



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 08:32 PM UTC

PDB ID : 8EC0 / pdb_00008ec0
EMDB ID : EMD-28011
Title : III2IV respiratory supercomplex from *Saccharomyces cerevisiae* cardiolipin-lacking mutant
Authors : Hryc, C.F.; Mileykovskaya, E.; Baker, M.; Dowhan, W.
Deposited on : 2022-08-31
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

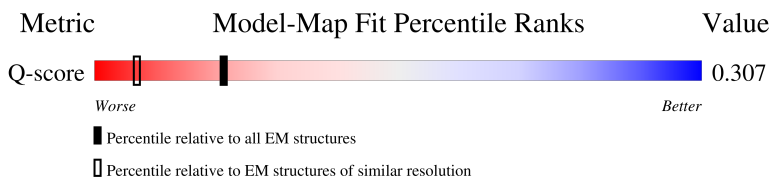
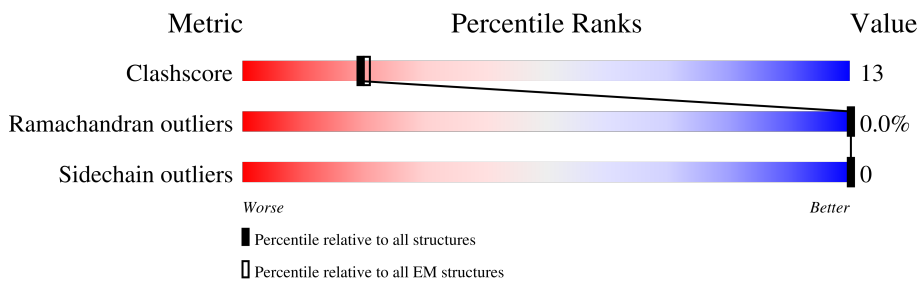
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	457	<p>71% 23% 6%</p>
1	a	457	<p>73% 21% 6%</p>
2	B	368	<p>69% 26% .</p>
2	b	368	<p>74% 21% .</p>


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Mol	Chain	Length	Quality of chain
3	C	215	42% 58% 28% 14%
3	c	215	47% 62% 24% 14%
4	E	66	32% 71% 15% 14%
4	e	66	20% 55% 30% 14%
5	F	127	71% 28%
5	f	127	74% 25%
6	G	147	10% 34% 16% 50%
6	g	147	12% 40% 10% 50%
7	H	94	5% 78% 21%
7	h	94	10% 77% 22%
8	J	385	7% 65% 35%
8	j	385	8% 62% 38%
9	K	534	64% 67% 33%
10	L	309	6% 61% 19% 20%
10	l	309	9% 57% 23% 20%
11	M	78	44% 49% 12% 40%
12	N	60	85% 77% 22%
13	O	269	77% 69% 31%
14	P	251	50% 57% 37% 6%
15	Q	148	24% 47% 22% 31%
16	R	59	53% 69% 24% 7%
17	S	129	78% 71% 17% 12%
18	T	155	46% 57% 21% 22%
19	U	83	86% 75% 18% 7%
20	V	66	23% 53% 8% 39%

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Mol	Chain	Length	Quality of chain
21	W	153	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	FES	C	301	-	-	X	-
24	FES	c	301	-	-	X	-

2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 46624 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	Total	C	N	O	S	0	0
			3345	2110	576	653	6		
1	a	431	Total	C	N	O	S	0	0
			3345	2110	576	653	6		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		
2	b	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		
3	c	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	57	Total	C	N	O	0	0
			465	310	77	78		
4	e	57	Total	C	N	O	0	0
			465	310	77	78		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		
5	f	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	74	Total	C	N	O	S	0	0
			624	391	108	123	2		
6	g	74	Total	C	N	O	S	0	0
			624	391	108	123	2		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	93	Total	C	N	O	S	0	0
			773	510	131	130	2		
7	h	93	Total	C	N	O	S	0	0
			773	510	131	130	2		

- Molecule 8 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		
8	j	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		

- Molecule 9 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	534	Total	C	N	O	S	0	0
			4162	2778	649	713	22		

- Molecule 10 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		
10	l	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	47	382	261	62	58	1	0	0

- Molecule 12 is a protein called Cytochrome c oxidase subunit 7, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	N	59	484	328	83	73	0	0

- Molecule 13 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	O	269	2146	1430	344	357	15	0	0

- Molecule 14 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	P	236	1889	1242	286	351	10	0	0

- Molecule 15 is a protein called Cytochrome c oxidase subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	Q	102	851	545	137	168	1	0	0

- Molecule 16 is a protein called Cytochrome c oxidase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	R	55	455	300	79	73	3	0	0

- Molecule 17 is a protein called Cytochrome c oxidase subunit 13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	S	113	928	605	160	160	3	0	0

- Molecule 18 is a protein called Cytochrome c oxidase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	T	121	913	576	151	181	5	0	0

- Molecule 19 is a protein called Cytochrome c oxidase subunit 12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U	77	642	410	109	118	5	0	0

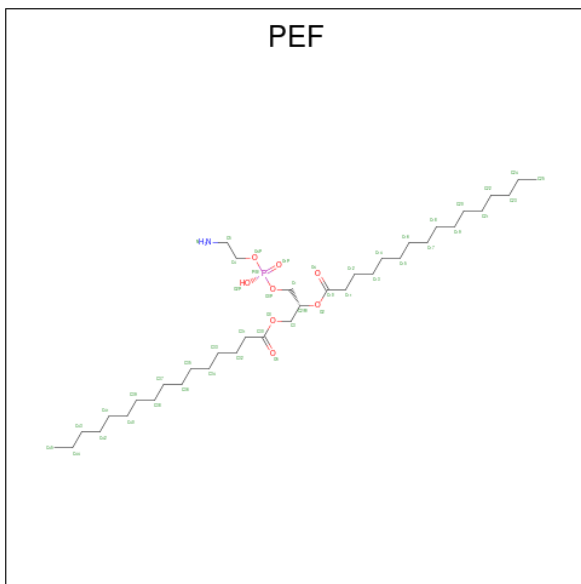
- Molecule 20 is a protein called Cytochrome c oxidase subunit 26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	40	321	214	53	53	1	0	0

- Molecule 21 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	133	1049	663	184	198	4	0	0

- Molecule 22 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: C₃₇H₇₄NO₈P) (labeled as "Ligand of Interest" by depositor).



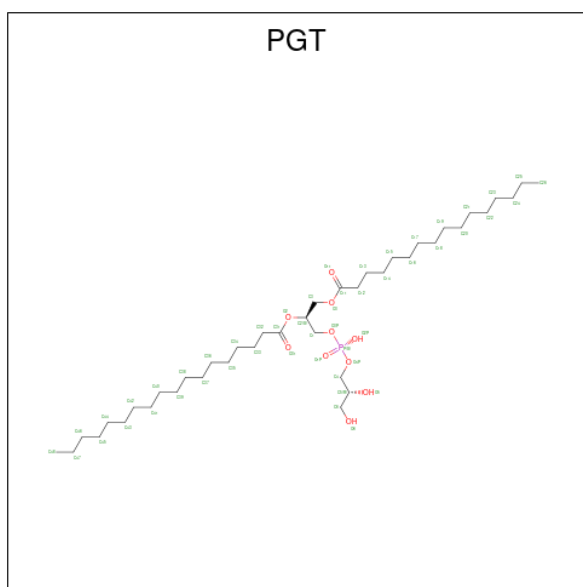
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
22	A	1	40	30	1	8	1	0

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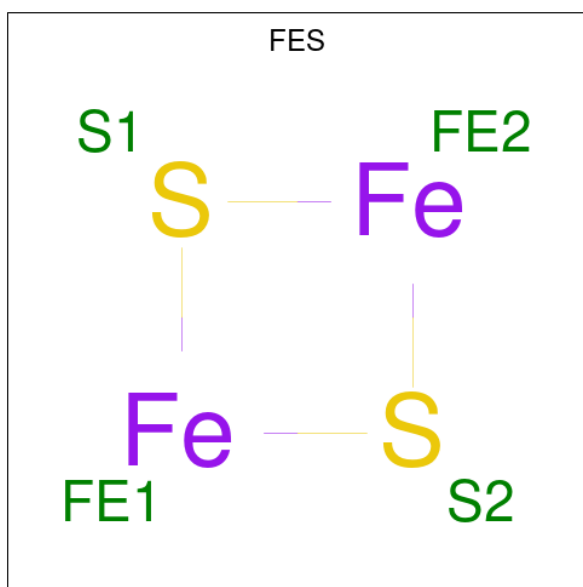
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
22	C	1	Total 43	C 33	N 1	O 8	P 1	0
22	H	1	Total 36	C 26	N 1	O 8	P 1	0
22	J	1	Total 45	C 35	N 1	O 8	P 1	0
22	J	1	Total 31	C 21	N 1	O 8	P 1	0
22	J	1	Total 31	C 21	N 1	O 8	P 1	0
22	J	1	Total 29	C 19	N 1	O 8	P 1	0
22	V	1	Total 33	C 23	N 1	O 8	P 1	0
22	V	1	Total 41	C 31	N 1	O 8	P 1	0
22	a	1	Total 40	C 30	N 1	O 8	P 1	0
22	c	1	Total 43	C 33	N 1	O 8	P 1	0
22	j	1	Total 45	C 35	N 1	O 8	P 1	0
22	j	1	Total 31	C 21	N 1	O 8	P 1	0
22	j	1	Total 31	C 21	N 1	O 8	P 1	0
22	j	1	Total 29	C 19	N 1	O 8	P 1	0

- Molecule 23 is (1S)-2-{{{(2R)-2,3-DIHYDROXYPROPYL}OXY}(HYDROXY)PHOSPHORYL}OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P) (labeled as "Ligand of Interest" by depositor).



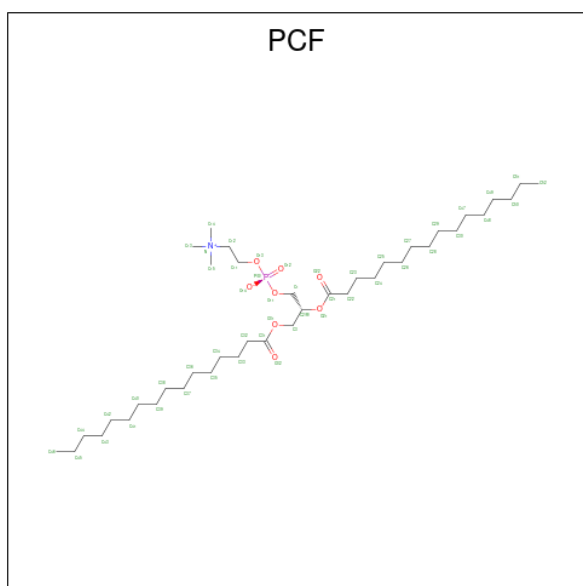
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
23	A	1	51	40	10	1	0
23	C	1	51	40	10	1	0
23	H	1	49	38	10	1	0
23	L	1	51	40	10	1	0
23	W	1	51	40	10	1	0
23	a	1	51	40	10	1	0
23	j	1	49	38	10	1	0

- Molecule 24 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
24	C	1	Total	Fe	S	0
			4	2	2	
24	c	1	Total	Fe	S	0
			4	2	2	

- Molecule 25 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



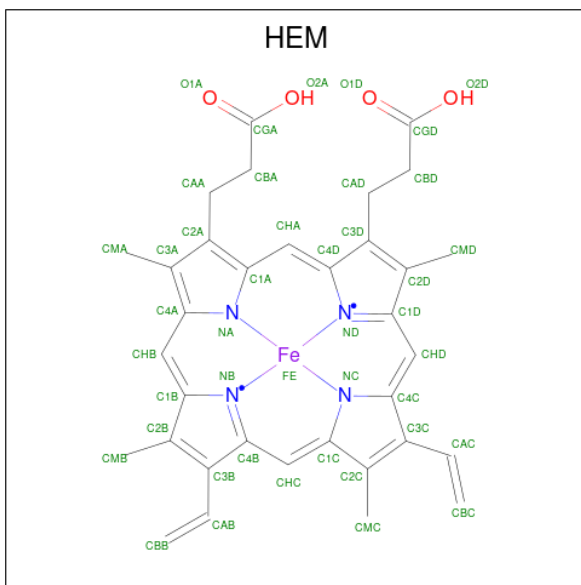
Mol	Chain	Residues	Atoms				AltConf	
25	E	1	Total	C	N	O	P	0
			47	37	1	8	1	

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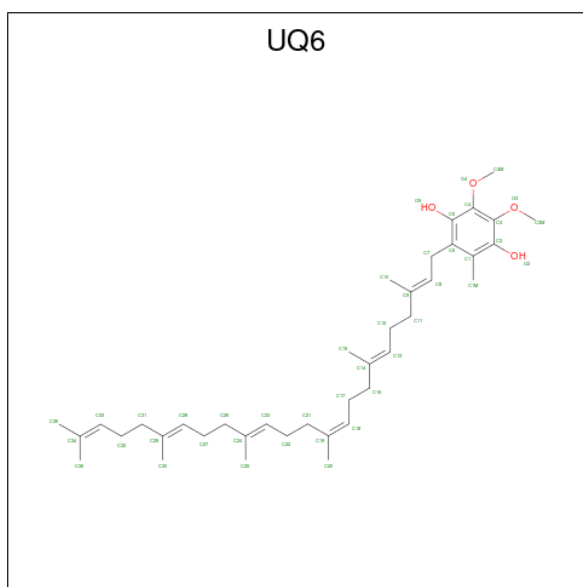
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
25	W	1	Total	C	N	O	P	0
			36	26	1	8	1	
25	W	1	Total	C	N	O	P	0
			50	40	1	8	1	
25	c	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 26 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
26	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
26	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
26	L	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
26	j	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
26	j	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
26	l	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 27 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: $C_{39}H_{60}O_4$) (labeled as "Ligand of Interest" by depositor).

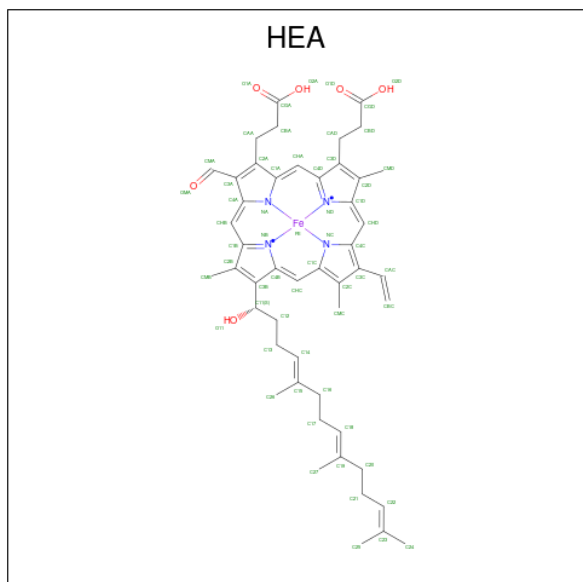


Mol	Chain	Residues	Atoms		AltConf
27	J	1	Total	C O	0
			43	39 4	
27	j	1	Total	C O	0
			43	39 4	

- Molecule 28 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

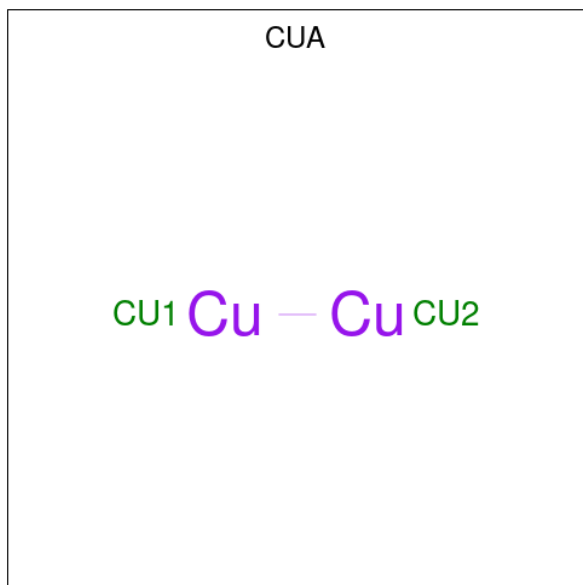
Mol	Chain	Residues	Atoms		AltConf
28	K	1	Total	Cu	0
			1	1	

- Molecule 29 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms				AltConf	
29	K	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
29	K	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 30 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).

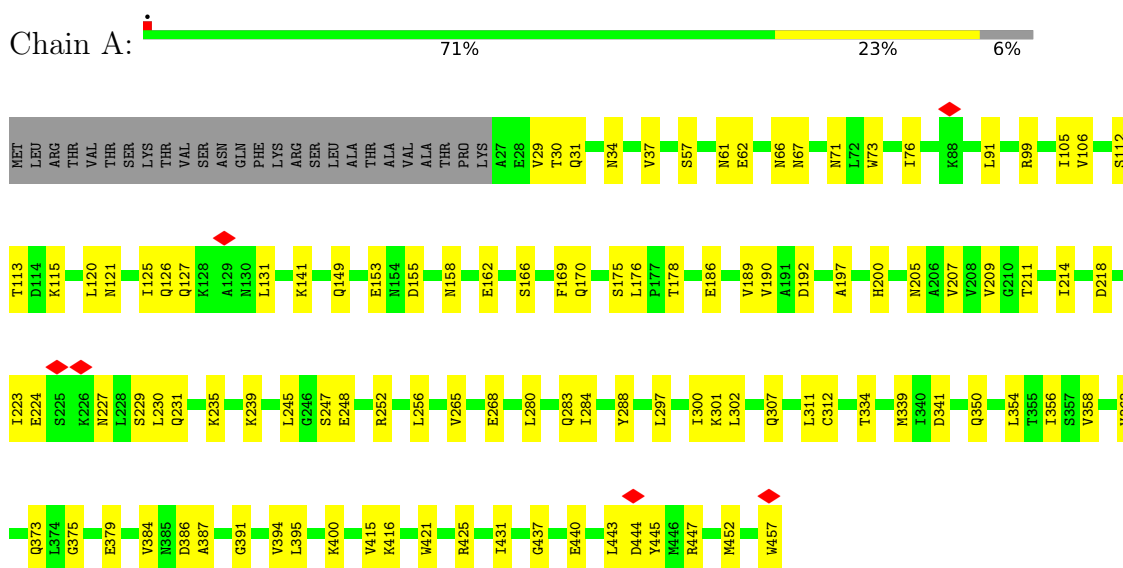


Mol	Chain	Residues	Atoms		AltConf
30	P	1	Total	Cu	0
			1	1	
30	P	1	Total	Cu	0
			1	1	

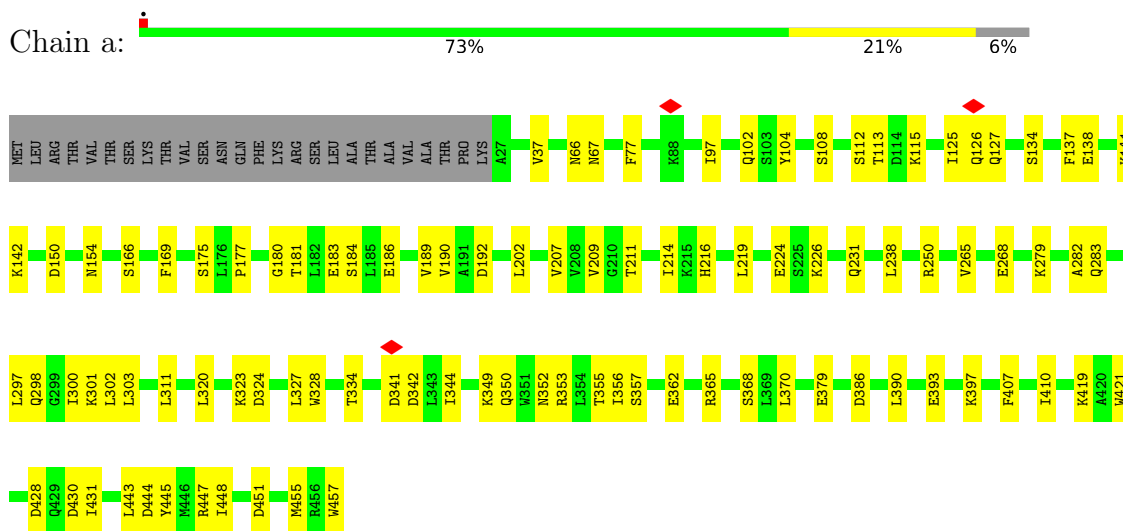
3 Residue-property plots

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

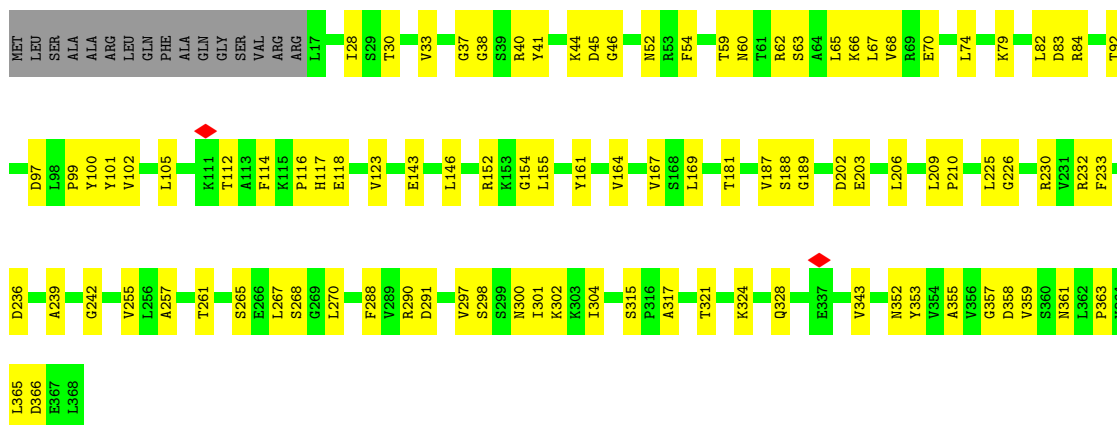
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



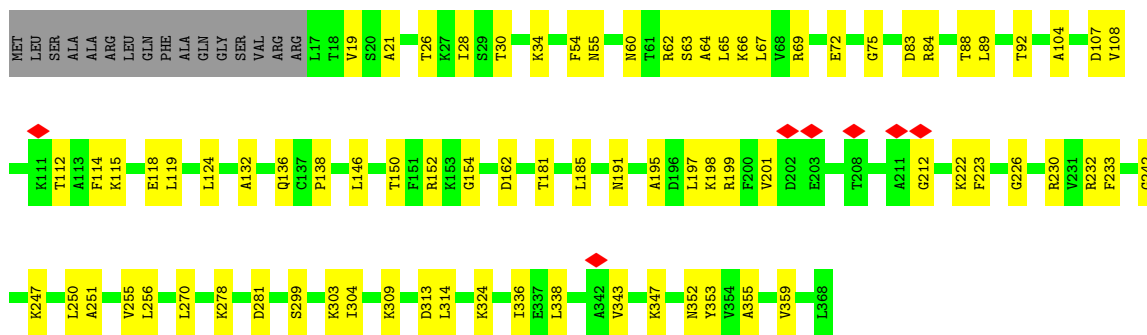
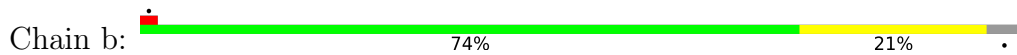
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



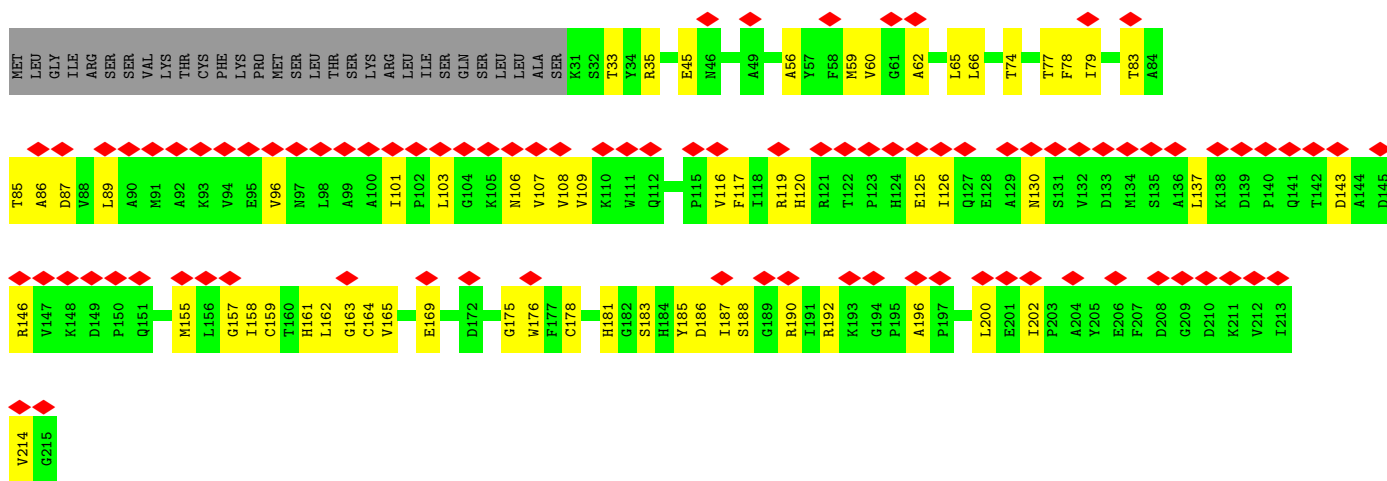
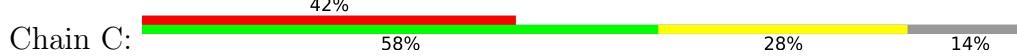
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



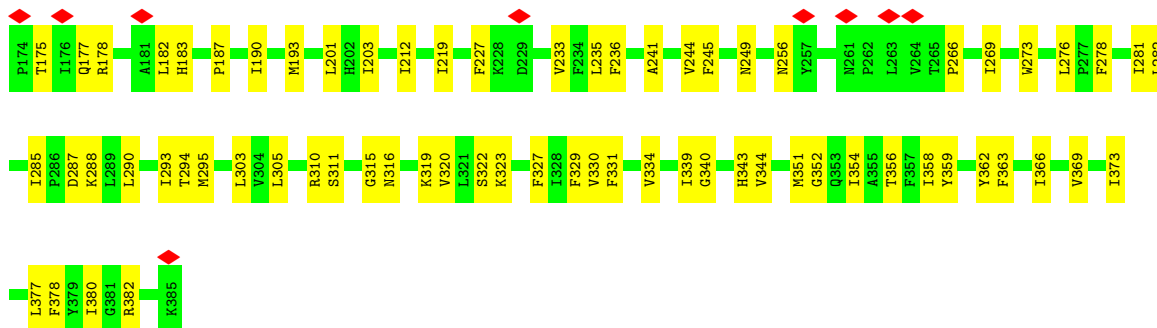
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



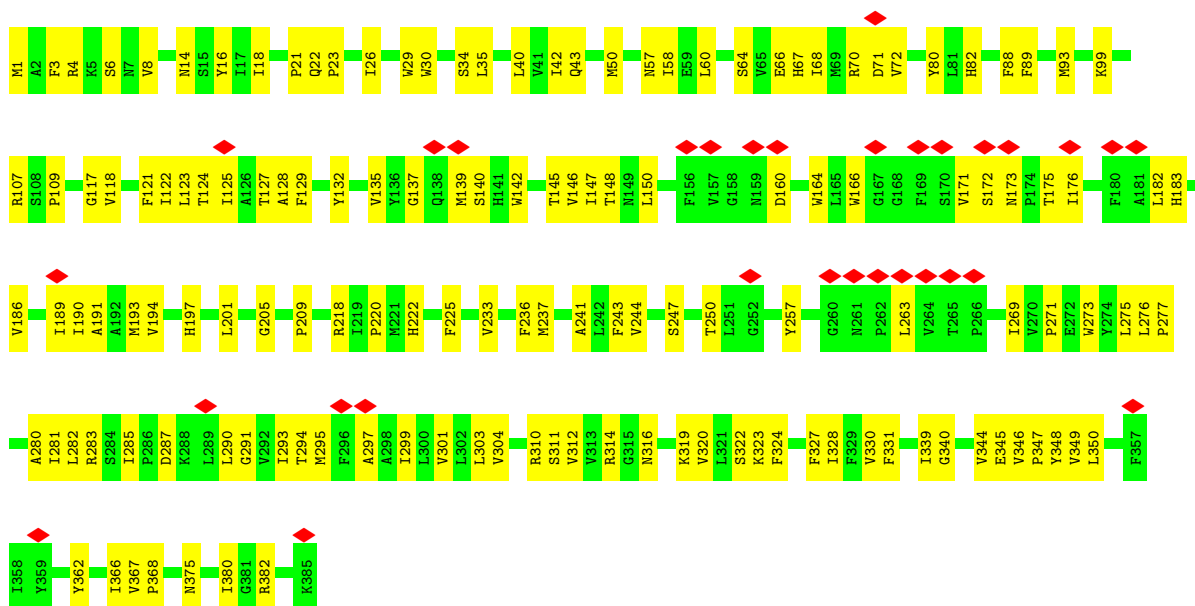
- Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial



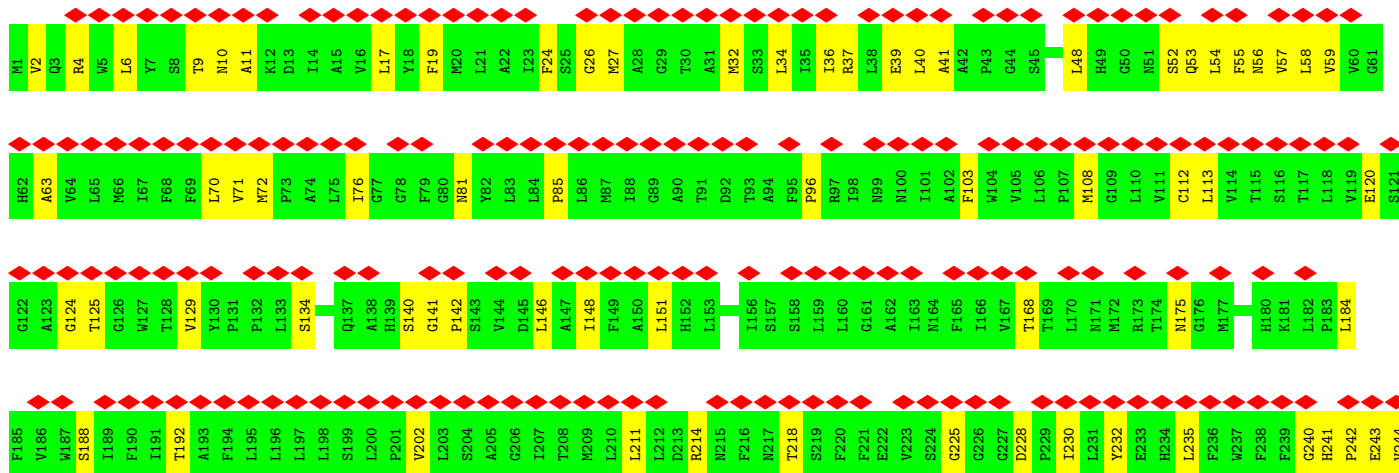
- Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

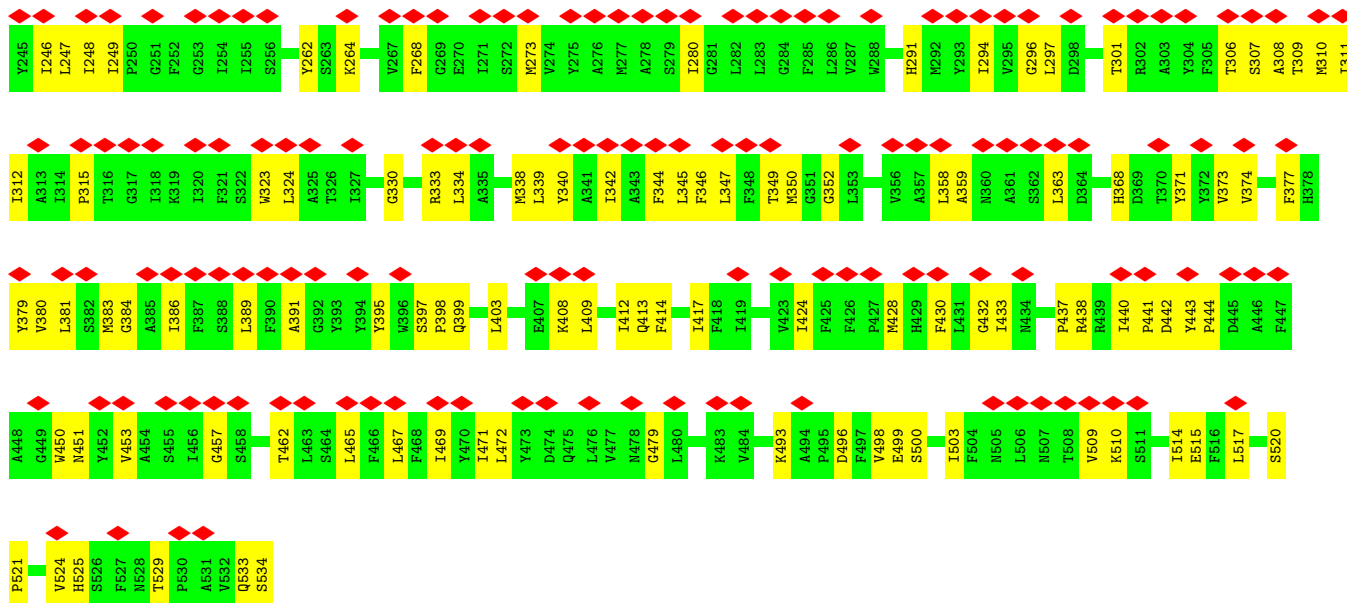


• Molecule 8: Cytochrome b



• Molecule 9: Cytochrome c oxidase subunit 1

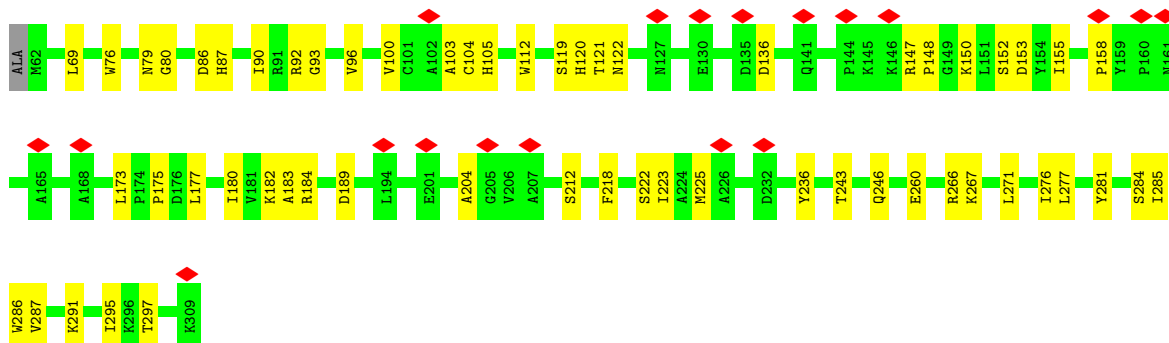




• Molecule 10: Cytochrome c1, heme protein, mitochondrial



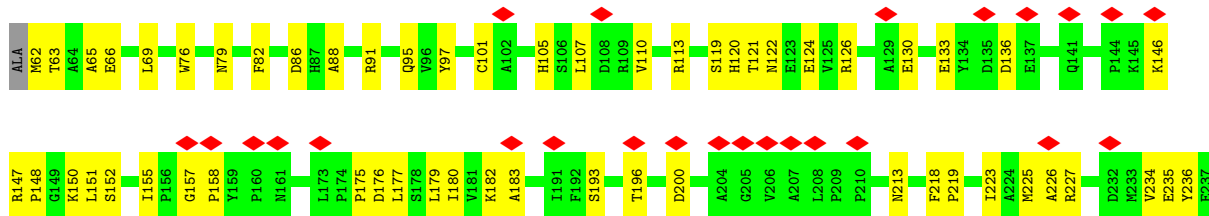
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• Molecule 10: Cytochrome c1, heme protein, mitochondrial

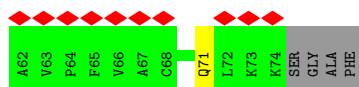
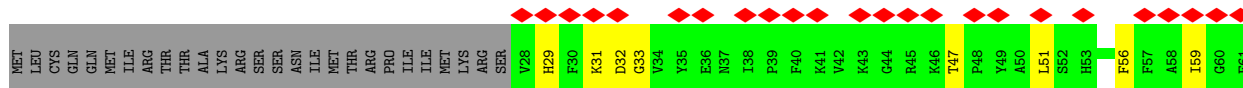
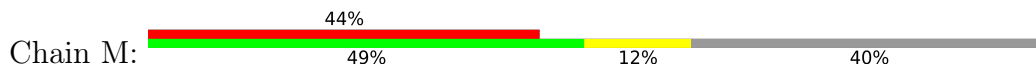


MET	PHE	SER	ASN	LEU	SER	LYS	ARG	TRP	ALA	GLN	ARC	THR	THR	LEU	SER	LYS	PHE	TYR	SER	THR	ALA	THR	GLY	ALA	ALA	SER	LYS	SER	GLY	LYS	LEU	THR	GLN	LYS	VAL	THR	ALA	GLY	VAL	ALA	ALA	ALA	GLY	ILE	THR	ALA	SER	THR	LEU	TYR	ALA	ASP	SER	LEU	THR	ALA	GLU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

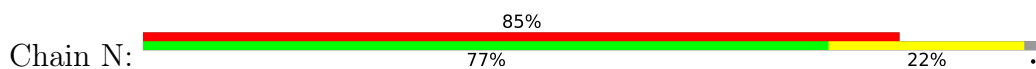




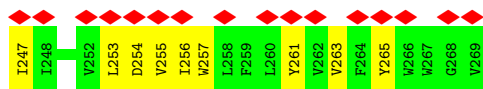
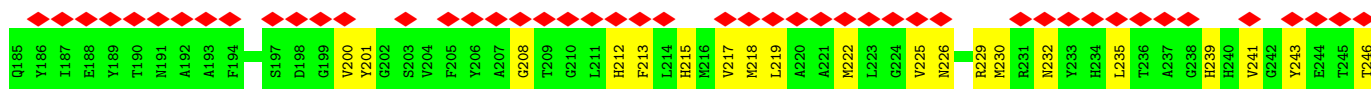
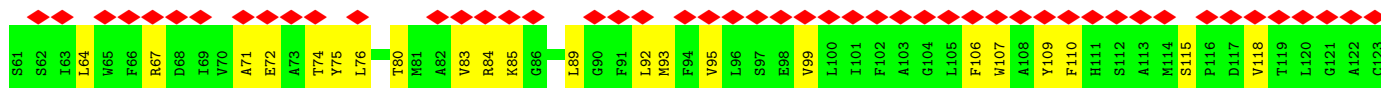
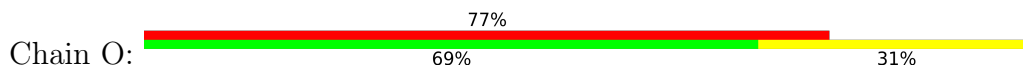
- Molecule 11: Cytochrome c oxidase subunit 8, mitochondrial



- Molecule 12: Cytochrome c oxidase subunit 7, mitochondrial

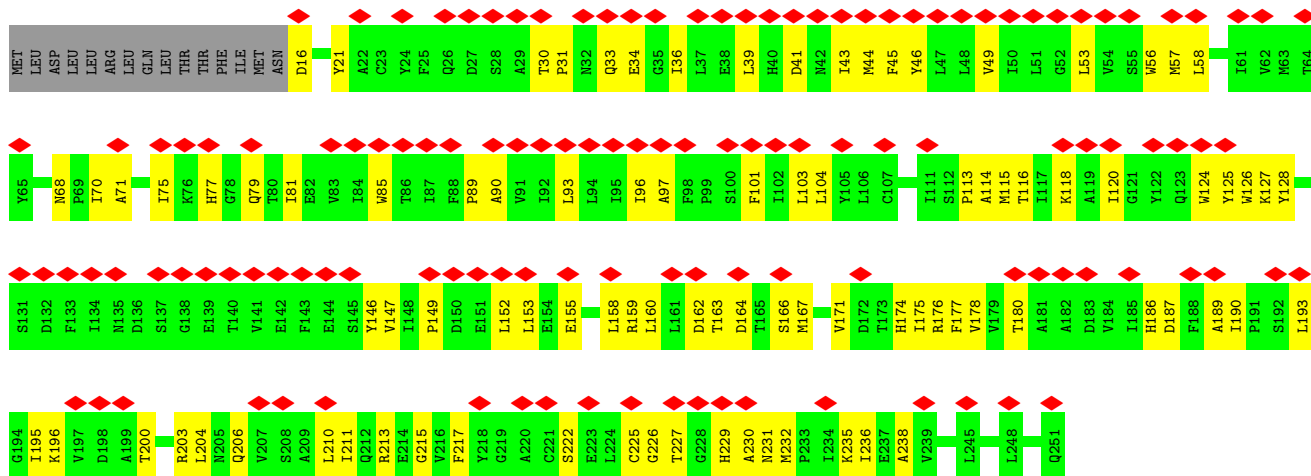


- Molecule 13: Cytochrome c oxidase subunit 3

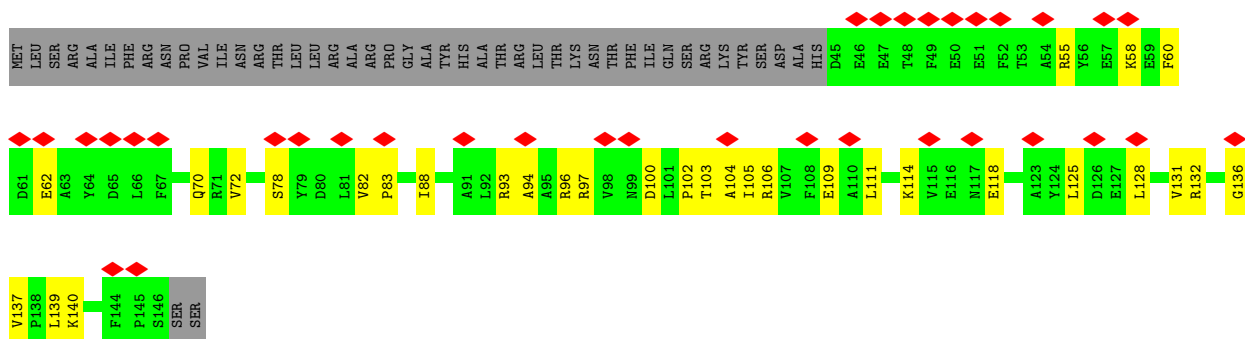


- Molecule 14: Cytochrome c oxidase subunit 2

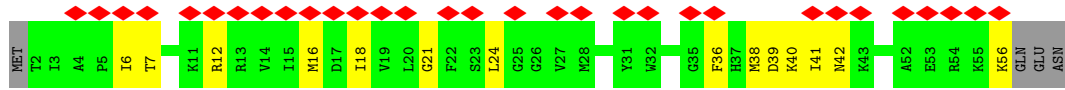




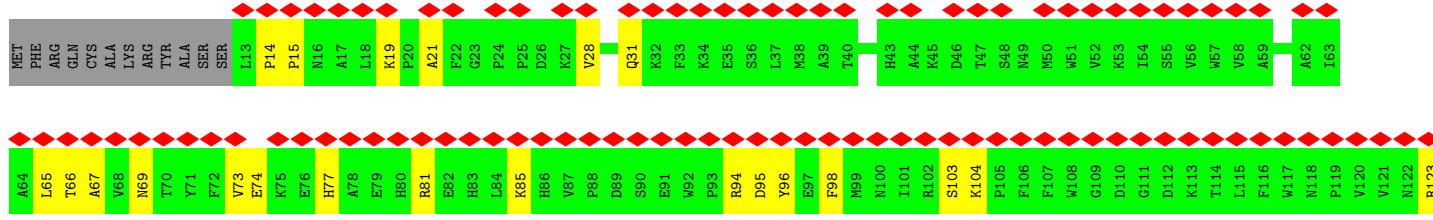
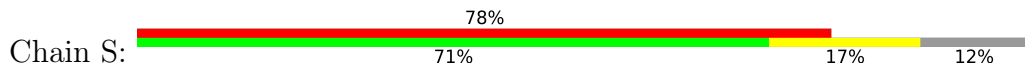
• Molecule 15: Cytochrome c oxidase subunit 6, mitochondrial

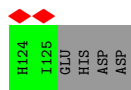


• Molecule 16: Cytochrome c oxidase subunit 9, mitochondrial

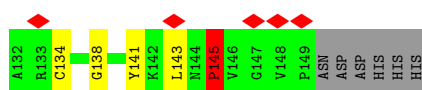
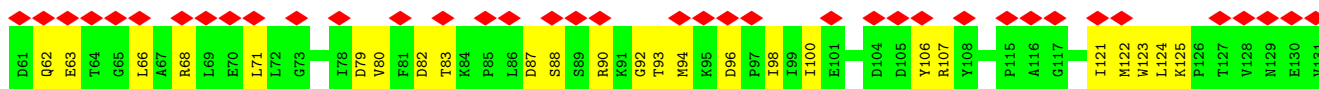
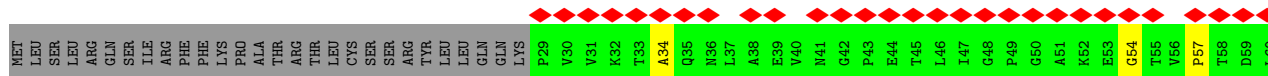


• Molecule 17: Cytochrome c oxidase subunit 13, mitochondrial

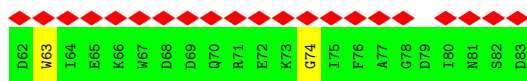
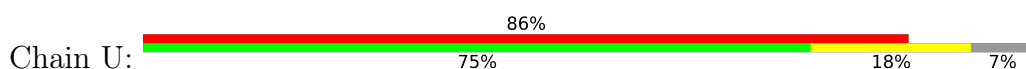




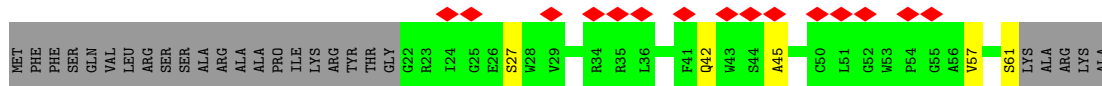
- Molecule 18: Cytochrome c oxidase subunit 4, mitochondrial



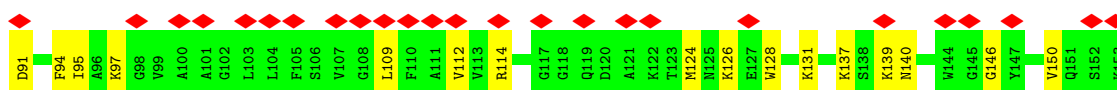
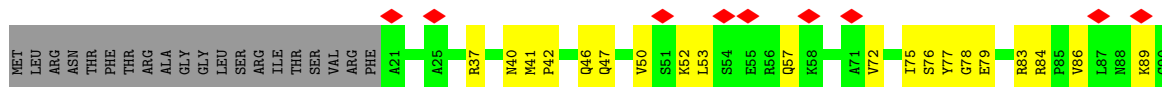
- Molecule 19: Cytochrome c oxidase subunit 12, mitochondrial



- Molecule 20: Cytochrome c oxidase subunit 26, mitochondrial



- Molecule 21: Cytochrome c oxidase subunit 5A, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	745670	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.361	Depositor
Minimum map value	-1.226	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEF, UQ6, PGT, HEA, CUA, FES, PCF, CU, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.11	0/3406	0.30	0/4615
1	a	0.11	0/3406	0.30	0/4615
2	B	0.11	0/2781	0.32	1/3764 (0.0%)
2	b	0.10	0/2781	0.30	0/3764
3	C	0.11	0/1444	0.31	0/1957
3	c	0.12	0/1444	0.31	0/1957
4	E	0.09	0/479	0.24	0/646
4	e	0.13	0/479	0.43	1/646 (0.2%)
5	F	0.13	0/1040	0.33	0/1408
5	f	0.12	0/1040	0.34	0/1408
6	G	0.12	0/638	0.38	0/858
6	g	0.11	0/638	0.30	0/858
7	H	0.11	0/804	0.29	0/1088
7	h	0.12	0/804	0.36	0/1088
8	J	0.14	0/3192	0.35	0/4354
8	j	0.14	0/3192	0.35	0/4354
9	K	0.14	0/4290	0.37	1/5857 (0.0%)
10	L	0.13	0/2022	0.35	0/2751
10	l	0.13	0/2022	0.32	0/2751
11	M	0.11	0/396	0.30	0/533
12	N	0.10	0/500	0.28	0/681
13	O	0.11	0/2218	0.32	0/3036
14	P	0.11	0/1941	0.32	0/2653
15	Q	0.13	0/868	0.34	0/1174
16	R	0.15	0/467	0.38	0/626
17	S	0.10	0/962	0.26	0/1310
18	T	0.11	0/932	0.33	1/1269 (0.1%)
19	U	0.09	0/664	0.23	0/899
20	V	0.09	0/332	0.28	0/452
21	W	0.12	0/1074	0.31	0/1451
All	All	0.12	0/46256	0.33	4/62823 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	e	56	ILE	N-CA-C	-5.72	108.28	113.71
9	K	437	PRO	CA-N-CD	-5.65	104.09	112.00
18	T	145	PRO	CA-N-CD	-5.54	104.24	112.00
2	B	68	VAL	N-CA-C	-5.49	108.49	113.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3345	0	3323	75	0
1	a	3345	0	3323	69	0
2	B	2735	0	2774	69	0
2	b	2735	0	2774	60	0
3	C	1411	0	1386	54	0
3	c	1411	0	1386	45	0
4	E	465	0	459	7	0
4	e	465	0	459	21	0
5	F	1019	0	1034	27	0
5	f	1019	0	1034	30	0
6	G	624	0	583	18	0
6	g	624	0	583	10	0
7	H	773	0	736	21	0
7	h	773	0	736	19	0
8	J	3090	0	3129	102	0
8	j	3090	0	3129	124	0
9	K	4162	0	4192	151	0
10	L	1961	0	1890	53	0
10	l	1961	0	1890	66	0
11	M	382	0	386	7	0
12	N	484	0	517	9	0
13	O	2146	0	2137	60	0
14	P	1889	0	1866	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	Q	851	0	822	28	0
16	R	455	0	469	13	0
17	S	928	0	906	17	0
18	T	913	0	912	29	0
19	U	642	0	586	11	0
20	V	321	0	314	5	0
21	W	1049	0	1030	33	0
22	A	40	0	53	2	0
22	C	43	0	62	1	0
22	H	36	0	48	4	0
22	J	136	0	167	2	0
22	V	74	0	97	2	0
22	a	40	0	53	1	0
22	c	43	0	62	5	0
22	j	136	0	167	6	0
23	A	51	0	78	4	0
23	C	51	0	78	1	0
23	H	49	0	71	1	0
23	L	51	0	78	0	0
23	W	51	0	78	3	0
23	a	51	0	78	2	0
23	j	49	0	71	1	0
24	C	4	0	0	2	0
24	c	4	0	0	2	0
25	E	47	0	71	0	0
25	W	86	0	126	1	0
25	c	47	0	71	1	0
26	J	86	0	60	9	0
26	L	43	0	30	6	0
26	j	86	0	60	12	0
26	l	43	0	30	13	0
27	J	43	0	58	4	0
27	j	43	0	58	4	0
28	K	1	0	0	0	0
29	K	120	0	108	23	0
30	P	2	0	0	0	0
All	All	46624	0	46678	1178	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 13.

All (1178) 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)
3:C:161:HIS:HE1	3:C:181:HIS:ND1	1.62	0.97
10:l:175:PRO:HD3	26:l:401:HEM:HAD2	1.52	0.90
1:a:302:LEU:HB3	1:a:350:GLN:HG3	1.59	0.84
2:B:52:ASN:HD22	2:B:82:LEU:HB2	1.42	0.84
4:e:48:LEU:HD22	4:e:50:LYS:HZ3	1.42	0.83
15:Q:82:VAL:H	16:R:6:ILE:HG21	1.41	0.83
3:C:178:CYS:HB3	3:C:183:SER:H	1.45	0.81
5:F:52:GLU:HG3	8:J:109:PRO:HG3	1.62	0.81
4:e:48:LEU:HD23	4:e:49:TRP:H	1.46	0.80
1:A:302:LEU:HB3	1:A:350:GLN:HG3	1.61	0.80
3:C:161:HIS:CE1	3:C:181:HIS:ND1	2.51	0.79
6:G:125:GLU:O	6:G:129:HIS:ND1	2.17	0.77
8:J:68:ILE:HD12	8:J:72:VAL:HG11	1.66	0.77
1:a:393:GLU:O	1:a:397:LYS:HB2	1.84	0.77
5:F:117:LYS:HB2	2:b:66:LYS:HE2	1.66	0.76
12:N:23:HIS:HB3	12:N:26:SER:HB3	1.68	0.76
3:c:178:CYS:CB	24:c:301:FES:S1	2.73	0.76
14:P:114:ALA:HB1	19:U:7:SER:HB2	1.67	0.76
10:L:260:GLU:OE2	10:L:266:ARG:NH1	2.19	0.75
8:j:345:GLU:OE1	10:l:62:MET:N	2.21	0.74
10:L:100:VAL:HG22	26:L:401:HEM:HBB1	1.70	0.73
2:B:54:PHE:HE2	2:B:114:PHE:HA	1.53	0.73
9:K:371:TYR:OH	9:K:428:MET:SD	2.47	0.73
1:A:211:THR:HG21	1:A:386:ASP:HB3	1.69	0.73
1:A:62:GLU:HG3	1:A:176:LEU:HD11	1.70	0.73
10:L:112:TRP:HE1	10:L:155:ILE:HG13	1.54	0.72
10:l:225:MET:HB3	10:l:227:ARG:HH22	1.52	0.72
3:c:117:PHE:N	3:c:155:MET:O	2.22	0.72
8:J:14:ASN:HA	8:J:18:ILE:HB	1.72	0.72
3:c:166:PRO:HB2	3:c:176:TRP:HB3	1.72	0.71
1:A:166:SER:HA	1:A:175:SER:HB2	1.72	0.71
21:W:53:LEU:O	21:W:57:GLN:NE2	2.25	0.70
1:a:108:SER:OG	1:a:112:SER:OG	2.09	0.70
8:J:51:ALA:HB2	26:J:403:HEM:HBC1	1.74	0.70
2:B:255:VAL:HG23	2:B:321:THR:HG21	1.73	0.69
5:F:120:LEU:HD23	2:b:66:LYS:HB3	1.74	0.69
19:U:55:TYR:HA	19:U:59:CYS:HB3	1.75	0.69
3:C:146:ARG:NH2	3:C:188:SER:O	2.25	0.69
14:P:41:ASP:OD2	16:R:40:LYS:NZ	2.25	0.69
16:R:6:ILE:HG22	16:R:7:THR:H	1.56	0.69
1:A:248:GLU:HB3	7:H:28:ALA:HB3	1.74	0.69
26:J:404:HEM:HBD1	26:J:404:HEM:HHA	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:529:THR:HG21	18:T:107:ARG:HH12	1.58	0.69
10:L:87:HIS:HB3	10:L:90:ILE:HD12	1.73	0.69
8:j:183:HIS:HE1	26:j:403:HEM:ND	1.91	0.68
10:l:101:CYS:HB3	26:l:401:HEM:HAB	1.75	0.68
8:J:169:PHE:HB2	3:c:112:GLN:HE22	1.59	0.68
1:a:67:ASN:ND2	1:a:177:PRO:O	2.27	0.68
9:K:125:THR:HG21	9:K:134:SER:HA	1.76	0.68
29:K:603:HEA:H242	14:P:89:PRO:HB3	1.76	0.68
14:P:118:LYS:HG2	14:P:178:VAL:HB	1.76	0.68
1:a:216:HIS:HA	1:a:219:LEU:HD23	1.76	0.67
2:b:28:ILE:O	2:b:191:ASN:ND2	2.22	0.67
1:A:297:LEU:HD12	2:B:65:LEU:HB3	1.76	0.67
6:G:129:HIS:HD2	10:L:69:LEU:HD23	1.59	0.67
5:F:101:PRO:HB3	8:J:382:ARG:HH12	1.60	0.67
9:K:142:PRO:HB3	13:O:41:MET:HG3	1.76	0.67
2:b:26:THR:HB	2:b:191:ASN:HD21	1.59	0.67
9:K:377:PHE:HB2	29:K:603:HEA:HMD2	1.76	0.67
13:O:118:VAL:HG11	14:P:203:ARG:HG2	1.76	0.67
1:a:169:PHE:HB2	1:a:175:SER:HB3	1.76	0.67
8:J:139:MET:SD	8:J:256:ASN:ND2	2.67	0.67
8:j:118:VAL:HG11	8:j:303:LEU:HD13	1.76	0.67
9:K:291:HIS:CE1	29:K:603:HEA:HBD1	2.30	0.67
1:A:169:PHE:HB2	1:A:175:SER:HB3	1.76	0.66
2:b:34:LYS:HG2	2:b:88:THR:HG23	1.76	0.66
14:P:215:GLY:H	14:P:238:ALA:HB3	1.60	0.66
1:A:230:LEU:HG	1:A:231:GLN:HG3	1.78	0.66
15:Q:106:ARG:NH2	21:W:76:SER:O	2.29	0.66
8:j:281:ILE:HG23	8:j:295:MET:HE1	1.78	0.66
2:B:59:THR:HG23	2:B:112:THR:HG21	1.76	0.66
14:P:190:ILE:HD13	14:P:236:ILE:HD13	1.77	0.66
10:l:76:TRP:HB2	10:l:79:ASN:HB2	1.77	0.66
7:H:34:GLN:HE22	10:L:297:THR:HG21	1.60	0.66
3:c:156:LEU:HD22	3:c:203:PRO:HD3	1.78	0.66
7:h:62:PRO:HB3	8:j:328:ILE:HD13	1.78	0.66
8:J:339:ILE:HD12	8:J:351:MET:HE3	1.78	0.65
29:K:603:HEA:HBA2	29:K:603:HEA:HMA	1.79	0.65
8:j:247:SER:HG	8:j:250:THR:HG1	1.43	0.65
2:B:30:THR:HG22	2:B:92:THR:HG22	1.77	0.65
3:C:59:MET:HE1	10:L:286:TRP:HE3	1.62	0.65
6:g:107:ILE:O	6:g:111:GLN:NE2	2.30	0.65
3:c:110:LYS:HA	3:c:115:PRO:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:180:ILE:HD13	26:l:401:HEM:HMA1	1.78	0.65
10:l:136:ASP:OD1	10:l:147:ARG:NH1	2.31	0.64
1:a:37:VAL:HB	1:a:207:VAL:HG22	1.79	0.64
14:P:36:ILE:HG22	14:P:103:LEU:HD21	1.79	0.64
2:B:324:LYS:O	2:B:328:GLN:HG2	1.97	0.64
9:K:374:VAL:HA	9:K:377:PHE:CE1	2.33	0.64
3:C:165:VAL:HB	8:j:142:TRP:HE1	1.63	0.63
5:F:75:ILE:HG23	8:J:212:ILE:HD12	1.79	0.63
13:O:99:VAL:HG13	13:O:256:ILE:HG21	1.79	0.63
8:J:241:ALA:HA	8:J:244:VAL:HG12	1.81	0.63
5:f:47:ASP:OD2	5:f:74:ARG:NH1	2.32	0.63
1:A:265:VAL:HG12	1:A:431:ILE:HG22	1.79	0.63
9:K:148:ILE:HG21	9:K:211:LEU:HB2	1.80	0.63
15:Q:100:ASP:O	15:Q:103:THR:OG1	2.16	0.63
1:a:368:SER:HB2	2:b:75:GLY:HA2	1.80	0.63
9:K:371:TYR:HB3	9:K:432:GLY:HA2	1.81	0.63
14:P:177:PHE:HE1	14:P:195:ILE:HG21	1.63	0.62
1:A:112:SER:HB2	1:A:115:LYS:HE2	1.81	0.62
9:K:381:LEU:HB3	29:K:602:HEA:HAC	1.80	0.62
8:j:310:ARG:O	8:j:375:ASN:ND2	2.33	0.62
2:B:298:SER:OG	2:B:302:LYS:NZ	2.32	0.62
8:J:29:TRP:HB3	8:J:99:LYS:HG3	1.81	0.62
5:f:20:VAL:HG13	5:f:21:LEU:HD12	1.80	0.62
2:B:62:ARG:NH1	2:B:67:LEU:O	2.32	0.62
1:A:312:CYS:HA	1:A:334:THR:HG22	1.82	0.62
8:j:148:THR:HG21	8:j:166:TRP:HE1	1.65	0.62
15:Q:132:ARG:HH22	15:Q:140:LYS:HE2	1.65	0.62
1:A:91:LEU:HD13	1:A:106:VAL:HG13	1.81	0.62
9:K:441:PRO:HD2	14:P:230:ALA:HB2	1.82	0.61
2:b:19:VAL:HG11	2:b:201:VAL:HG11	1.82	0.61
13:O:163:ASN:O	13:O:164:ARG:NH1	2.33	0.61
1:a:209:VAL:HG13	1:a:390:LEU:HD22	1.81	0.61
1:A:155:ASP:OD2	1:A:158:ASN:ND2	2.33	0.61
1:a:268:GLU:OE2	1:a:421:TRP:NE1	2.26	0.61
8:j:123:LEU:HD13	8:j:193:MET:HE1	1.83	0.61
14:P:166:SER:HB3	14:P:235:LYS:HE2	1.82	0.61
2:b:150:THR:HG22	2:b:352:ASN:HD22	1.66	0.61
8:J:111:VAL:O	8:J:115:ASN:ND2	2.33	0.61
9:K:399:GLN:NE2	9:K:515:GLU:O	2.34	0.61
14:P:187:ASP:OD2	14:P:222:SER:OG	2.19	0.61
8:j:21:PRO:O	8:j:218:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:67:HIS:ND1	8:j:71:ASP:OD2	2.34	0.61
8:j:287:ASP:HB2	8:j:290:LEU:HB2	1.83	0.61
7:H:6:GLY:HA2	8:j:1:MET:HE1	1.82	0.61
1:A:283:GLN:NE2	1:A:373:GLN:OE1	2.34	0.61
14:P:57:MET:HE1	16:R:18:ILE:HA	1.83	0.61
10:l:150:LYS:HD2	10:l:152:SER:H	1.66	0.61
8:J:287:ASP:HB3	8:J:290:LEU:HB3	1.81	0.61
26:J:403:HEM:HBC2	26:J:403:HEM:HHD	1.83	0.61
9:K:503:ILE:HG13	15:Q:70:GLN:HG3	1.82	0.61
1:A:268:GLU:OE2	1:A:421:TRP:NE1	2.31	0.60
9:K:268:PHE:HE1	14:P:75:ILE:HG22	1.66	0.60
14:P:39:LEU:HD13	14:P:103:LEU:HD22	1.82	0.60
3:c:146:ARG:HH11	3:c:155:MET:HE3	1.66	0.60
3:C:161:HIS:HB2	3:C:196:ALA:HB2	1.83	0.60
18:T:143:LEU:HD23	18:T:145:PRO:HD3	1.84	0.60
3:C:116:VAL:HG11	3:C:214:VAL:HG11	1.82	0.60
26:J:404:HEM:HHC	26:J:404:HEM:HBB2	1.82	0.60
9:K:11:ALA:O	9:K:81:ASN:ND2	2.35	0.60
10:l:63:THR:HG22	10:l:65:ALA:H	1.67	0.60
10:l:225:MET:HG2	26:l:401:HEM:C4C	2.36	0.60
1:A:288:TYR:OH	1:A:307:GLN:NE2	2.33	0.60
2:B:118:GLU:OE2	5:f:62:ARG:NH1	2.34	0.60
8:J:126:ALA:O	8:J:130:LEU:HG	2.02	0.60
8:J:290:LEU:HA	8:J:293:ILE:HG12	1.83	0.60
9:K:346:PHE:O	9:K:349:THR:OG1	2.17	0.60
9:K:368:HIS:CE1	14:P:196:LYS:HB3	2.36	0.60
1:a:166:SER:HA	1:a:175:SER:HB2	1.83	0.60
1:a:447:ARG:NH2	8:j:222:HIS:O	2.35	0.60
21:W:72:VAL:HA	21:W:75:ILE:HG12	1.83	0.60
2:b:21:ALA:HB2	2:b:197:LEU:HD13	1.84	0.59
8:j:123:LEU:HD22	8:j:190:ILE:HD11	1.85	0.59
8:j:123:LEU:HD21	8:j:186:VAL:HG22	1.84	0.59
14:P:149:PRO:HD2	14:P:152:LEU:HB2	1.84	0.59
9:K:244:VAL:CG1	29:K:603:HEA:HAC	2.32	0.59
1:a:451:ASP:HA	22:a:501:PEF:HN2	1.67	0.59
7:h:77:ASN:O	7:h:81:TYR:N	2.24	0.59
8:j:88:PHE:HB3	8:j:236:PHE:HZ	1.68	0.59
21:W:139:LYS:HG2	21:W:140:ASN:H	1.68	0.59
8:J:266:PRO:HD2	8:J:269:ILE:HD11	1.85	0.59
29:K:603:HEA:HHC	29:K:603:HEA:H122	1.84	0.59
2:b:226:GLY:N	2:b:352:ASN:OD1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:70:GLY:HA3	22:c:303:PEF:H142	1.84	0.59
1:A:300:ILE:HG12	1:A:301:LYS:H	1.68	0.58
23:A:502:PGT:H472	27:J:405:UQ6:H71	1.84	0.58
9:K:175:ASN:ND2	18:T:83:THR:O	2.36	0.58
15:Q:94:ALA:HA	15:Q:97:ARG:HD2	1.84	0.58
7:h:92:VAL:HG11	8:j:346:VAL:HG11	1.84	0.58
8:J:201:LEU:HD21	27:J:405:UQ6:H3M3	1.85	0.58
13:O:139:LEU:HA	13:O:142:THR:HG22	1.84	0.58
5:f:52:GLU:OE1	8:j:314:ARG:NH2	2.36	0.58
8:j:124:THR:HA	8:j:127:THR:HG22	1.84	0.58
9:K:430:PHE:HA	9:K:433:ILE:HG12	1.84	0.58
13:O:74:THR:HA	13:O:239:HIS:HE2	1.68	0.58
3:C:165:VAL:HB	8:j:142:TRP:NE1	2.18	0.58
9:K:85:PRO:HB3	9:K:168:THR:HG21	1.86	0.58
9:K:377:PHE:HA	9:K:380:VAL:HG22	1.86	0.58
2:B:38:GLY:H	2:B:41:TYR:HD2	1.50	0.58
2:b:222:LYS:NZ	2:b:223:PHE:O	2.36	0.58
4:e:44:ASN:HB3	4:e:47:LYS:HE2	1.85	0.58
13:O:226:ASN:O	13:O:230:MET:HG2	2.04	0.58
8:J:320:VAL:HA	8:J:323:LYS:HE2	1.86	0.58
8:j:349:VAL:HG13	8:j:350:LEU:HD12	1.86	0.57
10:l:133:GLU:N	10:l:133:GLU:OE1	2.36	0.57
2:b:230:ARG:HB3	2:b:359:VAL:HG21	1.85	0.57
13:O:67:ARG:HB2	13:O:229:ARG:HH21	1.69	0.57
1:a:447:ARG:HH21	8:j:220:PRO:HB2	1.69	0.57
8:j:172:SER:O	8:j:175:THR:OG1	2.20	0.57
2:B:230:ARG:NH2	2:B:363:PRO:O	2.37	0.57
3:c:161:HIS:HA	3:c:196:ALA:HB2	1.87	0.57
13:O:107:TRP:HA	13:O:110:PHE:HB3	1.87	0.57
3:c:166:PRO:HA	3:c:178:CYS:HA	1.85	0.57
14:P:200:THR:HB	14:P:203:ARG:HB2	1.87	0.57
7:h:43:ASN:OD1	7:h:47:ASN:ND2	2.38	0.57
14:P:155:GLU:HG3	21:W:131:LYS:HE2	1.85	0.57
3:C:143:ASP:H	3:C:190:ARG:HH21	1.53	0.57
9:K:134:SER:O	9:K:214:ARG:NH1	2.38	0.57
16:R:36:PHE:CE2	16:R:40:LYS:HD2	2.40	0.57
2:B:230:ARG:HH11	2:B:359:VAL:HG13	1.69	0.57
8:J:80:TYR:O	8:J:84:ASN:ND2	2.27	0.57
3:c:121:ARG:HG3	3:c:153:LEU:HB2	1.87	0.56
5:f:7:SER:O	5:f:11:ILE:HG13	2.04	0.56
8:J:127:THR:HA	8:J:130:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:310:MET:HG2	14:P:93:LEU:HD13	1.87	0.56
3:C:159:CYS:SG	3:C:161:HIS:HB3	2.46	0.56
5:F:43:LEU:HD21	5:F:78:ALA:HB2	1.88	0.56
8:J:13:VAL:HG13	8:J:17:ILE:HD13	1.87	0.56
8:J:57:ASN:O	8:J:61:ALA:N	2.38	0.56
8:J:121:PHE:HA	8:J:124:THR:HG22	1.87	0.56
21:W:83:ARG:HB2	21:W:83:ARG:NH1	2.20	0.56
2:b:63:SER:HB3	2:b:67:LEU:HD23	1.86	0.56
8:j:316:ASN:ND2	8:j:322:SER:OG	2.37	0.56
2:B:46:GLY:HA3	2:B:161:TYR:HB2	1.88	0.56
2:B:60:ASN:H	2:B:112:THR:HB	1.70	0.56
14:P:186:HIS:ND1	14:P:232:MET:HE1	2.21	0.56
15:Q:118:GLU:HB3	20:V:27:SER:HA	1.87	0.56
8:j:118:VAL:O	8:j:122:ILE:HG12	2.05	0.56
8:j:137:GLY:H	8:j:140:SER:HB3	1.71	0.56
1:A:37:VAL:HB	1:A:207:VAL:HG12	1.88	0.56
17:S:19:LYS:HD2	17:S:21:ALA:H	1.70	0.56
2:b:195:ALA:HB1	2:b:199:ARG:HH12	1.70	0.56
8:j:71:ASP:HA	10:l:113:ARG:HH21	1.71	0.56
6:G:101:CYS:HA	6:G:104:ARG:HG2	1.88	0.56
14:P:16:ASP:OD1	14:P:213:ARG:NH2	2.39	0.56
2:B:66:LYS:HA	5:f:120:LEU:HD22	1.88	0.56
1:A:311:LEU:HG	1:A:339:MET:HB3	1.88	0.56
8:J:273:TRP:HA	8:J:276:LEU:HD23	1.88	0.56
9:K:469:ILE:HA	9:K:472:LEU:HD12	1.87	0.56
3:c:178:CYS:HB3	24:c:301:FES:S1	2.42	0.56
4:e:48:LEU:HD23	4:e:49:TRP:N	2.17	0.56
5:f:88:LEU:HB2	5:f:93:TRP:HE1	1.70	0.56
2:B:206:LEU:HA	2:B:209:LEU:HD23	1.88	0.56
8:J:130:LEU:HD13	8:J:182:LEU:HD13	1.88	0.56
9:K:389:LEU:HD21	29:K:602:HEA:H253	1.87	0.56
18:T:57:PRO:HG2	18:T:62:GLN:HB3	1.88	0.56
3:c:109:VAL:O	3:c:116:VAL:N	2.36	0.55
6:G:129:HIS:CD2	10:L:69:LEU:HD23	2.39	0.55
14:P:174:HIS:HA	14:P:210:LEU:HB3	1.88	0.55
1:a:211:THR:HG21	1:a:386:ASP:HB3	1.87	0.55
2:B:52:ASN:ND2	2:B:82:LEU:HB2	2.18	0.55
3:C:86:ALA:HA	3:C:89:LEU:HD12	1.88	0.55
10:L:121:THR:HG23	10:L:122:ASN:H	1.70	0.55
4:e:55:ARG:HG2	4:e:56:ILE:HG13	1.88	0.55
8:j:88:PHE:HZ	8:j:243:PHE:HD2	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:315:GLY:O	8:J:319:LYS:NZ	2.40	0.55
13:O:215:HIS:HA	13:O:218:MET:HE3	1.89	0.55
22:c:303:PEF:H351	8:j:241:ALA:HB2	1.89	0.55
13:O:131:ALA:HB3	13:O:201:TYR:HD2	1.72	0.55
1:a:428:ASP:O	3:c:53:ARG:NH1	2.40	0.55
2:b:309:LYS:O	2:b:347:LYS:NZ	2.40	0.55
8:j:171:VAL:HA	8:j:175:THR:HG21	1.89	0.55
6:G:90:GLU:HA	6:G:93:ALA:HB2	1.88	0.54
1:a:362:GLU:HA	1:a:365:ARG:HG2	1.88	0.54
5:f:3:GLN:HB2	8:j:310:ARG:HB3	1.89	0.54
8:J:278:PHE:HA	8:J:281:ILE:HG22	1.89	0.54
14:P:53:LEU:O	14:P:57:MET:HG2	2.08	0.54
26:j:403:HEM:HHA	26:j:403:HEM:HBD1	1.88	0.54
4:E:55:ARG:HH21	4:E:56:ILE:HG22	1.72	0.54
13:O:243:TYR:HA	13:O:246:THR:HG22	1.89	0.54
14:P:93:LEU:HA	14:P:96:ILE:HG12	1.89	0.54
2:b:195:ALA:HB1	2:b:199:ARG:NH1	2.22	0.54
3:C:162:LEU:HD13	8:j:146:VAL:HG13	1.88	0.54
7:H:62:PRO:HB2	8:J:331:PHE:HD2	1.72	0.54
8:J:38:LEU:HD23	8:J:233:VAL:HG21	1.89	0.54
9:K:27:MET:HA	9:K:465:LEU:HD11	1.89	0.54
13:O:138:PRO:HG2	13:O:265:TYR:HE1	1.72	0.54
14:P:125:TYR:HE2	14:P:127:LYS:HZ1	1.55	0.54
6:g:132:HIS:HB3	10:l:69:LEU:HD21	1.88	0.54
9:K:19:PHE:CZ	29:K:602:HEA:H241	2.43	0.54
9:K:306:THR:HA	9:K:309:THR:HG22	1.88	0.54
2:b:256:LEU:HA	2:b:314:LEU:HD11	1.89	0.54
8:j:57:ASN:HB2	8:j:60:LEU:HB2	1.90	0.54
8:j:80:TYR:OH	10:l:182:LYS:NZ	2.39	0.54
10:l:225:MET:HG2	26:l:401:HEM:NC	2.23	0.54
9:K:19:PHE:HZ	29:K:602:HEA:H241	1.72	0.54
10:L:281:TYR:O	10:L:285:ILE:HG12	2.07	0.54
13:O:126:PRO:HG2	13:O:201:TYR:HE1	1.73	0.54
2:b:62:ARG:NH2	2:b:107:ASP:OD2	2.41	0.54
2:b:250:LEU:HD21	2:b:278:LYS:HE3	1.90	0.54
8:j:301:VAL:HA	8:j:304:VAL:HG12	1.90	0.54
9:K:34:LEU:HD22	9:K:462:THR:HG21	1.90	0.54
2:B:358:ASP:OD2	2:B:361:ASN:ND2	2.40	0.54
9:K:380:VAL:HB	29:K:603:HEA:HBC1	1.90	0.54
10:L:92:ARG:HB3	10:L:236:TYR:HE2	1.72	0.54
10:L:103:ALA:HA	10:L:158:PRO:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:120:ILE:HD12	14:P:180:THR:HG23	1.90	0.54
8:j:160:ASP:OD1	8:j:164:TRP:NE1	2.41	0.54
1:A:30:THR:O	1:A:31:GLN:NE2	2.41	0.54
9:K:241:HIS:HB3	9:K:242:PRO:HD3	1.90	0.54
5:f:95:LYS:HE3	5:f:96:ALA:H	1.72	0.54
9:K:413:GLN:HE22	9:K:467:LEU:HB3	1.73	0.54
9:K:498:VAL:HG23	9:K:499:GLU:HG2	1.89	0.54
10:L:184:ARG:NH1	26:L:401:HEM:O2A	2.41	0.53
3:c:166:PRO:HA	3:c:179:PRO:HD3	1.89	0.53
1:A:209:VAL:HG21	1:A:387:ALA:HB1	1.90	0.53
14:P:30:THR:HG23	14:P:33:GLN:H	1.73	0.53
2:B:63:SER:HB2	2:B:66:LYS:HG2	1.90	0.53
8:J:344:VAL:H	3:c:182:GLY:HA3	1.72	0.53
2:b:146:LEU:HD21	2:b:242:GLY:HA3	1.89	0.53
5:f:3:GLN:HE22	5:f:8:ILE:HG12	1.73	0.53
8:J:183:HIS:NE2	26:J:403:HEM:NC	2.55	0.53
9:K:403:LEU:HD12	9:K:479:GLY:HA3	1.90	0.53
11:M:47:THR:HG23	11:M:51:LEU:HB3	1.90	0.53
2:B:65:LEU:HD13	5:f:117:LYS:HZ2	1.73	0.53
9:K:324:LEU:HD21	14:P:57:MET:HB3	1.89	0.53
17:S:94:ARG:NH2	19:U:74:GLY:O	2.42	0.53
1:a:150:ASP:OD2	1:a:154:ASN:ND2	2.42	0.53
8:j:70:ARG:NH2	10:l:258:CYS:O	2.41	0.53
8:j:197:HIS:CE1	26:j:404:HEM:NA	2.77	0.53
2:B:232:ARG:NH2	2:b:162:ASP:OD2	2.41	0.53
5:F:29:ALA:O	5:F:33:ILE:HG12	2.09	0.53
6:g:106:LYS:NZ	6:g:122:ASP:OD1	2.42	0.53
3:C:45:GLU:HB3	23:C:302:PGT:H62	1.91	0.53
9:K:330:GLY:O	14:P:68:ASN:ND2	2.40	0.53
14:P:190:ILE:HD12	14:P:195:ILE:HD11	1.91	0.53
15:Q:60:PHE:CE1	15:Q:72:VAL:HG21	2.44	0.53
26:j:403:HEM:HBC2	26:j:403:HEM:HHD	1.89	0.53
2:B:70:GLU:OE2	2:B:100:TYR:OH	2.24	0.53
5:F:55:ILE:HD11	5:F:110:ALA:HB1	1.91	0.53
8:J:35:LEU:HD11	8:J:236:PHE:CD2	2.44	0.53
9:K:202:VAL:HG12	9:K:235:LEU:HG	1.89	0.53
2:b:313:ASP:OD1	2:b:314:LEU:N	2.41	0.53
23:A:502:PGT:H62	8:J:4:ARG:HH22	1.73	0.53
22:H:101:PEF:N	21:W:89:LYS:O	2.41	0.53
8:J:40:LEU:O	8:J:44:ILE:HG12	2.09	0.53
8:j:16:TYR:O	27:j:405:UQ6:O2	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:J:404:HEM:HHC	26:J:404:HEM:CBB	2.38	0.53
14:P:158:LEU:H	14:P:162:ASP:HB2	1.73	0.53
10:I:176:ASP:N	10:I:176:ASP:OD1	2.41	0.53
9:K:148:ILE:HA	9:K:151:LEU:HD12	1.91	0.52
10:L:119:SER:O	10:L:120:HIS:ND1	2.41	0.52
18:T:100:ILE:HG21	18:T:107:ARG:HD2	1.90	0.52
8:j:147:ILE:HA	8:j:150:LEU:HD23	1.89	0.52
2:B:366:ASP:OD2	2:b:152:ARG:NH2	2.31	0.52
13:O:84:ARG:HD3	13:O:239:HIS:HA	1.91	0.52
8:j:29:TRP:HB3	8:j:99:LYS:HG3	1.90	0.52
26:J:404:HEM:HBD1	26:J:404:HEM:CHA	2.40	0.52
9:K:374:VAL:HB	9:K:438:ARG:HH11	1.75	0.52
21:W:78:GLY:HA3	21:W:83:ARG:HH11	1.73	0.52
8:j:26:ILE:HG23	8:j:30:TRP:HB2	1.90	0.52
1:A:66:ASN:ND2	1:A:192:ASP:OD1	2.42	0.52
15:Q:96:ARG:HE	15:Q:104:ALA:HB2	1.74	0.52
3:c:177:PHE:CZ	3:c:182:GLY:HA2	2.44	0.52
5:f:16:LEU:HD21	8:j:380:ILE:HG13	1.90	0.52
10:l:235:GLU:H	10:l:241:PRO:HG2	1.75	0.52
5:F:3:GLN:HB2	8:J:310:ARG:HB2	1.90	0.52
12:N:22:ARG:NH2	13:O:72:GLU:OE2	2.43	0.52
19:U:41:LYS:HE2	19:U:44:ASP:H	1.74	0.52
1:A:375:GLY:O	1:A:379:GLU:HB2	2.10	0.52
8:J:285:ILE:O	3:c:195:PRO:HB3	2.10	0.52
10:l:101:CYS:HB3	26:l:401:HEM:CAB	2.39	0.52
13:O:6:ARG:HA	13:O:9:HIS:CE1	2.45	0.52
14:P:70:ILE:HD11	15:Q:78:SER:HA	1.91	0.52
15:Q:62:GLU:OE2	18:T:93:THR:OG1	2.28	0.52
5:f:3:GLN:NE2	5:f:7:SER:OG	2.43	0.52
10:l:180:ILE:CD1	26:l:401:HEM:HAA2	2.39	0.52
3:C:85:THR:OG1	3:C:87:ASP:OD1	2.26	0.52
3:C:106:ASN:OD1	3:C:119:ARG:NH1	2.37	0.52
8:J:249:ASN:O	10:L:182:LYS:NZ	2.38	0.52
9:K:40:LEU:O	9:K:443:TYR:OH	2.26	0.52
9:K:72:MET:O	9:K:76:ILE:HG12	2.10	0.52
9:K:218:THR:HA	13:O:200:VAL:HG11	1.91	0.52
13:O:212:HIS:HB3	13:O:257:TRP:HH2	1.75	0.52
15:Q:137:VAL:HG12	15:Q:139:LEU:HD23	1.90	0.52
1:A:61:ASN:ND2	1:A:235:LYS:HD2	2.25	0.51
12:N:38:ALA:HB1	13:O:28:PHE:HE2	1.75	0.51
14:P:81:ILE:HG22	14:P:85:TRP:CZ3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:225:CYS:H	14:P:229:HIS:HB2	1.75	0.51
17:S:66:THR:HA	17:S:69:ASN:HD21	1.76	0.51
5:f:87:LEU:HD23	7:h:50:ARG:HD2	1.92	0.51
8:J:203:ILE:HG13	8:j:8:VAL:HG11	1.92	0.51
1:a:323:LYS:NZ	1:a:324:ASP:OD1	2.41	0.51
4:e:40:TYR:CE1	10:l:268:ARG:HB3	2.46	0.51
2:B:117:HIS:HB3	5:f:62:ARG:HB3	1.93	0.51
1:A:444:ASP:OD1	1:A:445:TYR:N	2.40	0.51
2:B:265:SER:O	2:B:268:SER:OG	2.24	0.51
9:K:192:THR:HG23	9:K:246:ILE:HA	1.92	0.51
10:L:175:PRO:HB2	10:L:180:ILE:HD11	1.93	0.51
10:l:218:PHE:HD1	10:l:219:PRO:HD2	1.75	0.51
5:F:3:GLN:HG3	8:J:310:ARG:HD3	1.92	0.51
8:J:249:ASN:HB2	10:L:182:LYS:HE2	1.91	0.51
3:c:115:PRO:HG2	3:c:157:GLY:HA3	1.92	0.51
10:l:225:MET:SD	26:l:401:HEM:C4D	3.04	0.51
15:Q:83:PRO:HB2	15:Q:88:ILE:HG13	1.91	0.51
1:a:125:ILE:HG13	1:a:126:GLN:H	1.76	0.51
8:j:58:ILE:HG22	8:j:176:ILE:HD12	1.93	0.51
1:A:71:ASN:ND2	1:A:178:THR:O	2.29	0.51
1:A:113:THR:HG21	1:A:214:ILE:HG21	1.92	0.51
8:J:46:THR:HG23	8:J:82:HIS:CE1	2.45	0.51
9:K:36:ILE:HD11	9:K:58:LEU:HB2	1.93	0.51
9:K:359:ALA:HB2	29:K:603:HEA:HMB3	1.92	0.51
9:K:9:THR:HA	9:K:96:PRO:HB3	1.93	0.51
9:K:11:ALA:HB1	9:K:81:ASN:HB2	1.92	0.51
9:K:230:ILE:HD11	14:P:203:ARG:HD2	1.93	0.51
14:P:147:VAL:HG11	14:P:231:ASN:HB2	1.92	0.51
1:A:189:VAL:HG23	1:A:190:VAL:H	1.76	0.51
3:C:59:MET:HE1	10:L:286:TRP:CE3	2.43	0.51
9:K:228:ASP:OD2	9:K:228:ASP:N	2.44	0.51
9:K:363:LEU:HD11	14:P:43:ILE:HD12	1.93	0.51
14:P:116:THR:HG22	14:P:176:ARG:HB2	1.93	0.51
1:A:252:ARG:HH21	7:H:21:GLN:HE21	1.59	0.51
3:C:176:TRP:HB2	3:C:185:TYR:HB2	1.93	0.51
8:J:117:GLY:O	26:J:404:HEM:HMC2	2.10	0.51
8:J:142:TRP:HZ2	3:c:165:VAL:HB	1.76	0.51
8:j:285:ILE:HD12	8:j:290:LEU:HB3	1.93	0.51
9:K:4:ARG:HD2	11:M:31:LYS:HE3	1.93	0.50
5:f:101:PRO:HB3	8:j:382:ARG:HH21	1.76	0.50
8:j:271:PRO:HB3	8:j:275:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:44:ILE:O	8:J:48:ILE:HG12	2.12	0.50
8:J:170:SER:HB3	3:c:112:GLN:NE2	2.26	0.50
9:K:17:LEU:HD21	9:K:103:PHE:CE2	2.47	0.50
9:K:409:LEU:HD23	9:K:412:ILE:HD11	1.93	0.50
15:Q:83:PRO:HD3	15:Q:114:LYS:HE2	1.94	0.50
18:T:98:ILE:HG12	18:T:141:TYR:CE1	2.46	0.50
1:a:297:LEU:HB3	2:b:65:LEU:HD13	1.94	0.50
8:J:146:VAL:HG13	3:c:162:LEU:HB3	1.93	0.50
11:M:32:ASP:OD1	11:M:32:ASP:N	2.44	0.50
10:l:200:ASP:OD1	10:l:200:ASP:N	2.44	0.50
8:J:378:PHE:O	8:J:382:ARG:HG3	2.12	0.50
23:a:502:PGT:H221	23:a:502:PGT:H432	1.92	0.50
3:c:87:ASP:OD1	3:c:88:VAL:N	2.45	0.50
8:j:201:LEU:CD1	26:j:404:HEM:HAA1	2.41	0.50
2:B:202:ASP:OD1	2:B:203:GLU:N	2.44	0.50
5:F:71:ARG:O	5:F:75:ILE:HG12	2.11	0.50
9:K:63:ALA:HB2	29:K:602:HEA:HBD2	1.94	0.50
9:K:517:LEU:HD13	18:T:123:TRP:HZ2	1.76	0.50
14:P:147:VAL:HG21	14:P:231:ASN:HB2	1.94	0.50
8:j:58:ILE:HG21	8:j:173:ASN:HA	1.93	0.50
8:j:290:LEU:HA	8:j:293:ILE:HG12	1.93	0.50
1:A:57:SER:HB3	1:A:200:HIS:HD2	1.76	0.50
1:A:375:GLY:HA3	2:B:28:ILE:HG13	1.93	0.50
6:G:114:TYR:HE2	6:G:117:LEU:HD13	1.76	0.50
9:K:264:LYS:HE2	9:K:493:LYS:HD2	1.93	0.50
10:L:93:GLY:HA2	10:L:96:VAL:HG12	1.94	0.50
13:O:72:GLU:HB3	13:O:76:LEU:HD13	1.94	0.50
15:Q:88:ILE:HG21	15:Q:111:LEU:HD21	1.94	0.50
8:j:93:MET:HG3	26:j:404:HEM:HBB2	1.93	0.50
1:A:363:VAL:HG21	1:A:415:VAL:HG12	1.92	0.50
8:J:35:LEU:HD21	8:J:236:PHE:HB2	1.94	0.50
13:O:213:PHE:O	13:O:217:VAL:HG23	2.12	0.50
15:Q:109:GLU:OE1	15:Q:140:LYS:NZ	2.44	0.50
10:l:126:ARG:HH12	10:l:151:LEU:HA	1.76	0.50
3:C:159:CYS:HB3	3:C:163:GLY:H	1.75	0.50
6:G:139:ALA:O	6:G:141:ARG:N	2.41	0.50
8:J:62:PHE:HA	8:J:65:VAL:HG12	1.93	0.50
9:K:120:GLU:HA	11:M:71:GLN:HE21	1.76	0.50
14:P:126:TRP:CE2	14:P:232:MET:HE2	2.47	0.50
14:P:186:HIS:CG	14:P:232:MET:HE1	2.46	0.50
21:W:137:LYS:HD2	21:W:146:GLY:HA3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ILE:HG13	1:A:126:GLN:HG3	1.94	0.49
1:A:247:SER:HA	7:H:29:VAL:HA	1.93	0.49
9:K:339:LEU:HD13	9:K:414:PHE:CG	2.47	0.49
14:P:16:ASP:HA	14:P:217:PHE:HD1	1.76	0.49
3:c:159:CYS:SG	3:c:161:HIS:HB3	2.52	0.49
7:h:37:LEU:HD12	7:h:40:ILE:HB	1.93	0.49
10:l:223:ILE:HG22	10:l:225:MET:H	1.76	0.49
2:B:83:ASP:OD1	2:B:84:ARG:N	2.41	0.49
9:K:140:SER:OG	9:K:141:GLY:N	2.45	0.49
10:L:147:ARG:NH1	10:L:148:PRO:O	2.45	0.49
18:T:90:ARG:HG3	18:T:92:GLY:H	1.77	0.49
8:j:14:ASN:HA	8:j:18:ILE:HB	1.94	0.49
7:H:39:GLY:O	7:H:43:ASN:ND2	2.46	0.49
9:K:262:TYR:HB3	9:K:338:MET:CE	2.42	0.49
13:O:164:ARG:NE	18:T:54:GLY:O	2.39	0.49
13:O:222:MET:HA	13:O:225:VAL:HG12	1.92	0.49
15:Q:105:ILE:HG12	15:Q:139:LEU:HD22	1.94	0.49
19:U:28:TRP:HE1	19:U:63:TRP:HZ3	1.60	0.49
8:J:118:VAL:HG11	8:J:303:LEU:HG	1.94	0.49
15:Q:128:LEU:HA	15:Q:131:VAL:HG22	1.93	0.49
17:S:103:SER:OG	17:S:104:LYS:N	2.44	0.49
2:b:30:THR:HG22	2:b:92:THR:HG22	1.94	0.49
4:e:10:PHE:HA	4:e:13:ARG:HH22	1.77	0.49
7:h:53:LYS:HA	7:h:56:PHE:CE1	2.47	0.49
8:j:128:ALA:HB2	26:j:403:HEM:HMB1	1.93	0.49
8:j:324:PHE:O	8:j:328:ILE:HG12	2.12	0.49
22:j:406:PEF:H312	22:j:406:PEF:H141	1.93	0.49
2:B:65:LEU:HD22	5:f:117:LYS:HZ3	1.77	0.49
7:H:41:PHE:HZ	22:H:101:PEF:H392	1.77	0.49
8:J:107:ARG:NH2	8:J:311:SER:O	2.40	0.49
9:K:280:ILE:HD11	9:K:315:PRO:HB2	1.93	0.49
9:K:291:HIS:ND1	29:K:603:HEA:O1D	2.45	0.49
9:K:308:ALA:HA	9:K:311:ILE:HG22	1.95	0.49
10:L:212:SER:OG	10:L:222:SER:OG	2.24	0.49
14:P:163:THR:HG22	14:P:164:ASP:H	1.77	0.49
1:a:97:ILE:HG13	1:a:102:GLN:HA	1.95	0.49
2:b:247:LYS:HD2	2:b:336:ILE:HD11	1.94	0.49
1:A:443:LEU:HD13	1:A:447:ARG:HG3	1.94	0.49
3:C:74:THR:O	3:C:78:PHE:HD1	1.95	0.49
8:J:245:PHE:O	10:L:266:ARG:NE	2.45	0.49
8:J:354:ILE:O	8:J:358:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:181:THR:HG22	3:c:34:TYR:HD2	1.77	0.49
2:b:251:ALA:HB2	2:b:338:LEU:HB3	1.95	0.49
5:f:50:ALA:O	5:f:56:MET:HG3	2.12	0.49
14:P:180:THR:HB	14:P:204:LEU:HD12	1.93	0.49
7:h:50:ARG:HH12	7:h:51:ARG:HE	1.60	0.49
8:j:241:ALA:HA	8:j:244:VAL:HG22	1.95	0.49
5:F:62:ARG:NH1	2:b:118:GLU:OE2	2.45	0.49
9:K:296:GLY:O	19:U:22:ASN:ND2	2.46	0.49
1:a:297:LEU:HD22	2:b:65:LEU:HD22	1.95	0.49
3:c:195:PRO:O	3:c:197:PRO:HD3	2.12	0.49
2:B:188:SER:OG	2:B:189:GLY:N	2.44	0.49
5:F:41:LEU:HB3	5:F:43:LEU:HD23	1.94	0.49
7:H:62:PRO:HA	7:H:65:ILE:HG22	1.93	0.49
9:K:294:ILE:HG13	9:K:368:HIS:CD2	2.48	0.49
8:j:117:GLY:C	26:j:404:HEM:HBC2	2.38	0.49
10:l:260:GLU:HB2	10:l:262:GLU:HG3	1.95	0.49
1:A:73:TRP:CZ2	1:A:197:ALA:HB2	2.48	0.49
2:B:54:PHE:HD1	2:B:123:VAL:HG11	1.77	0.49
9:K:19:PHE:CZ	29:K:602:HEA:H251	2.48	0.49
9:K:500:SER:HA	15:Q:106:ARG:NH2	2.28	0.49
10:l:120:HIS:HB3	10:l:124:GLU:HG3	1.95	0.49
5:F:88:LEU:HD23	5:F:92:GLU:HB3	1.95	0.48
8:J:377:LEU:HA	8:J:380:ILE:HG22	1.94	0.48
14:P:153:LEU:HD21	21:W:124:MET:HE3	1.93	0.48
21:W:78:GLY:HA3	21:W:83:ARG:HD2	1.96	0.48
1:a:443:LEU:HD13	1:a:447:ARG:HB3	1.95	0.48
2:b:69:ARG:O	2:b:72:GLU:HG3	2.13	0.48
10:l:107:LEU:HG	10:l:177:LEU:HB2	1.95	0.48
1:A:149:GLN:O	1:A:153:GLU:HG3	2.12	0.48
3:C:164:CYS:HB2	8:j:142:TRP:HD1	1.78	0.48
7:H:36:PRO:HG2	10:L:286:TRP:CZ2	2.48	0.48
8:J:343:HIS:HB3	3:c:182:GLY:HA3	1.95	0.48
9:K:500:SER:N	15:Q:70:GLN:OE1	2.44	0.48
9:K:533:GLN:HG3	18:T:121:ILE:HD13	1.94	0.48
23:a:502:PGT:O1P	8:j:4:ARG:NH1	2.46	0.48
5:f:47:ASP:OD1	5:f:71:ARG:NE	2.46	0.48
1:A:239:LYS:HG2	21:W:42:PRO:HB3	1.94	0.48
6:G:95:VAL:HB	6:G:127:PHE:HE1	1.77	0.48
14:P:97:ALA:O	14:P:101:PHE:N	2.38	0.48
14:P:171:VAL:HA	14:P:211:ILE:HG23	1.95	0.48
19:U:33:ASP:N	19:U:33:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:280:ALA:HB2	8:j:340:GLY:HA3	1.94	0.48
10:l:193:SER:HA	10:l:196:THR:HG22	1.94	0.48
8:J:141:HIS:NE2	8:J:171:VAL:HG21	2.29	0.48
9:K:225:GLY:HA2	17:S:98:PHE:HE1	1.77	0.48
1:a:265:VAL:HG22	1:a:431:ILE:HG22	1.95	0.48
8:j:139:MET:HB3	8:j:269:ILE:HD12	1.95	0.48
1:A:34:ASN:HB3	1:A:223:ILE:HD12	1.95	0.48
1:A:224:GLU:HB2	1:A:227:ASN:HB2	1.96	0.48
5:F:47:ASP:OD2	5:F:102:TYR:OH	2.30	0.48
9:K:330:GLY:HA2	14:P:71:ALA:HA	1.95	0.48
13:O:143:ILE:HG12	17:S:67:ALA:HB2	1.96	0.48
16:R:6:ILE:HG22	16:R:7:THR:N	2.27	0.48
2:b:55:ASN:HD21	2:b:89:LEU:HD11	1.78	0.48
3:c:161:HIS:CD2	3:c:195:PRO:HD2	2.49	0.48
7:h:61:ILE:O	7:h:65:ILE:HG23	2.13	0.48
9:K:24:PHE:HA	9:K:27:MET:HE2	1.94	0.48
1:a:356:ILE:HD12	1:a:457:TRP:CZ3	2.48	0.48
8:j:330:VAL:HG21	22:j:401:PEF:H361	1.95	0.48
2:B:40:ARG:HG3	2:B:155:LEU:HA	1.94	0.48
3:C:56:ALA:O	3:C:60:VAL:HG23	2.14	0.48
3:C:146:ARG:HB3	3:C:202:ILE:HG13	1.96	0.48
8:J:124:THR:HA	8:J:127:THR:HG22	1.95	0.48
1:a:430:ASP:OD1	1:a:430:ASP:N	2.46	0.48
5:f:13:ASP:OD1	5:f:17:LYS:NZ	2.46	0.48
8:j:43:GLN:OE1	8:j:82:HIS:ND1	2.46	0.48
1:A:252:ARG:HH21	7:H:21:GLN:NE2	2.11	0.48
5:F:69:TYR:OH	7:H:22:LYS:NZ	2.46	0.48
8:J:282:LEU:HB2	8:J:295:MET:HE3	1.96	0.48
10:L:173:LEU:HD23	10:L:173:LEU:H	1.78	0.48
3:c:133:ASP:OD1	3:c:133:ASP:N	2.44	0.48
3:C:162:LEU:HD12	3:C:181:HIS:CE1	2.49	0.48
5:F:27:PRO:HA	5:F:30:ASN:HD21	1.79	0.48
9:K:534:SER:HB3	18:T:88:SER:HB3	1.96	0.48
13:O:208:GLY:O	13:O:212:HIS:ND1	2.47	0.48
2:B:270:LEU:HD23	2:B:270:LEU:H	1.77	0.47
3:C:74:THR:O	3:C:77:THR:OG1	2.24	0.47
8:J:327:PHE:HA	8:J:330:VAL:HG12	1.96	0.47
9:K:496:ASP:HB3	9:K:498:VAL:HG22	1.96	0.47
10:L:177:LEU:HA	10:L:180:ILE:HG12	1.96	0.47
13:O:235:LEU:HD11	13:O:241:VAL:H	1.79	0.47
21:W:109:LEU:HA	21:W:112:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:47:LYS:HG3	10:l:86:ASP:HA	1.95	0.47
1:A:170:GLN:HB2	1:A:245:LEU:HD21	1.95	0.47
9:K:509:VAL:HG12	18:T:123:TRP:HH2	1.79	0.47
10:L:243:THR:HG23	10:L:246:GLN:HG2	1.95	0.47
13:O:10:GLN:HG2	18:T:80:VAL:HB	1.96	0.47
18:T:34:ALA:HB1	18:T:68:ARG:HH22	1.79	0.47
1:a:189:VAL:HG23	1:a:190:VAL:H	1.78	0.47
3:C:126:ILE:O	3:C:130:ASN:ND2	2.47	0.47
6:G:124:VAL:HG21	10:L:204:ALA:HB3	1.96	0.47
8:J:227:PHE:HD1	10:L:291:LYS:HD2	1.79	0.47
29:K:602:HEA:H271	29:K:602:HEA:H212	1.69	0.47
13:O:71:ALA:O	13:O:75:TYR:HB3	2.14	0.47
14:P:177:PHE:O	14:P:206:GLN:HA	2.15	0.47
15:Q:60:PHE:HE1	15:Q:72:VAL:HG21	1.79	0.47
1:A:341:ASP:OD1	23:A:502:PGT:O5	2.32	0.47
8:J:91:MET:O	8:J:95:MET:HG3	2.14	0.47
15:Q:93:ARG:HD2	15:Q:94:ALA:N	2.29	0.47
21:W:41:MET:HE2	21:W:46:GLN:HG3	1.95	0.47
1:a:444:ASP:OD1	1:a:445:TYR:N	2.42	0.47
3:C:79:ILE:O	3:C:83:THR:HG23	2.14	0.47
9:K:307:SER:HA	9:K:310:MET:SD	2.55	0.47
9:K:408:LYS:HD2	21:W:94:PHE:HD2	1.80	0.47
13:O:156:HIS:ND1	13:O:246:THR:O	2.47	0.47
2:b:150:THR:HG22	2:b:352:ASN:ND2	2.28	0.47
3:c:126:ILE:O	3:c:130:ASN:ND2	2.46	0.47
8:j:201:LEU:HD11	26:j:404:HEM:HAA1	1.97	0.47
10:l:126:ARG:HH22	10:l:151:LEU:N	2.12	0.47
10:l:175:PRO:HG2	26:l:401:HEM:HAA1	1.95	0.47
1:A:105:ILE:HG21	1:A:384:VAL:HG12	1.96	0.47
9:K:10:ASN:HB3	9:K:524:VAL:HG12	1.95	0.47
13:O:89:LEU:O	13:O:93:MET:HG2	2.15	0.47
5:f:63:LEU:HD12	5:f:64:PRO:HD2	1.97	0.47
8:j:122:ILE:HD12	8:j:299:ILE:HD12	1.97	0.47
1:A:301:LYS:HB2	1:A:350:GLN:NE2	2.30	0.47
2:B:255:VAL:HG11	2:B:343:VAL:HG11	1.96	0.47
3:C:33:THR:HG23	7:H:25:THR:HG21	1.96	0.47
22:C:303:PEF:H432	22:C:303:PEF:H371	1.96	0.47
8:J:57:ASN:OD1	8:J:177:GLN:NE2	2.47	0.47
8:J:285:ILE:HG13	8:J:294:THR:HG21	1.96	0.47
9:K:39:GLU:HG3	9:K:48:LEU:HD12	1.96	0.47
13:O:254:ASP:OD1	13:O:255:VAL:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:457:TRP:HD1	4:e:14:ASN:HB2	1.80	0.47
10:l:82:PHE:CE2	10:l:271:LEU:HD11	2.50	0.47
8:j:339:ILE:HD11	8:j:348:TYR:CD1	2.49	0.47
22:j:406:PEF:H111	22:j:406:PEF:H142	1.70	0.47
2:B:66:LYS:HG3	2:B:67:LEU:HG	1.96	0.47
3:C:183:SER:OG	24:C:301:FES:S1	2.65	0.47
29:K:603:HEA:H211	29:K:603:HEA:H271	1.80	0.47
14:P:115:MET:SD	14:P:175:ILE:HG22	2.55	0.47
21:W:126:LYS:HG3	21:W:150:VAL:HG11	1.96	0.47
3:C:96:VAL:HG22	3:C:109:VAL:HG11	1.96	0.47
5:F:63:LEU:HD11	5:F:103:LEU:HD12	1.97	0.47
9:K:340:TYR:CE1	9:K:414:PHE:HB2	2.50	0.47
9:K:440:ILE:HG23	14:P:230:ALA:HB1	1.96	0.47
13:O:136:GLU:HB3	17:S:74:GLU:HG2	1.95	0.47
8:j:50:MET:HE1	8:j:68:ILE:HG21	1.96	0.47
2:B:353:TYR:HB3	2:B:365:LEU:HD12	1.95	0.46
3:C:181:HIS:CD2	8:j:282:LEU:HD22	2.50	0.46
8:J:60:LEU:O	8:J:64:SER:N	2.38	0.46
9:K:129:VAL:HG23	9:K:232:TYR:HE2	1.80	0.46
14:P:217:PHE:HD2	14:P:236:ILE:HD11	1.80	0.46
21:W:79:GLU:O	21:W:84:ARG:NH1	2.47	0.46
1:a:353:ARG:HA	1:a:356:ILE:HG22	1.97	0.46
6:g:82:ARG:HH12	6:g:139:ALA:HB2	1.80	0.46
6:g:107:ILE:C	6:g:111:GLN:HE22	2.23	0.46
1:A:158:ASN:O	1:A:162:GLU:HG2	2.15	0.46
1:A:447:ARG:NH2	8:J:18:ILE:O	2.49	0.46
2:B:225:LEU:HA	2:B:352:ASN:HD21	1.79	0.46
5:F:95:LYS:HB2	5:F:98:GLU:HG2	1.96	0.46
6:G:145:LYS:O	6:G:147:LYS:NZ	2.35	0.46
8:J:80:TYR:HB3	8:J:244:VAL:HG23	1.97	0.46
9:K:2:VAL:HG22	9:K:6:LEU:HG	1.97	0.46
9:K:397:SER:OG	9:K:398:PRO:HD3	2.15	0.46
13:O:106:PHE:HA	13:O:109:TYR:CZ	2.50	0.46
18:T:66:LEU:HD23	18:T:66:LEU:H	1.80	0.46
7:h:30:SER:O	7:h:32:TYR:N	2.48	0.46
27:j:405:UQ6:H272	27:j:405:UQ6:H311	1.69	0.46
3:C:159:CYS:HB2	3:C:164:CYS:O	2.16	0.46
4:E:26:PHE:O	4:E:29:GLN:HG2	2.14	0.46
9:K:521:PRO:O	11:M:33:GLY:HA3	2.15	0.46
3:c:162:LEU:HG	3:c:181:HIS:HE1	1.79	0.46
25:c:302:PCF:H461	25:c:302:PCF:H282	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:327:PHE:HA	8:j:330:VAL:HG12	1.96	0.46
6:G:121:GLU:HB3	7:H:86:ARG:HH11	1.81	0.46
8:J:58:ILE:HD12	8:J:58:ILE:H	1.80	0.46
2:b:270:LEU:HG	2:b:304:ILE:HD11	1.98	0.46
3:c:85:THR:OG1	3:c:86:ALA:N	2.47	0.46
7:h:76:TYR:HD2	8:j:347:PRO:HG3	1.81	0.46
8:j:129:PHE:HE2	8:j:147:ILE:HB	1.80	0.46
1:A:431:ILE:HG21	1:A:452:MET:HE1	1.97	0.46
7:H:62:PRO:HB2	8:J:331:PHE:CD2	2.50	0.46
8:J:36:LEU:HG	8:J:92:VAL:HG13	1.96	0.46
9:K:374:VAL:HA	9:K:377:PHE:CD1	2.50	0.46
9:K:386:ILE:HG21	29:K:602:HEA:H262	1.96	0.46
1:a:344:ILE:HG21	1:a:448:ILE:HG13	1.98	0.46
3:C:158:ILE:HG13	3:C:163:GLY:HA2	1.97	0.46
9:K:368:HIS:NE2	14:P:196:LYS:O	2.44	0.46
9:K:409:LEU:HD13	9:K:471:ILE:HG12	1.96	0.46
10:l:262:GLU:OE1	10:l:266:ARG:HB3	2.16	0.46
1:A:121:ASN:O	1:A:125:ILE:HG12	2.16	0.46
9:K:408:LYS:HA	21:W:95:ILE:HD11	1.97	0.46
10:L:76:TRP:H	10:L:79:ASN:HD21	1.64	0.46
12:N:31:TYR:HB3	12:N:32:PRO:HD3	1.98	0.46
1:A:356:ILE:HD12	1:A:457:TRP:NE1	2.30	0.46
27:J:405:UQ6:H172	27:J:405:UQ6:H151	1.60	0.46
9:K:442:ASP:OD1	9:K:442:ASP:N	2.46	0.46
13:O:140:LEU:O	13:O:144:ILE:HG12	2.16	0.46
2:b:104:ALA:O	2:b:108:VAL:HG23	2.15	0.46
10:l:264:ASP:OD1	10:l:264:ASP:N	2.49	0.46
2:B:33:VAL:HG23	2:B:187:VAL:HG22	1.97	0.46
2:B:255:VAL:HA	2:B:321:THR:HG21	1.98	0.46
10:L:284:SER:HA	10:L:287:VAL:HG12	1.98	0.46
8:j:273:TRP:HA	8:j:276:LEU:HD23	1.98	0.46
10:l:122:ASN:O	10:l:126:ARG:HG2	2.15	0.46
2:B:270:LEU:HD12	2:B:300:ASN:HB3	1.98	0.46
3:C:79:ILE:O	3:C:83:THR:N	2.49	0.46
3:C:119:ARG:HE	3:C:187:ILE:HD11	1.81	0.46
5:F:51:GLU:HG3	5:F:71:ARG:HH21	1.81	0.46
10:L:105:HIS:CE1	26:L:401:HEM:NA	2.82	0.46
1:a:341:ASP:OD1	1:a:342:ASP:N	2.48	0.46
6:g:94:LEU:HD12	6:g:98:TYR:CE2	2.51	0.46
8:j:257:TYR:HB3	10:l:179:LEU:HD23	1.97	0.46
10:l:97:TYR:CZ	10:l:107:LEU:HD12	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:164:CYS:HB2	8:j:142:TRP:CD1	2.51	0.45
3:C:169:GLU:N	3:C:175:GLY:O	2.49	0.45
3:C:186:ASP:OD1	3:C:190:ARG:N	2.49	0.45
7:H:39:GLY:HA2	22:H:101:PEF:H31	1.98	0.45
9:K:413:GLN:O	9:K:417:ILE:HD12	2.16	0.45
17:S:85:LYS:O	17:S:123:ARG:NH1	2.49	0.45
1:a:183:GLU:HA	1:a:186:GLU:HG3	1.98	0.45
1:a:300:ILE:HG12	1:a:301:LYS:H	1.81	0.45
8:j:182:LEU:O	8:j:186:VAL:HG12	2.16	0.45
10:l:91:ARG:NH2	10:l:119:SER:O	2.49	0.45
1:A:431:ILE:O	1:A:445:TYR:OH	2.32	0.45
2:B:54:PHE:CE2	2:B:114:PHE:HA	2.42	0.45
2:B:117:HIS:HB3	5:f:62:ARG:HD3	1.97	0.45
3:C:143:ASP:OD1	3:C:146:ARG:NH2	2.49	0.45
5:F:3:GLN:NE2	5:F:7:SER:OG	2.50	0.45
13:O:18:MET:O	13:O:20:SER:N	2.49	0.45
1:a:224:GLU:OE1	1:a:226:LYS:NZ	2.49	0.45
2:b:60:ASN:ND2	2:b:112:THR:O	2.46	0.45
5:f:34:ASN:HA	5:f:39:LYS:HD3	1.97	0.45
8:j:191:ALA:HA	8:j:194:VAL:HG12	1.99	0.45
9:K:380:VAL:HB	29:K:603:HEA:CBC	2.47	0.45
13:O:133:GLN:H	17:S:81:ARG:HH22	1.64	0.45
14:P:45:PHE:O	14:P:49:VAL:HG13	2.16	0.45
16:R:24:LEU:HD21	20:V:42:GLN:HG2	1.99	0.45
18:T:63:GLU:HB2	18:T:68:ARG:HB3	1.98	0.45
21:W:37:ARG:HG3	21:W:40:ASN:HB2	1.98	0.45
21:W:79:GLU:H	21:W:83:ARG:HD2	1.82	0.45
4:e:9:THR:O	4:e:13:ARG:NH1	2.46	0.45
2:B:233:PHE:HB3	2:B:357:GLY:HA2	1.99	0.45
3:C:83:THR:HG22	8:j:164:TRP:CD1	2.52	0.45
14:P:146:TYR:H	14:P:164:ASP:HB2	1.82	0.45
14:P:193:LEU:HB3	14:P:195:ILE:HG12	1.99	0.45
21:W:83:ARG:HB2	21:W:83:ARG:HH11	1.81	0.45
2:B:267:LEU:HD22	2:B:304:ILE:HG12	1.98	0.45
3:C:155:MET:SD	3:C:200:LEU:HB2	2.57	0.45
9:K:493:LYS:NZ	9:K:510:LYS:H	2.14	0.45
10:L:136:ASP:HB3	10:L:147:ARG:HB3	1.98	0.45
14:P:124:TRP:HE1	14:P:226:GLY:HA3	1.80	0.45
15:Q:55:ARG:O	15:Q:58:LYS:HG3	2.16	0.45
1:a:311:LEU:O	1:a:334:THR:OG1	2.26	0.45
8:j:35:LEU:HD13	8:j:233:VAL:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:18:VAL:O	4:E:21:ILE:HG22	2.17	0.45
9:K:262:TYR:HB3	9:K:338:MET:HE1	1.99	0.45
9:K:500:SER:HB2	9:K:503:ILE:HG12	1.98	0.45
10:L:276:ILE:HG23	10:L:277:LEU:HD22	1.99	0.45
14:P:41:ASP:HA	14:P:44:MET:HG2	1.98	0.45
18:T:134:CYS:HB3	18:T:138:GLY:H	1.81	0.45
5:f:5:PHE:HE2	8:j:312:VAL:HG21	1.82	0.45
8:j:30:TRP:NE1	26:j:404:HEM:O1D	2.50	0.45
8:j:121:PHE:O	8:j:125:ILE:HG12	2.17	0.45
10:L:86:ASP:OD1	10:L:86:ASP:N	2.50	0.45
7:h:62:PRO:HB2	8:j:331:PHE:CD2	2.52	0.45
8:j:257:TYR:HB2	10:l:183:ALA:HB2	1.98	0.45
8:J:305:LEU:HD22	8:J:363:PHE:HE2	1.82	0.45
27:J:405:UQ6:H322	27:J:405:UQ6:H301	1.77	0.45
9:K:374:VAL:HG23	9:K:377:PHE:CZ	2.52	0.45
1:a:202:LEU:HG	1:a:231:GLN:HB3	1.98	0.45
5:f:62:ARG:NH1	5:f:109:GLU:OE2	2.50	0.45
8:j:35:LEU:HD11	8:j:236:PHE:CD1	2.52	0.45
1:A:425:ARG:HA	1:A:425:ARG:HD2	1.85	0.45
8:J:38:LEU:O	8:J:42:ILE:HG12	2.17	0.45
10:L:218:PHE:HD2	10:L:223:ILE:HD11	1.82	0.45
14:P:77:HIS:ND1	14:P:79:GLN:HG3	2.32	0.45
1:A:57:SER:OG	1:A:205:ASN:ND2	2.50	0.45
8:J:116:VAL:O	8:J:120:ILE:HG13	2.17	0.45
8:J:352:GLY:O	8:J:356:THR:HG23	2.17	0.45
9:K:52:SER:OG	14:P:227:THR:O	2.30	0.45
9:K:54:LEU:O	9:K:58:LEU:HD12	2.16	0.45
21:W:128:TRP:HZ3	21:W:131:LYS:HZ1	1.64	0.45
1:a:443:LEU:HD13	1:a:447:ARG:HD2	1.99	0.45
2:b:132:ALA:O	2:b:136:GLN:HG2	2.17	0.45
3:c:111:TRP:CZ2	3:c:215:GLY:HA2	2.52	0.45
3:c:154:ILE:HD13	3:c:212:VAL:HG11	1.98	0.45
8:j:40:LEU:HD12	8:j:89:PHE:CZ	2.51	0.45
8:j:107:ARG:HA	8:j:107:ARG:HD3	1.70	0.45
1:A:61:ASN:HD21	1:A:235:LYS:HD2	1.82	0.44
8:J:316:ASN:HD21	8:J:322:SER:HB3	1.83	0.44
2:b:152:ARG:O	2:b:154:GLY:N	2.40	0.44
8:j:23:PRO:HG2	8:j:26:ILE:HD11	1.98	0.44
10:l:175:PRO:HD2	26:l:401:HEM:HAA1	2.00	0.44
2:B:33:VAL:HG11	2:B:105:LEU:HD21	1.98	0.44
9:K:32:MET:HE1	9:K:58:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:112:TRP:NE1	10:L:155:ILE:HG13	2.27	0.44
11:M:56:PHE:HA	11:M:59:ILE:HG12	1.98	0.44
13:O:219:LEU:O	13:O:222:MET:HG3	2.17	0.44
18:T:106:TYR:O	18:T:107:ARG:NE	2.50	0.44
8:j:145:THR:HA	8:j:148:THR:HG22	1.99	0.44
1:A:416:LYS:HD2	1:A:416:LYS:HA	1.78	0.44
23:H:102:PGT:H202	23:H:102:PGT:H172	1.87	0.44
9:K:380:VAL:HG23	9:K:381:LEU:HD22	2.00	0.44
16:R:12:ARG:HG2	16:R:16:MET:HE3	2.00	0.44
3:C:62:ALA:HA	3:C:65:LEU:HD12	1.98	0.44
3:C:143:ASP:N	3:C:190:ARG:HH21	2.16	0.44
8:J:30:TRP:HD1	26:J:404:HEM:CBA	2.30	0.44
9:K:333:ARG:O	9:K:338:MET:HG3	2.16	0.44
10:L:104:CYS:SG	26:L:401:HEM:HMC3	2.57	0.44
13:O:253:LEU:HG	13:O:257:TRP:CD1	2.52	0.44
14:P:90:ALA:O	14:P:93:LEU:HG	2.18	0.44
18:T:124:LEU:HG	18:T:141:TYR:HE2	1.82	0.44
21:W:91:ASP:O	21:W:95:ILE:HG12	2.18	0.44
8:j:123:LEU:HD22	8:j:190:ILE:CD1	2.47	0.44
10:l:95:GLN:HE22	10:l:234:VAL:HG13	1.82	0.44
8:J:278:PHE:O	8:J:281:ILE:HG22	2.17	0.44
9:K:108:MET:HE1	13:O:34:ALA:HB2	2.00	0.44
9:K:134:SER:O	9:K:134:SER:OG	2.30	0.44
9:K:339:LEU:HD12	9:K:340:TYR:N	2.32	0.44
10:L:121:THR:HG23	10:L:122:ASN:N	2.33	0.44
18:T:79:ASP:OD1	18:T:79:ASP:N	2.50	0.44
4:e:41:GLU:HG2	4:e:50:LYS:NZ	2.32	0.44
10:l:236:TYR:CD2	10:l:241:PRO:HG3	2.52	0.44
5:F:88:LEU:HB3	5:F:92:GLU:HG2	1.99	0.44
2:b:65:LEU:HD11	2:b:66:LYS:HE3	2.00	0.44
23:j:408:PGT:H412	23:j:408:PGT:H161	2.00	0.44
10:l:121:THR:OG1	10:l:122:ASN:N	2.47	0.44
10:l:281:TYR:O	10:l:285:ILE:HG12	2.18	0.44
2:B:70:GLU:O	2:B:74:LEU:N	2.49	0.44
3:C:108:VAL:HB	8:j:263:LEU:HD13	2.00	0.44
8:J:97:MET:HE1	8:J:121:PHE:CG	2.53	0.44
13:O:33:LEU:HB2	13:O:58:LEU:HD13	1.99	0.44
13:O:115:SER:O	13:O:115:SER:OG	2.30	0.44
1:a:282:ALA:HB2	1:a:328:TRP:HE1	1.83	0.44
3:c:180:CYS:HB2	3:c:181:HIS:CD2	2.53	0.44
2:B:226:GLY:N	2:B:352:ASN:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:42:GLY:HA2	5:F:94:ILE:HG12	1.99	0.44
8:J:95:MET:HE2	8:J:95:MET:HB3	1.88	0.44
8:J:132:TYR:CZ	8:J:140:SER:HA	2.53	0.44
2:B:79:LYS:HE3	2:B:79:LYS:HB3	1.76	0.44
9:K:17:LEU:HD21	9:K:103:PHE:CZ	2.52	0.44
10:L:173:LEU:O	26:L:401:HEM:HAD1	2.18	0.44
1:a:66:ASN:HD21	1:a:192:ASP:CG	2.26	0.44
2:B:152:ARG:O	2:B:154:GLY:N	2.43	0.43
7:H:84:ALA:HB1	7:H:88:GLU:HB3	1.99	0.43
8:J:369:VAL:O	8:J:373:ILE:HG12	2.18	0.43
12:N:17:LYS:HD2	12:N:17:LYS:HA	1.84	0.43
15:Q:88:ILE:HD13	15:Q:111:LEU:HD21	1.99	0.43
18:T:96:ASP:OD1	18:T:96:ASP:N	2.50	0.43
1:a:320:LEU:HD12	1:a:327:LEU:HD23	2.00	0.43
9:K:323:TRP:CE3	9:K:345:LEU:HD11	2.53	0.43
1:a:238:LEU:H	1:a:238:LEU:HD23	1.83	0.43
4:e:48:LEU:CD2	4:e:49:TRP:H	2.25	0.43
10:l:105:HIS:HE1	26:l:401:HEM:C4D	2.32	0.43
10:l:213:ASN:OD1	10:l:226:ALA:HA	2.18	0.43
2:B:315:SER:C	2:B:317:ALA:H	2.26	0.43
3:C:35:ARG:HH11	3:C:35:ARG:HG2	1.83	0.43
9:K:59:VAL:HG13	29:K:602:HEA:HBA1	1.99	0.43
13:O:85:LYS:HA	13:O:85:LYS:HD3	1.78	0.43
14:P:167:MET:HB2	14:P:236:ILE:HG22	2.00	0.43
17:S:95:ASP:OD1	17:S:95:ASP:N	2.50	0.43
1:a:297:LEU:HD13	2:b:65:LEU:HD22	2.00	0.43
2:b:19:VAL:HG23	2:b:198:LYS:NZ	2.33	0.43
4:e:42:ASN:O	4:e:45:LYS:NZ	2.48	0.43
10:l:130:GLU:HA	10:l:148:PRO:CB	2.48	0.43
1:A:214:ILE:HD12	1:A:218:ASP:HB2	1.99	0.43
2:B:239:ALA:HB3	2:B:301:ILE:HG21	2.01	0.43
22:J:407:PEF:H142	22:J:407:PEF:H111	1.73	0.43
9:K:347:LEU:HB3	9:K:383:MET:HE3	2.01	0.43
9:K:358:LEU:HD11	9:K:373:VAL:HG12	2.00	0.43
9:K:450:TRP:HA	9:K:453:VAL:HG22	1.99	0.43
12:N:46:LEU:HD23	12:N:46:LEU:H	1.83	0.43
13:O:37:THR:O	13:O:40:THR:OG1	2.27	0.43
16:R:38:MET:HA	16:R:41:ILE:HG22	2.00	0.43
1:a:447:ARG:HH12	8:j:222:HIS:HB3	1.83	0.43
2:b:83:ASP:CG	2:b:84:ARG:H	2.25	0.43
14:P:126:TRP:HB3	14:P:128:TYR:HE1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:53:LYS:HA	19:U:56:ASN:HB3	2.00	0.43
20:V:57:VAL:O	20:V:61:SER:OG	2.31	0.43
22:c:303:PEF:H412	8:j:237:MET:HG3	2.00	0.43
4:e:49:TRP:HZ2	10:l:121:THR:HA	1.84	0.43
1:A:391:GLY:HA2	1:A:394:VAL:HG12	2.00	0.43
9:K:53:GLN:O	9:K:57:VAL:HG23	2.19	0.43
9:K:240:GLY:O	9:K:244:VAL:N	2.47	0.43
13:O:143:ILE:HD12	13:O:146:LEU:HD12	2.01	0.43
15:Q:132:ARG:O	15:Q:136:GLY:N	2.52	0.43
16:R:39:ASP:HA	16:R:42:ASN:ND2	2.33	0.43
18:T:68:ARG:HA	18:T:71:LEU:HG	2.00	0.43
22:V:101:PEF:H152	22:V:101:PEF:H121	1.80	0.43
2:b:66:LYS:H	2:b:66:LYS:HD2	1.83	0.43
10:l:146:LYS:HB2	10:l:146:LYS:HE3	1.83	0.43
4:E:52:VAL:O	4:E:56:ILE:HG12	2.18	0.43
9:K:243:GLU:HA	9:K:246:ILE:HD12	1.99	0.43
14:P:56:TRP:CD1	16:R:21:GLY:HA2	2.54	0.43
14:P:193:LEU:HD23	14:P:195:ILE:HD13	2.00	0.43
1:a:125:ILE:HG13	1:a:126:GLN:N	2.33	0.43
2:b:195:ALA:HB1	2:b:199:ARG:NH2	2.34	0.43
6:g:76:ASP:N	6:g:76:ASP:OD1	2.52	0.43
7:h:88:GLU:O	7:h:92:VAL:HG23	2.18	0.43
8:j:3:PHE:HA	8:j:6:SER:HB3	2.01	0.43
1:A:29:VAL:HG21	1:A:400:LYS:HE3	2.00	0.43
2:B:45:ASP:OD1	2:B:45:ASP:N	2.52	0.43
5:F:88:LEU:HG	5:F:89:PRO:HD2	2.00	0.43
6:G:94:LEU:HA	6:G:97:HIS:HE1	1.84	0.43
9:K:112:CYS:HB2	9:K:146:LEU:HD22	2.01	0.43
9:K:344:PHE:CE1	9:K:384:GLY:HA2	2.53	0.43
13:O:4:LEU:HD23	13:O:8:ARG:HD3	2.00	0.43
18:T:82:ASP:OD1	18:T:82:ASP:N	2.50	0.43
18:T:93:THR:OG1	18:T:94:MET:N	2.50	0.43
1:a:447:ARG:HH22	8:j:222:HIS:HB3	1.84	0.43
1:a:455:MET:SD	1:a:455:MET:N	2.91	0.43
4:e:32:PHE:O	4:e:36:ILE:HG12	2.19	0.43
6:g:87:ASN:ND2	6:g:90:GLU:OE1	2.39	0.43
7:h:58:TYR:CE2	8:j:323:LYS:HD2	2.54	0.43
8:j:132:TYR:O	8:j:135:VAL:HG22	2.19	0.43
8:j:201:LEU:O	8:j:205:GLY:N	2.33	0.43
2:B:146:LEU:HD21	2:B:242:GLY:HA3	2.00	0.43
3:C:117:PHE:CE2	3:C:157:GLY:HA2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:7:SER:O	5:F:11:ILE:HG13	2.19	0.43
7:H:63:ALA:HB2	8:J:331:PHE:CZ	2.54	0.43
9:K:248:ILE:HG13	29:K:603:HEA:HBC2	1.99	0.43
9:K:342:ILE:HD12	14:P:58:LEU:HD11	2.01	0.43
14:P:46:TYR:O	14:P:49:VAL:HG22	2.18	0.43
15:Q:125:LEU:O	15:Q:128:LEU:HG	2.19	0.43
18:T:122:MET:HE2	18:T:122:MET:HB2	1.97	0.43
4:e:40:TYR:CD1	10:l:268:ARG:HB3	2.54	0.43
8:j:34:SER:OG	27:j:405:UQ6:O5	2.27	0.43
8:j:88:PHE:HB3	8:j:236:PHE:CZ	2.50	0.43
10:l:97:TYR:OH	10:l:107:LEU:HB2	2.19	0.43
10:l:235:GLU:N	10:l:241:PRO:HG2	2.32	0.43
1:A:252:ARG:HB3	1:A:252:ARG:NH1	2.33	0.43
8:J:362:TYR:HA	8:J:366:ILE:HG22	2.00	0.43
2:b:247:LYS:HE2	2:b:281:ASP:HA	2.01	0.43
3:c:106:ASN:OD1	3:c:119:ARG:NH1	2.44	0.43
5:f:13:ASP:O	5:f:17:LYS:HD3	2.18	0.43
8:j:82:HIS:HE1	26:j:403:HEM:NC	2.17	0.43
2:B:60:ASN:N	2:B:112:THR:HB	2.33	0.42
7:H:12:TRP:H	7:H:15:HIS:CD2	2.37	0.42
8:J:187:PRO:HA	8:J:190:ILE:HB	2.01	0.42
8:J:329:PHE:HE1	8:J:359:TYR:CD1	2.36	0.42
14:P:77:HIS:HD1	14:P:79:GLN:HG3	1.83	0.42
8:j:297:ALA:O	8:j:301:VAL:HG13	2.18	0.42
1:A:280:LEU:O	1:A:284:ILE:HG13	2.19	0.42
2:B:302:LYS:HZ2	2:B:363:PRO:HG3	1.84	0.42
3:C:161:HIS:CE1	3:C:181:HIS:CG	3.07	0.42
1:a:357:SER:HA	1:a:419:LYS:HE2	2.01	0.42
1:a:407:PHE:HA	1:a:410:ILE:HG22	2.01	0.42
2:b:181:THR:O	2:b:185:LEU:HG	2.19	0.42
2:b:281:ASP:OD1	2:b:281:ASP:N	2.52	0.42
22:c:303:PEF:H401	8:j:42:ILE:HG21	2.00	0.42
8:j:22:GLN:HB2	8:j:225:PHE:CE2	2.54	0.42
2:B:44:LYS:HD2	2:B:167:VAL:HG12	2.01	0.42
4:E:49:TRP:CE3	4:E:52:VAL:HG21	2.54	0.42
8:J:1:MET:HA	8:J:5:LYS:HG3	2.01	0.42
15:Q:102:PRO:HG3	21:W:72:VAL:HG13	2.01	0.42
1:a:67:ASN:HB3	1:a:180:GLY:HA2	2.02	0.42
1:a:138:GLU:O	1:a:142:LYS:HG2	2.19	0.42
2:b:255:VAL:HG11	2:b:343:VAL:HG11	2.01	0.42
2:b:353:TYR:HE1	2:b:355:ALA:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:52:VAL:HG13	10:l:88:ALA:HA	2.00	0.42
1:A:141:LYS:NZ	1:A:186:GLU:HA	2.34	0.42
1:A:356:ILE:HD12	1:A:457:TRP:CD1	2.54	0.42
8:J:102:TYR:OH	22:J:401:PEF:O2P	2.34	0.42
8:J:132:TYR:O	8:J:140:SER:HB2	2.19	0.42
10:L:150:LYS:HG2	10:L:153:ASP:HB2	2.02	0.42
14:P:31:PRO:HA	14:P:34:GLU:HG2	2.01	0.42
1:a:447:ARG:NH2	8:j:220:PRO:HB2	2.32	0.42
10:l:263:HIS:O	10:l:266:ARG:HG2	2.20	0.42
1:A:395:LEU:HD23	1:A:395:LEU:HA	1.88	0.42
6:G:125:GLU:HG2	6:G:126:GLU:N	2.34	0.42
8:J:42:ILE:O	8:J:46:THR:HG22	2.19	0.42
8:J:235:LEU:HD12	10:L:281:TYR:CZ	2.55	0.42
14:P:163:THR:HG22	14:P:164:ASP:N	2.33	0.42
21:W:97:LYS:HE2	23:W:201:PGT:H122	2.00	0.42
2:b:181:THR:HB	2:b:212:GLY:H	1.84	0.42
3:c:126:ILE:HD11	3:c:151:GLN:HA	2.02	0.42
4:e:48:LEU:CD2	4:e:50:LYS:HZ3	2.24	0.42
7:h:57:LEU:HD23	7:h:57:LEU:H	1.85	0.42
7:h:58:TYR:HB3	8:j:327:PHE:CE2	2.54	0.42
1:A:76:ILE:HG23	1:A:131:LEU:HD21	2.00	0.42
10:L:177:LEU:HD23	10:L:180:ILE:HG13	2.02	0.42
13:O:64:LEU:O	13:O:67:ARG:HG3	2.18	0.42
13:O:157:HIS:HA	13:O:160:ILE:HG22	2.01	0.42
14:P:177:PHE:CE1	14:P:195:ILE:HD13	2.54	0.42
1:a:113:THR:HG21	1:a:214:ILE:HG21	2.01	0.42
2:b:54:PHE:CE2	2:b:114:PHE:HA	2.55	0.42
2:b:324:LYS:HA	2:b:324:LYS:HD2	1.89	0.42
8:j:294:THR:HG23	8:j:295:MET:CE	2.49	0.42
1:A:67:ASN:CG	1:A:176:LEU:HD12	2.44	0.42
22:A:501:PEF:H341	22:A:501:PEF:H372	1.87	0.42
22:H:101:PEF:H382	23:W:201:PGT:H221	2.00	0.42
8:J:67:HIS:ND1	8:J:71:ASP:HB3	2.34	0.42
8:J:219:ILE:HG21	10:L:295:ILE:HD11	2.02	0.42
3:c:74:THR:HG21	22:c:303:PEF:H181	2.01	0.42
4:e:51:ASP:O	4:e:55:ARG:HB3	2.20	0.42
8:j:60:LEU:O	8:j:64:SER:HB2	2.19	0.42
8:J:4:ARG:HD2	8:J:18:ILE:HG21	2.02	0.42
8:J:43:GLN:OE1	8:J:82:HIS:ND1	2.53	0.42
1:a:379:GLU:HG3	2:b:26:THR:HG23	2.01	0.42
3:c:72:LYS:HE3	3:c:72:LYS:HB3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:f:5:PHE:CE2	8:j:312:VAL:HG21	2.54	0.42
8:j:291:GLY:O	8:j:295:MET:HG2	2.18	0.42
1:A:125:ILE:HG22	1:A:229:SER:HA	2.01	0.42
6:G:78:LEU:O	6:G:82:ARG:HG2	2.20	0.42
9:K:71:VAL:HG11	9:K:247:LEU:HD13	2.02	0.42
10:L:80:GLY:O	10:L:267:LYS:NZ	2.53	0.42
12:N:44:PRO:O	12:N:48:ILE:HG13	2.20	0.42
13:O:243:TYR:O	13:O:247:ILE:HG12	2.20	0.42
20:V:45:ALA:HA	22:V:102:PEF:H241	2.01	0.42
22:j:406:PEF:H312	22:j:406:PEF:H342	1.72	0.42
10:l:284:SER:HA	10:l:287:VAL:HG12	2.02	0.42
2:B:99:PRO:HA	2:B:102:VAL:HG12	2.02	0.42
7:H:34:GLN:NE2	10:L:297:THR:HG21	2.31	0.42
9:K:188:SER:OG	9:K:249:ILE:HG22	2.20	0.42
14:P:53:LEU:HD11	14:P:57:MET:HE2	2.01	0.42
17:S:28:VAL:O	17:S:31:GLN:HG3	2.20	0.42
2:b:115:LYS:HA	2:b:115:LYS:HD3	1.64	0.42
8:j:66:GLU:O	8:j:70:ARG:HG2	2.20	0.42
10:l:225:MET:HE2	10:l:227:ARG:NH2	2.34	0.42
1:A:256:LEU:HD12	1:A:437:GLY:HA2	2.02	0.41
1:A:354:LEU:HD12	1:A:358:VAL:HG11	2.02	0.41
1:A:375:GLY:O	1:A:379:GLU:CB	2.67	0.41
9:K:184:LEU:HD23	9:K:184:LEU:HA	1.95	0.41
9:K:334:LEU:O	21:W:86:VAL:HG21	2.20	0.41
10:L:180:ILE:HA	10:L:183:ALA:HB3	2.02	0.41
10:L:182:LYS:HG3	10:L:182:LYS:O	2.20	0.41
13:O:133:GLN:H	17:S:81:ARG:HH12	1.68	0.41
14:P:21:TYR:HD2	20:V:57:VAL:HG13	1.84	0.41
14:P:189:ALA:HA	14:P:196:LYS:HG3	2.02	0.41
17:S:96:TYR:CE2	17:S:98:PHE:HB2	2.55	0.41
1:a:349:LYS:HD3	1:a:349:LYS:HA	1.71	0.41
1:a:457:TRP:CD1	4:e:14:ASN:HB2	2.55	0.41
10:l:298:ARG:HE	10:l:300:PHE:HZ	1.67	0.41
2:B:37:GLY:HA2	2:B:41:TYR:CD2	2.55	0.41
2:B:236:ASP:OD2	2:B:290:ARG:NH2	2.53	0.41
9:K:347:LEU:HA	9:K:350:MET:HE2	2.02	0.41
10:L:281:TYR:CE1	10:L:285:ILE:HD11	2.54	0.41
13:O:21:PRO:O	13:O:24:ILE:HG22	2.20	0.41
14:P:113:PRO:HD2	19:U:13:GLY:O	2.20	0.41
6:g:99:GLU:HG3	6:g:127:PHE:CZ	2.55	0.41
8:j:118:VAL:N	26:j:404:HEM:HBC2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:247:SER:OG	8:j:250:THR:OG1	2.18	0.41
3:C:192:ARG:HE	3:C:192:ARG:HB3	1.67	0.41
9:K:40:LEU:HD11	9:K:55:PHE:HE1	1.85	0.41
9:K:525:HIS:CE1	11:M:29:HIS:HB2	2.56	0.41
13:O:263:VAL:C	13:O:265:TYR:H	2.28	0.41
17:S:65:LEU:O	17:S:69:ASN:ND2	2.53	0.41
17:S:73:VAL:O	17:S:77:HIS:ND1	2.40	0.41
1:a:77:PHE:CE2	1:a:104:TYR:HB3	2.56	0.41
1:a:250:ARG:NH2	1:a:444:ASP:HA	2.35	0.41
2:b:119:LEU:O	2:b:124:LEU:HD23	2.21	0.41
2:b:138:PRO:HG3	2:b:233:PHE:HE2	1.85	0.41
5:f:52:GLU:HG2	8:j:109:PRO:HG2	2.02	0.41
10:l:63:THR:O	10:l:66:GLU:HG3	2.20	0.41
10:l:101:CYS:HB3	26:l:401:HEM:C3B	2.55	0.41
10:l:260:GLU:N	10:l:260:GLU:OE1	2.53	0.41
10:l:260:GLU:O	10:l:260:GLU:HG2	2.19	0.41
1:A:67:ASN:HD21	1:A:176:LEU:HB2	1.85	0.41
2:B:353:TYR:CE2	2:B:355:ALA:HB2	2.55	0.41
9:K:37:ARG:NH2	9:K:451:ASN:OD1	2.54	0.41
9:K:297:LEU:HD12	9:K:301:THR:HB	2.01	0.41
9:K:391:ALA:O	9:K:395:TYR:HB3	2.20	0.41
9:K:413:GLN:NE2	9:K:467:LEU:HB3	2.35	0.41
10:L:225:MET:SD	26:L:401:HEM:C4D	3.13	0.41
13:O:3:HIS:HA	13:O:6:ARG:HG2	2.02	0.41
14:P:56:TRP:HD1	16:R:21:GLY:HA2	1.85	0.41
17:S:66:THR:HA	17:S:69:ASN:ND2	2.34	0.41
1:a:126:GLN:HA	1:a:127:GLN:HA	1.75	0.41
1:a:134:SER:O	1:a:137:PHE:N	2.52	0.41
1:a:183:GLU:HG2	1:a:184:SER:N	2.36	0.41
1:a:279:LYS:HG3	1:a:370:LEU:HD11	2.02	0.41
3:c:159:CYS:O	3:c:163:GLY:N	2.54	0.41
2:B:97:ASP:O	2:B:101:TYR:HD1	2.02	0.41
2:B:164:VAL:HG21	2:b:232:ARG:HB3	2.03	0.41
8:J:23:PRO:HG2	8:J:26:ILE:HD11	2.03	0.41
8:J:331:PHE:HA	8:J:334:VAL:HG22	2.01	0.41
9:K:37:ARG:O	9:K:41:ALA:N	2.54	0.41
9:K:297:LEU:HD23	9:K:297:LEU:H	1.85	0.41
13:O:75:TYR:CD2	13:O:76:LEU:HD12	2.56	0.41
15:Q:106:ARG:NH2	21:W:77:TYR:HA	2.35	0.41
1:a:298:GLN:O	1:a:303:LEU:HD23	2.20	0.41
8:j:189:ILE:O	8:j:193:MET:HE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:311:SER:OG	8:j:319:LYS:NZ	2.51	0.41
2:B:116:PRO:HB3	2:B:169:LEU:HD22	2.02	0.41
13:O:80:THR:H	13:O:83:VAL:HG12	1.85	0.41
14:P:206:GLN:HG2	19:U:21:GLN:O	2.20	0.41
17:S:14:PRO:HA	17:S:15:PRO:HD3	1.86	0.41
1:a:112:SER:HB2	1:a:115:LYS:HD2	2.03	0.41
7:h:61:ILE:HB	7:h:62:PRO:HD3	2.01	0.41
22:A:501:PEF:H321	22:A:501:PEF:H352	1.80	0.41
2:B:143:GLU:HG3	2:B:288:PHE:HZ	1.85	0.41
3:C:101:ILE:HG12	3:C:107:VAL:HG21	2.03	0.41
6:G:76:ASP:OD1	6:G:76:ASP:N	2.54	0.41
10:L:150:LYS:HG3	10:L:152:SER:H	1.84	0.41
12:N:4:LYS:HA	12:N:4:LYS:HD3	1.93	0.41
13:O:95:VAL:O	13:O:99:VAL:HG23	2.20	0.41
21:W:52:LYS:HD2	21:W:52:LYS:HA	1.76	0.41
23:W:201:PGT:H352	23:W:201:PGT:H321	1.84	0.41
5:f:32:PHE:HD1	8:j:320:VAL:HG21	1.85	0.41
8:j:362:TYR:HA	8:j:366:ILE:HB	2.02	0.41
6:G:77:GLN:HE22	6:G:145:LYS:HA	1.85	0.41
8:J:58:ILE:HG23	8:J:136:TYR:CE2	2.56	0.41
8:J:153:ALA:HB2	8:J:288:LYS:HD3	2.03	0.41
9:K:56:ASN:OD1	9:K:124:GLY:HA3	2.21	0.41
9:K:347:LEU:HB3	9:K:383:MET:HG2	2.02	0.41
7:h:51:ARG:HA	7:h:51:ARG:HD3	1.86	0.41
8:j:30:TRP:CH2	8:j:209:PRO:HG3	2.56	0.41
22:j:406:PEF:H161	22:j:406:PEF:H131	1.86	0.41
10:l:218:PHE:CD1	10:l:219:PRO:HD2	2.56	0.41
26:l:401:HEM:HHA	26:l:401:HEM:HBA1	2.02	0.41
1:A:126:GLN:HA	1:A:127:GLN:HA	1.55	0.41
2:B:74:LEU:HD22	2:B:101:TYR:CE1	2.56	0.41
3:C:119:ARG:HH21	3:C:125:GLU:CD	2.29	0.41
4:E:17:PHE:CE2	4:E:21:ILE:HD12	2.56	0.41
5:F:10:ARG:HA	5:F:13:ASP:OD2	2.21	0.41
5:F:32:PHE:HA	5:F:35:LEU:HG	2.03	0.41
8:J:175:THR:O	8:J:178:ARG:HG2	2.21	0.41
8:J:276:LEU:HD12	8:J:340:GLY:C	2.46	0.41
8:J:329:PHE:HE1	8:J:359:TYR:HD1	1.68	0.41
9:K:26:GLY:HA3	9:K:70:LEU:HD13	2.03	0.41
9:K:323:TRP:HE3	9:K:345:LEU:HD11	1.85	0.41
9:K:379:TYR:OH	9:K:428:MET:HB2	2.21	0.41
9:K:444:PRO:HD3	14:P:160:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:517:LEU:HD13	18:T:123:TRP:CZ2	2.54	0.41
10:L:189:ASP:OD1	10:L:189:ASP:N	2.53	0.41
12:N:43:THR:HB	12:N:47:TYR:CE2	2.56	0.41
13:O:92:LEU:HA	13:O:95:VAL:HG22	2.01	0.41
16:R:56:LYS:HD3	16:R:56:LYS:HA	1.83	0.41
19:U:15:ASP:N	19:U:15:ASP:OD1	2.54	0.41
21:W:47:GLN:HA	21:W:50:VAL:HG22	2.03	0.41
2:b:63:SER:OG	2:b:64:ALA:N	2.52	0.41
2:b:230:ARG:NH1	2:b:359:VAL:HG22	2.36	0.41
2:b:299:SER:O	2:b:303:LYS:HG2	2.21	0.41
3:c:80:SER:O	3:c:83:THR:HG22	2.20	0.41
3:c:116:VAL:HA	3:c:156:LEU:HA	2.03	0.41
6:g:141:ARG:HD3	6:g:141:ARG:HA	1.97	0.41
8:j:68:ILE:O	8:j:72:VAL:HG12	2.20	0.41
8:j:283:ARG:HH12	8:j:344:VAL:HB	1.85	0.41
1:A:252:ARG:HD2	1:A:440:GLU:CD	2.46	0.41
3:C:103:LEU:HD13	3:C:120:HIS:CE1	2.56	0.41
9:K:113:LEU:HD23	9:K:113:LEU:HA	1.88	0.41
9:K:347:LEU:CB	9:K:383:MET:HG2	2.51	0.41
9:K:352:GLY:HA3	29:K:603:HEA:H14	2.03	0.41
9:K:520:SER:O	9:K:521:PRO:C	2.65	0.41
1:a:283:GLN:O	1:a:283:GLN:NE2	2.54	0.41
1:a:352:ASN:HA	1:a:355:THR:HG22	2.02	0.41
2:b:195:ALA:HB1	2:b:199:ARG:HH22	1.85	0.41
3:c:105:LYS:HD2	3:c:105:LYS:HA	1.85	0.41
4:e:3:PHE:HB3	4:e:7:TYR:HB2	2.03	0.41
1:A:99:ARG:HA	1:A:99:ARG:HD3	1.84	0.40
2:B:181:THR:OG1	2:B:210:PRO:O	2.29	0.40
3:C:66:LEU:HD22	10:L:276:ILE:HD11	2.03	0.40
6:G:85:PHE:CE2	6:G:139:ALA:HA	2.56	0.40
6:G:94:LEU:HA	6:G:97:HIS:CE1	2.55	0.40
8:J:118:VAL:O	8:J:122:ILE:HG13	2.21	0.40
9:K:308:ALA:O	9:K:312:ILE:HG12	2.21	0.40
13:O:146:LEU:HD21	13:O:261:TYR:HD2	1.86	0.40
13:O:160:ILE:HB	13:O:247:ILE:HD11	2.03	0.40
18:T:87:ASP:OD1	18:T:87:ASP:N	2.54	0.40
21:W:41:MET:HE2	21:W:46:GLN:CG	2.50	0.40
1:A:120:LEU:HD12	1:A:120:LEU:HA	1.97	0.40
23:A:502:PGT:O1P	23:A:502:PGT:O6	2.35	0.40
2:B:291:ASP:HB2	2:B:297:VAL:HG23	2.03	0.40
9:K:273:MET:O	9:K:273:MET:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:101:PHE:O	14:P:104:LEU:HG	2.21	0.40
21:W:139:LYS:HG2	21:W:140:ASN:N	2.35	0.40
3:c:146:ARG:NH2	3:c:190:ARG:HG2	2.37	0.40
7:h:74:ASN:O	7:h:77:ASN:HB2	2.21	0.40
22:j:401:PEF:H191	22:j:401:PEF:H372	2.03	0.40
27:j:405:UQ6:H251	27:j:405:UQ6:H271	1.67	0.40
10:l:110:VAL:O	10:l:155:ILE:HG12	2.22	0.40
1:A:230:LEU:H	1:A:230:LEU:HD23	1.85	0.40
3:C:137:LEU:HD22	3:C:190:ARG:HD2	2.03	0.40
9:K:443:TYR:C	14:P:159:ARG:HH12	2.29	0.40
21:W:78:GLY:O	21:W:79:GLU:HG2	2.21	0.40
1:a:141:LYS:HE2	1:a:186:GLU:HA	2.03	0.40
5:f:15:ILE:HG13	5:f:16:LEU:HD22	2.03	0.40
8:j:367:VAL:HG23	8:j:368:PRO:HD3	2.03	0.40
2:B:257:ALA:O	2:B:261:THR:HG22	2.22	0.40
7:H:60:LEU:H	7:H:60:LEU:HD23	1.86	0.40
9:K:514:ILE:HD11	18:T:125:LYS:HD3	2.02	0.40
21:W:114:ARG:HG3	25:W:202:PCF:H122	2.04	0.40
8:j:276:LEU:N	8:j:277:PRO:HD2	2.37	0.40
10:l:157:GLY:HA2	10:l:158:PRO:HD3	1.92	0.40
3:C:178:CYS:CB	24:C:301:FES:S1	3.10	0.40
4:E:39:TRP:HZ3	10:L:271:LEU:HD21	1.85	0.40
8:J:193:MET:HE2	8:J:193:MET:HB2	1.94	0.40
9:K:34:LEU:HB2	9:K:462:THR:HG21	2.03	0.40
9:K:359:ALA:HB2	29:K:603:HEA:CMB	2.52	0.40
9:K:424:ILE:HG13	9:K:457:GLY:HA3	2.04	0.40
13:O:229:ARG:NH1	13:O:232:ASN:OD1	2.55	0.40
14:P:81:ILE:HG22	14:P:85:TRP:CE3	2.56	0.40
3:c:110:LYS:HB2	3:c:110:LYS:HE2	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/457 (94%)	394 (92%)	35 (8%)	0	100	100
1	a	429/457 (94%)	400 (93%)	29 (7%)	0	100	100
2	B	350/368 (95%)	330 (94%)	20 (6%)	0	100	100
2	b	350/368 (95%)	329 (94%)	21 (6%)	0	100	100
3	C	183/215 (85%)	173 (94%)	10 (6%)	0	100	100
3	c	183/215 (85%)	173 (94%)	10 (6%)	0	100	100
4	E	55/66 (83%)	54 (98%)	1 (2%)	0	100	100
4	e	55/66 (83%)	51 (93%)	4 (7%)	0	100	100
5	F	124/127 (98%)	119 (96%)	5 (4%)	0	100	100
5	f	124/127 (98%)	117 (94%)	7 (6%)	0	100	100
6	G	72/147 (49%)	65 (90%)	7 (10%)	0	100	100
6	g	72/147 (49%)	63 (88%)	9 (12%)	0	100	100
7	H	91/94 (97%)	82 (90%)	9 (10%)	0	100	100
7	h	91/94 (97%)	78 (86%)	13 (14%)	0	100	100
8	J	383/385 (100%)	365 (95%)	18 (5%)	0	100	100
8	j	383/385 (100%)	371 (97%)	12 (3%)	0	100	100
9	K	532/534 (100%)	509 (96%)	23 (4%)	0	100	100
10	L	246/309 (80%)	219 (89%)	27 (11%)	0	100	100
10	l	246/309 (80%)	211 (86%)	35 (14%)	0	100	100
11	M	45/78 (58%)	43 (96%)	2 (4%)	0	100	100
12	N	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
13	O	267/269 (99%)	249 (93%)	18 (7%)	0	100	100
14	P	234/251 (93%)	220 (94%)	14 (6%)	0	100	100
15	Q	100/148 (68%)	97 (97%)	3 (3%)	0	100	100
16	R	53/59 (90%)	49 (92%)	4 (8%)	0	100	100
17	S	111/129 (86%)	102 (92%)	9 (8%)	0	100	100
18	T	119/155 (77%)	112 (94%)	6 (5%)	1 (1%)	16	45
19	U	75/83 (90%)	71 (95%)	4 (5%)	0	100	100
20	V	38/66 (58%)	34 (90%)	4 (10%)	0	100	100
21	W	131/153 (86%)	117 (89%)	14 (11%)	0	100	100
All	All	5628/6321 (89%)	5250 (93%)	377 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	T	145	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/393 (94%)	370 (100%)	0	100	100
1	a	370/393 (94%)	370 (100%)	0	100	100
2	B	301/313 (96%)	301 (100%)	0	100	100
2	b	301/313 (96%)	301 (100%)	0	100	100
3	C	151/179 (84%)	151 (100%)	0	100	100
3	c	151/179 (84%)	151 (100%)	0	100	100
4	E	47/54 (87%)	47 (100%)	0	100	100
4	e	47/54 (87%)	47 (100%)	0	100	100
5	F	110/111 (99%)	110 (100%)	0	100	100
5	f	110/111 (99%)	110 (100%)	0	100	100
6	G	67/131 (51%)	67 (100%)	0	100	100
6	g	67/131 (51%)	67 (100%)	0	100	100
7	H	77/78 (99%)	77 (100%)	0	100	100
7	h	77/78 (99%)	77 (100%)	0	100	100
8	J	338/338 (100%)	338 (100%)	0	100	100
8	j	338/338 (100%)	338 (100%)	0	100	100
9	K	447/447 (100%)	447 (100%)	0	100	100
10	L	206/251 (82%)	206 (100%)	0	100	100
10	l	206/251 (82%)	206 (100%)	0	100	100
11	M	39/67 (58%)	39 (100%)	0	100	100
12	N	50/51 (98%)	50 (100%)	0	100	100
13	O	228/228 (100%)	228 (100%)	0	100	100
14	P	209/224 (93%)	209 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	Q	91/131 (70%)	91 (100%)	0	100	100
16	R	46/50 (92%)	46 (100%)	0	100	100
17	S	99/113 (88%)	99 (100%)	0	100	100
18	T	102/135 (76%)	102 (100%)	0	100	100
19	U	69/74 (93%)	69 (100%)	0	100	100
20	V	33/53 (62%)	33 (100%)	0	100	100
21	W	110/127 (87%)	110 (100%)	0	100	100
All	All	4857/5396 (90%)	4857 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	283	GLN
1	A	385	ASN
2	B	52	ASN
2	B	328	GLN
2	B	361	ASN
3	C	120	HIS
3	C	184	HIS
5	F	30	ASN
5	F	86	HIS
6	G	77	GLN
7	H	34	GLN
7	H	43	ASN
8	J	138	GLN
8	J	177	GLN
8	J	253	HIS
9	K	3	GLN
10	L	78	HIS
10	L	185	HIS
10	L	303	ASN
12	N	23	HIS
14	P	205	ASN
15	Q	117	ASN
17	S	16	ASN
17	S	100	ASN

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Mol	Chain	Res	Type
17	S	122	ASN
18	T	41	ASN
19	U	23	GLN
21	W	142	ASN
1	a	227	ASN
1	a	336	ASN
1	a	385	ASN
2	b	258	ASN
3	c	112	GLN
5	f	3	GLN
5	f	57	GLN
8	j	149	ASN
8	j	197	HIS
10	l	105	HIS
10	l	141	GLN
10	l	169	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 1 is monoatomic and 2 are modelled with single atom - leaving 38 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
22	PEF	j	402	-	30,30,46	0.50	0	33,35,51	1.31	4 (12%)
22	PEF	C	303	-	42,42,46	0.46	0	45,47,51	1.24	4 (8%)
22	PEF	J	402	-	30,30,46	0.50	0	33,35,51	1.33	4 (12%)
27	UQ6	J	405	-	43,43,43	0.42	0	54,55,55	1.65	14 (25%)
26	HEM	L	401	10	50,50,50	1.58	7 (14%)	67,82,82	1.15	7 (10%)
22	PEF	j	401	-	44,44,46	0.45	0	47,49,51	1.21	4 (8%)
23	PGT	a	502	-	50,50,50	0.48	0	53,56,56	0.48	0
29	HEA	K	603	9	67,67,67	1.28	8 (11%)	81,103,103	1.58	14 (17%)
26	HEM	j	404	8	50,50,50	1.58	7 (14%)	67,82,82	1.15	6 (8%)
22	PEF	c	303	-	42,42,46	0.46	0	45,47,51	1.26	4 (8%)
26	HEM	J	404	8	50,50,50	1.61	8 (16%)	67,82,82	1.14	5 (7%)
26	HEM	l	401	10	50,50,50	1.54	7 (14%)	67,82,82	1.11	5 (7%)
24	FES	C	301	3	0,4,4	-	-	-	-	-
22	PEF	J	407	-	28,28,46	0.51	0	31,33,51	1.30	4 (12%)
23	PGT	C	302	-	50,50,50	0.49	0	53,56,56	0.46	0
23	PGT	L	402	-	50,50,50	0.48	0	53,56,56	0.48	0
26	HEM	J	403	8	50,50,50	1.60	7 (14%)	67,82,82	1.12	5 (7%)
22	PEF	H	101	-	35,35,46	0.49	0	38,40,51	1.28	4 (10%)
22	PEF	V	101	-	32,32,46	0.49	0	35,37,51	1.31	4 (11%)
22	PEF	J	401	-	44,44,46	0.45	0	47,49,51	1.23	4 (8%)
22	PEF	a	501	-	39,39,46	0.47	0	42,44,51	1.25	4 (9%)
27	UQ6	j	405	-	43,43,43	0.43	0	54,55,55	1.65	14 (25%)
22	PEF	j	406	-	30,30,46	0.50	0	33,35,51	1.31	4 (12%)
29	HEA	K	602	9	67,67,67	1.26	7 (10%)	81,103,103	1.54	14 (17%)
22	PEF	J	406	-	30,30,46	0.50	0	33,35,51	1.35	4 (12%)
23	PGT	j	408	-	48,48,50	0.50	0	51,54,56	0.46	0
25	PCF	E	101	-	46,46,49	0.64	0	52,54,57	0.55	0
23	PGT	H	102	-	48,48,50	0.49	0	51,54,56	0.47	0
23	PGT	A	502	-	50,50,50	0.49	0	53,56,56	0.46	0
22	PEF	A	501	-	39,39,46	0.47	0	42,44,51	1.26	4 (9%)
24	FES	c	301	3	0,4,4	-	-	-	-	-
25	PCF	W	203	-	49,49,49	0.63	0	55,57,57	0.54	0
25	PCF	W	202	-	35,35,49	0.71	0	41,43,57	0.57	0
22	PEF	V	102	-	40,40,46	0.47	0	43,45,51	1.27	5 (11%)
22	PEF	j	407	-	28,28,46	0.51	0	31,33,51	1.35	4 (12%)
25	PCF	c	302	-	46,46,49	0.64	0	52,54,57	0.61	0
23	PGT	W	201	-	50,50,50	0.49	0	53,56,56	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	HEM	j	403	8	50,50,50	1.60	7 (14%)	67,82,82	1.11	6 (8%)

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
22	PEF	j	402	-	-	3/34/34/50	-
22	PEF	C	303	-	-	9/46/46/50	-
22	PEF	J	402	-	-	5/34/34/50	-
27	UQ6	J	405	-	-	10/39/39/39	0/1/1/1
26	HEM	L	401	10	-	6/14/54/54	-
22	PEF	j	401	-	-	9/48/48/50	-
23	PGT	a	502	-	-	21/55/55/55	-
29	HEA	K	603	9	-	18/36/76/76	-
26	HEM	j	404	8	-	7/14/54/54	-
22	PEF	c	303	-	-	10/46/46/50	-
26	HEM	J	404	8	-	8/14/54/54	-
26	HEM	l	401	10	-	10/14/54/54	-
24	FES	C	301	3	-	-	0/1/1/1
22	PEF	J	407	-	-	8/32/32/50	-
23	PGT	C	302	-	-	12/55/55/55	-
23	PGT	L	402	-	-	20/55/55/55	-
26	HEM	J	403	8	-	4/14/54/54	-
22	PEF	H	101	-	-	9/39/39/50	-
22	PEF	V	101	-	-	5/36/36/50	-
22	PEF	J	401	-	-	11/48/48/50	-
22	PEF	a	501	-	-	11/43/43/50	-
27	UQ6	j	405	-	-	11/39/39/39	0/1/1/1
22	PEF	j	406	-	-	3/34/34/50	-
29	HEA	K	602	9	-	19/36/76/76	-
22	PEF	J	406	-	-	4/34/34/50	-
23	PGT	j	408	-	-	18/53/53/55	-
25	PCF	E	101	-	-	13/50/50/53	-
23	PGT	H	102	-	-	13/53/53/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PGT	A	502	-	-	24/55/55/55	-
22	PEF	A	501	-	-	8/43/43/50	-
24	FES	c	301	3	-	-	0/1/1/1
25	PCF	W	203	-	-	11/53/53/53	-
25	PCF	W	202	-	-	8/39/39/53	-
22	PEF	V	102	-	-	9/44/44/50	-
22	PEF	j	407	-	-	6/32/32/50	-
25	PCF	c	302	-	-	14/50/50/53	-
23	PGT	W	201	-	-	22/55/55/55	-
26	HEM	j	403	8	-	12/14/54/54	-

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	l	401	HEM	FE-ND	5.65	2.12	1.94
26	J	403	HEM	FE-ND	5.64	2.12	1.94
26	L	401	HEM	FE-ND	5.60	2.12	1.94
26	j	403	HEM	FE-ND	5.60	2.12	1.94
26	J	404	HEM	FE-ND	5.56	2.12	1.94
26	j	404	HEM	FE-ND	5.46	2.11	1.94
29	K	603	HEA	CMA-C3A	-4.01	1.36	1.45
29	K	602	HEA	CMA-C3A	-3.97	1.36	1.45
26	l	401	HEM	FE-NC	3.47	2.06	1.95
26	j	403	HEM	FE-NC	3.36	2.06	1.95
26	j	404	HEM	FE-NC	3.35	2.06	1.95
26	L	401	HEM	FE-NC	3.33	2.06	1.95
26	J	404	HEM	FE-NC	3.32	2.06	1.95
26	J	403	HEM	FE-NC	3.30	2.06	1.95
26	J	404	HEM	CAB-C3B	3.01	1.55	1.47
29	K	603	HEA	CHC-C1C	-2.94	1.32	1.39
29	K	602	HEA	C4C-NC	-2.94	1.34	1.39
26	J	404	HEM	C3C-C2C	-2.91	1.31	1.37
29	K	602	HEA	CHC-C1C	-2.90	1.32	1.39
26	j	403	HEM	C3C-C2C	-2.88	1.31	1.37
29	K	603	HEA	C4C-NC	-2.88	1.34	1.39
26	J	403	HEM	C3C-C2C	-2.87	1.31	1.37
26	L	401	HEM	C3C-C2C	-2.86	1.31	1.37
26	L	401	HEM	CAB-C3B	2.83	1.54	1.47
26	l	401	HEM	CAB-C3B	2.82	1.54	1.47
26	J	403	HEM	CAB-C3B	2.82	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	j	404	HEM	CAB-C3B	2.78	1.54	1.47
26	j	404	HEM	C3C-C2C	-2.78	1.31	1.37
26	j	403	HEM	CAB-C3B	2.77	1.54	1.47
26	l	401	HEM	C3C-C2C	-2.74	1.31	1.37
26	L	401	HEM	FE-NB	-2.71	1.86	1.94
26	j	404	HEM	FE-NB	-2.69	1.86	1.94
26	j	403	HEM	FE-NB	-2.66	1.86	1.94
26	J	403	HEM	FE-NB	-2.65	1.86	1.94
26	J	404	HEM	FE-NB	-2.64	1.86	1.94
26	j	404	HEM	C2A-C3A	-2.62	1.32	1.38
26	J	403	HEM	C2A-C3A	-2.59	1.32	1.38
26	l	401	HEM	CAC-C3C	2.59	1.54	1.47
26	j	404	HEM	CAC-C3C	2.57	1.54	1.47
26	L	401	HEM	CAC-C3C	2.57	1.54	1.47
26	J	404	HEM	C2A-C3A	-2.54	1.32	1.38
26	l	401	HEM	C2A-C3A	-2.53	1.32	1.38
26	L	401	HEM	C2A-C3A	-2.52	1.32	1.38
29	K	603	HEA	C1D-C2D	2.51	1.49	1.44
26	J	404	HEM	CAC-C3C	2.50	1.54	1.47
26	j	403	HEM	CAC-C3C	2.49	1.54	1.47
26	J	403	HEM	CAC-C3C	2.47	1.54	1.47
29	K	602	HEA	C1D-C2D	2.46	1.49	1.44
26	j	403	HEM	C2A-C3A	-2.43	1.32	1.38
29	K	602	HEA	C3C-C2C	-2.40	1.33	1.41
29	K	603	HEA	C3C-C2C	-2.40	1.33	1.41
29	K	602	HEA	C1D-ND	-2.39	1.36	1.40
29	K	603	HEA	C1D-ND	-2.36	1.36	1.40
29	K	602	HEA	FE-NC	2.03	2.01	1.95
26	J	404	HEM	C3D-C2D	-2.02	1.32	1.36
29	K	603	HEA	FE-NC	2.01	2.01	1.95
29	K	603	HEA	CHA-C1A	-2.01	1.34	1.38
26	l	401	HEM	CMB-C2B	2.01	1.54	1.50

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	K	603	HEA	CMD-C2D-C1D	5.83	134.14	125.03
29	K	602	HEA	CMD-C2D-C1D	5.68	133.91	125.03
27	J	405	UQ6	C7-C8-C9	-5.04	120.19	127.42
27	j	405	UQ6	C7-C8-C9	-4.93	120.36	127.42
29	K	603	HEA	CHB-C4A-NA	-4.66	119.38	124.45
29	K	602	HEA	CHB-C4A-NA	-4.44	119.61	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	303	PEF	O2-C10-C11	4.11	120.38	111.48
22	J	406	PEF	O2-C10-C11	4.01	120.15	111.48
22	a	501	PEF	O2-C10-C11	3.95	120.03	111.48
22	J	401	PEF	O2-C10-C11	3.94	120.01	111.48
22	j	407	PEF	O2-C10-C11	3.94	120.01	111.48
22	C	303	PEF	O2-C10-C11	3.90	119.91	111.48
22	A	501	PEF	O2-C10-C11	3.89	119.91	111.48
22	j	401	PEF	O2-C10-C11	3.88	119.88	111.48
22	V	101	PEF	O2-C10-C11	3.87	119.86	111.48
22	H	101	PEF	O2-C10-C11	3.87	119.86	111.48
22	J	402	PEF	O2-C10-C11	3.83	119.76	111.48
22	j	402	PEF	O2-C10-C11	3.78	119.66	111.48
22	j	406	PEF	O2-C10-C11	3.69	119.46	111.48
22	J	407	PEF	O2-C10-C11	3.65	119.38	111.48
22	V	102	PEF	O2-C10-C11	3.36	118.75	111.48
26	L	401	HEM	CAC-C3C-C4C	3.26	132.59	124.82
26	j	403	HEM	CAC-C3C-C4C	3.26	132.59	124.82
26	J	404	HEM	CAC-C3C-C4C	3.24	132.55	124.82
27	J	405	UQ6	C12-C13-C14	-3.18	120.35	127.62
27	J	405	UQ6	C22-C23-C24	-3.14	120.43	127.62
29	K	603	HEA	C12-C11-C3B	3.10	116.97	112.12
22	H	101	PEF	P-O4P-C4	-3.09	106.56	121.26
22	J	406	PEF	P-O4P-C4	-3.08	106.62	121.26
26	l	401	HEM	CAC-C3C-C4C	3.07	132.14	124.82
22	j	402	PEF	P-O4P-C4	-3.06	106.67	121.26
26	j	404	HEM	CAC-C3C-C4C	3.06	132.12	124.82
22	C	303	PEF	P-O4P-C4	-3.05	106.73	121.26
22	j	406	PEF	P-O4P-C4	-3.04	106.77	121.26
22	c	303	PEF	P-O4P-C4	-3.04	106.80	121.26
27	j	405	UQ6	C17-C18-C19	-3.02	120.71	127.62
27	j	405	UQ6	C27-C28-C29	-3.01	120.73	127.62
22	j	407	PEF	P-O4P-C4	-3.01	106.93	121.26
22	J	407	PEF	P-O4P-C4	-3.01	106.94	121.26
22	J	401	PEF	P-O4P-C4	-3.01	106.94	121.26
22	A	501	PEF	P-O4P-C4	-3.00	106.98	121.26
27	J	405	UQ6	C27-C28-C29	-2.99	120.79	127.62
27	j	405	UQ6	C12-C13-C14	-2.98	120.80	127.62
22	V	101	PEF	P-O4P-C4	-2.98	107.06	121.26
22	J	402	PEF	P-O4P-C4	-2.98	107.08	121.26
27	j	405	UQ6	C22-C23-C24	-2.98	120.81	127.62
29	K	603	HEA	C2A-C1A-NA	2.97	113.19	110.32
22	V	102	PEF	P-O4P-C4	-2.97	107.13	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	K	602	HEA	C2A-C1A-NA	2.96	113.18	110.32
22	a	501	PEF	P-O4P-C4	-2.94	107.26	121.26
29	K	603	HEA	CHB-C4A-C3A	2.93	130.14	125.21
27	J	405	UQ6	C17-C18-C19	-2.92	120.94	127.62
22	V	102	PEF	C2-O2-C10	2.89	124.71	117.80
22	j	401	PEF	P-O4P-C4	-2.88	107.56	121.26
27	j	405	UQ6	C25-C24-C26	2.84	120.17	115.23
27	j	405	UQ6	C3M-O3-C3	-2.84	107.03	114.74
29	K	602	HEA	O1D-CGD-CBD	-2.82	114.14	123.09
27	J	405	UQ6	C30-C29-C31	2.81	120.11	115.23
29	K	603	HEA	CHD-C1D-ND	-2.80	120.90	124.37
26	j	404	HEM	CMB-C2B-C1B	-2.79	120.68	125.03
27	J	405	UQ6	C15-C14-C16	2.77	120.03	115.23
26	J	403	HEM	CAC-C3C-C4C	2.77	131.43	124.82
27	j	405	UQ6	C15-C14-C16	2.76	120.02	115.23
22	c	303	PEF	O3-C30-C31	2.76	120.24	111.83
27	J	405	UQ6	C3M-O3-C3	-2.75	107.28	114.74
22	J	402	PEF	O3-C30-C31	2.74	120.18	111.83
26	J	403	HEM	CMB-C2B-C1B	-2.72	120.78	125.03
22	J	406	PEF	O3-C30-C31	2.72	120.14	111.83
29	K	603	HEA	O1D-CGD-CBD	-2.72	114.46	123.09
22	C	303	PEF	O3-C30-C31	2.72	120.12	111.83
22	A	501	PEF	O3-C30-C31	2.71	120.11	111.83
27	j	405	UQ6	C4M-O4-C4	-2.69	107.43	114.74
29	K	602	HEA	CHD-C1D-ND	-2.69	121.04	124.37
22	j	402	PEF	O3-C30-C31	2.68	120.01	111.83
22	H	101	PEF	P-O3P-C1	-2.68	106.00	121.35
22	a	501	PEF	O3-C30-C31	2.68	120.00	111.83
26	j	403	HEM	CAC-C3C-C2C	-2.68	119.73	128.43
26	J	404	HEM	CMB-C2B-C1B	-2.67	120.85	125.03
26	l	401	HEM	CMB-C2B-C1B	-2.67	120.86	125.03
27	j	405	UQ6	C30-C29-C31	2.67	119.86	115.23
22	V	101	PEF	O3-C30-C31	2.67	119.97	111.83
22	j	406	PEF	O3-C30-C31	2.66	119.94	111.83
29	K	602	HEA	CHB-C4A-C3A	2.66	129.69	125.21
22	J	407	PEF	O3-C30-C31	2.64	119.89	111.83
22	J	401	PEF	O3-C30-C31	2.63	119.86	111.83
22	J	401	PEF	P-O3P-C1	-2.63	106.30	121.35
22	H	101	PEF	O3-C30-C31	2.62	119.82	111.83
27	J	405	UQ6	C4M-O4-C4	-2.62	107.64	114.74
22	V	101	PEF	P-O3P-C1	-2.62	106.36	121.35
27	J	405	UQ6	C20-C19-C21	2.61	119.76	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	102	PEF	P-O3P-C1	-2.61	106.42	121.35
22	j	401	PEF	O3-C30-C31	2.61	119.78	111.83
27	j	405	UQ6	C20-C19-C21	2.61	119.75	115.23
22	j	407	PEF	O3-C30-C31	2.60	119.77	111.83
26	L	401	HEM	CAC-C3C-C2C	-2.57	120.06	128.43
22	A	501	PEF	P-O3P-C1	-2.57	106.61	121.35
22	j	407	PEF	P-O3P-C1	-2.57	106.62	121.35
22	V	102	PEF	O3-C30-C31	2.57	119.67	111.83
22	j	406	PEF	P-O3P-C1	-2.57	106.64	121.35
27	J	405	UQ6	C25-C24-C26	2.56	119.67	115.23
22	j	401	PEF	P-O3P-C1	-2.54	106.79	121.35
26	J	404	HEM	CAC-C3C-C2C	-2.54	120.18	128.43
26	l	401	HEM	CAC-C3C-C2C	-2.53	120.19	128.43
22	C	303	PEF	P-O3P-C1	-2.53	106.84	121.35
22	J	402	PEF	P-O3P-C1	-2.52	106.89	121.35
22	J	406	PEF	P-O3P-C1	-2.51	106.97	121.35
27	J	405	UQ6	C10-C9-C11	2.51	119.58	115.23
27	j	405	UQ6	C10-C9-C11	2.50	119.57	115.23
22	j	402	PEF	P-O3P-C1	-2.50	107.01	121.35
29	K	603	HEA	CMB-C2B-C3B	-2.47	125.50	130.28
26	L	401	HEM	CMC-C2C-C3C	-2.47	122.46	128.43
26	j	404	HEM	CAC-C3C-C2C	-2.46	120.42	128.43
22	a	501	PEF	P-O3P-C1	-2.45	107.33	121.35
26	J	403	HEM	CMC-C2C-C3C	-2.43	122.54	128.43
26	j	404	HEM	CMC-C2C-C3C	-2.40	122.63	128.43
22	J	407	PEF	P-O3P-C1	-2.39	107.66	121.35
26	j	403	HEM	CMB-C2B-C1B	-2.38	121.31	125.03
29	K	602	HEA	C1D-C2D-C3D	-2.36	104.50	106.98
22	c	303	PEF	P-O3P-C1	-2.35	107.90	121.35
26	j	403	HEM	CMC-C2C-C3C	-2.33	122.80	128.43
26	J	403	HEM	CAC-C3C-C2C	-2.32	120.88	128.43
26	l	401	HEM	CMC-C2C-C3C	-2.30	122.85	128.43
26	J	403	HEM	CMC-C2C-C1C	2.29	128.76	124.73
29	K	602	HEA	C3D-C4D-ND	2.26	112.53	110.35
27	j	405	UQ6	C36-C34-C35	2.26	119.78	114.59
29	K	602	HEA	CMB-C2B-C3B	-2.23	125.96	130.28
27	J	405	UQ6	C36-C34-C35	2.23	119.72	114.59
29	K	602	HEA	C3C-C4C-NC	2.23	111.67	109.80
26	L	401	HEM	CMB-C2B-C1B	-2.22	121.56	125.03
29	K	602	HEA	C26-C15-C14	-2.22	117.93	123.63
26	L	401	HEM	C3C-C2C-C1C	2.20	109.13	107.05
26	J	404	HEM	CMC-C2C-C3C	-2.18	123.16	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	K	603	HEA	C1D-C2D-C3D	-2.16	104.70	106.98
29	K	602	HEA	C3B-C4B-NB	2.16	112.32	109.84
29	K	603	HEA	C3D-C4D-ND	2.15	112.43	110.35
29	K	602	HEA	C12-C11-C3B	2.14	115.46	112.12
26	j	403	HEM	CMC-C2C-C1C	2.13	128.48	124.73
26	j	403	HEM	CAA-CBA-CGA	-2.13	108.03	113.67
27	J	405	UQ6	C32-C33-C34	-2.11	120.61	127.64
26	j	404	HEM	CMC-C2C-C1C	2.10	128.43	124.73
27	j	405	UQ6	C32-C33-C34	-2.10	120.64	127.64
26	L	401	HEM	CMC-C2C-C1C	2.09	128.41	124.73
29	K	603	HEA	C3B-C4B-NB	2.08	112.23	109.84
29	K	603	HEA	OMA-CMA-C3A	-2.07	120.94	125.62
29	K	603	HEA	CHA-C1A-NA	-2.05	122.22	124.45
29	K	603	HEA	C4B-C3B-C2B	-2.05	104.00	107.44
26	l	401	HEM	CMC-C2C-C1C	2.04	128.33	124.73
26	J	404	HEM	C3C-C2C-C1C	2.03	108.97	107.05
29	K	602	HEA	C4B-C3B-C2B	-2.03	104.03	107.44
26	j	404	HEM	C3C-C2C-C1C	2.01	108.94	107.05
26	L	401	HEM	C1B-NB-C4B	2.00	107.58	105.21

There are no chirality outliers.

All (391) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	501	PEF	C31-C30-O3-C3
22	J	402	PEF	C31-C30-O3-C3
22	J	402	PEF	O5-C30-O3-C3
22	j	401	PEF	C4-O4P-P-O1P
22	j	401	PEF	C4-O4P-P-O3P
23	A	502	PGT	C32-C31-O2-C2
23	A	502	PGT	C1-O3P-P-O2P
23	A	502	PGT	C1-O3P-P-O4P
23	C	302	PGT	C1-O3P-P-O2P
23	C	302	PGT	C1-O3P-P-O4P
23	H	102	PGT	O4P-C4-C5-C6
23	L	402	PGT	C4-C5-C6-O6
23	W	201	PGT	C4-O4P-P-O3P
23	W	201	PGT	O4P-C4-C5-O5
23	a	502	PGT	C1-O3P-P-O1P
23	a	502	PGT	C1-O3P-P-O4P
23	a	502	PGT	C4-O4P-P-O3P
23	a	502	PGT	O4P-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
23	a	502	PGT	O11-C11-O3-C3
23	j	408	PGT	O31-C31-O2-C2
23	j	408	PGT	C1-O3P-P-O2P
23	j	408	PGT	C1-O3P-P-O4P
23	j	408	PGT	C4-O4P-P-O3P
23	j	408	PGT	C4-O4P-P-O1P
23	j	408	PGT	O4P-C4-C5-O5
23	j	408	PGT	C4-C5-C6-O6
25	E	101	PCF	C1-O11-P-O12
25	W	203	PCF	O21-C2-C3-O31
26	J	403	HEM	C3D-CAD-CBD-CGD
26	L	401	HEM	C2C-C3C-CAC-CBC
26	L	401	HEM	C4C-C3C-CAC-CBC
26	j	403	HEM	C2B-C3B-CAB-CBB
26	j	404	HEM	C2C-C3C-CAC-CBC
26	j	404	HEM	C4C-C3C-CAC-CBC
26	l	401	HEM	C2A-CAA-CBA-CGA
26	l	401	HEM	C2B-C3B-CAB-CBB
26	l	401	HEM	C2C-C3C-CAC-CBC
27	J	405	UQ6	C30-C29-C31-C32
27	j	405	UQ6	C23-C24-C26-C27
27	j	405	UQ6	C25-C24-C26-C27
29	K	602	HEA	C4C-C3C-CAC-CBC
29	K	602	HEA	C17-C18-C19-C20
29	K	602	HEA	C17-C18-C19-C27
29	K	602	HEA	C21-C22-C23-C24
29	K	603	HEA	C13-C14-C15-C26
29	K	603	HEA	C17-C18-C19-C27
22	A	501	PEF	O5-C30-O3-C3
29	K	602	HEA	C21-C22-C23-C25
23	L	402	PGT	O11-C11-O3-C3
25	W	202	PCF	O32-C31-O31-C3
23	A	502	PGT	O31-C31-O2-C2
22	H	101	PEF	C31-C30-O3-C3
23	L	402	PGT	C12-C11-O3-C3
23	a	502	PGT	C12-C11-O3-C3
25	W	202	PCF	C32-C31-O31-C3
23	j	408	PGT	C32-C31-O2-C2
27	J	405	UQ6	C15-C14-C16-C17
29	K	602	HEA	C26-C15-C16-C17
27	J	405	UQ6	C13-C14-C16-C17
27	J	405	UQ6	C28-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
29	K	602	HEA	C18-C19-C20-C21
29	K	603	HEA	C18-C19-C20-C21
29	K	603	HEA	C3A-C2A-CAA-CBA
29	K	602	HEA	C13-C14-C15-C26
22	H	101	PEF	O5-C30-O3-C3
23	W	201	PGT	O11-C11-O3-C3
29	K	603	HEA	C21-C22-C23-C25
23	H	102	PGT	O4P-C4-C5-O5
23	L	402	PGT	O4P-C4-C5-O5
23	a	502	PGT	O4P-C4-C5-O5
23	W	201	PGT	C12-C11-O3-C3
27	j	405	UQ6	C15-C14-C16-C17
29	K	602	HEA	C14-C15-C16-C17
27	J	405	UQ6	C9-C11-C12-C13
27	J	405	UQ6	C24-C26-C27-C28
27	j	405	UQ6	C9-C11-C12-C13
27	j	405	UQ6	C19-C21-C22-C23
27	j	405	UQ6	C29-C31-C32-C33
26	j	403	HEM	C1A-C2A-CAA-CBA
25	E	101	PCF	C2-C1-O11-P
26	j	403	HEM	C2A-CAA-CBA-CGA
29	K	602	HEA	C2A-CAA-CBA-CGA
23	L	402	PGT	C32-C31-O2-C2
23	a	502	PGT	C32-C31-O2-C2
29	K	603	HEA	C1A-C2A-CAA-CBA
23	L	402	PGT	O4P-C4-C5-C6
23	W	201	PGT	O4P-C4-C5-C6
23	H	102	PGT	C12-C11-O3-C3
25	E	101	PCF	C11-C12-N-C15
27	j	405	UQ6	C13-C14-C16-C17
25	c	302	PCF	C22-C23-C24-C25
23	j	408	PGT	C11-C12-C13-C14
22	A	501	PEF	O3P-C1-C2-O2
25	E	101	PCF	O21-C2-C3-O31
23	L	402	PGT	O5-C5-C6-O6
23	L	402	PGT	O31-C31-O2-C2
27	J	405	UQ6	C19-C21-C22-C23
27	j	405	UQ6	C14-C16-C17-C18
25	E	101	PCF	C11-C12-N-C13
22	j	407	PEF	C10-C11-C12-C13
23	W	201	PGT	C31-C32-C33-C34
23	H	102	PGT	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
23	A	502	PGT	C2-C1-O3P-P
22	J	401	PEF	C10-C11-C12-C13
22	V	101	PEF	C30-C31-C32-C33
22	a	501	PEF	C30-C31-C32-C33
26	j	403	HEM	C3A-C2A-CAA-CBA
23	A	502	PGT	O4P-C4-C5-O5
23	a	502	PGT	O31-C31-O2-C2
26	J	404	HEM	C4D-C3D-CAD-CBD
22	c	303	PEF	C10-C11-C12-C13
23	A	502	PGT	O4P-C4-C5-C6
25	c	302	PCF	C11-C12-N-C15
23	W	201	PGT	C11-C12-C13-C14
29	K	603	HEA	C27-C19-C20-C21
23	j	408	PGT	C5-C4-O4P-P
26	J	404	HEM	C2D-C3D-CAD-CBD
26	l	401	HEM	C3D-CAD-CBD-CGD
23	A	502	PGT	C4-C5-C6-O6
23	W	201	PGT	C32-C31-O2-C2
25	c	302	PCF	C11-C12-N-C13
25	c	302	PCF	C11-C12-N-C14
23	C	302	PGT	C15-C16-C17-C18
23	W	201	PGT	C43-C44-C45-C46
23	a	502	PGT	C18-C19-C20-C21
25	W	203	PCF	C22-C23-C24-C25
25	E	101	PCF	C25-C26-C27-C28
23	j	408	PGT	O5-C5-C6-O6
23	a	502	PGT	C35-C36-C37-C38
25	W	202	PCF	C24-C25-C26-C27
25	c	302	PCF	C32-C33-C34-C35
22	C	303	PEF	C34-C35-C36-C37
23	A	502	PGT	C13-C14-C15-C16
22	j	406	PEF	C12-C13-C14-C15
23	A	502	PGT	C36-C37-C38-C39
23	A	502	PGT	C35-C36-C37-C38
22	c	303	PEF	C38-C39-C40-C41
25	E	101	PCF	C11-C12-N-C14
29	K	602	HEA	C2C-C3C-CAC-CBC
23	C	302	PGT	C32-C31-O2-C2
22	c	303	PEF	C39-C40-C41-C42
29	K	603	HEA	C3D-CAD-CBD-CGD
22	V	102	PEF	C15-C16-C17-C18
23	H	102	PGT	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	c	303	PEF	C35-C36-C37-C38
23	W	201	PGT	O31-C31-O2-C2
22	C	303	PEF	C14-C15-C16-C17
22	J	401	PEF	C15-C16-C17-C18
22	C	303	PEF	C39-C40-C41-C42
23	H	102	PGT	C38-C39-C40-C41
26	J	404	HEM	C2C-C3C-CAC-CBC
26	L	401	HEM	C2B-C3B-CAB-CBB
26	j	404	HEM	C2B-C3B-CAB-CBB
26	j	403	HEM	C4B-C3B-CAB-CBB
26	l	401	HEM	C4B-C3B-CAB-CBB
22	j	406	PEF	O2-C2-C3-O3
26	j	403	HEM	C4D-C3D-CAD-CBD
22	A	501	PEF	O3P-C1-C2-C3
22	H	101	PEF	O3P-C1-C2-C3
22	J	402	PEF	O3P-C1-C2-C3
23	C	302	PGT	O3P-C1-C2-C3
23	C	302	PGT	O31-C31-O2-C2
22	a	501	PEF	C15-C16-C17-C18
22	J	407	PEF	C14-C15-C16-C17
23	j	408	PGT	C35-C36-C37-C38
22	A	501	PEF	C1-C2-C3-O3
22	j	407	PEF	C1-C2-C3-O3
25	E	101	PCF	C1-C2-C3-O31
25	W	203	PCF	C1-C2-C3-O31
22	C	303	PEF	C36-C37-C38-C39
23	C	302	PGT	O4P-C4-C5-O5
22	C	303	PEF	C10-C11-C12-C13
23	H	102	PGT	C31-C32-C33-C34
23	L	402	PGT	C3-C2-O2-C31
22	a	501	PEF	C16-C17-C18-C19
23	j	408	PGT	C33-C34-C35-C36
29	K	602	HEA	C2A-C3A-CMA-OMA
27	j	405	UQ6	C18-C19-C21-C22
22	A	501	PEF	O2-C2-C3-O3
22	C	303	PEF	O2-C2-C3-O3
22	V	101	PEF	O2-C2-C3-O3
22	j	407	PEF	O2-C2-C3-O3
23	L	402	PGT	C36-C37-C38-C39
22	H	101	PEF	C37-C38-C39-C40
29	K	603	HEA	C21-C22-C23-C24
22	A	501	PEF	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	j	405	UQ6	C20-C19-C21-C22
23	H	102	PGT	O5-C5-C6-O6
26	j	403	HEM	C2D-C3D-CAD-CBD
23	W	201	PGT	C23-C24-C25-C26
22	a	501	PEF	C33-C34-C35-C36
22	C	303	PEF	O3P-C1-C2-C3
23	L	402	PGT	O3P-C1-C2-C3
23	H	102	PGT	C13-C14-C15-C16
23	L	402	PGT	C11-C12-C13-C14
22	C	303	PEF	C1-C2-C3-O3
22	j	406	PEF	C1-C2-C3-O3
23	A	502	PGT	C1-C2-C3-O3
22	j	401	PEF	C37-C38-C39-C40
29	K	602	HEA	C27-C19-C20-C21
22	J	407	PEF	O3P-C1-C2-O2
22	V	102	PEF	O3P-C1-C2-O2
23	L	402	PGT	O3P-C1-C2-O2
26	J	403	HEM	C2A-CAA-CBA-CGA
26	j	403	HEM	C3D-CAD-CBD-CGD
22	J	406	PEF	O2-C2-C3-O3
23	A	502	PGT	O2-C2-C3-O3
22	c	303	PEF	C37-C38-C39-C40
22	j	401	PEF	C14-C15-C16-C17
23	A	502	PGT	C34-C35-C36-C37
27	J	405	UQ6	C14-C16-C17-C18
22	j	407	PEF	C30-C31-C32-C33
23	j	408	PGT	O4P-C4-C5-C6
22	J	407	PEF	O3P-C1-C2-C3
22	a	501	PEF	O3P-C1-C2-C3
23	A	502	PGT	O3P-C1-C2-C3
23	H	102	PGT	O3P-C1-C2-C3
22	A	501	PEF	C30-C31-C32-C33
22	V	102	PEF	C1-C2-O2-C10
23	a	502	PGT	C3-C2-O2-C31
22	j	401	PEF	C33-C34-C35-C36
22	C	303	PEF	O3P-C1-C2-O2
22	H	101	PEF	O3P-C1-C2-O2
23	A	502	PGT	O3P-C1-C2-O2
23	H	102	PGT	O3P-C1-C2-O2
22	a	501	PEF	C35-C36-C37-C38
22	V	102	PEF	C1-C2-C3-O3
23	W	201	PGT	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
22	a	501	PEF	C10-C11-C12-C13
26	J	403	HEM	C4C-C3C-CAC-CBC
26	j	403	HEM	C4C-C3C-CAC-CBC
26	j	404	HEM	C4B-C3B-CAB-CBB
26	l	401	HEM	C4C-C3C-CAC-CBC
25	W	203	PCF	C32-C31-O31-C3
23	L	402	PGT	C14-C15-C16-C17
22	j	402	PEF	O2-C2-C3-O3
23	W	201	PGT	O2-C2-C3-O3
25	W	202	PCF	O21-C2-C3-O31
22	J	401	PEF	C31-C32-C33-C34
23	a	502	PGT	C2-C1-O3P-P
25	E	101	PCF	O13-C11-C12-N
25	W	202	PCF	O13-C11-C12-N
25	W	203	PCF	O13-C11-C12-N
25	c	302	PCF	O13-C11-C12-N
23	A	502	PGT	O5-C5-C6-O6
22	J	401	PEF	O3P-C1-C2-C3
22	j	401	PEF	O3P-C1-C2-C3
22	j	407	PEF	O3P-C1-C2-C3
25	c	302	PCF	C34-C35-C36-C37
25	c	302	PCF	C21-C22-C23-C24
23	A	502	PGT	C5-C4-O4P-P
22	J	401	PEF	O3P-C1-C2-O2
22	J	402	PEF	O3P-C1-C2-O2
22	a	501	PEF	O3P-C1-C2-O2
22	j	401	PEF	O3P-C1-C2-O2
22	j	407	PEF	O3P-C1-C2-O2
23	C	302	PGT	O3P-C1-C2-O2
25	W	203	PCF	O32-C31-O31-C3
25	W	202	PCF	C22-C23-C24-C25
29	K	602	HEA	C4A-C3A-CMA-OMA
22	V	102	PEF	O2-C2-C3-O3
22	J	406	PEF	C1-C2-C3-O3
22	V	101	PEF	C1-C2-C3-O3
25	W	202	PCF	C1-C2-C3-O31
23	A	502	PGT	C37-C38-C39-C40
23	a	502	PGT	C12-C13-C14-C15
22	a	501	PEF	C37-C38-C39-C40
23	A	502	PGT	C32-C33-C34-C35
22	H	101	PEF	C31-C32-C33-C34
29	K	602	HEA	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
22	H	101	PEF	C1-O3P-P-O1P
22	J	401	PEF	C4-O4P-P-O1P
22	J	402	PEF	C4-O4P-P-O1P
22	c	303	PEF	C1-O3P-P-O4P
23	W	201	PGT	C1-O3P-P-O1P
23	W	201	PGT	C4-O4P-P-O1P
23	a	502	PGT	C1-O3P-P-O2P
23	a	502	PGT	C4-O4P-P-O1P
23	j	408	PGT	C4-O4P-P-O2P
25	E	101	PCF	C11-O13-P-O12
23	A	502	PGT	C17-C18-C19-C20
25	W	203	PCF	C25-C26-C27-C28
22	V	102	PEF	C11-C10-O2-C2
25	W	203	PCF	C2-C1-O11-P
25	W	202	PCF	C21-C22-C23-C24
23	a	502	PGT	C15-C16-C17-C18
22	V	102	PEF	C31-C32-C33-C34
22	V	101	PEF	O3P-C1-C2-C3
22	V	102	PEF	O4-C10-O2-C2
23	W	201	PGT	C5-C4-O4P-P
25	c	302	PCF	C2-C1-O11-P
23	L	402	PGT	O2-C2-C3-O3
23	A	502	PGT	C43-C44-C45-C46
22	j	401	PEF	C10-C11-C12-C13
23	a	502	PGT	C44-C45-C46-C47
23	j	408	PGT	C12-C11-O3-C3
26	J	404	HEM	C4C-C3C-CAC-CBC
26	L	401	HEM	C4B-C3B-CAB-CBB
23	C	302	PGT	C18-C19-C20-C21
25	c	302	PCF	C39-C40-C41-C42
22	c	303	PEF	C16-C17-C18-C19
23	j	408	PGT	O11-C11-O3-C3
23	W	201	PGT	C22-C23-C24-C25
22	J	407	PEF	C11-C12-C13-C14
22	c	303	PEF	C2-C1-O3P-P
29	K	603	HEA	CAD-CBD-CGD-O1D
23	a	502	PGT	C37-C38-C39-C40
26	j	404	HEM	CAA-CBA-CGA-O1A
29	K	603	HEA	CAA-CBA-CGA-O1A
23	A	502	PGT	C12-C13-C14-C15
23	A	502	PGT	C42-C43-C44-C45
26	J	404	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
23	H	102	PGT	C17-C18-C19-C20
26	j	403	HEM	CAD-CBD-CGD-O1D
29	K	603	HEA	CAD-CBD-CGD-O2D
25	c	302	PCF	C3-C2-O21-C21
29	K	602	HEA	CAA-CBA-CGA-O1A
29	K	603	HEA	C2C-C3C-CAC-CBC
26	J	404	HEM	CAD-CBD-CGD-O2D
26	L	401	HEM	CAA-CBA-CGA-O2A
22	j	402	PEF	C11-C12-C13-C14
23	L	402	PGT	C2-C1-O3P-P
29	K	602	HEA	C3D-CAD-CBD-CGD
29	K	603	HEA	C2A-CAA-CBA-CGA
26	j	403	HEM	CAA-CBA-CGA-O1A
26	l	401	HEM	CAA-CBA-CGA-O2A
23	W	201	PGT	C35-C36-C37-C38
26	j	403	HEM	CAD-CBD-CGD-O2D
26	l	401	HEM	CAD-CBD-CGD-O2D
27	J	405	UQ6	C20-C19-C21-C22
22	j	401	PEF	C13-C14-C15-C16
22	J	407	PEF	C15-C16-C17-C18
22	J	407	PEF	O4-C10-O2-C2
26	j	404	HEM	CAA-CBA-CGA-O2A
22	J	406	PEF	C13-C14-C15-C16
26	J	404	HEM	CAD-CBD-CGD-O1D
22	H	101	PEF	C36-C37-C38-C39
29	K	603	HEA	CAA-CBA-CGA-O2A
29	K	603	HEA	C16-C17-C18-C19
22	V	101	PEF	O3P-C1-C2-O2
29	K	603	HEA	C4C-C3C-CAC-CBC
26	J	404	HEM	CAA-CBA-CGA-O2A
29	K	603	HEA	C11-C12-C13-C14
26	l	401	HEM	CAD-CBD-CGD-O1D
25	W	203	PCF	O11-C1-C2-C3
23	L	402	PGT	O2-C31-C32-C33
22	a	501	PEF	C2-C1-O3P-P
25	E	101	PCF	C32-C33-C34-C35
22	c	303	PEF	C36-C37-C38-C39
23	a	502	PGT	C43-C44-C45-C46
23	C	302	PGT	C38-C39-C40-C41
23	W	201	PGT	C32-C33-C34-C35
26	l	401	HEM	CAA-CBA-CGA-O1A
23	L	402	PGT	C16-C17-C18-C19

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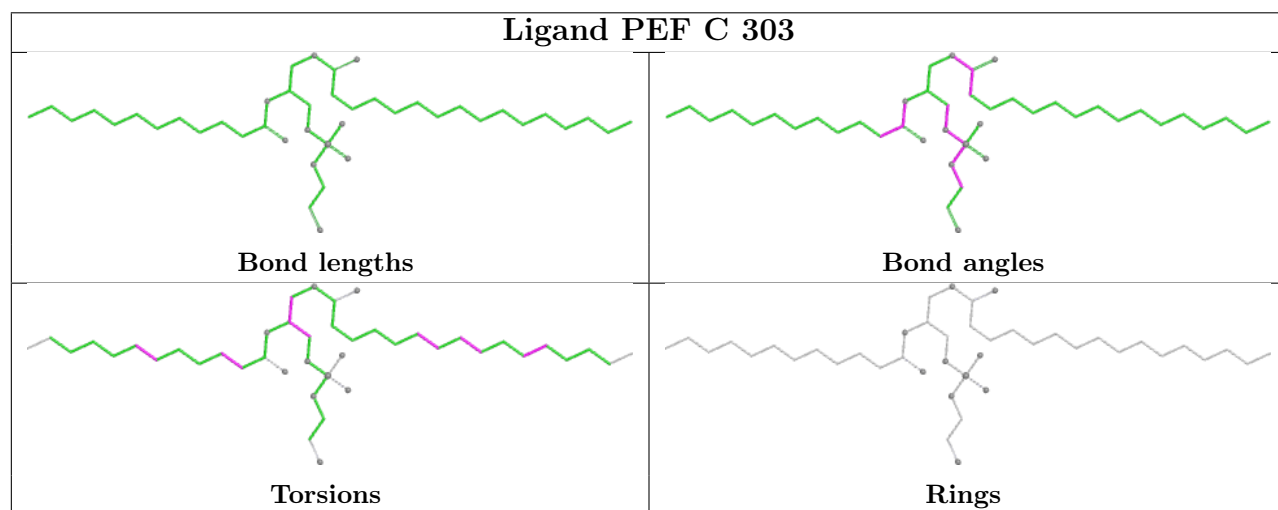
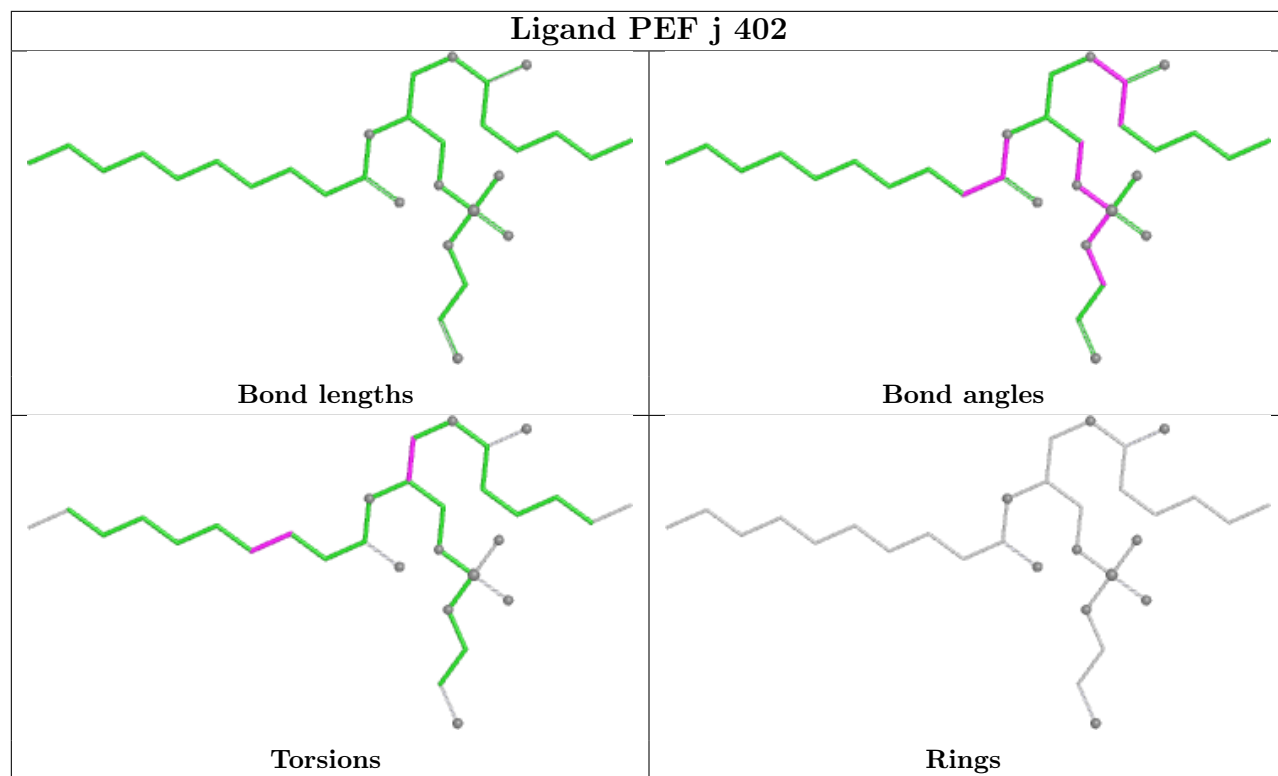
Mol	Chain	Res	Type	Atoms
23	L	402	PGT	C31-C32-C33-C34
22	V	102	PEF	O3P-C1-C2-C3
29	K	602	HEA	CAA-CBA-CGA-O2A
22	J	401	PEF	C36-C37-C38-C39
22	J	407	PEF	C11-C10-O2-C2
26	L	401	HEM	CAA-CBA-CGA-O1A
22	H	101	PEF	C34-C35-C36-C37
23	L	402	PGT	C13-C14-C15-C16
23	j	408	PGT	O3P-C1-C2-O2
22	j	402	PEF	C1-C2-C3-O3
23	W	201	PGT	C17-C18-C19-C20
23	W	201	PGT	C19-C20-C21-C22
23	H	102	PGT	C16-C17-C18-C19
22	J	406	PEF	O3P-C1-C2-C3
22	J	401	PEF	C33-C34-C35-C36
23	C	302	PGT	C1-C2-O2-C31
25	W	203	PCF	C23-C24-C25-C26
29	K	602	HEA	CAD-CBD-CGD-O2D
26	J	403	HEM	C1A-C2A-CAA-CBA
25	c	302	PCF	C33-C34-C35-C36
23	C	302	PGT	C20-C21-C22-C23
22	J	401	PEF	C13-C14-C15-C16
22	c	303	PEF	O3P-C1-C2-O2
25	E	101	PCF	C41-C42-C43-C44
23	W	201	PGT	C12-C13-C14-C15
27	J	405	UQ6	C18-C19-C21-C22
22	J	401	PEF	C38-C39-C40-C41
22	J	407	PEF	C10-C11-C12-C13
25	E	101	PCF	C22-C23-C24-C25
27	j	405	UQ6	C6-C7-C8-C9
22	J	401	PEF	C30-C31-C32-C33
22	a	501	PEF	C32-C33-C34-C35
23	a	502	PGT	C41-C42-C43-C44
25	W	203	PCF	C27-C28-C29-C30
25	c	302	PCF	C29-C30-C47-C48
26	j	404	HEM	CAD-CBD-CGD-O2D
25	c	302	PCF	C31-C32-C33-C34

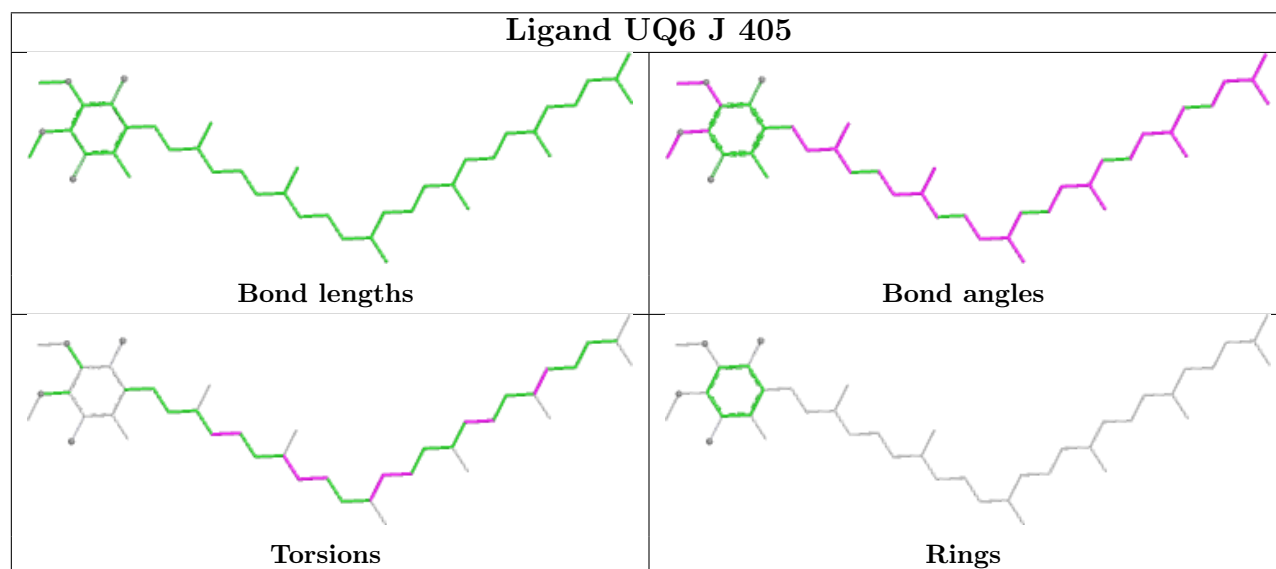
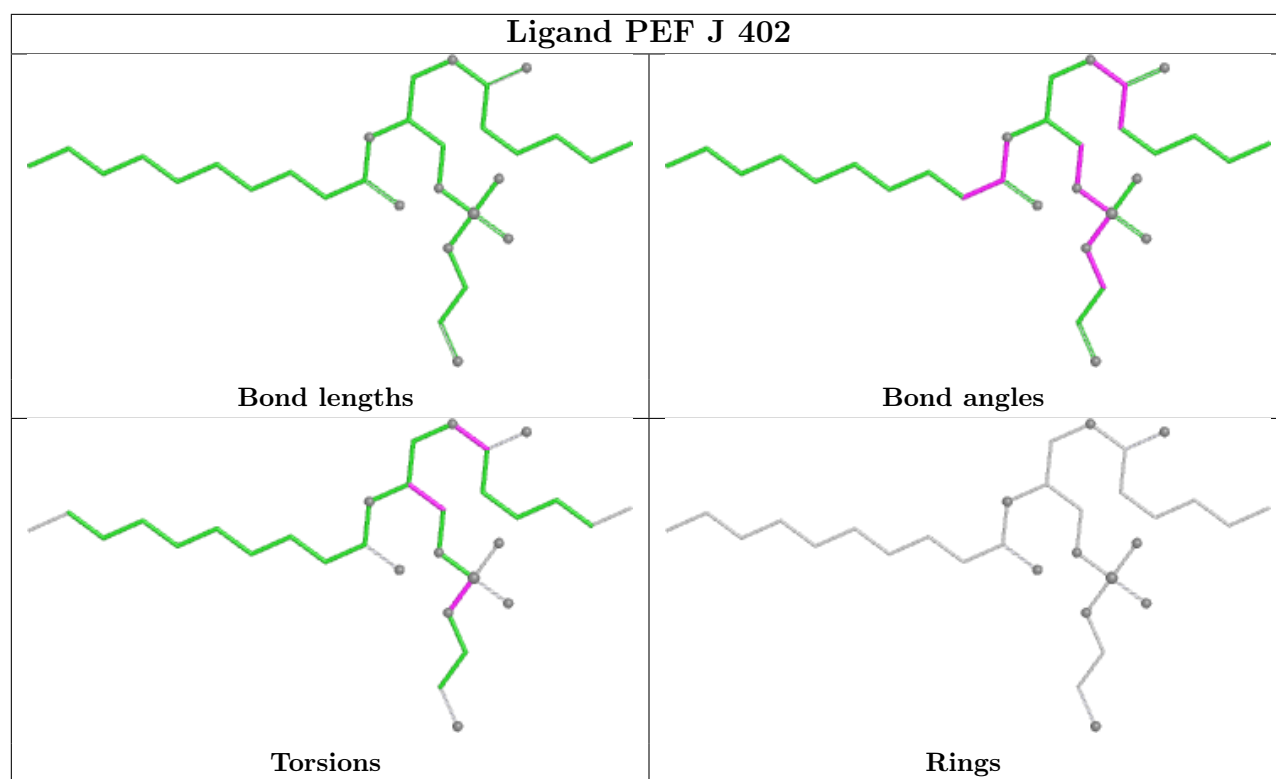
There are no ring outliers.

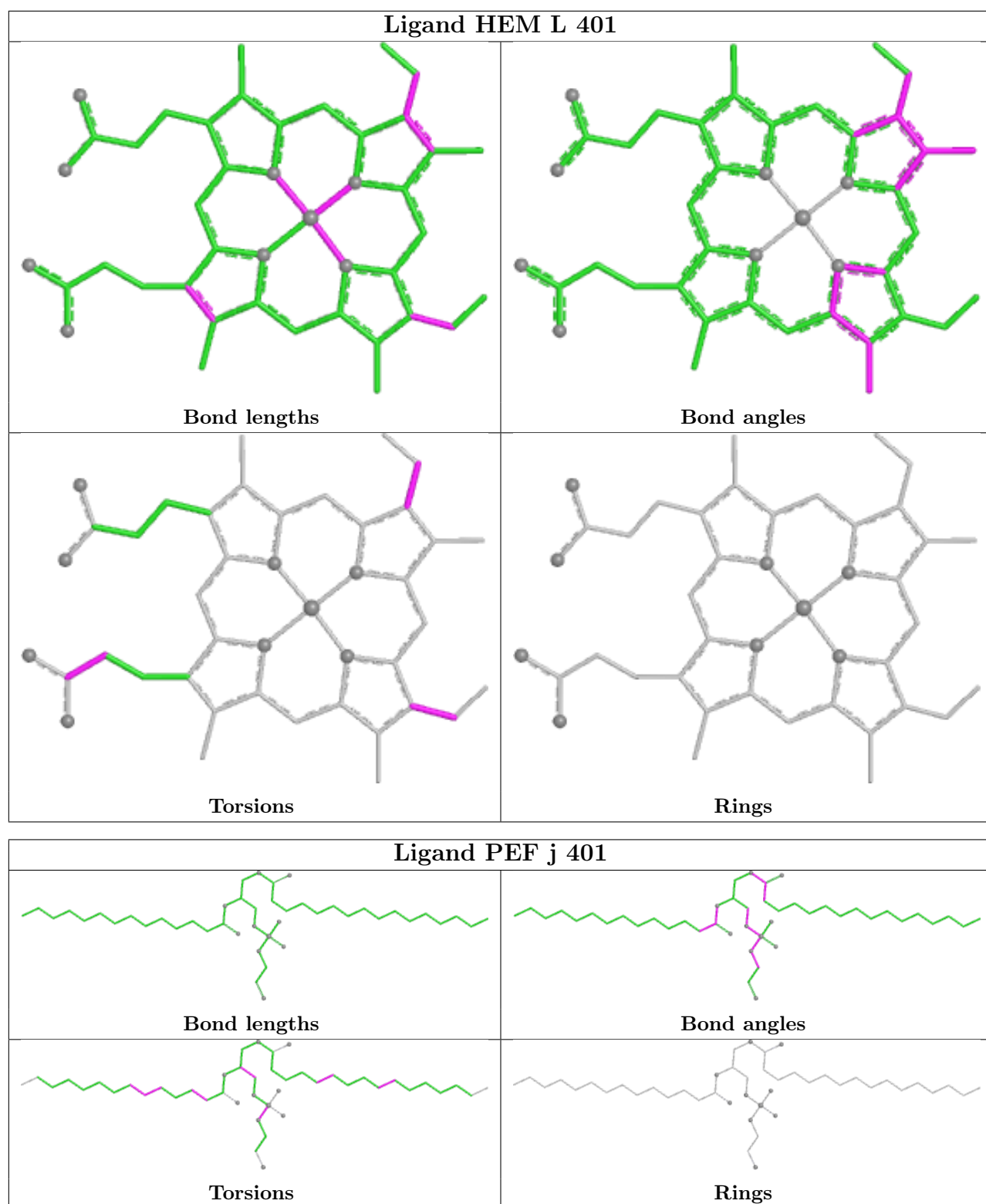
31 monomers are involved in 110 short contacts:

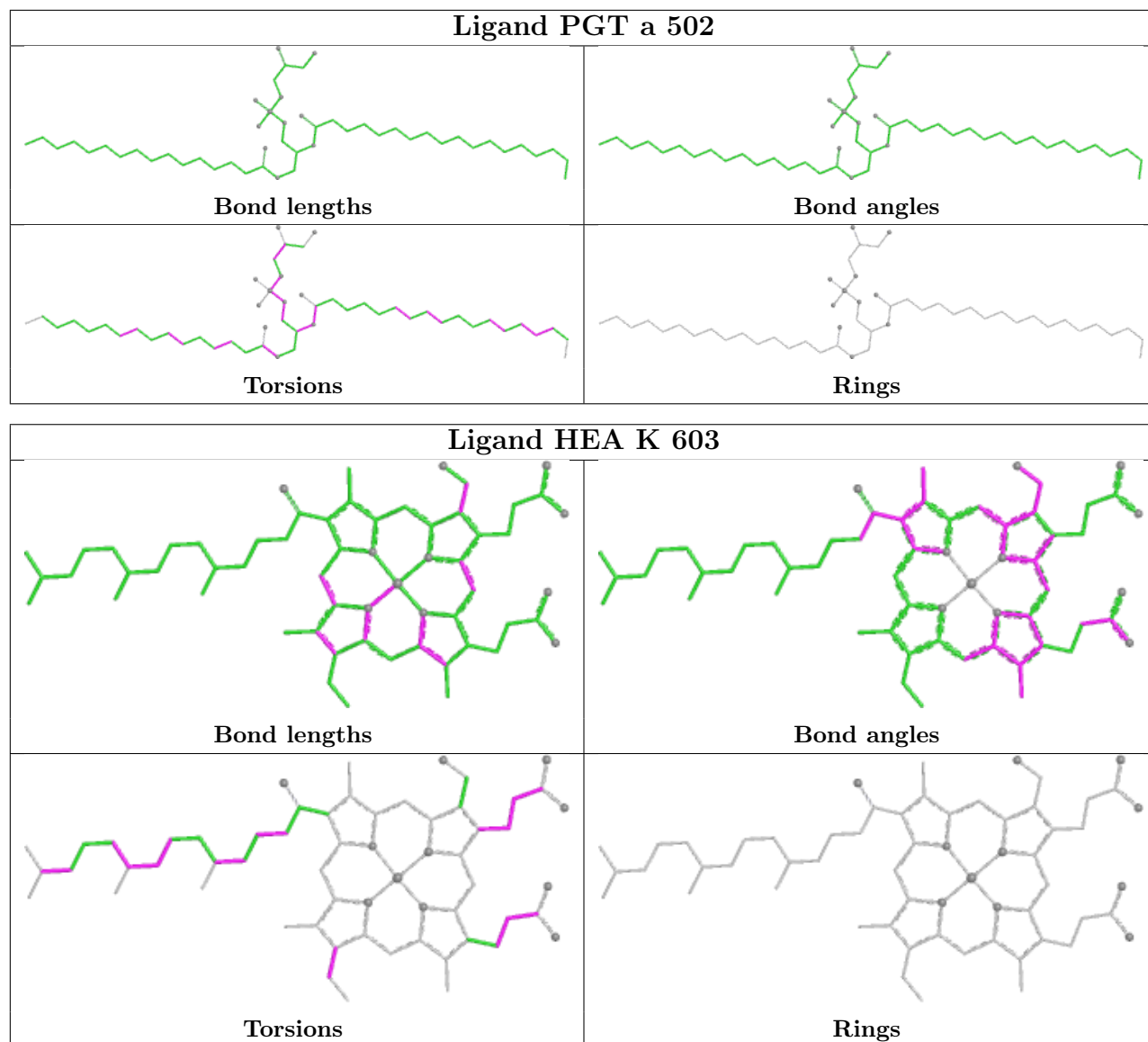
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	303	PEF	1	0
27	J	405	UQ6	4	0
26	L	401	HEM	6	0
22	j	401	PEF	2	0
23	a	502	PGT	2	0
29	K	603	HEA	14	0
26	j	404	HEM	7	0
22	c	303	PEF	5	0
26	J	404	HEM	6	0
26	l	401	HEM	13	0
24	C	301	FES	2	0
22	J	407	PEF	1	0
23	C	302	PGT	1	0
26	J	403	HEM	3	0
22	H	101	PEF	4	0
22	V	101	PEF	1	0
22	J	401	PEF	1	0
22	a	501	PEF	1	0
27	j	405	UQ6	4	0
22	j	406	PEF	4	0
29	K	602	HEA	9	0
23	j	408	PGT	1	0
23	H	102	PGT	1	0
23	A	502	PGT	4	0
22	A	501	PEF	2	0
24	c	301	FES	2	0
25	W	202	PCF	1	0
22	V	102	PEF	1	0
25	c	302	PCF	1	0
23	W	201	PGT	3	0
26	j	403	HEM	5	0

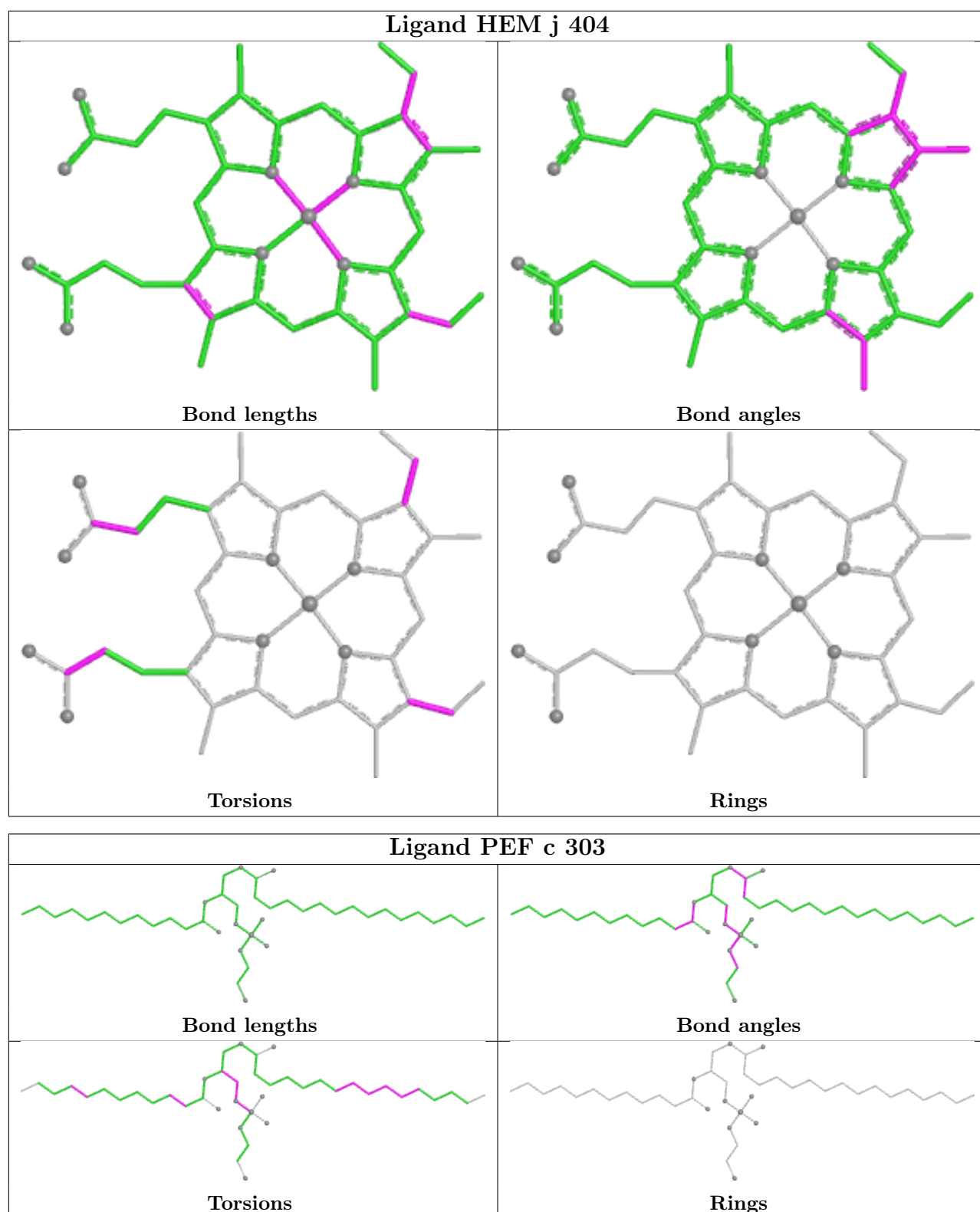
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

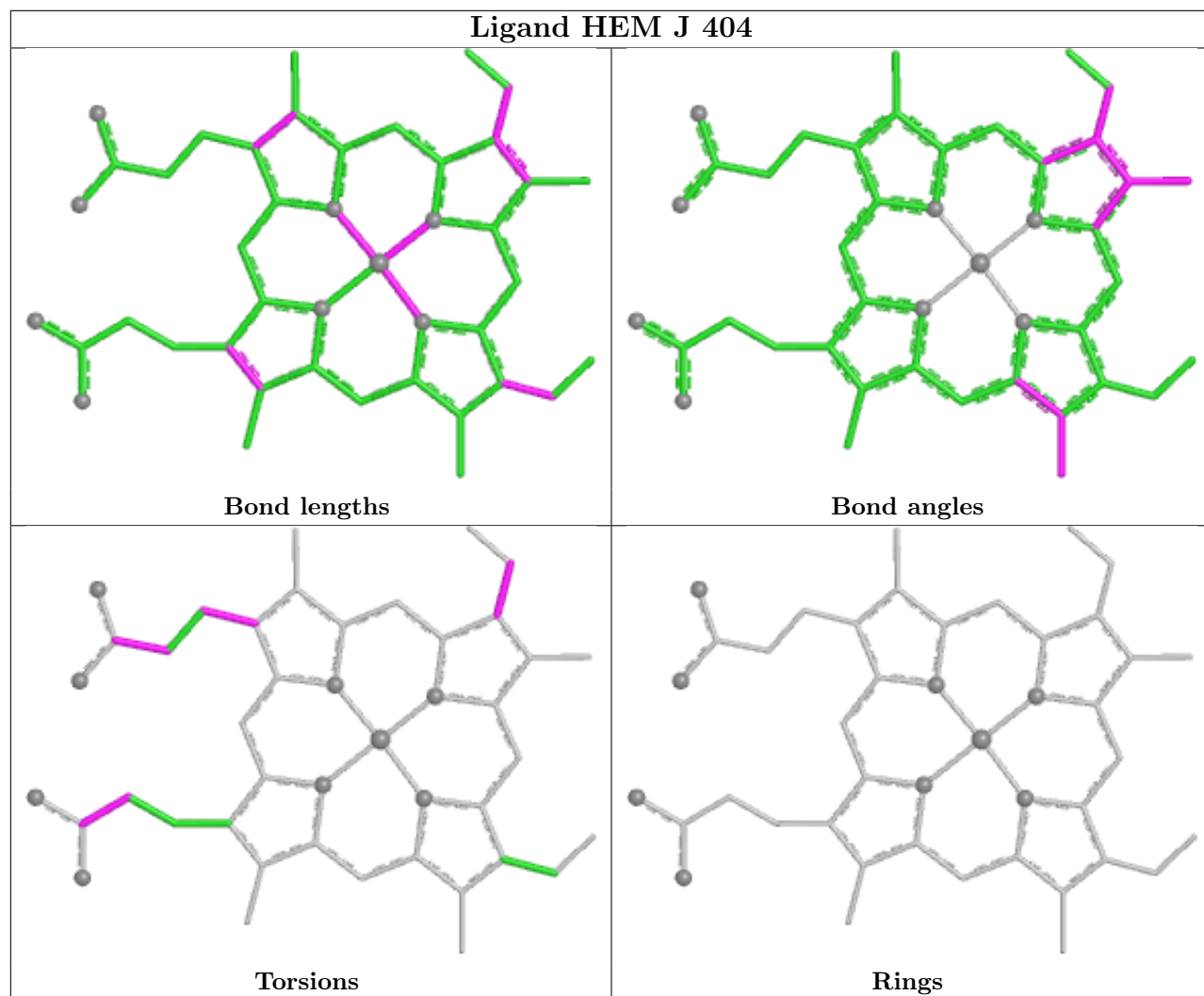


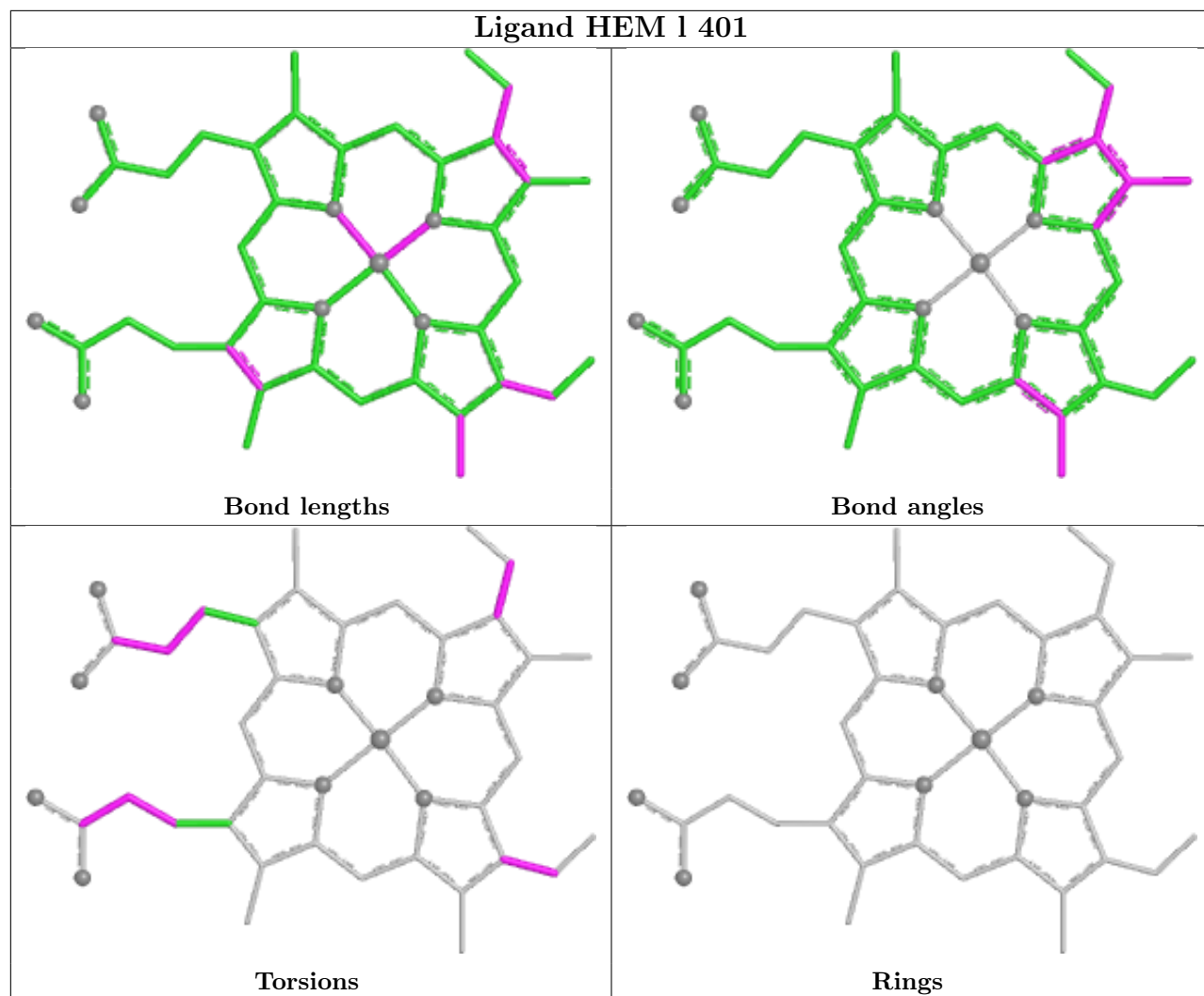


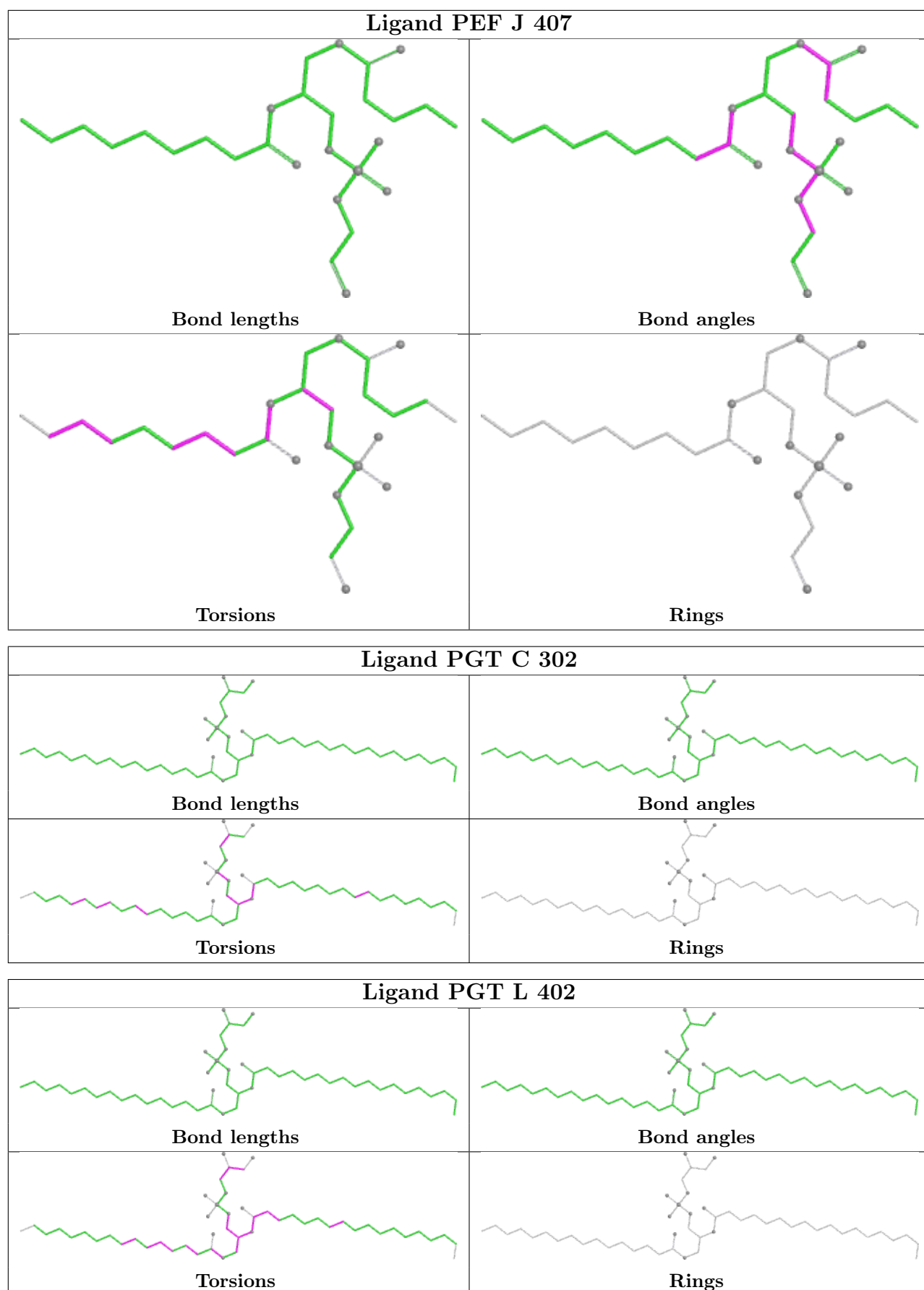


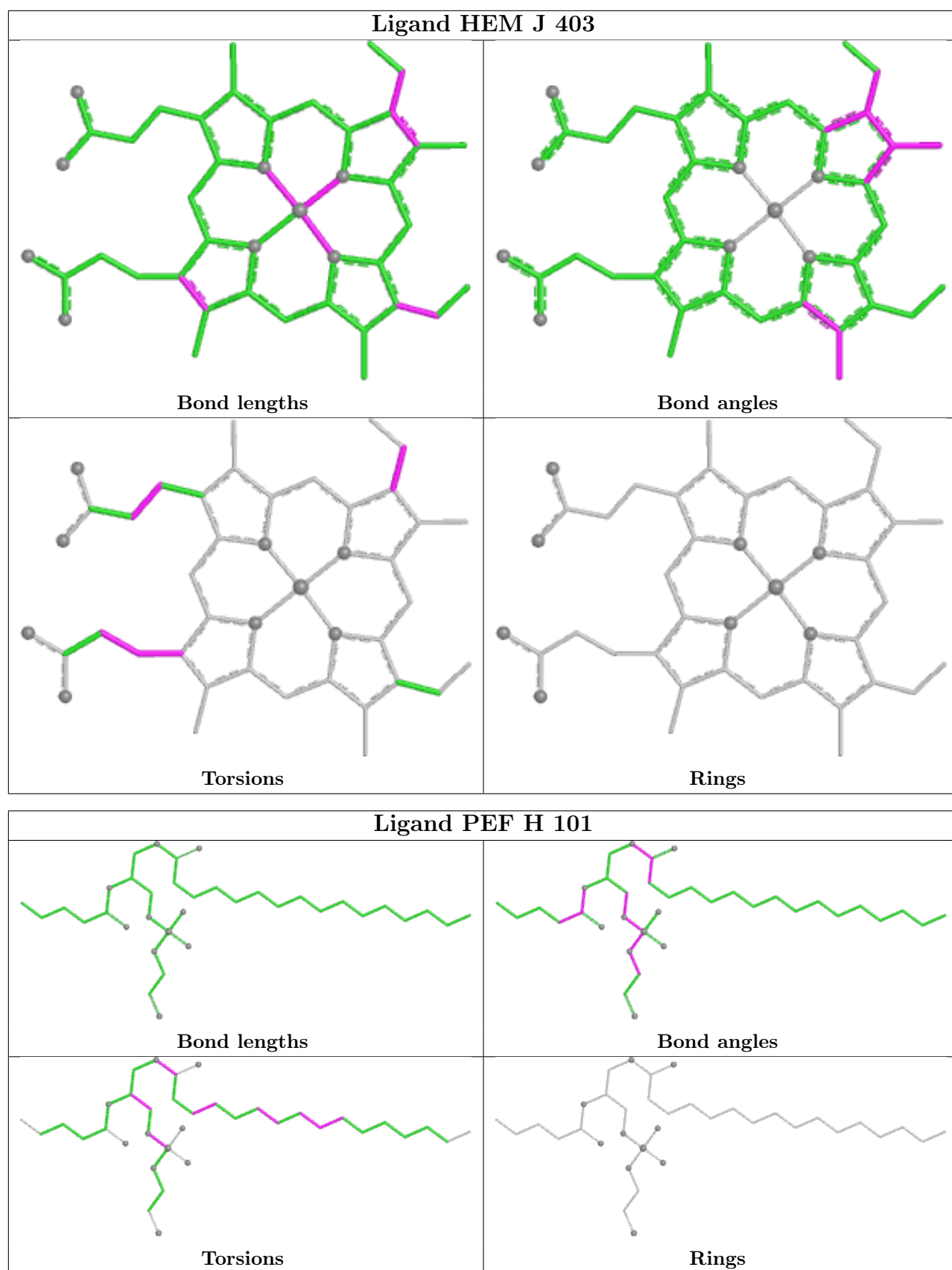


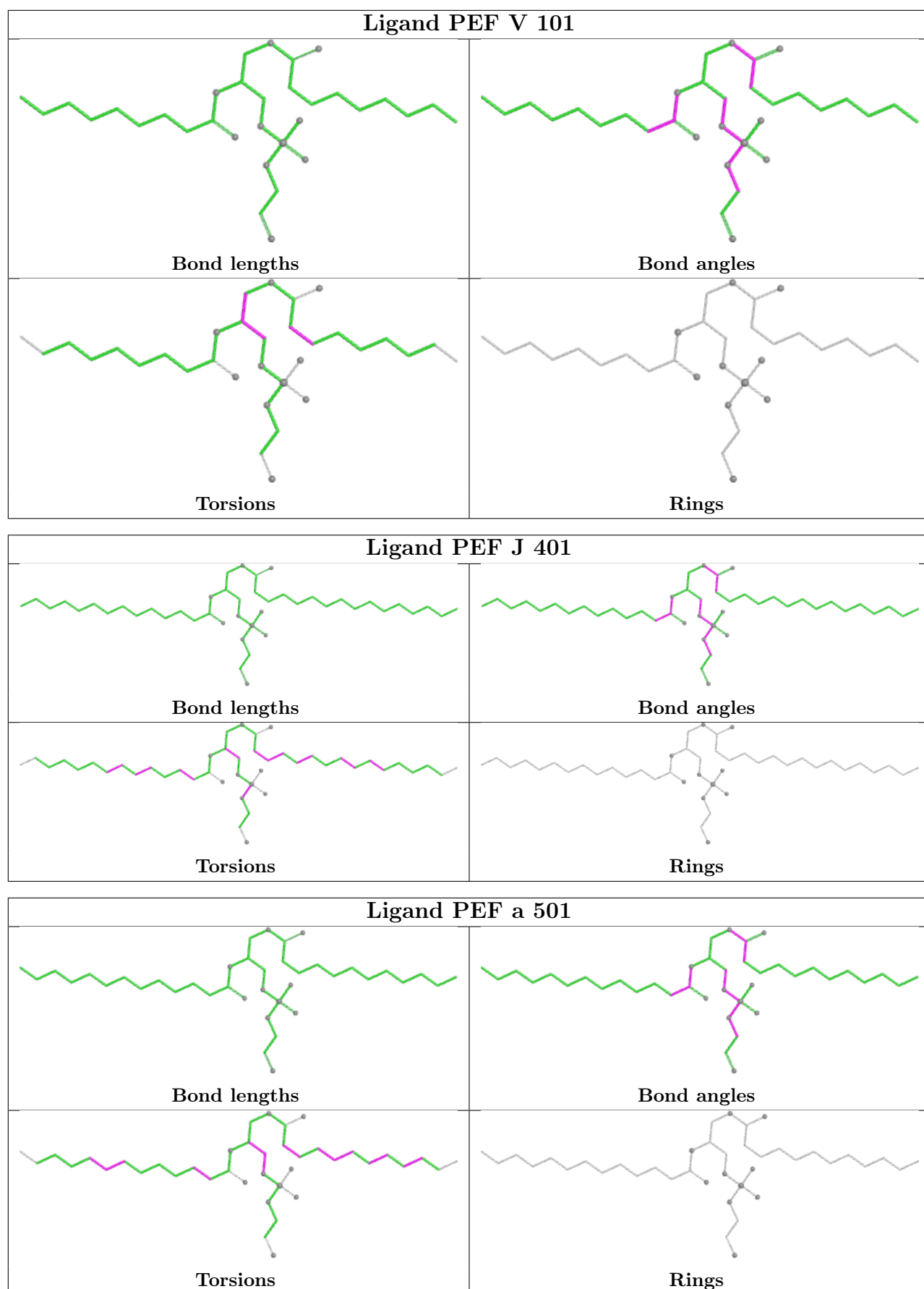


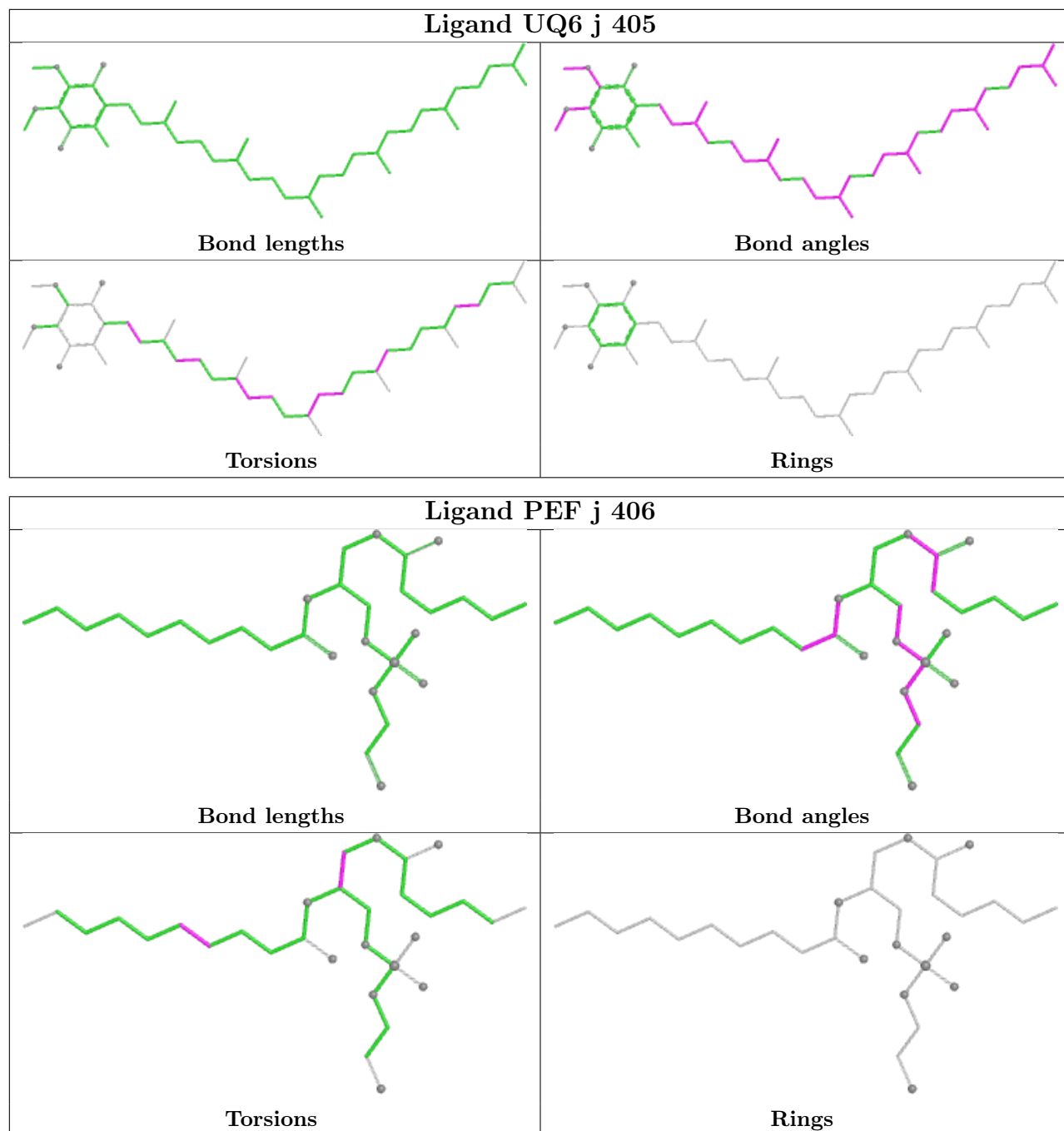


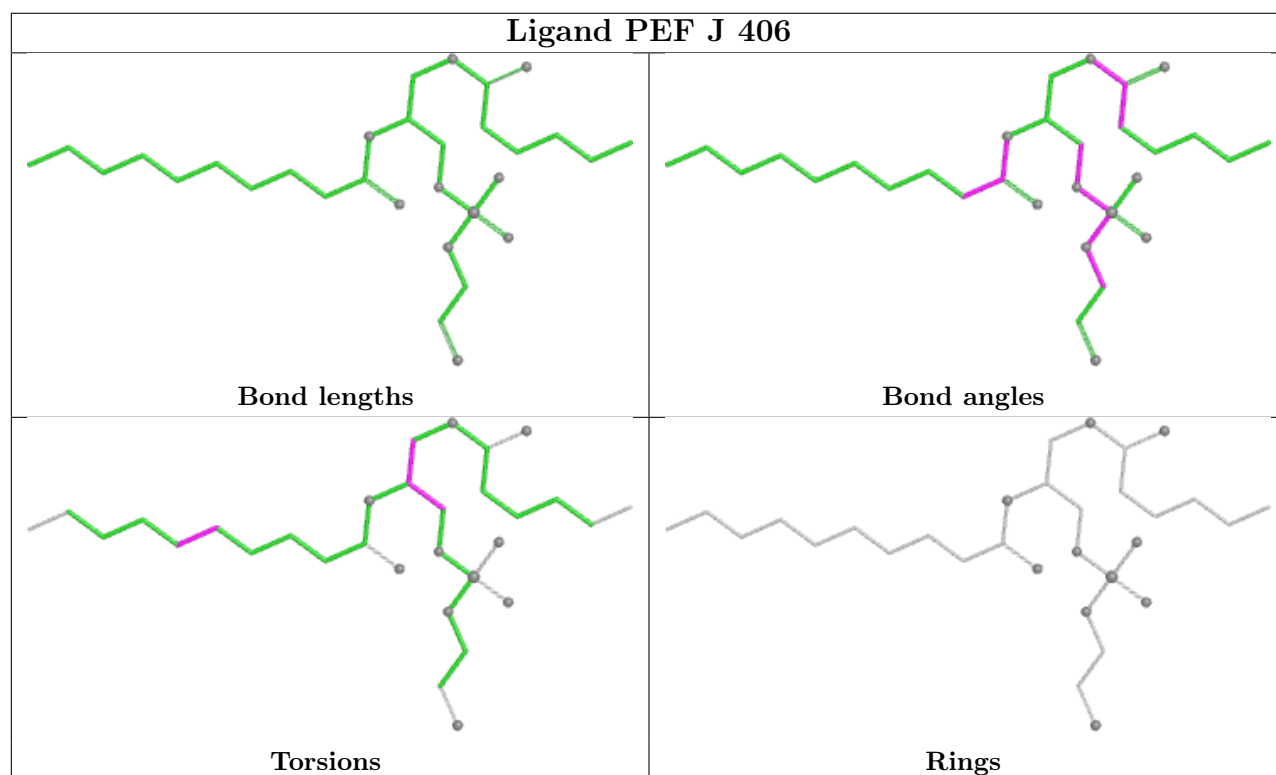
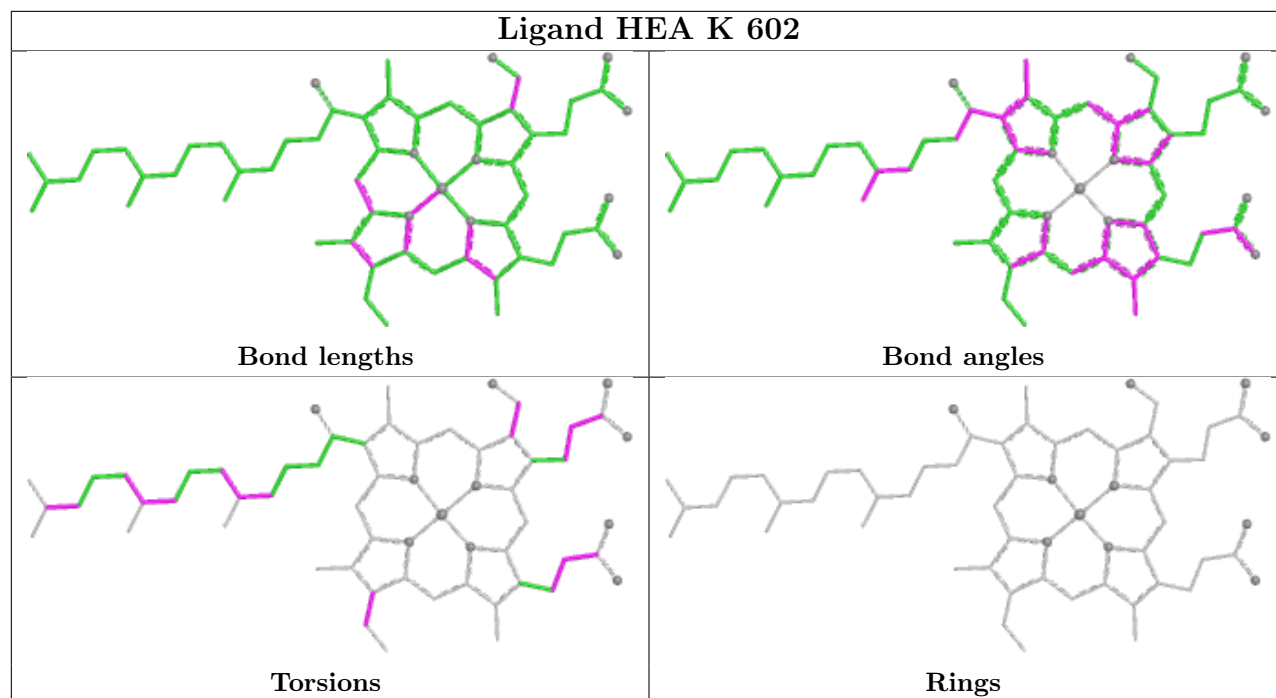


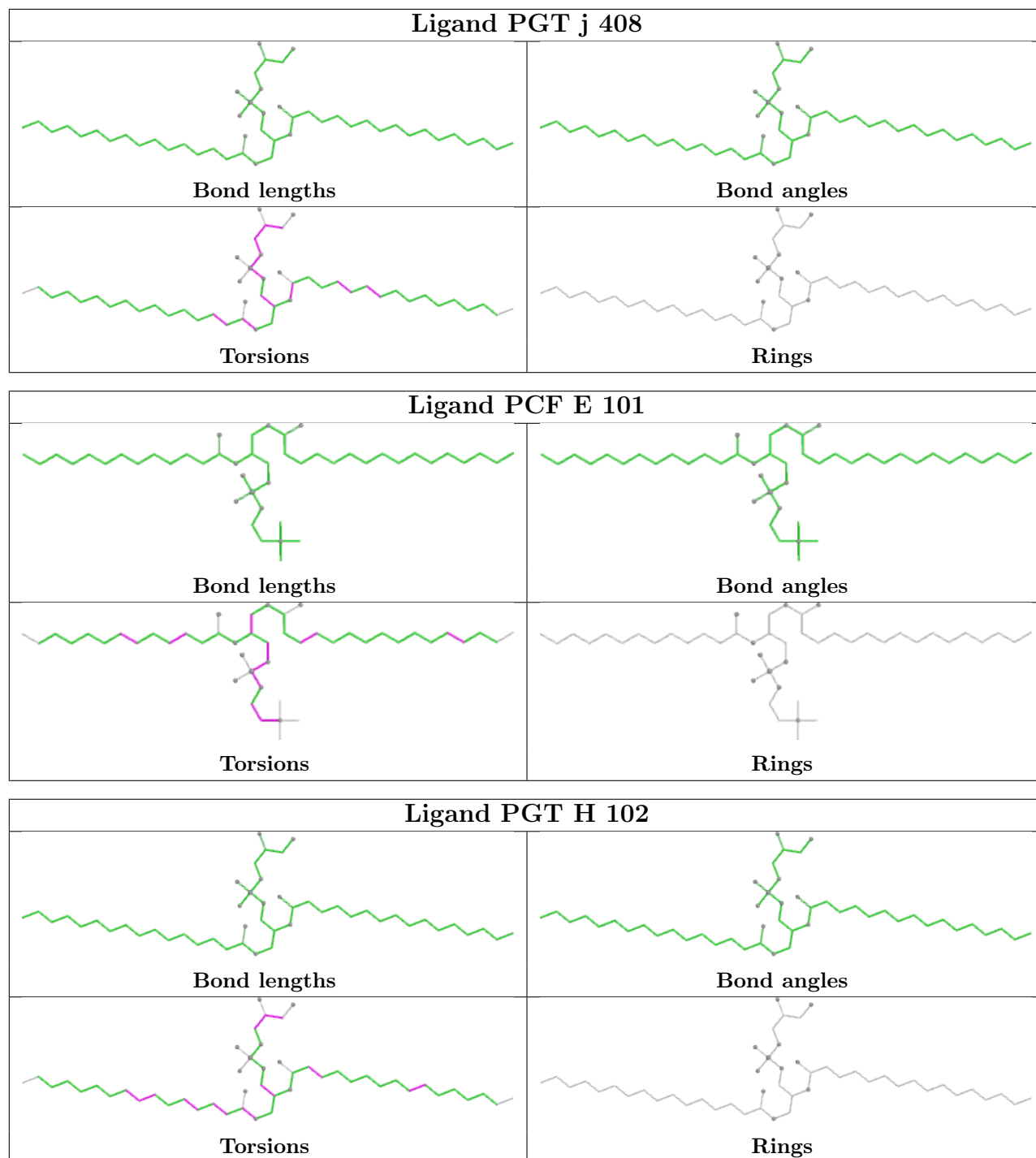


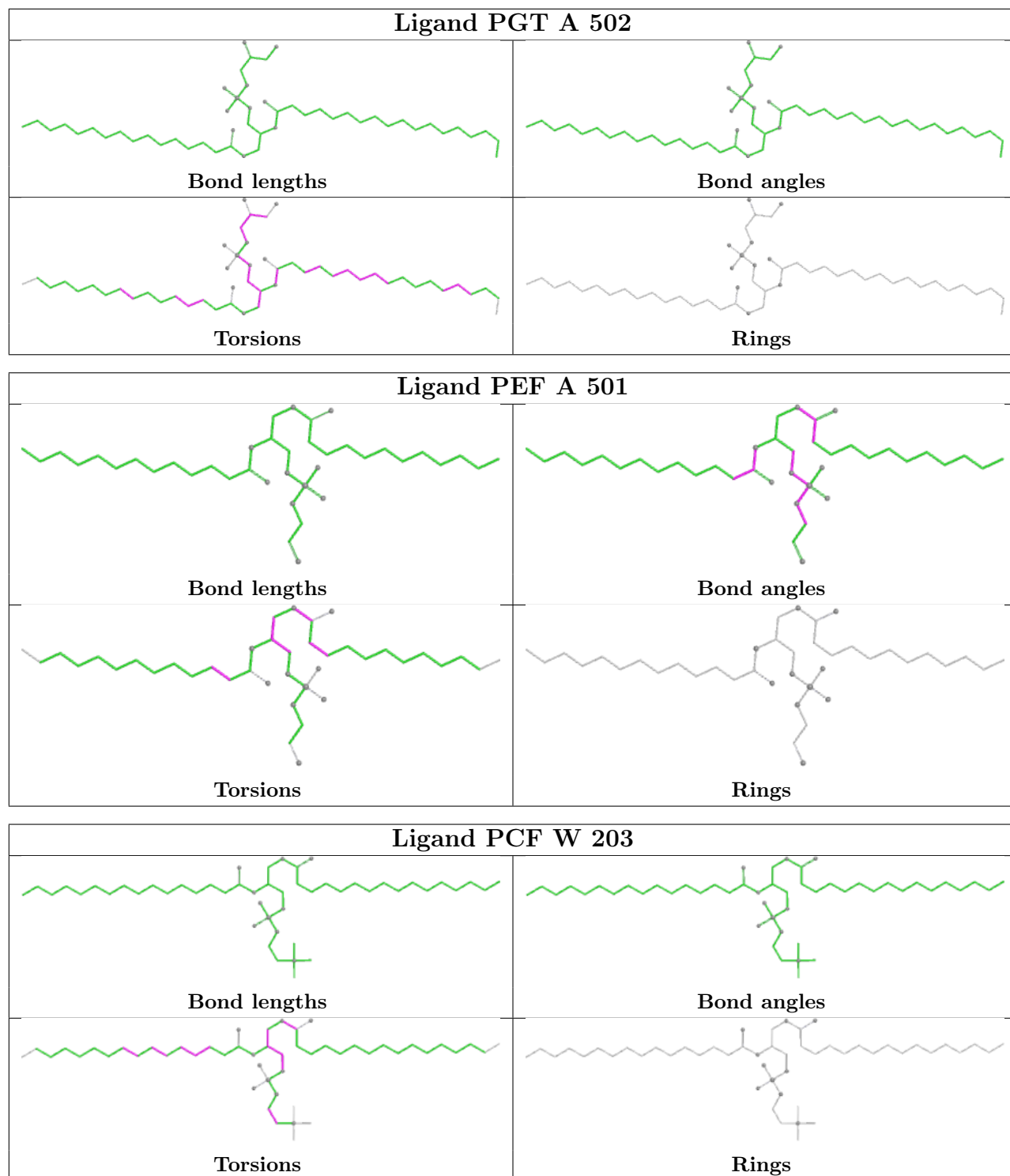


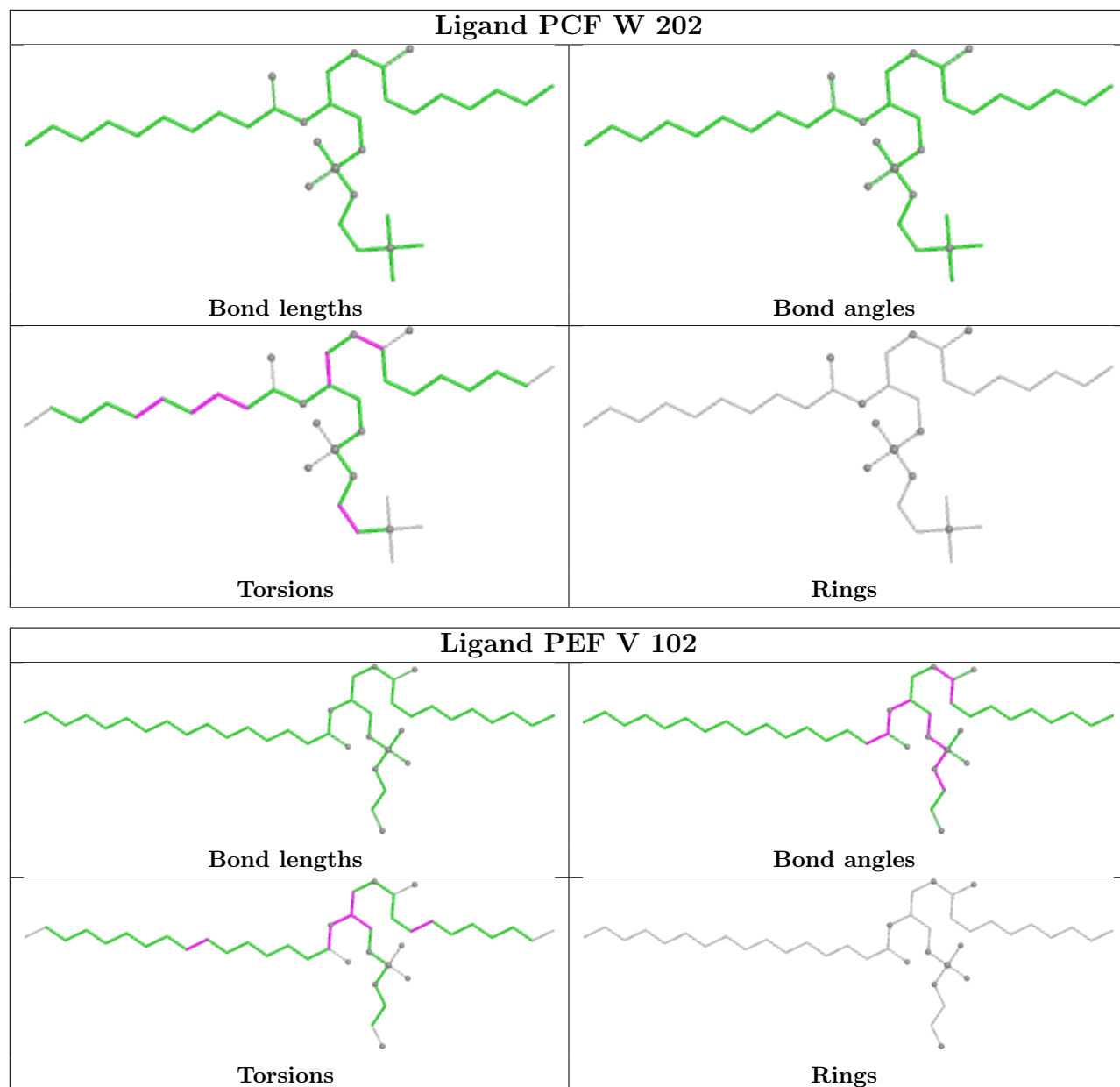


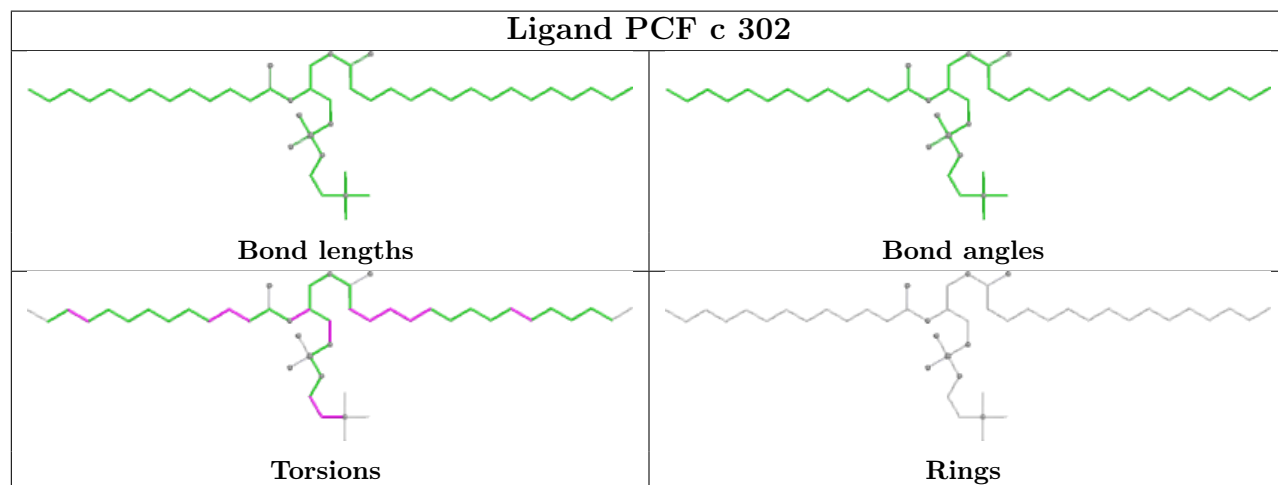
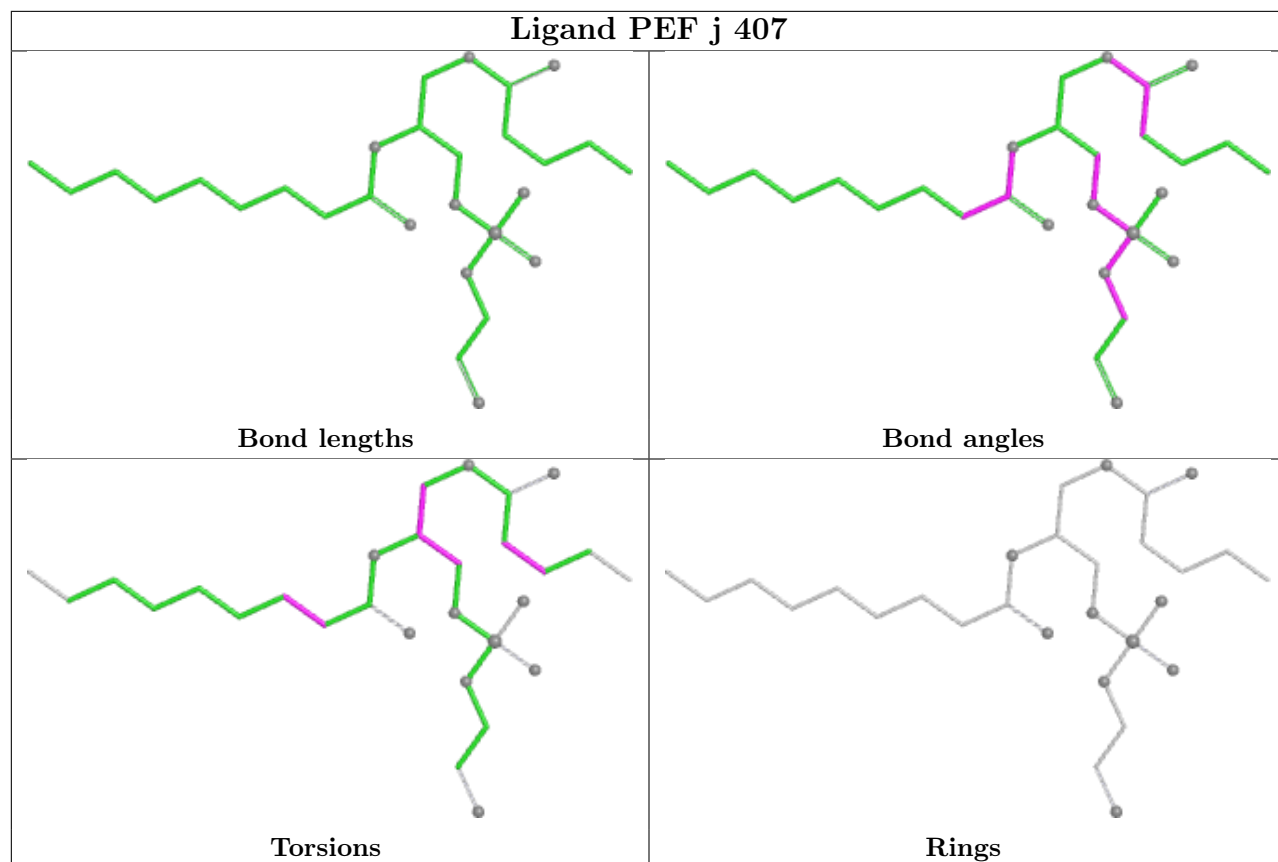


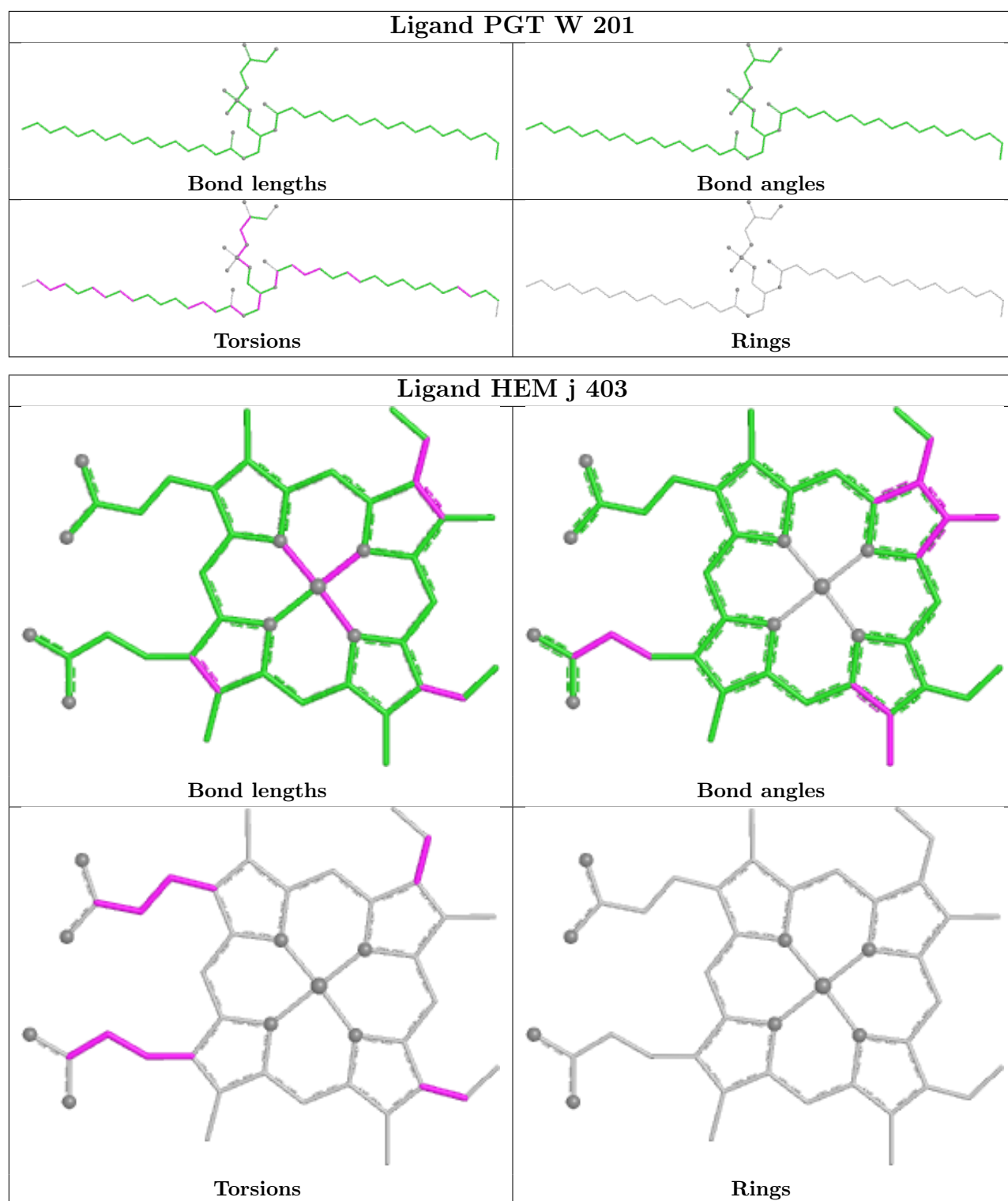












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

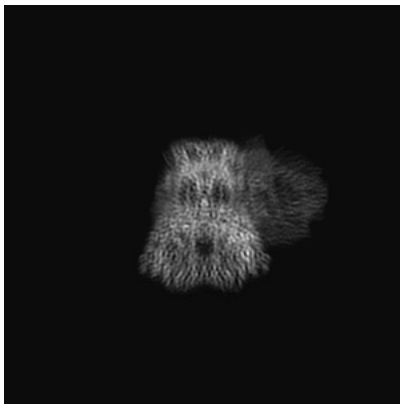
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28011. These allow visual inspection of the internal detail of the map and identification of artifacts.

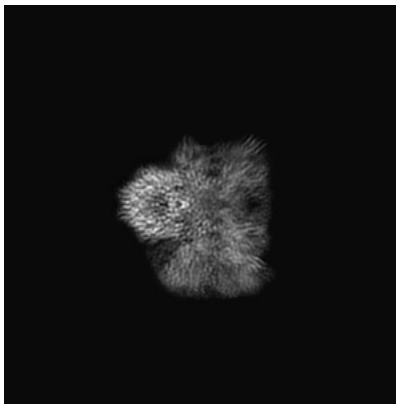
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

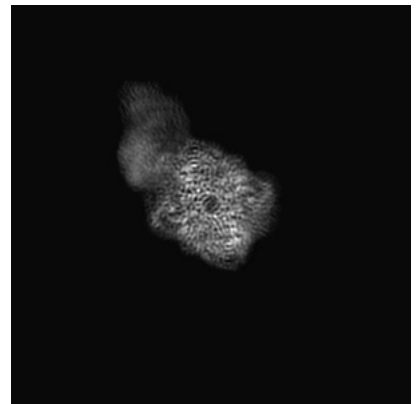
6.1.1 Primary map



X

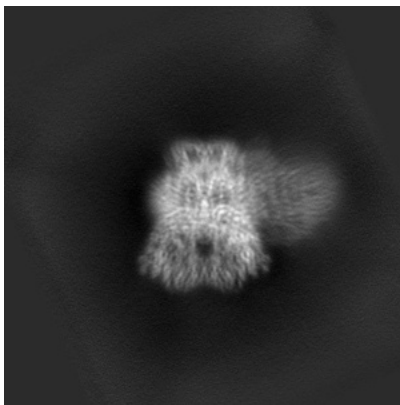


Y

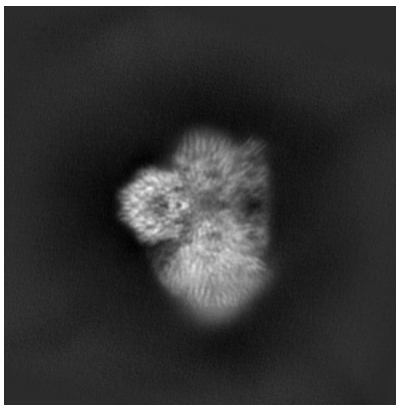


Z

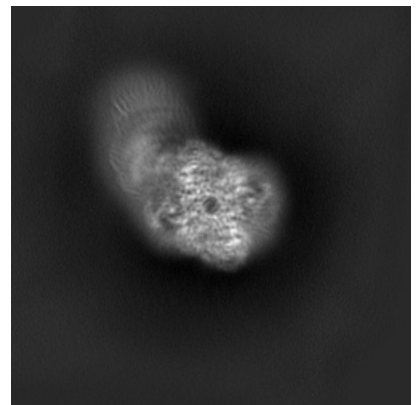
6.1.2 Raw map



X



Y

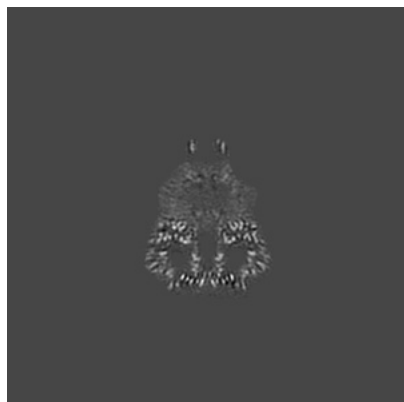


Z

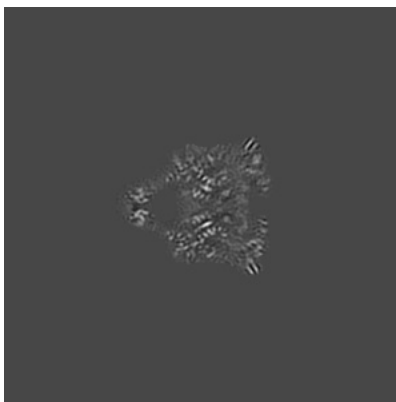
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

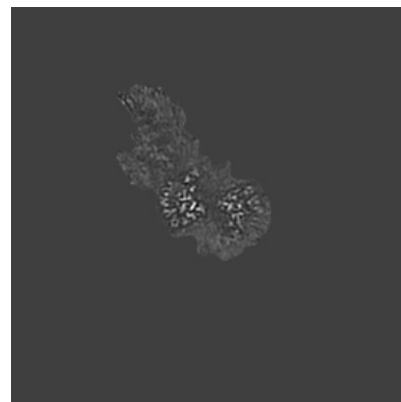
6.2.1 Primary map



X Index: 180

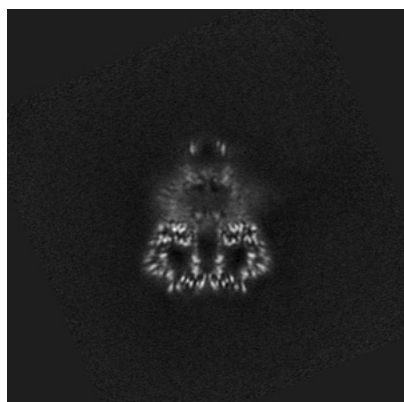


Y Index: 180

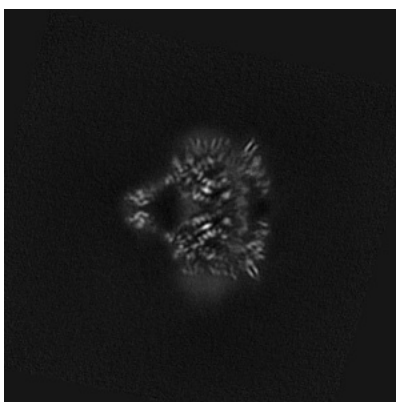


Z Index: 180

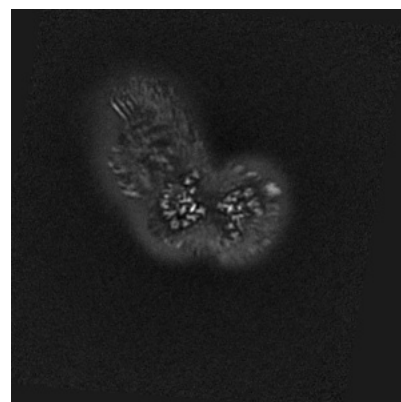
6.2.2 Raw map



X Index: 180



Y Index: 180

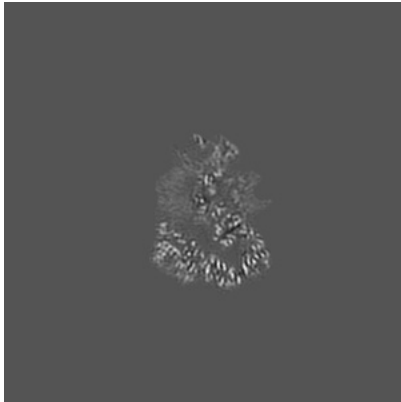


Z Index: 180

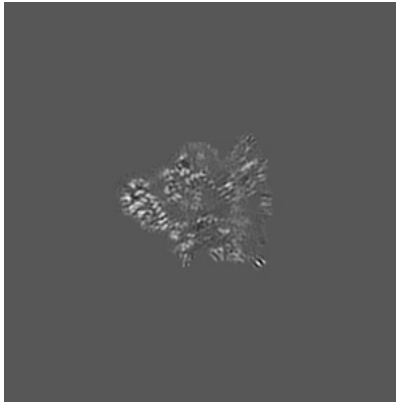
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

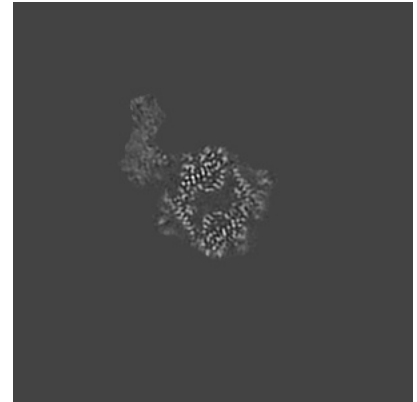
6.3.1 Primary map



X Index: 168

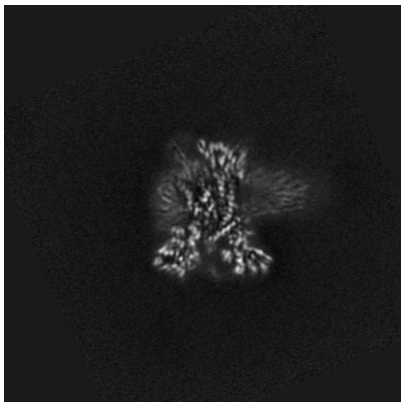


Y Index: 170

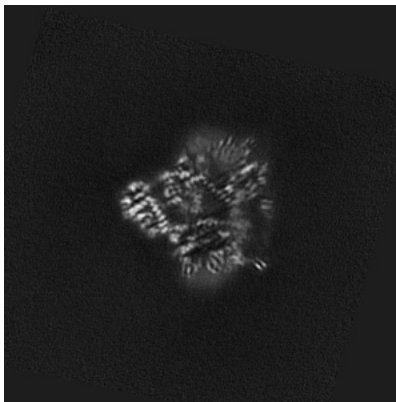


Z Index: 155

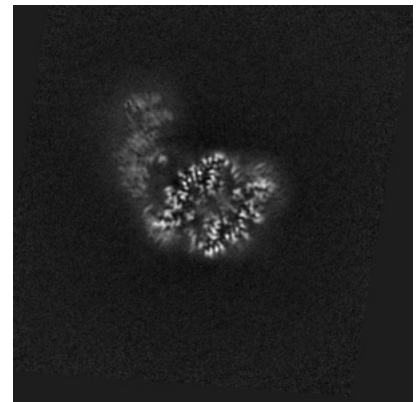
6.3.2 Raw map



X Index: 158



Y Index: 170

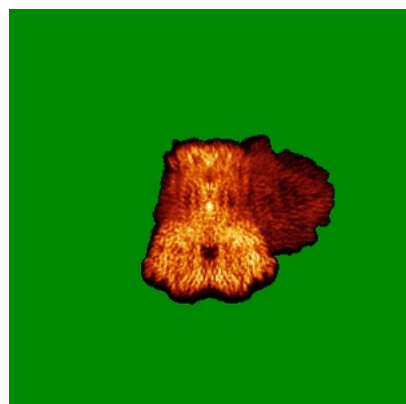


Z Index: 160

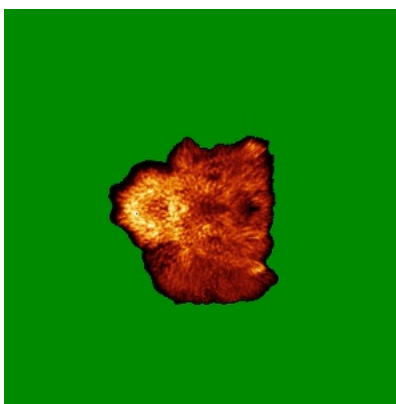
The images above show the largest variance slices of the map in three orthogonal directions.

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

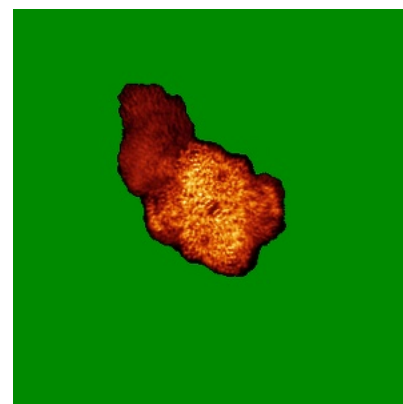
6.4.1 Primary map



X

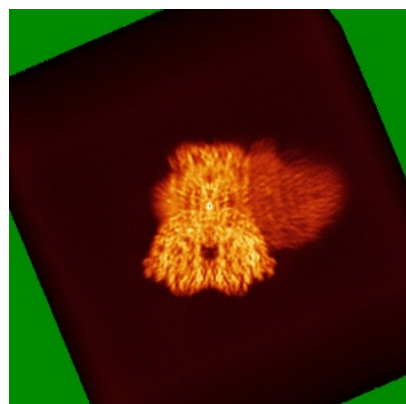


Y

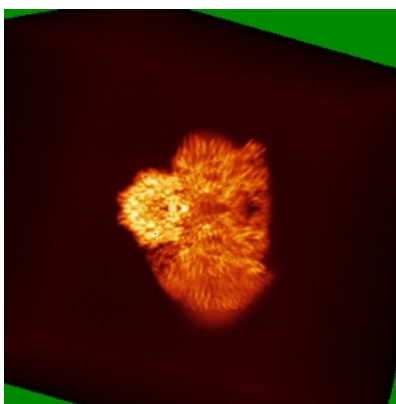


Z

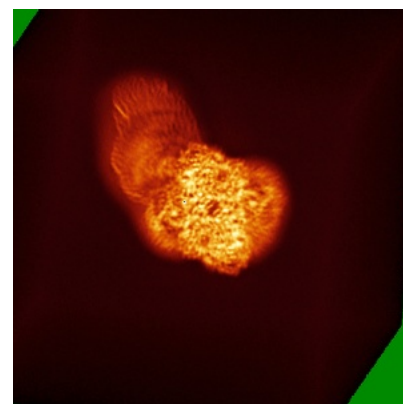
6.4.2 Raw map



X



Y

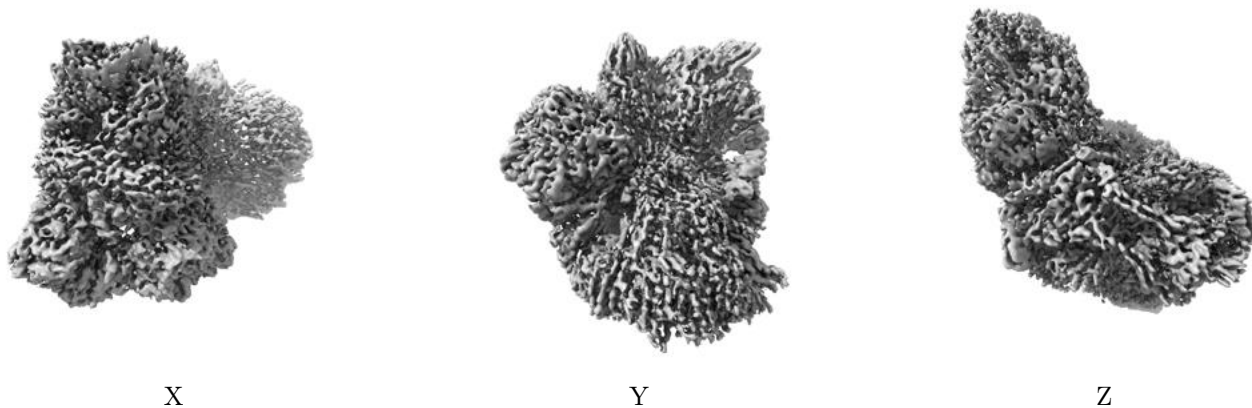


Z

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

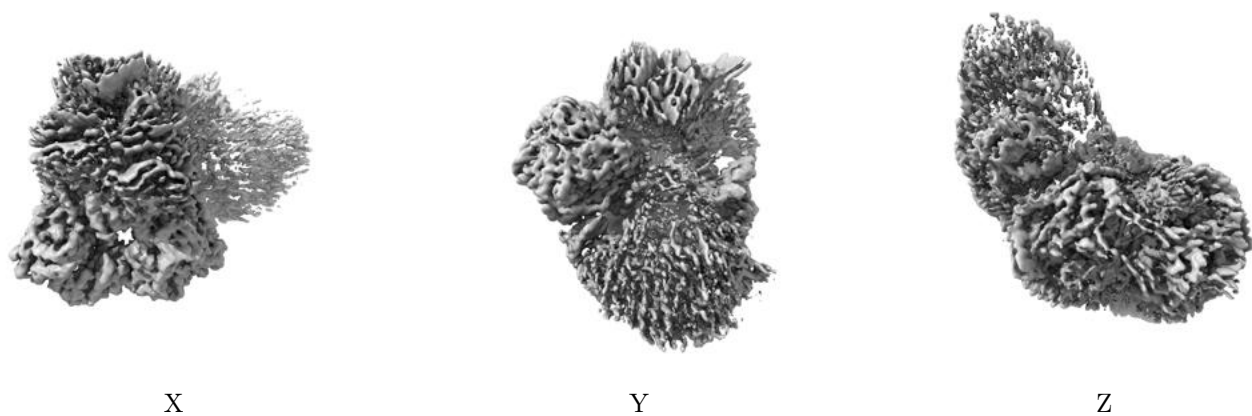
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

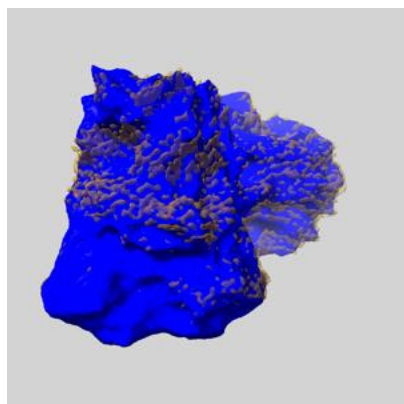
6.6 Mask visualisation [i](#)

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

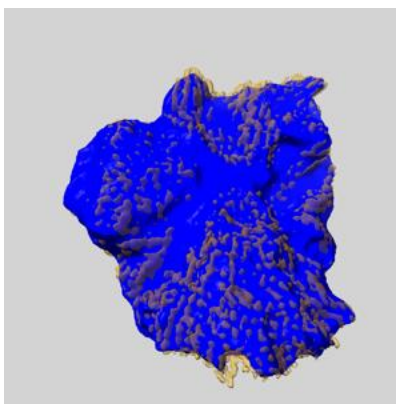
A mask typically either:

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

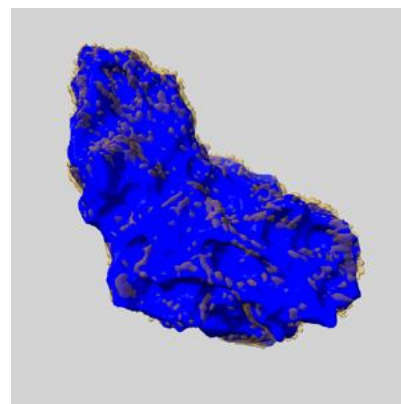
6.6.1 emd_28011_msk_1.map [i](#)



X



Y

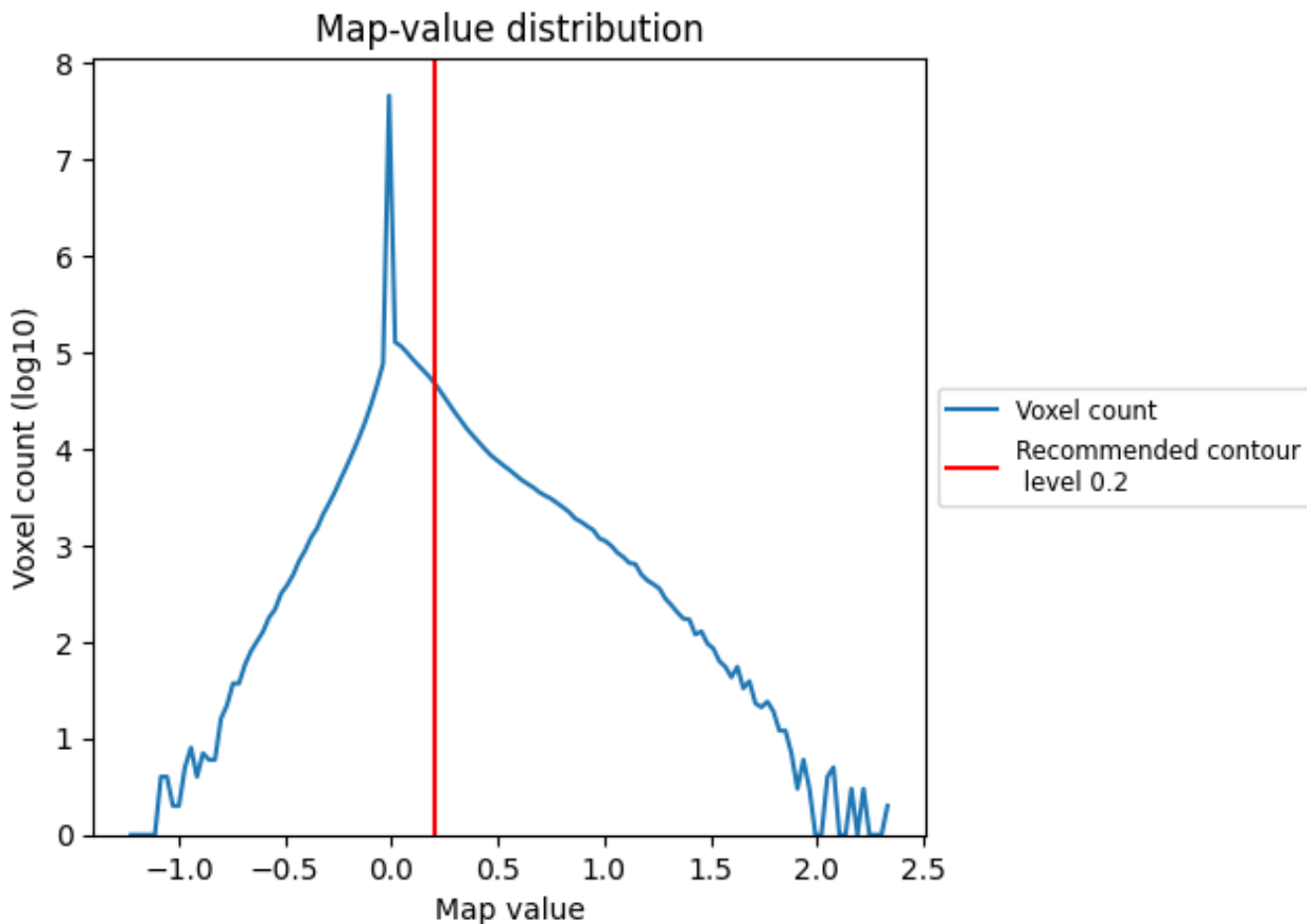


Z

7 Map analysis [i](#)

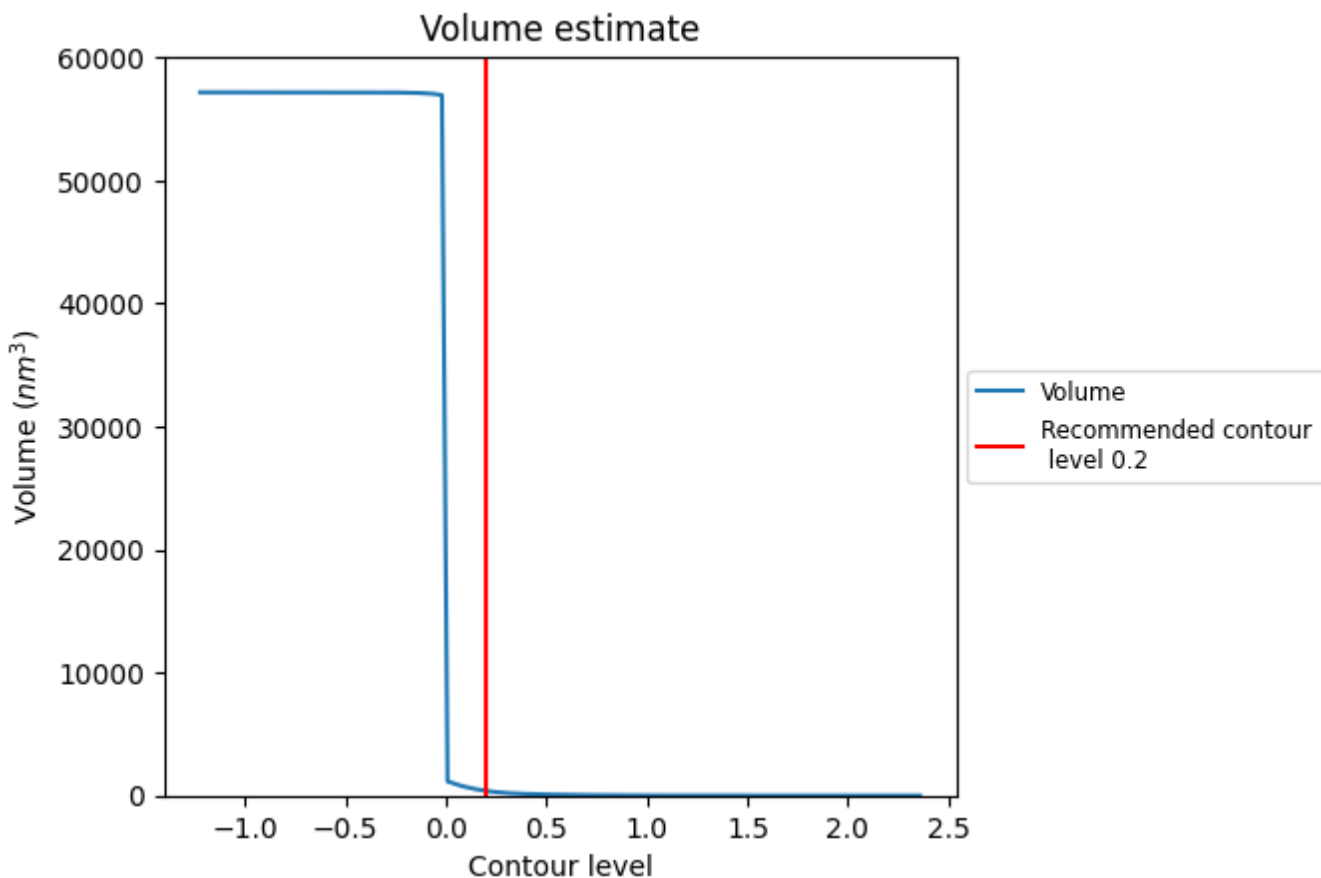
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

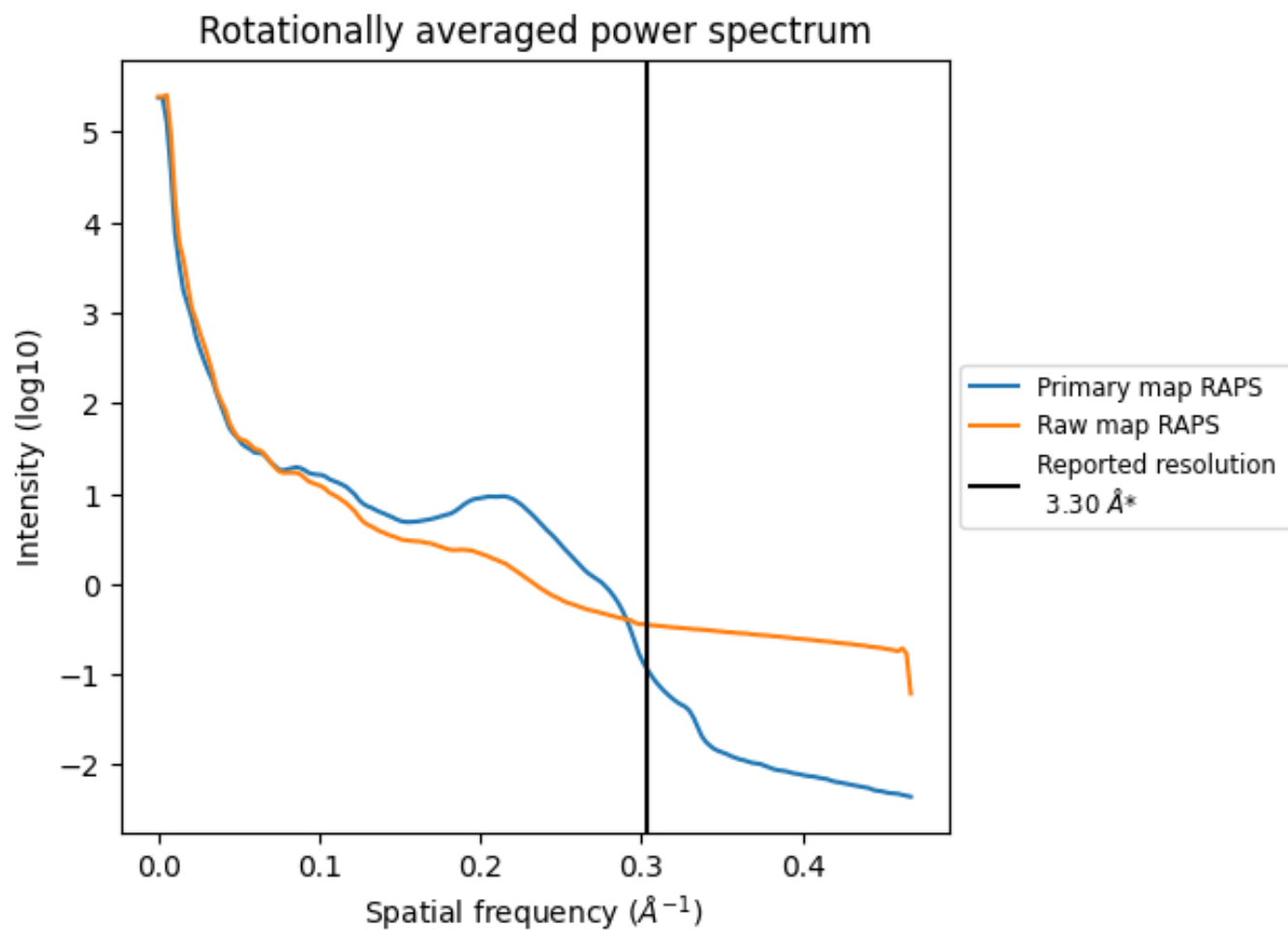
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 380 nm³; this corresponds to an approximate mass of 343 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

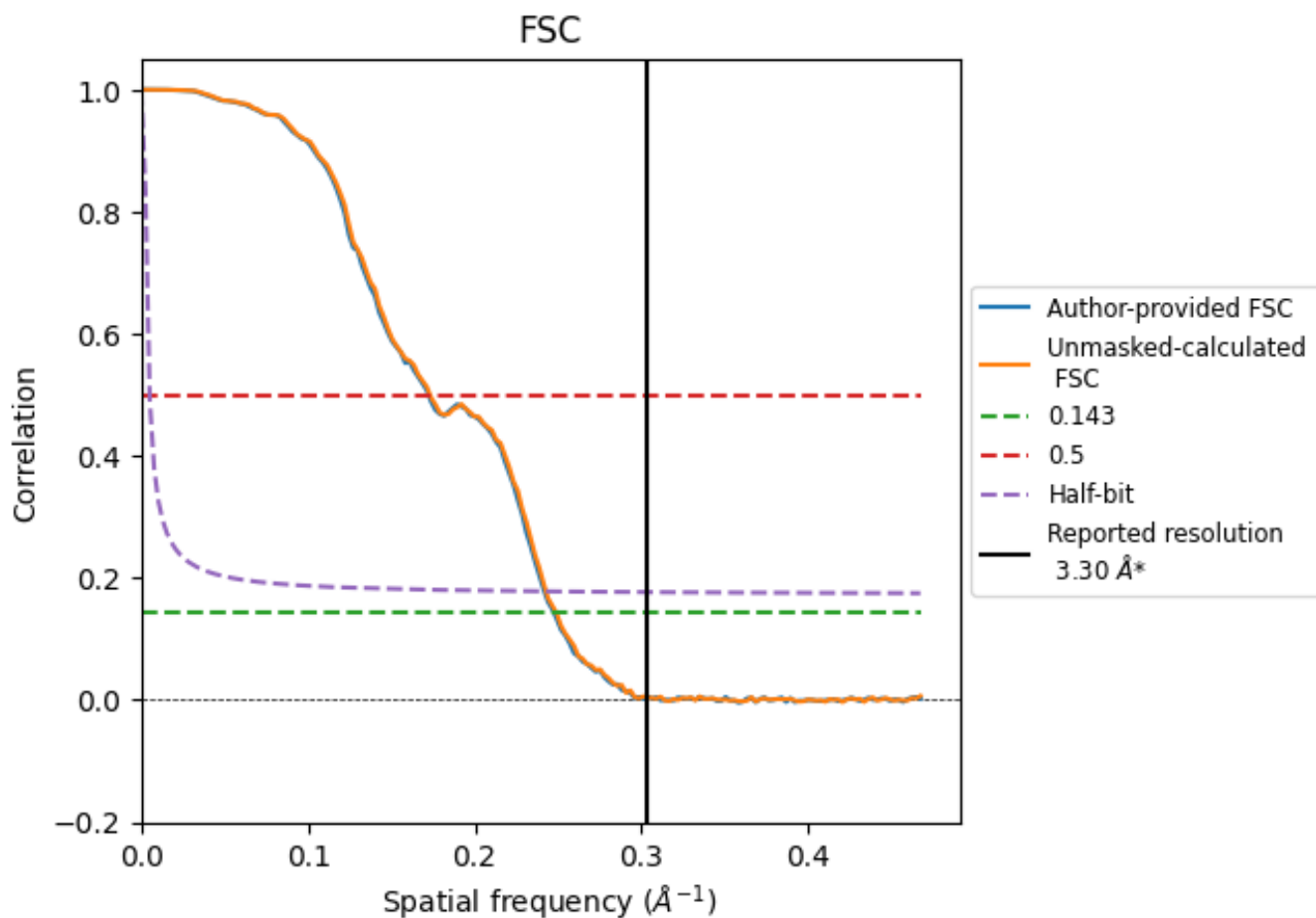


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	4.04	5.80	4.14
Unmasked-calculated*	4.02	5.77	4.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.04 differs from the reported value 3.3 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 3.3 by more than 10 %

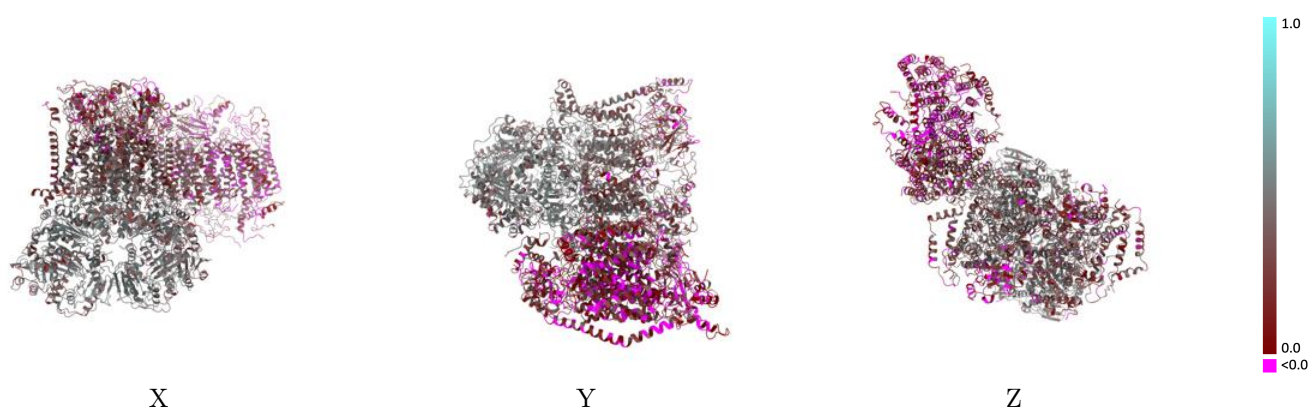
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28011 and PDB model 8EC0. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)

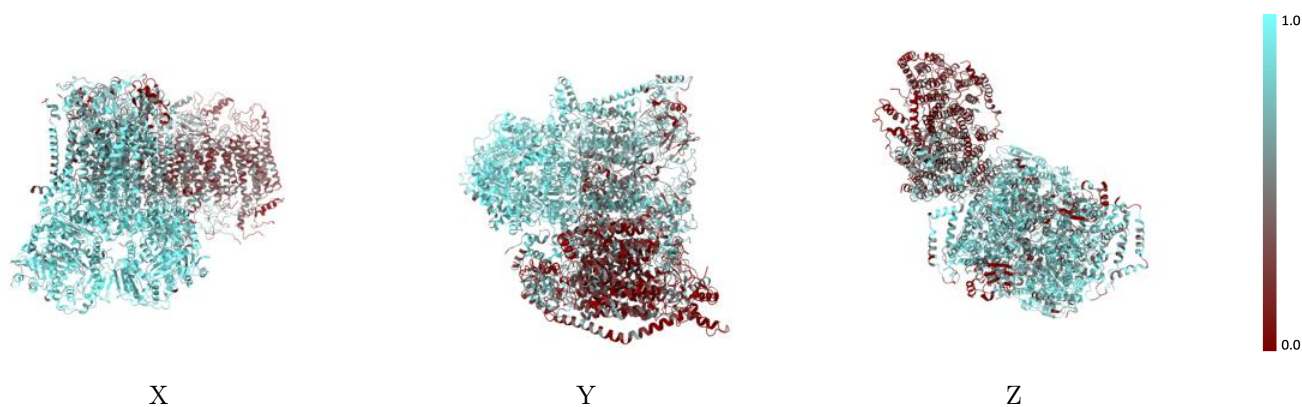
This section was not generated.

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



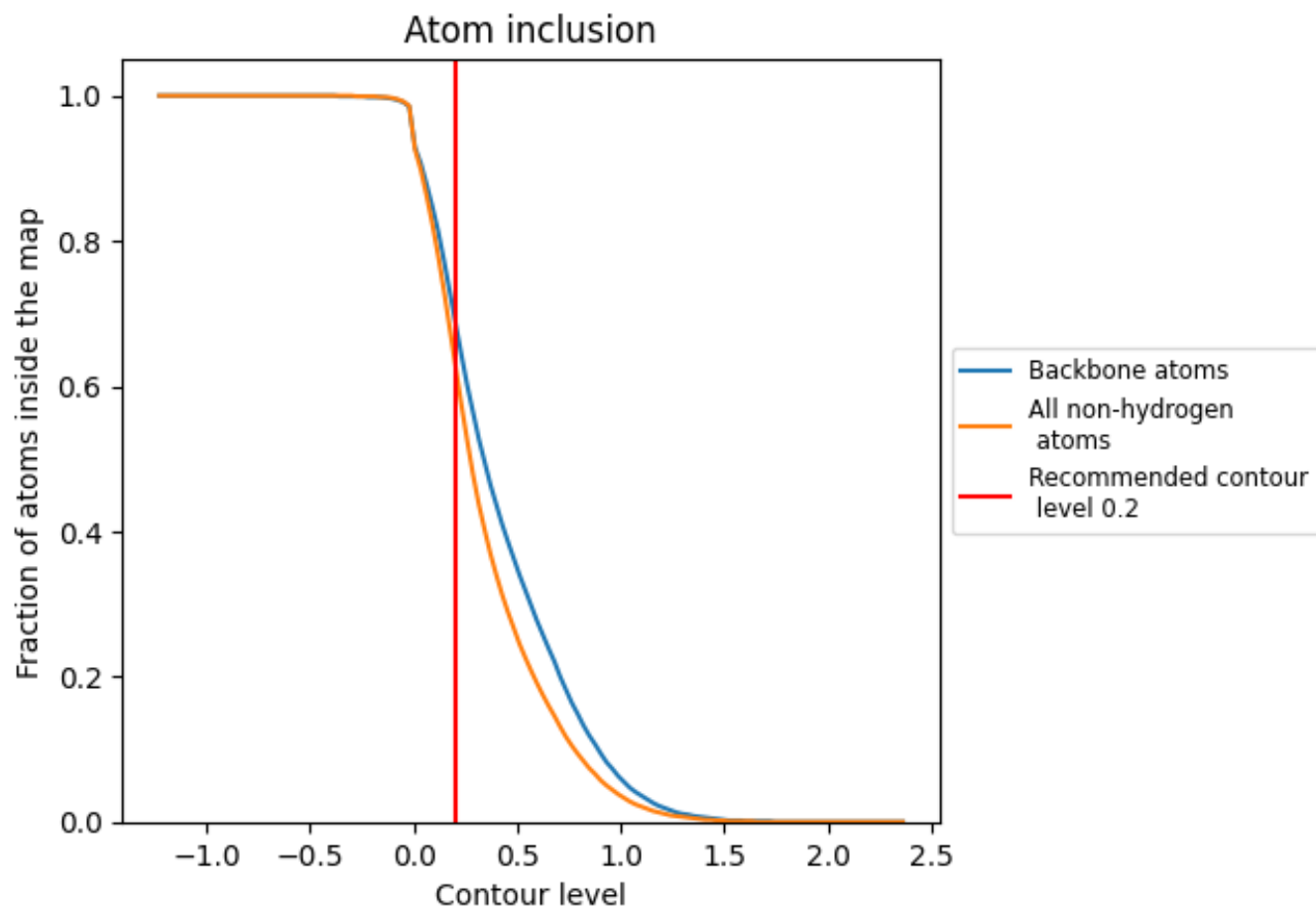
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 63% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6320	 0.3070
A	 0.8630	 0.4430
B	 0.9030	 0.4560
C	 0.4320	 0.2220
E	 0.5560	 0.2890
F	 0.8650	 0.4390
G	 0.6620	 0.2540
H	 0.7350	 0.3930
J	 0.7270	 0.3870
K	 0.3270	 0.1480
L	 0.7750	 0.3630
M	 0.1990	 0.1340
N	 0.1800	 0.1080
O	 0.2700	 0.1390
P	 0.4140	 0.1460
Q	 0.5600	 0.2060
R	 0.3710	 0.1330
S	 0.1110	 0.0390
T	 0.3650	 0.1360
U	 0.1050	 0.0640
V	 0.4880	 0.2790
W	 0.5720	 0.2760
a	 0.8700	 0.4390
b	 0.8860	 0.4460
c	 0.4160	 0.1850
e	 0.6430	 0.2290
f	 0.8540	 0.4190
g	 0.6470	 0.2620
h	 0.8100	 0.3540
j	 0.7370	 0.3660
l	 0.7200	 0.3220

