



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 09:48 PM UTC

PDB ID : 9G83 / pdb_00009g83
EMDB ID : EMD-51125
Title : Respiratory supercomplex CI1-CIII2-CIV2-(cbb3)1 from alphaproteobacterium
Authors : Yaikhomba, M.; Hirst, J.; Croll, T.I.; Spikes, T.E.; Agip, A.N.A.
Deposited on : 2024-07-22
Resolution : 6.98 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:

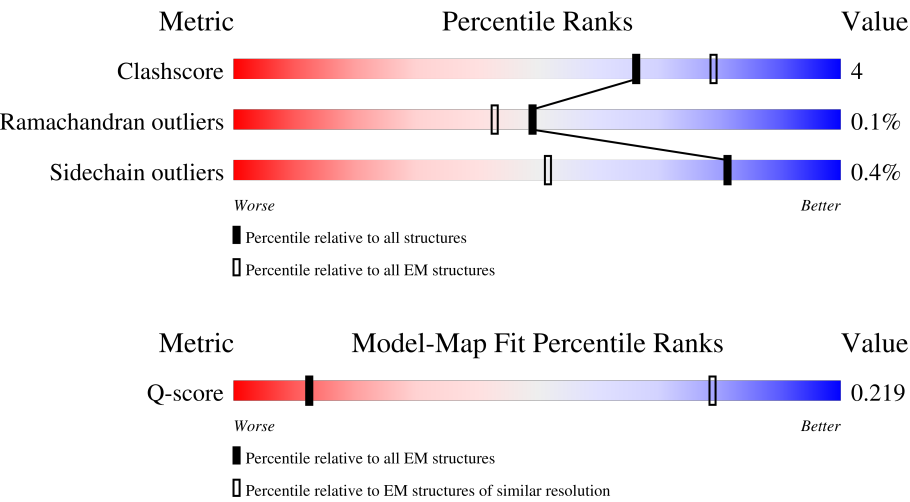
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 6.98 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.








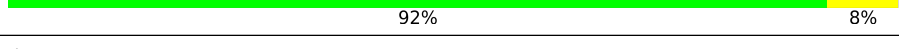
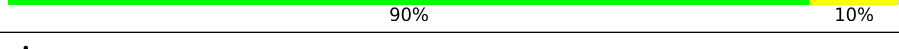
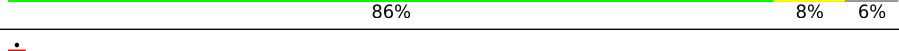
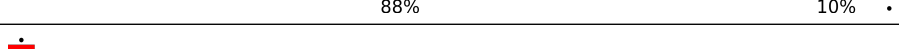
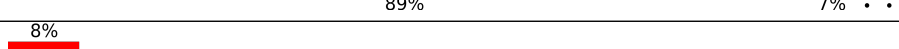
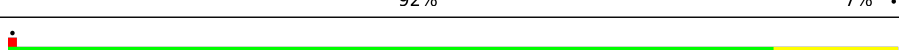

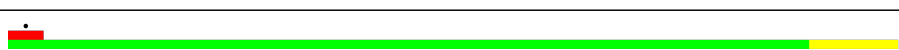

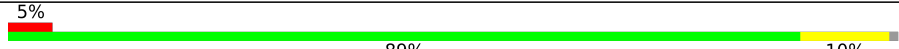
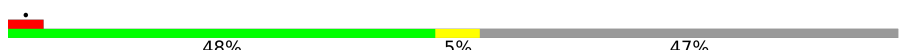




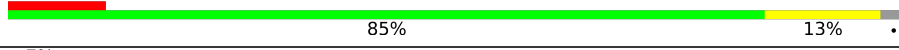
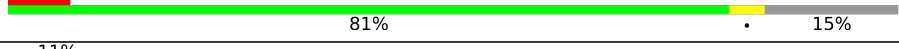

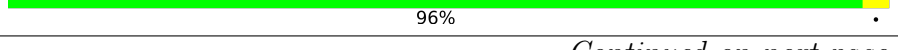

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	450 (6.48 - 7.46)

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	121	
2	B	175	
3	C	208	
4	D	412	

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Mol	Chain	Length	Quality of chain
5	E	239	
6	F	431	
7	G	674	
8	H	345	
9	I	163	
10	J	199	
11	K	101	
12	L	703	
13	M	513	
14	N	499	
15	P	330	
16	Q	103	
17	R	62	
18	Z	217	
19	a	440	
19	d	440	
20	b	450	
20	e	450	
21	c	195	
21	f	195	
22	g	558	
22	k	558	
23	h	298	
23	l	298	
24	i	274	

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Mol	Chain	Length	Quality of chain
24	m	274	
25	j	66	
25	n	66	
26	o	176	
26	p	176	
27	q	124	
28	r	35	
29	s	30	
30	t	539	
31	u	241	
32	v	349	

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
33	SF4	B	1001	-	-	X	-
33	SF4	F	501	-	-	X	-

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 83417 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	121	Total	C	N	O	S	0	0
			969	658	141	164	6		

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	162	Total	C	N	O	S	0	0
			1270	799	227	231	13		

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	194	Total	C	N	O	S	0	0
			1586	1020	274	290	2		

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	411	Total	C	N	O	S	0	0
			3277	2072	582	601	22		

- Molecule 5 is a protein called NADH dehydrogenase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	237	Total	C	N	O	S	0	0
			1822	1155	314	340	13		

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	422	Total	C	N	O	S	0	0
			3241	2027	583	600	31		

- Molecule 7 is a protein called NADH-quinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	665	Total	C	N	O	S	0	0
			5068	3149	917	969	33		

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	341	Total	C	N	O	S	0	0
			2722	1848	413	439	22		

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	162	Total	C	N	O	S	0	0
			1319	836	230	242	11		

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	199	Total	C	N	O	S	0	0
			1528	1014	246	257	11		

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			764	508	123	128	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	658	Total	C	N	O	S	0	0
			5193	3458	850	852	33		

- Molecule 13 is a protein called NADH dehydrogenase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	503	Total	C	N	O	S	0	0
			3915	2615	610	658	32		

- Molecule 14 is a protein called NADH-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	480	Total	C	N	O	S	0	0
			3556	2342	565	617	32		

- Molecule 15 is a protein called NAD-dependent epimerase/dehydratase.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	328	Total	C	N	O	S	0	0
			2468	1541	463	452	12		

- Molecule 16 is a protein called ETC complex I subunit conserved region.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	103	Total	C	N	O	S	0	0
			849	523	167	156	3		

- Molecule 17 is a protein called Zinc finger CHCC-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	61	Total	C	N	O	S	0	0
			488	304	90	91	3		

- Molecule 18 is a protein called Protein-L-isoaspartate O-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	216	Total	C	N	O	S	0	0
			1642	1033	294	306	9		

- Molecule 19 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	433	Total	C	N	O	S	0	0
			3504	2373	552	561	18		
19	d	434	Total	C	N	O	S	0	0
			3513	2378	553	564	18		

- Molecule 20 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	239	Total	C	N	O	S	0	0
			1855	1181	311	354	9		
20	e	239	Total	C	N	O	S	0	0
			1855	1181	311	354	9		

- Molecule 21 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	c	180	Total	C	N	O	S	0	0
			1353	838	245	263	7		
21	f	181	Total	C	N	O	S	0	0
			1361	842	246	266	7		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	g	544	Total	C	N	O	S	0	0
			4322	2890	684	715	33		
22	k	544	Total	C	N	O	S	0	0
			4322	2890	684	715	33		

- Molecule 23 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	h	252	Total	C	N	O	S	0	0
			1976	1295	319	354	8		
23	l	252	Total	C	N	O	S	0	0
			1976	1295	319	354	8		

- Molecule 24 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	i	273	Total	C	N	O	S	0	0
			2183	1483	341	348	11		
24	m	273	Total	C	N	O	S	0	0
			2183	1483	341	348	11		

- Molecule 25 is a protein called Aa3 type cytochrome c oxidase subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	43	Total	C	N	O	S	0	0
			332	214	58	59	1		
25	n	43	Total	C	N	O	S	0	0
			332	214	58	59	1		

- Molecule 26 is a protein called Cytochrome c, class I.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	o	43	Total	C	N	O	S	0	0
			315	210	48	55	2		
26	p	44	Total	C	N	O	S	0	0
			321	213	49	57	2		

- Molecule 27 is a protein called NADH:ubiquinone oxidoreductase 17.2 kD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	q	123	Total	C	N	O	S	0	0
			1018	651	181	185	1		

- Molecule 28 is a protein called Transmembrane helix of unknown identity.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	r	35	Total	C	N	O	0	0
			175	105	35	35		

- Molecule 29 is a protein called Transmembrane helix of unknown identity.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	s	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 30 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	t	470	Total	C	N	O	S	0	0
			3732	2498	596	616	22		

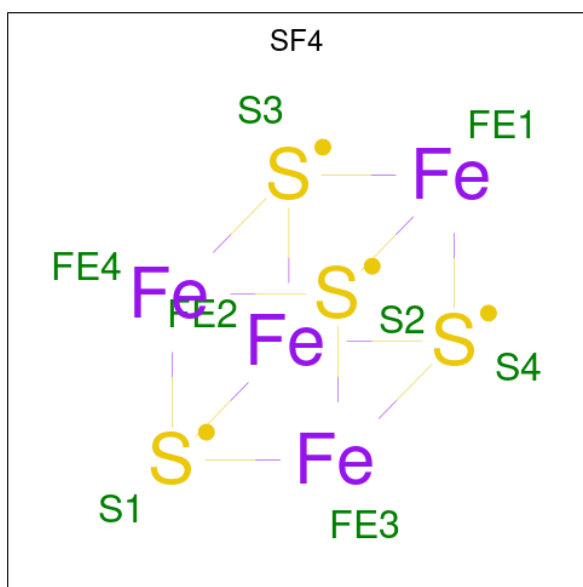
- Molecule 31 is a protein called Cytochrome c oxidase, cbb3-type, subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	u	191	Total	C	N	O	S	0	0
			1517	969	261	277	10		

- Molecule 32 is a protein called Cbb3-type cytochrome c oxidase subunit CcoP.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	v	276	Total	C	N	O	S	0	0
			2095	1326	356	406	7		

- Molecule 33 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

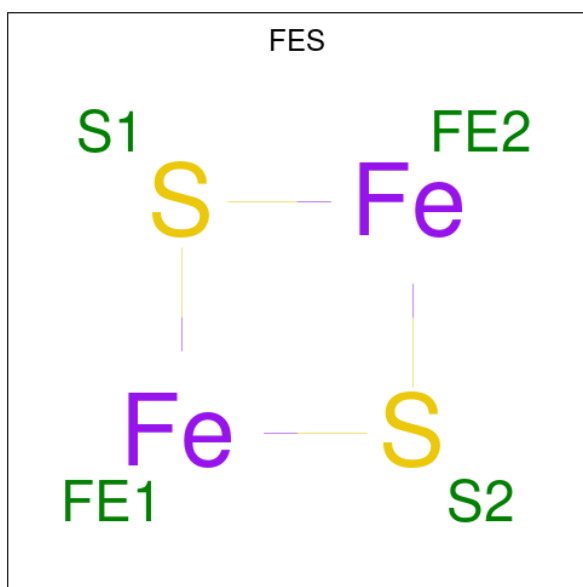


Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	Fe	S	0
			8	4	4	
33	F	1	Total	Fe	S	0
			8	4	4	
33	G	1	Total	Fe	S	0
			8	4	4	
33	G	1	Total	Fe	S	0
			8	4	4	
33	I	1	Total	Fe	S	0
			8	4	4	
33	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

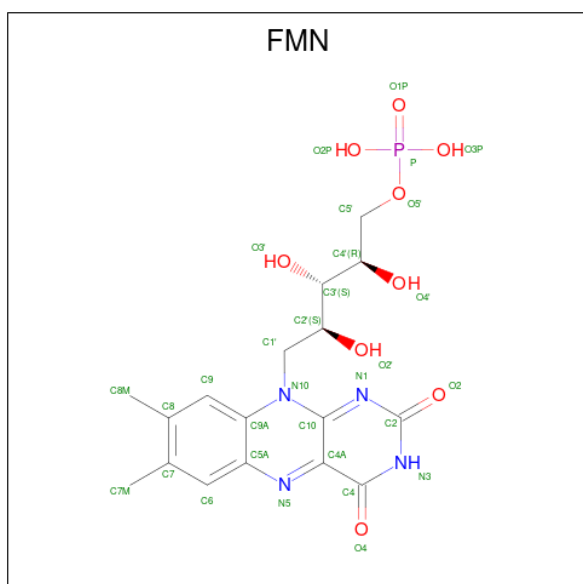
Mol	Chain	Residues	Atoms		AltConf
34	D	1	Total	Na	0
			1	1	

- Molecule 35 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



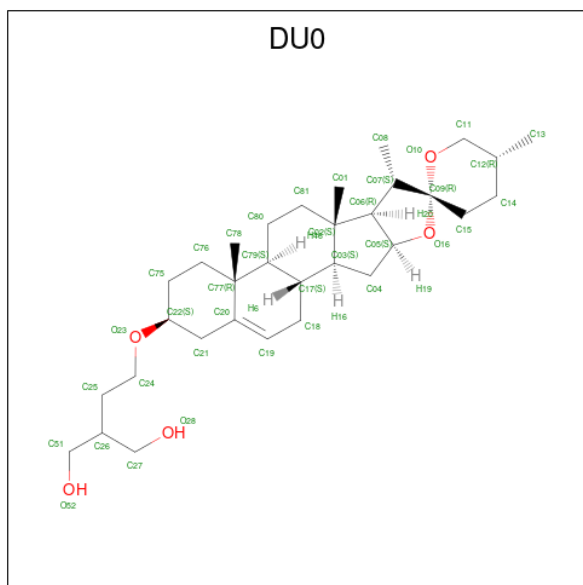
Mol	Chain	Residues	Atoms			AltConf
35	E	1	Total	Fe	S	0
			4	2	2	
35	G	1	Total	Fe	S	0
			4	2	2	
35	c	1	Total	Fe	S	0
			4	2	2	
35	f	1	Total	Fe	S	0
			4	2	2	

- Molecule 36 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



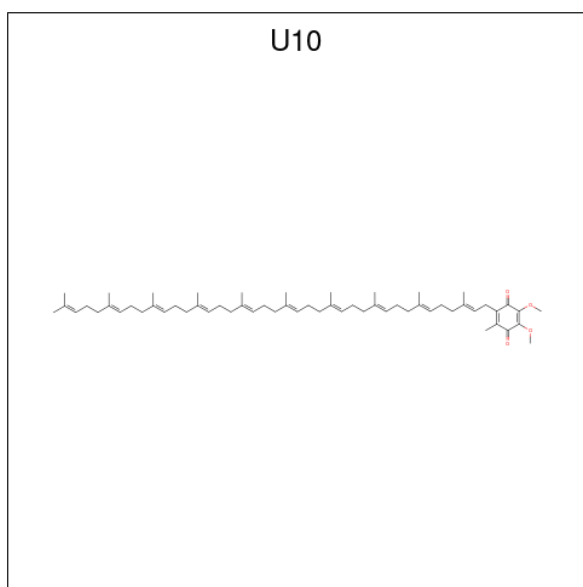
Mol	Chain	Residues	Atoms					AltConf
36	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 37 is 2-[2-[(1 {S},2 {S},4 {S},5' {R},6 {R},7 {S},8 {R},9 {S},12 {S},13 {R},16 {S})]-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.0.0^{2,9}.0^{4,8}.0^{13,18}]]icos-18-ene-6,2'-oxane]-16-yl]oxyethyl]propane-1,3-diol (CCD ID: DU0) (formula: C₃₂H₅₂O₅).



Mol	Chain	Residues	Atoms			AltConf
37	H	1	Total	C	O	0
			37	32	5	
37	N	1	Total	C	O	0
			37	32	5	
37	f	1	Total	C	O	0
			37	32	5	

- Molecule 38 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).

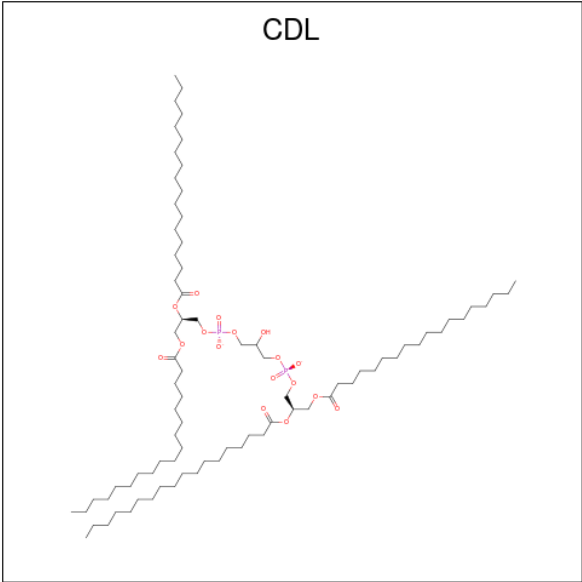


Mol	Chain	Residues	Atoms			AltConf
38	H	1	Total	C	O	0
			63	59	4	
38	a	1	Total	C	O	0
			63	59	4	
38	a	1	Total	C	O	0
			63	59	4	
38	d	1	Total	C	O	0
			63	59	4	
38	d	1	Total	C	O	0
			63	59	4	

- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn).

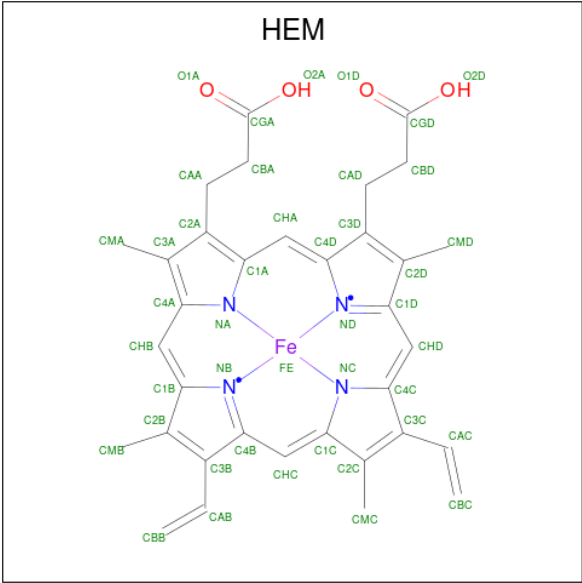
Mol	Chain	Residues	Atoms		AltConf
39	R	1	Total	Zn	0
			1	1	

- Molecule 40 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
40	a	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
41	a	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	a	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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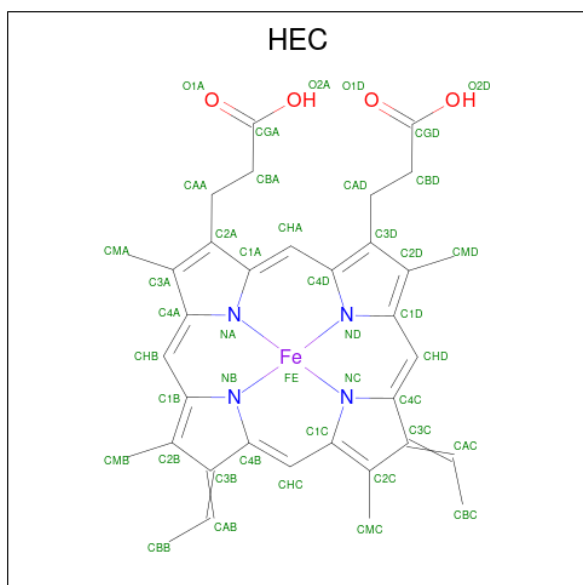
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Mol	Chain	Residues	Atoms					AltConf
41	d	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	d	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	t	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	t	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 42 is CALCIUM ION (CCD ID: CA) (formula: Ca).

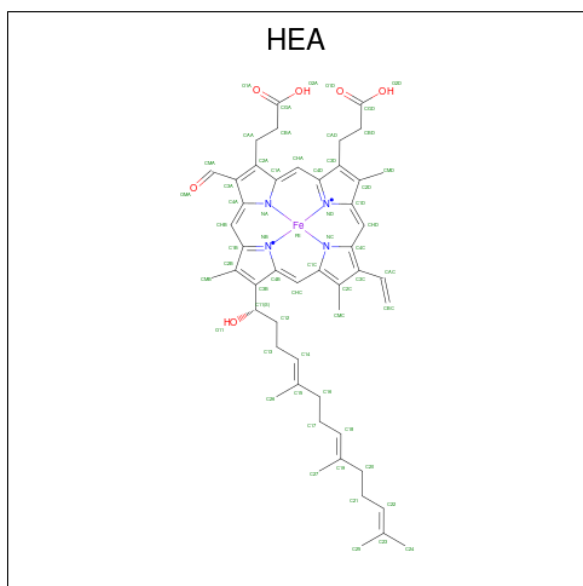
Mol	Chain	Residues	Atoms		AltConf
42	b	1	Total	Ca	0
			1	1	
42	e	1	Total	Ca	0
			1	1	
42	g	1	Total	Ca	0
			1	1	
42	k	1	Total	Ca	0
			1	1	
42	t	2	Total	Ca	0
			2	2	

- Molecule 43 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
43	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
43	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
43	u	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
43	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
43	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 44 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
44	g	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
44	g	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
44	k	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
44	k	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

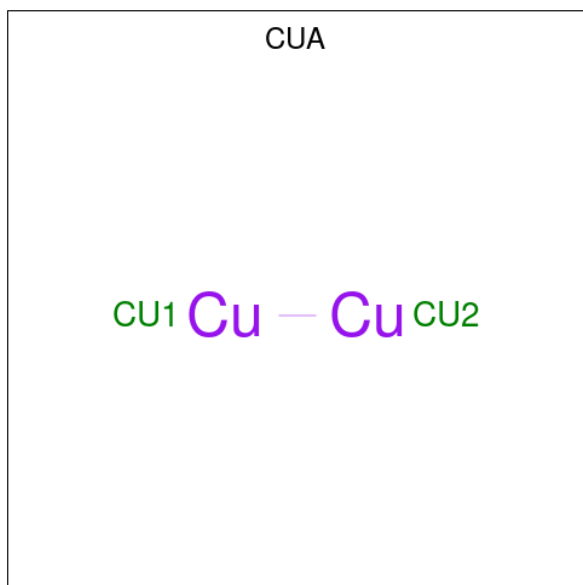
- Molecule 45 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
45	g	1	Total 1	Cu 1	0
45	k	1	Total 1	Cu 1	0
45	t	1	Total 1	Cu 1	0

- Molecule 46 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
46	g	1	Total 1	Mn 1	0

- Molecule 47 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).

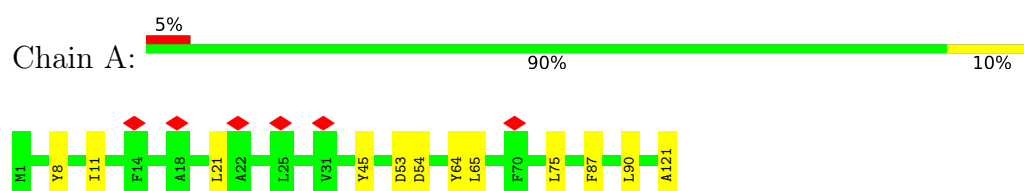


Mol	Chain	Residues	Atoms		AltConf
47	h	1	Total 2	Cu 2	0
47	l	1	Total 2	Cu 2	0

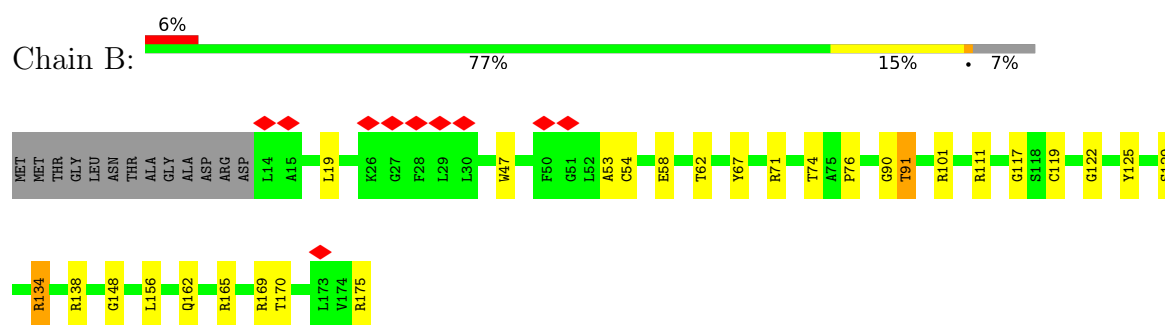
3 Residue-property plots [i](#)

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

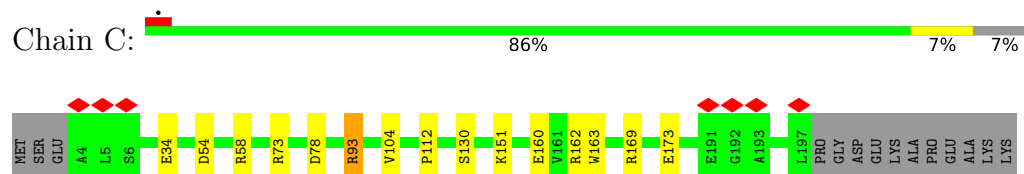
- Molecule 1: NADH-quinone oxidoreductase subunit A



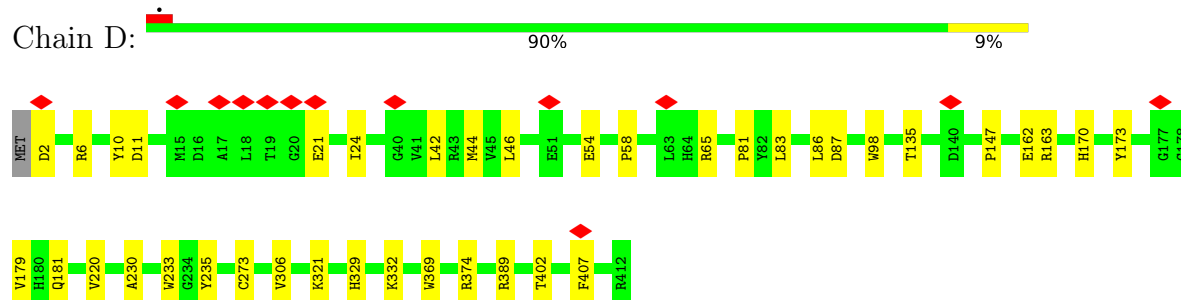
- Molecule 2: NADH-quinone oxidoreductase subunit B



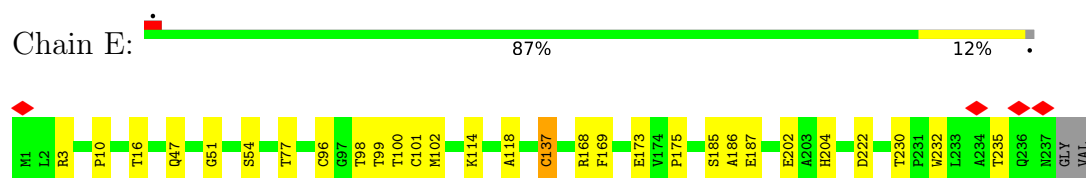
- Molecule 3: NADH-quinone oxidoreductase subunit C



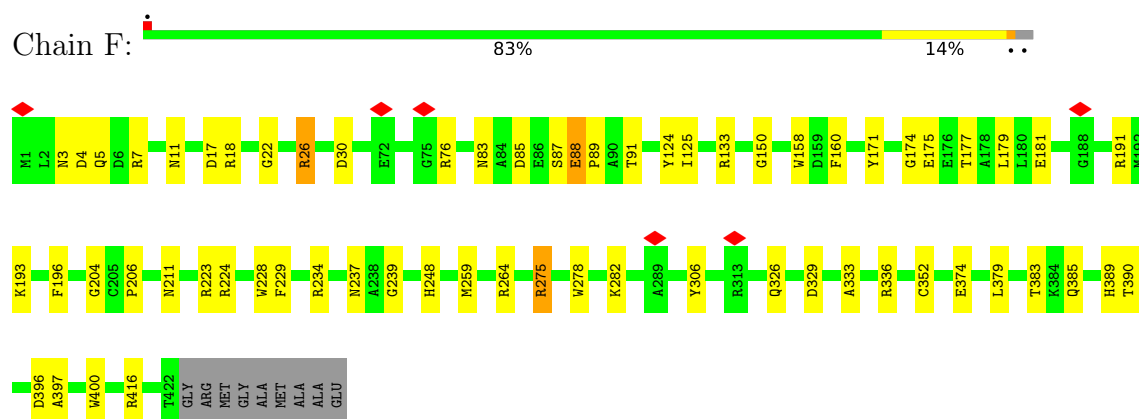
- Molecule 4: NADH-quinone oxidoreductase subunit D



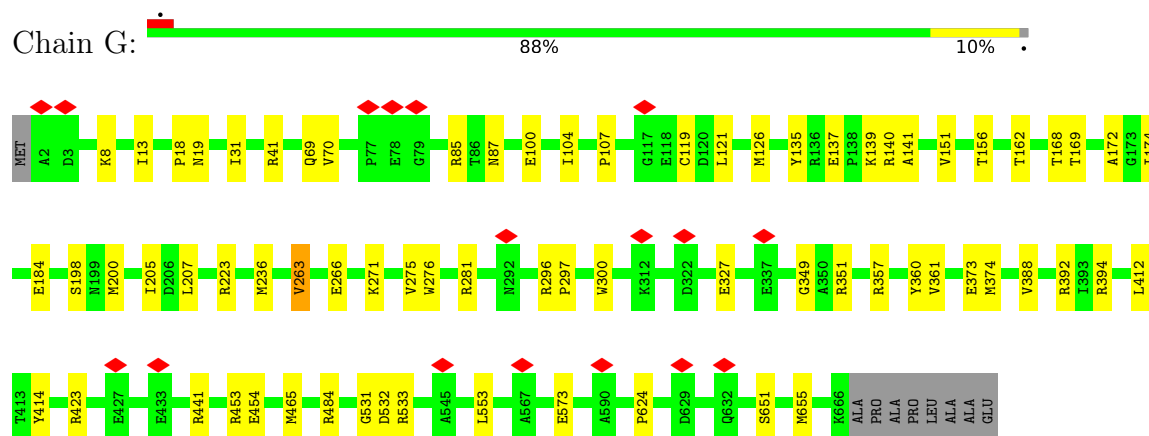
- Molecule 5: NADH dehydrogenase subunit E



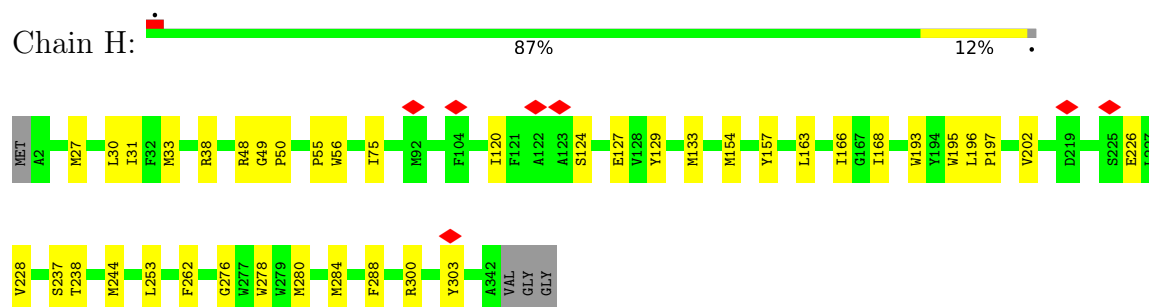
- Molecule 6: NADH-quinone oxidoreductase subunit F



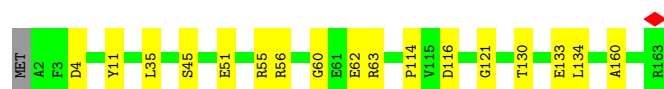
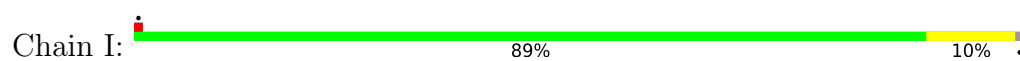
- Molecule 7: NADH-quinone oxidoreductase



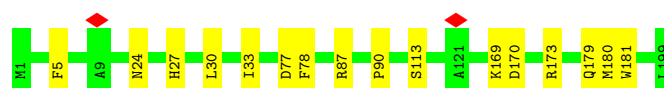
- Molecule 8: NADH-quinone oxidoreductase subunit H



- Molecule 9: NADH-quinone oxidoreductase subunit I



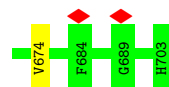
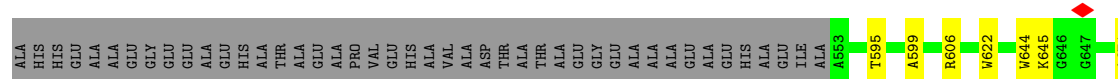
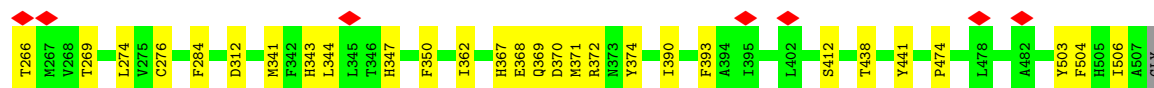
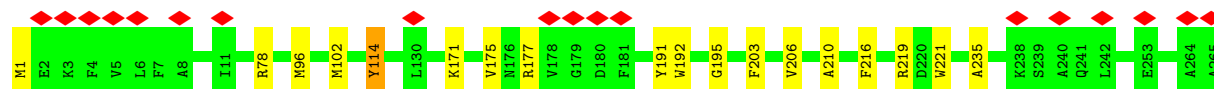
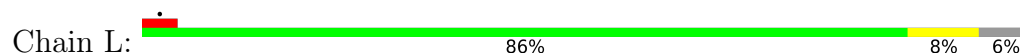
- Molecule 10: NADH-quinone oxidoreductase subunit J



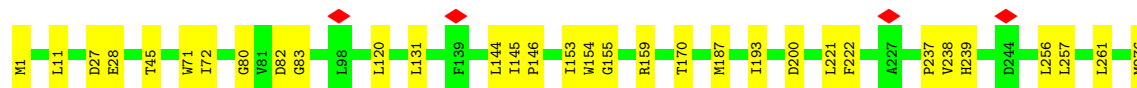
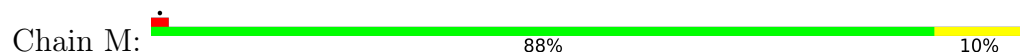
- Molecule 11: NADH-quinone oxidoreductase subunit K



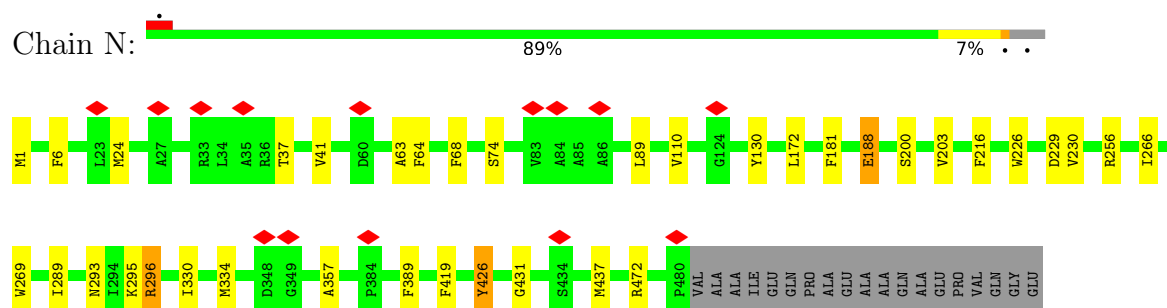
- Molecule 12: NADH dehydrogenase subunit L



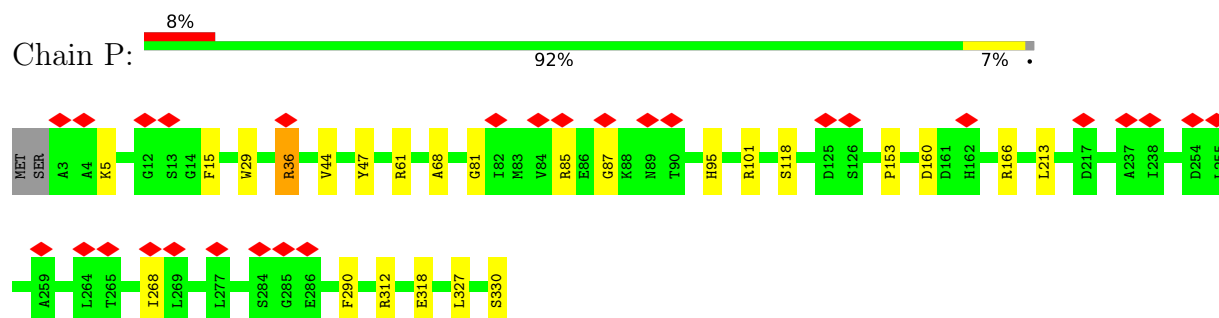
- Molecule 13: NADH dehydrogenase subunit M



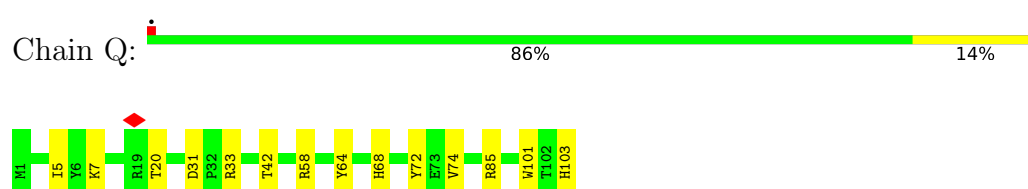
- Molecule 14: NADH-quinone oxidoreductase subunit N



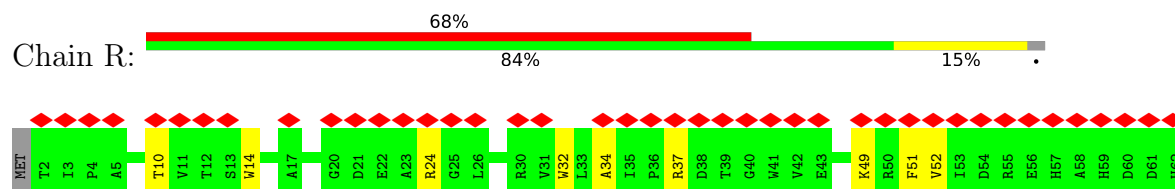
- Molecule 15: NAD-dependent epimerase/dehydratase



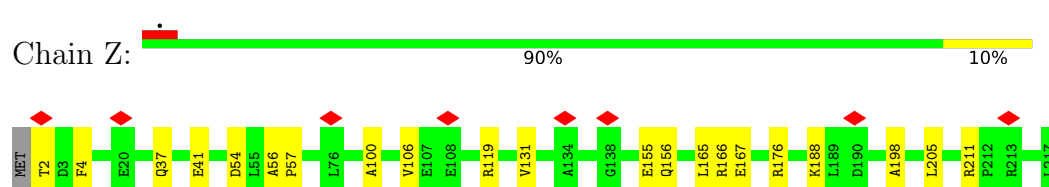
- Molecule 16: ETC complex I subunit conserved region



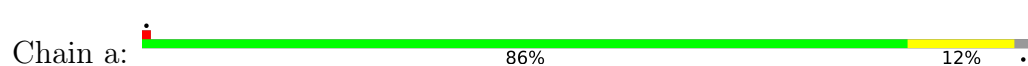
- Molecule 17: Zinc finger CHCC-type domain-containing protein

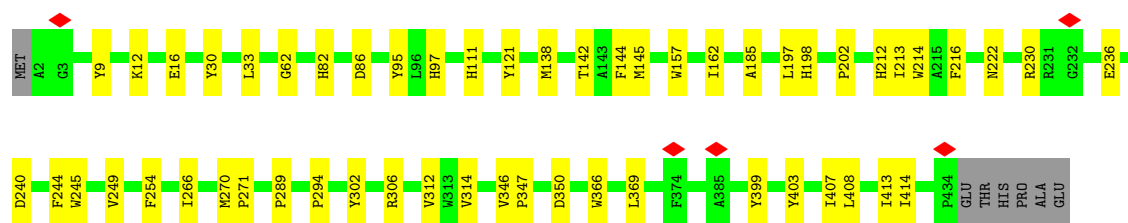


- Molecule 18: Protein-L-isoaspartate O-methyltransferase

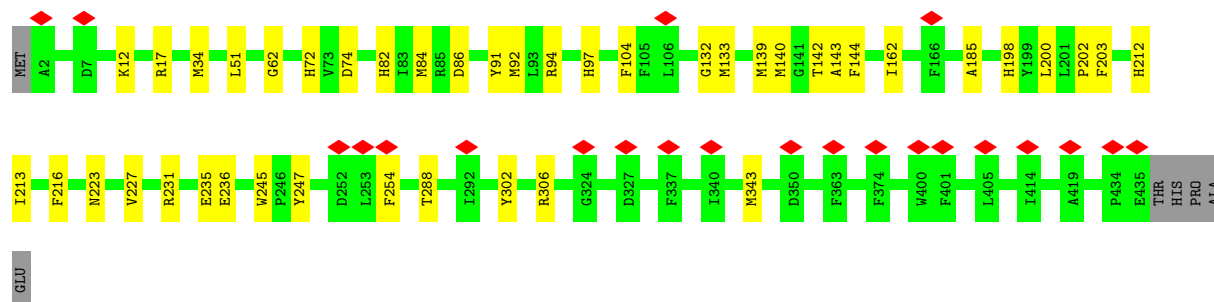
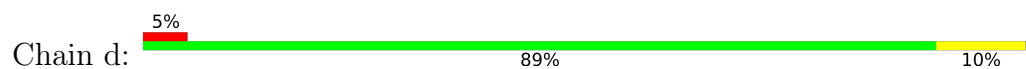


- Molecule 19: Cytochrome b

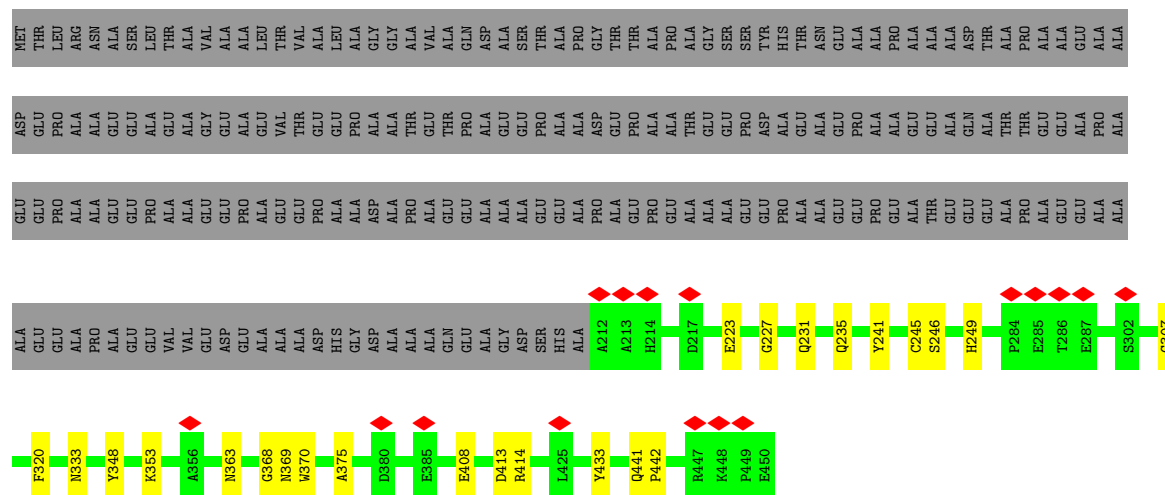




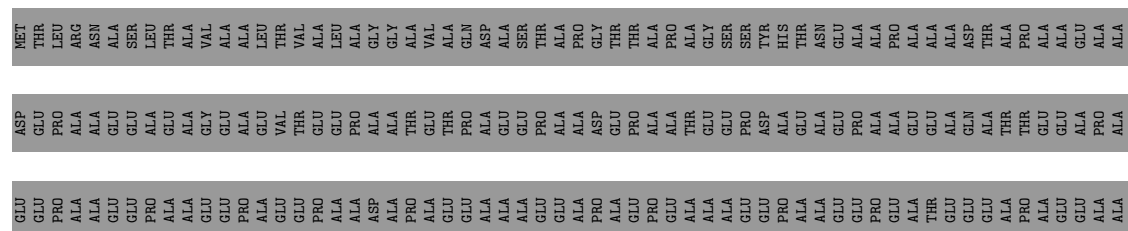
• Molecule 19: Cytochrome b

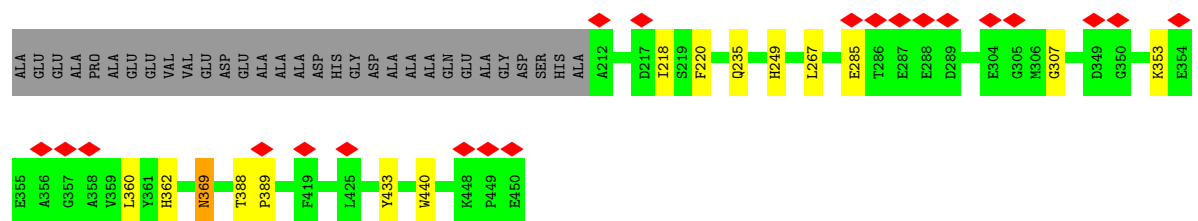


• Molecule 20: Cytochrome c1

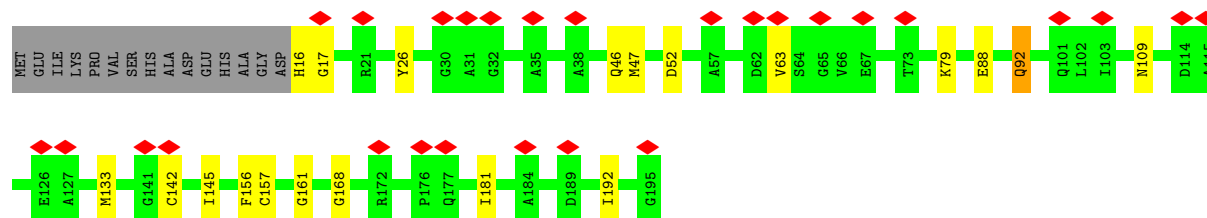
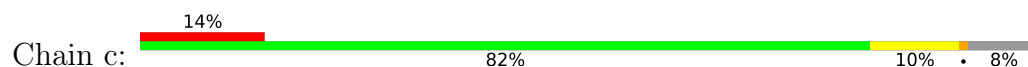


• Molecule 20: Cytochrome c1

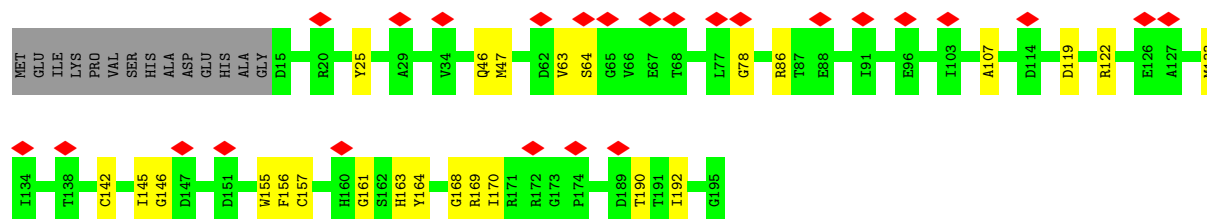
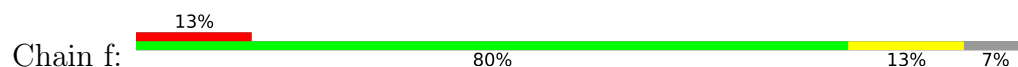




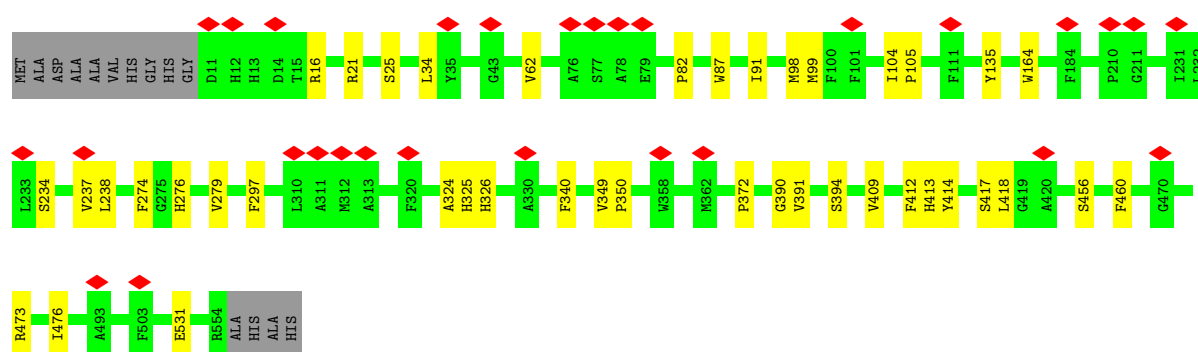
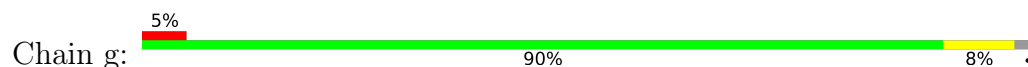
- Molecule 21: Ubiquinol-cytochrome c reductase iron-sulfur subunit



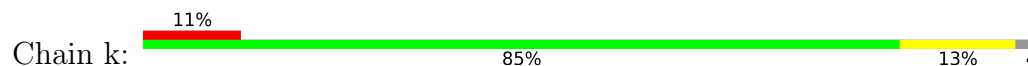
- Molecule 21: Ubiquinol-cytochrome c reductase iron-sulfur subunit

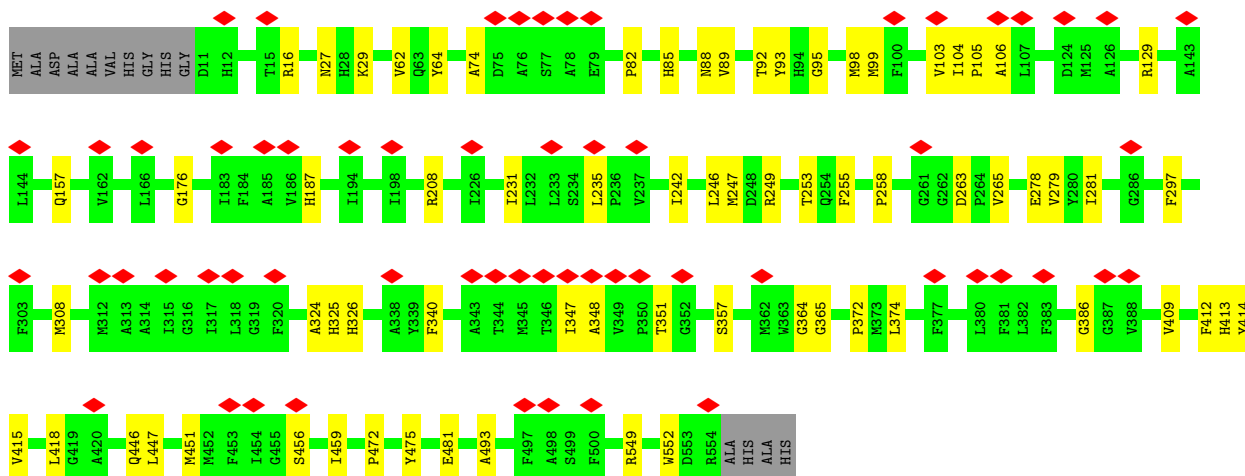


- Molecule 22: Cytochrome c oxidase subunit 1

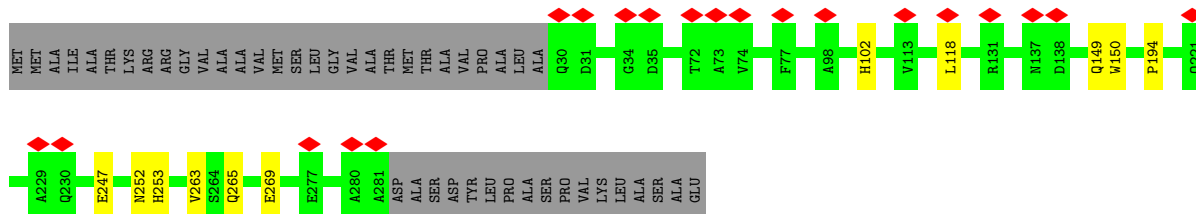
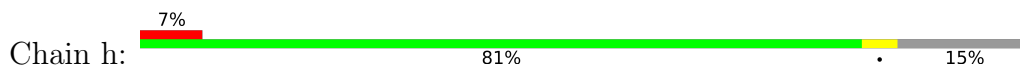


- Molecule 22: Cytochrome c oxidase subunit 1

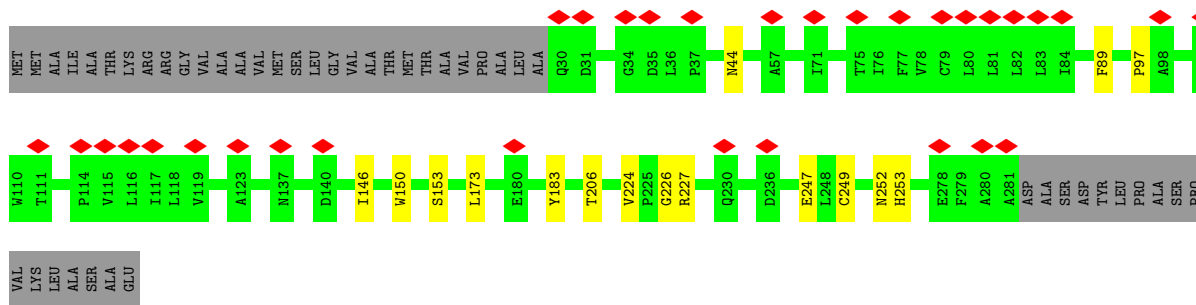
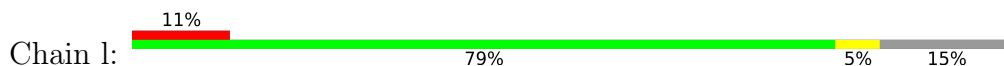




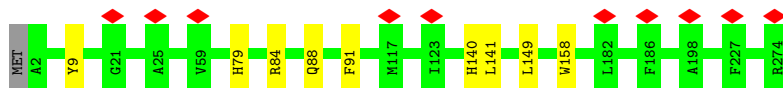
• Molecule 23: Cytochrome c oxidase subunit 2



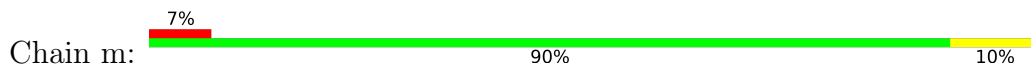
• Molecule 23: Cytochrome c oxidase subunit 2

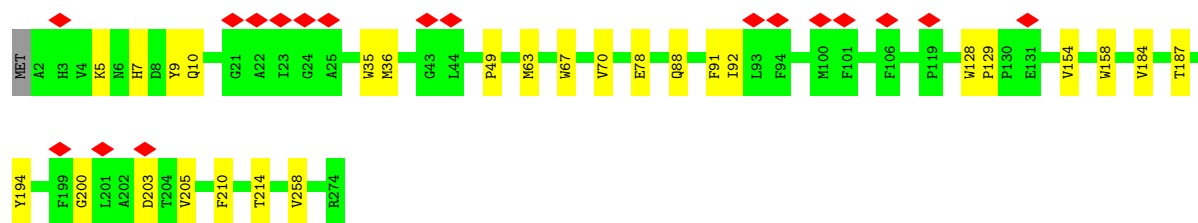


• Molecule 24: cytochrome-c oxidase

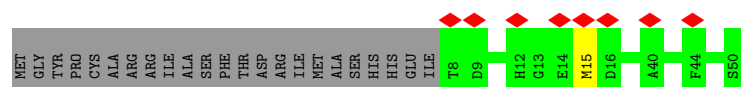


• Molecule 24: cytochrome-c oxidase

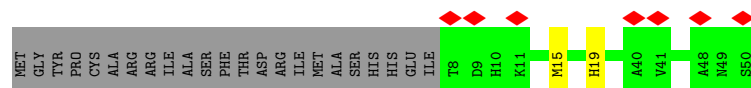




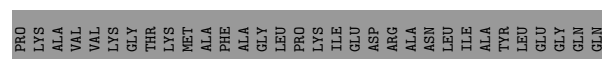
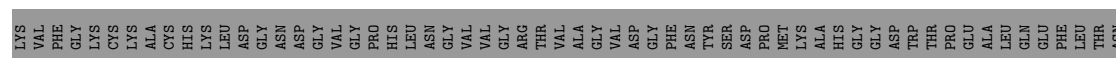
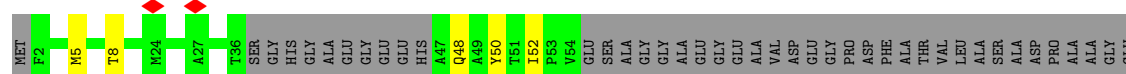
- Molecule 25: Aa3 type cytochrome c oxidase subunit IV



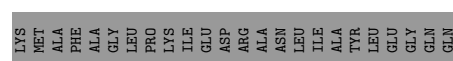
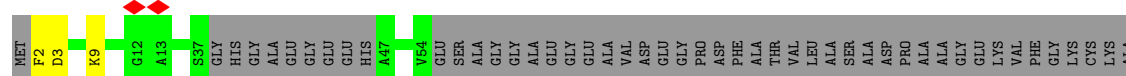
- Molecule 25: Aa3 type cytochrome c oxidase subunit IV



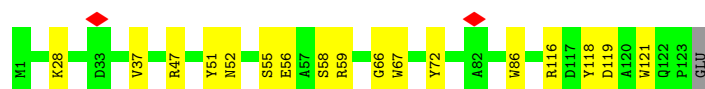
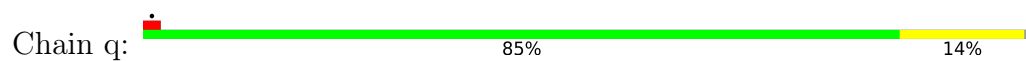
- Molecule 26: Cytochrome c, class I



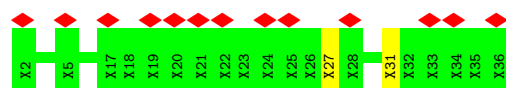
- Molecule 26: Cytochrome c, class I



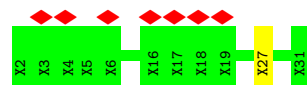
- Molecule 27: NADH:ubiquinone oxidoreductase 17.2 kD subunit



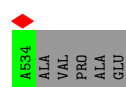
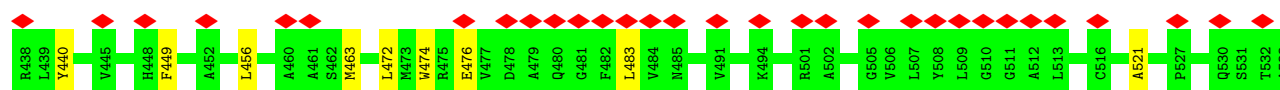
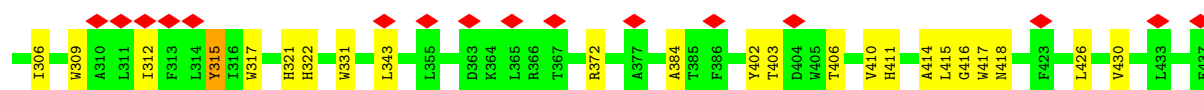
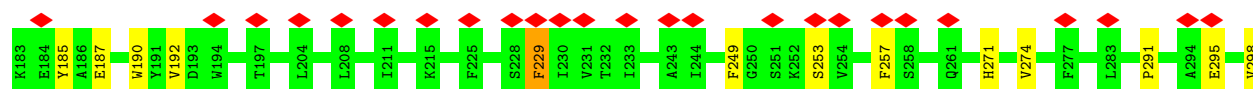
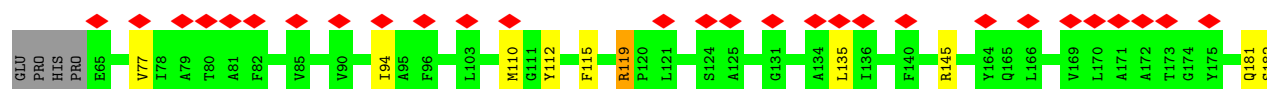
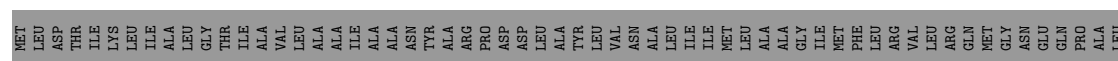
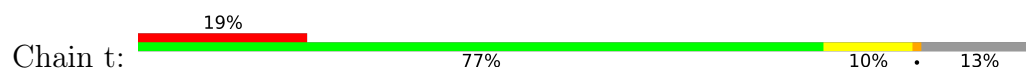
- Molecule 28: Transmembrane helix of unknown identity



- Molecule 29: Transmembrane helix of unknown identity



- Molecule 30: cytochrome-c oxidase



- Molecule 31: Cytochrome c oxidase, cbb3-type, subunit II





• Molecule 32: Cbb3-type cytochrome c oxidase subunit CcoP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4238	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.2	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.068	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0112	Depositor
Map size (\AA)	393.0, 393.0, 393.0	wwPDB
Map dimensions	375, 375, 375	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4, 2MR, CU, FMN, CDL, DU0, NA, U10, HEM, MN, HEC, FME, FES, CA, CUA, HEA

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	0.30	0/988	0.56	0/1345
2	B	0.32	0/1297	0.65	0/1758
3	C	0.32	0/1624	0.65	0/2208
4	D	0.32	0/3339	0.62	0/4520
5	E	0.25	0/1865	0.63	0/2537
6	F	0.28	0/3308	0.63	0/4456
7	G	0.28	0/5156	0.64	0/6982
8	H	0.32	0/2815	0.61	0/3837
9	I	0.33	0/1354	0.63	0/1828
10	J	0.31	0/1548	0.61	1/2104 (0.0%)
11	K	0.35	0/775	0.57	0/1050
12	L	0.25	0/5357	0.56	1/7293 (0.0%)
13	M	0.29	0/4010	0.58	0/5460
14	N	0.31	0/3634	0.56	0/4935
15	P	0.27	0/2511	0.65	1/3409 (0.0%)
16	Q	0.30	0/872	0.63	0/1181
17	R	0.23	0/503	0.67	0/685
18	Z	0.30	0/1669	0.62	0/2266
19	a	0.35	0/3641	0.60	0/4993
19	d	0.32	0/3650	0.62	0/5005
20	b	0.29	0/1906	0.54	0/2592
20	e	0.29	0/1906	0.63	0/2592
21	c	0.25	0/1382	0.55	0/1880
21	f	0.24	0/1390	0.55	0/1891
22	g	0.26	0/4483	0.62	0/6118
22	k	0.23	0/4483	0.60	0/6118
23	h	0.24	0/2033	0.60	0/2787
23	l	0.22	0/2033	0.60	0/2787
24	i	0.28	0/2270	0.52	0/3107
24	m	0.26	0/2270	0.56	0/3107
25	j	0.25	0/339	0.48	0/457
25	n	0.22	0/339	0.55	0/457

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	o	0.28	0/321	0.58	0/436
26	p	0.30	0/327	0.50	0/444
27	q	0.29	0/1049	0.63	0/1434
30	t	0.22	0/3863	0.62	0/5281
31	u	0.24	0/1551	0.59	0/2104
32	v	0.22	0/2154	0.60	0/2955
All	All	0.28	0/84015	0.60	3/114399 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	C	0	1
6	F	0	3
7	G	0	2
8	H	0	1
12	L	0	1
13	M	0	1
14	N	0	2
15	P	0	2
16	Q	0	1
19	d	0	1
22	g	0	2
30	t	0	3
31	u	0	1
All	All	0	22

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	87	ARG	CA-CB-CG	-5.35	103.40	114.10
12	L	266	THR	N-CA-C	5.10	118.95	111.04
15	P	327	LEU	N-CA-C	5.10	116.92	111.36

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	134	ARG	Sidechain
3	C	93	ARG	Sidechain
6	F	234	ARG	Sidechain
6	F	26	ARG	Sidechain
6	F	275	ARG	Sidechain
7	G	223	ARG	Sidechain
7	G	484	ARG	Sidechain
8	H	48	ARG	Sidechain
12	L	606	ARG	Sidechain
13	M	460	ARG	Sidechain
14	N	296	ARG	Sidechain
14	N	472	ARG	Sidechain
15	P	166	ARG	Sidechain
15	P	36	ARG	Sidechain
16	Q	85	ARG	Sidechain
19	d	231	ARG	Sidechain
22	g	16	ARG	Sidechain
22	g	473	ARG	Sidechain
30	t	119	ARG	Sidechain
30	t	145	ARG	Sidechain
30	t	271	HIS	Sidechain
31	u	108	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	969	0	970	9	0
2	B	1270	0	1268	21	0
3	C	1586	0	1562	11	0
4	D	3277	0	3217	27	0
5	E	1822	0	1796	21	0
6	F	3241	0	3188	47	0
7	G	5068	0	5037	42	0
8	H	2722	0	2744	25	0
9	I	1319	0	1259	14	0
10	J	1528	0	1612	14	0
11	K	764	0	817	6	0
12	L	5193	0	5152	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	3915	0	4024	30	0
14	N	3556	0	3656	24	0
15	P	2468	0	2498	13	0
16	Q	849	0	812	7	0
17	R	488	0	450	6	0
18	Z	1642	0	1643	13	0
19	a	3504	0	3483	48	0
19	d	3513	0	3489	33	0
20	b	1855	0	1773	16	0
20	e	1855	0	1773	9	0
21	c	1353	0	1295	14	0
21	f	1361	0	1299	14	0
22	g	4322	0	4225	24	0
22	k	4322	0	4226	49	0
23	h	1976	0	1960	6	0
23	l	1976	0	1960	14	0
24	i	2183	0	2144	6	0
24	m	2183	0	2144	17	0
25	j	332	0	331	1	0
25	n	332	0	331	2	0
26	o	315	0	324	4	0
26	p	321	0	329	4	0
27	q	1018	0	942	10	0
28	r	175	0	38	1	0
29	s	150	0	33	1	0
30	t	3732	0	3692	32	0
31	u	1517	0	1507	21	0
32	v	2095	0	1968	17	0
33	B	8	0	0	3	0
33	F	8	0	0	2	0
33	G	16	0	0	1	0
33	I	16	0	0	0	0
34	D	1	0	0	0	0
35	E	4	0	0	1	0
35	G	4	0	0	0	0
35	c	4	0	0	0	0
35	f	4	0	0	0	0
36	F	31	0	19	6	0
37	H	37	0	0	0	0
37	N	37	0	0	0	0
37	f	37	0	0	0	0
38	H	63	0	90	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	a	126	0	180	12	0
38	d	126	0	180	9	0
39	R	1	0	0	0	0
40	a	100	0	156	3	0
41	a	86	0	60	11	0
41	d	86	0	60	11	0
41	t	86	0	60	5	0
42	b	1	0	0	0	0
42	e	1	0	0	0	0
42	g	1	0	0	0	0
42	k	1	0	0	0	0
42	t	2	0	0	0	0
43	b	43	0	30	1	0
43	e	43	0	30	1	0
43	u	43	0	30	4	0
43	v	86	0	60	6	0
44	g	120	0	108	7	0
44	k	120	0	108	9	0
45	g	1	0	0	0	0
45	k	1	0	0	0	0
45	t	1	0	0	0	0
46	g	1	0	0	0	0
47	h	2	0	0	0	0
47	l	2	0	0	0	0
All	All	83417	0	82142	645	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (645) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:u:210:ARG:H	31:u:211:PRO:HD2	1.51	0.75
22:k:308:MET:HE3	22:k:357:SER:HB2	1.69	0.74
5:E:204:HIS:O	6:F:18:ARG:NH2	2.20	0.74
1:A:21:LEU:HD13	38:H:402:U10:H561	1.72	0.71
22:k:98:MET:HB3	44:k:601:HEA:CAC	2.24	0.68
1:A:75:LEU:HD11	11:K:71:ALA:HB3	1.76	0.68
30:t:415:LEU:HB2	30:t:456:LEU:HD13	1.77	0.66
31:u:210:ARG:H	31:u:211:PRO:CD	2.08	0.66
22:k:365:GLY:HA2	23:l:89:PHE:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:u:68:CYS:SG	43:u:1000:HEC:HHC	2.36	0.66
22:k:351:THR:HG21	44:k:602:HEA:H14	1.77	0.65
32:v:185:HIS:CE1	43:v:1001:HEC:ND	2.64	0.65
7:G:151:VAL:HG22	7:G:205:ILE:HD11	1.78	0.65
32:v:251:VAL:HG22	32:v:311:ILE:HG22	1.79	0.65
19:d:62:GLY:C	41:d:502:HEM:HBC2	2.23	0.64
22:k:98:MET:HB3	44:k:601:HEA:HAC	1.79	0.64
7:G:357:ARG:HA	7:G:360:TYR:CE2	2.33	0.63
8:H:31:ILE:HD11	38:H:402:U10:H252	1.79	0.63
22:k:549:ARG:HA	22:k:552:TRP:CE2	2.33	0.63
19:a:244:PHE:CD2	38:a:504:U10:H3M3	2.34	0.63
13:M:27:ASP:OD1	13:M:28:GLU:N	2.32	0.63
13:M:257:LEU:HA	13:M:261:LEU:HD12	1.79	0.63
23:l:146:ILE:HG23	23:l:153:SER:HG	1.63	0.62
21:f:107:ALA:O	21:f:122:ARG:NH1	2.27	0.62
15:P:81:GLY:HA3	15:P:95:HIS:HD2	1.64	0.62
22:g:21:ARG:O	22:g:25:SER:HB3	1.99	0.62
22:g:98:MET:HB3	44:g:603:HEA:CAC	2.29	0.61
6:F:385:GLN:O	6:F:389:HIS:ND1	2.30	0.61
13:M:430:SER:HA	13:M:433:TYR:CE2	2.35	0.61
30:t:410:VAL:HG22	41:t:602:HEM:C2D	2.36	0.61
19:d:140:MET:HE3	38:d:501:U10:H71	1.83	0.61
4:D:163:ARG:HG2	4:D:163:ARG:HH11	1.66	0.61
19:a:97:HIS:HE1	41:a:505:HEM:C1C	2.17	0.61
24:m:210:PHE:O	24:m:214:THR:HG22	1.99	0.61
24:m:35:TRP:CE2	24:m:49:PRO:HG3	2.35	0.61
26:o:48:GLN:NE2	26:o:50:TYR:O	2.34	0.61
12:L:347:HIS:HA	12:L:350:PHE:CE2	2.37	0.60
13:M:187:MET:HE1	13:M:221:LEU:HD11	1.82	0.60
12:L:438:THR:HA	12:L:441:TYR:CE2	2.35	0.60
20:b:249:HIS:CD2	43:b:502:HEC:NB	2.68	0.60
4:D:273:CYS:HB3	4:D:402:THR:HG21	1.84	0.60
5:E:98:THR:HG22	5:E:99:THR:H	1.67	0.60
6:F:17:ASP:O	6:F:26:ARG:NH2	2.35	0.60
19:a:142:THR:HG21	41:a:505:HEM:HBB2	1.82	0.59
2:B:47:TRP:CZ2	2:B:76:PRO:HB3	2.38	0.59
19:a:62:GLY:HA3	41:a:505:HEM:C4C	2.38	0.59
9:I:51:GLU:O	9:I:121:GLY:N	2.36	0.59
31:u:46:VAL:N	31:u:93:ALA:HB1	2.18	0.58
8:H:196:LEU:HB3	8:H:197:PRO:HD3	1.85	0.58
18:Z:165:LEU:HD23	18:Z:188:LYS:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:300:TRP:HE1	7:G:573:GLU:HB3	1.68	0.58
8:H:163:LEU:HA	8:H:166:ILE:HD12	1.84	0.58
30:t:94:ILE:HB	30:t:115:PHE:CE2	2.39	0.58
6:F:211:ASN:N	36:F:502:FMN:O2P	2.35	0.58
9:I:56:ARG:NH1	9:I:60:GLY:O	2.31	0.58
24:m:88:GLN:HA	24:m:91:PHE:CE2	2.39	0.57
7:G:8:LYS:HE2	7:G:13:ILE:HD11	1.85	0.57
21:f:145:ILE:N	21:f:156:PHE:O	2.36	0.57
8:H:202:VAL:HG22	8:H:262:PHE:CD1	2.40	0.57
22:k:176:GLY:O	22:k:249:ARG:NH2	2.37	0.57
31:u:176:ALA:O	31:u:209:ARG:NH2	2.35	0.57
5:E:137:CYS:SG	6:F:89:PRO:HA	2.45	0.57
14:N:357:ALA:HB1	14:N:437:MET:HG3	1.87	0.57
4:D:42:LEU:HB2	4:D:407:PHE:CZ	2.40	0.57
2:B:129:SER:O	2:B:134:ARG:NH2	2.37	0.57
16:Q:101:TRP:CH2	16:Q:103:HIS:HA	2.40	0.57
19:d:162:ILE:HG13	38:d:501:U10:H3M3	1.86	0.57
24:i:88:GLN:HA	24:i:91:PHE:CE2	2.40	0.57
15:P:330:SER:OG	18:Z:100:ALA:O	2.19	0.56
12:L:210:ALA:HB2	12:L:284:PHE:HB3	1.88	0.56
19:a:244:PHE:CE1	38:a:504:U10:H4M3	2.40	0.56
22:g:234:SER:O	22:g:237:VAL:HG22	2.05	0.56
6:F:229:PHE:CZ	6:F:239:GLY:HA3	2.40	0.56
6:F:352:CYS:HB3	33:F:501:SF4:S2	2.45	0.56
20:e:249:HIS:CE1	20:e:307:GLY:HA3	2.39	0.56
23:l:150:TRP:CD2	23:l:252:ASN:HB2	2.41	0.56
22:g:409:VAL:HA	22:g:412:PHE:CE2	2.41	0.56
30:t:426:LEU:O	30:t:430:VAL:HG23	2.05	0.56
12:L:595:THR:HA	12:L:599:ALA:HB3	1.88	0.56
17:R:14:TRP:CZ3	17:R:37:ARG:HA	2.40	0.56
19:a:144:PHE:HD2	38:a:502:U10:H202	1.70	0.56
21:c:26:TYR:CE1	26:p:9:LYS:HE3	2.41	0.56
22:g:62:VAL:HG21	22:g:82:PRO:HB3	1.87	0.56
3:C:151:LYS:HE3	4:D:369:TRP:CZ2	2.41	0.55
30:t:190:TRP:CD1	30:t:253:SER:HB3	2.39	0.55
32:v:314:ILE:HA	32:v:319:PRO:HD3	1.88	0.55
5:E:47:GLN:O	5:E:51:GLY:N	2.38	0.55
8:H:193:TRP:HB2	8:H:195:TRP:CD1	2.41	0.55
23:l:146:ILE:HD11	23:l:206:THR:HG23	1.87	0.55
30:t:384:ALA:HB1	41:t:602:HEM:HMC3	1.89	0.55
4:D:173:TYR:OH	4:D:181:GLN:O	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:v:177:PHE:CD2	32:v:181:CYS:HB2	2.42	0.55
4:D:220:VAL:HG11	10:J:179:GLN:HA	1.89	0.55
23:l:150:TRP:NE1	23:l:249:CYS:O	2.38	0.55
1:A:121:ALA:OXT	10:J:173:ARG:NH2	2.40	0.54
23:l:146:ILE:HG23	23:l:153:SER:OG	2.07	0.54
32:v:271:VAL:O	32:v:275:ALA:N	2.38	0.54
3:C:169:ARG:NH2	18:Z:198:ALA:O	2.41	0.54
30:t:321:HIS:CD2	30:t:322:HIS:CD2	2.95	0.54
2:B:169:ARG:HG3	2:B:170:THR:HG23	1.90	0.54
22:k:409:VAL:HA	22:k:412:PHE:CE2	2.43	0.54
6:F:76:ARG:NH1	6:F:204:GLY:O	2.35	0.54
19:d:12:LYS:O	19:d:17:ARG:NH2	2.35	0.54
19:a:9:TYR:HB2	19:a:30:TYR:CD1	2.42	0.54
24:i:79:HIS:O	24:i:84:ARG:NE	2.35	0.54
20:e:235:GLN:HG2	20:e:267:LEU:HD21	1.89	0.53
21:c:145:ILE:N	21:c:156:PHE:O	2.38	0.53
6:F:88:GLU:O	6:F:91:THR:OG1	2.19	0.53
31:u:9:VAL:HG23	31:u:10:LEU:H	1.73	0.53
22:k:208:ARG:HH21	25:n:19:HIS:CD2	2.27	0.53
31:u:72:HIS:CE1	31:u:109:GLY:HA3	2.44	0.53
7:G:85:ARG:NH1	7:G:87:ASN:OD1	2.38	0.53
7:G:349:GLY:O	7:G:351:ARG:NH1	2.42	0.53
22:g:418:LEU:HD21	22:g:456:SER:HB3	1.90	0.53
30:t:182:SER:HA	31:u:69:TYR:CE2	2.43	0.53
4:D:44:MET:HE2	4:D:46:LEU:HD21	1.91	0.53
7:G:374:MET:HE1	7:G:441:ARG:HB2	1.91	0.53
19:a:403:TYR:HA	19:a:407:ILE:HD12	1.91	0.53
13:M:288:VAL:HG11	13:M:329:PHE:CD1	2.44	0.53
15:P:44:VAL:HA	15:P:47:TYR:CE2	2.43	0.53
20:b:353:LYS:HE2	20:b:370:TRP:CD2	2.44	0.53
21:c:26:TYR:CZ	26:p:9:LYS:HE3	2.44	0.52
27:q:52:ASN:O	27:q:59:ARG:NH2	2.37	0.52
3:C:34:GLU:OE2	3:C:93:ARG:NH1	2.38	0.52
32:v:274:PHE:CD2	32:v:278:CYS:HB2	2.44	0.52
7:G:423:ARG:NH2	7:G:454:GLU:OE1	2.29	0.52
18:Z:2:THR:HB	18:Z:4:PHE:CE2	2.43	0.52
13:M:71:TRP:CG	13:M:72:ILE:H	2.27	0.52
17:R:49:LYS:HE2	17:R:51:PHE:CE2	2.45	0.52
18:Z:54:ASP:N	18:Z:54:ASP:OD1	2.39	0.52
5:E:98:THR:OG1	5:E:137:CYS:N	2.37	0.52
20:b:249:HIS:CE1	20:b:307:GLY:HA3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:t:411:HIS:HA	30:t:414:ALA:HB3	1.91	0.52
7:G:281:ARG:HA	27:q:119:ASP:HB3	1.92	0.52
12:L:177:ARG:NH1	13:M:427:VAL:O	2.41	0.52
44:g:602:HEA:H242	23:h:118:LEU:HG	1.92	0.52
24:i:9:TYR:CE2	25:j:15:MET:HE1	2.45	0.52
31:u:96:MET:HA	31:u:96:MET:HE2	1.91	0.52
19:d:202:PRO:HG2	41:d:502:HEM:HMC3	1.91	0.52
22:k:16:ARG:HG3	22:k:16:ARG:HH11	1.74	0.52
7:G:281:ARG:NH1	7:G:651:SER:O	2.37	0.52
14:N:74:SER:OG	14:N:256:ARG:NH2	2.43	0.52
19:a:33:LEU:HD21	38:a:504:U10:H1M1	1.91	0.52
21:c:79:LYS:HE3	19:d:185:ALA:HB2	1.92	0.52
7:G:140:ARG:NH1	7:G:184:GLU:OE1	2.34	0.51
12:L:192:TRP:CZ2	13:M:414:ARG:HB2	2.45	0.51
22:g:276:HIS:O	22:g:279:VAL:HG22	2.09	0.51
30:t:406:THR:O	30:t:410:VAL:HG23	2.10	0.51
7:G:351:ARG:NH1	7:G:453:ARG:O	2.43	0.51
38:d:501:U10:H152	38:d:501:U10:H112	1.90	0.51
22:k:412:PHE:CE1	22:k:413:HIS:CE1	2.99	0.51
7:G:174:ILE:HG21	7:G:198:SER:HB2	1.91	0.51
12:L:312:ASP:CG	12:L:369:GLN:HE21	2.18	0.51
24:m:10:GLN:HG3	24:m:78:GLU:HG3	1.93	0.51
22:k:62:VAL:HG21	22:k:82:PRO:HB3	1.93	0.51
22:k:89:VAL:HG13	22:k:93:TYR:CD2	2.46	0.51
23:l:173:LEU:HD11	23:l:183:TYR:HA	1.92	0.51
30:t:403:THR:HG22	30:t:474:TRP:CZ3	2.46	0.51
2:B:58:GLU:O	2:B:62:THR:HG23	2.10	0.51
2:B:111:ARG:O	2:B:175:ARG:NH2	2.40	0.51
22:k:187:HIS:NE2	22:k:242:ILE:HG13	2.25	0.51
22:k:447:LEU:HG	22:k:451:MET:HE2	1.93	0.51
20:b:408:GLU:OE2	20:b:414:ARG:NH1	2.38	0.51
5:E:230:THR:HG23	5:E:232:TRP:CZ2	2.45	0.50
13:M:82:ASP:OD1	13:M:83:GLY:N	2.44	0.50
21:c:109:ASN:HA	21:c:181:ILE:HB	1.92	0.50
5:E:96:CYS:HB3	5:E:101:CYS:SG	2.51	0.50
6:F:224:ARG:HD3	6:F:228:TRP:CE3	2.46	0.50
19:a:82:HIS:CE1	19:a:86:ASP:HB2	2.47	0.50
19:a:302:TYR:CZ	19:a:306:ARG:HD3	2.46	0.50
30:t:135:LEU:HD13	30:t:229:PHE:CZ	2.46	0.50
31:u:151:VAL:HB	31:u:210:ARG:HE	1.75	0.50
5:E:100:THR:HB	35:E:401:FES:S2	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:c:142:CYS:SG	19:d:288:THR:HG21	2.51	0.50
12:L:192:TRP:CE3	13:M:414:ARG:HD2	2.47	0.50
19:d:133:MET:HE1	19:d:343:MET:HE3	1.94	0.50
22:k:258:PRO:HB3	23:l:226:GLY:HA3	1.93	0.50
6:F:282:LYS:HD2	6:F:326:GLN:HA	1.94	0.50
6:F:379:LEU:O	6:F:383:THR:HG23	2.11	0.50
31:u:60:ARG:O	31:u:64:VAL:HG13	2.10	0.50
7:G:19:ASN:O	7:G:69:GLN:NE2	2.39	0.50
6:F:396:ASP:HB3	6:F:400:TRP:CZ2	2.47	0.50
9:I:56:ARG:HD2	27:q:86:TRP:CE3	2.46	0.50
12:L:203:PHE:HA	12:L:206:VAL:HG23	1.93	0.50
14:N:200:SER:HB3	14:N:203:VAL:HG23	1.94	0.50
5:E:185:SER:OG	5:E:186:ALA:N	2.45	0.49
22:g:99:MET:HG3	22:g:164:TRP:CZ3	2.47	0.49
9:I:130:THR:N	9:I:133:GLU:OE1	2.45	0.49
5:E:230:THR:O	5:E:230:THR:HG22	2.13	0.49
8:H:154:MET:HA	8:H:157:TYR:CE2	2.48	0.49
15:P:312:ARG:HB3	15:P:318:GLU:HG3	1.94	0.49
43:e:502:HEC:HMC1	43:e:502:HEC:HBC3	1.94	0.49
31:u:82:GLU:CD	31:u:107:ARG:HH12	2.20	0.49
22:k:414:TYR:CD1	22:k:418:LEU:HD12	2.47	0.49
8:H:31:ILE:CD1	38:H:402:U10:H252	2.43	0.49
5:E:202:GLU:HG2	6:F:18:ARG:NH2	2.27	0.49
6:F:22:GLY:C	6:F:26:ARG:HH21	2.21	0.49
19:d:235:GLU:OE2	19:d:236:GLU:HG2	2.13	0.49
22:k:255:PHE:HA	24:m:205:VAL:HG23	1.95	0.49
2:B:71:ARG:HA	8:H:50:PRO:HA	1.95	0.49
17:R:10:THR:HA	17:R:52:VAL:O	2.13	0.49
20:b:231:GLN:OE1	20:b:235:GLN:NE2	2.46	0.49
21:c:63:VAL:HG11	21:c:192:ILE:HD12	1.95	0.49
21:f:63:VAL:HG11	21:f:192:ILE:HD12	1.95	0.49
22:k:246:LEU:HD11	24:m:36:MET:HE1	1.95	0.49
30:t:181:GLN:HB2	30:t:187:GLU:HA	1.95	0.49
14:N:226:TRP:HE3	14:N:230:VAL:HG21	1.78	0.48
19:d:132:GLY:HA3	41:d:503:HEM:HBC2	1.95	0.48
21:f:64:SER:HB3	21:f:190:THR:HB	1.95	0.48
19:d:97:HIS:HE1	41:d:502:HEM:C1C	2.31	0.48
7:G:263:VAL:O	7:G:392:ARG:NH1	2.46	0.48
4:D:321:LYS:NZ	9:I:114:PRO:O	2.40	0.48
10:J:30:LEU:O	10:J:33:ILE:HG22	2.14	0.48
22:k:325:HIS:NE2	22:k:326:HIS:CD2	2.80	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:347:HIS:HA	12:L:350:PHE:CZ	2.48	0.48
30:t:274:VAL:HG11	41:t:602:HEM:C4C	2.49	0.48
43:u:1000:HEC:HBC3	43:u:1000:HEC:HHD	1.94	0.48
7:G:465:MET:SD	7:G:624:PRO:HA	2.54	0.48
14:N:216:PHE:CE2	14:N:226:TRP:CD1	3.02	0.48
19:d:82:HIS:CE1	19:d:86:ASP:HB2	2.49	0.48
21:f:156:PHE:CE1	21:f:161:GLY:HA2	2.49	0.48
22:k:364:GLY:O	23:l:97:PRO:HA	2.14	0.48
22:k:456:SER:HA	22:k:459:ILE:HD12	1.94	0.48
6:F:329:ASP:OD1	6:F:416:ARG:NH2	2.42	0.48
7:G:200:MET:HE1	7:G:388:VAL:HG22	1.95	0.48
9:I:4:ASP:HB3	10:J:181:TRP:CD1	2.49	0.48
19:a:97:HIS:HE1	41:a:505:HEM:CHC	2.27	0.48
19:a:162:ILE:HD11	38:a:502:U10:C4	2.43	0.48
19:d:254:PHE:CE1	20:e:433:TYR:HB2	2.49	0.48
20:e:353:LYS:HE3	20:e:360:LEU:HD12	1.96	0.48
22:k:297:PHE:CE2	22:k:372:PRO:HB2	2.48	0.48
38:a:504:U10:H211	38:d:501:U10:H38	1.96	0.48
22:k:88:ASN:O	22:k:92:THR:OG1	2.31	0.48
6:F:211:ASN:H	36:F:502:FMN:P	2.36	0.48
6:F:259:MET:HE1	6:F:306:TYR:CD2	2.48	0.48
8:H:276:GLY:HA3	8:H:278:TRP:CZ2	2.49	0.48
12:L:78:ARG:HD3	12:L:503:TYR:CE2	2.49	0.48
6:F:177:THR:HB	6:F:191:ARG:HG2	1.96	0.47
19:a:214:TRP:HE1	40:a:501:CDL:HB61	1.79	0.47
27:q:51:TYR:CG	27:q:55:SER:HA	2.49	0.47
30:t:110:MET:HB2	30:t:112:TYR:CZ	2.49	0.47
6:F:248:HIS:HA	6:F:275:ARG:NH1	2.30	0.47
14:N:266:ILE:HA	14:N:269:TRP:NE1	2.29	0.47
20:b:353:LYS:HE2	20:b:370:TRP:CG	2.49	0.47
22:g:414:TYR:CD1	22:g:418:LEU:HD12	2.50	0.47
7:G:532:ASP:CG	7:G:533:ARG:H	2.22	0.47
44:g:602:HEA:OMA	44:g:602:HEA:HBB	2.14	0.47
21:c:156:PHE:CE1	21:c:161:GLY:HA2	2.49	0.47
22:k:106:ALA:HB1	44:k:601:HEA:H243	1.95	0.47
43:v:1002:HEC:HBC2	43:v:1002:HEC:HHD	1.95	0.47
6:F:390:THR:HB	33:F:501:SF4:S1	2.54	0.47
13:M:145:ILE:HB	13:M:146:PRO:HD3	1.96	0.47
16:Q:58:ARG:CZ	16:Q:74:VAL:HG11	2.44	0.47
4:D:21:GLU:HA	4:D:24:ILE:HD12	1.97	0.47
19:a:12:LYS:H	19:a:16:GLU:CD	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:d:200:LEU:HD21	38:d:501:U10:H353	1.96	0.47
22:k:325:HIS:CD2	22:k:326:HIS:CD2	3.03	0.47
30:t:77:VAL:HG11	30:t:430:VAL:HG22	1.96	0.47
30:t:321:HIS:NE2	30:t:322:HIS:CD2	2.82	0.47
32:v:216:VAL:HG22	43:v:1001:HEC:HMB1	1.97	0.47
2:B:19:LEU:HD22	15:P:68:ALA:HB2	1.96	0.47
3:C:104:VAL:O	3:C:130:SER:N	2.46	0.47
12:L:235:ALA:HB2	12:L:274:LEU:HD23	1.96	0.47
16:Q:5:ILE:HD12	16:Q:72:TYR:CD1	2.49	0.47
30:t:463:MET:HA	30:t:463:MET:HE2	1.96	0.47
11:K:51:SER:HB2	11:K:56:ASP:O	2.15	0.47
19:d:223:ASN:ND2	19:d:227:VAL:O	2.47	0.47
21:f:146:GLY:HA2	21:f:155:TRP:CD1	2.50	0.47
38:a:502:U10:C33	38:a:502:U10:H402	2.44	0.47
6:F:175:GLU:OE1	6:F:177:THR:N	2.38	0.46
19:d:212:HIS:HE1	41:d:503:HEM:CHD	2.27	0.46
22:g:104:ILE:HB	22:g:105:PRO:HD3	1.97	0.46
22:k:89:VAL:HG13	22:k:93:TYR:CE2	2.50	0.46
21:c:16:HIS:CG	21:c:17:GLY:N	2.83	0.46
2:B:101:ARG:HG2	3:C:163:TRP:CE3	2.50	0.46
2:B:138:ARG:HG2	3:C:162:ARG:NH2	2.30	0.46
5:E:3:ARG:HD3	5:E:77:THR:O	2.15	0.46
20:e:285:GLU:CD	20:e:285:GLU:H	2.23	0.46
43:u:1000:HEC:HHD	43:u:1000:HEC:CBC	2.45	0.46
12:L:371:MET:HA	12:L:374:TYR:CD2	2.50	0.46
19:a:121:TYR:OH	19:a:350:ASP:OD2	2.28	0.46
22:g:412:PHE:CE1	22:g:413:HIS:CE1	3.04	0.46
3:C:54:ASP:O	3:C:58:ARG:N	2.49	0.46
7:G:169:THR:O	7:G:394:ARG:NH2	2.49	0.46
7:G:373:GLU:OE1	7:G:441:ARG:NE	2.43	0.46
18:Z:156:GLN:HB3	18:Z:211:ARG:CZ	2.46	0.46
32:v:209:LEU:H	32:v:209:LEU:HD12	1.80	0.46
5:E:10:PRO:HD2	5:E:54:SER:HB2	1.97	0.46
7:G:139:LYS:HB2	17:R:32:TRP:CD1	2.50	0.46
11:K:28:ASN:OD1	11:K:30:ILE:HG22	2.16	0.46
13:M:237:PRO:C	13:M:239:HIS:H	2.23	0.46
15:P:5:LYS:HB3	15:P:29:TRP:CZ3	2.50	0.46
19:a:202:PRO:HG2	41:a:505:HEM:HMC3	1.96	0.46
22:g:413:HIS:CG	22:g:460:PHE:CE1	3.04	0.46
19:a:294:PRO:HB3	38:a:502:U10:H4M2	1.97	0.46
8:H:27:MET:C	38:H:402:U10:H253	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:5:PHE:CZ	11:K:6:HIS:HB3	2.50	0.46
12:L:219:ARG:NH1	12:L:221:TRP:HA	2.31	0.46
13:M:71:TRP:CD1	13:M:72:ILE:H	2.33	0.46
14:N:229:ASP:OD1	14:N:296:ARG:NH2	2.31	0.46
19:d:213:ILE:HA	19:d:216:PHE:CE2	2.51	0.46
22:g:391:VAL:O	22:g:394:SER:OG	2.29	0.46
22:k:413:HIS:CE1	44:k:601:HEA:NA	2.83	0.46
32:v:282:HIS:O	32:v:288:GLY:N	2.42	0.46
4:D:162:GLU:OE2	9:I:45:SER:OG	2.31	0.46
27:q:66:GLY:HA3	27:q:72:TYR:CE2	2.51	0.46
1:A:45:TYR:HE2	8:H:228:VAL:HG21	1.81	0.46
7:G:531:GLY:HA3	27:q:121:TRP:CG	2.50	0.46
22:k:103:VAL:HG21	44:k:601:HEA:HBC2	1.98	0.46
8:H:244:MET:HB3	38:H:402:U10:H153	1.97	0.45
24:m:63:MET:HB3	24:m:67:TRP:CZ3	2.51	0.45
3:C:160:GLU:O	3:C:173:GLU:N	2.44	0.45
7:G:168:THR:HA	7:G:172:ALA:HB3	1.98	0.45
12:L:102:MET:HG3	12:L:114:TYR:HE2	1.81	0.45
12:L:276:CYS:SG	12:L:341:MET:HE3	2.56	0.45
18:Z:41:GLU:CD	18:Z:41:GLU:H	2.23	0.45
19:a:346:VAL:HG12	19:a:347:PRO:HD3	1.98	0.45
32:v:254:VAL:HG23	32:v:297:LEU:HD13	1.97	0.45
4:D:332:LYS:HG3	7:G:126:MET:HG3	1.99	0.45
19:d:34:MET:HE1	19:d:245:TRP:CD1	2.52	0.45
19:d:142:THR:HG21	41:d:502:HEM:HBB2	1.98	0.45
32:v:117:VAL:O	32:v:117:VAL:HG13	2.16	0.45
12:L:343:HIS:HA	12:L:412:SER:OG	2.16	0.45
21:c:133:MET:SD	21:c:168:GLY:HA3	2.56	0.45
19:d:91:TYR:CE2	19:d:92:MET:HG2	2.51	0.45
32:v:233:MET:HE1	43:v:1002:HEC:C4B	2.47	0.45
4:D:10:TYR:O	10:J:169:LYS:HE3	2.17	0.45
7:G:357:ARG:HA	7:G:360:TYR:CD2	2.52	0.45
9:I:116:ASP:OD1	9:I:116:ASP:N	2.50	0.45
15:P:36:ARG:HH11	15:P:85:ARG:HH22	1.64	0.45
22:k:324:ALA:HB3	22:k:340:PHE:CE2	2.52	0.45
24:m:9:TYR:CE2	25:n:15:MET:HE1	2.51	0.45
30:t:440:TYR:CD2	30:t:521:ALA:HB1	2.52	0.45
31:u:70:VAL:HG23	31:u:71:CYS:N	2.31	0.45
4:D:329:HIS:CD2	7:G:126:MET:SD	3.10	0.45
6:F:174:GLY:HA3	36:F:502:FMN:N5	2.32	0.45
19:a:62:GLY:HA3	41:a:505:HEM:C3C	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:363:ASN:O	20:b:369:ASN:HA	2.17	0.45
22:g:34:LEU:HB3	22:g:135:TYR:CZ	2.52	0.45
5:E:16:THR:OG1	5:E:222:ASP:O	2.33	0.45
6:F:193:LYS:HB3	6:F:196:PHE:CE1	2.51	0.45
8:H:30:LEU:HD21	38:H:402:U10:H161	1.99	0.45
19:a:408:LEU:HD23	19:a:408:LEU:HA	1.86	0.45
38:a:504:U10:H562	38:d:501:U10:H111	1.99	0.45
21:c:142:CYS:HB2	21:c:157:CYS:SG	2.57	0.45
12:L:368:GLU:O	12:L:374:TYR:OH	2.28	0.45
16:Q:33:ARG:HB3	16:Q:42:THR:HG23	1.99	0.45
24:m:194:TYR:OH	24:m:214:THR:HG23	2.17	0.45
5:E:102:MET:HE1	6:F:333:ALA:HA	1.99	0.45
6:F:397:ALA:HA	6:F:400:TRP:CE3	2.52	0.45
10:J:90:PRO:HB2	19:a:369:LEU:HD11	1.98	0.45
14:N:330:ILE:HG22	14:N:334:MET:HE2	1.99	0.45
18:Z:166:ARG:HD2	18:Z:167:GLU:O	2.16	0.45
19:a:230:ARG:HB3	19:a:236:GLU:CD	2.42	0.45
19:d:198:HIS:HE1	41:d:502:HEM:CHB	2.30	0.45
24:m:158:TRP:CG	26:o:5:MET:HE1	2.51	0.45
5:E:168:ARG:HE	5:E:173:GLU:CD	2.24	0.44
14:N:1:MET:SD	14:N:6:PHE:HB2	2.57	0.44
24:m:5:LYS:NZ	24:m:7:HIS:O	2.47	0.44
4:D:374:ARG:HD3	4:D:374:ARG:C	2.42	0.44
6:F:11:ASN:ND2	6:F:26:ARG:HH12	2.15	0.44
6:F:124:TYR:CG	6:F:179:LEU:HD11	2.52	0.44
6:F:181:GLU:OE2	6:F:191:ARG:NH1	2.47	0.44
13:M:120:LEU:HD23	13:M:256:LEU:HD13	1.99	0.44
13:M:131:LEU:HA	13:M:193:ILE:HD12	1.98	0.44
13:M:153:ILE:HB	13:M:154:TRP:CE3	2.53	0.44
19:a:138:MET:HA	38:d:504:U10:H501	1.99	0.44
10:J:90:PRO:HB3	19:a:366:TRP:CZ3	2.52	0.44
14:N:266:ILE:HA	14:N:269:TRP:CE2	2.52	0.44
18:Z:155:GLU:OE1	18:Z:211:ARG:N	2.35	0.44
19:a:111:HIS:CD2	41:a:503:HEM:C1C	3.05	0.44
19:d:302:TYR:CE2	19:d:306:ARG:HD3	2.53	0.44
12:L:269:THR:HG23	12:L:344:LEU:HD21	1.98	0.44
21:c:46:GLN:HE22	21:c:47:MET:HG3	1.82	0.44
19:d:72:HIS:NE2	19:d:74:ASP:OD2	2.45	0.44
22:k:324:ALA:HB3	22:k:340:PHE:CD2	2.51	0.44
23:l:247:GLU:C	23:l:253:HIS:CE1	2.95	0.44
6:F:248:HIS:HA	6:F:275:ARG:CZ	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:413:ILE:HG13	19:a:414:ILE:HG23	2.00	0.44
20:b:241:TYR:CE2	20:b:246:SER:HB3	2.53	0.44
20:b:413:ASP:OD1	20:b:413:ASP:N	2.51	0.44
16:Q:31:ASP:O	16:Q:33:ARG:NH1	2.45	0.44
22:g:390:GLY:C	44:g:602:HEA:HMB2	2.42	0.44
31:u:67:GLY:O	31:u:70:VAL:HG22	2.17	0.44
32:v:300:ALA:C	32:v:302:TRP:H	2.26	0.44
12:L:216:PHE:HB3	12:L:221:TRP:CD1	2.53	0.44
19:a:95:TYR:CD1	19:a:271:PRO:HB2	2.53	0.44
22:g:324:ALA:HB3	22:g:340:PHE:CG	2.52	0.44
23:h:247:GLU:C	23:h:253:HIS:CE1	2.96	0.44
30:t:119:ARG:CZ	31:u:70:VAL:HB	2.48	0.44
6:F:83:ASN:ND2	36:F:502:FMN:H2'	2.33	0.44
8:H:168:ILE:HD11	8:H:262:PHE:CE1	2.53	0.44
13:M:308:ASP:OD1	13:M:310:LYS:N	2.49	0.44
14:N:24:MET:HE2	14:N:24:MET:HA	2.00	0.44
19:a:213:ILE:HA	19:a:216:PHE:CE2	2.52	0.44
27:q:28:LYS:HE3	27:q:37:VAL:HG13	1.98	0.44
2:B:91:THR:HA	2:B:119:CYS:HB3	2.00	0.44
3:C:112:PRO:HB2	4:D:233:TRP:CH2	2.53	0.44
6:F:336:ARG:HD2	6:F:336:ARG:HA	1.84	0.44
7:G:135:TYR:CZ	7:G:137:GLU:HB2	2.53	0.44
10:J:113:SER:HB3	14:N:181:PHE:CZ	2.53	0.44
23:h:194:PRO:HA	23:h:263:VAL:O	2.18	0.44
4:D:135:THR:HB	4:D:147:PRO:HA	2.00	0.43
14:N:1:MET:HG2	14:N:64:PHE:CE2	2.53	0.43
19:d:84:MET:SD	19:d:94:ARG:HD3	2.58	0.43
24:m:184:VAL:O	24:m:187:THR:HG22	2.17	0.43
43:v:1002:HEC:HHD	43:v:1002:HEC:CBC	2.48	0.43
2:B:101:ARG:HG2	3:C:163:TRP:CZ3	2.53	0.43
6:F:264:ARG:HD3	6:F:278:TRP:CH2	2.52	0.43
19:a:270:MET:O	19:a:270:MET:HG2	2.18	0.43
19:d:132:GLY:HA3	41:d:503:HEM:C3C	2.53	0.43
22:g:531:GLU:N	22:g:531:GLU:OE1	2.48	0.43
22:k:459:ILE:HD11	22:k:493:ALA:HA	2.00	0.43
30:t:472:LEU:O	30:t:476:GLU:N	2.51	0.43
33:B:1001:SF4:S4	4:D:170:HIS:HE1	2.40	0.43
7:G:41:ARG:NE	7:G:266:GLU:OE1	2.39	0.43
19:a:145:MET:SD	19:a:197:LEU:HB2	2.59	0.43
21:f:46:GLN:HE22	21:f:47:MET:HG3	1.83	0.43
6:F:83:ASN:HD22	36:F:502:FMN:H2'	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:k:348:ALA:HB1	44:k:602:HEA:H262	2.00	0.43
4:D:11:ASP:HA	10:J:169:LYS:HE2	2.00	0.43
6:F:237:ASN:HB3	6:F:259:MET:HE2	2.00	0.43
12:L:191:TYR:O	12:L:195:GLY:N	2.41	0.43
13:M:276:MET:C	13:M:278:PRO:HD3	2.44	0.43
19:d:104:PHE:CD2	19:d:139:MET:HE3	2.53	0.43
21:f:163:HIS:O	21:f:170:ILE:HD12	2.18	0.43
29:s:27:UNK:HA	30:t:249:PHE:CZ	2.53	0.43
4:D:86:LEU:O	4:D:87:ASP:C	2.62	0.43
9:I:56:ARG:HA	9:I:62:GLU:HA	2.00	0.43
11:K:20:PHE:HA	11:K:23:PHE:CE2	2.54	0.43
12:L:370:ASP:OD2	12:L:372:ARG:NH2	2.46	0.43
19:a:312:VAL:HG12	19:a:314:VAL:HG12	2.00	0.43
22:k:27:ASN:OD1	22:k:29:LYS:HG2	2.19	0.43
22:k:365:GLY:CA	23:l:89:PHE:HB3	2.47	0.43
5:E:235:THR:HG22	6:F:150:GLY:HA2	1.99	0.43
14:N:130:TYR:CZ	14:N:172:LEU:HD11	2.54	0.43
15:P:268:ILE:HD12	15:P:268:ILE:H	1.84	0.43
19:d:247:TYR:HB3	20:e:440:TRP:CZ2	2.52	0.43
27:q:116:ARG:NH1	27:q:118:TYR:O	2.49	0.43
2:B:162:GLN:O	2:B:165:ARG:HG2	2.19	0.43
4:D:6:ARG:HA	4:D:54:GLU:OE1	2.19	0.43
6:F:4:ASP:HA	6:F:7:ARG:HE	1.83	0.43
7:G:100:GLU:O	7:G:104:ILE:HG23	2.19	0.43
13:M:458:THR:N	13:M:461:GLU:OE1	2.42	0.43
19:a:162:ILE:HD11	38:a:502:U10:C5	2.49	0.43
19:a:245:TRP:CE3	19:a:249:VAL:HG11	2.53	0.43
20:b:223:GLU:O	20:b:227:GLY:HA3	2.19	0.43
21:f:142:CYS:HB2	21:f:157:CYS:SG	2.59	0.43
22:g:87:TRP:HB2	22:g:476:ILE:HD12	2.00	0.43
27:q:47:ARG:HB2	27:q:67:TRP:CH2	2.53	0.43
30:t:331:TRP:HA	32:v:113:ALA:HA	2.01	0.43
4:D:273:CYS:CB	4:D:402:THR:HG21	2.47	0.43
7:G:357:ARG:O	7:G:361:VAL:HG22	2.19	0.43
14:N:293:ASN:OD1	14:N:295:LYS:N	2.51	0.43
15:P:15:PHE:HD2	15:P:160:ASP:HB2	1.83	0.43
16:Q:7:LYS:HE2	16:Q:20:THR:O	2.19	0.43
18:Z:56:ALA:HB1	18:Z:57:PRO:HD2	2.01	0.43
19:a:369:LEU:HB2	19:a:399:TYR:OH	2.19	0.43
2:B:67:TYR:CE1	9:I:35:LEU:HD21	2.53	0.43
5:E:169:PHE:CZ	5:E:175:PRO:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:H:402:U10:H272	38:H:402:U10:H251	1.69	0.43
13:M:155:GLY:C	13:M:159:ARG:HD3	2.44	0.43
22:k:64:TYR:CE2	22:k:74:ALA:HB2	2.53	0.43
28:r:27:UNK:O	28:r:31:UNK:N	2.52	0.43
30:t:417:TRP:CD1	30:t:418:ASN:OD1	2.71	0.43
1:A:53:ASP:OD1	1:A:54:ASP:N	2.49	0.42
1:A:75:LEU:HD13	11:K:68:THR:HA	2.01	0.42
8:H:129:TYR:HB3	8:H:133:MET:HE3	2.01	0.42
8:H:237:SER:OG	8:H:238:THR:N	2.52	0.42
10:J:24:ASN:HB3	10:J:27:HIS:CG	2.54	0.42
15:P:81:GLY:HA3	15:P:95:HIS:CD2	2.50	0.42
18:Z:176:ARG:HB2	18:Z:205:LEU:HD21	2.01	0.42
19:a:214:TRP:NE1	40:a:501:CDL:HB61	2.33	0.42
19:a:266:ILE:HA	19:a:270:MET:SD	2.58	0.42
20:e:388:THR:HG23	20:e:389:PRO:HD2	2.00	0.42
44:g:603:HEA:HBB	44:g:603:HEA:OMA	2.19	0.42
30:t:321:HIS:HB2	41:t:602:HEM:HMA3	2.00	0.42
30:t:415:LEU:HD21	41:t:603:HEM:CHC	2.48	0.42
15:P:61:ARG:HA	15:P:101:ARG:NH2	2.33	0.42
19:a:212:HIS:CE1	41:a:503:HEM:NC	2.87	0.42
1:A:87:PHE:HA	1:A:90:LEU:CD1	2.49	0.42
3:C:73:ARG:NH2	3:C:78:ASP:OD1	2.45	0.42
6:F:125:ILE:HD13	6:F:133:ARG:HB3	2.01	0.42
7:G:327:GLU:CD	7:G:553:LEU:H	2.27	0.42
20:b:320:PHE:CE2	20:b:333:ASN:HB3	2.54	0.42
21:c:52:ASP:N	21:c:52:ASP:OD1	2.53	0.42
19:d:97:HIS:CE1	41:d:502:HEM:C1C	3.07	0.42
22:g:297:PHE:CE2	22:g:372:PRO:HB2	2.54	0.42
23:h:150:TRP:CD2	23:h:252:ASN:HB2	2.54	0.42
24:m:154:VAL:HG13	26:o:8:THR:HG23	2.01	0.42
32:v:214:THR:HG21	32:v:222:ASP:HB3	2.02	0.42
7:G:271:LYS:HA	7:G:655:MET:HE1	2.01	0.42
14:N:188:GLU:N	14:N:188:GLU:CD	2.78	0.42
19:a:230:ARG:HH21	19:a:240:ASP:CG	2.27	0.42
19:a:294:PRO:HG3	38:a:502:U10:C3M	2.49	0.42
19:d:203:PHE:HB3	38:d:501:U10:H462	2.01	0.42
6:F:3:ASN:OD1	6:F:5:GLN:HG3	2.19	0.42
6:F:76:ARG:CZ	6:F:206:PRO:HD3	2.49	0.42
13:M:200:ASP:OD1	13:M:200:ASP:N	2.47	0.42
20:b:441:GLN:HB3	20:b:442:PRO:HD3	2.02	0.42
23:h:149:GLN:HG2	23:h:150:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2:ASP:CG	4:D:389:ARG:HH21	2.27	0.42
5:E:114:LYS:HA	5:E:118:ALA:O	2.20	0.42
6:F:85:ASP:O	36:F:502:FMN:N3	2.40	0.42
12:L:171:LYS:O	12:L:175:VAL:HG23	2.19	0.42
19:a:111:HIS:CD2	41:a:503:HEM:NC	2.87	0.42
20:e:362:HIS:CE1	20:e:369:ASN:HB3	2.55	0.42
24:i:140:HIS:CD2	24:i:141:LEU:HG	2.54	0.42
22:k:231:ILE:HG23	22:k:235:LEU:HD12	2.02	0.42
2:B:47:TRP:CD1	2:B:74:THR:HG22	2.54	0.42
22:k:129:ARG:NH2	24:m:70:VAL:HG22	2.35	0.42
24:m:200:GLY:N	24:m:203:ASP:OD2	2.42	0.42
26:p:2:PHE:CG	26:p:3:ASP:N	2.88	0.42
8:H:55:PRO:HB2	8:H:56:TRP:CE3	2.55	0.42
21:f:25:TYR:CD1	21:f:25:TYR:N	2.85	0.42
26:o:5:MET:HE3	26:o:8:THR:HB	2.01	0.42
6:F:224:ARG:HD3	6:F:228:TRP:CD2	2.55	0.42
13:M:11:LEU:HD23	13:M:45:THR:HG23	2.02	0.42
20:b:348:TYR:CE2	20:b:375:ALA:HA	2.55	0.42
22:k:481:GLU:OE1	23:l:44:ASN:N	2.49	0.42
30:t:483:LEU:HD13	31:u:85:ARG:CZ	2.50	0.42
32:v:290:ARG:HG3	32:v:290:ARG:HH11	1.85	0.42
2:B:117:GLY:HA2	2:B:148:GLY:O	2.20	0.42
14:N:188:GLU:CD	14:N:188:GLU:H	2.28	0.42
22:g:91:ILE:HG12	44:g:603:HEA:HBA1	2.01	0.42
22:k:85:HIS:CD2	22:k:157:GLN:HB2	2.55	0.42
4:D:42:LEU:HD11	4:D:58:PRO:HB3	2.02	0.41
4:D:230:ALA:HA	4:D:235:TYR:CD2	2.55	0.41
9:I:160:ALA:HB1	17:R:24:ARG:HD3	2.02	0.41
12:L:362:ILE:CG2	12:L:367:HIS:HA	2.50	0.41
13:M:72:ILE:HD11	14:N:389:PHE:CE1	2.54	0.41
14:N:426:TYR:CD1	14:N:426:TYR:C	2.97	0.41
18:Z:106:VAL:HA	18:Z:131:VAL:O	2.20	0.41
20:b:368:GLY:C	20:b:370:TRP:H	2.28	0.41
22:g:238:LEU:HD22	22:g:274:PHE:CZ	2.55	0.41
22:g:325:HIS:CD2	22:g:326:HIS:CD2	3.08	0.41
24:i:158:TRP:CH2	26:p:9:LYS:HG3	2.55	0.41
2:B:125:TYR:CE2	4:D:81:PRO:HB2	2.54	0.41
6:F:374:GLU:CD	6:F:374:GLU:N	2.78	0.41
8:H:226:GLU:OE2	8:H:300:ARG:NE	2.46	0.41
12:L:644:TRP:CZ3	12:L:645:LYS:HE2	2.54	0.41
19:a:222:ASN:H	41:a:503:HEM:CGD	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:t:317:TRP:CH2	31:u:31:VAL:HG21	2.55	0.41
31:u:9:VAL:HG23	31:u:10:LEU:N	2.35	0.41
2:B:62:THR:HG21	2:B:156:LEU:HD23	2.01	0.41
4:D:83:LEU:HG	4:D:98:TRP:HB2	2.02	0.41
7:G:119:CYS:SG	7:G:121:LEU:HB3	2.61	0.41
7:G:162:THR:N	33:G:701:SF4:S3	2.81	0.41
9:I:134:LEU:HA	9:I:134:LEU:HD23	1.84	0.41
10:J:170:ASP:OD1	10:J:170:ASP:N	2.53	0.41
13:M:222:PHE:CD1	13:M:222:PHE:C	2.98	0.41
40:a:501:CDL:OA7	40:a:501:CDL:HA32	2.20	0.41
19:d:72:HIS:CD2	19:d:74:ASP:HB2	2.55	0.41
22:g:417:SER:O	22:g:418:LEU:HD23	2.20	0.41
30:t:315:TYR:CD2	30:t:343:LEU:HD21	2.56	0.41
13:M:144:LEU:HD21	13:M:170:THR:HG21	2.00	0.41
19:a:266:ILE:HG12	19:a:270:MET:HE1	2.02	0.41
22:k:247:MET:HB3	22:k:253:THR:HG21	2.02	0.41
22:k:265:VAL:HG23	23:l:224:VAL:HG11	2.02	0.41
44:k:601:HEA:HMD1	44:k:601:HEA:HHD	1.88	0.41
6:F:30:ASP:O	6:F:223:ARG:NH1	2.53	0.41
8:H:33:MET:HG3	8:H:288:PHE:CZ	2.56	0.41
14:N:426:TYR:CE1	14:N:431:GLY:HA2	2.55	0.41
18:Z:37:GLN:O	18:Z:119:ARG:NE	2.50	0.41
19:a:244:PHE:CZ	38:a:504:U10:H4M3	2.55	0.41
22:k:104:ILE:HB	22:k:105:PRO:HD3	2.01	0.41
22:k:374:LEU:HD11	22:k:446:GLN:OE1	2.20	0.41
24:m:128:TRP:HA	24:m:129:PRO:C	2.46	0.41
30:t:372:ARG:HB3	30:t:449:PHE:CE1	2.55	0.41
2:B:71:ARG:HA	8:H:49:GLY:HA3	2.03	0.41
6:F:158:TRP:CD1	6:F:160:PHE:HB2	2.55	0.41
8:H:75:ILE:HD12	8:H:75:ILE:H	1.86	0.41
10:J:77:ASP:OD1	10:J:78:PHE:N	2.53	0.41
19:a:157:TRP:CD1	19:a:289:PRO:HD3	2.55	0.41
19:d:143:ALA:HA	41:d:502:HEM:HHB	2.03	0.41
21:f:86:ARG:HH22	21:f:119:ASP:CG	2.29	0.41
31:u:213:VAL:CG1	31:u:217:ASP:HB2	2.50	0.41
9:I:55:ARG:HB2	9:I:63:ARG:HD2	2.03	0.41
14:N:63:ALA:N	14:N:68:PHE:O	2.48	0.41
21:f:164:TYR:HA	21:f:169:ARG:O	2.20	0.41
44:g:602:HEA:H262	44:g:602:HEA:H273	2.03	0.41
22:k:95:GLY:O	22:k:99:MET:HG2	2.21	0.41
6:F:374:GLU:CD	6:F:374:GLU:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:38:ARG:HD2	38:H:402:U10:H4M3	2.02	0.41
12:L:390:ILE:HA	12:L:393:PHE:CD2	2.55	0.41
20:b:241:TYR:HD1	20:b:245:CYS:HB2	1.85	0.41
22:g:349:VAL:HB	22:g:350:PRO:HD3	2.03	0.41
22:k:263:ASP:OD2	23:l:227:ARG:NH1	2.50	0.41
2:B:90:GLY:HA2	33:B:1001:SF4:S3	2.60	0.41
2:B:169:ARG:CG	2:B:170:THR:HG23	2.51	0.41
4:D:179:VAL:HG22	4:D:306:VAL:CG1	2.51	0.41
12:L:504:PHE:HB2	12:L:506:ILE:HD11	2.03	0.41
12:L:622:TRP:N	12:L:622:TRP:CD1	2.89	0.41
13:M:326:MET:HE3	13:M:408:THR:HG22	2.02	0.41
13:M:361:TYR:O	13:M:365:HIS:HA	2.21	0.41
44:k:601:HEA:OMA	44:k:601:HEA:HHB	2.20	0.41
24:m:91:PHE:CE1	24:m:92:ILE:HG13	2.56	0.41
30:t:291:PRO:O	30:t:295:GLU:N	2.54	0.41
1:A:8:TYR:HA	1:A:11:ILE:HD12	2.02	0.41
7:G:107:PRO:HG3	7:G:156:THR:HG23	2.03	0.41
16:Q:64:TYR:CE1	16:Q:68:HIS:CD2	3.09	0.41
19:a:185:ALA:HB3	21:f:78:GLY:HA3	2.03	0.41
21:f:133:MET:SD	21:f:168:GLY:HA3	2.60	0.41
27:q:56:GLU:CD	27:q:58:SER:HG	2.28	0.41
1:A:64:TYR:CG	1:A:65:LEU:N	2.89	0.40
7:G:141:ALA:HB1	17:R:34:ALA:HB2	2.04	0.40
7:G:296:ARG:NH2	7:G:297:PRO:O	2.53	0.40
15:P:118:SER:O	15:P:153:PRO:HD2	2.21	0.40
19:a:198:HIS:HE1	41:a:505:HEM:CHB	2.34	0.40
22:k:386:GLY:HA3	22:k:415:VAL:HG13	2.03	0.40
7:G:412:LEU:HB3	7:G:414:TYR:CZ	2.56	0.40
9:I:11:TYR:CE2	10:J:180:MET:HB3	2.56	0.40
12:L:96:MET:HE3	12:L:474:PRO:HG3	2.04	0.40
13:M:80:GLY:HA3	13:M:131:LEU:HD11	2.04	0.40
23:h:265:GLN:O	23:h:269:GLU:HG2	2.21	0.40
31:u:123:TRP:HB2	43:v:1001:HEC:HBC1	2.03	0.40
6:F:87:SER:HB2	6:F:171:TYR:HD1	1.85	0.40
7:G:207:LEU:HA	7:G:207:LEU:HD23	1.91	0.40
7:G:236:MET:SD	7:G:275:VAL:HG21	2.62	0.40
8:H:280:MET:HG3	8:H:284:MET:HE2	2.02	0.40
12:L:192:TRP:CZ3	13:M:414:ARG:HD2	2.57	0.40
15:P:213:LEU:HB3	15:P:290:PHE:CZ	2.56	0.40
19:a:254:PHE:CZ	20:b:433:TYR:HB2	2.57	0.40
21:c:88:GLU:O	21:c:92:GLN:NE2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:d:51:LEU:HD13	41:d:503:HEM:C3B	2.57	0.40
20:e:218:ILE:HD11	20:e:220:PHE:CZ	2.56	0.40
30:t:309:TRP:CE3	30:t:312:ILE:HD11	2.56	0.40
31:u:140:MET:HE1	43:u:1000:HEC:C1B	2.51	0.40
5:E:187:GLU:OE1	5:E:187:GLU:N	2.53	0.40
7:G:18:PRO:HA	7:G:70:VAL:HB	2.02	0.40
7:G:276:TRP:CD1	7:G:276:TRP:C	2.99	0.40
8:H:120:ILE:HD11	8:H:253:LEU:HD21	2.03	0.40
8:H:124:SER:HA	8:H:127:GLU:OE2	2.21	0.40
12:L:644:TRP:CG	13:M:306:GLN:HE22	2.39	0.40
14:N:89:LEU:HD11	14:N:110:VAL:HG11	2.03	0.40
14:N:289:ILE:HD12	14:N:419:PHE:HD2	1.87	0.40
19:d:144:PHE:HB2	38:d:501:U10:H1M3	2.03	0.40
22:k:278:GLU:HA	22:k:281:ILE:HD12	2.03	0.40
32:v:215:THR:HG22	32:v:323:MET:HG2	2.04	0.40
2:B:53:ALA:HB3	33:B:1001:SF4:S3	2.61	0.40
5:E:96:CYS:SG	5:E:137:CYS:HA	2.61	0.40
12:L:671:ALA:O	12:L:674:VAL:HG22	2.22	0.40
14:N:37:THR:O	14:N:41:VAL:HG23	2.21	0.40
24:i:149:LEU:HD23	24:i:149:LEU:HA	1.92	0.40
22:k:472:PRO:HB2	22:k:475:TYR:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
2	B	160/175 (91%)	155 (97%)	4 (2%)	1 (1%)	21	59
3	C	192/208 (92%)	185 (96%)	7 (4%)	0	100	100
4	D	408/412 (99%)	394 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	235/239 (98%)	226 (96%)	8 (3%)	1 (0%)	30	67
6	F	420/431 (97%)	402 (96%)	18 (4%)	0	100	100
7	G	663/674 (98%)	635 (96%)	27 (4%)	1 (0%)	43	78
8	H	339/345 (98%)	328 (97%)	11 (3%)	0	100	100
9	I	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
10	J	197/199 (99%)	194 (98%)	3 (2%)	0	100	100
11	K	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
12	L	654/703 (93%)	625 (96%)	28 (4%)	1 (0%)	43	78
13	M	501/513 (98%)	494 (99%)	6 (1%)	1 (0%)	43	78
14	N	478/499 (96%)	468 (98%)	10 (2%)	0	100	100
15	P	326/330 (99%)	317 (97%)	8 (2%)	1 (0%)	36	72
16	Q	101/103 (98%)	101 (100%)	0	0	100	100
17	R	59/62 (95%)	54 (92%)	5 (8%)	0	100	100
18	Z	214/217 (99%)	206 (96%)	8 (4%)	0	100	100
19	a	431/440 (98%)	422 (98%)	9 (2%)	0	100	100
19	d	432/440 (98%)	425 (98%)	7 (2%)	0	100	100
20	b	237/450 (53%)	231 (98%)	6 (2%)	0	100	100
20	e	237/450 (53%)	234 (99%)	2 (1%)	1 (0%)	30	67
21	c	178/195 (91%)	171 (96%)	7 (4%)	0	100	100
21	f	179/195 (92%)	174 (97%)	5 (3%)	0	100	100
22	g	542/558 (97%)	528 (97%)	14 (3%)	0	100	100
22	k	542/558 (97%)	526 (97%)	16 (3%)	0	100	100
23	h	250/298 (84%)	240 (96%)	10 (4%)	0	100	100
23	l	250/298 (84%)	240 (96%)	10 (4%)	0	100	100
24	i	271/274 (99%)	263 (97%)	8 (3%)	0	100	100
24	m	271/274 (99%)	262 (97%)	9 (3%)	0	100	100
25	j	41/66 (62%)	40 (98%)	1 (2%)	0	100	100
25	n	41/66 (62%)	40 (98%)	1 (2%)	0	100	100
26	o	39/176 (22%)	39 (100%)	0	0	100	100
26	p	40/176 (23%)	40 (100%)	0	0	100	100
27	q	121/124 (98%)	116 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	t	468/539 (87%)	439 (94%)	27 (6%)	2 (0%)	30	67
31	u	187/241 (78%)	177 (95%)	8 (4%)	2 (1%)	11	46
32	v	274/349 (78%)	245 (89%)	25 (9%)	4 (2%)	8	40
All	All	10356/11662 (89%)	10005 (97%)	336 (3%)	15 (0%)	49	83

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	u	210	ARG
13	M	238	VAL
32	v	283	ALA
5	E	137	CYS
20	e	369	ASN
32	v	77	HIS
30	t	402	TYR
7	G	263	VAL
32	v	130	ARG
12	L	114	TYR
15	P	87	GLY
2	B	122	GLY
32	v	301	VAL
30	t	416	GLY
31	u	78	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/97 (100%)	97 (100%)	0	100	100
2	B	136/145 (94%)	134 (98%)	2 (2%)	57	72
3	C	172/183 (94%)	172 (100%)	0	100	100
4	D	341/342 (100%)	341 (100%)	0	100	100
5	E	189/190 (100%)	189 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	331/335 (99%)	330 (100%)	1 (0%)	86	86
7	G	530/535 (99%)	529 (100%)	1 (0%)	87	87
8	H	277/279 (99%)	276 (100%)	1 (0%)	84	84
9	I	136/137 (99%)	136 (100%)	0	100	100
10	J	158/158 (100%)	158 (100%)	0	100	100
11	K	81/81 (100%)	80 (99%)	1 (1%)	63	75
12	L	518/543 (95%)	518 (100%)	0	100	100
13	M	410/416 (99%)	408 (100%)	2 (0%)	81	83
14	N	357/369 (97%)	355 (99%)	2 (1%)	78	83
15	P	248/250 (99%)	248 (100%)	0	100	100
16	Q	87/87 (100%)	87 (100%)	0	100	100
17	R	51/52 (98%)	51 (100%)	0	100	100
18	Z	167/168 (99%)	167 (100%)	0	100	100
19	a	360/366 (98%)	360 (100%)	0	100	100
19	d	361/366 (99%)	361 (100%)	0	100	100
20	b	192/319 (60%)	192 (100%)	0	100	100
20	e	192/319 (60%)	192 (100%)	0	100	100
21	c	139/151 (92%)	138 (99%)	1 (1%)	76	81
21	f	140/151 (93%)	140 (100%)	0	100	100
22	g	447/454 (98%)	447 (100%)	0	100	100
22	k	447/454 (98%)	445 (100%)	2 (0%)	84	84
23	h	211/243 (87%)	210 (100%)	1 (0%)	81	83
23	l	211/243 (87%)	211 (100%)	0	100	100
24	i	220/221 (100%)	220 (100%)	0	100	100
24	m	220/221 (100%)	219 (100%)	1 (0%)	81	83
25	j	34/53 (64%)	34 (100%)	0	100	100
25	n	34/53 (64%)	34 (100%)	0	100	100
26	o	32/126 (25%)	31 (97%)	1 (3%)	35	56
26	p	33/126 (26%)	33 (100%)	0	100	100
27	q	103/104 (99%)	103 (100%)	0	100	100
30	t	376/428 (88%)	369 (98%)	7 (2%)	50	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	u	163/205 (80%)	159 (98%)	4 (2%)	42	63
32	v	211/269 (78%)	206 (98%)	5 (2%)	43	64
All	All	8412/9239 (91%)	8380 (100%)	32 (0%)	81	84

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	54	CYS
2	B	91	THR
6	F	88	GLU
7	G	31	ILE
8	H	303	TYR
11	K	25	ASN
13	M	365	HIS
13	M	471	MET
14	N	188	GLU
14	N	426	TYR
21	c	92	GLN
23	h	102	HIS
22	k	279	VAL
22	k	347	ILE
24	m	258	VAL
26	o	52	ILE
30	t	185	TYR
30	t	192	VAL
30	t	229	PHE
30	t	257	PHE
30	t	298	VAL
30	t	306	ILE
30	t	315	TYR
31	u	50	ARG
31	u	64	VAL
31	u	105	SER
31	u	125	LEU
32	v	92	TRP
32	v	117	VAL
32	v	162	ASP
32	v	256	GLU
32	v	338	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	29	GLN
3	C	38	ASN
4	D	28	ASN
4	D	329	HIS
4	D	330	HIS
5	E	83	GLN
6	F	83	ASN
6	F	348	GLN
7	G	259	ASN
7	G	260	HIS
7	G	619	GLN
8	H	60	GLN
10	J	167	HIS
12	L	198	GLN
12	L	241	GLN
12	L	263	HIS
13	M	393	ASN
13	M	498	ASN
14	N	65	HIS
14	N	291	GLN
14	N	323	ASN
15	P	78	ASN
15	P	95	HIS
15	P	116	HIS
15	P	226	GLN
16	Q	48	GLN
16	Q	78	HIS
18	Z	6	GLN
20	b	394	GLN
20	b	436	ASN
21	c	121	ASN
19	d	99	ASN
19	d	358	GLN
20	e	321	HIS
20	e	362	HIS
20	e	372	GLN
20	e	394	GLN
21	f	92	GLN
21	f	121	ASN
22	g	59	HIS
22	g	395	GLN
23	h	65	HIS
23	h	94	ASN

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Mol	Chain	Res	Type
23	h	158	ASN
24	i	140	HIS
24	i	244	GLN
25	j	21	GLN
22	k	12	HIS
22	k	269	HIS
22	k	526	HIS
23	l	94	ASN
23	l	158	ASN
23	l	221	GLN
24	m	256	HIS
30	t	155	ASN
30	t	322	HIS
32	v	218	HIS
32	v	252	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	2MR	D	65	4	10,12,13	2.49	2 (20%)	5,13,15	1.20	1 (20%)
1	FME	A	1	1	8,9,10	0.92	0	8,9,11	0.91	0
12	FME	L	1	12	8,9,10	0.91	0	8,9,11	1.37	1 (12%)
27	FME	q	1	27	8,9,10	1.00	0	8,9,11	0.86	0
10	FME	J	1	10	8,9,10	1.00	0	8,9,11	0.79	0
13	FME	M	1	13	8,9,10	1.02	0	8,9,11	1.07	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	2MR	D	65	4	-	1/10/13/15	-
1	FME	A	1	1	-	1/7/9/11	-
12	FME	L	1	12	-	0/7/9/11	-
27	FME	q	1	27	-	0/7/9/11	-
10	FME	J	1	10	-	1/7/9/11	-
13	FME	M	1	13	-	4/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	65	2MR	CZ-NH2	5.50	1.44	1.33
4	D	65	2MR	CZ-NE	4.83	1.44	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	1	FME	C-CA-N	2.82	114.94	109.50
4	D	65	2MR	NE-CZ-NH2	-2.63	117.07	119.48
13	M	1	FME	C-CA-N	2.28	113.91	109.50

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	65	2MR	O-C-CA-CB
10	J	1	FME	O-C-CA-CB
13	M	1	FME	O-C-CA-CB
13	M	1	FME	N-CA-CB-CG
13	M	1	FME	C-CA-CB-CG
1	A	1	FME	CB-CA-N-CN
13	M	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 12 are monoatomic - leaving 37 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	$\# Z > 2$
44	HEA	g	603	22	67,67,67	1.43	9 (13%)	81,103,103	2.38	31 (38%)
44	HEA	k	601	22	67,67,67	1.42	5 (7%)	81,103,103	2.46	29 (35%)
44	HEA	k	602	22	67,67,67	1.70	10 (14%)	81,103,103	2.07	27 (33%)
33	SF4	B	1001	2	0,12,12	-	-	-	-	-
43	HEC	v	1002	32	46,50,50	1.86	5 (10%)	58,82,82	1.43	6 (10%)
41	HEM	d	502	19	50,50,50	1.37	6 (12%)	67,82,82	1.12	6 (8%)
43	HEC	v	1001	32	46,50,50	1.88	4 (8%)	58,82,82	1.58	7 (12%)
33	SF4	I	1001	9	0,12,12	-	-	-	-	-
40	CDL	a	501	-	99,99,99	0.92	6 (6%)	105,111,111	0.93	5 (4%)
37	DU0	H	401	-	42,42,42	0.60	0	64,66,66	0.91	2 (3%)
47	CUA	h	301	23	0,1,1	-	-	-	-	-
43	HEC	e	502	20	46,50,50	1.95	6 (13%)	58,82,82	1.81	8 (13%)
33	SF4	F	501	6	0,12,12	-	-	-	-	-
35	FES	E	401	5	0,4,4	-	-	-	-	-
38	U10	H	402	-	63,63,63	0.69	0	78,79,79	1.23	7 (8%)
41	HEM	d	503	19	50,50,50	1.38	5 (10%)	67,82,82	1.00	4 (5%)
41	HEM	t	603	42,30	50,50,50	1.37	6 (12%)	67,82,82	0.99	2 (2%)
33	SF4	G	701	7	0,12,12	-	-	-	-	-
47	CUA	l	301	23	0,1,1	-	-	-	-	-
43	HEC	b	502	20	46,50,50	1.96	6 (13%)	58,82,82	1.74	4 (6%)
37	DU0	N	501	-	42,42,42	0.65	0	64,66,66	0.89	3 (4%)
35	FES	c	1000	21	0,4,4	-	-	-	-	-
38	U10	d	501	-	63,63,63	0.70	0	78,79,79	1.10	4 (5%)
38	U10	a	502	-	63,63,63	0.71	0	78,79,79	1.00	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	HEC	u	1000	31	46,50,50	1.86	5 (10%)	58,82,82	1.43	4 (6%)
41	HEM	a	505	19	50,50,50	1.46	8 (16%)	67,82,82	1.15	6 (8%)
38	U10	d	504	-	63,63,63	0.71	0	78,79,79	1.05	5 (6%)
44	HEA	g	602	22	67,67,67	1.37	7 (10%)	81,103,103	2.20	27 (33%)
41	HEM	a	503	19	50,50,50	1.43	6 (12%)	67,82,82	1.02	3 (4%)
37	DU0	f	201	-	42,42,42	0.65	0	64,66,66	0.94	5 (7%)
36	FMN	F	502	-	33,33,33	1.04	2 (6%)	48,50,50	1.28	9 (18%)
41	HEM	t	602	45,42,30	50,50,50	1.49	7 (14%)	67,82,82	1.02	2 (2%)
35	FES	G	703	7	0,4,4	-	-	-		
33	SF4	I	1002	9	0,12,12	-	-	-		
38	U10	a	504	-	63,63,63	0.70	0	78,79,79	0.97	3 (3%)
33	SF4	G	702	7	0,12,12	-	-	-		
35	FES	f	202	21	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	HEA	g	603	22	-	4/36/76/76	-
44	HEA	k	601	22	-	5/36/76/76	-
44	HEA	k	602	22	-	11/36/76/76	-
33	SF4	B	1001	2	-	-	0/6/5/5
43	HEC	v	1002	32	-	0/14/54/54	-
41	HEM	d	502	19	-	8/14/54/54	-
43	HEC	v	1001	32	-	2/14/54/54	-
33	SF4	I	1001	9	-	-	0/6/5/5
40	CDL	a	501	-	-	24/110/110/110	-
37	DU0	H	401	-	-	0/10/98/98	0/6/6/6
43	HEC	e	502	20	-	8/14/54/54	-
33	SF4	F	501	6	-	-	0/6/5/5
35	FES	E	401	5	-	-	0/1/1/1
41	HEM	d	503	19	-	8/14/54/54	-
38	U10	H	402	-	-	21/63/87/87	0/1/1/1
41	HEM	t	603	42,30	-	7/14/54/54	-
33	SF4	G	701	7	-	-	0/6/5/5
43	HEC	b	502	20	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DU0	N	501	-	-	0/10/98/98	0/6/6/6
38	U10	d	501	-	-	18/63/87/87	0/1/1/1
35	FES	c	1000	21	-	-	0/1/1/1
38	U10	a	502	-	-	12/63/87/87	0/1/1/1
43	HEC	u	1000	31	-	4/14/54/54	-
41	HEM	a	505	19	-	6/14/54/54	-
38	U10	d	504	-	-	8/63/87/87	0/1/1/1
44	HEA	g	602	22	-	12/36/76/76	-
41	HEM	a	503	19	-	6/14/54/54	-
37	DU0	f	201	-	-	2/10/98/98	0/6/6/6
36	FMN	F	502	-	-	2/18/18/18	0/3/3/3
41	HEM	t	602	45,42,30	-	5/14/54/54	-
35	FES	G	703	7	-	-	0/1/1/1
38	U10	a	504	-	-	7/63/87/87	0/1/1/1
33	SF4	I	1002	9	-	-	0/6/5/5
33	SF4	G	702	7	-	-	0/6/5/5
35	FES	f	202	21	-	-	0/1/1/1

All (103) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	v	1001	HEC	CAC-C3C	6.60	1.56	1.35
43	v	1002	HEC	CAC-C3C	6.38	1.55	1.35
43	u	1000	HEC	CAC-C3C	6.35	1.55	1.35
43	v	1001	HEC	CAB-C3B	6.33	1.55	1.35
43	u	1000	HEC	CAB-C3B	6.32	1.55	1.35
43	v	1002	HEC	CAB-C3B	6.18	1.55	1.35
43	e	502	HEC	CAB-C3B	6.13	1.54	1.35
43	b	502	HEC	CAC-C3C	6.11	1.54	1.35
43	e	502	HEC	CAC-C3C	6.06	1.54	1.35
43	b	502	HEC	CAB-C3B	6.03	1.54	1.35
44	k	602	HEA	FE-NB	6.03	2.13	1.94
43	v	1001	HEC	C3D-C2D	5.51	1.53	1.38
43	v	1002	HEC	C3D-C2D	5.45	1.53	1.38
44	k	602	HEA	FE-ND	5.29	2.11	1.94
43	u	1000	HEC	C3D-C2D	5.18	1.52	1.38
43	b	502	HEC	C3D-C2D	4.88	1.51	1.38
44	k	602	HEA	FE-NA	4.82	2.11	1.95
43	e	502	HEC	C3D-C2D	4.72	1.51	1.38
44	k	601	HEA	C3B-C2B	4.59	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	t	602	HEM	FE-NC	4.14	2.08	1.95
44	g	603	HEA	C3B-C2B	4.10	1.44	1.34
41	t	603	HEM	FE-NA	3.89	2.08	1.95
44	k	601	HEA	C3D-C2D	3.83	1.45	1.36
44	g	602	HEA	C3B-C2B	3.70	1.43	1.34
44	k	601	HEA	C3A-C2A	3.68	1.45	1.37
44	g	602	HEA	C3D-C2D	3.66	1.44	1.36
44	g	603	HEA	C3D-C2D	3.62	1.44	1.36
44	k	602	HEA	FE-NC	3.58	2.07	1.95
44	k	602	HEA	C4B-NB	-3.34	1.34	1.40
41	t	603	HEM	FE-ND	3.27	2.05	1.94
44	g	603	HEA	C1D-ND	-3.19	1.34	1.40
41	t	602	HEM	FE-NB	3.12	2.04	1.94
44	g	603	HEA	C11-C3B	-3.08	1.47	1.51
36	F	502	FMN	C4A-N5	3.04	1.37	1.30
40	a	501	CDL	OA8-CA7	3.01	1.42	1.33
41	t	602	HEM	FE-ND	2.98	2.04	1.94
44	k	601	HEA	C1D-ND	-2.86	1.35	1.40
41	d	502	HEM	C3C-C2C	-2.85	1.31	1.37
41	a	505	HEM	C2A-C3A	-2.81	1.31	1.38
44	g	602	HEA	C1D-ND	-2.80	1.35	1.40
44	g	602	HEA	C3A-C2A	2.78	1.43	1.37
44	g	602	HEA	C4B-C3B	2.76	1.49	1.44
41	t	602	HEM	CAB-C3B	2.76	1.54	1.47
44	g	603	HEA	C3A-C2A	2.75	1.43	1.37
41	t	603	HEM	CAC-C3C	2.75	1.54	1.47
41	t	602	HEM	FE-NA	2.74	2.04	1.95
41	t	602	HEM	CAC-C3C	2.71	1.54	1.47
41	a	505	HEM	C3C-C2C	-2.69	1.31	1.37
40	a	501	CDL	OB8-CB6	-2.69	1.39	1.45
44	k	602	HEA	C4A-NA	-2.68	1.34	1.39
41	d	503	HEM	CAB-C3B	2.68	1.54	1.47
41	a	503	HEM	C3C-C2C	-2.66	1.31	1.37
41	d	502	HEM	C2A-C3A	-2.64	1.32	1.38
41	a	503	HEM	C2A-C3A	-2.63	1.32	1.38
41	d	503	HEM	CAC-C3C	2.61	1.54	1.47
41	a	505	HEM	CAB-C3B	2.60	1.54	1.47
40	a	501	CDL	OA6-CA5	2.58	1.41	1.34
41	t	603	HEM	CAB-C3B	2.55	1.54	1.47
41	a	503	HEM	CAB-C3B	2.55	1.54	1.47
40	a	501	CDL	OB6-CB4	-2.50	1.40	1.46
44	k	602	HEA	CAC-C3C	2.50	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	d	502	HEM	CAB-C3B	2.48	1.54	1.47
41	d	502	HEM	CAC-C3C	2.46	1.54	1.47
44	g	603	HEA	C4A-NA	-2.43	1.35	1.39
41	d	503	HEM	C2A-C3A	-2.42	1.32	1.38
44	g	602	HEA	C4A-NA	-2.41	1.35	1.39
41	a	503	HEM	CAC-C3C	2.39	1.53	1.47
44	k	602	HEA	O2D-CGD	-2.39	1.22	1.30
41	d	503	HEM	C3C-C2C	-2.36	1.32	1.37
44	k	601	HEA	C4D-C3D	2.34	1.49	1.45
41	a	505	HEM	C3D-C2D	-2.32	1.31	1.36
43	v	1001	HEC	CMC-C2C	2.31	1.55	1.50
41	a	505	HEM	CAC-C3C	2.30	1.53	1.47
44	k	602	HEA	CMA-C3A	2.29	1.50	1.45
44	g	603	HEA	C4B-NB	-2.28	1.36	1.40
41	a	505	HEM	CHD-C1D	-2.28	1.34	1.39
43	b	502	HEC	C3B-C2B	-2.27	1.33	1.41
41	a	503	HEM	C3B-C2B	-2.26	1.32	1.37
44	g	603	HEA	C4C-NC	-2.24	1.35	1.39
41	d	502	HEM	C3D-C2D	-2.24	1.32	1.36
43	v	1002	HEC	CMB-C2B	2.22	1.55	1.50
40	a	501	CDL	OB8-CB7	2.22	1.39	1.33
41	a	503	HEM	CHB-C4A	-2.21	1.34	1.39
43	e	502	HEC	C3C-C2C	-2.21	1.33	1.41
40	a	501	CDL	OB6-CB5	2.19	1.40	1.34
41	a	505	HEM	C3B-C2B	-2.16	1.32	1.37
43	u	1000	HEC	CMB-C2B	2.16	1.55	1.50
41	d	503	HEM	C3B-C2B	-2.15	1.32	1.37
36	F	502	FMN	C10-N1	2.15	1.37	1.33
43	v	1002	HEC	C3C-C2C	-2.15	1.33	1.41
44	g	603	HEA	C1A-NA	-2.15	1.35	1.39
44	k	602	HEA	C3A-C2A	-2.14	1.32	1.37
43	u	1000	HEC	C3C-C2C	-2.14	1.33	1.41
41	d	502	HEM	C3B-C2B	-2.13	1.32	1.37
41	a	505	HEM	CHA-C1A	-2.13	1.34	1.39
43	e	502	HEC	C3B-C2B	-2.12	1.34	1.41
41	t	603	HEM	CMC-C2C	2.09	1.55	1.50
41	t	602	HEM	C2A-C3A	-2.08	1.33	1.38
43	b	502	HEC	CMC-C2C	2.08	1.55	1.50
43	e	502	HEC	C2A-C3A	-2.07	1.32	1.36
41	t	603	HEM	CMA-C3A	2.05	1.55	1.50
44	g	602	HEA	C4B-NB	-2.04	1.36	1.40
43	b	502	HEC	C3C-C2C	-2.04	1.34	1.41

All (214) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	b	502	HEC	CBB-CAB-C3B	-6.65	114.15	127.43
43	b	502	HEC	CBC-CAC-C3C	-6.53	114.38	127.43
43	e	502	HEC	CBC-CAC-C3C	-6.45	114.54	127.43
44	k	601	HEA	C3A-C2A-C1A	-6.44	100.95	107.05
44	g	602	HEA	C3A-C2A-C1A	-6.30	101.09	107.05
44	g	603	HEA	C3A-C2A-C1A	-6.25	101.13	107.05
43	e	502	HEC	CBB-CAB-C3B	-5.75	115.94	127.43
44	k	601	HEA	CBA-CAA-C2A	5.73	128.37	112.53
44	k	602	HEA	C4B-NB-C1B	5.55	111.78	105.21
43	v	1001	HEC	CBB-CAB-C3B	-5.53	116.39	127.43
43	u	1000	HEC	CBC-CAC-C3C	-5.28	116.89	127.43
43	v	1002	HEC	CBC-CAC-C3C	-5.27	116.90	127.43
44	k	601	HEA	CAA-CBA-CGA	-5.23	99.79	113.67
44	k	602	HEA	C2A-C1A-NA	-5.16	105.35	110.32
44	k	601	HEA	CMC-C2C-C3C	5.00	138.31	126.55
43	v	1001	HEC	CBC-CAC-C3C	-4.97	117.49	127.43
44	k	601	HEA	C2A-C1A-NA	4.88	115.03	110.32
44	g	603	HEA	CMC-C2C-C3C	4.87	138.01	126.55
38	d	501	U10	C6-C1-C2	4.81	122.97	119.17
43	b	502	HEC	CMC-C2C-C1C	-4.81	118.10	125.42
44	g	603	HEA	CAA-CBA-CGA	-4.76	101.05	113.67
44	g	602	HEA	CAA-CBA-CGA	-4.75	101.07	113.67
44	k	601	HEA	CMD-C2D-C1D	-4.72	117.66	125.03
44	g	603	HEA	C2A-C1A-NA	4.62	114.78	110.32
44	g	603	HEA	C3D-C4D-ND	4.62	114.82	110.35
44	k	601	HEA	C3D-C4D-ND	4.61	114.81	110.35
44	g	602	HEA	C3D-C4D-ND	4.59	114.79	110.35
38	a	504	U10	C6-C1-C2	4.58	122.79	119.17
43	e	502	HEC	CBD-CAD-C3D	-4.58	99.88	112.53
44	k	601	HEA	CMC-C2C-C1C	-4.52	118.54	125.42
44	k	601	HEA	C12-C11-C3B	4.51	119.17	112.12
44	g	603	HEA	C13-C14-C15	-4.47	117.40	127.62
44	g	602	HEA	C2A-C1A-NA	4.42	114.59	110.32
44	g	602	HEA	CMC-C2C-C3C	4.39	136.87	126.55
43	e	502	HEC	CMC-C2C-C1C	-4.38	118.76	125.42
44	k	601	HEA	CHA-C1A-C2A	-4.30	118.07	124.86
44	k	602	HEA	CAD-CBD-CGD	-4.26	102.36	113.67
44	g	603	HEA	CMD-C2D-C1D	-4.25	118.39	125.03
44	k	602	HEA	C3B-C4B-NB	-4.24	104.97	109.84
44	g	602	HEA	CHA-C4D-C3D	-4.15	118.72	124.77
38	H	402	U10	C6-C1-C2	4.14	122.43	119.17
40	a	501	CDL	CA4-OA6-CA5	4.12	127.65	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	k	601	HEA	C4D-C3D-C2D	-4.11	100.91	106.89
44	g	603	HEA	CMC-C2C-C1C	-4.09	119.19	125.42
44	k	602	HEA	CMC-C2C-C1C	-4.09	119.19	125.42
44	g	603	HEA	CHA-C1A-C2A	-4.08	118.42	124.86
44	g	602	HEA	CMC-C2C-C1C	-4.04	119.27	125.42
43	v	1002	HEC	CBB-CAB-C3B	-4.00	119.44	127.43
38	H	402	U10	C27-C28-C29	-3.98	118.52	127.62
44	k	602	HEA	O2A-CGA-O1A	-3.95	113.17	123.33
43	u	1000	HEC	CBB-CAB-C3B	-3.93	119.57	127.43
44	g	602	HEA	CMD-C2D-C1D	-3.89	118.96	125.03
44	g	603	HEA	CHA-C4D-C3D	-3.85	119.16	124.77
44	k	601	HEA	CBD-CAD-C3D	-3.82	101.97	112.53
44	g	603	HEA	C4D-C3D-C2D	-3.78	101.38	106.89
44	g	603	HEA	C13-C12-C11	-3.75	108.40	114.39
44	k	601	HEA	CAD-C3D-C4D	3.74	131.21	124.70
41	a	505	HEM	C1C-CHC-C4B	-3.72	118.12	126.02
44	g	603	HEA	C3C-C2C-C1C	-3.71	102.80	107.17
38	H	402	U10	C7-C8-C9	-3.65	120.54	126.83
44	k	601	HEA	CMB-C2B-C1B	-3.61	119.39	125.03
44	g	602	HEA	CHA-C1A-C2A	-3.60	119.17	124.86
44	g	602	HEA	C27-C19-C20	3.60	121.47	115.23
43	v	1001	HEC	CMC-C2C-C1C	-3.52	120.06	125.42
44	g	603	HEA	CMB-C2B-C1B	-3.52	119.54	125.03
44	g	602	HEA	CAD-CBD-CGD	-3.51	104.35	113.67
44	g	602	HEA	C4D-C3D-C2D	-3.50	101.79	106.89
44	k	602	HEA	C4A-NA-C1A	3.50	111.53	105.82
38	H	402	U10	C8-C7-C6	3.47	120.62	112.08
44	k	601	HEA	CMD-C2D-C3D	3.43	135.42	126.15
44	k	601	HEA	C3C-C2C-C1C	-3.41	103.15	107.17
44	g	603	HEA	CMD-C2D-C3D	3.39	135.32	126.15
44	k	602	HEA	CBD-CAD-C3D	3.34	121.78	112.53
44	k	602	HEA	C3C-C4C-NC	-3.34	106.98	109.80
36	F	502	FMN	C4A-C10-N10	3.34	121.27	116.48
38	a	502	U10	C6-C1-C2	3.32	121.79	119.17
44	k	602	HEA	C4A-C3A-C2A	3.29	109.67	106.81
38	a	502	U10	C7-C6-C5	-3.28	114.71	118.52
38	d	504	U10	C6-C1-C2	3.25	121.73	119.17
44	g	602	HEA	CMD-C2D-C3D	3.23	134.89	126.15
37	f	201	DU0	O10-C09-O16	-3.21	102.23	109.88
41	t	602	HEM	CAD-CBD-CGD	-3.21	105.14	113.67
44	k	602	HEA	C27-C19-C20	3.20	120.78	115.23
41	a	503	HEM	C4C-CHD-C1D	-3.19	119.24	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	F	502	FMN	C4-N3-C2	-3.17	120.02	125.64
41	a	505	HEM	CAD-CBD-CGD	-3.15	105.30	113.67
44	g	603	HEA	CBD-CAD-C3D	-3.14	103.85	112.53
43	v	1001	HEC	CBD-CAD-C3D	-3.10	103.95	112.53
44	k	601	HEA	CHA-C4D-C3D	-3.08	120.29	124.77
43	v	1002	HEC	C4D-ND-C1D	3.07	110.82	105.82
44	k	602	HEA	C2B-C1B-NB	-3.07	106.36	109.90
44	k	602	HEA	C13-C14-C15	-3.06	120.61	127.62
38	d	504	U10	C1-C6-C5	3.02	122.56	119.62
44	g	602	HEA	CHB-C1B-C2B	-2.99	120.31	125.03
44	k	602	HEA	C1D-ND-C4D	2.96	108.72	105.21
44	g	602	HEA	CMB-C2B-C1B	-2.93	120.46	125.03
43	v	1001	HEC	C4D-ND-C1D	2.92	110.58	105.82
44	g	603	HEA	CMB-C2B-C3B	2.91	135.91	130.28
44	k	601	HEA	CMB-C2B-C3B	2.86	135.80	130.28
43	e	502	HEC	CHD-C4C-NC	2.85	127.56	124.45
41	d	503	HEM	C4C-CHD-C1D	-2.85	119.97	126.02
41	d	502	HEM	CAD-CBD-CGD	-2.83	106.17	113.67
43	u	1000	HEC	C4D-ND-C1D	2.82	110.42	105.82
44	g	602	HEA	C3C-C2C-C1C	-2.81	103.85	107.17
44	k	601	HEA	C13-C14-C15	-2.79	121.23	127.62
41	d	502	HEM	C1C-CHC-C4B	-2.77	120.12	126.02
44	g	603	HEA	CAA-C2A-C1A	2.73	130.40	124.85
37	f	201	DU0	O10-C09-C07	2.73	115.39	107.26
44	k	602	HEA	O11-C11-C12	2.71	116.34	109.14
44	g	602	HEA	CAA-C2A-C1A	2.70	130.35	124.85
43	v	1001	HEC	CBA-CAA-C2A	-2.69	105.10	112.53
44	g	603	HEA	CAD-C3D-C4D	2.65	129.32	124.70
41	d	503	HEM	CAD-CBD-CGD	-2.64	106.66	113.67
38	H	402	U10	C22-C21-C19	2.63	121.91	113.19
44	k	602	HEA	CHB-C4A-NA	2.63	127.32	124.45
44	g	603	HEA	C12-C13-C14	2.63	119.06	112.16
43	u	1000	HEC	CMB-C2B-C1B	-2.62	121.43	125.42
43	b	502	HEC	CHD-C4C-NC	2.57	127.25	124.45
44	g	602	HEA	C20-C19-C18	-2.57	115.41	121.17
44	g	602	HEA	C2B-C1B-NB	2.57	112.87	109.90
41	d	503	HEM	C4A-CHB-C1B	-2.53	120.29	126.25
43	e	502	HEC	C1D-C2D-C3D	-2.52	103.93	106.82
41	a	503	HEM	CBA-CAA-C2A	-2.52	105.57	112.53
37	f	201	DU0	C11-O10-C09	2.49	117.99	113.69
44	g	603	HEA	CHC-C1C-C2C	-2.48	120.23	127.43
41	a	505	HEM	CAA-CBA-CGA	-2.48	107.09	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	k	601	HEA	CHC-C1C-C2C	-2.46	120.27	127.43
44	g	603	HEA	CHB-C1B-C2B	-2.46	121.14	125.03
44	k	601	HEA	C3B-C4B-NB	2.45	112.66	109.84
43	e	502	HEC	CMD-C2D-C1D	2.45	129.15	125.42
44	k	602	HEA	C2D-C1D-ND	-2.43	107.04	109.84
40	a	501	CDL	OB6-CB5-C51	2.43	116.73	111.48
38	d	501	U10	O2-C2-C3	2.41	126.14	121.03
36	F	502	FMN	C5A-C9A-N10	2.41	120.14	117.97
44	k	602	HEA	C4C-NC-C1C	2.41	109.75	105.82
41	d	502	HEM	CBA-CAA-C2A	-2.41	105.88	112.53
44	g	602	HEA	CHC-C1C-C2C	-2.40	120.46	127.43
44	k	602	HEA	CMB-C2B-C3B	-2.39	125.64	130.28
40	a	501	CDL	OA6-CA4-CA6	2.38	116.87	108.34
44	g	602	HEA	C4B-C3B-C2B	-2.36	103.47	107.44
41	t	603	HEM	C3B-C2B-C1B	2.36	108.18	106.41
36	F	502	FMN	C10-C4A-N5	-2.35	120.01	124.81
44	g	603	HEA	CBA-CAA-C2A	2.35	119.03	112.53
37	f	201	DU0	C08-C07-C09	2.34	118.71	114.94
37	N	501	DU0	O10-C09-O16	-2.33	104.33	109.88
41	a	503	HEM	C4A-CHB-C1B	-2.32	120.79	126.25
44	k	601	HEA	C12-C13-C14	2.30	118.22	112.16
44	k	602	HEA	CMC-C2C-C3C	2.30	131.96	126.55
41	d	502	HEM	C4A-CHB-C1B	-2.30	120.85	126.25
36	F	502	FMN	C4A-C4-N3	2.29	119.09	113.25
43	e	502	HEC	CAA-CBA-CGA	-2.27	107.65	113.67
44	g	602	HEA	C3B-C4B-NB	2.26	112.44	109.84
41	t	602	HEM	C3B-C2B-C1B	2.26	108.11	106.41
36	F	502	FMN	C1'-C2'-C3'	2.26	115.79	109.66
36	F	502	FMN	C4-C4A-C10	2.26	120.80	116.93
44	k	601	HEA	CHB-C1B-C2B	-2.26	121.47	125.03
44	k	601	HEA	CHA-C1A-NA	2.25	126.90	124.45
44	g	602	HEA	CHB-C1B-NB	2.23	126.82	124.42
44	k	602	HEA	CHC-C1C-NC	2.22	127.89	123.86
44	g	603	HEA	C3B-C4B-NB	2.22	112.39	109.84
41	a	505	HEM	CBC-CAC-C3C	-2.22	116.45	127.53
37	N	501	DU0	O16-C09-C07	2.21	107.49	104.56
44	g	602	HEA	C26-C15-C16	2.20	119.05	115.23
38	d	501	U10	O3-C3-C4	-2.19	115.34	123.64
38	d	504	U10	C7-C6-C5	-2.19	115.97	118.52
41	d	502	HEM	CHB-C1B-NB	2.19	127.07	124.37
44	g	603	HEA	C17-C18-C19	-2.18	122.64	127.62
44	k	601	HEA	C17-C18-C19	-2.18	122.64	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	k	602	HEA	C17-C18-C19	-2.18	122.64	127.62
41	d	503	HEM	CAA-CBA-CGA	-2.16	107.92	113.67
44	k	602	HEA	CAD-C3D-C4D	-2.16	120.93	124.70
38	H	402	U10	C21-C19-C18	2.16	126.02	121.17
36	F	502	FMN	O4-C4-C4A	-2.16	120.83	126.53
43	v	1002	HEC	CHD-C4C-C3C	2.16	128.85	125.21
38	d	501	U10	O3-C3-C2	2.16	123.92	116.64
44	g	602	HEA	CAD-C3D-C4D	2.15	128.44	124.70
38	a	502	U10	O4-C4-C5	2.15	123.88	116.64
41	a	505	HEM	CHB-C1B-NB	2.14	127.02	124.37
44	g	603	HEA	CHA-C1A-NA	2.13	126.78	124.45
44	k	602	HEA	CHA-C1A-C2A	2.13	128.23	124.86
37	N	501	DU0	C15-C09-C07	-2.13	111.81	115.66
41	d	502	HEM	CMC-C2C-C1C	2.12	128.47	124.73
44	g	603	HEA	C25-C23-C24	2.11	119.44	114.59
37	H	401	DU0	O16-C05-C06	2.11	107.98	105.12
36	F	502	FMN	C4A-C10-N1	-2.10	119.43	124.59
38	d	504	U10	O4-C4-C3	-2.10	115.70	123.64
38	a	502	U10	C4M-O4-C4	2.10	123.84	116.47
40	a	501	CDL	CA6-CA4-CA3	2.10	116.67	111.78
44	k	602	HEA	CHB-C1B-C2B	2.10	128.34	125.03
44	g	603	HEA	C2B-C1B-NB	2.09	112.32	109.90
43	v	1002	HEC	CMB-C2B-C1B	-2.08	122.25	125.42
44	k	601	HEA	C26-C15-C16	2.07	118.83	115.23
38	a	502	U10	O4-C4-C3	-2.07	115.82	123.64
44	g	603	HEA	C27-C19-C20	2.06	118.80	115.23
44	k	601	HEA	C4B-C3B-C2B	-2.06	103.98	107.44
38	a	504	U10	C1M-C1-C6	-2.05	121.08	124.45
37	H	401	DU0	O10-C09-O16	-2.05	105.00	109.88
44	k	602	HEA	O1D-CGD-CBD	-2.05	116.60	123.09
37	f	201	DU0	C22-C21-C20	2.05	114.47	111.45
38	H	402	U10	C11-C9-C8	2.04	125.75	121.17
43	v	1001	HEC	CMB-C2B-C1B	-2.04	122.32	125.42
44	k	602	HEA	CAD-C3D-C2D	2.03	131.67	127.87
38	d	504	U10	O4-C4-C5	2.03	123.49	116.64
43	v	1002	HEC	CAA-CBA-CGA	-2.03	108.29	113.67
44	g	603	HEA	C12-C11-C3B	2.03	115.29	112.12
40	a	501	CDL	CA6-OA8-CA7	2.02	124.50	117.12
41	t	603	HEM	C1B-NB-C4B	2.02	107.59	105.21
41	a	505	HEM	C1A-CHA-C4D	-2.02	121.51	126.25
44	g	602	HEA	C21-C22-C23	-2.01	120.93	127.64
44	k	601	HEA	C2B-C1B-NB	2.01	112.22	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	g	602	HEA	CMB-C2B-C3B	2.00	134.15	130.28
38	a	504	U10	C7-C8-C9	-2.00	123.38	126.83
44	g	603	HEA	O11-C11-C3B	-2.00	107.59	111.26
44	k	601	HEA	C2D-C1D-ND	2.00	112.14	109.84

There are no chirality outliers.

All (186) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	d	501	U10	C4-C3-O3-C3M
38	d	501	U10	C6-C7-C8-C9
40	a	501	CDL	C1-CA2-OA2-PA1
40	a	501	CDL	CA2-OA2-PA1-OA3
40	a	501	CDL	CA4-CA6-OA8-CA7
40	a	501	CDL	CB4-CB3-OB5-PB2
41	d	503	HEM	C2C-C3C-CAC-CBC
41	d	503	HEM	C4C-C3C-CAC-CBC
41	t	602	HEM	C2B-C3B-CAB-CBB
41	t	602	HEM	C4B-C3B-CAB-CBB
41	t	602	HEM	C2C-C3C-CAC-CBC
41	t	602	HEM	C4C-C3C-CAC-CBC
41	t	603	HEM	C2B-C3B-CAB-CBB
43	b	502	HEC	C2B-C3B-CAB-CBB
43	b	502	HEC	C4B-C3B-CAB-CBB
43	b	502	HEC	C2C-C3C-CAC-CBC
43	b	502	HEC	C4C-C3C-CAC-CBC
43	e	502	HEC	C2B-C3B-CAB-CBB
43	e	502	HEC	C4B-C3B-CAB-CBB
43	e	502	HEC	C2C-C3C-CAC-CBC
43	e	502	HEC	C4C-C3C-CAC-CBC
43	v	1001	HEC	C2B-C3B-CAB-CBB
43	v	1001	HEC	C4B-C3B-CAB-CBB
44	k	602	HEA	C2A-C3A-CMA-OMA
44	k	602	HEA	C4A-C3A-CMA-OMA
44	k	602	HEA	C2D-C3D-CAD-CBD
44	k	602	HEA	C4D-C3D-CAD-CBD
44	k	602	HEA	C21-C22-C23-C24
44	k	602	HEA	C21-C22-C23-C25
38	H	402	U10	C25-C24-C26-C27
44	g	602	HEA	C27-C19-C20-C21
38	H	402	U10	C23-C24-C26-C27
38	d	501	U10	C29-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
41	t	603	HEM	C3D-CAD-CBD-CGD
44	g	602	HEA	C18-C19-C20-C21
38	a	502	U10	C3-C4-O4-C4M
38	d	504	U10	C3-C4-O4-C4M
38	d	501	U10	C35-C34-C36-C37
41	a	503	HEM	C2C-C3C-CAC-CBC
41	a	505	HEM	C2C-C3C-CAC-CBC
41	d	502	HEM	C2C-C3C-CAC-CBC
41	t	603	HEM	C2C-C3C-CAC-CBC
41	t	603	HEM	C4B-C3B-CAB-CBB
41	t	602	HEM	C2A-CAA-CBA-CGA
38	H	402	U10	C13-C14-C16-C17
38	d	501	U10	C33-C34-C36-C37
40	a	501	CDL	C12-C13-C14-C15
40	a	501	CDL	OA5-CA3-CA4-CA6
38	H	402	U10	C15-C14-C16-C17
40	a	501	CDL	C1-CB2-OB2-PB2
40	a	501	CDL	CA3-CA4-OA6-CA5
40	a	501	CDL	C38-C39-C40-C41
40	a	501	CDL	OA6-CA4-CA6-OA8
37	f	201	DU0	O23-C24-C25-C26
44	g	602	HEA	C3B-C11-C12-C13
44	k	601	HEA	C3B-C11-C12-C13
38	a	504	U10	C14-C16-C17-C18
38	a	502	U10	C25-C24-C26-C27
38	H	402	U10	C45-C44-C46-C47
38	H	402	U10	C43-C44-C46-C47
38	a	502	U10	C23-C24-C26-C27
40	a	501	CDL	OB5-CB3-CB4-OB6
38	a	504	U10	C19-C21-C22-C23
40	a	501	CDL	C35-C36-C37-C38
40	a	501	CDL	OB5-CB3-CB4-CB6
38	d	501	U10	C1-C6-C7-C8
41	a	503	HEM	C2B-C3B-CAB-CBB
41	d	502	HEM	C2B-C3B-CAB-CBB
38	d	504	U10	C44-C46-C47-C48
41	d	502	HEM	C4C-C3C-CAC-CBC
41	t	603	HEM	C4C-C3C-CAC-CBC
38	H	402	U10	C5-C6-C7-C8
38	a	502	U10	C5-C6-C7-C8
38	d	501	U10	C5-C6-C7-C8
44	g	602	HEA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
44	g	602	HEA	C1A-C2A-CAA-CBA
38	d	501	U10	C12-C11-C9-C10
36	F	502	FMN	O4'-C4'-C5'-O5'
40	a	501	CDL	C39-C40-C41-C42
40	a	501	CDL	OA5-CA3-CA4-OA6
38	d	501	U10	C12-C11-C9-C8
38	a	502	U10	C2-C3-O3-C3M
38	a	502	U10	C5-C4-O4-C4M
40	a	501	CDL	CA2-OA2-PA1-OA5
40	a	501	CDL	CB2-OB2-PB2-OB3
40	a	501	CDL	CB2-OB2-PB2-OB5
40	a	501	CDL	CA2-C1-CB2-OB2
38	H	402	U10	C35-C34-C36-C37
40	a	501	CDL	C17-C18-C19-C20
38	H	402	U10	C16-C17-C18-C19
38	d	501	U10	C11-C12-C13-C14
38	d	501	U10	C46-C47-C48-C49
44	g	602	HEA	C2A-CAA-CBA-CGA
38	a	502	U10	C9-C11-C12-C13
38	a	504	U10	C29-C31-C32-C33
38	d	501	U10	C34-C36-C37-C38
38	a	502	U10	C26-C27-C28-C29
38	a	502	U10	C1-C6-C7-C8
38	d	501	U10	C21-C22-C23-C24
38	H	402	U10	C5-C4-O4-C4M
41	t	603	HEM	CAD-CBD-CGD-O2D
38	d	501	U10	C39-C41-C42-C43
41	a	503	HEM	C4C-C3C-CAC-CBC
41	a	505	HEM	C4C-C3C-CAC-CBC
38	a	504	U10	C50-C49-C51-C52
38	d	504	U10	C45-C44-C46-C47
41	a	503	HEM	CAA-CBA-CGA-O1A
41	d	502	HEM	CAD-CBD-CGD-O2D
41	d	503	HEM	CAA-CBA-CGA-O1A
38	a	504	U10	C5-C4-O4-C4M
38	d	501	U10	C2-C3-O3-C3M
41	t	603	HEM	CAD-CBD-CGD-O1D
38	H	402	U10	C24-C26-C27-C28
38	a	502	U10	C24-C26-C27-C28
43	e	502	HEC	CAA-CBA-CGA-O1A
44	g	603	HEA	CAA-CBA-CGA-O1A
38	H	402	U10	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
43	b	502	HEC	CAA-CBA-CGA-O1A
43	e	502	HEC	CAA-CBA-CGA-O2A
38	d	504	U10	C35-C34-C36-C37
38	a	504	U10	C48-C49-C51-C52
44	g	603	HEA	CAA-CBA-CGA-O2A
44	k	602	HEA	CAA-CBA-CGA-O1A
44	k	602	HEA	CAD-CBD-CGD-O1D
38	H	402	U10	C3-C4-O4-C4M
44	k	601	HEA	CAA-CBA-CGA-O1A
41	a	503	HEM	CAA-CBA-CGA-O2A
43	e	502	HEC	CAD-CBD-CGD-O1D
36	F	502	FMN	C4'-C5'-O5'-P
40	a	501	CDL	CA4-CA3-OA5-PA1
41	d	503	HEM	CAA-CBA-CGA-O2A
38	H	402	U10	C30-C29-C31-C32
38	d	501	U10	C40-C39-C41-C42
44	g	602	HEA	C26-C15-C16-C17
41	d	503	HEM	CAD-CBD-CGD-O2D
38	H	402	U10	C39-C41-C42-C43
44	g	602	HEA	CAA-CBA-CGA-O1A
38	H	402	U10	C33-C34-C36-C37
38	d	504	U10	C33-C34-C36-C37
44	k	601	HEA	CAA-CBA-CGA-O2A
44	g	602	HEA	CAD-CBD-CGD-O2D
38	H	402	U10	C51-C52-C53-C54
41	d	502	HEM	CAD-CBD-CGD-O1D
38	d	501	U10	C19-C21-C22-C23
44	k	601	HEA	CAD-CBD-CGD-O2D
38	H	402	U10	C28-C29-C31-C32
41	d	503	HEM	CAD-CBD-CGD-O1D
43	b	502	HEC	CAA-CBA-CGA-O2A
44	k	602	HEA	C11-C12-C13-C14
44	g	602	HEA	CAD-CBD-CGD-O1D
44	g	602	HEA	CAA-CBA-CGA-O2A
41	a	505	HEM	CAD-CBD-CGD-O1D
41	a	505	HEM	CAD-CBD-CGD-O2D
41	d	503	HEM	C2B-C3B-CAB-CBB
37	f	201	DU0	C75-C22-O23-C24
43	e	502	HEC	CAD-CBD-CGD-O2D
41	d	502	HEM	CAA-CBA-CGA-O2A
43	u	1000	HEC	CAA-CBA-CGA-O2A
44	g	603	HEA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
44	k	601	HEA	CAD-CBD-CGD-O1D
38	d	504	U10	C5-C4-O4-C4M
38	d	504	U10	C43-C44-C46-C47
43	u	1000	HEC	CAD-CBD-CGD-O1D
38	H	402	U10	C9-C11-C12-C13
41	a	503	HEM	C4B-C3B-CAB-CBB
41	a	505	HEM	C4B-C3B-CAB-CBB
41	d	502	HEM	C4B-C3B-CAB-CBB
41	d	503	HEM	C4B-C3B-CAB-CBB
38	d	501	U10	C16-C17-C18-C19
43	u	1000	HEC	CAD-CBD-CGD-O2D
43	u	1000	HEC	CAA-CBA-CGA-O1A
44	k	602	HEA	CAD-CBD-CGD-O2D
44	g	603	HEA	CAD-CBD-CGD-O1D
40	a	501	CDL	C52-C51-CB5-OB6
40	a	501	CDL	C53-C54-C55-C56
41	d	502	HEM	CAA-CBA-CGA-O1A
38	d	504	U10	C50-C49-C51-C52
38	a	502	U10	C4-C3-O3-C3M
44	k	602	HEA	CAA-CBA-CGA-O2A
38	H	402	U10	C11-C12-C13-C14
44	g	602	HEA	O11-C11-C12-C13
38	a	502	U10	C28-C29-C31-C32
38	a	504	U10	C33-C34-C36-C37
40	a	501	CDL	C52-C51-CB5-OB7
38	H	402	U10	C1-C6-C7-C8
41	a	505	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

26 monomers are involved in 98 short contacts:

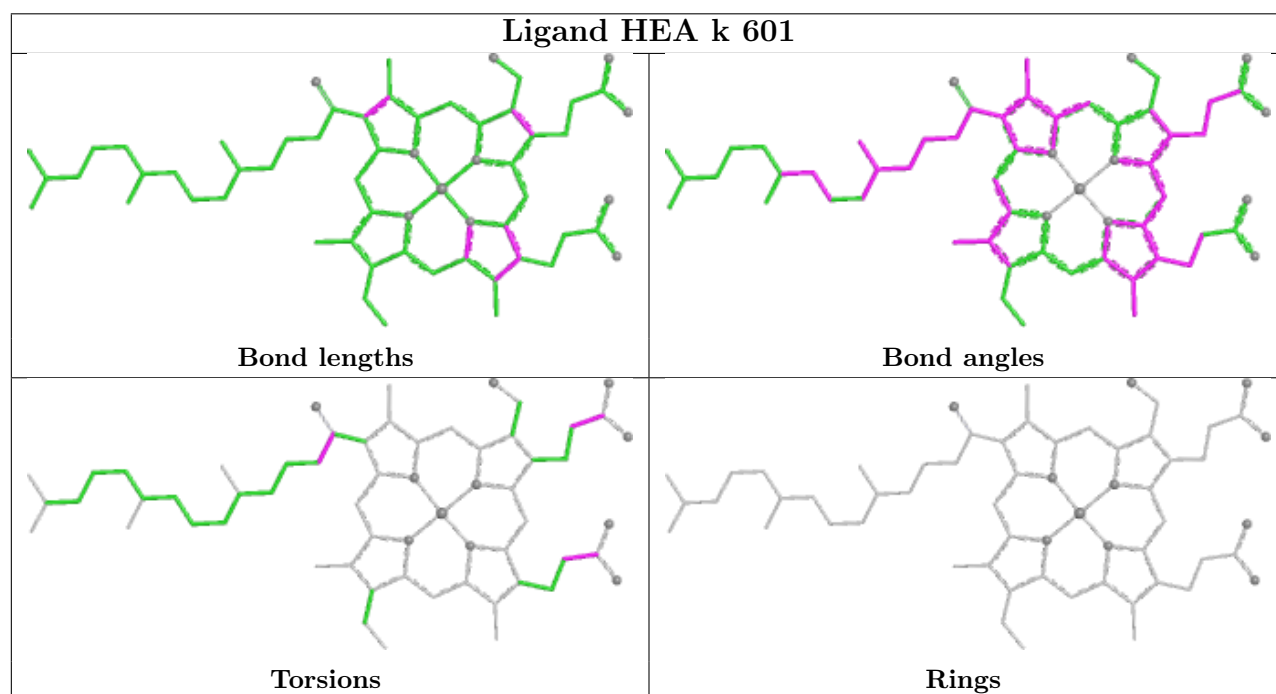
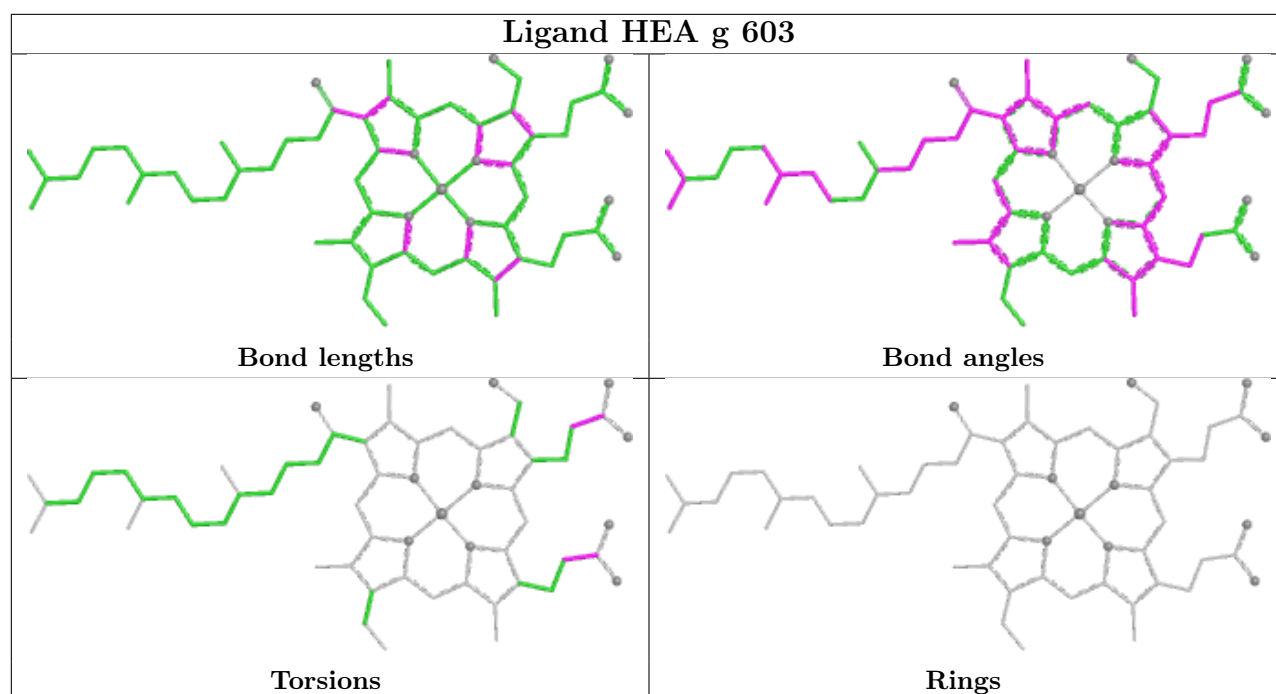
Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	g	603	HEA	3	0
44	k	601	HEA	7	0
44	k	602	HEA	2	0
33	B	1001	SF4	3	0
43	v	1002	HEC	3	0
41	d	502	HEM	7	0
43	v	1001	HEC	3	0
40	a	501	CDL	3	0
43	e	502	HEC	1	0
33	F	501	SF4	2	0

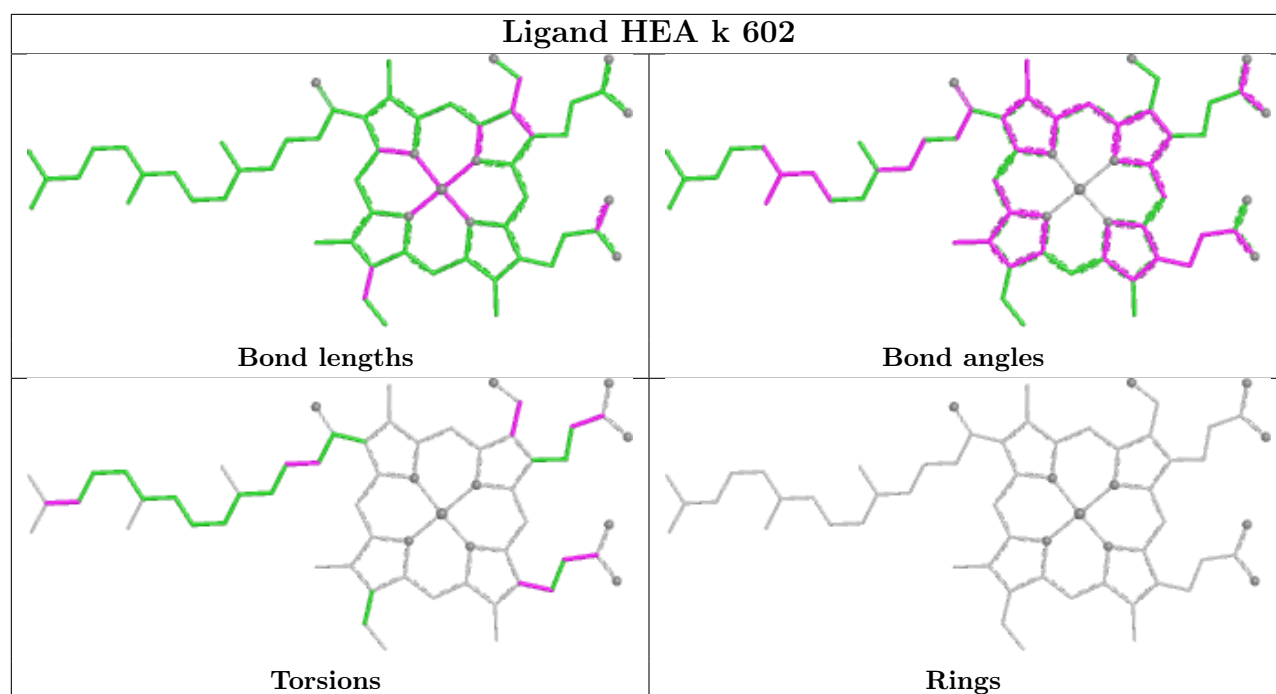
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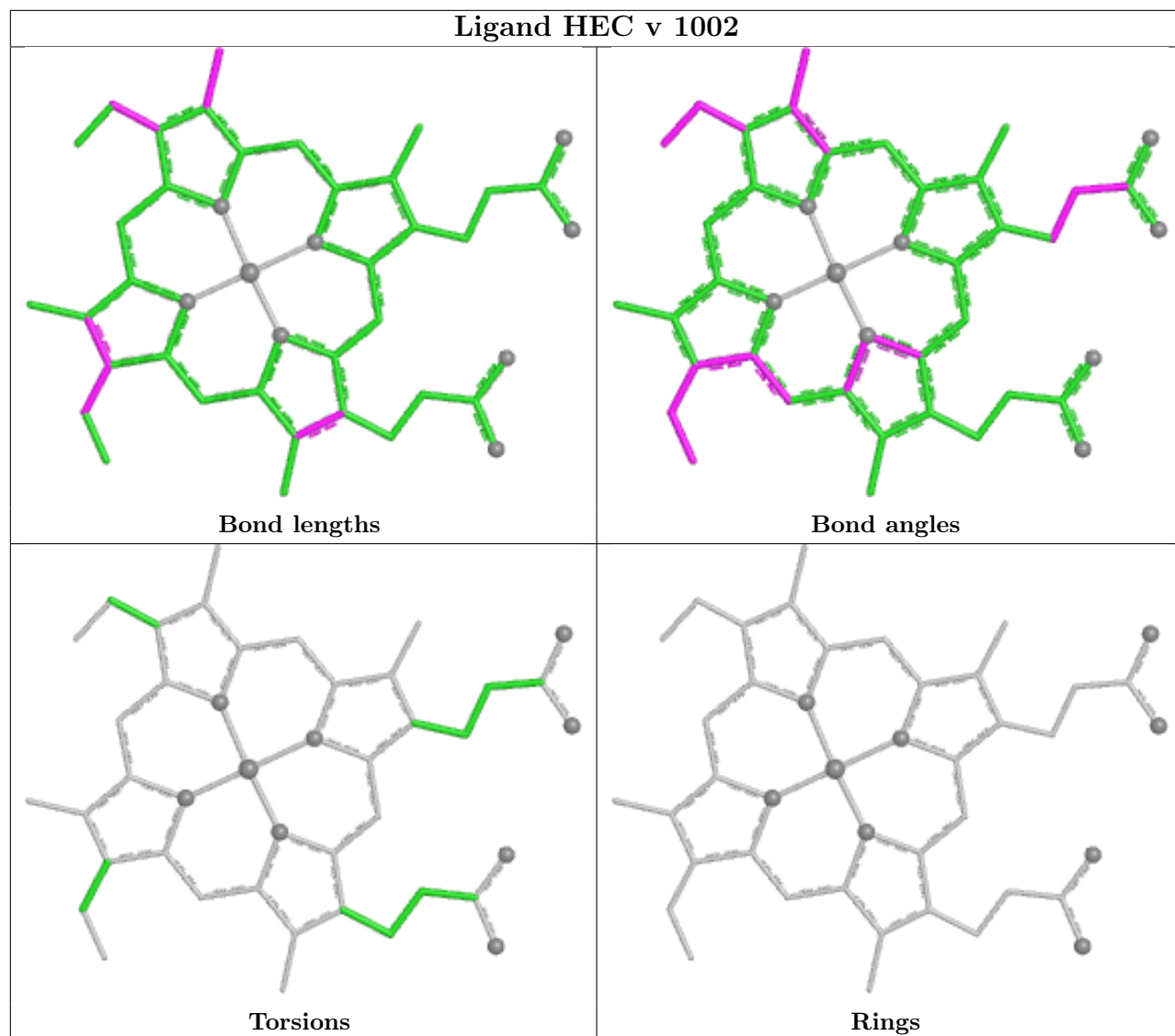
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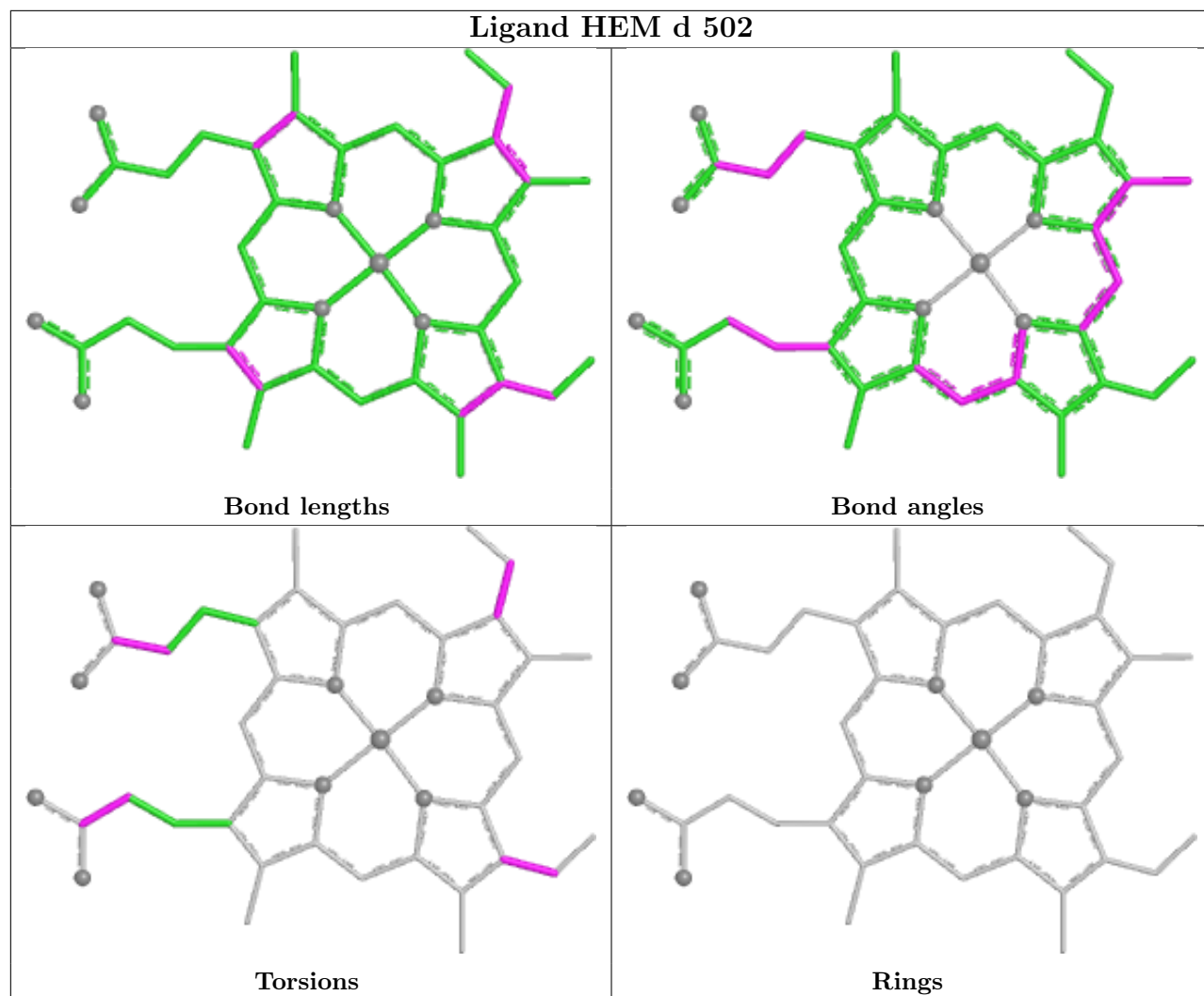
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	E	401	FES	1	0
38	H	402	U10	8	0
41	d	503	HEM	4	0
41	t	603	HEM	1	0
33	G	701	SF4	1	0
43	b	502	HEC	1	0
38	d	501	U10	8	0
38	a	502	U10	6	0
43	u	1000	HEC	4	0
41	a	505	HEM	7	0
38	d	504	U10	1	0
44	g	602	HEA	4	0
41	a	503	HEM	4	0
36	F	502	FMN	6	0
41	t	602	HEM	4	0
38	a	504	U10	6	0

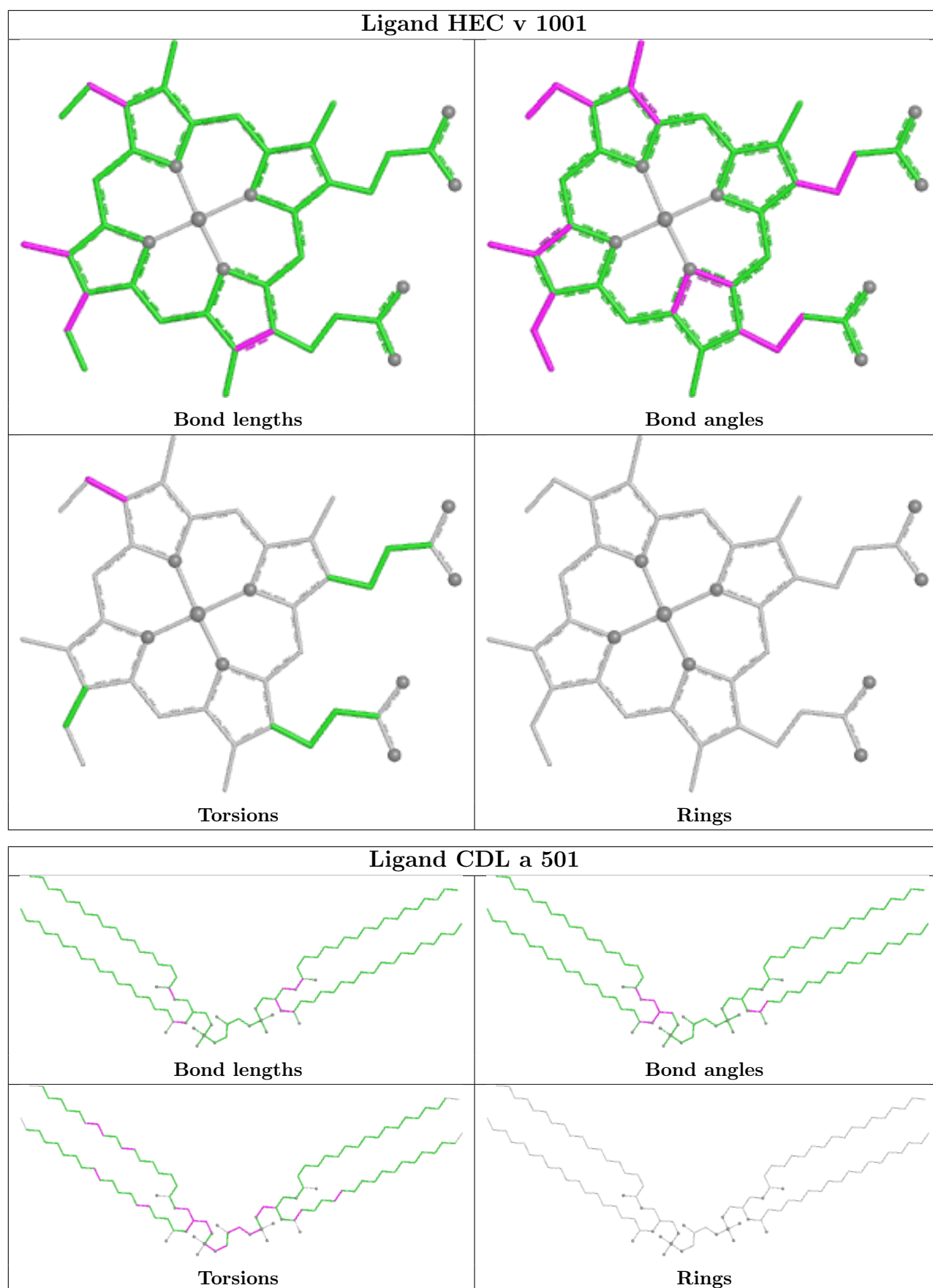
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



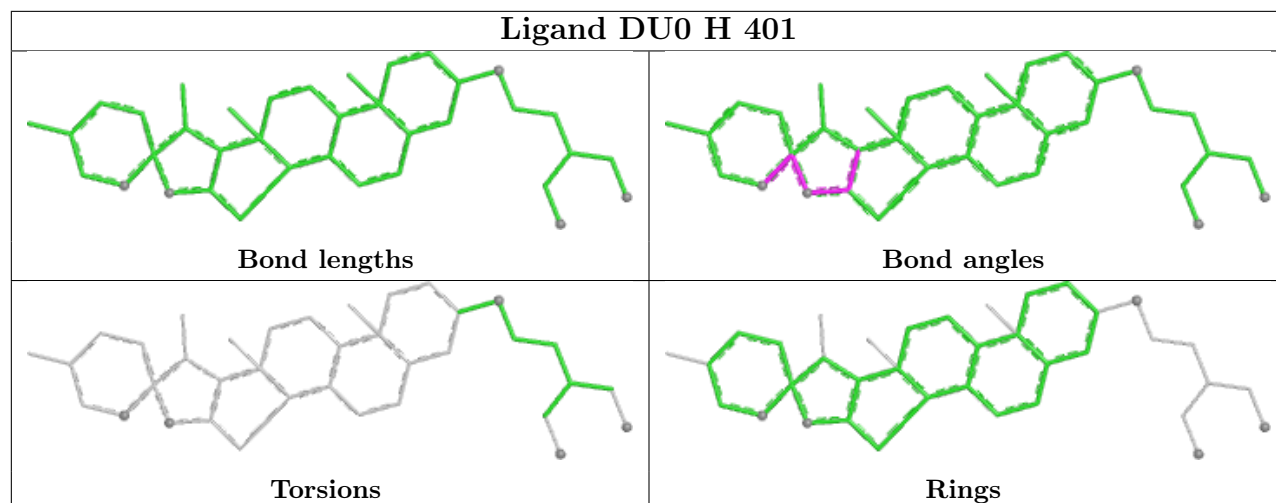




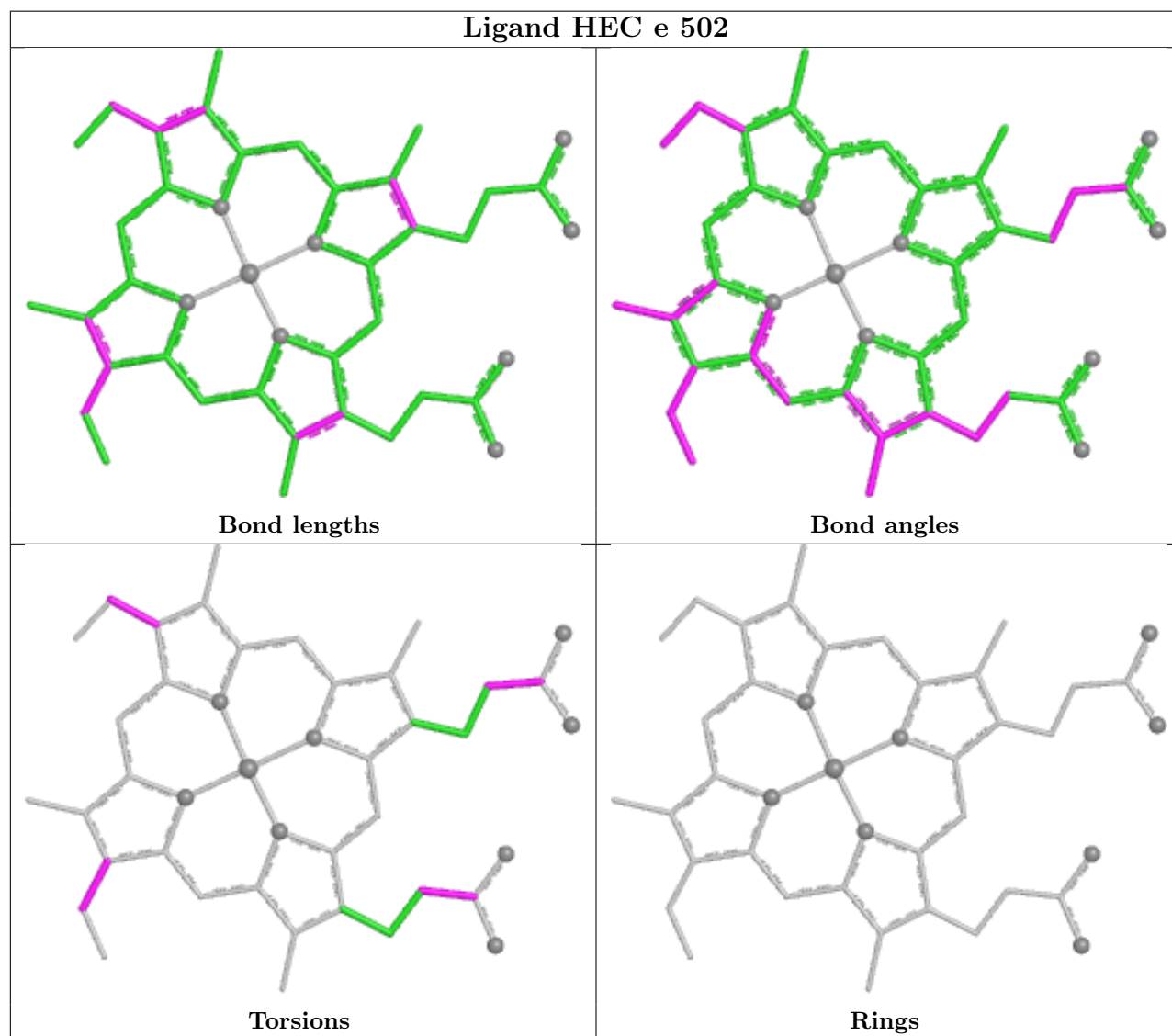


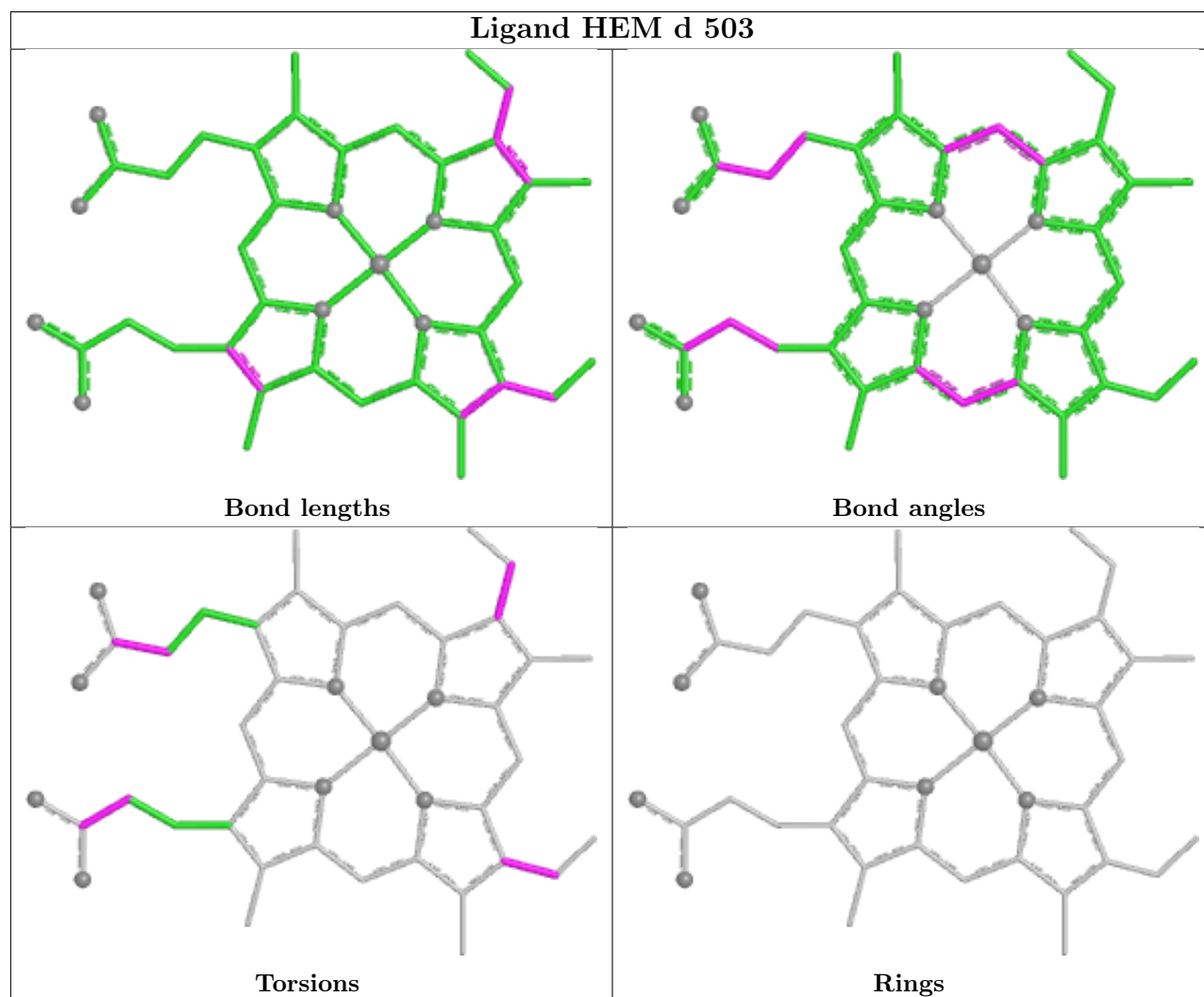
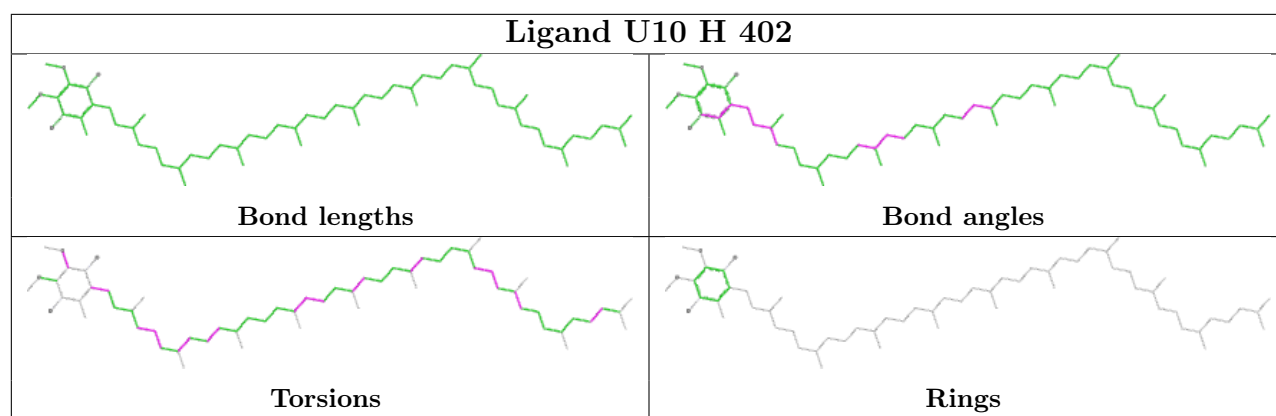


Ligand DU0 H 401

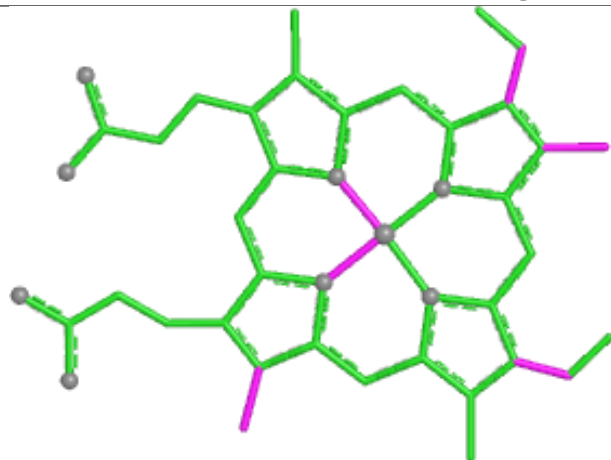


Ligand HEC e 502

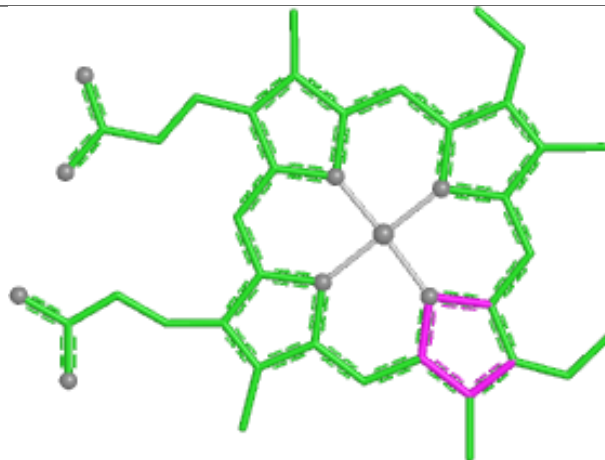




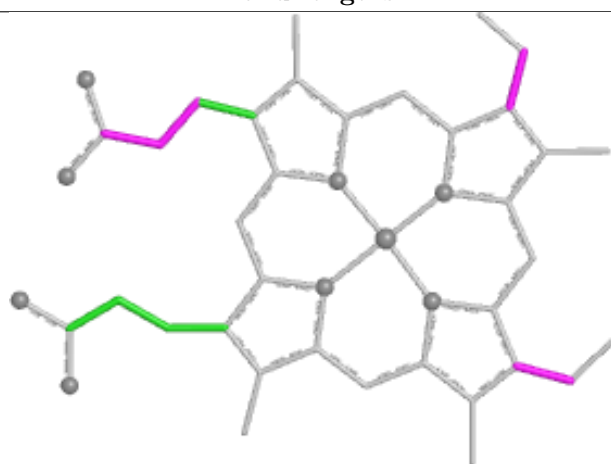
Ligand HEM t 603



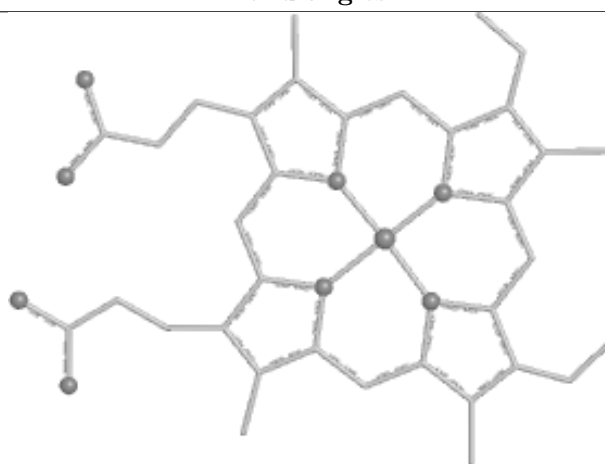
Bond lengths



Bond angles

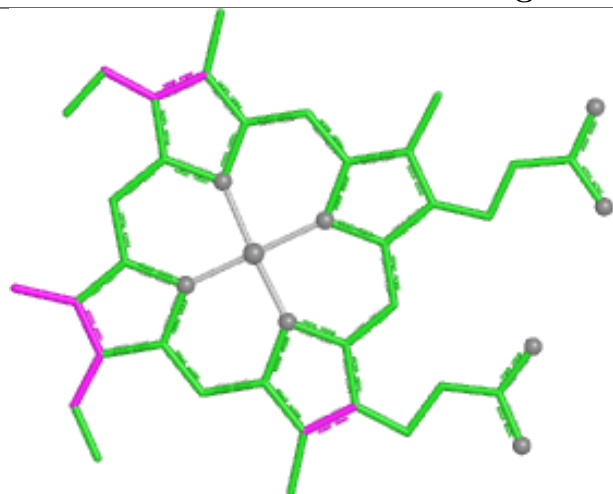


Torsions

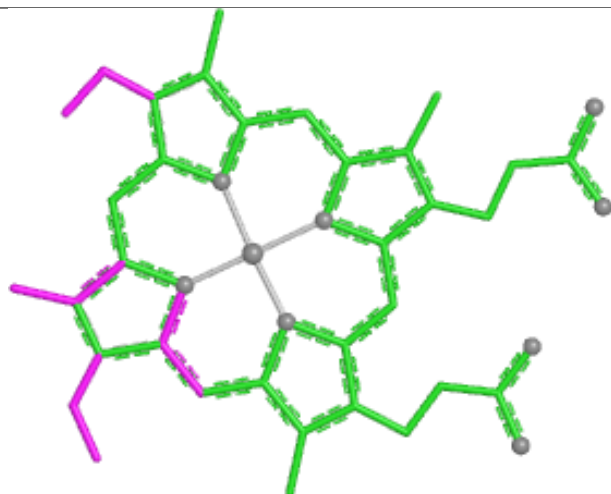


Rings

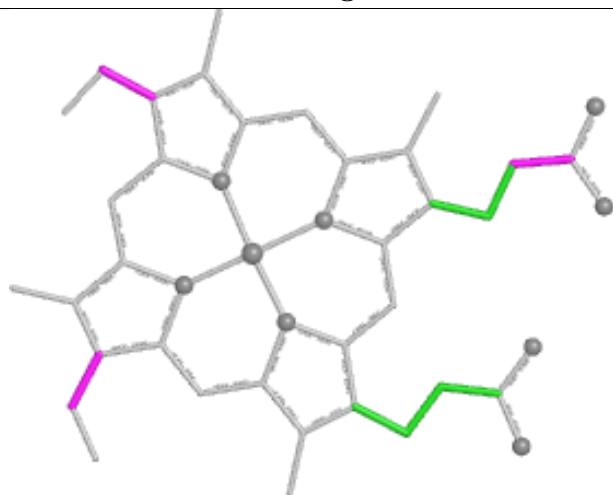
Ligand HEC b 502



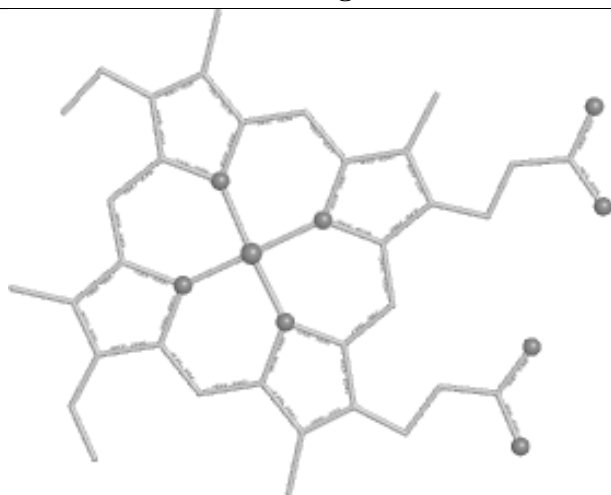
Bond lengths



Bond angles

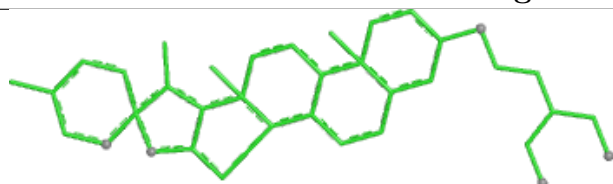


Torsions

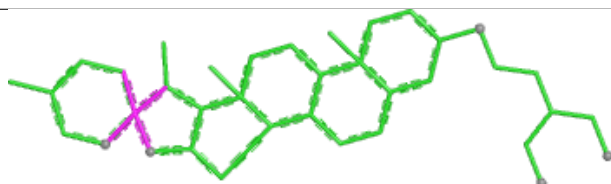


Rings

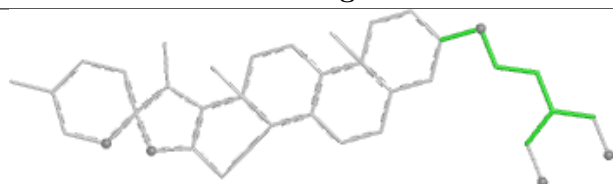
Ligand DU0 N 501



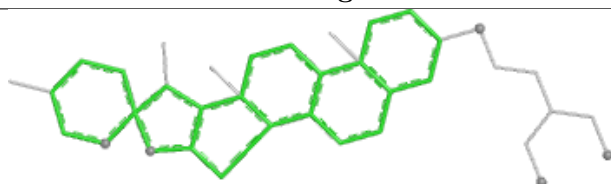
Bond lengths



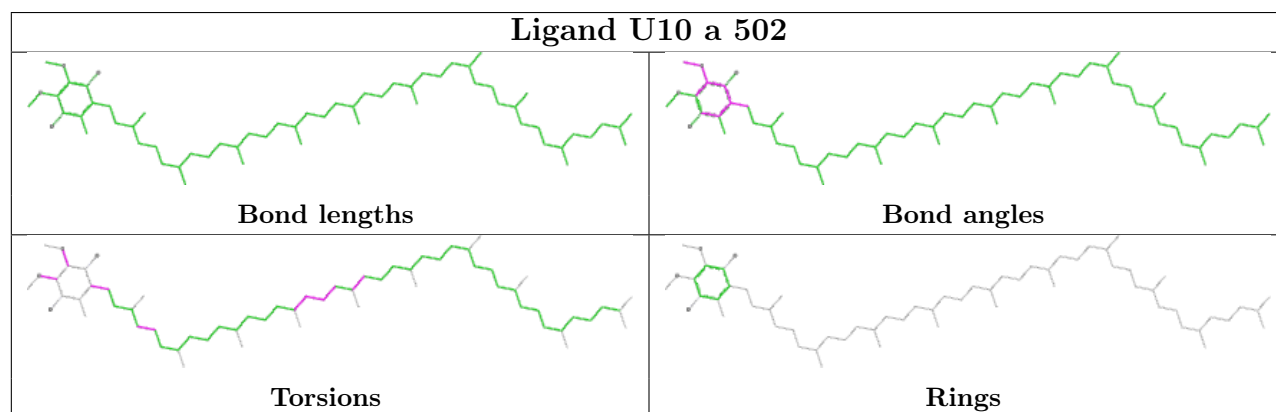
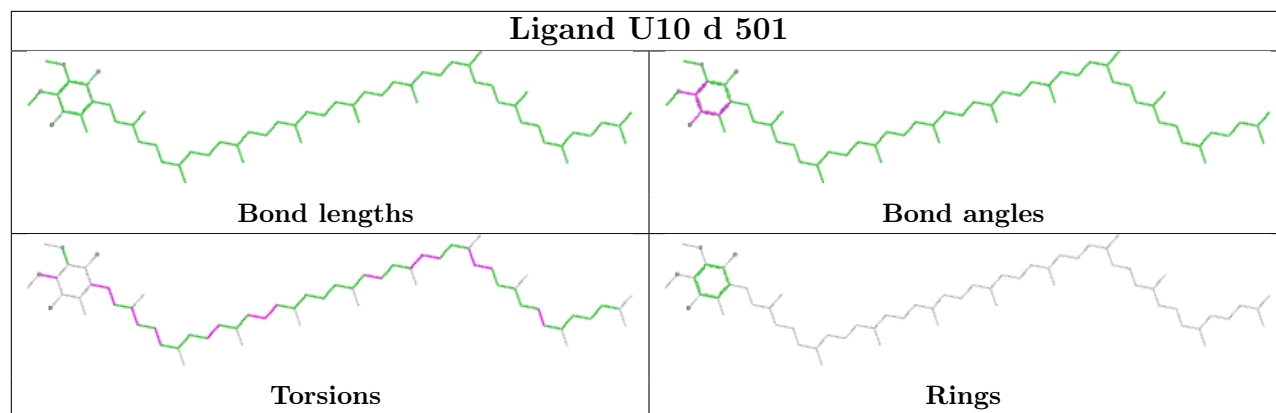
Bond angles

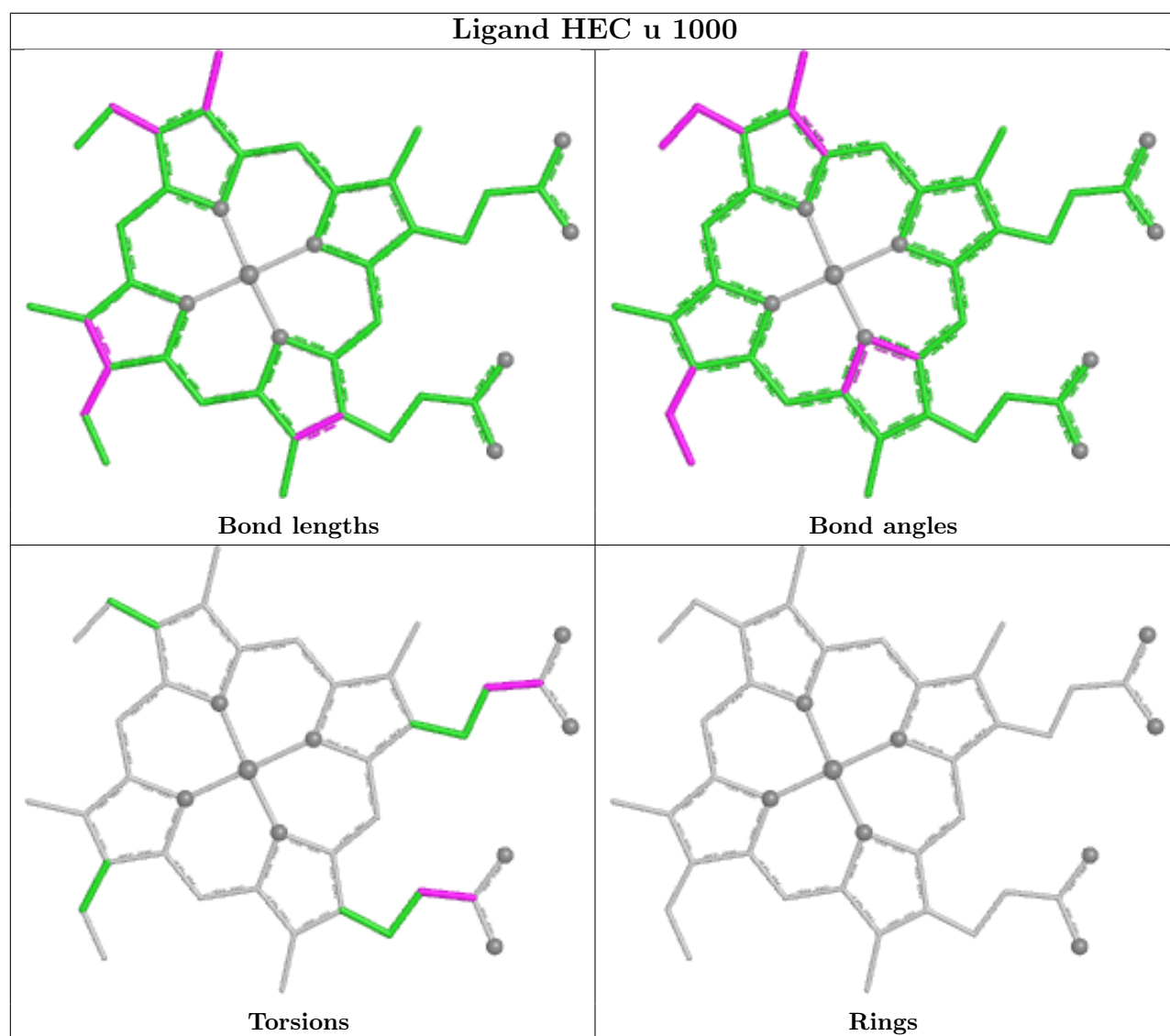


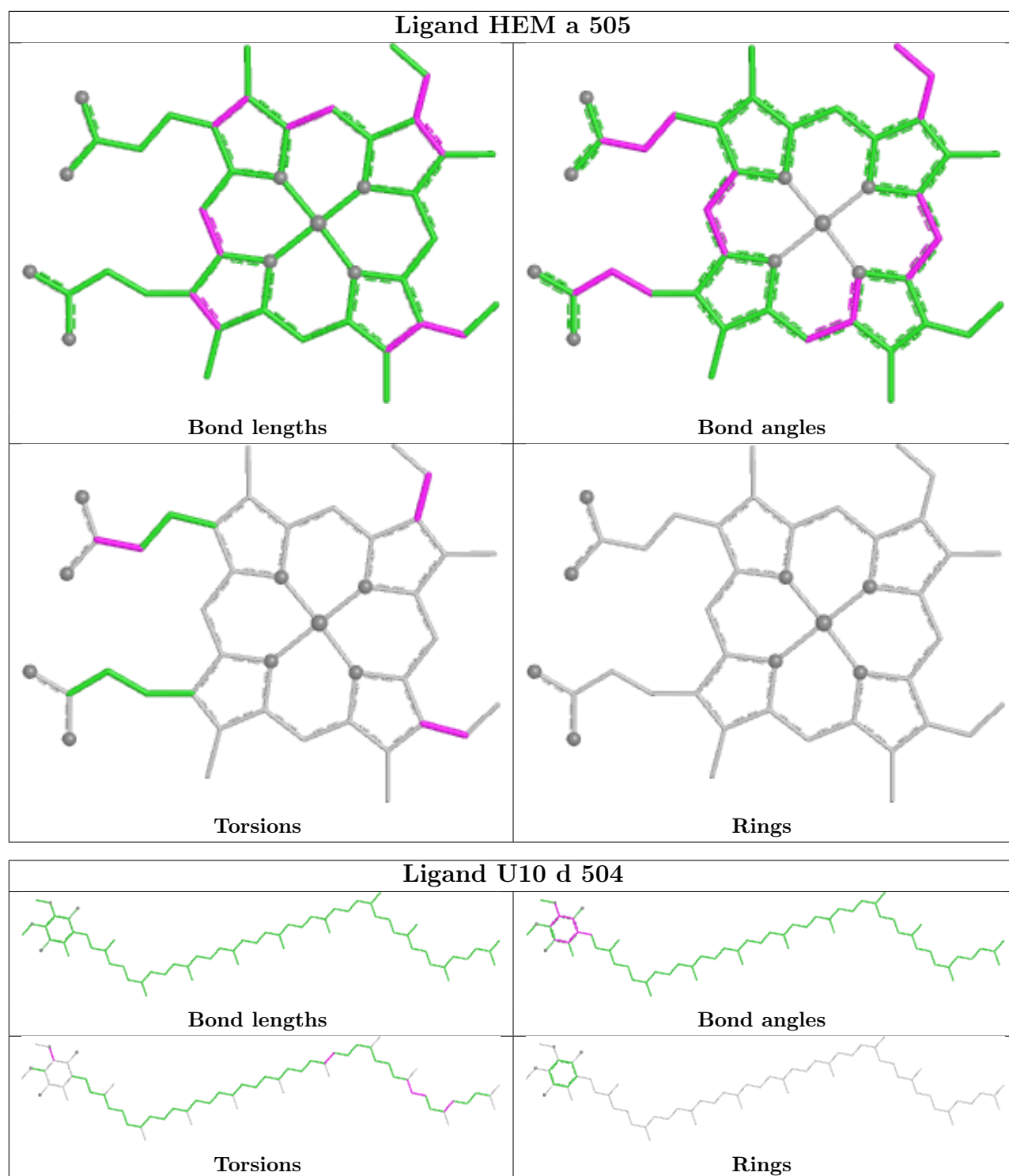
Torsions



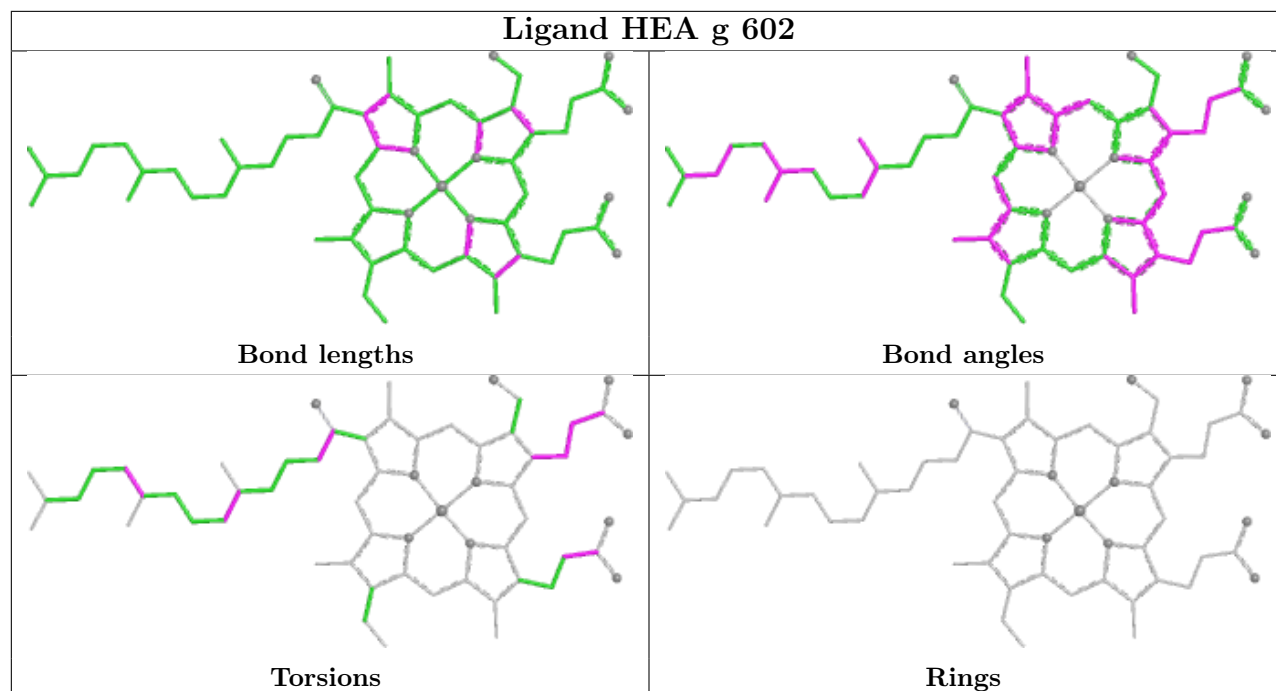
Rings



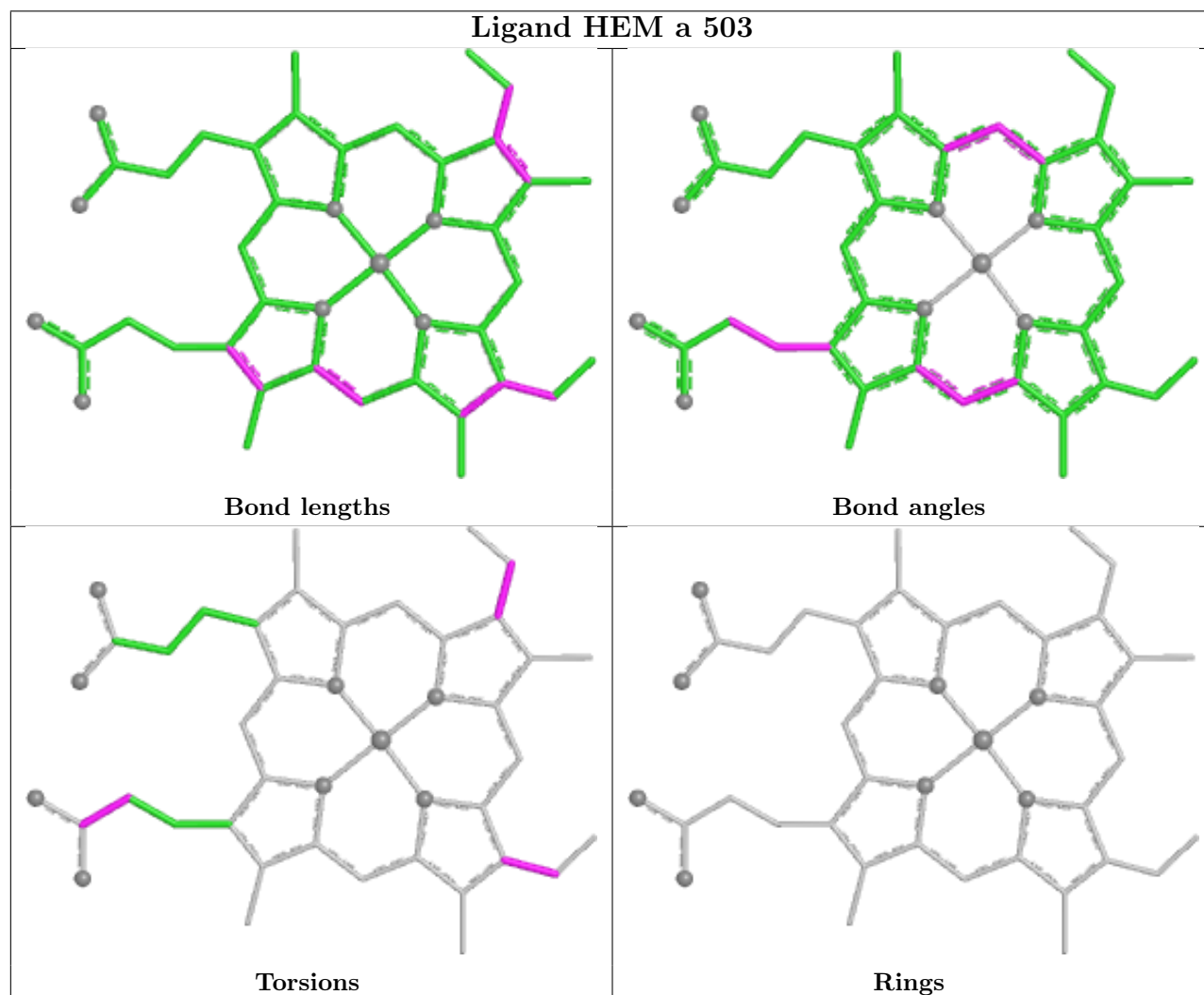




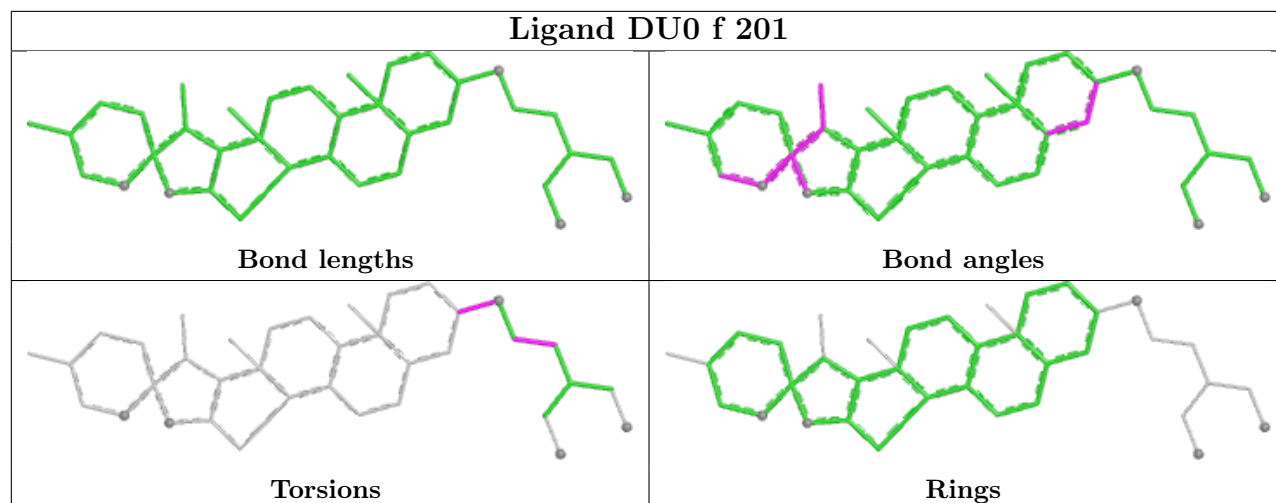
Ligand HEA g 602



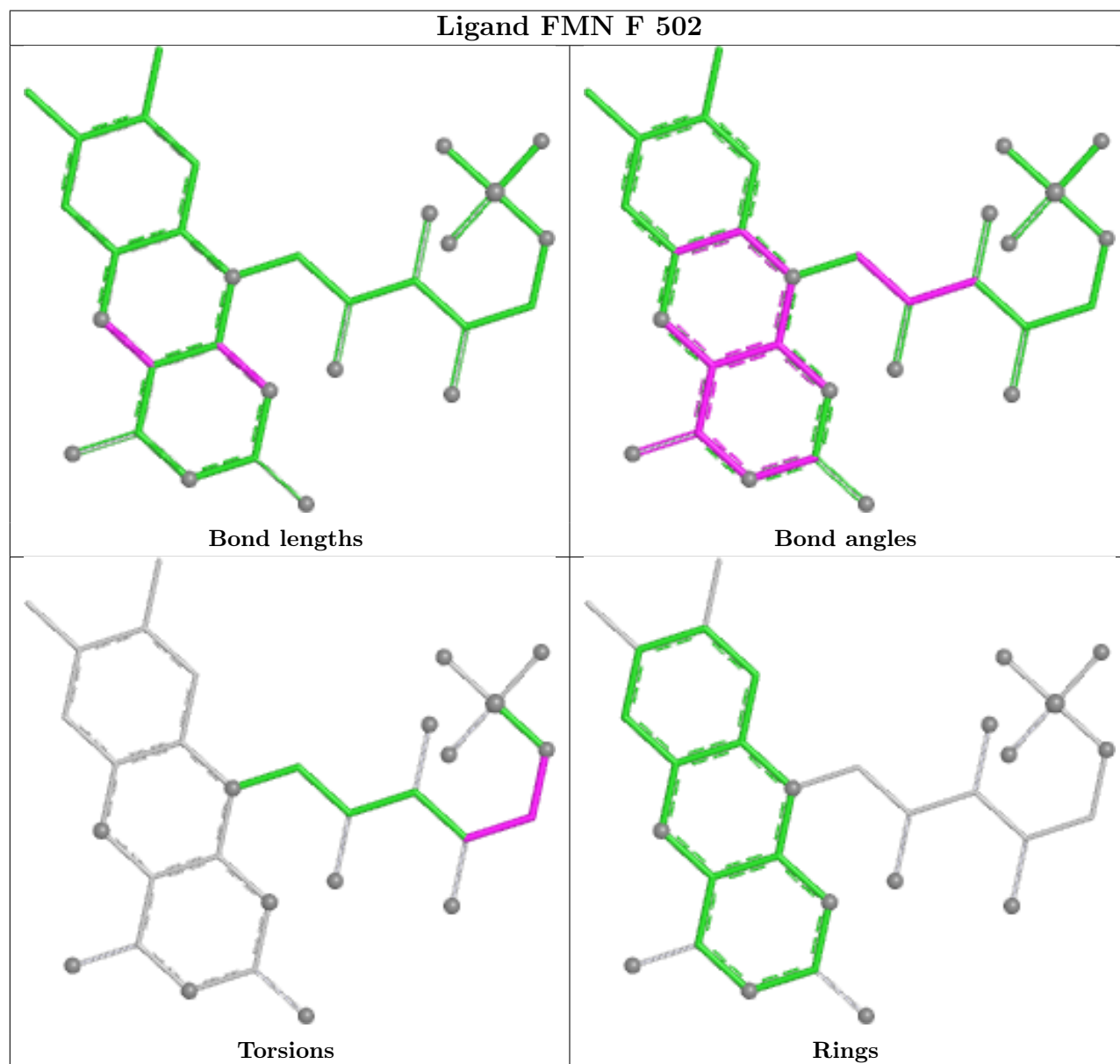
Ligand HEM a 503

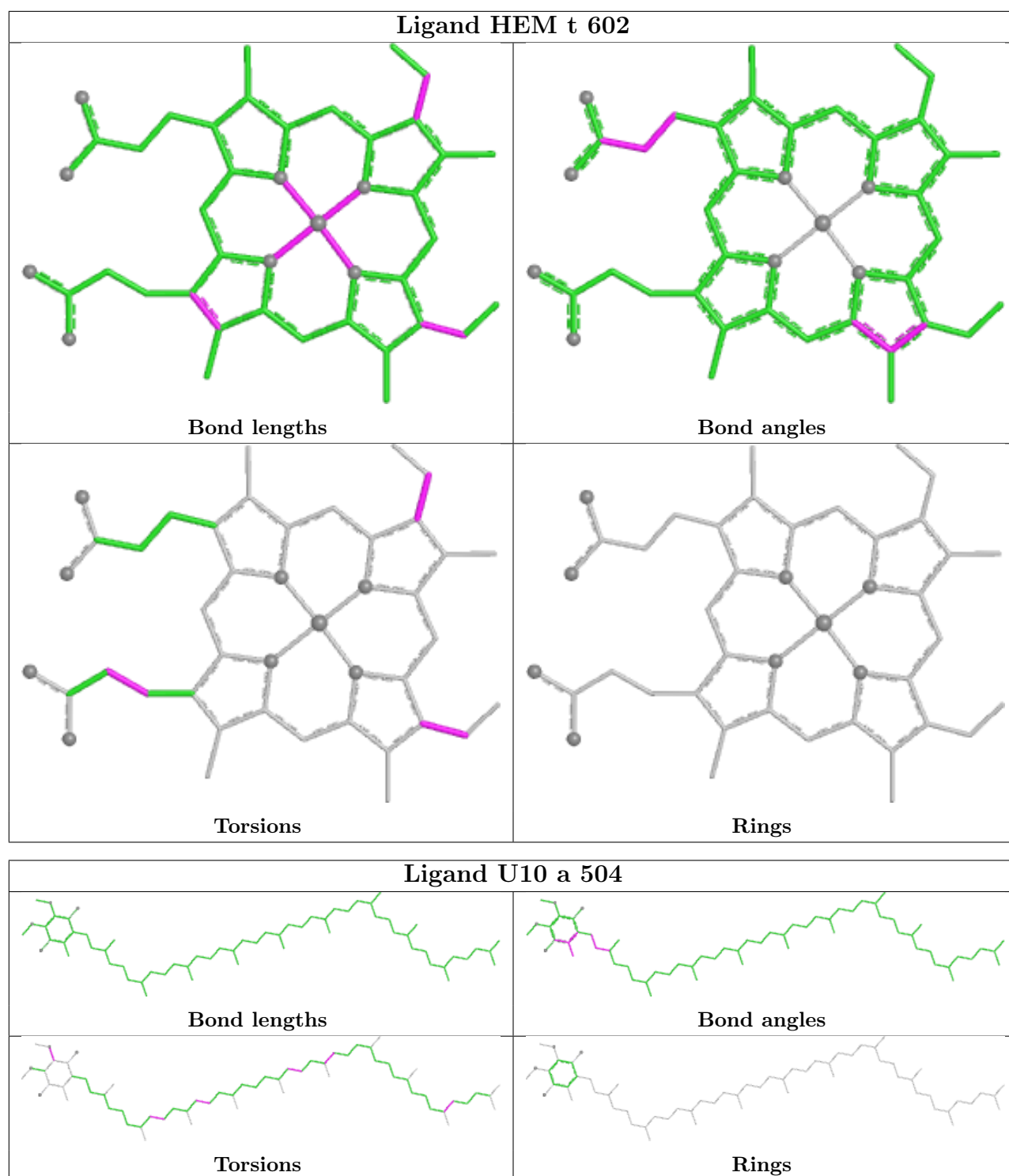


Ligand DU0 f 201



Ligand FMN F 502





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.

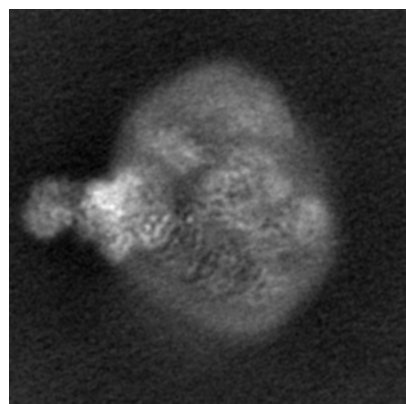
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51125. These allow visual inspection of the internal detail of the map and identification of artifacts.

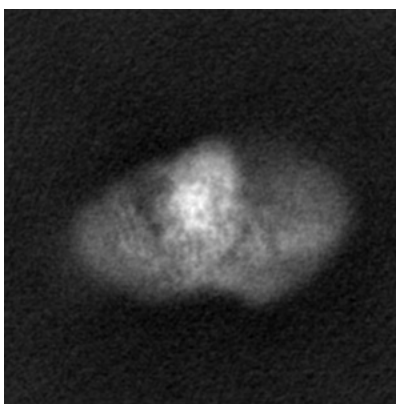
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

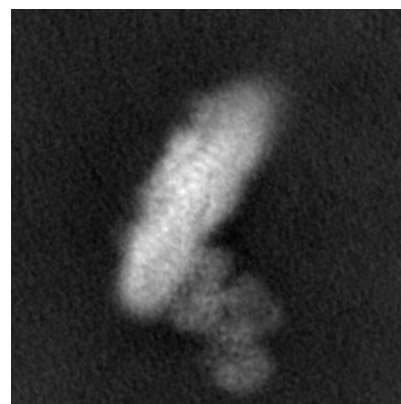
6.1.1 Primary map



X

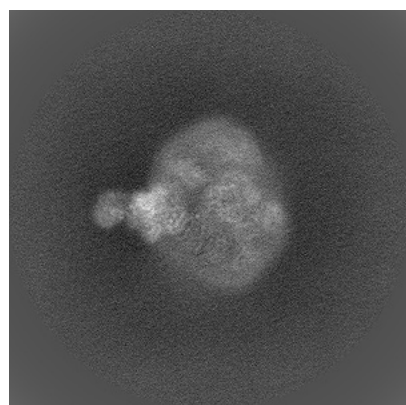


Y

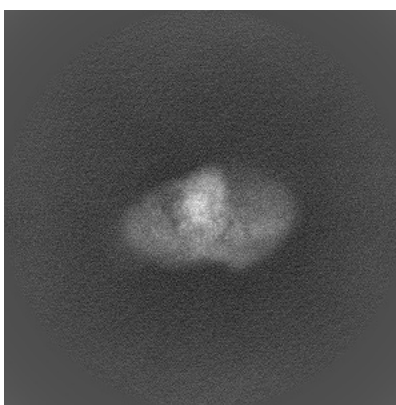


Z

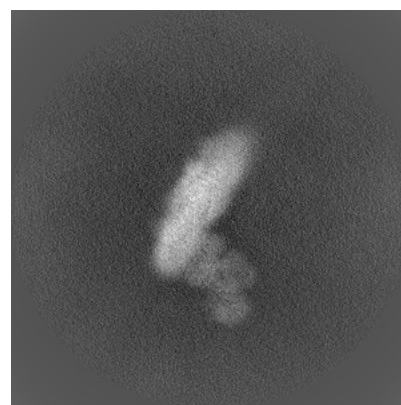
6.1.2 Raw map



X



Y

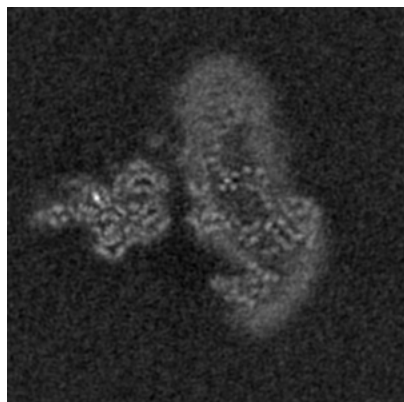


Z

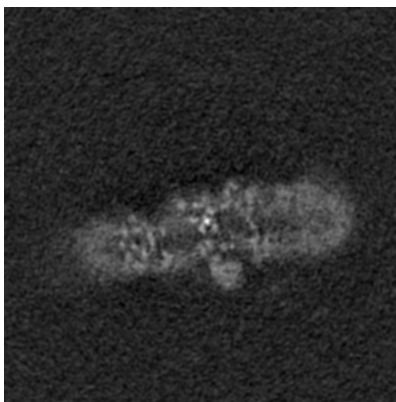
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

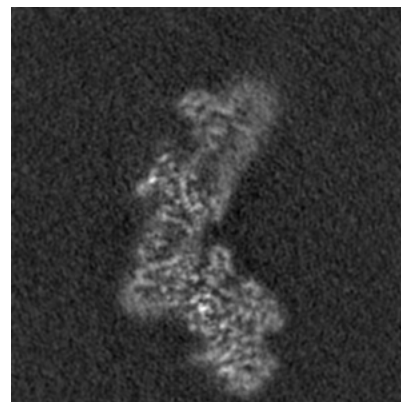
6.2.1 Primary map



X Index: 187

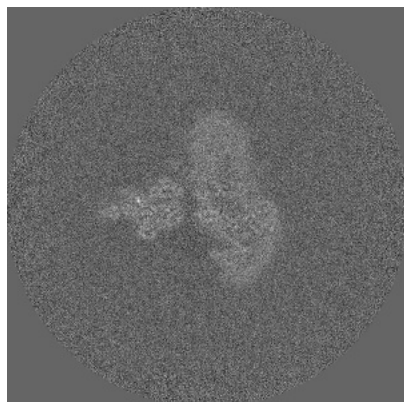


Y Index: 187

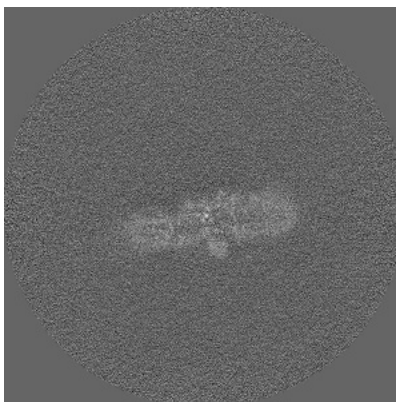


Z Index: 187

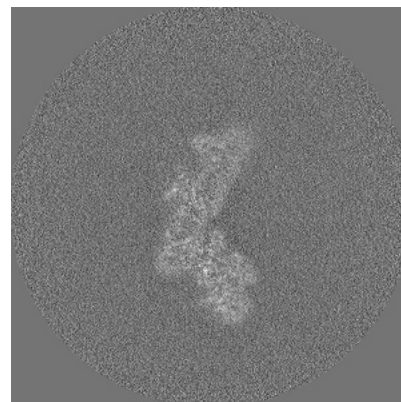
6.2.2 Raw map



X Index: 300



Y Index: 300

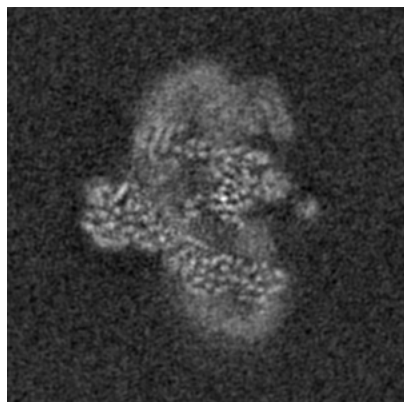


Z Index: 300

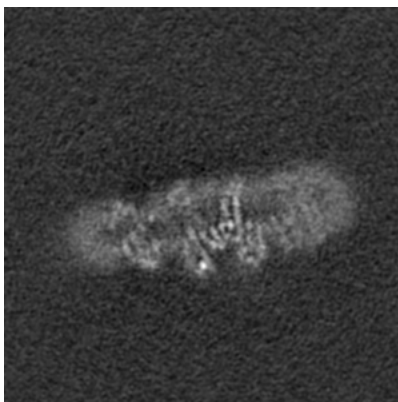
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

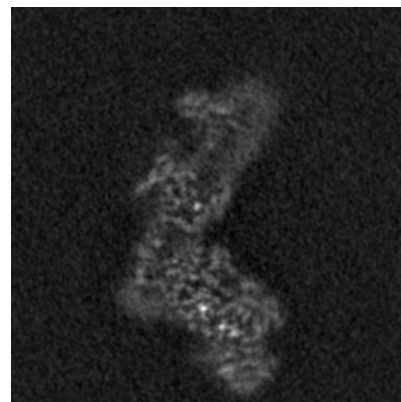
6.3.1 Primary map



X Index: 161

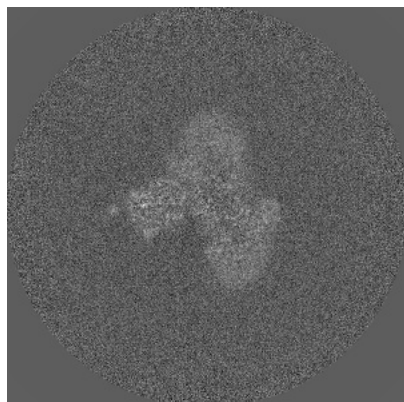


Y Index: 212

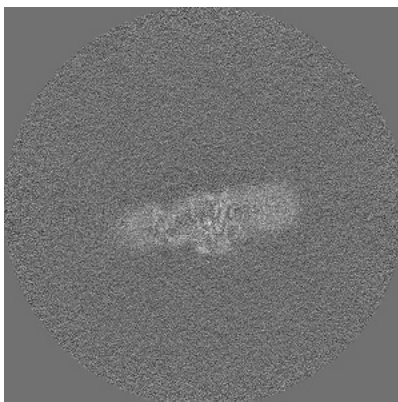


Z Index: 189

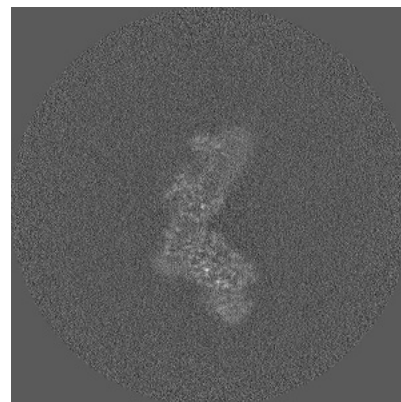
6.3.2 Raw map



X Index: 291



Y Index: 317



Z Index: 302

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

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

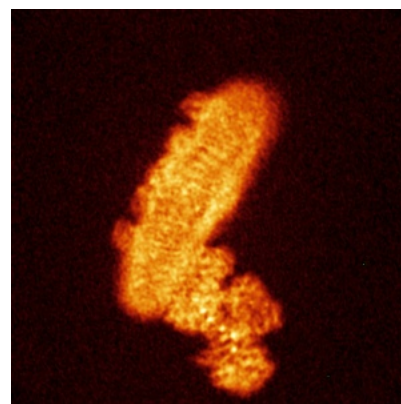
6.4.1 Primary map



X

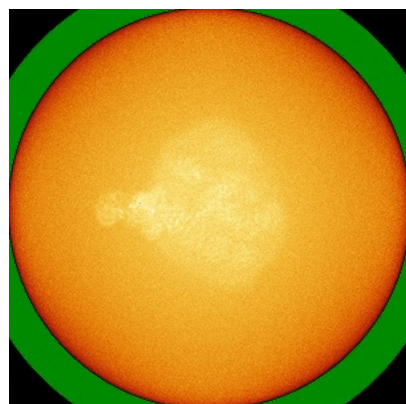


Y

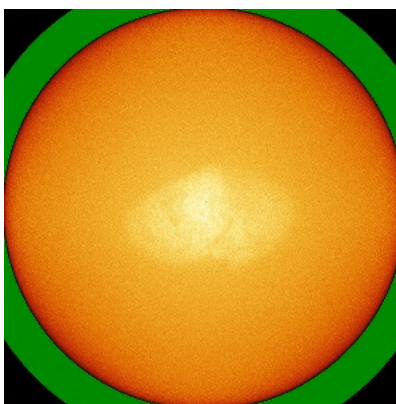


Z

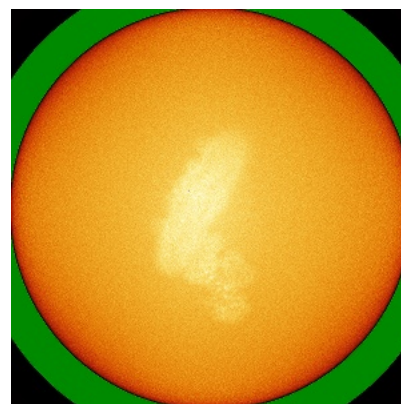
6.4.2 Raw map



X



Y

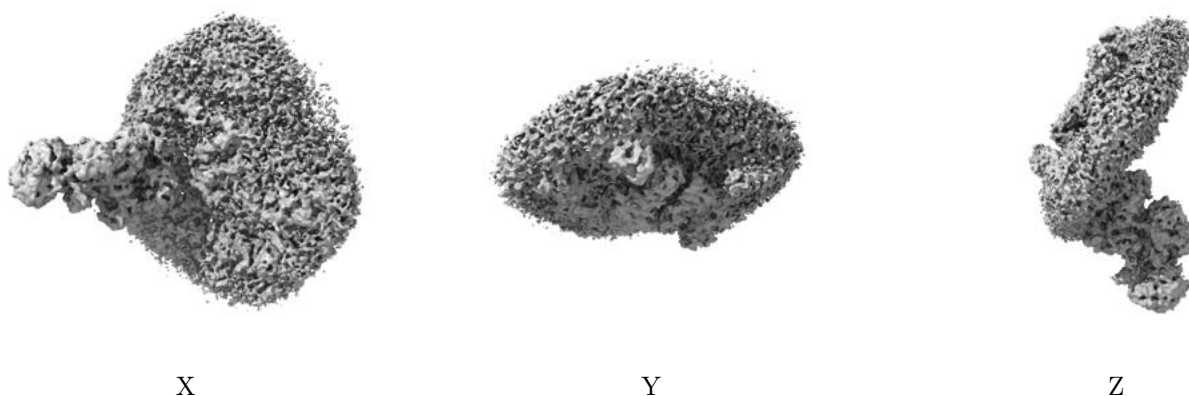


Z

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.

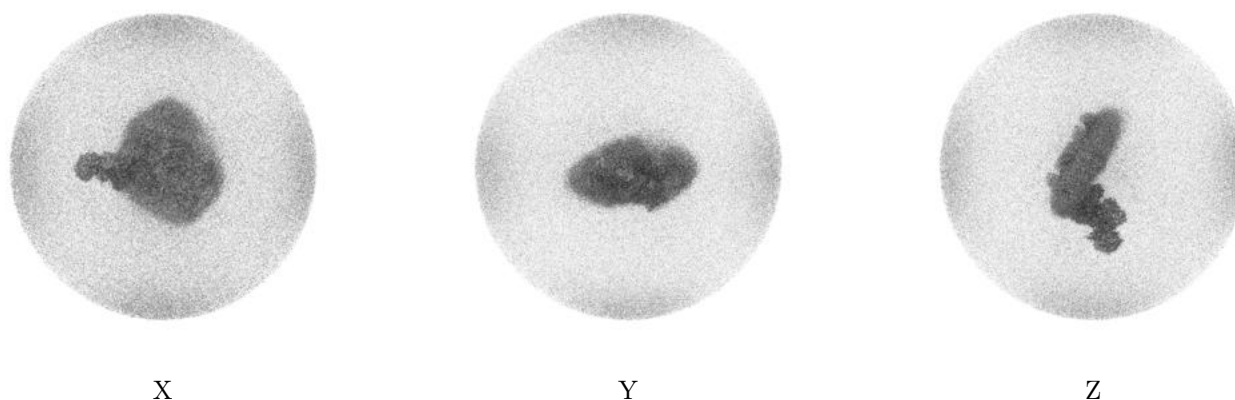
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0112. 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.

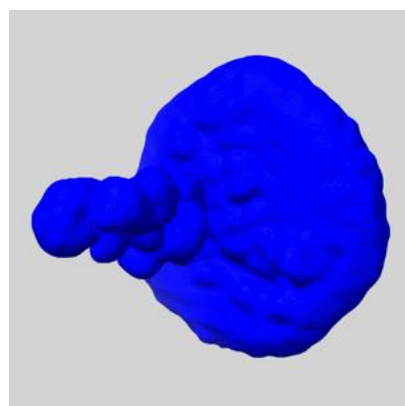
6.6 Mask visualisation [i](#)

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

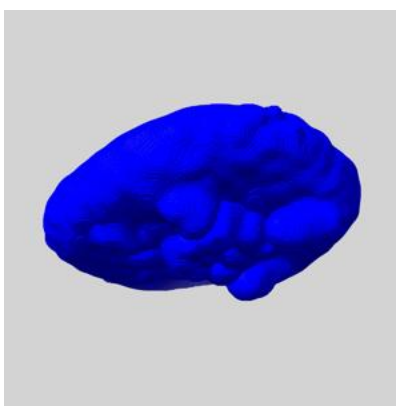
A mask typically either:

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

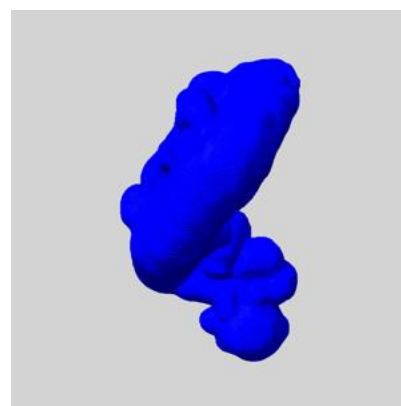
6.6.1 emd_51125_msk_1.map [i](#)



X



Y

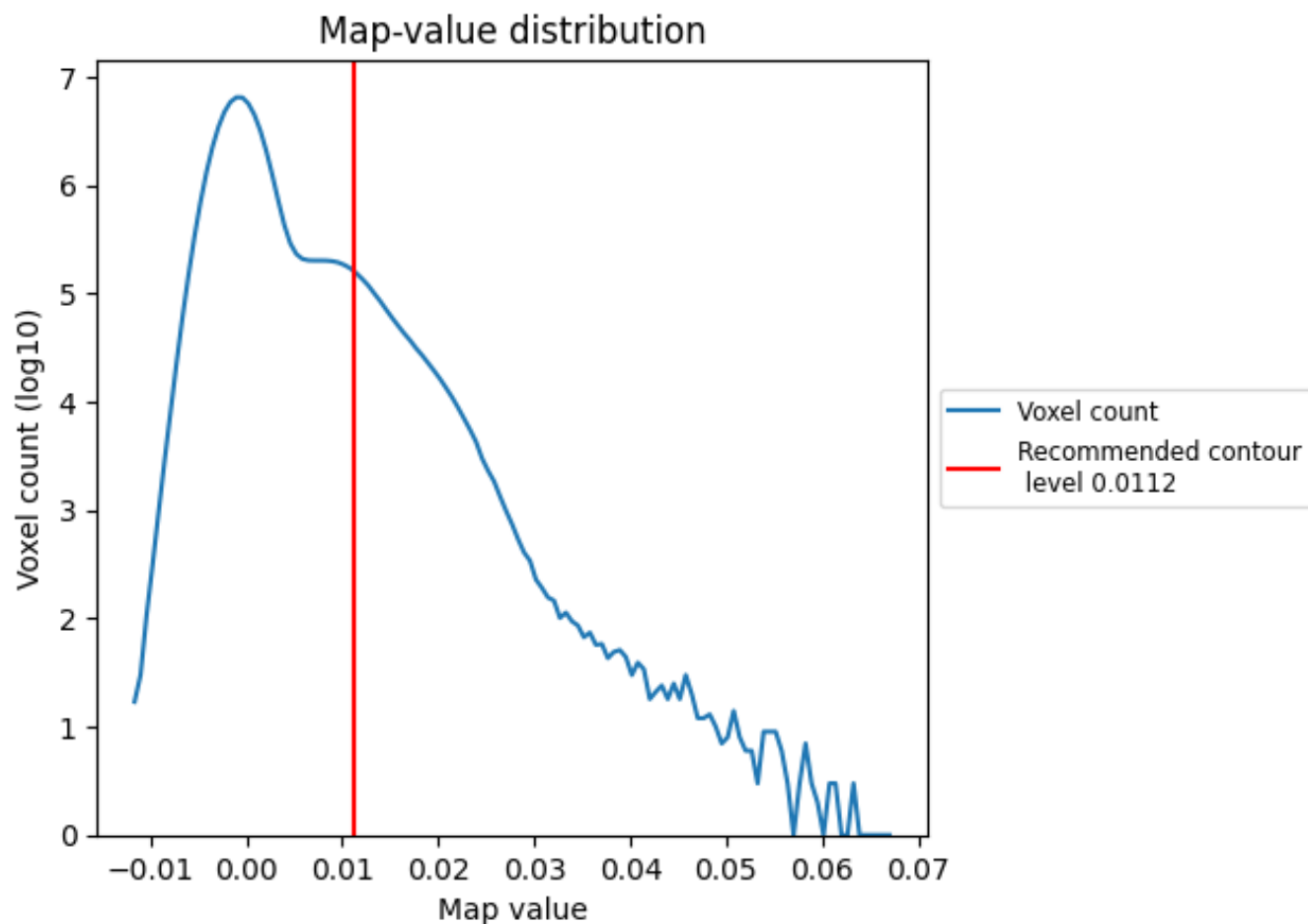


Z

7 Map analysis [i](#)

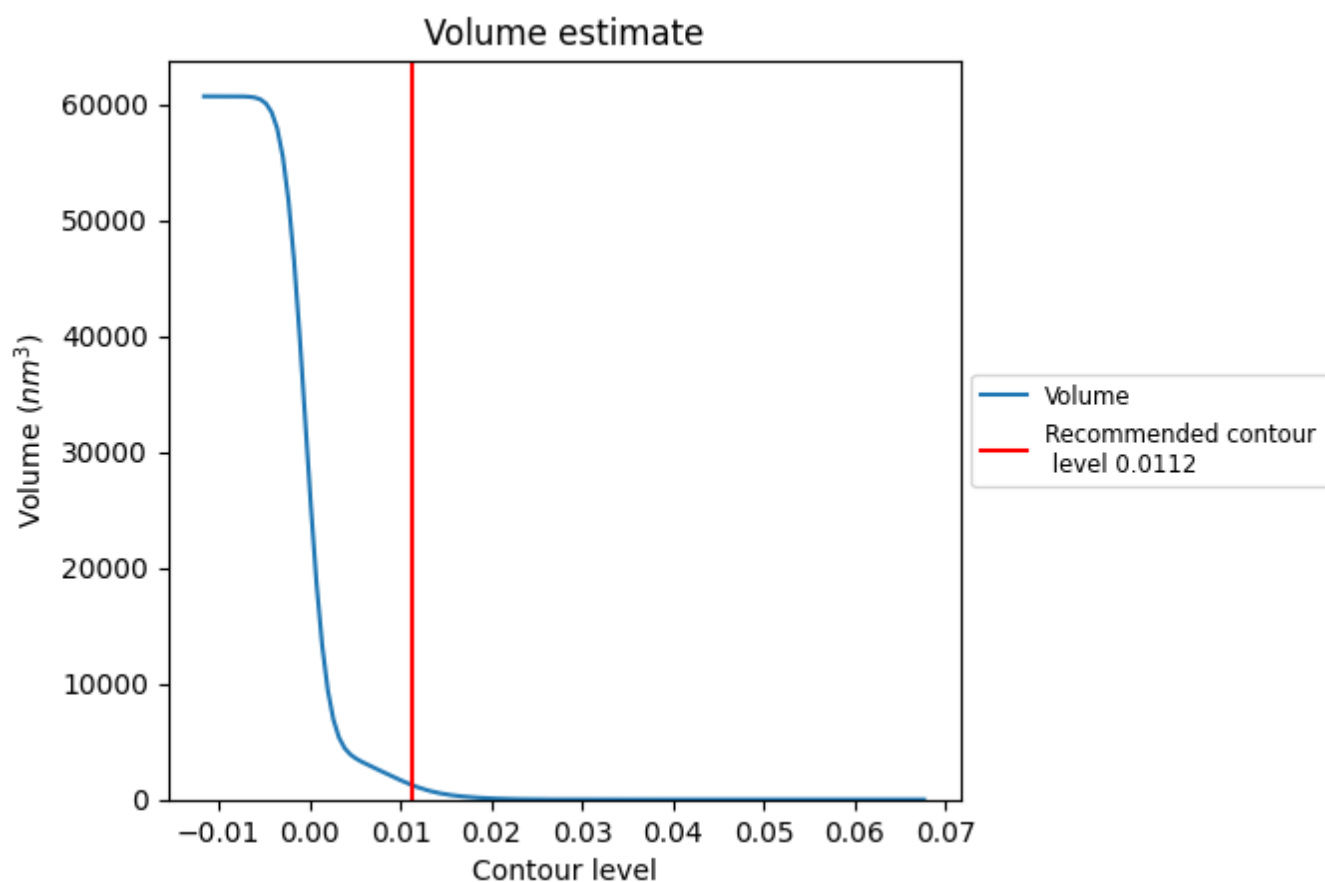
This section contains the results of statistical analysis of the map.

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.

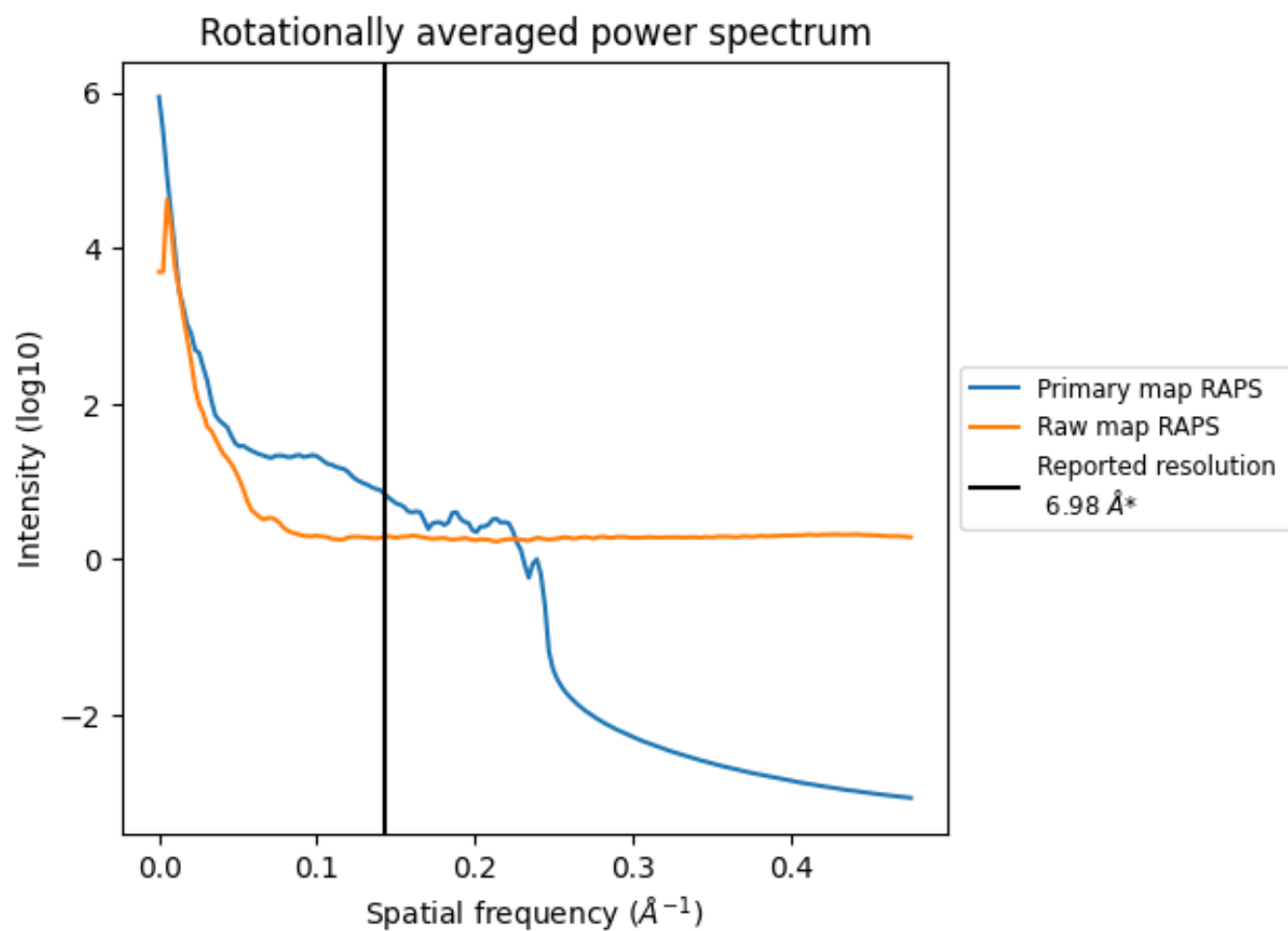
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1272 nm³; this corresponds to an approximate mass of 1149 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

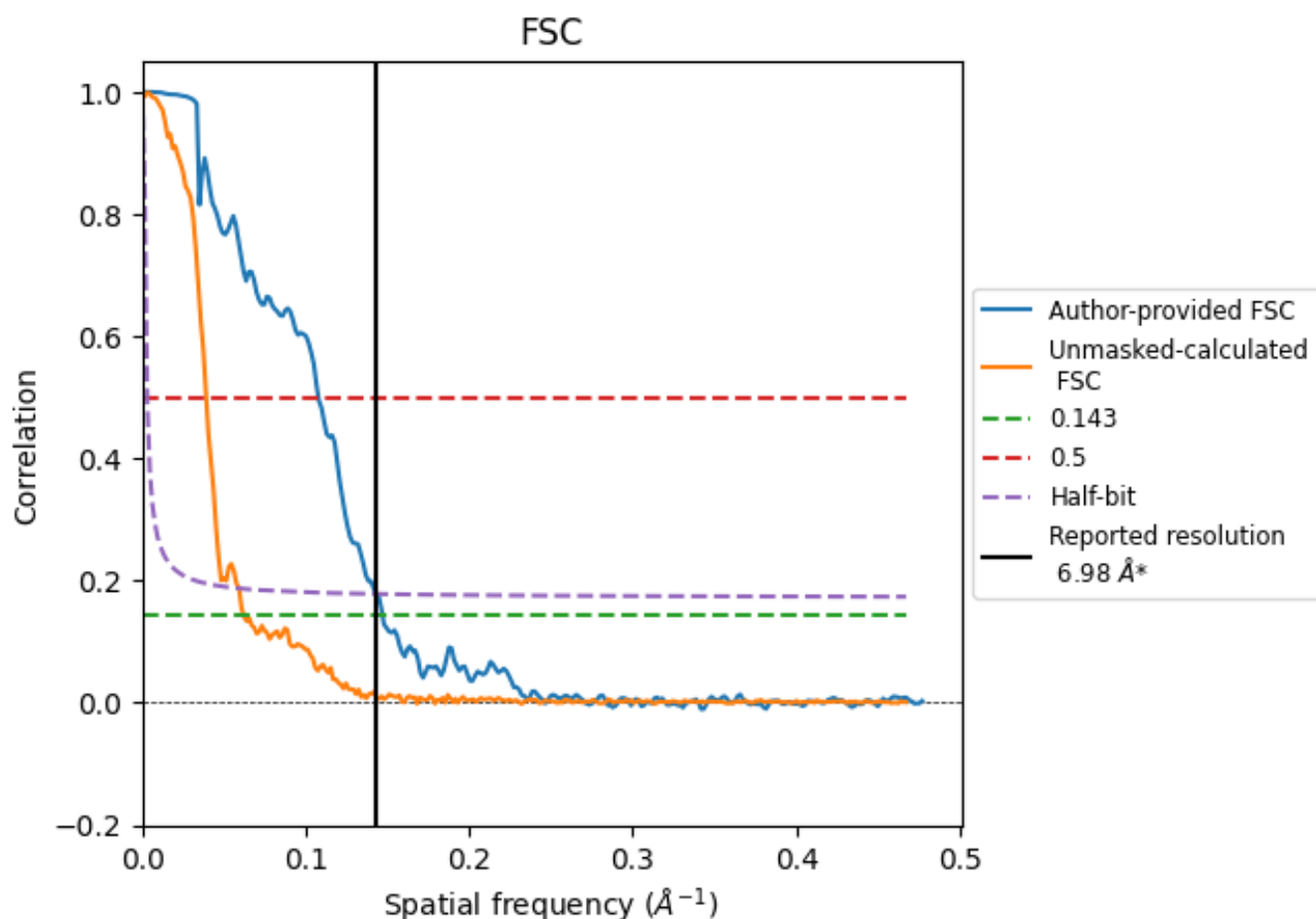


*Reported resolution corresponds to spatial frequency of 0.143 Å⁻¹

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 0.143 Å⁻¹

8.2 Resolution estimates [i](#)

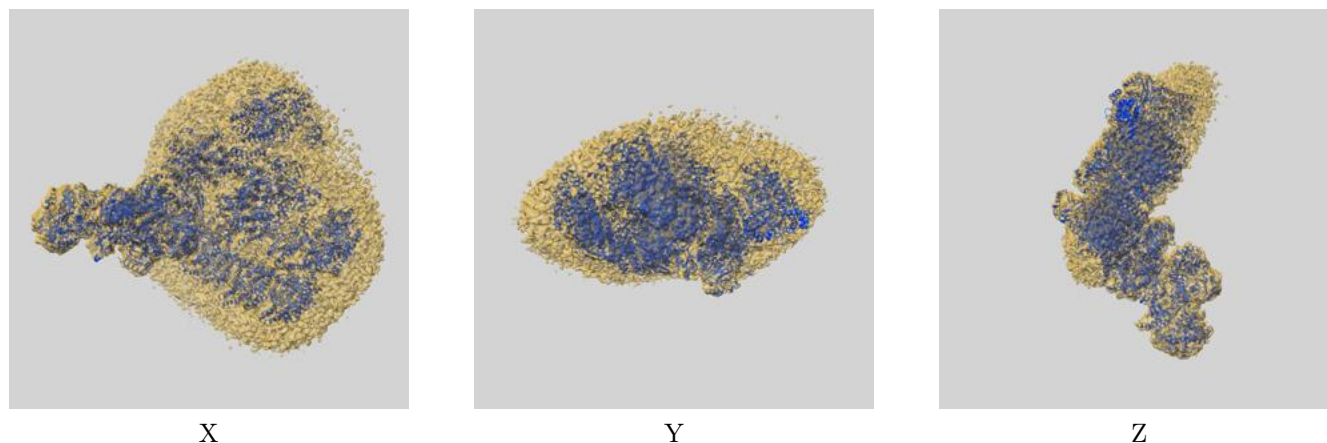
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.98	-	-
Author-provided FSC curve	6.80	9.28	7.00
Unmasked-calculated*	16.10	25.51	16.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 16.10 differs from the reported value 6.98 by more than 10 %

9 Map-model fit [i](#)

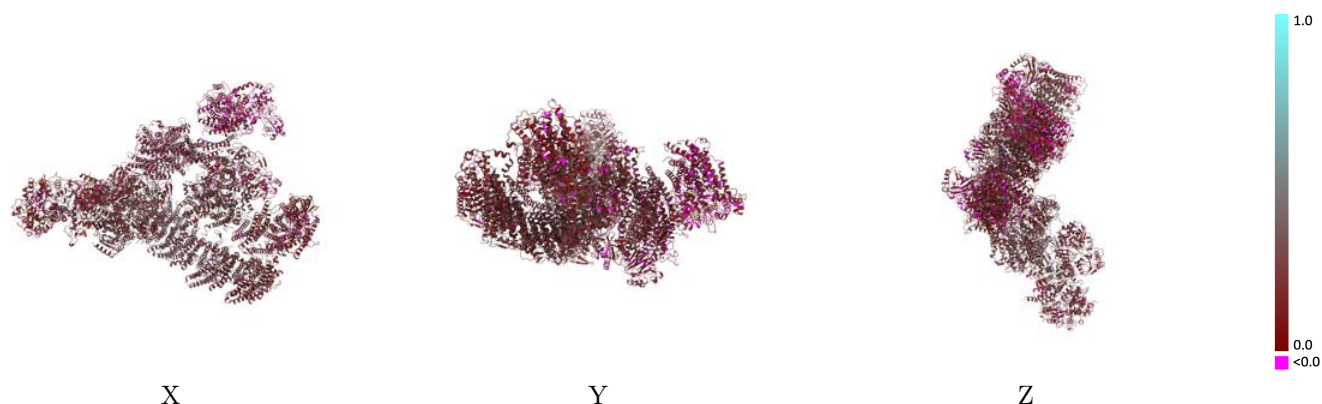
This section contains information regarding the fit between EMDB map EMD-51125 and PDB model 9G83. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



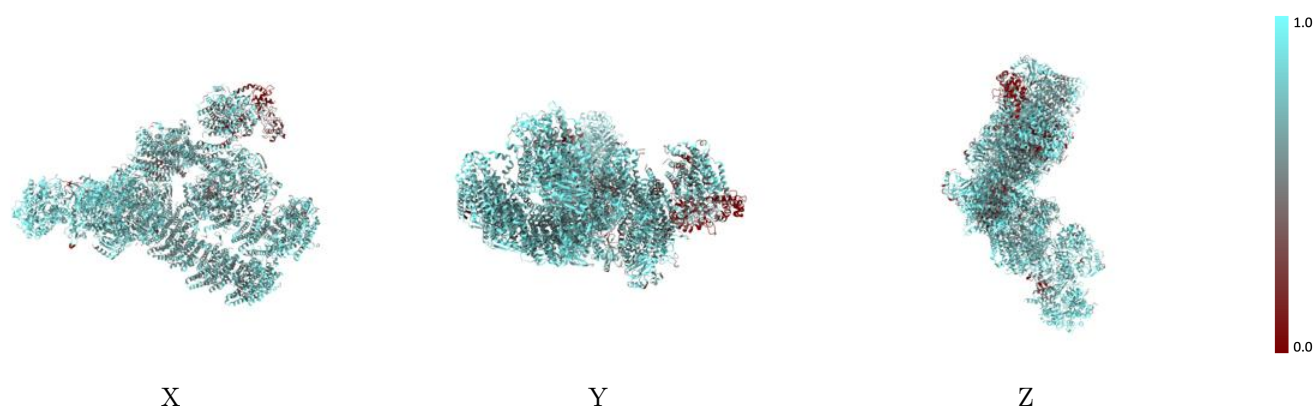
The images above show the 3D surface view of the map at the recommended contour level 0.0112 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



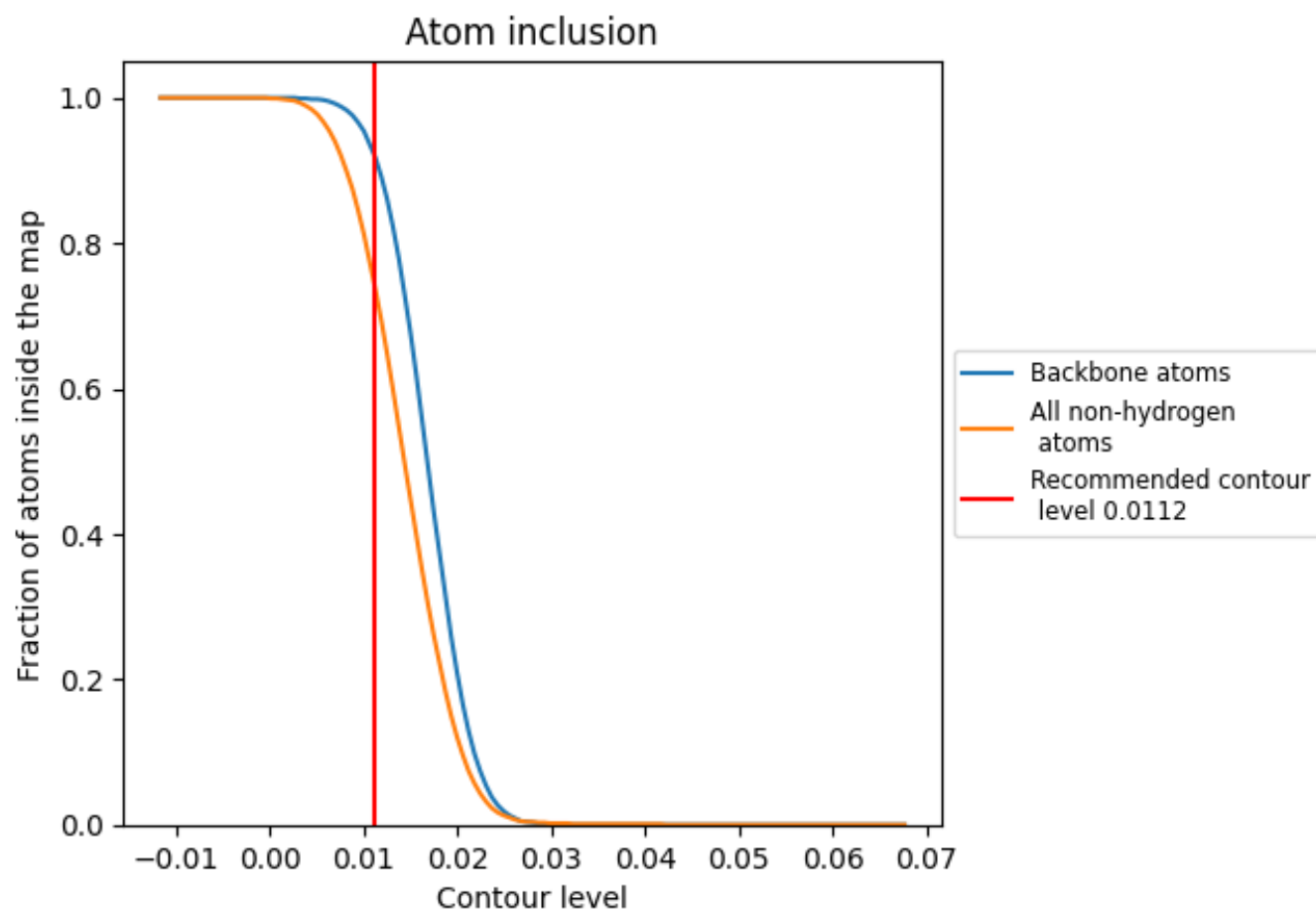
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0112).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ













The table lists the average atom inclusion at the recommended contour level (0.0112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7400	 0.2190
A	 0.7070	 0.2590
B	 0.7640	 0.2810
C	 0.7940	 0.2760
D	 0.7920	 0.2700
E	 0.8590	 0.2200
F	 0.8530	 0.2020
G	 0.8140	 0.2320
H	 0.7300	 0.2420
I	 0.8550	 0.2580
J	 0.7270	 0.2570
K	 0.7030	 0.2550
L	 0.7610	 0.2170
M	 0.7420	 0.2310
N	 0.7380	 0.2480
P	 0.7200	 0.2360
Q	 0.8440	 0.2770
R	 0.2860	 0.1840
Z	 0.7790	 0.2680
a	 0.7260	 0.2660
b	 0.7850	 0.2630
c	 0.7350	 0.1860
d	 0.7230	 0.2330
e	 0.7540	 0.2350
f	 0.7440	 0.1820
g	 0.7550	 0.1920
h	 0.7760	 0.1950
i	 0.7430	 0.2300
j	 0.6380	 0.2070
k	 0.7330	 0.1500
l	 0.7490	 0.1600
m	 0.7420	 0.1970
n	 0.6050	 0.2350
o	 0.7600	 0.2460
p	 0.8210	 0.2660



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Chain	Atom inclusion	Q-score
q	 0.8700	 0.2690
r	 0.6110	 0.2760
s	 0.6670	 0.2530
t	 0.6650	 0.1390
u	 0.5620	 0.1420
v	 0.3370	 0.1440