



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 11:42 PM EDT

PDB ID : 8E7S / pdb_00008e7s
EMDB ID : EMD-27940
Title : III2IV2 respiratory supercomplex from *Saccharomyces cerevisiae* with 4 bound UQ6
Authors : Hryc, C.F.; Mileykovskaya, E.; Baker, M.; Dowhan, W.
Deposited on : 2022-08-24
Resolution : 3.20 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.dev133
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) : 2.50

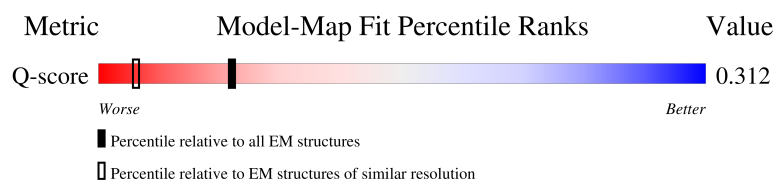
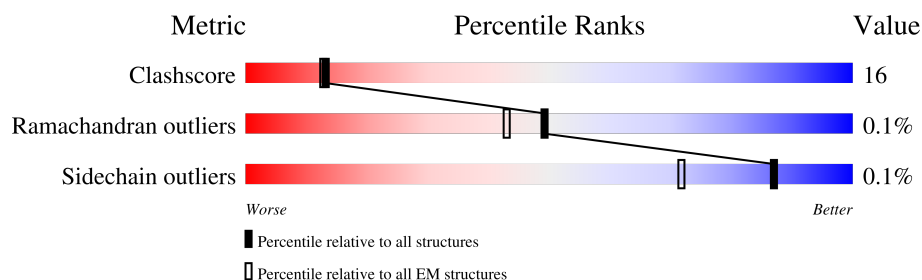
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

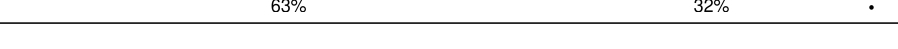
The reported resolution of this entry is 3.20 Å.

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	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	A	457	
1	a	457	
2	B	368	
2	b	368	

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Mol	Chain	Length	Quality of chain
3	C	215	
3	c	215	
4	D	77	
4	d	77	
5	E	66	
5	e	66	
6	F	127	
6	f	127	
7	G	147	
7	g	147	
8	H	94	
8	h	94	
9	J	385	
9	j	385	
10	K	534	
10	k	534	
11	L	309	
11	l	309	
12	M	78	
12	m	78	
13	N	60	
13	n	60	
14	O	269	
14	o	269	
15	P	251	

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Mol	Chain	Length	Quality of chain
15	p	251	
16	Q	148	
16	q	148	
17	R	59	
17	r	59	
18	S	129	
18	s	129	
19	T	155	
19	t	155	
20	U	83	
20	u	83	
21	V	66	
21	v	66	
22	W	153	
22	w	153	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	FES	C	301	-	-	X	-
24	FES	c	301	-	-	X	-
25	CDL	C	302	X	-	-	-
25	CDL	H	601	X	-	-	-
25	CDL	J	403	X	-	-	-
25	CDL	K	603	X	-	-	-
25	CDL	L	402	X	-	-	-
25	CDL	c	302	X	-	-	-
25	CDL	h	601	X	-	-	-
25	CDL	h	602	X	-	-	-
25	CDL	j	402	X	-	-	-
25	CDL	k	602	X	-	-	-

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 62847 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

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

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

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

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

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

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	66	Total	C	N	O	S	0	0
			521	344	84	91	2		
4	d	66	Total	C	N	O	S	0	0
			521	344	84	91	2		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

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

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7, mitochondrial.

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

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	75	Total	C	N	O	S	0	0
			633	396	109	126	2		
7	g	75	Total	C	N	O	S	0	0
			633	396	109	126	2		

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

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

- Molecule 9 is a protein called Cytochrome b.

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

- Molecule 10 is a protein called Cytochrome c oxidase subunit 1.

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

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

- Molecule 11 is a protein called Cytochrome c1, heme protein, mitochondrial.

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

- Molecule 12 is a protein called Cytochrome c oxidase subunit 8, mitochondrial.

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

- Molecule 13 is a protein called Cytochrome c oxidase subunit 7, mitochondrial.

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

- Molecule 14 is a protein called Cytochrome c oxidase subunit 3.

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

- Molecule 15 is a protein called Cytochrome c oxidase subunit 2.

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

- Molecule 16 is a protein called Cytochrome c oxidase subunit 6, mitochondrial.

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

- Molecule 17 is a protein called Cytochrome c oxidase subunit 9, mitochondrial.

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

- Molecule 18 is a protein called Cytochrome c oxidase subunit 13, mitochondrial.

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

- Molecule 19 is a protein called Cytochrome c oxidase subunit 4, mitochondrial.

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

- Molecule 20 is a protein called Cytochrome c oxidase subunit 12, mitochondrial.

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

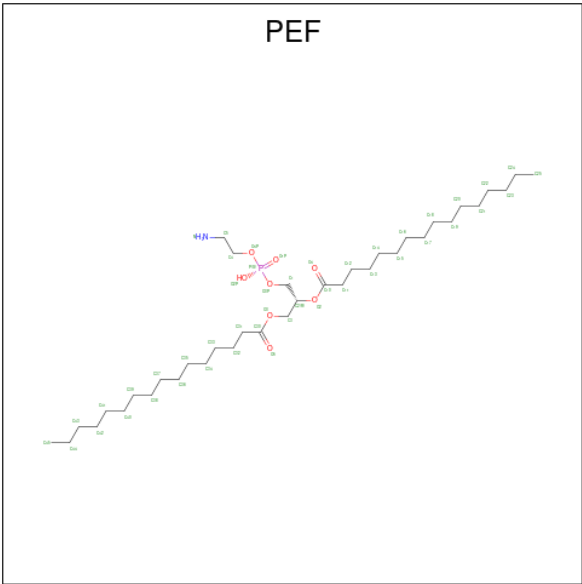
- Molecule 21 is a protein called Cytochrome c oxidase subunit 26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	45	Total	C	N	O	S	0	0
			361	238	63	59	1		
21	v	45	Total	C	N	O	S	0	0
			361	238	63	59	1		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

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

- Molecule 23 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: C₃₇H₇₄NO₈P) (labeled as "Ligand of Interest" by depositor).



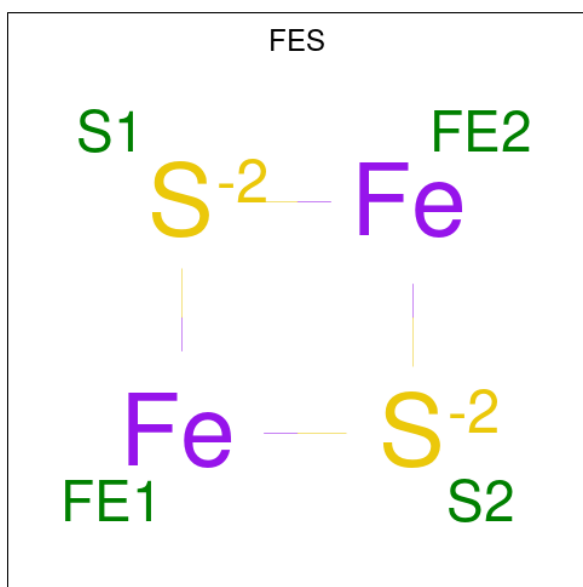
Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
23	A	1	Total	C	N	O	P	0
			31	21	1	8	1	
23	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
23	C	1	Total	C	N	O	P	0
			29	19	1	8	1	
23	C	1	Total	C	N	O	P	0
			32	22	1	8	1	

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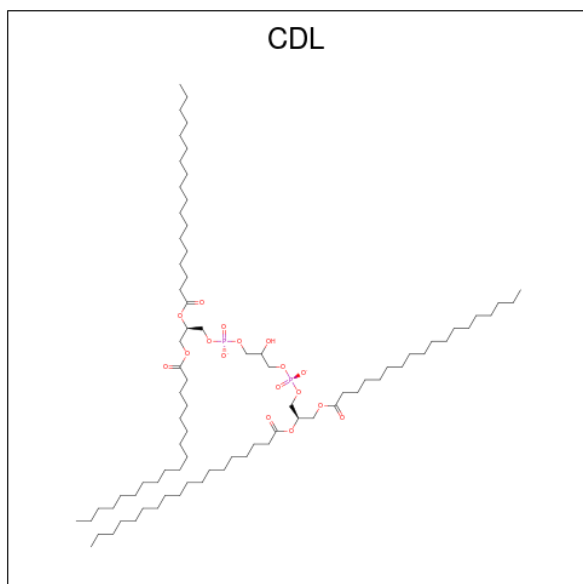
Mol	Chain	Residues	Atoms					AltConf
23	E	1	Total	C	N	O	P	0
			32	22	1	8	1	
23	J	1	Total	C	N	O	P	0
			45	35	1	8	1	
23	J	1	Total	C	N	O	P	0
			43	33	1	8	1	
23	J	1	Total	C	N	O	P	0
			29	19	1	8	1	
23	V	1	Total	C	N	O	P	0
			33	23	1	8	1	
23	W	1	Total	C	N	O	P	0
			36	26	1	8	1	
23	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
23	a	1	Total	C	N	O	P	0
			40	30	1	8	1	
23	a	1	Total	C	N	O	P	0
			31	21	1	8	1	
23	a	1	Total	C	N	O	P	0
			40	30	1	8	1	
23	c	1	Total	C	N	O	P	0
			29	19	1	8	1	
23	c	1	Total	C	N	O	P	0
			32	22	1	8	1	
23	e	1	Total	C	N	O	P	0
			32	22	1	8	1	
23	j	1	Total	C	N	O	P	0
			45	35	1	8	1	
23	j	1	Total	C	N	O	P	0
			43	33	1	8	1	
23	j	1	Total	C	N	O	P	0
			29	19	1	8	1	
23	v	1	Total	C	N	O	P	0
			33	23	1	8	1	
23	w	1	Total	C	N	O	P	0
			36	26	1	8	1	
23	w	1	Total	C	N	O	P	0
			41	31	1	8	1	

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



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

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



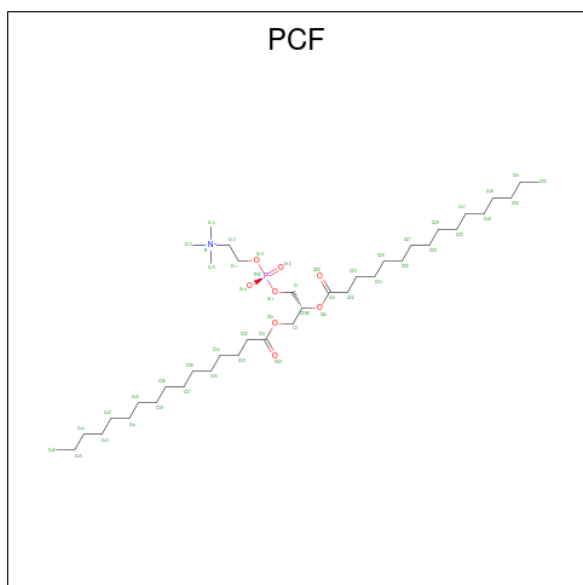
Mol	Chain	Residues	Atoms				AltConf
25	C	1	Total	C	O	P	0
			53	34	17	2	

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Mol	Chain	Residues	Atoms				AltConf
25	H	1	Total	C	O	P	0
			53	34	17	2	
25	J	1	Total	C	O	P	0
			56	37	17	2	
25	K	1	Total	C	O	P	0
			67	48	17	2	
25	L	1	Total	C	O	P	0
			67	48	17	2	
25	c	1	Total	C	O	P	0
			48	29	17	2	
25	h	1	Total	C	O	P	0
			53	34	17	2	
25	h	1	Total	C	O	P	0
			67	48	17	2	
25	j	1	Total	C	O	P	0
			56	37	17	2	
25	k	1	Total	C	O	P	0
			67	48	17	2	

- Molecule 26 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



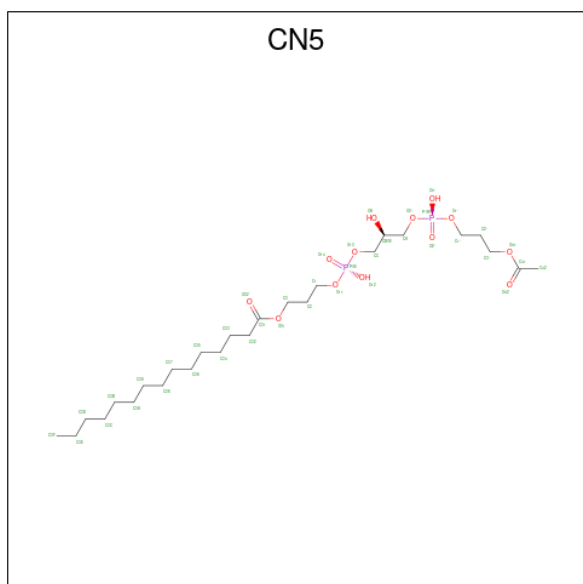
Mol	Chain	Residues	Atoms					AltConf
26	E	1	Total	C	N	O	P	0
			47	37	1	8	1	
26	H	1	Total	C	N	O	P	0
			50	40	1	8	1	

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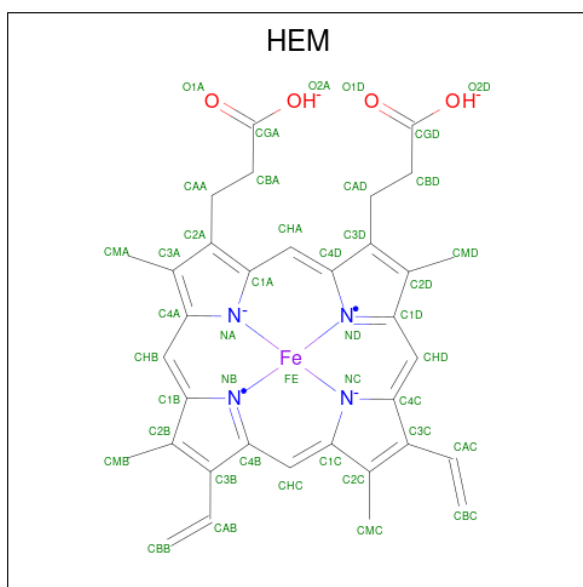
Mol	Chain	Residues	Atoms					AltConf
26	W	1	Total	C	N	O	P	0
			36	26	1	8	1	
26	a	1	Total	C	N	O	P	0
			47	37	1	8	1	
26	k	1	Total	C	N	O	P	0
			36	26	1	8	1	
26	w	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 27 is (5S,11R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-4,6,10,12,16-pentaoxa-5,11-di phosphaoctadec-1-yl pentadecanoate (CCD ID: CN5) (formula: $C_{26}H_{52}O_{13}P_2$).



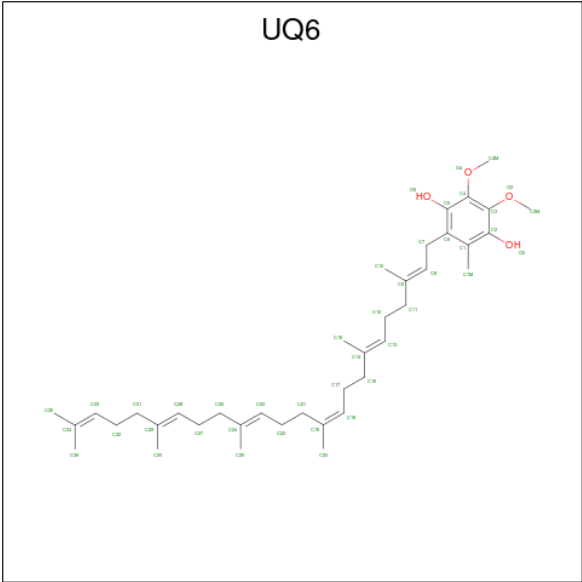
Mol	Chain	Residues	Atoms				AltConf
27	J	1	Total	C	O	P	0
			41	26	13	2	

- Molecule 28 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



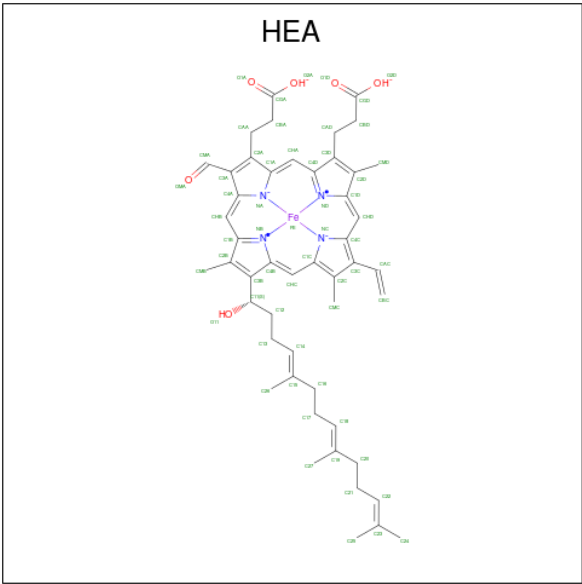
Mol	Chain	Residues	Atoms					AltConf
28	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
28	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
28	L	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
28	j	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
28	j	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
28	l	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 29 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXA ENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: $C_{39}H_{60}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	J	1	Total	C	O	0
			43	39	4	
29	J	1	Total	C	O	0
			20	16	4	
29	j	1	Total	C	O	0
			43	39	4	
29	j	1	Total	C	O	0
			43	39	4	

- Molecule 30 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

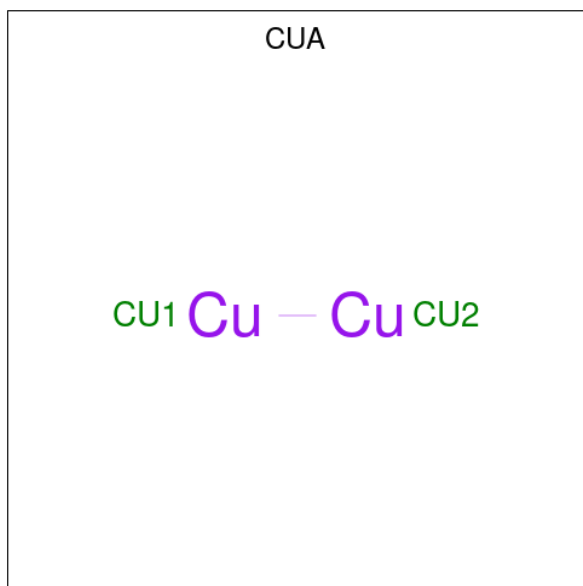


Mol	Chain	Residues	Atoms					AltConf
30	K	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
30	K	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
30	k	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
30	k	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 31 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
31	K	1	Total	Cu	0
			1	1	
31	k	1	Total	Cu	0
			1	1	

- Molecule 32 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).

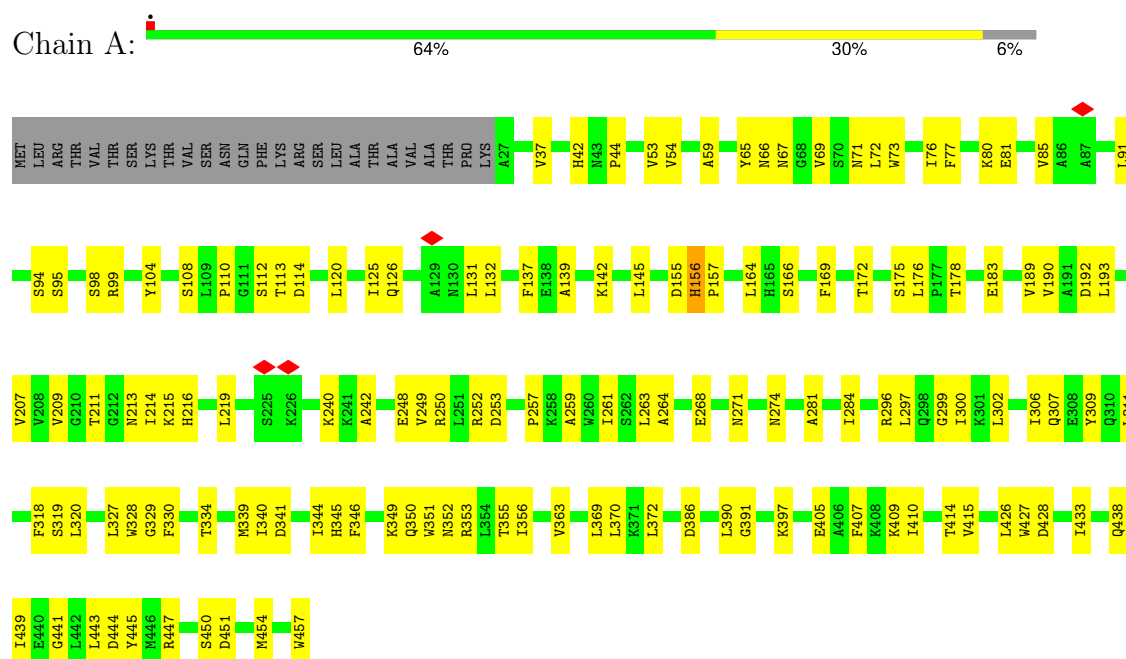


Mol	Chain	Residues	Atoms		AltConf
32	P	1	Total	Cu	0
			1	1	
32	P	1	Total	Cu	0
			1	1	
32	p	1	Total	Cu	0
			1	1	
32	p	1	Total	Cu	0
			1	1	

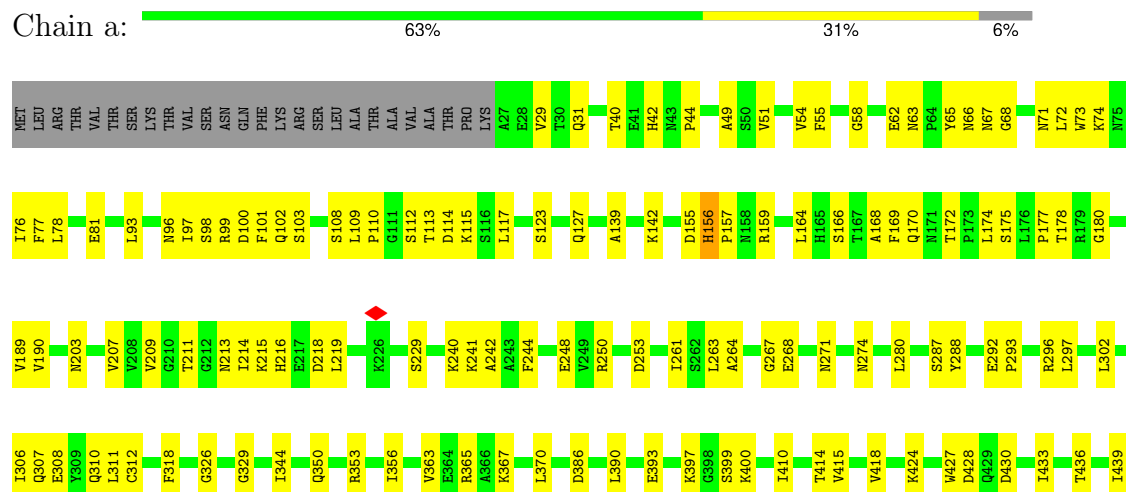
3 Residue-property plots

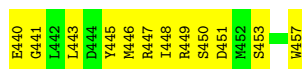
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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



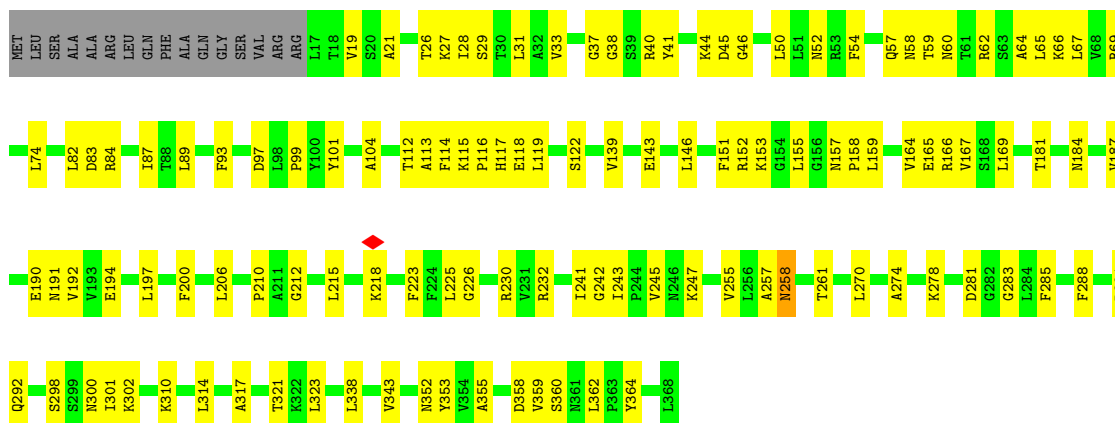
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial





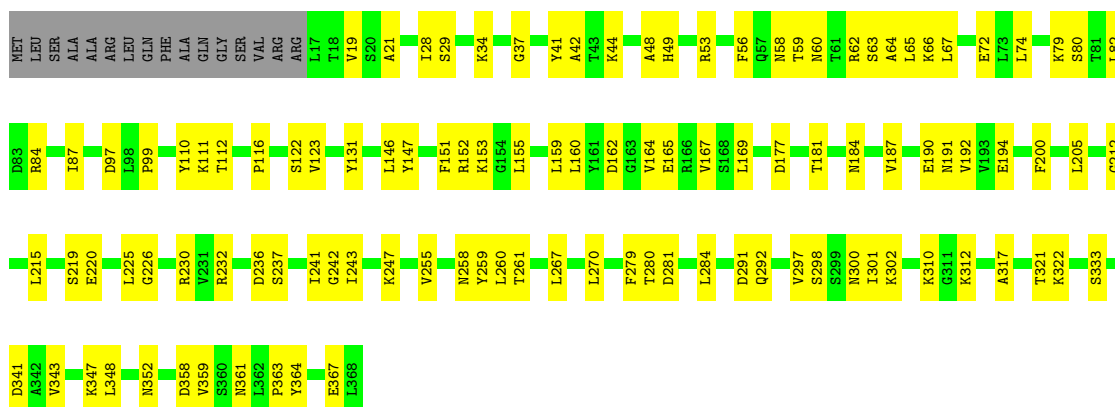
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:  63% 32%



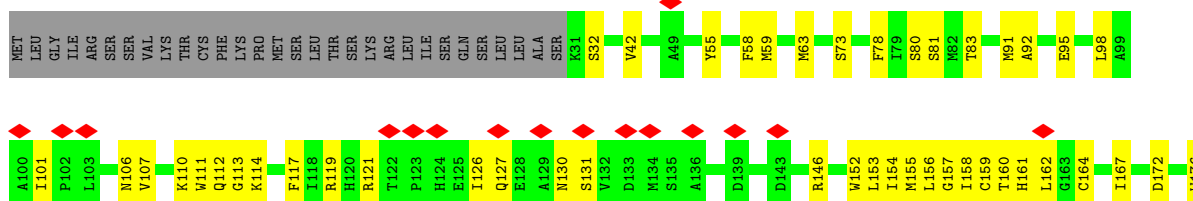
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

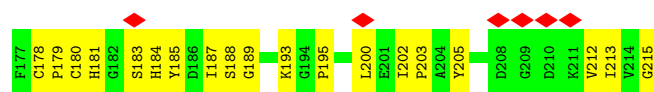
Chain b:  66% 30%



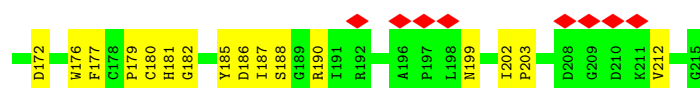
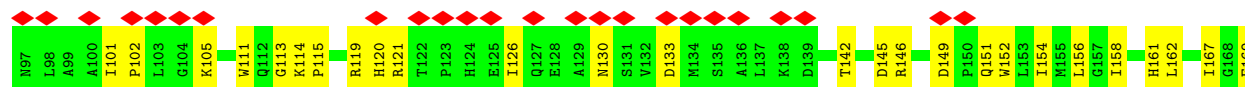
• Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain C:  10% 56% 30% 14%





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



- Molecule 4: Cytochrome b-c1 complex subunit 10, mitochondrial



- Molecule 4: Cytochrome b-c1 complex subunit 10, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit 9, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit 9, mitochondrial

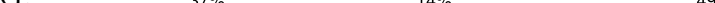


- Molecule 6: Cytochrome b-c1 complex subunit 7, mitochondrial

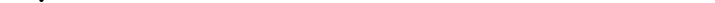
MET	P2	Q3	L16	S22	V26	P27	Y38	L43	L48	E51	E52	N53	M56	Q57	T58	R62	A70	R71	A72	Y73	R74	I75	T84	H85	H86	P101	E116	K117	L120	D121	N122	I123	E124	K127
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- Chain f: 83% 17%

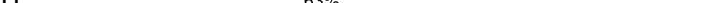
MET
P2
Q3
S4
F5
L3S
K39
D47
R62
Y73
R74
Q80
T81
E82
L83
T84
H85
D99
V100
P101
I107
K117
D118
E119
L120
D121
N122
I123
E124
K127

- Chain G: 

MET	GLY	ASP
MET	ASP	ASP
MET	LEU	ASP
LEU	ASP	ASP
LEU	GLU	ASP
VAL	ASP	ASP
GLY	GLU	GLU
TYR	GLU	GLU
TRP	GLU	GLU
GLN	GLU	E73
LEU	LYS	L78
ILE	THR	K92
VAL	VAL	V95
PRO	VAL	H96
VAL	VAL	E99
ALA	VAL	E100
ALA	ALA	E103
GLU	ASP	I107
ASP	ASP	Q108
ASN	ASP	G109
GLN	ASN	Q110
HIS	GLN	Q111
GLU	HIS	P112
GLU	GLU	G113
LYS	GLU	D116
ALA	LYS	L117
ALA	ALA	E118
GLU	GLU	H119
GLY	GLY	E126
GLU	GLU	F128
LYS	GLU	H129
GLU	GLU	A139
ASN	GLU	P140
GLY	ASN	F141
ASP	GLY	L142
ASP	ASP	F143
ASP	GLU	K147
ASP	ASP	
GLU	GLU	
ASP	ASP	
GLU	GLU	
ASP	ASP	
ASP	ASP	
ASP	ASP	

- Chain g: 

[illegible]

- Chain H:  63% 35%

NET

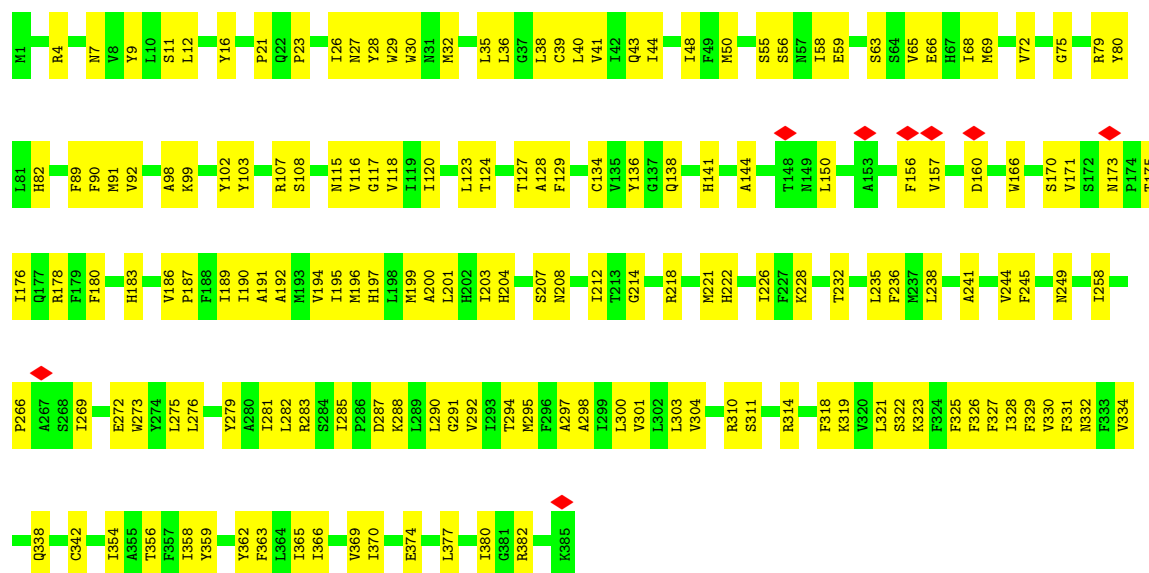
G2 S5 G6 K7 T8 Y9 M10 W13 Q21 I24 Y27 S30 Q34 K35 P36 L37 Q38 G39 I40 F41 H42 V45 Y58 I61 P62 Y66 W70 K71 N72 G73 E75 Y76 M77 L80 Y81 S82 K83 R86 L89 E90 N93 U94

- Chain h: 66% 31% .

MET	G2	K7	W12	W13	G14	H15	M16		Q21		I24		Y27	S30	P36	L37	Q38	G39	I40	N43		N47		R50		Y58		I61		I65	I66	A67	V68	V69	W70	K71	N72	G73	N74	E75		Y81		B86		E90	R91	V92	N93		H94
-----	----	----	-----	-----	-----	-----	-----	--	-----	--	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	--	-----	--	-----	--	-----	--	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	-----	--	-----	--	-----	-----	-----	-----	--	-----

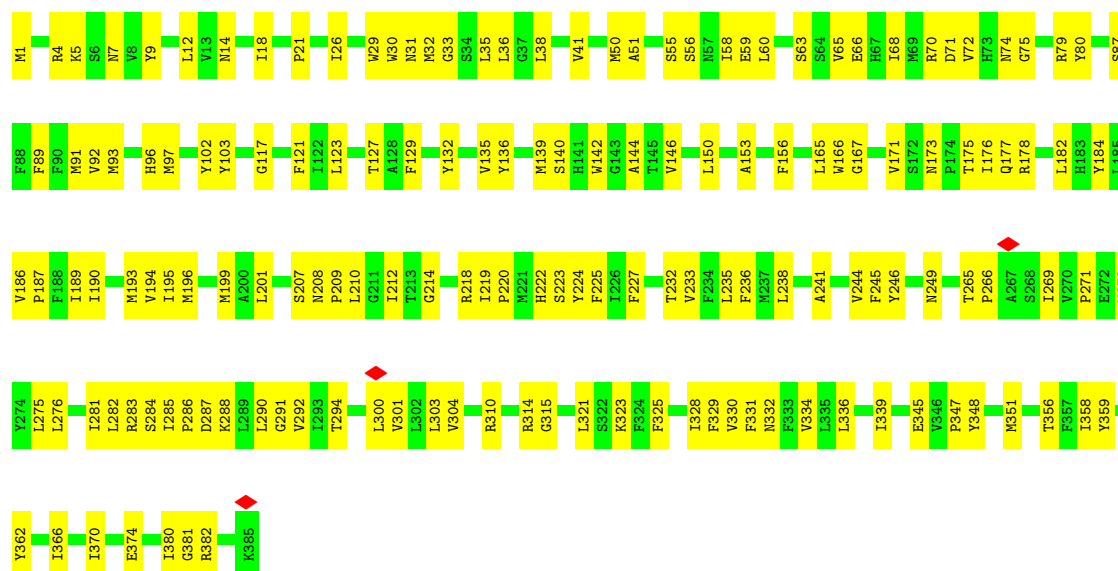
- 

Chain J:  57% 43%



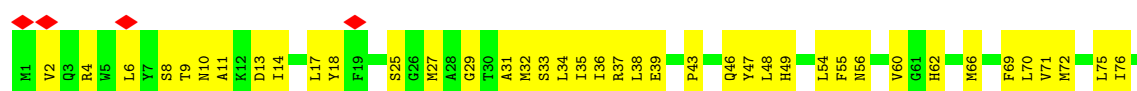
• Molecule 9: Cytochrome b

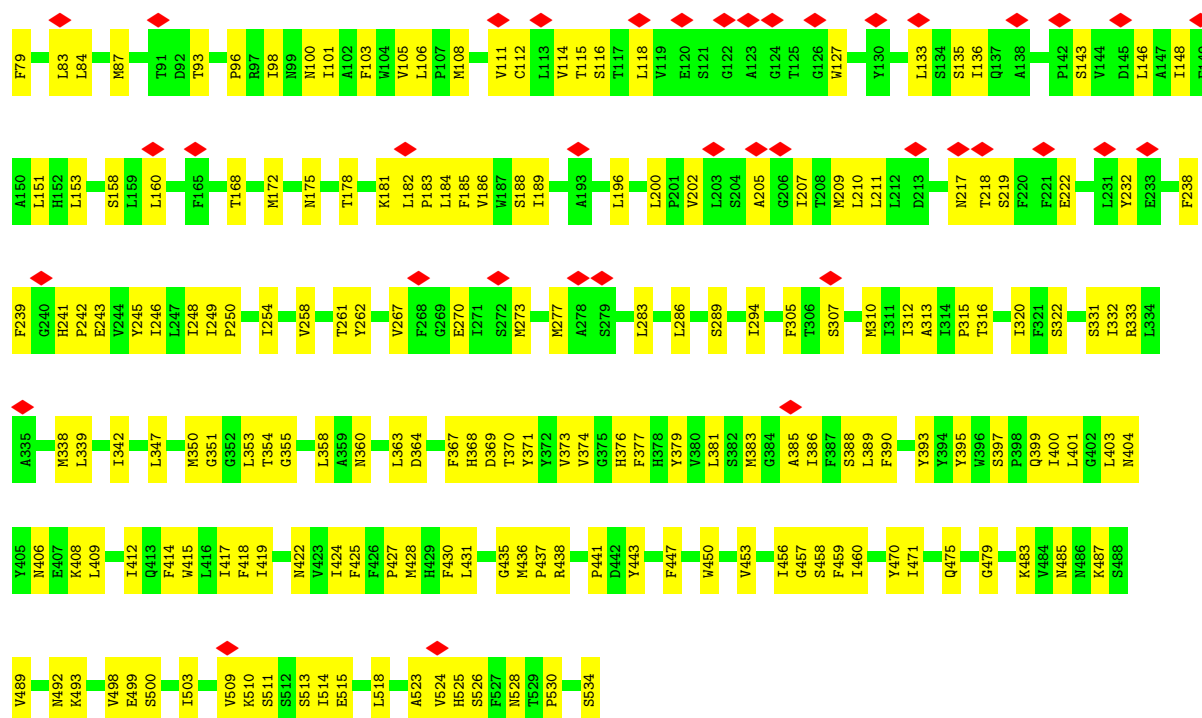
Chain j:  59% 41%



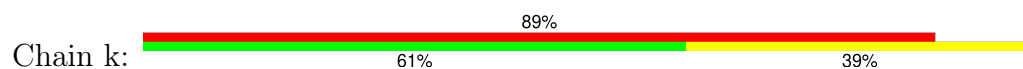
• Molecule 10: Cytochrome c oxidase subunit 1

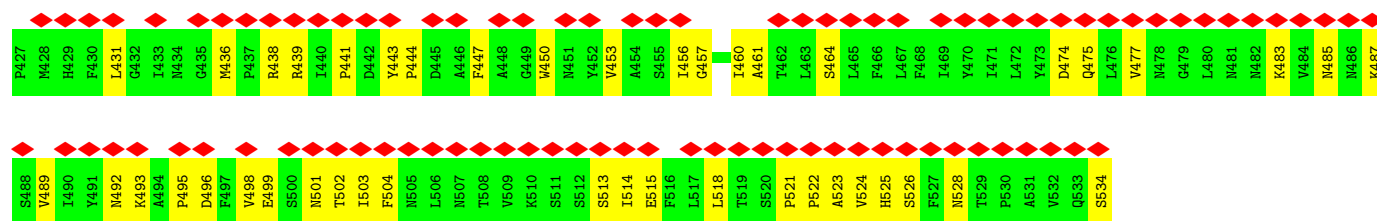
Chain K:  8% 58% 42%





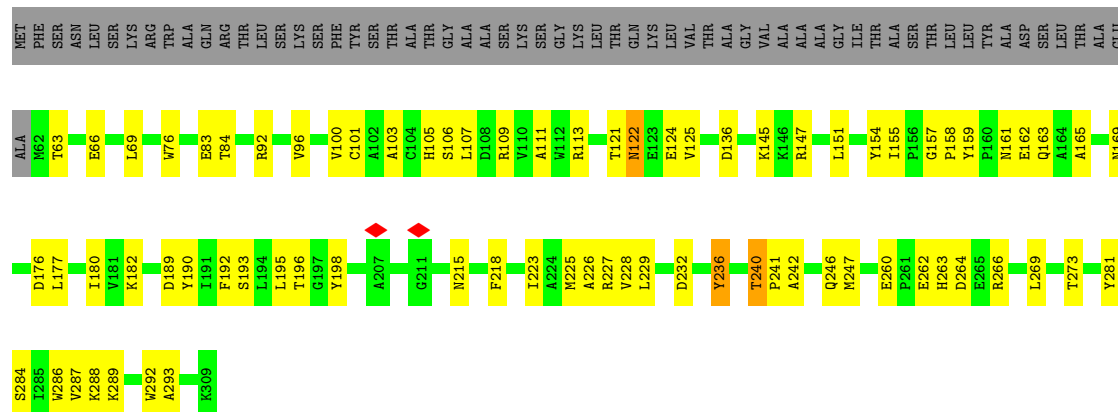
• Molecule 10: Cytochrome c oxidase subunit 1





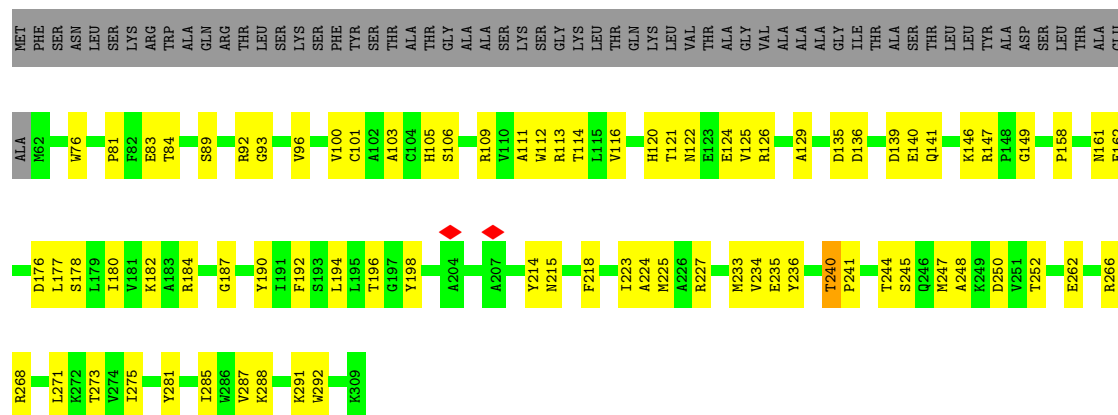
- Molecule 11: Cytochrome c1, heme protein, mitochondrial

Chain L: 56% 24% 20%



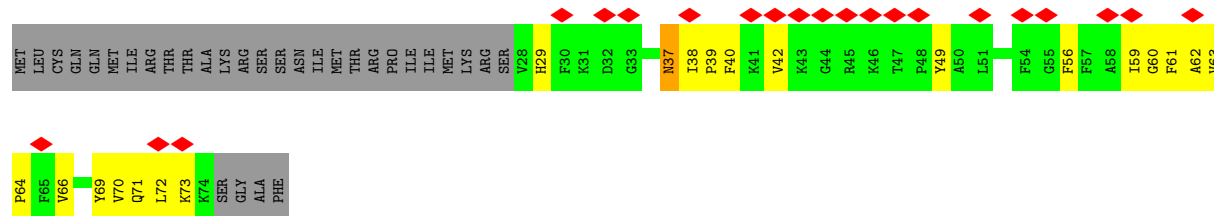
- Molecule 11: Cytochrome c1, heme protein, mitochondrial

Chain I: 54% 26% 20%

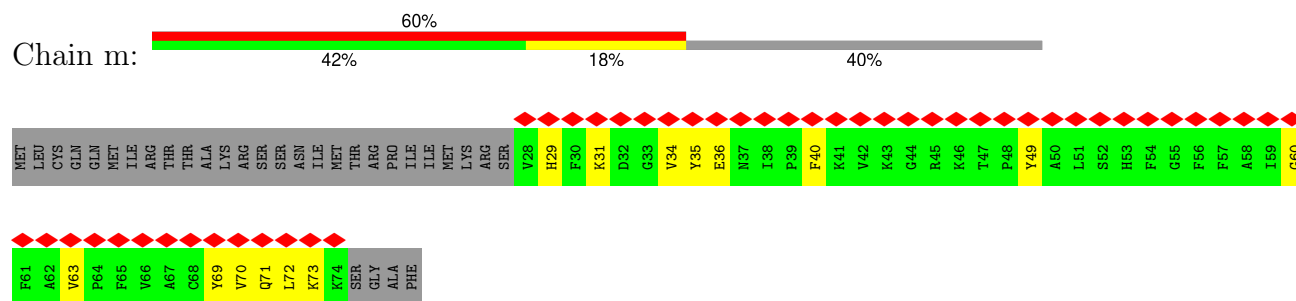


- Molecule 12: Cytochrome c oxidase subunit 8, mitochondrial

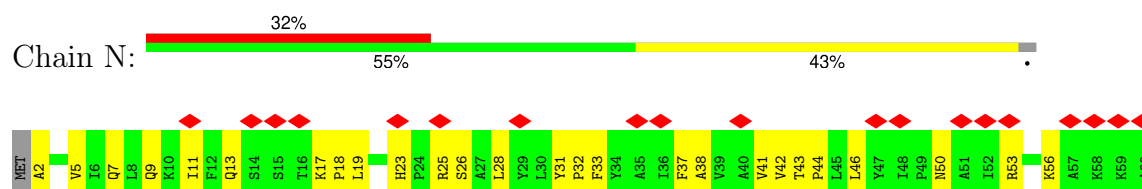
Chain M: 27% 35% 24% 40%



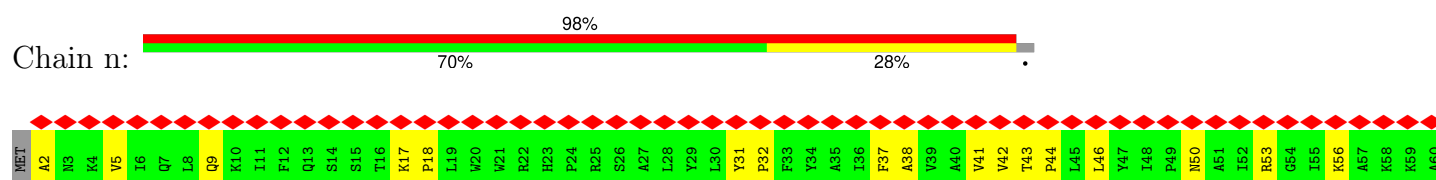
- Molecule 12: Cytochrome c oxidase subunit 8, mitochondrial



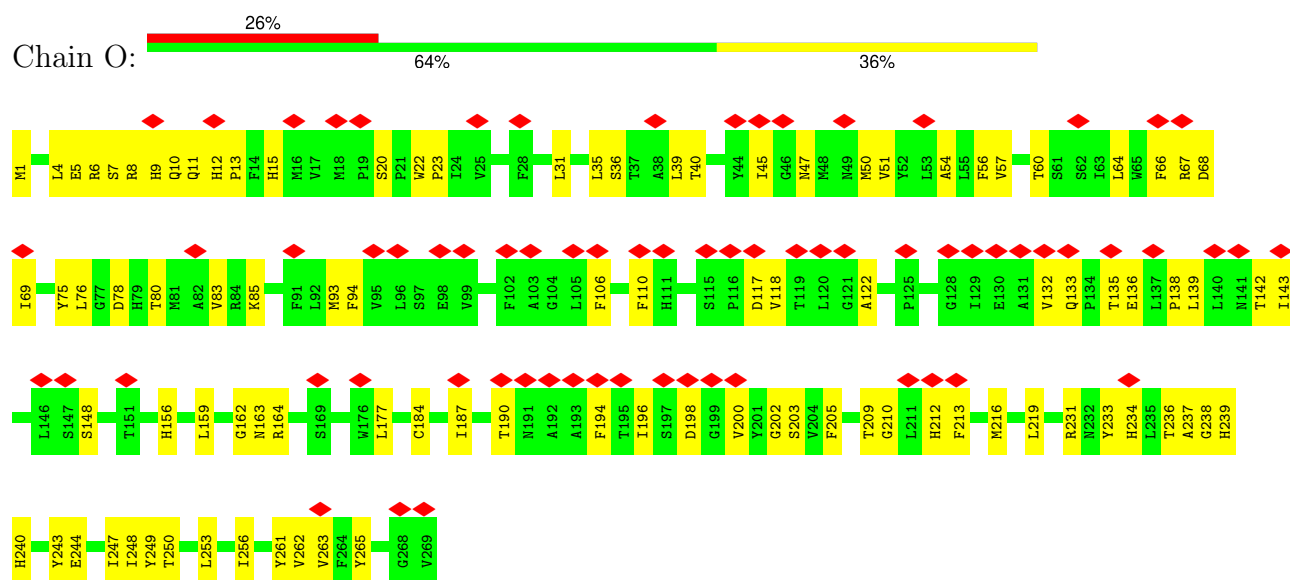
- Molecule 13: Cytochrome c oxidase subunit 7, mitochondrial



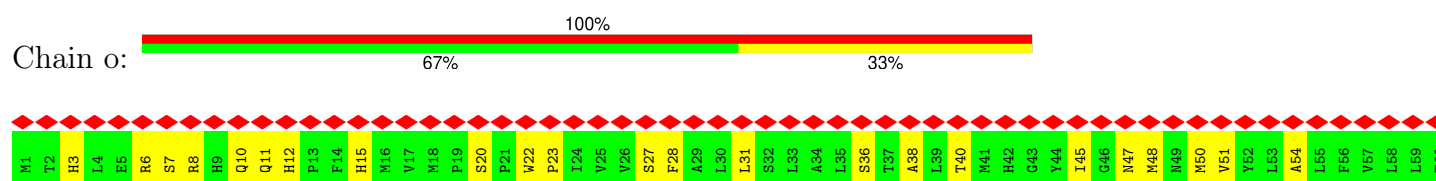
- Molecule 13: Cytochrome c oxidase subunit 7, mitochondrial



- Molecule 14: Cytochrome c oxidase subunit 3

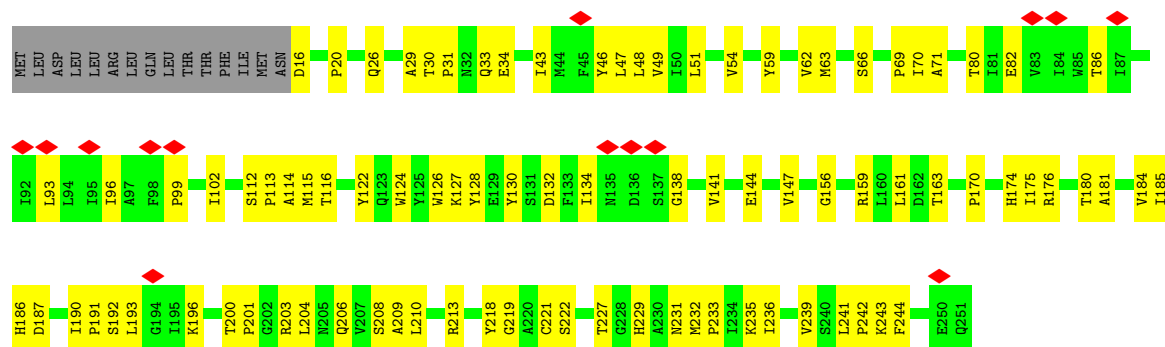


- Molecule 14: Cytochrome c oxidase subunit 3

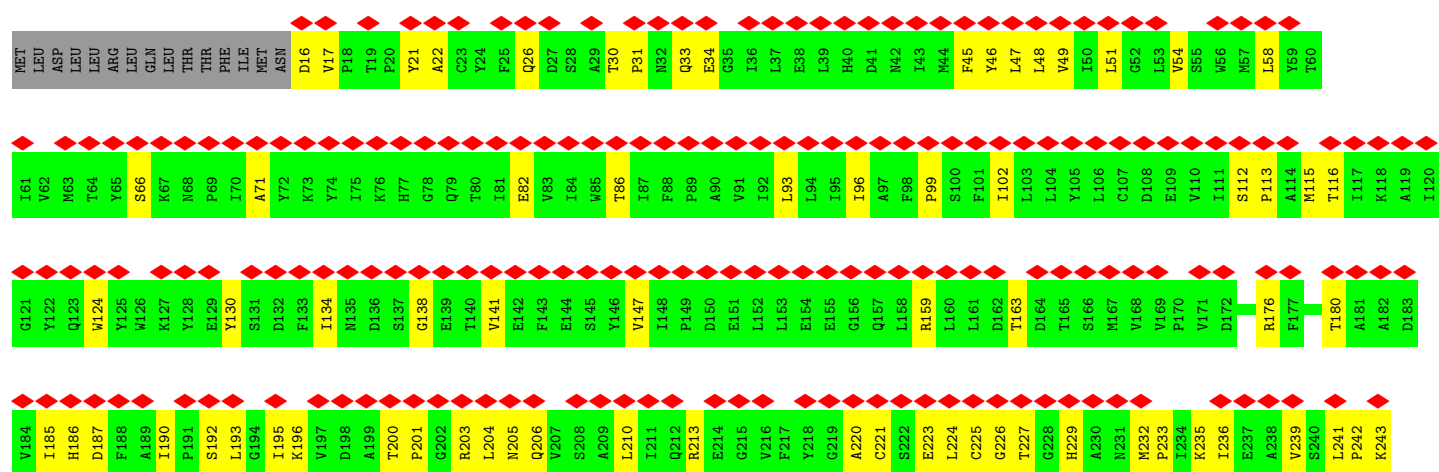
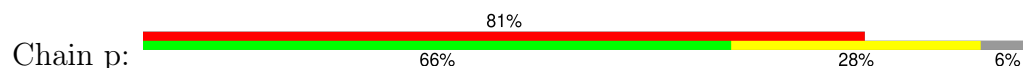


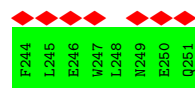


• Molecule 15: Cytochrome c oxidase subunit 2

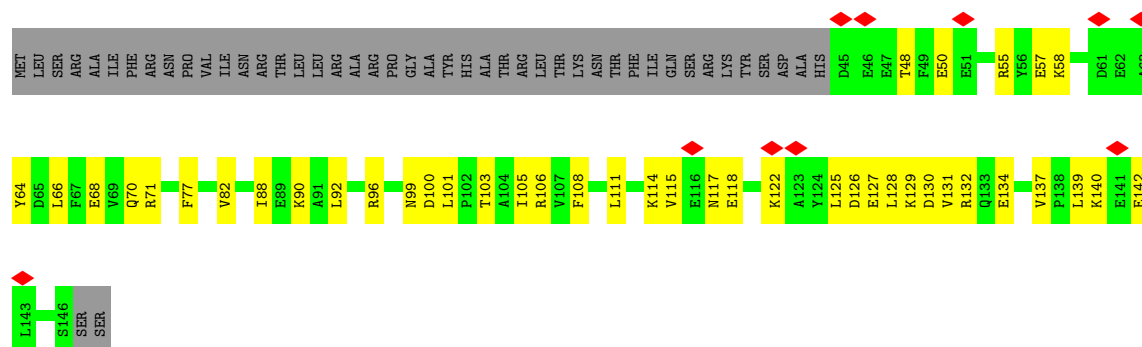
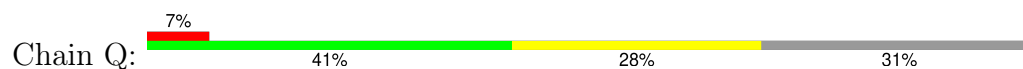


• Molecule 15: Cytochrome c oxidase subunit 2

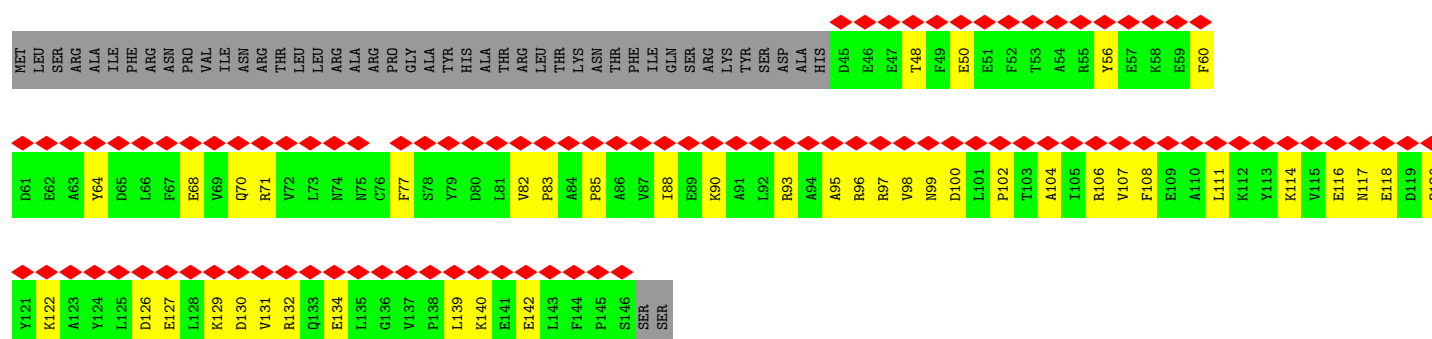




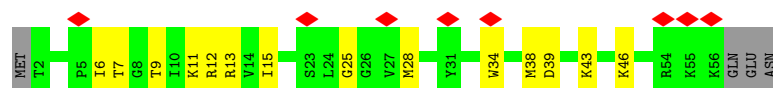
• Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial



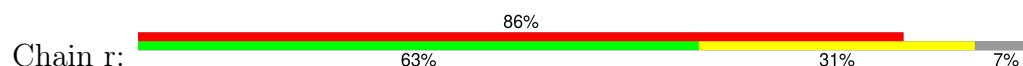
• Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial



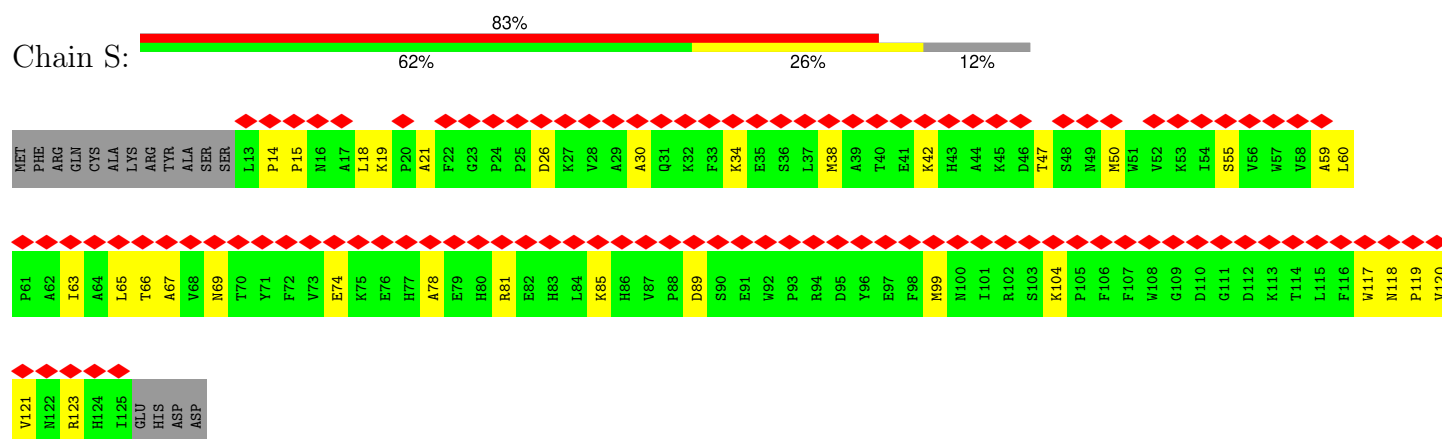
• Molecule 17: Cytochrome c oxidase subunit 9, mitochondrial



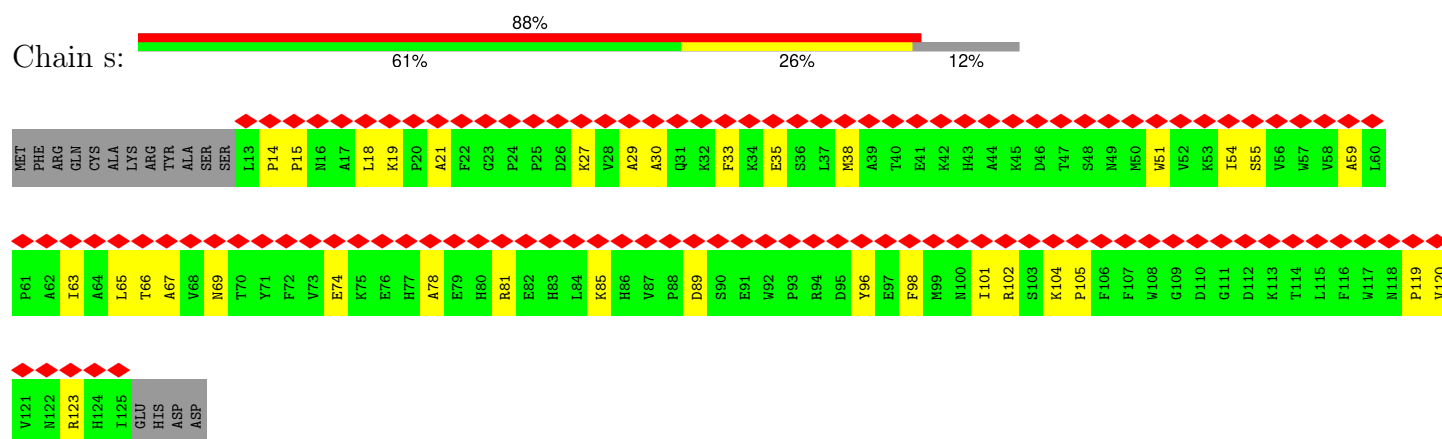
• Molecule 17: Cytochrome c oxidase subunit 9, mitochondrial



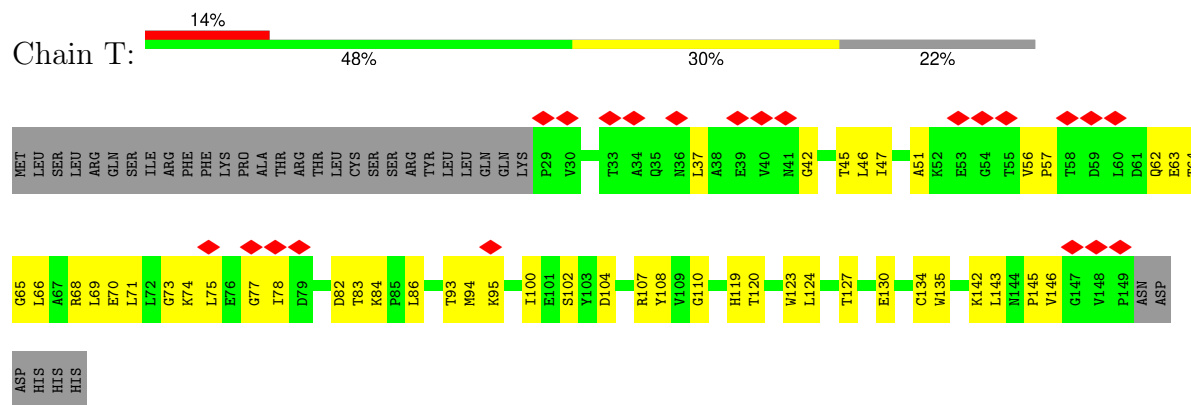
• Molecule 18: Cytochrome c oxidase subunit 13, mitochondrial



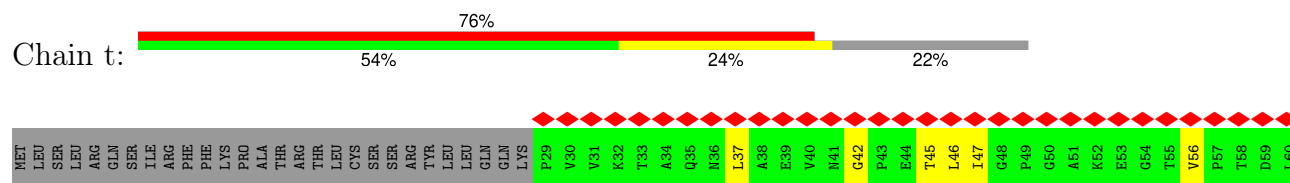
- Molecule 18: Cytochrome c oxidase subunit 13, mitochondrial

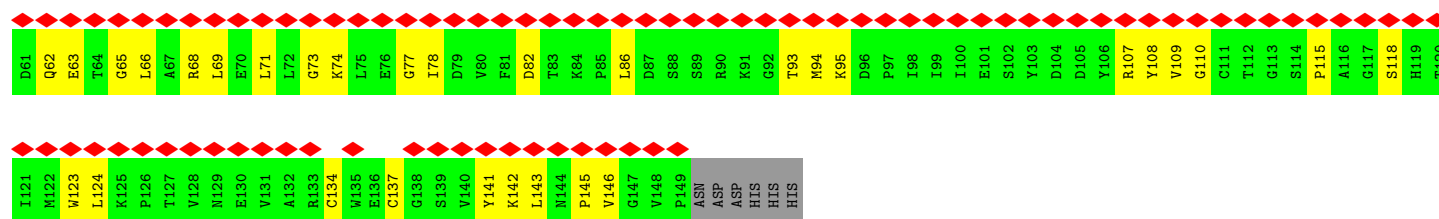


- Molecule 19: Cytochrome c oxidase subunit 4, mitochondrial

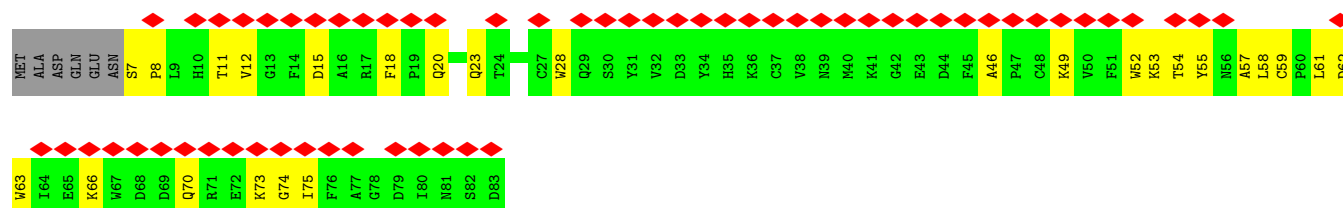
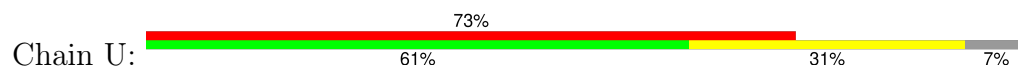


- Molecule 19: Cytochrome c oxidase subunit 4, mitochondrial

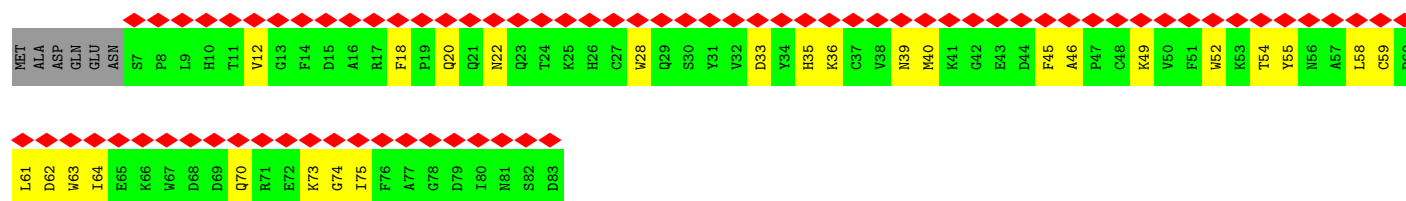




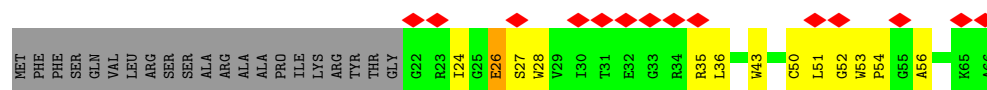
- Molecule 20: Cytochrome c oxidase subunit 12, mitochondrial



- Molecule 20: Cytochrome c oxidase subunit 12, mitochondrial



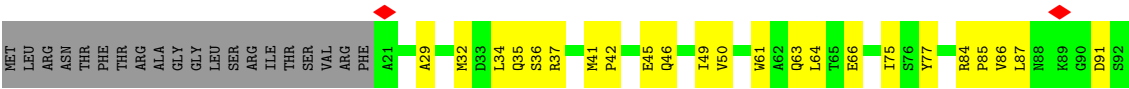
- Molecule 21: Cytochrome c oxidase subunit 26, mitochondrial



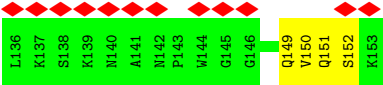
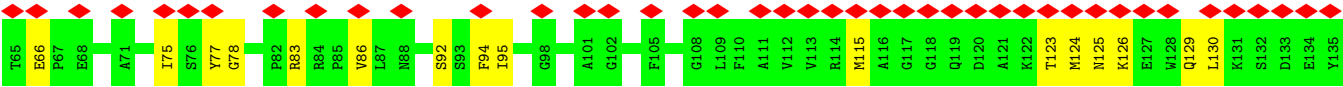
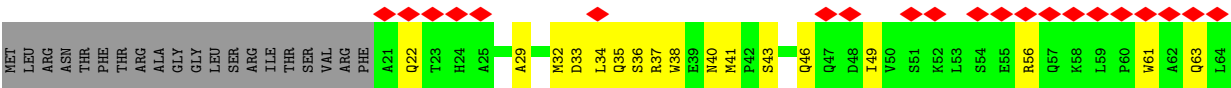
- Molecule 21: Cytochrome c oxidase subunit 26, mitochondrial



- Molecule 22: Cytochrome c oxidase subunit 5A, mitochondrial



● Molecule 22: Cytochrome c oxidase subunit 5A, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	493055	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.844	Depositor
Minimum map value	-0.873	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.245	Depositor
Map size (Å)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCF, PEF, CN5, HEA, CUA, UQ6, CDL, FES, CU, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/3406	0.40	0/4615
1	a	0.25	0/3406	0.42	0/4615
2	B	0.25	0/2781	0.37	0/3764
2	b	0.24	0/2781	0.37	0/3764
3	C	0.17	0/1444	0.37	0/1957
3	c	0.17	0/1444	0.34	0/1957
4	D	0.17	0/537	0.43	0/728
4	d	0.15	0/537	0.37	0/728
5	E	0.21	0/479	0.30	0/646
5	e	0.22	0/479	0.36	0/646
6	F	0.22	0/1040	0.39	0/1408
6	f	0.21	0/1040	0.35	0/1408
7	G	0.17	0/647	0.40	0/870
7	g	0.18	0/647	0.39	0/870
8	H	0.20	0/804	0.41	0/1088
8	h	0.27	0/804	0.51	0/1088
9	J	0.27	0/3192	0.45	0/4354
9	j	0.26	0/3192	0.41	0/4354
10	K	0.15	0/4290	0.36	0/5857
10	k	0.13	0/4290	0.36	0/5857
11	L	0.24	0/2022	0.38	0/2751
11	l	0.24	0/2022	0.42	0/2751
12	M	0.15	0/396	0.39	0/533
12	m	0.16	0/396	0.40	0/533
13	N	0.16	0/500	0.36	0/681
13	n	0.15	0/500	0.36	0/681
14	O	0.10	0/2218	0.31	0/3036
14	o	0.11	0/2218	0.33	0/3036
15	P	0.12	0/1941	0.30	0/2653
15	p	0.13	0/1941	0.33	0/2653
16	Q	0.15	0/868	0.36	0/1174
16	q	0.13	0/868	0.34	0/1174

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	R	0.12	0/467	0.33	0/626
17	r	0.12	0/467	0.33	0/626
18	S	0.10	0/962	0.26	0/1310
18	s	0.10	0/962	0.27	0/1310
19	T	0.13	0/932	0.30	0/1269
19	t	0.11	0/932	0.28	0/1269
20	U	0.09	0/664	0.23	0/899
20	u	0.11	0/664	0.28	0/899
21	V	0.16	0/372	0.46	2/502 (0.4%)
21	v	0.16	0/372	0.50	2/502 (0.4%)
22	W	0.16	0/1074	0.37	0/1451
22	w	0.13	0/1074	0.35	0/1451
All	All	0.19	0/62072	0.37	4/84344 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	v	26	GLU	CA-C-N	5.08	130.85	121.70
21	v	26	GLU	C-N-CA	5.08	130.85	121.70
21	V	26	GLU	CA-C-N	5.07	130.82	121.70
21	V	26	GLU	C-N-CA	5.07	130.82	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3345	0	3323	108	0
1	a	3345	0	3323	115	0
2	B	2735	0	2774	95	0
2	b	2735	0	2774	89	0
3	C	1411	0	1386	60	0
3	c	1411	0	1386	53	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	521	0	525	24	0
4	d	521	0	525	18	0
5	E	465	0	459	13	0
5	e	465	0	459	17	0
6	F	1019	0	1034	23	0
6	f	1019	0	1034	24	0
7	G	633	0	587	12	0
7	g	633	0	587	10	0
8	H	773	0	736	30	0
8	h	773	0	736	30	0
9	J	3090	0	3129	148	0
9	j	3090	0	3129	151	0
10	K	4162	0	4192	184	0
10	k	4162	0	4192	170	0
11	L	1961	0	1890	71	0
11	l	1961	0	1890	71	0
12	M	382	0	386	17	0
12	m	382	0	386	14	0
13	N	484	0	517	24	0
13	n	484	0	517	15	0
14	O	2146	0	2137	81	0
14	o	2146	0	2137	77	0
15	P	1889	0	1866	81	0
15	p	1889	0	1866	67	0
16	Q	851	0	822	38	0
16	q	851	0	822	31	0
17	R	455	0	469	13	0
17	r	455	0	469	13	0
18	S	928	0	906	29	0
18	s	928	0	906	24	0
19	T	913	0	912	43	0
19	t	913	0	912	30	0
20	U	642	0	586	26	0
20	u	642	0	586	22	0
21	V	361	0	363	14	0
21	v	361	0	363	13	0
22	W	1049	0	1030	37	0
22	w	1049	0	1030	39	0
23	A	111	0	141	15	0
23	C	61	0	68	6	0
23	E	32	0	37	2	0
23	J	117	0	159	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	V	33	0	39	0	0
23	W	77	0	106	7	0
23	a	111	0	141	8	0
23	c	61	0	68	6	0
23	e	32	0	37	1	0
23	j	117	0	159	8	0
23	v	33	0	39	0	0
23	w	77	0	106	5	0
24	C	4	0	0	3	0
24	c	4	0	0	3	0
25	C	53	0	50	5	0
25	H	53	0	50	3	0
25	J	56	0	56	3	0
25	K	67	0	78	6	0
25	L	67	0	78	5	0
25	c	48	0	40	5	0
25	h	120	0	128	4	0
25	j	56	0	56	2	0
25	k	67	0	78	4	0
26	E	47	0	71	3	0
26	H	50	0	80	2	0
26	W	36	0	46	2	0
26	a	47	0	71	2	0
26	k	36	0	46	1	0
26	w	50	0	80	0	0
27	J	41	0	50	6	0
28	J	86	0	60	14	0
28	L	43	0	30	9	0
28	j	86	0	60	17	0
28	l	43	0	30	9	0
29	J	63	0	77	11	0
29	j	86	0	116	9	0
30	K	120	0	108	28	0
30	k	120	0	108	23	0
31	K	1	0	0	0	0
31	k	1	0	0	0	0
32	P	2	0	0	0	0
32	p	2	0	0	0	0
All	All	62847	0	62805	2043	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 16.

All (2043) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:HIS:HE1	3:C:181:HIS:ND1	1.49	1.11
15:p:225:CYS:SG	15:p:229:HIS:CE1	2.51	1.04
3:C:161:HIS:CE1	3:C:181:HIS:ND1	2.26	1.03
4:d:48:TRP:H	4:d:51:PHE:HB3	1.34	0.92
9:J:50:MET:HE1	9:J:68:ILE:HG21	1.49	0.91
3:C:178:CYS:HB3	3:C:183:SER:H	1.35	0.90
9:J:27:ASN:H	9:J:30:TRP:HZ3	1.20	0.89
9:J:332:ASN:HD21	9:J:358:ILE:HG23	1.40	0.87
3:c:181:HIS:HE1	24:c:301:FES:S2	1.82	0.87
1:a:55:PHE:HB2	1:a:102:GLN:HB3	1.57	0.84
1:A:302:LEU:HB3	1:A:350:GLN:HG3	1.59	0.84
15:p:186:HIS:CE1	15:p:225:CYS:SG	2.69	0.84
14:o:6:ARG:O	14:o:10:GLN:HB2	1.79	0.83
9:j:36:LEU:HD11	9:j:93:MET:HE2	1.61	0.83
28:J:404:HEM:HBD2	28:J:404:HEM:HHA	1.62	0.81
14:O:198:ASP:HB3	18:S:99:MET:HB2	1.61	0.81
1:A:297:LEU:HD12	2:B:65:LEU:HB3	1.62	0.80
4:D:35:GLY:HA2	4:D:38:MET:HE3	1.63	0.80
11:L:105:HIS:NE2	28:L:401:HEM:C4C	2.38	0.80
14:O:6:ARG:O	14:O:10:GLN:HB2	1.82	0.80
19:t:110:GLY:HA3	19:t:123:TRP:HA	1.63	0.79
1:a:166:SER:HA	1:a:175:SER:HB2	1.65	0.79
18:S:34:LYS:HD3	19:T:75:LEU:HG	1.63	0.79
9:J:166:TRP:HE1	9:J:171:VAL:HG22	1.48	0.79
10:K:8:SER:O	10:K:100:ASN:ND2	2.16	0.79
8:H:39:GLY:O	8:H:41:PHE:N	2.16	0.78
9:J:35:LEU:HD11	9:J:236:PHE:HB2	1.67	0.77
11:L:236:TYR:H	11:L:241:PRO:HG2	1.49	0.77
14:O:148:SER:HB3	14:O:177:LEU:HD22	1.66	0.76
10:k:295:VAL:O	15:p:205:ASN:ND2	2.19	0.76
9:J:43:GLN:OE1	9:J:82:HIS:ND1	2.18	0.76
9:J:287:ASP:HB3	9:J:290:LEU:HB2	1.68	0.75
9:j:127:THR:HG21	9:j:190:ILE:HD11	1.68	0.75
2:b:225:LEU:HA	2:b:352:ASN:HD21	1.51	0.74
11:L:103:ALA:HA	11:L:158:PRO:HG2	1.69	0.74
14:o:20:SER:HB3	14:o:22:TRP:HD1	1.53	0.74
16:q:82:VAL:HG21	16:q:117:ASN:HD21	1.51	0.74
10:K:112:CYS:HB2	10:K:146:LEU:HD22	1.69	0.74
1:a:63:ASN:ND2	22:w:33:ASP:OD2	2.21	0.74
6:f:3:GLN:HB2	9:j:310:ARG:HB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:q:82:VAL:H	17:r:6:ILE:HG21	1.53	0.74
2:b:255:VAL:HG23	2:b:321:THR:HG21	1.70	0.74
2:B:255:VAL:HG23	2:B:321:THR:HG21	1.70	0.73
10:k:489:VAL:HG21	22:w:86:VAL:HG12	1.69	0.73
3:C:73:SER:HB3	23:C:304:PEF:H21	1.69	0.73
16:q:90:LYS:HG3	16:q:93:ARG:HH21	1.53	0.73
14:o:148:SER:HB3	14:o:177:LEU:HD22	1.68	0.73
22:w:35:GLN:NE2	22:w:36:SER:OG	2.22	0.72
9:J:127:THR:HG21	9:J:190:ILE:HD11	1.71	0.72
10:k:247:LEU:HD11	30:k:604:HEA:HBC2	1.71	0.72
1:A:65:TYR:HB3	22:W:29:ALA:HB1	1.70	0.72
6:F:117:LYS:HG3	2:b:65:LEU:HD11	1.70	0.72
11:L:136:ASP:HB3	11:L:147:ARG:HD2	1.70	0.72
9:j:187:PRO:HG2	28:j:403:HEM:HBB2	1.72	0.72
10:K:219:SER:HB2	10:K:222:GLU:HB2	1.70	0.72
1:a:297:LEU:HD12	2:b:65:LEU:HB3	1.69	0.72
19:t:68:ARG:HA	19:t:71:LEU:HG	1.72	0.72
11:l:136:ASP:OD2	11:l:147:ARG:NE	2.23	0.72
16:Q:96:ARG:NH1	16:Q:99:ASN:OD1	2.23	0.71
11:l:101:CYS:SG	28:l:401:HEM:HAB	2.30	0.71
11:l:147:ARG:HH12	11:l:149:GLY:HA2	1.55	0.71
15:p:220:ALA:HB1	15:p:232:MET:HE3	1.73	0.71
9:j:38:LEU:HD23	9:j:233:VAL:HG21	1.71	0.71
30:k:603:HEA:HBD2	30:k:603:HEA:HHA	1.71	0.71
3:c:146:ARG:HB2	3:c:202:ILE:HG13	1.73	0.71
9:j:362:TYR:HA	9:j:366:ILE:HB	1.73	0.71
9:J:26:ILE:HG23	9:J:30:TRP:HE3	1.54	0.71
16:Q:106:ARG:HH21	22:W:77:TYR:HA	1.55	0.71
9:J:208:ASN:ND2	9:J:212:ILE:O	2.23	0.71
30:K:604:HEA:H161	30:K:604:HEA:HMC1	1.72	0.71
18:S:55:SER:HA	18:S:59:ALA:HB3	1.72	0.70
23:c:304:PEF:H112	11:l:273:THR:HG23	1.71	0.70
2:B:113:ALA:HB1	2:B:115:LYS:HE3	1.71	0.70
1:A:248:GLU:HG2	1:A:250:ARG:HH21	1.55	0.70
30:K:604:HEA:HBD2	30:K:604:HEA:HHA	1.71	0.70
20:u:35:HIS:O	20:u:39:ASN:ND2	2.23	0.70
3:C:78:PHE:O	3:C:81:SER:OG	2.10	0.70
9:j:50:MET:HE1	9:j:68:ILE:HG12	1.72	0.70
14:o:200:VAL:HG23	14:o:203:SER:HB3	1.72	0.70
2:b:60:ASN:H	2:b:112:THR:HB	1.56	0.70
9:j:281:ILE:HG22	9:j:356:THR:HG22	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:l:121:THR:HG23	11:l:122:ASN:H	1.57	0.70
3:C:114:LYS:HE2	3:C:158:ILE:HD12	1.74	0.69
9:j:97:MET:HE1	9:j:121:PHE:CG	2.26	0.69
6:F:75:ILE:HD13	9:J:212:ILE:HD13	1.74	0.69
10:K:32:MET:HE3	10:K:62:HIS:HA	1.75	0.69
10:k:142:PRO:HB3	14:o:38:ALA:HB1	1.73	0.69
15:p:113:PRO:HG2	20:u:58:LEU:HA	1.72	0.69
18:s:55:SER:HA	18:s:59:ALA:HB3	1.75	0.69
28:J:405:HEM:HBB2	28:J:405:HEM:HMB2	1.74	0.69
20:U:11:THR:HG21	20:U:53:LYS:HZ2	1.58	0.69
5:e:13:ARG:HB3	5:e:16:VAL:HG12	1.74	0.69
9:j:68:ILE:HD12	9:j:72:VAL:HG11	1.73	0.69
16:q:118:GLU:HB3	21:v:26:GLU:HB2	1.75	0.69
14:O:200:VAL:HG23	14:O:203:SER:HB2	1.74	0.69
16:Q:64:TYR:OH	19:T:95:LYS:NZ	2.26	0.68
9:j:7:ASN:ND2	23:j:406:PEF:O4	2.26	0.68
1:A:164:LEU:HD21	1:A:264:ALA:HB2	1.73	0.68
23:A:502:PEF:H312	25:J:403:CDL:HA32	1.76	0.68
6:F:124:GLU:OE2	4:d:21:ARG:NH2	2.26	0.68
17:R:6:ILE:HG22	17:R:7:THR:H	1.57	0.68
6:f:82:GLU:HG3	9:j:210:LEU:HD21	1.73	0.68
9:j:70:ARG:NH1	11:l:109:ARG:O	2.21	0.68
15:p:204:LEU:HD12	20:u:63:TRP:CD1	2.28	0.68
2:B:298:SER:OG	2:B:302:LYS:NZ	2.27	0.68
11:L:84:THR:OG1	11:L:264:ASP:OD1	2.10	0.68
15:P:30:THR:OG1	15:P:210:LEU:O	2.11	0.68
1:A:125:ILE:HG13	1:A:126:GLN:HG3	1.75	0.68
15:P:113:PRO:HD2	20:U:58:LEU:HG	1.77	0.68
6:f:39:LYS:NZ	6:f:99:ASP:OD2	2.27	0.67
9:J:12:LEU:HD11	27:J:402:CN5:H2'	1.75	0.67
17:R:34:TRP:CD1	17:R:38:MET:HE3	2.29	0.67
14:O:162:GLY:HA2	19:T:56:VAL:HB	1.76	0.67
16:Q:111:LEU:O	16:Q:114:LYS:NZ	2.25	0.67
3:C:121:ARG:NH1	3:C:187:ILE:O	2.27	0.67
9:J:362:TYR:HA	9:J:366:ILE:HB	1.75	0.67
2:b:28:ILE:O	2:b:191:ASN:ND2	2.27	0.67
2:B:40:ARG:NH2	2:B:41:TYR:OH	2.26	0.67
2:B:66:LYS:HA	6:f:120:LEU:HD22	1.77	0.67
15:P:16:ASP:O	15:P:26:GLN:NE2	2.28	0.67
1:a:447:ARG:NH2	9:j:222:HIS:O	2.28	0.67
1:A:261:ILE:HD12	1:A:344:ILE:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:513:SER:OG	10:K:515:GLU:OE1	2.12	0.67
9:j:301:VAL:HA	9:j:304:VAL:HG12	1.75	0.67
8:h:43:ASN:OD1	8:h:47:ASN:ND2	2.27	0.67
13:n:37:PHE:HE1	14:o:50:MET:HB2	1.60	0.67
17:r:6:ILE:HG22	17:r:7:THR:H	1.60	0.67
9:J:338:GLN:NE2	9:J:342:CYS:SG	2.68	0.66
1:a:67:ASN:HD21	1:a:177:PRO:HD2	1.60	0.66
4:d:43:VAL:HG22	5:e:26:PHE:HB2	1.78	0.66
10:k:8:SER:O	10:k:100:ASN:ND2	2.27	0.66
11:l:161:ASN:OD1	11:l:162:GLU:N	2.27	0.66
19:T:68:ARG:HA	19:T:71:LEU:HG	1.78	0.66
1:A:443:LEU:HD22	1:A:447:ARG:HG2	1.76	0.66
9:J:187:PRO:HG2	28:J:404:HEM:HMC1	1.77	0.66
30:K:601:HEA:HHA	30:K:601:HEA:O2A	1.95	0.66
14:O:20:SER:HB3	14:O:22:TRP:HD1	1.59	0.66
10:k:267:VAL:HG21	10:k:270:GLU:HB3	1.77	0.66
4:D:50:LYS:NZ	9:j:156:PHE:O	2.28	0.66
10:K:158:SER:HB3	10:K:196:LEU:HD21	1.76	0.66
15:p:225:CYS:SG	15:p:229:HIS:HE1	2.18	0.66
19:t:142:LYS:NZ	19:t:143:LEU:O	2.29	0.66
1:A:346:PHE:HE1	23:A:502:PEF:H41	1.60	0.66
1:A:263:LEU:HA	1:A:433:ILE:HG22	1.77	0.66
1:a:216:HIS:HA	1:a:219:LEU:HD23	1.78	0.66
1:a:248:GLU:HG2	1:a:250:ARG:HH21	1.60	0.66
9:j:4:ARG:HD2	9:j:18:ILE:HG21	1.77	0.66
1:A:108:SER:OG	1:A:112:SER:OG	2.14	0.66
14:O:78:ASP:H	19:T:65:GLY:HA2	1.60	0.66
2:b:298:SER:OG	2:b:302:LYS:NZ	2.26	0.66
2:B:225:LEU:HA	2:B:352:ASN:HD21	1.61	0.66
11:L:223:ILE:HG22	11:L:225:MET:H	1.60	0.66
13:N:25:ARG:HH21	13:N:28:LEU:HD22	1.59	0.66
16:Q:68:GLU:HA	16:Q:71:ARG:HG2	1.77	0.66
10:k:320:ILE:HA	10:k:323:TRP:HE3	1.61	0.66
9:J:201:LEU:HD11	28:J:405:HEM:HAA1	1.78	0.66
22:w:129:GLN:NE2	22:w:149:GLN:O	2.23	0.66
10:k:158:SER:HB3	10:k:196:LEU:HD11	1.77	0.65
10:k:406:ASN:HB3	10:k:409:LEU:HB2	1.77	0.65
22:W:129:GLN:NE2	22:W:149:GLN:O	2.19	0.65
10:k:409:LEU:HD13	10:k:412:ILE:HD11	1.79	0.65
10:k:450:TRP:HE1	15:p:21:TYR:HA	1.62	0.65
15:p:30:THR:HG23	15:p:33:GLN:H	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:64:TYR:N	16:Q:68:GLU:OE2	2.29	0.65
9:J:116:VAL:O	9:J:120:ILE:HD12	1.96	0.65
3:c:51:LYS:NZ	25:c:302:CDL:OA4	2.28	0.65
9:j:330:VAL:HG23	23:j:401:PEF:H402	1.77	0.65
10:k:368:HIS:HB3	15:p:196:LYS:HE2	1.78	0.65
3:C:181:HIS:CD2	9:j:282:LEU:HD22	2.32	0.65
15:P:30:THR:HG23	15:P:33:GLN:H	1.60	0.65
15:p:147:VAL:HB	15:p:233:PRO:HD3	1.79	0.65
3:C:155:MET:HE1	3:C:189:GLY:HA3	1.77	0.65
2:B:54:PHE:HA	2:B:57:GLN:HE22	1.60	0.65
1:a:457:TRP:HZ3	5:e:13:ARG:HE	1.45	0.65
28:j:404:HEM:HMC2	28:j:404:HEM:HBC2	1.78	0.65
2:B:117:HIS:O	6:f:62:ARG:NH1	2.29	0.65
14:o:156:HIS:HB3	14:o:247:ILE:HG22	1.78	0.65
1:a:113:THR:HG21	1:a:214:ILE:HG21	1.80	0.64
10:k:390:PHE:HE2	10:k:417:ILE:HD13	1.62	0.64
13:N:2:ALA:HB2	14:O:233:TYR:HB2	1.79	0.64
11:l:190:TYR:OH	28:l:401:HEM:O2A	2.11	0.64
15:p:31:PRO:HA	15:p:34:GLU:HG2	1.78	0.64
23:A:503:PEF:H211	23:C:304:PEF:H192	1.79	0.64
10:K:409:LEU:HD13	10:K:412:ILE:HD11	1.79	0.64
10:k:443:TYR:O	15:p:159:ARG:NH2	2.30	0.64
11:l:83:GLU:O	11:l:267:LYS:NZ	2.30	0.64
30:K:601:HEA:H241	15:P:93:LEU:HD11	1.79	0.64
15:P:113:PRO:HG2	20:U:58:LEU:HA	1.80	0.64
16:Q:118:GLU:OE2	21:V:28:TRP:NE1	2.30	0.64
19:t:107:ARG:HD2	19:t:108:TYR:H	1.62	0.64
3:C:55:TYR:OH	25:C:302:CDL:OB9	2.15	0.64
9:J:68:ILE:HD12	9:J:72:VAL:HG11	1.80	0.64
10:K:62:HIS:O	10:K:66:MET:HG2	1.98	0.64
9:j:285:ILE:HD12	9:j:290:LEU:HB3	1.80	0.64
2:B:28:ILE:O	2:B:191:ASN:ND2	2.24	0.64
15:P:114:ALA:H	15:P:174:HIS:HB2	1.62	0.64
10:K:374:VAL:HA	10:K:377:PHE:CE1	2.33	0.64
2:b:59:THR:OG1	2:b:62:ARG:O	2.16	0.64
9:J:35:LEU:HD12	9:J:232:THR:HG22	1.78	0.64
10:K:108:MET:HA	10:K:111:VAL:HG22	1.79	0.64
9:j:195:ILE:O	9:j:199:MET:HG3	1.96	0.64
10:k:261:THR:O	10:k:493:LYS:NZ	2.23	0.64
2:B:37:GLY:HA2	2:B:41:TYR:HD2	1.62	0.63
2:b:358:ASP:OD2	2:b:361:ASN:ND2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:259:VAL:HG21	10:k:323:TRP:HD1	1.63	0.63
12:m:69:TYR:O	13:n:56:LYS:NZ	2.31	0.63
9:J:160:ASP:HB3	23:c:303:PEF:HN2	1.61	0.63
19:T:62:GLN:NE2	19:T:63:GLU:OE2	2.31	0.63
2:b:255:VAL:HG11	2:b:343:VAL:HG11	1.79	0.63
15:p:16:ASP:N	15:p:192:SER:HG	1.95	0.63
1:a:261:ILE:HD12	1:a:344:ILE:HD11	1.77	0.63
3:c:70:GLY:HA3	23:c:304:PEF:H142	1.80	0.63
11:l:240:THR:H	11:l:241:PRO:HD2	1.62	0.63
15:p:115:MET:O	15:p:176:ARG:N	2.29	0.63
1:A:369:LEU:HD23	1:A:372:LEU:HD21	1.80	0.63
9:J:36:LEU:HD12	9:J:92:VAL:HG13	1.80	0.63
9:J:196:MET:HB3	9:j:9:TYR:CE2	2.34	0.63
1:a:353:ARG:NH1	4:d:26:TYR:OH	2.31	0.63
10:k:320:ILE:HD12	30:k:604:HEA:H171	1.79	0.63
11:l:106:SER:OG	11:l:176:ASP:OD1	2.15	0.63
1:A:98:SER:O	1:A:99:ARG:NH1	2.29	0.63
1:A:353:ARG:NH1	23:A:501:PEF:O3	2.32	0.63
16:Q:122:LYS:HG2	21:V:24:ILE:HG12	1.79	0.63
8:H:81:TYR:HB3	11:L:63:THR:HG22	1.81	0.63
11:l:235:GLU:HA	11:l:241:PRO:HG3	1.80	0.63
10:K:489:VAL:HG21	22:W:86:VAL:HG12	1.80	0.63
5:e:42:ASN:HD21	22:w:115:MET:HE1	1.63	0.63
10:K:406:ASN:HB3	10:K:409:LEU:HB2	1.79	0.62
10:k:319:LYS:HG3	10:k:323:TRP:CZ3	2.34	0.62
10:k:332:ILE:HB	15:p:66:SER:HA	1.81	0.62
2:B:353:TYR:HE1	2:B:355:ALA:HB2	1.63	0.62
10:K:37:ARG:NH1	30:K:604:HEA:OMA	2.32	0.62
10:K:377:PHE:CD1	30:K:601:HEA:HBD1	2.34	0.62
15:P:156:GLY:HA2	22:W:131:LYS:HB3	1.81	0.62
9:j:241:ALA:HA	9:j:244:VAL:HG12	1.81	0.62
9:j:287:ASP:HB2	9:j:290:LEU:HB2	1.81	0.62
10:k:310:MET:HB2	15:p:93:LEU:HD22	1.81	0.62
1:A:252:ARG:CZ	8:H:21:GLN:HE22	2.12	0.62
9:J:58:ILE:HG22	9:J:176:ILE:HD12	1.79	0.62
15:P:200:THR:OG1	15:P:203:ARG:O	2.18	0.62
1:a:211:THR:HG21	1:a:386:ASP:HB3	1.80	0.62
2:b:37:GLY:HA2	2:b:41:TYR:HD2	1.64	0.62
3:c:190:ARG:HA	3:c:199:ASN:HD21	1.63	0.62
9:J:23:PRO:HG2	9:J:26:ILE:HD11	1.80	0.62
19:T:142:LYS:NZ	19:T:143:LEU:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:l:190:TYR:CZ	11:l:194:LEU:HD11	2.34	0.62
9:J:266:PRO:HD2	9:J:269:ILE:HD11	1.80	0.62
6:f:101:PRO:HB3	9:j:382:ARG:HH12	1.63	0.62
17:R:25:GLY:HA2	17:R:28:MET:HE3	1.81	0.62
15:p:221:CYS:O	15:p:232:MET:HE1	1.99	0.62
1:A:352:ASN:ND2	1:A:454:MET:HG3	2.13	0.62
2:B:116:PRO:HA	2:B:169:LEU:HD13	1.81	0.62
15:P:115:MET:O	15:P:176:ARG:N	2.32	0.62
16:q:68:GLU:HA	16:q:71:ARG:HG2	1.81	0.62
10:k:342:ILE:HD12	15:p:58:LEU:HD11	1.80	0.62
9:J:325:PHE:O	9:J:328:ILE:HG22	2.00	0.62
11:L:195:LEU:HD11	28:L:401:HEM:HMB3	1.82	0.62
8:h:58:TYR:CE1	9:j:323:LYS:HD2	2.35	0.62
11:L:225:MET:SD	28:L:401:HEM:C4C	2.92	0.62
20:U:73:LYS:HE3	20:U:75:ILE:HB	1.82	0.62
7:g:137:ALA:O	7:g:141:ARG:NH1	2.33	0.62
9:j:266:PRO:HD2	9:j:269:ILE:HD11	1.82	0.62
11:L:161:ASN:OD1	11:L:162:GLU:N	2.26	0.61
3:c:176:TRP:HB2	3:c:185:TYR:HB2	1.81	0.61
16:q:88:ILE:HG13	16:q:111:LEU:HD21	1.81	0.61
10:K:530:PRO:O	19:T:107:ARG:NH2	2.33	0.61
16:Q:82:VAL:H	17:R:6:ILE:HG21	1.65	0.61
21:V:52:GLY:O	21:V:56:ALA:N	2.30	0.61
1:a:71:ASN:ND2	1:a:178:THR:O	2.28	0.61
1:a:110:PRO:HB3	1:a:213:ASN:HD21	1.66	0.61
14:o:78:ASP:H	19:t:65:GLY:HA2	1.64	0.61
16:q:122:LYS:HG2	21:v:24:ILE:HG12	1.82	0.61
10:k:108:MET:HA	10:k:111:VAL:HG22	1.83	0.61
1:a:393:GLU:OE1	1:a:397:LYS:NZ	2.33	0.61
10:k:112:CYS:HB2	10:k:146:LEU:HD22	1.80	0.61
10:k:400:ILE:HG13	10:k:401:LEU:HG	1.82	0.61
15:p:203:ARG:HH12	15:p:205:ASN:HB2	1.66	0.61
1:A:66:ASN:ND2	1:A:192:ASP:OD1	2.33	0.61
9:J:30:TRP:CD1	9:J:99:LYS:HZ1	2.18	0.61
9:J:370:ILE:O	9:J:374:GLU:HG2	2.01	0.61
10:K:184:LEU:HD12	10:K:277:MET:HE1	1.81	0.61
1:a:112:SER:HB2	1:a:115:LYS:HE2	1.81	0.61
2:b:84:ARG:HG2	2:b:279:PHE:CZ	2.36	0.61
8:h:40:ILE:HD11	25:h:602:CDL:H512	1.83	0.61
11:l:89:SER:OG	11:l:92:ARG:NH2	2.31	0.61
9:J:241:ALA:HA	9:J:244:VAL:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:254:ILE:HD11	10:K:388:SER:HB3	1.82	0.61
11:L:215:ASN:HB2	11:L:227:ARG:HH22	1.64	0.61
30:K:604:HEA:HBA2	30:K:604:HEA:HMA	1.82	0.61
9:j:123:LEU:O	9:j:127:THR:HG23	2.00	0.61
3:C:172:ASP:OD1	8:h:93:ASN:ND2	2.33	0.61
8:H:8:THR:HG22	8:H:10:MET:H	1.65	0.61
25:H:601:CDL:H372	9:J:91:MET:HE1	1.81	0.61
10:K:151:LEU:HD11	10:K:207:ILE:HG21	1.83	0.61
9:J:9:TYR:CE2	9:j:196:MET:HB3	2.36	0.60
1:a:189:VAL:HG23	1:a:190:VAL:H	1.65	0.60
3:c:115:PRO:HD2	3:c:158:ILE:HD11	1.81	0.60
14:o:162:GLY:HA2	19:t:56:VAL:HB	1.83	0.60
2:B:119:LEU:HD13	2:B:169:LEU:HD21	1.82	0.60
2:b:29:SER:OG	2:b:190:GLU:O	2.17	0.60
22:w:22:GLN:HE22	22:w:56:ARG:HA	1.65	0.60
2:B:181:THR:OG1	2:B:212:GLY:N	2.31	0.60
2:B:247:LYS:HE2	2:B:281:ASP:HA	1.83	0.60
6:F:101:PRO:HB3	9:J:382:ARG:HH12	1.66	0.60
22:W:36:SER:O	22:W:37:ARG:NE	2.34	0.60
3:c:92:ALA:O	3:c:111:TRP:NE1	2.34	0.60
9:j:165:LEU:O	9:j:178:ARG:NH1	2.34	0.60
14:o:168:LEU:HD23	14:o:171:LEU:HD21	1.83	0.60
14:o:225:VAL:HG13	14:o:229:ARG:HH21	1.66	0.60
1:A:166:SER:HA	1:A:175:SER:HB2	1.83	0.60
10:K:217:ASN:OD1	18:S:104:LYS:NZ	2.30	0.60
14:o:240:HIS:HB2	14:o:243:TYR:HB2	1.83	0.60
2:B:258:ASN:HB3	2:B:321:THR:HG22	1.83	0.60
9:J:9:TYR:HE2	9:j:196:MET:HB3	1.65	0.60
9:J:107:ARG:HH21	9:J:314:ARG:HA	1.67	0.60
14:O:194:PHE:HB2	18:S:121:VAL:HB	1.82	0.60
1:a:271:ASN:HD21	1:a:397:LYS:HA	1.66	0.60
4:D:21:ARG:NH1	6:f:124:GLU:OE2	2.34	0.60
10:K:485:ASN:HD21	10:K:487:LYS:HB2	1.67	0.60
9:j:208:ASN:ND2	9:j:212:ILE:O	2.34	0.60
22:w:29:ALA:HA	22:w:32:MET:HE3	1.84	0.60
30:K:604:HEA:H161	30:K:604:HEA:CMC	2.32	0.60
1:a:310:GLN:NE2	1:a:312:CYS:O	2.35	0.60
3:c:120:HIS:CE1	3:c:151:GLN:HB3	2.37	0.60
2:B:164:VAL:HG13	2:B:165:GLU:OE1	2.02	0.60
15:P:112:SER:OG	20:U:53:LYS:NZ	2.35	0.60
21:V:26:GLU:HA	21:V:27:SER:OG	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:170:GLN:HG2	3:c:36:THR:HG21	1.82	0.60
1:a:430:ASP:OD1	1:a:449:ARG:NH1	2.32	0.60
3:c:154:ILE:HD13	3:c:212:VAL:HG21	1.84	0.60
2:b:291:ASP:OD1	2:b:292:GLN:N	2.32	0.59
11:l:92:ARG:HB2	11:l:236:TYR:CD2	2.37	0.59
11:L:63:THR:OG1	11:L:66:GLU:OE1	2.20	0.59
22:W:136:LEU:HA	22:W:139:LYS:HZ2	1.67	0.59
29:j:405:UQ6:H201	29:j:405:UQ6:H253	1.83	0.59
10:k:254:ILE:HD11	10:k:388:SER:HB3	1.84	0.59
1:A:257:PRO:O	1:A:438:GLN:NE2	2.35	0.59
1:A:370:LEU:HD22	1:A:410:ILE:HD11	1.83	0.59
2:B:243:ILE:HB	2:B:285:PHE:HB3	1.84	0.59
3:c:73:SER:HB2	23:c:304:PEF:H21	1.84	0.59
9:j:30:TRP:CH2	9:j:209:PRO:HG3	2.36	0.59
14:o:175:PHE:HE1	14:o:223:LEU:HB3	1.67	0.59
15:p:48:LEU:HD23	15:p:51:LEU:HD21	1.84	0.59
2:B:66:LYS:HZ2	6:f:117:LYS:HB2	1.67	0.59
1:a:169:PHE:HB2	1:a:175:SER:HB3	1.84	0.59
9:j:146:VAL:HG11	29:j:407:UQ6:H3M3	1.84	0.59
23:E:102:PEF:H312	26:W:203:PCF:H222	1.85	0.59
6:F:121:ASP:OD1	6:F:122:ASN:N	2.35	0.59
10:K:443:TYR:O	15:P:159:ARG:NH2	2.36	0.59
22:w:34:LEU:HD12	22:w:49:ILE:HD12	1.84	0.59
1:A:189:VAL:HG23	1:A:190:VAL:H	1.67	0.59
25:C:302:CDL:H121	25:K:603:CDL:H132	1.83	0.59
9:J:117:GLY:O	28:J:405:HEM:HMC2	2.03	0.59
22:W:91:ASP:N	22:W:91:ASP:OD1	2.34	0.59
6:f:121:ASP:OD1	6:f:122:ASN:N	2.35	0.59
10:k:399:GLN:NE2	10:k:515:GLU:O	2.36	0.59
3:C:156:LEU:H	3:C:203:PRO:HD3	1.65	0.59
23:E:102:PEF:H182	26:W:203:PCF:H362	1.85	0.59
10:K:399:GLN:NE2	10:K:515:GLU:O	2.36	0.59
1:A:211:THR:HG21	1:A:386:ASP:HB3	1.83	0.59
9:J:150:LEU:HD22	9:J:292:VAL:HG22	1.85	0.59
10:k:114:VAL:HG23	12:m:63:VAL:HG23	1.85	0.59
10:k:374:VAL:HA	10:k:377:PHE:CE1	2.38	0.59
9:J:26:ILE:HG23	9:J:30:TRP:CE3	2.37	0.59
10:K:360:ASN:HB3	10:K:363:LEU:HB2	1.83	0.59
10:K:389:LEU:HD23	30:K:604:HEA:H251	1.84	0.59
14:O:240:HIS:HB2	14:O:243:TYR:HB2	1.84	0.59
15:P:176:ARG:NH1	20:U:57:ALA:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:93:MET:SD	9:j:97:MET:HE3	2.42	0.59
14:o:67:ARG:NH1	14:o:68:ASP:OD1	2.36	0.59
2:B:29:SER:OG	2:B:190:GLU:O	2.19	0.58
2:B:364:TYR:CZ	2:b:152:ARG:HD2	2.38	0.58
7:G:117:LEU:O	7:G:119:HIS:ND1	2.35	0.58
10:K:188:SER:HB2	10:K:249:ILE:HG22	1.85	0.58
10:K:320:ILE:HD12	30:K:601:HEA:H171	1.83	0.58
3:c:120:HIS:HE1	3:c:151:GLN:HB3	1.68	0.58
10:k:4:ARG:NH2	10:k:13:ASP:OD2	2.36	0.58
11:l:105:HIS:NE2	28:l:401:HEM:C1C	2.57	0.58
15:p:30:THR:OG1	15:p:210:LEU:O	2.20	0.58
9:J:48:ILE:HD13	28:J:404:HEM:HBC1	1.84	0.58
1:a:436:THR:C	1:a:439:ILE:HD11	2.28	0.58
9:j:87:SER:OG	9:j:273:TRP:NE1	2.32	0.58
15:p:204:LEU:HB2	20:u:63:TRP:HE1	1.68	0.58
2:B:45:ASP:HB2	2:B:158:PRO:HG2	1.84	0.58
10:K:270:GLU:HA	10:K:273:MET:HG2	1.85	0.58
21:V:53:TRP:CG	21:V:54:PRO:HD3	2.39	0.58
10:k:52:SER:HB2	10:k:441:PRO:HG3	1.85	0.58
10:k:344:PHE:HD1	10:k:345:LEU:HD22	1.68	0.58
10:k:377:PHE:CD1	30:k:604:HEA:HBD1	2.38	0.58
11:l:92:ARG:HB2	11:l:236:TYR:HD2	1.68	0.58
15:p:163:THR:HG22	15:p:235:LYS:HD3	1.84	0.58
18:s:119:PRO:O	18:s:123:ARG:NH2	2.36	0.58
10:K:114:VAL:HG23	12:M:63:VAL:HG23	1.86	0.58
17:R:39:ASP:O	17:R:43:LYS:HG2	2.04	0.58
1:a:365:ARG:NE	2:b:72:GLU:OE2	2.35	0.58
6:F:85:HIS:NE2	25:H:601:CDL:OA4	2.32	0.58
9:J:178:ARG:NH2	3:c:82:MET:O	2.35	0.58
9:j:300:LEU:HD23	9:j:303:LEU:HD22	1.86	0.58
10:k:515:GLU:HA	10:k:518:LEU:HD13	1.85	0.58
9:J:200:ALA:O	9:J:203:ILE:HG12	2.03	0.58
18:S:85:LYS:HA	18:S:120:VAL:HG23	1.85	0.58
1:a:164:LEU:HD21	1:a:264:ALA:HB2	1.85	0.58
10:k:431:LEU:HG	10:k:447:PHE:HD2	1.69	0.58
14:o:75:TYR:HD2	14:o:76:LEU:HD22	1.68	0.58
16:q:96:ARG:NH1	16:q:99:ASN:OD1	2.37	0.58
18:s:85:LYS:HA	18:s:120:VAL:HG23	1.85	0.58
10:K:105:VAL:O	10:K:153:LEU:HD13	2.04	0.58
10:K:245:TYR:HA	10:K:248:ILE:HG22	1.86	0.58
10:K:310:MET:HB2	15:P:93:LEU:HD22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:50:VAL:HG12	22:W:75:ILE:HD13	1.86	0.58
1:a:58:GLY:H	1:a:100:ASP:HA	1.67	0.58
10:k:30:THR:HG22	30:k:603:HEA:H14	1.86	0.58
9:J:28:TYR:OH	25:L:402:CDL:OA3	2.20	0.58
10:K:267:VAL:HG21	10:K:270:GLU:HB3	1.85	0.58
10:K:418:PHE:O	10:K:422:ASN:ND2	2.29	0.58
1:a:209:VAL:HG13	1:a:390:LEU:HD22	1.86	0.58
1:a:441:GLY:HA2	8:h:13:TRP:HB3	1.84	0.58
2:b:84:ARG:NH2	2:b:159:LEU:HD21	2.19	0.58
3:c:156:LEU:H	3:c:203:PRO:HD3	1.68	0.58
11:L:215:ASN:HD22	11:L:227:ARG:NH2	2.02	0.58
16:q:126:ASP:HA	16:q:129:LYS:HG2	1.85	0.58
9:J:221:MET:HE1	29:J:406:UQ6:H4M2	1.86	0.58
11:L:288:LYS:NZ	25:L:402:CDL:OA3	2.27	0.58
15:P:122:TYR:O	15:P:186:HIS:NE2	2.37	0.58
22:W:42:PRO:HD2	22:W:45:GLU:OE2	2.04	0.58
1:a:248:GLU:HG3	1:a:433:ILE:HG13	1.86	0.58
14:o:47:ASN:HB2	14:o:50:MET:HE3	1.86	0.58
11:L:122:ASN:O	11:L:125:VAL:HG22	2.04	0.57
3:c:55:TYR:CZ	3:c:59:MET:HE1	2.39	0.57
11:l:215:ASN:HD22	11:l:218:PHE:HB2	1.69	0.57
14:O:143:ILE:HD11	18:S:63:ILE:HG23	1.85	0.57
9:j:36:LEU:HD12	9:j:92:VAL:HG22	1.85	0.57
15:p:200:THR:OG1	15:p:203:ARG:O	2.22	0.57
21:v:53:TRP:CG	21:v:54:PRO:HD3	2.39	0.57
6:F:53:ASN:HB2	6:F:56:MET:HE2	1.85	0.57
7:G:117:LEU:O	7:G:118:GLU:HG3	2.05	0.57
9:J:123:LEU:O	9:J:127:THR:HG23	2.04	0.57
10:K:241:HIS:NE2	10:K:245:TYR:OH	2.37	0.57
10:K:347:LEU:HD21	10:K:379:TYR:CD1	2.39	0.57
1:A:441:GLY:HA2	8:H:13:TRP:HB3	1.85	0.57
2:B:82:LEU:HD12	2:B:83:ASP:H	1.69	0.57
8:H:9:TYR:H	9:J:204:HIS:CD2	2.22	0.57
10:k:245:TYR:HA	10:k:248:ILE:HG22	1.86	0.57
2:B:60:ASN:H	2:B:112:THR:HB	1.69	0.57
7:G:147:LYS:OXT	11:L:246:GLN:NE2	2.35	0.57
9:J:228:LYS:HG3	11:L:292:TRP:HE1	1.70	0.57
14:O:156:HIS:HB3	14:O:247:ILE:HG22	1.85	0.57
15:P:163:THR:HG22	15:P:235:LYS:HD3	1.86	0.57
10:k:131:PRO:HG2	10:k:229:PRO:HB3	1.86	0.57
10:K:313:ALA:O	10:K:316:THR:OG1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:364:ASP:HB2	10:K:368:HIS:HB2	1.87	0.57
11:L:263:HIS:CD2	11:L:266:ARG:HH21	2.22	0.57
22:W:109:LEU:HA	22:W:112:VAL:HG22	1.86	0.57
10:k:4:ARG:O	10:k:8:SER:OG	2.20	0.57
10:k:75:LEU:HA	10:k:79:PHE:HD2	1.70	0.57
1:A:42:HIS:CE1	1:A:44:PRO:HG3	2.38	0.57
1:A:427:TRP:NE1	5:E:12:LYS:O	2.36	0.57
9:J:300:LEU:HD23	9:J:303:LEU:HD12	1.87	0.57
14:O:36:SER:HB3	14:O:51:VAL:HG12	1.87	0.57
15:P:126:TRP:HE1	15:P:232:MET:HG3	1.70	0.57
9:j:50:MET:HE2	9:j:50:MET:HA	1.87	0.57
10:k:485:ASN:HD21	10:k:487:LYS:HB2	1.70	0.57
15:p:112:SER:HB2	20:u:12:VAL:HG22	1.87	0.57
9:J:279:TYR:OH	9:J:283:ARG:NH1	2.38	0.57
16:Q:126:ASP:HA	16:Q:129:LYS:HG2	1.86	0.57
9:J:26:ILE:HA	9:J:30:TRP:CZ3	2.40	0.57
23:c:303:PEF:H32	23:c:303:PEF:HN1	1.70	0.57
9:j:142:TRP:CD1	9:j:265:THR:HG1	2.23	0.57
10:k:32:MET:HE1	10:k:62:HIS:N	2.19	0.57
10:K:425:PHE:HA	10:K:428:MET:HE2	1.87	0.56
1:A:139:ALA:O	1:A:142:LYS:HG3	2.06	0.56
2:B:181:THR:OG1	2:B:210:PRO:O	2.17	0.56
9:J:178:ARG:HH21	3:c:82:MET:HB3	1.70	0.56
22:W:129:GLN:HG3	22:W:150:VAL:HA	1.87	0.56
22:w:129:GLN:HG3	22:w:150:VAL:HA	1.87	0.56
2:B:19:VAL:HG12	2:B:187:VAL:HB	1.86	0.56
25:H:601:CDL:H111	25:L:402:CDL:H312	1.87	0.56
9:J:354:ILE:O	9:J:358:ILE:HG22	2.05	0.56
10:K:127:TRP:CD1	30:K:604:HEA:HBD1	2.40	0.56
10:K:307:SER:HA	10:K:310:MET:HE2	1.87	0.56
16:Q:88:ILE:HG13	16:Q:111:LEU:HD21	1.86	0.56
16:Q:96:ARG:NH1	16:Q:96:ARG:O	2.33	0.56
2:b:226:GLY:N	2:b:352:ASN:OD1	2.37	0.56
10:k:98:ILE:HG23	10:k:160:LEU:HB3	1.87	0.56
14:o:8:ARG:O	14:o:12:HIS:ND1	2.36	0.56
16:q:108:PHE:HD2	16:q:139:LEU:HD11	1.71	0.56
22:w:34:LEU:HD11	22:w:75:ILE:HD11	1.87	0.56
22:w:36:SER:O	22:w:37:ARG:NE	2.37	0.56
9:J:170:SER:HB3	3:c:113:GLY:HA3	1.86	0.56
10:K:178:THR:OG1	10:K:181:LYS:NZ	2.34	0.56
10:K:457:GLY:HA2	10:K:460:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:239:HIS:CE1	19:T:63:GLU:HB3	2.40	0.56
9:j:201:LEU:HD11	28:j:404:HEM:HAA1	1.87	0.56
11:l:288:LYS:O	11:l:292:TRP:HB2	2.05	0.56
22:w:123:THR:HG23	22:w:124:MET:SD	2.44	0.56
3:C:195:PRO:HG3	9:j:286:PRO:HA	1.86	0.56
9:J:16:TYR:HB3	29:J:406:UQ6:H1M1	1.86	0.56
13:N:5:VAL:HG12	19:T:47:ILE:HD13	1.88	0.56
15:P:185:ILE:HG12	15:P:201:PRO:HD3	1.88	0.56
19:T:143:LEU:HD23	19:T:145:PRO:HD3	1.88	0.56
6:F:117:LYS:HB2	2:b:66:LYS:HD2	1.88	0.56
22:W:34:LEU:HD12	22:W:49:ILE:HD12	1.88	0.56
1:a:263:LEU:HA	1:a:433:ILE:HG22	1.87	0.56
3:C:95:GLU:HG3	3:C:213:ILE:HG22	1.87	0.56
4:D:53:ASP:OD1	4:D:57:LYS:NZ	2.39	0.56
10:K:39:GLU:HG3	10:K:47:TYR:HB2	1.88	0.56
10:K:428:MET:HA	10:K:431:LEU:HD13	1.88	0.56
13:N:5:VAL:HG13	14:O:234:HIS:CD2	2.41	0.56
15:P:113:PRO:HB3	15:P:208:SER:HB2	1.86	0.56
18:S:47:THR:HA	18:S:50:MET:HE2	1.87	0.56
11:l:218:PHE:CD1	11:l:223:ILE:HD11	2.41	0.56
1:A:110:PRO:HB3	1:A:213:ASN:HD21	1.71	0.56
6:F:120:LEU:HD22	2:b:66:LYS:HA	1.88	0.56
15:P:181:ALA:HB3	15:P:201:PRO:HA	1.88	0.56
1:A:81:GLU:OE1	1:A:81:GLU:N	2.38	0.56
9:J:321:LEU:HB2	9:J:374:GLU:OE1	2.06	0.56
11:L:288:LYS:O	11:L:292:TRP:HB2	2.05	0.56
10:k:418:PHE:O	10:k:422:ASN:ND2	2.31	0.56
1:A:450:SER:O	23:A:503:PEF:N	2.38	0.56
9:J:359:TYR:CE1	9:J:363:PHE:HE2	2.24	0.56
10:K:534:SER:HB3	19:T:86:LEU:HB2	1.87	0.56
1:a:302:LEU:HB3	1:a:350:GLN:HG3	1.88	0.56
11:l:93:GLY:HA2	11:l:250:ASP:HB3	1.87	0.56
11:l:96:VAL:HG21	11:l:247:MET:HG2	1.88	0.56
11:l:126:ARG:O	11:l:129:ALA:N	2.38	0.56
8:H:86:ARG:NH2	8:H:90:GLU:OE2	2.39	0.55
11:L:155:ILE:H	11:L:155:ILE:HD12	1.70	0.55
9:j:59:GLU:HG2	9:j:60:LEU:HG	1.88	0.55
10:k:75:LEU:HD13	10:k:250:PRO:HB2	1.88	0.55
3:C:179:PRO:HG2	9:j:265:THR:HG21	1.88	0.55
10:K:342:ILE:HG22	23:W:202:PEF:H212	1.88	0.55
14:O:239:HIS:HE1	19:T:63:GLU:HB3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:70:LEU:HD21	30:k:603:HEA:H273	1.88	0.55
1:A:59:ALA:N	1:A:99:ARG:O	2.39	0.55
2:B:62:ARG:HH12	2:B:104:ALA:HA	1.72	0.55
3:C:180:CYS:HB2	24:C:301:FES:S2	2.46	0.55
10:K:217:ASN:HA	18:S:104:LYS:HD2	1.87	0.55
15:P:116:THR:HG21	20:U:61:LEU:H	1.71	0.55
10:k:105:VAL:O	10:k:153:LEU:HD13	2.06	0.55
2:B:184:ASN:ND2	2:B:215:LEU:H	2.04	0.55
14:O:15:HIS:HE1	14:O:76:LEU:HB3	1.71	0.55
20:U:54:THR:HA	20:U:58:LEU:HB2	1.89	0.55
15:p:213:ARG:HH21	17:r:47:PHE:HB3	1.72	0.55
9:J:273:TRP:HA	9:J:276:LEU:HD23	1.88	0.55
10:K:390:PHE:HE2	10:K:417:ILE:HD13	1.71	0.55
10:K:390:PHE:HE1	30:K:604:HEA:H242	1.71	0.55
10:k:347:LEU:HB3	10:k:383:MET:SD	2.47	0.55
1:A:77:PHE:HB3	1:A:104:TYR:CE2	2.42	0.55
9:J:192:ALA:O	9:J:195:ILE:HG22	2.06	0.55
16:Q:48:THR:OG1	16:Q:50:GLU:OE1	2.23	0.55
7:g:78:LEU:HD13	7:g:142:LEU:HD22	1.88	0.55
22:w:61:TRP:CD1	22:w:63:GLN:H	2.25	0.55
28:J:405:HEM:HMC2	28:J:405:HEM:HBC2	1.89	0.55
29:J:406:UQ6:H33	29:j:407:UQ6:H272	1.89	0.55
10:K:27:MET:HE3	12:M:60:GLY:HA3	1.88	0.55
16:Q:118:GLU:HB3	21:V:26:GLU:HB2	1.88	0.55
11:l:180:ILE:HG12	28:l:401:HEM:HMA1	1.88	0.55
15:p:185:ILE:HG12	15:p:201:PRO:HD3	1.87	0.55
2:B:230:ARG:HG2	2:B:355:ALA:HB3	1.87	0.55
4:D:48:TRP:HB2	4:D:51:PHE:HB2	1.89	0.55
7:G:78:LEU:HD13	7:G:142:LEU:HD22	1.89	0.55
13:N:50:ASN:HA	13:N:53:ARG:HD3	1.89	0.55
7:g:117:LEU:O	7:g:118:GLU:HG3	2.06	0.55
14:O:118:VAL:HG13	20:U:28:TRP:HE1	1.71	0.55
16:Q:106:ARG:NH2	22:W:77:TYR:HA	2.21	0.55
19:T:42:GLY:O	19:T:45:THR:OG1	2.25	0.55
10:k:334:LEU:HD21	23:w:202:PEF:H142	1.89	0.55
2:B:139:VAL:HG13	2:B:288:PHE:CE2	2.42	0.55
9:J:69:MET:HE1	9:J:80:TYR:CZ	2.42	0.55
1:a:293:PRO:HG2	2:b:53:ARG:HD2	1.88	0.55
10:k:495:PRO:HD2	22:w:83:ARG:HD3	1.89	0.55
10:k:514:ILE:HA	19:t:123:TRP:HE1	1.72	0.55
13:n:37:PHE:CE1	14:o:50:MET:HB2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s:19:LYS:HD2	18:s:21:ALA:H	1.72	0.55
1:A:268:GLU:HG3	1:A:274:ASN:HB3	1.90	0.54
2:B:146:LEU:HD21	2:B:242:GLY:HA3	1.89	0.54
10:K:243:GLU:HA	10:K:246:ILE:HD12	1.88	0.54
9:j:300:LEU:HA	9:j:303:LEU:HD13	1.89	0.54
10:k:331:SER:H	15:p:71:ALA:HB2	1.72	0.54
22:w:34:LEU:HG	22:w:38:TRP:CD1	2.41	0.54
1:A:53:VAL:HG13	1:A:120:LEU:HD21	1.89	0.54
1:A:318:PHE:CZ	1:A:329:GLY:HA3	2.42	0.54
1:A:353:ARG:HA	1:A:356:ILE:HG22	1.89	0.54
2:B:190:GLU:OE1	2:B:190:GLU:N	2.40	0.54
5:E:18:VAL:O	5:E:21:ILE:HG22	2.07	0.54
8:H:77:ASN:HA	8:H:80:LEU:HD12	1.89	0.54
23:J:407:PEF:H401	29:j:407:UQ6:H312	1.89	0.54
30:K:601:HEA:H202	30:K:601:HEA:H242	1.88	0.54
14:O:143:ILE:HG12	18:S:67:ALA:HB2	1.90	0.54
8:h:68:TYR:O	8:h:72:ASN:ND2	2.41	0.54
10:K:83:LEU:HD22	10:K:185:PHE:HD2	1.72	0.54
10:K:358:LEU:HA	10:K:363:LEU:HD23	1.89	0.54
14:O:117:ASP:HB3	14:O:122:ALA:HB2	1.88	0.54
11:l:215:ASN:ND2	11:l:218:PHE:HB2	2.22	0.54
8:H:70:TRP:O	8:H:74:ASN:ND2	2.40	0.54
9:J:330:VAL:HG23	23:J:401:PEF:H391	1.88	0.54
10:K:218:THR:HB	14:O:196:ILE:HG21	1.90	0.54
15:P:204:LEU:HD12	20:U:63:TRP:CD1	2.42	0.54
18:S:34:LYS:O	18:S:38:MET:HG2	2.07	0.54
2:B:37:GLY:HA2	2:B:41:TYR:CD2	2.42	0.54
10:K:101:ILE:HG13	10:K:160:LEU:HD13	1.89	0.54
22:W:99:VAL:HG11	23:W:202:PEF:H352	1.88	0.54
1:a:98:SER:O	1:a:99:ARG:NH1	2.35	0.54
1:a:114:ASP:OD1	1:a:115:LYS:N	2.41	0.54
16:q:77:PHE:HE1	16:q:83:PRO:HG2	1.72	0.54
10:K:172:MET:HE1	14:O:13:PRO:HG3	1.90	0.54
12:M:42:VAL:HG22	12:M:49:TYR:HE1	1.71	0.54
19:T:102:SER:OG	19:T:107:ARG:NH1	2.40	0.54
1:a:108:SER:OG	1:a:112:SER:OG	2.25	0.54
2:B:54:PHE:HE2	2:B:114:PHE:HA	1.73	0.54
10:K:29:GLY:HA2	10:K:32:MET:HG2	1.89	0.54
2:b:247:LYS:NZ	2:b:280:THR:O	2.37	0.54
10:k:218:THR:HB	14:o:196:ILE:HG21	1.90	0.54
14:o:136:GLU:HA	14:o:139:LEU:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:CYS:SG	3:C:161:HIS:HB3	2.48	0.54
27:J:402:CN5:H37	29:j:405:UQ6:H8	1.90	0.54
10:K:4:ARG:NH2	10:K:13:ASP:OD2	2.39	0.54
14:O:163:ASN:O	14:O:164:ARG:NE	2.41	0.54
1:a:96:ASN:OD1	1:a:97:ILE:N	2.41	0.54
15:p:113:PRO:HD2	20:u:58:LEU:HG	1.89	0.54
19:t:62:GLN:NE2	19:t:63:GLU:OE2	2.40	0.54
21:v:52:GLY:O	21:v:56:ALA:N	2.31	0.54
2:B:166:ARG:NH1	2:B:167:VAL:O	2.40	0.54
10:K:71:VAL:HG21	10:K:385:ALA:HB1	1.90	0.54
30:K:604:HEA:HBA2	30:K:604:HEA:CMA	2.38	0.54
1:a:240:LYS:NZ	22:w:40:ASN:OD1	2.24	0.54
23:j:406:PEF:N	23:j:406:PEF:O1P	2.39	0.54
10:k:37:ARG:NH1	30:k:603:HEA:HMA	2.23	0.54
25:k:602:CDL:H762	25:k:602:CDL:H571	1.90	0.54
14:o:11:GLN:HG2	14:o:12:HIS:CD2	2.42	0.54
14:o:209:THR:O	14:o:212:HIS:ND1	2.41	0.54
2:B:270:LEU:HD12	2:B:300:ASN:HB3	1.90	0.54
9:j:332:ASN:ND2	9:j:358:ILE:HG13	2.22	0.54
16:q:48:THR:OG1	16:q:50:GLU:OE1	2.26	0.54
3:c:161:HIS:O	3:c:162:LEU:HD12	2.08	0.53
28:j:403:HEM:HAA1	28:j:403:HEM:O1D	2.07	0.53
10:K:69:PHE:CD1	10:K:106:LEU:HD12	2.43	0.53
15:P:31:PRO:HA	15:P:34:GLU:HG2	1.90	0.53
16:Q:137:VAL:HG12	16:Q:139:LEU:HD23	1.90	0.53
8:h:69:TRP:NE1	9:j:351:MET:SD	2.81	0.53
11:l:224:ALA:HB3	28:l:401:HEM:HBD2	1.90	0.53
17:r:39:ASP:O	17:r:43:LYS:HG2	2.09	0.53
10:K:523:ALA:O	10:K:526:SER:OG	2.24	0.53
19:T:37:LEU:HD11	19:T:69:LEU:HA	1.90	0.53
2:b:58:ASN:H	2:b:64:ALA:HA	1.74	0.53
9:j:173:ASN:OD1	9:j:177:GLN:NE2	2.41	0.53
2:B:31:LEU:HD13	2:B:197:LEU:HD21	1.89	0.53
1:a:433:ILE:HD13	1:a:448:ILE:HD13	1.90	0.53
26:a:502:PCF:H31	23:a:504:PEF:H111	1.89	0.53
3:c:85:THR:OG1	9:j:71:ASP:O	2.25	0.53
9:j:26:ILE:HG23	9:j:30:TRP:CE3	2.43	0.53
15:p:193:LEU:HD12	15:p:236:ILE:HD13	1.91	0.53
19:t:37:LEU:HD11	19:t:69:LEU:HA	1.90	0.53
20:u:36:LYS:HB3	20:u:40:MET:HE1	1.91	0.53
1:A:252:ARG:NH1	8:H:21:GLN:HE22	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:HIS:HE1	3:C:181:HIS:CE1	2.23	0.53
7:g:109:GLN:HA	7:g:114:TYR:CD2	2.44	0.53
1:A:216:HIS:HA	1:A:219:LEU:HD23	1.90	0.53
11:l:136:ASP:HB2	11:l:147:ARG:HD2	1.91	0.53
14:o:40:THR:HG21	14:o:51:VAL:HG11	1.90	0.53
2:B:38:GLY:HA2	2:B:87:ILE:HD11	1.91	0.53
22:W:136:LEU:HA	22:W:139:LYS:HG2	1.91	0.53
2:b:151:PHE:HD2	2:b:155:LEU:HD22	1.73	0.53
10:k:18:TYR:HE1	10:k:103:PHE:HB2	1.74	0.53
16:q:130:ASP:OD1	16:q:131:VAL:N	2.42	0.53
21:v:26:GLU:HA	21:v:27:SER:OG	2.09	0.53
1:A:271:ASN:HD21	1:A:397:LYS:HA	1.73	0.53
1:A:341:ASP:OD2	9:J:4:ARG:NH2	2.42	0.53
14:O:244:GLU:HA	14:O:247:ILE:HG12	1.91	0.53
15:P:187:ASP:N	15:P:221:CYS:SG	2.77	0.53
22:W:29:ALA:HA	22:W:32:MET:HE2	1.91	0.53
1:a:447:ARG:HH21	9:j:222:HIS:HB3	1.74	0.53
11:l:140:GLU:OE1	11:l:141:GLN:NE2	2.31	0.53
1:A:311:LEU:HD13	1:A:339:MET:HB3	1.91	0.53
6:F:73:TYR:HB2	8:H:24:ILE:HD11	1.91	0.53
10:K:503:ILE:HG12	16:Q:66:LEU:HD11	1.90	0.53
11:L:121:THR:HG1	11:L:124:GLU:CD	2.17	0.53
14:O:142:THR:HB	14:O:261:TYR:CZ	2.44	0.53
22:W:61:TRP:CD1	22:W:63:GLN:H	2.26	0.53
3:c:51:LYS:HD3	25:c:302:CDL:HA61	1.91	0.53
10:k:200:LEU:HD23	10:k:239:PHE:HE1	1.74	0.53
9:J:27:ASN:N	9:J:30:TRP:HZ3	1.99	0.53
9:J:171:VAL:HA	9:J:175:THR:HG21	1.90	0.53
1:a:450:SER:OG	23:a:504:PEF:O4P	2.23	0.53
9:j:171:VAL:HA	9:j:175:THR:HG21	1.89	0.53
9:j:193:MET:HA	9:j:193:MET:HE3	1.90	0.53
13:n:50:ASN:HA	13:n:53:ARG:HD3	1.90	0.53
14:o:163:ASN:O	14:o:164:ARG:NE	2.42	0.53
22:w:32:MET:O	22:w:35:GLN:NE2	2.38	0.53
3:C:63:MET:HE1	11:L:287:VAL:HG11	1.90	0.52
7:G:92:LYS:HA	7:G:95:VAL:HG12	1.89	0.52
9:J:138:GLN:HB2	9:J:258:ILE:HB	1.91	0.52
14:O:262:VAL:HG12	14:O:263:VAL:HG13	1.90	0.52
9:j:80:TYR:OH	11:l:182:LYS:NZ	2.40	0.52
9:j:331:PHE:HA	9:j:334:VAL:HG12	1.92	0.52
22:w:150:VAL:HG13	22:w:151:GLN:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:73:GLY:O	19:T:77:GLY:N	2.42	0.52
1:a:68:GLY:O	1:a:72:LEU:HG	2.09	0.52
8:h:70:TRP:NE1	8:h:74:ASN:HD21	2.07	0.52
3:C:161:HIS:CG	24:C:301:FES:S2	2.90	0.52
6:F:38:TYR:HB2	6:F:43:LEU:HB2	1.90	0.52
8:H:58:TYR:CE2	9:J:323:LYS:HD2	2.45	0.52
9:J:72:VAL:HG13	9:J:75:GLY:HA3	1.90	0.52
1:a:318:PHE:CE2	1:a:329:GLY:HA3	2.44	0.52
14:o:80:THR:H	14:o:83:VAL:HG12	1.74	0.52
1:A:76:ILE:HG13	1:A:77:PHE:N	2.25	0.52
9:J:63:SER:O	9:J:66:GLU:HG3	2.08	0.52
11:L:232:ASP:H	11:L:242:ALA:HA	1.73	0.52
19:T:107:ARG:HE	19:T:108:TYR:H	1.55	0.52
2:b:131:TYR:HA	2:b:160:LEU:HD22	1.91	0.52
4:d:47:GLY:HA2	4:d:51:PHE:HD2	1.75	0.52
10:K:369:ASP:O	15:P:222:SER:OG	2.28	0.52
10:K:403:LEU:HB3	10:K:475:GLN:HG3	1.91	0.52
12:M:40:PHE:CD2	12:M:49:TYR:HE2	2.28	0.52
6:f:101:PRO:HA	9:j:382:ARG:HH22	1.74	0.52
10:k:95:PHE:HD2	10:k:98:ILE:HG13	1.75	0.52
2:B:310:LYS:HE2	2:B:310:LYS:HA	1.90	0.52
9:J:327:PHE:HA	9:J:330:VAL:HG12	1.91	0.52
10:K:29:GLY:HA2	10:K:32:MET:HE2	1.92	0.52
14:O:136:GLU:HA	14:O:139:LEU:HD13	1.91	0.52
15:P:206:GLN:NE2	20:U:23:GLN:O	2.43	0.52
20:U:55:TYR:HA	20:U:59:CYS:HB3	1.91	0.52
21:V:35:ARG:HE	21:V:36:LEU:HD22	1.75	0.52
9:j:51:ALA:HB2	28:j:403:HEM:HMB1	1.91	0.52
10:k:37:ARG:HG3	30:k:603:HEA:HMB2	1.92	0.52
10:K:105:VAL:HG22	10:K:153:LEU:HB2	1.92	0.52
11:L:169:ASN:ND2	28:L:401:HEM:HMD1	2.25	0.52
1:A:37:VAL:HB	1:A:207:VAL:HG12	1.91	0.52
1:A:320:LEU:O	1:A:327:LEU:N	2.34	0.52
1:A:447:ARG:NH2	9:J:222:HIS:O	2.42	0.52
10:K:33:SER:OG	10:K:62:HIS:ND1	2.43	0.52
15:P:124:TRP:HA	15:P:232:MET:HE1	1.92	0.52
1:A:215:LYS:O	1:A:216:HIS:ND1	2.42	0.52
4:D:17:ARG:NH2	6:f:121:ASP:OD2	2.43	0.52
10:K:331:SER:H	15:P:71:ALA:HB2	1.75	0.52
10:K:400:ILE:HG13	10:K:401:LEU:HG	1.92	0.52
14:o:20:SER:HB3	14:o:22:TRP:CD1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:p:124:TRP:HZ2	15:p:227:THR:H	1.58	0.52
2:B:255:VAL:HG11	2:B:343:VAL:HG11	1.90	0.52
2:B:257:ALA:HB1	2:B:274:ALA:O	2.09	0.52
3:C:101:ILE:HG12	3:C:107:VAL:HG21	1.92	0.52
9:J:50:MET:SD	9:J:68:ILE:HG12	2.49	0.52
15:P:134:ILE:HD12	15:P:138:GLY:H	1.75	0.52
22:w:32:MET:HA	22:w:35:GLN:HG3	1.92	0.52
15:P:115:MET:HA	15:P:115:MET:HE2	1.91	0.51
18:S:119:PRO:O	18:S:123:ARG:NH2	2.43	0.51
1:a:155:ASP:OD1	1:a:156:HIS:N	2.43	0.51
10:k:11:ALA:HA	10:k:14:ILE:HG22	1.91	0.51
10:k:333:ARG:NH1	10:k:492:ASN:O	2.43	0.51
19:t:124:LEU:HD11	19:t:134:CYS:HA	1.92	0.51
1:A:369:LEU:O	1:A:372:LEU:HG	2.10	0.51
16:Q:130:ASP:OD1	16:Q:131:VAL:N	2.43	0.51
9:j:29:TRP:O	9:j:32:MET:HB3	2.11	0.51
9:j:127:THR:HG22	9:j:186:VAL:CG1	2.40	0.51
9:j:214:GLY:O	9:j:218:ARG:NE	2.42	0.51
11:l:184:ARG:HH21	28:l:401:HEM:CGA	2.23	0.51
15:p:99:PRO:HA	15:p:102:ILE:HG22	1.91	0.51
1:A:351:TRP:HB3	1:A:426:LEU:HD11	1.93	0.51
5:E:47:LYS:NZ	11:L:83:GLU:OE1	2.43	0.51
7:G:100:GLU:O	7:G:103:GLU:HG3	2.10	0.51
13:N:9:GLN:OE1	13:N:13:GLN:NE2	2.33	0.51
14:O:11:GLN:HG2	14:O:12:HIS:CD2	2.44	0.51
10:k:151:LEU:HD11	10:k:207:ILE:HG21	1.92	0.51
13:n:2:ALA:HB2	14:o:233:TYR:HB2	1.92	0.51
12:M:38:ILE:HD12	12:M:39:PRO:HD2	1.91	0.51
12:M:62:ALA:O	12:M:66:VAL:HG22	2.10	0.51
15:P:115:MET:HG3	15:P:175:ILE:HG23	1.92	0.51
15:P:175:ILE:O	15:P:209:ALA:N	2.39	0.51
22:W:136:LEU:O	22:W:140:ASN:N	2.43	0.51
4:d:3:TYR:OH	4:d:8:SER:OG	2.27	0.51
8:h:16:MET:HE2	8:h:16:MET:HA	1.92	0.51
8:h:81:TYR:OH	9:j:345:GLU:OE1	2.28	0.51
14:o:222:MET:HE1	14:o:245:THR:HB	1.91	0.51
2:B:45:ASP:OD1	2:B:46:GLY:N	2.42	0.51
3:C:111:TRP:HE1	3:C:215:GLY:HA2	1.76	0.51
13:N:9:GLN:NE2	14:O:75:TYR:O	2.44	0.51
1:a:29:VAL:HG11	1:a:400:LYS:HD3	1.91	0.51
1:a:65:TYR:HB3	22:w:29:ALA:HB1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:202:VAL:HG21	10:k:238:PHE:HD2	1.74	0.51
10:k:319:LYS:HD2	10:k:322:SER:OG	2.10	0.51
10:k:498:VAL:HG23	16:q:70:GLN:HE21	1.75	0.51
13:N:23:HIS:HB3	13:N:26:SER:HB3	1.91	0.51
2:b:341:ASP:OD2	2:b:341:ASP:N	2.43	0.51
9:j:186:VAL:HA	9:j:189:ILE:HD13	1.93	0.51
10:k:95:PHE:CD2	10:k:98:ILE:HG13	2.46	0.51
12:m:72:LEU:HD23	12:m:73:LYS:N	2.25	0.51
1:A:263:LEU:HB2	1:A:330:PHE:HD2	1.76	0.51
10:K:56:ASN:O	10:K:60:VAL:HG23	2.10	0.51
12:M:72:LEU:HD23	12:M:73:LYS:N	2.25	0.51
14:O:132:VAL:HG13	18:S:81:ARG:HD3	1.92	0.51
1:a:203:ASN:OD1	1:a:229:SER:N	2.44	0.51
25:c:302:CDL:H121	25:k:602:CDL:H152	1.93	0.51
1:A:349:LYS:NZ	1:A:454:MET:HB3	2.26	0.51
26:H:602:PCF:H321	23:W:202:PEF:H312	1.92	0.51
1:a:443:LEU:HD22	1:a:447:ARG:HD2	1.93	0.51
10:k:178:THR:OG1	10:k:181:LYS:NZ	2.30	0.51
19:t:94:MET:HG2	19:t:95:LYS:HD3	1.92	0.51
22:w:41:MET:HE3	22:w:46:GLN:HE22	1.76	0.51
3:C:161:HIS:NE2	3:C:181:HIS:HB2	2.25	0.51
6:F:26:VAL:N	6:F:27:PRO:HD2	2.25	0.51
10:K:108:MET:N	10:K:108:MET:SD	2.83	0.51
2:b:364:TYR:N	2:b:367:GLU:OE2	2.44	0.51
11:l:135:ASP:OD2	11:l:146:LYS:HG2	2.10	0.51
2:B:26:THR:O	2:B:191:ASN:ND2	2.35	0.51
16:Q:131:VAL:HA	16:Q:134:GLU:HG2	1.92	0.51
22:W:84:ARG:HD2	22:W:85:PRO:O	2.11	0.51
2:b:181:THR:OG1	2:b:212:GLY:N	2.41	0.51
19:t:63:GLU:HG3	19:t:71:LEU:HD21	1.92	0.51
10:K:10:ASN:HB3	10:K:524:VAL:HG11	1.91	0.50
10:K:509:VAL:C	10:K:510:LYS:HD2	2.35	0.50
12:M:37:ASN:O	12:M:37:ASN:ND2	2.41	0.50
3:c:114:LYS:HD2	3:c:158:ILE:HG13	1.93	0.50
11:l:105:HIS:HB3	11:l:177:LEU:HD13	1.92	0.50
1:A:319:SER:HA	1:A:328:TRP:HA	1.93	0.50
3:C:146:ARG:NH2	3:C:188:SER:O	2.44	0.50
10:K:111:VAL:HA	10:K:114:VAL:HG12	1.94	0.50
15:P:93:LEU:HA	15:P:96:ILE:HG12	1.93	0.50
16:Q:57:GLU:HG3	16:Q:90:LYS:HG2	1.93	0.50
1:a:318:PHE:O	1:a:329:GLY:N	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:77:THR:HG23	9:j:74:ASN:CG	2.37	0.50
3:c:161:HIS:CE1	3:c:162:LEU:HD13	2.45	0.50
9:j:332:ASN:HD21	9:j:358:ILE:HG13	1.75	0.50
10:k:56:ASN:O	10:k:60:VAL:HG23	2.11	0.50
19:t:115:PRO:HG2	19:t:118:SER:HB2	1.93	0.50
10:K:358:LEU:HD13	10:K:367:PHE:HB2	1.92	0.50
14:O:8:ARG:O	14:O:12:HIS:ND1	2.44	0.50
1:a:297:LEU:H	1:a:297:LEU:HD23	1.76	0.50
2:b:259:TYR:HD1	2:b:260:LEU:HD12	1.75	0.50
15:p:134:ILE:HD12	15:p:138:GLY:H	1.76	0.50
22:w:34:LEU:HG	22:w:38:TRP:HD1	1.76	0.50
25:C:302:CDL:H721	25:L:402:CDL:H602	1.92	0.50
10:K:261:THR:HG21	10:K:395:TYR:CE1	2.46	0.50
10:K:339:LEU:HD23	10:K:414:PHE:CD2	2.46	0.50
9:j:190:ILE:O	9:j:194:VAL:HG23	2.11	0.50
10:K:438:ARG:NH1	30:K:604:HEA:O2D	2.44	0.50
14:O:133:GLN:HG3	14:O:135:THR:H	1.77	0.50
9:J:157:VAL:HG23	4:d:50:LYS:HD3	1.93	0.50
9:j:30:TRP:HH2	9:j:209:PRO:HG3	1.77	0.50
2:B:232:ARG:NH2	2:b:162:ASP:OD2	2.36	0.50
9:J:275:LEU:HD23	29:J:408:UQ6:H71	1.92	0.50
1:a:353:ARG:NE	23:a:501:PEF:O1P	2.36	0.50
8:h:21:GLN:OE1	8:h:21:GLN:N	2.44	0.50
25:h:601:CDL:H341	9:j:32:MET:HE1	1.94	0.50
9:j:127:THR:HG22	9:j:186:VAL:HG13	1.94	0.50
6:F:51:GLU:OE2	6:F:56:MET:HB3	2.12	0.50
9:J:29:TRP:HB3	9:J:99:LYS:HG3	1.94	0.50
10:K:283:LEU:HD13	10:K:286:LEU:HD13	1.94	0.50
10:K:371:TYR:O	10:K:374:VAL:HG22	2.11	0.50
10:K:500:SER:HB2	10:K:503:ILE:HD13	1.94	0.50
11:L:247:MET:N	11:L:247:MET:SD	2.85	0.50
12:M:69:TYR:O	13:N:56:LYS:NZ	2.39	0.50
14:O:56:PHE:O	14:O:60:THR:HG23	2.12	0.50
2:b:230:ARG:NH1	2:b:359:VAL:HG12	2.26	0.50
10:k:310:MET:HE2	15:p:93:LEU:HB3	1.93	0.50
10:k:312:ILE:O	10:k:315:PRO:HD2	2.11	0.50
1:A:94:SER:OG	1:A:95:SER:N	2.45	0.50
3:C:167:ILE:HG23	3:C:179:PRO:HG3	1.92	0.50
9:J:294:THR:HA	9:J:297:ALA:HB3	1.93	0.50
10:K:175:ASN:HB2	19:T:83:THR:HA	1.93	0.50
16:Q:132:ARG:NH2	16:Q:140:LYS:HG3	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:317:ALA:O	2:b:321:THR:HG23	2.12	0.50
3:c:101:ILE:HG21	3:c:152:TRP:HZ3	1.77	0.50
9:j:63:SER:O	9:j:66:GLU:HG3	2.11	0.50
10:k:436:MET:HE1	10:k:444:PRO:HD2	1.93	0.50
30:k:604:HEA:H241	15:p:93:LEU:HD11	1.93	0.50
11:l:187:GLY:HA2	11:l:190:TYR:HB3	1.93	0.50
13:N:38:ALA:HA	13:N:41:VAL:HG12	1.94	0.49
18:S:89:ASP:OD1	18:S:89:ASP:N	2.45	0.49
19:T:124:LEU:HD11	19:T:134:CYS:HA	1.93	0.49
22:W:126:LYS:HE3	22:W:153:LYS:HA	1.93	0.49
1:a:42:HIS:CE1	1:a:44:PRO:HG3	2.46	0.49
2:b:21:ALA:N	2:b:194:GLU:OE2	2.45	0.49
5:e:48:LEU:HD21	11:l:84:THR:HG21	1.94	0.49
6:f:85:HIS:O	8:h:50:ARG:NH2	2.45	0.49
1:A:155:ASP:OD1	1:A:156:HIS:N	2.45	0.49
1:A:443:LEU:H	1:A:443:LEU:HD12	1.77	0.49
2:B:355:ALA:HB1	2:B:362:LEU:HD12	1.94	0.49
6:F:101:PRO:HB3	9:J:382:ARG:NH1	2.27	0.49
9:J:186:VAL:HA	9:J:189:ILE:HD13	1.94	0.49
16:Q:77:PHE:HZ	16:Q:111:LEU:HD12	1.76	0.49
20:U:70:GLN:HA	20:U:73:LYS:HG2	1.94	0.49
3:c:162:LEU:HB2	24:c:301:FES:S2	2.53	0.49
9:j:4:ARG:NH1	25:j:402:CDL:OB3	2.35	0.49
9:j:32:MET:SD	9:j:92:VAL:HG23	2.53	0.49
9:j:182:LEU:O	9:j:186:VAL:HG12	2.12	0.49
10:k:25:SER:HB2	10:k:65:LEU:HD21	1.94	0.49
28:l:401:HEM:HBC2	28:l:401:HEM:HMC1	1.94	0.49
18:s:66:THR:HA	18:s:69:ASN:HD21	1.77	0.49
21:v:37:ILE:HA	21:v:40:ILE:HG12	1.94	0.49
4:D:63:GLY:N	4:D:64:PRO:HD3	2.27	0.49
10:k:219:SER:HB3	10:k:222:GLU:HB2	1.93	0.49
10:k:298:ASP:OD1	20:u:22:ASN:ND2	2.46	0.49
9:J:192:ALA:O	9:J:196:MET:HG3	2.12	0.49
15:P:29:ALA:HA	15:P:213:ARG:HE	1.77	0.49
10:k:2:VAL:HG13	10:k:6:LEU:HD12	1.93	0.49
11:l:76:TRP:HH2	11:l:252:THR:HG21	1.78	0.49
14:o:64:LEU:O	14:o:67:ARG:HG3	2.12	0.49
14:o:238:GLY:O	14:o:240:HIS:ND1	2.46	0.49
17:r:28:MET:HE1	21:v:47:LEU:HD13	1.94	0.49
19:t:42:GLY:O	19:t:45:THR:OG1	2.29	0.49
9:J:98:ALA:HB2	23:J:401:PEF:H412	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:269:LEU:O	11:L:273:THR:HG23	2.12	0.49
14:O:238:GLY:O	14:O:240:HIS:ND1	2.45	0.49
20:U:18:PHE:CE2	20:U:20:GLN:HB3	2.47	0.49
1:a:42:HIS:HD2	1:a:215:LYS:HB3	1.77	0.49
1:a:214:ILE:HD12	1:a:218:ASP:HB2	1.95	0.49
2:b:37:GLY:HA2	2:b:41:TYR:CD2	2.46	0.49
10:k:230:ILE:HD11	15:p:200:THR:HG21	1.93	0.49
12:m:72:LEU:HD23	12:m:73:LYS:H	1.77	0.49
15:p:17:VAL:O	15:p:26:GLN:NE2	2.46	0.49
16:q:56:TYR:O	16:q:60:PHE:HD2	1.94	0.49
23:A:503:PEF:H192	23:C:304:PEF:H181	1.94	0.49
2:B:52:ASN:ND2	2:B:82:LEU:HB2	2.28	0.49
2:B:66:LYS:NZ	6:f:117:LYS:HB2	2.27	0.49
9:J:129:PHE:HZ	9:J:144:ALA:HA	1.78	0.49
27:J:402:CN5:H32	9:j:12:LEU:HD11	1.94	0.49
17:R:28:MET:HE1	21:V:43:TRP:CH2	2.47	0.49
14:o:142:THR:HB	14:o:261:TYR:CZ	2.48	0.49
2:B:245:VAL:HG22	2:B:283:GLY:O	2.13	0.49
8:H:72:ASN:O	8:H:75:GLU:HG3	2.12	0.49
9:J:29:TRP:O	9:J:32:MET:HB3	2.12	0.49
9:J:65:VAL:O	9:J:68:ILE:HG22	2.12	0.49
9:J:300:LEU:HA	9:J:303:LEU:HD12	1.95	0.49
9:J:331:PHE:HA	9:J:334:VAL:HG12	1.93	0.49
28:J:405:HEM:HBB2	28:J:405:HEM:CMB	2.41	0.49
10:K:43:PRO:O	10:K:46:GLN:NE2	2.34	0.49
11:L:288:LYS:HG2	11:L:292:TRP:HD1	1.78	0.49
14:O:213:PHE:HD1	14:O:216:MET:HE1	1.78	0.49
16:Q:82:VAL:HG13	16:Q:114:LYS:HE2	1.93	0.49
3:c:190:ARG:HA	3:c:199:ASN:ND2	2.28	0.49
14:o:15:HIS:HE1	14:o:76:LEU:HB3	1.76	0.49
15:P:126:TRP:CG	15:P:128:TYR:HH	2.31	0.49
15:P:239:VAL:HB	15:P:243:LYS:HB3	1.95	0.49
16:Q:100:ASP:OD2	16:Q:103:THR:HG23	2.12	0.49
8:h:12:TRP:H	8:h:15:HIS:CD2	2.30	0.49
10:k:108:MET:HE1	14:o:27:SER:HB2	1.95	0.49
10:k:261:THR:HG21	10:k:395:TYR:OH	2.12	0.49
11:l:223:ILE:HG22	11:l:225:MET:H	1.77	0.49
20:u:54:THR:HA	20:u:58:LEU:HB2	1.95	0.49
2:B:59:THR:OG1	2:B:62:ARG:O	2.25	0.49
10:K:70:LEU:HD21	30:K:604:HEA:H273	1.95	0.49
23:e:101:PEF:H312	26:k:605:PCF:H222	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:h:601:CDL:H391	9:j:91:MET:HG2	1.95	0.49
10:k:342:ILE:HG23	15:p:58:LEU:HD11	1.94	0.49
10:k:360:ASN:HB3	10:k:363:LEU:HB2	1.94	0.49
19:t:73:GLY:O	19:t:78:ILE:N	2.38	0.49
9:J:58:ILE:HG12	9:J:173:ASN:OD1	2.12	0.49
9:J:99:LYS:C	9:J:99:LYS:HD3	2.38	0.49
11:L:198:TYR:HB3	11:L:227:ARG:HE	1.78	0.49
2:b:84:ARG:CZ	2:b:159:LEU:HD21	2.42	0.49
4:d:10:LYS:HD3	4:d:11:THR:O	2.11	0.49
5:e:18:VAL:HA	5:e:21:ILE:HG22	1.95	0.49
10:k:105:VAL:HG22	10:k:153:LEU:HB2	1.95	0.49
14:o:72:GLU:HG3	14:o:76:LEU:HD23	1.95	0.49
16:q:122:LYS:HE3	21:v:24:ILE:HD11	1.95	0.49
15:P:46:TYR:HA	15:P:49:VAL:HG22	1.95	0.48
1:a:62:GLU:OE2	1:a:66:ASN:HB3	2.13	0.48
1:a:457:TRP:HE3	5:e:13:ARG:HG3	1.77	0.48
5:e:55:ARG:HH21	5:e:56:ILE:HD12	1.78	0.48
9:j:219:ILE:HG13	9:j:225:PHE:HE1	1.79	0.48
10:k:144:VAL:O	10:k:148:ILE:HG12	2.13	0.48
10:k:162:ALA:HB2	10:k:196:LEU:HD22	1.95	0.48
11:l:100:VAL:HG23	11:l:233:MET:HE1	1.95	0.48
14:o:117:ASP:HB3	14:o:122:ALA:HB2	1.95	0.48
14:o:132:VAL:HG13	18:s:81:ARG:HD3	1.95	0.48
1:A:405:GLU:C	1:A:409:LYS:HZ1	2.22	0.48
3:C:106:ASN:OD1	3:C:119:ARG:NH1	2.46	0.48
3:C:181:HIS:HB3	9:j:283:ARG:HG2	1.93	0.48
10:K:18:TYR:CE1	10:K:103:PHE:HB2	2.48	0.48
1:a:49:ALA:HB2	1:a:110:PRO:HA	1.95	0.48
2:b:110:TYR:CD2	2:b:205:LEU:HD21	2.48	0.48
11:l:121:THR:HG23	11:l:122:ASN:N	2.27	0.48
3:C:146:ARG:HB3	3:C:202:ILE:HG13	1.96	0.48
16:Q:105:ILE:HA	16:Q:139:LEU:HD13	1.94	0.48
18:S:65:LEU:O	18:S:69:ASN:ND2	2.46	0.48
18:S:74:GLU:HA	18:S:78:ALA:HB3	1.94	0.48
7:g:146:LEU:HD21	11:l:245:SER:HB3	1.95	0.48
9:j:117:GLY:O	28:j:404:HEM:HMC2	2.13	0.48
10:k:404:ASN:HD22	10:k:483:LYS:HG2	1.78	0.48
15:p:116:THR:HG21	20:u:61:LEU:H	1.78	0.48
10:K:437:PRO:HB3	15:P:222:SER:HA	1.95	0.48
1:a:445:TYR:HA	1:a:448:ILE:HG22	1.95	0.48
23:a:503:PEF:H122	25:j:402:CDL:H512	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:325:PHE:O	9:j:328:ILE:HG22	2.14	0.48
10:k:213:ASP:HA	10:k:218:THR:HG23	1.96	0.48
10:k:293:TYR:HA	10:k:302:ARG:HH11	1.77	0.48
1:A:299:GLY:N	2:B:69:ARG:HH21	2.11	0.48
2:B:84:ARG:CZ	2:B:159:LEU:HD21	2.43	0.48
4:D:39:LEU:O	4:D:43:VAL:HG23	2.13	0.48
10:K:353:LEU:HB2	15:P:47:LEU:HD12	1.95	0.48
3:c:142:THR:HG23	3:c:145:ASP:H	1.78	0.48
7:g:92:LYS:HA	7:g:95:VAL:HG12	1.96	0.48
9:j:271:PRO:HB2	9:j:275:LEU:HB2	1.94	0.48
9:j:345:GLU:HB2	9:j:348:TYR:CD2	2.48	0.48
16:q:104:ALA:HA	16:q:107:VAL:HG12	1.96	0.48
16:q:106:ARG:HH21	22:w:77:TYR:HA	1.79	0.48
21:v:53:TRP:CD1	21:v:54:PRO:HD3	2.49	0.48
4:D:58:LYS:HD3	4:D:58:LYS:HA	1.72	0.48
8:H:66:TYR:OH	9:J:328:ILE:HG13	2.12	0.48
2:b:84:ARG:NH1	2:b:159:LEU:HD21	2.29	0.48
9:j:321:LEU:HB2	9:j:374:GLU:OE2	2.14	0.48
10:k:186:VAL:HA	10:k:189:ILE:HG12	1.96	0.48
10:K:135:SER:OG	10:K:136:ILE:N	2.47	0.48
13:N:31:TYR:HB3	13:N:32:PRO:HD3	1.96	0.48
19:T:110:GLY:HA3	19:T:123:TRP:HA	1.96	0.48
1:a:440:GLU:OE1	1:a:440:GLU:N	2.41	0.48
4:d:39:LEU:O	4:d:43:VAL:HG23	2.14	0.48
10:k:17:LEU:HB3	10:k:103:PHE:CZ	2.49	0.48
10:k:18:TYR:CE1	10:k:103:PHE:HB2	2.49	0.48
1:A:113:THR:HG21	1:A:214:ILE:HG21	1.96	0.48
23:A:502:PEF:H121	25:J:403:CDL:HA31	1.96	0.48
2:B:52:ASN:HD22	2:B:82:LEU:HB2	1.79	0.48
3:C:176:TRP:HB2	3:C:185:TYR:HB2	1.96	0.48
8:H:42:HIS:NE2	26:H:602:PCF:H122	2.29	0.48
9:J:365:ILE:O	9:J:369:VAL:HG12	2.13	0.48
10:K:242:PRO:O	10:K:246:ILE:HG13	2.13	0.48
2:b:230:ARG:HH11	2:b:359:VAL:HG12	1.78	0.48
9:j:59:GLU:H	9:j:59:GLU:CD	2.22	0.48
9:j:153:ALA:HB2	9:j:288:LYS:HE2	1.96	0.48
9:j:166:TRP:HE1	9:j:171:VAL:HG22	1.78	0.48
10:k:135:SER:OG	10:k:136:ILE:N	2.47	0.48
10:k:439:ARG:HE	15:p:224:LEU:HB2	1.79	0.48
25:k:602:CDL:H311	22:w:94:PHE:CE1	2.49	0.48
1:A:349:LYS:HZ3	1:A:454:MET:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:353:LEU:HD13	15:P:47:LEU:HD12	1.96	0.48
1:a:353:ARG:NH2	23:a:501:PEF:H31	2.29	0.48
10:k:320:ILE:HA	10:k:323:TRP:CE3	2.46	0.48
2:B:66:LYS:NZ	6:f:117:LYS:HE2	2.29	0.47
4:D:29:ASN:HA	5:E:13:ARG:NH2	2.28	0.47
10:K:289:SER:HB3	10:K:305:PHE:CZ	2.48	0.47
10:K:294:ILE:HD12	15:P:196:LYS:HE3	1.95	0.47
11:L:121:THR:OG1	11:L:122:ASN:N	2.47	0.47
15:P:147:VAL:HG11	15:P:231:ASN:HB2	1.96	0.47
2:b:310:LYS:O	2:b:347:LYS:NZ	2.46	0.47
1:A:172:THR:HG21	1:A:242:ALA:HA	1.95	0.47
2:B:116:PRO:HG2	2:B:117:HIS:CE1	2.49	0.47
7:G:96:HIS:O	7:G:99:GLU:HG3	2.14	0.47
15:P:113:PRO:HA	15:P:174:HIS:HB3	1.95	0.47
22:W:41:MET:HE3	22:W:46:GLN:HE22	1.79	0.47
5:e:18:VAL:O	5:e:21:ILE:HG22	2.15	0.47
10:k:152:HIS:O	10:k:156:ILE:HG12	2.14	0.47
2:B:50:LEU:HD21	2:B:119:LEU:HD11	1.95	0.47
9:J:191:ALA:HA	9:J:194:VAL:HG22	1.96	0.47
25:K:603:CDL:H311	22:W:94:PHE:CE1	2.48	0.47
1:a:51:VAL:HG21	1:a:117:LEU:HD21	1.96	0.47
1:a:287:SER:OG	1:a:288:TYR:N	2.48	0.47
3:c:102:PRO:HB2	3:c:105:LYS:HB2	1.95	0.47
10:k:66:MET:HB3	30:k:603:HEA:CAC	2.44	0.47
14:o:64:LEU:HD11	14:o:67:ARG:HH21	1.80	0.47
1:A:54:VAL:HG21	1:A:391:GLY:HA3	1.96	0.47
9:J:39:CYS:SG	9:J:89:PHE:HB2	2.55	0.47
10:K:202:VAL:HG21	10:K:238:PHE:HD2	1.80	0.47
9:j:50:MET:HE1	9:j:68:ILE:CG1	2.43	0.47
9:j:50:MET:CE	9:j:68:ILE:HG12	2.43	0.47
9:j:246:TYR:CE2	11:l:81:PRO:HB3	2.49	0.47
12:m:34:VAL:HG12	12:m:35:TYR:HD2	1.78	0.47
14:o:66:PHE:O	14:o:69:ILE:HG22	2.14	0.47
1:A:91:LEU:HA	2:B:323:LEU:HD13	1.97	0.47
1:A:345:HIS:O	1:A:349:LYS:HG2	2.15	0.47
9:J:245:PHE:HA	11:L:266:ARG:HD3	1.96	0.47
10:K:115:THR:HA	10:K:118:LEU:HB2	1.96	0.47
10:K:312:ILE:O	10:K:315:PRO:HD2	2.14	0.47
14:O:106:PHE:O	14:O:110:PHE:HB2	2.14	0.47
19:T:73:GLY:O	19:T:78:ILE:N	2.35	0.47
1:a:139:ALA:O	1:a:142:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:248:GLU:HA	1:a:433:ILE:O	2.15	0.47
4:d:4:THR:HA	4:d:5:SER:HA	1.51	0.47
9:j:284:SER:OG	9:j:285:ILE:N	2.48	0.47
10:k:453:VAL:HA	10:k:456:ILE:HG22	1.95	0.47
11:l:214:TYR:O	11:l:227:ARG:NH2	2.48	0.47
1:A:328:TRP:CZ3	1:A:426:LEU:HD12	2.50	0.47
4:D:29:ASN:HA	5:E:13:ARG:HH21	1.79	0.47
10:K:368:HIS:HB3	15:P:196:LYS:HE2	1.97	0.47
16:Q:101:LEU:HD23	16:Q:105:ILE:HD11	1.97	0.47
19:T:119:HIS:ND1	19:T:120:THR:O	2.42	0.47
1:a:127:GLN:OE1	1:a:127:GLN:N	2.46	0.47
5:e:27:VAL:O	5:e:31:VAL:HG22	2.15	0.47
9:j:129:PHE:HZ	9:j:144:ALA:HA	1.78	0.47
1:A:155:ASP:O	1:A:156:HIS:ND1	2.48	0.47
1:A:253:ASP:N	1:A:253:ASP:OD1	2.45	0.47
2:B:291:ASP:OD1	2:B:292:GLN:N	2.47	0.47
8:H:36:PRO:HG2	11:L:286:TRP:CZ2	2.50	0.47
10:K:273:MET:HE1	10:K:322:SER:HB2	1.96	0.47
11:L:92:ARG:HD2	11:L:236:TYR:CD2	2.49	0.47
13:N:37:PHE:HE1	14:O:50:MET:HB3	1.79	0.47
14:O:118:VAL:HG13	20:U:28:TRP:NE1	2.30	0.47
15:P:63:MET:HA	15:P:63:MET:HE3	1.97	0.47
15:P:130:TYR:N	15:P:141:VAL:O	2.41	0.47
20:U:46:ALA:HA	20:U:49:LYS:HE3	1.97	0.47
2:b:37:GLY:O	2:b:87:ILE:HG12	2.15	0.47
6:f:5:PHE:CD2	6:f:107:ILE:HG21	2.50	0.47
9:j:235:LEU:O	9:j:238:LEU:HG	2.15	0.47
10:k:27:MET:SD	12:m:60:GLY:HA3	2.54	0.47
25:k:602:CDL:H511	25:k:602:CDL:H731	1.96	0.47
19:t:46:LEU:HD23	19:t:68:ARG:NE	2.30	0.47
9:J:196:MET:HB3	9:j:9:TYR:HE2	1.79	0.47
11:L:176:ASP:N	11:L:176:ASP:OD1	2.47	0.47
1:a:108:SER:OG	1:a:109:LEU:N	2.48	0.47
1:a:363:VAL:HG21	1:a:415:VAL:HG12	1.96	0.47
2:b:42:ALA:HB2	2:b:48:ALA:HB2	1.96	0.47
3:c:55:TYR:CD2	25:c:302:CDL:H1	2.49	0.47
2:B:151:PHE:HE1	2:B:223:PHE:HB3	1.79	0.47
10:K:389:LEU:CD2	30:K:604:HEA:H251	2.44	0.47
10:K:409:LEU:HB3	10:K:471:ILE:HG12	1.97	0.47
1:a:267:GLY:N	1:a:326:GLY:O	2.44	0.47
3:c:177:PHE:O	3:c:179:PRO:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:111:VAL:HA	10:k:114:VAL:HG12	1.97	0.47
10:k:534:SER:HB3	19:t:86:LEU:HB2	1.97	0.47
15:p:159:ARG:HD3	22:w:123:THR:HG21	1.97	0.47
3:C:91:MET:SD	3:C:92:ALA:N	2.88	0.47
10:K:75:LEU:HA	10:K:79:PHE:HD2	1.80	0.47
10:K:116:SER:HB2	10:K:143:SER:HA	1.96	0.47
10:K:493:LYS:HZ3	10:K:511:SER:HB3	1.80	0.47
11:L:96:VAL:O	11:L:100:VAL:HG12	2.15	0.47
15:P:161:LEU:HD22	15:P:218:TYR:CD1	2.50	0.47
16:Q:92:LEU:HD11	16:Q:108:PHE:HE1	1.80	0.47
28:j:403:HEM:O1D	28:j:403:HEM:HHA	2.14	0.47
30:k:603:HEA:CMA	30:k:603:HEA:HBA2	2.45	0.47
20:u:73:LYS:HE3	20:u:75:ILE:HB	1.97	0.47
1:A:407:PHE:O	1:A:410:ILE:HG22	2.15	0.46
10:K:98:ILE:HG23	10:K:160:LEU:HB3	1.96	0.46
22:W:130:LEU:HA	22:W:133:ASP:OD2	2.15	0.46
9:j:93:MET:HE2	9:j:93:MET:HA	1.96	0.46
10:k:54:LEU:O	10:k:58:LEU:HD23	2.14	0.46
19:t:73:GLY:O	19:t:77:GLY:N	2.48	0.46
23:A:503:PEF:H371	9:J:226:ILE:HD11	1.97	0.46
2:B:292:GLN:O	2:B:292:GLN:NE2	2.48	0.46
6:F:16:LEU:HB2	9:J:380:ILE:HD11	1.97	0.46
10:K:185:PHE:O	10:K:188:SER:OG	2.24	0.46
11:L:286:TRP:HB2	25:L:402:CDL:H581	1.97	0.46
14:O:64:LEU:O	14:O:67:ARG:HG3	2.15	0.46
15:P:193:LEU:HD12	15:P:236:ILE:HD13	1.96	0.46
1:a:168:ALA:HB1	1:a:244:PHE:CE1	2.50	0.46
1:a:451:ASP:HA	23:a:504:PEF:HN2	1.79	0.46
6:f:101:PRO:HB3	9:j:382:ARG:NH1	2.29	0.46
9:j:249:ASN:OD1	11:l:182:LYS:HE2	2.14	0.46
10:k:389:LEU:HD23	30:k:603:HEA:H241	1.97	0.46
11:l:121:THR:N	11:l:124:GLU:OE2	2.45	0.46
14:o:219:LEU:HD13	14:o:249:TYR:HD2	1.80	0.46
3:C:55:TYR:CZ	25:C:302:CDL:H122	2.51	0.46
3:C:162:LEU:HD12	3:C:181:HIS:CE1	2.50	0.46
10:K:75:LEU:HD13	10:K:250:PRO:HB2	1.96	0.46
10:K:87:MET:SD	10:K:186:VAL:HG11	2.55	0.46
14:O:253:LEU:HA	14:O:256:ILE:HG12	1.96	0.46
19:T:63:GLU:HG3	19:T:71:LEU:HD21	1.97	0.46
2:b:243:ILE:O	2:b:284:LEU:HD12	2.15	0.46
4:d:26:TYR:HB3	4:d:30:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:167:GLY:HA3	9:j:178:ARG:HH22	1.78	0.46
11:l:192:PHE:O	11:l:196:THR:HG22	2.15	0.46
11:L:180:ILE:HG12	28:L:401:HEM:CMA	2.45	0.46
15:P:159:ARG:HD3	22:W:123:THR:HG21	1.97	0.46
2:b:29:SER:OG	2:b:192:VAL:HG13	2.14	0.46
2:b:225:LEU:HA	2:b:352:ASN:ND2	2.25	0.46
15:p:130:TYR:N	15:p:141:VAL:O	2.44	0.46
20:u:46:ALA:HA	20:u:49:LYS:HE3	1.97	0.46
7:G:125:GLU:OE2	7:G:129:HIS:NE2	2.48	0.46
9:J:300:LEU:O	9:J:303:LEU:HB2	2.15	0.46
25:K:603:CDL:H712	25:K:603:CDL:H142	1.97	0.46
16:Q:55:ARG:HG2	16:Q:58:LYS:HZ3	1.80	0.46
1:a:306:ILE:HG23	1:a:311:LEU:HB2	1.96	0.46
3:c:146:ARG:HH11	3:c:202:ILE:HD11	1.80	0.46
5:e:55:ARG:NH2	5:e:56:ILE:HA	2.31	0.46
13:n:38:ALA:HA	13:n:41:VAL:HG12	1.98	0.46
14:o:135:THR:HG23	14:o:265:TYR:HD1	1.80	0.46
15:p:187:ASP:N	15:p:221:CYS:SG	2.87	0.46
1:A:309:TYR:OH	8:h:7:LYS:N	2.48	0.46
2:B:258:ASN:HA	2:B:261:THR:HG22	1.97	0.46
9:J:235:LEU:HD12	11:L:281:TYR:OH	2.15	0.46
10:K:485:ASN:HD21	10:K:487:LYS:HE3	1.81	0.46
11:L:121:THR:N	11:L:124:GLU:OE2	2.35	0.46
14:o:143:ILE:HD11	18:s:63:ILE:HG23	1.98	0.46
1:A:156:HIS:HB2	1:A:157:PRO:HD3	1.98	0.46
1:A:320:LEU:N	1:A:327:LEU:O	2.49	0.46
2:B:226:GLY:N	2:B:352:ASN:OD1	2.47	0.46
7:G:107:ILE:O	7:G:110:GLN:NE2	2.49	0.46
9:J:207:SER:H	28:J:405:HEM:CGD	2.29	0.46
15:P:163:THR:HB	15:P:233:PRO:HB2	1.98	0.46
18:S:42:LYS:HA	18:S:42:LYS:HD2	1.72	0.46
1:a:77:PHE:CZ	1:a:93:LEU:HD13	2.50	0.46
2:b:19:VAL:HG12	2:b:187:VAL:HB	1.98	0.46
2:b:34:LYS:NZ	2:b:333:SER:OG	2.43	0.46
3:c:156:LEU:HD23	3:c:158:ILE:H	1.81	0.46
5:e:43:HIS:ND1	5:e:43:HIS:O	2.48	0.46
9:j:285:ILE:HD11	9:j:294:THR:HG21	1.98	0.46
9:j:347:PRO:O	9:j:351:MET:HG2	2.15	0.46
23:j:401:PEF:H342	23:j:401:PEF:H152	1.98	0.46
10:k:87:MET:SD	10:k:186:VAL:HG11	2.56	0.46
10:k:125:THR:HG22	10:k:133:LEU:HG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:316:THR:HG21	30:k:604:HEA:H132	1.97	0.46
10:k:450:TRP:NE1	15:p:21:TYR:HA	2.29	0.46
10:k:461:ALA:HB1	30:k:603:HEA:H263	1.97	0.46
11:l:109:ARG:HB2	11:l:178:SER:HB3	1.98	0.46
14:o:28:PHE:O	14:o:31:LEU:HG	2.16	0.46
14:o:45:ILE:HG22	14:o:47:ASN:H	1.81	0.46
1:A:444:ASP:OD1	1:A:445:TYR:N	2.43	0.46
9:J:118:VAL:HG11	9:J:303:LEU:CD2	2.45	0.46
9:J:291:GLY:HA2	9:J:294:THR:HG22	1.98	0.46
10:K:69:PHE:HD1	10:K:106:LEU:HD12	1.80	0.46
10:K:148:ILE:HG21	10:K:211:LEU:HD22	1.97	0.46
14:O:5:GLU:HA	14:O:8:ARG:HG2	1.97	0.46
14:O:135:THR:HG23	14:O:265:TYR:HD1	1.81	0.46
15:P:26:GLN:OE1	15:P:192:SER:OG	2.34	0.46
16:Q:115:VAL:HG13	16:Q:117:ASN:HB2	1.97	0.46
16:Q:142:GLU:CD	22:W:66:GLU:HG2	2.40	0.46
18:S:66:THR:HA	18:S:69:ASN:HD21	1.79	0.46
19:T:100:ILE:HG12	19:T:107:ARG:HD3	1.97	0.46
9:j:93:MET:SD	28:j:404:HEM:HMC3	2.56	0.46
10:k:525:HIS:NE2	12:m:29:HIS:HB3	2.30	0.46
11:l:116:VAL:HG22	11:l:125:VAL:HG21	1.98	0.46
11:l:281:TYR:O	11:l:285:ILE:HG12	2.15	0.46
14:o:36:SER:HB3	14:o:51:VAL:HG12	1.97	0.46
17:r:14:VAL:O	17:r:18:ILE:HG12	2.15	0.46
1:A:114:ASP:OD1	1:A:114:ASP:N	2.45	0.46
2:B:117:HIS:HB2	6:f:62:ARG:HD3	1.98	0.46
10:K:100:ASN:ND2	14:O:23:PRO:HG3	2.31	0.46
22:W:147:TYR:O	22:W:149:GLN:NE2	2.49	0.46
2:b:164:VAL:HG13	2:b:165:GLU:OE1	2.15	0.46
20:u:55:TYR:HA	20:u:59:CYS:HB3	1.96	0.46
22:w:35:GLN:NE2	22:w:36:SER:HG	2.14	0.46
1:A:296:ARG:HH21	1:A:307:GLN:NE2	2.14	0.46
9:J:377:LEU:HA	9:J:380:ILE:HG22	1.97	0.46
10:K:436:MET:HE1	10:K:447:PHE:HB2	1.97	0.46
12:M:70:VAL:HG13	12:M:71:GLN:CD	2.41	0.46
14:O:66:PHE:O	14:O:69:ILE:HG22	2.16	0.46
14:O:164:ARG:NH2	19:T:51:ALA:O	2.41	0.46
1:a:155:ASP:O	1:a:156:HIS:ND1	2.48	0.46
23:a:501:PEF:H362	4:d:26:TYR:HD2	1.81	0.46
7:g:134:LEU:O	7:g:138:THR:HG23	2.16	0.46
9:j:72:VAL:HG13	9:j:75:GLY:HA3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:j:405:UQ6:H301	29:j:405:UQ6:H322	1.64	0.46
10:k:108:MET:N	10:k:108:MET:SD	2.88	0.46
10:k:342:ILE:HG23	15:p:58:LEU:HD21	1.98	0.46
30:k:604:HEA:O2A	30:k:604:HEA:HHa	2.16	0.46
11:l:112:TRP:CZ3	11:l:129:ALA:HA	2.51	0.46
15:p:34:GLU:HB2	17:r:44:ARG:NH2	2.31	0.46
15:p:45:PHE:O	15:p:49:VAL:HG13	2.15	0.46
1:A:334:THR:HG21	1:A:340:ILE:HD11	1.97	0.45
2:B:360:SER:HA	2:b:153:LYS:HE3	1.98	0.45
9:J:235:LEU:O	9:J:238:LEU:HG	2.15	0.45
10:K:17:LEU:HB3	10:K:103:PHE:CZ	2.51	0.45
10:K:127:TRP:HD1	30:K:604:HEA:HBD1	1.81	0.45
10:K:493:LYS:NZ	10:K:511:SER:HB3	2.32	0.45
11:L:159:TYR:CD2	11:L:165:ALA:HA	2.51	0.45
15:P:99:PRO:HA	15:P:102:ILE:HG22	1.98	0.45
26:a:502:PCF:H382	4:d:44:PHE:HZ	1.81	0.45
3:c:177:PHE:CZ	3:c:182:GLY:HA2	2.52	0.45
8:h:91:ARG:HG3	8:h:92:VAL:HG23	1.98	0.45
1:A:249:VAL:HG22	8:H:27:TYR:CE1	2.51	0.45
2:B:65:LEU:HD23	2:B:65:LEU:H	1.81	0.45
2:B:93:PHE:HB3	2:B:101:TYR:CE2	2.52	0.45
2:B:153:LYS:NZ	2:B:157:ASN:HD21	2.14	0.45
10:K:386:ILE:HG21	30:K:604:HEA:H171	1.97	0.45
13:N:37:PHE:CZ	14:O:54:ALA:HB2	2.52	0.45
1:a:427:TRP:NE1	5:e:12:LYS:HG3	2.31	0.45
6:f:85:HIS:NE2	25:h:601:CDL:OA4	2.50	0.45
13:n:31:TYR:HB3	13:n:32:PRO:HD3	1.98	0.45
14:o:3:HIS:ND1	18:s:19:LYS:O	2.50	0.45
15:p:82:GLU:O	15:p:86:THR:OG1	2.21	0.45
2:B:37:GLY:O	2:B:87:ILE:HG12	2.17	0.45
4:D:4:THR:HA	4:D:5:SER:HA	1.63	0.45
14:O:40:THR:HG21	14:O:51:VAL:HG11	1.98	0.45
20:U:70:GLN:O	20:U:74:GLY:N	2.49	0.45
3:c:126:ILE:O	3:c:130:ASN:ND2	2.49	0.45
9:j:194:VAL:HG22	28:j:404:HEM:HBB2	1.98	0.45
11:l:271:LEU:O	11:l:275:ILE:HG12	2.17	0.45
14:o:244:GLU:HA	14:o:247:ILE:HG12	1.97	0.45
9:J:272:GLU:OE2	9:J:272:GLU:HA	2.17	0.45
9:J:287:ASP:OD1	9:J:288:LYS:N	2.50	0.45
10:K:93:THR:OG1	10:K:168:THR:OG1	2.34	0.45
10:K:453:VAL:HA	10:K:456:ILE:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:525:HIS:O	10:K:525:HIS:ND1	2.46	0.45
1:a:428:ASP:OD2	3:c:57:TYR:OH	2.28	0.45
2:b:241:ILE:HD11	2:b:301:ILE:HD11	1.99	0.45
9:j:166:TRP:O	9:j:175:THR:HG22	2.15	0.45
10:k:438:ARG:NH1	30:k:603:HEA:O2D	2.49	0.45
11:l:291:LYS:HE2	11:l:291:LYS:HB3	1.64	0.45
1:A:80:LYS:HA	1:A:80:LYS:HD2	1.79	0.45
8:H:45:VAL:HG21	23:W:201:PEF:H362	1.97	0.45
9:J:118:VAL:HG11	9:J:303:LEU:HD21	1.99	0.45
29:J:408:UQ6:H122	29:J:408:UQ6:H101	1.65	0.45
10:K:381:LEU:HD22	30:K:601:HEA:CAC	2.47	0.45
14:O:1:MET:O	14:O:4:LEU:HG	2.16	0.45
15:P:112:SER:HA	20:U:58:LEU:HD11	1.97	0.45
22:W:143:PRO:HD2	22:W:144:TRP:CZ3	2.51	0.45
4:d:11:THR:OG1	4:d:12:GLY:N	2.49	0.45
10:k:136:ILE:HG21	18:s:104:LYS:HE2	1.98	0.45
12:m:40:PHE:HB3	12:m:49:TYR:CE1	2.52	0.45
14:o:15:HIS:NE2	14:o:78:ASP:OD2	2.29	0.45
1:A:67:ASN:OD1	1:A:176:LEU:HD12	2.17	0.45
2:B:40:ARG:HD3	2:B:155:LEU:HG	1.98	0.45
10:K:498:VAL:O	16:Q:70:GLN:NE2	2.43	0.45
30:K:604:HEA:H212	30:K:604:HEA:H271	1.23	0.45
11:L:113:ARG:HA	11:L:151:LEU:HD12	1.97	0.45
14:O:209:THR:O	14:O:212:HIS:ND1	2.49	0.45
16:Q:55:ARG:HA	16:Q:58:LYS:HG2	1.98	0.45
19:T:46:LEU:HD23	19:T:68:ARG:NE	2.31	0.45
2:b:84:ARG:HH22	2:b:159:LEU:HD21	1.81	0.45
10:k:386:ILE:HD11	30:k:603:HEA:HMC3	1.97	0.45
5:E:27:VAL:O	5:E:31:VAL:HG22	2.16	0.45
6:F:22:SER:O	6:F:26:VAL:HG12	2.17	0.45
2:b:258:ASN:HD22	2:b:321:THR:HA	1.81	0.45
3:c:63:MET:HE1	11:l:287:VAL:HG11	1.99	0.45
3:c:167:ILE:HG23	3:c:179:PRO:HG3	1.99	0.45
14:o:64:LEU:HD12	14:o:67:ARG:HE	1.81	0.45
18:s:18:LEU:HD22	19:t:146:VAL:HG23	1.99	0.45
2:B:218:LYS:H	2:B:218:LYS:HG2	1.59	0.45
4:D:62:LEU:C	4:D:64:PRO:HD3	2.42	0.45
9:J:91:MET:HB2	9:J:273:TRP:CZ2	2.52	0.45
9:J:311:SER:OG	9:J:319:LYS:HE2	2.17	0.45
10:K:9:THR:HG22	10:K:96:PRO:HB2	1.98	0.45
10:K:62:HIS:HE1	30:K:604:HEA:NC	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:138:PRO:O	14:O:142:THR:HG23	2.17	0.45
19:T:82:ASP:HB2	19:T:84:LYS:HE2	1.99	0.45
2:b:44:LYS:HD2	2:b:167:VAL:HG12	1.98	0.45
10:k:223:VAL:HG21	15:p:201:PRO:HB2	1.97	0.45
30:k:604:HEA:H202	30:k:604:HEA:H242	1.98	0.45
15:p:113:PRO:HB2	15:p:176:ARG:HG2	1.98	0.45
15:p:190:ILE:HB	15:p:195:ILE:HG13	1.99	0.45
2:B:255:VAL:HG13	2:B:314:LEU:HD21	1.99	0.45
5:E:44:ASN:HB3	5:E:47:LYS:HB2	1.98	0.45
9:J:301:VAL:O	9:J:304:VAL:HG12	2.17	0.45
10:K:377:PHE:CE1	30:K:601:HEA:HBD1	2.52	0.45
14:O:202:GLY:HA2	14:O:205:PHE:CD2	2.52	0.45
15:P:147:VAL:HG21	15:P:231:ASN:HB2	1.98	0.45
1:a:365:ARG:HE	2:b:72:GLU:CD	2.24	0.45
1:a:453:SER:O	1:a:453:SER:OG	2.34	0.45
2:b:258:ASN:HA	2:b:261:THR:HG22	1.99	0.45
3:c:180:CYS:SG	3:c:181:HIS:ND1	2.90	0.45
10:k:525:HIS:CE1	12:m:29:HIS:HB3	2.50	0.45
14:o:262:VAL:HG12	14:o:263:VAL:HG13	1.98	0.45
18:s:51:TRP:HA	18:s:54:ILE:HG12	1.99	0.45
18:s:96:TYR:CE1	18:s:98:PHE:HB2	2.52	0.45
9:J:90:PHE:CE2	9:J:128:ALA:HB2	2.51	0.45
23:J:409:PEF:H121	23:J:409:PEF:H152	1.50	0.45
10:K:347:LEU:HB3	10:K:383:MET:SD	2.57	0.45
11:L:105:HIS:HD1	11:L:177:LEU:HD21	1.81	0.45
11:L:106:SER:OG	11:L:107:LEU:N	2.50	0.45
17:R:12:ARG:NH1	17:R:13:ARG:HB2	2.31	0.45
8:h:58:TYR:HE1	9:j:323:LYS:HD2	1.81	0.45
9:j:1:MET:HE1	9:j:5:LYS:O	2.17	0.45
9:j:96:HIS:NE2	28:j:404:HEM:ND	2.65	0.45
9:j:132:TYR:OH	9:j:139:MET:SD	2.56	0.45
10:k:244:VAL:HB	30:k:604:HEA:CAC	2.47	0.45
16:q:93:ARG:HH11	16:q:97:ARG:HE	1.64	0.45
16:q:142:GLU:CD	22:w:66:GLU:HG2	2.42	0.45
18:s:33:PHE:CD2	19:t:74:LYS:HB2	2.52	0.45
18:s:104:LYS:HD3	18:s:105:PRO:O	2.18	0.45
20:u:61:LEU:HD12	20:u:64:ILE:HG13	1.99	0.45
2:B:58:ASN:H	2:B:64:ALA:HA	1.81	0.44
3:C:92:ALA:HB3	3:C:112:GLN:H	1.82	0.44
4:D:39:LEU:HD21	5:E:23:ALA:HB2	1.99	0.44
7:G:139:ALA:HB3	7:G:140:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:228:LYS:HD2	11:L:292:TRP:CZ2	2.52	0.44
10:K:49:HIS:N	12:M:72:LEU:HD11	2.33	0.44
10:K:499:GLU:HG3	19:T:135:TRP:CH2	2.51	0.44
11:L:229:LEU:HD12	11:L:229:LEU:HA	1.87	0.44
11:L:240:THR:HB	11:L:241:PRO:HD3	1.98	0.44
15:P:82:GLU:O	15:P:86:THR:OG1	2.22	0.44
17:R:28:MET:HE1	21:V:43:TRP:HH2	1.83	0.44
19:T:70:GLU:HG2	19:T:71:LEU:N	2.32	0.44
1:a:42:HIS:CD2	1:a:215:LYS:HB3	2.52	0.44
2:b:66:LYS:O	2:b:67:LEU:HD23	2.16	0.44
2:b:146:LEU:HD21	2:b:242:GLY:HA3	1.99	0.44
2:b:270:LEU:HD12	2:b:300:ASN:HB3	1.99	0.44
23:j:401:PEF:H391	23:j:401:PEF:H361	1.74	0.44
6:F:84:THR:HG23	6:F:86:HIS:H	1.82	0.44
9:J:90:PHE:CZ	9:J:124:THR:HG22	2.53	0.44
10:K:105:VAL:HA	10:K:108:MET:HE1	1.98	0.44
10:K:424:ILE:HD11	10:K:458:SER:HA	1.98	0.44
13:N:7:GLN:O	13:N:11:ILE:HG12	2.18	0.44
15:P:204:LEU:HD11	20:U:62:ASP:HB3	1.99	0.44
1:a:58:GLY:N	1:a:100:ASP:HA	2.30	0.44
4:d:47:GLY:HA2	4:d:51:PHE:CD2	2.52	0.44
9:j:103:TYR:CE1	9:j:209:PRO:HB3	2.53	0.44
10:k:88:ILE:HG22	10:k:90:ALA:H	1.82	0.44
10:k:523:ALA:O	10:k:526:SER:OG	2.27	0.44
13:n:17:LYS:HE3	13:n:18:PRO:HD2	1.98	0.44
14:o:85:LYS:HD2	14:o:85:LYS:HA	1.79	0.44
15:p:180:THR:HB	15:p:204:LEU:CD2	2.47	0.44
15:p:224:LEU:HG	15:p:226:GLY:H	1.81	0.44
18:s:65:LEU:O	18:s:69:ASN:ND2	2.49	0.44
3:C:162:LEU:HD13	9:j:146:VAL:HG13	1.99	0.44
9:J:23:PRO:HG2	9:J:26:ILE:CD1	2.47	0.44
23:J:401:PEF:N	23:J:401:PEF:O1P	2.50	0.44
10:K:404:ASN:HD22	10:K:483:LYS:HG2	1.82	0.44
14:O:93:MET:SD	14:O:94:PHE:N	2.90	0.44
15:P:170:PRO:HD3	15:P:244:PHE:CE1	2.52	0.44
9:j:33:GLY:O	9:j:36:LEU:HB3	2.18	0.44
10:k:33:SER:OG	10:k:62:HIS:ND1	2.50	0.44
10:k:495:PRO:HG3	10:k:504:PHE:CG	2.52	0.44
11:l:240:THR:H	11:l:241:PRO:CD	2.29	0.44
21:v:32:GLU:OE2	21:v:36:LEU:HD12	2.17	0.44
4:D:26:TYR:HB3	4:D:30:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:189:ILE:H	9:J:189:ILE:HD12	1.82	0.44
10:K:4:ARG:NH2	10:K:10:ASN:OD1	2.50	0.44
10:K:248:ILE:HD13	30:K:601:HEA:CB	2.47	0.44
14:O:7:SER:O	14:O:11:GLN:NE2	2.51	0.44
16:Q:125:LEU:O	16:Q:128:LEU:HG	2.16	0.44
1:a:156:HIS:HB2	1:a:157:PRO:HD3	1.99	0.44
2:b:62:ARG:HB2	2:b:67:LEU:HB2	1.99	0.44
2:b:147:TYR:HE1	2:b:284:LEU:HB3	1.82	0.44
2:b:255:VAL:HA	2:b:321:THR:HG21	2.00	0.44
10:k:95:PHE:HE1	10:k:97:ARG:HH21	1.66	0.44
10:k:218:THR:OG1	14:o:196:ILE:HG12	2.17	0.44
10:k:360:ASN:HD22	10:k:363:LEU:HB2	1.82	0.44
10:k:457:GLY:HA2	10:k:460:ILE:HD12	2.00	0.44
19:t:93:THR:OG1	19:t:94:MET:SD	2.75	0.44
1:A:407:PHE:CD2	2:B:27:LYS:HD2	2.53	0.44
4:D:60:PRO:O	4:D:64:PRO:HG3	2.18	0.44
8:H:81:TYR:HE1	8:H:89:LEU:HD13	1.83	0.44
10:K:447:PHE:CG	10:K:450:TRP:HD1	2.36	0.44
1:a:54:VAL:HB	1:a:207:VAL:HG12	2.00	0.44
1:a:271:ASN:ND2	1:a:397:LYS:HD3	2.32	0.44
9:j:136:TYR:CD1	9:j:176:ILE:HD11	2.52	0.44
10:k:45:SER:HB3	10:k:49:HIS:HA	1.99	0.44
10:k:502:THR:HG23	10:k:503:ILE:HD12	2.00	0.44
2:B:74:LEU:HD21	2:B:97:ASP:HB3	1.99	0.44
4:D:17:ARG:NH2	6:f:118:ASP:OD1	2.47	0.44
11:L:145:LYS:HE3	11:L:145:LYS:HB3	1.81	0.44
14:O:159:LEU:O	14:O:163:ASN:N	2.48	0.44
14:O:210:GLY:HA2	14:O:213:PHE:CD2	2.53	0.44
20:U:15:ASP:OD1	20:U:15:ASP:N	2.50	0.44
22:W:61:TRP:O	22:W:64:LEU:HD12	2.17	0.44
1:a:31:GLN:HE21	1:a:399:SER:HA	1.82	0.44
1:a:81:GLU:OE1	1:a:123:SER:OG	2.31	0.44
23:a:504:PEF:H42	9:j:222:HIS:HE1	1.82	0.44
8:h:70:TRP:CD1	8:h:74:ASN:HD21	2.36	0.44
10:k:31:ALA:O	10:k:34:LEU:HB3	2.17	0.44
10:k:338:MET:O	10:k:342:ILE:HG12	2.17	0.44
16:q:100:ASP:OD1	16:q:102:PRO:HD2	2.17	0.44
1:A:428:ASP:OD2	26:E:101:PCF:H133	2.17	0.44
3:C:98:LEU:HB2	3:C:152:TRP:CZ2	2.53	0.44
3:C:126:ILE:O	3:C:130:ASN:ND2	2.50	0.44
3:C:180:CYS:HB3	3:C:181:HIS:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:304:PEF:H142	23:C:304:PEF:H171	1.74	0.44
10:K:514:ILE:N	19:T:123:TRP:HZ2	2.16	0.44
11:L:289:LYS:HE3	11:L:289:LYS:HB3	1.72	0.44
14:O:133:GLN:HB3	18:S:81:ARG:HH21	1.82	0.44
19:T:66:LEU:HA	19:T:68:ARG:NH1	2.32	0.44
1:a:356:ILE:HD12	1:a:457:TRP:HA	2.00	0.44
2:b:49:HIS:HA	2:b:82:LEU:HD13	2.00	0.44
10:k:130:TYR:CE1	10:k:233:GLU:HG3	2.53	0.44
10:k:513:SER:OG	10:k:515:GLU:OE1	2.33	0.44
13:n:43:THR:OG1	13:n:44:PRO:HD3	2.18	0.44
1:A:306:ILE:HG23	1:A:311:LEU:HB2	2.00	0.44
1:A:352:ASN:OD1	1:A:427:TRP:HZ3	2.01	0.44
3:C:80:SER:O	3:C:83:THR:HG22	2.18	0.44
3:C:161:HIS:CG	24:C:301:FES:S1	3.00	0.44
4:D:20:LEU:HD12	4:D:20:LEU:HA	1.84	0.44
11:L:111:ALA:HB2	11:L:154:TYR:CE1	2.52	0.44
18:S:14:PRO:HA	18:S:15:PRO:HD3	1.92	0.44
1:a:370:LEU:HD22	1:a:410:ILE:CD1	2.48	0.44
3:c:59:MET:HE2	3:c:59:MET:HB2	1.87	0.44
5:e:40:TYR:CE2	11:l:268:ARG:HB2	2.53	0.44
9:j:38:LEU:O	9:j:41:VAL:HG12	2.18	0.44
10:k:514:ILE:HD11	19:t:108:TYR:CD1	2.52	0.44
11:l:96:VAL:HG23	11:l:234:VAL:HG21	1.98	0.44
11:l:225:MET:HE1	28:l:401:HEM:NA	2.33	0.44
1:A:370:LEU:HD22	1:A:410:ILE:CD1	2.48	0.44
1:A:439:ILE:HD12	1:A:439:ILE:H	1.83	0.44
2:B:44:LYS:HD2	2:B:167:VAL:HG12	2.00	0.44
2:B:358:ASP:OD1	2:B:359:VAL:N	2.51	0.44
10:K:18:TYR:HE1	10:K:103:PHE:HB2	1.83	0.44
10:K:33:SER:HA	10:K:36:ILE:HD12	2.00	0.44
10:K:525:HIS:CE1	12:M:29:HIS:HB3	2.52	0.44
12:M:56:PHE:HA	12:M:59:ILE:HG12	2.00	0.44
3:c:133:ASP:OD1	3:c:133:ASP:N	2.50	0.44
4:d:51:PHE:HE2	4:d:55:LEU:HD12	1.82	0.44
9:j:187:PRO:HB3	28:j:403:HEM:HMC2	2.00	0.44
10:k:159:LEU:O	10:k:163:ILE:HG13	2.17	0.44
10:k:501:ASN:HD21	22:w:83:ARG:HG2	1.83	0.44
16:q:85:PRO:HG3	16:q:127:GLU:HG3	1.99	0.44
20:u:70:GLN:HA	20:u:73:LYS:HG2	1.99	0.44
23:A:501:PEF:H371	4:D:30:LEU:HD21	1.99	0.43
2:B:317:ALA:O	2:B:321:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:79:ARG:NH1	28:J:404:HEM:O2D	2.50	0.43
10:K:351:GLY:O	10:K:354:THR:OG1	2.28	0.43
28:L:401:HEM:HBD1	28:L:401:HEM:CMD	2.48	0.43
18:S:26:ASP:HA	19:T:77:GLY:HA3	1.99	0.43
21:V:53:TRP:CD1	21:V:54:PRO:HD3	2.53	0.43
1:a:363:VAL:HG12	1:a:367:LYS:HE2	1.99	0.43
9:j:194:VAL:HG13	28:j:404:HEM:HMB3	2.00	0.43
10:k:255:ILE:HA	10:k:258:VAL:HG22	1.99	0.43
10:k:380:VAL:HB	30:k:604:HEA:HBC1	2.00	0.43
12:m:31:LYS:HB3	12:m:36:GLU:HG3	1.99	0.43
17:r:38:MET:HE3	17:r:42:ASN:HB2	1.99	0.43
1:A:99:ARG:HD3	1:A:99:ARG:HA	1.73	0.43
1:A:261:ILE:CD1	1:A:344:ILE:HD11	2.46	0.43
2:B:84:ARG:NE	2:B:159:LEU:HD21	2.32	0.43
9:J:40:LEU:O	9:J:44:ILE:HG12	2.18	0.43
10:K:55:PHE:CG	10:K:441:PRO:HB3	2.54	0.43
10:K:525:HIS:NE2	12:M:29:HIS:HB3	2.33	0.43
11:L:180:ILE:HG12	28:L:401:HEM:HMA1	2.00	0.43
11:L:218:PHE:CZ	11:L:223:ILE:HD11	2.53	0.43
11:L:284:SER:HA	11:L:287:VAL:HG12	1.99	0.43
13:N:17:LYS:HA	13:N:17:LYS:HD2	1.69	0.43
15:P:59:TYR:CE2	21:V:43:TRP:HB2	2.52	0.43
15:P:69:PRO:HB2	15:P:70:ILE:HD12	2.00	0.43
15:P:127:LYS:HA	15:P:144:GLU:HA	2.01	0.43
16:Q:105:ILE:HG23	16:Q:139:LEU:HD13	2.01	0.43
9:j:55:SER:OG	9:j:56:SER:N	2.51	0.43
10:k:10:ASN:HB3	10:k:524:VAL:HG11	1.99	0.43
10:k:100:ASN:ND2	14:o:23:PRO:HG3	2.33	0.43
14:o:219:LEU:HB2	14:o:249:TYR:HE2	1.83	0.43
15:p:205:ASN:OD1	15:p:206:GLN:N	2.51	0.43
23:A:501:PEF:H141	23:A:501:PEF:H111	1.70	0.43
3:C:185:TYR:CD2	3:C:200:LEU:HD11	2.52	0.43
10:K:83:LEU:O	10:K:87:MET:N	2.36	0.43
13:N:38:ALA:O	13:N:42:VAL:HG13	2.18	0.43
1:a:159:ARG:NH1	1:a:436:THR:HG21	2.34	0.43
2:b:322:LYS:HB2	2:b:322:LYS:HE3	1.79	0.43
3:c:156:LEU:N	3:c:203:PRO:HD3	2.34	0.43
7:g:117:LEU:O	7:g:117:LEU:HD23	2.18	0.43
9:j:281:ILE:HA	9:j:284:SER:HB3	2.00	0.43
10:k:72:MET:O	10:k:76:ILE:HB	2.18	0.43
11:l:109:ARG:HB2	11:l:178:SER:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:l:120:HIS:HB3	11:l:124:GLU:CG	2.48	0.43
15:p:26:GLN:HA	15:p:26:GLN:OE1	2.18	0.43
15:p:93:LEU:HA	15:p:96:ILE:HG12	2.00	0.43
1:A:69:VAL:HG23	1:A:193:LEU:HD12	2.00	0.43
14:O:190:THR:HG21	18:S:117:TRP:CE2	2.53	0.43
1:a:248:GLU:OE2	1:a:445:TYR:HD1	2.02	0.43
2:b:122:SER:OG	2:b:123:VAL:N	2.51	0.43
9:j:79:ARG:NH1	28:j:403:HEM:O2D	2.37	0.43
9:j:334:VAL:HG23	23:j:408:PEF:H131	1.99	0.43
10:k:307:SER:O	10:k:310:MET:HG3	2.19	0.43
10:k:319:LYS:HG3	10:k:323:TRP:CH2	2.52	0.43
10:k:413:GLN:HE22	10:k:464:SER:HB2	1.82	0.43
19:t:134:CYS:HB3	19:t:137:CYS:HB3	2.00	0.43
2:B:152:ARG:HD2	2:b:364:TYR:CE2	2.53	0.43
9:J:214:GLY:O	9:J:218:ARG:NE	2.51	0.43
10:K:389:LEU:HD21	30:K:604:HEA:H241	2.00	0.43
13:N:46:LEU:HD23	13:N:46:LEU:H	1.83	0.43
15:P:126:TRP:HE1	15:P:232:MET:CG	2.30	0.43
1:a:268:GLU:HG3	1:a:274:ASN:HB3	2.00	0.43
2:b:236:ASP:CG	2:b:292:GLN:HA	2.42	0.43
3:c:119:ARG:NH2	3:c:169:GLU:OE1	2.36	0.43
8:h:66:TYR:CE1	9:j:328:ILE:HD11	2.54	0.43
13:n:46:LEU:HD23	13:n:46:LEU:H	1.84	0.43
14:o:138:PRO:O	14:o:142:THR:HG23	2.19	0.43
21:v:43:TRP:CZ2	21:v:47:LEU:HD11	2.53	0.43
1:A:71:ASN:ND2	1:A:178:THR:O	2.34	0.43
2:B:29:SER:OG	2:B:192:VAL:HG13	2.18	0.43
2:B:230:ARG:HD3	2:B:359:VAL:CG1	2.49	0.43
10:K:370:THR:O	10:K:373:VAL:HG22	2.18	0.43
10:K:427:PRO:HA	10:K:430:PHE:CD2	2.54	0.43
8:h:65:ILE:HG22	8:h:66:TYR:HD1	1.83	0.43
9:j:65:VAL:HA	9:j:68:ILE:HG22	2.00	0.43
14:o:159:LEU:O	14:o:163:ASN:N	2.48	0.43
15:p:204:LEU:HD12	20:u:63:TRP:NE1	2.33	0.43
16:q:131:VAL:HA	16:q:134:GLU:HG2	1.98	0.43
23:C:304:PEF:O2	11:L:273:THR:HG22	2.18	0.43
10:K:72:MET:O	10:K:76:ILE:HB	2.18	0.43
10:K:205:ALA:O	10:K:209:MET:HG3	2.19	0.43
10:K:397:SER:OG	10:K:475:GLN:NE2	2.35	0.43
15:P:124:TRP:HZ2	15:P:227:THR:H	1.67	0.43
1:a:29:VAL:HA	1:a:40:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:67:ASN:ND2	1:a:180:GLY:HA2	2.33	0.43
1:a:73:TRP:CE3	1:a:76:ILE:HD11	2.53	0.43
2:b:74:LEU:HD21	2:b:97:ASP:CB	2.49	0.43
9:j:245:PHE:HA	11:l:266:ARG:HD3	2.00	0.43
10:k:148:ILE:HD12	10:k:207:ILE:HG23	2.00	0.43
10:k:287:VAL:HB	10:k:290:HIS:CG	2.54	0.43
14:o:200:VAL:HG13	14:o:200:VAL:O	2.19	0.43
15:p:239:VAL:HB	15:p:243:LYS:HB3	2.00	0.43
18:s:89:ASP:OD1	18:s:89:ASP:N	2.48	0.43
22:w:41:MET:HE3	22:w:46:GLN:OE1	2.19	0.43
9:J:102:TYR:HD1	9:J:326:PHE:CD2	2.37	0.43
10:K:427:PRO:HA	10:K:430:PHE:HD2	1.83	0.43
11:L:109:ARG:HD2	11:L:109:ARG:O	2.19	0.43
11:L:189:ASP:O	11:L:190:TYR:HB3	2.17	0.43
14:O:231:ARG:HD2	14:O:231:ARG:HA	1.78	0.43
19:T:93:THR:OG1	19:T:94:MET:N	2.51	0.43
2:b:56:PHE:CD2	2:b:80:SER:HB3	2.54	0.43
9:j:135:VAL:HA	28:j:403:HEM:O1A	2.19	0.43
10:k:150:ALA:O	10:k:153:LEU:HG	2.19	0.43
10:k:191:ILE:HA	10:k:194:PHE:HD2	1.83	0.43
14:o:247:ILE:HG13	14:o:248:ILE:N	2.33	0.43
17:r:16:MET:HA	17:r:19:VAL:HG12	2.01	0.43
22:w:150:VAL:HG13	22:w:151:GLN:N	2.33	0.43
9:J:329:PHE:HE1	9:J:359:TYR:CE1	2.36	0.43
23:J:407:PEF:H391	23:J:407:PEF:H362	1.84	0.43
14:O:67:ARG:NH1	14:O:68:ASP:OD1	2.51	0.43
15:P:16:ASP:OD2	22:W:142:ASN:N	2.42	0.43
15:P:180:THR:HB	15:P:204:LEU:HD23	2.01	0.43
1:a:96:ASN:HB3	1:a:103:SER:HB2	2.00	0.43
1:a:248:GLU:O	8:h:27:TYR:HA	2.19	0.43
3:c:77:THR:HG23	9:j:74:ASN:ND2	2.33	0.43
8:h:13:TRP:CE2	9:j:21:PRO:HG3	2.54	0.43
9:j:71:ASP:HB3	11:l:113:ARG:HH22	1.84	0.43
10:k:447:PHE:HZ	15:p:22:ALA:HB3	1.83	0.43
12:m:40:PHE:HB3	12:m:49:TYR:CZ	2.54	0.43
15:p:193:LEU:HD23	15:p:193:LEU:HA	1.85	0.43
17:r:47:PHE:O	17:r:50:GLU:HG3	2.19	0.43
19:t:66:LEU:HA	19:t:68:ARG:NH1	2.34	0.43
1:A:169:PHE:HB2	1:A:175:SER:HB3	2.00	0.43
10:K:262:TYR:CE1	10:K:492:ASN:HB2	2.53	0.43
10:K:470:TYR:CE2	25:K:603:CDL:H521	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:61:PHE:O	12:M:64:PRO:HD2	2.19	0.43
15:P:51:LEU:HA	15:P:54:VAL:HG22	2.00	0.43
9:j:329:PHE:HE1	9:j:359:TYR:CD1	2.37	0.43
14:o:253:LEU:HA	14:o:256:ILE:HG12	2.01	0.43
16:q:95:ALA:HA	16:q:98:VAL:HG22	2.00	0.43
19:t:109:VAL:HG13	19:t:141:TYR:HD2	1.83	0.43
1:A:73:TRP:CE3	1:A:76:ILE:HD11	2.54	0.42
1:A:183:GLU:OE1	3:C:32:SER:HB2	2.19	0.42
1:A:300:ILE:HD12	23:A:501:PEF:H42	2.01	0.42
3:C:155:MET:HE3	3:C:200:LEU:HB2	2.01	0.42
23:C:303:PEF:H311	4:D:48:TRP:HE1	1.84	0.42
4:D:41:LEU:O	4:D:45:THR:HG22	2.18	0.42
6:F:48:LEU:HD21	9:J:318:PHE:CD2	2.54	0.42
9:J:107:ARG:HG3	9:J:108:SER:H	1.84	0.42
14:O:190:THR:O	18:S:118:ASN:ND2	2.36	0.42
20:U:7:SER:HA	20:U:8:PRO:HD3	1.83	0.42
23:W:201:PEF:H341	23:W:201:PEF:H311	1.72	0.42
23:W:201:PEF:H431	23:W:201:PEF:H402	1.87	0.42
1:a:280:LEU:HD22	1:a:418:VAL:HG21	2.01	0.42
3:c:121:ARG:NH2	3:c:187:ILE:HG13	2.34	0.42
7:g:139:ALA:HB3	7:g:140:PRO:HD3	2.01	0.42
9:j:26:ILE:HD12	9:j:30:TRP:CD2	2.53	0.42
9:j:290:LEU:HD23	9:j:290:LEU:HA	1.82	0.42
29:j:407:UQ6:H222	29:j:407:UQ6:H201	1.90	0.42
10:k:93:THR:OG1	10:k:164:ASN:ND2	2.50	0.42
18:s:101:ILE:HG13	18:s:102:ARG:HD3	2.00	0.42
21:v:65:LYS:NZ	22:w:126:LYS:HD2	2.33	0.42
1:A:125:ILE:HG13	1:A:126:GLN:N	2.33	0.42
3:C:154:ILE:HD12	3:C:205:TYR:CG	2.53	0.42
10:K:84:LEU:HA	10:K:87:MET:HG3	2.01	0.42
10:K:133:LEU:HD22	15:P:184:VAL:HG11	2.00	0.42
10:K:435:GLY:HA3	15:P:191:PRO:HG2	2.01	0.42
11:L:105:HIS:NE2	28:L:401:HEM:C1C	2.56	0.42
14:O:231:ARG:NH1	14:O:233:TYR:OH	2.53	0.42
15:P:161:LEU:HD22	15:P:218:TYR:CE1	2.54	0.42
20:U:46:ALA:HA	20:U:49:LYS:HB2	2.01	0.42
9:j:31:ASN:HB3	9:j:232:THR:HG21	1.99	0.42
10:k:389:LEU:CD2	30:k:603:HEA:H251	2.49	0.42
13:n:37:PHE:CE2	14:o:54:ALA:HB2	2.54	0.42
14:o:7:SER:O	14:o:11:GLN:NE2	2.51	0.42
22:w:92:SER:HA	22:w:95:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:w:201:PEF:H311	23:w:201:PEF:H341	1.48	0.42
1:A:281:ALA:HA	1:A:284:ILE:HD12	2.01	0.42
8:H:71:LYS:HD3	8:H:71:LYS:HA	1.72	0.42
28:J:404:HEM:HMC2	28:J:404:HEM:HBC2	2.01	0.42
10:K:393:TYR:OH	10:K:475:GLN:OE1	2.25	0.42
11:L:163:GLN:HG2	11:l:139:ASP:O	2.20	0.42
13:N:17:LYS:HE3	13:N:18:PRO:HD2	2.01	0.42
21:V:51:LEU:C	21:V:54:PRO:HD2	2.44	0.42
1:a:288:TYR:OH	1:a:307:GLN:OE1	2.32	0.42
2:b:53:ARG:HA	2:b:53:ARG:HD3	1.66	0.42
6:f:35:LEU:HD23	6:f:35:LEU:O	2.19	0.42
10:k:353:LEU:HB2	15:p:47:LEU:HD12	2.01	0.42
20:u:18:PHE:CE2	20:u:20:GLN:HB3	2.53	0.42
20:u:70:GLN:O	20:u:74:GLY:N	2.52	0.42
22:w:43:SER:HA	22:w:46:GLN:HG2	2.01	0.42
3:C:117:PHE:CE1	3:C:157:GLY:HA3	2.54	0.42
3:C:187:ILE:HD12	3:C:187:ILE:HA	1.93	0.42
4:D:43:VAL:HG22	5:E:26:PHE:HB2	2.01	0.42
6:F:70:ALA:HB1	6:F:74:ARG:HH12	1.84	0.42
9:J:298:ALA:HA	9:J:301:VAL:HG12	2.01	0.42
10:K:14:ILE:HD11	10:K:103:PHE:HB3	2.00	0.42
10:K:31:ALA:O	10:K:34:LEU:HB3	2.18	0.42
11:L:190:TYR:HA	11:L:193:SER:HB2	2.02	0.42
15:P:80:THR:H	17:R:11:LYS:NZ	2.18	0.42
2:b:28:ILE:C	2:b:191:ASN:HD22	2.24	0.42
11:l:111:ALA:O	11:l:114:THR:HG22	2.20	0.42
1:A:81:GLU:O	1:A:85:VAL:HG22	2.19	0.42
3:C:110:LYS:HE2	3:C:110:LYS:HA	2.01	0.42
26:E:101:PCF:H143	26:E:101:PCF:H111	1.81	0.42
8:H:93:ASN:ND2	3:c:172:ASP:OD2	2.44	0.42
9:J:102:TYR:HD2	9:J:103:TYR:CD1	2.36	0.42
9:J:285:ILE:HD12	9:J:290:LEU:HB3	2.01	0.42
10:K:2:VAL:HG13	10:K:6:LEU:HB2	2.02	0.42
10:K:29:GLY:C	10:K:66:MET:HE1	2.44	0.42
11:L:218:PHE:CE1	11:L:223:ILE:HD11	2.54	0.42
2:b:56:PHE:CE2	2:b:80:SER:HB3	2.54	0.42
3:c:121:ARG:HH12	3:c:188:SER:HA	1.83	0.42
5:e:44:ASN:HB3	5:e:47:LYS:HD2	2.01	0.42
9:j:271:PRO:HG2	9:j:276:LEU:HD22	2.00	0.42
11:l:198:TYR:CG	11:l:227:ARG:HG3	2.55	0.42
18:s:27:LYS:HG3	18:s:29:ALA:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:30:THR:O	5:E:34:THR:HG23	2.20	0.42
11:L:101:CYS:SG	28:L:401:HEM:CAB	3.08	0.42
12:M:63:VAL:CG1	12:M:64:PRO:HD3	2.50	0.42
15:P:176:ARG:NH2	20:U:58:LEU:O	2.52	0.42
2:b:79:LYS:HB3	2:b:79:LYS:HE3	1.90	0.42
2:b:184:ASN:HD21	2:b:215:LEU:HB2	1.84	0.42
3:c:42:VAL:HG12	8:h:38:GLN:CB	2.50	0.42
8:h:40:ILE:HD12	8:h:40:ILE:HA	1.75	0.42
8:h:72:ASN:HA	8:h:75:GLU:HG2	2.01	0.42
10:k:358:LEU:HG	30:k:604:HEA:HMA	2.02	0.42
2:B:118:GLU:O	2:B:122:SER:OG	2.33	0.42
5:E:55:ARG:NH2	5:E:56:ILE:HA	2.35	0.42
8:H:37:LEU:HD23	8:H:40:ILE:HD13	2.02	0.42
25:J:403:CDL:H562	25:J:403:CDL:H531	1.83	0.42
29:J:406:UQ6:H222	29:J:406:UQ6:H201	1.72	0.42
10:K:377:PHE:O	10:K:381:LEU:HD23	2.19	0.42
13:N:43:THR:OG1	13:N:44:PRO:HD3	2.19	0.42
14:O:80:THR:H	14:O:83:VAL:HG12	1.84	0.42
14:O:237:ALA:HB3	19:T:57:PRO:HD2	2.02	0.42
15:P:221:CYS:HB3	15:P:232:MET:HG2	2.00	0.42
15:P:241:LEU:HB3	15:P:242:PRO:HD3	2.01	0.42
2:b:258:ASN:HB2	2:b:321:THR:HG22	2.02	0.42
23:c:303:PEF:H51	4:d:48:TRP:HB3	2.02	0.42
6:f:47:ASP:OD2	6:f:74:ARG:NH1	2.50	0.42
9:j:35:LEU:HD11	9:j:236:PHE:CG	2.55	0.42
9:j:184:TYR:O	9:j:187:PRO:HD2	2.20	0.42
10:k:72:MET:HB2	10:k:73:PRO:HD3	2.00	0.42
16:q:117:ASN:HB3	16:q:120:GLN:HG2	2.00	0.42
18:s:35:GLU:HA	18:s:38:MET:HG3	2.01	0.42
1:A:259:ALA:HB3	1:A:334:THR:HG22	2.02	0.42
1:A:346:PHE:CE1	23:A:502:PEF:H41	2.48	0.42
9:J:107:ARG:HG3	9:J:108:SER:N	2.35	0.42
9:J:156:PHE:HB2	9:J:157:VAL:H	1.71	0.42
9:J:282:LEU:HD12	9:J:295:MET:HE2	2.01	0.42
9:J:298:ALA:O	9:J:301:VAL:HG12	2.19	0.42
29:J:406:UQ6:H151	29:J:406:UQ6:H172	1.84	0.42
10:K:133:LEU:HD13	15:P:184:VAL:HG21	2.01	0.42
10:K:200:LEU:HD23	10:K:239:PHE:HE1	1.85	0.42
25:K:603:CDL:H322	25:K:603:CDL:H351	1.92	0.42
15:P:62:VAL:O	15:P:66:SER:HB3	2.20	0.42
18:S:30:ALA:HA	19:T:74:LYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:63:ASN:OD1	1:a:63:ASN:N	2.51	0.42
1:a:172:THR:O	1:a:174:LEU:N	2.49	0.42
1:a:424:LYS:HE2	1:a:424:LYS:HB3	1.76	0.42
10:k:163:ILE:HG12	14:o:93:MET:CE	2.50	0.42
3:C:58:PHE:HD2	3:C:59:MET:HE2	1.84	0.42
3:C:121:ARG:CZ	3:C:153:LEU:HD22	2.50	0.42
6:F:3:GLN:HB2	9:J:310:ARG:HB2	2.01	0.42
9:J:55:SER:OG	9:J:56:SER:N	2.52	0.42
9:J:281:ILE:HG22	9:J:356:THR:HG22	2.02	0.42
10:K:332:ILE:HG23	10:K:338:MET:HE2	2.02	0.42
10:K:528:ASN:HB3	19:T:104:ASP:OD2	2.20	0.42
17:R:11:LYS:O	17:R:15:ILE:HG12	2.20	0.42
21:V:50:CYS:HA	21:V:53:TRP:HD1	1.85	0.42
22:W:85:PRO:HG2	22:W:87:LEU:O	2.19	0.42
2:b:348:LEU:HD12	2:b:348:LEU:HA	1.89	0.42
8:h:86:ARG:NH2	8:h:90:GLU:OE2	2.52	0.42
9:j:370:ILE:O	9:j:374:GLU:HG2	2.20	0.42
10:k:49:HIS:N	12:m:72:LEU:HD11	2.35	0.42
10:k:350:MET:O	10:k:353:LEU:HG	2.20	0.42
11:l:198:TYR:CD2	11:l:227:ARG:HG3	2.55	0.42
14:o:133:GLN:HG3	14:o:135:THR:H	1.84	0.42
14:o:143:ILE:HG12	18:s:67:ALA:HB2	2.02	0.42
1:A:457:TRP:C	4:D:29:ASN:HD21	2.27	0.42
25:C:302:CDL:H551	25:C:302:CDL:H521	1.90	0.42
8:H:83:LYS:HA	8:H:83:LYS:HD2	1.86	0.42
9:J:157:VAL:HG13	9:J:157:VAL:O	2.20	0.42
10:K:182:LEU:HD12	10:K:183:PRO:HD2	2.01	0.42
10:K:333:ARG:NH1	10:K:492:ASN:O	2.53	0.42
30:K:601:HEA:HHA	30:K:601:HEA:CGA	2.50	0.42
11:L:125:VAL:HG21	11:L:151:LEU:HD11	2.02	0.42
13:N:33:PHE:CE2	14:O:57:VAL:HG11	2.55	0.42
14:O:247:ILE:HG13	14:O:248:ILE:N	2.34	0.42
2:b:302:LYS:HZ2	2:b:363:PRO:HG3	1.85	0.42
4:d:63:GLY:N	4:d:64:PRO:HD3	2.34	0.42
9:j:207:SER:OG	28:j:404:HEM:O2D	2.35	0.42
9:j:223:SER:HA	9:j:227:PHE:HE2	1.85	0.42
10:k:474:ASP:HA	10:k:477:VAL:HG12	2.02	0.42
11:l:103:ALA:HA	11:l:158:PRO:HG2	2.02	0.42
18:s:14:PRO:HA	18:s:15:PRO:HD3	1.92	0.42
3:C:55:TYR:CE1	3:C:59:MET:HE3	2.55	0.41
3:C:159:CYS:HB2	3:C:164:CYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:71:ARG:O	6:F:75:ILE:HG22	2.20	0.41
7:G:143:PHE:CE2	11:L:76:TRP:HA	2.55	0.41
9:J:38:LEU:HA	9:J:41:VAL:HG12	2.02	0.41
9:J:136:TYR:CD2	9:J:176:ILE:HD11	2.55	0.41
10:K:381:LEU:HD22	30:K:601:HEA:CBC	2.49	0.41
14:O:236:THR:OG1	14:O:237:ALA:N	2.53	0.41
17:R:9:THR:HA	17:R:12:ARG:CD	2.50	0.41
1:a:253:ASP:N	1:a:253:ASP:OD1	2.53	0.41
2:b:111:LYS:HD2	2:b:177:ASP:OD1	2.20	0.41
8:h:43:ASN:O	8:h:47:ASN:HB2	2.20	0.41
9:j:58:ILE:HG22	9:j:176:ILE:HD12	2.02	0.41
10:k:289:SER:HB3	10:k:305:PHE:CZ	2.55	0.41
10:k:528:ASN:O	14:o:11:GLN:NE2	2.53	0.41
14:o:80:THR:O	14:o:84:ARG:NE	2.34	0.41
15:p:51:LEU:HA	15:p:54:VAL:HG22	2.02	0.41
17:r:12:ARG:NH1	17:r:13:ARG:HB2	2.35	0.41
18:s:74:GLU:HA	18:s:78:ALA:HB3	2.01	0.41
1:A:209:VAL:HG13	1:A:390:LEU:HD22	2.01	0.41
1:A:271:ASN:ND2	1:A:397:LYS:HG2	2.35	0.41
23:A:503:PEF:H371	23:A:503:PEF:H341	1.94	0.41
2:B:206:LEU:HD12	2:B:206:LEU:HA	1.86	0.41
8:H:62:PRO:HB3	9:J:328:ILE:HD12	2.03	0.41
8:H:66:TYR:HE1	9:J:332:ASN:N	2.17	0.41
10:K:25:SER:HB3	10:K:69:PHE:CE2	2.55	0.41
11:L:260:GLU:O	11:L:262:GLU:N	2.46	0.41
18:S:18:LEU:HD22	19:T:146:VAL:HG23	2.01	0.41
9:j:102:TYR:HE2	23:j:401:PEF:H32	1.85	0.41
9:j:132:TYR:O	9:j:140:SER:OG	2.22	0.41
10:k:334:LEU:HG	10:k:339:LEU:HD11	2.01	0.41
11:l:244:THR:HA	11:l:247:MET:HE3	2.01	0.41
13:n:38:ALA:O	13:n:42:VAL:HG13	2.20	0.41
14:o:236:THR:OG1	14:o:237:ALA:N	2.52	0.41
1:A:72:LEU:HD11	1:A:137:PHE:HE1	1.85	0.41
2:B:33:VAL:CG1	2:B:89:LEU:HB2	2.49	0.41
2:B:230:ARG:NH2	2:B:364:TYR:HA	2.35	0.41
3:C:42:VAL:HG12	8:H:38:GLN:HG2	2.02	0.41
5:E:50:LYS:HA	5:E:53:LYS:NZ	2.35	0.41
9:J:249:ASN:ND2	11:L:182:LYS:HD2	2.34	0.41
10:K:186:VAL:HA	10:K:189:ILE:HG12	2.00	0.41
30:K:604:HEA:HBC1	30:K:604:HEA:HMC3	2.02	0.41
14:O:156:HIS:O	14:O:159:LEU:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:112:SER:HB2	20:U:12:VAL:HG22	2.01	0.41
15:P:116:THR:O	15:P:132:ASP:HB2	2.20	0.41
19:T:66:LEU:HA	19:T:68:ARG:HH11	1.85	0.41
1:a:292:GLU:O	1:a:296:ARG:HG3	2.20	0.41
2:b:58:ASN:CG	2:b:64:ALA:HB2	2.44	0.41
2:b:151:PHE:CD2	2:b:155:LEU:HD22	2.53	0.41
2:b:219:SER:OG	2:b:220:GLU:N	2.53	0.41
9:j:14:ASN:HA	9:j:18:ILE:HB	2.02	0.41
9:j:89:PHE:CD2	28:j:403:HEM:HBC1	2.55	0.41
9:j:93:MET:HE1	28:j:404:HEM:HHC	2.01	0.41
10:k:396:TRP:NE1	10:k:515:GLU:OE2	2.51	0.41
14:o:202:GLY:HA2	14:o:205:PHE:CD2	2.56	0.41
19:t:143:LEU:HD23	19:t:145:PRO:HD3	2.01	0.41
20:u:33:ASP:OD1	20:u:33:ASP:N	2.53	0.41
1:A:131:LEU:HG	1:A:132:LEU:HD22	2.03	0.41
1:A:352:ASN:HD22	1:A:454:MET:HG3	1.84	0.41
2:B:62:ARG:HB2	2:B:67:LEU:HB2	2.02	0.41
2:B:241:ILE:HD11	2:B:301:ILE:HD11	2.03	0.41
3:C:160:THR:HG23	3:C:200:LEU:HD23	2.03	0.41
3:C:184:HIS:CD2	3:C:193:LYS:HB3	2.55	0.41
6:F:116:GLU:O	2:b:66:LYS:HG2	2.20	0.41
8:H:36:PRO:HB2	8:H:37:LEU:HD12	2.02	0.41
10:K:210:LEU:HD11	10:K:232:TYR:CZ	2.56	0.41
10:K:350:MET:O	10:K:353:LEU:HG	2.20	0.41
10:K:355:GLY:HA3	10:K:376:HIS:CE1	2.55	0.41
25:K:603:CDL:H561	25:K:603:CDL:H742	2.01	0.41
11:L:157:GLY:HA2	11:L:158:PRO:HD3	1.96	0.41
14:O:4:LEU:HD12	14:O:5:GLU:N	2.36	0.41
14:O:9:HIS:CD2	19:T:66:LEU:HD13	2.56	0.41
14:O:39:LEU:HD21	14:O:45:ILE:HB	2.03	0.41
18:S:55:SER:HB3	18:S:60:LEU:HD23	2.02	0.41
1:a:447:ARG:HH22	9:j:220:PRO:HB2	1.86	0.41
6:f:80:GLN:OE1	6:f:80:GLN:HA	2.21	0.41
9:j:314:ARG:HG2	9:j:315:GLY:N	2.35	0.41
10:k:188:SER:HB2	10:k:249:ILE:HG22	2.02	0.41
10:k:342:ILE:HG22	23:w:202:PEF:H212	2.01	0.41
13:n:9:GLN:NE2	14:o:75:TYR:O	2.53	0.41
16:q:126:ASP:OD1	16:q:127:GLU:N	2.54	0.41
22:w:125:ASN:O	22:w:129:GLN:HG2	2.21	0.41
1:A:137:PHE:CZ	1:A:189:VAL:HA	2.55	0.41
23:A:502:PEF:H172	23:A:502:PEF:H142	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:184:HIS:HD2	3:C:193:LYS:HB3	1.85	0.41
9:J:134:CYS:SG	9:J:180:PHE:HA	2.60	0.41
10:K:515:GLU:HA	10:K:518:LEU:HD13	2.03	0.41
11:L:125:VAL:HG23	11:L:151:LEU:HD21	2.01	0.41
16:Q:126:ASP:OD1	16:Q:127:GLU:N	2.53	0.41
18:S:47:THR:HA	18:S:50:MET:HG2	2.03	0.41
2:b:28:ILE:HD12	2:b:28:ILE:HA	1.87	0.41
3:c:149:ASP:HB3	3:c:152:TRP:HD1	1.85	0.41
3:c:180:CYS:SG	3:c:181:HIS:CE1	3.14	0.41
10:k:370:THR:O	10:k:373:VAL:HG22	2.21	0.41
12:m:34:VAL:HG12	12:m:35:TYR:CD2	2.55	0.41
22:w:126:LYS:O	22:w:130:LEU:HD23	2.20	0.41
23:A:501:PEF:H311	23:A:501:PEF:H342	1.69	0.41
9:J:319:LYS:HB2	9:J:322:SER:HB3	2.02	0.41
29:J:408:UQ6:H1M1	29:J:408:UQ6:H72	1.84	0.41
10:K:108:MET:HG3	14:O:31:LEU:HB3	2.03	0.41
10:K:408:LYS:HG2	22:W:94:PHE:HD2	1.85	0.41
14:O:219:LEU:HD13	14:O:249:TYR:HD2	1.84	0.41
15:P:221:CYS:HB3	15:P:229:HIS:CE1	2.56	0.41
20:U:49:LYS:HG2	20:U:52:TRP:HE1	1.84	0.41
1:a:446:MET:HG2	9:j:224:TYR:CE1	2.55	0.41
8:h:61:ILE:HD13	8:h:61:ILE:HA	1.93	0.41
30:k:603:HEA:H271	30:k:603:HEA:H212	1.33	0.41
13:n:5:VAL:HG12	19:t:47:ILE:HD13	2.01	0.41
14:o:239:HIS:CE1	19:t:63:GLU:HB3	2.55	0.41
15:p:241:LEU:HB3	15:p:242:PRO:HD3	2.02	0.41
2:B:278:LYS:NZ	2:B:338:LEU:HD11	2.35	0.41
3:C:154:ILE:HD11	3:C:212:VAL:HG21	2.01	0.41
3:C:178:CYS:SG	3:C:180:CYS:HB2	2.60	0.41
15:P:190:ILE:HD13	15:P:219:GLY:HA3	2.03	0.41
18:S:30:ALA:O	18:S:34:LYS:HG2	2.21	0.41
1:a:77:PHE:CD2	1:a:78:LEU:HD12	2.55	0.41
2:b:63:SER:OG	2:b:66:LYS:HE2	2.19	0.41
3:c:186:ASP:OD1	3:c:190:ARG:N	2.34	0.41
8:h:58:TYR:CD1	9:j:323:LYS:HD2	2.55	0.41
23:j:406:PEF:H182	23:j:406:PEF:H151	1.91	0.41
10:k:174:THR:HG23	10:k:177:MET:H	1.85	0.41
10:k:314:ILE:HB	10:k:315:PRO:HD3	2.03	0.41
10:k:493:LYS:HA	10:k:493:LYS:HD3	1.82	0.41
14:o:48:MET:O	14:o:48:MET:HE3	2.20	0.41
17:r:9:THR:HA	17:r:12:ARG:NE	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s:30:ALA:HA	19:t:74:LYS:O	2.21	0.41
18:s:66:THR:HA	18:s:69:ASN:ND2	2.36	0.41
21:v:50:CYS:HA	21:v:53:TRP:HD1	1.86	0.41
22:w:78:GLY:HA3	22:w:83:ARG:HG3	2.02	0.41
23:w:202:PEF:H251	23:w:202:PEF:H221	1.94	0.41
1:A:240:LYS:HA	1:A:240:LYS:HD2	1.71	0.41
1:A:355:THR:HG21	1:A:427:TRP:CE3	2.56	0.41
2:B:143:GLU:HG2	2:B:288:PHE:HZ	1.86	0.41
28:J:404:HEM:HBC2	28:J:404:HEM:CMC	2.50	0.41
29:J:406:UQ6:H212	29:J:406:UQ6:H171	1.80	0.41
14:O:47:ASN:HD22	14:O:50:MET:HG2	1.85	0.41
14:O:85:LYS:HA	14:O:85:LYS:HD2	1.90	0.41
15:P:20:PRO:HG3	22:W:149:GLN:HA	2.03	0.41
16:Q:90:LYS:HD2	16:Q:90:LYS:HA	1.84	0.41
18:S:19:LYS:HD2	18:S:21:ALA:H	1.85	0.41
2:b:116:PRO:CB	2:b:169:LEU:HD13	2.51	0.41
2:b:247:LYS:HE3	2:b:281:ASP:HA	2.03	0.41
6:f:73:TYR:HB2	8:h:24:ILE:HD11	2.03	0.41
9:j:5:LYS:HG2	9:j:14:ASN:HD22	1.86	0.41
10:k:412:ILE:HG22	22:w:95:ILE:HG23	2.03	0.41
14:o:118:VAL:HG13	20:u:28:TRP:HE1	1.84	0.41
16:q:90:LYS:HD2	16:q:93:ARG:HE	1.85	0.41
2:B:21:ALA:N	2:B:194:GLU:OE2	2.54	0.41
3:C:113:GLY:O	3:C:114:LYS:HD2	2.21	0.41
4:D:7:LEU:HD11	4:D:9:SER:HB3	2.03	0.41
7:G:128:PHE:CD1	11:L:69:LEU:HD11	2.56	0.41
9:J:7:ASN:O	9:J:11:SER:N	2.42	0.41
9:J:26:ILE:HA	9:J:30:TRP:HZ3	1.81	0.41
9:J:58:ILE:HG13	9:J:59:GLU:N	2.36	0.41
9:J:91:MET:HB2	9:J:273:TRP:HZ2	1.86	0.41
9:J:115:ASN:O	9:J:118:VAL:HG12	2.21	0.41
9:J:195:ILE:HD11	27:J:402:CN5:C3'	2.51	0.41
28:J:405:HEM:HMA2	29:J:406:UQ6:O4	2.20	0.41
29:J:406:UQ6:H322	29:J:406:UQ6:H301	1.91	0.41
10:K:60:VAL:HG13	10:K:127:TRP:HA	2.03	0.41
10:K:218:THR:OG1	14:O:196:ILE:HG12	2.20	0.41
12:M:72:LEU:HD23	12:M:73:LYS:H	1.84	0.41
15:P:48:LEU:HA	15:P:51:LEU:HG	2.03	0.41
16:Q:96:ARG:HD2	16:Q:96:ARG:HA	1.84	0.41
19:T:47:ILE:HG23	19:T:64:THR:HG22	2.03	0.41
20:U:66:LYS:HA	20:U:66:LYS:HD2	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:101:ALA:HA	22:W:104:LEU:HG	2.01	0.41
23:W:202:PEF:H221	23:W:202:PEF:H251	1.81	0.41
1:a:99:ARG:HD3	1:a:99:ARG:HA	1.87	0.41
1:a:271:ASN:ND2	1:a:397:LYS:HA	2.35	0.41
1:a:308:GLU:OE2	9:j:1:MET:N	2.36	0.41
2:b:237:SER:OG	2:b:297:VAL:HG21	2.21	0.41
9:j:336:LEU:O	9:j:339:ILE:HG22	2.21	0.41
10:k:62:HIS:O	10:k:66:MET:HG2	2.21	0.41
10:k:108:MET:HG3	14:o:31:LEU:HB3	2.02	0.41
10:k:283:LEU:HD13	10:k:286:LEU:HD13	2.03	0.41
12:m:70:VAL:HG13	12:m:71:GLN:CD	2.46	0.41
14:o:80:THR:C	14:o:84:ARG:HE	2.22	0.41
16:q:64:TYR:N	16:q:68:GLU:OE2	2.54	0.41
22:w:150:VAL:HG22	22:w:152:SER:O	2.21	0.41
23:w:202:PEF:H142	23:w:202:PEF:H111	1.88	0.41
26:E:101:PCF:H262	26:E:101:PCF:H231	1.78	0.41
9:J:197:HIS:CD2	28:J:405:HEM:NB	2.89	0.41
13:N:5:VAL:HG22	14:O:234:HIS:CE1	2.55	0.41
14:O:238:GLY:HA2	19:T:62:GLN:HE22	1.85	0.41
1:a:430:ASP:HA	1:a:449:ARG:CZ	2.51	0.41
2:b:267:LEU:HD12	2:b:312:LYS:HZ1	1.86	0.41
5:e:44:ASN:HB3	5:e:47:LYS:HB2	2.03	0.41
9:j:150:LEU:HD22	9:j:292:VAL:HG22	2.02	0.41
9:j:345:GLU:HB2	9:j:348:TYR:HD2	1.86	0.41
11:l:105:HIS:NE2	28:l:401:HEM:C4B	2.88	0.41
13:n:17:LYS:HA	13:n:17:LYS:HD2	1.67	0.41
14:o:168:LEU:HA	14:o:171:LEU:HG	2.02	0.41
15:p:204:LEU:HD11	20:u:62:ASP:HB3	2.03	0.41
15:p:223:GLU:O	15:p:229:HIS:NE2	2.54	0.41
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.88	0.40
2:B:164:VAL:HG11	2:b:232:ARG:NH2	2.36	0.40
3:C:117:PHE:CD1	3:C:157:GLY:HA3	2.56	0.40
3:C:127:GLN:O	3:C:131:SER:OG	2.28	0.40
6:F:58:THR:HG22	6:F:62:ARG:HE	1.85	0.40
8:H:13:TRP:CZ2	9:J:21:PRO:HG3	2.55	0.40
9:J:183:HIS:O	9:J:187:PRO:HD3	2.21	0.40
9:J:195:ILE:HD11	27:J:402:CN5:H3'	2.03	0.40
10:K:35:ILE:O	10:K:38:LEU:N	2.53	0.40
10:K:258:VAL:HA	10:K:261:THR:HG22	2.03	0.40
10:K:403:LEU:CD1	10:K:479:GLY:HA3	2.51	0.40
11:L:226:ALA:O	11:L:228:VAL:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:241:LYS:HG3	1:a:242:ALA:H	1.86	0.40
2:b:347:LYS:HE2	2:b:347:LYS:HB2	1.89	0.40
25:c:302:CDL:HB21	8:h:36:PRO:HD2	2.03	0.40
9:j:380:ILE:HG13	9:j:381:GLY:N	2.35	0.40
10:k:6:LEU:HD22	10:k:104:TRP:HH2	1.86	0.40
10:k:496:ASP:O	10:k:499:GLU:HG2	2.21	0.40
10:k:521:PRO:HA	10:k:522:PRO:HD3	1.93	0.40
15:p:46:TYR:O	15:p:49:VAL:HG22	2.21	0.40
16:q:111:LEU:O	16:q:114:LYS:NZ	2.52	0.40
16:q:116:GLU:HG2	16:q:117:ASN:N	2.35	0.40
1:A:66:ASN:HB2	22:W:29:ALA:HB3	2.03	0.40
1:A:363:VAL:HG21	1:A:415:VAL:HG12	2.03	0.40
2:B:255:VAL:HA	2:B:321:THR:HG21	2.04	0.40
3:C:119:ARG:HD2	3:C:176:TRP:HH2	1.86	0.40
9:J:208:ASN:HD21	9:J:214:GLY:CA	2.33	0.40
10:K:415:TRP:O	10:K:419:ILE:HG12	2.21	0.40
15:P:43:ILE:O	15:P:47:LEU:HD23	2.21	0.40
17:R:46:LYS:HA	17:R:46:LYS:HD2	1.73	0.40
19:T:127:THR:HG23	19:T:130:GLU:H	1.86	0.40
21:V:51:LEU:HD23	21:V:51:LEU:HA	1.89	0.40
1:a:100:ASP:O	1:a:101:PHE:HD2	2.04	0.40
2:b:99:PRO:HB3	2:b:200:PHE:CE1	2.56	0.40
3:c:51:LYS:HE3	3:c:51:LYS:HB3	1.92	0.40
6:f:84:THR:O	6:f:85:HIS:HB2	2.21	0.40
29:j:405:UQ6:H112	29:j:405:UQ6:H72	1.75	0.40
29:j:405:UQ6:H13	29:j:405:UQ6:H171	1.71	0.40
11:l:89:SER:O	11:l:93:GLY:N	2.47	0.40
22:w:129:GLN:HG3	22:w:150:VAL:HG23	2.03	0.40
1:A:414:THR:HG22	1:A:415:VAL:N	2.36	0.40
8:H:34:GLN:NE2	11:L:293:ALA:HB1	2.36	0.40
10:K:111:VAL:O	10:K:114:VAL:HG12	2.20	0.40
11:L:227:ARG:HD3	11:L:227:ARG:HA	1.96	0.40
13:N:5:VAL:HG22	14:O:234:HIS:ND1	2.37	0.40
13:N:18:PRO:O	13:N:19:LEU:HB2	2.21	0.40
14:O:184:CYS:O	14:O:187:ILE:HG22	2.22	0.40
14:O:250:THR:HA	14:O:253:LEU:HG	2.03	0.40
22:W:93:SER:O	22:W:97:LYS:HG2	2.21	0.40
1:a:293:PRO:O	1:a:297:LEU:HD22	2.22	0.40
5:e:51:ASP:OD2	5:e:51:ASP:C	2.63	0.40
2:B:99:PRO:HG3	2:B:200:PHE:CE2	2.56	0.40
2:B:230:ARG:HD3	2:B:359:VAL:HG13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:18:VAL:HA	5:E:21:ILE:HG22	2.03	0.40
8:H:61:ILE:HB	8:H:62:PRO:HD3	2.02	0.40
27:J:402:CN5:H37	27:J:402:CN5:H34A	1.96	0.40
11:L:192:PHE:O	11:L:196:THR:HG22	2.22	0.40
16:Q:108:PHE:HB3	16:Q:140:LYS:HD3	2.04	0.40
17:R:12:ARG:HH11	17:R:13:ARG:HB2	1.86	0.40
1:a:414:THR:HG22	1:a:415:VAL:N	2.37	0.40
3:c:161:HIS:HB3	24:c:301:FES:S2	2.61	0.40
10:k:249:ILE:HD13	10:k:249:ILE:HA	1.90	0.40
11:l:89:SER:O	11:l:92:ARG:HG2	2.21	0.40
11:l:198:TYR:HB2	11:l:227:ARG:NH1	2.36	0.40
14:o:15:HIS:CE1	14:o:76:LEU:HD12	2.57	0.40
1:A:451:ASP:OD1	1:A:451:ASP:N	2.55	0.40
2:B:58:ASN:CG	2:B:64:ALA:HB2	2.47	0.40
9:J:35:LEU:CD1	9:J:232:THR:HG22	2.49	0.40
9:J:136:TYR:CE2	9:J:141:HIS:HB2	2.56	0.40
9:J:195:ILE:O	9:J:199:MET:HG3	2.22	0.40
10:K:11:ALA:HA	10:K:14:ILE:HG22	2.02	0.40
10:K:48:LEU:HD11	10:K:54:LEU:HD23	2.03	0.40
10:K:459:PHE:CZ	22:W:113:VAL:HG11	2.56	0.40
10:K:485:ASN:ND2	10:K:487:LYS:HB2	2.36	0.40
13:N:42:VAL:HG12	14:O:35:LEU:HD11	2.04	0.40
1:a:74:LYS:HZ1	1:a:96:ASN:C	2.29	0.40
1:a:215:LYS:HG3	1:a:216:HIS:N	2.36	0.40
7:g:73:GLU:HG3	7:g:74:VAL:HG23	2.03	0.40
9:j:291:GLY:HA2	9:j:294:THR:HG22	2.02	0.40
10:k:403:LEU:HB3	10:k:475:GLN:HG3	2.03	0.40
11:l:248:ALA:O	11:l:252:THR:HG22	2.22	0.40
11:l:262:GLU:O	11:l:266:ARG:HB2	2.22	0.40
14:o:148:SER:HA	14:o:151:THR:HG22	2.04	0.40
14:o:231:ARG:HA	14:o:231:ARG:HD2	1.83	0.40
16:q:132:ARG:NH2	16:q:140:LYS:HG3	2.37	0.40
17:r:3:ILE:O	17:r:3:ILE:HG13	2.21	0.40
19:t:82:ASP:N	19:t:82:ASP:OD1	2.55	0.40
20:u:45:PHE:HD2	20:u:52:TRP:HH2	1.70	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	429/457 (94%)	368 (86%)	60 (14%)	1 (0%)	43	73
1	a	429/457 (94%)	366 (85%)	62 (14%)	1 (0%)	43	73
2	B	350/368 (95%)	324 (93%)	26 (7%)	0	100	100
2	b	350/368 (95%)	319 (91%)	31 (9%)	0	100	100
3	C	183/215 (85%)	166 (91%)	17 (9%)	0	100	100
3	c	183/215 (85%)	167 (91%)	16 (9%)	0	100	100
4	D	64/77 (83%)	59 (92%)	5 (8%)	0	100	100
4	d	64/77 (83%)	61 (95%)	3 (5%)	0	100	100
5	E	55/66 (83%)	55 (100%)	0	0	100	100
5	e	55/66 (83%)	54 (98%)	1 (2%)	0	100	100
6	F	124/127 (98%)	116 (94%)	8 (6%)	0	100	100
6	f	124/127 (98%)	116 (94%)	8 (6%)	0	100	100
7	G	73/147 (50%)	72 (99%)	1 (1%)	0	100	100
7	g	73/147 (50%)	71 (97%)	2 (3%)	0	100	100
8	H	91/94 (97%)	84 (92%)	5 (6%)	2 (2%)	5	29
8	h	91/94 (97%)	82 (90%)	8 (9%)	1 (1%)	11	43
9	J	383/385 (100%)	352 (92%)	31 (8%)	0	100	100
9	j	383/385 (100%)	363 (95%)	20 (5%)	0	100	100
10	K	532/534 (100%)	493 (93%)	39 (7%)	0	100	100
10	k	532/534 (100%)	506 (95%)	26 (5%)	0	100	100
11	L	246/309 (80%)	210 (85%)	33 (13%)	3 (1%)	10	42
11	l	246/309 (80%)	211 (86%)	34 (14%)	1 (0%)	30	62
12	M	45/78 (58%)	43 (96%)	2 (4%)	0	100	100
12	m	45/78 (58%)	40 (89%)	5 (11%)	0	100	100
13	N	57/60 (95%)	50 (88%)	7 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	n	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
14	O	267/269 (99%)	245 (92%)	22 (8%)	0	100	100
14	o	267/269 (99%)	246 (92%)	21 (8%)	0	100	100
15	P	234/251 (93%)	218 (93%)	16 (7%)	0	100	100
15	p	234/251 (93%)	222 (95%)	12 (5%)	0	100	100
16	Q	100/148 (68%)	92 (92%)	8 (8%)	0	100	100
16	q	100/148 (68%)	92 (92%)	8 (8%)	0	100	100
17	R	53/59 (90%)	50 (94%)	3 (6%)	0	100	100
17	r	53/59 (90%)	52 (98%)	1 (2%)	0	100	100
18	S	111/129 (86%)	103 (93%)	8 (7%)	0	100	100
18	s	111/129 (86%)	102 (92%)	9 (8%)	0	100	100
19	T	119/155 (77%)	109 (92%)	10 (8%)	0	100	100
19	t	119/155 (77%)	110 (92%)	9 (8%)	0	100	100
20	U	75/83 (90%)	72 (96%)	3 (4%)	0	100	100
20	u	75/83 (90%)	72 (96%)	3 (4%)	0	100	100
21	V	43/66 (65%)	41 (95%)	2 (5%)	0	100	100
21	v	43/66 (65%)	39 (91%)	4 (9%)	0	100	100
22	W	131/153 (86%)	115 (88%)	16 (12%)	0	100	100
22	w	131/153 (86%)	119 (91%)	12 (9%)	0	100	100
All	All	7530/8460 (89%)	6898 (92%)	623 (8%)	9 (0%)	49	79

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	40	ILE
11	L	240	THR
11	l	240	THR
11	L	122	ASN
1	A	156	HIS
1	a	156	HIS
11	L	236	TYR
8	H	30	SER
8	h	30	SER

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	370/393 (94%)	370 (100%)	0	100	100
1	a	370/393 (94%)	370 (100%)	0	100	100
2	B	301/313 (96%)	300 (100%)	1 (0%)	86	88
2	b	301/313 (96%)	301 (100%)	0	100	100
3	C	151/179 (84%)	151 (100%)	0	100	100
3	c	151/179 (84%)	151 (100%)	0	100	100
4	D	56/66 (85%)	56 (100%)	0	100	100
4	d	56/66 (85%)	56 (100%)	0	100	100
5	E	47/54 (87%)	47 (100%)	0	100	100
5	e	47/54 (87%)	47 (100%)	0	100	100
6	F	110/111 (99%)	110 (100%)	0	100	100
6	f	110/111 (99%)	110 (100%)	0	100	100
7	G	68/131 (52%)	67 (98%)	1 (2%)	57	76
7	g	68/131 (52%)	68 (100%)	0	100	100
8	H	77/78 (99%)	77 (100%)	0	100	100
8	h	77/78 (99%)	75 (97%)	2 (3%)	40	69
9	J	338/338 (100%)	338 (100%)	0	100	100
9	j	338/338 (100%)	338 (100%)	0	100	100
10	K	447/447 (100%)	447 (100%)	0	100	100
10	k	447/447 (100%)	447 (100%)	0	100	100
11	L	206/251 (82%)	206 (100%)	0	100	100
11	l	206/251 (82%)	206 (100%)	0	100	100
12	M	39/67 (58%)	38 (97%)	1 (3%)	40	69
12	m	39/67 (58%)	39 (100%)	0	100	100
13	N	50/51 (98%)	50 (100%)	0	100	100
13	n	50/51 (98%)	50 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	O	228/228 (100%)	228 (100%)	0	100	100
14	o	228/228 (100%)	228 (100%)	0	100	100
15	P	209/224 (93%)	209 (100%)	0	100	100
15	p	209/224 (93%)	209 (100%)	0	100	100
16	Q	91/131 (70%)	91 (100%)	0	100	100
16	q	91/131 (70%)	91 (100%)	0	100	100
17	R	46/50 (92%)	46 (100%)	0	100	100
17	r	46/50 (92%)	46 (100%)	0	100	100
18	S	99/113 (88%)	99 (100%)	0	100	100
18	s	99/113 (88%)	99 (100%)	0	100	100
19	T	102/135 (76%)	102 (100%)	0	100	100
19	t	102/135 (76%)	102 (100%)	0	100	100
20	U	69/74 (93%)	69 (100%)	0	100	100
20	u	69/74 (93%)	69 (100%)	0	100	100
21	V	36/53 (68%)	36 (100%)	0	100	100
21	v	36/53 (68%)	36 (100%)	0	100	100
22	W	110/127 (87%)	109 (99%)	1 (1%)	70	81
22	w	110/127 (87%)	110 (100%)	0	100	100
All	All	6500/7228 (90%)	6494 (100%)	6 (0%)	87	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	258	ASN
7	G	108	GLN
12	M	37	ASN
22	W	35	GLN
8	h	38	GLN
8	h	40	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	310	GLN

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Mol	Chain	Res	Type
1	A	317	HIS
2	B	157	ASN
2	B	184	ASN
3	C	161	HIS
7	G	84	HIS
8	H	21	GLN
8	H	47	ASN
8	H	74	ASN
8	H	77	ASN
9	J	138	GLN
9	J	208	ASN
9	J	256	ASN
9	J	261	ASN
9	J	332	ASN
9	J	338	GLN
10	K	137	GLN
10	K	482	ASN
10	K	485	ASN
11	L	169	ASN
11	L	303	ASN
14	O	191	ASN
14	O	234	HIS
18	S	122	ASN
20	U	23	GLN
20	U	35	HIS
22	W	46	GLN
1	a	67	ASN
1	a	102	GLN
1	a	154	ASN
1	a	199	ASN
1	a	385	ASN
2	b	52	ASN
2	b	145	GLN
2	b	258	ASN
2	b	361	ASN
3	c	106	ASN
3	c	130	ASN
3	c	181	HIS
6	f	86	HIS
7	g	119	HIS
8	h	38	GLN
8	h	42	HIS

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Mol	Chain	Res	Type
8	h	47	ASN
8	h	74	ASN
9	j	27	ASN
9	j	82	HIS
9	j	115	ASN
9	j	253	HIS
10	k	99	ASN
10	k	100	ASN
10	k	164	ASN
10	k	217	ASN
10	k	399	GLN
10	k	482	ASN
10	k	485	ASN
11	l	163	GLN
11	l	169	ASN
11	l	213	ASN
11	l	246	GLN
14	o	141	ASN
16	q	70	GLN
16	q	117	ASN
18	s	69	ASN
18	s	86	HIS
18	s	100	ASN
18	s	124	HIS
20	u	35	HIS
20	u	56	ASN
22	w	22	GLN
22	w	35	GLN
22	w	57	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 63 ligands modelled in this entry, 2 are monoatomic and 4 are modelled with single atom - leaving 57 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	$\# Z > 2$
26	PCF	E	101	-	46,46,49	0.63	0	52,54,57	0.62	1 (1%)
25	CDL	L	402	-	66,66,99	1.09	6 (9%)	72,78,111	0.89	4 (5%)
23	PEF	J	407	-	42,42,46	0.46	0	45,47,51	1.30	5 (11%)
25	CDL	C	302	-	52,52,99	1.22	6 (11%)	58,64,111	0.94	3 (5%)
23	PEF	w	201	-	35,35,46	0.48	0	38,40,51	1.32	4 (10%)
25	CDL	h	602	-	66,66,99	1.09	6 (9%)	72,78,111	0.89	4 (5%)
23	PEF	W	201	-	35,35,46	0.46	0	38,40,51	1.32	4 (10%)
26	PCF	W	203	-	35,35,49	0.71	0	41,43,57	0.55	0
29	UQ6	j	407	-	43,43,43	0.47	0	54,55,55	1.57	13 (24%)
25	CDL	k	602	-	66,66,99	1.09	6 (9%)	72,78,111	0.87	2 (2%)
23	PEF	w	202	-	40,40,46	0.46	0	43,45,51	1.24	4 (9%)
23	PEF	W	202	-	40,40,46	0.45	0	43,45,51	1.27	4 (9%)
29	UQ6	j	405	-	43,43,43	0.46	0	54,55,55	1.60	14 (25%)
23	PEF	A	502	-	30,30,46	0.48	0	33,35,51	1.38	4 (12%)
23	PEF	e	101	-	31,31,46	0.51	0	34,36,51	1.33	5 (14%)
23	PEF	j	406	-	42,42,46	0.44	0	45,47,51	1.29	4 (8%)
25	CDL	h	601	-	52,52,99	1.23	6 (11%)	58,64,111	0.97	4 (6%)
30	HEA	K	604	10	67,67,67	2.17	23 (34%)	81,103,103	2.48	34 (41%)
28	HEM	J	404	9	50,50,50	1.85	14 (28%)	67,82,82	1.86	15 (22%)
23	PEF	E	102	-	31,31,46	0.49	0	34,36,51	1.34	5 (14%)
25	CDL	j	402	-	55,55,99	1.20	6 (10%)	61,67,111	0.93	4 (6%)
23	PEF	C	303	-	28,28,46	0.52	0	31,33,51	1.38	5 (16%)
24	FES	C	301	3	0,4,4	-	-	-	-	-
28	HEM	l	401	11	50,50,50	1.82	15 (30%)	67,82,82	1.73	15 (22%)
29	UQ6	J	408	-	20,20,43	0.59	0	25,27,55	1.67	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PEF	a	503	-	30,30,46	0.49	0	33,35,51	1.32	4 (12%)
30	HEA	K	601	10	67,67,67	2.19	23 (34%)	81,103,103	2.48	35 (43%)
28	HEM	L	401	11	50,50,50	1.81	13 (26%)	67,82,82	1.79	14 (20%)
24	FES	c	301	3	0,4,4	-	-	-	-	-
23	PEF	A	503	-	39,39,46	0.44	0	42,44,51	1.28	4 (9%)
30	HEA	k	604	10	67,67,67	2.21	23 (34%)	81,103,103	2.48	34 (41%)
23	PEF	c	303	-	28,28,46	0.49	0	31,33,51	1.33	4 (12%)
23	PEF	A	501	-	39,39,46	0.45	0	42,44,51	1.27	4 (9%)
23	PEF	j	408	-	28,28,46	0.51	0	31,33,51	1.32	4 (12%)
25	CDL	c	302	-	47,47,99	1.28	6 (12%)	53,59,111	1.02	5 (9%)
29	UQ6	J	406	-	43,43,43	0.50	0	54,55,55	1.70	13 (24%)
26	PCF	a	502	-	46,46,49	0.63	0	52,54,57	0.58	0
23	PEF	c	304	-	31,31,46	0.47	0	34,36,51	1.34	4 (11%)
26	PCF	H	602	-	49,49,49	0.62	0	55,57,57	0.50	0
23	PEF	v	101	-	32,32,46	0.48	0	35,37,51	1.31	5 (14%)
26	PCF	k	605	-	35,35,49	0.71	0	41,43,57	0.54	0
26	PCF	w	203	-	49,49,49	0.63	0	55,57,57	0.53	0
25	CDL	H	601	-	52,52,99	1.22	6 (11%)	58,64,111	0.96	4 (6%)
28	HEM	J	405	9	50,50,50	1.85	15 (30%)	67,82,82	1.91	16 (23%)
30	HEA	k	603	10	67,67,67	2.22	24 (35%)	81,103,103	2.42	34 (41%)
28	HEM	j	404	9	50,50,50	1.84	14 (28%)	67,82,82	1.91	16 (23%)
25	CDL	J	403	-	55,55,99	1.19	6 (10%)	61,67,111	0.97	4 (6%)
28	HEM	j	403	9	50,50,50	1.84	14 (28%)	67,82,82	1.85	15 (22%)
23	PEF	J	401	-	44,44,46	0.45	0	47,49,51	1.21	4 (8%)
23	PEF	J	409	-	28,28,46	0.50	0	31,33,51	1.39	4 (12%)
23	PEF	a	501	-	39,39,46	0.46	0	42,44,51	1.36	5 (11%)
25	CDL	K	603	-	66,66,99	1.08	6 (9%)	72,78,111	0.89	2 (2%)
27	CN5	J	402	-	40,40,40	0.50	0	44,48,48	0.92	1 (2%)
23	PEF	j	401	-	44,44,46	0.44	0	47,49,51	1.20	4 (8%)
23	PEF	a	504	-	39,39,46	0.45	0	42,44,51	1.24	4 (9%)
23	PEF	C	304	-	31,31,46	0.48	0	34,36,51	1.32	4 (11%)
23	PEF	V	101	-	32,32,46	0.49	0	35,37,51	1.34	5 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PCF	E	101	-	-	12/50/50/53	-
25	CDL	L	402	-	1/1/9/9	33/77/77/110	-
23	PEF	J	407	-	-	10/46/46/50	-
25	CDL	C	302	-	1/1/9/9	27/63/63/110	-
23	PEF	w	201	-	-	10/39/39/50	-
25	CDL	h	602	-	1/1/9/9	26/77/77/110	-
23	PEF	W	201	-	-	7/39/39/50	-
26	PCF	W	203	-	-	10/39/39/53	-
29	UQ6	j	407	-	-	9/39/39/39	0/1/1/1
25	CDL	k	602	-	1/1/9/9	33/77/77/110	-
23	PEF	w	202	-	-	6/44/44/50	-
23	PEF	W	202	-	-	8/44/44/50	-
29	UQ6	j	405	-	-	7/39/39/39	0/1/1/1
23	PEF	A	502	-	-	1/34/34/50	-
23	PEF	e	101	-	-	6/35/35/50	-
25	CDL	h	601	-	1/1/9/9	26/63/63/110	-
23	PEF	j	406	-	-	14/46/46/50	-
30	HEA	K	604	10	-	16/36/76/76	-
28	HEM	J	404	9	-	5/14/54/54	-
23	PEF	E	102	-	-	8/35/35/50	-
25	CDL	j	402	-	1/1/9/9	23/66/66/110	-
23	PEF	C	303	-	-	9/32/32/50	-
28	HEM	l	401	11	-	4/14/54/54	-
29	UQ6	J	408	-	-	2/12/12/39	0/1/1/1
30	HEA	K	601	10	-	16/36/76/76	-
23	PEF	a	503	-	-	6/34/34/50	-
24	FES	C	301	3	-	-	0/1/1/1
28	HEM	L	401	11	-	6/14/54/54	-
24	FES	c	301	3	-	-	0/1/1/1
23	PEF	A	503	-	-	11/43/43/50	-
30	HEA	k	604	10	-	16/36/76/76	-
23	PEF	c	303	-	-	8/32/32/50	-
23	PEF	A	501	-	-	8/43/43/50	-
25	CDL	c	302	-	1/1/9/9	22/58/58/110	-
23	PEF	j	408	-	-	5/32/32/50	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	UQ6	J	406	-	-	11/39/39/39	0/1/1/1
26	PCF	a	502	-	-	13/50/50/53	-
23	PEF	c	304	-	-	10/35/35/50	-
26	PCF	H	602	-	-	16/53/53/53	-
23	PEF	v	101	-	-	7/36/36/50	-
26	PCF	k	605	-	-	7/39/39/53	-
26	PCF	w	203	-	-	15/53/53/53	-
25	CDL	H	601	-	1/1/9/9	28/63/63/110	-
28	HEM	J	405	9	-	7/14/54/54	-
30	HEA	k	603	10	-	17/36/76/76	-
28	HEM	j	404	9	-	6/14/54/54	-
25	CDL	J	403	-	1/1/9/9	27/66/66/110	-
28	HEM	j	403	9	-	8/14/54/54	-
23	PEF	J	401	-	-	16/48/48/50	-
23	PEF	J	409	-	-	11/32/32/50	-
23	PEF	a	501	-	-	9/43/43/50	-
25	CDL	K	603	-	1/1/9/9	34/77/77/110	-
27	CN5	J	402	-	-	8/44/44/44	-
23	PEF	j	401	-	-	11/48/48/50	-
23	PEF	a	504	-	-	7/43/43/50	-
23	PEF	C	304	-	-	8/35/35/50	-
23	PEF	V	101	-	-	9/36/36/50	-

All (238) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	k	604	HEA	FE-ND	4.97	2.10	1.94
28	L	401	HEM	FE-NB	4.97	2.10	1.94
30	k	604	HEA	FE-NB	4.95	2.10	1.94
28	J	405	HEM	FE-NB	4.90	2.10	1.94
28	j	404	HEM	FE-NB	4.87	2.09	1.94
30	K	601	HEA	FE-ND	4.85	2.09	1.94
30	k	603	HEA	FE-NB	4.83	2.09	1.94
28	J	404	HEM	FE-NB	4.83	2.09	1.94
30	k	603	HEA	FE-ND	4.82	2.09	1.94
30	K	601	HEA	FE-NB	4.79	2.09	1.94
28	j	403	HEM	FE-NB	4.73	2.09	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	l	401	HEM	FE-NB	4.64	2.09	1.94
30	K	604	HEA	FE-NB	4.62	2.09	1.94
30	K	604	HEA	FE-ND	4.57	2.09	1.94
30	k	604	HEA	FE-NC	4.48	2.09	1.95
30	k	603	HEA	C3A-C2A	4.47	1.47	1.37
30	k	604	HEA	C3A-C2A	4.46	1.47	1.37
30	K	601	HEA	C3D-C2D	4.46	1.46	1.36
30	k	603	HEA	C3D-C2D	4.45	1.46	1.36
30	K	601	HEA	FE-NC	4.39	2.09	1.95
30	K	604	HEA	C3D-C2D	4.38	1.46	1.36
30	K	604	HEA	C3A-C2A	4.37	1.47	1.37
30	K	601	HEA	C3A-C2A	4.37	1.47	1.37
30	k	604	HEA	C3D-C2D	4.37	1.46	1.36
30	k	603	HEA	FE-NC	4.37	2.09	1.95
30	k	603	HEA	C3B-C2B	4.32	1.44	1.34
30	k	604	HEA	C3B-C2B	4.27	1.44	1.34
30	K	604	HEA	FE-NC	4.19	2.09	1.95
30	K	601	HEA	C3B-C2B	4.18	1.44	1.34
30	k	603	HEA	CHB-C4A	4.15	1.46	1.38
30	k	603	HEA	CHC-C4B	4.15	1.46	1.38
30	K	604	HEA	C3B-C2B	4.15	1.44	1.34
28	L	401	HEM	FE-NC	4.04	2.08	1.95
28	l	401	HEM	FE-NC	4.03	2.08	1.95
30	K	601	HEA	CHD-C1D	4.02	1.46	1.38
28	j	403	HEM	FE-NC	4.00	2.08	1.95
30	k	604	HEA	CHB-C4A	3.99	1.46	1.38
28	j	404	HEM	C1B-NB	-3.97	1.33	1.40
30	k	603	HEA	CHD-C1D	3.97	1.46	1.38
30	k	604	HEA	CHD-C1D	3.96	1.46	1.38
30	K	604	HEA	CHC-C4B	3.95	1.46	1.38
30	k	604	HEA	CHC-C4B	3.95	1.46	1.38
28	J	404	HEM	C1B-NB	-3.89	1.33	1.40
28	J	405	HEM	C1B-NB	-3.86	1.33	1.40
28	j	404	HEM	FE-NC	3.85	2.07	1.95
28	J	405	HEM	FE-NC	3.85	2.07	1.95
28	J	404	HEM	FE-NC	3.83	2.07	1.95
30	K	601	HEA	CHC-C4B	3.82	1.46	1.38
30	K	601	HEA	CHB-C4A	3.82	1.45	1.38
28	j	403	HEM	C1B-NB	-3.82	1.33	1.40
30	K	604	HEA	CHB-C4A	3.79	1.45	1.38
30	K	604	HEA	CHD-C1D	3.78	1.46	1.38
28	l	401	HEM	C1B-NB	-3.72	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	604	HEA	C11-C3B	-3.67	1.46	1.51
30	K	601	HEA	C11-C3B	-3.64	1.46	1.51
28	L	401	HEM	C1B-NB	-3.58	1.34	1.40
30	K	604	HEA	C1D-ND	-3.55	1.34	1.40
30	k	604	HEA	CHA-C1A	3.49	1.45	1.38
30	k	603	HEA	CHA-C1A	3.44	1.45	1.38
30	k	603	HEA	CHC-C1C	3.40	1.47	1.39
28	J	404	HEM	C3C-C4C	-3.38	1.40	1.46
28	L	401	HEM	C3C-C4C	-3.37	1.40	1.46
28	J	405	HEM	C1C-C2C	-3.37	1.38	1.45
30	K	604	HEA	CHA-C1A	3.37	1.45	1.38
30	K	601	HEA	C4B-NB	-3.36	1.34	1.40
30	k	603	HEA	C1D-ND	-3.35	1.34	1.40
30	K	601	HEA	CHA-C1A	3.34	1.44	1.38
28	J	405	HEM	C4D-ND	-3.33	1.34	1.40
28	J	404	HEM	C4D-ND	-3.32	1.34	1.40
30	K	601	HEA	C1D-ND	-3.32	1.34	1.40
25	h	601	CDL	PA1-OA4	-3.30	1.40	1.55
28	l	401	HEM	C4D-ND	-3.30	1.34	1.40
28	J	405	HEM	C3C-C4C	-3.28	1.40	1.46
28	j	403	HEM	C4D-ND	-3.28	1.34	1.40
30	k	604	HEA	CHC-C1C	3.28	1.46	1.39
25	L	402	CDL	PA1-OA4	-3.28	1.40	1.55
28	j	404	HEM	C4D-ND	-3.27	1.34	1.40
25	h	602	CDL	PA1-OA4	-3.27	1.40	1.55
28	l	401	HEM	C3C-C4C	-3.26	1.40	1.46
28	j	404	HEM	C3C-C4C	-3.26	1.40	1.46
30	k	604	HEA	C1D-ND	-3.25	1.34	1.40
25	J	403	CDL	PA1-OA4	-3.25	1.40	1.55
30	K	604	HEA	C4B-NB	-3.24	1.34	1.40
25	j	402	CDL	PA1-OA4	-3.24	1.40	1.55
25	H	601	CDL	PA1-OA4	-3.23	1.40	1.55
30	k	603	HEA	CHD-C4C	3.22	1.46	1.39
25	K	603	CDL	PA1-OA4	-3.21	1.40	1.55
30	K	604	HEA	CHC-C1C	3.21	1.46	1.39
30	k	604	HEA	CHD-C4C	3.21	1.46	1.39
25	C	302	CDL	PA1-OA4	-3.20	1.40	1.55
25	k	602	CDL	PA1-OA4	-3.19	1.40	1.55
30	K	601	HEA	CHD-C4C	3.18	1.46	1.39
25	c	302	CDL	PA1-OA4	-3.18	1.40	1.55
30	k	604	HEA	C1A-NA	3.17	1.45	1.39
28	j	403	HEM	C3C-C4C	-3.14	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	k	604	HEA	C4A-NA	3.12	1.45	1.39
28	j	404	HEM	C1D-ND	-3.11	1.32	1.38
28	L	401	HEM	C4D-ND	-3.11	1.34	1.40
28	j	403	HEM	C1C-C2C	-3.11	1.39	1.45
30	K	601	HEA	CHC-C1C	3.10	1.46	1.39
28	J	404	HEM	C1C-C2C	-3.08	1.39	1.45
28	j	404	HEM	C1C-C2C	-3.06	1.39	1.45
28	J	405	HEM	C1D-ND	-3.05	1.32	1.38
30	k	604	HEA	C11-C3B	-3.04	1.47	1.51
25	h	602	CDL	PB2-OB4	-3.04	1.41	1.55
28	J	404	HEM	C1D-ND	-3.04	1.32	1.38
30	k	603	HEA	C4A-NA	3.04	1.45	1.39
25	J	403	CDL	PB2-OB4	-3.03	1.41	1.55
25	h	601	CDL	PB2-OB4	-3.03	1.41	1.55
25	L	402	CDL	PA1-OA3	-3.02	1.40	1.50
25	H	601	CDL	PB2-OB4	-3.01	1.41	1.55
25	c	302	CDL	PB2-OB4	-3.00	1.41	1.55
30	k	603	HEA	C4B-NB	-3.00	1.35	1.40
30	K	601	HEA	C4A-NA	3.00	1.45	1.39
25	j	402	CDL	PB2-OB4	-2.99	1.41	1.55
25	C	302	CDL	PB2-OB4	-2.99	1.41	1.55
30	k	603	HEA	C1A-NA	2.98	1.45	1.39
30	K	604	HEA	CHD-C4C	2.97	1.46	1.39
25	h	602	CDL	PA1-OA3	-2.97	1.40	1.50
25	j	402	CDL	PB2-OB3	-2.96	1.40	1.50
25	L	402	CDL	PB2-OB3	-2.96	1.40	1.50
25	L	402	CDL	PB2-OB4	-2.96	1.41	1.55
30	K	604	HEA	C1A-NA	2.96	1.45	1.39
25	h	601	CDL	PA1-OA3	-2.96	1.40	1.50
25	h	602	CDL	PB2-OB3	-2.96	1.40	1.50
25	h	601	CDL	PB2-OB3	-2.95	1.40	1.50
25	H	601	CDL	PA1-OA3	-2.95	1.40	1.50
25	K	603	CDL	PB2-OB4	-2.95	1.41	1.55
28	l	401	HEM	FE-ND	-2.95	1.85	1.94
30	k	604	HEA	C4B-NB	-2.95	1.35	1.40
28	j	403	HEM	FE-ND	-2.95	1.85	1.94
25	k	602	CDL	PB2-OB4	-2.94	1.41	1.55
25	C	302	CDL	PB2-OB3	-2.94	1.40	1.50
30	k	603	HEA	C11-C3B	-2.93	1.47	1.51
25	J	403	CDL	PA1-OA3	-2.93	1.40	1.50
28	j	403	HEM	C1D-ND	-2.93	1.33	1.38
25	c	302	CDL	PA1-OA3	-2.92	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	l	401	HEM	C1D-ND	-2.92	1.33	1.38
28	l	401	HEM	C1C-C2C	-2.92	1.39	1.45
25	j	402	CDL	PA1-OA3	-2.91	1.40	1.50
25	c	302	CDL	PB2-OB3	-2.91	1.40	1.50
28	J	405	HEM	C4B-NB	-2.91	1.33	1.38
25	H	601	CDL	PB2-OB3	-2.90	1.40	1.50
25	J	403	CDL	PB2-OB3	-2.90	1.40	1.50
30	K	601	HEA	C1A-NA	2.90	1.45	1.39
25	K	603	CDL	PB2-OB3	-2.90	1.40	1.50
30	k	604	HEA	CHA-C4D	2.89	1.45	1.39
25	k	602	CDL	PB2-OB3	-2.89	1.40	1.50
30	k	603	HEA	CHB-C1B	2.89	1.45	1.39
28	J	404	HEM	C4B-NB	-2.88	1.33	1.38
25	C	302	CDL	PA1-OA3	-2.88	1.40	1.50
30	K	604	HEA	C4A-NA	2.87	1.45	1.39
25	k	602	CDL	PA1-OA3	-2.86	1.40	1.50
28	J	404	HEM	FE-ND	-2.86	1.86	1.94
25	K	603	CDL	PA1-OA3	-2.86	1.40	1.50
30	k	603	HEA	CHA-C4D	2.86	1.45	1.39
28	j	404	HEM	FE-ND	-2.85	1.86	1.94
28	j	404	HEM	C4B-NB	-2.85	1.33	1.38
28	j	403	HEM	C4B-NB	-2.84	1.33	1.38
28	J	405	HEM	FE-ND	-2.83	1.86	1.94
28	j	403	HEM	C1A-C2A	-2.81	1.39	1.44
28	L	401	HEM	C1D-ND	-2.79	1.33	1.38
30	K	601	HEA	CHA-C4D	2.79	1.45	1.39
30	K	604	HEA	C4C-NC	-2.79	1.34	1.39
28	L	401	HEM	C1C-C2C	-2.77	1.39	1.45
28	l	401	HEM	C1A-C2A	-2.74	1.39	1.44
30	K	604	HEA	CHA-C4D	2.72	1.45	1.39
28	L	401	HEM	FE-ND	-2.70	1.86	1.94
28	l	401	HEM	C4B-NB	-2.69	1.33	1.38
30	k	604	HEA	CHB-C1B	2.68	1.45	1.39
30	K	604	HEA	C1C-NC	-2.67	1.34	1.39
28	L	401	HEM	C1A-C2A	-2.64	1.39	1.44
28	J	405	HEM	C1A-C2A	-2.60	1.39	1.44
30	K	604	HEA	CHB-C1B	2.58	1.45	1.39
30	k	603	HEA	C4C-NC	-2.58	1.34	1.39
30	K	601	HEA	CHB-C1B	2.57	1.45	1.39
28	J	404	HEM	C1A-C2A	-2.56	1.39	1.44
30	K	604	HEA	C1B-NB	-2.55	1.33	1.38
25	k	602	CDL	PB2-OB5	2.54	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	j	402	CDL	PB2-OB5	2.53	1.69	1.59
30	K	601	HEA	C4C-NC	-2.53	1.34	1.39
30	k	603	HEA	C1C-NC	-2.53	1.34	1.39
25	K	603	CDL	PB2-OB5	2.52	1.69	1.59
25	L	402	CDL	PB2-OB5	2.52	1.69	1.59
30	K	601	HEA	C1C-NC	-2.50	1.34	1.39
25	c	302	CDL	PB2-OB5	2.50	1.69	1.59
28	l	401	HEM	C1A-NA	-2.49	1.34	1.39
25	c	302	CDL	PA1-OA5	2.49	1.69	1.59
25	K	603	CDL	PA1-OA5	2.49	1.69	1.59
30	k	604	HEA	C4C-NC	-2.49	1.34	1.39
30	K	601	HEA	C1B-NB	-2.49	1.34	1.38
28	j	404	HEM	C1A-C2A	-2.48	1.39	1.44
25	k	602	CDL	PA1-OA5	2.46	1.69	1.59
25	H	601	CDL	PB2-OB5	2.45	1.69	1.59
25	C	302	CDL	PA1-OA5	2.44	1.69	1.59
25	J	403	CDL	PB2-OB5	2.43	1.68	1.59
25	C	302	CDL	PB2-OB5	2.43	1.68	1.59
25	h	601	CDL	PB2-OB5	2.43	1.68	1.59
30	k	604	HEA	C1C-NC	-2.42	1.35	1.39
25	J	403	CDL	PA1-OA5	2.41	1.68	1.59
28	j	403	HEM	C1A-NA	-2.41	1.35	1.39
28	J	404	HEM	C1A-NA	-2.40	1.35	1.39
25	h	602	CDL	PB2-OB5	2.40	1.68	1.59
30	k	603	HEA	C1B-NB	-2.38	1.34	1.38
28	L	401	HEM	C4B-NB	-2.38	1.34	1.38
25	h	602	CDL	PA1-OA5	2.37	1.68	1.59
28	l	401	HEM	C4A-NA	-2.37	1.35	1.39
30	K	604	HEA	C4D-ND	-2.36	1.34	1.38
25	j	402	CDL	PA1-OA5	2.36	1.68	1.59
30	k	604	HEA	C1B-NB	-2.36	1.34	1.38
28	J	405	HEM	C1A-NA	-2.32	1.35	1.39
25	L	402	CDL	PA1-OA5	2.31	1.68	1.59
28	j	404	HEM	C1A-NA	-2.31	1.35	1.39
28	J	405	HEM	C1C-NC	-2.29	1.35	1.39
28	L	401	HEM	C1A-NA	-2.27	1.35	1.39
30	k	604	HEA	C4B-C3B	2.26	1.48	1.44
25	h	601	CDL	PA1-OA5	2.26	1.68	1.59
30	k	603	HEA	C4B-C3B	2.25	1.48	1.44
28	J	404	HEM	C4A-NA	-2.25	1.35	1.39
28	L	401	HEM	C4A-NA	-2.25	1.35	1.39
25	H	601	CDL	PA1-OA5	2.22	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	J	404	HEM	C2A-C3A	-2.19	1.33	1.38
28	l	401	HEM	C4C-NC	-2.15	1.35	1.39
28	l	401	HEM	C1C-NC	-2.14	1.35	1.39
30	k	603	HEA	C4D-ND	-2.13	1.34	1.38
28	j	404	HEM	C4A-NA	-2.13	1.35	1.39
28	J	405	HEM	C4C-NC	-2.12	1.35	1.39
28	j	403	HEM	C1C-NC	-2.12	1.35	1.39
28	J	405	HEM	C4A-NA	-2.12	1.35	1.39
28	j	403	HEM	C4A-NA	-2.11	1.35	1.39
28	J	405	HEM	C2A-C3A	-2.11	1.33	1.38
28	j	403	HEM	C2A-C3A	-2.09	1.33	1.38
30	K	601	HEA	C4D-ND	-2.08	1.34	1.38
28	J	404	HEM	C4C-NC	-2.07	1.35	1.39
28	j	404	HEM	C4C-NC	-2.06	1.35	1.39
28	L	401	HEM	C2A-C3A	-2.05	1.33	1.38
28	l	401	HEM	C2A-C3A	-2.02	1.33	1.38
28	j	404	HEM	C1C-NC	-2.00	1.35	1.39

All (414) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	601	HEA	C3D-C4D-ND	6.70	116.82	110.35
30	k	603	HEA	C3D-C4D-ND	6.60	116.73	110.35
30	k	604	HEA	C3D-C4D-ND	6.50	116.63	110.35
28	j	404	HEM	CAD-C3D-C4D	6.45	135.95	124.70
30	K	604	HEA	C3D-C4D-ND	6.42	116.56	110.35
29	J	408	UQ6	C7-C8-C9	-6.14	118.62	127.42
28	J	405	HEM	CAD-C3D-C4D	6.01	135.18	124.70
29	J	406	UQ6	C7-C8-C9	-5.79	119.13	127.42
30	K	604	HEA	C13-C12-C11	-5.71	105.28	114.39
30	k	604	HEA	C2B-C1B-NB	5.64	116.42	109.90
30	K	601	HEA	C2B-C1B-NB	5.55	116.32	109.90
30	k	604	HEA	C13-C12-C11	-5.40	105.77	114.39
30	K	604	HEA	C2B-C1B-NB	5.39	116.14	109.90
28	J	404	HEM	CAD-C3D-C4D	5.36	134.04	124.70
30	K	601	HEA	C3B-C4B-NB	5.27	115.89	109.84
30	k	604	HEA	C3B-C4B-NB	5.16	115.77	109.84
30	K	601	HEA	C13-C12-C11	-5.15	106.17	114.39
28	j	403	HEM	CAD-C3D-C4D	5.12	133.62	124.70
30	k	603	HEA	C13-C12-C11	-5.07	106.29	114.39
28	j	403	HEM	CHC-C4B-NB	5.07	129.88	124.42
30	K	601	HEA	C3C-C2C-C1C	-5.03	101.24	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	k	603	HEA	C2B-C1B-NB	5.01	115.70	109.90
30	k	604	HEA	C2D-C1D-ND	5.01	115.60	109.84
30	K	604	HEA	C3C-C4C-NC	5.00	114.01	109.80
30	k	603	HEA	C3C-C4C-NC	4.95	113.97	109.80
30	k	604	HEA	C3C-C2C-C1C	-4.95	101.34	107.17
30	K	604	HEA	C3C-C2C-C1C	-4.93	101.35	107.17
28	J	405	HEM	CHC-C4B-NB	4.91	129.71	124.42
28	J	404	HEM	CHC-C4B-NB	4.90	129.69	124.42
30	K	604	HEA	C2D-C1D-ND	4.89	115.47	109.84
30	k	604	HEA	C3C-C4C-NC	4.85	113.88	109.80
30	k	603	HEA	C2D-C1D-ND	4.83	115.39	109.84
28	j	404	HEM	CHC-C4B-NB	4.81	129.60	124.42
28	L	401	HEM	CAD-C3D-C4D	4.78	133.04	124.70
30	K	601	HEA	C2D-C1D-ND	4.77	115.32	109.84
30	k	603	HEA	C3B-C4B-NB	4.76	115.31	109.84
30	k	603	HEA	C3C-C2C-C1C	-4.74	101.58	107.17
30	K	604	HEA	C3B-C4B-NB	4.73	115.28	109.84
29	j	407	UQ6	C7-C8-C9	-4.64	120.77	127.42
30	K	601	HEA	C3C-C4C-NC	4.64	113.71	109.80
29	j	405	UQ6	C7-C8-C9	-4.52	120.94	127.42
28	j	404	HEM	CAD-C3D-C2D	-4.50	119.43	127.87
28	l	401	HEM	CAD-C3D-C4D	4.45	132.45	124.70
28	l	401	HEM	CHC-C4B-NB	4.38	129.14	124.42
28	j	403	HEM	CHD-C1D-ND	4.27	129.01	124.42
30	K	601	HEA	CAD-C3D-C4D	4.24	132.09	124.70
28	j	403	HEM	CHB-C1B-NB	4.22	129.59	124.37
30	k	603	HEA	C26-C15-C16	4.20	122.52	115.23
28	j	404	HEM	CBD-CAD-C3D	4.19	124.11	112.53
28	J	405	HEM	CAD-C3D-C2D	-4.18	120.04	127.87
28	J	405	HEM	CHD-C1D-ND	4.18	128.92	124.42
23	w	201	PEF	O2-C10-C11	4.16	120.49	111.48
23	a	504	PEF	O2-C10-C11	4.15	120.45	111.48
30	k	604	HEA	C26-C15-C16	4.14	122.42	115.23
30	k	604	HEA	CAD-C3D-C4D	4.12	131.88	124.70
28	J	404	HEM	CHD-C1D-ND	4.09	128.82	124.42
28	l	401	HEM	C1B-NB-C4B	4.07	110.03	105.21
23	W	202	PEF	O2-C10-C11	4.05	120.24	111.48
28	J	405	HEM	CBD-CAD-C3D	4.04	123.70	112.53
28	J	404	HEM	CHB-C1B-NB	4.03	129.35	124.37
28	L	401	HEM	CHD-C1D-ND	4.02	128.75	124.42
23	W	201	PEF	O2-C10-C11	3.99	120.11	111.48
23	A	503	PEF	O2-C10-C11	3.98	120.09	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	401	HEM	CHC-C4B-NB	3.95	128.68	124.42
28	j	404	HEM	CHD-C1D-ND	3.95	128.68	124.42
30	K	601	HEA	C4D-C3D-C2D	-3.95	101.14	106.89
23	A	502	PEF	O2-C10-C11	3.94	120.00	111.48
30	k	603	HEA	CAD-C3D-C4D	3.90	131.50	124.70
23	j	406	PEF	O2-C10-C11	3.89	119.90	111.48
30	K	601	HEA	C26-C15-C16	3.87	121.94	115.23
23	C	304	PEF	O2-C10-C11	3.87	119.85	111.48
23	A	501	PEF	O2-C10-C11	3.86	119.84	111.48
28	L	401	HEM	CHB-C1B-NB	3.86	129.14	124.37
23	w	202	PEF	O2-C10-C11	3.85	119.81	111.48
30	K	601	HEA	C2C-C1C-NC	3.84	116.30	110.14
23	J	409	PEF	O2-C10-C11	3.84	119.79	111.48
30	k	603	HEA	C4D-C3D-C2D	-3.84	101.31	106.89
28	L	401	HEM	C3B-C4B-NB	-3.81	106.73	109.47
23	c	304	PEF	O2-C10-C11	3.78	119.66	111.48
23	j	408	PEF	O2-C10-C11	3.75	119.60	111.48
23	j	401	PEF	O2-C10-C11	3.73	119.56	111.48
30	k	604	HEA	C2C-C1C-NC	3.73	116.13	110.14
30	K	604	HEA	C4D-C3D-C2D	-3.70	101.50	106.89
23	a	503	PEF	O2-C10-C11	3.70	119.49	111.48
30	k	604	HEA	C4D-C3D-C2D	-3.69	101.53	106.89
23	C	303	PEF	O2-C10-C11	3.68	119.43	111.48
23	J	401	PEF	O2-C10-C11	3.68	119.43	111.48
30	K	604	HEA	C2C-C1C-NC	3.66	116.01	110.14
30	K	604	HEA	C3A-C2A-C1A	-3.66	103.58	107.05
30	K	601	HEA	CHB-C1B-C2B	-3.62	119.31	125.03
23	v	101	PEF	O2-C10-C11	3.62	119.31	111.48
28	L	401	HEM	C1B-NB-C4B	3.61	109.49	105.21
30	k	604	HEA	CHB-C1B-C2B	-3.61	119.33	125.03
23	V	101	PEF	O2-C10-C11	3.59	119.24	111.48
28	J	404	HEM	CHD-C4C-NC	3.58	128.35	124.45
28	J	404	HEM	CAD-C3D-C2D	-3.58	121.17	127.87
30	k	603	HEA	C3A-C2A-C1A	-3.57	103.67	107.05
28	l	401	HEM	C3B-C4B-NB	-3.56	106.91	109.47
28	l	401	HEM	CHD-C1D-ND	3.55	128.24	124.42
30	K	604	HEA	CHB-C1B-C2B	-3.54	119.43	125.03
23	E	102	PEF	O2-C10-C11	3.54	119.14	111.48
30	K	604	HEA	C2A-C1A-NA	3.51	113.71	110.32
29	j	405	UQ6	C12-C13-C14	-3.50	119.61	127.62
28	j	403	HEM	CAD-C3D-C2D	-3.50	121.31	127.87
30	k	603	HEA	C2C-C1C-NC	3.50	115.75	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	J	405	HEM	CHB-C1B-NB	3.48	128.67	124.37
23	J	407	PEF	C2-O2-C10	3.46	126.08	117.80
23	a	501	PEF	C2-O2-C10	3.45	126.06	117.80
30	K	604	HEA	CAD-C3D-C4D	3.44	130.69	124.70
28	j	404	HEM	CHB-C1B-NB	3.44	128.62	124.37
30	K	604	HEA	C26-C15-C16	3.44	121.19	115.23
23	c	303	PEF	O2-C10-C11	3.43	118.90	111.48
30	k	603	HEA	C2A-C1A-NA	3.42	113.63	110.32
30	K	604	HEA	C17-C18-C19	-3.42	119.80	127.62
23	a	501	PEF	P-O4P-C4	-3.38	105.17	121.26
30	k	604	HEA	C3A-C2A-C1A	-3.36	103.87	107.05
28	l	401	HEM	CHB-C1B-NB	3.35	128.51	124.37
30	K	601	HEA	C2A-C1A-NA	3.34	113.54	110.32
23	J	407	PEF	O2-C10-C11	3.33	118.68	111.48
30	K	604	HEA	C1D-C2D-C3D	-3.33	103.48	106.98
28	j	404	HEM	C1B-NB-C4B	3.32	109.13	105.21
28	j	403	HEM	C1B-NB-C4B	3.30	109.12	105.21
23	e	101	PEF	O2-C10-C11	3.30	118.61	111.48
30	k	604	HEA	C2A-C1A-NA	3.29	113.50	110.32
25	H	601	CDL	OA4-PA1-OA3	3.29	127.74	112.44
29	j	405	UQ6	C22-C23-C24	-3.29	120.10	127.62
30	K	601	HEA	C3A-C2A-C1A	-3.28	103.94	107.05
23	j	406	PEF	P-O4P-C4	-3.26	105.73	121.26
30	k	604	HEA	C1D-C2D-C3D	-3.24	103.57	106.98
23	A	502	PEF	P-O4P-C4	-3.24	105.84	121.26
25	j	402	CDL	OA4-PA1-OA3	3.23	127.48	112.44
29	j	405	UQ6	C27-C28-C29	-3.22	120.24	127.62
29	J	406	UQ6	C22-C23-C24	-3.22	120.25	127.62
25	h	601	CDL	OA4-PA1-OA3	3.21	127.40	112.44
28	L	401	HEM	CHD-C4C-NC	3.20	127.94	124.45
25	L	402	CDL	OA4-PA1-OA3	3.19	127.28	112.44
29	J	406	UQ6	C27-C28-C29	-3.19	120.33	127.62
23	J	401	PEF	P-O4P-C4	-3.17	106.15	121.26
30	k	604	HEA	C4B-C3B-C2B	-3.17	102.11	107.44
25	K	603	CDL	OA4-PA1-OA3	3.17	127.17	112.44
23	J	407	PEF	P-O4P-C4	-3.17	106.19	121.26
23	W	201	PEF	P-O4P-C4	-3.16	106.20	121.26
25	k	602	CDL	OA4-PA1-OA3	3.16	127.14	112.44
29	j	407	UQ6	C27-C28-C29	-3.16	120.39	127.62
28	J	404	HEM	C1B-NB-C4B	3.16	108.95	105.21
30	k	603	HEA	CHB-C1B-C2B	-3.14	120.07	125.03
28	J	404	HEM	CBD-CAD-C3D	3.14	121.22	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	J	403	CDL	OA4-PA1-OA3	3.14	127.05	112.44
23	j	401	PEF	P-O4P-C4	-3.14	106.31	121.26
25	C	302	CDL	OA4-PA1-OA3	3.14	127.04	112.44
30	K	601	HEA	C1B-C2B-C3B	-3.13	103.17	106.80
30	k	603	HEA	C1D-C2D-C3D	-3.12	103.69	106.98
29	j	407	UQ6	C10-C9-C11	3.12	120.65	115.23
30	k	603	HEA	C4B-C3B-C2B	-3.12	102.19	107.44
23	A	503	PEF	P-O4P-C4	-3.12	106.42	121.26
30	K	604	HEA	C1B-C2B-C3B	-3.12	103.19	106.80
23	a	501	PEF	O2-C10-C11	3.11	118.22	111.48
23	c	304	PEF	P-O4P-C4	-3.11	106.45	121.26
25	h	602	CDL	OA4-PA1-OA3	3.10	126.86	112.44
28	J	405	HEM	CHD-C4C-NC	3.09	127.82	124.45
25	c	302	CDL	OA4-PA1-OA3	3.08	126.76	112.44
23	W	202	PEF	P-O4P-C4	-3.07	106.63	121.26
30	K	601	HEA	C4B-C3B-C2B	-3.06	102.29	107.44
28	L	401	HEM	CAD-C3D-C2D	-3.06	122.13	127.87
30	K	604	HEA	CAD-CBD-CGD	-3.06	105.54	113.67
23	a	503	PEF	P-O4P-C4	-3.06	106.70	121.26
30	K	604	HEA	C27-C19-C20	3.05	120.52	115.23
25	C	302	CDL	OB4-PB2-OB3	3.04	126.58	112.44
28	L	401	HEM	CBD-CAD-C3D	3.04	120.93	112.53
23	V	101	PEF	P-O4P-C4	-3.03	106.83	121.26
23	j	408	PEF	P-O4P-C4	-3.03	106.85	121.26
23	w	202	PEF	P-O4P-C4	-3.03	106.86	121.26
23	C	304	PEF	P-O4P-C4	-3.02	106.89	121.26
28	J	405	HEM	C1B-NB-C4B	3.01	108.78	105.21
23	c	303	PEF	P-O4P-C4	-3.01	106.91	121.26
25	c	302	CDL	OB4-PB2-OB3	3.01	126.44	112.44
23	v	101	PEF	P-O4P-C4	-3.01	106.95	121.26
29	J	406	UQ6	C3M-O3-C3	-3.00	106.59	114.74
23	A	501	PEF	P-O4P-C4	-3.00	106.99	121.26
23	J	409	PEF	O3-C30-C31	2.99	120.94	111.83
30	k	604	HEA	C27-C19-C20	2.98	120.41	115.23
30	K	601	HEA	C1D-C2D-C3D	-2.97	103.85	106.98
30	k	603	HEA	C17-C18-C19	-2.97	120.82	127.62
23	E	102	PEF	P-O4P-C4	-2.97	107.12	121.26
29	J	406	UQ6	C12-C13-C14	-2.97	120.83	127.62
28	j	403	HEM	CHD-C4C-NC	2.96	127.68	124.45
23	J	409	PEF	P-O4P-C4	-2.96	107.16	121.26
28	j	403	HEM	CBD-CAD-C3D	2.95	120.69	112.53
30	k	604	HEA	CHA-C4D-C3D	-2.94	120.49	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	604	HEA	CHA-C4D-C3D	-2.94	120.49	124.77
23	e	101	PEF	P-O4P-C4	-2.93	107.33	121.26
29	j	407	UQ6	C17-C18-C19	-2.92	120.93	127.62
30	K	604	HEA	C13-C14-C15	-2.92	120.94	127.62
30	k	604	HEA	C17-C18-C19	-2.92	120.95	127.62
23	w	201	PEF	P-O4P-C4	-2.92	107.38	121.26
28	l	401	HEM	CBD-CAD-C3D	2.90	120.55	112.53
30	k	604	HEA	C1B-C2B-C3B	-2.90	103.44	106.80
30	K	601	HEA	C27-C19-C20	2.90	120.26	115.23
30	K	604	HEA	C16-C15-C14	-2.90	114.66	121.17
29	J	406	UQ6	C25-C24-C26	2.89	120.24	115.23
25	j	402	CDL	OB4-PB2-OB3	2.89	125.88	112.44
23	C	303	PEF	P-O4P-C4	-2.88	107.53	121.26
29	j	405	UQ6	C17-C18-C19	-2.88	121.03	127.62
30	K	604	HEA	C4B-C3B-C2B	-2.88	102.60	107.44
25	h	601	CDL	OB4-PB2-OB3	2.87	125.80	112.44
23	C	303	PEF	O3-C30-C31	2.86	120.56	111.83
30	K	601	HEA	CBD-CAD-C3D	2.85	120.43	112.53
30	k	604	HEA	CAD-CBD-CGD	-2.85	106.09	113.67
28	l	401	HEM	CAD-C3D-C2D	-2.84	122.55	127.87
25	J	403	CDL	OB4-PB2-OB3	2.83	125.59	112.44
30	k	603	HEA	CAD-CBD-CGD	-2.82	106.18	113.67
25	h	602	CDL	OB4-PB2-OB3	2.82	125.54	112.44
23	j	406	PEF	O3-C30-C31	2.81	120.42	111.83
25	k	602	CDL	OB4-PB2-OB3	2.81	125.52	112.44
23	A	503	PEF	P-O3P-C1	-2.81	105.24	121.35
25	H	601	CDL	OB4-PB2-OB3	2.80	125.46	112.44
25	L	402	CDL	OB4-PB2-OB3	2.80	125.45	112.44
30	K	601	HEA	CBA-CAA-C2A	-2.79	104.81	112.53
23	a	501	PEF	P-O3P-C1	-2.79	105.37	121.35
29	j	405	UQ6	C4M-O4-C4	-2.78	107.19	114.74
25	K	603	CDL	OB4-PB2-OB3	2.78	125.39	112.44
30	k	603	HEA	C27-C19-C20	2.78	120.05	115.23
29	J	406	UQ6	C15-C14-C16	2.78	120.05	115.23
23	a	503	PEF	O3-C30-C31	2.77	120.29	111.83
23	V	101	PEF	C2-O2-C10	2.77	124.43	117.80
23	c	303	PEF	O3-C30-C31	2.76	120.25	111.83
29	j	407	UQ6	C15-C14-C16	2.76	120.02	115.23
28	l	401	HEM	CHD-C4C-NC	2.75	127.45	124.45
30	k	604	HEA	CHC-C1C-C2C	-2.75	119.44	127.43
23	j	401	PEF	P-O3P-C1	-2.75	105.61	121.35
29	j	405	UQ6	C3M-O3-C3	-2.75	107.29	114.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	304	PEF	O3-C30-C31	2.75	120.21	111.83
30	K	604	HEA	C12-C13-C14	-2.74	104.95	112.16
29	J	408	UQ6	C4M-O4-C4	-2.73	107.34	114.74
30	K	601	HEA	CHC-C1C-C2C	-2.73	119.51	127.43
30	K	601	HEA	CHA-C4D-C3D	-2.72	120.81	124.77
23	e	101	PEF	C2-O2-C10	2.72	124.31	117.80
28	j	404	HEM	CHD-C4C-NC	2.72	127.41	124.45
23	J	401	PEF	O3-C30-C31	2.72	120.11	111.83
30	K	604	HEA	C21-C20-C19	-2.71	104.19	113.19
23	E	102	PEF	O3-C30-C31	2.71	120.10	111.83
23	j	406	PEF	P-O3P-C1	-2.70	105.86	121.35
30	K	601	HEA	CAD-CBD-CGD	-2.70	106.50	113.67
23	c	304	PEF	P-O3P-C1	-2.70	105.87	121.35
23	A	501	PEF	O3-C30-C31	2.70	120.07	111.83
23	e	101	PEF	O3-C30-C31	2.70	120.07	111.83
23	J	401	PEF	P-O3P-C1	-2.70	105.89	121.35
30	K	601	HEA	C17-C18-C19	-2.70	121.45	127.62
23	a	504	PEF	P-O4P-C4	-2.68	108.50	121.26
23	A	502	PEF	O3-C30-C31	2.68	120.00	111.83
23	j	401	PEF	O3-C30-C31	2.67	119.98	111.83
29	j	407	UQ6	C4M-O4-C4	-2.67	107.49	114.74
23	c	303	PEF	P-O3P-C1	-2.65	106.14	121.35
30	k	603	HEA	C1B-C2B-C3B	-2.65	103.73	106.80
28	J	405	HEM	CHD-C1D-C2D	-2.65	120.84	125.03
23	a	501	PEF	O3-C30-C31	2.65	119.91	111.83
23	A	502	PEF	P-O3P-C1	-2.64	106.21	121.35
28	L	401	HEM	CHD-C1D-C2D	-2.64	120.86	125.03
27	J	402	CN5	O31-C31-C32	2.63	119.85	111.83
29	J	406	UQ6	C30-C29-C31	2.62	119.78	115.23
30	K	604	HEA	CHC-C1C-C2C	-2.62	119.82	127.43
23	w	202	PEF	O3-C30-C31	2.62	119.83	111.83
28	L	401	HEM	C4C-CHD-C1D	-2.61	120.47	126.02
23	a	504	PEF	O3-C30-C31	2.61	119.79	111.83
25	c	302	CDL	CA4-OA6-CA5	2.61	124.03	117.80
23	V	101	PEF	P-O3P-C1	-2.60	106.43	121.35
23	j	408	PEF	O3-C30-C31	2.60	119.76	111.83
30	k	604	HEA	C21-C20-C19	-2.60	104.58	113.19
30	k	603	HEA	CHA-C4D-C3D	-2.60	120.99	124.77
23	w	202	PEF	P-O3P-C1	-2.58	106.55	121.35
23	w	201	PEF	O3-C30-C31	2.58	119.71	111.83
23	v	101	PEF	O3-C30-C31	2.58	119.70	111.83
23	V	101	PEF	O3-C30-C31	2.58	119.69	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	202	PEF	P-O3P-C1	-2.57	106.62	121.35
23	C	304	PEF	O3-C30-C31	2.56	119.65	111.83
23	E	102	PEF	P-O3P-C1	-2.56	106.67	121.35
23	W	201	PEF	P-O3P-C1	-2.56	106.68	121.35
28	j	403	HEM	CHA-C4D-ND	2.55	127.53	124.37
23	e	101	PEF	P-O3P-C1	-2.55	106.73	121.35
23	j	408	PEF	P-O3P-C1	-2.55	106.75	121.35
23	J	409	PEF	P-O3P-C1	-2.55	106.76	121.35
23	a	503	PEF	P-O3P-C1	-2.55	106.76	121.35
23	J	407	PEF	P-O3P-C1	-2.54	106.79	121.35
30	k	603	HEA	C12-C13-C14	-2.54	105.49	112.16
29	J	406	UQ6	C17-C18-C19	-2.54	121.82	127.62
23	v	101	PEF	P-O3P-C1	-2.54	106.81	121.35
23	W	202	PEF	O3-C30-C31	2.53	119.56	111.83
30	k	603	HEA	C21-C20-C19	-2.53	104.80	113.19
23	C	304	PEF	P-O3P-C1	-2.53	106.86	121.35
29	j	405	UQ6	C20-C19-C21	2.53	119.62	115.23
29	J	406	UQ6	C10-C9-C11	2.52	119.60	115.23
28	j	403	HEM	CHD-C1D-C2D	-2.51	121.07	125.03
28	J	404	HEM	CHD-C1D-C2D	-2.50	121.08	125.03
30	k	603	HEA	C13-C14-C15	-2.49	121.92	127.62
30	k	604	HEA	C4B-NB-C1B	-2.49	102.26	105.21
30	k	604	HEA	C12-C13-C14	-2.49	105.62	112.16
23	A	503	PEF	O3-C30-C31	2.49	119.42	111.83
30	K	601	HEA	C21-C20-C19	-2.49	104.94	113.19
23	J	407	PEF	O3-C30-C31	2.48	119.39	111.83
29	j	407	UQ6	C20-C19-C21	2.48	119.53	115.23
28	L	401	HEM	CHA-C4D-ND	2.47	127.42	124.37
29	j	407	UQ6	C12-C13-C14	-2.46	122.00	127.62
25	h	602	CDL	OB6-CB5-OB7	-2.45	117.97	123.70
26	E	101	PCF	C11-C12-N	-2.45	107.96	115.82
23	a	504	PEF	P-O3P-C1	-2.43	107.41	121.35
30	K	601	HEA	C4B-NB-C1B	-2.43	102.33	105.21
29	j	407	UQ6	C30-C29-C31	2.42	119.43	115.23
28	j	404	HEM	C3B-C4B-NB	-2.42	107.73	109.47
23	W	201	PEF	O3-C30-C31	2.42	119.20	111.83
28	j	403	HEM	C3B-C4B-NB	-2.42	107.73	109.47
29	J	408	UQ6	C10-C9-C11	2.42	119.42	115.23
29	j	405	UQ6	C10-C9-C11	2.41	119.41	115.23
28	j	404	HEM	CHD-C1D-C2D	-2.41	121.22	125.03
23	E	102	PEF	C2-O2-C10	2.40	123.55	117.80
28	j	404	HEM	C4C-CHD-C1D	-2.40	120.92	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	303	PEF	P-O3P-C1	-2.40	107.61	121.35
30	k	603	HEA	CHC-C1C-C2C	-2.39	120.49	127.43
29	j	407	UQ6	C25-C24-C26	2.39	119.38	115.23
29	J	406	UQ6	C4M-O4-C4	-2.38	108.27	114.74
28	J	404	HEM	CHA-C4D-ND	2.37	127.30	124.37
30	K	601	HEA	C16-C15-C14	-2.37	115.86	121.17
23	C	303	PEF	C2-O2-C10	2.37	123.46	117.80
29	J	406	UQ6	C20-C19-C21	2.36	119.33	115.23
25	J	403	CDL	OA6-CA5-OA7	-2.36	118.19	123.70
23	A	501	PEF	P-O3P-C1	-2.36	107.83	121.35
29	j	407	UQ6	C36-C34-C35	2.36	120.02	114.59
29	j	405	UQ6	C25-C24-C26	2.35	119.31	115.23
30	K	601	HEA	C12-C13-C14	-2.35	105.98	112.16
28	l	401	HEM	CAA-CBA-CGA	-2.35	107.43	113.67
30	k	603	HEA	CMB-C2B-C1B	2.34	128.69	125.03
29	j	405	UQ6	C36-C34-C35	2.33	119.96	114.59
29	j	407	UQ6	C3M-O3-C3	-2.33	108.42	114.74
28	J	405	HEM	CHA-C1A-NA	2.33	128.08	123.86
30	K	604	HEA	C21-C22-C23	-2.32	119.91	127.64
28	J	404	HEM	C4C-CHD-C1D	-2.32	121.09	126.02
23	v	101	PEF	C2-O2-C10	2.31	123.33	117.80
28	j	403	HEM	CHA-C1A-NA	2.31	128.04	123.86
30	k	604	HEA	CMD-C2D-C1D	2.30	128.62	125.03
29	J	408	UQ6	C3M-O3-C3	-2.29	108.52	114.74
29	j	407	UQ6	C22-C23-C24	-2.28	122.40	127.62
28	j	403	HEM	C4C-CHD-C1D	-2.28	121.17	126.02
30	k	604	HEA	C13-C14-C15	-2.27	122.43	127.62
28	j	404	HEM	CHA-C1A-NA	2.26	127.95	123.86
28	J	404	HEM	CHB-C1B-C2B	-2.25	120.55	126.95
28	j	403	HEM	CHB-C1B-C2B	-2.25	120.56	126.95
30	K	601	HEA	CMB-C2B-C1B	2.25	128.54	125.03
28	J	405	HEM	C4C-CHD-C1D	-2.24	121.26	126.02
30	k	603	HEA	CHB-C4A-NA	-2.24	122.02	124.45
30	k	604	HEA	CBA-CAA-C2A	-2.23	106.35	112.53
30	K	601	HEA	C13-C14-C15	-2.23	122.51	127.62
25	c	302	CDL	OB6-CB5-OB7	-2.23	118.49	123.70
30	K	604	HEA	CHD-C1D-C2D	-2.23	120.62	126.95
29	J	406	UQ6	C36-C34-C35	2.23	119.71	114.59
29	j	405	UQ6	C15-C14-C16	2.22	119.08	115.23
25	j	402	CDL	OB6-CB5-OB7	-2.22	118.53	123.70
28	J	404	HEM	C1C-CHC-C4B	-2.20	121.33	126.02
30	k	603	HEA	C4C-C3C-C2C	-2.20	104.56	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	401	HEM	CHB-C1B-C2B	-2.20	120.68	126.95
23	w	201	PEF	P-O3P-C1	-2.20	108.75	121.35
28	J	405	HEM	C1C-CHC-C4B	-2.20	121.35	126.02
25	L	402	CDL	OB6-CB5-OB7	-2.19	118.58	123.70
30	K	604	HEA	CMB-C2B-C1B	2.19	128.46	125.03
29	j	405	UQ6	C32-C33-C34	-2.19	120.33	127.64
25	h	601	CDL	OB6-CB5-OB7	-2.19	118.58	123.70
25	J	403	CDL	OB6-CB5-OB7	-2.19	118.59	123.70
28	l	401	HEM	C4C-CHD-C1D	-2.19	121.37	126.02
28	j	404	HEM	C1C-CHC-C4B	-2.18	121.39	126.02
28	l	401	HEM	CHA-C4D-ND	2.17	127.06	124.37
30	k	603	HEA	C27-C19-C18	-2.16	118.07	123.63
28	L	401	HEM	CHA-C1A-NA	2.16	127.78	123.86
30	k	603	HEA	CHC-C4B-NB	-2.16	121.70	124.37
29	j	405	UQ6	C30-C29-C31	2.16	118.97	115.23
30	k	604	HEA	C1D-ND-C4D	-2.15	102.67	105.21
25	H	601	CDL	OA6-CA5-OA7	-2.14	118.70	123.70
30	k	604	HEA	CBD-CAD-C3D	2.14	118.44	112.53
28	l	401	HEM	C1C-CHC-C4B	-2.14	121.48	126.02
28	J	405	HEM	CBA-CAA-C2A	-2.13	106.64	112.53
30	k	603	HEA	CMD-C2D-C1D	2.12	128.35	125.03
30	k	604	HEA	CMB-C2B-C1B	2.12	128.34	125.03
25	h	601	CDL	OA6-CA5-OA7	-2.12	118.75	123.70
30	k	604	HEA	CHD-C1D-C2D	-2.12	120.94	126.95
25	C	302	CDL	OB6-CB5-OB7	-2.11	118.76	123.70
30	K	604	HEA	C25-C23-C24	2.11	119.45	114.59
30	K	601	HEA	CMD-C2D-C1D	2.11	128.33	125.03
25	h	602	CDL	OA6-CA5-OA7	-2.11	118.78	123.70
30	K	601	HEA	CHD-C1D-C2D	-2.10	120.97	126.95
25	L	402	CDL	OA6-CA5-OA7	-2.10	118.79	123.70
30	K	604	HEA	C4C-C3C-C2C	-2.10	104.69	107.30
30	k	603	HEA	C16-C15-C14	-2.10	116.46	121.17
28	l	401	HEM	CHD-C1D-C2D	-2.10	121.72	125.03
28	j	403	HEM	CAA-CBA-CGA	-2.09	108.12	113.67
30	K	604	HEA	CMC-C2C-C3C	2.09	131.47	126.55
28	j	404	HEM	C4A-CHB-C1B	-2.09	121.34	126.25
28	J	404	HEM	C3B-C4B-NB	-2.08	107.97	109.47
30	k	603	HEA	CBD-CAD-C3D	2.08	118.29	112.53
30	K	604	HEA	C26-C15-C14	-2.07	118.30	123.63
25	H	601	CDL	OB6-CB5-OB7	-2.07	118.86	123.70
28	j	404	HEM	CHB-C1B-C2B	-2.07	121.07	126.95
30	K	601	HEA	C27-C19-C18	-2.06	118.32	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	J	405	HEM	CHB-C1B-C2B	-2.06	121.10	126.95
30	k	604	HEA	C16-C15-C14	-2.06	116.55	121.17
29	J	408	UQ6	C6-C7-C8	2.05	115.57	112.06
28	l	401	HEM	O2A-CGA-O1A	-2.05	118.05	123.33
28	J	404	HEM	CHA-C1A-NA	2.05	127.58	123.86
30	k	603	HEA	CHD-C1D-C2D	-2.05	121.12	126.95
28	j	404	HEM	C2A-C1A-NA	-2.04	107.89	110.15
28	J	405	HEM	CHA-C4D-ND	2.04	126.89	124.37
25	c	302	CDL	OA6-CA5-OA7	-2.04	118.94	123.70
30	K	604	HEA	C4B-NB-C1B	-2.03	102.80	105.21
30	K	601	HEA	C25-C23-C24	2.02	119.25	114.59
25	j	402	CDL	OA6-CA5-OA7	-2.02	118.98	123.70
30	K	601	HEA	O11-C11-C3B	-2.01	107.58	111.26
30	k	604	HEA	C27-C19-C18	-2.01	118.48	123.63
28	J	405	HEM	C2A-C1A-NA	-2.01	107.93	110.15

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	C	302	CDL	CA4
25	H	601	CDL	CA4
25	J	403	CDL	CA4
25	K	603	CDL	CA4
25	L	402	CDL	CA4
25	c	302	CDL	CA4
25	h	601	CDL	CA4
25	h	602	CDL	CA4
25	j	402	CDL	CA4
25	k	602	CDL	CA4

All (695) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	501	PEF	O2-C2-C3-O3
23	A	503	PEF	O4P-C4-C5-N
23	A	503	PEF	C4-O4P-P-O3P
23	C	303	PEF	C11-C10-O2-C2
23	E	102	PEF	C1-O3P-P-O1P
23	J	401	PEF	C4-O4P-P-O1P
23	J	401	PEF	C4-O4P-P-O3P
23	J	409	PEF	C11-C10-O2-C2
23	J	409	PEF	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
23	J	409	PEF	O5-C30-O3-C3
23	W	201	PEF	O2-C2-C3-O3
23	a	501	PEF	O2-C2-C3-O3
23	a	501	PEF	O4P-C4-C5-N
23	a	504	PEF	C4-O4P-P-O1P
23	a	504	PEF	C4-O4P-P-O3P
23	j	401	PEF	C11-C10-O2-C2
25	C	302	CDL	CA2-OA2-PA1-OA3
25	C	302	CDL	CA2-OA2-PA1-OA5
25	C	302	CDL	CA3-OA5-PA1-OA2
25	C	302	CDL	CA3-OA5-PA1-OA3
25	C	302	CDL	OA6-CA4-CA6-OA8
25	C	302	CDL	CB3-OB5-PB2-OB2
25	C	302	CDL	CB3-OB5-PB2-OB3
25	C	302	CDL	CB3-OB5-PB2-OB4
25	C	302	CDL	C51-CB5-OB6-CB4
25	H	601	CDL	O1-C1-CB2-OB2
25	H	601	CDL	CA2-C1-CB2-OB2
25	H	601	CDL	CA2-OA2-PA1-OA4
25	H	601	CDL	CA2-OA2-PA1-OA5
25	H	601	CDL	CA3-OA5-PA1-OA3
25	H	601	CDL	OA7-CA5-OA6-CA4
25	H	601	CDL	C11-CA5-OA6-CA4
25	H	601	CDL	OB6-CB4-CB6-OB8
25	J	403	CDL	CA3-OA5-PA1-OA3
25	J	403	CDL	OA7-CA5-OA6-CA4
25	J	403	CDL	CB2-OB2-PB2-OB4
25	J	403	CDL	CB2-OB2-PB2-OB5
25	J	403	CDL	CB3-OB5-PB2-OB2
25	J	403	CDL	CB3-OB5-PB2-OB3
25	J	403	CDL	CB3-OB5-PB2-OB4
25	K	603	CDL	CA2-OA2-PA1-OA3
25	K	603	CDL	CA2-OA2-PA1-OA5
25	K	603	CDL	CA3-OA5-PA1-OA2
25	K	603	CDL	CA3-OA5-PA1-OA4
25	K	603	CDL	OA7-CA5-OA6-CA4
25	K	603	CDL	C11-CA5-OA6-CA4
25	K	603	CDL	CB2-OB2-PB2-OB3
25	K	603	CDL	CB2-OB2-PB2-OB5
25	K	603	CDL	CB3-OB5-PB2-OB3
25	L	402	CDL	CA2-OA2-PA1-OA3
25	L	402	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
25	L	402	CDL	CA3-OA5-PA1-OA2
25	L	402	CDL	CA3-OA5-PA1-OA3
25	L	402	CDL	CA3-OA5-PA1-OA4
25	L	402	CDL	CB2-OB2-PB2-OB5
25	L	402	CDL	CB3-OB5-PB2-OB3
25	L	402	CDL	CB3-OB5-PB2-OB4
25	c	302	CDL	O1-C1-CA2-OA2
25	c	302	CDL	CA3-OA5-PA1-OA2
25	c	302	CDL	CA3-OA5-PA1-OA3
25	c	302	CDL	CA3-OA5-PA1-OA4
25	c	302	CDL	C11-CA5-OA6-CA4
25	c	302	CDL	CB3-OB5-PB2-OB4
25	c	302	CDL	CB4-CB3-OB5-PB2
25	h	601	CDL	OA7-CA5-OA6-CA4
25	h	601	CDL	C11-CA5-OA6-CA4
25	h	601	CDL	CB2-OB2-PB2-OB3
25	h	601	CDL	CB2-OB2-PB2-OB4
25	h	601	CDL	CB3-OB5-PB2-OB2
25	h	601	CDL	CB3-OB5-PB2-OB3
25	h	601	CDL	CB3-OB5-PB2-OB4
25	h	601	CDL	C51-CB5-OB6-CB4
25	h	602	CDL	CA3-OA5-PA1-OA2
25	h	602	CDL	OA7-CA5-OA6-CA4
25	h	602	CDL	C11-CA5-OA6-CA4
25	h	602	CDL	CB2-OB2-PB2-OB3
25	h	602	CDL	CB2-OB2-PB2-OB4
25	h	602	CDL	CB2-OB2-PB2-OB5
25	j	402	CDL	CA2-OA2-PA1-OA3
25	j	402	CDL	CA2-OA2-PA1-OA4
25	j	402	CDL	CA3-OA5-PA1-OA2
25	j	402	CDL	CA4-CA3-OA5-PA1
25	j	402	CDL	CB2-OB2-PB2-OB3
25	j	402	CDL	CB2-OB2-PB2-OB5
25	k	602	CDL	CA2-OA2-PA1-OA3
25	k	602	CDL	CA2-OA2-PA1-OA4
25	k	602	CDL	CA2-OA2-PA1-OA5
25	k	602	CDL	CA3-OA5-PA1-OA2
25	k	602	CDL	CA3-OA5-PA1-OA4
25	k	602	CDL	CB2-OB2-PB2-OB3
25	k	602	CDL	CB3-OB5-PB2-OB2
25	k	602	CDL	CB3-OB5-PB2-OB3
26	E	101	PCF	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
26	E	101	PCF	C11-O13-P-O12
26	E	101	PCF	O21-C2-C3-O31
26	H	602	PCF	C1-O11-P-O12
26	a	502	PCF	C1-O11-P-O12
26	a	502	PCF	O13-C11-C12-N
26	w	203	PCF	C1-O11-P-O12
27	J	402	CN5	CC-O13-P-O11
27	J	402	CN5	CC-O13-P-O12
27	J	402	CN5	CC-O13-P-O14
27	J	402	CN5	C1'-O1'-P'-O2'
28	J	404	HEM	C2D-C3D-CAD-CBD
28	J	404	HEM	C4D-C3D-CAD-CBD
28	J	405	HEM	C2D-C3D-CAD-CBD
28	J	405	HEM	C4D-C3D-CAD-CBD
28	j	403	HEM	C2D-C3D-CAD-CBD
28	j	403	HEM	C4D-C3D-CAD-CBD
28	j	404	HEM	C2D-C3D-CAD-CBD
28	j	404	HEM	C4D-C3D-CAD-CBD
28	l	401	HEM	C2B-C3B-CAB-CBB
28	l	401	HEM	C4B-C3B-CAB-CBB
29	J	408	UQ6	C12-C11-C9-C8
29	J	408	UQ6	C12-C11-C9-C10
29	j	405	UQ6	C9-C11-C12-C13
29	j	407	UQ6	C20-C19-C21-C22
30	K	601	HEA	C2A-C3A-CMA-OMA
30	K	601	HEA	C4A-C3A-CMA-OMA
30	K	601	HEA	C13-C14-C15-C26
30	K	601	HEA	C20-C21-C22-C23
30	K	601	HEA	C21-C22-C23-C24
30	k	603	HEA	C2A-C3A-CMA-OMA
30	k	603	HEA	C4A-C3A-CMA-OMA
30	k	604	HEA	C2A-C3A-CMA-OMA
30	k	604	HEA	C4A-C3A-CMA-OMA
30	k	604	HEA	C21-C22-C23-C24
25	K	603	CDL	OB9-CB7-OB8-CB6
25	h	602	CDL	OB9-CB7-OB8-CB6
25	j	402	CDL	OB9-CB7-OB8-CB6
25	k	602	CDL	OB9-CB7-OB8-CB6
30	K	601	HEA	C21-C22-C23-C25
30	k	604	HEA	C21-C22-C23-C25
25	K	603	CDL	C71-CB7-OB8-CB6
25	h	602	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
25	k	602	CDL	C71-CB7-OB8-CB6
25	J	403	CDL	OA9-CA7-OA8-CA6
25	L	402	CDL	OA9-CA7-OA8-CA6
25	h	602	CDL	OA9-CA7-OA8-CA6
26	W	203	PCF	O32-C31-O31-C3
26	k	605	PCF	O32-C31-O31-C3
23	j	401	PEF	O4-C10-O2-C2
25	K	603	CDL	OB7-CB5-OB6-CB4
25	h	601	CDL	OB7-CB5-OB6-CB4
25	L	402	CDL	C31-CA7-OA8-CA6
25	h	602	CDL	C71-CB7-OB8-CB6
25	j	402	CDL	C71-CB7-OB8-CB6
26	W	203	PCF	C32-C31-O31-C3
26	k	605	PCF	C32-C31-O31-C3
25	J	403	CDL	C11-CA5-OA6-CA4
25	K	603	CDL	C51-CB5-OB6-CB4
29	J	406	UQ6	C25-C24-C26-C27
29	j	407	UQ6	C25-C24-C26-C27
30	k	603	HEA	C27-C19-C20-C21
29	j	407	UQ6	C18-C19-C21-C22
29	j	407	UQ6	C23-C24-C26-C27
30	k	603	HEA	C18-C19-C20-C21
28	L	401	HEM	C2D-C3D-CAD-CBD
30	k	603	HEA	C2D-C3D-CAD-CBD
25	J	403	CDL	C31-CA7-OA8-CA6
30	K	601	HEA	C17-C18-C19-C27
30	k	604	HEA	C17-C18-C19-C27
30	K	601	HEA	C17-C18-C19-C20
30	k	604	HEA	C17-C18-C19-C20
25	H	601	CDL	OB9-CB7-OB8-CB6
28	L	401	HEM	C4D-C3D-CAD-CBD
30	K	604	HEA	C4D-C3D-CAD-CBD
30	k	603	HEA	C4D-C3D-CAD-CBD
23	C	303	PEF	O4-C10-O2-C2
23	J	409	PEF	O4-C10-O2-C2
25	C	302	CDL	OB7-CB5-OB6-CB4
25	c	302	CDL	OA7-CA5-OA6-CA4
25	C	302	CDL	O1-C1-CA2-OA2
25	c	302	CDL	O1-C1-CB2-OB2
25	h	601	CDL	O1-C1-CB2-OB2
25	k	602	CDL	C11-CA5-OA6-CA4
25	k	602	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
25	H	601	CDL	C71-CB7-OB8-CB6
25	c	302	CDL	C31-CA7-OA8-CA6
29	j	405	UQ6	C30-C29-C31-C32
30	K	604	HEA	C27-C19-C20-C21
29	J	406	UQ6	C23-C24-C26-C27
29	J	406	UQ6	C24-C26-C27-C28
29	j	407	UQ6	C9-C11-C12-C13
29	j	407	UQ6	C24-C26-C27-C28
30	K	601	HEA	C19-C20-C21-C22
30	K	604	HEA	C15-C16-C17-C18
30	K	604	HEA	C19-C20-C21-C22
30	k	603	HEA	C15-C16-C17-C18
30	k	604	HEA	C19-C20-C21-C22
30	K	604	HEA	C3A-C2A-CAA-CBA
28	j	404	HEM	C2A-CAA-CBA-CGA
30	K	601	HEA	C2A-CAA-CBA-CGA
30	k	603	HEA	C3D-CAD-CBD-CGD
30	k	604	HEA	C2A-CAA-CBA-CGA
25	c	302	CDL	OA9-CA7-OA8-CA6
30	K	604	HEA	C1A-C2A-CAA-CBA
25	k	602	CDL	OA7-CA5-OA6-CA4
25	k	602	CDL	OB7-CB5-OB6-CB4
25	C	302	CDL	CB2-C1-CA2-OA2
25	J	403	CDL	CA2-C1-CB2-OB2
25	L	402	CDL	C71-CB7-OB8-CB6
29	j	405	UQ6	C28-C29-C31-C32
30	K	604	HEA	C18-C19-C20-C21
25	J	403	CDL	O1-C1-CB2-OB2
25	L	402	CDL	O1-C1-CB2-OB2
25	L	402	CDL	OB9-CB7-OB8-CB6
23	J	407	PEF	O2-C2-C3-O3
23	j	406	PEF	O2-C2-C3-O3
25	L	402	CDL	OB6-CB4-CB6-OB8
29	J	406	UQ6	C9-C11-C12-C13
29	J	406	UQ6	C19-C21-C22-C23
29	j	405	UQ6	C19-C21-C22-C23
30	k	603	HEA	C19-C20-C21-C22
23	c	304	PEF	C10-C11-C12-C13
25	c	302	CDL	C51-CB5-OB6-CB4
26	w	203	PCF	C2-C1-O11-P
23	J	409	PEF	C30-C31-C32-C33
25	J	403	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
25	h	601	CDL	CB5-C51-C52-C53
25	h	602	CDL	O1-C1-CA2-OA2
25	j	402	CDL	O1-C1-CB2-OB2
25	H	601	CDL	C51-CB5-OB6-CB4
23	A	501	PEF	C30-C31-C32-C33
25	H	601	CDL	OB7-CB5-OB6-CB4
25	c	302	CDL	OB7-CB5-OB6-CB4
25	L	402	CDL	CA2-C1-CB2-OB2
25	c	302	CDL	CA2-C1-CB2-OB2
25	h	602	CDL	CB2-C1-CA2-OA2
26	H	602	PCF	C11-C12-N-C14
26	H	602	PCF	C11-C12-N-C15
26	W	203	PCF	C11-C12-N-C13
26	W	203	PCF	C11-C12-N-C14
26	W	203	PCF	C11-C12-N-C15
26	k	605	PCF	C11-C12-N-C15
26	w	203	PCF	C11-C12-N-C13
26	w	203	PCF	C11-C12-N-C14
26	w	203	PCF	C11-C12-N-C15
25	j	402	CDL	C51-CB5-OB6-CB4
25	j	402	CDL	OB7-CB5-OB6-CB4
23	e	101	PEF	C10-C11-C12-C13
30	k	604	HEA	C15-C16-C17-C18
25	H	601	CDL	O1-C1-CA2-OA2
27	J	402	CN5	O1'-C1'-C2'-C3'
26	H	602	PCF	C2-C1-O11-P
30	K	604	HEA	C2D-C3D-CAD-CBD
28	J	404	HEM	C3D-CAD-CBD-CGD
26	H	602	PCF	C11-C12-N-C13
26	k	605	PCF	C11-C12-N-C13
26	k	605	PCF	C11-C12-N-C14
23	j	406	PEF	C31-C32-C33-C34
23	j	408	PEF	C11-C12-C13-C14
26	E	101	PCF	C33-C34-C35-C36
23	C	304	PEF	C10-C11-C12-C13
23	J	409	PEF	C11-C12-C13-C14
23	W	202	PEF	C19-C20-C21-C22
23	j	401	PEF	C13-C14-C15-C16
28	J	405	HEM	C2A-CAA-CBA-CGA
28	L	401	HEM	C3D-CAD-CBD-CGD
23	w	202	PEF	C19-C20-C21-C22
25	K	603	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
25	k	602	CDL	C33-C34-C35-C36
26	H	602	PCF	C34-C35-C36-C37
30	K	601	HEA	C14-C15-C16-C17
25	k	602	CDL	CA5-C11-C12-C13
26	H	602	PCF	C31-C32-C33-C34
26	w	203	PCF	C22-C23-C24-C25
23	c	303	PEF	C12-C13-C14-C15
23	j	406	PEF	C11-C12-C13-C14
25	j	402	CDL	C52-C53-C54-C55
23	J	401	PEF	C11-C10-O2-C2
23	c	304	PEF	C11-C10-O2-C2
23	v	101	PEF	C11-C10-O2-C2
25	C	302	CDL	C11-CA5-OA6-CA4
25	L	402	CDL	C51-CB5-OB6-CB4
25	C	302	CDL	CB7-C71-C72-C73
28	L	401	HEM	C2B-C3B-CAB-CBB
23	J	401	PEF	C16-C17-C18-C19
26	w	203	PCF	C25-C26-C27-C28
25	C	302	CDL	OA5-CA3-CA4-OA6
25	h	602	CDL	C11-C12-C13-C14
26	H	602	PCF	C27-C28-C29-C30
26	H	602	PCF	C25-C26-C27-C28
25	K	603	CDL	CB5-C51-C52-C53
23	J	401	PEF	O2-C2-C3-O3
23	w	201	PEF	O2-C2-C3-O3
25	J	403	CDL	OB6-CB4-CB6-OB8
25	h	601	CDL	OA6-CA4-CA6-OA8
23	j	406	PEF	C18-C19-C20-C21
26	E	101	PCF	C2-C1-O11-P
23	a	503	PEF	C11-C12-C13-C14
30	k	603	HEA	C1A-C2A-CAA-CBA
23	c	304	PEF	O4-C10-O2-C2
23	v	101	PEF	O4-C10-O2-C2
25	K	603	CDL	CA2-C1-CB2-OB2
25	c	302	CDL	CB2-C1-CA2-OA2
23	E	102	PEF	C11-C10-O2-C2
23	C	303	PEF	O3P-C1-C2-C3
23	W	201	PEF	O3P-C1-C2-C3
23	j	406	PEF	O3P-C1-C2-C3
25	C	302	CDL	OA5-CA3-CA4-CA6
26	a	502	PCF	O11-C1-C2-C3
26	w	203	PCF	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
23	J	407	PEF	C35-C36-C37-C38
25	L	402	CDL	C53-C54-C55-C56
23	A	501	PEF	C12-C13-C14-C15
23	j	401	PEF	C12-C13-C14-C15
23	j	408	PEF	C10-C11-C12-C13
23	W	201	PEF	C1-C2-C3-O3
23	a	501	PEF	C1-C2-C3-O3
23	a	504	PEF	C1-C2-C3-O3
23	j	406	PEF	C1-C2-C3-O3
25	h	601	CDL	CA3-CA4-CA6-OA8
25	j	402	CDL	CB3-CB4-CB6-OB8
26	E	101	PCF	C1-C2-C3-O31
26	W	203	PCF	C23-C24-C25-C26
25	C	302	CDL	O1-C1-CB2-OB2
25	K	603	CDL	CA7-C31-C32-C33
23	J	401	PEF	C30-C31-C32-C33
26	w	203	PCF	C31-C32-C33-C34
29	J	406	UQ6	C30-C29-C31-C32
25	L	402	CDL	OB7-CB5-OB6-CB4
30	k	603	HEA	C3A-C2A-CAA-CBA
23	E	102	PEF	C3-C2-O2-C10
25	k	602	CDL	CA6-CA4-OA6-CA5
23	j	406	PEF	C32-C33-C34-C35
26	w	203	PCF	C34-C35-C36-C37
25	h	602	CDL	C52-C53-C54-C55
25	j	402	CDL	CA2-C1-CB2-OB2
23	E	102	PEF	O3P-C1-C2-O2
25	J	403	CDL	OA5-CA3-CA4-OA6
26	a	502	PCF	O11-C1-C2-O21
23	a	503	PEF	C30-C31-C32-C33
26	w	203	PCF	C27-C28-C29-C30
23	j	401	PEF	C40-C41-C42-C43
30	k	604	HEA	C20-C21-C22-C23
26	H	602	PCF	C24-C25-C26-C27
25	K	603	CDL	C12-C13-C14-C15
25	K	603	CDL	C52-C53-C54-C55
30	K	604	HEA	C3B-C11-C12-C13
23	V	101	PEF	C31-C32-C33-C34
23	a	503	PEF	C32-C33-C34-C35
23	J	401	PEF	O4-C10-O2-C2
25	C	302	CDL	OA7-CA5-OA6-CA4
25	H	601	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
25	h	602	CDL	C1-CB2-OB2-PB2
25	k	602	CDL	C52-C53-C54-C55
23	E	102	PEF	O3P-C1-C2-C3
23	J	407	PEF	O3P-C1-C2-C3
23	V	101	PEF	O3P-C1-C2-C3
23	c	303	PEF	O3P-C1-C2-C3
23	j	408	PEF	O3P-C1-C2-C3
23	v	101	PEF	O3P-C1-C2-C3
25	L	402	CDL	OB5-CB3-CB4-CB6
25	c	302	CDL	OB5-CB3-CB4-CB6
25	j	402	CDL	OB5-CB3-CB4-CB6
23	J	409	PEF	C10-C11-C12-C13
25	K	603	CDL	CB7-C71-C72-C73
23	w	201	PEF	C37-C38-C39-C40
25	k	602	CDL	C31-C32-C33-C34
26	a	502	PCF	C21-C22-C23-C24
23	J	401	PEF	C41-C42-C43-C44
25	H	601	CDL	CB2-C1-CA2-OA2
25	k	602	CDL	CA2-C1-CB2-OB2
25	C	302	CDL	C31-CA7-OA8-CA6
23	J	409	PEF	C12-C13-C14-C15
23	J	401	PEF	C1-C2-C3-O3
23	J	407	PEF	C1-C2-C3-O3
23	J	409	PEF	C1-C2-C3-O3
23	w	201	PEF	C1-C2-C3-O3
25	L	402	CDL	CB3-CB4-CB6-OB8
25	h	601	CDL	CB3-CB4-CB6-OB8
23	e	101	PEF	C14-C15-C16-C17
23	c	303	PEF	C30-C31-C32-C33
25	k	602	CDL	C54-C55-C56-C57
29	J	406	UQ6	C20-C19-C21-C22
26	w	203	PCF	C26-C27-C28-C29
23	C	303	PEF	O3P-C1-C2-O2
23	C	304	PEF	O3P-C1-C2-O2
23	W	201	PEF	O3P-C1-C2-O2
23	W	202	PEF	O3P-C1-C2-O2
23	c	303	PEF	O3P-C1-C2-O2
23	j	401	PEF	O3P-C1-C2-O2
23	j	406	PEF	O3P-C1-C2-O2
23	j	408	PEF	O3P-C1-C2-O2
23	v	101	PEF	O3P-C1-C2-O2
23	w	202	PEF	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
25	L	402	CDL	OA5-CA3-CA4-OA6
25	c	302	CDL	OB5-CB3-CB4-OB6
25	h	602	CDL	OB5-CB3-CB4-OB6
25	j	402	CDL	OB5-CB3-CB4-OB6
23	a	504	PEF	C34-C35-C36-C37
23	j	406	PEF	C10-C11-C12-C13
28	j	403	HEM	C3D-CAD-CBD-CGD
23	J	409	PEF	O2-C2-C3-O3
25	h	602	CDL	OA6-CA4-CA6-OA8
25	j	402	CDL	OB6-CB4-CB6-OB8
23	E	102	PEF	O4-C10-O2-C2
26	E	101	PCF	C21-C22-C23-C24
23	A	503	PEF	C33-C34-C35-C36
23	A	503	PEF	C36-C37-C38-C39
29	j	405	UQ6	C25-C24-C26-C27
25	C	302	CDL	OB5-CB3-CB4-CB6
25	H	601	CDL	OA5-CA3-CA4-CA6
25	h	602	CDL	OB5-CB3-CB4-CB6
25	J	403	CDL	C1-CA2-OA2-PA1
25	k	602	CDL	CB7-C71-C72-C73
23	W	201	PEF	C35-C36-C37-C38
28	j	403	HEM	C2B-C3B-CAB-CBB
23	a	501	PEF	C1-C2-O2-C10
23	e	101	PEF	C3-C2-O2-C10
25	H	601	CDL	CA3-CA4-OA6-CA5
25	K	603	CDL	CA6-CA4-OA6-CA5
25	K	603	CDL	CB6-CB4-OB6-CB5
25	c	302	CDL	CA3-CA4-OA6-CA5
25	h	601	CDL	CA3-CA4-OA6-CA5
26	a	502	PCF	C26-C27-C28-C29
23	V	101	PEF	O3P-C1-C2-O2
23	e	101	PEF	O3P-C1-C2-O2
23	w	201	PEF	O3P-C1-C2-O2
25	C	302	CDL	OB5-CB3-CB4-OB6
25	L	402	CDL	OB5-CB3-CB4-OB6
25	C	302	CDL	OA9-CA7-OA8-CA6
23	A	501	PEF	C1-C2-C3-O3
23	A	503	PEF	C1-C2-C3-O3
23	v	101	PEF	C1-C2-C3-O3
25	C	302	CDL	CA3-CA4-CA6-OA8
25	H	601	CDL	CB3-CB4-CB6-OB8
25	h	602	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
25	k	602	CDL	CA3-CA4-CA6-OA8
30	K	601	HEA	C15-C16-C17-C18
25	h	601	CDL	CB7-C71-C72-C73
28	j	403	HEM	C4B-C3B-CAB-CBB
30	K	601	HEA	O11-C11-C12-C13
30	K	604	HEA	O11-C11-C12-C13
30	k	604	HEA	O11-C11-C12-C13
29	j	405	UQ6	C23-C24-C26-C27
26	k	605	PCF	C23-C24-C25-C26
23	a	504	PEF	O2-C2-C3-O3
25	h	601	CDL	OB6-CB4-CB6-OB8
25	k	602	CDL	OA6-CA4-CA6-OA8
23	J	407	PEF	C16-C17-C18-C19
25	H	601	CDL	CB5-C51-C52-C53
23	j	408	PEF	C13-C14-C15-C16
23	E	102	PEF	C2-C1-O3P-P
23	E	102	PEF	C16-C17-C18-C19
26	E	101	PCF	O13-C11-C12-N
26	H	602	PCF	O13-C11-C12-N
26	W	203	PCF	O13-C11-C12-N
26	k	605	PCF	O13-C11-C12-N
26	w	203	PCF	O13-C11-C12-N
25	h	601	CDL	CA2-C1-CB2-OB2
23	A	501	PEF	C15-C16-C17-C18
27	J	402	CN5	C32-C31-O31-C3
23	w	201	PEF	C31-C32-C33-C34
23	C	304	PEF	C31-C30-O3-C3
29	j	407	UQ6	C12-C11-C9-C10
23	C	304	PEF	O3P-C1-C2-C3
23	J	401	PEF	O3P-C1-C2-C3
23	W	202	PEF	O3P-C1-C2-C3
23	a	501	PEF	O3P-C1-C2-C3
23	c	304	PEF	O3P-C1-C2-C3
23	e	101	PEF	O3P-C1-C2-C3
23	w	201	PEF	O3P-C1-C2-C3
23	w	202	PEF	O3P-C1-C2-C3
25	J	403	CDL	OA5-CA3-CA4-CA6
25	L	402	CDL	OA5-CA3-CA4-CA6
25	h	601	CDL	OA5-CA3-CA4-CA6
25	j	402	CDL	OA5-CA3-CA4-CA6
25	K	603	CDL	C32-C33-C34-C35
25	k	602	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
23	J	401	PEF	O3P-C1-C2-O2
23	c	304	PEF	O3P-C1-C2-O2
25	H	601	CDL	OA5-CA3-CA4-OA6
25	h	601	CDL	OA5-CA3-CA4-OA6
25	j	402	CDL	OA5-CA3-CA4-OA6
26	w	203	PCF	O11-C1-C2-O21
30	K	604	HEA	C3D-CAD-CBD-CGD
23	w	201	PEF	C32-C33-C34-C35
26	a	502	PCF	C11-C12-N-C15
23	A	502	PEF	C11-C12-C13-C14
26	E	101	PCF	C23-C24-C25-C26
27	J	402	CN5	O32-C31-O31-C3
23	w	202	PEF	C1-C2-C3-O3
25	J	403	CDL	CB3-CB4-CB6-OB8
25	K	603	CDL	CA3-CA4-CA6-OA8
25	h	602	CDL	O1-C1-CB2-OB2
23	C	304	PEF	O5-C30-O3-C3
23	A	503	PEF	C32-C33-C34-C35
23	J	401	PEF	C14-C15-C16-C17
23	A	503	PEF	C4-O4P-P-O2P
23	V	101	PEF	C4-O4P-P-O1P
23	W	201	PEF	C1-O3P-P-O1P
23	W	202	PEF	C1-O3P-P-O1P
23	W	202	PEF	C4-O4P-P-O1P
23	a	504	PEF	C4-O4P-P-O2P
23	c	304	PEF	C4-O4P-P-O1P
23	j	401	PEF	C4-O4P-P-O1P
23	j	406	PEF	C1-O3P-P-O1P
23	j	406	PEF	C1-O3P-P-O4P
23	w	201	PEF	C1-O3P-P-O1P
23	w	202	PEF	C1-O3P-P-O1P
25	H	601	CDL	CA2-OA2-PA1-OA3
25	H	601	CDL	CA3-OA5-PA1-OA2
25	H	601	CDL	CA3-OA5-PA1-OA4
25	K	603	CDL	CA2-OA2-PA1-OA4
25	K	603	CDL	CB2-OB2-PB2-OB4
25	L	402	CDL	CA2-OA2-PA1-OA4
25	L	402	CDL	CB2-OB2-PB2-OB3
25	L	402	CDL	CB3-OB5-PB2-OB2
25	h	601	CDL	CB2-OB2-PB2-OB5
25	h	602	CDL	CA3-OA5-PA1-OA3
25	j	402	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
25	j	402	CDL	CA3-OA5-PA1-OA3
25	j	402	CDL	CB2-OB2-PB2-OB4
26	E	101	PCF	C11-O13-P-O11
30	K	604	HEA	C11-C12-C13-C14
30	k	603	HEA	C11-C12-C13-C14
23	j	401	PEF	C35-C36-C37-C38
29	J	406	UQ6	C28-C29-C31-C32
25	C	302	CDL	C1-CA2-OA2-PA1
25	J	403	CDL	CA4-CA3-OA5-PA1
25	c	302	CDL	C1-CA2-OA2-PA1
25	c	302	CDL	C1-CB2-OB2-PB2
25	h	601	CDL	CA4-CA3-OA5-PA1
25	h	602	CDL	CB4-CB3-OB5-PB2
23	j	401	PEF	C30-C31-C32-C33
25	k	602	CDL	CB5-C51-C52-C53
25	L	402	CDL	CB5-C51-C52-C53
23	a	501	PEF	C13-C14-C15-C16
23	J	407	PEF	C3-C2-O2-C10
23	V	101	PEF	C3-C2-O2-C10
23	v	101	PEF	C3-C2-O2-C10
25	J	403	CDL	CA3-CA4-OA6-CA5
25	k	602	CDL	CB6-CB4-OB6-CB5
23	j	406	PEF	C35-C36-C37-C38
29	j	405	UQ6	C14-C16-C17-C18
26	a	502	PCF	C11-C12-N-C13
23	j	401	PEF	O3P-C1-C2-C3
26	H	602	PCF	O11-C1-C2-C3
25	K	603	CDL	C34-C35-C36-C37
23	a	501	PEF	O3P-C1-C2-O2
23	c	303	PEF	C10-C11-C12-C13
23	J	407	PEF	C18-C19-C20-C21
23	J	401	PEF	C11-C12-C13-C14
23	A	503	PEF	O2-C2-C3-O3
25	J	403	CDL	OA6-CA4-CA6-OA8
25	K	603	CDL	OA6-CA4-CA6-OA8
28	J	404	HEM	C2A-CAA-CBA-CGA
23	c	304	PEF	C31-C30-O3-C3
23	A	501	PEF	C31-C32-C33-C34
26	H	602	PCF	C26-C27-C28-C29
25	C	302	CDL	C72-C73-C74-C75
25	H	601	CDL	C32-C33-C34-C35
23	C	304	PEF	C2-C1-O3P-P

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Mol	Chain	Res	Type	Atoms
25	k	602	CDL	CA4-CA3-OA5-PA1
23	J	407	PEF	C13-C14-C15-C16
23	c	304	PEF	O5-C30-O3-C3
25	L	402	CDL	CB7-C71-C72-C73
28	L	401	HEM	C4B-C3B-CAB-CBB
25	H	601	CDL	C36-C37-C38-C39
25	K	603	CDL	O1-C1-CB2-OB2
25	L	402	CDL	O1-C1-CA2-OA2
26	a	502	PCF	C22-C23-C24-C25
29	J	406	UQ6	C15-C14-C16-C17
23	J	407	PEF	C12-C13-C14-C15
25	h	602	CDL	C1-CA2-OA2-PA1
26	W	203	PCF	C24-C25-C26-C27
30	k	604	HEA	CAA-CBA-CGA-O1A
26	a	502	PCF	C24-C25-C26-C27
25	C	302	CDL	CA2-C1-CB2-OB2
26	a	502	PCF	C34-C35-C36-C37
23	W	202	PEF	C1-C2-C3-O3
29	j	407	UQ6	C29-C31-C32-C33
23	c	304	PEF	C11-C12-C13-C14
25	k	602	CDL	C52-C51-CB5-OB6
23	C	303	PEF	C1-C2-O2-C10
23	j	406	PEF	C30-C31-C32-C33
30	K	604	HEA	C14-C15-C16-C17
23	a	503	PEF	C12-C13-C14-C15
26	a	502	PCF	C11-C12-N-C14
26	W	203	PCF	C21-C22-C23-C24
23	C	304	PEF	C30-C31-C32-C33
28	l	401	HEM	CAA-CBA-CGA-O2A
23	e	101	PEF	C2-C1-O3P-P
25	c	302	CDL	CA4-CA3-OA5-PA1
27	J	402	CN5	CB-CC-O13-P
23	a	501	PEF	C30-C31-C32-C33
28	J	405	HEM	CAA-CBA-CGA-O1A
23	A	503	PEF	O3P-C1-C2-C3
30	K	601	HEA	CAA-CBA-CGA-O2A
30	k	603	HEA	CAA-CBA-CGA-O1A
23	J	401	PEF	C32-C33-C34-C35
23	A	501	PEF	C34-C35-C36-C37
23	W	202	PEF	C20-C21-C22-C23
28	j	404	HEM	CAA-CBA-CGA-O2A
29	J	406	UQ6	C18-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
30	k	603	HEA	C14-C15-C16-C17
30	K	604	HEA	CAA-CBA-CGA-O1A
25	h	601	CDL	CA5-C11-C12-C13
28	j	403	HEM	CAD-CBD-CGD-O1D
28	j	404	HEM	CAA-CBA-CGA-O1A
30	K	601	HEA	CAA-CBA-CGA-O1A
30	k	603	HEA	C26-C15-C16-C17
30	k	604	HEA	CAD-CBD-CGD-O2D
23	a	504	PEF	C2-C1-O3P-P
23	c	304	PEF	C2-C1-O3P-P
25	C	302	CDL	CB4-CB3-OB5-PB2
29	j	407	UQ6	C12-C11-C9-C8
23	j	406	PEF	C12-C13-C14-C15
26	w	203	PCF	C30-C47-C48-C49
28	J	405	HEM	CAA-CBA-CGA-O2A
23	V	101	PEF	C1-C2-C3-O3
25	J	403	CDL	CA3-CA4-CA6-OA8
25	j	402	CDL	O1-C1-CA2-OA2
23	V	101	PEF	O4-C10-O2-C2
26	H	602	PCF	O11-C1-C2-O21
25	c	302	CDL	C52-C51-CB5-OB6
25	L	402	CDL	C31-C32-C33-C34
26	W	203	PCF	C22-C23-C24-C25
25	h	602	CDL	C74-C75-C76-C77
30	k	603	HEA	CAA-CBA-CGA-O2A
28	j	404	HEM	CAD-CBD-CGD-O2D
25	J	403	CDL	C52-C53-C54-C55
25	H	601	CDL	OB5-CB3-CB4-CB6
26	E	101	PCF	O11-C1-C2-C3
23	c	303	PEF	O2-C2-C3-O3
23	J	401	PEF	C40-C41-C42-C43
25	J	403	CDL	C53-C54-C55-C56
23	j	401	PEF	C33-C34-C35-C36
23	C	304	PEF	C15-C16-C17-C18
30	k	604	HEA	C27-C19-C20-C21
28	j	403	HEM	CAA-CBA-CGA-O2A
28	l	401	HEM	CAD-CBD-CGD-O2D
25	k	602	CDL	C34-C35-C36-C37
23	a	503	PEF	C1-C2-C3-O3
30	k	604	HEA	CAA-CBA-CGA-O2A
23	W	201	PEF	C11-C12-C13-C14
26	a	502	PCF	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
28	L	401	HEM	CAD-CBD-CGD-O1D
25	h	601	CDL	C72-C71-CB7-OB8
25	K	603	CDL	C55-C56-C57-C58
30	K	604	HEA	CAA-CBA-CGA-O2A
25	J	403	CDL	C32-C31-CA7-OA8
23	V	101	PEF	C11-C10-O2-C2
30	K	601	HEA	C3B-C11-C12-C13
23	J	401	PEF	C35-C36-C37-C38
25	k	602	CDL	O1-C1-CB2-OB2
28	j	403	HEM	CAD-CBD-CGD-O2D
23	c	303	PEF	O4-C10-O2-C2
23	A	501	PEF	O3P-C1-C2-O2
29	J	406	UQ6	C13-C14-C16-C17
30	k	604	HEA	CAD-CBD-CGD-O1D
23	C	303	PEF	O2-C10-C11-C12
25	K	603	CDL	C61-C62-C63-C64
23	C	303	PEF	O2-C2-C3-O3
30	K	604	HEA	CAD-CBD-CGD-O2D
25	h	602	CDL	C52-C51-CB5-OB6
25	H	601	CDL	CB7-C71-C72-C73
23	A	503	PEF	C15-C16-C17-C18
23	W	202	PEF	C35-C36-C37-C38
23	J	409	PEF	C1-C2-O2-C10
25	J	403	CDL	CA6-CA4-OA6-CA5
26	H	602	PCF	C48-C49-C50-C51
26	E	101	PCF	C40-C41-C42-C43
23	J	407	PEF	C2-C1-O3P-P
23	a	503	PEF	C2-C1-O3P-P
25	L	402	CDL	C52-C53-C54-C55
25	K	603	CDL	C62-C63-C64-C65
25	h	602	CDL	C52-C51-CB5-OB7
23	C	303	PEF	C12-C13-C14-C15
23	C	303	PEF	O4-C10-C11-C12
25	h	601	CDL	C72-C71-CB7-OB9
23	v	101	PEF	C31-C32-C33-C34
23	w	201	PEF	O4-C10-O2-C2
23	w	202	PEF	O2-C2-C3-O3
25	L	402	CDL	OA6-CA4-CA6-OA8
23	A	503	PEF	C34-C35-C36-C37
23	V	101	PEF	C33-C34-C35-C36
25	J	403	CDL	C11-C12-C13-C14
25	H	601	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
25	K	603	CDL	C52-C51-CB5-OB6
23	a	501	PEF	C12-C13-C14-C15
26	H	602	PCF	C1-C2-C3-O31
28	J	405	HEM	CAD-CBD-CGD-O2D
25	L	402	CDL	C72-C71-CB7-OB8
28	J	405	HEM	CAD-CBD-CGD-O1D
25	h	601	CDL	CA7-C31-C32-C33
25	k	602	CDL	C12-C11-CA5-OA6
25	k	602	CDL	C72-C71-CB7-OB8
23	c	303	PEF	C11-C10-O2-C2
23	w	201	PEF	C11-C10-O2-C2
25	K	603	CDL	C72-C71-CB7-OB8
28	J	404	HEM	CAD-CBD-CGD-O1D
30	k	603	HEA	CAD-CBD-CGD-O1D

There are no ring outliers.

54 monomers are involved in 225 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	E	101	PCF	3	0
25	L	402	CDL	5	0
23	J	407	PEF	2	0
25	C	302	CDL	5	0
23	w	201	PEF	1	0
25	h	602	CDL	1	0
23	W	201	PEF	3	0
26	W	203	PCF	2	0
29	j	407	UQ6	4	0
25	k	602	CDL	4	0
23	w	202	PEF	4	0
23	W	202	PEF	4	0
29	j	405	UQ6	5	0
23	A	502	PEF	5	0
23	e	101	PEF	1	0
23	j	406	PEF	3	0
25	h	601	CDL	3	0
30	K	604	HEA	18	0
28	J	404	HEM	6	0
23	E	102	PEF	2	0
25	j	402	CDL	2	0
23	C	303	PEF	1	0
24	C	301	FES	3	0

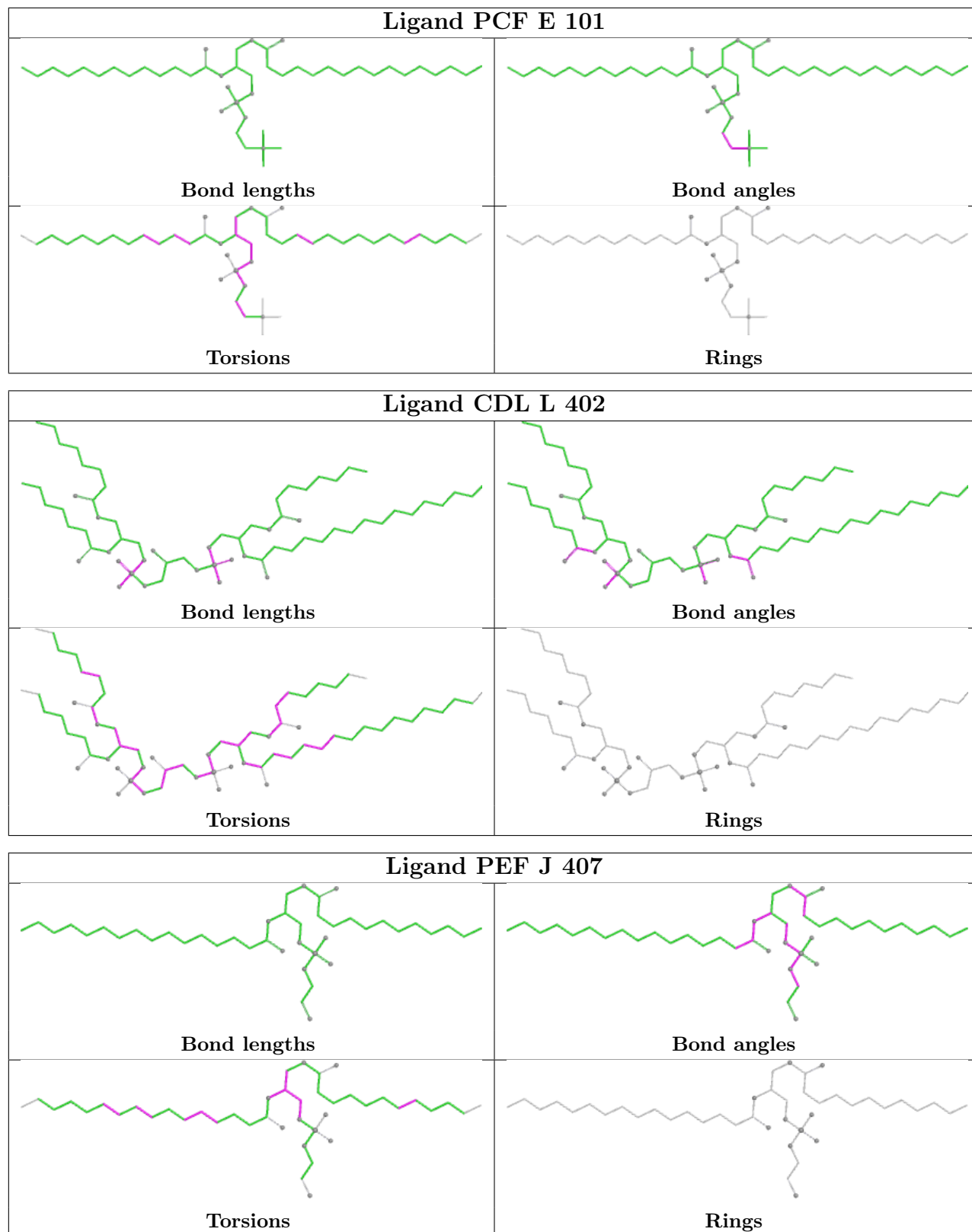
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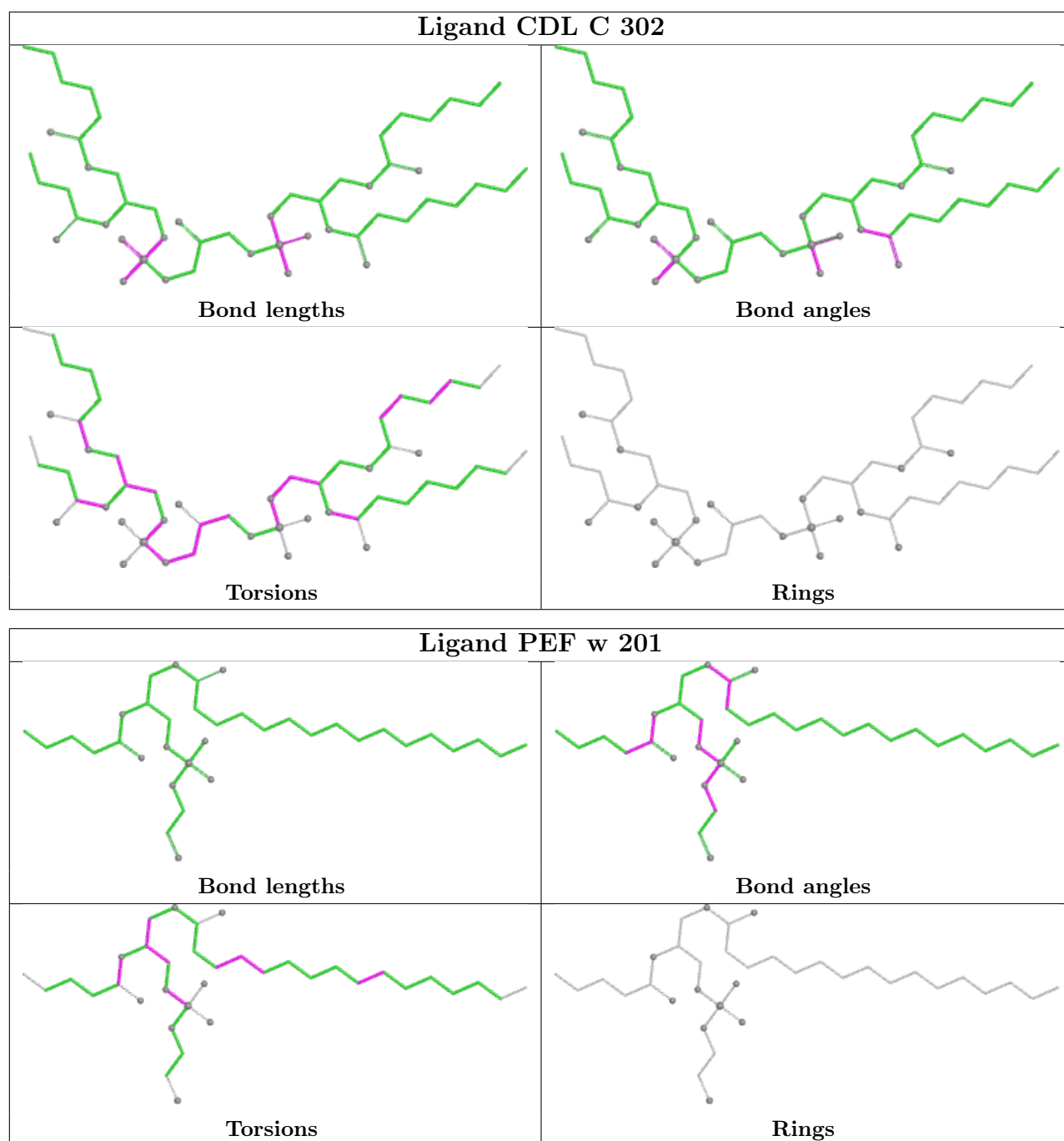
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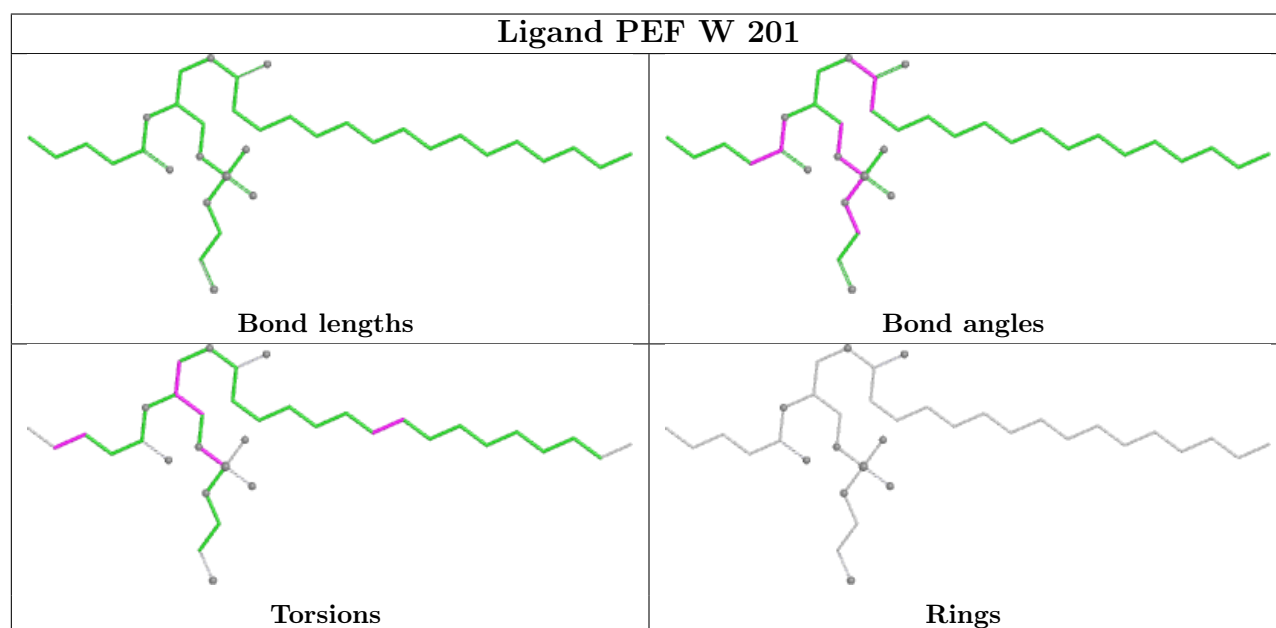
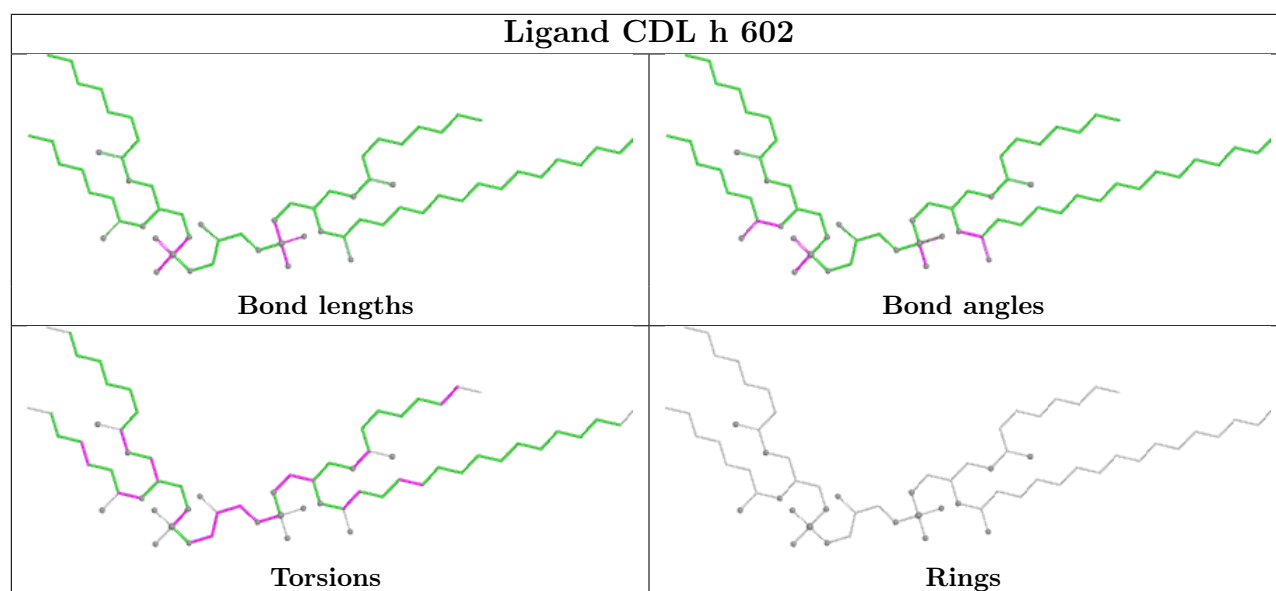
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	l	401	HEM	9	0
29	J	408	UQ6	3	0
23	a	503	PEF	1	0
30	K	601	HEA	10	0
28	L	401	HEM	9	0
24	c	301	FES	3	0
23	A	503	PEF	5	0
30	k	604	HEA	10	0
23	c	303	PEF	3	0
23	A	501	PEF	5	0
23	j	408	PEF	1	0
25	c	302	CDL	5	0
29	J	406	UQ6	8	0
26	a	502	PCF	2	0
23	c	304	PEF	3	0
26	H	602	PCF	2	0
26	k	605	PCF	1	0
25	H	601	CDL	3	0
28	J	405	HEM	8	0
30	k	603	HEA	13	0
28	j	404	HEM	9	0
25	J	403	CDL	3	0
28	j	403	HEM	8	0
23	J	401	PEF	3	0
23	J	409	PEF	1	0
23	a	501	PEF	3	0
25	K	603	CDL	6	0
27	J	402	CN5	6	0
23	j	401	PEF	4	0
23	a	504	PEF	4	0
23	C	304	PEF	5	0

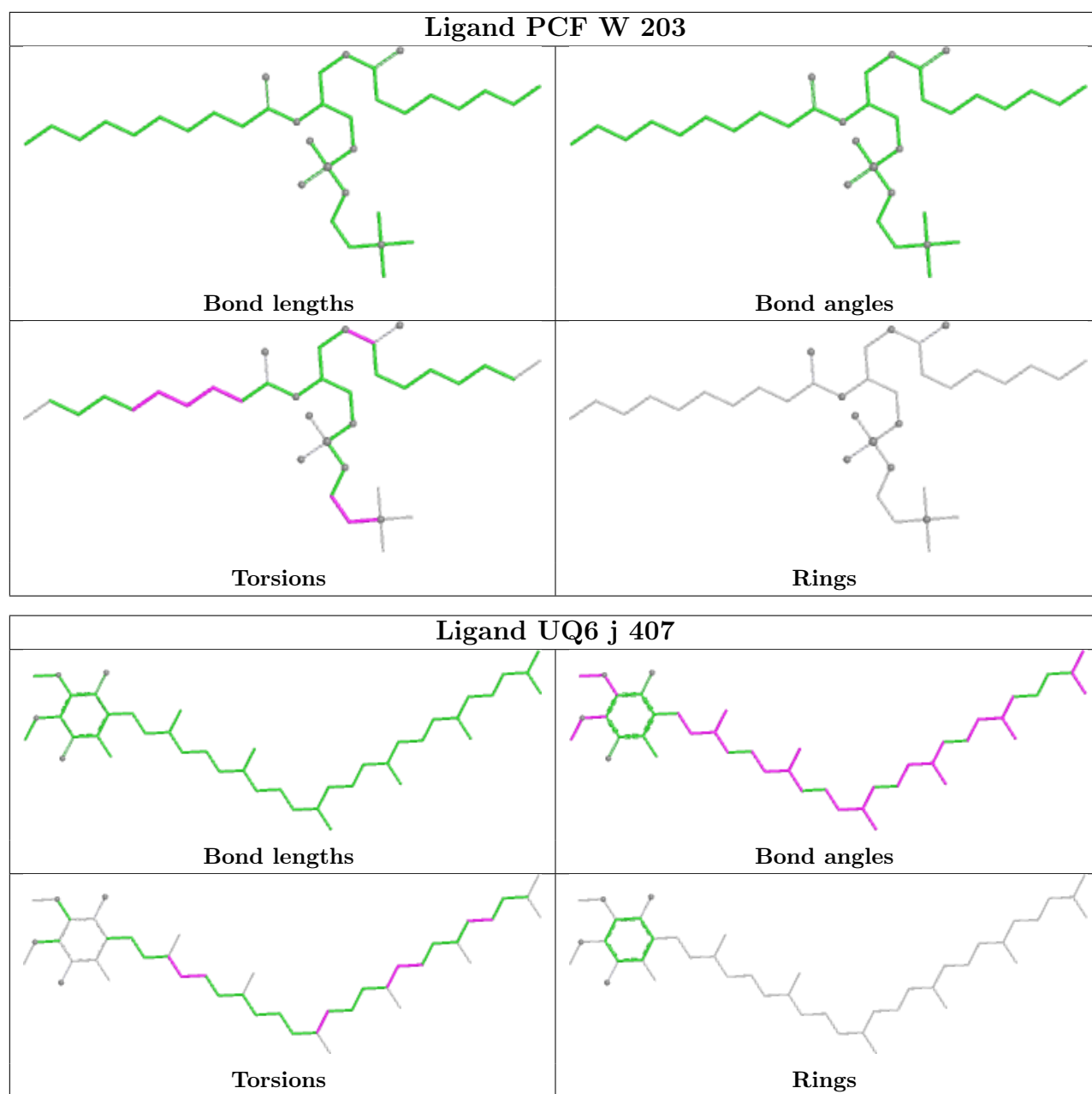
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

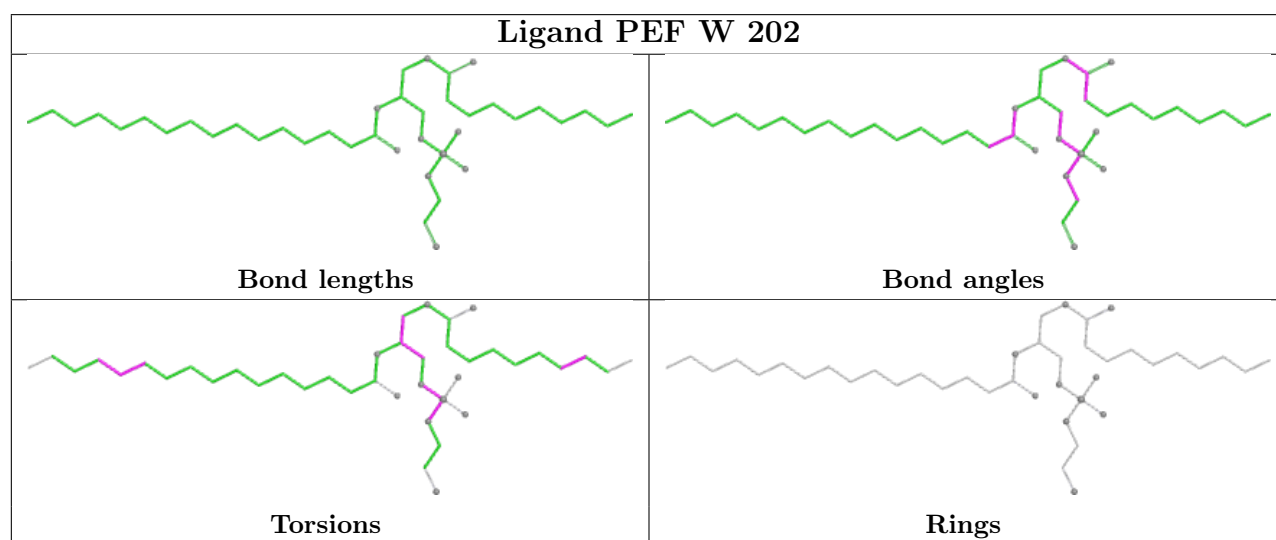
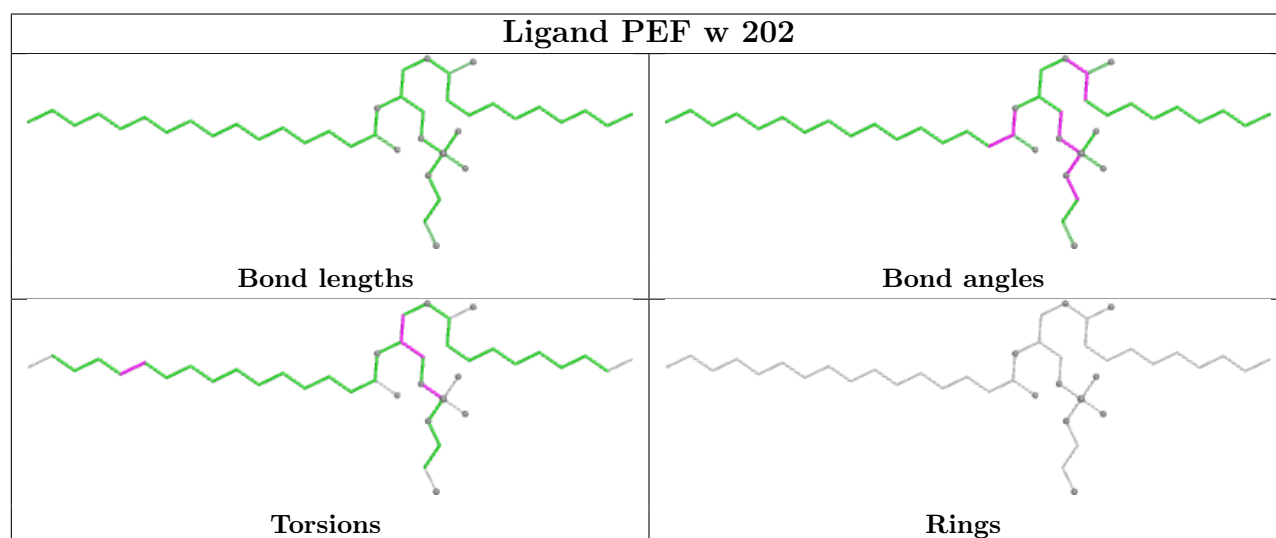
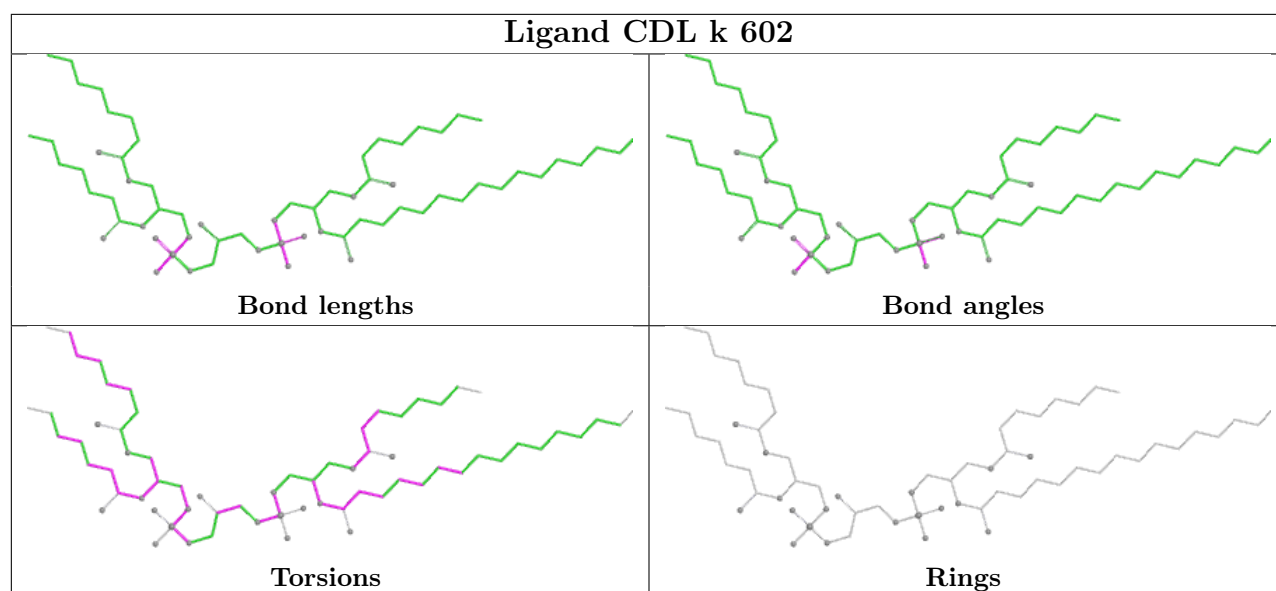
equivalents in the CSD to analyse the geometry.

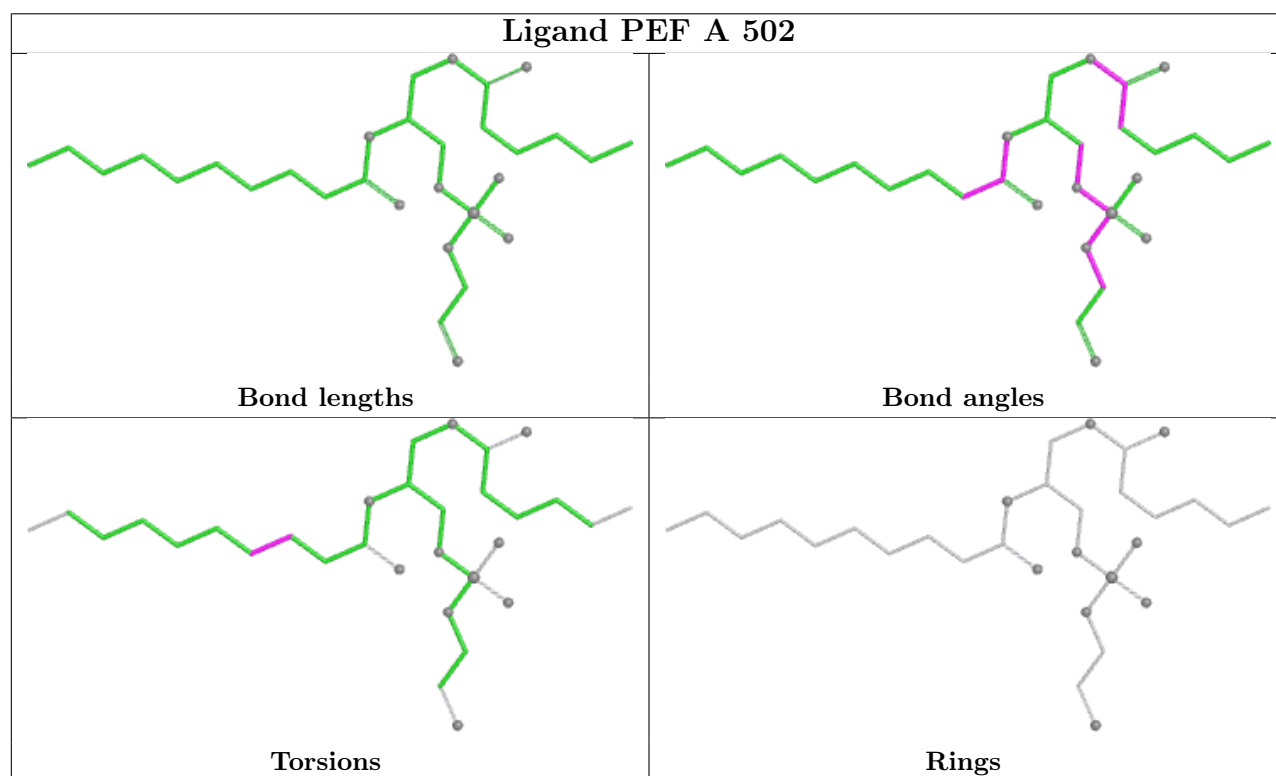
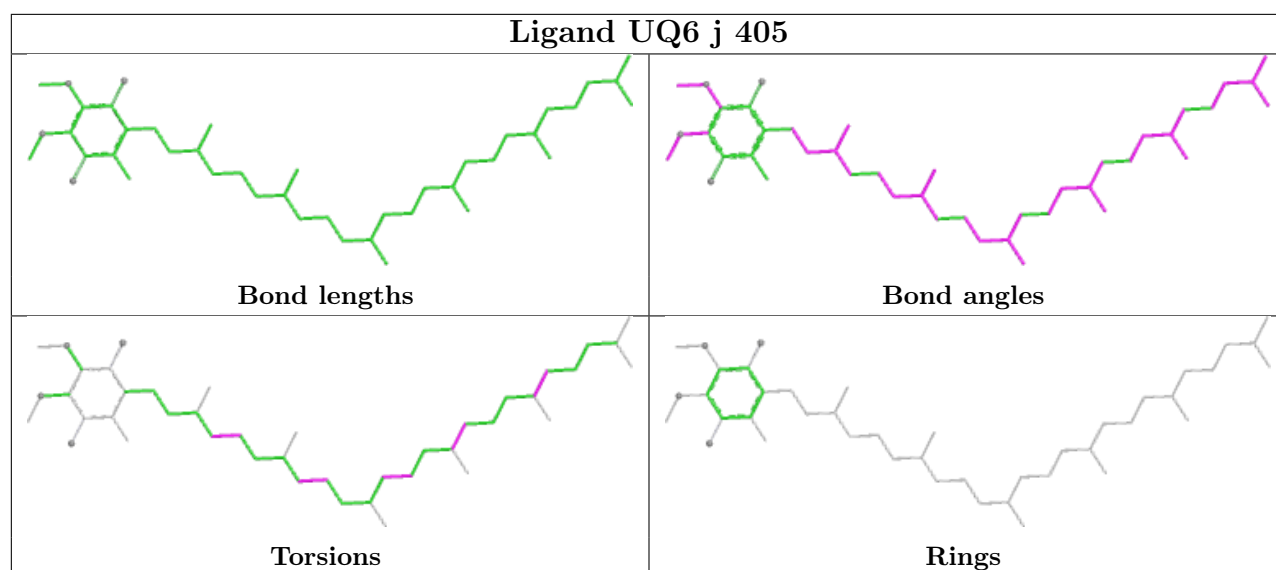


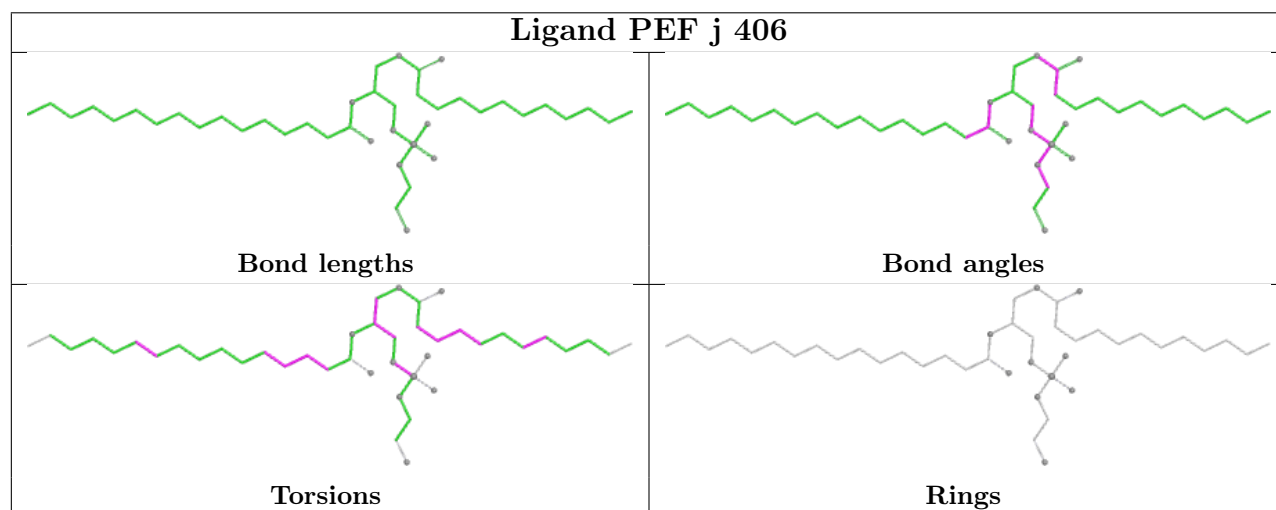
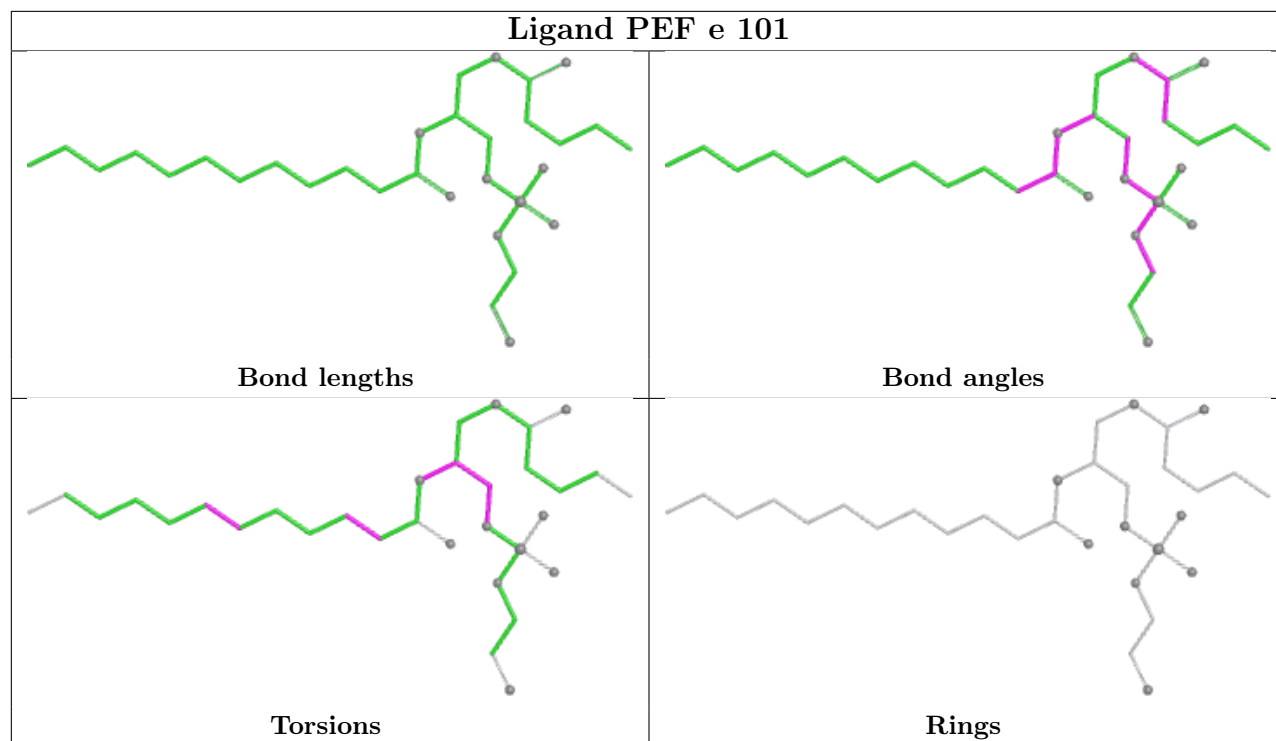


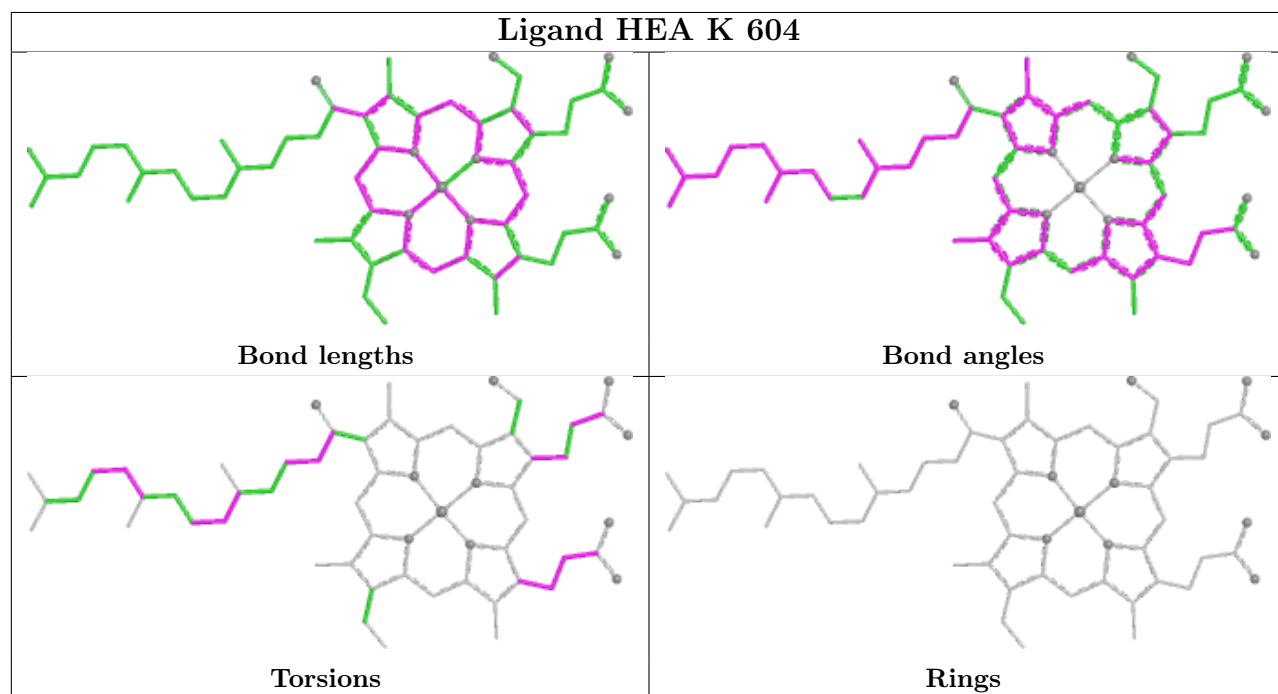
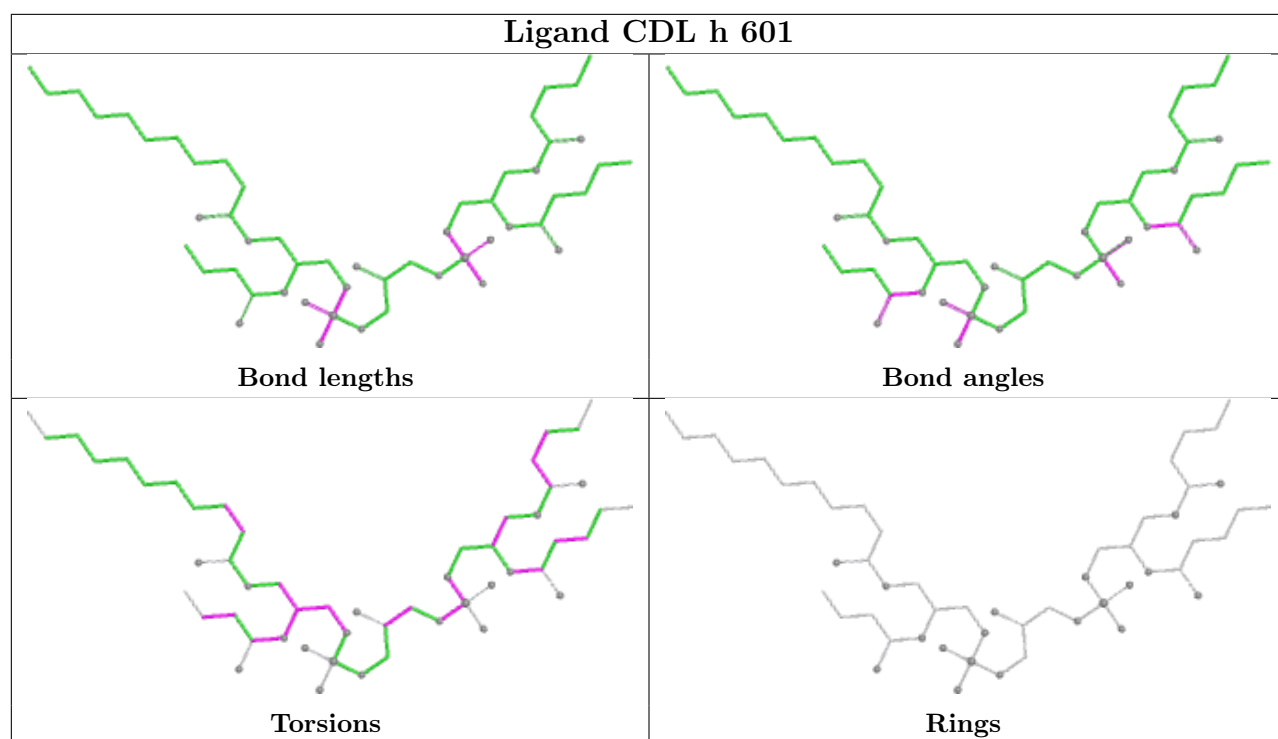




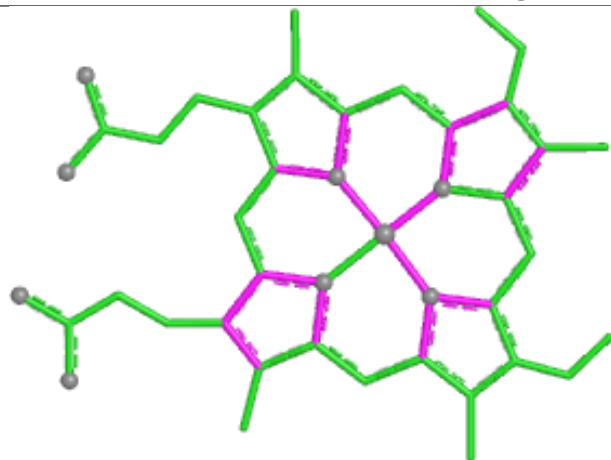




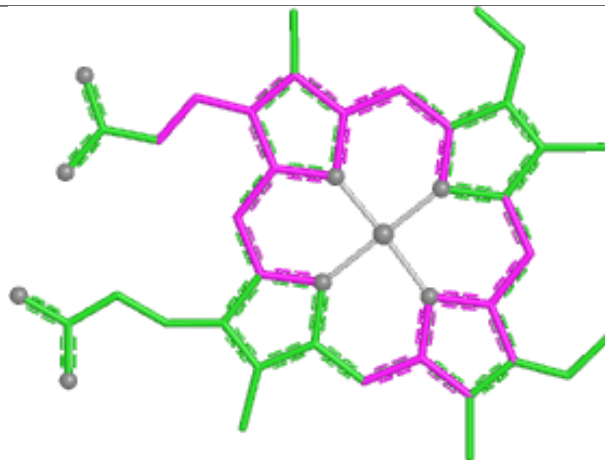




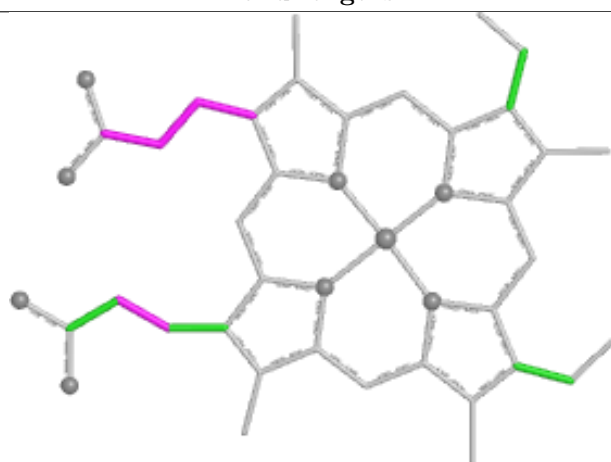
Ligand HEM J 404



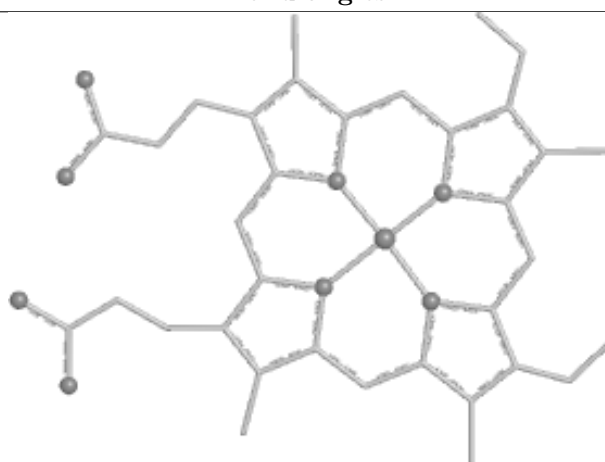
Bond lengths



Bond angles

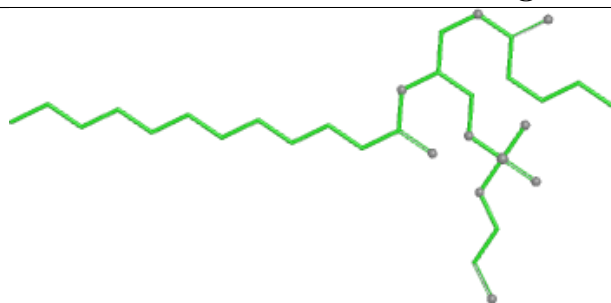


Torsions

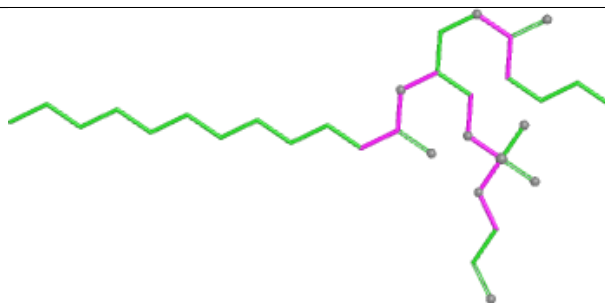


Rings

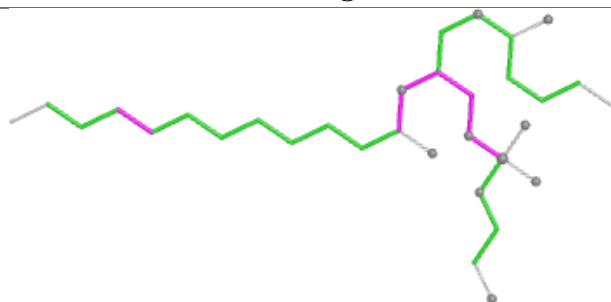
Ligand PEF E 102



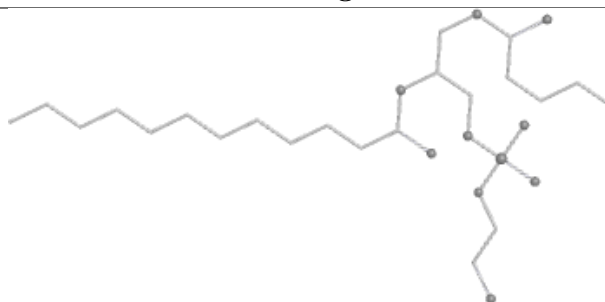
Bond lengths



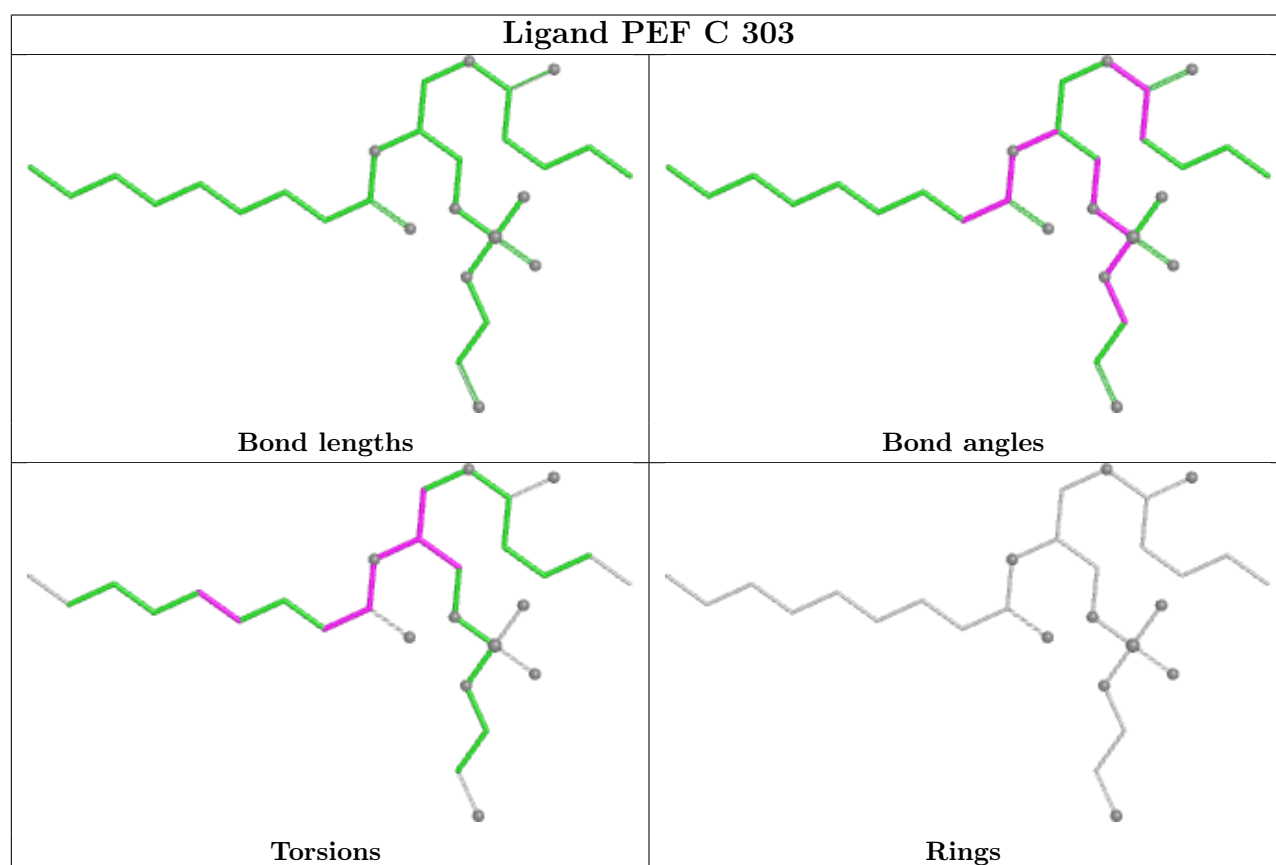
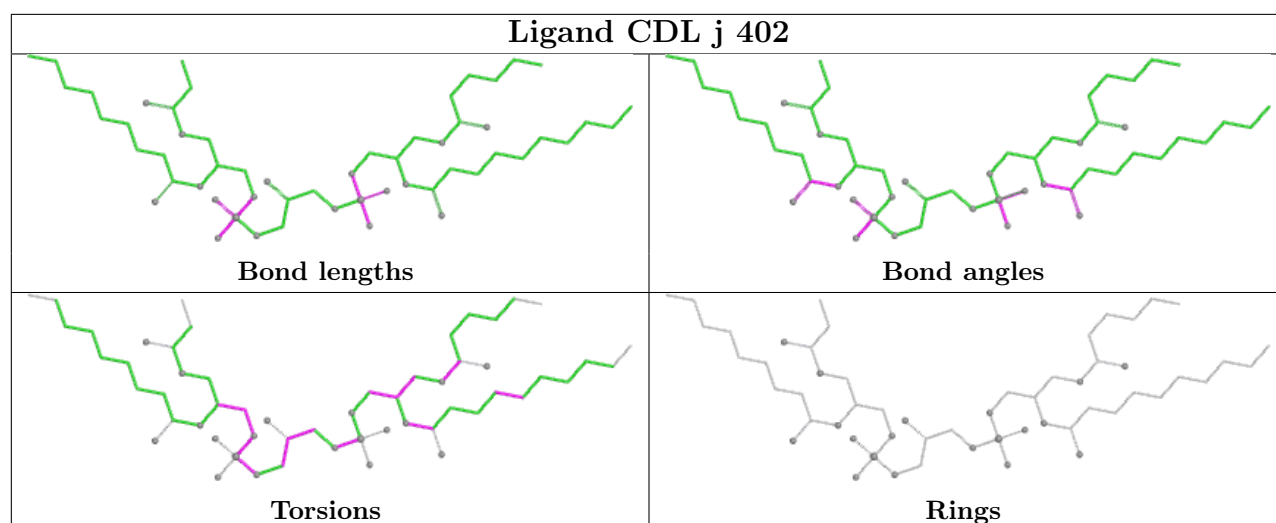
Bond angles



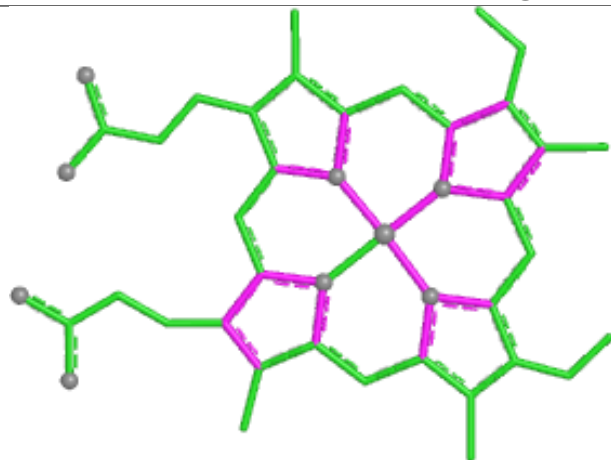
Torsions



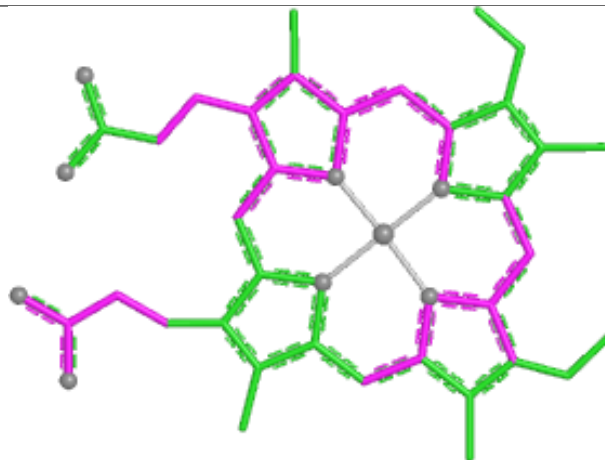
Rings



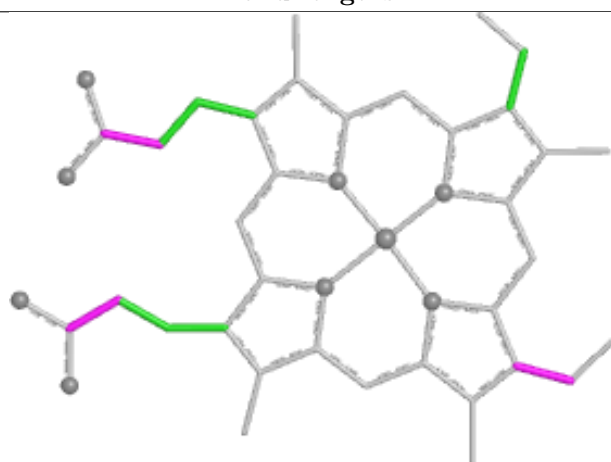
Ligand HEM 1 401



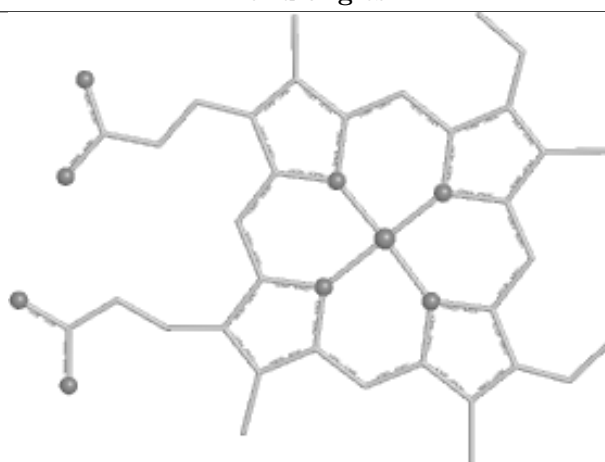
Bond lengths



Bond angles

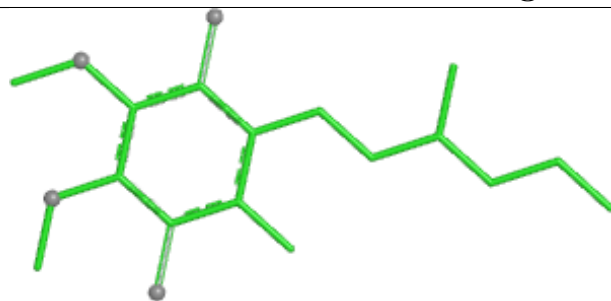


Torsions

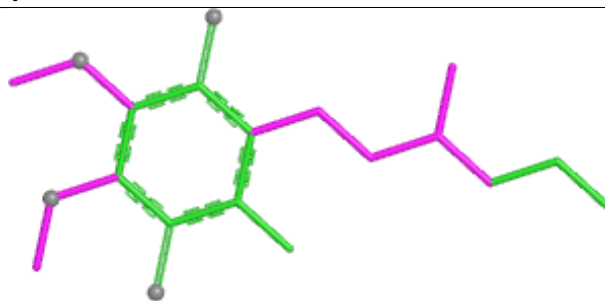


Rings

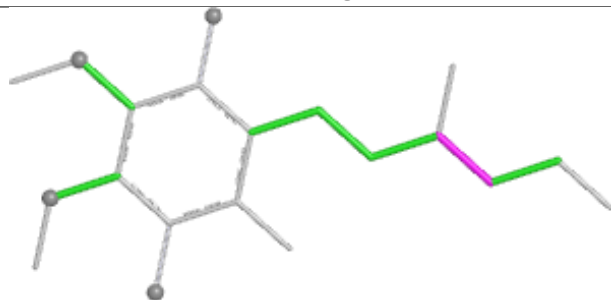
Ligand UQ6 J 408



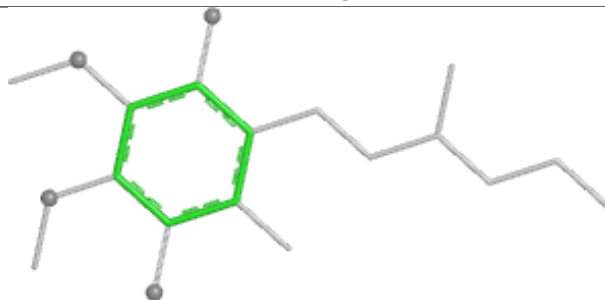
Bond lengths



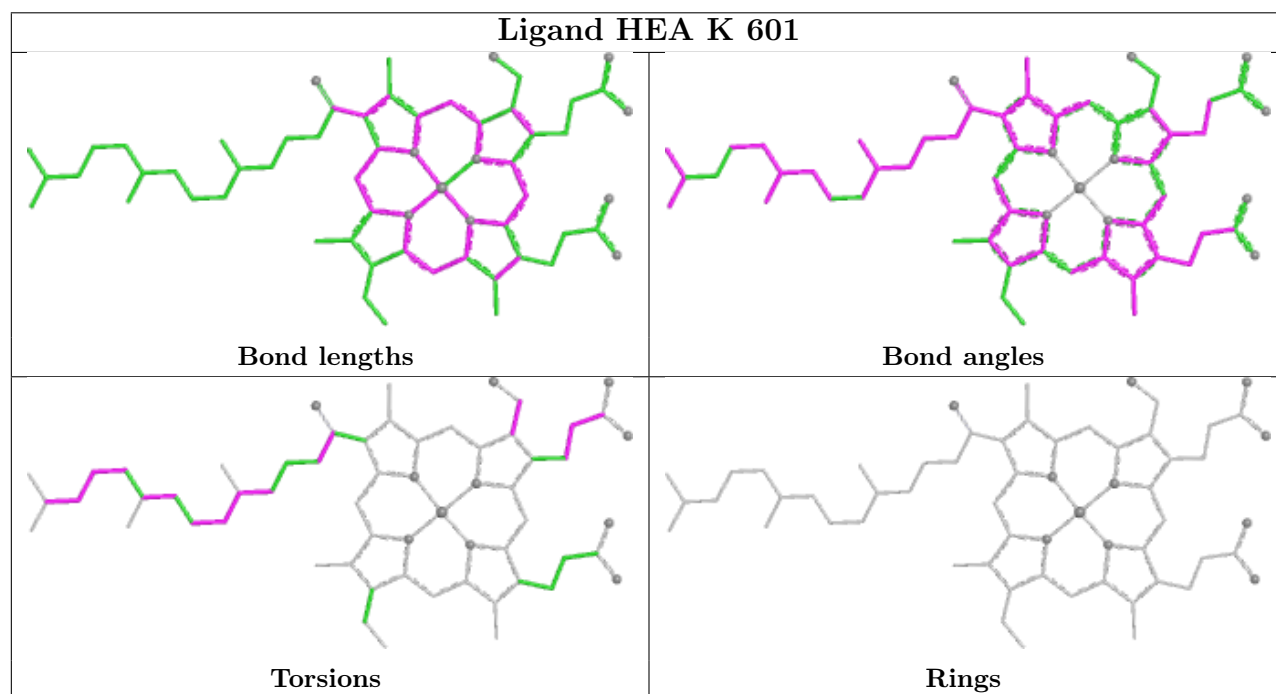
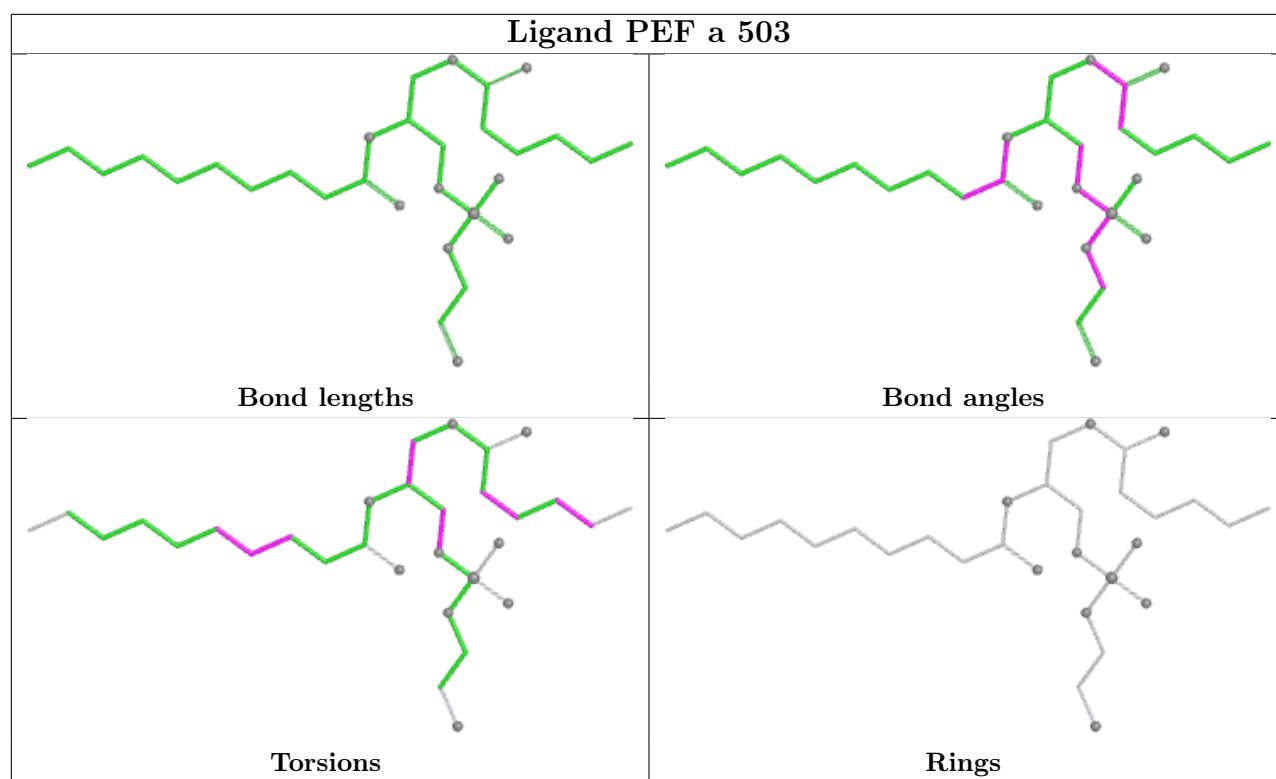
Bond angles

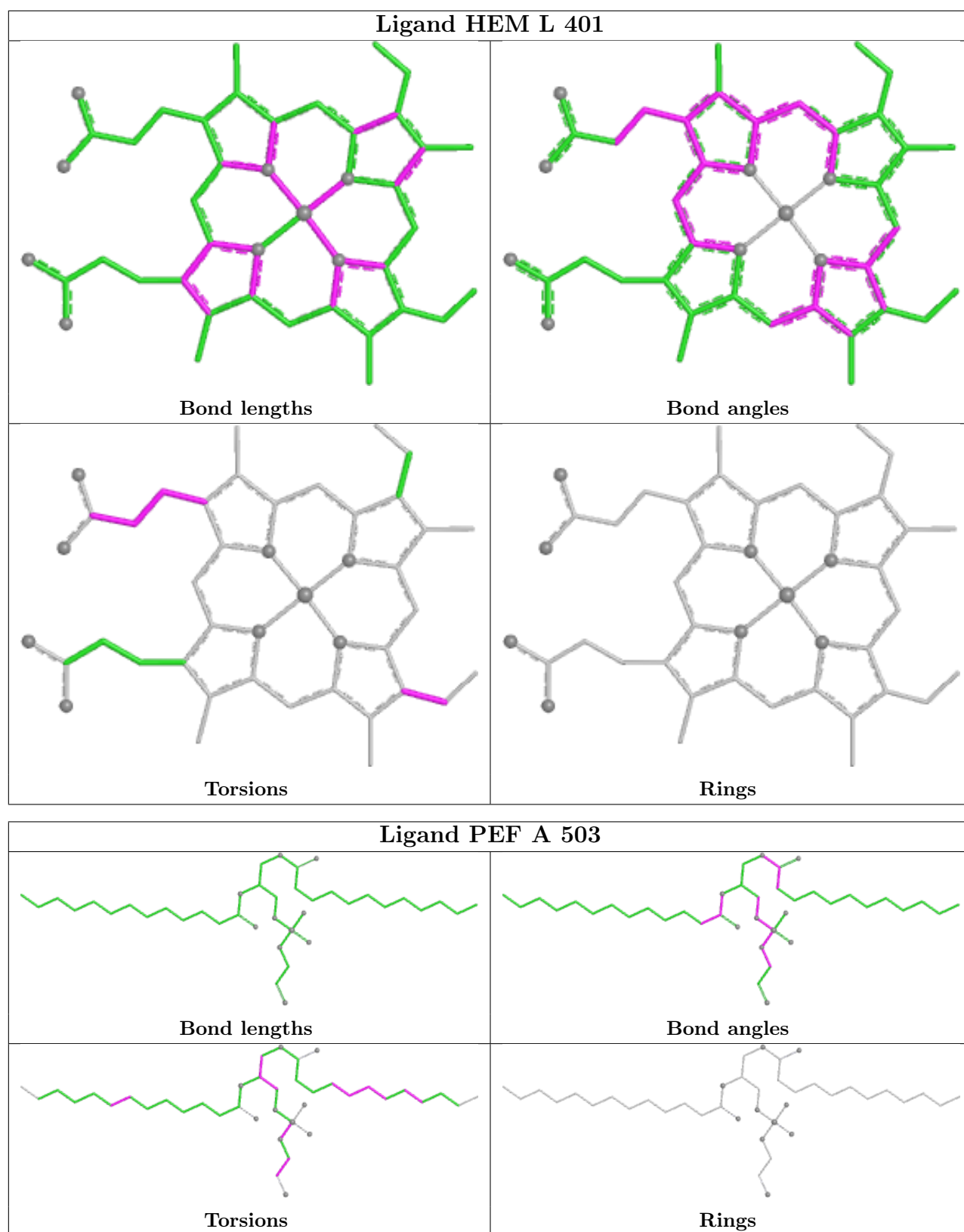


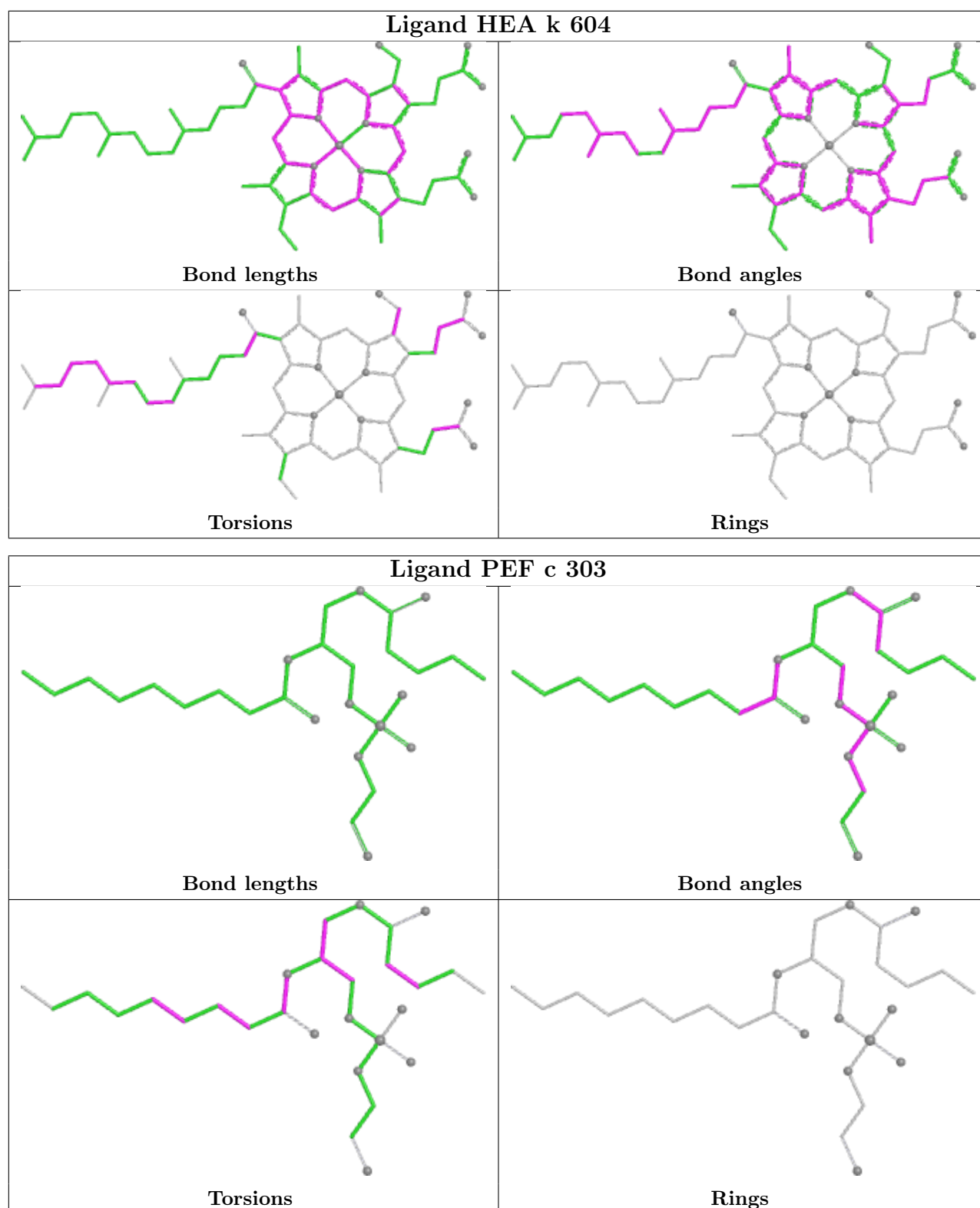
Torsions

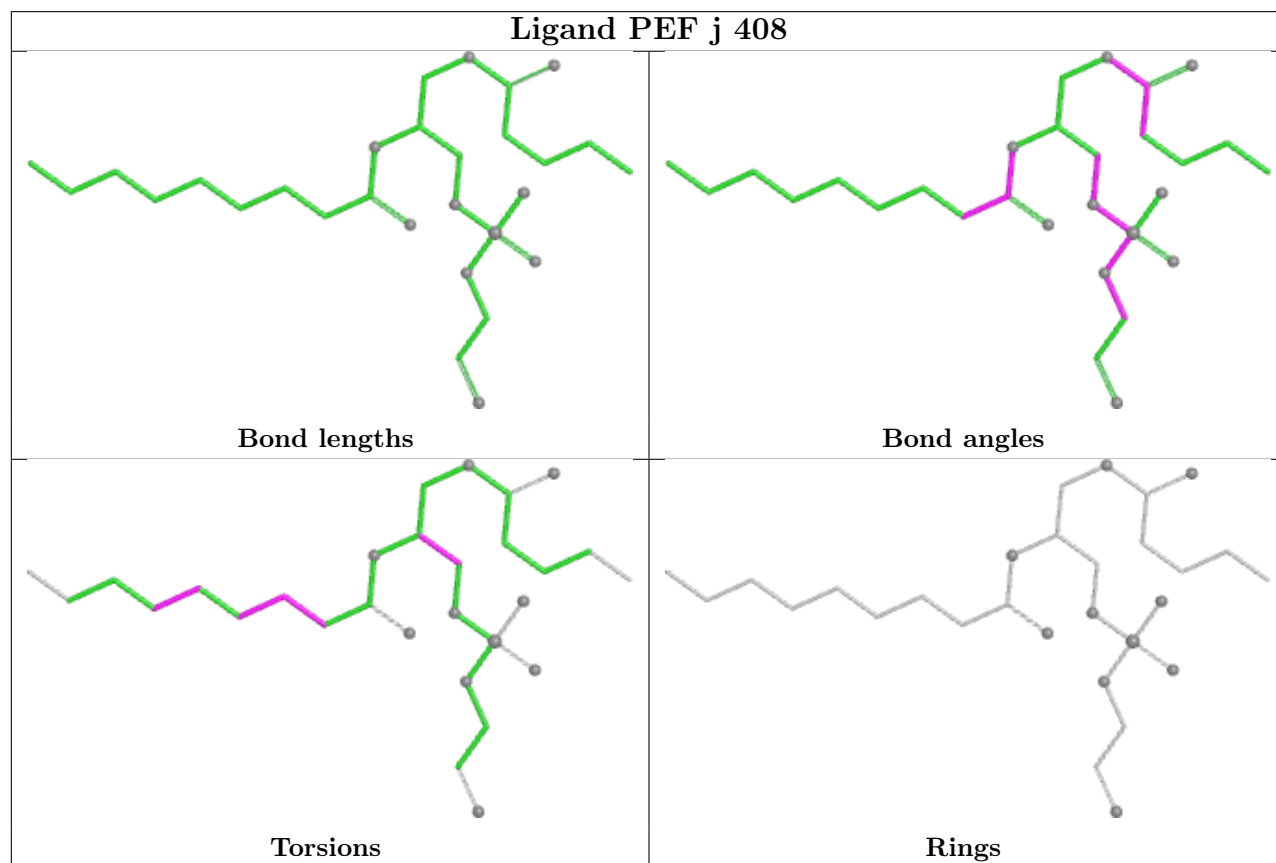
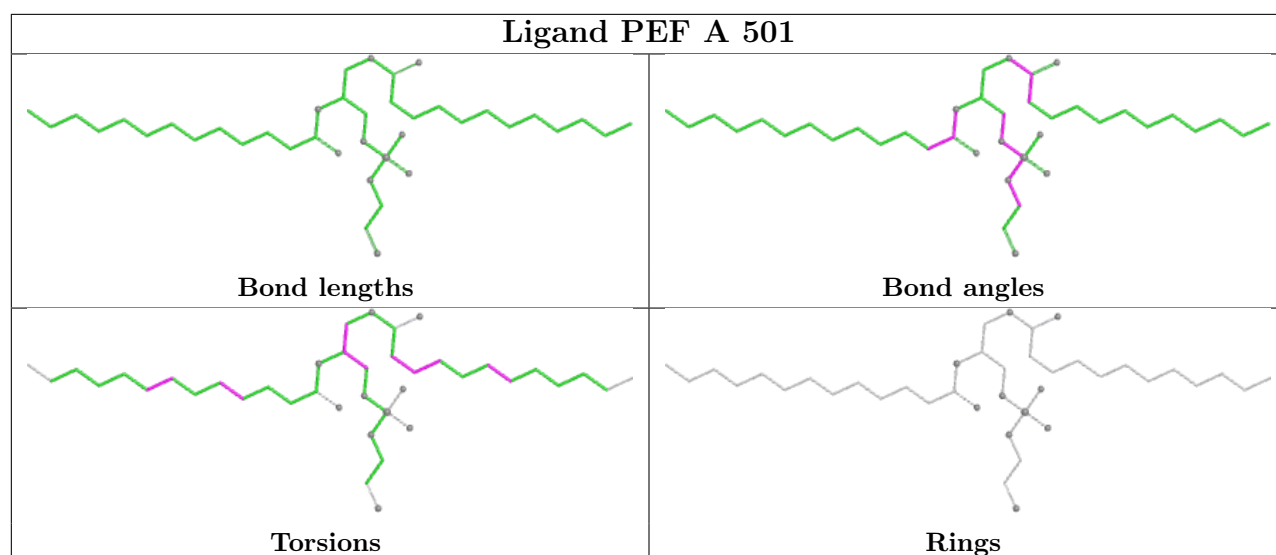


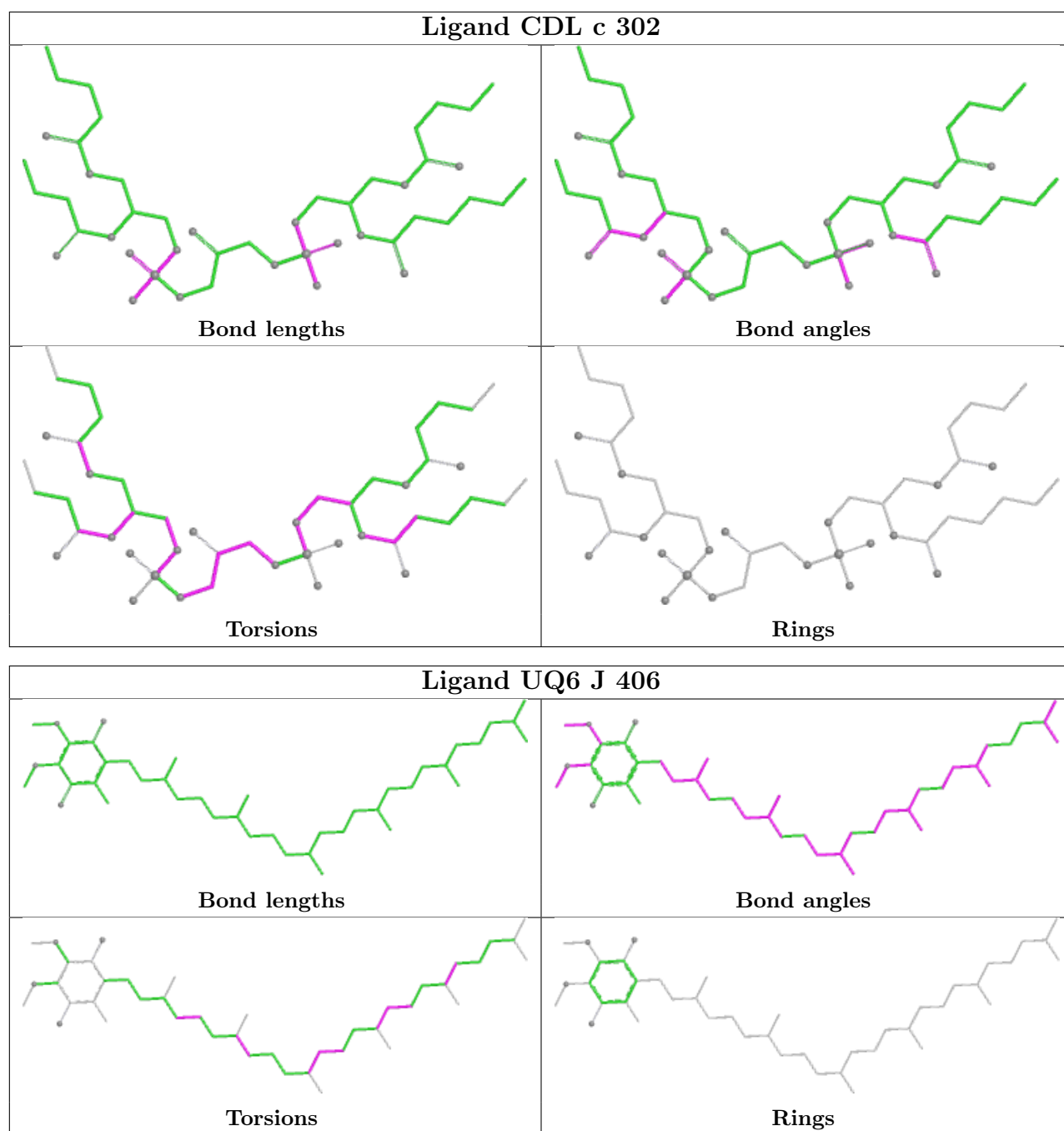
Rings

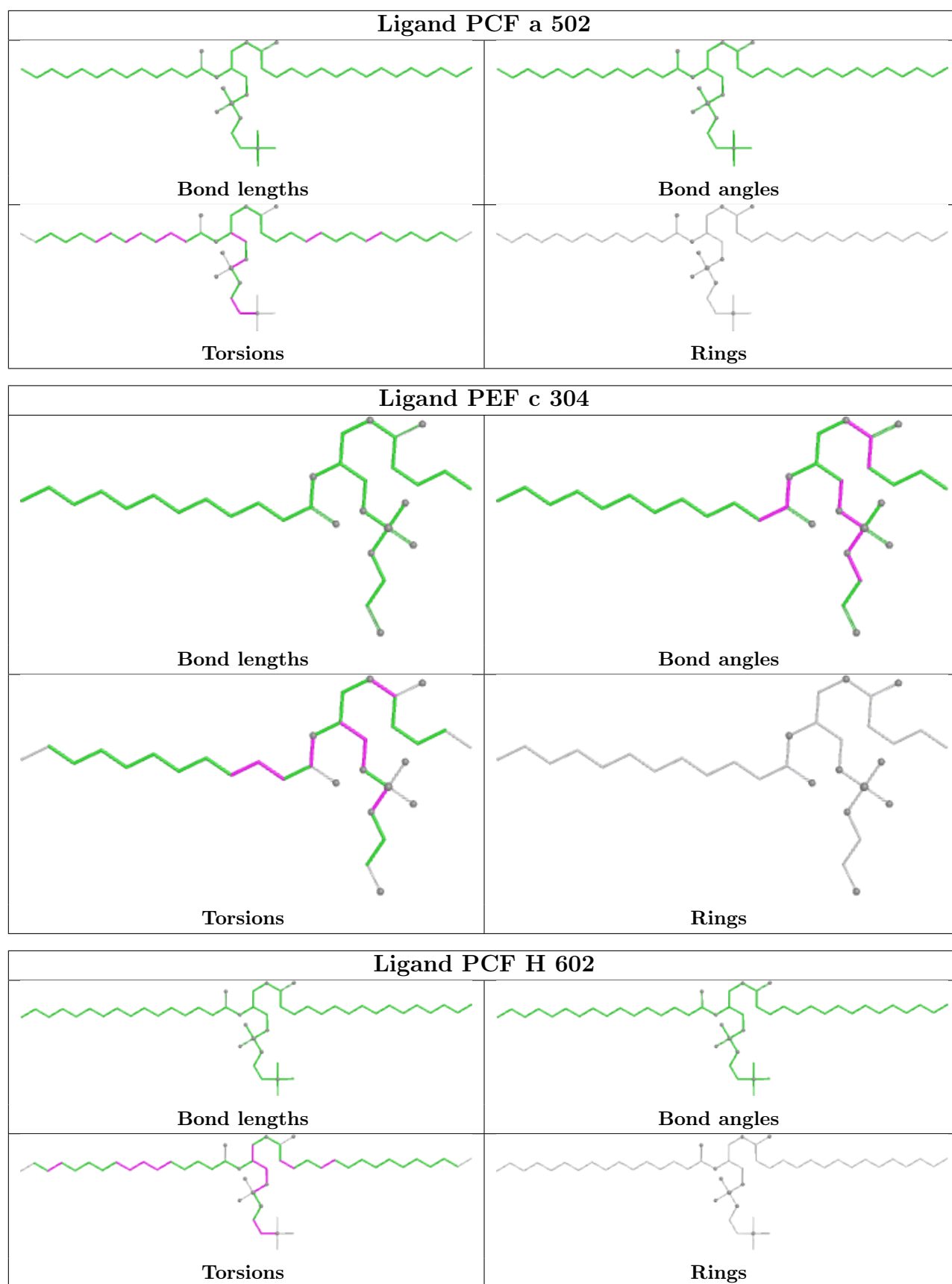


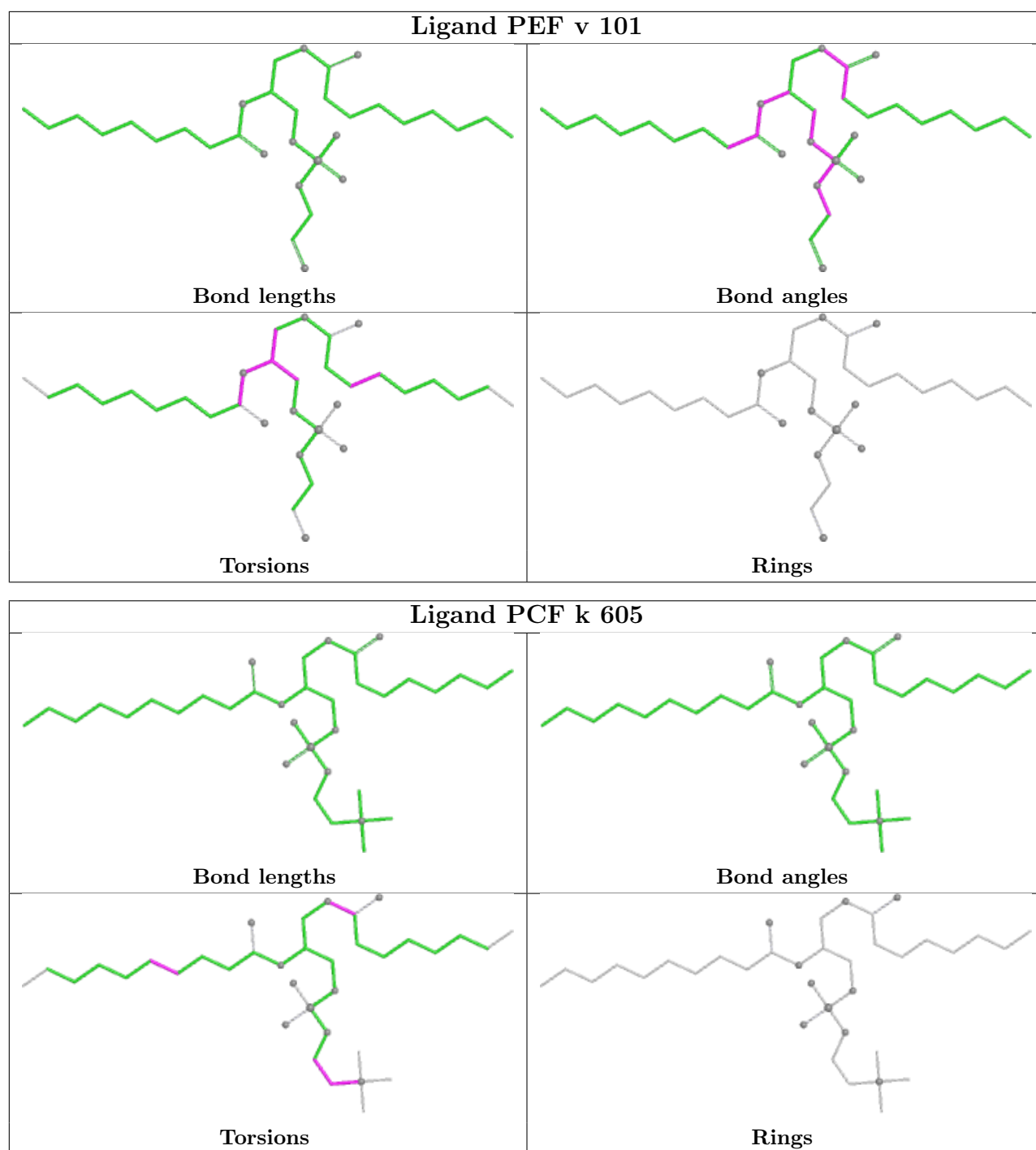


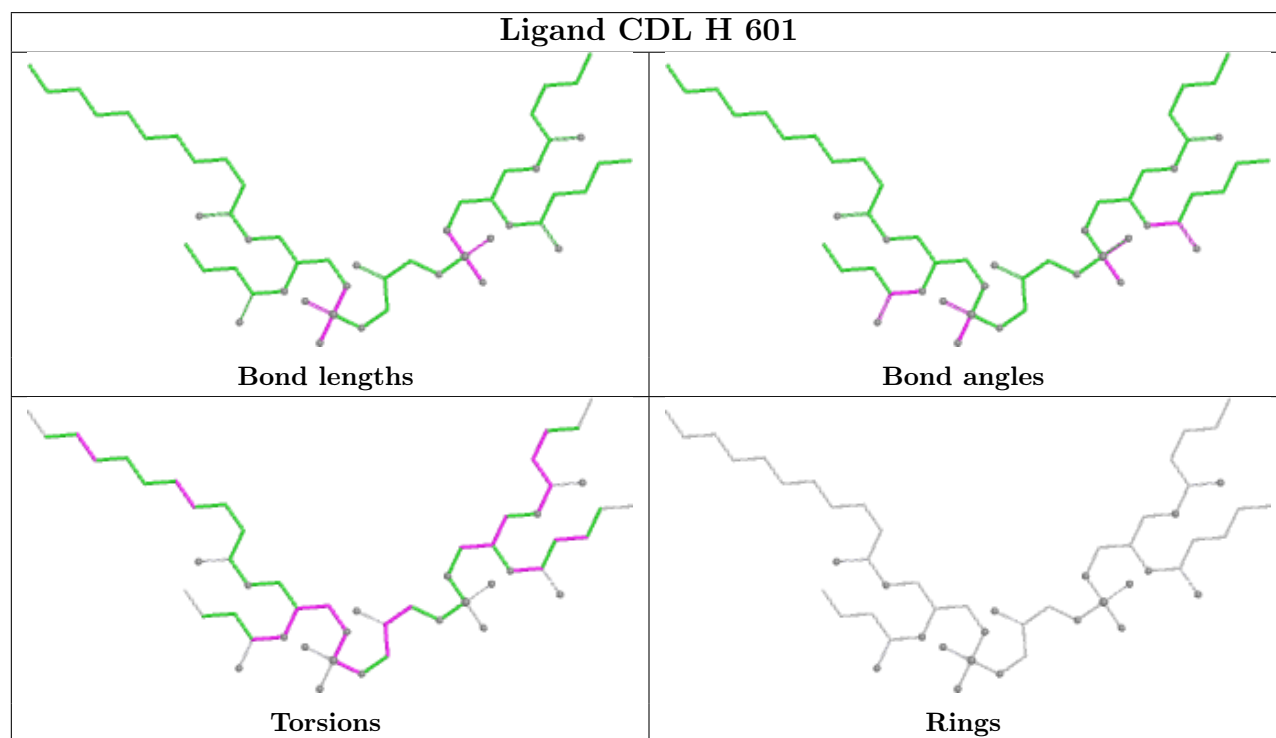
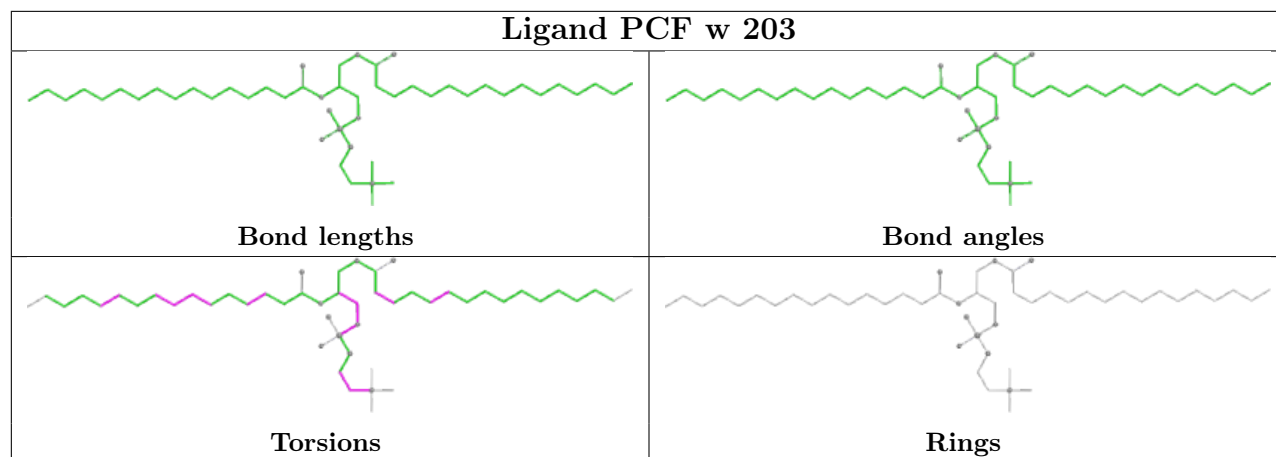


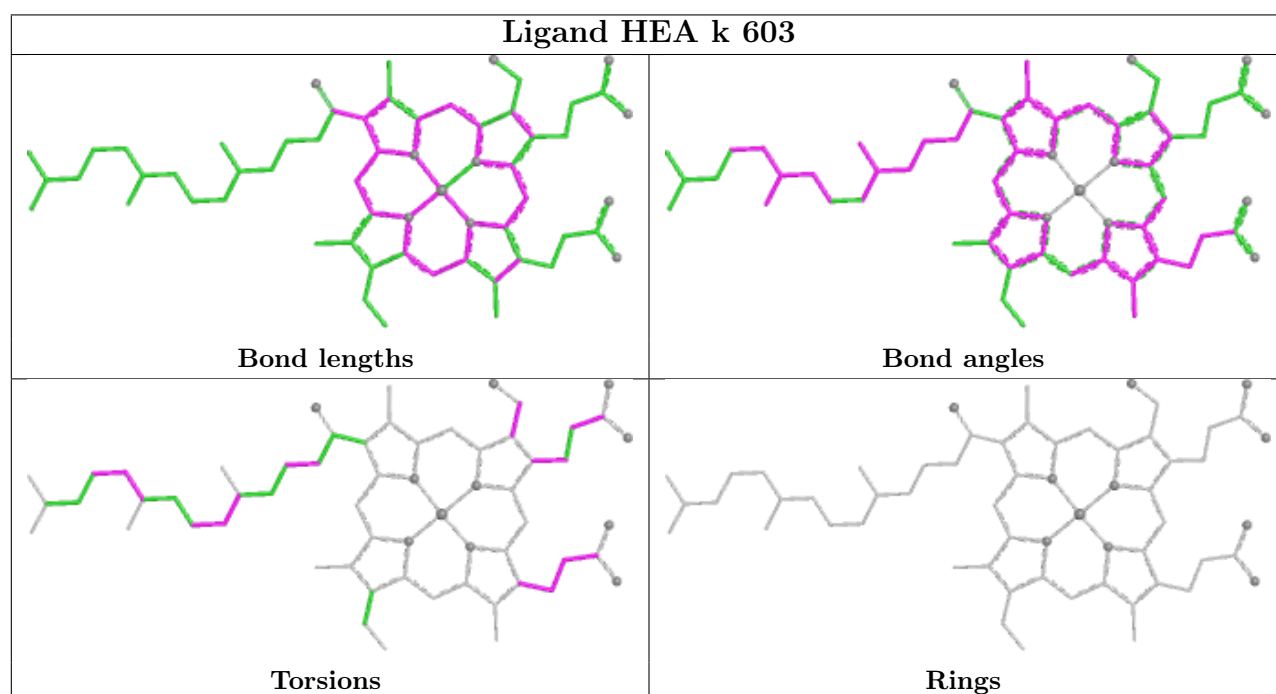
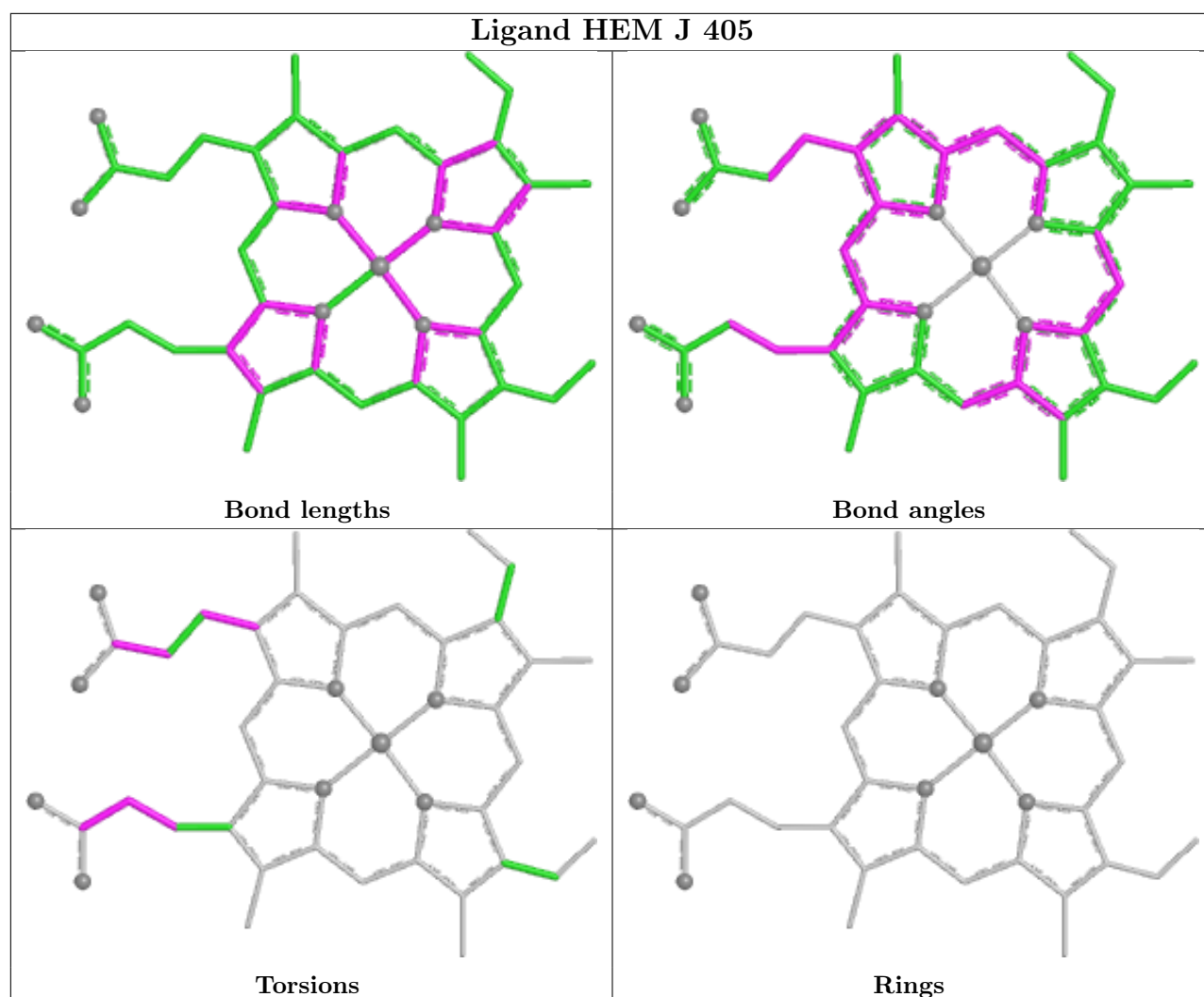




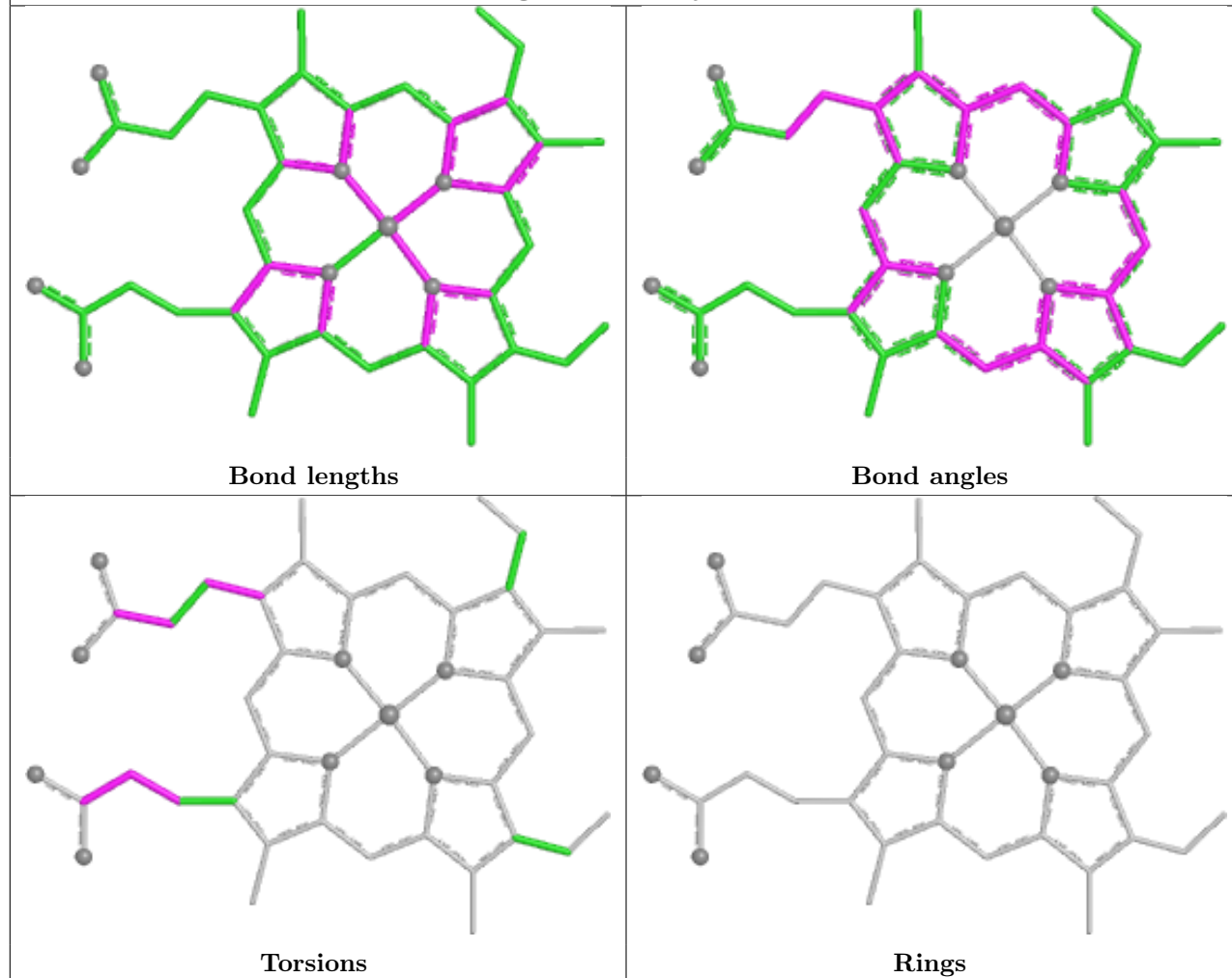




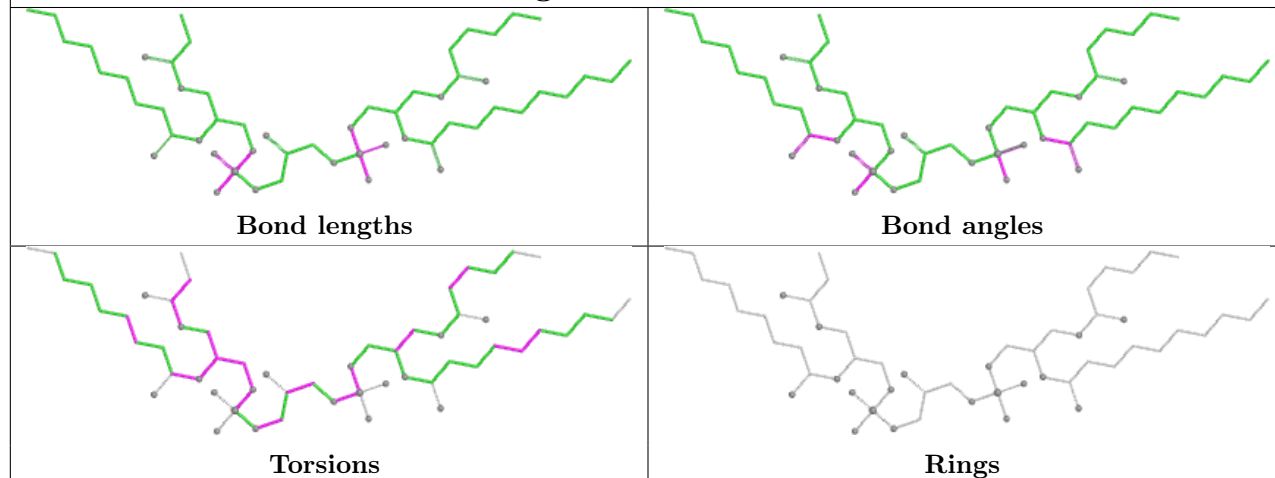




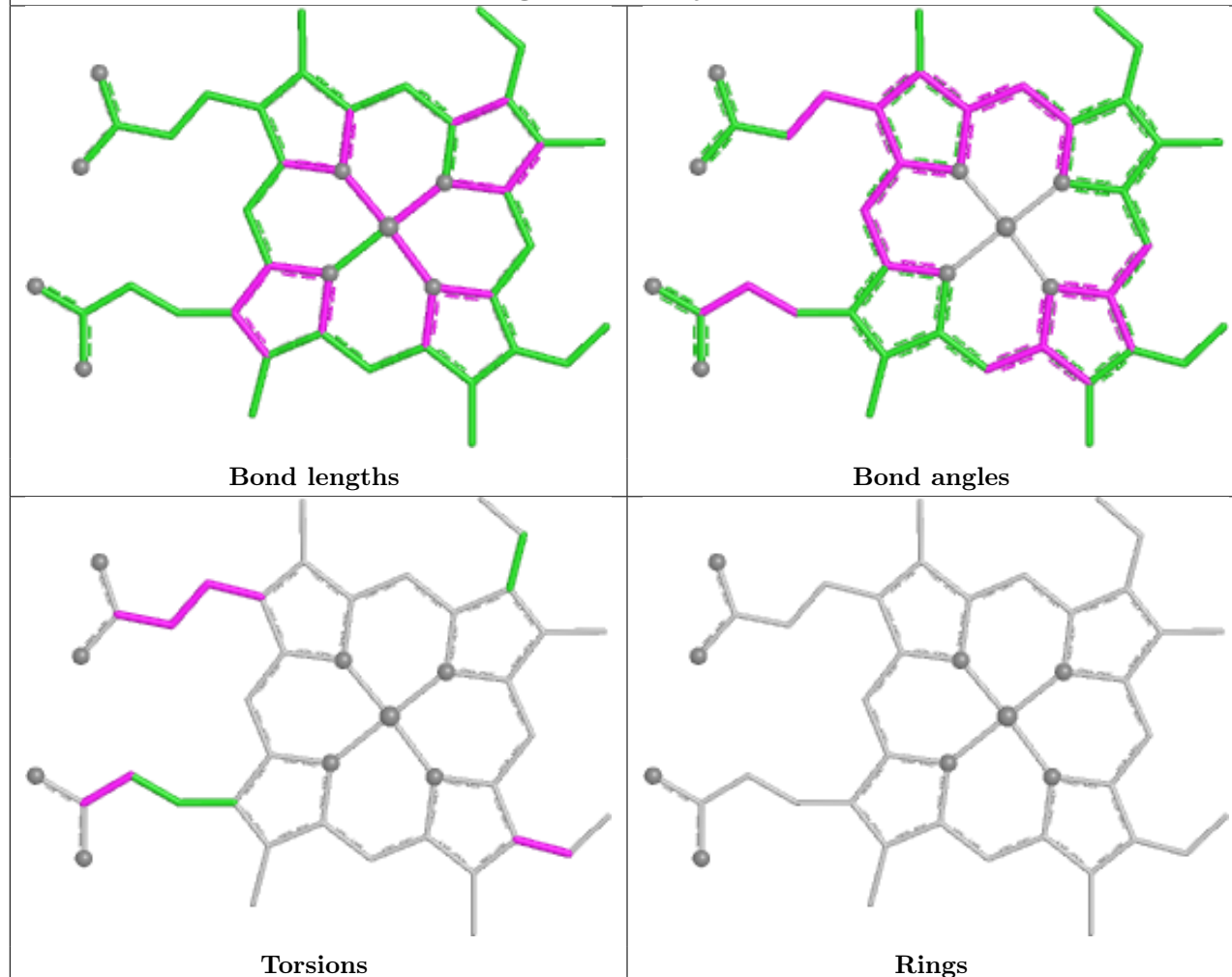
Ligand HEM j 404



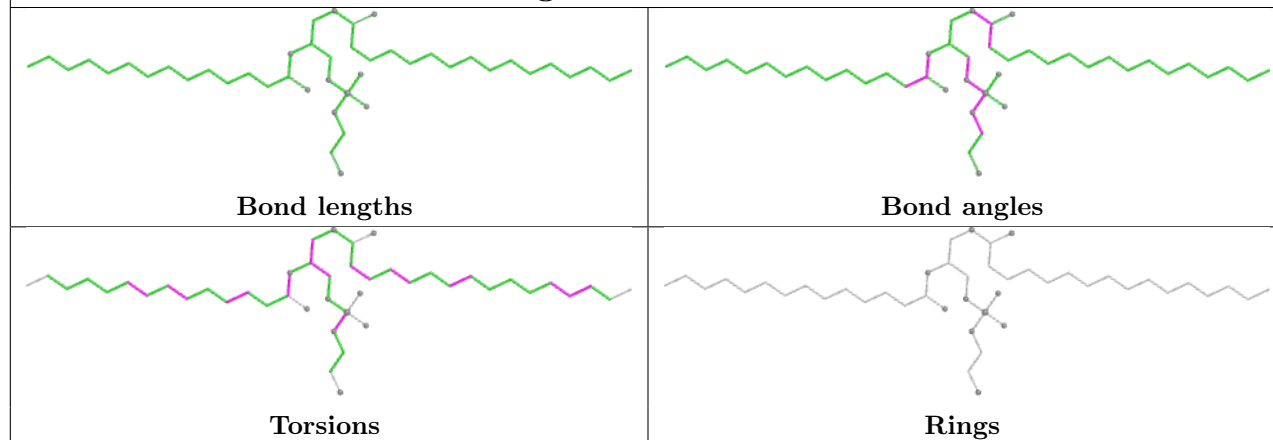
Ligand CDL J 403

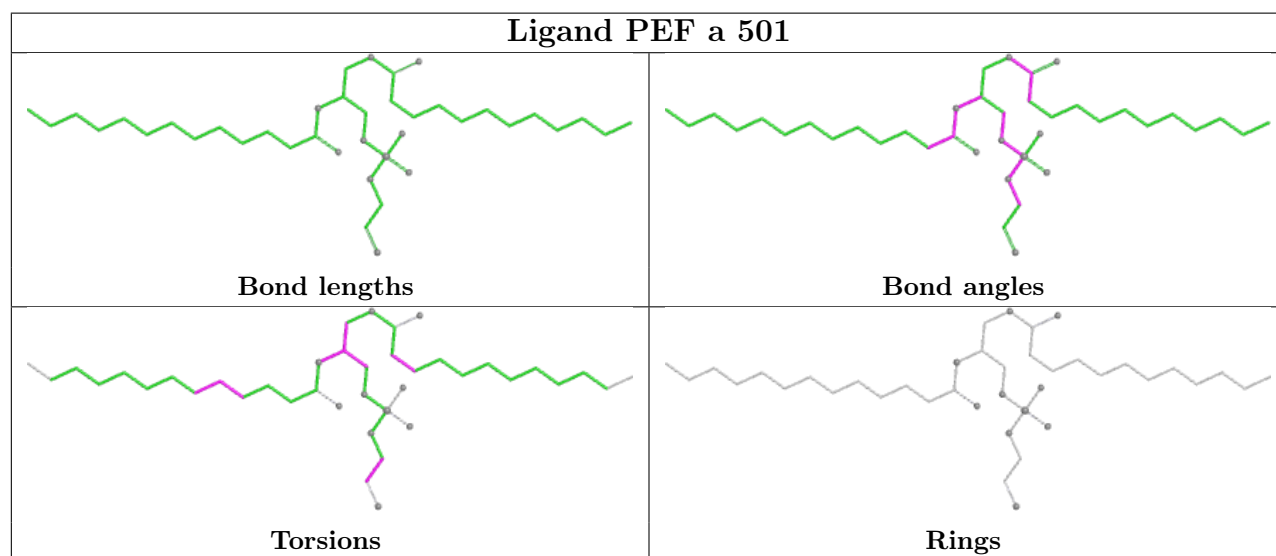
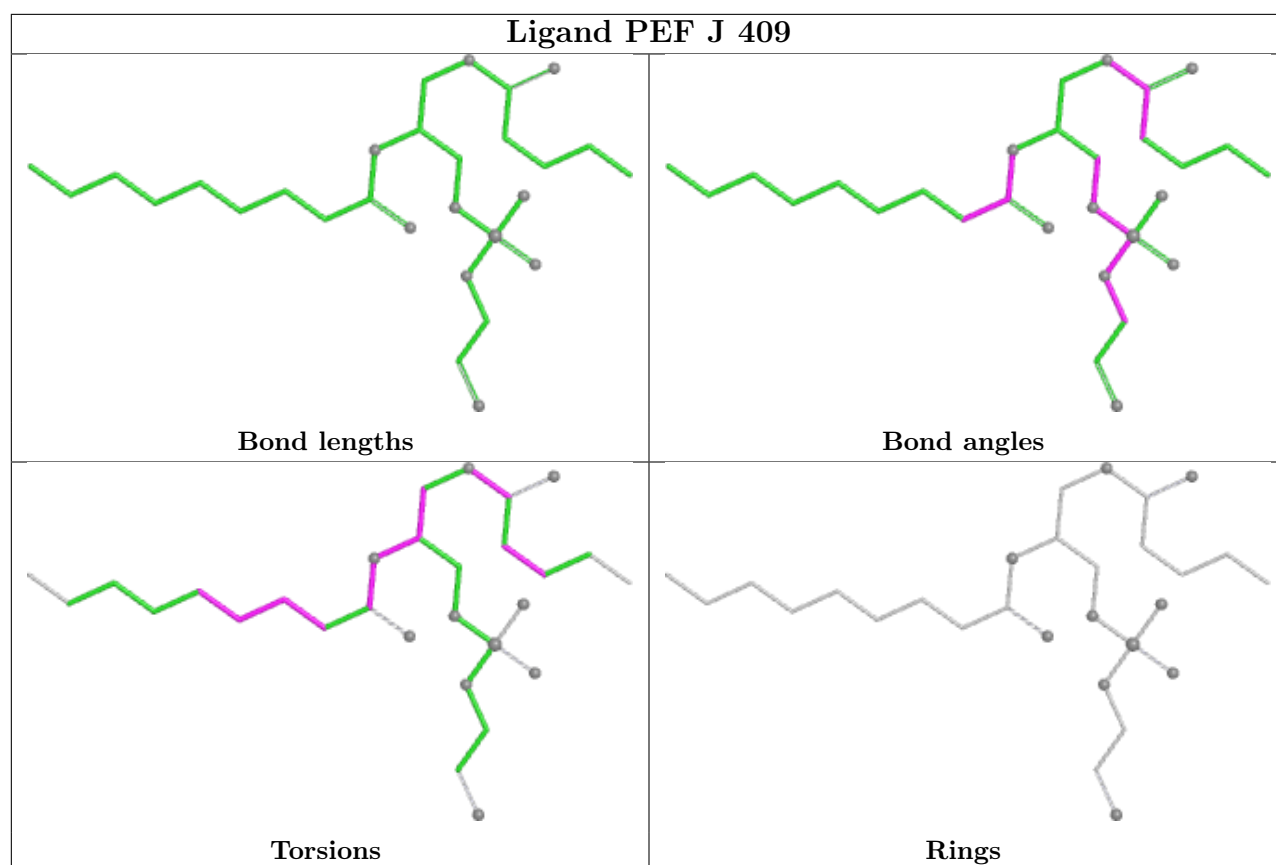


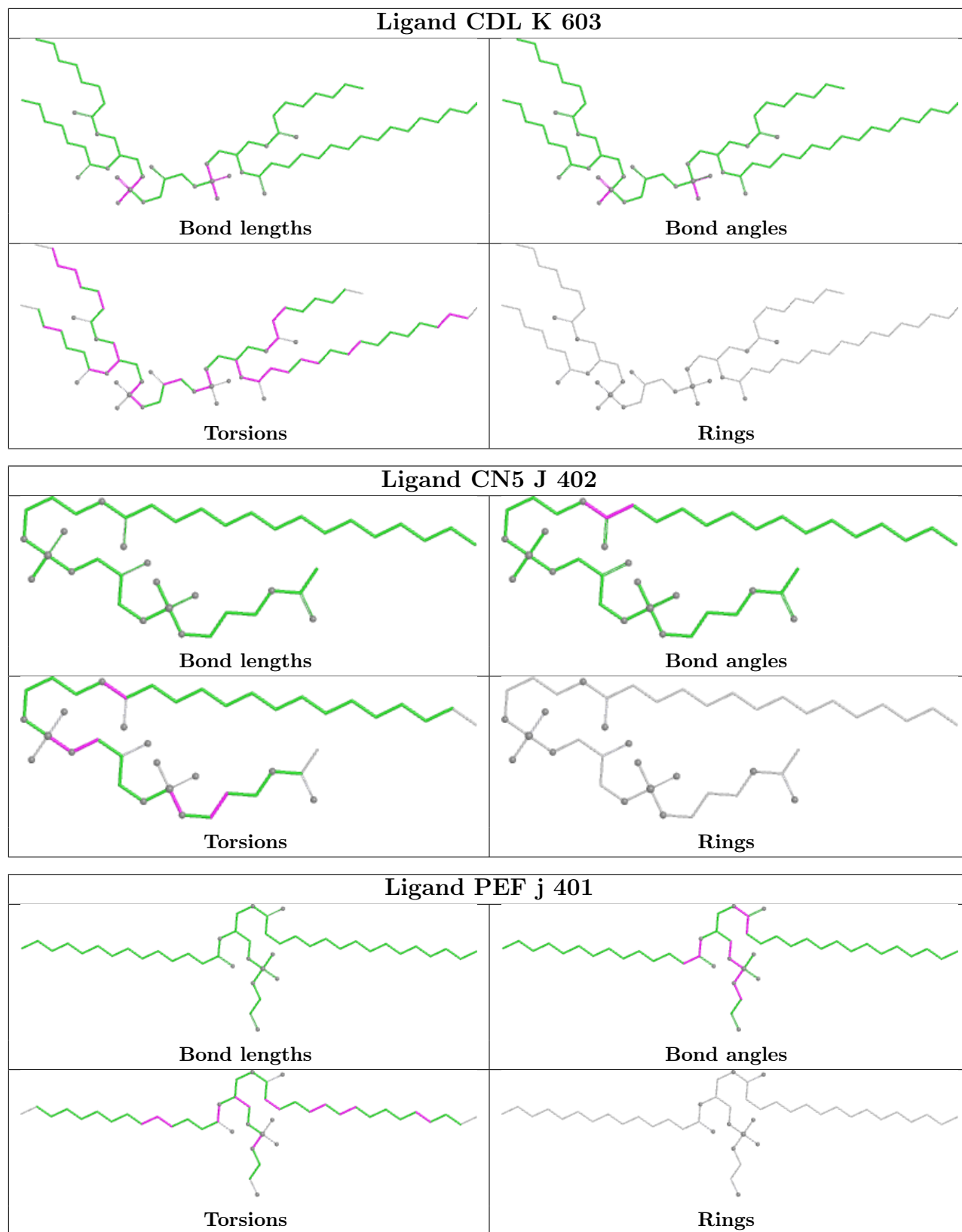
Ligand HEM j 403

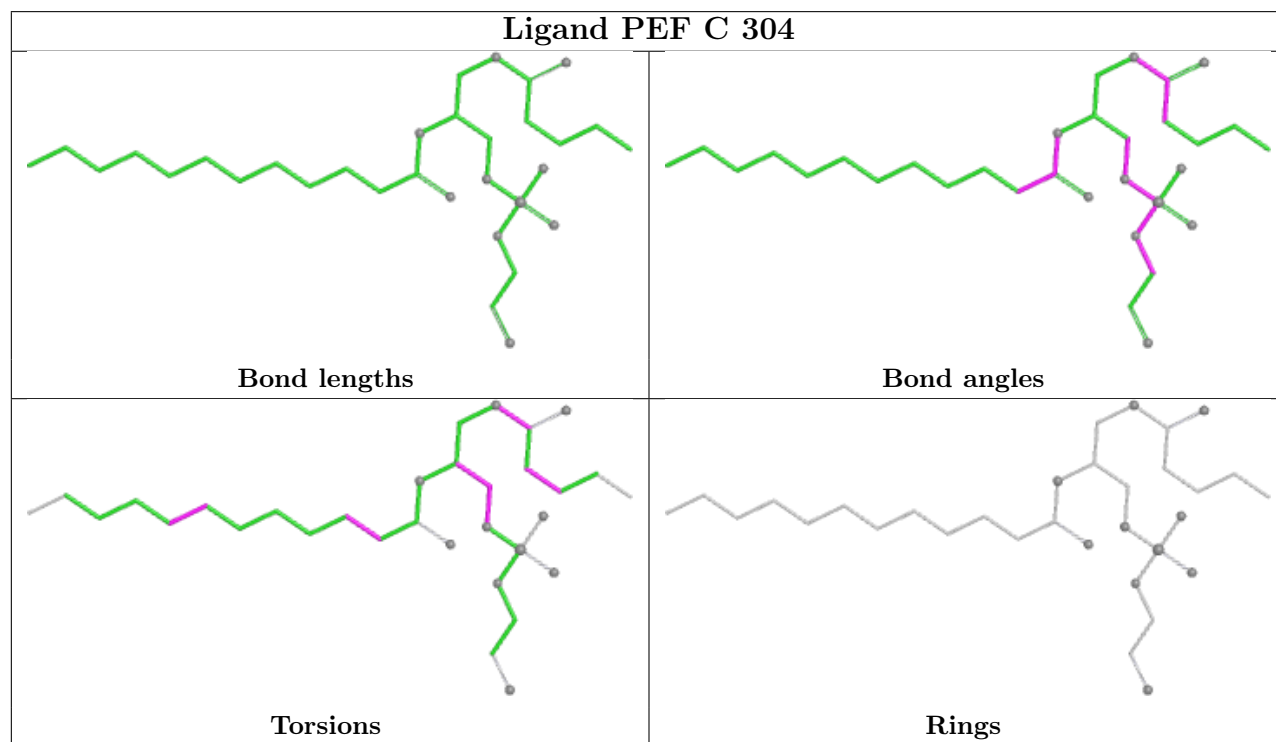
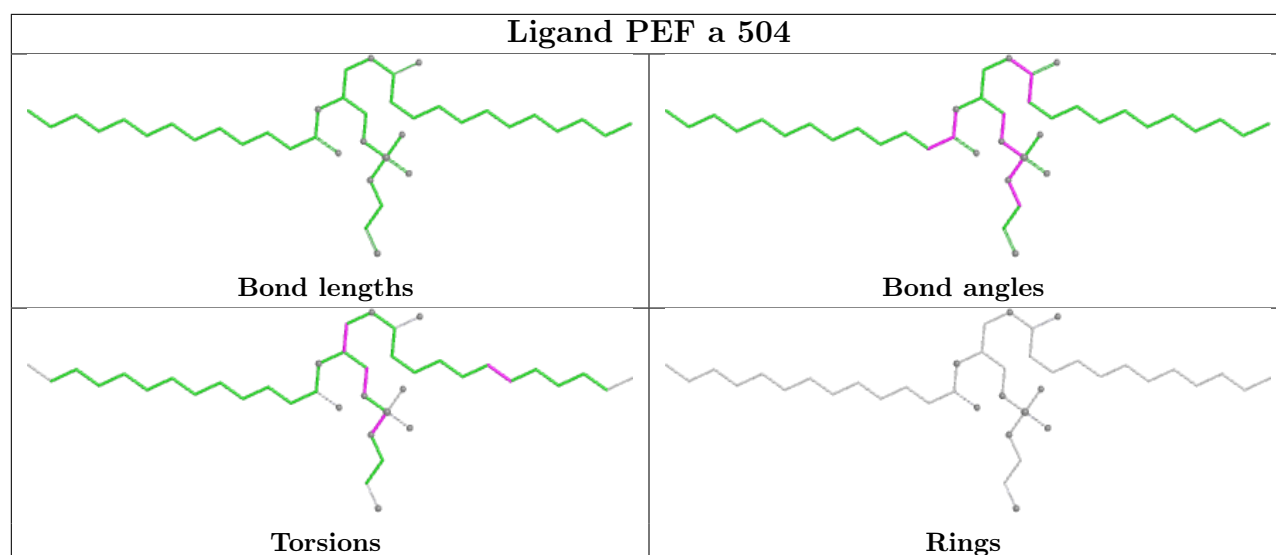


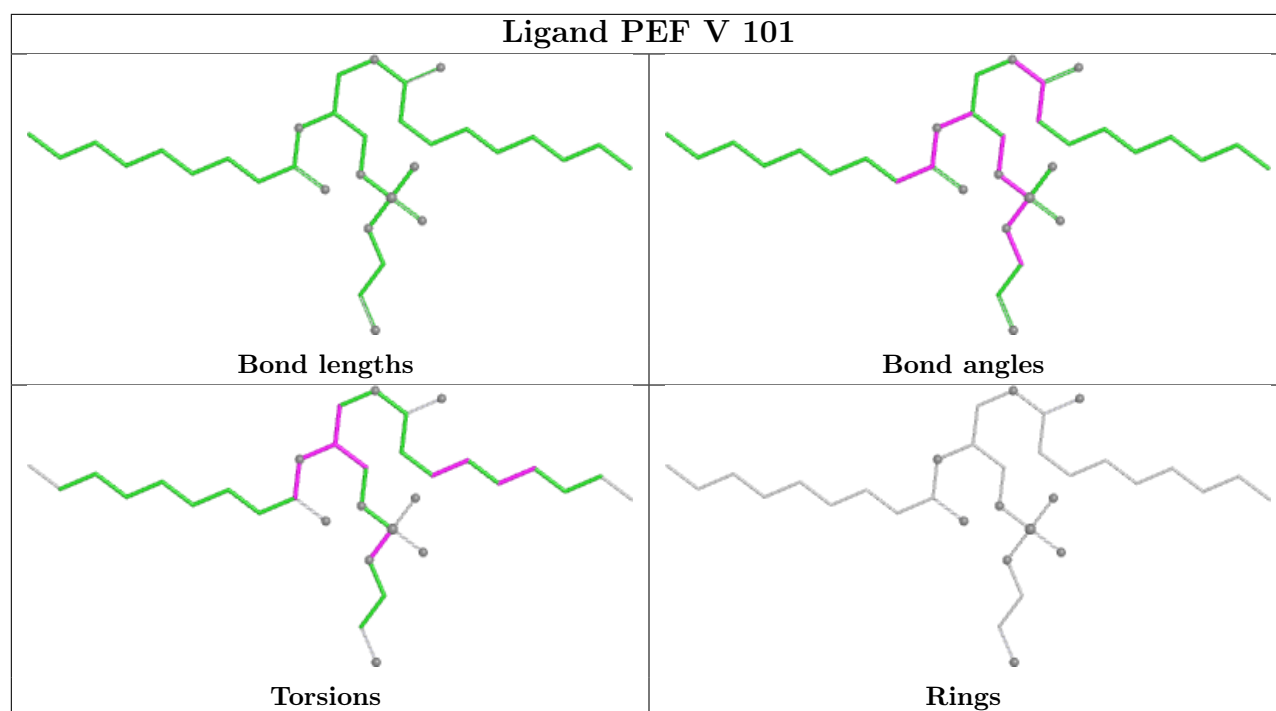
Ligand PEF J 401











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

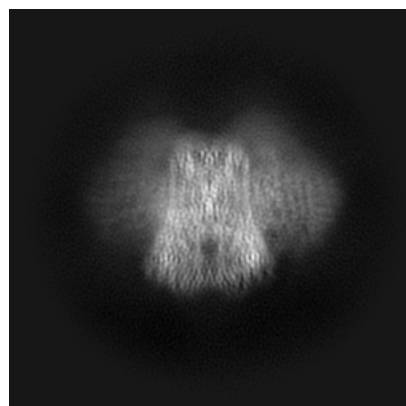
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27940. These allow visual inspection of the internal detail of the map and identification of artifacts.

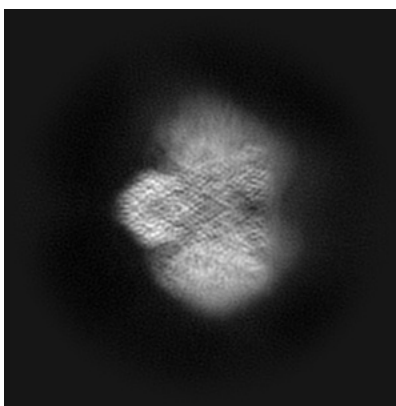
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

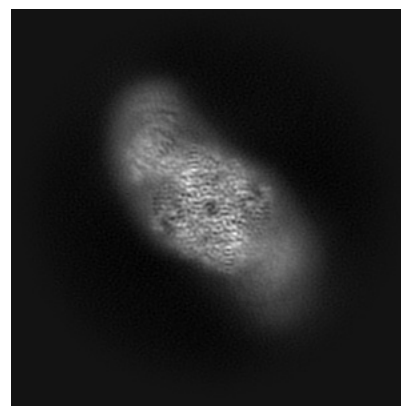
6.1.1 Primary map



X

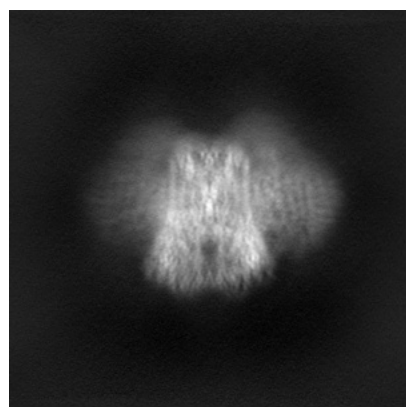


Y

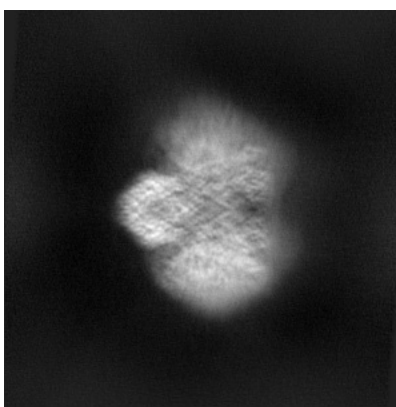


Z

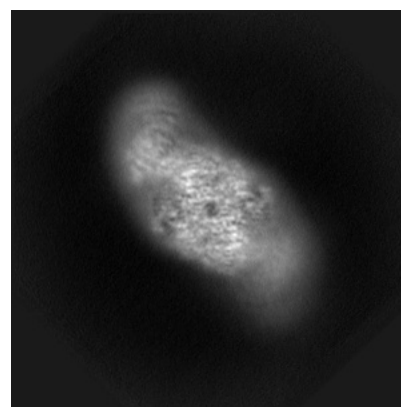
6.1.2 Raw map



X



Y

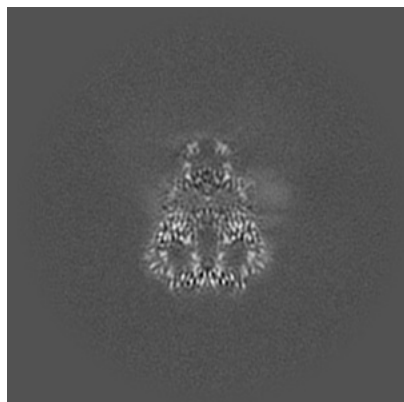


Z

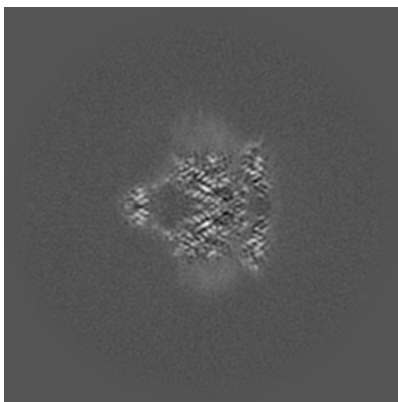
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

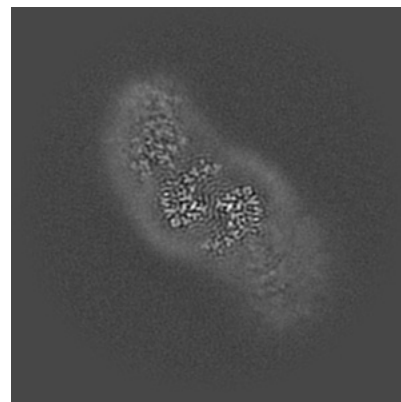
6.2.1 Primary map



X Index: 180

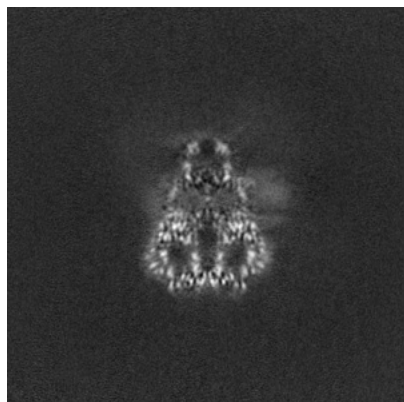


Y Index: 180

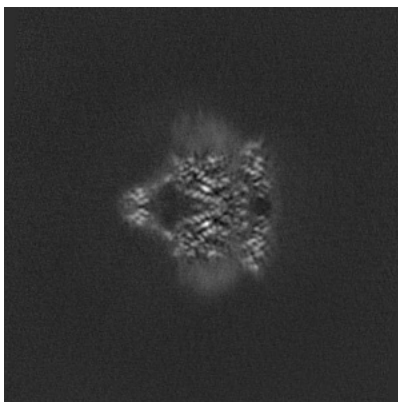


Z Index: 180

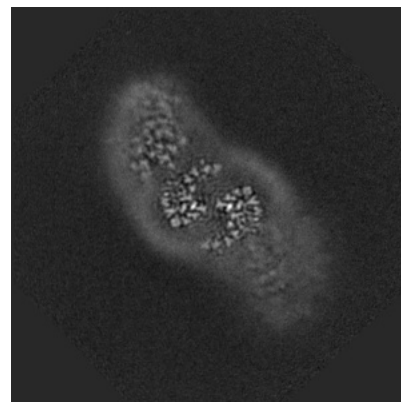
6.2.2 Raw map



X Index: 180



Y Index: 180

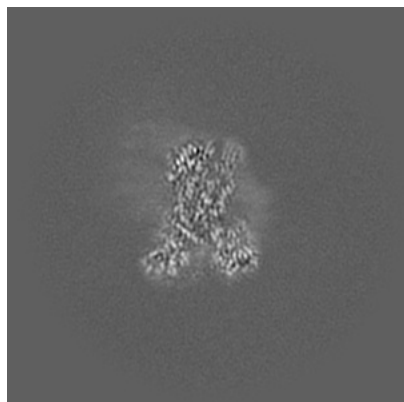


Z Index: 180

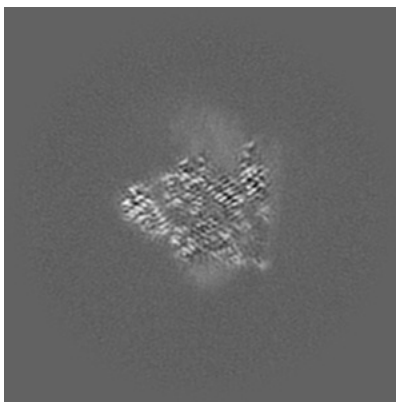
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

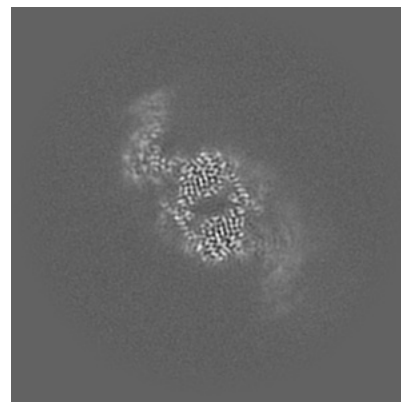
6.3.1 Primary map



X Index: 202

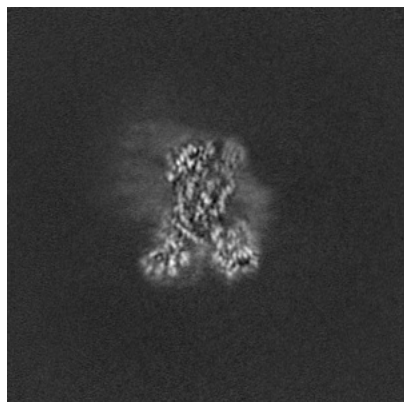


Y Index: 170

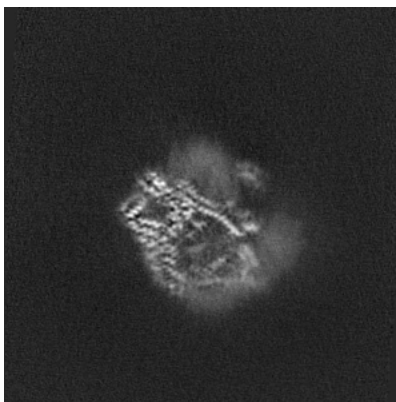


Z Index: 153

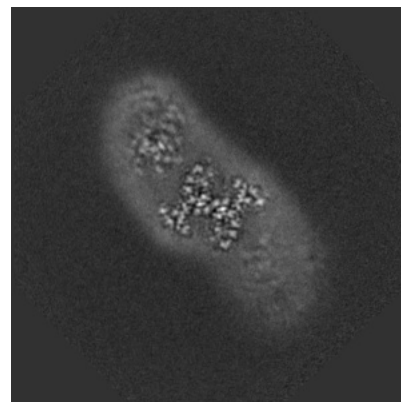
6.3.2 Raw map



X Index: 202



Y Index: 214

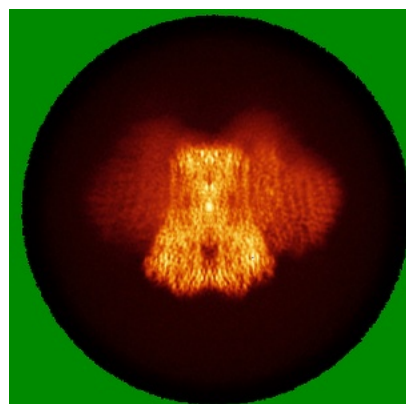


Z Index: 197

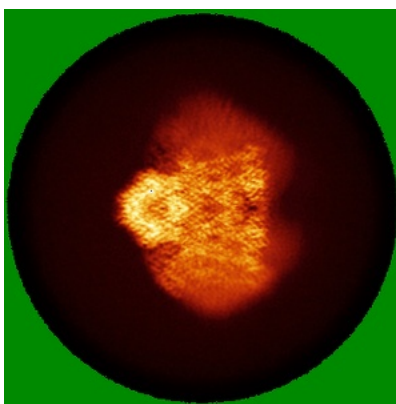
The images above show the largest variance slices of the map in three orthogonal directions.

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

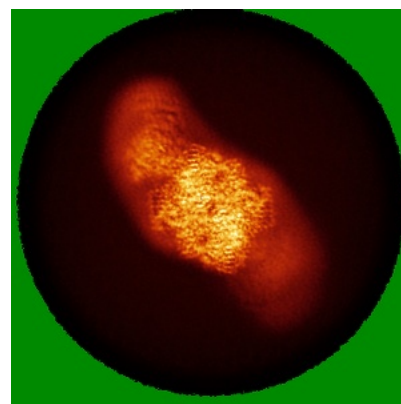
6.4.1 Primary map



X

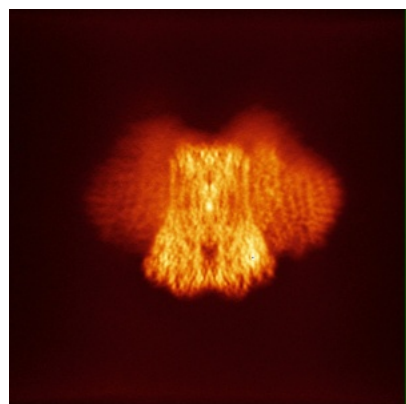


Y

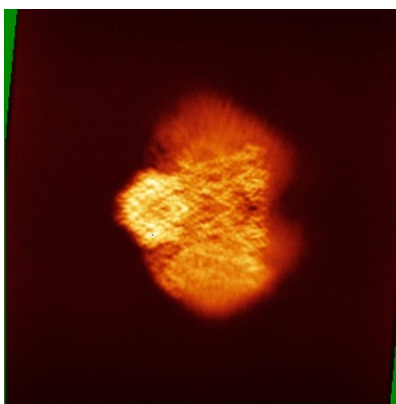


Z

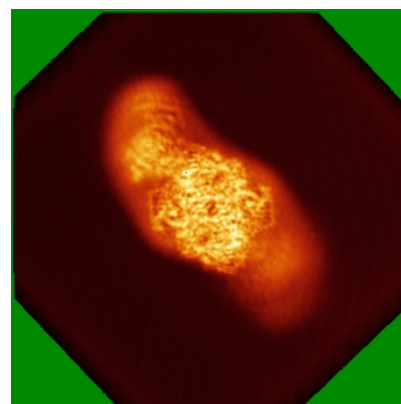
6.4.2 Raw map



X



Y

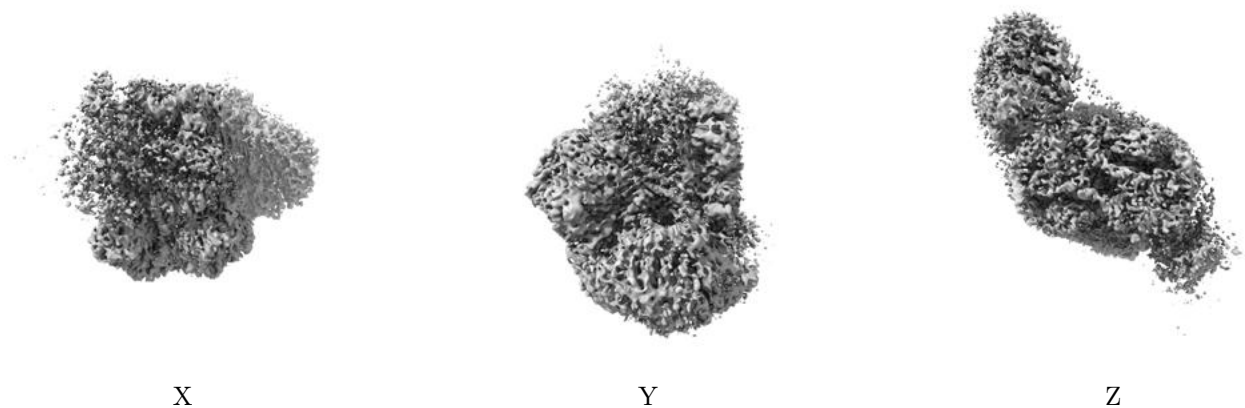


Z

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.

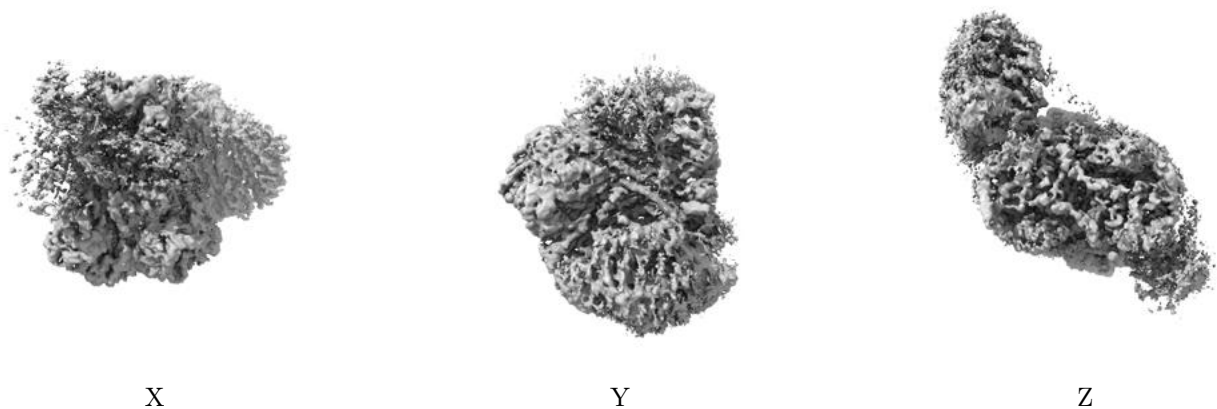
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.245. 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.

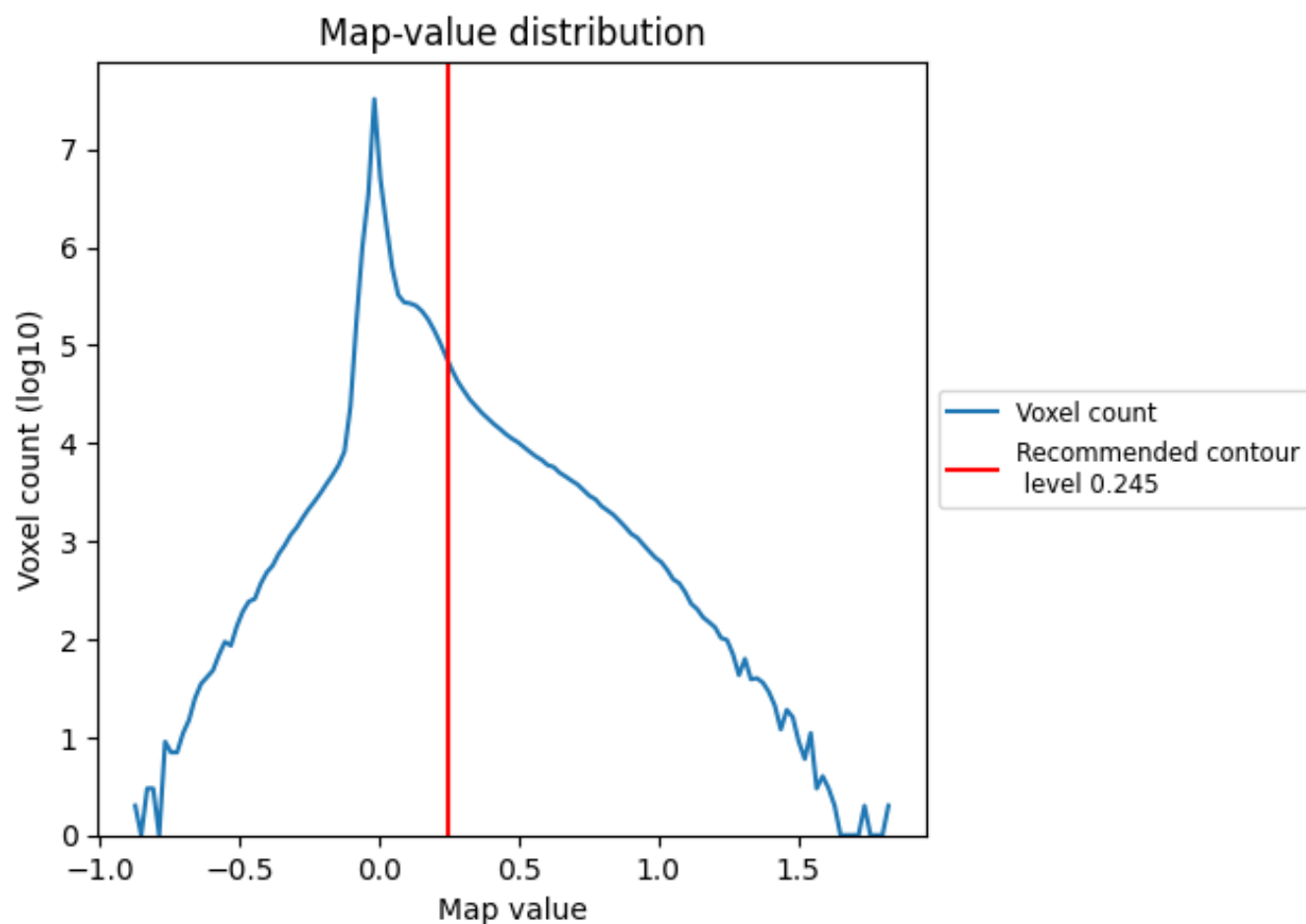
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

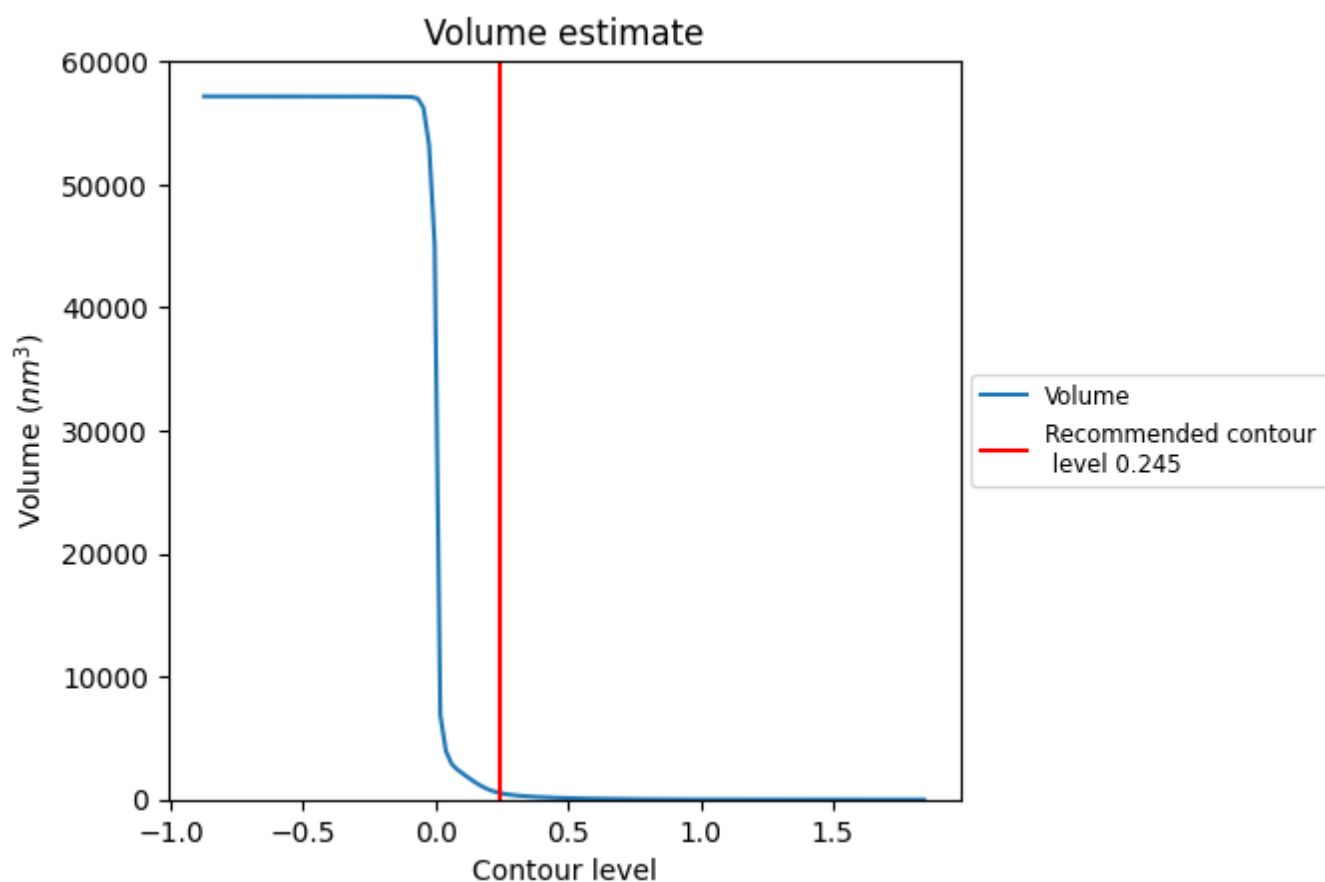
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

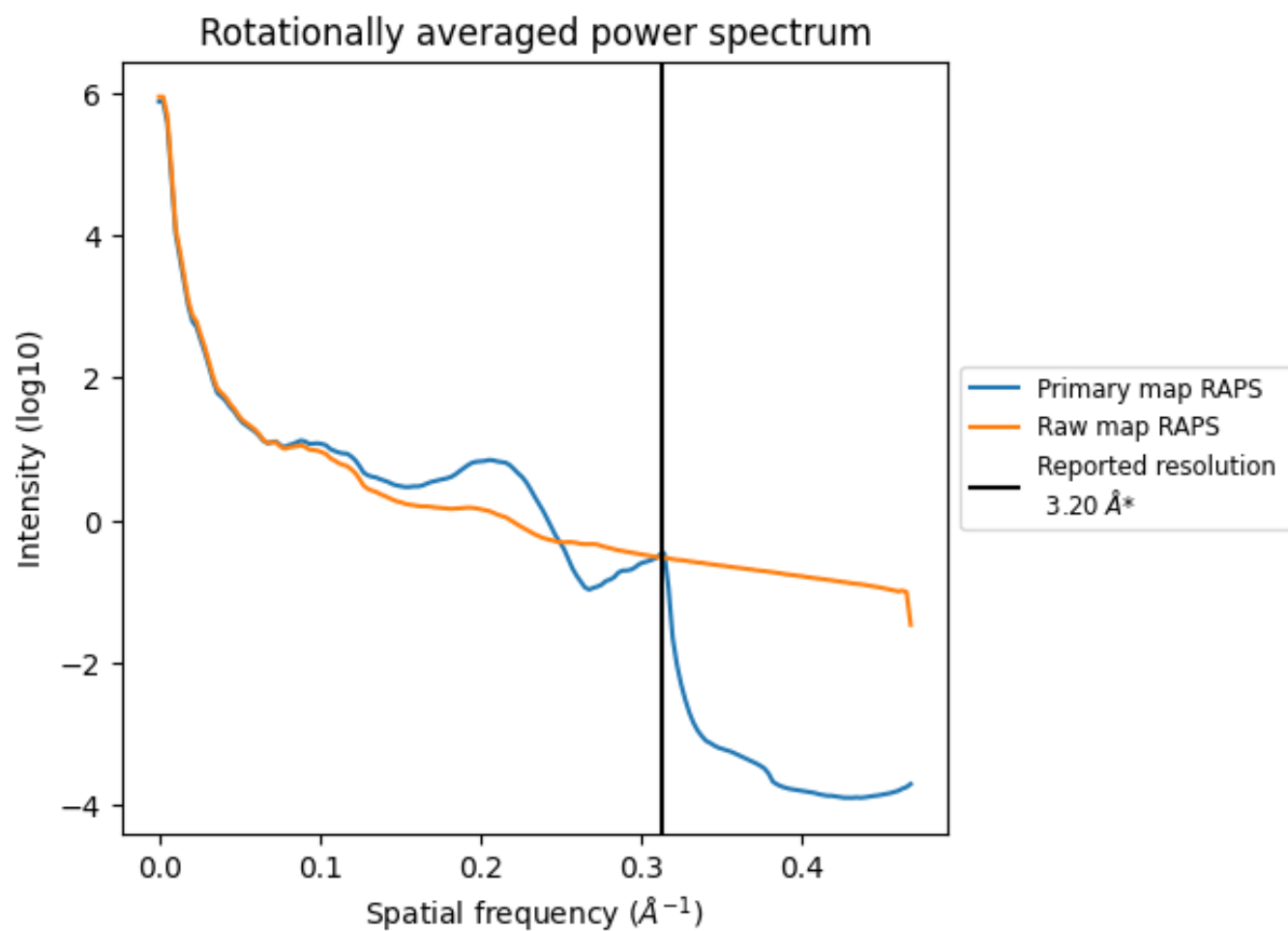
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 525 nm³; this corresponds to an approximate mass of 474 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 ⓘ

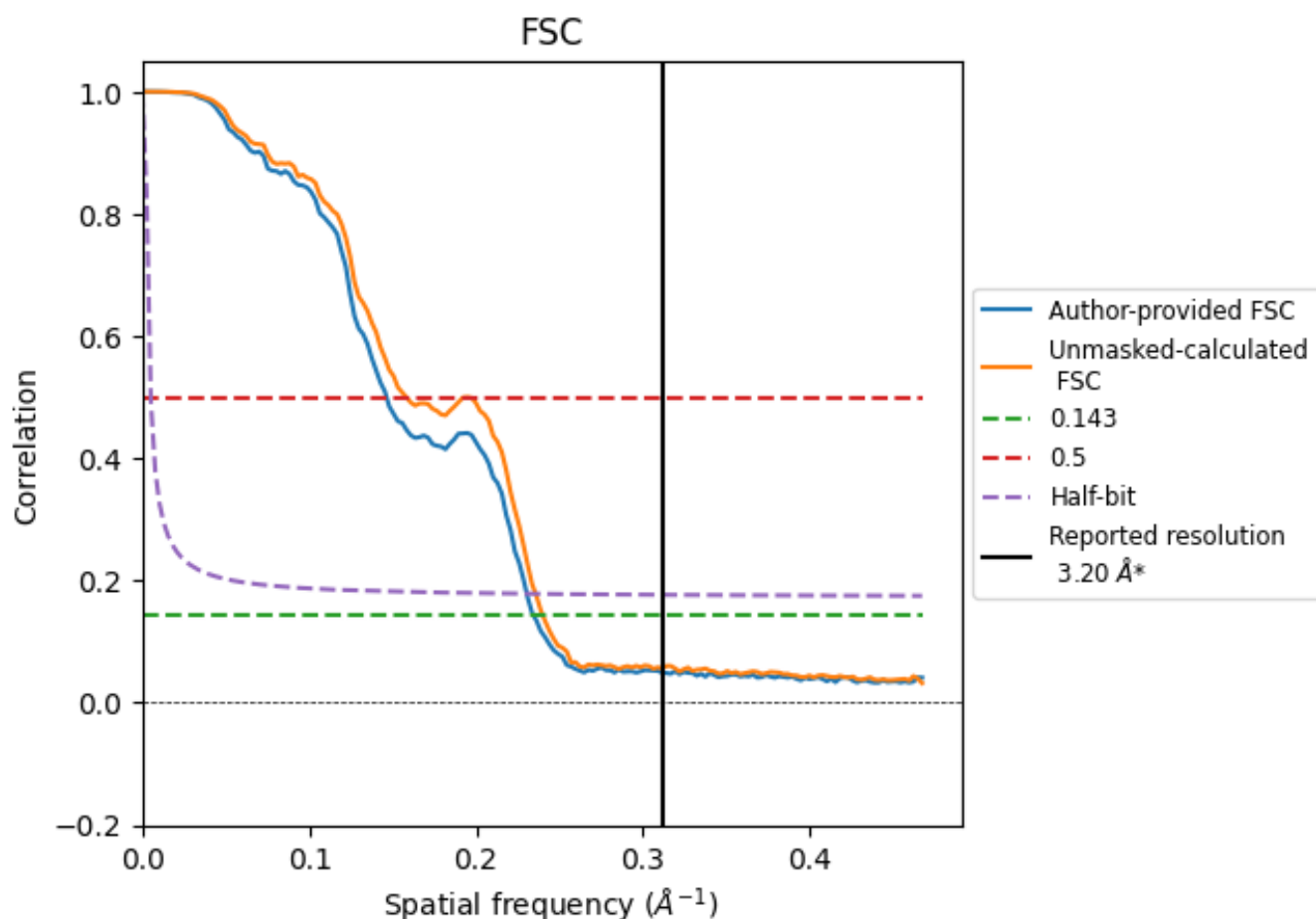


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	4.27	6.84	4.34
Unmasked-calculated*	4.17	6.32	4.24

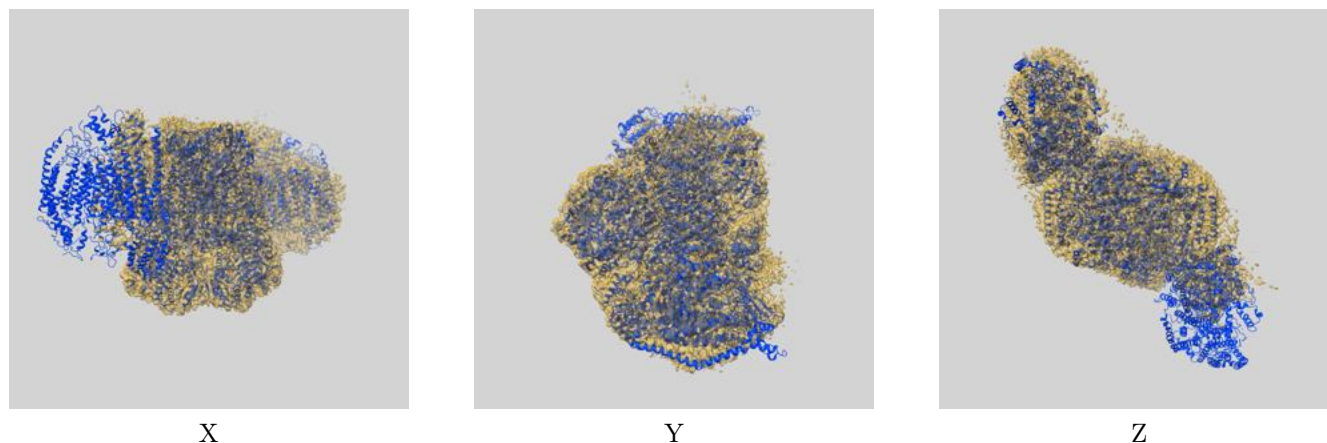
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.27 differs from the reported value 3.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.17 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

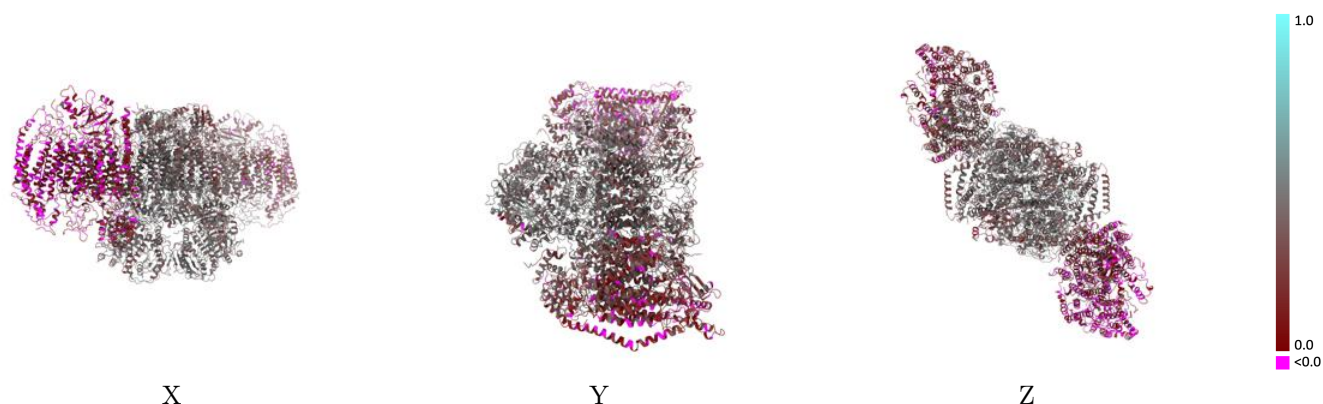
This section contains information regarding the fit between EMDB map EMD-27940 and PDB model 8E7S. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

9.1 Map-model overlay [i](#)



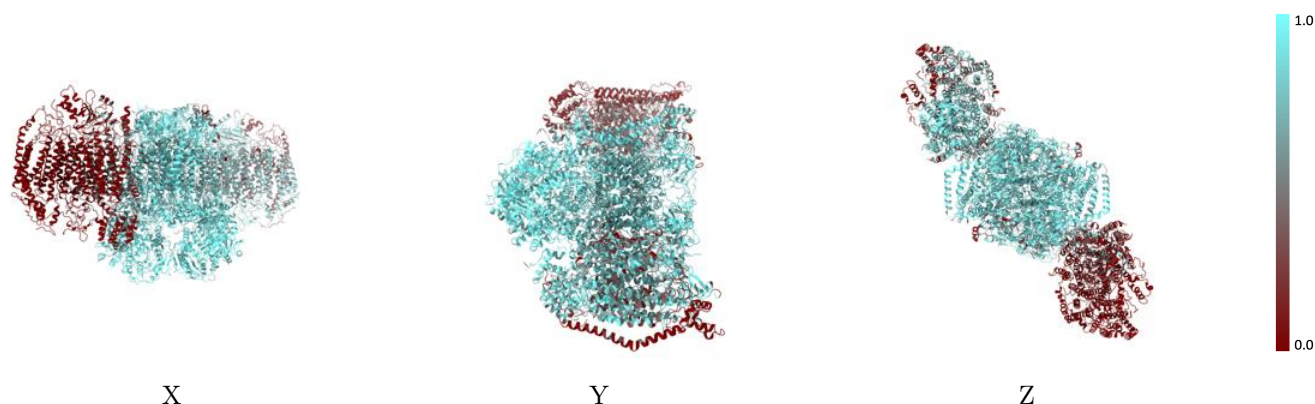
The images above show the 3D surface view of the map at the recommended contour level 0.245 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



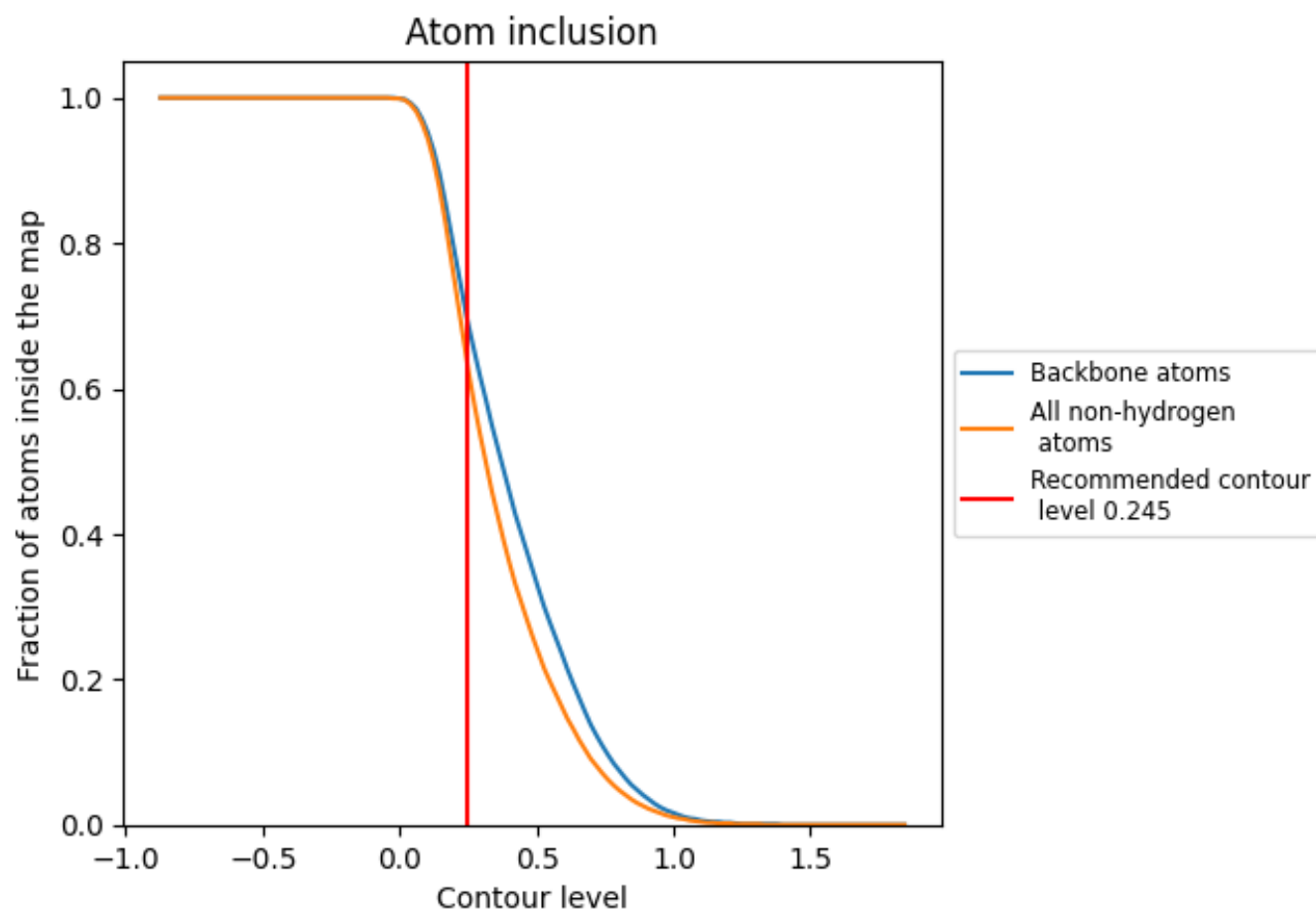
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.245).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 64% 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 (0.245) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6380	 0.3120
A	 0.9260	 0.4260
B	 0.9380	 0.4330
C	 0.7330	 0.3570
D	 0.7440	 0.3710
E	 0.7950	 0.4000
F	 0.9010	 0.4340
G	 0.8490	 0.3690
H	 0.8320	 0.4310
J	 0.8400	 0.4220
K	 0.7100	 0.3240
L	 0.9050	 0.4290
M	 0.4320	 0.2750
N	 0.5230	 0.2610
O	 0.6000	 0.1920
P	 0.8130	 0.2850
Q	 0.7890	 0.2870
R	 0.7200	 0.2440
S	 0.0580	 0.1440
T	 0.7080	 0.2960
U	 0.1840	 0.1570
V	 0.5940	 0.2850
W	 0.7810	 0.3480
a	 0.9270	 0.4310
b	 0.9430	 0.4290
c	 0.6810	 0.3420
d	 0.5920	 0.3560
e	 0.7970	 0.3840
f	 0.9050	 0.4280
g	 0.8450	 0.3860
h	 0.8990	 0.4320
j	 0.8680	 0.4220
k	 0.1350	 0.1560
l	 0.9090	 0.4210
m	 0.0000	 0.1350



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Chain	Atom inclusion	Q-score
n	 0.0000	 0.0710
o	 0.0010	 0.0460
p	 0.1510	 0.1210
q	 0.0530	 0.1440
r	 0.1020	 0.0670
s	 0.0000	 0.0210
t	 0.0280	 0.0850
u	 0.0000	 0.0380
v	 0.2750	 0.1630
w	 0.3370	 0.2200