIS
28	Z	123	ASN
29	k	190	HIS
29	k	251	GLN
29	k	287	HIS
30	l	15	HIS
30	l	76	ASN
33	o	97	HIS
35	q	60	GLN
35	q	75	GLN
36	r	13	GLN
36	r	25	GLN
38	t	12	GLN
38	t	13	GLN
38	t	77	GLN
41	w	119	GLN
42	x	13	ASN
44	z	44	GLN

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$
29	SEP	k	36	29	8,9,10	1.56	1 (12%)	7,12,14	1.33	1 (14%)
23	FME	M	1	23	8,9,10	1.08	1 (12%)	8,9,11	1.14	1 (12%)
4	2MR	4	85	4	10,12,13	2.45	2 (20%)	5,13,15	0.99	0
25	AYA	V	1	25	6,7,8	1.27	1 (16%)	6,8,10	1.83	2 (33%)
22	FME	L	1	22	8,9,10	0.99	0	8,9,11	0.96	1 (12%)
15	AYA	h	1	15	6,7,8	1.31	1 (16%)	6,8,10	1.24	1 (16%)
21	FME	K	1	21	8,9,10	0.99	0	8,9,11	1.04	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SEP	k	36	29	-	3/6/8/10	-
23	FME	M	1	23	-	4/7/9/11	-
4	2MR	4	85	4	-	3/10/13/15	-
25	AYA	V	1	25	-	3/5/6/8	-
22	FME	L	1	22	-	2/7/9/11	-
15	AYA	h	1	15	-	0/5/6/8	-
21	FME	K	1	21	-	3/7/9/11	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	85	2MR	CZ-NH2	5.15	1.44	1.33
4	4	85	2MR	CZ-NE	5.08	1.45	1.34
29	k	36	SEP	P-O1P	3.42	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	h	1	AYA	CA-N	-2.56	1.43	1.46
25	V	1	AYA	CA-N	-2.52	1.43	1.46
23	M	1	FME	CA-N	-2.41	1.43	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	V	1	AYA	CB-CA-N	3.46	113.59	109.68
29	k	36	SEP	OG-CB-CA	2.86	110.93	108.14
15	h	1	AYA	CB-CA-N	2.80	112.84	109.68
25	V	1	AYA	CA-N-CT	2.46	124.68	121.50
21	K	1	FME	C-CA-N	2.10	113.56	109.50
22	L	1	FME	C-CA-N	2.03	113.41	109.50
23	M	1	FME	CA-N-CN	-2.00	119.74	122.82

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	4	85	2MR	C-CA-CB-CG
23	M	1	FME	C-CA-CB-CG
25	V	1	AYA	O-C-CA-CB
23	M	1	FME	CA-CB-CG-SD
25	V	1	AYA	OT-CT-N-CA
25	V	1	AYA	CM-CT-N-CA
21	K	1	FME	N-CA-CB-CG
22	L	1	FME	CA-CB-CG-SD
23	M	1	FME	CB-CG-SD-CE
21	K	1	FME	CB-CG-SD-CE
22	L	1	FME	CB-CG-SD-CE
29	k	36	SEP	CB-OG-P-O1P
23	M	1	FME	N-CA-CB-CG
21	K	1	FME	C-CA-CB-CG
4	4	85	2MR	NE-CD-CG-CB
4	4	85	2MR	CA-CB-CG-CD
29	k	36	SEP	CB-OG-P-O3P
29	k	36	SEP	CA-CB-OG-P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	M	1	FME	2	0
21	K	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 2 are monoatomic - leaving 30 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	$\# Z > 2$
50	3PE	V	201	-	26,26,50	0.48	0	29,31,55	0.50	1 (3%)
50	3PE	A	201	-	50,50,50	0.30	0	53,55,55	0.33	0
54	ZMP	X	101	17	25,30,36	0.79	1 (4%)	29,37,45	1.02	2 (6%)
50	3PE	H	401	-	50,50,50	0.31	0	53,55,55	0.34	0
45	SF4	6	201	6	0,12,12	-	-	-	-	-
50	3PE	o	501	-	30,30,50	0.38	0	33,35,55	0.37	0
45	SF4	1	501	1	0,12,12	-	-	-	-	-
50	3PE	6	203	-	50,50,50	0.30	0	53,55,55	0.30	0
50	3PE	L	1001	-	50,50,50	0.30	0	53,55,55	0.32	0
55	AMP	k	501	-	25,25,25	1.41	4 (16%)	37,38,38	1.93	9 (24%)
45	SF4	9	403	7	0,12,12	-	-	-	-	-
45	SF4	9	402	7	0,12,12	-	-	-	-	-
50	3PE	M	501	-	43,43,50	0.32	0	46,48,55	0.33	0
51	PC1	9	401	-	53,53,53	0.30	0	59,61,61	0.46	0
51	PC1	L	1002	-	53,53,53	0.30	0	59,61,61	0.53	1 (1%)
53	NDP	d	401	-	51,52,52	0.34	0	71,80,80	0.37	0
50	3PE	J	201	-	39,39,50	0.35	0	42,44,55	0.32	0
56	MYR	s	201	37	13,14,15	0.15	0	12,13,15	0.15	0
48	FES	3	803	3	0,4,4	-	-	-	-	-
51	PC1	6	202	-	45,45,53	0.31	0	51,53,61	0.32	0
51	PC1	L	1003	-	53,53,53	0.29	0	59,61,61	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SF4	3	801	3	0,12,12	-	-	-		
48	FES	2	300	2	0,4,4	-	-	-		
50	3PE	V	202	-	36,36,50	0.35	0	39,41,55	0.30	0
45	SF4	3	802	3	0,12,12	-	-	-		
51	PC1	M	502	-	53,53,53	0.30	0	59,61,61	0.35	0
50	3PE	4	501	-	39,39,50	0.33	0	42,44,55	0.35	0
46	FMN	1	502	-	33,33,33	1.06	2 (6%)	48,50,50	1.27	7 (14%)
54	ZMP	j	101	17	28,33,36	0.66	1 (3%)	32,40,45	1.10	3 (9%)
47	NAI	1	503	-	47,48,48	0.40	1 (2%)	64,73,73	1.79	4 (6%)

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
50	3PE	V	201	-	-	2/27/27/54	-
50	3PE	A	201	-	-	13/54/54/54	-
54	ZMP	X	101	17	-	15/35/37/43	-
50	3PE	H	401	-	-	7/54/54/54	-
50	3PE	o	501	-	-	5/34/34/54	-
45	SF4	6	201	6	-	-	0/6/5/5
45	SF4	1	501	1	-	-	0/6/5/5
50	3PE	6	203	-	-	11/54/54/54	-
50	3PE	L	1001	-	-	12/54/54/54	-
55	AMP	k	501	-	-	0/10/26/26	0/3/3/3
45	SF4	9	403	7	-	-	0/6/5/5
45	SF4	9	402	7	-	-	0/6/5/5
50	3PE	M	501	-	-	8/47/47/54	-
51	PC1	9	401	-	-	8/57/57/57	-
51	PC1	L	1002	-	-	14/57/57/57	-
53	NDP	d	401	-	-	10/34/77/77	0/5/5/5
50	3PE	J	201	-	-	9/43/43/54	-
56	MYR	s	201	37	-	0/12/12/13	-
48	FES	3	803	3	-	-	0/1/1/1
51	PC1	6	202	-	-	9/49/49/57	-
51	PC1	L	1003	-	-	8/57/57/57	-
45	SF4	3	801	3	-	-	0/6/5/5
48	FES	2	300	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	3PE	V	202	-	-	12/40/40/54	-
45	SF4	3	802	3	-	-	0/6/5/5
51	PC1	M	502	-	-	13/57/57/57	-
50	3PE	4	501	-	-	5/43/43/54	-
46	FMN	1	502	-	-	7/18/18/18	0/3/3/3
54	ZMP	j	101	17	-	10/38/40/43	-
47	NAI	1	503	-	-	8/29/72/72	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	k	501	AMP	C5-C4	4.66	1.47	1.39
46	1	502	FMN	C4A-N5	3.19	1.37	1.30
55	k	501	AMP	C5-C6	2.77	1.48	1.41
54	j	101	ZMP	C9-C10	2.42	1.53	1.50
54	X	101	ZMP	C9-C10	2.32	1.53	1.50
55	k	501	AMP	C8-N7	2.31	1.36	1.31
55	k	501	AMP	C5-N7	-2.25	1.35	1.39
46	1	502	FMN	C10-N1	2.05	1.37	1.33
47	1	503	NAI	PA-O5B	2.01	1.67	1.59

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	1	503	NAI	O5B-PA-O1A	-9.60	70.88	108.94
47	1	503	NAI	O2A-PA-O1A	-8.25	74.05	112.44
55	k	501	AMP	C5-C4-N3	-6.05	118.39	126.72
47	1	503	NAI	O3-PA-O1A	-5.83	93.18	110.70
55	k	501	AMP	N3-C4-N9	4.70	135.16	127.17
55	k	501	AMP	C2-N3-C4	3.83	121.18	111.83
55	k	501	AMP	C4-C5-N7	-3.68	106.38	110.58
46	1	502	FMN	C4-N3-C2	-3.42	119.57	125.64
55	k	501	AMP	N3-C2-N1	-3.29	123.61	128.58
46	1	502	FMN	C4A-C10-N10	3.22	121.09	116.48
55	k	501	AMP	C5-N7-C8	2.69	107.67	103.45
54	X	101	ZMP	O1-C10-C9	-2.64	120.93	123.98
46	1	502	FMN	C4A-C4-N3	2.63	119.95	113.25
55	k	501	AMP	C4-N9-C8	2.58	108.45	105.74
54	j	101	ZMP	C14-C15-N2	-2.54	106.59	112.00
47	1	503	NAI	O2A-PA-O5B	2.50	118.92	107.57
54	j	101	ZMP	C15-C14-C13	-2.48	108.26	112.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	1	502	FMN	O4-C4-C4A	-2.46	120.04	126.53
46	1	502	FMN	C10-C4A-N5	-2.45	119.80	124.81
54	j	101	ZMP	O1-C10-C9	-2.44	121.17	123.98
54	X	101	ZMP	C15-C14-C13	-2.35	108.48	112.39
55	k	501	AMP	C6-C5-N7	2.19	136.31	132.09
46	1	502	FMN	C4'-C3'-C2'	-2.17	109.97	113.57
51	L	1002	PC1	C2-O21-C21	2.13	122.89	117.80
50	V	201	3PE	O12-P-O14	2.12	119.09	110.83
55	k	501	AMP	N9-C8-N7	-2.03	111.06	113.94
46	1	502	FMN	C4A-C10-N1	-2.01	119.66	124.59

There are no chirality outliers.

All (186) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1	502	FMN	N10-C1'-C2'-O2'
46	1	502	FMN	N10-C1'-C2'-C3'
46	1	502	FMN	C5'-O5'-P-O2P
46	1	502	FMN	C5'-O5'-P-O3P
50	4	501	3PE	C11-O13-P-O12
50	4	501	3PE	O13-C11-C12-N
50	6	203	3PE	C1-O11-P-O12
50	6	203	3PE	C1-O11-P-O13
50	6	203	3PE	C11-O13-P-O11
50	A	201	3PE	C1-O11-P-O13
50	A	201	3PE	C1-O11-P-O14
50	A	201	3PE	C11-O13-P-O11
50	A	201	3PE	C11-O13-P-O14
50	A	201	3PE	O13-C11-C12-N
50	H	401	3PE	C1-O11-P-O12
50	H	401	3PE	C1-O11-P-O13
50	H	401	3PE	O13-C11-C12-N
50	J	201	3PE	C1-O11-P-O14
50	L	1001	3PE	C1-O11-P-O13
50	L	1001	3PE	C1-O11-P-O14
50	L	1001	3PE	C11-O13-P-O11
50	L	1001	3PE	O13-C11-C12-N
50	V	202	3PE	C1-O11-P-O12
50	V	202	3PE	C1-O11-P-O13
50	V	202	3PE	C11-O13-P-O11
50	V	202	3PE	C11-O13-P-O12
50	V	202	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
50	V	202	3PE	O13-C11-C12-N
50	o	501	3PE	C1-O11-P-O12
50	o	501	3PE	C1-O11-P-O13
50	o	501	3PE	C1-O11-P-O14
51	6	202	PC1	C1-O11-P-O12
51	6	202	PC1	C1-O11-P-O13
51	9	401	PC1	C11-O13-P-O12
51	9	401	PC1	C11-O13-P-O11
51	L	1002	PC1	C1-O11-P-O12
51	L	1003	PC1	C11-O13-P-O12
51	L	1003	PC1	C11-O13-P-O11
51	M	502	PC1	C11-O13-P-O12
51	M	502	PC1	C11-O13-P-O14
51	M	502	PC1	C11-O13-P-O11
53	d	401	NDP	C5D-O5D-PN-O3
53	d	401	NDP	C5D-O5D-PN-O1N
53	d	401	NDP	C2N-C3N-C7N-N7N
54	j	101	ZMP	C16-C17-C18-C21
54	j	101	ZMP	S1-C11-C12-N1
54	X	101	ZMP	C19-C18-C21-O5
54	X	101	ZMP	C17-C18-C21-O5
54	X	101	ZMP	C16-C17-C18-C21
54	X	101	ZMP	C17-C16-N2-C15
54	X	101	ZMP	C7-C8-C9-C10
54	X	101	ZMP	O3-C16-N2-C15
51	M	502	PC1	C11-C12-N-C14
51	L	1002	PC1	C31-C32-C33-C34
51	M	502	PC1	C11-C12-N-C15
51	L	1002	PC1	C2-C1-O11-P
47	1	503	NAI	C2D-C1D-N1N-C2N
47	1	503	NAI	C2D-C1D-N1N-C6N
50	V	201	3PE	C22-C23-C24-C25
50	L	1001	3PE	O11-C1-C2-C3
51	9	401	PC1	C3D-C3E-C3F-C3G
50	A	201	3PE	C2C-C2D-C2E-C2F
54	X	101	ZMP	C6-C7-C8-C9
50	A	201	3PE	C2E-C2F-C2G-C2H
51	M	502	PC1	C3A-C3B-C3C-C3D
51	6	202	PC1	C11-C12-N-C14
51	M	502	PC1	C11-C12-N-C13
54	X	101	ZMP	O3-C16-C17-O4
51	L	1002	PC1	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
51	9	401	PC1	C2B-C2C-C2D-C2E
50	J	201	3PE	C1-C2-C3-O31
51	L	1002	PC1	C38-C39-C3A-C3B
51	6	202	PC1	C11-C12-N-C13
46	1	502	FMN	C5'-O5'-P-O1P
51	L	1002	PC1	O11-C1-C2-O21
54	j	101	ZMP	C5-C6-C7-C8
51	6	202	PC1	C11-C12-N-C15
50	J	201	3PE	C26-C27-C28-C29
54	X	101	ZMP	C5-C6-C7-C8
51	M	502	PC1	C25-C26-C27-C28
50	M	501	3PE	C31-C32-C33-C34
50	A	201	3PE	C1-C2-C3-O31
51	L	1002	PC1	C32-C33-C34-C35
50	L	1001	3PE	O11-C1-C2-O21
51	9	401	PC1	C3B-C3C-C3D-C3E
50	6	203	3PE	C3C-C3D-C3E-C3F
50	A	201	3PE	O21-C2-C3-O31
54	j	101	ZMP	C6-C7-C8-C9
53	d	401	NDP	PN-O3-PA-O5B
54	j	101	ZMP	C7-C8-C9-C10
50	M	501	3PE	C39-C3A-C3B-C3C
50	H	401	3PE	C27-C28-C29-C2A
51	L	1003	PC1	C11-C12-N-C13
47	1	503	NAI	O4D-C1D-N1N-C2N
50	L	1001	3PE	C34-C35-C36-C37
51	9	401	PC1	O13-C11-C12-N
51	L	1002	PC1	O13-C11-C12-N
51	L	1003	PC1	C11-C12-N-C14
54	j	101	ZMP	O3-C16-C17-O4
47	1	503	NAI	O4D-C1D-N1N-C6N
54	X	101	ZMP	C20-C18-C21-O5
50	J	201	3PE	C31-C32-C33-C34
51	M	502	PC1	C2-C1-O11-P
53	d	401	NDP	C2N-C3N-C7N-O7N
47	1	503	NAI	C5B-O5B-PA-O1A
47	1	503	NAI	C5B-O5B-PA-O3
50	4	501	3PE	C11-O13-P-O11
50	6	203	3PE	C1-O11-P-O14
50	6	203	3PE	C11-O13-P-O14
50	A	201	3PE	C1-O11-P-O12
50	J	201	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
50	L	1001	3PE	C1-O11-P-O12
50	L	1001	3PE	C11-O13-P-O14
50	M	501	3PE	C1-O11-P-O12
50	M	501	3PE	C1-O11-P-O13
50	M	501	3PE	C1-O11-P-O14
50	M	501	3PE	C11-O13-P-O12
50	V	202	3PE	C1-O11-P-O14
51	9	401	PC1	C11-O13-P-O14
51	L	1002	PC1	C1-O11-P-O14
51	L	1002	PC1	C1-O11-P-O13
53	d	401	NDP	C5D-O5D-PN-O2N
54	j	101	ZMP	O4-C17-C18-C21
54	X	101	ZMP	O4-C17-C18-C21
50	M	501	3PE	C2-C1-O11-P
50	V	201	3PE	C1-O11-P-O14
54	X	101	ZMP	C2-C3-C4-C5
50	J	201	3PE	C21-C22-C23-C24
50	J	201	3PE	C25-C26-C27-C28
50	6	203	3PE	C33-C34-C35-C36
50	J	201	3PE	O21-C2-C3-O31
51	L	1003	PC1	C11-C12-N-C15
54	X	101	ZMP	S1-C11-C12-N1
51	L	1002	PC1	C23-C24-C25-C26
50	L	1001	3PE	C36-C37-C38-C39
51	M	502	PC1	C39-C3A-C3B-C3C
51	9	401	PC1	C3-C2-O21-C21
51	L	1003	PC1	C3E-C3F-C3G-C3H
53	d	401	NDP	O4D-C1D-N1N-C6N
54	X	101	ZMP	O1-C10-S1-C11
47	1	503	NAI	C2N-C3N-C7N-N7N
50	V	202	3PE	C32-C33-C34-C35
46	1	502	FMN	O2'-C2'-C3'-C4'
50	A	201	3PE	C2-C1-O11-P
54	j	101	ZMP	C13-C14-C15-N2
50	H	401	3PE	O21-C2-C3-O31
50	o	501	3PE	C31-C32-C33-C34
50	6	203	3PE	C23-C24-C25-C26
51	L	1002	PC1	C1-C2-O21-C21
46	1	502	FMN	O2'-C2'-C3'-O3'
54	j	101	ZMP	C16-C17-C18-C20
51	6	202	PC1	O31-C31-C32-C33
51	M	502	PC1	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
50	A	201	3PE	O31-C31-C32-C33
53	d	401	NDP	C2D-C1D-N1N-C6N
53	d	401	NDP	O4B-C4B-C5B-O5B
50	6	203	3PE	O21-C21-C22-C23
50	J	201	3PE	C27-C28-C29-C2A
47	1	503	NAI	PN-O3-PA-O1A
50	V	202	3PE	O31-C31-C32-C33
50	6	203	3PE	C3D-C3E-C3F-C3G
50	M	501	3PE	C33-C34-C35-C36
51	6	202	PC1	O21-C21-C22-C23
53	d	401	NDP	C2B-O2B-P2B-O3X
50	4	501	3PE	O21-C21-C22-C23
51	L	1002	PC1	C24-C25-C26-C27
50	L	1001	3PE	O31-C31-C32-C33
51	L	1003	PC1	C39-C3A-C3B-C3C
50	o	501	3PE	C25-C26-C27-C28
50	H	401	3PE	C33-C34-C35-C36
50	6	203	3PE	C37-C38-C39-C3A
51	6	202	PC1	C22-C23-C24-C25
50	A	201	3PE	O32-C31-C32-C33
50	V	202	3PE	C31-C32-C33-C34
51	L	1003	PC1	C31-C32-C33-C34
50	4	501	3PE	O22-C21-C22-C23
54	j	101	ZMP	N2-C16-C17-O4
54	X	101	ZMP	N2-C16-C17-O4
50	V	202	3PE	O32-C31-C32-C33
51	6	202	PC1	O22-C21-C22-C23
50	H	401	3PE	O21-C21-C22-C23
50	V	202	3PE	O21-C21-C22-C23
51	M	502	PC1	C3B-C3C-C3D-C3E
51	L	1002	PC1	O21-C21-C22-C23
51	M	502	PC1	O31-C31-C32-C33
50	L	1001	3PE	O21-C21-C22-C23

There are no ring outliers.

13 monomers are involved in 24 short contacts:

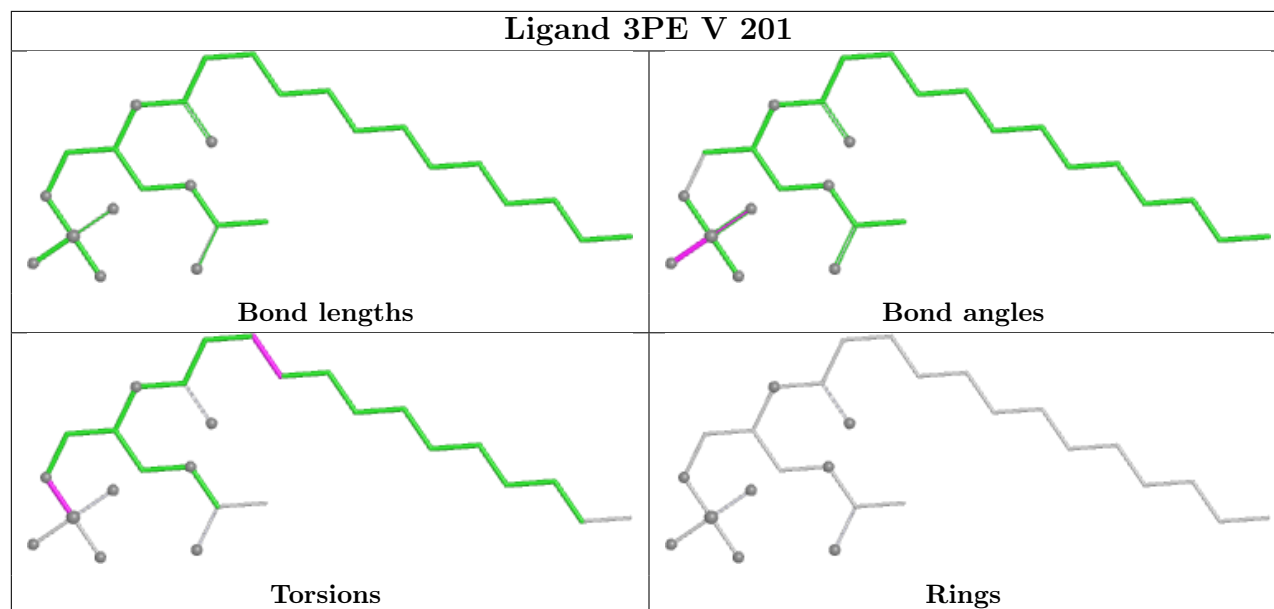
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	A	201	3PE	1	0
50	H	401	3PE	1	0
50	6	203	3PE	1	0
50	L	1001	3PE	1	0

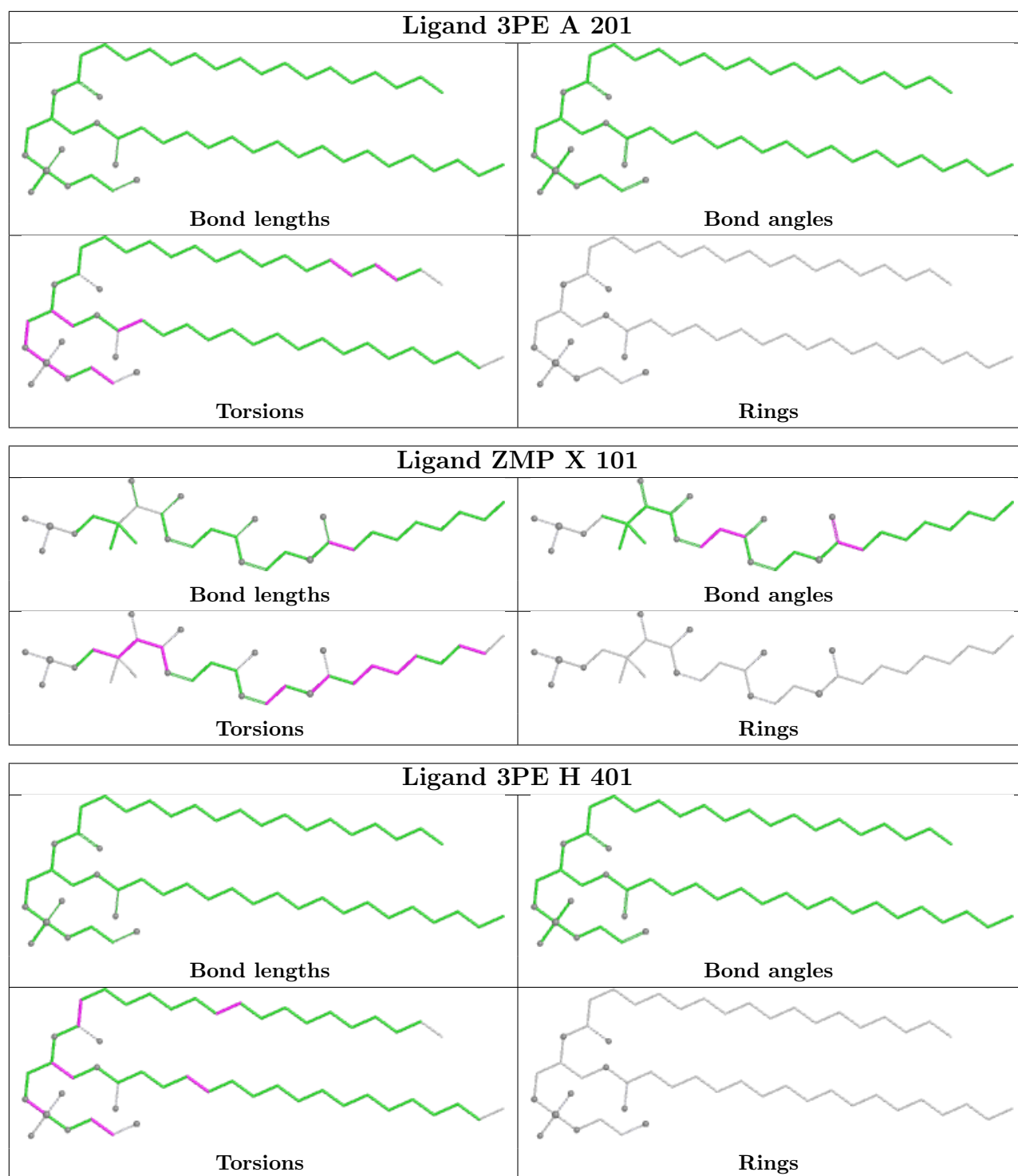
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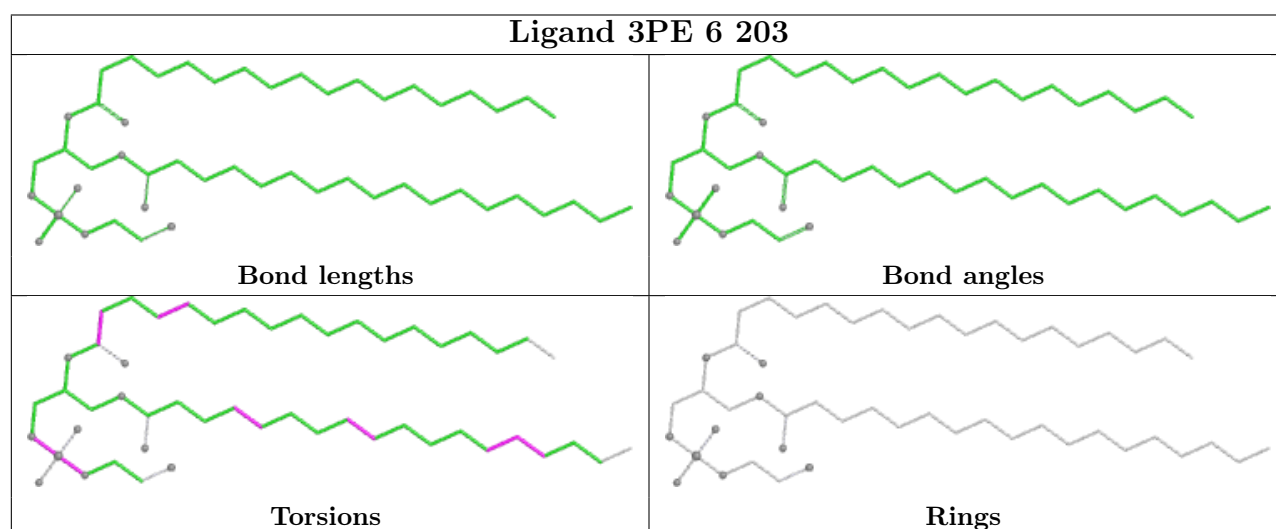
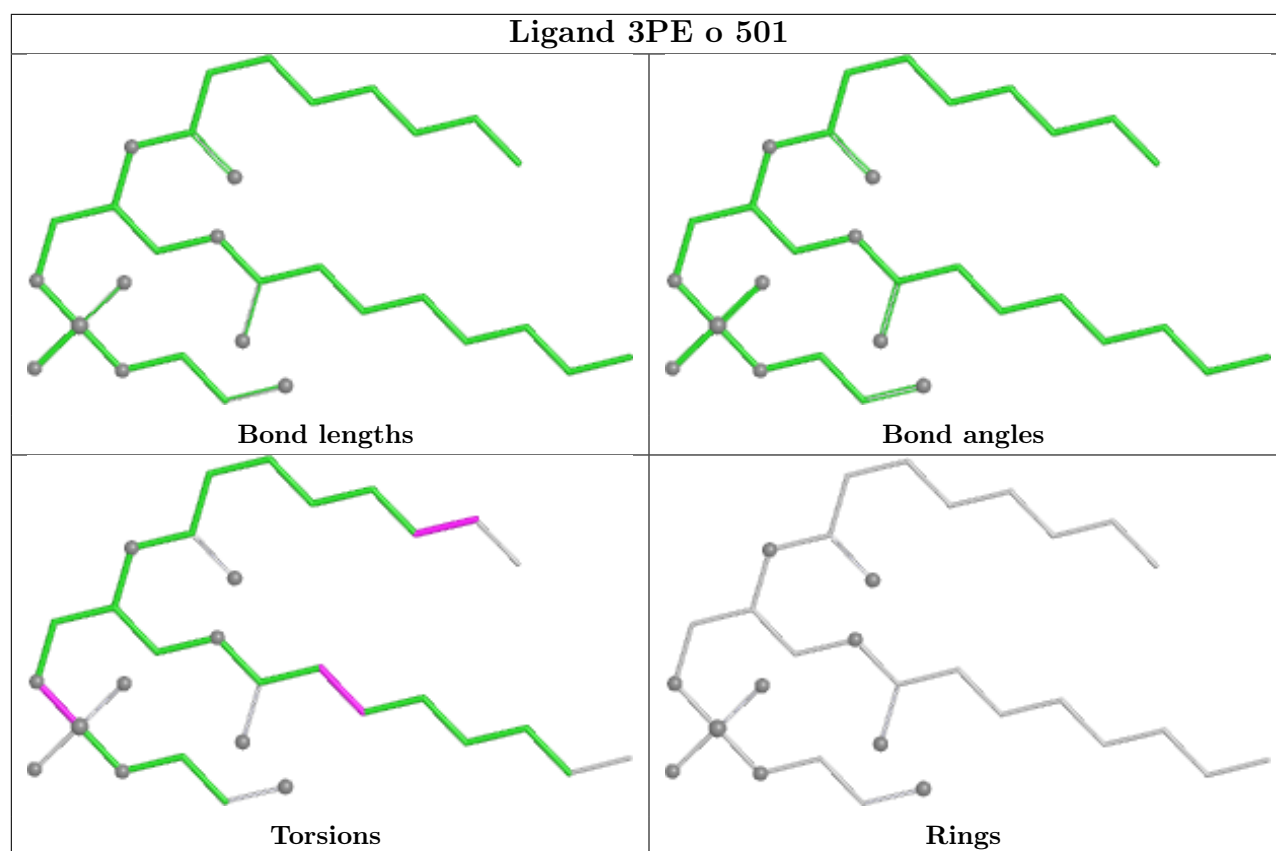
Continued from previous page...

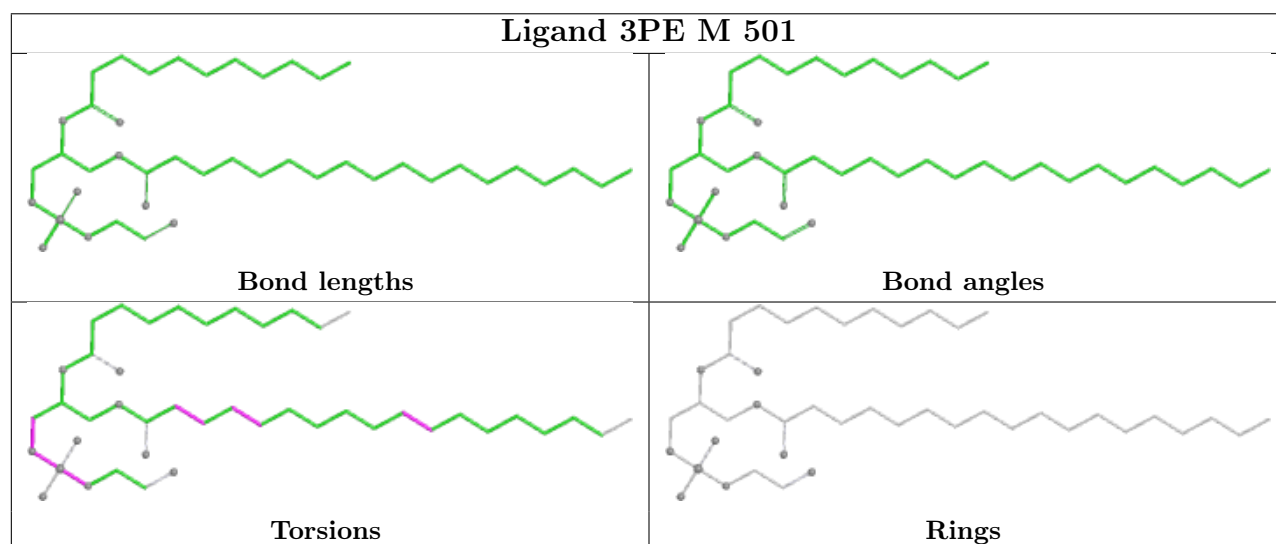
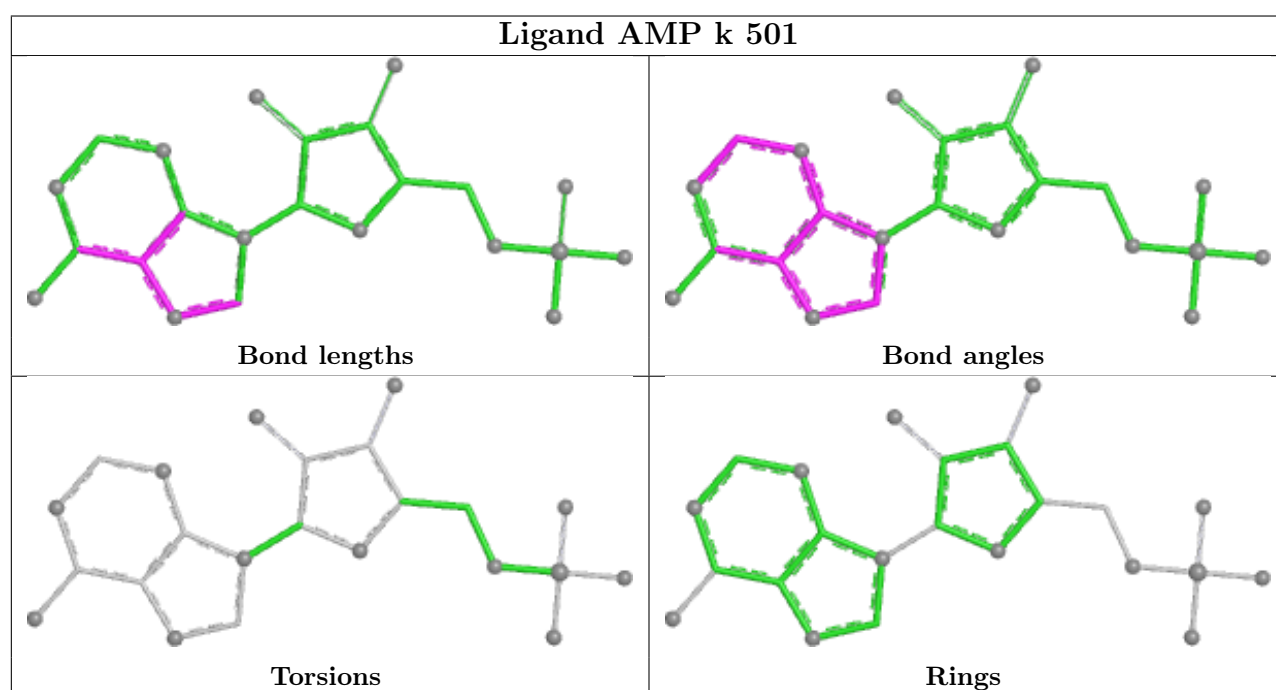
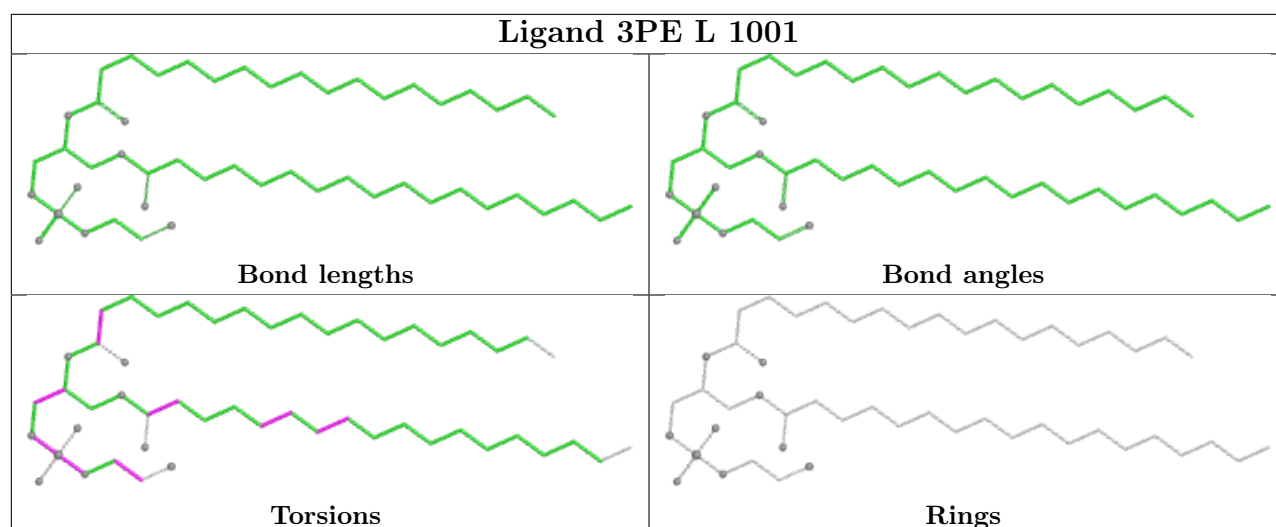
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	k	501	AMP	3	0
51	L	1002	PC1	2	0
53	d	401	NDP	3	0
50	J	201	3PE	2	0
51	L	1003	PC1	2	0
50	V	202	3PE	2	0
51	M	502	PC1	4	0
54	j	101	ZMP	1	0
47	1	503	NAI	3	0

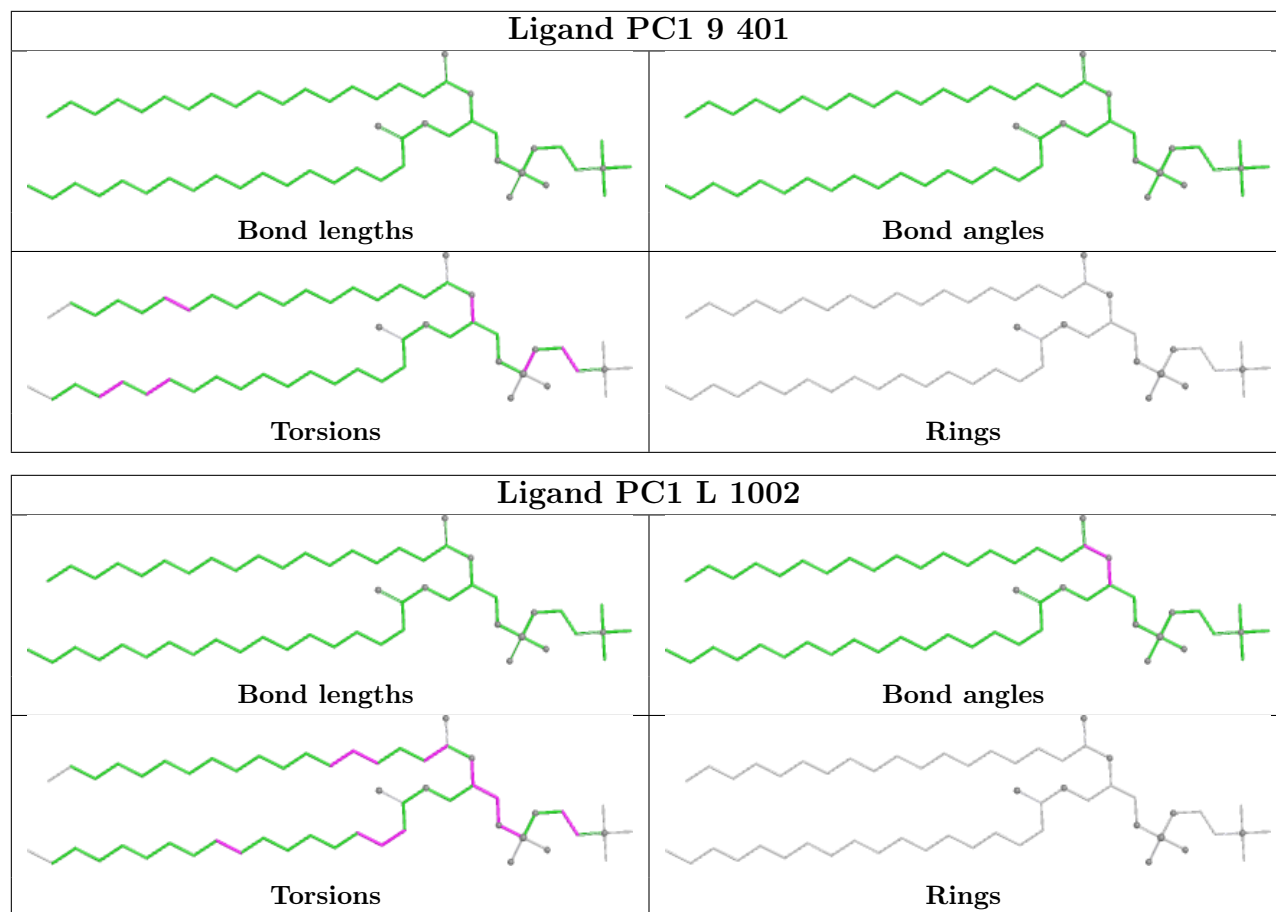
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



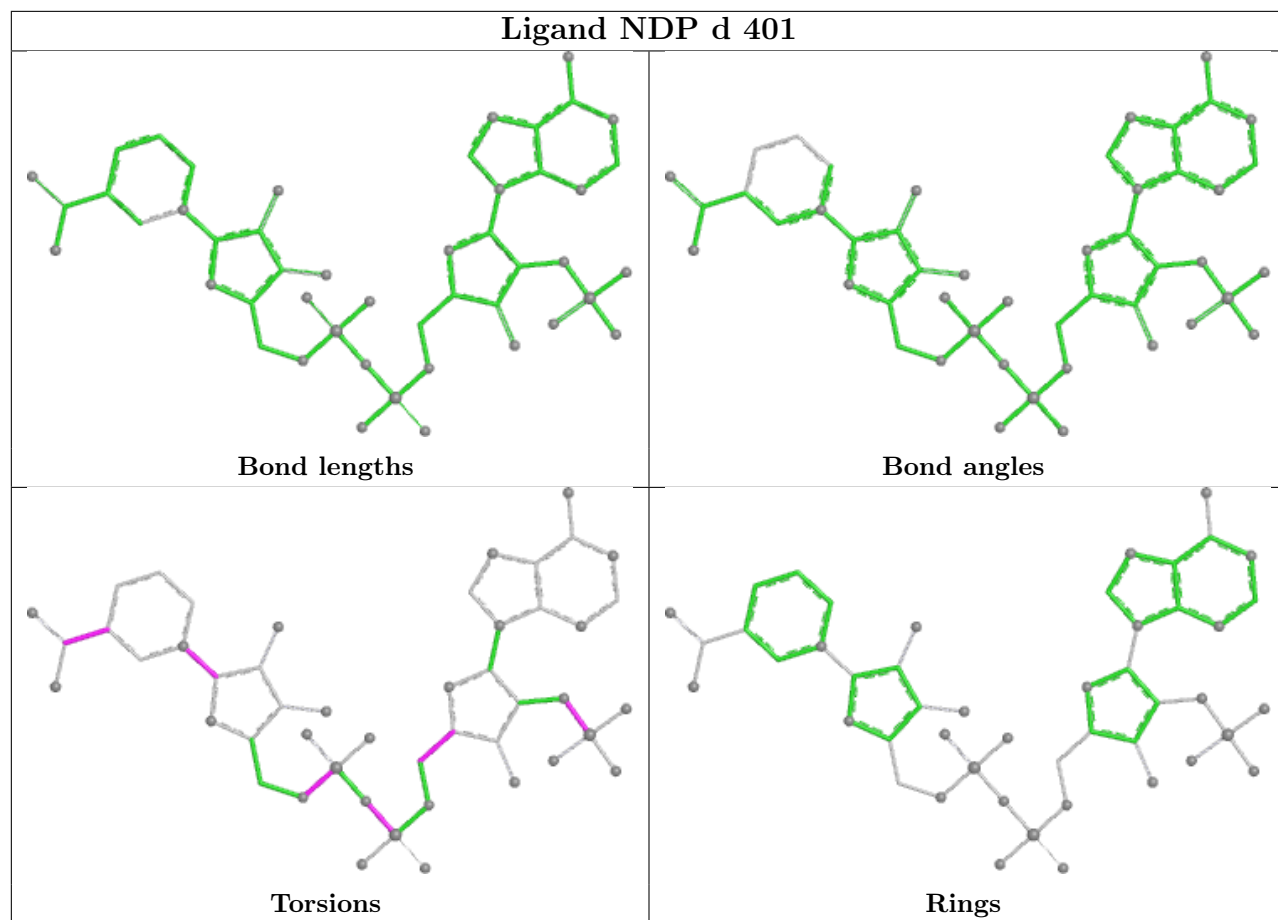




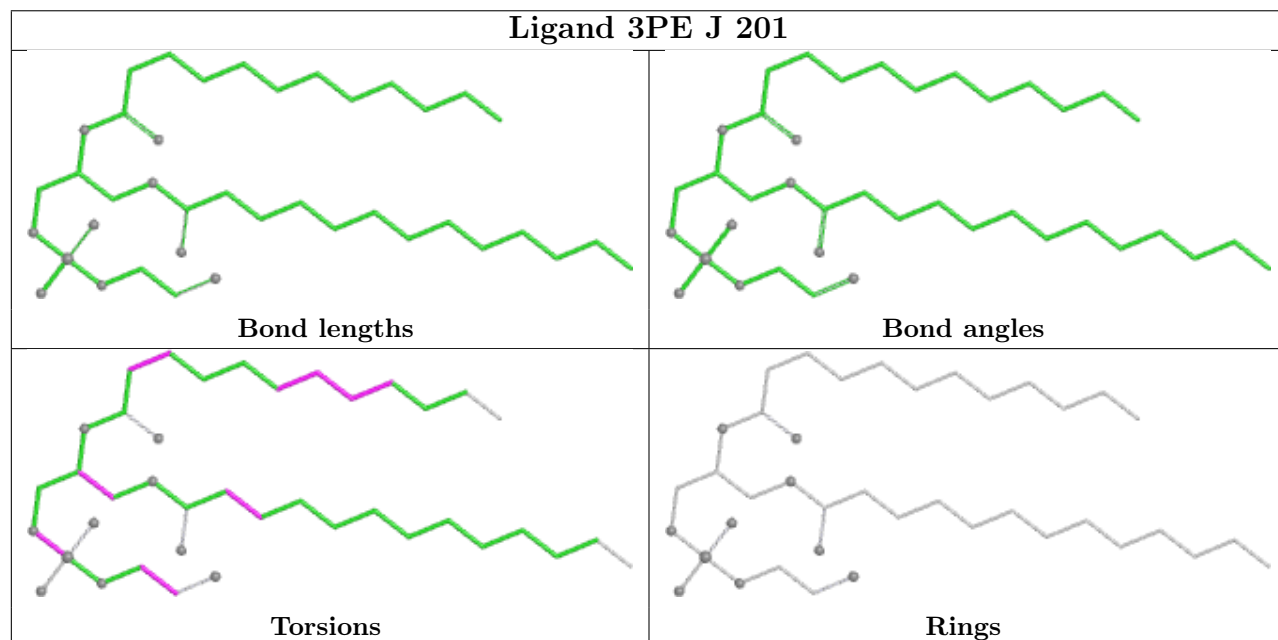


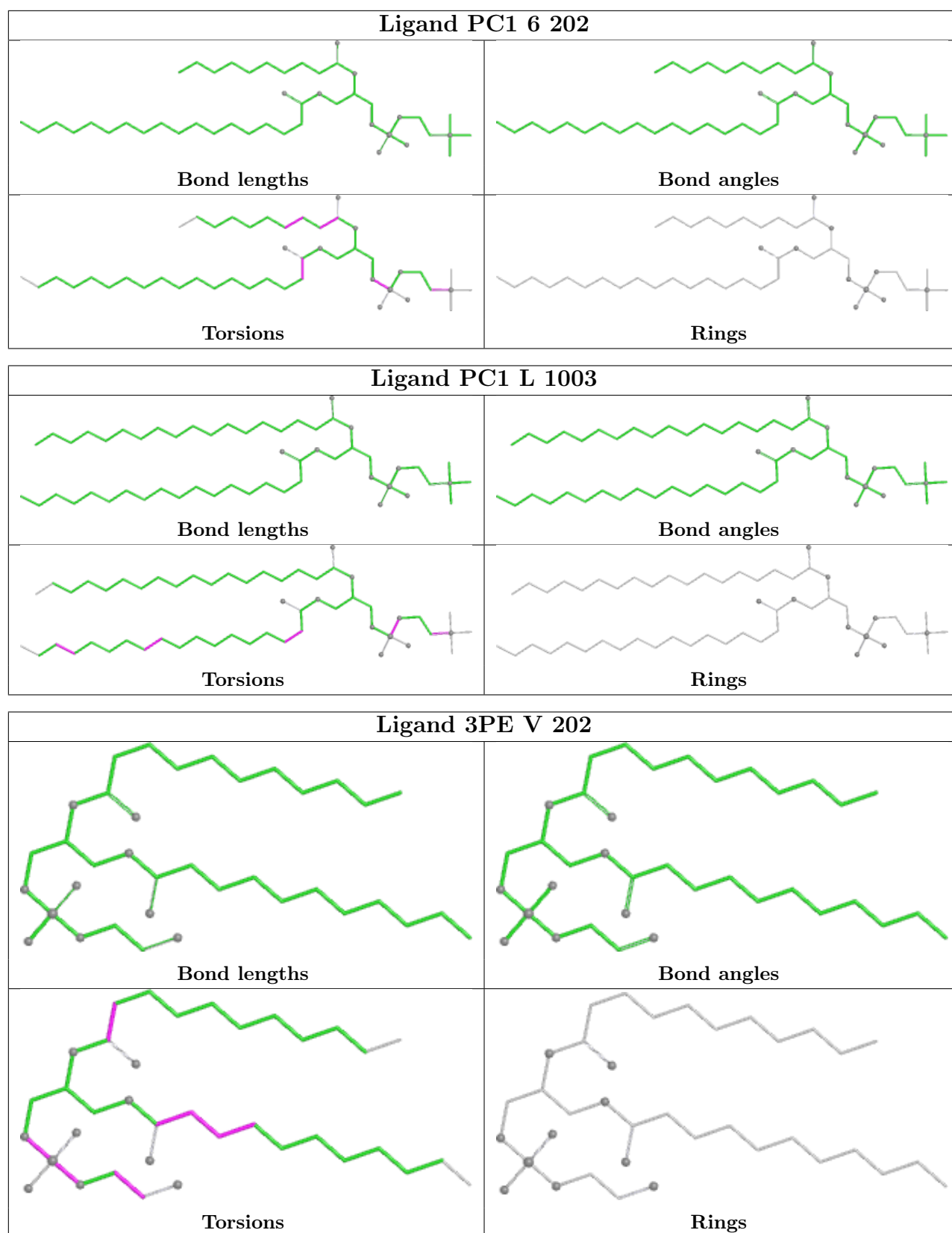


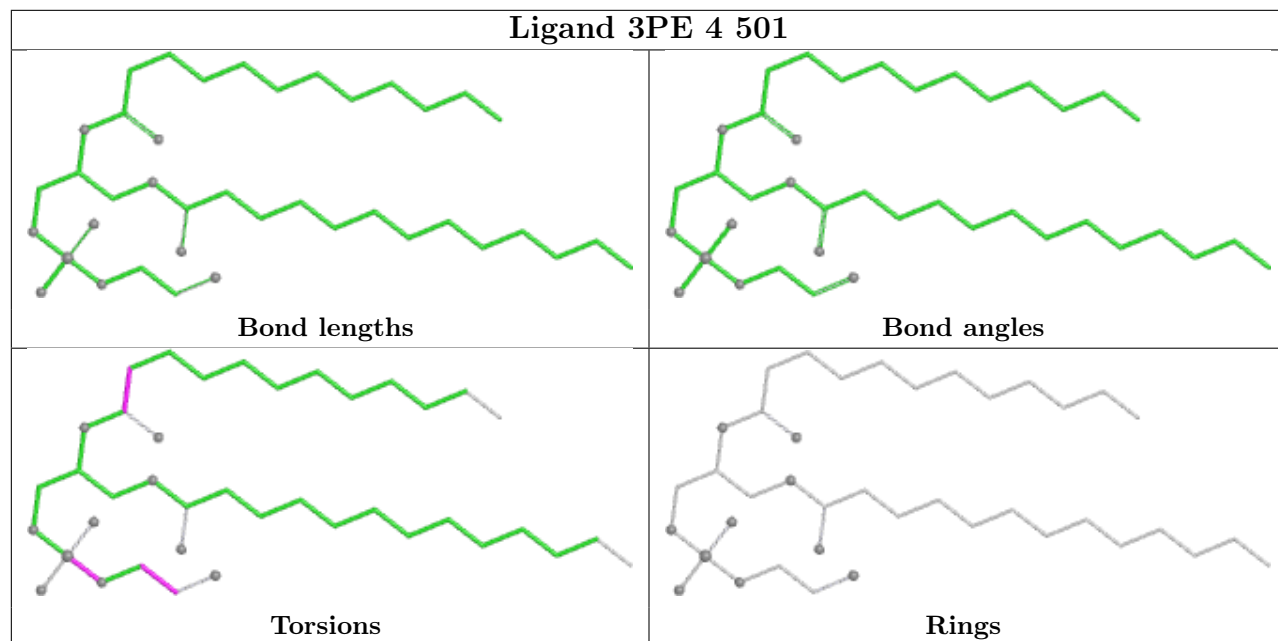
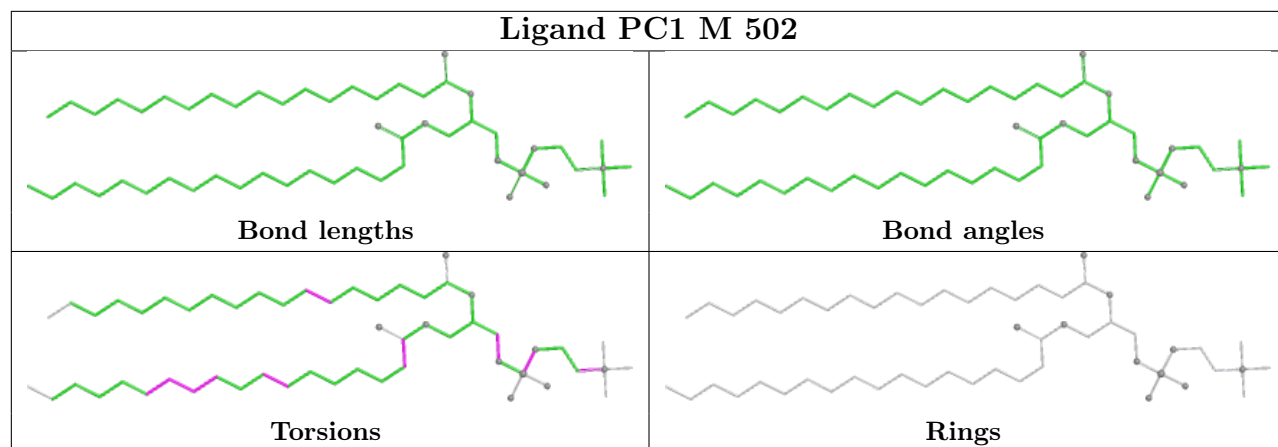
Ligand NDP d 401

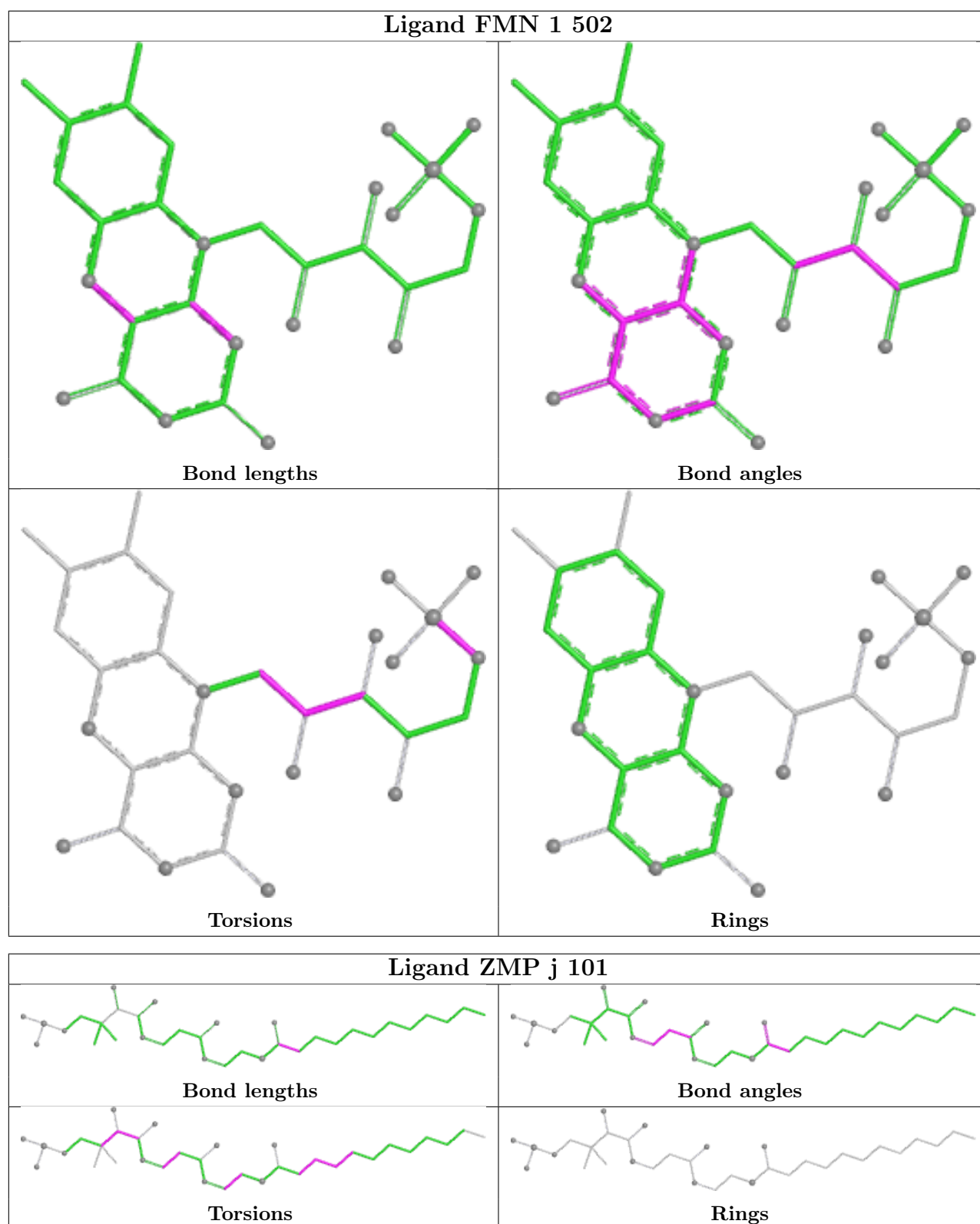


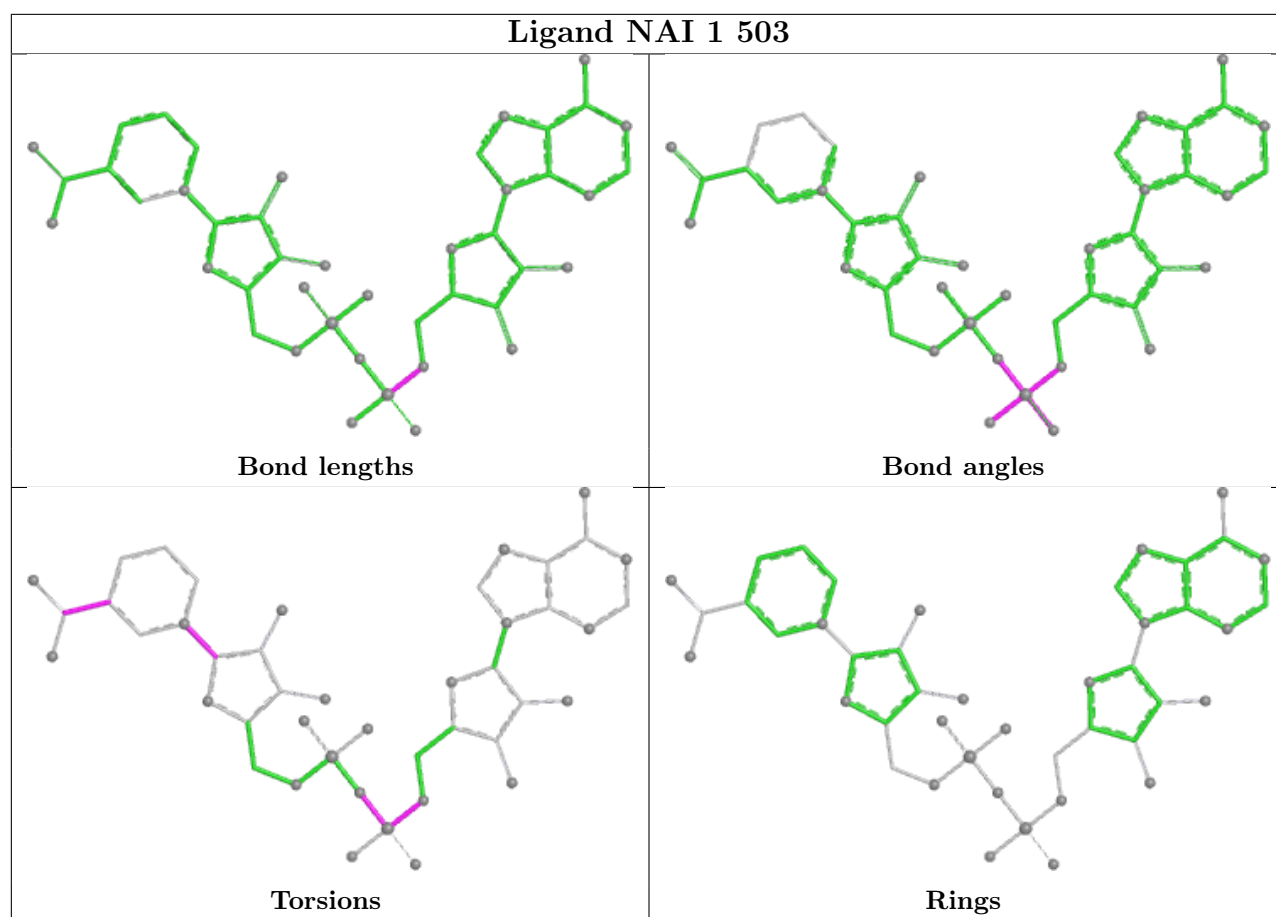
Ligand 3PE J 201











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.

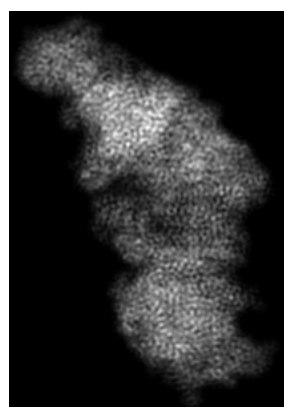
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14658. These allow visual inspection of the internal detail of the map and identification of artifacts.

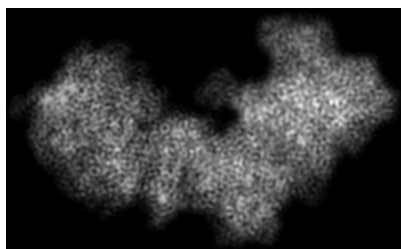
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

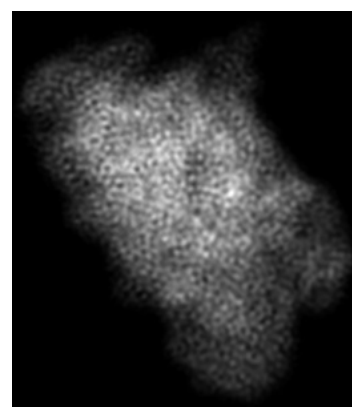
6.1.1 Primary map



X



Y



Z

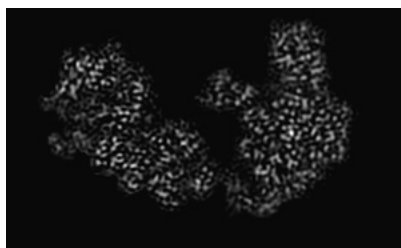
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 71



Y Index: 81



Z Index: 117

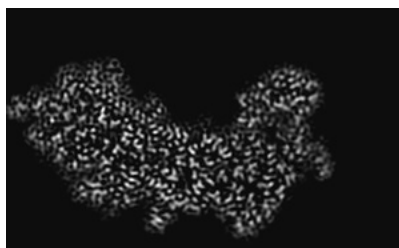
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

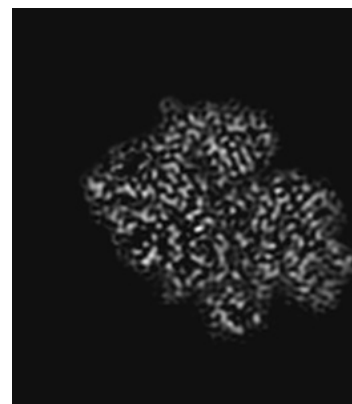
6.3.1 Primary map



X Index: 89



Y Index: 106

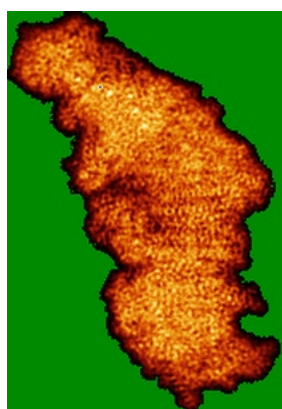


Z Index: 172

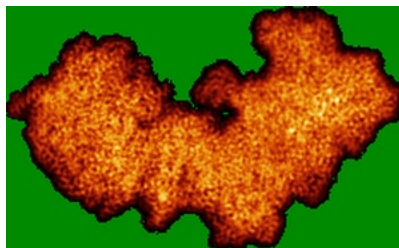
The images above show the largest variance slices of the map in three orthogonal directions.

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

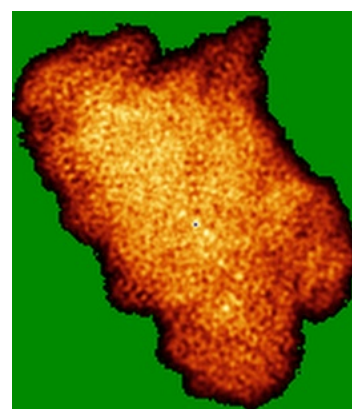
6.4.1 Primary map



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

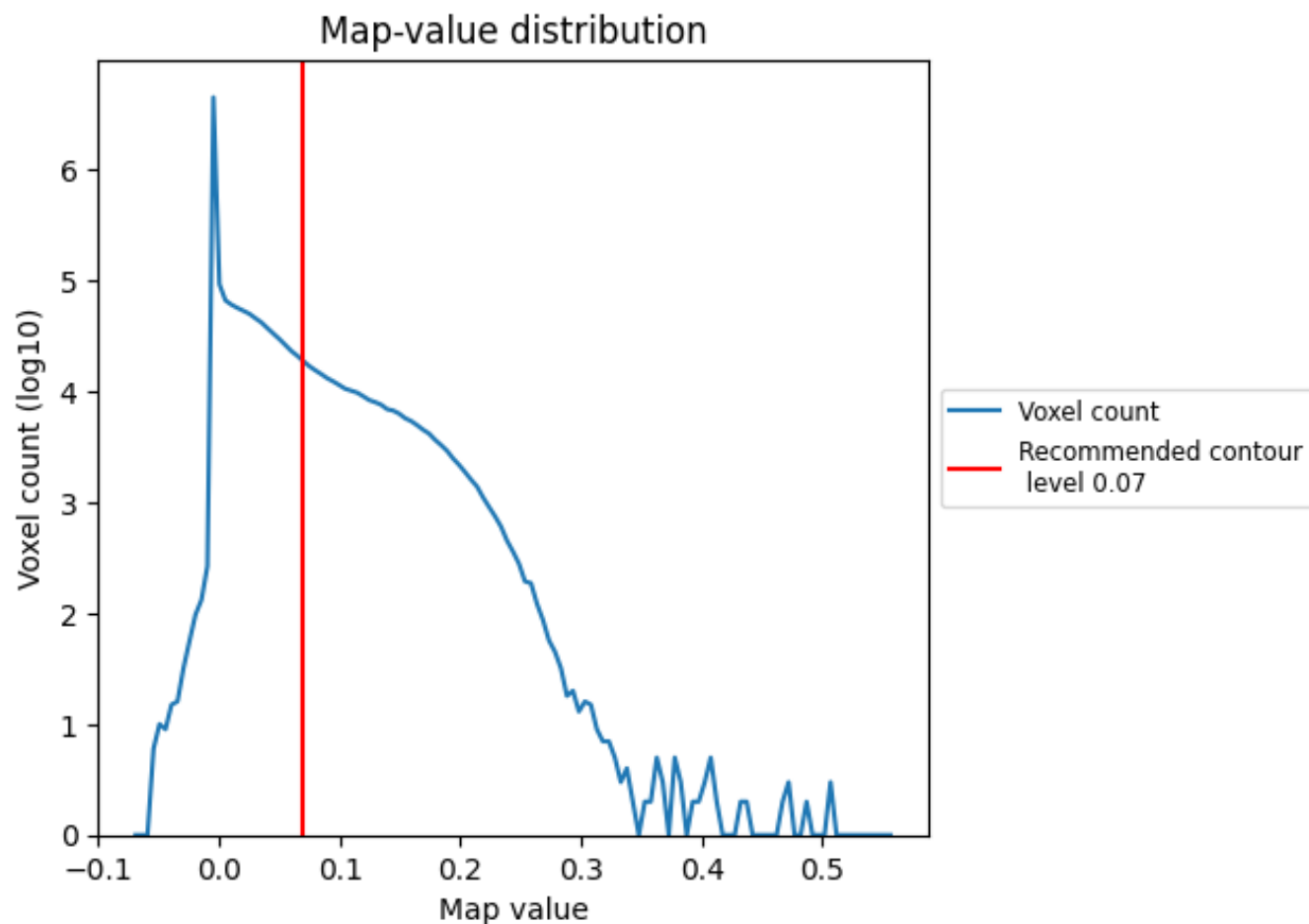
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

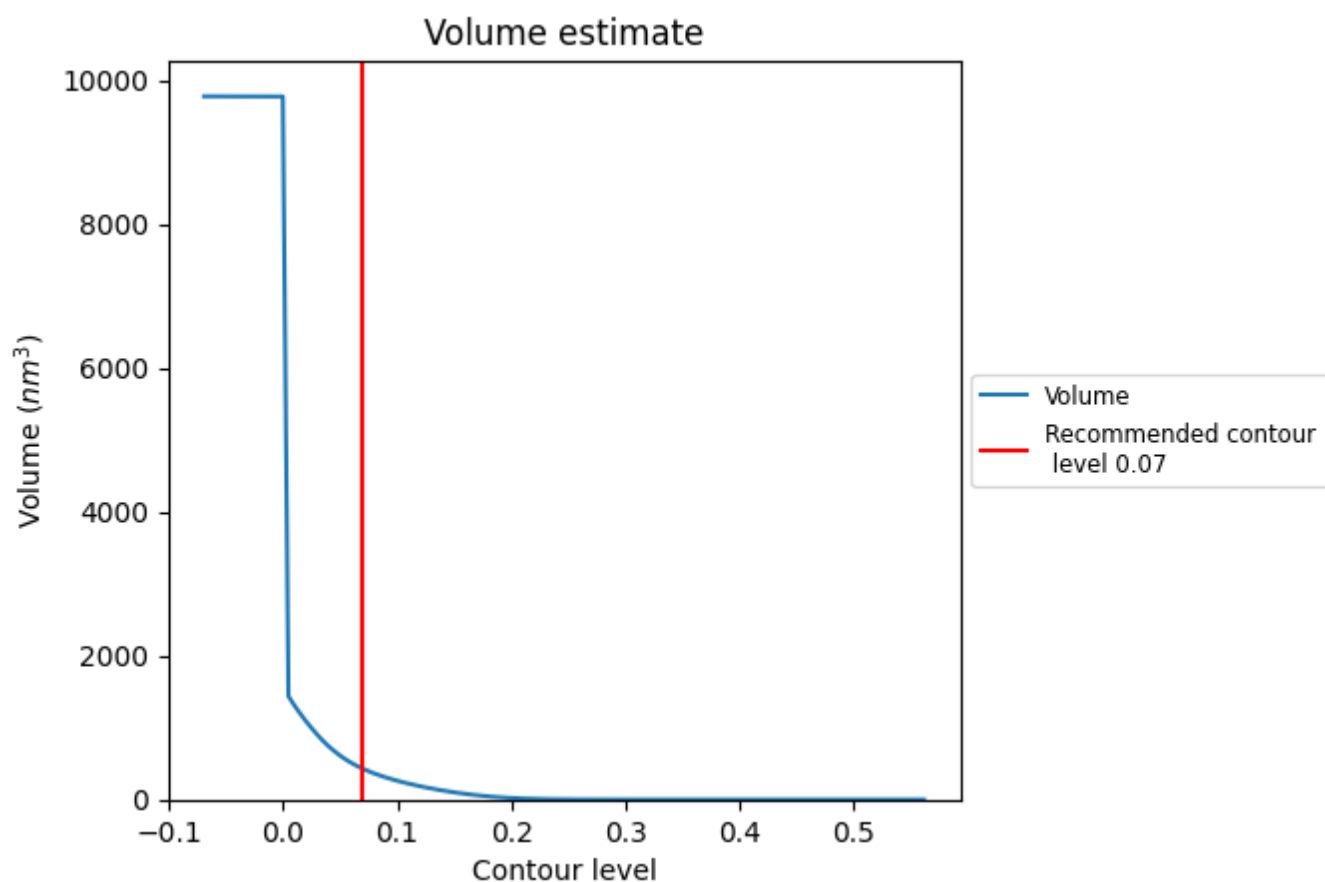
This section contains the results of statistical analysis of the map.

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 427 nm³; this corresponds to an approximate mass of 385 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.

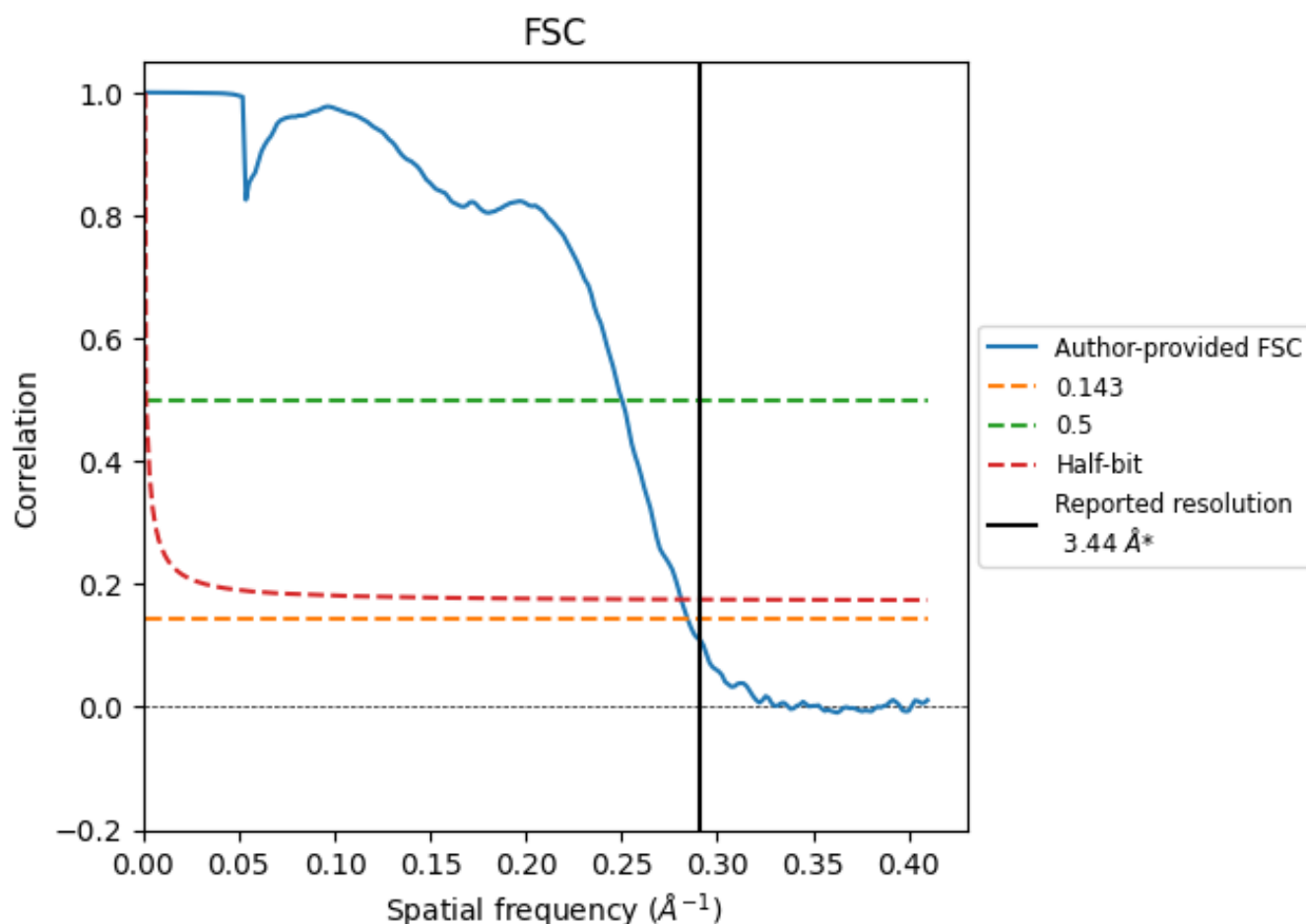
7.3 Rotationally averaged power spectrum [i](#)

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 0.291 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

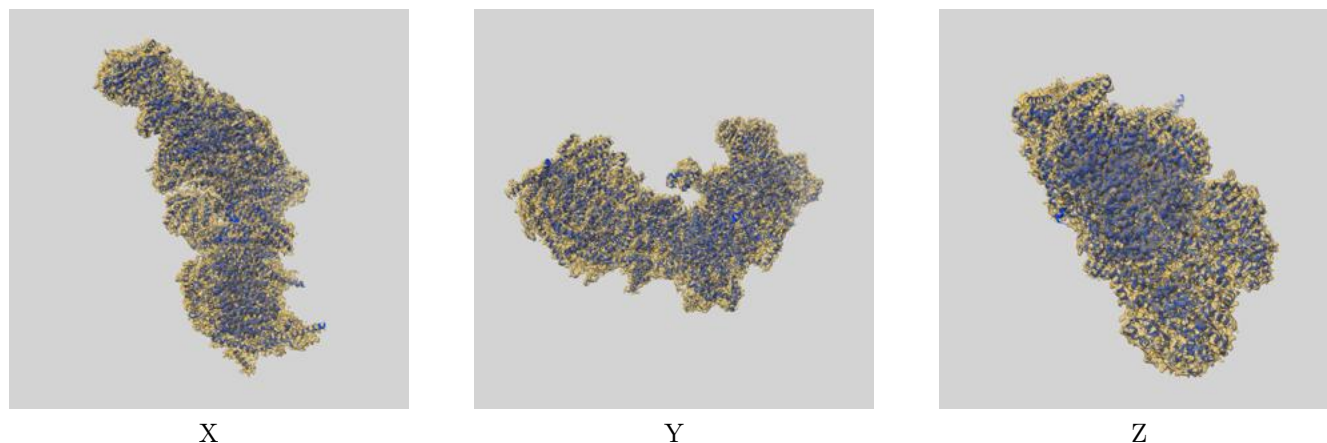
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	3.51	4.00	3.56
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

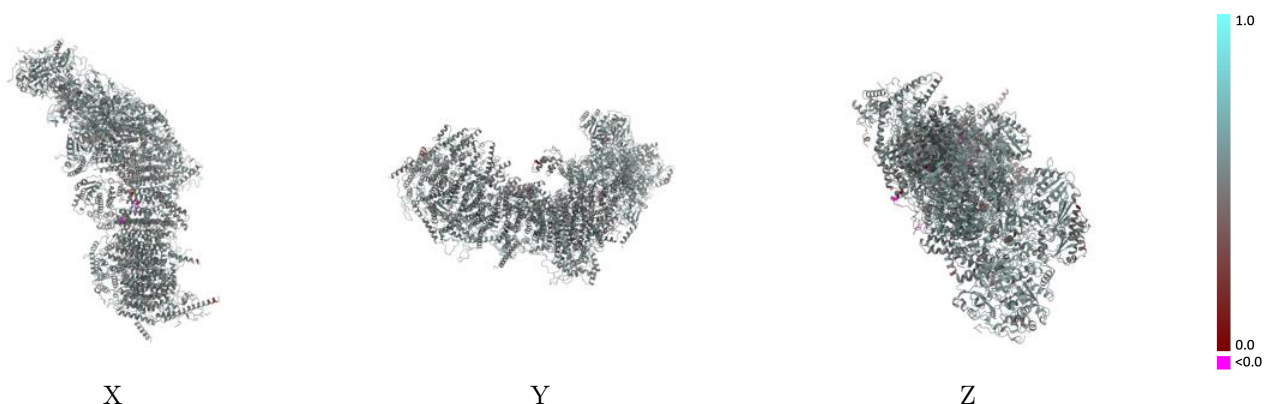
This section contains information regarding the fit between EMDB map EMD-14658 and PDB model 7ZDM. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



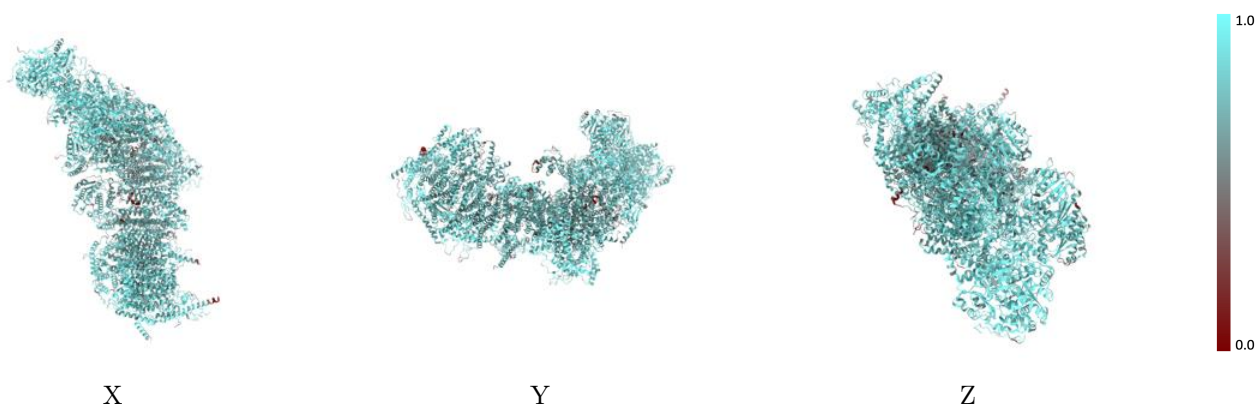
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



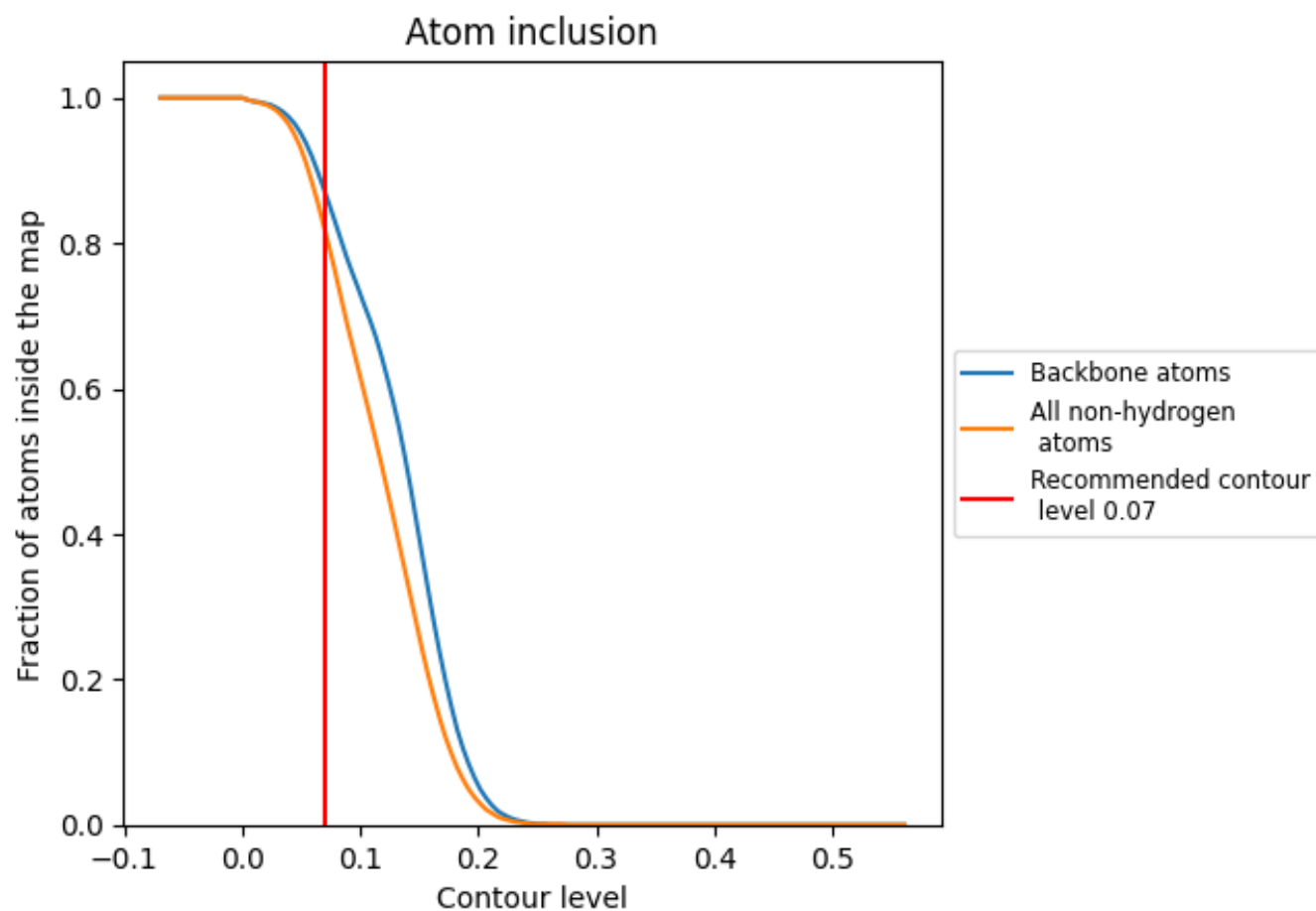
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 82% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.5240
1	 0.8900	 0.5310
2	 0.8620	 0.5300
3	 0.8460	 0.5330
4	 0.7970	 0.5180
5	 0.8610	 0.5550
6	 0.8400	 0.5440
9	 0.8320	 0.5280
A	 0.6360	 0.4750
H	 0.7410	 0.5040
J	 0.7750	 0.5110
K	 0.8060	 0.5270
L	 0.8200	 0.5220
M	 0.8440	 0.5460
N	 0.8450	 0.5390
V	 0.7690	 0.5060
W	 0.8670	 0.5430
X	 0.8280	 0.5100
Y	 0.8390	 0.5260
Z	 0.8250	 0.5240
a	 0.8400	 0.5190
b	 0.8190	 0.5480
c	 0.8040	 0.5410
d	 0.8250	 0.5320
e	 0.8230	 0.5090
f	 0.7960	 0.5220
g	 0.7890	 0.5290
h	 0.8180	 0.5260
i	 0.8430	 0.5450
j	 0.6360	 0.4420
k	 0.7960	 0.5200
l	 0.8170	 0.5200
m	 0.7900	 0.5100
n	 0.8090	 0.5030
o	 0.8330	 0.5330



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Chain	Atom inclusion	Q-score
p	 0.7910	 0.5190
q	 0.8210	 0.5130
r	 0.7970	 0.5170
s	 0.7990	 0.4910
t	 0.8240	 0.5170
u	 0.8430	 0.5040
v	 0.8180	 0.5240
w	 0.8030	 0.5250
x	 0.7590	 0.5110
y	 0.7230	 0.4980
z	 0.8160	 0.5020