Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:15 pm BST

PDB ID	:	1W5C
Title	:	Photosystem II from Thermosynechococcus elongatus
Authors	:	Biesiadka, J.; Loll, B.; Kern, J.; Irrgang, K.-D.; Saenger, W.
Deposited on	:	2004-08-06
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

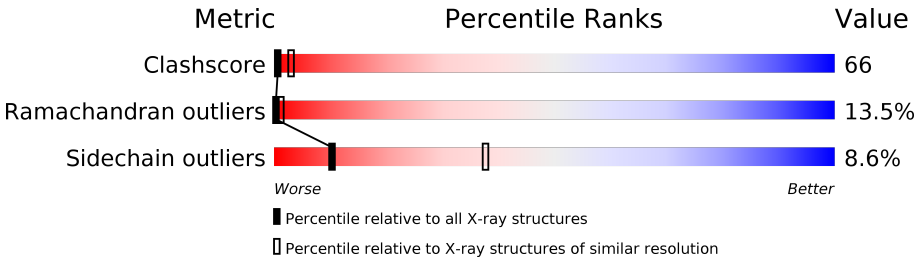
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	360	23% 54% 13% • 8%
1	G	360	25% 54% 12% • 8%
2	B	510	32% 49% 11% • 6%
2	H	510	32% 49% 11% • 6%
3	C	473	30% 49% 12% • 7%
3	I	473	29% 48% 14% • 7%
4	D	352	24% 59% 14% ••
4	J	352	26% 59% 14% ••

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Mol	Chain	Length	Quality of chain
5	E	84	24% 49% 14% • 10%
5	K	84	23% 49% 15% • 10%
6	F	44	14% 52% 14% 5% 16%
6	L	44	16% 45% 16% 7% 16%
7	O	179	68% 32%
7	P	179	66% 34%
8	S	100	43% 57%
8	U	100	39% 61%
9	T	163	56% 26% • 17%
9	V	163	53% 29% • 17%
10	X	359	52% 48%
10	Y	359	53% 47%

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
11	CLA	A	1342	X	-	-	-
11	CLA	A	1343	X	-	-	-
11	CLA	A	1344	X	-	-	-
11	CLA	A	1346	X	-	-	-
11	CLA	B	1482	X	-	-	-
11	CLA	B	1483	X	-	-	-
11	CLA	B	1484	X	-	-	-
11	CLA	B	1485	X	-	-	-
11	CLA	B	1486	X	-	-	-
11	CLA	B	1487	X	-	-	-
11	CLA	B	1488	X	-	-	-
11	CLA	B	1489	X	-	-	-
11	CLA	B	1490	X	-	-	-
11	CLA	B	1491	X	-	-	-
11	CLA	B	1492	X	-	-	-
11	CLA	B	1493	X	-	-	-
11	CLA	B	1494	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	B	1495	X	-	-	-
11	CLA	B	1496	X	-	-	-
11	CLA	B	1497	X	-	-	-
11	CLA	C	1459	X	-	-	-
11	CLA	C	1460	X	-	-	-
11	CLA	C	1461	X	-	-	-
11	CLA	C	1462	X	-	-	-
11	CLA	C	1463	X	-	-	-
11	CLA	C	1464	X	-	-	-
11	CLA	C	1465	X	-	-	-
11	CLA	C	1466	X	-	-	-
11	CLA	C	1467	X	-	-	-
11	CLA	C	1468	X	-	-	-
11	CLA	C	1469	X	-	-	-
11	CLA	C	1470	X	-	-	-
11	CLA	C	1471	X	-	-	-
11	CLA	D	1351	X	-	-	-
11	CLA	D	1353	X	-	-	-
11	CLA	G	1342	X	-	-	-
11	CLA	G	1343	X	-	-	-
11	CLA	G	1344	X	-	-	-
11	CLA	G	1346	X	-	-	-
11	CLA	H	1482	X	-	-	-
11	CLA	H	1483	X	-	-	-
11	CLA	H	1484	X	-	-	-
11	CLA	H	1485	X	-	-	-
11	CLA	H	1486	X	-	-	-
11	CLA	H	1487	X	-	-	-
11	CLA	H	1488	X	-	-	-
11	CLA	H	1489	X	-	-	-
11	CLA	H	1490	X	-	-	-
11	CLA	H	1491	X	-	-	-
11	CLA	H	1492	X	-	-	-
11	CLA	H	1493	X	-	-	-
11	CLA	H	1494	X	-	-	-
11	CLA	H	1495	X	-	-	-
11	CLA	H	1496	X	-	-	-
11	CLA	H	1497	X	-	-	-
11	CLA	I	1459	X	-	-	-
11	CLA	I	1460	X	-	-	-
11	CLA	I	1461	X	-	-	-
11	CLA	I	1462	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	I	1463	X	-	-	-
11	CLA	I	1464	X	-	-	-
11	CLA	I	1465	X	-	-	-
11	CLA	I	1466	X	-	-	-
11	CLA	I	1467	X	-	-	-
11	CLA	I	1468	X	-	-	-
11	CLA	I	1469	X	-	-	-
11	CLA	I	1470	X	-	-	-
11	CLA	I	1471	X	-	-	-
11	CLA	J	1351	X	-	-	-
11	CLA	J	1353	X	-	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 35614 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 PHOTOSYSTEM Q(B) PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	31
			2279	1505	370	390	14			
1	G	332	Total	C	N	O	S	0	0	31
			2279	1505	370	390	14			

- Molecule 2 is a protein called PHOTOSYSTEM II CORE LIGHT HARVESTING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	479	Total	C	N	O	S	0	0	66
			3053	2027	504	510	12			
2	H	479	Total	C	N	O	S	0	0	66
			3053	2027	504	510	12			

- Molecule 3 is a protein called PHOTOSYSTEM II CP43 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	438	Total	C	N	O	S	0	0	73
			2791	1861	467	452	11			
3	I	438	Total	C	N	O	S	0	0	73
			2791	1861	467	452	11			

- Molecule 4 is a protein called PHOTOSYSTEM II REACTION CENTER D2 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	350	Total	C	N	O	S	0	0	0
			2602	1719	421	450	12			
4	J	350	Total	C	N	O	S	0	0	0
			2602	1719	421	450	12			

- Molecule 5 is a protein called CYTOCHROME B559 ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	76	Total	C	N	O	0	0	5
			536	354	89	93			
5	K	76	Total	C	N	O	0	0	5
			536	354	89	93			

- Molecule 6 is a protein called CYTOCHROME B559 BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	37	Total	C	N	O	S	0	0	0
			297	202	48	46	1			
6	L	37	Total	C	N	O	S	0	0	0
			297	202	48	46	1			

- Molecule 7 is a protein called PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	O	179	Total	C	N	O	0	0	3
			883	531	176	176			
7	P	179	Total	C	N	O	0	0	3
			883	531	176	176			

- Molecule 8 is a protein called PHOTOSYSTEM II 12 KDA EXTRINSIC PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	S	100	Total	C	N	O	0	0	0
			499	299	100	100			
8	U	100	Total	C	N	O	0	0	0
			499	299	100	100			

- Molecule 9 is a protein called CYTOCHROME C-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	T	136	Total	C	N	O	S	0	0	0
			1058	672	176	206	4			
9	V	136	Total	C	N	O	S	0	0	0
			1058	672	176	206	4			

- Molecule 10 is a protein called UNASSIGNED SUBUNITS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	X	359	Total	C	N	O	0	0	0
			1791	1073	359	359			

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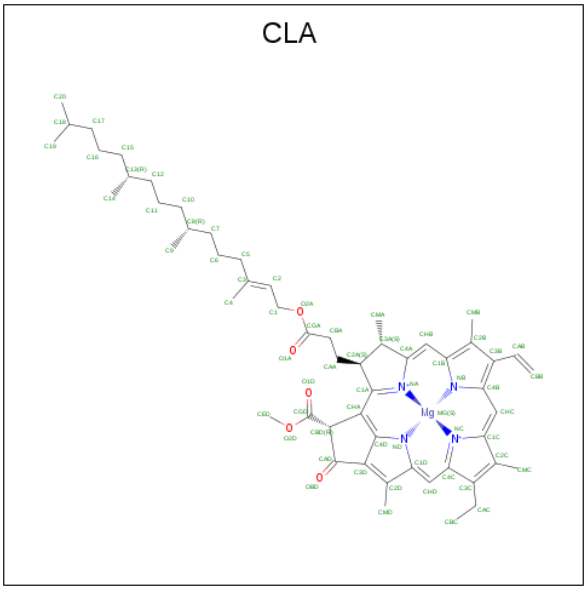
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	Y	359	Total	C	N	O	0	0	0
			1791	1073	359	359			

- Molecule 11 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C Mg N O 65 55 1 4 5	0	0
11	B	1	Total C Mg N O 50 40 1 4 5	0	0
11	B	1	Total C Mg N O 45 35 1 4 5	0	0
11	B	1	Total C Mg N 27 22 1 4	0	0
11	B	1	Total C Mg N O 65 55 1 4 5	0	0
11	B	1	Total C Mg N O 45 35 1 4 5	0	0
11	B	1	Total C Mg N O 65 55 1 4 5	0	0
11	B	1	Total C Mg N O 55 45 1 4 5	0	0
11	B	1	Total C Mg N O 65 55 1 4 5	0	0
11	B	1	Total C Mg N O 41 33 1 4 3	0	0
11	C	1	Total C Mg N O 45 35 1 4 5	0	0
11	C	1	Total C Mg N O 47 37 1 4 5	0	0
11	C	1	Total C Mg N 27 22 1 4	0	0
11	C	1	Total C Mg N O 56 46 1 4 5	0	0
11	C	1	Total C Mg N O 55 45 1 4 5	0	0
11	C	1	Total C Mg N O 56 46 1 4 5	0	0
11	C	1	Total C Mg N O 65 55 1 4 5	0	0
11	C	1	Total C Mg N O 50 40 1 4 5	0	0
11	C	1	Total C Mg N O 47 37 1 4 5	0	0
11	C	1	Total C Mg N 27 22 1 4	0	0
11	C	1	Total C Mg N O 41 33 1 4 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
11	C	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
11	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	D	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	G	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
11	G	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
11	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	H	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	H	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	H	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	H	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
11	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	H	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	H	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	H	1	Total	C	Mg	N		0	0
			27	22	1	4			
11	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	H	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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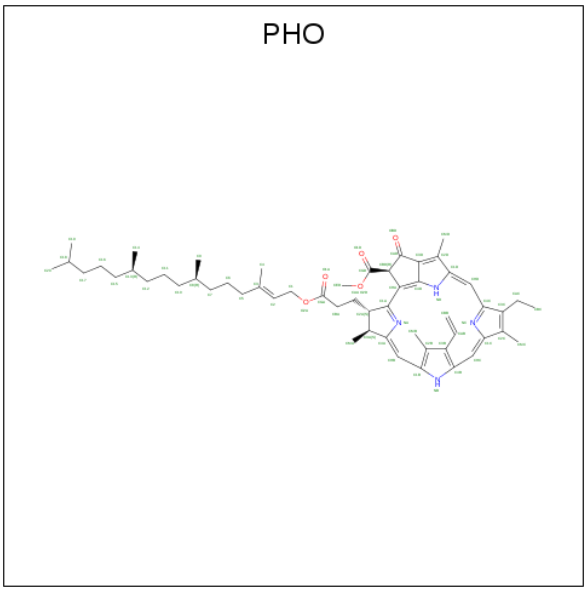
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	H	1	Total C Mg N O 55 45 1 4 5	0	0
11	H	1	Total C Mg N O 65 55 1 4 5	0	0
11	H	1	Total C Mg N O 41 33 1 4 3	0	0
11	I	1	Total C Mg N O 45 35 1 4 5	0	0
11	I	1	Total C Mg N O 47 37 1 4 5	0	0
11	I	1	Total C Mg N 27 22 1 4	0	0
11	I	1	Total C Mg N O 56 46 1 4 5	0	0
11	I	1	Total C Mg N O 55 45 1 4 5	0	0
11	I	1	Total C Mg N O 56 46 1 4 5	0	0
11	I	1	Total C Mg N O 65 55 1 4 5	0	0
11	I	1	Total C Mg N O 50 40 1 4 5	0	0
11	I	1	Total C Mg N O 47 37 1 4 5	0	0
11	I	1	Total C Mg N 27 22 1 4	0	0
11	I	1	Total C Mg N O 41 33 1 4 3	0	0
11	I	1	Total C Mg N O 41 33 1 4 3	0	0
11	I	1	Total C Mg N O 41 33 1 4 3	0	0
11	J	1	Total C Mg N O 65 55 1 4 5	0	0
11	J	1	Total C Mg N O 50 40 1 4 5	0	0

- Molecule 12 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C N O 64 55 4 5	0	0
12	D	1	Total C N O 54 45 4 5	0	0
12	G	1	Total C N O 64 55 4 5	0	0
12	J	1	Total C N O 54 45 4 5	0	0

- Molecule 13 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

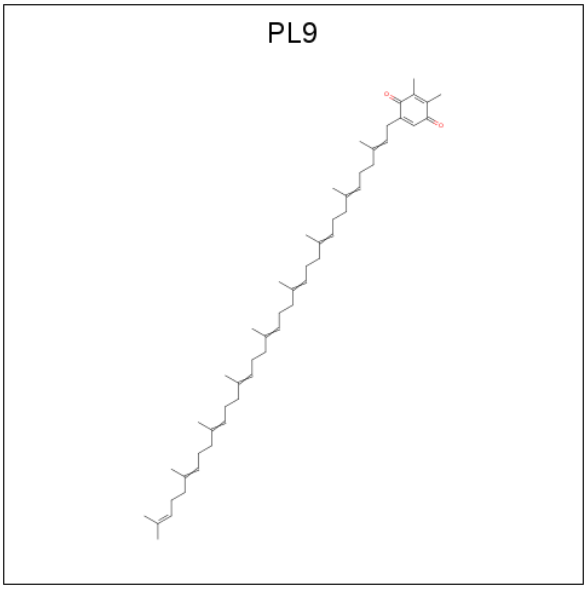
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	G	4	Total Mn 4 4	0	0
13	A	4	Total Mn 4 4	0	0

- Molecule 14 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	G	1	Total Fe 1 1	0	0
14	A	1	Total Fe 1 1	0	0

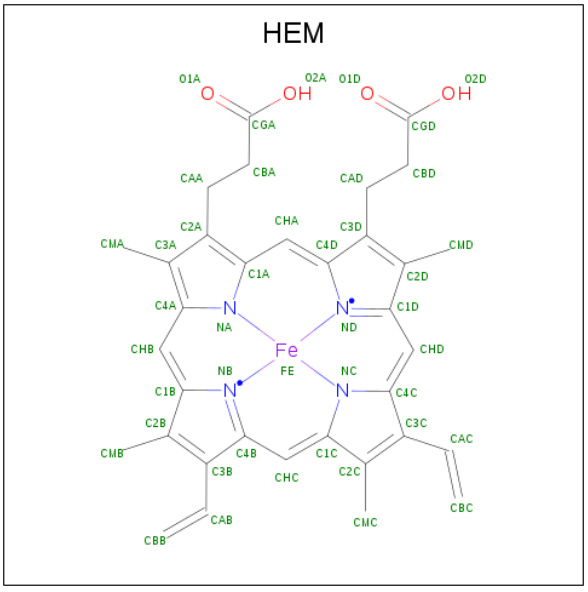
- Molecule 15 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18 ,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,

3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



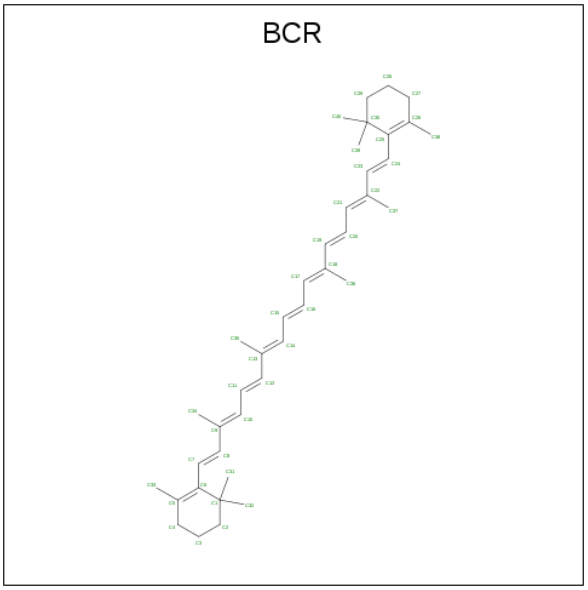
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	D	1	Total C 6 6	0	0
15	J	1	Total C 6 6	0	0

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



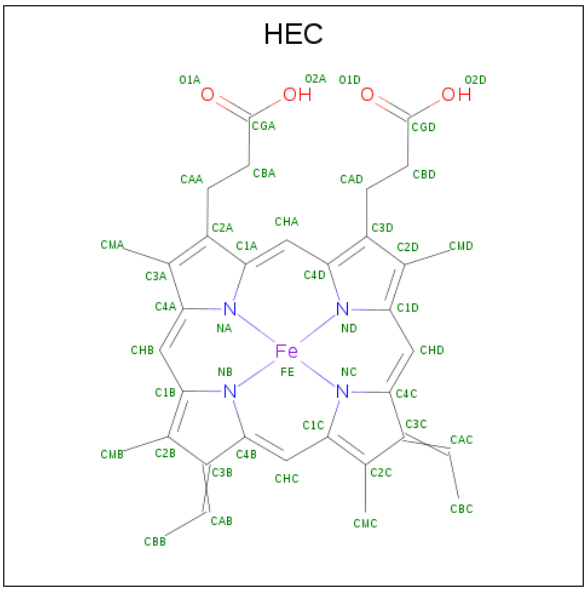
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	E	1	Total	C	Fe	N	0	0
			25	20	1	4		
16	L	1	Total	C	Fe	N	0	0
			25	20	1	4		

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	F	1	Total	C	0	0
			40	40		
17	L	1	Total	C	0	0
			40	40		

- Molecule 18 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	T	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
18	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

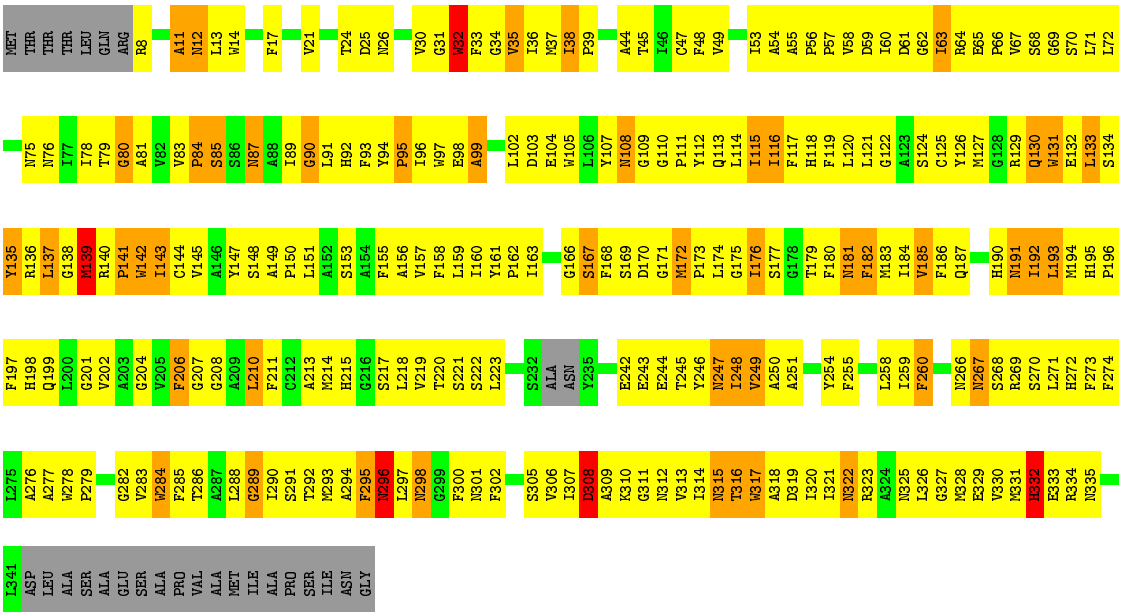
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

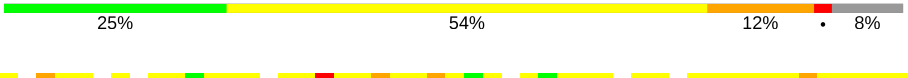
- Molecule 1: PHOTOSYSTEM Q(B) PROTEIN 1

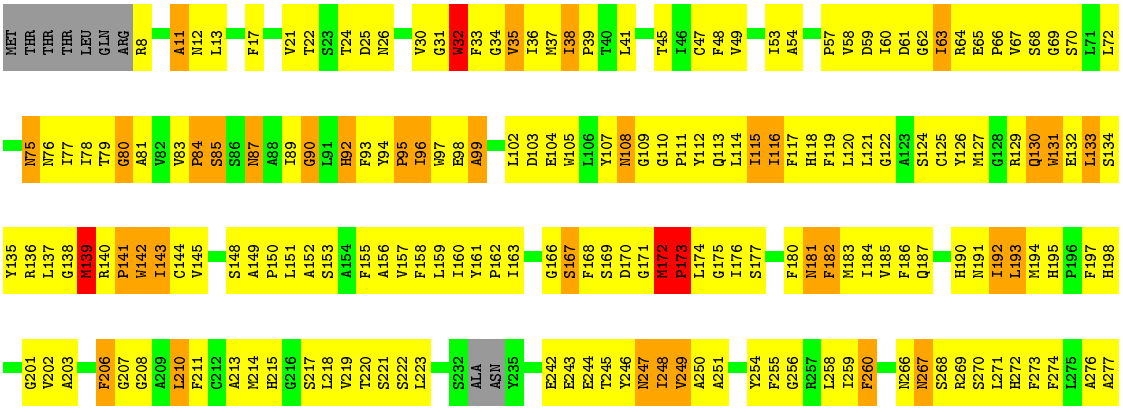
Chain A:

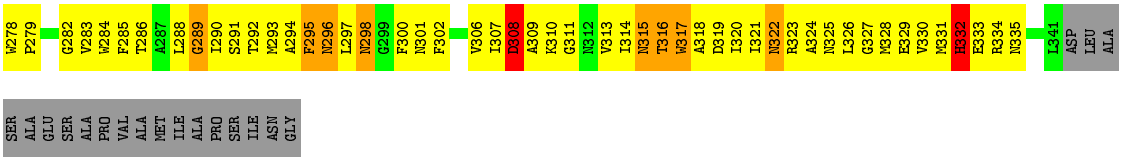


- Molecule 1: PHOTOSYSTEM Q(B) PROTEIN 1

Chain G:

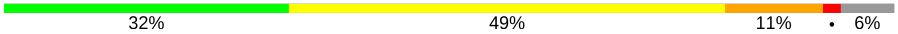


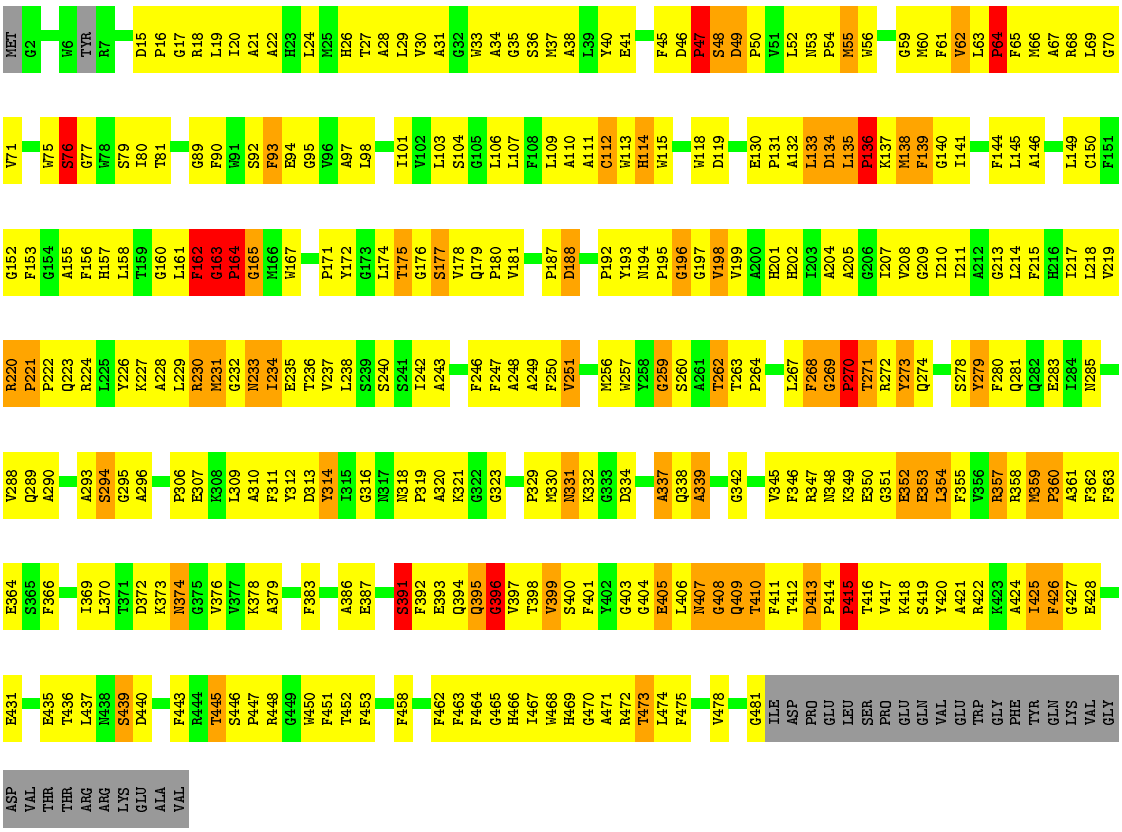




• Molecule 2: PHOTOSYSTEM II CORE LIGHT HARVESTING PROTEIN

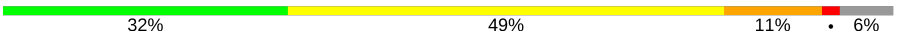
Chain B:

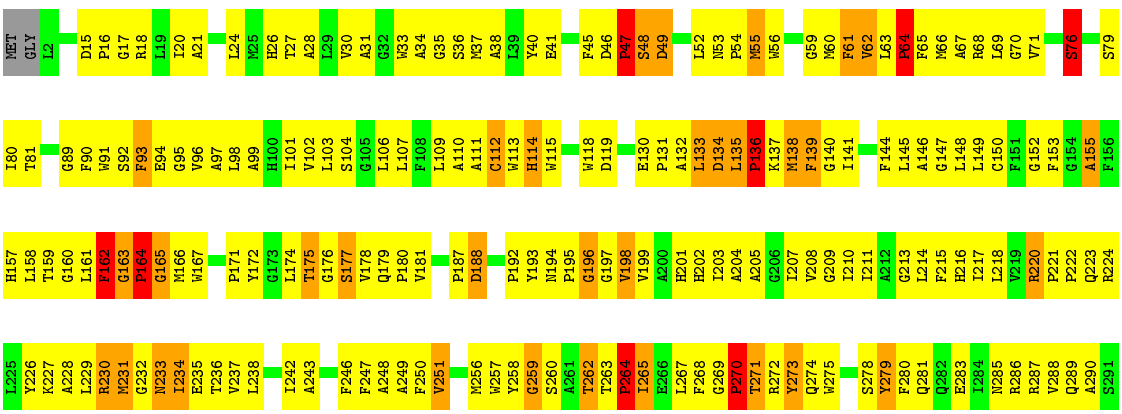


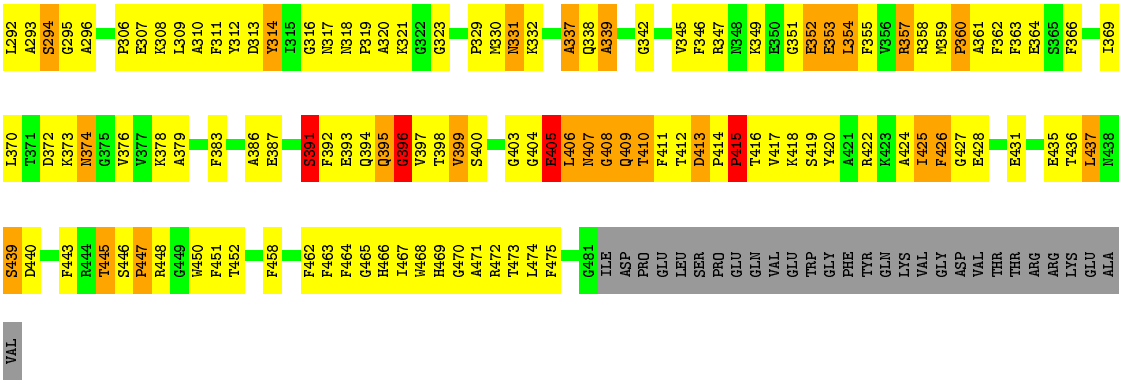


• Molecule 2: PHOTOSYSTEM II CORE LIGHT HARVESTING PROTEIN

Chain H:

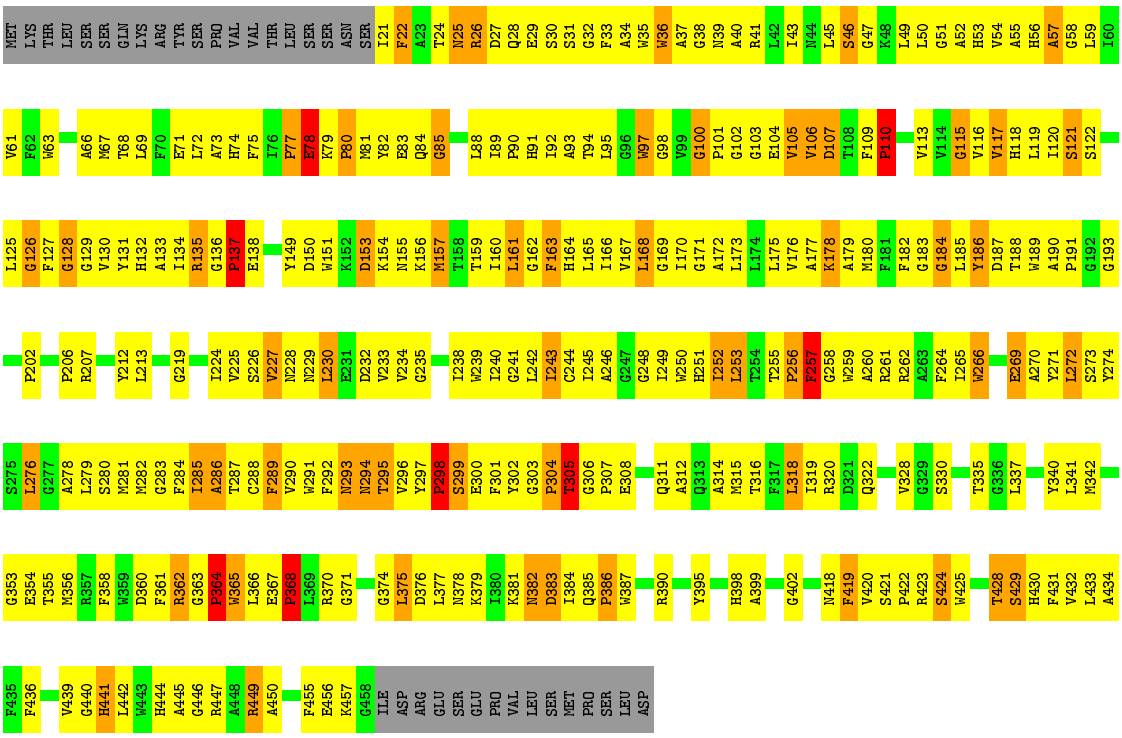






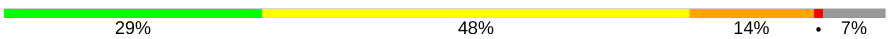
• Molecule 3: PHOTOSYSTEM II CP43 PROTEIN

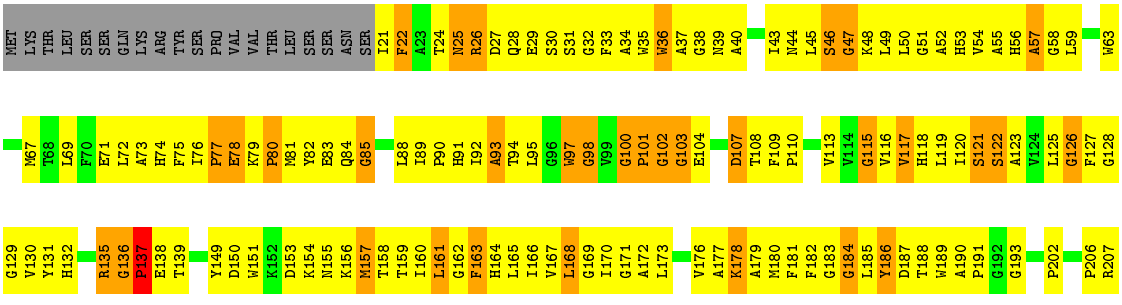
Chain C:

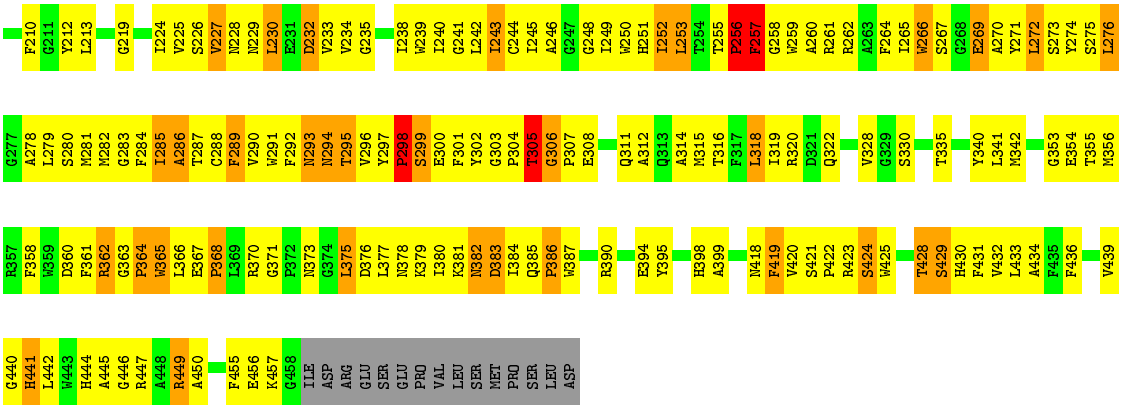


• Molecule 3: PHOTOSYSTEM II CP43 PROTEIN

Chain I:

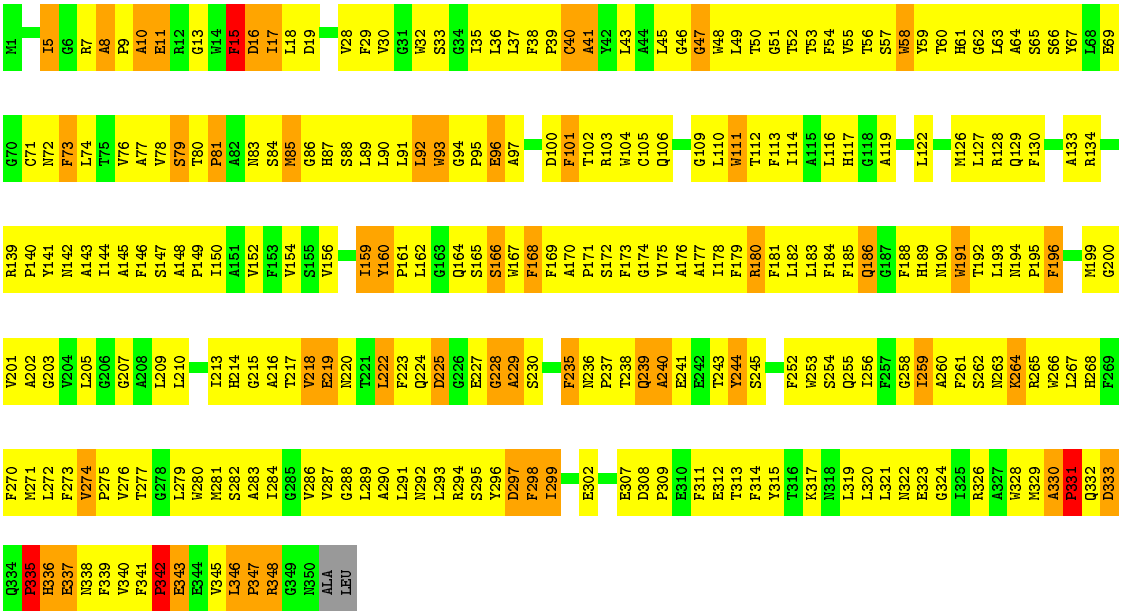






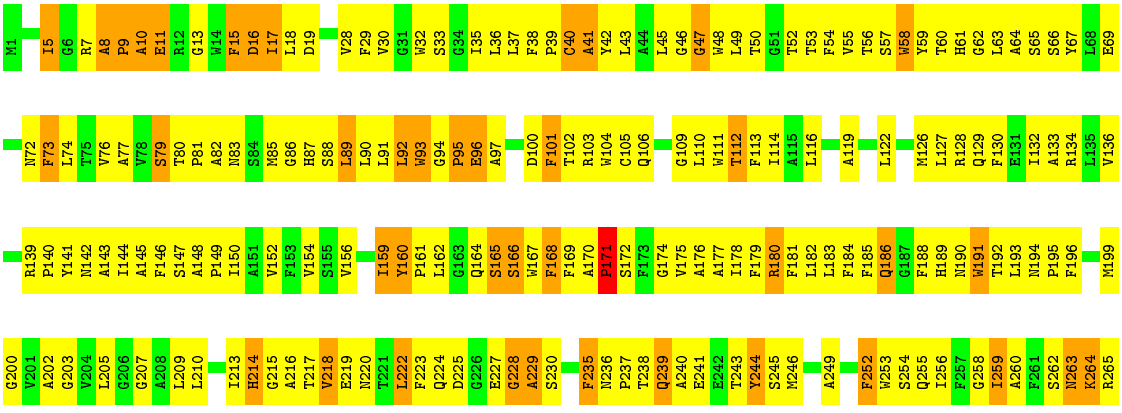
• Molecule 4: PHOTOSYSTEM II REACTION CENTER D2 PROTEIN

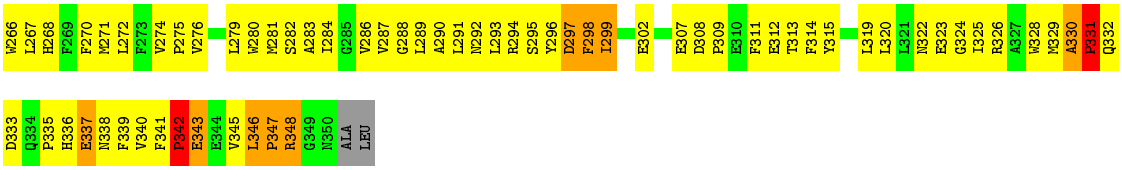
Chain D:



• Molecule 4: PHOTOSYSTEM II REACTION CENTER D2 PROTEIN

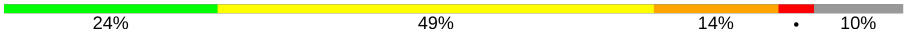
Chain J:

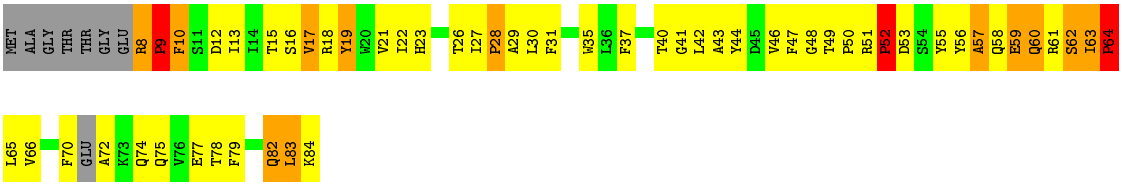




• Molecule 5: CYTOCHROME B559 ALPHA SUBUNIT

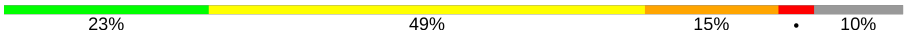
Chain E:

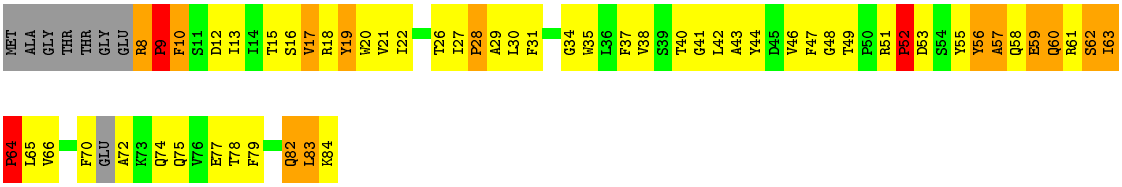




• Molecule 5: CYTOCHROME B559 ALPHA SUBUNIT

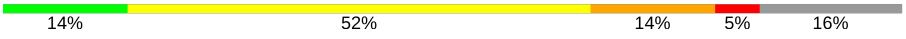
Chain K:





• Molecule 6: CYTOCHROME B559 BETA SUBUNIT

Chain F:

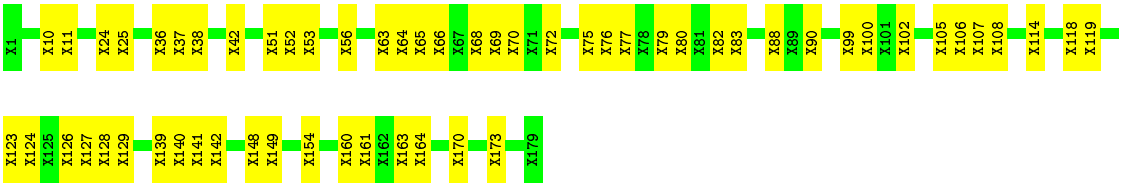


• Molecule 6: CYTOCHROME B559 BETA SUBUNIT

Chain L:

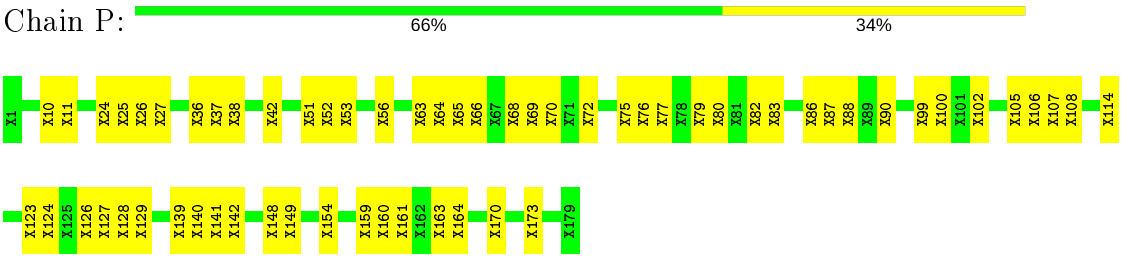
• Molecule 7: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE

Chain O:



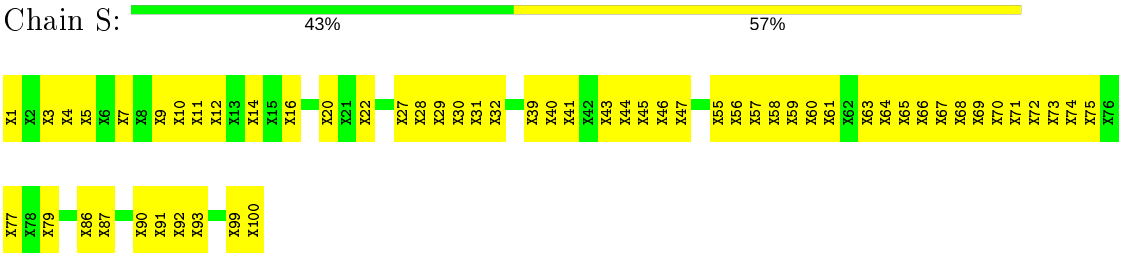
• Molecule 7: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE

Chain P:



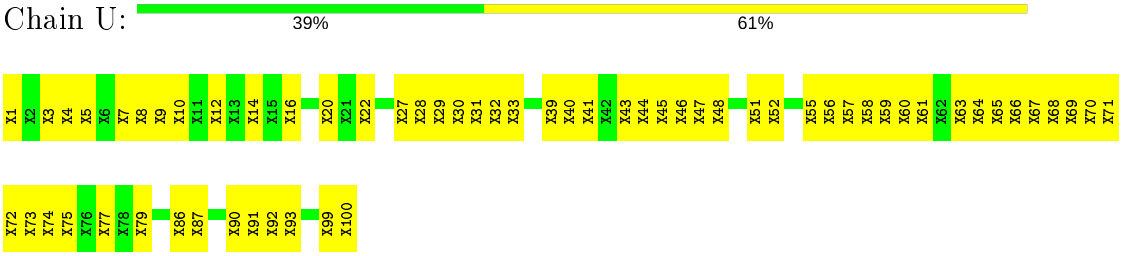
• Molecule 8: PHOTOSYSTEM II 12 KDA EXTRINSIC PROTEIN

Chain S:



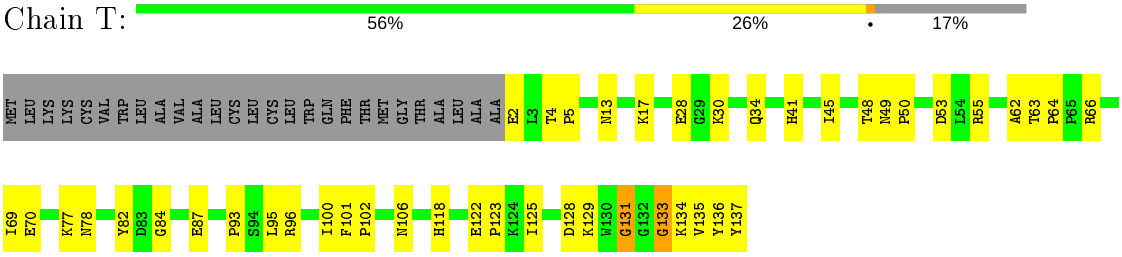
• Molecule 8: PHOTOSYSTEM II 12 KDA EXTRINSIC PROTEIN

Chain U:



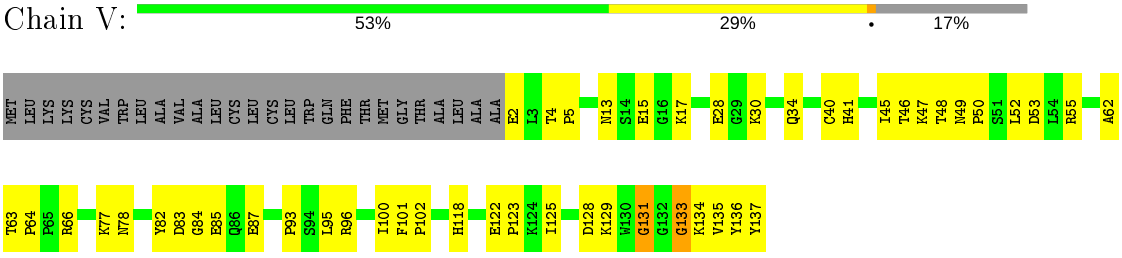
• Molecule 9: CYTOCHROME C-550

Chain T:



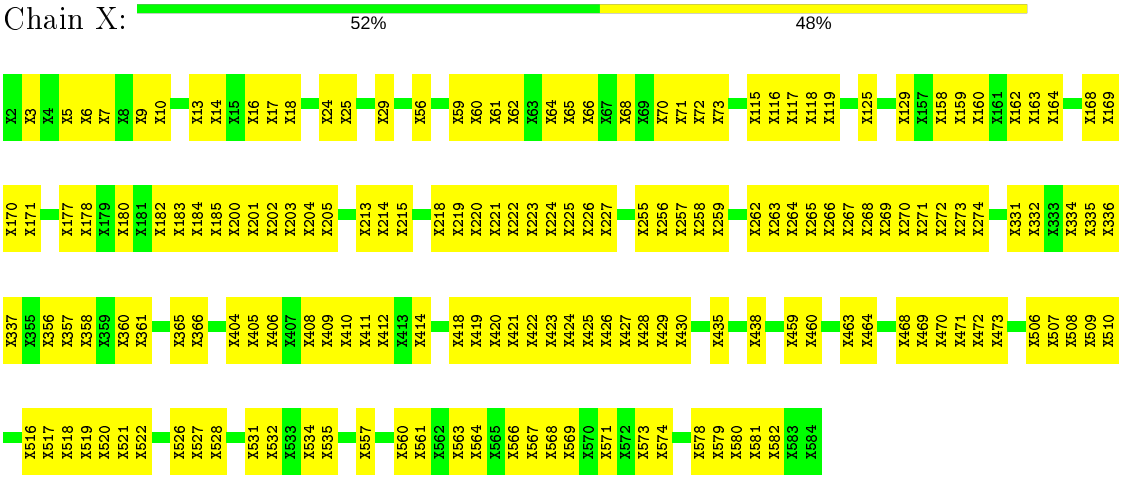
• Molecule 9: CYTOCHROME C-550

Chain V:



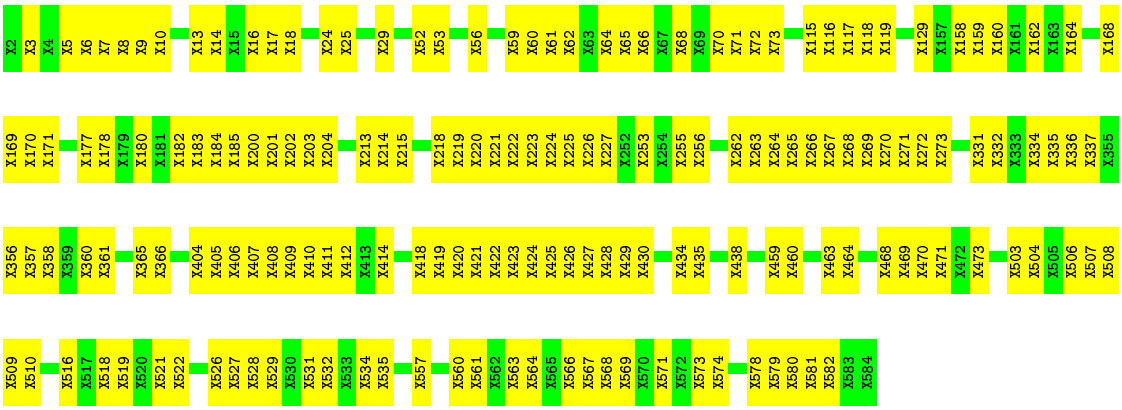
- Molecule 10: UNASSIGNED SUBUNITS

Chain X:



- Molecule 10: UNASSIGNED SUBUNITS

Chain Y:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	127.52Å 224.61Å 305.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20	Depositor
% Data completeness (in resolution range)	75.6 (10.00-3.20)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	35614	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PHO, MN, CLA, PL9, FE2, HEC, HEM, BCR

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	0.69	0/2315	0.88	1/3161 (0.0%)
1	G	0.66	0/2315	0.91	2/3161 (0.1%)
2	B	0.69	0/3081	0.98	9/4202 (0.2%)
2	H	0.67	0/3081	0.99	9/4202 (0.2%)
3	C	0.62	0/2806	0.90	3/3822 (0.1%)
3	I	0.62	0/2806	0.89	5/3822 (0.1%)
4	D	0.70	0/2688	0.96	4/3678 (0.1%)
4	J	0.69	0/2688	0.97	5/3678 (0.1%)
5	E	0.62	0/547	0.89	0/751
5	K	0.66	0/547	0.95	1/751 (0.1%)
6	F	0.77	0/307	1.19	4/421 (1.0%)
6	L	0.79	0/307	1.21	4/421 (1.0%)
9	T	0.65	0/1079	0.81	0/1466
9	V	0.69	0/1079	0.81	0/1466
All	All	0.67	0/25646	0.94	47/35002 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	1
2	B	0	1
2	H	0	1
All	All	0	4

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	270	PRO	CA-N-CD	-14.97	90.54	111.50
2	B	270	PRO	CA-N-CD	-13.49	92.62	111.50
4	J	171	PRO	CA-N-CD	-11.70	95.12	111.50
2	B	47	PRO	CA-N-CD	-11.20	95.81	111.50
2	B	396	GLY	N-CA-C	-10.89	85.88	113.10
2	H	396	GLY	N-CA-C	-10.79	86.13	113.10
3	C	110	PRO	CA-N-CD	-10.78	96.40	111.50
4	J	342	PRO	CA-N-CD	-10.54	96.75	111.50
2	B	76	SER	N-CA-C	-10.36	83.02	111.00
2	H	76	SER	N-CA-C	-10.32	83.12	111.00
4	D	342	PRO	CA-N-CD	-10.27	97.12	111.50
2	H	264	PRO	CA-N-CD	-10.23	97.17	111.50
1	G	173	PRO	CA-N-CD	-9.94	97.59	111.50
4	D	335	PRO	CA-N-CD	-9.80	97.78	111.50
6	L	14	PRO	CA-N-CD	-9.77	97.82	111.50
6	L	10	PRO	CA-N-CD	-9.54	98.15	111.50
2	H	47	PRO	CA-N-CD	-9.29	98.50	111.50
6	F	14	PRO	CA-N-CD	-8.87	99.08	111.50
3	C	137	PRO	CA-N-CD	-8.62	99.43	111.50
5	K	64	PRO	CA-N-CD	-8.15	100.09	111.50
3	I	137	PRO	CA-N-CD	-8.12	100.13	111.50
6	F	45	ARG	N-CA-C	-7.97	89.49	111.00
2	H	162	PHE	C-N-CA	6.87	136.72	122.30
2	B	162	PHE	C-N-CA	6.26	135.44	122.30
2	B	164	PRO	CA-N-CD	-6.04	103.04	111.50
3	C	100	GLY	N-CA-C	-5.95	98.23	113.10
3	I	256	PRO	CA-N-CD	-5.88	103.26	111.50
2	B	391	SER	N-CA-C	5.84	126.77	111.00
6	F	13	TYR	N-CA-C	5.82	126.71	111.00
2	H	391	SER	N-CA-C	5.81	126.68	111.00
3	I	100	GLY	N-CA-C	-5.79	98.61	113.10
6	L	13	TYR	N-CA-C	5.75	126.52	111.00
2	H	91	TRP	CA-CB-CG	-5.72	102.84	113.70
2	B	268	PHE	CB-CA-C	-5.68	99.03	110.40
2	H	164	PRO	CA-N-CD	-5.67	103.56	111.50
6	F	13	TYR	C-N-CD	-5.59	108.29	120.60
6	L	9	GLU	C-N-CD	-5.59	108.31	120.60
4	D	5	ILE	N-CA-C	5.57	126.04	111.00
3	I	107	ASP	CB-CA-C	-5.46	99.47	110.40
1	G	172	MET	C-N-CD	-5.41	108.70	120.60
4	J	5	ILE	N-CA-C	5.35	125.44	111.00
1	A	137	LEU	CA-CB-CG	5.16	127.16	115.30
2	B	163	GLY	N-CA-C	5.15	125.99	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	331	PRO	CA-N-CD	-5.15	104.29	111.50
3	I	136	GLY	N-CA-C	-5.09	100.37	113.10
4	J	9	PRO	N-CA-CB	5.06	109.37	103.30
4	D	15	PHE	N-CA-C	5.02	124.55	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	332	HIS	Sidechain
2	B	273	TYR	Sidechain
1	G	332	HIS	Sidechain
2	H	273	TYR	Sidechain

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	2279	0	2113	445	0
1	G	2279	0	2113	452	0
2	B	3053	0	2666	441	0
2	H	3053	0	2666	456	0
3	C	2791	0	2530	447	0
3	I	2791	0	2530	445	0
4	D	2602	0	2383	463	0
4	J	2602	0	2383	473	0
5	E	536	0	480	87	0
5	K	536	0	480	91	0
6	F	297	0	304	56	0
6	L	297	0	304	62	0
7	O	883	0	221	43	0
7	P	883	0	219	45	0
8	S	499	0	116	50	0
8	U	499	0	115	52	0
9	T	1058	0	1066	59	0
9	V	1058	0	1066	62	0
10	X	1791	0	396	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	Y	1791	0	393	135	0
11	A	222	0	207	37	0
11	B	846	0	774	84	0
11	C	598	0	458	69	0
11	D	115	0	111	19	0
11	G	222	0	207	33	0
11	H	846	0	774	91	0
11	I	598	0	458	69	0
11	J	115	0	111	16	0
12	A	64	0	74	14	0
12	D	54	0	51	4	0
12	G	64	0	74	17	0
12	J	54	0	51	9	0
13	A	4	0	0	0	0
13	G	4	0	0	0	0
14	A	1	0	0	0	0
14	G	1	0	0	0	0
15	D	6	0	1	1	0
15	J	6	0	1	1	0
16	E	25	0	4	2	0
16	L	25	0	4	2	0
17	F	40	0	56	4	0
17	L	40	0	56	3	0
18	T	43	0	31	3	0
18	V	43	0	31	2	0
All	All	35614	0	28078	4207	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 66.

All (4207) 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)
4:D:330:ALA:HB1	4:D:331:PRO:CD	1.48	1.42
4:J:330:ALA:HB1	4:J:331:PRO:CD	1.54	1.36
1:G:84:PRO:CG	1:G:173:PRO:HG3	1.56	1.35
4:D:330:ALA:CB	4:D:331:PRO:CD	1.99	1.33
4:J:330:ALA:CB	4:J:331:PRO:CD	2.07	1.28
1:G:84:PRO:CD	1:G:173:PRO:HG3	1.64	1.26
1:A:309:ALA:O	9:V:2:GLU:HA	1.27	1.23
4:J:171:PRO:HD3	4:J:181:PHE:CE2	1.75	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:45:PHE:CD2	2:H:47:PRO:HD3	1.75	1.21
1:A:309:ALA:O	9:V:2:GLU:CA	1.91	1.17
6:L:12:SER:O	6:L:14:PRO:HD2	1.43	1.17
4:J:331:PRO:CG	4:J:339:PHE:HB3	1.74	1.17
2:B:45:PHE:CD2	2:B:47:PRO:HD3	1.80	1.15
2:H:61:PHE:O	2:H:64:PRO:HD2	1.44	1.15
5:K:62:SER:C	5:K:64:PRO:HD3	1.67	1.14
3:I:296:VAL:CG1	11:I:1459:CLA:HAA1	1.77	1.14
6:F:12:SER:O	6:F:14:PRO:HD2	1.48	1.13
3:I:449:ARG:HG3	3:I:449:ARG:HH11	1.08	1.13
4:D:331:PRO:CG	4:D:339:PHE:HB3	1.78	1.13
4:J:330:ALA:HB3	4:J:331:PRO:HD2	1.28	1.13
4:D:52:THR:HG22	4:D:67:TYR:HE1	1.09	1.12
4:J:171:PRO:HD3	4:J:181:PHE:CD2	1.83	1.12
4:D:126:MET:HA	4:D:129:GLN:HE21	1.11	1.12
4:J:330:ALA:CB	4:J:331:PRO:HD2	1.74	1.10
1:A:142:TRP:HB3	4:D:220:ASN:OD1	1.49	1.10
4:J:331:PRO:HG3	4:J:339:PHE:CB	1.79	1.10
4:J:126:MET:HA	4:J:129:GLN:HE21	1.03	1.10
1:G:186:PHE:HD2	1:G:192:ILE:HD11	1.16	1.09
4:J:331:PRO:CG	4:J:339:PHE:CB	2.29	1.09
3:I:228:ASN:HA	3:I:295:THR:HG21	1.34	1.09
4:J:113:PHE:HA	11:J:1353:CLA:HED1	1.34	1.09
1:A:47:CYS:SG	1:A:114:LEU:HD23	1.93	1.08
1:A:143:ILE:HG13	4:D:220:ASN:HD22	1.12	1.08
3:C:296:VAL:CG1	11:C:1459:CLA:HAA1	1.81	1.08
1:G:142:TRP:HB3	4:J:220:ASN:OD1	1.51	1.08
4:D:330:ALA:CB	4:D:331:PRO:HD2	1.73	1.08
1:A:186:PHE:HD2	1:A:192:ILE:HD11	1.13	1.08
3:C:449:ARG:HH11	3:C:449:ARG:HG3	1.07	1.08
1:G:84:PRO:HG2	1:G:173:PRO:HG3	1.26	1.07
4:J:52:THR:HG22	4:J:67:TYR:HE1	1.12	1.07
3:C:228:ASN:HA	3:C:295:THR:HG21	1.37	1.07
4:D:113:PHE:HA	11:D:1353:CLA:HED1	1.35	1.07
5:K:62:SER:O	5:K:64:PRO:HD3	1.50	1.07
1:A:127:MET:HE2	1:A:151:LEU:HD22	1.28	1.07
4:D:331:PRO:HG3	4:D:339:PHE:CB	1.84	1.07
3:I:296:VAL:HG11	11:I:1459:CLA:CAA	1.85	1.06
2:B:61:PHE:O	2:B:64:PRO:HD2	1.52	1.06
3:C:296:VAL:HG11	11:C:1459:CLA:CAA	1.86	1.06
1:G:114:LEU:HA	11:G:1346:CLA:HED1	1.35	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:45:PHE:CE2	2:H:47:PRO:HD3	1.90	1.05
4:J:126:MET:O	4:J:129:GLN:HG2	1.55	1.05
4:J:331:PRO:HG2	4:J:339:PHE:HB3	1.24	1.05
4:D:330:ALA:HB3	4:D:331:PRO:HD2	1.21	1.05
3:C:187:ASP:HB3	3:C:230:LEU:HD23	1.37	1.04
1:G:47:CYS:SG	1:G:114:LEU:HD23	1.97	1.04
3:I:296:VAL:HG11	11:I:1459:CLA:HAA1	1.04	1.04
4:D:330:ALA:CB	4:D:331:PRO:HD3	1.75	1.04
2:B:400:SER:HB3	2:B:410:THR:HB	1.38	1.03
3:C:106:VAL:O	3:C:107:ASP:CB	1.98	1.03
1:A:138:GLY:HA2	3:C:455:PHE:CE1	1.93	1.03
4:D:126:MET:O	4:D:129:GLN:HG2	1.58	1.03
1:A:63:ILE:HG12	1:A:64:ARG:H	1.20	1.02
1:G:63:ILE:HG12	1:G:64:ARG:H	1.23	1.02
4:D:331:PRO:HG2	4:D:339:PHE:HB3	1.39	1.01
1:G:84:PRO:HG2	1:G:173:PRO:CG	1.89	1.01
4:D:122:LEU:HD21	11:D:1351:CLA:H92	1.39	1.01
1:A:309:ALA:O	9:V:2:GLU:CB	2.09	1.01
3:I:187:ASP:HB3	3:I:230:LEU:HD23	1.43	1.01
2:H:400:SER:HB3	2:H:410:THR:HB	1.38	1.00
1:G:138:GLY:HA2	3:I:455:PHE:CE1	1.96	1.00
2:H:30:VAL:HG12	11:H:1486:CLA:HAC1	1.39	1.00
1:G:143:ILE:HG13	4:J:220:ASN:HD22	1.26	1.00
4:J:330:ALA:HB1	4:J:331:PRO:HD3	1.01	1.00
1:A:63:ILE:HG13	3:C:335:THR:CG2	1.91	1.00
6:F:37:ILE:HA	6:F:40:MET:HE2	1.42	0.99
5:E:22:ILE:HG23	10:X:568:UNK:CB	1.92	0.99
3:C:43:ILE:HG22	11:C:1467:CLA:HMC1	1.43	0.99
4:J:171:PRO:CD	4:J:181:PHE:CE2	2.44	0.99
3:C:296:VAL:HG11	11:C:1459:CLA:HAA1	1.00	0.99
4:J:122:LEU:HD21	11:J:1351:CLA:H92	1.41	0.99
1:G:310:LYS:HA	9:T:2:GLU:HA	1.43	0.99
1:A:183:MET:HE1	11:A:1343:CLA:HHD	1.45	0.98
2:B:347:ARG:HB3	2:B:351:GLY:HA2	1.41	0.98
4:J:86:GLY:HA2	4:J:166:SER:HB3	1.44	0.98
3:C:37:ALA:HA	11:C:1466:CLA:HBA2	1.45	0.98
4:D:86:GLY:HA2	4:D:166:SER:HB3	1.44	0.98
2:H:347:ARG:HB3	2:H:351:GLY:HA2	1.46	0.98
3:I:311:GLN:HG2	3:I:355:THR:CG2	1.94	0.98
1:G:63:ILE:HG13	3:I:335:THR:CG2	1.93	0.97
3:C:311:GLN:HG2	3:C:355:THR:CG2	1.94	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:160:TYR:HB3	4:D:161:PRO:HD3	1.47	0.97
5:K:22:ILE:HG23	10:Y:568:UNK:CB	1.94	0.97
1:A:114:LEU:HA	11:A:1346:CLA:HED1	1.43	0.97
1:G:278:TRP:HB3	1:G:279:PRO:HD3	1.42	0.97
3:I:43:ILE:HG22	11:I:1467:CLA:HMC1	1.46	0.97
1:G:310:LYS:HB2	9:T:2:GLU:N	1.78	0.97
4:D:331:PRO:CG	4:D:339:PHE:CB	2.43	0.97
2:H:30:VAL:CG1	11:H:1486:CLA:HAC1	1.93	0.97
4:J:340:VAL:O	4:J:342:PRO:CD	2.13	0.97
3:I:311:GLN:HG2	3:I:355:THR:HG21	1.44	0.97
4:D:52:THR:HG22	4:D:67:TYR:CE1	2.00	0.96
3:I:37:ALA:HA	11:I:1466:CLA:HBA2	1.45	0.96
5:K:65:LEU:C	5:K:66:VAL:CA	2.33	0.96
7:P:65:UNK:C	7:P:66:UNK:CA	2.42	0.96
2:H:135:LEU:HB2	2:H:136:PRO:HD3	1.44	0.96
3:I:107:ASP:O	3:I:110:PRO:HD2	1.63	0.96
3:I:363:GLY:O	3:I:367:GLU:HG2	1.65	0.96
4:J:340:VAL:O	4:J:342:PRO:HD2	1.64	0.96
9:T:129:LYS:HE3	9:T:135:VAL:HG21	1.45	0.96
1:A:310:LYS:HB2	9:V:2:GLU:N	1.81	0.96
7:O:65:UNK:C	7:O:66:UNK:CA	2.44	0.96
2:B:149:LEU:HG	11:B:1484:CLA:HBC1	1.47	0.96
1:A:186:PHE:CD2	1:A:192:ILE:HD11	2.00	0.95
2:B:135:LEU:HB2	2:B:136:PRO:HD3	1.49	0.95
4:D:345:VAL:O	4:D:345:VAL:HG12	1.63	0.95
6:F:41:GLN:HB3	10:X:331:UNK:CB	1.96	0.95
1:G:221:SER:HA	4:J:139:ARG:HB2	1.49	0.95
4:J:52:THR:HG22	4:J:67:TYR:CE1	2.01	0.95
3:I:398:HIS:C	3:I:399:ALA:CA	2.36	0.95
6:L:41:GLN:HB3	10:Y:331:UNK:CB	1.96	0.94
4:J:160:TYR:HB3	4:J:161:PRO:HD3	1.47	0.94
9:V:133:GLY:O	9:V:137:TYR:HB2	1.67	0.94
2:B:45:PHE:CE2	2:B:47:PRO:HD3	2.01	0.94
1:G:272:HIS:CD2	4:J:218:VAL:HG21	2.02	0.94
1:A:221:SER:HA	4:D:139:ARG:HB2	1.48	0.94
3:I:173:LEU:O	3:I:176:VAL:HG12	1.67	0.94
4:J:253:TRP:HB2	4:J:260:ALA:HB2	1.50	0.94
1:G:186:PHE:CD2	1:G:192:ILE:HD11	2.03	0.93
2:H:149:LEU:HG	11:H:1484:CLA:HBC1	1.51	0.93
2:H:31:ALA:H	11:H:1486:CLA:HBC3	1.31	0.93
3:C:363:GLY:O	3:C:367:GLU:HG2	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.04	0.93
4:J:345:VAL:O	4:J:345:VAL:HG12	1.68	0.93
4:J:148:ALA:HB3	4:J:149:PRO:HD3	1.51	0.93
3:C:106:VAL:O	3:C:107:ASP:HB2	1.13	0.93
4:D:307:GLU:O	4:D:309:PRO:HD3	1.67	0.93
5:E:26:THR:HG21	16:E:1085:HEM:C2C	2.03	0.93
3:C:398:HIS:C	3:C:399:ALA:CA	2.37	0.93
3:C:224:ILE:CA	3:C:225:VAL:N	2.32	0.92
6:L:10:PRO:HB2	6:L:19:ARG:HH11	1.34	0.92
4:D:164:GLN:HE22	4:D:189:HIS:HE1	1.13	0.92
1:G:84:PRO:CG	1:G:173:PRO:CG	2.44	0.92
3:I:224:ILE:CA	3:I:225:VAL:N	2.32	0.92
3:I:449:ARG:HH11	3:I:449:ARG:CG	1.82	0.92
3:C:311:GLN:HG2	3:C:355:THR:HG21	1.51	0.92
2:H:150:CYS:HB2	11:H:1484:CLA:HMC3	1.51	0.92
2:B:59:GLY:CA	11:B:1488:CLA:HED1	1.98	0.92
2:B:263:THR:HG22	2:B:263:THR:O	1.69	0.92
3:C:173:LEU:O	3:C:176:VAL:HG12	1.70	0.92
3:I:155:ASN:O	3:I:159:THR:HG23	1.70	0.91
5:K:62:SER:O	5:K:64:PRO:CD	2.18	0.91
2:H:53:ASN:N	2:H:54:PRO:HD3	1.83	0.91
2:B:60:MET:CA	2:B:61:PHE:N	2.33	0.91
3:C:155:ASN:HB2	3:C:255:THR:HG22	1.53	0.91
2:B:53:ASN:N	2:B:54:PRO:HD3	1.83	0.91
1:A:330:VAL:HG12	4:D:347:PRO:HA	1.53	0.91
9:V:129:LYS:HE3	9:V:135:VAL:HG21	1.50	0.91
1:A:175:GLY:H	12:A:1345:PHO:H192	1.35	0.91
3:C:294:ASN:O	3:C:295:THR:HG23	1.70	0.91
4:J:307:GLU:O	4:J:309:PRO:HD3	1.71	0.91
1:A:310:LYS:HA	9:V:2:GLU:HA	1.51	0.91
1:A:81:ALA:HB3	1:A:174:LEU:O	1.70	0.90
1:A:129:ARG:HH21	4:D:256:ILE:HG23	1.33	0.90
1:G:129:ARG:HH21	4:J:256:ILE:HG23	1.32	0.90
5:K:26:THR:HG21	16:L:1046:HEM:C2C	2.06	0.90
9:T:133:GLY:O	9:T:137:TYR:HB2	1.71	0.90
3:I:95:LEU:O	3:I:185:LEU:HA	1.71	0.90
2:H:60:MET:CA	2:H:61:PHE:N	2.35	0.90
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.54	0.90
1:A:278:TRP:HB3	1:A:279:PRO:HD3	1.53	0.90
1:G:286:THR:HG22	11:G:1342:CLA:O1D	1.72	0.90
2:H:263:THR:O	2:H:263:THR:HG22	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:331:PRO:HG3	4:J:339:PHE:CG	2.07	0.90
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.52	0.89
1:G:92:HIS:HA	3:I:219:GLY:CA	2.02	0.89
2:H:397:VAL:HA	2:H:417:VAL:HG21	1.54	0.89
1:A:222:SER:C	1:A:223:LEU:CA	2.40	0.89
2:H:180:PRO:C	2:H:181:VAL:CA	2.41	0.89
4:J:126:MET:HA	4:J:129:GLN:NE2	1.86	0.89
4:D:253:TRP:HB2	4:D:260:ALA:HB2	1.54	0.89
4:J:323:GLU:HG2	4:J:326:ARG:HH21	1.36	0.89
4:D:102:THR:HG22	5:E:46:VAL:O	1.71	0.89
1:G:63:ILE:HG13	3:I:335:THR:HG21	1.54	0.89
3:I:155:ASN:HB2	3:I:255:THR:HG22	1.54	0.89
1:G:81:ALA:HB3	1:G:174:LEU:O	1.74	0.88
2:B:180:PRO:C	2:B:181:VAL:CA	2.41	0.88
1:G:175:GLY:H	12:G:1345:PHO:H192	1.39	0.88
5:E:59:GLU:O	5:E:60:GLN:HB3	1.72	0.88
1:G:24:THR:C	1:G:25:ASP:CA	2.42	0.87
3:I:242:LEU:O	3:I:245:ILE:HG13	1.74	0.87
1:A:127:MET:HE2	1:A:151:LEU:CD2	2.04	0.87
2:H:59:GLY:CA	11:H:1488:CLA:HED1	2.04	0.87
1:A:286:THR:HG22	11:A:1342:CLA:O1D	1.73	0.87
3:C:95:LEU:O	3:C:185:LEU:HA	1.75	0.87
5:K:62:SER:C	5:K:64:PRO:CD	2.43	0.87
2:B:80:ILE:C	2:B:81:THR:CA	2.43	0.87
4:J:323:GLU:HG2	4:J:326:ARG:NH2	1.90	0.87
1:A:24:THR:C	1:A:25:ASP:CA	2.43	0.87
3:C:190:ALA:C	3:C:191:PRO:CA	2.43	0.87
1:G:57:PRO:HG3	1:G:68:SER:HB3	1.54	0.87
1:G:330:VAL:HG12	4:J:347:PRO:HA	1.53	0.87
1:G:309:ALA:O	9:T:2:GLU:HA	1.75	0.87
3:C:242:LEU:O	3:C:245:ILE:HG13	1.75	0.86
2:H:80:ILE:C	2:H:81:THR:CA	2.43	0.86
3:I:273:SER:HB2	3:I:445:ALA:HB2	1.57	0.86
4:J:102:THR:HG22	5:K:46:VAL:O	1.74	0.86
3:C:341:LEU:C	3:C:342:MET:CA	2.43	0.86
3:C:149:TYR:CA	3:C:150:ASP:N	2.39	0.86
1:A:92:HIS:HA	3:C:219:GLY:CA	2.05	0.86
3:C:212:TYR:C	3:C:213:LEU:CA	2.43	0.86
2:H:329:PRO:CA	2:H:330:MET:N	2.39	0.86
3:C:245:ILE:HD12	3:C:246:ALA:N	1.90	0.86
4:D:330:ALA:HB1	4:D:331:PRO:HD3	0.87	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:65:LEU:C	5:E:66:VAL:CA	2.44	0.86
1:A:334:ARG:C	1:A:335:ASN:CA	2.44	0.85
3:C:449:ARG:HH11	3:C:449:ARG:CG	1.86	0.85
4:D:323:GLU:HG2	4:D:326:ARG:HH21	1.41	0.85
1:G:222:SER:C	1:G:223:LEU:CA	2.44	0.85
4:D:258:GLY:O	4:D:259:ILE:HG13	1.76	0.85
3:I:190:ALA:C	3:I:191:PRO:CA	2.44	0.85
2:B:329:PRO:CA	2:B:330:MET:N	2.39	0.85
2:H:135:LEU:HB2	2:H:136:PRO:CD	2.06	0.85
2:H:31:ALA:HA	2:H:34:ALA:HB3	1.56	0.85
2:B:150:CYS:HB2	11:B:1484:CLA:HMC3	1.57	0.85
4:J:331:PRO:HG3	4:J:339:PHE:HB2	1.59	0.85
2:H:354:LEU:HD11	2:H:378:LYS:CB	2.06	0.85
3:C:82:TYR:HA	3:C:422:PRO:HG2	1.57	0.85
2:H:414:PRO:HB2	2:H:415:PRO:HD3	1.59	0.85
3:I:212:TYR:C	3:I:213:LEU:CA	2.45	0.85
1:A:254:TYR:OH	4:D:129:GLN:HB2	1.77	0.85
3:I:341:LEU:C	3:I:342:MET:CA	2.45	0.85
1:G:334:ARG:C	1:G:335:ASN:CA	2.45	0.85
3:I:353:GLY:CA	3:I:354:GLU:N	2.40	0.84
3:I:82:TYR:HA	3:I:422:PRO:HG2	1.59	0.84
7:P:68:UNK:CA	7:P:69:UNK:N	2.40	0.84
6:F:10:PRO:HB2	6:F:19:ARG:HH11	1.40	0.84
3:I:376:ASP:HB2	3:I:379:LYS:HG3	1.57	0.84
3:I:449:ARG:HG3	3:I:449:ARG:NH1	1.87	0.84
4:J:223:PHE:CE2	4:J:245:SER:HB3	2.13	0.84
3:C:353:GLY:CA	3:C:354:GLU:N	2.40	0.84
3:C:376:ASP:HB2	3:C:379:LYS:HG3	1.56	0.84
1:G:254:TYR:OH	4:J:129:GLN:HB2	1.78	0.84
2:H:263:THR:H	2:H:264:PRO:CD	1.91	0.84
2:B:320:ALA:C	2:B:321:LYS:CA	2.46	0.84
5:E:70:PHE:CA	5:E:72:ALA:N	2.41	0.84
4:D:103:ARG:HG2	4:D:106:GLN:OE1	1.78	0.84
4:D:164:GLN:HE22	4:D:189:HIS:CE1	1.96	0.84
4:D:274:VAL:HB	4:D:275:PRO:HD3	1.57	0.84
2:H:271:THR:HG1	2:H:274:GLN:HG3	1.43	0.84
3:I:228:ASN:CA	3:I:295:THR:HG21	2.07	0.84
7:O:68:UNK:CA	7:O:69:UNK:N	2.41	0.84
4:J:343:GLU:OE1	4:J:343:GLU:N	2.11	0.83
1:G:34:GLY:HA2	1:G:37:MET:HB3	1.61	0.83
3:I:53:HIS:HB3	11:I:1470:CLA:OBD	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:248:ILE:HD12	4:J:235:PHE:HZ	1.43	0.83
5:K:70:PHE:CA	5:K:72:ALA:N	2.41	0.83
10:Y:334:UNK:C	10:Y:335:UNK:O	2.22	0.83
2:B:425:ILE:HG23	2:B:425:ILE:O	1.78	0.83
4:J:164:GLN:HE22	4:J:189:HIS:HE1	1.23	0.83
1:A:63:ILE:HG13	3:C:335:THR:HG21	1.59	0.83
3:C:155:ASN:O	3:C:159:THR:HG23	1.78	0.83
2:H:55:MET:C	2:H:56:TRP:CA	2.47	0.83
3:I:149:TYR:CA	3:I:150:ASP:N	2.41	0.83
5:K:59:GLU:O	5:K:60:GLN:HB3	1.75	0.83
2:H:320:ALA:C	2:H:321:LYS:CA	2.47	0.83
3:I:40:ALA:O	3:I:43:ILE:HG12	1.78	0.83
1:G:176:ILE:HG12	11:G:1343:CLA:HED3	1.61	0.83
2:H:271:THR:OG1	2:H:274:GLN:HG3	1.78	0.83
2:H:316:GLY:HA2	2:H:443:PHE:CD1	2.13	0.83
2:B:316:GLY:HA2	2:B:443:PHE:CD1	2.14	0.82
2:B:397:VAL:HA	2:B:417:VAL:HG21	1.61	0.82
2:H:130:GLU:CA	2:H:131:PRO:N	2.42	0.82
3:I:280:SER:HB2	3:I:434:ALA:O	1.79	0.82
3:I:456:GLU:C	3:I:457:LYS:CA	2.48	0.82
1:A:307:ILE:O	1:A:309:ALA:N	2.09	0.82
2:H:31:ALA:N	11:H:1486:CLA:HBC3	1.94	0.82
1:G:217:SER:OG	4:J:142:ASN:HA	1.79	0.82
2:H:355:PHE:O	2:H:370:LEU:HA	1.80	0.82
2:B:161:LEU:O	2:B:162:PHE:HB2	1.80	0.82
2:H:236:THR:HB	2:H:473:THR:CG2	2.09	0.82
4:J:274:VAL:HB	4:J:275:PRO:HD3	1.61	0.82
2:H:141:ILE:HB	2:H:217:ILE:HD12	1.62	0.82
3:I:294:ASN:O	3:I:295:THR:HG23	1.80	0.82
2:H:89:GLY:CA	2:H:90:PHE:N	2.43	0.82
1:A:290:ILE:HD11	11:A:1342:CLA:OBD	1.80	0.81
6:F:12:SER:O	6:F:14:PRO:CD	2.26	0.81
2:H:24:LEU:HD23	2:H:111:ALA:N	1.96	0.81
4:J:61:HIS:HB3	4:J:63:LEU:HD13	1.61	0.81
4:J:171:PRO:HG3	4:J:181:PHE:CG	2.15	0.81
2:B:130:GLU:CA	2:B:131:PRO:N	2.43	0.81
2:B:236:THR:HB	2:B:473:THR:CG2	2.11	0.81
2:H:45:PHE:CD2	2:H:47:PRO:CD	2.60	0.81
3:I:266:TRP:HB3	3:I:271:TYR:OH	1.81	0.81
3:I:89:ILE:HB	3:I:90:PRO:HD3	1.62	0.81
4:J:258:GLY:O	4:J:259:ILE:HG13	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:445:ALA:HB1	11:C:1463:CLA:HED1	1.61	0.81
3:C:456:GLU:C	3:C:457:LYS:CA	2.48	0.81
2:H:306:PRO:CA	2:H:307:GLU:N	2.43	0.81
1:A:242:GLU:CA	1:A:243:GLU:N	2.43	0.81
3:I:260:ALA:HB1	11:I:1464:CLA:HAA2	1.60	0.81
8:U:5:UNK:C	8:U:7:UNK:N	2.40	0.81
2:B:163:GLY:O	2:B:165:GLY:N	2.13	0.81
2:B:15:ASP:CA	2:B:16:PRO:N	2.43	0.81
2:B:354:LEU:HD11	2:B:378:LYS:CB	2.09	0.81
2:B:89:GLY:CA	2:B:90:PHE:N	2.43	0.81
4:D:86:GLY:HA2	4:D:166:SER:CB	2.10	0.81
3:I:95:LEU:HD23	3:I:97:TRP:HZ3	1.45	0.81
2:B:414:PRO:HB2	2:B:415:PRO:HD3	1.63	0.81
2:B:55:MET:C	2:B:56:TRP:CA	2.49	0.81
2:H:15:ASP:CA	2:H:16:PRO:N	2.44	0.81
1:A:34:GLY:HA2	1:A:37:MET:HB3	1.61	0.80
1:A:63:ILE:HG12	1:A:64:ARG:N	1.96	0.80
3:C:228:ASN:CA	3:C:295:THR:HG21	2.11	0.80
4:D:223:PHE:CE2	4:D:245:SER:HB3	2.15	0.80
2:B:306:PRO:CA	2:B:307:GLU:N	2.43	0.80
1:A:39:PRO:HB2	11:A:1346:CLA:HAB	1.63	0.80
2:H:187:PRO:CA	2:H:188:ASP:N	2.44	0.80
1:A:202:VAL:O	1:A:206:PHE:HB2	1.82	0.80
2:B:236:THR:HB	2:B:473:THR:HG23	1.64	0.80
3:C:53:HIS:HB3	11:C:1470:CLA:OBD	1.80	0.80
4:D:53:THR:HG22	4:D:67:TYR:CD1	2.16	0.80
2:H:295:GLY:C	2:H:296:ALA:CA	2.50	0.80
4:J:122:LEU:HD21	11:J:1351:CLA:C9	2.11	0.80
2:B:295:GLY:C	2:B:296:ALA:CA	2.50	0.80
1:A:217:SER:OG	4:D:142:ASN:HA	1.80	0.80
3:C:185:LEU:O	3:C:230:LEU:HD21	1.82	0.80
3:C:449:ARG:HG3	3:C:449:ARG:NH1	1.88	0.80
6:F:19:ARG:O	6:F:23:VAL:HG23	1.80	0.80
1:G:30:VAL:CA	1:G:31:GLY:N	2.45	0.80
3:I:154:LYS:NZ	3:I:261:ARG:HD3	1.97	0.80
10:X:334:UNK:C	10:X:335:UNK:O	2.26	0.80
4:D:126:MET:HA	4:D:129:GLN:NE2	1.95	0.80
1:G:141:PRO:HG2	3:I:446:GLY:O	1.81	0.80
1:A:141:PRO:HG2	3:C:446:GLY:O	1.82	0.80
1:A:30:VAL:CA	1:A:31:GLY:N	2.45	0.79
1:G:63:ILE:HG12	1:G:64:ARG:N	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:THR:HG22	2:B:107:LEU:HD13	1.63	0.79
3:C:56:HIS:HE1	11:C:1467:CLA:HMA1	1.47	0.79
1:G:39:PRO:HB2	11:G:1346:CLA:HAB	1.64	0.79
1:G:84:PRO:CD	1:G:173:PRO:CG	2.55	0.79
4:J:103:ARG:HG2	4:J:106:GLN:OE1	1.82	0.79
1:G:193:LEU:HB3	4:J:179:PHE:CD1	2.18	0.79
2:B:187:PRO:CA	2:B:188:ASP:N	2.46	0.79
1:A:142:TRP:CB	4:D:220:ASN:OD1	2.31	0.79
2:H:61:PHE:O	2:H:64:PRO:CD	2.29	0.79
3:C:260:ALA:HB1	11:C:1464:CLA:HAA2	1.63	0.79
2:H:161:LEU:O	2:H:162:PHE:HB2	1.81	0.79
1:G:219:VAL:HG21	4:J:268:HIS:CD2	2.16	0.79
3:C:266:TRP:HB3	3:C:271:TYR:OH	1.81	0.79
1:G:222:SER:O	1:G:246:TYR:HA	1.83	0.79
2:H:270:PRO:O	2:H:271:THR:HG23	1.82	0.79
3:I:56:HIS:HE1	11:I:1467:CLA:HMA1	1.47	0.79
3:I:100:GLY:O	3:I:101:PRO:C	2.17	0.79
2:B:135:LEU:HB2	2:B:136:PRO:CD	2.11	0.79
4:J:196:PHE:CE1	4:J:284:ILE:HB	2.18	0.79
6:L:12:SER:O	6:L:14:PRO:CD	2.30	0.79
1:A:176:ILE:HG12	11:A:1343:CLA:HED3	1.65	0.79
2:B:474:LEU:HD11	11:B:1489:CLA:HAA2	1.65	0.79
2:H:45:PHE:O	2:H:47:PRO:HD2	1.84	0.78
4:J:164:GLN:HE22	4:J:189:HIS:CE1	2.00	0.78
4:J:74:LEU:HD23	4:J:175:VAL:HG11	1.62	0.78
4:J:86:GLY:HA2	4:J:166:SER:CB	2.12	0.78
3:C:206:PRO:CA	3:C:207:ARG:N	2.46	0.78
1:G:258:LEU:HA	4:J:128:ARG:HH12	1.49	0.78
4:D:69:GLU:HG2	5:E:55:TYR:OH	1.83	0.78
10:X:59:UNK:O	10:X:60:UNK:C	2.31	0.78
3:I:245:ILE:HD12	3:I:246:ALA:N	1.99	0.78
3:I:52:ALA:HA	11:I:1469:CLA:HMB3	1.66	0.78
9:T:129:LYS:HE3	9:T:135:VAL:CG2	2.14	0.78
1:A:143:ILE:HG13	4:D:220:ASN:ND2	1.96	0.78
4:D:196:PHE:CE1	4:D:284:ILE:HB	2.18	0.78
2:H:383:PHE:O	7:P:107:UNK:HA	1.82	0.78
3:I:206:PRO:CA	3:I:207:ARG:N	2.46	0.78
3:I:305:THR:OG1	3:I:307:PRO:HD2	1.84	0.78
3:I:304:PRO:HG2	3:I:398:HIS:O	1.83	0.78
1:G:161:TYR:CE2	1:G:186:PHE:HE1	2.00	0.78
6:L:19:ARG:O	6:L:23:VAL:HG23	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:261:ARG:HA	3:C:266:TRP:HZ2	1.49	0.77
11:H:1496:CLA:H152	11:H:1497:CLA:HMD3	1.64	0.77
1:A:297:LEU:CD2	3:C:428:THR:HG21	2.14	0.77
1:A:193:LEU:HB3	4:D:179:PHE:CD1	2.19	0.77
3:C:273:SER:HB2	3:C:445:ALA:HB2	1.65	0.77
4:D:331:PRO:HG3	4:D:339:PHE:CG	2.19	0.77
1:G:187:GLN:HB2	11:G:1342:CLA:HAC2	1.66	0.77
1:G:183:MET:HG2	11:G:1342:CLA:HBC2	1.65	0.77
2:B:330:MET:HE2	2:B:446:SER:HB3	1.66	0.77
3:C:305:THR:OG1	3:C:307:PRO:HD2	1.84	0.77
6:F:12:SER:C	6:F:14:PRO:HD2	2.03	0.77
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.66	0.77
2:H:248:ALA:O	2:H:251:VAL:HG23	1.85	0.77
1:A:248:ILE:HD12	4:D:235:PHE:HZ	1.49	0.77
4:D:323:GLU:HG2	4:D:326:ARG:NH2	1.99	0.77
6:L:28:VAL:HB	6:L:29:PRO:HD3	1.66	0.77
4:D:122:LEU:HD21	11:D:1351:CLA:C9	2.14	0.77
2:H:229:LEU:C	2:H:231:MET:H	1.86	0.77
2:H:474:LEU:HD11	11:H:1489:CLA:HAA2	1.67	0.77
4:J:87:HIS:CE1	4:J:162:LEU:HA	2.19	0.77
3:C:167:VAL:O	3:C:170:ILE:HG22	1.85	0.77
1:G:294:ALA:C	1:G:296:ASN:H	1.88	0.77
3:I:261:ARG:HA	3:I:266:TRP:HZ2	1.50	0.77
1:A:330:VAL:CG1	4:D:347:PRO:HA	2.14	0.77
7:P:11:UNK:HA	7:P:173:UNK:CB	2.14	0.77
4:D:343:GLU:OE1	4:D:343:GLU:N	2.16	0.76
2:B:215:PHE:CZ	11:B:1490:CLA:HMD3	2.20	0.76
1:G:242:GLU:CA	1:G:243:GLU:N	2.48	0.76
4:J:267:LEU:O	4:J:271:MET:HG3	1.84	0.76
6:L:37:ILE:HA	6:L:40:MET:HE2	1.67	0.76
1:A:149:ALA:HB3	1:A:150:PRO:HD3	1.66	0.76
2:B:24:LEU:HD23	2:B:111:ALA:N	2.00	0.76
2:H:24:LEU:HD11	11:H:1497:CLA:HBC2	1.64	0.76
2:H:236:THR:HB	2:H:473:THR:HG23	1.66	0.76
2:B:355:PHE:O	2:B:370:LEU:HA	1.84	0.76
4:D:340:VAL:O	4:D:342:PRO:HD2	1.86	0.76
4:J:176:ALA:HA	4:J:179:PHE:HD2	1.49	0.76
4:D:87:HIS:CE1	4:D:162:LEU:HA	2.21	0.76
2:H:134:ASP:O	2:H:136:PRO:HD2	1.85	0.76
4:J:53:THR:HG22	4:J:67:TYR:CD1	2.20	0.76
7:O:11:UNK:HA	7:O:173:UNK:CB	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:THR:OG1	2:B:274:GLN:HG3	1.84	0.76
2:B:383:PHE:O	7:O:107:UNK:HA	1.85	0.76
2:B:45:PHE:CD2	2:B:47:PRO:CD	2.65	0.76
3:C:52:ALA:HA	11:C:1469:CLA:HMB3	1.68	0.76
1:G:62:GLY:CA	1:G:87:ASN:HB3	2.16	0.76
4:J:345:VAL:O	4:J:346:LEU:CB	2.32	0.76
5:K:27:ILE:HB	5:K:28:PRO:HD3	1.67	0.76
6:L:10:PRO:HB2	6:L:19:ARG:NH1	2.00	0.76
2:B:160:GLY:HA2	2:B:163:GLY:HA2	1.66	0.76
1:G:206:PHE:HE1	11:G:1342:CLA:HMB1	1.51	0.76
2:H:118:TRP:C	2:H:119:ASP:CA	2.54	0.76
10:X:470:UNK:O	10:X:473:UNK:N	2.19	0.76
1:A:206:PHE:HE1	11:A:1342:CLA:HMB1	1.51	0.76
2:B:141:ILE:HB	2:B:217:ILE:HD12	1.66	0.76
1:G:290:ILE:HD11	11:G:1342:CLA:OBD	1.85	0.75
8:U:59:UNK:O	8:U:61:UNK:N	2.20	0.75
1:A:64:ARG:O	1:A:66:PRO:HD3	1.86	0.75
2:B:31:ALA:HA	2:B:34:ALA:HB3	1.66	0.75
1:G:143:ILE:HD11	4:J:217:THR:HA	1.68	0.75
2:H:246:PHE:HE1	2:H:463:PHE:HB2	1.51	0.75
2:H:52:LEU:HD22	2:H:337:ALA:HB1	1.68	0.75
3:I:169:GLY:HA2	3:I:244:CYS:SG	2.26	0.75
1:A:62:GLY:CA	1:A:87:ASN:HB3	2.16	0.75
2:B:229:LEU:C	2:B:231:MET:H	1.89	0.75
3:I:116:VAL:HG23	3:I:117:VAL:N	2.01	0.75
6:L:37:ILE:HA	6:L:40:MET:CE	2.16	0.75
8:S:59:UNK:O	8:S:61:UNK:N	2.18	0.75
4:D:340:VAL:O	4:D:342:PRO:CD	2.34	0.75
2:H:138:MET:SD	11:H:1496:CLA:HBC2	2.26	0.75
1:G:330:VAL:CG1	4:J:347:PRO:HA	2.16	0.75
2:B:263:THR:N	2:B:264:PRO:HD3	2.02	0.75
3:I:185:LEU:O	3:I:230:LEU:HD21	1.86	0.75
5:K:13:ILE:HG22	5:K:19:TYR:CD2	2.21	0.75
2:B:118:TRP:C	2:B:119:ASP:CA	2.55	0.75
2:B:248:ALA:O	2:B:251:VAL:HG23	1.86	0.75
2:B:270:PRO:O	2:B:271:THR:HG23	1.86	0.75
3:C:225:VAL:HG13	3:C:289:PHE:HA	1.67	0.75
3:C:35:TRP:CE2	3:C:36:TRP:HD1	2.05	0.75
2:H:229:LEU:O	2:H:231:MET:N	2.20	0.75
7:O:83:UNK:HA	7:O:90:UNK:CB	2.16	0.75
1:A:143:ILE:N	4:D:220:ASN:ND2	2.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ALA:C	1:A:296:ASN:H	1.87	0.75
4:D:167:TRP:O	4:D:168:PHE:HB2	1.86	0.75
5:E:13:ILE:HG22	5:E:19:TYR:CD2	2.21	0.75
5:E:62:SER:O	5:E:64:PRO:N	2.20	0.75
2:H:31:ALA:H	11:H:1486:CLA:CBC	1.99	0.75
1:A:222:SER:O	1:A:246:TYR:HA	1.86	0.74
3:C:315:MET:HG3	3:C:365:TRP:HZ3	1.52	0.74
4:J:69:GLU:HG2	5:K:55:TYR:OH	1.86	0.74
8:S:5:UNK:C	8:S:7:UNK:N	2.42	0.74
9:V:48:THR:OG1	18:V:1138:HEC:HMD3	1.87	0.74
2:B:268:PHE:HB2	2:B:448:ARG:HH11	1.52	0.74
11:B:1496:CLA:H152	11:B:1497:CLA:HMD3	1.68	0.74
3:C:189:TRP:HE1	3:C:295:THR:HG22	1.50	0.74
4:D:61:HIS:HB3	4:D:63:LEU:HD13	1.68	0.74
2:B:246:PHE:HE1	2:B:463:PHE:HB2	1.53	0.74
4:D:74:LEU:HD23	4:D:175:VAL:HG11	1.67	0.74
1:G:142:TRP:CB	4:J:220:ASN:OD1	2.32	0.74
1:G:84:PRO:HG2	1:G:173:PRO:CD	2.16	0.74
9:T:48:THR:OG1	18:T:1138:HEC:HMD3	1.88	0.74
2:B:271:THR:HG1	2:B:274:GLN:HG3	1.50	0.74
9:V:129:LYS:HE3	9:V:135:VAL:CG2	2.17	0.74
2:B:138:MET:SD	11:B:1496:CLA:HBC2	2.27	0.74
1:A:258:LEU:HD12	4:D:128:ARG:NH1	2.02	0.74
4:D:308:ASP:HB3	4:D:311:PHE:HB2	1.68	0.74
2:H:330:MET:CE	2:H:446:SER:HB3	2.18	0.74
2:B:257:TRP:HB2	2:B:452:THR:HG21	1.69	0.74
4:D:329:MET:O	4:D:330:ALA:O	2.06	0.74
1:A:247:ASN:ND2	1:A:247:ASN:O	2.20	0.74
2:H:263:THR:N	2:H:264:PRO:HD2	2.03	0.74
3:C:304:PRO:HG2	3:C:398:HIS:O	1.87	0.74
1:G:258:LEU:HD12	4:J:128:ARG:NH1	2.03	0.74
5:K:62:SER:O	5:K:63:ILE:C	2.26	0.74
3:C:278:ALA:O	3:C:282:MET:HG3	1.87	0.74
3:C:78:GLU:OE2	3:C:104:GLU:HA	1.88	0.74
1:G:310:LYS:NZ	5:K:58:GLN:HG2	2.03	0.74
2:H:52:LEU:C	2:H:54:PRO:HD3	2.08	0.74
10:Y:507:UNK:O	10:Y:509:UNK:N	2.21	0.74
2:B:134:ASP:O	2:B:136:PRO:HD2	1.88	0.73
3:C:370:ARG:HE	3:C:371:GLY:H	1.34	0.73
1:A:107:TYR:C	1:A:109:GLY:H	1.91	0.73
1:A:309:ALA:O	9:V:2:GLU:CG	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:HG13	3:C:335:THR:HG23	1.68	0.73
2:B:229:LEU:O	2:B:231:MET:N	2.21	0.73
1:A:258:LEU:HD12	4:D:128:ARG:CZ	2.18	0.73
1:G:81:ALA:HB3	1:G:174:LEU:C	2.08	0.73
11:H:1488:CLA:H171	4:J:281:MET:HE1	1.68	0.73
1:A:62:GLY:HA2	1:A:87:ASN:HB3	1.70	0.73
3:C:81:MET:HE3	3:C:301:PHE:HA	1.69	0.73
1:G:306:VAL:HG12	1:G:313:VAL:HG22	1.69	0.73
4:J:308:ASP:HB3	4:J:311:PHE:HB2	1.69	0.73
2:B:167:TRP:CG	2:B:267:LEU:HD11	2.23	0.73
3:C:120:ILE:O	3:C:122:SER:N	2.21	0.73
1:G:149:ALA:HB3	1:G:150:PRO:HD3	1.71	0.73
4:J:196:PHE:HE1	4:J:284:ILE:HB	1.52	0.73
4:J:292:ASN:O	4:J:294:ARG:HG2	1.88	0.73
2:B:24:LEU:HD11	11:B:1497:CLA:HBC2	1.69	0.73
3:C:100:GLY:O	3:C:101:PRO:C	2.23	0.73
5:E:62:SER:O	5:E:63:ILE:C	2.26	0.73
1:G:62:GLY:HA2	1:G:87:ASN:HB3	1.69	0.73
3:I:315:MET:HG3	3:I:365:TRP:HZ3	1.54	0.73
4:J:15:PHE:O	4:J:18:LEU:N	2.21	0.73
1:A:309:ALA:O	9:V:2:GLU:HG2	1.88	0.73
1:A:332:HIS:CD2	1:A:333:GLU:H	2.06	0.73
3:I:113:VAL:O	3:I:117:VAL:HG23	1.89	0.73
1:G:258:LEU:HD12	4:J:128:ARG:CZ	2.17	0.73
6:F:43:ILE:CG2	6:F:45:ARG:O	2.36	0.73
2:H:347:ARG:HB2	2:H:398:THR:CB	2.19	0.73
4:D:37:LEU:HD23	4:D:37:LEU:C	2.10	0.73
1:G:202:VAL:O	1:G:206:PHE:HB2	1.89	0.73
1:G:248:ILE:HD12	4:J:235:PHE:CZ	2.24	0.73
3:I:445:ALA:HB1	11:I:1463:CLA:HED1	1.71	0.73
4:J:340:VAL:O	4:J:342:PRO:HD3	1.87	0.73
9:V:133:GLY:O	9:V:137:TYR:CB	2.37	0.73
1:G:222:SER:O	1:G:246:TYR:CA	2.37	0.73
4:D:83:ASN:CG	4:D:336:HIS:HD2	1.92	0.72
1:G:219:VAL:HG11	4:J:268:HIS:CG	2.24	0.72
2:H:247:PHE:O	2:H:251:VAL:HG22	1.89	0.72
3:C:423:ARG:HG3	3:C:423:ARG:O	1.89	0.72
4:J:171:PRO:CD	4:J:181:PHE:CD2	2.67	0.72
4:J:343:GLU:OE2	9:T:134:LYS:NZ	2.22	0.72
2:B:52:LEU:C	2:B:54:PRO:HD3	2.08	0.72
3:C:187:ASP:CB	3:C:230:LEU:HD23	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:ARG:O	1:G:66:PRO:HD3	1.89	0.72
7:O:42:UNK:CB	7:O:53:UNK:HA	2.18	0.72
2:H:263:THR:N	2:H:264:PRO:CD	2.52	0.72
3:C:89:ILE:HB	3:C:90:PRO:HD3	1.69	0.72
2:H:395:GLN:CB	2:H:397:VAL:H	2.02	0.72
3:I:315:MET:O	3:I:319:ILE:HG13	1.88	0.72
7:O:68:UNK:CA	7:O:69:UNK:H	2.03	0.72
7:P:83:UNK:HA	7:P:90:UNK:CB	2.20	0.72
3:C:287:THR:HG22	3:C:430:HIS:CB	2.19	0.72
4:D:290:ALA:C	4:D:291:LEU:HD12	2.09	0.72
1:G:38:ILE:HB	1:G:39:PRO:HD3	1.70	0.72
2:H:172:TYR:HA	2:H:280:PHE:HE1	1.55	0.72
3:I:287:THR:HG22	3:I:430:HIS:CB	2.20	0.72
1:A:81:ALA:HB3	1:A:174:LEU:C	2.09	0.72
2:B:31:ALA:HB2	11:B:1486:CLA:HBC3	1.70	0.72
2:B:172:TYR:HA	2:B:280:PHE:HE1	1.55	0.72
3:C:95:LEU:HD23	3:C:97:TRP:HZ3	1.55	0.72
2:H:257:TRP:HB2	2:H:452:THR:HG21	1.71	0.72
4:D:145:ALA:HA	4:D:276:VAL:HG22	1.70	0.72
2:H:349:LYS:HD2	2:H:394:GLN:HA	1.71	0.72
11:G:1344:CLA:HAB	11:J:1351:CLA:H62	1.70	0.72
4:J:83:ASN:CG	4:J:336:HIS:HD2	1.92	0.72
1:A:258:LEU:HA	4:D:128:ARG:HH12	1.54	0.72
2:B:61:PHE:O	2:B:64:PRO:CD	2.33	0.72
2:B:69:LEU:HD23	11:B:1487:CLA:HMA1	1.72	0.72
1:G:94:TYR:OH	1:G:108:ASN:ND2	2.22	0.72
3:I:102:GLY:H	3:I:193:GLY:CA	2.03	0.72
4:J:152:VAL:HG13	11:J:1351:CLA:HED3	1.72	0.72
1:G:129:ARG:NH2	4:J:256:ILE:HG23	2.04	0.72
10:Y:509:UNK:O	10:Y:510:UNK:C	2.35	0.72
3:C:169:GLY:HA2	3:C:244:CYS:SG	2.29	0.71
4:D:331:PRO:HG3	4:D:339:PHE:HB2	1.72	0.71
3:I:167:VAL:O	3:I:170:ILE:HG22	1.90	0.71
4:J:329:MET:O	4:J:330:ALA:O	2.08	0.71
1:A:112:TYR:CZ	1:A:116:ILE:HD11	2.25	0.71
1:G:247:ASN:O	1:G:247:ASN:ND2	2.22	0.71
4:J:37:LEU:C	4:J:37:LEU:HD23	2.11	0.71
10:X:177:UNK:O	10:X:178:UNK:C	2.38	0.71
3:C:56:HIS:CE1	11:C:1467:CLA:HMA1	2.25	0.71
1:A:143:ILE:HD11	4:D:217:THR:HA	1.72	0.71
1:A:133:LEU:HA	1:A:136:ARG:HB2	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:MET:HE2	4:D:346:LEU:O	1.90	0.71
1:A:143:ILE:H	4:D:220:ASN:ND2	1.89	0.71
3:C:113:VAL:O	3:C:117:VAL:HG23	1.90	0.71
5:E:26:THR:O	5:E:29:ALA:HB3	1.90	0.71
1:G:297:LEU:CD2	3:I:428:THR:HG21	2.21	0.71
3:I:423:ARG:O	3:I:423:ARG:HG3	1.90	0.71
4:J:290:ALA:C	4:J:291:LEU:HD12	2.10	0.71
5:K:10:PHE:HE2	6:L:19:ARG:NE	1.88	0.71
2:H:106:LEU:HB3	11:H:1496:CLA:H121	1.72	0.71
3:I:304:PRO:O	3:I:305:THR:HG23	1.90	0.71
4:J:88:SER:C	4:J:90:LEU:H	1.91	0.71
2:B:163:GLY:O	2:B:164:PRO:C	2.25	0.71
4:D:196:PHE:HE1	4:D:284:ILE:HB	1.53	0.71
1:A:129:ARG:NH2	4:D:256:ILE:HG23	2.05	0.71
5:E:56:TYR:O	5:E:57:ALA:HB2	1.90	0.71
1:G:63:ILE:O	1:G:64:ARG:HD2	1.89	0.71
2:B:31:ALA:H	11:B:1486:CLA:HBC3	1.56	0.71
3:C:116:VAL:HG23	3:C:117:VAL:N	2.04	0.71
3:C:154:LYS:NZ	3:C:261:ARG:HD3	2.05	0.71
2:H:425:ILE:O	2:H:425:ILE:HG23	1.90	0.71
4:D:176:ALA:HA	4:D:179:PHE:HD2	1.55	0.71
2:H:330:MET:HE2	2:H:446:SER:HB3	1.72	0.71
1:G:295:PHE:O	3:I:291:TRP:CZ3	2.44	0.71
2:H:233:ASN:O	2:H:233:ASN:CG	2.28	0.71
3:I:50:LEU:HD23	3:I:132:HIS:CD2	2.26	0.71
7:P:42:UNK:CB	7:P:53:UNK:HA	2.21	0.71
2:H:391:SER:O	2:H:392:PHE:CB	2.38	0.70
4:J:253:TRP:O	4:J:256:ILE:N	2.22	0.70
4:J:72:ASN:O	4:J:74:LEU:N	2.23	0.70
1:G:310:LYS:CA	9:T:2:GLU:HA	2.20	0.70
2:B:247:PHE:O	2:B:251:VAL:HG22	1.91	0.70
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.72	0.70
3:I:370:ARG:HE	3:I:371:GLY:H	1.37	0.70
1:G:219:VAL:HG21	4:J:268:HIS:HD2	1.53	0.70
2:B:330:MET:CE	2:B:446:SER:HB3	2.21	0.70
4:D:15:PHE:O	4:D:18:LEU:N	2.25	0.70
3:I:278:ALA:O	3:I:282:MET:HG3	1.91	0.70
3:I:225:VAL:HG13	3:I:289:PHE:HA	1.73	0.70
4:J:235:PHE:CE1	4:J:237:PRO:HB3	2.26	0.70
1:G:310:LYS:CB	9:T:2:GLU:N	2.52	0.70
4:D:113:PHE:CA	11:D:1353:CLA:HED1	2.19	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:148:ALA:HA	4:D:280:TRP:NE1	2.06	0.70
5:E:10:PHE:HE2	6:F:19:ARG:NE	1.89	0.70
2:H:27:THR:HG22	2:H:107:LEU:HD13	1.74	0.70
3:I:189:TRP:HE1	3:I:295:THR:HG22	1.55	0.70
2:B:233:ASN:O	2:B:233:ASN:CG	2.30	0.70
2:H:69:LEU:HD23	11:H:1487:CLA:HMA1	1.72	0.70
4:J:38:PHE:O	4:J:39:PRO:C	2.27	0.70
1:A:219:VAL:HG21	4:D:268:HIS:CD2	2.26	0.70
1:A:84:PRO:HD3	1:A:173:PRO:HB3	1.72	0.70
2:B:45:PHE:O	2:B:47:PRO:HD2	1.91	0.70
3:C:261:ARG:HA	3:C:266:TRP:CZ2	2.26	0.70
9:V:55:ARG:HH21	9:V:128:ASP:HA	1.57	0.70
10:Y:59:UNK:O	10:Y:60:UNK:C	2.38	0.70
1:A:187:GLN:HB2	11:A:1342:CLA:HAC2	1.73	0.70
1:G:307:ILE:O	1:G:309:ALA:N	2.24	0.70
2:H:398:THR:C	2:H:400:SER:H	1.93	0.70
2:H:468:TRP:O	2:H:471:ALA:HB3	1.92	0.70
7:P:68:UNK:CA	7:P:69:UNK:H	2.04	0.70
1:G:206:PHE:CE1	11:G:1342:CLA:HMB1	2.26	0.70
1:G:331:MET:HE2	4:J:346:LEU:O	1.92	0.70
1:G:60:ILE:HD12	1:G:83:VAL:CG1	2.22	0.70
4:J:111:TRP:O	4:J:114:ILE:N	2.25	0.70
4:J:291:LEU:HD12	4:J:291:LEU:N	2.06	0.70
2:H:215:PHE:CZ	11:H:1490:CLA:HMD3	2.27	0.70
3:I:178:LYS:HA	3:I:182:PHE:HB2	1.74	0.70
3:I:52:ALA:HB2	11:I:1469:CLA:HMA1	1.74	0.70
2:B:263:THR:HG22	2:B:448:ARG:CZ	2.22	0.69
4:J:188:PHE:CZ	4:J:326:ARG:HG2	2.27	0.69
2:B:79:SER:C	2:B:80:ILE:HG13	2.13	0.69
1:G:314:ILE:HG23	4:J:58:TRP:CZ3	2.27	0.69
2:H:94:GLU:HG3	2:H:95:GLY:N	2.07	0.69
3:I:56:HIS:CE1	11:I:1467:CLA:HMA1	2.26	0.69
3:I:178:LYS:HD3	3:I:178:LYS:C	2.13	0.69
3:I:187:ASP:OD1	3:I:187:ASP:O	2.10	0.69
5:K:58:GLN:HE22	9:T:4:THR:HG23	1.57	0.69
1:A:60:ILE:HB	1:A:83:VAL:CG1	2.22	0.69
4:D:88:SER:C	4:D:90:LEU:H	1.94	0.69
1:G:107:TYR:C	1:G:109:GLY:H	1.94	0.69
3:I:390:ARG:HD2	9:T:100:ILE:HD12	1.73	0.69
10:Y:71:UNK:C	10:Y:73:UNK:N	2.54	0.69
2:B:360:PRO:HB2	2:B:363:PHE:HD2	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:SER:O	1:G:75:ASN:HB2	1.93	0.69
4:J:145:ALA:HA	4:J:276:VAL:HG22	1.74	0.69
9:T:93:PRO:HA	9:T:101:PHE:CD2	2.27	0.69
3:C:189:TRP:CH2	3:C:363:GLY:HA2	2.27	0.69
1:A:129:ARG:HH22	4:D:256:ILE:HA	1.58	0.69
1:A:127:MET:CE	1:A:151:LEU:HD22	2.16	0.69
1:G:129:ARG:NH2	4:J:256:ILE:HA	2.06	0.69
4:J:91:LEU:HA	11:J:1353:CLA:O1D	1.93	0.69
7:P:142:UNK:HA	7:P:149:UNK:CB	2.22	0.69
3:C:318:LEU:O	3:C:318:LEU:HD12	1.92	0.69
2:H:360:PRO:HB2	2:H:363:PHE:HD2	1.57	0.69
1:G:330:VAL:HG11	4:J:328:TRP:CZ2	2.28	0.69
1:A:309:ALA:C	9:V:2:GLU:HA	2.11	0.69
4:D:209:LEU:HD23	4:D:209:LEU:C	2.12	0.69
1:A:38:ILE:HB	1:A:39:PRO:HD3	1.74	0.69
2:B:221:PRO:HB3	11:B:1490:CLA:HED3	1.74	0.69
2:B:233:ASN:O	2:B:235:GLU:N	2.26	0.69
3:C:280:SER:HB2	3:C:434:ALA:O	1.92	0.69
2:H:468:TRP:CD1	4:J:144:ILE:HD11	2.27	0.69
2:B:332:LYS:O	2:B:439:SER:HA	1.93	0.69
1:A:129:ARG:NH2	4:D:256:ILE:HA	2.07	0.69
4:D:39:PRO:O	4:D:43:LEU:HB2	1.93	0.69
2:H:330:MET:O	2:H:331:ASN:CG	2.32	0.69
3:I:376:ASP:CB	3:I:379:LYS:HG3	2.23	0.69
4:J:235:PHE:CD1	4:J:235:PHE:O	2.46	0.69
1:A:141:PRO:O	1:A:143:ILE:N	2.26	0.68
2:B:468:TRP:O	2:B:471:ALA:HB3	1.91	0.68
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.75	0.68
4:J:61:HIS:HB3	4:J:63:LEU:CD1	2.22	0.68
1:A:310:LYS:CB	9:V:2:GLU:N	2.53	0.68
1:A:113:GLN:O	1:A:117:PHE:HD2	1.75	0.68
9:V:93:PRO:HA	9:V:101:PHE:CD2	2.29	0.68
3:C:176:VAL:O	3:C:180:MET:HG2	1.93	0.68
4:D:169:PHE:O	4:D:181:PHE:HE2	1.76	0.68
3:C:376:ASP:CB	3:C:379:LYS:HG3	2.22	0.68
3:C:377:LEU:O	3:C:381:LYS:HD3	1.93	0.68
4:J:209:LEU:C	4:J:209:LEU:HD23	2.14	0.68
9:T:78:ASN:OD1	9:T:96:ARG:NH2	2.26	0.68
2:B:234:ILE:O	2:B:235:GLU:C	2.30	0.68
2:B:66:MET:O	2:B:71:VAL:HB	1.93	0.68
4:D:343:GLU:OE2	9:V:134:LYS:NZ	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:ARG:HH22	4:J:256:ILE:HA	1.57	0.68
2:H:256:MET:SD	2:H:263:THR:HG23	2.34	0.68
4:J:176:ALA:HA	4:J:179:PHE:CD2	2.27	0.68
2:B:349:LYS:HD2	2:B:394:GLN:HA	1.75	0.68
2:B:468:TRP:CD1	4:D:144:ILE:HD11	2.29	0.68
1:G:133:LEU:HA	1:G:136:ARG:HB2	1.76	0.68
3:I:128:GLY:HA3	11:I:1471:CLA:CMC	2.24	0.68
3:I:35:TRP:CE2	3:I:36:TRP:HD1	2.11	0.68
3:I:37:ALA:HA	11:I:1466:CLA:CBA	2.21	0.68
11:A:1344:CLA:HAB	11:D:1351:CLA:H62	1.74	0.68
2:H:234:ILE:O	2:H:235:GLU:C	2.32	0.68
2:H:61:PHE:O	2:H:63:LEU:N	2.26	0.68
3:I:225:VAL:O	3:I:225:VAL:HG12	1.94	0.68
4:J:79:SER:HA	4:J:172:SER:HB3	1.76	0.68
1:G:143:ILE:N	4:J:220:ASN:ND2	2.41	0.68
7:O:142:UNK:HA	7:O:149:UNK:CB	2.22	0.68
1:A:121:LEU:O	1:A:121:LEU:HD23	1.94	0.68
1:A:206:PHE:CE1	11:A:1342:CLA:HMB1	2.28	0.68
2:B:52:LEU:HD22	2:B:337:ALA:HB1	1.75	0.68
3:I:261:ARG:HA	3:I:266:TRP:CZ2	2.28	0.68
3:I:154:LYS:HZ1	3:I:261:ARG:HD3	1.58	0.68
1:G:136:ARG:HE	10:Y:29:UNK:CB	2.07	0.68
3:C:187:ASP:O	3:C:187:ASP:OD1	2.11	0.68
4:D:345:VAL:CG1	4:D:345:VAL:O	2.36	0.68
5:K:13:ILE:HG22	5:K:19:TYR:HD2	1.59	0.68
3:C:128:GLY:HA3	11:C:1471:CLA:CMC	2.23	0.68
3:C:170:ILE:HG23	3:C:171:GLY:N	2.08	0.68
1:A:175:GLY:N	12:A:1345:PHO:H192	2.08	0.67
3:C:178:LYS:HD3	3:C:178:LYS:C	2.14	0.67
1:A:330:VAL:HG11	4:D:328:TRP:CZ2	2.29	0.67
1:G:96:ILE:HG22	11:G:1346:CLA:OBD	1.94	0.67
1:A:94:TYR:OH	1:A:108:ASN:ND2	2.27	0.67
2:B:64:PRO:O	2:B:67:ALA:HB3	1.95	0.67
3:C:225:VAL:HG12	3:C:225:VAL:O	1.95	0.67
3:C:354:GLU:C	3:C:356:MET:H	1.97	0.67
1:A:133:LEU:HD12	4:D:256:ILE:CG1	2.23	0.67
6:L:10:PRO:CB	6:L:19:ARG:HH11	2.07	0.67
3:C:240:ILE:HD12	11:C:1465:CLA:H91	1.76	0.67
5:E:41:GLY:O	5:E:44:TYR:N	2.27	0.67
2:H:318:ASN:O	2:H:320:ALA:N	2.27	0.67
3:I:260:ALA:O	3:I:264:PHE:HD2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:SER:O	1:A:246:TYR:CA	2.41	0.67
4:D:291:LEU:HD12	4:D:291:LEU:N	2.09	0.67
3:I:54:VAL:O	3:I:57:ALA:HB3	1.94	0.67
2:B:201:HIS:HD2	2:B:202:HIS:ND1	1.92	0.67
3:C:186:TYR:HE2	3:C:188:THR:HG23	1.60	0.67
1:G:315:ASN:O	1:G:316:THR:OG1	2.13	0.67
1:G:60:ILE:HD12	1:G:83:VAL:HG13	1.76	0.67
2:H:214:LEU:O	2:H:217:ILE:HG22	1.95	0.67
4:J:289:LEU:CD2	4:J:294:ARG:HB3	2.24	0.67
4:J:331:PRO:CG	4:J:339:PHE:CG	2.74	0.67
8:S:59:UNK:O	8:S:60:UNK:C	2.42	0.67
10:X:71:UNK:C	10:X:73:UNK:N	2.57	0.67
3:C:52:ALA:HB2	11:C:1469:CLA:HMA1	1.77	0.67
1:A:331:MET:CE	4:D:346:LEU:O	2.42	0.67
1:G:332:HIS:CD2	1:G:333:GLU:H	2.12	0.67
2:B:347:ARG:HB2	2:B:398:THR:CB	2.24	0.67
1:A:219:VAL:HG11	4:D:268:HIS:CG	2.29	0.67
4:J:126:MET:O	4:J:129:GLN:CG	2.37	0.67
1:A:297:LEU:HD23	3:C:428:THR:HG21	1.75	0.67
11:B:1495:CLA:HBD	11:B:1495:CLA:HBA1	1.76	0.67
3:C:37:ALA:HA	11:C:1466:CLA:CBA	2.23	0.67
1:G:214:MET:HA	1:G:217:SER:HB3	1.77	0.67
1:G:99:ALA:CB	1:G:104:GLU:OE1	2.43	0.67
11:H:1495:CLA:HBA1	11:H:1495:CLA:HBD	1.77	0.67
10:Y:177:UNK:O	10:Y:178:UNK:C	2.42	0.67
1:A:8:ARG:N	1:A:11:ALA:HB3	2.10	0.67
3:C:269:GLU:O	3:C:272:LEU:HB3	1.93	0.67
4:D:145:ALA:HA	4:D:276:VAL:CG2	2.24	0.67
1:G:84:PRO:HD3	1:G:173:PRO:HG3	1.73	0.67
2:H:233:ASN:O	2:H:235:GLU:N	2.27	0.67
2:H:462:PHE:CE1	11:H:1494:CLA:HMB3	2.30	0.67
1:A:267:ASN:O	1:A:270:SER:N	2.27	0.67
2:B:395:GLN:CB	2:B:397:VAL:H	2.08	0.67
2:H:288:VAL:O	2:H:292:LEU:HB2	1.95	0.67
2:H:61:PHE:O	2:H:62:VAL:C	2.33	0.67
3:I:82:TYR:CD2	3:I:302:TYR:O	2.48	0.67
1:A:127:MET:CE	1:A:151:LEU:CD2	2.72	0.66
1:A:70:SER:O	1:A:75:ASN:HB2	1.93	0.66
2:B:106:LEU:HB3	11:B:1496:CLA:H121	1.77	0.66
2:B:30:VAL:O	2:B:34:ALA:N	2.21	0.66
4:D:126:MET:O	4:D:129:GLN:CG	2.41	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:8:ARG:HB2	5:E:9:PRO:HD2	1.76	0.66
4:J:113:PHE:CA	11:J:1353:CLA:HED1	2.21	0.66
2:B:256:MET:SD	2:B:263:THR:HG23	2.35	0.66
1:A:63:ILE:CG1	3:C:335:THR:HG23	2.25	0.66
3:C:79:LYS:HE2	3:C:83:GLU:HG2	1.75	0.66
4:D:38:PHE:O	4:D:39:PRO:C	2.32	0.66
1:G:316:THR:HG22	1:G:318:ALA:H	1.60	0.66
2:H:49:ASP:OD2	2:H:52:LEU:N	2.29	0.66
3:I:176:VAL:O	3:I:180:MET:HG2	1.94	0.66
1:G:286:THR:CG2	11:G:1342:CLA:O1D	2.43	0.66
2:H:64:PRO:O	2:H:67:ALA:HB3	1.96	0.66
3:I:187:ASP:CB	3:I:230:LEU:HD23	2.21	0.66
3:I:315:MET:O	3:I:319:ILE:CG1	2.43	0.66
1:G:214:MET:CE	12:J:1352:PHO:HED1	2.25	0.66
2:B:413:ASP:N	2:B:413:ASP:OD1	2.27	0.66
3:C:298:PRO:O	3:C:299:SER:CB	2.44	0.66
4:D:61:HIS:HB3	4:D:63:LEU:CD1	2.24	0.66
2:H:167:TRP:CG	2:H:267:LEU:HD11	2.30	0.66
10:X:509:UNK:O	10:X:510:UNK:C	2.43	0.66
4:D:188:PHE:CZ	4:D:326:ARG:HG2	2.30	0.66
4:D:72:ASN:O	4:D:74:LEU:N	2.29	0.66
6:F:9:GLU:N	6:F:10:PRO:HD3	2.10	0.66
1:G:218:LEU:HD11	1:G:255:PHE:HD2	1.60	0.66
6:L:12:SER:C	6:L:14:PRO:HD2	2.14	0.66
1:A:99:ALA:CB	1:A:104:GLU:OE1	2.44	0.66
1:A:131:TRP:CH2	11:C:1463:CLA:HAA2	2.30	0.66
1:G:8:ARG:N	1:G:11:ALA:HB3	2.10	0.66
3:I:318:LEU:HD12	3:I:318:LEU:O	1.96	0.66
1:A:63:ILE:O	1:A:64:ARG:HD2	1.96	0.66
1:A:143:ILE:CG1	4:D:220:ASN:HD22	2.00	0.66
2:H:332:LYS:O	2:H:439:SER:HA	1.94	0.66
6:L:33:PHE:O	6:L:36:ALA:N	2.29	0.66
11:A:1346:CLA:HBB1	11:A:1346:CLA:HMB1	1.78	0.66
3:C:77:PRO:C	3:C:79:LYS:H	1.99	0.66
1:G:113:GLN:O	1:G:117:PHE:HD2	1.79	0.66
1:G:133:LEU:HD12	4:J:256:ILE:CG1	2.26	0.66
4:J:263:ASN:O	4:J:266:TRP:N	2.28	0.66
3:C:50:LEU:O	3:C:54:VAL:HG23	1.96	0.66
4:J:235:PHE:HE1	4:J:237:PRO:HB3	1.61	0.66
1:A:315:ASN:O	1:A:316:THR:CB	2.44	0.66
3:C:40:ALA:O	3:C:43:ILE:HG12	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ASN:O	1:A:267:ASN:O	2.14	0.65
3:C:312:ALA:O	3:C:316:THR:HG23	1.96	0.65
6:F:10:PRO:HB2	6:F:19:ARG:NH1	2.10	0.65
2:H:16:PRO:HG3	2:H:132:ALA:O	1.96	0.65
3:I:170:ILE:HG23	3:I:171:GLY:N	2.11	0.65
1:A:316:THR:HG22	1:A:318:ALA:H	1.61	0.65
2:B:139:PHE:CG	2:B:139:PHE:O	2.49	0.65
2:H:263:THR:H	2:H:264:PRO:HD2	1.58	0.65
1:G:142:TRP:HB3	4:J:220:ASN:CG	2.17	0.65
2:B:398:THR:C	2:B:400:SER:H	1.98	0.65
3:C:189:TRP:HE1	3:C:295:THR:CG2	2.09	0.65
1:G:84:PRO:HD2	1:G:173:PRO:HG3	1.71	0.65
2:H:397:VAL:HA	2:H:417:VAL:CG2	2.26	0.65
3:C:50:LEU:HD23	3:C:132:HIS:CD2	2.31	0.65
1:G:315:ASN:O	1:G:316:THR:CB	2.45	0.65
1:G:63:ILE:HG13	3:I:335:THR:HG23	1.79	0.65
2:H:217:ILE:HG12	2:H:217:ILE:O	1.96	0.65
5:K:56:TYR:O	5:K:57:ALA:HB2	1.96	0.65
1:A:310:LYS:CA	9:V:2:GLU:HA	2.22	0.65
1:A:134:SER:HA	1:A:139:MET:HB3	1.78	0.65
2:B:352:GLU:O	2:B:354:LEU:N	2.29	0.65
2:B:94:GLU:HG3	2:B:95:GLY:N	2.11	0.65
3:C:315:MET:O	3:C:319:ILE:HG13	1.95	0.65
3:C:45:LEU:O	3:C:46:SER:C	2.35	0.65
11:G:1344:CLA:CED	4:J:175:VAL:HG13	2.27	0.65
2:H:372:ASP:N	2:H:376:VAL:O	2.24	0.65
1:A:137:LEU:HD12	1:A:139:MET:HE1	1.79	0.65
2:B:195:PRO:O	2:B:196:GLY:C	2.35	0.65
1:A:248:ILE:HD12	4:D:235:PHE:CZ	2.31	0.65
3:I:180:MET:HG3	3:I:181:PHE:H	1.62	0.65
4:J:253:TRP:HB2	4:J:260:ALA:CB	2.24	0.65
1:A:286:THR:CG2	11:A:1342:CLA:O1D	2.45	0.65
1:A:315:ASN:O	1:A:316:THR:OG1	2.14	0.65
2:B:229:LEU:C	2:B:231:MET:N	2.50	0.65
4:D:253:TRP:HB2	4:D:260:ALA:CB	2.27	0.65
2:H:194:ASN:OD1	2:H:196:GLY:N	2.30	0.65
3:I:289:PHE:O	3:I:293:ASN:CB	2.45	0.65
10:Y:470:UNK:O	10:Y:473:UNK:N	2.29	0.65
2:B:288:VAL:HG23	2:B:289:GLN:N	2.12	0.65
2:B:330:MET:O	2:B:331:ASN:CG	2.36	0.65
4:D:167:TRP:O	4:D:168:PHE:CB	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:263:THR:HG22	2:H:448:ARG:CZ	2.26	0.65
1:G:180:PHE:CD2	4:J:192:THR:HB	2.32	0.65
4:J:148:ALA:HA	4:J:280:TRP:NE1	2.12	0.65
1:A:314:ILE:HG23	4:D:58:TRP:CZ3	2.31	0.65
1:A:60:ILE:HD12	1:A:83:VAL:HG13	1.79	0.65
2:B:17:GLY:O	2:B:20:ILE:HB	1.96	0.65
3:C:128:GLY:HA2	11:C:1471:CLA:HBC2	1.78	0.65
4:D:176:ALA:HA	4:D:179:PHE:CD2	2.32	0.65
1:G:143:ILE:H	4:J:220:ASN:ND2	1.95	0.65
2:H:109:LEU:O	2:H:112:CYS:HB2	1.97	0.65
9:T:133:GLY:O	9:T:137:TYR:CB	2.42	0.65
1:A:136:ARG:HE	10:X:29:UNK:CB	2.10	0.65
2:B:268:PHE:O	2:B:269:GLY:O	2.15	0.65
1:G:141:PRO:O	1:G:143:ILE:N	2.29	0.65
5:K:26:THR:O	5:K:29:ALA:HB3	1.97	0.65
10:Y:506:UNK:O	10:Y:507:UNK:C	2.44	0.65
10:Y:71:UNK:O	10:Y:73:UNK:N	2.29	0.65
2:B:79:SER:O	2:B:80:ILE:HG13	1.97	0.64
4:D:91:LEU:HA	11:D:1353:CLA:O1D	1.97	0.64
1:G:159:LEU:O	1:G:163:ILE:HG13	1.96	0.64
1:G:166:GLY:O	1:G:167:SER:HB2	1.97	0.64
1:G:58:VAL:N	1:G:67:VAL:O	2.29	0.64
1:G:83:VAL:HG22	4:J:314:PHE:HE1	1.62	0.64
4:J:39:PRO:O	4:J:43:LEU:HB2	1.96	0.64
4:J:88:SER:C	4:J:90:LEU:N	2.50	0.64
1:A:258:LEU:HG	4:D:128:ARG:HH22	1.62	0.64
3:C:235:GLY:O	3:C:238:ILE:HB	1.97	0.64
3:C:304:PRO:O	3:C:305:THR:HG23	1.97	0.64
1:A:160:ILE:HD12	3:C:431:PHE:HE1	1.62	0.64
11:A:1344:CLA:CED	4:D:175:VAL:HG13	2.27	0.64
4:D:274:VAL:CB	4:D:275:PRO:HD3	2.26	0.64
1:G:307:ILE:C	1:G:309:ALA:H	2.01	0.64
2:H:452:THR:HG22	2:H:452:THR:O	1.96	0.64
3:I:298:PRO:O	3:I:299:SER:CB	2.44	0.64
4:J:161:PRO:HB3	4:J:167:TRP:HA	1.79	0.64
6:L:16:PHE:HZ	10:Y:557:UNK:HA	1.63	0.64
3:C:120:ILE:C	3:C:122:SER:H	2.01	0.64
4:D:193:LEU:O	4:D:195:PRO:HD3	1.97	0.64
1:G:289:GLY:O	1:G:292:THR:HB	1.97	0.64
2:H:229:LEU:C	2:H:231:MET:N	2.49	0.64
3:I:78:GLU:OE2	3:I:104:GLU:HA	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:193:LEU:O	4:J:195:PRO:HD3	1.96	0.64
5:K:62:SER:O	5:K:64:PRO:N	2.30	0.64
9:T:55:ARG:HH21	9:T:128:ASP:HA	1.61	0.64
1:A:60:ILE:HD12	1:A:83:VAL:CG1	2.27	0.64
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.80	0.64
2:B:235:GLU:OE1	2:B:472:ARG:HD3	1.97	0.64
1:G:214:MET:O	1:G:215:HIS:C	2.34	0.64
1:G:217:SER:HG	4:J:142:ASN:HA	1.63	0.64
3:I:162:GLY:HA2	3:I:248:GLY:HA2	1.78	0.64
10:X:507:UNK:O	10:X:509:UNK:N	2.31	0.64
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.77	0.64
2:B:362:PHE:CE2	4:D:184:PHE:HZ	2.15	0.64
2:B:452:THR:O	2:B:452:THR:HG22	1.98	0.64
4:D:347:PRO:O	4:D:348:ARG:CB	2.46	0.64
1:G:36:ILE:O	1:G:39:PRO:HD2	1.96	0.64
2:H:223:GLN:O	2:H:227:LYS:N	2.31	0.64
2:H:236:THR:HB	2:H:473:THR:HG21	1.79	0.64
4:J:7:ARG:O	4:J:8:ALA:O	2.14	0.64
2:B:135:LEU:O	2:B:138:MET:N	2.31	0.64
4:D:272:LEU:HD23	4:D:272:LEU:C	2.17	0.64
1:G:180:PHE:CE2	4:J:192:THR:HB	2.32	0.64
1:G:307:ILE:C	1:G:309:ALA:N	2.46	0.64
3:I:77:PRO:C	3:I:79:LYS:H	2.01	0.64
1:A:309:ALA:O	9:V:2:GLU:HB3	1.95	0.64
10:X:331:UNK:O	10:X:334:UNK:N	2.31	0.64
1:A:269:ARG:NE	4:D:222:LEU:HD13	2.12	0.64
4:D:235:PHE:CD1	4:D:235:PHE:O	2.50	0.64
4:D:152:VAL:HG21	4:D:279:LEU:HD13	1.80	0.64
6:F:29:PRO:O	6:F:32:PHE:HB3	1.97	0.64
3:I:122:SER:O	3:I:125:LEU:N	2.31	0.64
1:A:142:TRP:HB3	4:D:220:ASN:CG	2.16	0.64
3:C:40:ALA:O	3:C:43:ILE:HG23	1.96	0.64
5:E:58:GLN:HE22	9:V:4:THR:HG23	1.63	0.64
11:H:1496:CLA:ND	11:H:1497:CLA:HBB2	2.13	0.64
2:H:354:LEU:CD1	2:H:378:LYS:CB	2.75	0.64
1:G:309:ALA:O	9:T:2:GLU:CA	2.46	0.64
1:A:283:VAL:HG21	12:A:1345:PHO:HMC1	1.80	0.64
2:B:217:ILE:O	2:B:217:ILE:HG12	1.97	0.64
5:E:8:ARG:HB2	5:E:9:PRO:CD	2.28	0.64
6:F:16:PHE:HZ	10:X:557:UNK:HA	1.62	0.64
1:G:117:PHE:HZ	1:G:168:PHE:CZ	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:326:LEU:O	1:G:329:GLU:N	2.31	0.64
3:I:260:ALA:CB	11:I:1464:CLA:HAA2	2.28	0.64
5:K:37:PHE:CE1	5:K:42:LEU:HB2	2.33	0.64
6:L:29:PRO:O	6:L:32:PHE:HB3	1.97	0.64
8:U:55:UNK:O	8:U:56:UNK:C	2.46	0.64
3:C:164:HIS:HA	3:C:167:VAL:HG23	1.80	0.64
4:D:126:MET:HE2	4:D:146:PHE:HB3	1.79	0.64
4:D:57:SER:O	4:D:59:TYR:N	2.31	0.64
4:D:7:ARG:O	4:D:8:ALA:O	2.16	0.64
1:G:137:LEU:HD12	1:G:139:MET:CE	2.29	0.64
1:G:78:ILE:HG23	1:G:176:ILE:HG21	1.79	0.64
3:I:424:SER:O	3:I:428:THR:OG1	2.15	0.64
2:B:214:LEU:O	2:B:217:ILE:HG22	1.97	0.63
3:C:54:VAL:O	3:C:57:ALA:HB3	1.99	0.63
5:E:13:ILE:HG22	5:E:19:TYR:HD2	1.59	0.63
4:J:126:MET:HE2	4:J:146:PHE:HB3	1.79	0.63
4:J:167:TRP:O	4:J:168:PHE:HB2	1.98	0.63
4:J:253:TRP:CB	4:J:260:ALA:HB2	2.27	0.63
1:A:307:ILE:C	1:A:309:ALA:H	2.01	0.63
1:A:34:GLY:O	1:A:36:ILE:N	2.32	0.63
3:C:176:VAL:HG13	3:C:177:ALA:N	2.13	0.63
4:D:289:LEU:CD2	4:D:294:ARG:HB3	2.28	0.63
1:G:269:ARG:NE	4:J:222:LEU:HD13	2.12	0.63
3:I:189:TRP:CH2	3:I:363:GLY:HA2	2.32	0.63
4:J:74:LEU:CD2	4:J:175:VAL:HG11	2.29	0.63
1:A:161:TYR:CE2	1:A:186:PHE:HE1	2.16	0.63
3:C:287:THR:HG22	3:C:430:HIS:HB3	1.79	0.63
3:C:35:TRP:C	3:C:37:ALA:H	2.01	0.63
1:G:85:SER:OG	1:G:113:GLN:HG3	1.99	0.63
4:J:145:ALA:HA	4:J:276:VAL:CG2	2.27	0.63
3:C:289:PHE:O	3:C:293:ASN:CB	2.47	0.63
11:G:1346:CLA:HMB1	11:G:1346:CLA:HBB1	1.79	0.63
1:G:331:MET:CE	4:J:346:LEU:O	2.46	0.63
1:G:258:LEU:O	4:J:128:ARG:NH2	2.32	0.63
4:J:330:ALA:O	4:J:332:GLN:N	2.30	0.63
1:A:104:GLU:HG2	1:A:108:ASN:ND2	2.14	0.63
2:B:194:ASN:OD1	2:B:196:GLY:N	2.31	0.63
3:C:362:ARG:HG3	3:C:362:ARG:HH11	1.64	0.63
2:H:139:PHE:CG	2:H:139:PHE:O	2.51	0.63
8:U:59:UNK:O	8:U:60:UNK:C	2.46	0.63
10:X:71:UNK:O	10:X:73:UNK:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ASN:O	1:A:182:PHE:C	2.36	0.63
4:D:45:LEU:HD22	4:D:49:LEU:HD11	1.81	0.63
4:D:65:SER:HB2	4:D:77:ALA:O	1.98	0.63
1:G:98:GLU:O	1:G:99:ALA:HB3	1.99	0.63
2:H:233:ASN:O	2:H:233:ASN:ND2	2.32	0.63
3:I:50:LEU:O	3:I:54:VAL:HG23	1.99	0.63
1:G:104:GLU:OE2	7:P:36:UNK:CB	2.46	0.63
1:A:310:LYS:HA	9:V:2:GLU:CA	2.27	0.63
1:A:84:PRO:HA	1:A:112:TYR:CG	2.34	0.63
4:D:263:ASN:O	4:D:266:TRP:N	2.28	0.63
4:J:15:PHE:O	4:J:16:ASP:C	2.36	0.63
1:A:297:LEU:HD22	3:C:428:THR:HG21	1.79	0.63
2:B:233:ASN:O	2:B:233:ASN:ND2	2.32	0.63
2:B:391:SER:O	2:B:392:PHE:CB	2.46	0.63
1:G:84:PRO:HG2	1:G:173:PRO:HD3	1.78	0.63
1:G:181:ASN:O	1:G:182:PHE:C	2.37	0.63
1:G:60:ILE:HB	1:G:83:VAL:CG1	2.28	0.63
1:G:85:SER:HA	1:G:109:GLY:O	1.97	0.63
3:I:188:THR:HG21	3:I:298:PRO:HB3	1.81	0.63
1:A:117:PHE:HZ	1:A:168:PHE:CZ	2.17	0.63
11:B:1496:CLA:ND	11:B:1497:CLA:HBB2	2.13	0.63
3:I:97:TRP:CZ3	3:I:178:LYS:NZ	2.66	0.63
3:I:45:LEU:O	3:I:46:SER:C	2.37	0.63
5:K:37:PHE:CD1	5:K:42:LEU:HB2	2.33	0.63
8:S:55:UNK:O	8:S:56:UNK:C	2.47	0.63
1:A:201:GLY:HA3	1:A:286:THR:OG1	1.98	0.62
2:B:263:THR:CG2	2:B:263:THR:O	2.43	0.62
2:B:93:PHE:O	2:B:94:GLU:C	2.37	0.62
3:I:186:TYR:HE2	3:I:188:THR:HG23	1.64	0.62
4:J:171:PRO:CD	4:J:181:PHE:CZ	2.82	0.62
4:J:62:GLY:HA3	5:K:63:ILE:CG2	2.29	0.62
1:A:294:ALA:C	1:A:296:ASN:N	2.51	0.62
3:C:264:PHE:HD1	3:C:274:TYR:HE1	1.48	0.62
4:D:253:TRP:CB	4:D:260:ALA:HB2	2.29	0.62
4:D:63:LEU:N	4:D:63:LEU:HD12	2.14	0.62
3:I:202:PRO:CA	3:I:235:GLY:HA3	2.29	0.62
3:I:95:LEU:HD23	3:I:97:TRP:CZ3	2.32	0.62
7:O:51:UNK:O	7:O:82:UNK:HA	1.99	0.62
9:T:129:LYS:CE	9:T:135:VAL:HG21	2.23	0.62
1:A:137:LEU:HD12	1:A:139:MET:CE	2.29	0.62
6:F:43:ILE:HG23	6:F:45:ARG:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:201:GLY:HA3	1:G:286:THR:OG1	2.00	0.62
3:I:91:HIS:HE1	11:I:1460:CLA:O1D	1.81	0.62
7:P:99:UNK:O	7:P:102:UNK:N	2.31	0.62
9:V:129:LYS:CE	9:V:135:VAL:HG21	2.26	0.62
3:C:91:HIS:HE1	11:C:1460:CLA:O1D	1.81	0.62
4:D:329:MET:O	4:D:330:ALA:C	2.36	0.62
2:H:138:MET:C	2:H:140:GLY:H	2.02	0.62
2:H:195:PRO:O	2:H:196:GLY:C	2.37	0.62
2:H:288:VAL:O	2:H:292:LEU:CB	2.48	0.62
3:I:69:LEU:CD1	3:I:115:GLY:HA3	2.30	0.62
10:X:225:UNK:C	10:X:227:UNK:N	2.62	0.62
2:B:16:PRO:HG3	2:B:132:ALA:O	2.00	0.62
2:B:338:GLN:O	2:B:339:ALA:O	2.17	0.62
3:C:250:TRP:HA	3:C:253:LEU:HD12	1.80	0.62
3:C:260:ALA:O	3:C:264:PHE:HD2	1.82	0.62
4:D:235:PHE:CE1	4:D:237:PRO:HB3	2.33	0.62
2:H:201:HIS:HD2	2:H:202:HIS:ND1	1.98	0.62
5:K:58:GLN:CD	9:T:2:GLU:N	2.53	0.62
10:X:6:UNK:O	10:X:7:UNK:C	2.48	0.62
1:G:112:TYR:CZ	1:G:116:ILE:HD11	2.34	0.62
3:I:312:ALA:O	3:I:316:THR:HG23	1.99	0.62
5:K:8:ARG:HB2	5:K:9:PRO:CD	2.30	0.62
10:Y:200:UNK:O	10:Y:204:UNK:N	2.32	0.62
3:C:307:PRO:HA	3:C:358:PHE:CD1	2.34	0.62
1:G:151:LEU:HG	1:G:155:PHE:CE2	2.35	0.62
2:H:158:LEU:HB3	2:H:199:VAL:HG22	1.81	0.62
3:I:189:TRP:HE1	3:I:295:THR:CG2	2.13	0.62
4:J:272:LEU:HD23	4:J:272:LEU:C	2.20	0.62
4:J:274:VAL:CB	4:J:275:PRO:HD3	2.30	0.62
7:O:88:UNK:O	7:O:139:UNK:HA	2.00	0.62
1:A:96:ILE:HG22	11:A:1346:CLA:OBD	1.99	0.62
2:B:397:VAL:HA	2:B:417:VAL:CG2	2.29	0.62
3:C:161:LEU:O	3:C:164:HIS:HB2	1.99	0.62
11:H:1488:CLA:H171	4:J:281:MET:CE	2.30	0.62
2:H:79:SER:C	2:H:80:ILE:HG13	2.20	0.62
3:I:269:GLU:O	3:I:272:LEU:HB3	1.99	0.62
3:I:287:THR:HG22	3:I:430:HIS:HB3	1.79	0.62
8:U:90:UNK:O	8:U:91:UNK:C	2.43	0.62
3:C:287:THR:HG22	3:C:430:HIS:HB2	1.81	0.62
4:D:238:THR:O	4:D:239:GLN:CB	2.48	0.62
3:I:63:TRP:HE1	11:I:1462:CLA:C2C	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:131:TRP:CH2	11:I:1463:CLA:HAA2	2.35	0.62
3:I:240:ILE:HD12	11:I:1465:CLA:H91	1.81	0.62
4:J:110:LEU:O	4:J:114:ILE:HG13	1.99	0.62
10:Y:6:UNK:O	10:Y:7:UNK:C	2.48	0.62
2:B:354:LEU:CD1	2:B:378:LYS:CB	2.78	0.62
1:G:326:LEU:C	1:G:328:MET:H	2.04	0.62
3:I:58:GLY:HA2	3:I:125:LEU:HD12	1.82	0.62
3:I:135:ARG:C	3:I:136:GLY:O	2.36	0.62
4:J:323:GLU:CG	4:J:326:ARG:HH21	2.10	0.62
4:J:345:VAL:O	4:J:345:VAL:CG1	2.41	0.62
3:C:276:LEU:CD1	11:C:1466:CLA:HBB1	2.29	0.61
2:H:403:GLY:H	2:H:407:ASN:HB2	1.65	0.61
1:G:311:GLY:HA3	9:T:125:ILE:HG21	1.80	0.61
10:X:224:UNK:O	10:X:227:UNK:N	2.33	0.61
4:J:152:VAL:HG21	4:J:279:LEU:HD13	1.82	0.61
1:A:183:MET:CE	11:A:1343:CLA:HHD	2.25	0.61
4:D:46:GLY:HA2	4:D:49:LEU:HD12	1.82	0.61
1:G:96:ILE:HG12	1:G:96:ILE:O	1.99	0.61
3:I:188:THR:CG2	3:I:298:PRO:HB3	2.30	0.61
3:I:354:GLU:C	3:I:356:MET:H	2.02	0.61
4:J:104:TRP:CE2	4:J:109:GLY:HA3	2.35	0.61
11:A:1342:CLA:H122	12:A:1345:PHO:H3A	1.82	0.61
1:A:266:ASN:O	1:A:267:ASN:C	2.37	0.61
2:B:197:GLY:O	2:B:198:VAL:C	2.39	0.61
3:C:58:GLY:HA2	3:C:125:LEU:HD12	1.81	0.61
1:G:160:ILE:HD12	3:I:431:PHE:HE1	1.65	0.61
1:G:63:ILE:CG1	3:I:335:THR:HG23	2.30	0.61
3:I:176:VAL:HG13	3:I:177:ALA:N	2.15	0.61
2:B:138:MET:C	2:B:140:GLY:H	2.04	0.61
3:C:260:ALA:CB	11:C:1464:CLA:HAA2	2.30	0.61
5:E:16:SER:O	5:E:17:VAL:HB	2.00	0.61
1:G:133:LEU:HD12	4:J:256:ILE:HG13	1.83	0.61
1:G:278:TRP:HB3	1:G:279:PRO:CD	2.24	0.61
2:H:18:ARG:NH1	2:H:115:TRP:CZ2	2.69	0.61
3:I:284:PHE:HE1	3:I:431:PHE:CD1	2.18	0.61
1:G:63:ILE:CG1	3:I:335:THR:CG2	2.74	0.61
3:I:390:ARG:CD	9:T:100:ILE:HD12	2.30	0.61
1:A:102:LEU:HD11	1:A:105:TRP:CE3	2.35	0.61
1:A:180:PHE:CE2	4:D:192:THR:HB	2.36	0.61
2:B:403:GLY:H	2:B:407:ASN:HB2	1.64	0.61
2:B:316:GLY:HA2	2:B:443:PHE:HD1	1.62	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:GLY:H	3:C:193:GLY:CA	2.13	0.61
4:D:104:TRP:CE2	4:D:109:GLY:HA3	2.35	0.61
4:D:189:HIS:HA	4:D:294:ARG:HH11	1.65	0.61
2:H:235:GLU:OE1	2:H:472:ARG:HD3	2.01	0.61
2:H:263:THR:O	2:H:263:THR:CG2	2.47	0.61
3:I:116:VAL:CG2	3:I:117:VAL:N	2.64	0.61
3:I:54:VAL:HB	3:I:129:GLY:HA2	1.81	0.61
1:A:214:MET:O	1:A:215:HIS:C	2.38	0.61
3:C:315:MET:HG3	3:C:365:TRP:CZ3	2.36	0.61
4:D:88:SER:C	4:D:90:LEU:N	2.52	0.61
1:G:289:GLY:O	1:G:293:MET:HG3	2.00	0.61
2:H:24:LEU:HB3	2:H:111:ALA:HB2	1.82	0.61
2:H:163:GLY:O	2:H:164:PRO:C	2.38	0.61
11:A:1342:CLA:HBD	11:A:1343:CLA:HAC2	1.83	0.61
1:A:218:LEU:HD11	1:A:255:PHE:HD2	1.66	0.61
1:A:58:VAL:N	1:A:67:VAL:O	2.33	0.61
2:B:31:ALA:CB	11:B:1486:CLA:HBC3	2.30	0.61
2:B:458:PHE:CG	11:B:1485:CLA:HMC3	2.35	0.61
1:A:295:PHE:O	3:C:291:TRP:CZ3	2.53	0.61
3:C:82:TYR:CD2	3:C:302:TYR:O	2.53	0.61
1:G:294:ALA:C	1:G:296:ASN:N	2.50	0.61
2:H:135:LEU:O	2:H:138:MET:N	2.34	0.61
2:H:316:GLY:HA2	2:H:443:PHE:HD1	1.66	0.61
3:I:259:TRP:HZ3	11:I:1464:CLA:H12	1.66	0.61
7:P:51:UNK:O	7:P:82:UNK:HA	1.99	0.61
3:C:367:GLU:O	3:C:368:PRO:C	2.38	0.61
4:D:111:TRP:O	4:D:114:ILE:N	2.34	0.61
3:I:230:LEU:O	3:I:234:VAL:HG23	2.01	0.61
4:J:171:PRO:HD2	4:J:181:PHE:CZ	2.36	0.61
4:J:223:PHE:HE2	4:J:245:SER:HB3	1.63	0.61
2:H:364:GLU:OE1	4:J:296:TYR:CD2	2.54	0.61
7:P:10:UNK:O	7:P:173:UNK:CB	2.49	0.61
1:A:157:VAL:O	1:A:157:VAL:HG12	2.01	0.60
1:A:306:VAL:HG23	1:A:308:ASP:H	1.65	0.60
2:B:445:THR:OG1	2:B:446:SER:N	2.33	0.60
3:C:162:GLY:HA2	3:C:248:GLY:HA2	1.82	0.60
2:H:288:VAL:O	2:H:292:LEU:N	2.25	0.60
7:O:105:UNK:O	7:O:106:UNK:CB	2.49	0.60
8:S:27:UNK:O	8:S:28:UNK:C	2.48	0.60
10:Y:468:UNK:O	10:Y:469:UNK:C	2.49	0.60
2:B:68:ARG:HB3	2:B:267:LEU:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:337:GLU:HG3	4:D:339:PHE:HE2	1.65	0.60
5:E:41:GLY:O	5:E:44:TYR:HB2	2.01	0.60
1:G:99:ALA:HB2	1:G:104:GLU:OE1	2.01	0.60
1:G:297:LEU:HD22	3:I:428:THR:HG21	1.82	0.60
2:H:268:PHE:HB2	2:H:448:ARG:HH11	1.66	0.60
3:I:315:MET:HG3	3:I:365:TRP:CZ3	2.36	0.60
1:A:151:LEU:HG	1:A:155:PHE:CE2	2.36	0.60
2:B:285:ASN:O	2:B:289:GLN:HB2	2.01	0.60
4:D:87:HIS:HE1	4:D:162:LEU:HA	1.64	0.60
1:G:156:ALA:HA	1:G:160:ILE:HB	1.83	0.60
8:S:12:UNK:C	8:S:14:UNK:N	2.60	0.60
8:S:1:UNK:O	8:S:3:UNK:N	2.32	0.60
3:C:73:ALA:HB3	3:C:74:HIS:HD2	1.66	0.60
1:G:121:LEU:HD23	1:G:121:LEU:O	2.01	0.60
2:H:93:PHE:O	2:H:94:GLU:C	2.40	0.60
7:O:75:UNK:O	7:O:76:UNK:C	2.50	0.60
2:B:149:LEU:HG	11:B:1484:CLA:CBC	2.28	0.60
2:B:462:PHE:CE1	11:B:1494:CLA:HMB3	2.35	0.60
3:I:128:GLY:HA2	11:I:1471:CLA:HBC2	1.83	0.60
10:Y:225:UNK:C	10:Y:227:UNK:N	2.62	0.60
10:Y:560:UNK:O	10:Y:561:UNK:C	2.50	0.60
1:A:143:ILE:N	4:D:220:ASN:HD21	1.99	0.60
1:A:207:GLY:O	1:A:210:LEU:HB3	2.02	0.60
2:B:223:GLN:O	2:B:227:LYS:N	2.34	0.60
6:F:36:ALA:O	6:F:39:ALA:HB3	2.01	0.60
2:H:352:GLU:O	2:H:354:LEU:N	2.35	0.60
2:B:318:ASN:O	2:B:320:ALA:N	2.35	0.60
2:B:33:TRP:HE1	11:B:1488:CLA:HBC2	1.65	0.60
2:B:346:PHE:O	2:B:354:LEU:HB3	2.02	0.60
4:D:253:TRP:O	4:D:256:ILE:N	2.29	0.60
6:F:33:PHE:O	6:F:36:ALA:N	2.34	0.60
3:I:52:ALA:CA	11:I:1469:CLA:HMB3	2.32	0.60
3:I:225:VAL:HG22	3:I:289:PHE:HD1	1.67	0.60
3:I:35:TRP:C	3:I:37:ALA:H	2.04	0.60
4:J:102:THR:O	4:J:105:CYS:HB2	2.02	0.60
4:J:191:TRP:HZ3	4:J:194:ASN:ND2	1.98	0.60
1:A:166:GLY:O	1:A:167:SER:HB2	2.02	0.60
3:C:226:SER:OG	3:C:227:VAL:N	2.34	0.60
4:D:74:LEU:CD2	4:D:175:VAL:HG11	2.32	0.60
1:G:137:LEU:HD12	1:G:139:MET:HE1	1.84	0.60
1:G:310:LYS:HD2	5:K:58:GLN:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:264:PHE:HD1	3:I:274:TYR:HE1	1.50	0.60
3:I:367:GLU:O	3:I:368:PRO:C	2.39	0.60
3:C:362:ARG:HG3	3:C:362:ARG:NH1	2.16	0.60
4:D:102:THR:O	4:D:105:CYS:HB2	2.02	0.60
1:G:314:ILE:HG23	4:J:58:TRP:HZ3	1.67	0.60
5:K:13:ILE:HA	5:K:16:SER:HB2	1.84	0.60
5:K:8:ARG:HB2	5:K:9:PRO:HD2	1.84	0.60
8:U:30:UNK:O	8:U:31:UNK:C	2.49	0.60
2:B:238:LEU:HD21	2:B:469:HIS:CD2	2.37	0.60
3:C:319:ILE:HD11	3:C:384:ILE:HD11	1.83	0.60
4:D:152:VAL:HG13	11:D:1351:CLA:HED3	1.83	0.60
4:D:62:GLY:HA3	5:E:63:ILE:CG2	2.32	0.60
1:G:127:MET:O	1:G:130:GLN:HB3	2.02	0.60
1:G:244:GLU:OE2	1:G:246:TYR:CE1	2.55	0.60
3:I:363:GLY:O	3:I:364:PRO:O	2.20	0.60
4:J:331:PRO:HG2	4:J:339:PHE:CB	2.07	0.60
4:D:223:PHE:HE2	4:D:245:SER:HB3	1.67	0.59
1:G:267:ASN:O	1:G:270:SER:N	2.34	0.59
1:G:211:PHE:CE2	1:G:274:PHE:HE2	2.19	0.59
2:H:362:PHE:CE2	4:J:184:PHE:HZ	2.19	0.59
4:J:61:HIS:CB	4:J:63:LEU:HD13	2.30	0.59
6:L:33:PHE:O	6:L:35:GLY:N	2.34	0.59
1:A:180:PHE:CD2	4:D:192:THR:HB	2.37	0.59
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.83	0.59
4:D:235:PHE:O	4:D:237:PRO:HD3	2.02	0.59
1:G:62:GLY:O	1:G:63:ILE:HB	2.01	0.59
2:H:135:LEU:HD12	2:H:232:GLY:HA2	1.83	0.59
2:H:445:THR:OG1	2:H:446:SER:N	2.34	0.59
3:I:287:THR:HG22	3:I:430:HIS:HB2	1.82	0.59
4:J:235:PHE:O	4:J:237:PRO:HD3	2.01	0.59
1:A:104:GLU:OE2	7:O:36:UNK:CB	2.50	0.59
11:G:1344:CLA:HED3	4:J:175:VAL:HG13	1.82	0.59
1:G:175:GLY:N	12:G:1345:PHO:H192	2.13	0.59
1:G:143:ILE:HG13	4:J:220:ASN:ND2	2.08	0.59
2:H:135:LEU:HD22	2:H:237:VAL:HG21	1.83	0.59
2:H:272:ARG:HG2	2:H:273:TYR:CD2	2.36	0.59
3:C:390:ARG:HD2	9:V:100:ILE:HD12	1.84	0.59
1:A:99:ALA:HB2	1:A:104:GLU:OE1	2.02	0.59
2:B:172:TYR:HA	2:B:280:PHE:CE1	2.37	0.59
3:C:54:VAL:HB	3:C:129:GLY:HA2	1.84	0.59
4:D:236:ASN:C	4:D:238:THR:H	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:113:TRP:HD1	11:H:1496:CLA:H191	1.67	0.59
2:H:446:SER:HB2	2:H:447:PRO:HD2	1.85	0.59
2:H:458:PHE:CG	11:H:1485:CLA:HMC3	2.37	0.59
3:I:297:TYR:HD1	3:I:302:TYR:CZ	2.20	0.59
6:L:16:PHE:CZ	10:Y:557:UNK:HA	2.37	0.59
10:X:200:UNK:O	10:X:204:UNK:N	2.35	0.59
1:A:159:LEU:O	1:A:163:ILE:HG13	2.03	0.59
3:C:49:LEU:O	3:C:50:LEU:C	2.40	0.59
3:C:63:TRP:HE1	11:C:1462:CLA:C2C	2.15	0.59
2:H:347:ARG:HD2	2:H:398:THR:CB	2.32	0.59
1:A:311:GLY:HA3	9:V:125:ILE:HG21	1.83	0.59
10:X:182:UNK:O	10:X:184:UNK:N	2.36	0.59
10:Y:331:UNK:O	10:Y:334:UNK:N	2.35	0.59
1:A:192:ILE:O	1:A:195:HIS:N	2.35	0.59
1:A:214:MET:HA	1:A:217:SER:HB3	1.85	0.59
2:B:313:ASP:O	2:B:314:TYR:O	2.18	0.59
2:B:347:ARG:HD2	2:B:398:THR:CB	2.33	0.59
3:C:188:THR:HG21	3:C:298:PRO:HB3	1.84	0.59
5:E:37:PHE:CE1	5:E:42:LEU:HB3	2.38	0.59
1:G:104:GLU:HG2	1:G:108:ASN:ND2	2.18	0.59
2:H:106:LEU:HD22	11:H:1496:CLA:H143	1.84	0.59
1:G:297:LEU:HD23	3:I:428:THR:HG21	1.84	0.59
4:J:87:HIS:HE1	4:J:161:PRO:O	1.85	0.59
5:K:10:PHE:CD2	6:L:19:ARG:NH2	2.70	0.59
7:O:82:UNK:O	7:O:90:UNK:CB	2.50	0.59
10:Y:357:UNK:O	10:Y:361:UNK:N	2.36	0.59
1:A:96:ILE:O	1:A:96:ILE:HG12	2.01	0.59
2:B:236:THR:HB	2:B:473:THR:HG21	1.85	0.59
2:B:415:PRO:O	2:B:419:SER:N	2.32	0.59
3:C:248:GLY:O	3:C:252:ILE:HG13	2.03	0.59
3:C:52:ALA:CA	11:C:1469:CLA:HMB3	2.32	0.59
4:D:152:VAL:CG2	4:D:279:LEU:HB3	2.32	0.59
4:D:61:HIS:CB	4:D:63:LEU:HD13	2.32	0.59
5:E:74:GLN:O	5:E:77:GLU:N	2.36	0.59
7:O:123:UNK:O	7:O:124:UNK:C	2.50	0.59
1:A:78:ILE:HG23	1:A:176:ILE:HG21	1.84	0.59
2:B:193:TYR:CE1	2:B:259:GLY:HA2	2.38	0.59
2:B:220:ARG:HB3	2:B:221:PRO:HD2	1.83	0.59
1:A:83:VAL:HG22	4:D:314:PHE:HE1	1.66	0.59
5:E:42:LEU:O	5:E:43:ALA:C	2.41	0.59
6:F:16:PHE:CZ	10:X:557:UNK:HA	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:1342:CLA:HBD	11:G:1343:CLA:HAC2	1.85	0.59
7:P:75:UNK:O	7:P:76:UNK:C	2.51	0.59
8:S:30:UNK:O	8:S:31:UNK:C	2.51	0.59
10:Y:357:UNK:O	10:Y:360:UNK:N	2.35	0.59
3:C:126:GLY:O	3:C:130:VAL:HG23	2.03	0.59
3:C:188:THR:CG2	3:C:298:PRO:HB3	2.32	0.59
4:D:161:PRO:HB3	4:D:167:TRP:HA	1.85	0.59
4:D:209:LEU:HD21	4:D:213:ILE:HD11	1.85	0.59
1:G:131:TRP:HB2	1:G:144:CYS:HB2	1.85	0.59
1:G:134:SER:HA	1:G:139:MET:HB3	1.84	0.59
1:G:49:VAL:O	1:G:53:ILE:HG13	2.03	0.59
3:I:116:VAL:HG23	3:I:117:VAL:H	1.68	0.59
3:I:266:TRP:CD1	3:I:266:TRP:N	2.71	0.59
10:Y:118:UNK:O	10:Y:119:UNK:C	2.49	0.59
1:A:90:GLY:O	1:A:167:SER:HA	2.02	0.59
2:B:353:GLU:O	2:B:354:LEU:O	2.21	0.59
1:G:84:PRO:HA	1:G:112:TYR:CG	2.38	0.59
4:J:347:PRO:O	4:J:348:ARG:CB	2.51	0.59
6:L:18:VAL:O	6:L:21:VAL:N	2.36	0.59
7:P:88:UNK:O	7:P:139:UNK:HA	2.02	0.59
8:S:44:UNK:O	8:S:45:UNK:C	2.50	0.59
1:A:60:ILE:HB	1:A:83:VAL:HG12	1.85	0.58
1:A:63:ILE:CG1	1:A:64:ARG:N	2.64	0.58
1:A:85:SER:HA	1:A:109:GLY:O	2.03	0.58
2:B:470:GLY:O	2:B:473:THR:HB	2.03	0.58
3:C:250:TRP:CD1	3:C:250:TRP:O	2.56	0.58
2:H:145:LEU:O	2:H:146:ALA:C	2.41	0.58
3:I:163:PHE:O	11:I:1470:CLA:HBB1	2.03	0.58
4:J:171:PRO:HG3	4:J:181:PHE:CD1	2.38	0.58
5:K:58:GLN:HE22	9:T:4:THR:CG2	2.15	0.58
2:B:167:TRP:CB	2:B:267:LEU:HD11	2.33	0.58
2:B:31:ALA:N	11:B:1486:CLA:HBC3	2.18	0.58
4:D:274:VAL:HB	4:D:275:PRO:CD	2.32	0.58
1:G:114:LEU:HA	11:G:1346:CLA:CED	2.24	0.58
2:H:351:GLY:O	2:H:353:GLU:N	2.36	0.58
4:J:46:GLY:HA2	4:J:49:LEU:HD12	1.85	0.58
4:J:52:THR:CG2	4:J:67:TYR:HE1	2.01	0.58
9:T:4:THR:HB	9:T:5:PRO:CD	2.33	0.58
5:E:58:GLN:HE22	9:V:4:THR:CG2	2.16	0.58
10:Y:224:UNK:O	10:Y:227:UNK:N	2.36	0.58
1:A:131:TRP:O	1:A:134:SER:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:LEU:O	2:B:112:CYS:HB2	2.03	0.58
3:C:286:ALA:HB2	11:C:1460:CLA:HMD3	1.84	0.58
3:C:264:PHE:HD1	3:C:274:TYR:CE1	2.21	0.58
1:G:137:LEU:HB2	1:G:139:MET:CE	2.33	0.58
2:H:172:TYR:O	2:H:174:LEU:HG	2.03	0.58
2:H:353:GLU:O	2:H:354:LEU:O	2.21	0.58
3:I:276:LEU:CD1	11:I:1466:CLA:HBB1	2.33	0.58
2:B:201:HIS:CD2	2:B:202:HIS:ND1	2.71	0.58
2:B:76:SER:O	7:P:66:UNK:CA	2.52	0.58
3:C:228:ASN:OD1	3:C:229:ASN:N	2.36	0.58
4:D:79:SER:HA	4:D:172:SER:HB3	1.85	0.58
4:D:191:TRP:CZ2	4:D:286:VAL:HG22	2.39	0.58
5:E:10:PHE:CD2	6:F:19:ARG:NH2	2.72	0.58
1:G:90:GLY:O	1:G:167:SER:HA	2.03	0.58
2:H:197:GLY:O	2:H:198:VAL:C	2.42	0.58
2:H:17:GLY:O	2:H:20:ILE:HB	2.03	0.58
2:H:332:LYS:O	2:H:439:SER:CA	2.51	0.58
4:J:152:VAL:HG11	11:J:1351:CLA:HBA1	1.84	0.58
4:D:302:GLU:OE1	7:O:114:UNK:CB	2.52	0.58
7:P:105:UNK:O	7:P:106:UNK:CB	2.50	0.58
10:X:578:UNK:C	10:X:580:UNK:N	2.64	0.58
4:D:36:LEU:HD23	11:D:1353:CLA:HBB2	1.84	0.58
4:D:16:ASP:O	4:D:17:ILE:C	2.41	0.58
11:G:1342:CLA:H143	12:G:1345:PHO:H62	1.85	0.58
1:G:183:MET:HA	11:G:1342:CLA:HMD2	1.83	0.58
3:I:156:LYS:O	3:I:160:ILE:HG13	2.03	0.58
4:J:87:HIS:HE1	4:J:162:LEU:HA	1.66	0.58
4:J:191:TRP:CZ2	4:J:286:VAL:HG22	2.39	0.58
4:J:65:SER:HB2	4:J:77:ALA:O	2.02	0.58
3:C:320:ARG:NH1	9:V:49:ASN:OD1	2.36	0.58
1:A:157:VAL:CG1	1:A:172:MET:HB3	2.34	0.58
2:B:372:ASP:N	2:B:376:VAL:O	2.31	0.58
2:B:435:GLU:O	2:B:436:THR:CB	2.48	0.58
5:E:59:GLU:O	5:E:60:GLN:CB	2.49	0.58
1:G:161:TYR:CE2	1:G:186:PHE:CE1	2.89	0.58
1:G:161:TYR:HB3	1:G:162:PRO:HD3	1.86	0.58
1:G:157:VAL:CG1	1:G:172:MET:HB3	2.34	0.58
2:H:53:ASN:N	2:H:54:PRO:CD	2.62	0.58
3:I:291:TRP:HD1	3:I:292:PHE:CD2	2.21	0.58
3:I:362:ARG:HG3	3:I:362:ARG:HH11	1.69	0.58
1:A:244:GLU:OE2	1:A:246:TYR:CE1	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:TRP:O	11:C:1466:CLA:H43	2.04	0.58
4:J:16:ASP:O	4:J:17:ILE:C	2.42	0.58
1:A:85:SER:OG	1:A:113:GLN:HG3	2.04	0.58
1:A:98:GLU:O	1:A:99:ALA:HB3	2.02	0.58
3:C:283:GLY:O	3:C:286:ALA:HB3	2.02	0.58
3:C:315:MET:O	3:C:319:ILE:CG1	2.52	0.58
4:D:93:TRP:HH2	11:D:1353:CLA:HBA2	1.69	0.58
2:H:163:GLY:O	2:H:165:GLY:N	2.35	0.58
2:H:398:THR:C	2:H:400:SER:N	2.57	0.58
3:I:286:ALA:HB2	11:I:1460:CLA:HMD3	1.86	0.58
5:K:15:THR:HG22	5:K:15:THR:O	2.02	0.58
10:Y:519:UNK:O	10:Y:522:UNK:N	2.36	0.58
1:A:207:GLY:O	1:A:210:LEU:N	2.37	0.58
2:B:425:ILE:O	2:B:426:PHE:HB3	2.03	0.58
3:C:235:GLY:HA2	3:C:238:ILE:HD12	1.84	0.58
3:C:363:GLY:O	3:C:364:PRO:O	2.21	0.58
3:C:56:HIS:ND1	11:C:1467:CLA:HHB	2.18	0.58
1:G:131:TRP:O	1:G:134:SER:HB2	2.03	0.58
1:G:176:ILE:HG23	1:G:180:PHE:CE1	2.39	0.58
2:H:30:VAL:HB	11:H:1486:CLA:HBC1	1.86	0.58
2:H:31:ALA:HA	2:H:34:ALA:CB	2.29	0.58
3:I:109:PHE:HB3	3:I:110:PRO:HD3	1.85	0.58
3:I:73:ALA:HB3	3:I:74:HIS:HD2	1.69	0.58
4:J:148:ALA:HB3	4:J:149:PRO:CD	2.30	0.58
4:J:91:LEU:C	4:J:93:TRP:H	2.06	0.58
1:A:63:ILE:CG1	3:C:335:THR:CG2	2.75	0.58
4:D:52:THR:CG2	4:D:67:TYR:HE1	2.00	0.58
5:E:63:ILE:HG22	5:E:63:ILE:O	2.03	0.58
2:H:243:ALA:O	2:H:246:PHE:HB3	2.04	0.58
2:H:425:ILE:O	2:H:426:PHE:HB3	2.02	0.58
3:I:248:GLY:O	3:I:252:ILE:HG13	2.03	0.58
4:J:225:ASP:O	4:J:225:ASP:OD1	2.21	0.58
7:O:64:UNK:HA	7:O:70:UNK:O	2.04	0.58
9:V:4:THR:HB	9:V:5:PRO:CD	2.33	0.58
2:B:394:GLN:O	2:B:395:GLN:CB	2.51	0.57
2:B:53:ASN:N	2:B:54:PRO:CD	2.62	0.57
4:D:91:LEU:C	4:D:93:TRP:H	2.08	0.57
1:G:310:LYS:HA	9:T:2:GLU:CA	2.27	0.57
2:H:161:LEU:O	2:H:162:PHE:CB	2.52	0.57
2:H:280:PHE:CZ	2:H:312:TYR:HD2	2.22	0.57
3:I:49:LEU:O	3:I:50:LEU:C	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:263:ASN:O	4:J:264:LYS:C	2.42	0.57
8:U:1:UNK:O	8:U:3:UNK:N	2.36	0.57
2:B:161:LEU:O	2:B:162:PHE:CB	2.51	0.57
3:C:116:VAL:CG2	3:C:117:VAL:N	2.67	0.57
3:C:97:TRP:CZ3	3:C:178:LYS:NZ	2.72	0.57
3:C:21:ILE:O	3:C:22:PHE:CB	2.53	0.57
3:C:355:THR:HG22	3:C:355:THR:O	2.04	0.57
4:D:160:TYR:HB3	4:D:161:PRO:CD	2.28	0.57
2:H:265:ILE:HD12	2:H:270:PRO:HA	1.87	0.57
2:H:313:ASP:O	2:H:314:TYR:O	2.21	0.57
2:H:94:GLU:CG	2:H:95:GLY:N	2.66	0.57
3:I:225:VAL:HG22	3:I:289:PHE:CD1	2.39	0.57
1:G:288:LEU:HD13	3:I:432:VAL:HG22	1.86	0.57
4:J:152:VAL:CG2	4:J:279:LEU:HB3	2.34	0.57
12:G:1345:PHO:CBB	4:J:205:LEU:HD21	2.34	0.57
1:A:126:TYR:O	1:A:130:GLN:HB2	2.05	0.57
1:A:131:TRP:HB2	1:A:144:CYS:HB2	1.86	0.57
1:A:142:TRP:CH2	1:A:273:PHE:CE1	2.92	0.57
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.32	0.57
4:D:235:PHE:HD2	4:D:243:THR:CG2	2.17	0.57
4:D:330:ALA:O	4:D:332:GLN:N	2.37	0.57
4:D:56:THR:N	5:E:49:THR:HG22	2.19	0.57
2:H:18:ARG:O	2:H:21:ALA:HB3	2.05	0.57
2:H:221:PRO:HB3	11:H:1490:CLA:HED3	1.85	0.57
2:H:68:ARG:HB3	2:H:267:LEU:HD13	1.85	0.57
4:J:302:GLU:OE1	7:P:114:UNK:CB	2.51	0.57
3:C:250:TRP:CD1	3:C:250:TRP:C	2.77	0.57
3:C:35:TRP:C	3:C:37:ALA:N	2.57	0.57
4:D:267:LEU:O	4:D:271:MET:HG3	2.04	0.57
4:D:52:THR:O	4:D:66:SER:HA	2.04	0.57
1:G:142:TRP:CH2	1:G:273:PHE:CE1	2.93	0.57
1:G:98:GLU:O	1:G:99:ALA:CB	2.52	0.57
2:H:27:THR:O	11:H:1486:CLA:HBC1	2.05	0.57
4:J:179:PHE:HA	4:J:182:LEU:HD12	1.87	0.57
7:O:10:UNK:O	7:O:173:UNK:CB	2.53	0.57
8:S:59:UNK:C	8:S:61:UNK:N	2.67	0.57
1:A:114:LEU:HA	11:A:1346:CLA:CED	2.28	0.57
1:A:210:LEU:HD12	1:A:210:LEU:C	2.24	0.57
1:A:35:VAL:HG12	1:A:35:VAL:O	2.04	0.57
2:B:24:LEU:HB3	2:B:111:ALA:HB2	1.87	0.57
2:B:113:TRP:HD1	11:B:1496:CLA:H191	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:PHE:O	11:C:1470:CLA:HBB1	2.05	0.57
4:D:152:VAL:CG2	4:D:279:LEU:HD13	2.34	0.57
2:H:424:ALA:O	2:H:426:PHE:N	2.37	0.57
3:I:154:LYS:HZ3	3:I:261:ARG:HD3	1.70	0.57
4:J:156:VAL:HG12	4:J:156:VAL:O	2.04	0.57
7:P:24:UNK:O	7:P:25:UNK:O	2.23	0.57
8:U:27:UNK:O	8:U:28:UNK:C	2.51	0.57
2:B:293:ALA:O	2:B:295:GLY:N	2.37	0.57
2:B:360:PRO:O	2:B:361:ALA:HB3	2.05	0.57
3:C:154:LYS:HZ1	3:C:261:ARG:HD3	1.68	0.57
4:D:15:PHE:O	4:D:16:ASP:C	2.43	0.57
1:G:283:VAL:HG21	12:G:1345:PHO:HMC1	1.87	0.57
2:H:24:LEU:HD23	2:H:111:ALA:CA	2.33	0.57
3:I:235:GLY:O	3:I:238:ILE:HB	2.05	0.57
4:J:296:TYR:HE1	4:J:322:ASN:HD22	1.51	0.57
7:O:107:UNK:O	7:O:108:UNK:CB	2.52	0.57
8:S:90:UNK:O	8:S:91:UNK:C	2.51	0.57
10:X:468:UNK:O	10:X:469:UNK:C	2.52	0.57
2:B:249:ALA:HA	11:B:1485:CLA:HMD3	1.87	0.57
2:B:272:ARG:HG2	2:B:273:TYR:CD2	2.39	0.57
3:C:259:TRP:HZ3	11:C:1464:CLA:H12	1.69	0.57
4:D:191:TRP:HZ3	4:D:194:ASN:ND2	2.03	0.57
1:A:219:VAL:HG21	4:D:268:HIS:HD2	1.68	0.57
4:D:323:GLU:CG	4:D:326:ARG:HH21	2.13	0.57
1:G:192:ILE:O	1:G:195:HIS:N	2.38	0.57
1:G:298:ASN:N	1:G:298:ASN:OD1	2.38	0.57
1:G:331:MET:O	1:G:332:HIS:O	2.21	0.57
3:I:161:LEU:O	3:I:164:HIS:HB2	2.04	0.57
3:I:279:LEU:O	3:I:280:SER:C	2.43	0.57
4:J:235:PHE:HD2	4:J:243:THR:CG2	2.16	0.57
4:J:63:LEU:N	4:J:63:LEU:HD12	2.19	0.57
1:A:183:MET:HA	11:A:1342:CLA:HMD2	1.87	0.57
12:G:1345:PHO:CAB	4:J:205:LEU:HD21	2.34	0.57
1:G:207:GLY:O	1:G:210:LEU:N	2.38	0.57
2:H:435:GLU:O	2:H:436:THR:CB	2.50	0.57
3:I:21:ILE:O	3:I:22:PHE:CB	2.52	0.57
3:I:228:ASN:OD1	3:I:229:ASN:N	2.38	0.57
3:I:264:PHE:HD1	3:I:274:TYR:CE1	2.23	0.57
4:J:57:SER:O	4:J:59:TYR:N	2.38	0.57
8:S:64:UNK:O	8:S:65:UNK:C	2.52	0.57
8:U:92:UNK:O	8:U:93:UNK:CB	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ILE:HG22	1:A:117:PHE:N	2.19	0.57
3:C:276:LEU:HD12	3:C:276:LEU:O	2.05	0.57
3:C:318:LEU:C	3:C:318:LEU:HD12	2.24	0.57
1:A:276:ALA:HB2	4:D:215:GLY:C	2.26	0.57
2:H:458:PHE:HB3	11:H:1485:CLA:HBC2	1.86	0.57
3:I:377:LEU:O	3:I:381:LYS:HD3	2.05	0.57
4:J:325:ILE:O	4:J:329:MET:HB3	2.05	0.57
4:J:331:PRO:CG	4:J:339:PHE:HB2	2.24	0.57
6:L:36:ALA:O	6:L:39:ALA:HB3	2.05	0.57
1:A:309:ALA:C	9:V:2:GLU:HG2	2.24	0.57
3:C:266:TRP:CD1	3:C:266:TRP:N	2.73	0.57
4:D:191:TRP:HA	4:D:191:TRP:CE3	2.40	0.57
6:F:33:PHE:O	6:F:35:GLY:N	2.37	0.57
1:G:214:MET:HE2	12:J:1352:PHO:HED1	1.87	0.57
2:H:474:LEU:HG	11:H:1489:CLA:HED1	1.86	0.57
3:I:116:VAL:CG2	3:I:117:VAL:H	2.18	0.57
3:I:244:CYS:HA	11:I:1464:CLA:HMC3	1.86	0.57
3:I:283:GLY:O	3:I:286:ALA:HB3	2.04	0.57
4:J:152:VAL:CG2	4:J:279:LEU:HD13	2.34	0.57
7:P:82:UNK:O	7:P:90:UNK:CB	2.53	0.57
8:U:12:UNK:C	8:U:14:UNK:N	2.66	0.57
9:V:133:GLY:O	9:V:137:TYR:CA	2.53	0.57
1:A:156:ALA:HA	1:A:160:ILE:HB	1.87	0.56
1:G:151:LEU:HG	1:G:155:PHE:HE2	1.70	0.56
1:G:248:ILE:CD1	4:J:235:PHE:CZ	2.88	0.56
2:H:270:PRO:C	2:H:271:THR:HG23	2.24	0.56
2:H:360:PRO:O	2:H:361:ALA:HB3	2.05	0.56
5:K:59:GLU:O	5:K:60:GLN:CB	2.50	0.56
8:S:57:UNK:C	8:S:59:UNK:N	2.62	0.56
8:U:40:UNK:O	8:U:41:UNK:C	2.53	0.56
8:U:71:UNK:O	8:U:74:UNK:N	2.38	0.56
1:A:107:TYR:O	1:A:109:GLY:N	2.38	0.56
2:B:27:THR:O	11:B:1486:CLA:HBC1	2.05	0.56
2:B:474:LEU:HG	11:B:1489:CLA:HED1	1.86	0.56
2:B:54:PRO:O	2:B:55:MET:C	2.42	0.56
4:D:235:PHE:HE1	4:D:237:PRO:HB3	1.70	0.56
1:G:207:GLY:O	1:G:210:LEU:HB3	2.05	0.56
1:G:214:MET:O	1:G:217:SER:N	2.38	0.56
2:H:397:VAL:O	2:H:411:PHE:O	2.23	0.56
4:J:263:ASN:O	4:J:265:ARG:N	2.38	0.56
6:L:37:ILE:HG12	6:L:40:MET:CE	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:92:UNK:O	8:S:93:UNK:CB	2.51	0.56
8:U:59:UNK:C	8:U:61:UNK:N	2.69	0.56
10:X:357:UNK:O	10:X:361:UNK:N	2.38	0.56
1:A:248:ILE:CD1	4:D:235:PHE:CZ	2.88	0.56
2:B:473:THR:HG21	11:B:1489:CLA:HED3	1.86	0.56
2:B:458:PHE:HB3	11:B:1485:CLA:HBC2	1.87	0.56
3:C:297:TYR:HD1	3:C:302:TYR:CZ	2.23	0.56
2:B:364:GLU:OE1	4:D:296:TYR:CD2	2.58	0.56
2:H:394:GLN:O	2:H:395:GLN:CB	2.53	0.56
3:I:297:TYR:HD1	3:I:302:TYR:CE2	2.23	0.56
4:J:337:GLU:HG3	4:J:339:PHE:HE2	1.69	0.56
8:S:69:UNK:O	8:S:70:UNK:C	2.53	0.56
2:B:144:PHE:HE1	2:B:210:ILE:HG23	1.69	0.56
2:B:450:TRP:NE1	11:B:1488:CLA:HBA1	2.19	0.56
3:C:284:PHE:HE1	3:C:431:PHE:CD1	2.24	0.56
1:G:116:ILE:CD1	1:G:158:PHE:HD1	2.18	0.56
1:G:157:VAL:O	1:G:157:VAL:HG12	2.05	0.56
1:G:258:LEU:HG	4:J:128:ARG:HH22	1.69	0.56
2:H:172:TYR:HA	2:H:280:PHE:CE1	2.37	0.56
2:H:174:LEU:HD11	2:H:309:LEU:HD21	1.87	0.56
2:H:369:ILE:O	2:H:379:ALA:O	2.23	0.56
9:T:87:GLU:CD	9:T:96:ARG:HH22	2.07	0.56
8:U:57:UNK:C	8:U:59:UNK:N	2.65	0.56
10:Y:404:UNK:O	10:Y:408:UNK:CB	2.54	0.56
1:A:310:LYS:NZ	5:E:58:GLN:HG2	2.20	0.56
11:B:1482:CLA:HBD	11:B:1482:CLA:CGA	2.35	0.56
3:C:258:GLY:O	3:C:262:ARG:NE	2.37	0.56
2:B:475:PHE:CE1	4:D:140:PRO:HG3	2.39	0.56
1:G:267:ASN:O	1:G:268:SER:C	2.44	0.56
2:H:144:PHE:HE1	2:H:210:ILE:HG23	1.69	0.56
2:H:236:THR:CB	2:H:473:THR:HG21	2.35	0.56
2:H:54:PRO:O	2:H:55:MET:C	2.43	0.56
3:I:258:GLY:O	3:I:262:ARG:NE	2.39	0.56
3:I:362:ARG:NH1	3:I:362:ARG:HG3	2.21	0.56
4:J:289:LEU:HD22	4:J:294:ARG:HB3	1.87	0.56
4:J:96:GLU:HA	4:J:96:GLU:OE1	2.05	0.56
4:D:164:GLN:NE2	4:D:189:HIS:HE1	1.95	0.56
2:H:270:PRO:O	2:H:271:THR:CG2	2.53	0.56
2:H:392:PHE:O	2:H:395:GLN:HA	2.05	0.56
4:J:89:LEU:O	4:J:90:LEU:C	2.44	0.56
10:Y:182:UNK:O	10:Y:184:UNK:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ASN:OD1	1:A:298:ASN:N	2.38	0.56
2:B:332:LYS:O	2:B:439:SER:CA	2.54	0.56
3:C:120:ILE:C	3:C:122:SER:N	2.57	0.56
3:C:270:ALA:O	3:C:274:TYR:HD2	1.86	0.56
1:G:218:LEU:CD1	1:G:255:PHE:HD2	2.18	0.56
2:H:285:ASN:O	2:H:289:GLN:HB2	2.06	0.56
3:I:367:GLU:HB2	3:I:368:PRO:HD3	1.87	0.56
4:J:37:LEU:C	4:J:37:LEU:CD2	2.74	0.56
7:P:107:UNK:O	7:P:108:UNK:CB	2.52	0.56
3:C:69:LEU:CD1	3:C:115:GLY:HA3	2.35	0.56
1:A:133:LEU:HD12	4:D:256:ILE:HG13	1.87	0.56
1:G:266:ASN:O	1:G:267:ASN:C	2.44	0.56
1:G:93:PHE:CE1	1:G:95:PRO:CG	2.88	0.56
2:H:134:ASP:O	2:H:136:PRO:CD	2.53	0.56
3:I:51:GLY:O	3:I:52:ALA:C	2.44	0.56
6:L:37:ILE:HG22	6:L:41:GLN:HE21	1.69	0.56
8:S:5:UNK:O	8:S:7:UNK:N	2.37	0.56
8:U:90:UNK:C	8:U:91:UNK:O	2.52	0.56
1:A:151:LEU:HG	1:A:155:PHE:HE2	1.71	0.56
3:C:189:TRP:NE1	3:C:295:THR:HG22	2.18	0.56
3:C:376:ASP:C	3:C:378:ASN:N	2.58	0.56
4:D:171:PRO:HG3	4:D:181:PHE:CG	2.40	0.56
1:G:34:GLY:O	1:G:36:ILE:N	2.39	0.56
2:H:61:PHE:HZ	11:H:1488:CLA:HBB1	1.71	0.56
3:I:39:ASN:ND2	11:I:1466:CLA:H11	2.20	0.56
10:X:118:UNK:O	10:X:119:UNK:C	2.51	0.56
4:D:184:PHE:O	4:D:188:PHE:HB2	2.06	0.56
1:G:315:ASN:HA	1:G:319:ASP:OD2	2.05	0.56
4:J:16:ASP:O	4:J:19:ASP:N	2.39	0.56
2:B:318:ASN:OD1	2:B:318:ASN:C	2.44	0.56
3:C:367:GLU:O	3:C:370:ARG:HB2	2.06	0.56
4:D:263:ASN:O	4:D:265:ARG:N	2.39	0.56
4:D:292:ASN:O	4:D:294:ARG:HG2	2.05	0.56
4:D:45:LEU:CD2	4:D:49:LEU:HD11	2.37	0.56
2:H:293:ALA:O	2:H:295:GLY:N	2.39	0.56
2:H:413:ASP:OD1	2:H:413:ASP:N	2.33	0.56
8:S:40:UNK:O	8:S:41:UNK:C	2.54	0.56
1:A:62:GLY:O	1:A:63:ILE:HB	2.04	0.55
2:B:92:SER:O	2:B:93:PHE:C	2.44	0.55
3:C:297:TYR:HD1	3:C:302:TYR:CE2	2.24	0.55
3:C:36:TRP:O	3:C:36:TRP:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:LEU:O	3:C:75:PHE:N	2.38	0.55
1:G:126:TYR:O	1:G:130:GLN:HB2	2.06	0.55
2:H:278:SER:O	2:H:281:GLN:HG2	2.06	0.55
2:H:338:GLN:O	2:H:339:ALA:O	2.23	0.55
2:H:338:GLN:O	2:H:431:GLU:O	2.24	0.55
4:J:160:TYR:HB3	4:J:161:PRO:CD	2.29	0.55
4:J:171:PRO:HD2	4:J:181:PHE:CE2	2.36	0.55
9:T:55:ARG:NH2	9:T:128:ASP:OD1	2.39	0.55
10:X:404:UNK:O	10:X:408:UNK:CB	2.54	0.55
3:C:424:SER:O	3:C:428:THR:OG1	2.23	0.55
1:G:210:LEU:O	1:G:213:ALA:HB3	2.06	0.55
2:H:238:LEU:HD21	2:H:469:HIS:CD2	2.41	0.55
3:I:43:ILE:CG2	11:I:1467:CLA:HMC1	2.29	0.55
3:I:377:LEU:O	3:I:381:LYS:HB2	2.07	0.55
4:J:216:ALA:O	4:J:220:ASN:ND2	2.39	0.55
5:K:42:LEU:O	5:K:43:ALA:C	2.45	0.55
8:U:5:UNK:O	8:U:7:UNK:N	2.38	0.55
1:A:174:LEU:HD22	12:A:1345:PHO:H151	1.88	0.55
1:A:195:HIS:HE1	1:A:197:PHE:CD1	2.25	0.55
2:B:138:MET:HA	2:B:141:ILE:HG22	1.89	0.55
11:B:1486:CLA:HMC1	11:B:1486:CLA:HBC2	1.87	0.55
2:B:338:GLN:O	2:B:431:GLU:O	2.23	0.55
3:C:167:VAL:HG22	11:C:1470:CLA:HMB2	1.87	0.55
3:C:227:VAL:HG11	3:C:233:VAL:HG23	1.88	0.55
3:C:56:HIS:O	3:C:57:ALA:C	2.44	0.55
2:H:144:PHE:CE1	2:H:210:ILE:HG23	2.41	0.55
3:I:186:TYR:HE2	3:I:188:THR:CG2	2.20	0.55
3:I:318:LEU:HD12	3:I:318:LEU:C	2.27	0.55
3:I:307:PRO:HA	3:I:358:PHE:CD1	2.42	0.55
3:C:284:PHE:HE1	3:C:431:PHE:CE1	2.25	0.55
4:D:263:ASN:O	4:D:264:LYS:C	2.45	0.55
5:E:15:THR:O	5:E:15:THR:HG22	2.05	0.55
2:H:103:LEU:HD23	2:H:103:LEU:N	2.20	0.55
3:I:167:VAL:HG22	11:I:1470:CLA:HMB2	1.87	0.55
4:J:169:PHE:O	4:J:181:PHE:HE2	1.90	0.55
4:J:189:HIS:HA	4:J:294:ARG:HH11	1.71	0.55
9:T:134:LYS:C	9:T:137:TYR:H	2.10	0.55
3:C:230:LEU:O	3:C:234:VAL:HG23	2.06	0.55
3:I:67:MET:O	3:I:71:GLU:N	2.39	0.55
1:A:331:MET:O	1:A:332:HIS:C	2.45	0.55
2:B:426:PHE:O	2:B:426:PHE:HD1	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:345:VAL:O	4:D:346:LEU:CB	2.54	0.55
1:G:157:VAL:HG13	1:G:172:MET:HB3	1.89	0.55
1:G:195:HIS:HE1	1:G:197:PHE:CD1	2.24	0.55
2:H:92:SER:O	2:H:93:PHE:C	2.45	0.55
3:I:164:HIS:HA	3:I:167:VAL:HG23	1.87	0.55
4:J:36:LEU:HD23	11:J:1353:CLA:HBB2	1.88	0.55
5:K:37:PHE:CE1	5:K:42:LEU:CB	2.89	0.55
10:Y:568:UNK:O	10:Y:569:UNK:C	2.54	0.55
1:A:176:ILE:HG23	1:A:180:PHE:CE1	2.41	0.55
3:C:135:ARG:HG3	3:C:136:GLY:H	1.70	0.55
3:C:37:ALA:CA	11:C:1466:CLA:HBA2	2.30	0.55
3:C:202:PRO:CA	3:C:235:GLY:HA3	2.37	0.55
4:D:126:MET:HE1	4:D:143:ALA:O	2.07	0.55
6:F:18:VAL:O	6:F:21:VAL:N	2.39	0.55
1:G:116:ILE:HG12	1:G:158:PHE:HD1	1.72	0.55
2:H:24:LEU:HD23	2:H:110:ALA:C	2.26	0.55
3:I:276:LEU:HD12	3:I:276:LEU:O	2.06	0.55
3:I:320:ARG:NH1	9:T:49:ASN:OD1	2.39	0.55
4:J:238:THR:O	4:J:239:GLN:CB	2.54	0.55
7:P:123:UNK:O	7:P:124:UNK:C	2.55	0.55
9:V:136:TYR:O	9:V:137:TYR:CG	2.59	0.55
5:E:58:GLN:CD	9:V:2:GLU:N	2.61	0.55
2:B:172:TYR:O	2:B:174:LEU:HG	2.06	0.55
2:B:193:TYR:OH	2:B:259:GLY:HA2	2.07	0.55
4:D:37:LEU:CD2	4:D:37:LEU:C	2.75	0.55
4:D:56:THR:CB	5:E:49:THR:HG22	2.37	0.55
1:G:116:ILE:HG22	1:G:117:PHE:N	2.21	0.55
2:H:201:HIS:HB2	11:H:1483:CLA:C1B	2.37	0.55
2:H:94:GLU:CG	2:H:95:GLY:H	2.20	0.55
3:I:56:HIS:ND1	11:I:1467:CLA:HHB	2.22	0.55
3:I:226:SER:OG	3:I:227:VAL:N	2.38	0.55
3:I:189:TRP:NE1	3:I:295:THR:HG22	2.22	0.55
4:J:62:GLY:C	4:J:63:LEU:HD12	2.27	0.55
5:K:16:SER:O	5:K:17:VAL:HB	2.07	0.55
5:K:35:TRP:CE3	6:L:39:ALA:HB2	2.42	0.55
10:Y:214:UNK:O	10:Y:218:UNK:N	2.40	0.55
3:C:166:ILE:HD11	3:C:249:ILE:HD13	1.88	0.55
3:C:284:PHE:O	3:C:285:ILE:C	2.45	0.55
4:D:58:TRP:HA	4:D:62:GLY:HA2	1.89	0.55
1:G:220:THR:C	1:G:222:SER:H	2.10	0.55
11:H:1496:CLA:H171	11:H:1497:CLA:CMD	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:271:THR:HG22	2:H:448:ARG:HE	1.70	0.55
3:I:135:ARG:HG3	3:I:136:GLY:H	1.72	0.55
3:I:36:TRP:O	3:I:36:TRP:HE3	1.89	0.55
7:O:99:UNK:O	7:O:102:UNK:N	2.39	0.55
8:U:44:UNK:O	8:U:45:UNK:C	2.54	0.55
1:A:332:HIS:HD2	1:A:333:GLU:H	1.54	0.55
2:B:193:TYR:CZ	2:B:259:GLY:HA2	2.42	0.55
2:B:94:GLU:CG	2:B:95:GLY:N	2.69	0.55
3:C:298:PRO:O	3:C:299:SER:HB3	2.06	0.55
4:D:190:ASN:HB2	4:D:296:TYR:HD1	1.71	0.55
1:G:95:PRO:O	1:G:105:TRP:NE1	2.40	0.55
1:G:89:ILE:HD11	1:G:108:ASN:HB3	1.89	0.55
2:H:30:VAL:HG12	11:H:1486:CLA:HHD	1.87	0.55
2:H:37:MET:O	2:H:40:TYR:N	2.40	0.55
8:S:73:UNK:O	8:S:74:UNK:C	2.54	0.55
10:X:13:UNK:O	10:X:14:UNK:C	2.54	0.55
10:X:225:UNK:O	10:X:226:UNK:C	2.55	0.55
1:A:331:MET:O	1:A:332:HIS:O	2.25	0.54
2:B:246:PHE:CZ	2:B:463:PHE:HD1	2.24	0.54
4:D:152:VAL:HG11	11:D:1351:CLA:HBA1	1.89	0.54
4:D:56:THR:HB	5:E:49:THR:HG22	1.90	0.54
1:G:198:HIS:O	1:G:201:GLY:N	2.37	0.54
2:H:323:GLY:CA	4:J:293:LEU:HD22	2.38	0.54
2:H:396:GLY:C	2:H:398:THR:N	2.60	0.54
3:I:330:SER:HB3	7:P:56:UNK:O	2.07	0.54
4:J:46:GLY:O	4:J:47:GLY:C	2.45	0.54
10:X:420:UNK:O	10:X:421:UNK:C	2.55	0.54
2:B:153:PHE:O	2:B:157:HIS:HB3	2.07	0.54
2:B:398:THR:C	2:B:400:SER:N	2.60	0.54
3:C:119:LEU:O	3:C:122:SER:OG	2.25	0.54
3:C:240:ILE:HA	3:C:243:ILE:HB	1.89	0.54
3:C:284:PHE:O	3:C:286:ALA:N	2.40	0.54
3:C:33:PHE:O	3:C:34:ALA:HB3	2.07	0.54
4:D:239:GLN:O	4:D:240:ALA:HB3	2.06	0.54
4:D:72:ASN:OD1	4:D:72:ASN:O	2.24	0.54
1:G:13:LEU:O	1:G:17:PHE:N	2.39	0.54
2:H:346:PHE:O	2:H:354:LEU:HB3	2.07	0.54
3:I:120:ILE:O	3:I:122:SER:N	2.40	0.54
3:I:259:TRP:CZ3	11:I:1464:CLA:H12	2.42	0.54
3:I:447:ARG:HG2	3:I:447:ARG:HH11	1.72	0.54
9:V:133:GLY:O	9:V:137:TYR:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:PRO:C	2:B:271:THR:HG23	2.27	0.54
1:A:217:SER:HG	4:D:142:ASN:HA	1.70	0.54
4:D:272:LEU:O	4:D:272:LEU:HD23	2.06	0.54
1:G:107:TYR:C	1:G:109:GLY:N	2.59	0.54
11:G:1342:CLA:H122	12:G:1345:PHO:H3A	1.88	0.54
1:G:248:ILE:CD1	4:J:235:PHE:HZ	2.18	0.54
4:J:56:THR:HB	5:K:49:THR:HG22	1.88	0.54
5:K:10:PHE:HD2	6:L:19:ARG:NH2	2.06	0.54
8:S:27:UNK:O	8:S:28:UNK:O	2.24	0.54
1:A:220:THR:C	1:A:222:SER:H	2.10	0.54
1:A:310:LYS:HD2	5:E:58:GLN:HG3	1.89	0.54
2:B:107:LEU:HD23	11:B:1497:CLA:HBC1	1.88	0.54
2:B:144:PHE:CE1	2:B:210:ILE:HG23	2.42	0.54
2:B:52:LEU:HD23	2:B:311:PHE:CD2	2.42	0.54
2:B:359:MET:HB3	2:B:426:PHE:HB3	1.88	0.54
3:C:150:ASP:O	3:C:151:TRP:C	2.46	0.54
3:C:377:LEU:O	3:C:381:LYS:HB2	2.08	0.54
3:C:433:LEU:O	3:C:434:ALA:C	2.44	0.54
3:C:74:HIS:CD2	3:C:74:HIS:H	2.26	0.54
4:D:89:LEU:O	4:D:90:LEU:C	2.46	0.54
1:G:278:TRP:CB	1:G:279:PRO:HD3	2.27	0.54
2:H:193:TYR:CE1	2:H:259:GLY:HA2	2.42	0.54
2:H:450:TRP:NE1	11:H:1488:CLA:HBA1	2.22	0.54
3:I:116:VAL:O	3:I:117:VAL:C	2.46	0.54
3:I:137:PRO:O	3:I:138:GLU:HB2	2.08	0.54
4:J:126:MET:HE1	4:J:143:ALA:O	2.08	0.54
6:L:33:PHE:C	6:L:35:GLY:N	2.60	0.54
8:U:64:UNK:O	8:U:65:UNK:C	2.55	0.54
9:V:55:ARG:HG3	9:V:131:GLY:HA2	1.90	0.54
1:A:267:ASN:O	1:A:268:SER:C	2.45	0.54
2:B:68:ARG:NH1	2:B:262:THR:O	2.40	0.54
3:C:168:LEU:HD23	11:C:1459:CLA:HMC2	1.90	0.54
3:C:75:PHE:CZ	3:C:77:PRO:HG3	2.42	0.54
1:G:135:TYR:O	1:G:136:ARG:HG2	2.07	0.54
2:H:446:SER:HB2	2:H:447:PRO:CD	2.37	0.54
2:H:475:PHE:CE1	4:J:140:PRO:HG3	2.42	0.54
3:I:355:THR:O	3:I:355:THR:HG22	2.07	0.54
5:K:12:ASP:O	5:K:16:SER:N	2.40	0.54
1:G:311:GLY:HA3	9:T:125:ILE:CG2	2.38	0.54
2:B:134:ASP:O	2:B:136:PRO:CD	2.55	0.54
2:B:194:ASN:O	2:B:195:PRO:C	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ALA:H	11:B:1486:CLA:CBC	2.19	0.54
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.90	0.54
2:B:271:THR:HG22	2:B:448:ARG:HE	1.72	0.54
4:D:279:LEU:HD11	12:D:1352:PHO:HBC3	1.90	0.54
11:H:1482:CLA:CGA	11:H:1482:CLA:HBD	2.38	0.54
2:H:422:ARG:O	2:H:425:ILE:HG22	2.07	0.54
4:J:191:TRP:HA	4:J:191:TRP:CE3	2.42	0.54
4:J:45:LEU:HD22	4:J:49:LEU:HD11	1.88	0.54
1:G:310:LYS:HZ1	5:K:58:GLN:HG2	1.71	0.54
7:O:148:UNK:O	7:O:149:UNK:CB	2.53	0.54
8:S:57:UNK:O	8:S:58:UNK:C	2.56	0.54
8:U:67:UNK:O	8:U:68:UNK:C	2.55	0.54
1:A:210:LEU:O	1:A:213:ALA:HB3	2.08	0.54
1:A:271:LEU:O	1:A:271:LEU:HG	2.08	0.54
2:B:205:ALA:O	2:B:209:GLY:N	2.41	0.54
3:C:170:ILE:CG2	3:C:171:GLY:N	2.71	0.54
3:C:186:TYR:HE2	3:C:188:THR:CG2	2.21	0.54
2:H:31:ALA:N	11:H:1486:CLA:CBC	2.66	0.54
2:H:468:TRP:HD1	4:J:144:ILE:HD11	1.71	0.54
2:H:470:GLY:O	2:H:473:THR:HB	2.07	0.54
3:I:376:ASP:C	3:I:378:ASN:N	2.59	0.54
10:X:17:UNK:O	10:X:18:UNK:C	2.55	0.54
10:X:506:UNK:O	10:X:507:UNK:C	2.55	0.54
10:X:5:UNK:O	10:X:6:UNK:C	2.56	0.54
11:A:1344:CLA:HED3	4:D:175:VAL:HG13	1.89	0.54
1:A:326:LEU:C	1:A:328:MET:H	2.09	0.54
2:B:211:ILE:O	2:B:214:LEU:HG	2.08	0.54
2:B:215:PHE:HZ	11:B:1490:CLA:HMD3	1.71	0.54
2:B:280:PHE:CZ	2:B:312:TYR:HD2	2.26	0.54
2:B:346:PHE:O	2:B:353:GLU:O	2.25	0.54
3:C:116:VAL:O	3:C:117:VAL:C	2.46	0.54
3:C:135:ARG:C	3:C:136:GLY:O	2.44	0.54
3:C:291:TRP:HD1	3:C:292:PHE:CD2	2.26	0.54
3:C:318:LEU:CD1	3:C:328:VAL:HG21	2.38	0.54
5:E:13:ILE:HA	5:E:16:SER:HB2	1.89	0.54
2:H:202:HIS:HE1	11:H:1484:CLA:NB	2.04	0.54
2:H:462:PHE:HA	11:H:1492:CLA:HMC1	1.90	0.54
2:H:167:TRP:CB	2:H:267:LEU:HD11	2.38	0.54
1:A:134:SER:C	1:A:136:ARG:H	2.10	0.54
2:B:63:LEU:O	2:B:64:PRO:C	2.45	0.54
4:D:183:LEU:O	4:D:184:PHE:C	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:209:LEU:O	4:D:209:LEU:HD23	2.07	0.54
6:F:40:MET:O	6:F:43:ILE:HG13	2.07	0.54
3:I:127:PHE:CE2	11:I:1471:CLA:HBC1	2.43	0.54
3:I:449:ARG:NH1	11:I:1463:CLA:O1D	2.41	0.54
4:J:139:ARG:HB3	4:J:141:TYR:HD1	1.73	0.54
8:S:55:UNK:O	8:S:58:UNK:N	2.40	0.54
8:S:67:UNK:O	8:S:68:UNK:C	2.56	0.54
9:V:134:LYS:O	9:V:137:TYR:O	2.26	0.54
12:A:1345:PHO:CBB	4:D:205:LEU:HD21	2.37	0.54
1:A:78:ILE:HD12	1:A:78:ILE:H	1.73	0.54
1:A:98:GLU:O	1:A:99:ALA:CB	2.56	0.54
2:B:24:LEU:HD23	2:B:111:ALA:CA	2.36	0.54
1:A:258:LEU:CD1	4:D:128:ARG:NH2	2.71	0.54
4:D:313:THR:C	4:D:315:TYR:N	2.60	0.54
2:H:269:GLY:H	2:H:448:ARG:HB2	1.73	0.54
3:I:250:TRP:CD1	3:I:250:TRP:C	2.81	0.54
3:I:82:TYR:HB3	3:I:302:TYR:C	2.28	0.54
4:J:313:THR:C	4:J:315:TYR:N	2.61	0.54
5:K:16:SER:HB3	5:K:19:TYR:HB3	1.90	0.54
11:B:1494:CLA:OBD	11:B:1495:CLA:HHC	2.08	0.53
2:B:33:TRP:NE1	11:B:1488:CLA:HBC2	2.22	0.53
1:G:210:LEU:HD13	12:J:1352:PHO:ND	2.24	0.53
2:H:280:PHE:O	2:H:283:GLU:HB3	2.07	0.53
3:I:126:GLY:O	3:I:130:VAL:HG23	2.08	0.53
3:I:37:ALA:CA	11:I:1466:CLA:HBA2	2.29	0.53
4:J:33:SER:OG	4:J:128:ARG:HA	2.08	0.53
1:G:324:ALA:HB2	4:J:329:MET:HE2	1.89	0.53
4:J:40:CYS:O	4:J:41:ALA:C	2.46	0.53
9:V:13:ASN:HD21	9:V:17:LYS:CG	2.22	0.53
10:X:270:UNK:O	10:X:271:UNK:C	2.57	0.53
10:X:59:UNK:C	10:X:61:UNK:N	2.70	0.53
10:X:59:UNK:O	10:X:61:UNK:N	2.41	0.53
10:Y:425:UNK:O	10:Y:429:UNK:CB	2.56	0.53
10:Y:578:UNK:C	10:Y:580:UNK:N	2.65	0.53
1:A:288:LEU:O	1:A:290:ILE:N	2.41	0.53
2:B:201:HIS:HB2	11:B:1483:CLA:C1B	2.38	0.53
4:D:74:LEU:HA	4:D:175:VAL:HG11	1.90	0.53
4:D:179:PHE:HA	4:D:182:LEU:HD12	1.89	0.53
5:E:56:TYR:O	5:E:57:ALA:CB	2.55	0.53
1:G:219:VAL:HG11	4:J:268:HIS:CD2	2.44	0.53
1:G:84:PRO:O	1:G:85:SER:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:27:THR:O	2:H:30:VAL:N	2.37	0.53
2:H:318:ASN:OD1	2:H:318:ASN:C	2.47	0.53
3:I:33:PHE:O	3:I:34:ALA:HB3	2.09	0.53
1:G:302:PHE:HE1	4:J:74:LEU:HD12	1.73	0.53
7:P:64:UNK:HA	7:P:70:UNK:O	2.09	0.53
9:V:134:LYS:C	9:V:137:TYR:H	2.12	0.53
9:V:4:THR:HB	9:V:5:PRO:HD2	1.89	0.53
10:X:435:UNK:O	10:X:438:UNK:N	2.41	0.53
2:B:323:GLY:CA	4:D:293:LEU:HD22	2.39	0.53
2:B:475:PHE:CZ	4:D:134:ARG:HB2	2.43	0.53
3:C:179:ALA:O	3:C:184:GLY:HA2	2.09	0.53
3:C:290:VAL:HA	3:C:297:TYR:CD2	2.43	0.53
4:D:110:LEU:O	4:D:114:ILE:HG13	2.09	0.53
1:G:174:LEU:HD22	12:G:1345:PHO:H151	1.89	0.53
4:J:279:LEU:HD11	12:J:1352:PHO:HBC3	1.90	0.53
1:G:26:ASN:CA	4:J:255:GLN:NE2	2.72	0.53
5:K:55:TYR:O	5:K:56:TYR:HB2	2.07	0.53
8:S:31:UNK:O	8:S:32:UNK:C	2.57	0.53
10:X:519:UNK:O	10:X:522:UNK:N	2.41	0.53
10:Y:336:UNK:O	10:Y:337:UNK:CB	2.56	0.53
1:A:201:GLY:HA2	1:A:282:GLY:O	2.07	0.53
11:B:1496:CLA:H171	11:B:1497:CLA:CMD	2.39	0.53
2:B:309:LEU:O	2:B:312:TYR:N	2.42	0.53
2:B:314:TYR:OH	2:B:334:ASP:OD1	2.25	0.53
2:B:396:GLY:C	2:B:398:THR:N	2.60	0.53
3:C:82:TYR:HB3	3:C:302:TYR:C	2.29	0.53
5:E:16:SER:HB3	5:E:19:TYR:HB3	1.90	0.53
1:G:132:GLU:O	1:G:134:SER:N	2.41	0.53
2:H:139:PHE:HB2	11:H:1491:CLA:CHD	2.38	0.53
3:I:173:LEU:O	3:I:176:VAL:CG1	2.51	0.53
4:J:184:PHE:O	4:J:188:PHE:HB2	2.09	0.53
1:G:133:LEU:HB2	4:J:252:PHE:CE2	2.43	0.53
5:K:17:VAL:O	5:K:21:VAL:HG23	2.08	0.53
4:J:56:THR:N	5:K:49:THR:HG22	2.23	0.53
1:A:186:PHE:CD2	1:A:192:ILE:CD1	2.84	0.53
1:A:218:LEU:CD1	1:A:255:PHE:HD2	2.20	0.53
1:A:218:LEU:HA	1:A:221:SER:OG	2.09	0.53
3:C:376:ASP:HB2	3:C:379:LYS:CG	2.34	0.53
3:C:455:PHE:O	3:C:456:GLU:CG	2.56	0.53
3:C:72:LEU:O	3:C:75:PHE:HB3	2.08	0.53
4:D:181:PHE:CZ	4:D:185:PHE:HE1	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:191:TRP:HA	4:D:191:TRP:HE3	1.74	0.53
4:D:296:TYR:HE1	4:D:322:ASN:HD22	1.56	0.53
6:F:33:PHE:C	6:F:35:GLY:N	2.62	0.53
1:G:255:PHE:CZ	1:G:259:ILE:HD12	2.44	0.53
2:H:135:LEU:CD1	2:H:232:GLY:HA2	2.38	0.53
2:H:220:ARG:HD2	2:H:221:PRO:HD2	1.90	0.53
2:H:33:TRP:HE1	11:H:1488:CLA:HBC2	1.73	0.53
3:I:284:PHE:HE1	3:I:431:PHE:CE1	2.25	0.53
4:J:210:LEU:HD11	4:J:270:PHE:CD2	2.43	0.53
9:V:55:ARG:NH2	9:V:128:ASP:OD1	2.41	0.53
2:B:24:LEU:HD23	2:B:110:ALA:C	2.28	0.53
2:B:220:ARG:HD2	2:B:221:PRO:HD2	1.90	0.53
2:B:446:SER:HB2	2:B:447:PRO:CD	2.39	0.53
3:C:39:ASN:ND2	11:C:1466:CLA:H11	2.23	0.53
4:D:184:PHE:C	4:D:184:PHE:CD1	2.80	0.53
1:G:140:ARG:O	4:J:220:ASN:HB3	2.08	0.53
1:G:271:LEU:O	1:G:271:LEU:HG	2.09	0.53
1:G:285:PHE:O	1:G:289:GLY:N	2.33	0.53
2:H:98:LEU:O	2:H:101:ILE:N	2.41	0.53
3:I:270:ALA:O	3:I:274:TYR:HD2	1.91	0.53
3:I:40:ALA:HA	3:I:43:ILE:HG23	1.91	0.53
9:V:78:ASN:OD1	9:V:96:ARG:NH2	2.41	0.53
1:A:36:ILE:O	1:A:39:PRO:HD2	2.09	0.53
2:B:135:LEU:HD12	2:B:232:GLY:HA2	1.90	0.53
2:B:106:LEU:HD22	11:B:1496:CLA:H143	1.89	0.53
2:B:15:ASP:CA	2:B:16:PRO:CD	2.87	0.53
3:C:367:GLU:HB2	3:C:368:PRO:HD3	1.89	0.53
4:D:289:LEU:HD22	4:D:294:ARG:HB3	1.90	0.53
5:E:17:VAL:O	5:E:21:VAL:HG23	2.09	0.53
1:G:168:PHE:O	1:G:170:ASP:O	2.26	0.53
2:H:107:LEU:HD23	11:H:1497:CLA:HBC1	1.90	0.53
3:I:287:THR:OG1	3:I:288:CYS:N	2.41	0.53
3:I:320:ARG:HD2	9:T:49:ASN:ND2	2.24	0.53
3:I:318:LEU:CD1	3:I:328:VAL:HG21	2.38	0.53
10:Y:262:UNK:O	10:Y:263:UNK:C	2.57	0.53
1:A:132:GLU:O	1:A:134:SER:N	2.42	0.53
1:A:211:PHE:CE2	1:A:274:PHE:HE2	2.26	0.53
1:A:288:LEU:O	1:A:291:SER:N	2.42	0.53
2:B:236:THR:CB	2:B:473:THR:HG21	2.39	0.53
3:C:240:ILE:HD12	11:C:1465:CLA:C9	2.39	0.53
4:D:148:ALA:HA	4:D:280:TRP:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:272:LEU:CD2	4:D:276:VAL:HG21	2.39	0.53
4:D:283:ALA:O	4:D:287:VAL:HG23	2.09	0.53
4:D:71:CYS:CB	4:D:76:VAL:HG22	2.38	0.53
1:G:290:ILE:C	1:G:292:THR:N	2.59	0.53
2:H:220:ARG:HB3	2:H:221:PRO:HD2	1.90	0.53
2:H:52:LEU:HD23	2:H:311:PHE:CD2	2.44	0.53
3:I:290:VAL:HA	3:I:297:TYR:CD2	2.43	0.53
3:I:79:LYS:HE2	3:I:83:GLU:HG2	1.90	0.53
4:J:339:PHE:HD1	4:J:341:PHE:CE1	2.27	0.53
8:S:71:UNK:O	8:S:74:UNK:N	2.41	0.53
3:C:156:LYS:O	3:C:160:ILE:HG13	2.09	0.53
4:D:216:ALA:O	4:D:220:ASN:ND2	2.42	0.53
4:D:46:GLY:O	4:D:47:GLY:C	2.46	0.53
1:G:255:PHE:CE1	1:G:259:ILE:HD12	2.44	0.53
3:I:252:ILE:O	3:I:253:LEU:C	2.46	0.53
3:I:433:LEU:O	3:I:434:ALA:C	2.47	0.53
9:T:100:ILE:C	9:T:102:PRO:HD3	2.29	0.53
9:T:13:ASN:HD21	9:T:17:LYS:CG	2.22	0.53
10:X:357:UNK:O	10:X:360:UNK:N	2.41	0.53
10:Y:13:UNK:O	10:Y:14:UNK:C	2.57	0.53
10:Y:184:UNK:O	10:Y:185:UNK:C	2.57	0.53
10:Y:5:UNK:O	10:Y:6:UNK:C	2.56	0.53
1:A:302:PHE:HE1	4:D:74:LEU:HD12	1.73	0.53
1:A:34:GLY:C	1:A:36:ILE:H	2.12	0.53
2:B:462:PHE:HA	11:B:1492:CLA:HMC1	1.91	0.53
2:B:135:LEU:HD22	2:B:237:VAL:HG21	1.91	0.53
2:B:49:ASP:OD2	2:B:52:LEU:N	2.41	0.53
4:D:139:ARG:HB3	4:D:141:TYR:HD1	1.74	0.53
2:B:362:PHE:HE2	4:D:184:PHE:HZ	1.57	0.53
4:D:209:LEU:CD2	4:D:209:LEU:C	2.77	0.53
1:A:314:ILE:HG23	4:D:58:TRP:HZ3	1.74	0.53
5:E:16:SER:O	5:E:17:VAL:CB	2.57	0.53
1:G:142:TRP:O	1:G:145:VAL:N	2.41	0.53
2:H:76:SER:O	7:O:66:UNK:CA	2.57	0.53
4:J:283:ALA:O	4:J:287:VAL:HG23	2.08	0.53
1:A:289:GLY:O	1:A:292:THR:HB	2.09	0.52
1:A:97:TRP:O	1:A:98:GLU:C	2.47	0.52
1:G:246:TYR:O	1:G:247:ASN:CG	2.47	0.52
2:H:246:PHE:CZ	2:H:463:PHE:HD1	2.27	0.52
2:H:473:THR:HG21	11:H:1489:CLA:HED3	1.92	0.52
3:I:318:LEU:HD11	3:I:328:VAL:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:52:THR:O	4:J:67:TYR:HD1	1.92	0.52
4:J:58:TRP:HA	4:J:62:GLY:HA2	1.90	0.52
4:J:76:VAL:HG12	4:J:77:ALA:N	2.23	0.52
8:S:99:UNK:O	8:S:100:UNK:C	2.58	0.52
8:U:14:UNK:C	8:U:16:UNK:N	2.70	0.52
10:X:200:UNK:O	10:X:201:UNK:C	2.57	0.52
10:Y:420:UNK:O	10:Y:421:UNK:C	2.56	0.52
1:A:142:TRP:O	1:A:145:VAL:N	2.42	0.52
1:A:93:PHE:CE1	1:A:95:PRO:CG	2.92	0.52
3:C:259:TRP:CZ3	11:C:1464:CLA:H12	2.44	0.52
3:C:67:MET:O	3:C:71:GLU:N	2.42	0.52
4:D:313:THR:C	4:D:315:TYR:H	2.12	0.52
2:H:247:PHE:HB2	11:H:1489:CLA:HBC1	1.91	0.52
4:J:32:TRP:O	4:J:35:ILE:N	2.43	0.52
4:J:56:THR:CB	5:K:49:THR:HG22	2.39	0.52
9:T:4:THR:HB	9:T:5:PRO:HD2	1.90	0.52
10:X:356:UNK:O	10:X:357:UNK:C	2.57	0.52
4:D:16:ASP:O	4:D:19:ASP:N	2.42	0.52
4:D:340:VAL:O	4:D:342:PRO:HD3	2.07	0.52
6:F:19:ARG:O	6:F:23:VAL:CG2	2.54	0.52
1:G:330:VAL:HG12	4:J:347:PRO:CA	2.35	0.52
3:I:74:HIS:CD2	3:I:74:HIS:N	2.77	0.52
4:J:239:GLN:O	4:J:240:ALA:HB3	2.09	0.52
7:P:148:UNK:O	7:P:149:UNK:CB	2.57	0.52
2:B:61:PHE:HZ	11:B:1488:CLA:HBB1	1.73	0.52
2:B:62:VAL:HG13	11:B:1486:CLA:O2D	2.10	0.52
3:C:137:PRO:O	3:C:138:GLU:HB2	2.08	0.52
6:F:15:ILE:HG22	6:F:15:ILE:O	2.09	0.52
2:H:263:THR:CG2	2:H:448:ARG:CZ	2.87	0.52
4:J:111:TRP:O	4:J:112:THR:C	2.47	0.52
10:Y:272:UNK:O	10:Y:273:UNK:C	2.57	0.52
1:A:294:ALA:O	1:A:296:ASN:N	2.43	0.52
4:D:80:THR:HB	4:D:168:PHE:HA	1.91	0.52
4:D:35:ILE:O	4:D:35:ILE:CG2	2.57	0.52
4:D:32:TRP:O	4:D:35:ILE:N	2.42	0.52
1:G:193:LEU:HD13	4:J:179:PHE:HB3	1.92	0.52
1:G:214:MET:HE1	12:J:1352:PHO:HED1	1.91	0.52
3:I:183:GLY:O	3:I:184:GLY:O	2.28	0.52
12:G:1345:PHO:HAB	4:J:205:LEU:HD21	1.90	0.52
10:Y:459:UNK:O	10:Y:460:UNK:C	2.56	0.52
1:A:122:GLY:O	1:A:125:CYS:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:VAL:O	1:A:53:ILE:HG13	2.10	0.52
3:C:116:VAL:HG23	3:C:117:VAL:H	1.73	0.52
3:C:244:CYS:HA	11:C:1464:CLA:HMC3	1.90	0.52
3:C:35:TRP:O	3:C:37:ALA:N	2.43	0.52
2:H:415:PRO:O	2:H:418:LYS:N	2.43	0.52
3:I:376:ASP:HB3	3:I:379:LYS:H	1.75	0.52
4:J:174:GLY:O	4:J:178:ILE:HG13	2.10	0.52
4:J:72:ASN:OD1	4:J:72:ASN:O	2.27	0.52
4:J:80:THR:HB	4:J:168:PHE:HA	1.92	0.52
7:P:37:UNK:O	7:P:38:UNK:CB	2.58	0.52
8:U:31:UNK:O	8:U:32:UNK:C	2.55	0.52
8:U:46:UNK:O	8:U:47:UNK:C	2.55	0.52
1:A:34:GLY:C	1:A:36:ILE:N	2.62	0.52
2:B:309:LEU:O	2:B:310:ALA:C	2.48	0.52
4:D:88:SER:O	4:D:167:TRP:HZ3	1.92	0.52
1:G:331:MET:O	1:G:332:HIS:C	2.46	0.52
2:H:138:MET:C	2:H:140:GLY:N	2.63	0.52
2:H:66:MET:O	2:H:71:VAL:HB	2.10	0.52
3:I:39:ASN:HB2	11:I:1466:CLA:HAA2	1.90	0.52
4:J:167:TRP:O	4:J:168:PHE:CB	2.58	0.52
4:J:45:LEU:CD2	4:J:49:LEU:HD11	2.40	0.52
4:J:88:SER:O	4:J:90:LEU:N	2.43	0.52
1:G:309:ALA:HB2	5:K:52:PRO:O	2.10	0.52
9:V:2:GLU:O	9:V:4:THR:N	2.41	0.52
10:X:158:UNK:O	10:X:162:UNK:N	2.42	0.52
10:Y:3:UNK:O	10:Y:6:UNK:N	2.43	0.52
2:B:18:ARG:NH1	2:B:115:TRP:CZ2	2.78	0.52
2:B:37:MET:O	2:B:40:TYR:N	2.43	0.52
6:F:28:VAL:HB	6:F:29:PRO:CD	2.37	0.52
1:G:102:LEU:HD11	1:G:105:TRP:CE3	2.45	0.52
2:H:314:TYR:H	2:H:427:GLY:HA3	1.75	0.52
3:I:69:LEU:HD13	3:I:115:GLY:HA3	1.91	0.52
4:J:91:LEU:O	4:J:93:TRP:N	2.42	0.52
10:Y:219:UNK:O	10:Y:220:UNK:C	2.58	0.52
10:Y:59:UNK:O	10:Y:61:UNK:N	2.43	0.52
1:A:142:TRP:CH2	1:A:273:PHE:HE1	2.28	0.52
11:B:1485:CLA:HMC2	11:B:1492:CLA:H191	1.92	0.52
2:B:149:LEU:C	11:B:1484:CLA:HBC2	2.30	0.52
2:B:94:GLU:CG	2:B:95:GLY:H	2.23	0.52
3:C:252:ILE:O	3:C:253:LEU:C	2.49	0.52
3:C:25:ASN:O	3:C:26:ARG:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:54:PHE:HB3	5:E:47:PHE:CG	2.44	0.52
5:E:51:ARG:O	5:E:53:ASP:N	2.43	0.52
5:E:62:SER:C	5:E:64:PRO:HD3	2.30	0.52
1:G:129:ARG:HH22	4:J:256:ILE:CA	2.22	0.52
1:G:310:LYS:HZ2	5:K:58:GLN:HG2	1.75	0.52
2:H:279:TYR:O	2:H:281:GLN:N	2.43	0.52
2:H:425:ILE:HG23	2:H:426:PHE:HD2	1.75	0.52
2:H:64:PRO:HG3	2:H:267:LEU:O	2.09	0.52
2:H:79:SER:O	2:H:80:ILE:HG13	2.09	0.52
3:I:429:SER:O	3:I:432:VAL:HB	2.10	0.52
6:L:15:ILE:O	6:L:15:ILE:HG22	2.09	0.52
1:A:151:LEU:CG	1:A:155:PHE:HE2	2.23	0.52
1:A:290:ILE:C	1:A:292:THR:N	2.62	0.52
2:B:103:LEU:HD23	2:B:103:LEU:N	2.24	0.52
2:B:247:PHE:HB2	11:B:1489:CLA:HBC1	1.92	0.52
2:B:362:PHE:HE2	4:D:184:PHE:CZ	2.27	0.52
3:C:450:ALA:O	3:C:455:PHE:N	2.41	0.52
3:C:77:PRO:C	3:C:79:LYS:N	2.64	0.52
4:D:279:LEU:CD1	12:D:1352:PHO:HBC3	2.40	0.52
4:D:57:SER:O	4:D:58:TRP:C	2.47	0.52
1:G:184:ILE:HA	11:G:1342:CLA:HBC1	1.92	0.52
2:H:33:TRP:O	2:H:36:SER:HB3	2.10	0.52
3:I:227:VAL:HG11	3:I:233:VAL:HG23	1.92	0.52
4:J:236:ASN:C	4:J:238:THR:H	2.12	0.52
9:V:46:THR:OG1	9:V:52:LEU:O	2.26	0.52
10:X:268:UNK:O	10:X:269:UNK:C	2.58	0.52
10:Y:200:UNK:O	10:Y:201:UNK:C	2.58	0.52
3:C:376:ASP:HB3	3:C:379:LYS:H	1.76	0.51
1:A:323:ARG:HG3	4:D:329:MET:HA	1.91	0.51
6:F:37:ILE:HG22	6:F:41:GLN:HE21	1.75	0.51
2:H:201:HIS:CD2	2:H:202:HIS:ND1	2.76	0.51
2:H:426:PHE:O	2:H:426:PHE:HD1	1.93	0.51
2:H:314:TYR:HA	2:H:427:GLY:HA3	1.92	0.51
3:I:168:LEU:HD23	11:I:1459:CLA:HMC2	1.92	0.51
3:I:450:ALA:O	3:I:455:PHE:N	2.43	0.51
10:Y:158:UNK:O	10:Y:162:UNK:N	2.43	0.51
1:A:129:ARG:HH22	4:D:256:ILE:CA	2.24	0.51
1:A:132:GLU:C	1:A:134:SER:N	2.63	0.51
1:A:248:ILE:O	1:A:251:ALA:N	2.38	0.51
1:A:60:ILE:HG23	1:A:61:ASP:N	2.25	0.51
2:B:138:MET:O	2:B:140:GLY:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:PRO:CB	11:B:1487:CLA:O1D	2.58	0.51
2:B:49:ASP:OD2	2:B:52:LEU:HB2	2.10	0.51
3:C:176:VAL:HG23	3:C:234:VAL:HG12	1.92	0.51
4:D:16:ASP:O	4:D:18:LEU:N	2.44	0.51
5:E:37:PHE:CD1	5:E:42:LEU:HB2	2.46	0.51
1:G:151:LEU:CG	1:G:155:PHE:HE2	2.23	0.51
1:G:162:PRO:HB3	1:G:168:PHE:HA	1.93	0.51
2:H:166:MET:HE3	11:H:1484:CLA:HED2	1.93	0.51
3:I:162:GLY:CA	3:I:248:GLY:HA2	2.40	0.51
3:I:35:TRP:C	3:I:37:ALA:N	2.59	0.51
5:K:63:ILE:N	5:K:64:PRO:CD	2.73	0.51
9:V:28:GLU:HA	9:V:28:GLU:OE1	2.10	0.51
1:A:84:PRO:HG2	1:A:173:PRO:HG3	1.92	0.51
3:C:176:VAL:CG1	3:C:177:ALA:N	2.73	0.51
3:C:227:VAL:HG12	3:C:227:VAL:O	2.09	0.51
3:C:282:MET:O	3:C:285:ILE:HB	2.10	0.51
3:C:35:TRP:CE3	3:C:36:TRP:HB3	2.45	0.51
4:D:100:ASP:CB	4:D:103:ARG:HB2	2.40	0.51
1:G:134:SER:C	1:G:136:ARG:H	2.12	0.51
1:G:60:ILE:HB	1:G:83:VAL:HG12	1.91	0.51
2:H:138:MET:HA	2:H:141:ILE:HG22	1.92	0.51
3:I:280:SER:O	3:I:434:ALA:HB1	2.10	0.51
3:I:80:PRO:HB2	3:I:83:GLU:HB3	1.92	0.51
8:U:43:UNK:O	8:U:47:UNK:N	2.42	0.51
8:U:55:UNK:O	8:U:58:UNK:N	2.43	0.51
10:X:563:UNK:O	10:X:566:UNK:N	2.43	0.51
2:B:164:PRO:HB2	11:B:1487:CLA:O1D	2.10	0.51
2:B:263:THR:CG2	2:B:448:ARG:CZ	2.88	0.51
11:C:1466:CLA:HBD	11:C:1466:CLA:HBA1	1.93	0.51
5:E:37:PHE:CE1	5:E:42:LEU:CB	2.93	0.51
2:H:110:ALA:HA	11:H:1496:CLA:C20	2.40	0.51
2:H:220:ARG:CD	2:H:221:PRO:HD2	2.41	0.51
3:I:418:ASN:CA	3:I:419:PHE:N	2.74	0.51
4:J:291:LEU:N	4:J:291:LEU:CD1	2.73	0.51
5:K:51:ARG:O	5:K:53:ASP:N	2.43	0.51
9:V:30:LYS:HG2	9:V:118:HIS:CE1	2.45	0.51
10:X:177:UNK:O	10:X:180:UNK:N	2.43	0.51
10:X:516:UNK:O	10:X:518:UNK:N	2.44	0.51
1:A:122:GLY:C	1:A:124:SER:N	2.64	0.51
2:B:37:MET:HG2	2:B:62:VAL:HG21	1.92	0.51
3:C:109:PHE:O	3:C:113:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:152:VAL:HG23	4:D:279:LEU:HB3	1.91	0.51
1:G:60:ILE:HG23	1:G:61:ASP:N	2.25	0.51
1:G:69:GLY:C	1:G:75:ASN:OD1	2.49	0.51
2:H:138:MET:O	2:H:140:GLY:N	2.44	0.51
11:H:1486:CLA:HMB1	11:H:1486:CLA:HBB1	1.93	0.51
3:I:280:SER:HA	3:I:434:ALA:HA	1.92	0.51
4:J:274:VAL:HB	4:J:275:PRO:CD	2.37	0.51
5:K:8:ARG:CB	5:K:9:PRO:CD	2.88	0.51
6:L:29:PRO:O	6:L:33:PHE:HD1	1.92	0.51
7:P:160:UNK:O	7:P:161:UNK:C	2.59	0.51
1:A:107:TYR:C	1:A:109:GLY:N	2.56	0.51
1:A:159:LEU:HD11	1:A:163:ILE:HD11	1.91	0.51
1:A:326:LEU:O	1:A:329:GLU:N	2.43	0.51
1:A:54:ALA:CB	1:A:72:LEU:HD12	2.40	0.51
1:A:93:PHE:C	1:A:95:PRO:HD3	2.31	0.51
2:B:288:VAL:HG23	2:B:289:GLN:H	1.75	0.51
3:C:116:VAL:CG2	3:C:117:VAL:H	2.23	0.51
3:C:74:HIS:CD2	3:C:74:HIS:N	2.78	0.51
4:D:152:VAL:HG12	11:D:1351:CLA:H43	1.92	0.51
4:D:181:PHE:CZ	4:D:185:PHE:CE1	2.98	0.51
1:G:122:GLY:C	1:G:124:SER:N	2.64	0.51
1:G:32:TRP:O	1:G:35:VAL:N	2.42	0.51
4:J:9:PRO:O	4:J:10:ALA:CB	2.58	0.51
4:J:136:VAL:HG12	4:J:136:VAL:O	2.09	0.51
1:G:193:LEU:HB3	4:J:179:PHE:CE1	2.45	0.51
4:J:329:MET:O	4:J:330:ALA:C	2.47	0.51
5:K:31:PHE:CE1	6:L:35:GLY:HA2	2.46	0.51
5:K:35:TRP:CD2	6:L:39:ALA:HB2	2.45	0.51
9:T:30:LYS:O	9:T:34:GLN:HG3	2.10	0.51
10:X:422:UNK:O	10:X:423:UNK:C	2.58	0.51
1:A:132:GLU:C	1:A:134:SER:H	2.13	0.51
1:A:93:PHE:O	1:A:95:PRO:HD3	2.11	0.51
3:C:430:HIS:NE2	11:C:1460:CLA:ND	2.59	0.51
1:A:83:VAL:HG22	4:D:314:PHE:CE1	2.45	0.51
4:D:330:ALA:O	4:D:333:ASP:N	2.37	0.51
1:G:120:LEU:O	1:G:124:SER:N	2.44	0.51
1:G:143:ILE:N	4:J:220:ASN:HD21	2.08	0.51
1:G:210:LEU:HD12	1:G:210:LEU:C	2.31	0.51
2:H:68:ARG:CG	2:H:69:LEU:N	2.74	0.51
3:I:367:GLU:O	3:I:370:ARG:HB2	2.11	0.51
4:J:296:TYR:O	4:J:296:TYR:CD2	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:296:TYR:CE1	4:J:319:LEU:HD23	2.46	0.51
6:L:37:ILE:HA	6:L:40:MET:HE3	1.91	0.51
7:O:160:UNK:O	7:O:161:UNK:C	2.59	0.51
10:X:184:UNK:O	10:X:185:UNK:C	2.59	0.51
10:Y:422:UNK:O	10:Y:423:UNK:C	2.59	0.51
10:Y:59:UNK:C	10:Y:61:UNK:N	2.72	0.51
2:B:246:PHE:CE1	2:B:463:PHE:HB2	2.40	0.51
3:C:225:VAL:HG22	3:C:289:PHE:HD1	1.76	0.51
3:C:330:SER:HB3	7:O:56:UNK:O	2.10	0.51
3:C:80:PRO:HB2	3:C:83:GLU:CB	2.41	0.51
4:D:62:GLY:C	4:D:63:LEU:HD12	2.31	0.51
1:G:132:GLU:C	1:G:134:SER:H	2.15	0.51
2:H:40:TYR:O	2:H:41:GLU:C	2.48	0.51
3:I:235:GLY:HA2	3:I:238:ILE:HD12	1.93	0.51
10:X:568:UNK:O	10:X:569:UNK:C	2.58	0.51
10:Y:264:UNK:O	10:Y:265:UNK:C	2.57	0.51
1:A:112:TYR:CE1	1:A:116:ILE:CD1	2.93	0.51
1:A:54:ALA:HB2	1:A:72:LEU:HD12	1.93	0.51
3:C:322:GLN:HE22	3:C:381:LYS:HA	1.76	0.51
3:C:385:GLN:HB3	3:C:386:PRO:HD2	1.93	0.51
1:A:140:ARG:O	4:D:220:ASN:HB3	2.10	0.51
4:D:210:LEU:HD11	4:D:270:PHE:CD2	2.46	0.51
1:G:118:HIS:O	1:G:119:PHE:C	2.49	0.51
2:H:280:PHE:CE2	2:H:312:TYR:HB3	2.46	0.51
2:H:475:PHE:CZ	4:J:134:ARG:HB2	2.46	0.51
2:H:61:PHE:CZ	11:H:1488:CLA:HBB1	2.45	0.51
3:I:35:TRP:O	3:I:37:ALA:N	2.43	0.51
3:I:449:ARG:NH1	3:I:449:ARG:CG	2.53	0.51
4:J:209:LEU:C	4:J:209:LEU:CD2	2.80	0.51
8:U:63:UNK:O	8:U:64:UNK:CB	2.58	0.51
10:X:203:UNK:O	10:X:204:UNK:C	2.58	0.51
10:X:459:UNK:O	10:X:460:UNK:C	2.56	0.51
2:B:220:ARG:CB	2:B:221:PRO:HD2	2.41	0.51
2:B:314:TYR:HA	2:B:427:GLY:HA3	1.92	0.51
2:B:67:ALA:HA	2:B:71:VAL:O	2.11	0.51
3:C:127:PHE:CE2	11:C:1471:CLA:HBC1	2.45	0.51
3:C:281:MET:O	3:C:282:MET:C	2.49	0.51
1:A:220:THR:O	4:D:139:ARG:HD2	2.11	0.51
4:D:172:SER:O	4:D:173:PHE:HB2	2.11	0.51
5:E:74:GLN:O	5:E:75:GLN:C	2.47	0.51
1:G:132:GLU:C	1:G:134:SER:N	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:GLY:O	1:G:208:GLY:C	2.49	0.51
1:G:317:TRP:CG	4:J:177:ALA:HB2	2.46	0.51
1:G:93:PHE:C	1:G:95:PRO:HD3	2.32	0.51
2:H:462:PHE:HE1	11:H:1494:CLA:HMB3	1.76	0.51
3:I:36:TRP:O	11:I:1466:CLA:H43	2.10	0.51
3:I:24:THR:O	3:I:25:ASN:CB	2.58	0.51
3:I:455:PHE:O	3:I:456:GLU:CG	2.59	0.51
3:I:93:ALA:O	3:I:94:THR:C	2.49	0.51
10:X:264:UNK:O	10:X:265:UNK:C	2.59	0.51
10:X:64:UNK:O	10:X:65:UNK:C	2.57	0.51
1:A:315:ASN:HA	1:A:319:ASP:OD2	2.11	0.50
2:B:202:HIS:HE1	11:B:1484:CLA:NB	2.09	0.50
2:B:194:ASN:OD1	2:B:194:ASN:C	2.50	0.50
2:B:61:PHE:O	2:B:62:VAL:C	2.48	0.50
11:C:1463:CLA:HAC1	11:C:1463:CLA:H92	1.92	0.50
3:C:72:LEU:O	3:C:73:ALA:C	2.49	0.50
4:D:39:PRO:O	4:D:43:LEU:CB	2.59	0.50
2:H:24:LEU:HB3	2:H:111:ALA:CB	2.41	0.50
2:H:424:ALA:C	2:H:426:PHE:H	2.13	0.50
4:J:213:ILE:O	4:J:214:HIS:C	2.49	0.50
4:J:52:THR:O	4:J:66:SER:HA	2.10	0.50
5:K:38:VAL:HG11	6:L:40:MET:HG2	1.91	0.50
7:O:127:UNK:O	7:O:129:UNK:N	2.44	0.50
10:X:262:UNK:O	10:X:263:UNK:C	2.58	0.50
10:Y:201:UNK:O	10:Y:202:UNK:C	2.59	0.50
10:Y:412:UNK:C	10:Y:414:UNK:N	2.72	0.50
1:A:116:ILE:CD1	1:A:158:PHE:HD1	2.24	0.50
1:A:145:VAL:HA	1:A:148:SER:HB3	1.93	0.50
3:C:39:ASN:HB2	11:C:1466:CLA:HAA2	1.92	0.50
3:C:455:PHE:O	3:C:456:GLU:CB	2.59	0.50
4:D:126:MET:CE	4:D:146:PHE:HB3	2.42	0.50
1:A:193:LEU:HD13	4:D:179:PHE:HB3	1.91	0.50
1:A:248:ILE:CD1	4:D:235:PHE:HZ	2.17	0.50
1:G:176:ILE:HG23	1:G:180:PHE:HE1	1.76	0.50
1:G:211:PHE:CE2	1:G:274:PHE:CE2	2.99	0.50
3:I:156:LYS:O	3:I:157:MET:C	2.50	0.50
3:I:370:ARG:HA	3:I:375:LEU:H	1.76	0.50
3:I:376:ASP:HB2	3:I:379:LYS:CG	2.35	0.50
4:J:16:ASP:O	4:J:18:LEU:N	2.45	0.50
9:V:64:PRO:HD2	9:V:66:ARG:NH2	2.26	0.50
9:V:87:GLU:CD	9:V:96:ARG:HH22	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:THR:CG2	2:B:107:LEU:HD13	2.37	0.50
2:B:37:MET:HG2	2:B:62:VAL:CG2	2.42	0.50
3:C:150:ASP:CB	3:C:271:TYR:HE2	2.25	0.50
3:C:308:GLU:O	3:C:311:GLN:HB2	2.12	0.50
5:E:18:ARG:O	5:E:21:VAL:HB	2.11	0.50
2:H:193:TYR:CZ	2:H:259:GLY:HA2	2.46	0.50
3:I:180:MET:HG3	3:I:181:PHE:N	2.27	0.50
4:J:222:LEU:HA	4:J:244:TYR:HA	1.93	0.50
4:J:93:TRP:HH2	11:J:1353:CLA:HBA2	1.76	0.50
7:P:163:UNK:O	7:P:164:UNK:O	2.29	0.50
9:T:134:LYS:O	9:T:137:TYR:N	2.43	0.50
10:Y:270:UNK:O	10:Y:271:UNK:C	2.60	0.50
1:A:60:ILE:HB	1:A:83:VAL:HG11	1.91	0.50
2:B:197:GLY:O	2:B:199:VAL:N	2.43	0.50
2:B:270:PRO:O	2:B:271:THR:CG2	2.59	0.50
2:B:397:VAL:O	2:B:399:VAL:N	2.44	0.50
1:G:141:PRO:HG2	3:I:446:GLY:C	2.30	0.50
1:G:177:SER:O	1:G:180:PHE:N	2.44	0.50
3:I:56:HIS:O	3:I:57:ALA:C	2.50	0.50
4:J:313:THR:C	4:J:315:TYR:H	2.13	0.50
5:K:74:GLN:O	5:K:75:GLN:C	2.49	0.50
5:K:10:PHE:HE2	6:L:19:ARG:CZ	2.24	0.50
8:U:66:UNK:O	8:U:70:UNK:N	2.45	0.50
10:Y:356:UNK:O	10:Y:357:UNK:C	2.59	0.50
10:Y:573:UNK:O	10:Y:574:UNK:C	2.60	0.50
1:A:305:SER:O	1:A:313:VAL:HG13	2.11	0.50
1:G:288:LEU:O	1:G:289:GLY:C	2.48	0.50
2:H:68:ARG:HH22	11:H:1485:CLA:HED3	1.76	0.50
3:I:188:THR:HG21	3:I:298:PRO:CB	2.41	0.50
3:I:281:MET:O	3:I:282:MET:C	2.50	0.50
3:I:298:PRO:O	3:I:299:SER:HB3	2.10	0.50
3:I:53:HIS:NE2	11:I:1467:CLA:NB	2.60	0.50
4:J:330:ALA:O	4:J:333:ASP:N	2.37	0.50
6:L:21:VAL:O	6:L:25:THR:HG23	2.12	0.50
8:S:14:UNK:C	8:S:16:UNK:N	2.72	0.50
10:X:68:UNK:C	10:X:70:UNK:N	2.74	0.50
1:A:255:PHE:CZ	1:A:259:ILE:HD12	2.46	0.50
2:B:397:VAL:C	2:B:399:VAL:H	2.15	0.50
3:C:188:THR:CG2	3:C:300:GLU:OE1	2.60	0.50
3:C:230:LEU:HD12	3:C:230:LEU:O	2.12	0.50
4:D:159:ILE:O	4:D:160:TYR:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:88:SER:O	4:D:167:TRP:CZ3	2.65	0.50
4:D:272:LEU:HD21	4:D:276:VAL:HG21	1.93	0.50
5:E:37:PHE:CE2	5:E:43:ALA:HA	2.47	0.50
5:E:8:ARG:CB	5:E:9:PRO:CD	2.87	0.50
1:G:142:TRP:CH2	1:G:273:PHE:HE1	2.30	0.50
1:G:258:LEU:CD1	4:J:128:ARG:NH2	2.75	0.50
1:G:37:MET:O	1:G:38:ILE:C	2.49	0.50
2:H:15:ASP:CA	2:H:16:PRO:CD	2.88	0.50
2:H:290:ALA:O	2:H:294:SER:HB3	2.12	0.50
2:H:68:ARG:HG3	2:H:69:LEU:N	2.27	0.50
3:I:80:PRO:HB2	3:I:83:GLU:CB	2.40	0.50
1:G:323:ARG:HG3	4:J:329:MET:HA	1.94	0.50
7:P:127:UNK:O	7:P:129:UNK:N	2.45	0.50
1:A:311:GLY:HA3	9:V:125:ILE:CG2	2.41	0.50
10:X:168:UNK:O	10:X:169:UNK:C	2.59	0.50
10:X:412:UNK:C	10:X:414:UNK:N	2.73	0.50
1:A:84:PRO:HG3	1:A:112:TYR:CE2	2.47	0.50
2:B:366:PHE:HD2	2:B:425:ILE:HD11	1.75	0.50
1:A:288:LEU:HD13	3:C:432:VAL:HG22	1.92	0.50
5:E:82:GLN:O	5:E:84:LYS:N	2.43	0.50
1:G:60:ILE:HB	1:G:83:VAL:HG11	1.93	0.50
11:H:1485:CLA:HMC2	11:H:1492:CLA:H191	1.93	0.50
2:H:397:VAL:C	2:H:399:VAL:H	2.15	0.50
3:I:119:LEU:O	3:I:122:SER:OG	2.30	0.50
3:I:178:LYS:CA	3:I:182:PHE:HB2	2.40	0.50
3:I:366:LEU:HD12	3:I:366:LEU:O	2.12	0.50
4:J:183:LEU:O	4:J:184:PHE:C	2.49	0.50
4:J:190:ASN:HB2	4:J:296:TYR:HD1	1.76	0.50
4:J:209:LEU:HD21	4:J:213:ILE:HD11	1.92	0.50
6:L:33:PHE:HA	6:L:36:ALA:HB3	1.94	0.50
7:O:123:UNK:O	7:O:126:UNK:N	2.45	0.50
8:S:29:UNK:O	8:S:30:UNK:C	2.59	0.50
10:Y:168:UNK:O	10:Y:169:UNK:C	2.60	0.50
11:A:1342:CLA:H143	12:A:1345:PHO:H62	1.93	0.50
2:B:135:LEU:O	2:B:137:LYS:N	2.45	0.50
2:B:351:GLY:O	2:B:353:GLU:N	2.45	0.50
1:G:266:ASN:O	1:G:267:ASN:O	2.30	0.50
11:H:1496:CLA:H171	11:H:1497:CLA:HMD1	1.93	0.50
2:H:346:PHE:O	2:H:353:GLU:O	2.29	0.50
1:G:276:ALA:HB2	4:J:215:GLY:C	2.32	0.50
10:Y:17:UNK:O	10:Y:18:UNK:C	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:203:UNK:O	10:Y:204:UNK:C	2.59	0.50
10:Y:526:UNK:O	10:Y:529:UNK:N	2.45	0.50
1:A:118:HIS:O	1:A:119:PHE:C	2.47	0.50
1:A:184:ILE:HA	11:A:1342:CLA:HBC1	1.94	0.50
1:A:290:ILE:CD1	11:A:1342:CLA:OBD	2.58	0.50
12:A:1345:PHO:CAB	4:D:205:LEU:HD21	2.41	0.50
2:B:220:ARG:CD	2:B:221:PRO:HD2	2.41	0.50
2:B:400:SER:HB3	2:B:410:THR:CB	2.27	0.50
3:C:159:THR:HA	3:C:252:ILE:HA	1.94	0.50
3:C:318:LEU:HD11	3:C:328:VAL:HG21	1.93	0.50
4:D:53:THR:HG21	6:F:37:ILE:HD11	1.93	0.50
5:E:10:PHE:HD2	6:F:19:ARG:NH2	2.09	0.50
5:E:10:PHE:HE2	6:F:19:ARG:HE	1.60	0.50
5:E:18:ARG:NH1	10:X:564:UNK:CB	2.75	0.50
1:G:107:TYR:O	1:G:109:GLY:N	2.44	0.50
11:H:1486:CLA:HMC1	11:H:1486:CLA:HBC2	1.94	0.50
2:H:178:VAL:O	2:H:179:GLN:HG3	2.11	0.50
2:H:418:LYS:O	2:H:419:SER:C	2.48	0.50
2:H:63:LEU:O	2:H:64:PRO:C	2.48	0.50
3:I:322:GLN:HE22	3:I:381:LYS:HA	1.77	0.50
4:J:209:LEU:O	4:J:209:LEU:HD23	2.12	0.50
5:K:41:GLY:O	5:K:44:TYR:HB2	2.11	0.50
6:L:14:PRO:O	6:L:15:ILE:HB	2.12	0.50
10:X:423:UNK:O	10:X:424:UNK:C	2.60	0.50
10:Y:225:UNK:O	10:Y:226:UNK:C	2.59	0.50
1:A:114:LEU:O	1:A:115:ILE:C	2.49	0.49
1:A:183:MET:HE2	11:A:1343:CLA:HBC3	1.92	0.49
1:A:210:LEU:HD12	1:A:210:LEU:O	2.12	0.49
1:A:69:GLY:C	1:A:75:ASN:OD1	2.51	0.49
2:B:236:THR:HG23	2:B:237:VAL:N	2.27	0.49
2:B:408:GLY:O	2:B:409:GLN:HB2	2.12	0.49
3:C:449:ARG:NH1	11:C:1463:CLA:O1D	2.45	0.49
1:A:65:GLU:CD	4:D:312:GLU:OE1	2.50	0.49
1:G:34:GLY:C	1:G:36:ILE:N	2.65	0.49
2:H:211:ILE:O	2:H:214:LEU:HG	2.10	0.49
2:H:415:PRO:O	2:H:419:SER:N	2.37	0.49
2:H:437:LEU:O	2:H:439:SER:N	2.43	0.49
3:I:120:ILE:C	3:I:122:SER:N	2.66	0.49
3:I:170:ILE:CG2	3:I:171:GLY:N	2.75	0.49
3:I:169:GLY:CA	3:I:244:CYS:SG	3.00	0.49
3:I:74:HIS:H	3:I:74:HIS:CD2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:276:VAL:O	4:J:280:TRP:HD1	1.95	0.49
5:K:37:PHE:CE2	5:K:43:ALA:HA	2.47	0.49
8:S:72:UNK:O	8:S:73:UNK:C	2.57	0.49
10:X:263:UNK:O	10:X:264:UNK:C	2.60	0.49
10:X:526:UNK:C	10:X:528:UNK:N	2.73	0.49
10:Y:405:UNK:O	10:Y:409:UNK:N	2.44	0.49
1:A:133:LEU:HB2	4:D:252:PHE:CE2	2.47	0.49
1:A:279:PRO:HB2	12:A:1345:PHO:HBC1	1.94	0.49
2:B:139:PHE:HB2	11:B:1491:CLA:CHD	2.42	0.49
2:B:478:VAL:O	2:B:481:GLY:N	2.45	0.49
3:C:40:ALA:HA	3:C:43:ILE:HG23	1.94	0.49
2:B:468:TRP:HD1	4:D:144:ILE:HD11	1.73	0.49
6:F:29:PRO:O	6:F:33:PHE:HD1	1.95	0.49
12:G:1345:PHO:HBB2	4:J:205:LEU:HD21	1.93	0.49
1:G:60:ILE:HD12	1:G:84:PRO:HD2	1.94	0.49
3:I:166:ILE:HD11	3:I:249:ILE:HD13	1.95	0.49
4:J:191:TRP:HA	4:J:191:TRP:HE3	1.76	0.49
4:J:235:PHE:CD2	4:J:243:THR:HG21	2.47	0.49
10:X:214:UNK:O	10:X:218:UNK:N	2.44	0.49
10:X:24:UNK:O	10:X:25:UNK:C	2.61	0.49
10:Y:221:UNK:O	10:Y:222:UNK:C	2.60	0.49
10:Y:225:UNK:O	10:Y:227:UNK:N	2.46	0.49
10:Y:255:UNK:O	10:Y:256:UNK:C	2.61	0.49
10:Y:418:UNK:O	10:Y:419:UNK:C	2.59	0.49
1:A:172:MET:SD	1:A:179:THR:HG23	2.53	0.49
1:A:285:PHE:O	1:A:289:GLY:N	2.35	0.49
3:C:242:LEU:HD12	3:C:245:ILE:HD11	1.95	0.49
3:C:279:LEU:O	3:C:280:SER:C	2.50	0.49
4:D:276:VAL:O	4:D:280:TRP:HD1	1.95	0.49
4:D:296:TYR:O	4:D:297:ASP:HB3	2.12	0.49
1:G:277:ALA:O	1:G:278:TRP:C	2.50	0.49
1:G:35:VAL:O	1:G:35:VAL:HG12	2.11	0.49
2:H:264:PRO:HB2	2:H:267:LEU:HD12	1.94	0.49
2:H:69:LEU:HB3	11:H:1487:CLA:CMA	2.42	0.49
3:I:272:LEU:O	3:I:273:SER:C	2.49	0.49
8:S:91:UNK:O	8:S:92:UNK:CB	2.59	0.49
9:V:122:GLU:N	9:V:123:PRO:HD2	2.27	0.49
10:X:426:UNK:O	10:X:427:UNK:C	2.60	0.49
10:Y:526:UNK:C	10:Y:528:UNK:N	2.72	0.49
1:A:330:VAL:HG12	4:D:347:PRO:CA	2.36	0.49
2:B:397:VAL:O	2:B:411:PHE:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:370:ARG:HE	3:C:371:GLY:N	2.06	0.49
3:C:440:GLY:O	3:C:441:HIS:C	2.50	0.49
4:D:96:GLU:HA	4:D:96:GLU:OE1	2.12	0.49
1:G:145:VAL:HA	1:G:148:SER:HB3	1.93	0.49
1:G:34:GLY:C	1:G:36:ILE:H	2.15	0.49
2:H:94:GLU:HG3	2:H:95:GLY:H	1.76	0.49
3:I:284:PHE:O	3:I:285:ILE:C	2.50	0.49
9:T:136:TYR:O	9:T:137:TYR:CG	2.65	0.49
2:B:136:PRO:HG2	2:B:221:PRO:HG3	1.94	0.49
2:B:145:LEU:O	2:B:146:ALA:C	2.50	0.49
11:B:1496:CLA:H13	11:B:1497:CLA:HMD2	1.94	0.49
2:B:243:ALA:O	2:B:246:PHE:HB3	2.13	0.49
2:B:280:PHE:O	2:B:283:GLU:HB3	2.13	0.49
3:C:109:PHE:HD2	3:C:110:PRO:HD3	1.77	0.49
3:C:235:GLY:HA2	3:C:238:ILE:CD1	2.43	0.49
3:C:270:ALA:C	3:C:274:TYR:HD2	2.16	0.49
3:C:287:THR:OG1	3:C:288:CYS:N	2.46	0.49
3:C:299:SER:HB2	3:C:303:GLY:O	2.11	0.49
3:C:387:TRP:O	3:C:390:ARG:HG2	2.11	0.49
4:D:296:TYR:CD2	4:D:296:TYR:O	2.65	0.49
17:F:1046:BCR:H331	17:F:1046:BCR:H343	1.94	0.49
1:G:309:ALA:O	9:T:2:GLU:CB	2.60	0.49
3:I:240:ILE:HA	3:I:243:ILE:HB	1.93	0.49
3:I:299:SER:HB2	3:I:303:GLY:O	2.13	0.49
4:J:181:PHE:CZ	4:J:185:PHE:HE1	2.31	0.49
4:J:186:GLN:HB2	11:J:1351:CLA:HBC1	1.93	0.49
1:A:142:TRP:O	1:A:143:ILE:C	2.50	0.49
1:A:219:VAL:HG11	4:D:268:HIS:CD2	2.47	0.49
1:A:278:TRP:CB	1:A:279:PRO:HD3	2.36	0.49
1:A:58:VAL:HB	1:A:83:VAL:HB	1.94	0.49
2:B:138:MET:C	2:B:140:GLY:N	2.65	0.49
2:B:263:THR:O	2:B:448:ARG:NH1	2.45	0.49
2:B:278:SER:O	2:B:281:GLN:HG2	2.13	0.49
2:B:424:ALA:C	2:B:426:PHE:H	2.16	0.49
3:C:109:PHE:CD2	3:C:110:PRO:HD3	2.47	0.49
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.48	0.49
4:D:313:THR:OG1	4:D:315:TYR:HB3	2.13	0.49
1:G:93:PHE:CE1	1:G:95:PRO:HG2	2.48	0.49
2:H:160:GLY:HA2	2:H:163:GLY:HA2	1.94	0.49
2:H:272:ARG:NH1	4:J:164:GLN:HA	2.27	0.49
6:L:17:THR:O	6:L:20:TRP:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:418:UNK:O	10:X:419:UNK:C	2.61	0.49
1:A:184:ILE:O	1:A:185:VAL:C	2.51	0.49
2:B:18:ARG:O	2:B:21:ALA:HB3	2.13	0.49
2:B:24:LEU:HD12	11:B:1496:CLA:HED2	1.94	0.49
2:B:466:HIS:O	2:B:468:TRP:N	2.45	0.49
11:C:1471:CLA:HHD	11:C:1471:CLA:HBC3	1.95	0.49
4:D:199:MET:O	4:D:200:GLY:C	2.51	0.49
1:A:26:ASN:CA	4:D:255:GLN:NE2	2.76	0.49
4:D:291:LEU:CD1	4:D:291:LEU:N	2.76	0.49
1:G:330:VAL:HG11	4:J:328:TRP:HZ2	1.78	0.49
2:H:149:LEU:C	11:H:1484:CLA:HBC2	2.32	0.49
3:I:430:HIS:NE2	11:I:1460:CLA:ND	2.61	0.49
3:I:265:ILE:H	3:I:274:TYR:HH	1.58	0.49
7:O:163:UNK:O	7:O:164:UNK:O	2.31	0.49
10:X:170:UNK:O	10:X:171:UNK:C	2.61	0.49
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.95	0.49
1:A:330:VAL:HG21	4:D:328:TRP:CZ2	2.48	0.49
11:C:1464:CLA:HMC2	11:C:1465:CLA:H121	1.94	0.49
3:C:156:LYS:O	3:C:157:MET:C	2.51	0.49
3:C:250:TRP:O	3:C:250:TRP:HD1	1.94	0.49
1:A:141:PRO:HG2	3:C:446:GLY:C	2.33	0.49
4:D:253:TRP:O	4:D:254:SER:C	2.51	0.49
1:A:330:VAL:HG11	4:D:328:TRP:HZ2	1.76	0.49
2:H:205:ALA:O	2:H:209:GLY:N	2.45	0.49
2:H:309:LEU:O	2:H:310:ALA:C	2.50	0.49
3:I:176:VAL:HG23	3:I:234:VAL:HG12	1.94	0.49
3:I:319:ILE:HD11	3:I:384:ILE:HD11	1.95	0.49
4:J:186:GLN:CB	11:J:1351:CLA:HBC1	2.43	0.49
4:J:188:PHE:CE1	4:J:326:ARG:HG2	2.48	0.49
4:J:253:TRP:O	4:J:254:SER:C	2.50	0.49
1:G:83:VAL:HG13	4:J:314:PHE:CZ	2.47	0.49
9:T:55:ARG:HG3	9:T:131:GLY:HA2	1.95	0.49
8:U:20:UNK:C	8:U:22:UNK:H	2.26	0.49
10:Y:357:UNK:O	10:Y:358:UNK:C	2.60	0.49
1:A:137:LEU:HB2	1:A:139:MET:CE	2.42	0.49
1:A:326:LEU:C	1:A:328:MET:N	2.66	0.49
1:A:330:VAL:CG1	4:D:347:PRO:CA	2.89	0.49
2:B:347:ARG:HB3	2:B:351:GLY:CA	2.28	0.49
2:B:463:PHE:C	2:B:465:GLY:N	2.66	0.49
2:B:61:PHE:CZ	11:B:1488:CLA:HBB1	2.48	0.49
3:C:259:TRP:O	3:C:260:ALA:C	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:429:SER:O	3:C:432:VAL:HB	2.12	0.49
4:D:174:GLY:O	4:D:178:ILE:HG13	2.12	0.49
5:E:63:ILE:N	5:E:64:PRO:HD3	2.28	0.49
1:G:186:PHE:CD2	1:G:192:ILE:CD1	2.86	0.49
1:G:326:LEU:C	1:G:328:MET:N	2.64	0.49
1:G:76:ASN:OD1	1:G:76:ASN:C	2.51	0.49
1:G:58:VAL:HB	1:G:83:VAL:HB	1.95	0.49
2:H:230:ARG:O	2:H:231:MET:C	2.51	0.49
3:I:27:ASP:O	3:I:31:SER:HB2	2.12	0.49
4:J:122:LEU:CD2	11:J:1351:CLA:H92	2.28	0.49
4:J:181:PHE:CZ	4:J:185:PHE:CE1	3.01	0.49
4:J:263:ASN:C	4:J:265:ARG:N	2.66	0.49
4:J:53:THR:HG21	6:L:37:ILE:HD11	1.95	0.49
9:T:128:ASP:HB3	9:T:134:LYS:HG3	1.95	0.49
10:X:168:UNK:O	10:X:170:UNK:N	2.46	0.49
10:Y:64:UNK:O	10:Y:65:UNK:C	2.60	0.49
2:B:69:LEU:HB3	11:B:1487:CLA:CMA	2.43	0.49
4:D:116:LEU:O	4:D:119:ALA:HB3	2.12	0.49
5:E:41:GLY:O	5:E:42:LEU:C	2.50	0.49
1:G:290:ILE:O	1:G:292:THR:N	2.45	0.49
2:H:24:LEU:HD23	2:H:111:ALA:HA	1.94	0.49
2:H:52:LEU:HD23	2:H:311:PHE:CE2	2.48	0.49
2:H:397:VAL:O	2:H:399:VAL:N	2.43	0.49
3:I:159:THR:HA	3:I:252:ILE:HA	1.94	0.49
3:I:35:TRP:CE3	3:I:36:TRP:HB3	2.47	0.49
3:I:442:LEU:HD21	11:I:1463:CLA:C1B	2.43	0.49
4:J:199:MET:O	4:J:200:GLY:C	2.51	0.49
4:J:57:SER:O	4:J:58:TRP:C	2.50	0.49
4:J:54:PHE:HB3	5:K:47:PHE:CG	2.48	0.49
6:L:11:VAL:CG1	6:L:12:SER:N	2.76	0.49
7:O:141:UNK:O	7:O:149:UNK:CB	2.61	0.49
8:S:43:UNK:O	8:S:47:UNK:N	2.46	0.49
8:U:99:UNK:O	8:U:100:UNK:C	2.59	0.49
8:U:4:UNK:O	8:U:7:UNK:CB	2.61	0.49
10:X:219:UNK:O	10:X:220:UNK:C	2.60	0.49
10:X:405:UNK:O	10:X:409:UNK:N	2.46	0.49
10:X:573:UNK:O	10:X:574:UNK:C	2.61	0.49
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.34	0.48
2:B:415:PRO:O	2:B:418:LYS:N	2.46	0.48
2:B:263:THR:O	2:B:448:ARG:NH2	2.46	0.48
2:B:462:PHE:HA	11:B:1492:CLA:CMC	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:445:ALA:CB	11:C:1463:CLA:HED1	2.36	0.48
3:C:178:LYS:CA	3:C:182:PHE:HB2	2.42	0.48
3:C:28:GLN:O	3:C:30:SER:N	2.46	0.48
4:D:235:PHE:CD2	4:D:243:THR:HG21	2.47	0.48
1:G:122:GLY:O	1:G:125:CYS:N	2.45	0.48
2:H:113:TRP:CD1	11:H:1496:CLA:H191	2.48	0.48
3:I:82:TYR:HD2	3:I:302:TYR:O	1.96	0.48
3:I:304:PRO:C	3:I:305:THR:CG2	2.81	0.48
4:J:126:MET:CE	4:J:146:PHE:HB3	2.43	0.48
4:J:279:LEU:CD1	12:J:1352:PHO:HBC3	2.42	0.48
5:K:63:ILE:O	5:K:63:ILE:HG22	2.12	0.48
8:S:63:UNK:O	8:S:64:UNK:CB	2.60	0.48
10:Y:59:UNK:O	10:Y:62:UNK:N	2.46	0.48
1:A:142:TRP:CZ2	1:A:273:PHE:CE1	3.01	0.48
1:A:161:TYR:HA	1:A:294:ALA:HB1	1.95	0.48
2:B:24:LEU:HB3	2:B:111:ALA:CB	2.43	0.48
3:C:449:ARG:HH12	11:C:1463:CLA:HAA1	1.78	0.48
4:D:48:TRP:O	4:D:52:THR:OG1	2.20	0.48
1:G:301:ASN:C	1:G:301:ASN:OD1	2.51	0.48
2:H:263:THR:O	2:H:448:ARG:NH2	2.45	0.48
3:I:52:ALA:HA	11:I:1469:CLA:CMB	2.41	0.48
1:G:214:MET:CE	12:J:1352:PHO:CED	2.91	0.48
4:J:184:PHE:CD1	4:J:184:PHE:C	2.86	0.48
6:L:40:MET:O	6:L:43:ILE:HG13	2.13	0.48
10:X:425:UNK:O	10:X:429:UNK:CB	2.61	0.48
10:X:64:UNK:C	10:X:66:UNK:N	2.74	0.48
10:Y:410:UNK:O	10:Y:411:UNK:C	2.60	0.48
1:A:301:ASN:C	1:A:301:ASN:OD1	2.51	0.48
2:B:178:VAL:O	2:B:179:GLN:HG3	2.12	0.48
2:B:314:TYR:H	2:B:427:GLY:HA3	1.79	0.48
4:D:171:PRO:HG3	4:D:181:PHE:CD1	2.48	0.48
4:D:225:ASP:O	4:D:225:ASP:OD1	2.32	0.48
4:D:263:ASN:C	4:D:265:ARG:N	2.65	0.48
4:D:57:SER:HB2	4:D:63:LEU:O	2.13	0.48
5:E:10:PHE:HE2	6:F:19:ARG:CZ	2.25	0.48
1:G:201:GLY:HA2	1:G:282:GLY:O	2.13	0.48
2:H:135:LEU:CB	2:H:136:PRO:CD	2.86	0.48
2:H:149:LEU:HG	11:H:1484:CLA:CBC	2.34	0.48
2:H:360:PRO:HB2	2:H:363:PHE:CD2	2.44	0.48
2:H:415:PRO:O	2:H:416:THR:C	2.49	0.48
11:I:1466:CLA:HBA1	11:I:1466:CLA:HBD	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:150:ASP:CB	3:I:271:TYR:HE2	2.25	0.48
3:I:265:ILE:N	3:I:274:TYR:HH	2.11	0.48
3:I:43:ILE:HG22	11:I:1467:CLA:HBC2	1.96	0.48
3:I:75:PHE:CZ	3:I:77:PRO:HG3	2.48	0.48
4:J:9:PRO:O	4:J:10:ALA:HB2	2.12	0.48
1:G:83:VAL:HG22	4:J:314:PHE:CE1	2.44	0.48
5:K:74:GLN:O	5:K:77:GLU:N	2.45	0.48
8:S:39:UNK:O	8:S:40:UNK:O	2.31	0.48
8:S:69:UNK:C	8:S:71:UNK:N	2.77	0.48
10:Y:268:UNK:O	10:Y:269:UNK:C	2.61	0.48
10:Y:426:UNK:O	10:Y:427:UNK:C	2.60	0.48
3:C:442:LEU:HD21	11:C:1463:CLA:C1B	2.43	0.48
3:C:225:VAL:HG22	3:C:289:PHE:CD1	2.48	0.48
3:C:354:GLU:C	3:C:356:MET:N	2.63	0.48
3:C:382:ASN:O	3:C:383:ASP:HB2	2.13	0.48
4:D:192:THR:OG1	4:D:193:LEU:N	2.46	0.48
4:D:222:LEU:HA	4:D:244:TYR:HA	1.94	0.48
1:G:142:TRP:O	1:G:143:ILE:C	2.52	0.48
1:G:332:HIS:HD2	1:G:333:GLU:H	1.60	0.48
2:H:236:THR:CB	2:H:473:THR:CG2	2.88	0.48
3:I:28:GLN:O	3:I:30:SER:N	2.46	0.48
1:G:142:TRP:CG	4:J:220:ASN:OD1	2.67	0.48
7:P:42:UNK:CB	7:P:52:UNK:O	2.61	0.48
8:S:71:UNK:O	8:S:72:UNK:C	2.58	0.48
8:U:73:UNK:O	8:U:74:UNK:C	2.59	0.48
8:U:74:UNK:O	8:U:75:UNK:C	2.61	0.48
1:A:258:LEU:HD12	4:D:128:ARG:NH2	2.28	0.48
1:A:255:PHE:CE1	1:A:259:ILE:HD12	2.47	0.48
2:B:114:HIS:NE2	11:B:1497:CLA:NB	2.62	0.48
3:C:288:CYS:O	3:C:289:PHE:C	2.50	0.48
3:C:358:PHE:C	3:C:360:ASP:H	2.17	0.48
3:C:81:MET:O	3:C:84:GLN:N	2.37	0.48
4:D:48:TRP:HB2	4:D:114:ILE:HD13	1.95	0.48
2:H:263:THR:H	2:H:264:PRO:HD3	1.72	0.48
2:H:362:PHE:HE2	4:J:184:PHE:CZ	2.32	0.48
3:I:122:SER:O	3:I:123:ALA:C	2.52	0.48
3:I:440:GLY:O	3:I:441:HIS:C	2.51	0.48
4:J:340:VAL:HG12	4:J:340:VAL:O	2.14	0.48
4:J:81:PRO:O	4:J:168:PHE:HD1	1.97	0.48
4:J:95:PRO:O	4:J:96:GLU:O	2.31	0.48
5:K:16:SER:O	5:K:17:VAL:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:567:UNK:O	10:X:571:UNK:N	2.47	0.48
10:Y:435:UNK:O	10:Y:438:UNK:N	2.46	0.48
4:D:46:GLY:O	4:D:49:LEU:N	2.47	0.48
4:D:53:THR:HG22	4:D:67:TYR:CE1	2.48	0.48
4:D:76:VAL:HG12	4:D:77:ALA:N	2.28	0.48
6:F:33:PHE:HA	6:F:36:ALA:HB3	1.96	0.48
1:G:221:SER:HB2	4:J:139:ARG:O	2.14	0.48
2:H:393:GLU:C	2:H:395:GLN:N	2.64	0.48
2:H:65:PHE:O	2:H:66:MET:C	2.50	0.48
3:I:382:ASN:O	3:I:383:ASP:HB2	2.12	0.48
3:I:49:LEU:O	3:I:52:ALA:N	2.47	0.48
4:J:46:GLY:O	4:J:49:LEU:N	2.45	0.48
4:J:88:SER:O	4:J:167:TRP:HZ3	1.96	0.48
7:P:127:UNK:O	7:P:128:UNK:C	2.61	0.48
8:S:46:UNK:O	8:S:47:UNK:C	2.61	0.48
10:X:272:UNK:O	10:X:273:UNK:C	2.61	0.48
10:Y:263:UNK:O	10:Y:264:UNK:C	2.61	0.48
1:A:127:MET:HB2	1:A:147:TYR:HD1	1.77	0.48
1:A:192:ILE:HG23	1:A:293:MET:HE1	1.95	0.48
2:B:30:VAL:HG12	11:B:1486:CLA:HHD	1.96	0.48
2:B:75:TRP:C	2:B:77:GLY:H	2.11	0.48
4:D:159:ILE:O	4:D:162:LEU:N	2.46	0.48
4:D:87:HIS:HE1	4:D:161:PRO:O	1.96	0.48
6:F:22:ALA:O	6:F:24:HIS:N	2.47	0.48
1:G:330:VAL:CG1	4:J:347:PRO:CA	2.90	0.48
2:H:372:ASP:O	2:H:374:ASN:N	2.43	0.48
3:I:161:LEU:HD21	11:I:1464:CLA:HBB1	1.95	0.48
3:I:171:GLY:O	3:I:172:ALA:C	2.50	0.48
3:I:178:LYS:O	3:I:178:LYS:HD3	2.14	0.48
3:I:385:GLN:HB3	3:I:386:PRO:HD2	1.96	0.48
4:J:298:PHE:O	10:Y:129:UNK:O	2.31	0.48
4:J:54:PHE:HE1	6:L:33:PHE:CE2	2.32	0.48
9:T:48:THR:HG1	18:T:1138:HEC:HMD3	1.79	0.48
8:U:71:UNK:C	8:U:73:UNK:N	2.76	0.48
10:Y:218:UNK:O	10:Y:219:UNK:C	2.62	0.48
1:A:214:MET:O	1:A:217:SER:N	2.47	0.48
1:A:35:VAL:O	1:A:35:VAL:CG1	2.62	0.48
2:B:98:LEU:O	2:B:101:ILE:N	2.46	0.48
2:B:24:LEU:HD23	2:B:111:ALA:HA	1.95	0.48
2:B:426:PHE:O	2:B:426:PHE:CD1	2.67	0.48
2:B:471:ALA:O	2:B:472:ARG:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:227:VAL:CG1	3:C:233:VAL:HG23	2.44	0.48
4:D:298:PHE:O	4:D:299:ILE:HB	2.14	0.48
1:G:159:LEU:HD11	1:G:163:ILE:HD11	1.95	0.48
1:G:222:SER:O	1:G:246:TYR:CB	2.62	0.48
1:G:32:TRP:O	1:G:35:VAL:HB	2.14	0.48
2:H:258:TYR:O	2:H:259:GLY:O	2.32	0.48
2:H:263:THR:O	2:H:448:ARG:NH1	2.46	0.48
2:H:52:LEU:O	2:H:337:ALA:HB3	2.13	0.48
3:I:32:GLY:O	3:I:34:ALA:N	2.43	0.48
4:J:224:GLN:HE21	4:J:227:GLU:CB	2.27	0.48
8:S:57:UNK:O	8:S:59:UNK:N	2.47	0.48
1:A:198:HIS:O	1:A:201:GLY:N	2.47	0.48
3:C:69:LEU:HD13	3:C:115:GLY:HA3	1.94	0.48
3:C:75:PHE:CE2	3:C:77:PRO:HG3	2.49	0.48
1:A:258:LEU:O	4:D:128:ARG:NH2	2.46	0.48
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.14	0.48
2:H:215:PHE:HZ	11:H:1490:CLA:HMD3	1.78	0.48
11:H:1494:CLA:OBD	11:H:1495:CLA:HHC	2.13	0.48
3:I:176:VAL:CG1	3:I:177:ALA:N	2.77	0.48
4:J:116:LEU:O	4:J:119:ALA:HB3	2.14	0.48
4:J:152:VAL:HG23	4:J:279:LEU:HB3	1.95	0.48
5:K:18:ARG:O	5:K:21:VAL:HB	2.14	0.48
7:P:141:UNK:O	7:P:149:UNK:CB	2.62	0.48
8:U:71:UNK:O	8:U:72:UNK:C	2.61	0.48
10:X:331:UNK:O	10:X:332:UNK:C	2.61	0.48
10:Y:168:UNK:O	10:Y:170:UNK:N	2.47	0.48
10:Y:578:UNK:O	10:Y:579:UNK:C	2.62	0.48
2:B:52:LEU:O	2:B:337:ALA:HB3	2.13	0.48
3:C:170:ILE:HG23	3:C:171:GLY:H	1.78	0.48
3:C:53:HIS:NE2	11:C:1467:CLA:NB	2.62	0.48
4:D:113:PHE:CZ	17:F:1046:BCR:HC41	2.49	0.48
1:G:133:LEU:HB2	4:J:252:PHE:HE2	1.79	0.48
1:G:330:VAL:HG21	4:J:328:TRP:CZ2	2.49	0.48
2:H:234:ILE:O	2:H:237:VAL:N	2.46	0.48
3:I:109:PHE:O	3:I:113:VAL:HG23	2.14	0.48
3:I:188:THR:HG21	3:I:298:PRO:CA	2.44	0.48
4:J:159:ILE:O	4:J:160:TYR:C	2.51	0.48
4:J:313:THR:OG1	4:J:315:TYR:HB3	2.12	0.48
8:U:90:UNK:O	8:U:91:UNK:O	2.32	0.48
10:X:159:UNK:O	10:X:160:UNK:C	2.61	0.48
5:K:18:ARG:NH1	10:Y:564:UNK:CB	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:SER:O	1:A:136:ARG:N	2.42	0.47
2:B:195:PRO:O	2:B:197:GLY:N	2.46	0.47
3:C:185:LEU:O	3:C:186:TYR:O	2.31	0.47
4:D:111:TRP:O	4:D:112:THR:C	2.52	0.47
4:D:213:ILE:O	4:D:214:HIS:C	2.52	0.47
4:D:342:PRO:O	4:D:345:VAL:CG2	2.62	0.47
1:G:258:LEU:HD12	4:J:128:ARG:NH2	2.29	0.47
1:G:279:PRO:HB2	12:G:1345:PHO:HBC1	1.96	0.47
1:G:58:VAL:CG1	1:G:109:GLY:HA3	2.44	0.47
3:I:188:THR:CG2	3:I:300:GLU:OE1	2.61	0.47
3:I:51:GLY:HA2	3:I:54:VAL:HB	1.96	0.47
3:I:72:LEU:O	3:I:75:PHE:HB3	2.14	0.47
4:J:101:PHE:O	4:J:104:TRP:HB3	2.13	0.47
11:G:1344:CLA:HBB2	12:J:1352:PHO:H91	1.96	0.47
7:P:26:UNK:O	7:P:27:UNK:C	2.62	0.47
10:X:405:UNK:O	10:X:406:UNK:C	2.61	0.47
10:Y:404:UNK:O	10:Y:405:UNK:CB	2.62	0.47
1:A:181:ASN:O	1:A:183:MET:N	2.48	0.47
1:A:288:LEU:O	1:A:289:GLY:C	2.52	0.47
2:B:162:PHE:CB	11:B:1487:CLA:HMD3	2.44	0.47
2:B:33:TRP:O	2:B:36:SER:HB3	2.14	0.47
2:B:40:TYR:O	2:B:41:GLU:C	2.50	0.47
3:C:118:HIS:HA	3:C:121:SER:HB3	1.95	0.47
3:C:276:LEU:HD11	11:C:1466:CLA:HBB1	1.94	0.47
3:C:43:ILE:CG2	11:C:1467:CLA:HMC1	2.29	0.47
4:D:103:ARG:O	4:D:104:TRP:C	2.50	0.47
4:D:122:LEU:CD2	11:D:1351:CLA:H92	2.28	0.47
4:D:189:HIS:ND1	4:D:294:ARG:NH1	2.62	0.47
4:D:73:PHE:CE2	4:D:175:VAL:HG21	2.48	0.47
4:D:88:SER:O	4:D:90:LEU:N	2.48	0.47
1:G:137:LEU:HD12	1:G:139:MET:HE3	1.97	0.47
1:G:84:PRO:CG	1:G:173:PRO:HD3	2.43	0.47
2:H:194:ASN:O	2:H:195:PRO:C	2.51	0.47
2:H:345:VAL:O	2:H:345:VAL:HG23	2.13	0.47
2:H:408:GLY:O	2:H:409:GLN:HB2	2.13	0.47
3:I:284:PHE:O	3:I:286:ALA:N	2.48	0.47
4:J:111:TRP:O	4:J:113:PHE:N	2.47	0.47
4:J:279:LEU:O	4:J:283:ALA:HB2	2.14	0.47
4:J:296:TYR:O	4:J:297:ASP:HB3	2.15	0.47
6:L:24:HIS:HA	6:L:27:ALA:HB3	1.95	0.47
8:S:9:UNK:O	8:S:11:UNK:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:41:HIS:HA	9:T:45:ILE:O	2.15	0.47
8:U:27:UNK:O	8:U:28:UNK:O	2.32	0.47
10:Y:8:UNK:O	10:Y:9:UNK:C	2.62	0.47
1:A:112:TYR:OH	1:A:116:ILE:HD11	2.14	0.47
1:A:127:MET:HB2	1:A:147:TYR:CD1	2.49	0.47
1:A:244:GLU:HG3	1:A:245:THR:N	2.30	0.47
5:E:31:PHE:CE1	6:F:35:GLY:HA2	2.49	0.47
2:H:76:SER:HA	7:O:69:UNK:CB	2.44	0.47
3:I:243:ILE:HG22	3:I:244:CYS:N	2.30	0.47
3:I:455:PHE:O	3:I:456:GLU:CB	2.61	0.47
1:G:143:ILE:CG1	4:J:220:ASN:HD22	2.12	0.47
5:K:41:GLY:O	5:K:44:TYR:N	2.47	0.47
5:K:82:GLN:O	5:K:84:LYS:N	2.47	0.47
6:L:18:VAL:O	6:L:19:ARG:C	2.51	0.47
7:P:142:UNK:CA	7:P:149:UNK:CB	2.91	0.47
9:V:100:ILE:C	9:V:102:PRO:HD3	2.34	0.47
3:C:390:ARG:CD	9:V:100:ILE:HD12	2.43	0.47
10:Y:428:UNK:C	10:Y:430:UNK:N	2.77	0.47
10:Y:526:UNK:O	10:Y:527:UNK:C	2.61	0.47
10:Y:563:UNK:O	10:Y:566:UNK:N	2.47	0.47
1:A:84:PRO:O	1:A:85:SER:O	2.31	0.47
2:B:263:THR:N	2:B:264:PRO:CD	2.76	0.47
2:B:424:ALA:O	2:B:426:PHE:N	2.44	0.47
3:C:264:PHE:CD2	3:C:264:PHE:N	2.82	0.47
4:D:52:THR:O	4:D:67:TYR:HD1	1.98	0.47
1:G:84:PRO:HG3	1:G:112:TYR:CE2	2.49	0.47
1:G:190:HIS:ND1	1:G:298:ASN:ND2	2.61	0.47
1:G:63:ILE:CG1	1:G:64:ARG:N	2.65	0.47
2:H:33:TRP:NE1	11:H:1488:CLA:HBC2	2.28	0.47
2:H:372:ASP:C	2:H:374:ASN:H	2.18	0.47
11:I:1464:CLA:HBA2	11:I:1464:CLA:H3A	1.49	0.47
3:I:227:VAL:O	3:I:227:VAL:HG12	2.13	0.47
3:I:40:ALA:O	3:I:43:ILE:HG23	2.14	0.47
4:J:127:LEU:C	4:J:129:GLN:H	2.18	0.47
4:J:54:PHE:HE1	6:L:33:PHE:CD2	2.31	0.47
10:X:115:UNK:O	10:X:119:UNK:N	2.47	0.47
10:X:225:UNK:O	10:X:227:UNK:N	2.47	0.47
10:X:526:UNK:O	10:X:527:UNK:C	2.63	0.47
10:Y:24:UNK:O	10:Y:25:UNK:C	2.62	0.47
12:A:1345:PHO:HBB2	4:D:205:LEU:HD21	1.95	0.47
11:B:1496:CLA:H171	11:B:1497:CLA:HMD1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:TYR:HB3	2:B:309:LEU:CD2	2.44	0.47
3:C:154:LYS:HZ3	3:C:261:ARG:HD3	1.75	0.47
3:C:187:ASP:HB3	3:C:230:LEU:CD2	2.27	0.47
3:C:376:ASP:C	3:C:378:ASN:H	2.17	0.47
5:E:35:TRP:CE3	6:F:39:ALA:HB2	2.49	0.47
1:G:129:ARG:NH2	4:J:256:ILE:CA	2.74	0.47
3:I:81:MET:SD	3:I:90:PRO:HG3	2.54	0.47
4:J:191:TRP:CZ2	4:J:286:VAL:CG2	2.97	0.47
7:P:79:UNK:O	7:P:80:UNK:C	2.62	0.47
10:X:357:UNK:O	10:X:358:UNK:C	2.63	0.47
10:Y:170:UNK:O	10:Y:171:UNK:C	2.60	0.47
10:Y:334:UNK:O	10:Y:335:UNK:O	2.31	0.47
1:A:290:ILE:HD11	11:A:1342:CLA:CAD	2.44	0.47
1:A:292:THR:HG23	3:C:428:THR:CG2	2.44	0.47
2:B:278:SER:C	2:B:279:TYR:O	2.50	0.47
2:B:425:ILE:HG23	2:B:426:PHE:HD2	1.79	0.47
3:C:32:GLY:O	3:C:34:ALA:N	2.46	0.47
3:C:376:ASP:OD2	3:C:379:LYS:HE3	2.14	0.47
4:D:224:GLN:HE21	4:D:227:GLU:CB	2.27	0.47
1:G:104:GLU:HG2	1:G:108:ASN:HD21	1.79	0.47
1:G:248:ILE:O	1:G:250:ALA:N	2.47	0.47
1:G:294:ALA:O	1:G:296:ASN:N	2.48	0.47
2:H:137:LYS:O	2:H:141:ILE:HG22	2.14	0.47
3:I:311:GLN:HA	3:I:355:THR:HG21	1.95	0.47
3:I:398:HIS:O	3:I:399:ALA:CA	2.63	0.47
4:J:235:PHE:CD1	4:J:235:PHE:C	2.87	0.47
5:K:15:THR:O	5:K:15:THR:CG2	2.63	0.47
10:X:470:UNK:O	10:X:471:UNK:C	2.62	0.47
1:A:104:GLU:HG2	1:A:108:ASN:HD21	1.80	0.47
1:A:137:LEU:CD1	1:A:139:MET:HE1	2.44	0.47
1:A:53:ILE:O	1:A:71:LEU:HB2	2.14	0.47
2:B:135:LEU:O	2:B:136:PRO:C	2.53	0.47
2:B:162:PHE:HB3	11:B:1487:CLA:HMD3	1.97	0.47
2:B:207:ILE:CG1	2:B:208:VAL:N	2.78	0.47
2:B:68:ARG:CG	2:B:69:LEU:N	2.76	0.47
3:C:127:PHE:C	3:C:129:GLY:H	2.17	0.47
3:C:304:PRO:C	3:C:305:THR:CG2	2.83	0.47
3:C:370:ARG:HA	3:C:375:LEU:H	1.79	0.47
4:D:188:PHE:CE1	4:D:326:ARG:HG2	2.48	0.47
1:G:259:ILE:O	1:G:260:PHE:CB	2.62	0.47
1:G:65:GLU:HG2	1:G:65:GLU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:ALA:HB2	1:G:72:LEU:HD12	1.97	0.47
2:H:192:PRO:HG3	11:H:1483:CLA:HBA2	1.95	0.47
3:I:425:TRP:CZ2	11:I:1462:CLA:O1A	2.68	0.47
3:I:188:THR:HG21	3:I:298:PRO:HA	1.96	0.47
3:I:364:PRO:O	3:I:365:TRP:C	2.51	0.47
4:J:339:PHE:CD1	4:J:341:PHE:CE1	3.03	0.47
4:J:72:ASN:C	4:J:76:VAL:HG23	2.35	0.47
6:L:28:VAL:HB	6:L:29:PRO:CD	2.39	0.47
7:O:42:UNK:CB	7:O:52:UNK:O	2.63	0.47
7:O:79:UNK:O	7:O:80:UNK:C	2.62	0.47
10:X:578:UNK:O	10:X:579:UNK:C	2.63	0.47
1:A:127:MET:O	1:A:130:GLN:HB3	2.14	0.47
1:A:153:SER:HB3	11:A:1342:CLA:H43	1.96	0.47
2:B:288:VAL:CG2	2:B:289:GLN:N	2.78	0.47
2:B:392:PHE:O	2:B:395:GLN:HA	2.14	0.47
4:D:156:VAL:HG12	4:D:156:VAL:O	2.14	0.47
4:D:337:GLU:HG3	4:D:339:PHE:CE2	2.49	0.47
4:D:55:VAL:O	4:D:66:SER:HB3	2.15	0.47
1:G:137:LEU:HB2	1:G:139:MET:HE3	1.97	0.47
2:H:243:ALA:C	2:H:246:PHE:HB3	2.34	0.47
2:H:310:ALA:O	2:H:428:GLU:HB2	2.15	0.47
3:I:387:TRP:O	3:I:390:ARG:HG2	2.15	0.47
3:I:50:LEU:O	3:I:54:VAL:N	2.46	0.47
4:J:39:PRO:O	4:J:43:LEU:CB	2.62	0.47
8:U:69:UNK:O	8:U:70:UNK:C	2.63	0.47
10:X:560:UNK:O	10:X:561:UNK:C	2.62	0.47
10:Y:115:UNK:O	10:Y:119:UNK:N	2.47	0.47
11:A:1342:CLA:HAB	11:A:1344:CLA:HMD2	1.97	0.47
1:A:246:TYR:O	1:A:247:ASN:CG	2.52	0.47
1:A:58:VAL:CG1	1:A:109:GLY:HA3	2.45	0.47
2:B:415:PRO:O	2:B:416:THR:C	2.54	0.47
3:C:162:GLY:CA	3:C:248:GLY:HA2	2.43	0.47
3:C:314:ALA:O	3:C:315:MET:C	2.53	0.47
4:D:43:LEU:HG	4:D:113:PHE:CZ	2.50	0.47
4:D:56:THR:OG1	4:D:57:SER:N	2.48	0.47
1:G:79:THR:O	1:G:80:GLY:O	2.32	0.47
2:H:132:ALA:O	2:H:133:LEU:CB	2.62	0.47
2:H:203:ILE:O	2:H:207:ILE:HG23	2.14	0.47
3:I:245:ILE:O	3:I:249:ILE:HG12	2.15	0.47
4:J:166:SER:O	4:J:167:TRP:C	2.50	0.47
5:K:30:LEU:HD13	6:L:28:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:NH2	4:D:256:ILE:CA	2.75	0.47
11:A:1342:CLA:HBB1	11:D:1351:CLA:NC	2.30	0.47
1:A:196:PRO:O	1:A:199:GLN:HB2	2.14	0.47
2:B:179:GLN:HB3	2:B:180:PRO:HD2	1.96	0.47
2:B:372:ASP:O	2:B:374:ASN:N	2.46	0.47
3:C:172:ALA:O	3:C:175:LEU:N	2.47	0.47
1:A:221:SER:HB2	4:D:139:ARG:O	2.15	0.47
1:G:218:LEU:HD11	1:G:255:PHE:CD2	2.45	0.47
2:H:147:GLY:O	2:H:148:LEU:C	2.53	0.47
2:H:24:LEU:HD12	11:H:1496:CLA:HED2	1.97	0.47
2:H:155:ALA:O	2:H:159:THR:CB	2.63	0.47
2:H:463:PHE:C	2:H:465:GLY:N	2.68	0.47
3:I:82:TYR:HB3	3:I:302:TYR:O	2.14	0.47
4:J:159:ILE:O	4:J:162:LEU:N	2.45	0.47
4:J:74:LEU:HA	4:J:175:VAL:HG11	1.97	0.47
4:J:57:SER:HB2	4:J:63:LEU:O	2.15	0.47
9:T:122:GLU:N	9:T:123:PRO:HD2	2.29	0.47
10:Y:177:UNK:O	10:Y:180:UNK:N	2.47	0.47
1:G:181:ASN:O	1:G:183:MET:N	2.48	0.47
1:G:62:GLY:CA	1:G:87:ASN:CB	2.90	0.47
1:G:93:PHE:O	1:G:95:PRO:HD3	2.14	0.47
2:H:136:PRO:HG2	2:H:221:PRO:HG3	1.97	0.47
2:H:309:LEU:O	2:H:312:TYR:N	2.48	0.47
2:H:330:MET:O	2:H:331:ASN:CB	2.63	0.47
3:I:436:PHE:O	3:I:439:VAL:HB	2.15	0.47
4:J:189:HIS:ND1	4:J:294:ARG:NH1	2.63	0.47
5:K:78:THR:O	5:K:79:PHE:C	2.53	0.47
6:L:37:ILE:HG12	6:L:40:MET:HE2	1.97	0.47
8:S:90:UNK:C	8:S:91:UNK:O	2.62	0.47
9:T:133:GLY:O	9:T:137:TYR:CA	2.62	0.47
8:U:7:UNK:O	8:U:9:UNK:N	2.48	0.47
1:A:59:ASP:O	1:A:60:ILE:C	2.52	0.46
2:B:174:LEU:O	2:B:175:THR:O	2.32	0.46
2:B:214:LEU:O	2:B:217:ILE:CG2	2.63	0.46
3:C:57:ALA:O	3:C:58:GLY:C	2.52	0.46
4:D:190:ASN:CG	4:D:322:ASN:HD21	2.18	0.46
6:F:17:THR:O	6:F:20:TRP:HB3	2.15	0.46
1:G:320:ILE:O	1:G:321:ILE:C	2.53	0.46
1:G:45:THR:HA	12:G:1345:PHO:H93	1.97	0.46
1:G:57:PRO:HA	1:G:67:VAL:O	2.14	0.46
3:I:229:ASN:CB	3:I:232:ASP:OD1	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:113:PHE:CZ	17:L:1047:BCR:HC41	2.50	0.46
4:J:192:THR:OG1	4:J:193:LEU:N	2.48	0.46
4:J:342:PRO:O	4:J:345:VAL:CG2	2.63	0.46
4:J:48:TRP:HB2	4:J:114:ILE:HD13	1.97	0.46
5:K:10:PHE:CE2	6:L:19:ARG:CZ	2.98	0.46
8:U:39:UNK:O	8:U:40:UNK:O	2.33	0.46
10:X:221:UNK:O	10:X:222:UNK:C	2.63	0.46
1:A:13:LEU:O	1:A:17:PHE:N	2.40	0.46
1:A:79:THR:O	1:A:80:GLY:O	2.33	0.46
2:B:113:TRP:CD1	11:B:1496:CLA:H191	2.49	0.46
3:C:122:SER:O	3:C:125:LEU:N	2.48	0.46
3:C:188:THR:HG21	3:C:298:PRO:CB	2.45	0.46
4:D:274:VAL:CB	4:D:275:PRO:CD	2.91	0.46
4:D:335:PRO:O	4:D:337:GLU:N	2.48	0.46
4:D:83:ASN:CG	4:D:336:HIS:CD2	2.81	0.46
2:H:193:TYR:CE1	2:H:260:SER:N	2.84	0.46
2:H:462:PHE:HA	11:H:1492:CLA:CMC	2.45	0.46
3:I:135:ARG:O	3:I:136:GLY:O	2.34	0.46
3:I:179:ALA:O	3:I:184:GLY:HA2	2.14	0.46
3:I:225:VAL:CG1	3:I:225:VAL:O	2.62	0.46
3:I:242:LEU:HD12	3:I:245:ILE:HD11	1.97	0.46
3:I:273:SER:CB	3:I:445:ALA:HB2	2.37	0.46
4:J:111:TRP:C	4:J:113:PHE:N	2.66	0.46
4:J:191:TRP:HZ2	4:J:286:VAL:CG2	2.29	0.46
4:J:87:HIS:C	4:J:167:TRP:CZ3	2.88	0.46
7:O:99:UNK:O	7:O:100:UNK:C	2.62	0.46
9:T:2:GLU:O	9:T:4:THR:N	2.45	0.46
1:A:122:GLY:C	1:A:124:SER:H	2.19	0.46
2:B:193:TYR:CE1	2:B:260:SER:N	2.83	0.46
2:B:61:PHE:O	2:B:63:LEU:N	2.48	0.46
3:C:245:ILE:O	3:C:249:ILE:HG12	2.15	0.46
5:E:12:ASP:O	5:E:16:SER:N	2.48	0.46
5:E:37:PHE:HE1	5:E:42:LEU:HB3	1.79	0.46
5:E:35:TRP:CD2	6:F:39:ALA:HB2	2.50	0.46
1:G:166:GLY:O	1:G:167:SER:CB	2.59	0.46
1:G:327:GLY:O	4:J:324:GLY:HA3	2.16	0.46
3:I:207:ARG:HA	3:I:210:PHE:CB	2.45	0.46
3:I:244:CYS:HA	11:I:1464:CLA:CMC	2.45	0.46
3:I:267:SER:O	3:I:271:TYR:N	2.40	0.46
3:I:370:ARG:HE	3:I:371:GLY:N	2.09	0.46
4:J:148:ALA:HB2	4:J:276:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:336:UNK:O	10:X:337:UNK:CB	2.64	0.46
10:X:410:UNK:O	10:X:411:UNK:C	2.64	0.46
10:X:580:UNK:C	10:X:582:UNK:N	2.77	0.46
1:A:110:GLY:O	1:A:111:PRO:C	2.53	0.46
1:A:166:GLY:O	1:A:167:SER:CB	2.63	0.46
1:A:167:SER:OG	1:A:169:SER:HB2	2.15	0.46
1:A:248:ILE:O	1:A:250:ALA:N	2.48	0.46
1:A:87:ASN:O	1:A:87:ASN:ND2	2.48	0.46
2:B:450:TRP:O	2:B:451:PHE:C	2.51	0.46
2:B:50:PRO:O	2:B:54:PRO:HG3	2.15	0.46
3:C:61:VAL:HG21	3:C:125:LEU:HD12	1.97	0.46
3:C:276:LEU:CD2	11:C:1466:CLA:HBB1	2.46	0.46
3:C:418:ASN:CA	3:C:419:PHE:N	2.78	0.46
3:C:95:LEU:HD23	3:C:97:TRP:CZ3	2.42	0.46
4:D:298:PHE:O	10:X:129:UNK:O	2.33	0.46
11:G:1342:CLA:HAB	11:G:1344:CLA:HMD2	1.97	0.46
1:G:292:THR:HG23	3:I:428:THR:CG2	2.44	0.46
1:G:65:GLU:CD	4:J:312:GLU:OE1	2.54	0.46
2:H:471:ALA:O	2:H:472:ARG:C	2.54	0.46
3:I:170:ILE:HG23	3:I:171:GLY:H	1.78	0.46
3:I:318:LEU:HD21	3:I:380:ILE:HG21	1.97	0.46
3:I:72:LEU:O	3:I:73:ALA:C	2.54	0.46
8:S:66:UNK:O	8:S:70:UNK:N	2.48	0.46
10:X:182:UNK:O	10:X:183:UNK:C	2.62	0.46
10:Y:158:UNK:O	10:Y:159:UNK:C	2.62	0.46
1:A:142:TRP:CZ2	1:A:273:PHE:CD1	3.04	0.46
1:A:32:TRP:O	1:A:35:VAL:HB	2.15	0.46
2:B:31:ALA:HA	2:B:34:ALA:CB	2.41	0.46
2:B:419:SER:HA	2:B:422:ARG:HE	1.80	0.46
2:B:68:ARG:HG3	2:B:69:LEU:N	2.30	0.46
4:D:279:LEU:O	4:D:283:ALA:HB2	2.15	0.46
4:D:9:PRO:O	4:D:10:ALA:CB	2.64	0.46
1:G:142:TRP:CZ2	1:G:273:PHE:CE1	3.04	0.46
3:I:257:PHE:HB3	3:I:258:GLY:H	1.58	0.46
3:I:270:ALA:C	3:I:274:TYR:HD2	2.19	0.46
3:I:298:PRO:O	3:I:299:SER:OG	2.34	0.46
1:G:220:THR:O	4:J:139:ARG:HD2	2.15	0.46
4:J:154:VAL:O	4:J:159:ILE:HG13	2.15	0.46
4:J:88:SER:O	4:J:167:TRP:CZ3	2.68	0.46
4:J:57:SER:O	4:J:60:THR:HG22	2.16	0.46
5:K:27:ILE:HB	5:K:28:PRO:CD	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:38:VAL:CG1	6:L:40:MET:HG2	2.46	0.46
1:A:160:ILE:HD12	3:C:431:PHE:CE1	2.47	0.46
2:B:219:VAL:HG12	2:B:219:VAL:O	2.16	0.46
3:C:280:SER:HA	3:C:434:ALA:HA	1.96	0.46
3:C:370:ARG:O	3:C:375:LEU:N	2.49	0.46
3:C:93:ALA:O	3:C:94:THR:C	2.52	0.46
1:G:116:ILE:CG1	1:G:158:PHE:HD1	2.29	0.46
2:H:26:HIS:HB2	11:H:1493:CLA:HMB2	1.97	0.46
3:I:120:ILE:C	3:I:122:SER:H	2.18	0.46
3:I:150:ASP:CB	3:I:271:TYR:CE2	2.99	0.46
4:J:126:MET:HE1	4:J:147:SER:N	2.31	0.46
5:K:37:PHE:CZ	5:K:43:ALA:HA	2.50	0.46
8:S:71:UNK:C	8:S:73:UNK:N	2.74	0.46
10:Y:412:UNK:O	10:Y:414:UNK:N	2.49	0.46
1:A:157:VAL:O	1:A:157:VAL:CG1	2.64	0.46
3:C:41:ARG:HB2	11:C:1469:CLA:O1D	2.16	0.46
4:D:92:LEU:HA	4:D:104:TRP:CD1	2.51	0.46
1:G:153:SER:HB3	11:G:1342:CLA:H43	1.98	0.46
1:G:142:TRP:CZ2	1:G:273:PHE:CD1	3.04	0.46
2:H:174:LEU:O	2:H:175:THR:O	2.34	0.46
3:I:282:MET:O	3:I:285:ILE:HB	2.16	0.46
5:K:19:TYR:CD1	5:K:19:TYR:C	2.88	0.46
8:S:74:UNK:O	8:S:75:UNK:C	2.61	0.46
9:T:134:LYS:O	9:T:137:TYR:O	2.34	0.46
9:V:62:ALA:HB2	9:V:82:TYR:CE1	2.50	0.46
10:Y:160:UNK:O	10:Y:164:UNK:CB	2.64	0.46
10:Y:534:UNK:O	10:Y:535:UNK:C	2.64	0.46
2:B:422:ARG:O	2:B:425:ILE:HG22	2.16	0.46
6:F:27:ALA:O	6:F:28:VAL:C	2.54	0.46
1:G:114:LEU:O	1:G:115:ILE:C	2.54	0.46
1:G:32:TRP:O	1:G:33:PHE:C	2.54	0.46
1:G:97:TRP:O	1:G:98:GLU:C	2.53	0.46
2:H:194:ASN:OD1	2:H:194:ASN:C	2.54	0.46
2:H:218:LEU:O	2:H:218:LEU:HD12	2.16	0.46
2:H:246:PHE:CE1	2:H:463:PHE:HB2	2.40	0.46
3:I:91:HIS:CE1	11:I:1460:CLA:O1D	2.66	0.46
3:I:273:SER:OG	3:I:274:TYR:N	2.49	0.46
4:J:164:GLN:NE2	4:J:189:HIS:HE1	2.01	0.46
4:J:272:LEU:CD2	4:J:276:VAL:HG21	2.44	0.46
4:J:73:PHE:CE2	4:J:175:VAL:HG21	2.51	0.46
4:J:93:TRP:CD1	4:J:93:TRP:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:41:GLY:O	5:K:42:LEU:C	2.54	0.46
9:V:83:ASP:OD1	9:V:85:GLU:HB2	2.16	0.46
10:X:428:UNK:C	10:X:430:UNK:N	2.77	0.46
1:A:176:ILE:HG23	1:A:180:PHE:HE1	1.79	0.46
1:A:187:GLN:NE2	1:A:325:ASN:OD1	2.49	0.46
1:A:193:LEU:HB3	4:D:179:PHE:CE1	2.50	0.46
1:A:76:ASN:C	1:A:76:ASN:OD1	2.54	0.46
3:C:164:HIS:O	3:C:167:VAL:N	2.49	0.46
3:C:171:GLY:O	3:C:172:ALA:C	2.55	0.46
3:C:270:ALA:O	3:C:271:TYR:C	2.53	0.46
1:A:210:LEU:HD13	12:D:1352:PHO:ND	2.31	0.46
4:D:71:CYS:HB2	4:D:76:VAL:HG22	1.98	0.46
4:D:71:CYS:HB3	4:D:76:VAL:HG22	1.98	0.46
1:G:244:GLU:HG3	1:G:245:THR:N	2.31	0.46
1:G:54:ALA:CB	1:G:72:LEU:HD12	2.46	0.46
2:H:135:LEU:O	2:H:136:PRO:C	2.54	0.46
2:H:197:GLY:O	2:H:199:VAL:N	2.49	0.46
3:I:240:ILE:HD12	11:I:1465:CLA:C9	2.46	0.46
4:J:139:ARG:HH11	4:J:141:TYR:HE1	1.64	0.46
6:L:19:ARG:O	6:L:23:VAL:CG2	2.59	0.46
8:S:27:UNK:C	8:S:28:UNK:O	2.64	0.46
9:V:77:LYS:HG2	9:V:95:LEU:HD22	1.97	0.46
10:X:218:UNK:O	10:X:219:UNK:C	2.64	0.46
10:X:469:UNK:O	10:X:470:UNK:C	2.63	0.46
10:X:580:UNK:O	10:X:581:UNK:C	2.64	0.46
10:Y:365:UNK:O	10:Y:366:UNK:C	2.64	0.46
10:Y:516:UNK:O	10:Y:518:UNK:N	2.49	0.46
1:A:134:SER:CA	1:A:139:MET:HB3	2.44	0.46
1:A:244:GLU:HG3	1:A:245:THR:H	1.81	0.46
1:A:32:TRP:O	1:A:35:VAL:N	2.49	0.46
2:B:293:ALA:O	2:B:294:SER:C	2.54	0.46
2:B:52:LEU:HD23	2:B:311:PHE:CE2	2.51	0.46
3:C:381:LYS:O	3:C:382:ASN:HB3	2.15	0.46
4:D:139:ARG:HH11	4:D:141:TYR:HE1	1.64	0.46
4:D:52:THR:CG2	4:D:76:VAL:HG11	2.46	0.46
4:D:91:LEU:O	4:D:93:TRP:N	2.49	0.46
4:D:9:PRO:O	4:D:10:ALA:HB2	2.16	0.46
1:G:137:LEU:CD1	1:G:139:MET:HE1	2.46	0.46
2:H:207:ILE:CG1	2:H:208:VAL:N	2.78	0.46
2:H:249:ALA:HA	11:H:1485:CLA:HMD3	1.97	0.46
2:H:49:ASP:OD2	2:H:52:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:449:ARG:HH12	11:I:1463:CLA:HAA1	1.81	0.46
3:I:288:CYS:O	3:I:289:PHE:C	2.55	0.46
4:J:10:ALA:O	4:J:11:GLU:CB	2.64	0.46
4:J:156:VAL:CG1	4:J:156:VAL:O	2.64	0.46
4:J:55:VAL:O	4:J:66:SER:HB3	2.16	0.46
8:U:72:UNK:O	8:U:73:UNK:C	2.62	0.46
10:X:3:UNK:O	10:X:6:UNK:N	2.49	0.46
10:Y:3:UNK:C	10:Y:5:UNK:N	2.77	0.46
2:B:272:ARG:NH1	4:D:164:GLN:HA	2.31	0.45
2:B:70:GLY:HA2	2:B:178:VAL:HG11	1.97	0.45
3:C:164:HIS:O	3:C:167:VAL:HG23	2.15	0.45
1:A:141:PRO:CG	3:C:446:GLY:O	2.58	0.45
4:D:203:GLY:O	4:D:207:GLY:N	2.46	0.45
4:D:32:TRP:O	4:D:33:SER:C	2.54	0.45
4:D:57:SER:O	4:D:60:THR:HG22	2.16	0.45
6:F:35:GLY:O	6:F:36:ALA:C	2.52	0.45
2:H:27:THR:CG2	2:H:107:LEU:HD13	2.43	0.45
3:I:118:HIS:HA	3:I:121:SER:HB3	1.98	0.45
11:I:1464:CLA:HMC2	11:I:1465:CLA:H121	1.97	0.45
3:I:431:PHE:O	3:I:432:VAL:C	2.54	0.45
4:J:139:ARG:NH1	4:J:141:TYR:HE1	2.13	0.45
8:S:9:UNK:O	8:S:10:UNK:C	2.55	0.45
10:X:266:UNK:O	10:X:267:UNK:C	2.63	0.45
2:B:132:ALA:O	2:B:133:LEU:CB	2.64	0.45
2:B:450:TRP:O	2:B:453:PHE:N	2.29	0.45
3:C:398:HIS:O	3:C:399:ALA:CA	2.62	0.45
4:D:186:GLN:CB	11:D:1351:CLA:HBC1	2.47	0.45
4:D:64:ALA:HB1	4:D:69:GLU:HB3	1.98	0.45
1:G:131:TRP:O	1:G:134:SER:CB	2.64	0.45
1:G:176:ILE:CG2	1:G:180:PHE:HE1	2.29	0.45
1:G:171:GLY:HA2	1:G:182:PHE:CE1	2.51	0.45
1:G:215:HIS:O	1:G:219:VAL:HG23	2.16	0.45
1:G:288:LEU:O	1:G:290:ILE:N	2.50	0.45
3:I:128:GLY:HA3	11:I:1471:CLA:HMC3	1.97	0.45
3:I:376:ASP:OD2	3:I:379:LYS:HE3	2.16	0.45
4:J:87:HIS:CE1	4:J:161:PRO:O	2.69	0.45
5:K:61:ARG:O	5:K:62:SER:HB2	2.15	0.45
8:U:86:UNK:O	8:U:87:UNK:C	2.65	0.45
3:C:66:ALA:HB1	10:X:517:UNK:HA	1.97	0.45
10:Y:331:UNK:O	10:Y:334:UNK:CB	2.64	0.45
10:Y:419:UNK:O	10:Y:423:UNK:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:567:UNK:O	10:Y:571:UNK:N	2.48	0.45
1:A:172:MET:HA	1:A:173:PRO:HD3	1.44	0.45
1:A:190:HIS:ND1	1:A:298:ASN:ND2	2.63	0.45
1:A:290:ILE:O	1:A:292:THR:N	2.50	0.45
2:B:450:TRP:CE2	11:B:1488:CLA:HBA1	2.51	0.45
2:B:110:ALA:HA	11:B:1496:CLA:C20	2.45	0.45
2:B:395:GLN:CB	2:B:397:VAL:CB	2.95	0.45
2:B:62:VAL:HG12	2:B:66:MET:HE2	1.98	0.45
3:C:167:VAL:CG2	11:C:1470:CLA:HMB2	2.47	0.45
3:C:242:LEU:O	3:C:243:ILE:C	2.55	0.45
3:C:24:THR:O	3:C:25:ASN:CB	2.64	0.45
4:D:33:SER:OG	4:D:128:ARG:HA	2.16	0.45
4:D:40:CYS:O	4:D:41:ALA:C	2.54	0.45
6:F:9:GLU:N	6:F:10:PRO:CD	2.79	0.45
2:H:145:LEU:CD1	11:H:1496:CLA:HMB2	2.47	0.45
2:H:214:LEU:HD12	2:H:215:PHE:N	2.31	0.45
3:I:250:TRP:CD1	3:I:250:TRP:O	2.69	0.45
3:I:304:PRO:O	3:I:305:THR:CG2	2.63	0.45
1:G:206:PHE:CZ	11:J:1351:CLA:HAA1	2.51	0.45
9:T:64:PRO:HD2	9:T:66:ARG:NH2	2.30	0.45
10:X:202:UNK:O	10:X:203:UNK:C	2.64	0.45
10:Y:531:UNK:O	10:Y:532:UNK:C	2.62	0.45
2:B:309:LEU:O	2:B:311:PHE:N	2.50	0.45
4:D:126:MET:HE1	4:D:147:SER:N	2.32	0.45
4:D:81:PRO:O	4:D:168:PHE:HD1	1.99	0.45
4:D:199:MET:O	4:D:202:ALA:N	2.50	0.45
4:D:83:ASN:OD1	4:D:336:HIS:HD2	1.98	0.45
4:D:87:HIS:C	4:D:167:TRP:CZ3	2.90	0.45
5:E:37:PHE:CZ	5:E:43:ALA:HA	2.52	0.45
5:E:82:GLN:O	5:E:83:LEU:C	2.54	0.45
1:G:222:SER:O	1:G:246:TYR:O	2.34	0.45
2:H:193:TYR:OH	2:H:259:GLY:HA2	2.15	0.45
2:H:396:GLY:O	2:H:398:THR:N	2.50	0.45
3:I:25:ASN:O	3:I:26:ARG:CB	2.64	0.45
3:I:358:PHE:C	3:I:360:ASP:H	2.18	0.45
3:I:77:PRO:C	3:I:79:LYS:N	2.66	0.45
4:J:191:TRP:O	4:J:194:ASN:N	2.38	0.45
11:H:1488:CLA:H203	4:J:281:MET:SD	2.57	0.45
1:A:176:ILE:CG2	1:A:180:PHE:HE1	2.29	0.45
1:A:171:GLY:HA2	1:A:182:PHE:CE1	2.51	0.45
2:B:204:ALA:O	2:B:205:ALA:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:LEU:HD21	11:C:1464:CLA:HBB1	1.98	0.45
3:C:167:VAL:HG13	11:C:1470:CLA:HMB2	1.98	0.45
3:C:366:LEU:O	3:C:366:LEU:HD12	2.17	0.45
3:C:55:ALA:O	3:C:56:HIS:C	2.55	0.45
4:D:186:GLN:HB2	11:D:1351:CLA:HBC1	1.99	0.45
4:D:56:THR:HG22	5:E:49:THR:HG22	1.99	0.45
1:G:180:PHE:CZ	4:J:192:THR:HB	2.51	0.45
2:H:193:TYR:HD1	2:H:260:SER:CB	2.29	0.45
3:I:228:ASN:HA	3:I:295:THR:CG2	2.25	0.45
3:I:267:SER:H	3:I:270:ALA:HB3	1.82	0.45
4:J:103:ARG:O	4:J:104:TRP:C	2.55	0.45
4:J:129:GLN:OE1	4:J:143:ALA:HA	2.16	0.45
4:J:264:LYS:C	4:J:266:TRP:H	2.20	0.45
7:O:127:UNK:O	7:O:128:UNK:C	2.64	0.45
7:O:154:UNK:HA	7:O:170:UNK:HA	1.98	0.45
10:Y:202:UNK:O	10:Y:203:UNK:C	2.64	0.45
10:Y:503:UNK:O	10:Y:504:UNK:C	2.65	0.45
10:Y:64:UNK:C	10:Y:66:UNK:N	2.75	0.45
1:A:104:GLU:O	1:A:104:GLU:HG2	2.17	0.45
1:A:32:TRP:O	1:A:33:PHE:C	2.55	0.45
1:A:62:GLY:CA	1:A:87:ASN:CB	2.92	0.45
2:B:152:GLY:O	2:B:153:PHE:C	2.53	0.45
2:B:192:PRO:HG3	11:B:1483:CLA:HBA2	1.98	0.45
2:B:234:ILE:O	2:B:237:VAL:N	2.49	0.45
2:B:280:PHE:CE2	2:B:312:TYR:HB3	2.52	0.45
3:C:129:GLY:C	3:C:131:TYR:N	2.70	0.45
3:C:82:TYR:CA	3:C:422:PRO:HG2	2.38	0.45
3:C:273:SER:CB	3:C:445:ALA:HB2	2.42	0.45
3:C:84:GLN:O	3:C:85:GLY:C	2.55	0.45
4:D:35:ILE:O	4:D:35:ILE:HG22	2.15	0.45
2:H:114:HIS:NE2	11:H:1497:CLA:NB	2.65	0.45
2:H:267:LEU:H	2:H:267:LEU:HG	1.57	0.45
2:H:398:THR:O	2:H:400:SER:N	2.50	0.45
2:H:64:PRO:CB	2:H:268:PHE:CZ	2.99	0.45
3:I:227:VAL:CG1	3:I:233:VAL:HG23	2.47	0.45
1:G:141:PRO:CG	3:I:446:GLY:O	2.60	0.45
3:I:56:HIS:O	3:I:59:LEU:HB3	2.16	0.45
2:H:464:PHE:CE1	4:J:144:ILE:HG23	2.51	0.45
4:J:315:TYR:CE1	4:J:319:LEU:HD12	2.52	0.45
4:J:53:THR:HG22	4:J:67:TYR:CE1	2.52	0.45
17:L:1047:BCR:H331	17:L:1047:BCR:H343	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:63:UNK:O	7:O:72:UNK:N	2.49	0.45
9:T:30:LYS:HG2	9:T:118:HIS:CE1	2.51	0.45
9:T:93:PRO:HG3	9:T:101:PHE:CD1	2.52	0.45
10:X:213:UNK:O	10:X:214:UNK:C	2.65	0.45
1:A:157:VAL:HG13	1:A:172:MET:HB3	1.99	0.45
3:C:109:PHE:HB3	3:C:110:PRO:CD	2.47	0.45
3:C:244:CYS:HA	11:C:1464:CLA:CMC	2.47	0.45
3:C:37:ALA:C	3:C:39:ASN:H	2.19	0.45
3:C:402:GLY:CA	3:C:420:VAL:HG13	2.47	0.45
4:D:139:ARG:NH1	4:D:141:TYR:HE1	2.14	0.45
4:D:148:ALA:CB	4:D:276:VAL:HA	2.46	0.45
1:A:317:TRP:CG	4:D:177:ALA:HB2	2.51	0.45
4:D:171:PRO:HG3	4:D:181:PHE:CD2	2.52	0.45
1:A:215:HIS:HB3	4:D:271:MET:CE	2.46	0.45
1:G:290:ILE:HD11	11:G:1342:CLA:CAD	2.46	0.45
1:G:320:ILE:O	1:G:322:ASN:N	2.50	0.45
2:H:150:CYS:N	11:H:1484:CLA:HBC2	2.32	0.45
2:H:18:ARG:O	2:H:21:ALA:N	2.48	0.45
2:H:215:PHE:CD2	2:H:216:HIS:N	2.84	0.45
2:H:220:ARG:CB	2:H:221:PRO:HD2	2.47	0.45
2:H:67:ALA:HA	2:H:71:VAL:O	2.17	0.45
2:H:68:ARG:NH1	2:H:262:THR:O	2.49	0.45
3:I:127:PHE:C	3:I:129:GLY:H	2.20	0.45
3:I:270:ALA:O	3:I:271:TYR:C	2.54	0.45
4:J:272:LEU:HD23	4:J:272:LEU:O	2.17	0.45
4:J:48:TRP:O	4:J:52:THR:OG1	2.23	0.45
5:K:27:ILE:O	5:K:28:PRO:C	2.54	0.45
7:O:142:UNK:CA	7:O:149:UNK:CB	2.93	0.45
7:O:24:UNK:O	7:O:25:UNK:O	2.34	0.45
8:S:4:UNK:O	8:S:7:UNK:CB	2.65	0.45
8:U:69:UNK:C	8:U:71:UNK:N	2.80	0.45
10:X:200:UNK:O	10:X:203:UNK:N	2.50	0.45
10:X:269:UNK:O	10:X:270:UNK:C	2.63	0.45
10:X:470:UNK:C	10:X:472:UNK:N	2.78	0.45
10:Y:519:UNK:C	10:Y:521:UNK:N	2.80	0.45
2:B:393:GLU:C	2:B:395:GLN:N	2.69	0.45
2:B:310:ALA:O	2:B:428:GLU:HB2	2.17	0.45
3:C:169:GLY:CA	3:C:244:CYS:SG	3.03	0.45
3:C:80:PRO:HB2	3:C:83:GLU:HB2	1.99	0.45
2:B:357:ARG:NH1	4:D:338:ASN:O	2.50	0.45
4:D:54:PHE:HE1	6:F:33:PHE:CD2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:33:PHE:CE1	17:F:1046:BCR:H14C	2.52	0.45
6:F:10:PRO:CB	6:F:19:ARG:HH11	2.20	0.45
3:I:230:LEU:O	3:I:230:LEU:HD12	2.16	0.45
4:J:287:VAL:O	4:J:290:ALA:HB3	2.16	0.45
4:J:83:ASN:O	4:J:83:ASN:OD1	2.34	0.45
5:K:51:ARG:O	5:K:52:PRO:C	2.56	0.45
8:U:57:UNK:O	8:U:58:UNK:C	2.63	0.45
1:A:119:PHE:CD2	12:A:1345:PHO:H111	2.52	0.45
2:B:345:VAL:HG23	2:B:345:VAL:O	2.17	0.45
2:B:360:PRO:HB2	2:B:363:PHE:CD2	2.43	0.45
2:B:396:GLY:O	2:B:398:THR:N	2.50	0.45
4:D:315:TYR:CE1	4:D:319:LEU:HD12	2.51	0.45
11:H:1488:CLA:H143	4:J:281:MET:HE1	1.98	0.45
2:H:238:LEU:CD2	2:H:469:HIS:CG	3.00	0.45
2:H:31:ALA:CB	11:H:1486:CLA:HBC3	2.46	0.45
2:H:426:PHE:O	2:H:426:PHE:CD1	2.70	0.45
3:I:56:HIS:O	3:I:59:LEU:CB	2.65	0.45
1:G:180:PHE:CG	4:J:192:THR:HB	2.52	0.45
10:X:201:UNK:O	10:X:202:UNK:C	2.63	0.45
2:B:45:PHE:C	2:B:47:PRO:HD2	2.37	0.45
3:C:364:PRO:O	3:C:365:TRP:C	2.55	0.45
5:E:18:ARG:NE	5:E:22:ILE:HD11	2.32	0.45
1:G:48:PHE:CD2	1:G:48:PHE:C	2.90	0.45
3:I:81:MET:HB3	3:I:301:PHE:O	2.17	0.45
3:I:82:TYR:CA	3:I:422:PRO:HG2	2.39	0.45
4:J:43:LEU:HG	4:J:113:PHE:CZ	2.52	0.45
5:K:18:ARG:NE	5:K:22:ILE:HD11	2.32	0.45
5:K:35:TRP:O	5:K:35:TRP:CD1	2.70	0.45
6:L:14:PRO:O	6:L:15:ILE:CB	2.65	0.45
7:P:142:UNK:C	7:P:149:UNK:CB	2.95	0.45
10:Y:507:UNK:O	10:Y:508:UNK:C	2.64	0.45
1:A:120:LEU:O	1:A:124:SER:N	2.49	0.44
1:A:207:GLY:O	1:A:208:GLY:C	2.54	0.44
2:B:133:LEU:O	2:B:134:ASP:CB	2.65	0.44
2:B:358:ARG:O	2:B:360:PRO:HD3	2.17	0.44
2:B:425:ILE:O	2:B:426:PHE:CB	2.65	0.44
4:D:294:ARG:HB2	4:D:295:SER:H	1.56	0.44
4:D:74:LEU:HA	4:D:175:VAL:CG1	2.46	0.44
5:E:49:THR:HA	5:E:50:PRO:HD3	1.79	0.44
1:G:122:GLY:C	1:G:124:SER:H	2.20	0.44
1:G:93:PHE:CZ	1:G:95:PRO:HG3	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:174:LEU:HD23	2:H:308:LYS:HB3	1.98	0.44
2:H:49:ASP:CG	2:H:49:ASP:O	2.55	0.44
3:I:305:THR:O	3:I:306:GLY:C	2.55	0.44
3:I:370:ARG:O	3:I:375:LEU:N	2.49	0.44
3:I:447:ARG:HG2	3:I:447:ARG:NH1	2.32	0.44
1:G:258:LEU:O	4:J:128:ARG:CZ	2.65	0.44
4:J:32:TRP:O	4:J:35:ILE:HB	2.18	0.44
10:Y:224:UNK:O	10:Y:225:UNK:C	2.64	0.44
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.00	0.44
2:B:222:PRO:O	2:B:226:TYR:N	2.42	0.44
3:C:164:HIS:HA	3:C:167:VAL:CG2	2.47	0.44
3:C:150:ASP:CB	3:C:271:TYR:CE2	3.00	0.44
3:C:311:GLN:HA	3:C:355:THR:HG21	1.99	0.44
3:C:35:TRP:CZ3	3:C:36:TRP:HB3	2.52	0.44
3:C:431:PHE:O	3:C:432:VAL:C	2.53	0.44
4:D:235:PHE:CD1	4:D:235:PHE:C	2.90	0.44
2:H:280:PHE:O	2:H:283:GLU:N	2.50	0.44
2:H:286:ARG:HG3	2:H:287:ARG:N	2.31	0.44
11:I:1471:CLA:HHD	11:I:1471:CLA:HBC3	1.99	0.44
3:I:167:VAL:CG2	11:I:1470:CLA:HMB2	2.46	0.44
3:I:229:ASN:HB2	3:I:232:ASP:OD1	2.18	0.44
3:I:188:THR:HG21	3:I:300:GLU:OE1	2.17	0.44
4:J:302:GLU:HB3	7:P:114:UNK:CB	2.47	0.44
4:J:96:GLU:OE1	4:J:96:GLU:CA	2.66	0.44
5:K:10:PHE:HE2	6:L:19:ARG:HE	1.62	0.44
7:P:11:UNK:CA	7:P:173:UNK:CB	2.90	0.44
8:S:77:UNK:C	8:S:79:UNK:N	2.79	0.44
10:Y:200:UNK:O	10:Y:203:UNK:N	2.51	0.44
1:A:105:TRP:CZ3	1:A:111:PRO:HG3	2.53	0.44
1:A:131:TRP:O	1:A:134:SER:CB	2.65	0.44
1:A:320:ILE:O	1:A:321:ILE:C	2.56	0.44
1:A:78:ILE:HB	4:D:298:PHE:HZ	1.81	0.44
2:B:139:PHE:CD1	2:B:139:PHE:O	2.70	0.44
2:B:418:LYS:O	2:B:419:SER:C	2.53	0.44
1:A:206:PHE:CZ	11:D:1351:CLA:HAA1	2.52	0.44
4:D:273:PHE:O	4:D:277:THR:OG1	2.24	0.44
1:G:112:TYR:CE1	1:G:116:ILE:CD1	3.00	0.44
1:G:176:ILE:CG1	11:G:1343:CLA:HED3	2.41	0.44
11:G:1346:CLA:HMB1	11:G:1346:CLA:CBB	2.46	0.44
1:G:279:PRO:CB	12:G:1345:PHO:HBC1	2.48	0.44
1:G:288:LEU:O	1:G:291:SER:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:425:ILE:O	2:H:426:PHE:CB	2.64	0.44
3:I:88:LEU:O	3:I:89:ILE:C	2.56	0.44
4:J:203:GLY:O	4:J:207:GLY:N	2.48	0.44
4:J:210:LEU:HD11	4:J:270:PHE:HD2	1.81	0.44
10:X:9:UNK:O	10:X:10:UNK:C	2.62	0.44
10:X:223:UNK:O	10:X:224:UNK:C	2.65	0.44
1:A:55:ALA:HA	1:A:56:PRO:HD3	1.75	0.44
1:A:57:PRO:CG	1:A:68:SER:HB3	2.36	0.44
2:B:172:TYR:HB3	2:B:309:LEU:HD21	1.98	0.44
2:B:372:ASP:C	2:B:374:ASN:H	2.19	0.44
3:C:109:PHE:HB3	3:C:110:PRO:HD2	1.98	0.44
3:C:243:ILE:HG22	3:C:244:CYS:N	2.32	0.44
3:C:43:ILE:HG22	11:C:1467:CLA:CMC	2.31	0.44
3:C:49:LEU:O	3:C:52:ALA:N	2.51	0.44
4:D:235:PHE:CD2	4:D:243:THR:CG2	2.99	0.44
5:E:10:PHE:CE2	6:F:19:ARG:CZ	3.01	0.44
2:H:265:ILE:HD13	2:H:265:ILE:HA	1.77	0.44
11:H:1488:CLA:C17	4:J:281:MET:HE1	2.43	0.44
7:O:142:UNK:C	7:O:149:UNK:CB	2.96	0.44
2:B:145:LEU:CD1	11:B:1496:CLA:HMB2	2.48	0.44
3:C:177:ALA:O	3:C:178:LYS:C	2.56	0.44
4:D:339:PHE:HD1	4:D:341:PHE:CE1	2.35	0.44
4:D:337:GLU:CG	4:D:339:PHE:HE2	2.28	0.44
5:E:23:HIS:HD2	16:E:1085:HEM:NB	2.14	0.44
6:F:33:PHE:C	6:F:35:GLY:H	2.21	0.44
1:G:218:LEU:HA	1:G:221:SER:OG	2.17	0.44
2:H:196:GLY:O	2:H:197:GLY:C	2.54	0.44
2:H:270:PRO:O	2:H:271:THR:CB	2.65	0.44
3:I:92:ILE:O	3:I:93:ALA:C	2.55	0.44
4:J:52:THR:CG2	4:J:76:VAL:HG11	2.47	0.44
10:X:158:UNK:O	10:X:159:UNK:C	2.63	0.44
10:X:331:UNK:O	10:X:334:UNK:CB	2.65	0.44
2:B:272:ARG:CG	2:B:273:TYR:N	2.80	0.44
3:C:168:LEU:O	11:C:1459:CLA:HMC1	2.17	0.44
3:C:172:ALA:O	3:C:173:LEU:C	2.56	0.44
3:C:269:GLU:N	11:C:1467:CLA:HBC1	2.32	0.44
3:C:188:THR:HG21	3:C:300:GLU:OE1	2.18	0.44
3:C:38:GLY:HA3	11:C:1469:CLA:C2D	2.47	0.44
3:C:430:HIS:O	3:C:434:ALA:N	2.46	0.44
3:C:51:GLY:O	3:C:52:ALA:C	2.56	0.44
3:C:91:HIS:O	3:C:92:ILE:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:18:VAL:O	6:F:21:VAL:HB	2.17	0.44
2:H:31:ALA:HB2	11:H:1486:CLA:HBC3	1.99	0.44
2:H:172:TYR:CE1	2:H:279:TYR:CZ	3.05	0.44
2:H:35:GLY:O	2:H:38:ALA:HB3	2.18	0.44
2:H:445:THR:HG23	2:H:450:TRP:NE1	2.33	0.44
3:I:276:LEU:HD13	11:I:1466:CLA:HBB1	1.99	0.44
3:I:225:VAL:HA	3:I:289:PHE:CE1	2.52	0.44
4:J:93:TRP:HA	4:J:97:ALA:HB2	2.00	0.44
9:T:28:GLU:OE1	9:T:28:GLU:HA	2.18	0.44
9:T:77:LYS:HG2	9:T:95:LEU:HD22	1.99	0.44
9:V:40:CYS:SG	9:V:47:LYS:HB2	2.58	0.44
10:X:255:UNK:O	10:X:256:UNK:C	2.65	0.44
10:Y:68:UNK:C	10:Y:70:UNK:N	2.74	0.44
1:A:13:LEU:O	1:A:14:TRP:C	2.55	0.44
1:A:222:SER:O	1:A:246:TYR:CB	2.65	0.44
1:A:259:ILE:O	1:A:260:PHE:CB	2.65	0.44
2:B:238:LEU:CD2	2:B:469:HIS:CG	3.01	0.44
2:B:280:PHE:O	2:B:283:GLU:N	2.50	0.44
2:B:445:THR:HG23	2:B:450:TRP:NE1	2.33	0.44
2:B:468:TRP:O	2:B:471:ALA:CB	2.64	0.44
2:B:65:PHE:O	2:B:66:MET:C	2.56	0.44
3:C:91:HIS:CE1	11:C:1460:CLA:O1D	2.67	0.44
3:C:271:TYR:O	3:C:272:LEU:C	2.54	0.44
3:C:56:HIS:O	3:C:59:LEU:HB3	2.18	0.44
4:D:111:TRP:HB3	4:D:112:THR:H	1.67	0.44
4:D:148:ALA:HB2	4:D:276:VAL:HA	2.00	0.44
4:D:191:TRP:CZ2	4:D:286:VAL:CG2	3.01	0.44
1:A:83:VAL:HG13	4:D:314:PHE:CZ	2.53	0.44
4:D:331:PRO:CG	4:D:339:PHE:CG	2.93	0.44
4:D:51:GLY:O	4:D:52:THR:C	2.56	0.44
1:G:248:ILE:O	1:G:249:VAL:C	2.55	0.44
1:G:258:LEU:HG	4:J:128:ARG:NH2	2.33	0.44
2:H:309:LEU:O	2:H:311:PHE:N	2.50	0.44
3:I:43:ILE:HG13	3:I:44:ASN:N	2.32	0.44
4:J:330:ALA:HB3	4:J:331:PRO:CD	2.00	0.44
4:J:56:THR:OG1	4:J:57:SER:N	2.50	0.44
4:J:91:LEU:C	4:J:93:TRP:N	2.69	0.44
1:A:112:TYR:CE1	1:A:116:ILE:HD12	2.53	0.44
1:A:112:TYR:CE1	1:A:116:ILE:HD11	2.53	0.44
1:A:134:SER:C	1:A:136:ARG:N	2.71	0.44
1:A:273:PHE:CD2	1:A:273:PHE:C	2.92	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLY:O	1:A:312:ASN:C	2.56	0.44
3:C:46:SER:O	3:C:47:GLY:C	2.56	0.44
4:D:122:LEU:HA	4:D:122:LEU:HD23	1.80	0.44
4:D:296:TYR:CE1	4:D:319:LEU:HD23	2.53	0.44
4:D:335:PRO:O	4:D:336:HIS:C	2.56	0.44
1:G:167:SER:OG	1:G:169:SER:HB2	2.18	0.44
1:G:47:CYS:SG	1:G:114:LEU:CD2	2.89	0.44
2:H:195:PRO:O	2:H:198:VAL:N	2.50	0.44
2:H:425:ILE:CG2	2:H:426:PHE:CD2	3.01	0.44
2:H:45:PHE:CE2	2:H:47:PRO:CD	2.82	0.44
2:H:468:TRP:O	2:H:471:ALA:CB	2.64	0.44
3:I:242:LEU:O	3:I:243:ILE:C	2.56	0.44
3:I:46:SER:O	3:I:47:GLY:C	2.56	0.44
7:P:154:UNK:HA	7:P:170:UNK:HA	2.00	0.44
9:T:69:ILE:O	9:T:70:GLU:C	2.56	0.44
10:X:168:UNK:C	10:X:170:UNK:N	2.81	0.44
10:X:463:UNK:O	10:X:464:UNK:C	2.66	0.44
10:Y:159:UNK:O	10:Y:160:UNK:C	2.63	0.44
11:A:1346:CLA:CBB	11:A:1346:CLA:HMB1	2.43	0.44
1:A:192:ILE:C	1:A:194:MET:N	2.71	0.44
1:A:258:LEU:HG	4:D:128:ARG:NH2	2.31	0.44
1:A:57:PRO:HA	1:A:67:VAL:O	2.18	0.44
4:D:261:PHE:CD1	4:D:266:TRP:HD1	2.36	0.44
4:D:342:PRO:O	4:D:345:VAL:HG23	2.17	0.44
5:E:19:TYR:CD1	5:E:19:TYR:C	2.90	0.44
5:E:51:ARG:O	5:E:52:PRO:C	2.54	0.44
1:G:157:VAL:O	1:G:157:VAL:CG1	2.65	0.44
1:G:21:VAL:O	1:G:22:THR:C	2.56	0.44
1:G:211:PHE:CD2	1:G:274:PHE:HE2	2.36	0.44
1:G:34:GLY:O	1:G:38:ILE:N	2.51	0.44
2:H:396:GLY:O	2:H:397:VAL:C	2.56	0.44
2:H:97:ALA:O	2:H:98:LEU:C	2.52	0.44
3:I:420:VAL:HG12	3:I:421:SER:N	2.33	0.44
3:I:97:TRP:O	3:I:98:GLY:C	2.56	0.44
1:G:258:LEU:O	4:J:128:ARG:NH1	2.51	0.44
4:J:160:TYR:CZ	4:J:164:GLN:OE1	2.70	0.44
1:G:320:ILE:HD11	4:J:63:LEU:HD21	1.98	0.44
18:V:1138:HEC:HHA	18:V:1138:HEC:HAD2	1.61	0.44
1:A:176:ILE:CG2	1:A:180:PHE:CE1	3.01	0.43
1:A:91:LEU:HA	1:A:91:LEU:HD12	1.88	0.43
2:B:176:GLY:O	2:B:177:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:GLY:O	2:B:214:LEU:C	2.57	0.43
2:B:425:ILE:CG2	2:B:426:PHE:CD2	3.00	0.43
3:C:170:ILE:CG2	3:C:171:GLY:H	2.29	0.43
3:C:189:TRP:HH2	3:C:363:GLY:HA2	1.80	0.43
3:C:341:LEU:CD2	3:C:375:LEU:HD13	2.48	0.43
3:C:395:TYR:O	3:C:398:HIS:N	2.37	0.43
4:D:111:TRP:C	4:D:113:PHE:N	2.68	0.43
4:D:286:VAL:C	4:D:288:GLY:N	2.69	0.43
4:D:72:ASN:C	4:D:76:VAL:HG23	2.38	0.43
1:G:307:ILE:O	1:G:308:ASP:C	2.53	0.43
3:I:318:LEU:HA	3:I:340:TYR:CD1	2.53	0.43
4:J:148:ALA:HA	4:J:280:TRP:HE1	1.80	0.43
12:G:1345:PHO:HAB	4:J:205:LEU:CD2	2.47	0.43
4:J:320:LEU:HA	4:J:320:LEU:HD23	1.73	0.43
4:J:61:HIS:CE1	4:J:80:THR:OG1	2.71	0.43
8:S:20:UNK:C	8:S:22:UNK:H	2.29	0.43
9:T:62:ALA:HB2	9:T:82:TYR:CE1	2.53	0.43
1:A:78:ILE:HD12	10:X:125:UNK:CB	2.48	0.43
10:Y:423:UNK:O	10:Y:424:UNK:C	2.65	0.43
1:A:177:SER:O	1:A:180:PHE:N	2.51	0.43
2:B:18:ARG:O	2:B:21:ALA:N	2.51	0.43
2:B:19:LEU:O	2:B:22:ALA:HB3	2.18	0.43
2:B:29:LEU:HD12	11:B:1495:CLA:HBB2	2.00	0.43
2:B:419:SER:OG	2:B:420:TYR:N	2.51	0.43
4:D:127:LEU:O	4:D:130:PHE:N	2.51	0.43
4:D:218:VAL:O	4:D:219:GLU:C	2.55	0.43
1:A:142:TRP:CG	4:D:220:ASN:OD1	2.71	0.43
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.98	0.43
1:G:77:ILE:H	1:G:77:ILE:HG13	1.64	0.43
2:H:153:PHE:O	2:H:157:HIS:HB3	2.19	0.43
2:H:316:GLY:HA2	2:H:443:PHE:CE1	2.51	0.43
2:H:450:TRP:CE2	11:H:1488:CLA:HBA1	2.54	0.43
7:O:37:UNK:O	7:O:38:UNK:CB	2.66	0.43
2:B:24:LEU:HD21	2:B:110:ALA:HB1	2.01	0.43
2:B:218:LEU:HD12	2:B:218:LEU:O	2.18	0.43
3:C:170:ILE:O	3:C:171:GLY:C	2.56	0.43
4:D:200:GLY:O	4:D:201:VAL:C	2.56	0.43
1:A:331:MET:HE3	4:D:346:LEU:O	2.15	0.43
1:G:116:ILE:HG12	1:G:158:PHE:CD1	2.51	0.43
1:G:202:VAL:O	1:G:206:PHE:N	2.47	0.43
2:H:222:PRO:O	2:H:223:GLN:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:278:SER:C	2:H:279:TYR:O	2.56	0.43
2:H:400:SER:HB3	2:H:410:THR:CB	2.28	0.43
2:H:62:VAL:HG13	11:H:1486:CLA:O2D	2.18	0.43
4:J:103:ARG:HA	4:J:106:GLN:HG3	2.01	0.43
4:J:218:VAL:O	4:J:219:GLU:C	2.56	0.43
9:V:134:LYS:O	9:V:137:TYR:N	2.50	0.43
10:X:56:UNK:O	10:X:59:UNK:N	2.50	0.43
10:Y:200:UNK:O	10:Y:203:UNK:CB	2.66	0.43
10:Y:265:UNK:O	10:Y:266:UNK:C	2.66	0.43
2:B:135:LEU:CD1	2:B:232:GLY:HA2	2.48	0.43
2:B:29:LEU:HA	2:B:29:LEU:HD23	1.70	0.43
2:B:309:LEU:C	2:B:311:PHE:N	2.68	0.43
2:B:359:MET:CE	2:B:366:PHE:HB2	2.49	0.43
3:C:188:THR:HG21	3:C:298:PRO:CA	2.48	0.43
3:C:319:ILE:CD1	3:C:384:ILE:HD11	2.47	0.43
3:C:61:VAL:HG21	3:C:125:LEU:CD1	2.48	0.43
3:C:82:TYR:HB3	3:C:302:TYR:O	2.18	0.43
4:D:117:HIS:NE2	11:D:1353:CLA:NA	2.66	0.43
2:B:464:PHE:CE1	4:D:144:ILE:HG23	2.53	0.43
4:D:252:PHE:O	4:D:256:ILE:HG13	2.17	0.43
1:G:121:LEU:HD23	1:G:121:LEU:C	2.39	0.43
1:G:172:MET:N	1:G:182:PHE:CD1	2.75	0.43
1:G:300:PHE:CE2	11:I:1462:CLA:H93	2.54	0.43
2:H:18:ARG:NH2	2:H:118:TRP:CE3	2.87	0.43
2:H:68:ARG:NH2	11:H:1485:CLA:CED	2.82	0.43
2:H:162:PHE:HB3	11:H:1487:CLA:HHD	2.00	0.43
3:I:445:ALA:CB	11:I:1463:CLA:HED1	2.45	0.43
3:I:282:MET:SD	11:I:1465:CLA:H42	2.57	0.43
3:I:165:LEU:O	3:I:169:GLY:N	2.50	0.43
4:J:59:TYR:N	4:J:59:TYR:CD1	2.87	0.43
6:L:34:LEU:HD12	6:L:34:LEU:HA	1.84	0.43
10:X:470:UNK:O	10:X:472:UNK:N	2.51	0.43
10:X:59:UNK:O	10:X:62:UNK:N	2.50	0.43
1:A:116:ILE:HG12	1:A:158:PHE:HD1	1.82	0.43
1:A:215:HIS:HB3	4:D:271:MET:HE2	2.00	0.43
1:A:218:LEU:HD11	1:A:255:PHE:CD2	2.50	0.43
1:A:38:ILE:CB	1:A:39:PRO:HD3	2.46	0.43
2:B:63:LEU:CB	2:B:64:PRO:CD	2.97	0.43
2:B:68:ARG:HH22	11:B:1485:CLA:HED3	1.84	0.43
2:B:92:SER:O	2:B:95:GLY:N	2.50	0.43
3:C:271:TYR:O	3:C:274:TYR:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:272:LEU:O	3:C:276:LEU:N	2.51	0.43
3:C:32:GLY:O	3:C:33:PHE:HB2	2.17	0.43
11:A:1344:CLA:HBB2	12:D:1352:PHO:H91	2.00	0.43
1:A:320:ILE:HD11	4:D:63:LEU:HD21	2.01	0.43
5:E:35:TRP:CD1	5:E:35:TRP:O	2.72	0.43
1:G:210:LEU:HD12	1:G:210:LEU:O	2.19	0.43
1:G:84:PRO:HD3	1:G:173:PRO:HB3	2.00	0.43
2:H:18:ARG:NH2	2:H:118:TRP:CZ3	2.86	0.43
2:H:309:LEU:C	2:H:311:PHE:N	2.69	0.43
2:H:63:LEU:CB	2:H:64:PRO:CD	2.96	0.43
3:I:115:GLY:O	3:I:116:VAL:C	2.56	0.43
3:I:241:GLY:O	3:I:245:ILE:HG23	2.18	0.43
5:K:34:GLY:O	5:K:38:VAL:HG23	2.19	0.43
6:L:33:PHE:C	6:L:35:GLY:H	2.22	0.43
10:X:160:UNK:O	10:X:164:UNK:CB	2.66	0.43
2:B:230:ARG:O	2:B:231:MET:C	2.57	0.43
2:B:396:GLY:O	2:B:397:VAL:C	2.56	0.43
3:C:240:ILE:CD1	11:C:1465:CLA:H91	2.48	0.43
3:C:225:VAL:HA	3:C:289:PHE:CE1	2.54	0.43
3:C:318:LEU:HA	3:C:340:TYR:CD1	2.54	0.43
3:C:376:ASP:O	3:C:378:ASN:N	2.51	0.43
4:D:91:LEU:HD13	4:D:93:TRP:CZ3	2.52	0.43
5:E:13:ILE:CG2	5:E:19:TYR:HD2	2.29	0.43
5:E:27:ILE:O	5:E:28:PRO:C	2.56	0.43
1:G:110:GLY:O	1:G:111:PRO:C	2.53	0.43
1:G:160:ILE:HD12	3:I:431:PHE:CE1	2.49	0.43
1:G:161:TYR:HA	1:G:294:ALA:HB1	2.00	0.43
1:G:59:ASP:O	1:G:60:ILE:C	2.57	0.43
2:H:242:ILE:HD11	11:H:1492:CLA:HBB1	2.00	0.43
3:I:290:VAL:HA	3:I:297:TYR:CE2	2.54	0.43
3:I:90:PRO:O	3:I:93:ALA:HB3	2.19	0.43
4:J:249:ALA:O	4:J:252:PHE:HB3	2.17	0.43
4:J:298:PHE:O	4:J:299:ILE:HB	2.19	0.43
7:O:11:UNK:CA	7:O:173:UNK:CB	2.93	0.43
2:B:332:LYS:O	2:B:440:ASP:N	2.52	0.43
3:C:115:GLY:O	3:C:116:VAL:C	2.56	0.43
3:C:421:SER:HA	3:C:422:PRO:HD3	1.81	0.43
4:D:154:VAL:O	4:D:159:ILE:HG13	2.18	0.43
4:D:185:PHE:O	4:D:186:GLN:C	2.56	0.43
4:D:56:THR:H	5:E:49:THR:HG22	1.82	0.43
5:E:10:PHE:CE2	6:F:19:ARG:NH2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:24:HIS:HA	6:F:27:ALA:HB3	1.99	0.43
1:G:105:TRP:CZ3	1:G:111:PRO:HG3	2.54	0.43
1:G:222:SER:O	1:G:246:TYR:HB2	2.19	0.43
2:H:152:GLY:O	2:H:153:PHE:C	2.55	0.43
2:H:204:ALA:O	2:H:205:ALA:C	2.56	0.43
3:I:150:ASP:O	3:I:151:TRP:C	2.56	0.43
3:I:264:PHE:CD2	3:I:264:PHE:N	2.87	0.43
3:I:38:GLY:HA3	11:I:1469:CLA:C2D	2.49	0.43
3:I:85:GLY:N	3:I:419:PHE:CE2	2.87	0.43
4:J:127:LEU:O	4:J:130:PHE:N	2.51	0.43
4:J:190:ASN:ND2	4:J:193:LEU:HD12	2.34	0.43
6:L:33:PHE:HB2	17:L:1047:BCR:H363	2.00	0.43
8:U:57:UNK:O	8:U:59:UNK:N	2.52	0.43
10:Y:580:UNK:O	10:Y:581:UNK:C	2.66	0.43
1:A:214:MET:O	1:A:217:SER:HB3	2.19	0.43
2:B:462:PHE:HE1	11:B:1494:CLA:HMB3	1.84	0.43
2:B:279:TYR:O	2:B:281:GLN:N	2.51	0.43
2:B:359:MET:HE3	2:B:366:PHE:CB	2.49	0.43
3:C:27:ASP:O	3:C:31:SER:HB2	2.19	0.43
4:D:279:LEU:HD22	11:D:1351:CLA:HBA2	2.01	0.43
1:A:272:HIS:HD2	4:D:218:VAL:HG21	1.73	0.43
5:E:15:THR:O	5:E:15:THR:CG2	2.66	0.43
6:F:14:PRO:O	6:F:15:ILE:HB	2.18	0.43
1:G:119:PHE:CD2	12:G:1345:PHO:H111	2.54	0.43
2:H:64:PRO:HB3	2:H:268:PHE:CZ	2.53	0.43
4:J:46:GLY:O	4:J:48:TRP:N	2.52	0.43
6:L:11:VAL:HG12	6:L:12:SER:N	2.34	0.43
8:U:77:UNK:C	8:U:79:UNK:N	2.80	0.43
1:A:121:LEU:HD23	1:A:121:LEU:C	2.38	0.43
1:A:8:ARG:N	1:A:11:ALA:CB	2.80	0.43
2:B:71:VAL:CG1	2:B:93:PHE:H	2.32	0.43
2:B:94:GLU:O	2:B:97:ALA:HB3	2.19	0.43
3:C:425:TRP:CZ2	11:C:1462:CLA:O1A	2.72	0.43
3:C:188:THR:HG21	3:C:298:PRO:HA	2.00	0.43
4:D:228:GLY:O	4:D:229:ALA:HB3	2.19	0.43
4:D:85:MET:HE2	4:D:85:MET:HB2	1.82	0.43
1:G:131:TRP:CE3	1:G:132:GLU:N	2.86	0.43
11:G:1342:CLA:HBB1	11:J:1351:CLA:NC	2.33	0.43
1:G:75:ASN:HA	1:G:75:ASN:HD22	1.59	0.43
2:H:70:GLY:HA2	2:H:178:VAL:HG11	2.00	0.43
2:H:410:THR:OG1	2:H:411:PHE:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:75:PHE:CE1	3:I:76:ILE:O	2.72	0.43
4:J:246:MET:O	4:J:249:ALA:HB3	2.19	0.43
4:J:272:LEU:HD21	4:J:276:VAL:HG21	2.00	0.43
18:T:1138:HEC:HHA	18:T:1138:HEC:HAD2	1.60	0.43
1:A:142:TRP:C	1:A:144:CYS:N	2.70	0.43
1:A:180:PHE:CZ	4:D:192:THR:HB	2.54	0.43
1:A:277:ALA:O	1:A:278:TRP:C	2.56	0.43
2:B:26:HIS:HB2	11:B:1493:CLA:HMB2	1.99	0.43
3:C:128:GLY:HA3	11:C:1471:CLA:HMC3	1.99	0.43
4:D:111:TRP:O	4:D:113:PHE:N	2.52	0.43
4:D:190:ASN:HD22	4:D:193:LEU:HD12	1.84	0.43
4:D:213:ILE:O	4:D:216:ALA:N	2.52	0.43
4:D:91:LEU:C	4:D:93:TRP:N	2.71	0.43
1:G:187:GLN:CB	11:G:1342:CLA:HAC2	2.43	0.43
2:H:162:PHE:CB	11:H:1487:CLA:HMD3	2.49	0.43
2:H:201:HIS:CE1	11:H:1484:CLA:HMB3	2.54	0.43
2:H:96:VAL:O	2:H:99:ALA:HB3	2.19	0.43
4:J:127:LEU:C	4:J:129:GLN:N	2.72	0.43
4:J:160:TYR:CB	4:J:161:PRO:HD3	2.34	0.43
4:J:336:HIS:C	4:J:336:HIS:ND1	2.73	0.43
8:U:51:UNK:O	8:U:52:UNK:O	2.37	0.43
9:V:13:ASN:HB2	9:V:15:GLU:OE1	2.19	0.43
10:X:116:UNK:O	10:X:117:UNK:C	2.67	0.43
1:A:211:PHE:CE2	1:A:274:PHE:CE2	3.06	0.42
2:B:158:LEU:CB	2:B:199:VAL:HG22	2.48	0.42
3:C:280:SER:O	3:C:434:ALA:HB1	2.19	0.42
3:C:35:TRP:CE2	3:C:36:TRP:CD1	2.96	0.42
3:C:374:GLY:O	3:C:375:LEU:HB2	2.19	0.42
4:D:288:GLY:C	4:D:290:ALA:N	2.73	0.42
6:F:33:PHE:HB2	17:F:1046:BCR:H363	2.00	0.42
1:G:210:LEU:HD13	12:J:1352:PHO:C1D	2.48	0.42
2:H:139:PHE:CD1	2:H:139:PHE:O	2.71	0.42
2:H:347:ARG:O	2:H:396:GLY:HA2	2.19	0.42
2:H:407:ASN:O	2:H:408:GLY:O	2.37	0.42
2:H:466:HIS:O	2:H:468:TRP:N	2.52	0.42
11:I:1463:CLA:HMD3	11:I:1465:CLA:HAB	2.01	0.42
3:I:170:ILE:CG2	3:I:171:GLY:H	2.33	0.42
4:J:149:PRO:O	4:J:150:ILE:C	2.57	0.42
9:T:133:GLY:O	9:T:137:TYR:N	2.51	0.42
10:X:516:UNK:O	10:X:517:UNK:C	2.67	0.42
1:A:323:ARG:O	1:A:326:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PHE:CE1	1:A:95:PRO:HG2	2.54	0.42
1:A:95:PRO:O	1:A:105:TRP:NE1	2.52	0.42
3:C:322:GLN:NE2	3:C:381:LYS:HA	2.34	0.42
3:C:269:GLU:OE1	3:C:447:ARG:HD3	2.19	0.42
4:D:93:TRP:HA	4:D:97:ALA:HB2	2.00	0.42
1:G:192:ILE:O	1:G:194:MET:N	2.52	0.42
2:H:395:GLN:CB	2:H:397:VAL:CB	2.97	0.42
3:I:226:SER:O	3:I:227:VAL:C	2.57	0.42
3:I:85:GLY:N	3:I:419:PHE:HE2	2.18	0.42
3:I:89:ILE:HB	3:I:90:PRO:CD	2.42	0.42
4:J:296:TYR:CZ	4:J:319:LEU:CD2	3.02	0.42
7:P:86:UNK:O	7:P:87:UNK:CB	2.67	0.42
9:V:41:HIS:HA	9:V:45:ILE:O	2.18	0.42
10:X:412:UNK:O	10:X:414:UNK:N	2.52	0.42
10:Y:266:UNK:O	10:Y:267:UNK:C	2.67	0.42
1:A:95:PRO:HB3	11:A:1346:CLA:OBD	2.19	0.42
1:A:204:GLY:HA3	1:A:282:GLY:HA3	2.00	0.42
1:A:222:SER:O	1:A:246:TYR:O	2.37	0.42
1:A:322:ASN:O	1:A:323:ARG:C	2.56	0.42
2:B:359:MET:HE3	2:B:366:PHE:HB2	2.02	0.42
3:C:178:LYS:O	3:C:182:PHE:HB2	2.19	0.42
3:C:56:HIS:O	3:C:59:LEU:CB	2.67	0.42
3:C:80:PRO:HB2	3:C:83:GLU:HB3	2.00	0.42
4:D:161:PRO:HG2	4:D:170:ALA:HB2	2.02	0.42
4:D:59:TYR:CD1	4:D:59:TYR:N	2.85	0.42
1:G:244:GLU:OE2	4:J:264:LYS:NZ	2.52	0.42
1:G:290:ILE:C	1:G:292:THR:H	2.23	0.42
2:H:213:GLY:O	2:H:214:LEU:C	2.57	0.42
2:H:275:TRP:HZ2	2:H:359:MET:O	2.03	0.42
2:H:314:TYR:N	2:H:427:GLY:HA3	2.35	0.42
2:H:332:LYS:O	2:H:440:ASP:N	2.52	0.42
3:I:178:LYS:CD	3:I:178:LYS:C	2.85	0.42
3:I:272:LEU:O	3:I:276:LEU:N	2.52	0.42
3:I:299:SER:C	3:I:301:PHE:N	2.70	0.42
2:H:357:ARG:NH1	4:J:338:ASN:O	2.52	0.42
7:P:63:UNK:O	7:P:72:UNK:N	2.53	0.42
10:X:531:UNK:O	10:X:532:UNK:C	2.66	0.42
10:Y:507:UNK:C	10:Y:509:UNK:N	2.80	0.42
10:Y:52:UNK:O	10:Y:53:UNK:C	2.66	0.42
2:B:242:ILE:HD11	11:B:1492:CLA:HBB1	2.00	0.42
2:B:425:ILE:HG23	2:B:426:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:186:TYR:CE2	3:C:188:THR:HG23	2.49	0.42
3:C:33:PHE:CZ	3:C:40:ALA:HB1	2.54	0.42
3:C:420:VAL:HG12	3:C:421:SER:N	2.35	0.42
1:A:258:LEU:CD1	4:D:128:ARG:CZ	2.95	0.42
4:D:43:LEU:O	4:D:113:PHE:HE1	2.03	0.42
6:F:23:VAL:O	6:F:23:VAL:HG12	2.19	0.42
5:E:30:LEU:HD13	6:F:28:VAL:HG13	2.01	0.42
1:G:41:LEU:HD13	12:G:1345:PHO:C2	2.50	0.42
2:H:208:VAL:HG21	11:H:1483:CLA:HMC1	2.01	0.42
2:H:195:PRO:O	2:H:197:GLY:N	2.52	0.42
2:H:214:LEU:HG	2:H:215:PHE:H	1.85	0.42
3:I:264:PHE:CE2	11:I:1464:CLA:HBA1	2.53	0.42
4:J:200:GLY:HA3	4:J:282:SER:HB3	2.02	0.42
4:J:286:VAL:C	4:J:288:GLY:N	2.68	0.42
4:J:82:ALA:HB3	4:J:85:MET:HE3	2.01	0.42
5:E:58:GLN:NE2	9:V:4:THR:OG1	2.53	0.42
10:X:215:UNK:O	10:X:219:UNK:N	2.52	0.42
10:Y:563:UNK:O	10:Y:564:UNK:C	2.68	0.42
1:A:65:GLU:HG2	1:A:65:GLU:O	2.19	0.42
2:B:214:LEU:HD12	2:B:215:PHE:N	2.34	0.42
3:C:163:PHE:CE2	3:C:252:ILE:HD13	2.53	0.42
3:C:269:GLU:OE2	3:C:447:ARG:NH1	2.52	0.42
3:C:299:SER:C	3:C:301:PHE:N	2.71	0.42
3:C:445:ALA:HB1	11:C:1463:CLA:CED	2.41	0.42
3:C:52:ALA:HA	11:C:1469:CLA:CMB	2.41	0.42
3:C:88:LEU:O	3:C:89:ILE:C	2.57	0.42
12:A:1345:PHO:HAB	4:D:205:LEU:HD21	2.01	0.42
1:G:192:ILE:C	1:G:194:MET:N	2.69	0.42
2:H:135:LEU:O	2:H:137:LYS:N	2.52	0.42
2:H:452:THR:CG2	2:H:452:THR:O	2.65	0.42
3:I:113:VAL:O	3:I:116:VAL:HG22	2.19	0.42
3:I:55:ALA:O	3:I:56:HIS:C	2.57	0.42
4:J:223:PHE:HD2	4:J:243:THR:O	2.03	0.42
4:J:244:TYR:HB2	4:J:245:SER:H	1.66	0.42
6:L:9:GLU:N	6:L:10:PRO:HD2	2.34	0.42
9:V:30:LYS:O	9:V:34:GLN:HG3	2.20	0.42
9:V:40:CYS:O	9:V:40:CYS:SG	2.77	0.42
1:A:102:LEU:O	1:A:105:TRP:HB3	2.20	0.42
1:A:64:ARG:C	1:A:66:PRO:HD3	2.38	0.42
2:B:248:ALA:O	2:B:251:VAL:CG2	2.63	0.42
2:B:464:PHE:HD2	11:B:1492:CLA:HAC2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:468:TRP:CD1	4:D:144:ILE:CD1	2.99	0.42
3:C:160:ILE:O	3:C:161:LEU:C	2.58	0.42
3:C:272:LEU:O	3:C:273:SER:C	2.55	0.42
3:C:286:ALA:O	3:C:287:THR:C	2.58	0.42
4:D:223:PHE:HB3	4:D:225:ASP:OD1	2.20	0.42
4:D:193:LEU:HD11	4:D:315:TYR:HE2	1.83	0.42
1:A:327:GLY:O	4:D:324:GLY:HA3	2.19	0.42
4:D:93:TRP:CD1	4:D:93:TRP:N	2.86	0.42
2:H:176:GLY:O	2:H:177:SER:HB3	2.19	0.42
2:H:263:THR:HG22	2:H:448:ARG:NH2	2.34	0.42
2:H:425:ILE:HG23	2:H:426:PHE:CD2	2.52	0.42
4:J:191:TRP:CZ3	4:J:194:ASN:ND2	2.85	0.42
4:J:64:ALA:HB1	4:J:69:GLU:HB3	2.00	0.42
7:P:123:UNK:O	7:P:126:UNK:N	2.53	0.42
10:X:365:UNK:O	10:X:366:UNK:C	2.63	0.42
1:A:134:SER:HA	1:A:139:MET:CB	2.47	0.42
2:B:330:MET:O	2:B:331:ASN:CB	2.68	0.42
3:C:51:GLY:HA2	3:C:54:VAL:CG2	2.50	0.42
4:D:194:ASN:HA	4:D:195:PRO:HD3	1.84	0.42
1:G:116:ILE:HD13	1:G:158:PHE:HB3	2.01	0.42
1:G:176:ILE:CG2	1:G:180:PHE:CE1	3.02	0.42
1:G:195:HIS:CE1	1:G:197:PHE:CD1	3.06	0.42
2:H:236:THR:N	2:H:473:THR:OG1	2.52	0.42
3:I:265:ILE:C	3:I:266:TRP:CD1	2.93	0.42
3:I:450:ALA:HB1	3:I:455:PHE:HB2	2.02	0.42
4:J:190:ASN:CG	4:J:322:ASN:HD21	2.23	0.42
4:J:235:PHE:CZ	4:J:237:PRO:HA	2.55	0.42
4:J:92:LEU:C	4:J:93:TRP:CD1	2.93	0.42
5:K:13:ILE:CG2	5:K:19:TYR:HD2	2.28	0.42
8:U:31:UNK:O	8:U:33:UNK:N	2.53	0.42
10:X:507:UNK:C	10:X:509:UNK:N	2.83	0.42
10:X:71:UNK:O	10:X:72:UNK:C	2.67	0.42
2:B:362:PHE:CE2	4:D:184:PHE:CZ	3.00	0.42
2:B:401:PHE:CD1	2:B:401:PHE:N	2.87	0.42
3:C:165:LEU:O	3:C:169:GLY:N	2.51	0.42
3:C:172:ALA:N	11:C:1459:CLA:CAC	2.83	0.42
3:C:187:ASP:CB	3:C:230:LEU:CD2	2.94	0.42
3:C:225:VAL:CG1	3:C:225:VAL:O	2.64	0.42
3:C:50:LEU:O	3:C:54:VAL:N	2.50	0.42
4:D:127:LEU:C	4:D:129:GLN:H	2.22	0.42
2:B:464:PHE:HE1	4:D:144:ILE:HG23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ILE:CA	4:D:220:ASN:ND2	2.83	0.42
4:D:264:LYS:C	4:D:266:TRP:H	2.23	0.42
5:E:27:ILE:HB	5:E:28:PRO:CD	2.45	0.42
1:A:310:LYS:HZ1	5:E:58:GLN:HG2	1.84	0.42
1:G:187:GLN:NE2	1:G:325:ASN:OD1	2.53	0.42
11:H:1496:CLA:HMA3	11:H:1497:CLA:HMC2	2.02	0.42
3:I:107:ASP:O	3:I:110:PRO:CD	2.52	0.42
4:J:148:ALA:CB	4:J:276:VAL:HA	2.50	0.42
5:K:10:PHE:CE2	6:L:19:ARG:NH2	2.88	0.42
6:L:27:ALA:O	6:L:28:VAL:C	2.58	0.42
7:O:75:UNK:O	7:O:77:UNK:N	2.53	0.42
5:K:58:GLN:NE2	9:T:2:GLU:O	2.53	0.42
10:X:266:UNK:O	10:X:268:UNK:N	2.53	0.42
10:Y:16:UNK:O	10:Y:17:UNK:C	2.64	0.42
10:Y:213:UNK:O	10:Y:214:UNK:C	2.67	0.42
1:A:133:LEU:HB2	4:D:252:PHE:HE2	1.85	0.42
1:A:81:ALA:CB	1:A:174:LEU:O	2.56	0.42
2:B:30:VAL:HB	11:B:1486:CLA:HAC1	2.02	0.42
2:B:167:TRP:HA	2:B:177:SER:O	2.19	0.42
2:B:243:ALA:C	2:B:246:PHE:HB3	2.39	0.42
2:B:369:ILE:O	2:B:379:ALA:O	2.38	0.42
2:B:397:VAL:C	2:B:399:VAL:N	2.73	0.42
3:C:41:ARG:NH1	11:C:1469:CLA:OBD	2.50	0.42
3:C:367:GLU:HB2	3:C:368:PRO:CD	2.50	0.42
3:C:95:LEU:HA	3:C:95:LEU:HD12	1.89	0.42
4:D:200:GLY:O	4:D:203:GLY:N	2.52	0.42
4:D:193:LEU:HB3	4:D:295:SER:HB3	2.02	0.42
1:G:244:GLU:HG3	1:G:245:THR:H	1.85	0.42
1:G:323:ARG:O	1:G:326:LEU:HB2	2.20	0.42
1:G:83:VAL:HA	1:G:84:PRO:HD3	1.87	0.42
2:H:167:TRP:CH2	2:H:177:SER:HA	2.55	0.42
2:H:98:LEU:O	2:H:99:ALA:C	2.58	0.42
3:I:239:TRP:O	3:I:243:ILE:N	2.37	0.42
3:I:305:THR:C	3:I:307:PRO:HD2	2.40	0.42
3:I:305:THR:O	3:I:307:PRO:N	2.53	0.42
3:I:314:ALA:O	3:I:315:MET:C	2.58	0.42
3:I:315:MET:O	3:I:319:ILE:CB	2.68	0.42
4:J:128:ARG:O	4:J:128:ARG:HG2	2.18	0.42
4:J:213:ILE:O	4:J:216:ALA:N	2.53	0.42
7:P:75:UNK:O	7:P:77:UNK:N	2.53	0.42
9:T:106:ASN:HD22	9:T:106:ASN:N	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:253:UNK:C	10:Y:255:UNK:N	2.82	0.42
10:Y:405:UNK:O	10:Y:408:UNK:N	2.53	0.42
10:Y:463:UNK:O	10:Y:464:UNK:C	2.68	0.42
10:Y:9:UNK:O	10:Y:10:UNK:C	2.67	0.42
11:A:1344:CLA:HBC3	4:D:178:ILE:HG23	2.02	0.42
1:A:167:SER:OG	1:A:169:SER:CB	2.68	0.42
2:B:18:ARG:NH2	2:B:115:TRP:O	2.52	0.42
2:B:208:VAL:HG21	11:B:1483:CLA:HMC1	2.02	0.42
2:B:222:PRO:O	2:B:223:GLN:C	2.57	0.42
2:B:240:SER:HB3	11:B:1491:CLA:C4B	2.50	0.42
2:B:35:GLY:O	2:B:38:ALA:HB3	2.20	0.42
3:C:73:ALA:HB3	3:C:74:HIS:CD2	2.50	0.42
4:D:161:PRO:CG	4:D:170:ALA:HB2	2.50	0.42
1:A:330:VAL:HG21	4:D:328:TRP:CH2	2.55	0.42
4:D:63:LEU:N	4:D:63:LEU:CD1	2.80	0.42
1:G:150:PRO:HB3	11:G:1342:CLA:H62	2.01	0.42
2:H:164:PRO:CB	11:H:1487:CLA:O1D	2.68	0.42
2:H:386:ALA:O	2:H:387:GLU:C	2.58	0.42
2:H:37:MET:HG2	2:H:62:VAL:HG21	2.01	0.42
3:I:373:ASN:N	3:I:373:ASN:OD1	2.53	0.42
3:I:376:ASP:C	3:I:378:ASN:H	2.22	0.42
3:I:37:ALA:C	3:I:39:ASN:H	2.22	0.42
3:I:47:GLY:O	3:I:48:LYS:C	2.56	0.42
3:I:75:PHE:CE2	3:I:77:PRO:HG3	2.55	0.42
4:J:100:ASP:CB	4:J:103:ARG:H	2.33	0.42
4:J:190:ASN:HD22	4:J:193:LEU:HD12	1.83	0.42
4:J:35:ILE:CG2	4:J:35:ILE:O	2.68	0.42
5:K:19:TYR:HE2	16:L:1046:HEM:C2A	2.38	0.42
8:U:9:UNK:O	8:U:10:UNK:C	2.62	0.42
10:X:224:UNK:O	10:X:225:UNK:C	2.68	0.42
10:X:272:UNK:C	10:X:274:UNK:N	2.82	0.42
10:Y:182:UNK:O	10:Y:183:UNK:C	2.67	0.42
3:C:133:ALA:C	3:C:134:ILE:HG13	2.40	0.41
4:D:236:ASN:C	4:D:238:THR:N	2.71	0.41
4:D:54:PHE:HE1	6:F:33:PHE:CE2	2.38	0.41
5:E:82:GLN:C	5:E:84:LYS:N	2.72	0.41
6:F:18:VAL:HA	6:F:21:VAL:HG23	2.02	0.41
1:G:193:LEU:HD22	4:J:179:PHE:CD1	2.55	0.41
1:G:256:GLY:HA2	1:G:260:PHE:O	2.20	0.41
11:H:1492:CLA:CMA	11:H:1493:CLA:HBC2	2.49	0.41
11:H:1496:CLA:H171	11:H:1497:CLA:HMD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:293:ALA:O	2:H:294:SER:C	2.56	0.41
2:H:463:PHE:C	2:H:465:GLY:H	2.23	0.41
2:H:45:PHE:C	2:H:47:PRO:HD2	2.40	0.41
11:I:1463:CLA:CMD	11:I:1465:CLA:HAB	2.50	0.41
4:J:337:GLU:HG3	4:J:339:PHE:CE2	2.53	0.41
5:K:19:TYR:HD1	5:K:20:TRP:N	2.18	0.41
9:T:63:THR:O	9:T:84:GLY:HA3	2.20	0.41
10:X:204:UNK:O	10:X:205:UNK:C	2.68	0.41
1:A:21:VAL:O	1:A:24:THR:CB	2.68	0.41
1:A:93:PHE:CZ	1:A:95:PRO:HG3	2.55	0.41
2:B:468:TRP:HD1	4:D:144:ILE:CD1	2.34	0.41
3:C:51:GLY:HA2	3:C:54:VAL:HB	2.01	0.41
4:D:149:PRO:O	4:D:150:ILE:C	2.57	0.41
4:D:191:TRP:HZ2	4:D:286:VAL:CG2	2.32	0.41
4:D:320:LEU:HD23	4:D:320:LEU:HA	1.78	0.41
1:G:110:GLY:N	1:G:111:PRO:CD	2.82	0.41
1:G:290:ILE:CD1	11:G:1342:CLA:OBD	2.63	0.41
1:G:152:ALA:O	1:G:155:PHE:N	2.53	0.41
1:G:323:ARG:HA	1:G:326:LEU:HD12	2.01	0.41
1:G:84:PRO:HD3	1:G:173:PRO:CB	2.50	0.41
2:H:397:VAL:C	2:H:399:VAL:N	2.73	0.41
2:H:414:PRO:HB2	2:H:415:PRO:CD	2.41	0.41
2:H:316:GLY:CA	2:H:443:PHE:CE1	3.04	0.41
3:I:122:SER:O	3:I:126:GLY:N	2.48	0.41
3:I:160:ILE:O	3:I:161:LEU:C	2.57	0.41
3:I:259:TRP:O	3:I:260:ALA:C	2.58	0.41
4:J:100:ASP:CB	4:J:103:ARG:HB2	2.50	0.41
4:J:199:MET:O	4:J:202:ALA:N	2.53	0.41
4:J:235:PHE:HD2	4:J:243:THR:HG21	1.83	0.41
4:J:191:TRP:CE3	4:J:289:LEU:HD11	2.55	0.41
6:L:36:ALA:O	6:L:40:MET:HG3	2.21	0.41
8:S:69:UNK:O	8:S:71:UNK:N	2.53	0.41
9:V:53:ASP:OD1	9:V:53:ASP:C	2.58	0.41
10:X:578:UNK:O	10:X:580:UNK:N	2.54	0.41
10:Y:470:UNK:O	10:Y:471:UNK:C	2.68	0.41
1:A:192:ILE:O	1:A:194:MET:N	2.53	0.41
11:B:1496:CLA:HMA3	11:B:1497:CLA:HMC2	2.02	0.41
2:B:348:ASN:C	2:B:350:GLU:N	2.73	0.41
2:B:94:GLU:HG3	2:B:95:GLY:H	1.79	0.41
4:D:10:ALA:O	4:D:11:GLU:CB	2.67	0.41
1:G:102:LEU:O	1:G:105:TRP:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:157:VAL:HG21	11:G:1343:CLA:CMC	2.49	0.41
2:H:236:THR:HG23	2:H:237:VAL:N	2.34	0.41
2:H:366:PHE:HD2	2:H:425:ILE:HD11	1.86	0.41
2:H:451:PHE:CD2	2:H:451:PHE:C	2.94	0.41
11:I:1465:CLA:HBA1	11:I:1465:CLA:H3A	1.83	0.41
3:I:276:LEU:HD13	3:I:276:LEU:HA	1.86	0.41
3:I:84:GLN:O	3:I:85:GLY:C	2.58	0.41
4:J:180:ARG:CD	4:J:180:ARG:C	2.88	0.41
4:J:286:VAL:O	4:J:287:VAL:C	2.55	0.41
4:J:335:PRO:O	4:J:336:HIS:C	2.58	0.41
4:J:337:GLU:CG	4:J:339:PHE:HE2	2.31	0.41
4:J:50:THR:O	4:J:54:PHE:N	2.45	0.41
6:L:33:PHE:O	6:L:34:LEU:C	2.57	0.41
10:Y:331:UNK:O	10:Y:332:UNK:C	2.66	0.41
1:A:157:VAL:HG21	11:A:1343:CLA:CMC	2.50	0.41
2:B:201:HIS:HA	11:B:1483:CLA:C4B	2.49	0.41
2:B:162:PHE:HB3	11:B:1487:CLA:HHD	2.02	0.41
2:B:421:ALA:O	2:B:424:ALA:N	2.53	0.41
3:C:105:VAL:O	3:C:107:ASP:N	2.54	0.41
3:C:382:ASN:OD1	3:C:382:ASN:N	2.52	0.41
3:C:450:ALA:HB1	3:C:455:PHE:HB2	2.01	0.41
4:D:253:TRP:HE1	15:D:1354:PL9:C1	2.32	0.41
4:D:262:SER:O	4:D:263:ASN:HB2	2.20	0.41
4:D:55:VAL:CG1	4:D:56:THR:N	2.82	0.41
4:D:83:ASN:O	4:D:84:SER:C	2.59	0.41
1:G:267:ASN:O	1:G:271:LEU:N	2.38	0.41
2:H:405:GLU:O	2:H:406:LEU:HB2	2.20	0.41
3:I:156:LYS:HD2	3:I:156:LYS:HA	1.89	0.41
3:I:97:TRP:CE3	3:I:178:LYS:NZ	2.88	0.41
3:I:275:SER:HB2	11:I:1465:CLA:HAA1	2.03	0.41
4:J:179:PHE:O	4:J:182:LEU:HB2	2.20	0.41
4:J:288:GLY:C	4:J:290:ALA:N	2.72	0.41
8:U:5:UNK:O	8:U:8:UNK:N	2.54	0.41
10:Y:116:UNK:O	10:Y:117:UNK:C	2.68	0.41
10:Y:56:UNK:O	10:Y:59:UNK:N	2.54	0.41
1:A:300:PHE:CE2	11:C:1462:CLA:H93	2.56	0.41
1:A:58:VAL:HG13	1:A:109:GLY:HA3	2.02	0.41
2:B:195:PRO:O	2:B:198:VAL:N	2.53	0.41
3:C:153:ASP:OD1	3:C:155:ASN:N	2.51	0.41
3:C:56:HIS:O	3:C:57:ALA:O	2.39	0.41
4:D:180:ARG:C	4:D:180:ARG:CD	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:58:GLN:OE1	9:V:2:GLU:HB2	2.19	0.41
1:G:69:GLY:HA2	1:G:75:ASN:OD1	2.21	0.41
1:G:84:PRO:CG	1:G:173:PRO:CD	2.88	0.41
11:H:1483:CLA:H143	11:H:1483:CLA:H111	1.94	0.41
2:H:419:SER:OG	2:H:420:TYR:N	2.53	0.41
2:H:59:GLY:CA	11:H:1488:CLA:CED	2.88	0.41
2:H:69:LEU:HD23	11:H:1487:CLA:CMA	2.46	0.41
3:I:395:TYR:O	3:I:398:HIS:N	2.37	0.41
4:J:152:VAL:CG1	11:J:1351:CLA:HBA1	2.51	0.41
4:J:228:GLY:O	4:J:229:ALA:HB3	2.20	0.41
5:K:65:LEU:O	5:K:66:VAL:CA	2.68	0.41
7:P:99:UNK:O	7:P:100:UNK:C	2.68	0.41
10:X:3:UNK:C	10:X:5:UNK:N	2.78	0.41
11:A:1342:CLA:H201	12:A:1345:PHO:H43	2.03	0.41
1:A:135:TYR:O	1:A:136:ARG:HG2	2.20	0.41
1:A:168:PHE:O	1:A:170:ASP:O	2.38	0.41
11:B:1496:CLA:H13	11:B:1497:CLA:CMD	2.50	0.41
2:B:471:ALA:O	2:B:473:THR:N	2.53	0.41
3:C:188:THR:HG22	3:C:300:GLU:OE1	2.19	0.41
4:D:194:ASN:OD1	4:D:196:PHE:HB2	2.20	0.41
1:G:45:THR:CA	12:G:1345:PHO:H93	2.50	0.41
1:G:139:MET:HE3	1:G:139:MET:HB2	1.80	0.41
1:G:255:PHE:O	1:G:256:GLY:C	2.58	0.41
2:H:464:PHE:HD2	11:H:1492:CLA:HAC2	1.86	0.41
11:H:1496:CLA:H13	11:H:1497:CLA:HMD2	2.02	0.41
2:H:21:ALA:CB	2:H:115:TRP:HD1	2.34	0.41
2:H:24:LEU:HD21	2:H:110:ALA:HB1	2.01	0.41
2:H:71:VAL:CG1	2:H:93:PHE:H	2.34	0.41
3:I:129:GLY:C	3:I:131:TYR:N	2.74	0.41
3:I:35:TRP:CZ3	3:I:36:TRP:HB3	2.56	0.41
4:J:132:ILE:O	4:J:133:ALA:C	2.58	0.41
7:O:118:UNK:O	7:O:119:UNK:C	2.68	0.41
8:S:12:UNK:O	8:S:14:UNK:N	2.53	0.41
9:T:128:ASP:HB3	9:T:134:LYS:CG	2.50	0.41
8:U:29:UNK:O	8:U:30:UNK:C	2.67	0.41
10:X:16:UNK:O	10:X:17:UNK:C	2.68	0.41
10:X:256:UNK:O	10:X:257:UNK:C	2.69	0.41
10:Y:71:UNK:O	10:Y:72:UNK:C	2.68	0.41
1:A:248:ILE:O	1:A:249:VAL:C	2.59	0.41
2:B:157:HIS:CE1	2:B:164:PRO:O	2.73	0.41
2:B:201:HIS:CE1	11:B:1484:CLA:HMB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:THR:HG22	2:B:448:ARG:NH2	2.36	0.41
2:B:236:THR:CB	2:B:473:THR:CG2	2.89	0.41
2:B:75:TRP:O	2:B:76:SER:CB	2.68	0.41
11:C:1464:CLA:HBA2	11:C:1464:CLA:H3A	1.46	0.41
3:C:265:ILE:C	3:C:266:TRP:CD1	2.94	0.41
4:D:200:GLY:HA3	4:D:282:SER:HB3	2.03	0.41
6:F:11:VAL:CG1	6:F:12:SER:N	2.83	0.41
1:G:48:PHE:HA	1:G:115:ILE:HD11	2.02	0.41
1:G:273:PHE:CD2	1:G:273:PHE:C	2.93	0.41
1:G:320:ILE:C	1:G:322:ASN:N	2.73	0.41
11:H:1486:CLA:CBB	11:H:1486:CLA:HMB1	2.50	0.41
2:H:237:VAL:HG22	11:H:1491:CLA:C3C	2.50	0.41
2:H:224:ARG:O	2:H:228:ALA:HB2	2.19	0.41
3:I:95:LEU:C	3:I:185:LEU:HA	2.39	0.41
3:I:308:GLU:O	3:I:311:GLN:HB2	2.21	0.41
4:J:122:LEU:HD23	4:J:122:LEU:HA	1.76	0.41
4:J:126:MET:HG2	4:J:130:PHE:HE1	1.85	0.41
1:G:272:HIS:HD2	4:J:218:VAL:HG21	1.74	0.41
4:J:224:GLN:O	4:J:225:ASP:C	2.58	0.41
4:J:262:SER:O	4:J:263:ASN:HB2	2.21	0.41
4:J:298:PHE:O	10:Y:129:UNK:CB	2.69	0.41
4:J:83:ASN:CG	4:J:336:HIS:CD2	2.83	0.41
7:P:88:UNK:CB	7:P:140:UNK:O	2.69	0.41
8:S:7:UNK:O	8:S:9:UNK:N	2.53	0.41
10:Y:215:UNK:O	10:Y:219:UNK:N	2.54	0.41
1:A:84:PRO:CD	1:A:173:PRO:HB3	2.46	0.41
1:A:191:ASN:O	1:A:192:ILE:C	2.59	0.41
1:A:45:THR:HA	12:A:1345:PHO:H93	2.02	0.41
1:A:48:PHE:CD2	1:A:48:PHE:C	2.94	0.41
1:A:69:GLY:HA2	1:A:75:ASN:OD1	2.20	0.41
2:B:466:HIS:C	2:B:468:TRP:N	2.73	0.41
2:B:64:PRO:HG3	2:B:267:LEU:O	2.21	0.41
3:C:257:PHE:HB3	3:C:258:GLY:H	1.59	0.41
3:C:92:ILE:O	3:C:93:ALA:C	2.59	0.41
4:D:101:PHE:O	4:D:104:TRP:HB3	2.20	0.41
4:D:281:MET:HA	4:D:281:MET:HE3	2.03	0.41
1:G:167:SER:OG	1:G:169:SER:CB	2.69	0.41
2:H:193:TYR:O	2:H:195:PRO:HD3	2.20	0.41
2:H:37:MET:HG2	2:H:62:VAL:CG2	2.51	0.41
2:H:349:LYS:HG3	2:H:394:GLN:O	2.21	0.41
2:H:64:PRO:HB2	2:H:268:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:168:LEU:O	11:I:1459:CLA:HMC1	2.20	0.41
3:I:272:LEU:HD21	11:I:1466:CLA:C1B	2.51	0.41
3:I:35:TRP:O	3:I:36:TRP:CG	2.74	0.41
4:J:199:MET:SD	4:J:281:MET:HE3	2.61	0.41
6:L:35:GLY:O	6:L:36:ALA:C	2.58	0.41
10:Y:223:UNK:O	10:Y:224:UNK:C	2.68	0.41
1:A:176:ILE:HG23	11:A:1343:CLA:HED1	2.03	0.41
1:A:142:TRP:HH2	1:A:273:PHE:CE1	2.38	0.41
2:B:21:ALA:CB	2:B:115:TRP:HD1	2.34	0.41
2:B:141:ILE:O	2:B:144:PHE:HB3	2.21	0.41
2:B:18:ARG:NH2	2:B:118:TRP:CE3	2.89	0.41
2:B:18:ARG:NH2	2:B:118:TRP:CZ3	2.89	0.41
2:B:214:LEU:HA	2:B:217:ILE:HG22	2.02	0.41
2:B:220:ARG:CB	2:B:221:PRO:CD	2.99	0.41
2:B:224:ARG:O	2:B:228:ALA:HB2	2.21	0.41
2:B:63:LEU:HA	2:B:66:MET:CE	2.51	0.41
3:C:183:GLY:O	3:C:184:GLY:O	2.38	0.41
3:C:436:PHE:O	3:C:439:VAL:HB	2.21	0.41
4:D:190:ASN:ND2	4:D:193:LEU:HD12	2.36	0.41
4:D:50:THR:O	4:D:54:PHE:HB2	2.21	0.41
1:G:202:VAL:O	1:G:203:ALA:C	2.59	0.41
1:G:214:MET:O	1:G:217:SER:HB3	2.20	0.41
2:H:166:MET:HE1	2:H:198:VAL:HG11	2.03	0.41
2:H:217:ILE:CG1	2:H:217:ILE:O	2.66	0.41
2:H:238:LEU:HD23	2:H:469:HIS:CG	2.56	0.41
2:H:31:ALA:HB3	2:H:104:SER:HB2	2.03	0.41
2:H:317:ASN:HA	2:H:330:MET:HE3	2.03	0.41
2:H:358:ARG:O	2:H:360:PRO:HD3	2.21	0.41
2:H:95:GLY:O	2:H:96:VAL:C	2.58	0.41
3:I:102:GLY:O	3:I:103:GLY:O	2.38	0.41
3:I:322:GLN:NE2	3:I:381:LYS:HA	2.36	0.41
3:I:394:GLU:OE2	3:I:398:HIS:CD2	2.74	0.41
3:I:57:ALA:O	3:I:58:GLY:C	2.58	0.41
10:X:258:UNK:O	10:X:259:UNK:C	2.68	0.41
10:Y:406:UNK:O	10:Y:407:UNK:C	2.68	0.41
10:Y:580:UNK:C	10:Y:582:UNK:N	2.79	0.41
1:A:150:PRO:HB3	11:A:1342:CLA:H62	2.02	0.41
2:B:31:ALA:HB3	2:B:104:SER:HB2	2.02	0.41
2:B:30:VAL:CG1	11:B:1486:CLA:HAC1	2.51	0.41
2:B:263:THR:O	2:B:448:ARG:CZ	2.69	0.41
3:C:122:SER:O	3:C:126:GLY:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:1465:CLA:HBA1	11:C:1465:CLA:H3A	1.80	0.41
3:C:238:ILE:O	3:C:239:TRP:C	2.58	0.41
3:C:245:ILE:C	3:C:245:ILE:HD12	2.41	0.41
3:C:305:THR:C	3:C:307:PRO:HD2	2.41	0.41
3:C:39:ASN:O	3:C:40:ALA:C	2.59	0.41
4:D:100:ASP:CB	4:D:103:ARG:H	2.34	0.41
4:D:298:PHE:O	10:X:129:UNK:CB	2.68	0.41
1:G:60:ILE:HD12	1:G:83:VAL:HG12	1.99	0.41
2:H:133:LEU:O	2:H:134:ASP:CB	2.68	0.41
2:H:263:THR:O	2:H:448:ARG:CZ	2.69	0.41
2:H:359:MET:HB3	2:H:426:PHE:HB3	2.02	0.41
2:H:69:LEU:HA	2:H:69:LEU:HD12	1.84	0.41
3:I:63:TRP:NE1	11:I:1462:CLA:C2C	2.83	0.41
11:I:1463:CLA:H93	11:I:1464:CLA:H51	2.02	0.41
4:J:161:PRO:HG2	4:J:170:ALA:HB2	2.03	0.41
4:J:253:TRP:HE1	15:J:1354:PL9:C1	2.33	0.41
4:J:313:THR:O	4:J:315:TYR:N	2.54	0.41
4:J:188:PHE:CE2	4:J:326:ARG:HG2	2.56	0.41
4:J:76:VAL:O	4:J:77:ALA:HB2	2.20	0.41
10:X:268:UNK:O	10:X:271:UNK:N	2.54	0.41
10:X:519:UNK:C	10:X:521:UNK:N	2.82	0.41
10:X:563:UNK:O	10:X:564:UNK:C	2.68	0.41
10:Y:532:UNK:C	10:Y:534:UNK:N	2.83	0.41
1:A:184:ILE:HD11	4:D:186:GLN:CD	2.42	0.41
1:A:296:ASN:ND2	1:A:298:ASN:OD1	2.54	0.41
2:B:196:GLY:O	2:B:197:GLY:C	2.59	0.41
2:B:347:ARG:H	2:B:398:THR:CB	2.34	0.41
2:B:238:LEU:HD23	2:B:469:HIS:CG	2.56	0.41
3:C:164:HIS:C	3:C:166:ILE:N	2.74	0.41
3:C:36:TRP:O	3:C:36:TRP:CE3	2.73	0.41
4:D:286:VAL:O	4:D:287:VAL:C	2.58	0.41
4:D:321:LEU:O	4:D:324:GLY:N	2.54	0.41
1:G:104:GLU:HG2	1:G:104:GLU:O	2.20	0.41
1:G:134:SER:HA	1:G:139:MET:CB	2.51	0.41
1:G:151:LEU:CD2	1:G:155:PHE:HE2	2.33	0.41
1:G:176:ILE:HG22	1:G:177:SER:N	2.36	0.41
2:H:222:PRO:O	2:H:226:TYR:N	2.45	0.41
2:H:92:SER:O	2:H:95:GLY:N	2.54	0.41
3:I:161:LEU:O	3:I:164:HIS:N	2.46	0.41
4:J:294:ARG:HB2	4:J:295:SER:H	1.51	0.41
5:K:82:GLN:O	5:K:83:LEU:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:47:UNK:O	8:U:48:UNK:C	2.69	0.41
1:A:290:ILE:C	1:A:292:THR:H	2.25	0.40
11:B:1486:CLA:CBB	11:B:1486:CLA:HMB1	2.51	0.40
2:B:37:MET:O	2:B:38:ALA:C	2.59	0.40
3:C:241:GLY:O	3:C:245:ILE:HG23	2.21	0.40
3:C:250:TRP:HA	3:C:253:LEU:CD1	2.50	0.40
4:D:32:TRP:O	4:D:35:ILE:HB	2.21	0.40
4:D:62:GLY:HA3	5:E:63:ILE:HG23	2.03	0.40
1:G:131:TRP:C	1:G:131:TRP:CD2	2.91	0.40
1:G:248:ILE:O	1:G:251:ALA:N	2.48	0.40
1:G:256:GLY:O	1:G:260:PHE:O	2.38	0.40
1:G:307:ILE:O	1:G:310:LYS:N	2.40	0.40
3:I:298:PRO:HB3	3:I:300:GLU:OE1	2.22	0.40
3:I:33:PHE:CZ	3:I:40:ALA:HB1	2.56	0.40
3:I:365:TRP:CG	3:I:366:LEU:N	2.90	0.40
3:I:382:ASN:OD1	3:I:382:ASN:N	2.53	0.40
3:I:73:ALA:HB3	3:I:74:HIS:CD2	2.52	0.40
4:J:42:TYR:O	4:J:43:LEU:C	2.60	0.40
4:J:72:ASN:O	4:J:73:PHE:C	2.60	0.40
5:K:37:PHE:CE1	5:K:42:LEU:HB3	2.56	0.40
8:S:86:UNK:O	8:S:87:UNK:C	2.68	0.40
10:X:162:UNK:O	10:X:163:UNK:C	2.65	0.40
10:X:519:UNK:O	10:X:520:UNK:C	2.69	0.40
10:Y:268:UNK:O	10:Y:271:UNK:N	2.53	0.40
1:A:133:LEU:HD12	4:D:256:ILE:HG12	1.99	0.40
1:A:44:ALA:O	1:A:45:THR:C	2.58	0.40
1:A:67:VAL:HG21	4:D:317:LYS:NZ	2.35	0.40
2:B:150:CYS:N	11:B:1484:CLA:HBC2	2.36	0.40
2:B:290:ALA:O	2:B:294:SER:HB3	2.21	0.40
3:C:67:MET:O	3:C:68:THR:C	2.59	0.40
4:D:335:PRO:C	4:D:337:GLU:N	2.74	0.40
4:D:56:THR:CG2	5:E:49:THR:HG22	2.51	0.40
1:G:142:TRP:HH2	1:G:273:PHE:CE1	2.38	0.40
2:H:18:ARG:HH21	2:H:118:TRP:HE3	1.69	0.40
2:H:193:TYR:CD1	2:H:260:SER:CB	3.03	0.40
2:H:347:ARG:CB	2:H:398:THR:CB	2.95	0.40
2:H:416:THR:O	2:H:420:TYR:HB2	2.21	0.40
3:I:185:LEU:O	3:I:186:TYR:O	2.38	0.40
3:I:189:TRP:C	3:I:190:ALA:O	2.58	0.40
4:J:56:THR:H	5:K:49:THR:HG22	1.86	0.40
7:O:88:UNK:CB	7:O:140:UNK:O	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:159:UNK:C	7:P:161:UNK:N	2.81	0.40
1:A:110:GLY:N	1:A:111:PRO:CD	2.85	0.40
1:A:12:ASN:C	1:A:14:TRP:N	2.75	0.40
11:B:1483:CLA:H41	11:B:1483:CLA:H62	1.92	0.40
2:B:346:PHE:O	2:B:354:LEU:CB	2.68	0.40
3:C:297:TYR:CD1	3:C:302:TYR:CZ	3.05	0.40
5:E:78:THR:O	5:E:79:PHE:C	2.57	0.40
11:G:1344:CLA:HED1	4:J:179:PHE:CZ	2.56	0.40
1:G:87:ASN:O	1:G:87:ASN:ND2	2.55	0.40
2:H:468:TRP:CD1	4:J:144:ILE:CD1	3.02	0.40
3:I:138:GLU:C	3:I:139:THR:CA	2.90	0.40
3:I:265:ILE:N	3:I:274:TYR:OH	2.47	0.40
3:I:275:SER:HA	3:I:278:ALA:HB2	2.03	0.40
4:J:91:LEU:HD13	4:J:93:TRP:CZ3	2.56	0.40
9:T:53:ASP:OD1	9:T:53:ASP:C	2.59	0.40
10:Y:168:UNK:C	10:Y:170:UNK:N	2.82	0.40
1:A:119:PHE:O	1:A:120:LEU:C	2.57	0.40
1:A:316:THR:O	1:A:318:ALA:N	2.55	0.40
2:B:156:PHE:CB	11:B:1487:CLA:HAC1	2.51	0.40
2:B:237:VAL:HG22	11:B:1491:CLA:C3C	2.50	0.40
2:B:386:ALA:O	2:B:387:GLU:C	2.60	0.40
1:A:254:TYR:CE2	4:D:133:ALA:HB2	2.56	0.40
11:D:1351:CLA:HAB	11:D:1351:CLA:HMB1	1.85	0.40
1:G:112:TYR:OH	1:G:116:ILE:HD11	2.20	0.40
1:G:180:PHE:CD2	4:J:192:THR:CG2	3.04	0.40
1:G:326:LEU:O	1:G:328:MET:N	2.53	0.40
2:H:407:ASN:O	2:H:408:GLY:C	2.60	0.40
2:H:99:ALA:O	2:H:103:LEU:HG	2.21	0.40
3:I:170:ILE:O	3:I:171:GLY:C	2.59	0.40
4:J:92:LEU:HA	4:J:104:TRP:CD1	2.56	0.40
4:J:127:LEU:O	4:J:129:GLN:N	2.54	0.40
4:J:185:PHE:O	4:J:186:GLN:C	2.59	0.40
4:J:335:PRO:O	4:J:337:GLU:N	2.54	0.40
8:U:27:UNK:C	8:U:28:UNK:O	2.70	0.40
8:U:1:UNK:C	8:U:3:UNK:N	2.85	0.40
10:X:507:UNK:O	10:X:508:UNK:C	2.69	0.40
10:Y:434:UNK:O	10:Y:435:UNK:C	2.70	0.40
11:A:1343:CLA:H143	11:A:1343:CLA:H112	1.93	0.40
1:A:161:TYR:CE2	1:A:186:PHE:CE1	3.05	0.40
1:A:172:MET:N	1:A:182:PHE:CD1	2.83	0.40
1:A:283:VAL:O	1:A:284:TRP:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:TRP:N	4:D:63:LEU:HD23	2.37	0.40
11:B:1486:CLA:HBB1	11:B:1486:CLA:HMB1	2.03	0.40
2:B:174:LEU:HD11	2:B:309:LEU:HD21	2.02	0.40
2:B:97:ALA:O	2:B:98:LEU:C	2.59	0.40
4:D:78:VAL:HG12	4:D:78:VAL:O	2.20	0.40
5:E:61:ARG:O	5:E:62:SER:HB2	2.22	0.40
1:G:157:VAL:C	1:G:158:PHE:CD2	2.95	0.40
1:G:317:TRP:CE3	1:G:320:ILE:HD12	2.56	0.40
11:H:1482:CLA:H61	11:H:1482:CLA:H41	1.91	0.40
2:H:464:PHE:HE1	4:J:144:ILE:HG23	1.86	0.40
3:I:244:CYS:HB3	11:I:1465:CLA:H93	2.02	0.40
3:I:376:ASP:O	3:I:377:LEU:C	2.60	0.40
4:J:136:VAL:CG1	4:J:136:VAL:O	2.69	0.40
6:L:18:VAL:O	6:L:21:VAL:HB	2.21	0.40
3:I:320:ARG:HD2	9:T:49:ASN:CG	2.42	0.40
9:V:63:THR:O	9:V:84:GLY:HA3	2.22	0.40
10:X:534:UNK:O	10:X:535:UNK:C	2.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	295/360 (82%)	188 (64%)	67 (23%)	40 (14%)	0 1
1	G	295/360 (82%)	184 (62%)	71 (24%)	40 (14%)	0 1
2	B	399/510 (78%)	244 (61%)	94 (24%)	61 (15%)	0 1
2	H	399/510 (78%)	246 (62%)	94 (24%)	59 (15%)	0 1
3	C	353/473 (75%)	205 (58%)	96 (27%)	52 (15%)	0 1
3	I	353/473 (75%)	206 (58%)	99 (28%)	48 (14%)	0 1
4	D	348/352 (99%)	223 (64%)	76 (22%)	49 (14%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	J	348/352 (99%)	222 (64%)	79 (23%)	47 (14%)	0 1
5	E	67/84 (80%)	40 (60%)	13 (19%)	14 (21%)	0 0
5	K	67/84 (80%)	43 (64%)	10 (15%)	14 (21%)	0 0
6	F	35/44 (80%)	24 (69%)	4 (11%)	7 (20%)	0 0
6	L	35/44 (80%)	22 (63%)	6 (17%)	7 (20%)	0 0
9	T	134/163 (82%)	121 (90%)	11 (8%)	2 (2%)	10 44
9	V	134/163 (82%)	124 (92%)	8 (6%)	2 (2%)	10 44
All	All	3262/3972 (82%)	2092 (64%)	728 (22%)	442 (14%)	0 1

All (442) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	12	ASN
1	A	63	ILE
1	A	80	GLY
1	A	85	SER
1	A	95	PRO
1	A	139	MET
1	A	141	PRO
1	A	142	TRP
1	A	172	MET
1	A	248	ILE
1	A	249	VAL
1	A	260	PHE
1	A	267	ASN
1	A	308	ASP
1	A	315	ASN
1	A	316	THR
1	A	332	HIS
2	B	46	ASP
2	B	62	VAL
2	B	93	PHE
2	B	133	LEU
2	B	134	ASP
2	B	135	LEU
2	B	163	GLY
2	B	171	PRO
2	B	175	THR
2	B	198	VAL

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Mol	Chain	Res	Type
2	B	230	ARG
2	B	234	ILE
2	B	269	GLY
2	B	314	TYR
2	B	339	ALA
2	B	353	GLU
2	B	354	LEU
2	B	395	GLN
2	B	404	GLY
2	B	405	GLU
2	B	425	ILE
3	C	22	PHE
3	C	25	ASN
3	C	26	ARG
3	C	46	SER
3	C	107	ASP
3	C	135	ARG
3	C	184	GLY
3	C	186	TYR
3	C	227	VAL
3	C	253	LEU
3	C	256	PRO
3	C	295	THR
3	C	364	PRO
3	C	365	TRP
3	C	382	ASN
3	C	383	ASP
4	D	5	ILE
4	D	8	ALA
4	D	10	ALA
4	D	11	GLU
4	D	15	PHE
4	D	16	ASP
4	D	40	CYS
4	D	58	TRP
4	D	73	PHE
4	D	96	GLU
4	D	166	SER
4	D	218	VAL
4	D	222	LEU
4	D	230	SER
4	D	239	GLN

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Mol	Chain	Res	Type
4	D	241	GLU
4	D	297	ASP
4	D	330	ALA
4	D	331	PRO
4	D	346	LEU
4	D	347	PRO
5	E	9	PRO
5	E	10	PHE
5	E	17	VAL
5	E	57	ALA
5	E	59	GLU
5	E	60	GLN
5	E	62	SER
6	F	13	TYR
6	F	14	PRO
6	F	15	ILE
1	G	11	ALA
1	G	12	ASN
1	G	63	ILE
1	G	80	GLY
1	G	85	SER
1	G	95	PRO
1	G	139	MET
1	G	141	PRO
1	G	142	TRP
1	G	182	PHE
1	G	248	ILE
1	G	249	VAL
1	G	260	PHE
1	G	267	ASN
1	G	315	ASN
1	G	316	THR
1	G	332	HIS
2	H	46	ASP
2	H	62	VAL
2	H	93	PHE
2	H	133	LEU
2	H	134	ASP
2	H	135	LEU
2	H	163	GLY
2	H	171	PRO
2	H	175	THR

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Mol	Chain	Res	Type
2	H	198	VAL
2	H	230	ARG
2	H	234	ILE
2	H	262	THR
2	H	314	TYR
2	H	339	ALA
2	H	353	GLU
2	H	354	LEU
2	H	395	GLN
2	H	404	GLY
2	H	405	GLU
2	H	406	LEU
2	H	425	ILE
3	I	22	PHE
3	I	25	ASN
3	I	26	ARG
3	I	46	SER
3	I	135	ARG
3	I	184	GLY
3	I	186	TYR
3	I	227	VAL
3	I	253	LEU
3	I	256	PRO
3	I	295	THR
3	I	364	PRO
3	I	365	TRP
3	I	383	ASP
4	J	5	ILE
4	J	8	ALA
4	J	10	ALA
4	J	11	GLU
4	J	16	ASP
4	J	40	CYS
4	J	58	TRP
4	J	73	PHE
4	J	96	GLU
4	J	166	SER
4	J	218	VAL
4	J	222	LEU
4	J	230	SER
4	J	239	GLN
4	J	241	GLU

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Mol	Chain	Res	Type
4	J	330	ALA
4	J	331	PRO
4	J	346	LEU
4	J	347	PRO
5	K	9	PRO
5	K	10	PHE
5	K	17	VAL
5	K	57	ALA
5	K	59	GLU
5	K	60	GLN
5	K	62	SER
6	L	13	TYR
6	L	14	PRO
6	L	15	ILE
1	A	35	VAL
1	A	90	GLY
1	A	108	ASN
1	A	116	ILE
1	A	182	PHE
1	A	185	VAL
1	A	192	ILE
1	A	289	GLY
2	B	76	SER
2	B	139	PHE
2	B	164	PRO
2	B	165	GLY
2	B	196	GLY
2	B	231	MET
2	B	259	GLY
2	B	262	THR
2	B	279	TYR
2	B	294	SER
2	B	331	ASN
2	B	337	ALA
2	B	406	LEU
2	B	408	GLY
2	B	409	GLN
2	B	426	PHE
2	B	437	LEU
2	B	439	SER
2	B	445	THR
3	C	80	PRO

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Mol	Chain	Res	Type
3	C	103	GLY
3	C	117	VAL
3	C	121	SER
3	C	243	ILE
3	C	299	SER
3	C	305	THR
3	C	306	GLY
3	C	361	PHE
3	C	362	ARG
4	D	28	VAL
4	D	92	LEU
4	D	165	SER
4	D	168	PHE
4	D	259	ILE
4	D	299	ILE
4	D	348	ARG
5	E	40	THR
6	F	23	VAL
6	F	34	LEU
1	G	32	TRP
1	G	35	VAL
1	G	90	GLY
1	G	99	ALA
1	G	115	ILE
1	G	116	ILE
1	G	130	GLN
1	G	181	ASN
1	G	192	ILE
1	G	289	GLY
2	H	48	SER
2	H	76	SER
2	H	155	ALA
2	H	162	PHE
2	H	164	PRO
2	H	196	GLY
2	H	231	MET
2	H	259	GLY
2	H	271	THR
2	H	279	TYR
2	H	294	SER
2	H	331	ASN
2	H	337	ALA

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Mol	Chain	Res	Type
2	H	391	SER
2	H	408	GLY
2	H	409	GLN
2	H	426	PHE
2	H	437	LEU
2	H	439	SER
2	H	445	THR
3	I	80	PRO
3	I	103	GLY
3	I	117	VAL
3	I	121	SER
3	I	243	ILE
3	I	252	ILE
3	I	299	SER
3	I	306	GLY
3	I	361	PHE
3	I	362	ARG
3	I	382	ASN
4	J	15	PHE
4	J	28	VAL
4	J	92	LEU
4	J	165	SER
4	J	168	PHE
4	J	259	ILE
4	J	297	ASP
4	J	299	ILE
4	J	343	GLU
4	J	348	ARG
5	K	48	GLY
6	L	34	LEU
1	A	32	TRP
1	A	99	ALA
1	A	115	ILE
1	A	130	GLN
1	A	133	LEU
1	A	167	SER
1	A	181	ASN
2	B	155	ALA
2	B	162	PHE
2	B	220	ARG
2	B	271	THR
2	B	342	GLY

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Mol	Chain	Res	Type
2	B	352	GLU
2	B	373	LYS
2	B	374	ASN
2	B	391	SER
3	C	36	TRP
3	C	57	ALA
3	C	106	VAL
3	C	153	ASP
3	C	257	PHE
3	C	293	ASN
3	C	298	PRO
3	C	375	LEU
3	C	441	HIS
4	D	41	ALA
4	D	94	GLY
4	D	225	ASP
4	D	228	GLY
4	D	336	HIS
4	D	343	GLU
5	E	83	LEU
6	F	27	ALA
1	G	92	HIS
1	G	108	ASN
1	G	133	LEU
1	G	167	SER
1	G	172	MET
1	G	193	LEU
1	G	308	ASP
2	H	139	PHE
2	H	220	ARG
2	H	342	GLY
2	H	352	GLU
2	H	373	LYS
3	I	98	GLY
3	I	257	PHE
3	I	298	PRO
3	I	305	THR
3	I	375	LEU
4	J	13	GLY
4	J	41	ALA
4	J	47	GLY
4	J	94	GLY

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Mol	Chain	Res	Type
5	K	40	THR
9	T	133	GLY
9	V	133	GLY
1	A	193	LEU
1	A	295	PHE
1	A	317	TRP
2	B	48	SER
2	B	177	SER
2	B	319	PRO
2	B	360	PRO
2	B	396	GLY
2	B	473	THR
3	C	29	GLU
3	C	285	ILE
3	C	286	ALA
3	C	294	ASN
4	D	17	ILE
4	D	29	PHE
4	D	47	GLY
4	D	79	SER
4	D	333	ASP
5	E	82	GLN
1	G	185	VAL
2	H	28	ALA
2	H	165	GLY
2	H	177	SER
2	H	319	PRO
2	H	360	PRO
2	H	374	ASN
2	H	396	GLY
3	I	57	ALA
3	I	153	ASP
3	I	441	HIS
4	J	17	ILE
4	J	29	PHE
4	J	228	GLY
4	J	264	LYS
5	K	82	GLN
5	K	83	LEU
9	T	131	GLY
9	V	131	GLY
1	A	135	TYR

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Mol	Chain	Res	Type
1	A	296	ASN
2	B	28	ALA
3	C	78	GLU
3	C	252	ILE
3	C	337	LEU
3	C	386	PRO
4	D	13	GLY
4	D	219	GLU
4	D	240	ALA
4	D	264	LYS
5	E	63	ILE
1	G	295	PHE
1	G	317	TRP
2	H	415	PRO
3	I	29	GLU
3	I	36	TRP
3	I	93	ALA
3	I	102	GLY
3	I	272	LEU
3	I	286	ALA
3	I	294	ASN
3	I	386	PRO
4	J	30	VAL
4	J	79	SER
4	J	89	LEU
4	J	112	THR
4	J	159	ILE
4	J	229	ALA
4	J	252	PHE
5	K	56	TYR
5	K	63	ILE
6	L	27	ALA
2	B	64	PRO
2	B	136	PRO
2	B	415	PRO
3	C	126	GLY
3	C	272	LEU
4	D	30	VAL
4	D	111	TRP
4	D	229	ALA
5	E	52	PRO
5	E	64	PRO

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Mol	Chain	Res	Type
1	G	247	ASN
2	H	64	PRO
3	I	285	ILE
3	I	293	ASN
4	J	214	HIS
4	J	263	ASN
5	K	52	PRO
6	L	23	VAL
1	A	38	ILE
4	D	274	VAL
2	H	399	VAL
6	L	11	VAL
3	C	128	GLY
4	D	159	ILE
6	F	11	VAL
1	G	38	ILE
2	H	136	PRO
2	H	467	ILE
3	I	101	PRO
2	B	467	ILE
3	C	115	GLY
5	E	48	GLY
1	G	96	ILE
3	I	115	GLY
3	I	126	GLY
4	J	160	TYR
1	A	176	ILE
3	C	85	GLY
3	C	98	GLY
3	C	105	VAL
3	C	304	PRO
3	C	368	PRO
4	D	160	TYR
3	I	47	GLY
3	I	85	GLY
2	B	399	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	217/291 (75%)	201 (93%)	16 (7%)	13 46
1	G	217/291 (75%)	200 (92%)	17 (8%)	12 43
2	B	256/407 (63%)	232 (91%)	24 (9%)	8 33
2	H	256/407 (63%)	229 (90%)	27 (10%)	7 28
3	C	243/374 (65%)	213 (88%)	30 (12%)	4 21
3	I	243/374 (65%)	212 (87%)	31 (13%)	4 20
4	D	239/283 (84%)	223 (93%)	16 (7%)	16 50
4	J	239/283 (84%)	225 (94%)	14 (6%)	19 54
5	E	49/73 (67%)	43 (88%)	6 (12%)	5 22
5	K	49/73 (67%)	43 (88%)	6 (12%)	5 22
6	F	31/38 (82%)	27 (87%)	4 (13%)	4 19
6	L	31/38 (82%)	26 (84%)	5 (16%)	2 11
9	T	117/138 (85%)	116 (99%)	1 (1%)	78 91
9	V	117/138 (85%)	116 (99%)	1 (1%)	78 91
All	All	2304/3208 (72%)	2106 (91%)	198 (9%)	10 38

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	TRP
1	A	84	PRO
1	A	87	ASN
1	A	103	ASP
1	A	131	TRP
1	A	139	MET
1	A	143	ILE
1	A	191	ASN
1	A	206	PHE
1	A	210	LEU
1	A	247	ASN
1	A	284	TRP
1	A	296	ASN
1	A	298	ASN
1	A	308	ASP
1	A	322	ASN

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Mol	Chain	Res	Type
2	B	47	PRO
2	B	48	SER
2	B	49	ASP
2	B	55	MET
2	B	64	PRO
2	B	112	CYS
2	B	114	HIS
2	B	136	PRO
2	B	138	MET
2	B	164	PRO
2	B	188	ASP
2	B	221	PRO
2	B	233	ASN
2	B	250	PHE
2	B	251	VAL
2	B	270	PRO
2	B	357	ARG
2	B	359	MET
2	B	405	GLU
2	B	407	ASN
2	B	410	THR
2	B	412	THR
2	B	413	ASP
2	B	415	PRO
3	C	77	PRO
3	C	78	GLU
3	C	97	TRP
3	C	110	PRO
3	C	137	PRO
3	C	157	MET
3	C	161	LEU
3	C	163	PHE
3	C	168	LEU
3	C	178	LYS
3	C	230	LEU
3	C	232	ASP
3	C	251	HIS
3	C	256	PRO
3	C	257	PHE
3	C	266	TRP
3	C	269	GLU
3	C	276	LEU

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Mol	Chain	Res	Type
3	C	289	PHE
3	C	298	PRO
3	C	305	THR
3	C	318	LEU
3	C	364	PRO
3	C	368	PRO
3	C	419	PHE
3	C	424	SER
3	C	428	THR
3	C	429	SER
3	C	444	HIS
3	C	449	ARG
4	D	81	PRO
4	D	85	MET
4	D	93	TRP
4	D	95	PRO
4	D	101	PHE
4	D	180	ARG
4	D	186	GLN
4	D	191	TRP
4	D	196	PHE
4	D	235	PHE
4	D	244	TYR
4	D	298	PHE
4	D	331	PRO
4	D	335	PRO
4	D	337	GLU
4	D	342	PRO
5	E	8	ARG
5	E	9	PRO
5	E	19	TYR
5	E	28	PRO
5	E	52	PRO
5	E	64	PRO
6	F	11	VAL
6	F	14	PRO
6	F	29	PRO
6	F	44	GLN
1	G	32	TRP
1	G	75	ASN
1	G	84	PRO
1	G	87	ASN

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Mol	Chain	Res	Type
1	G	103	ASP
1	G	131	TRP
1	G	139	MET
1	G	143	ILE
1	G	173	PRO
1	G	191	ASN
1	G	206	PHE
1	G	210	LEU
1	G	284	TRP
1	G	296	ASN
1	G	298	ASN
1	G	308	ASP
1	G	322	ASN
2	H	47	PRO
2	H	48	SER
2	H	49	ASP
2	H	55	MET
2	H	61	PHE
2	H	64	PRO
2	H	102	VAL
2	H	112	CYS
2	H	114	HIS
2	H	136	PRO
2	H	138	MET
2	H	164	PRO
2	H	188	ASP
2	H	233	ASN
2	H	250	PHE
2	H	251	VAL
2	H	264	PRO
2	H	265	ILE
2	H	270	PRO
2	H	357	ARG
2	H	405	GLU
2	H	407	ASN
2	H	410	THR
2	H	412	THR
2	H	413	ASP
2	H	415	PRO
2	H	447	PRO
3	I	77	PRO
3	I	78	GLU

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Mol	Chain	Res	Type
3	I	97	TRP
3	I	108	THR
3	I	122	SER
3	I	137	PRO
3	I	157	MET
3	I	158	THR
3	I	161	LEU
3	I	163	PHE
3	I	168	LEU
3	I	178	LYS
3	I	230	LEU
3	I	232	ASP
3	I	251	HIS
3	I	256	PRO
3	I	257	PHE
3	I	266	TRP
3	I	269	GLU
3	I	276	LEU
3	I	289	PHE
3	I	298	PRO
3	I	305	THR
3	I	318	LEU
3	I	368	PRO
3	I	419	PHE
3	I	424	SER
3	I	428	THR
3	I	429	SER
3	I	444	HIS
3	I	449	ARG
4	J	93	TRP
4	J	95	PRO
4	J	101	PHE
4	J	165	SER
4	J	171	PRO
4	J	180	ARG
4	J	186	GLN
4	J	191	TRP
4	J	235	PHE
4	J	244	TYR
4	J	298	PHE
4	J	331	PRO
4	J	337	GLU

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Mol	Chain	Res	Type
4	J	342	PRO
5	K	8	ARG
5	K	9	PRO
5	K	19	TYR
5	K	28	PRO
5	K	52	PRO
5	K	64	PRO
6	L	10	PRO
6	L	11	VAL
6	L	14	PRO
6	L	29	PRO
6	L	44	GLN
9	T	50	PRO
9	V	50	PRO

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

Mol	Chain	Res	Type
1	A	87	ASN
1	A	108	ASN
1	A	118	HIS
1	A	195	HIS
1	A	296	ASN
1	A	322	ASN
1	A	332	HIS
2	B	157	HIS
2	B	233	ASN
3	C	74	HIS
3	C	91	HIS
3	C	229	ASN
3	C	322	GLN
3	C	398	HIS
4	D	61	HIS
4	D	72	ASN
4	D	87	HIS
4	D	129	GLN
4	D	164	GLN
4	D	186	GLN
4	D	220	ASN
4	D	224	GLN
4	D	336	HIS
5	E	58	GLN

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Mol	Chain	Res	Type
6	F	41	GLN
1	G	75	ASN
1	G	87	ASN
1	G	108	ASN
1	G	118	HIS
1	G	195	HIS
1	G	267	ASN
1	G	296	ASN
1	G	322	ASN
2	H	157	HIS
2	H	233	ASN
2	H	289	GLN
3	I	74	HIS
3	I	91	HIS
3	I	132	HIS
3	I	229	ASN
3	I	322	GLN
3	I	398	HIS
4	J	61	HIS
4	J	72	ASN
4	J	87	HIS
4	J	129	GLN
4	J	164	GLN
4	J	186	GLN
4	J	220	ASN
4	J	224	GLN
4	J	255	GLN
4	J	336	HIS
5	K	58	GLN
6	L	41	GLN
9	T	106	ASN
9	T	118	HIS
9	V	106	ASN
9	V	118	HIS

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 92 ligands modelled in this entry, 10 are monoatomic - leaving 82 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	$\#\|Z\| > 2$
17	BCR	L	1047	-	41,41,41	1.64	7 (17%)	56,56,56	2.16	22 (39%)
15	PL9	D	1354	-	6,6,55	2.17	2 (33%)	6,6,69	1.00	0
11	CLA	C	1471	-	35,49,73	1.88	8 (22%)	38,84,113	2.50	7 (18%)
11	CLA	I	1465	-	59,73,73	1.26	7 (11%)	67,113,113	2.00	16 (23%)
11	CLA	C	1463	3	49,63,73	1.82	10 (20%)	55,101,113	2.28	12 (21%)
11	CLA	J	1353	4	44,58,73	1.55	8 (18%)	49,95,113	2.19	13 (26%)
18	HEC	T	1138	9	26,50,50	2.21	11 (42%)	18,82,82	2.39	3 (16%)
11	CLA	A	1342	1	59,73,73	1.34	7 (11%)	67,113,113	2.04	15 (22%)
11	CLA	B	1487	-	59,73,73	1.65	10 (16%)	67,113,113	1.92	15 (22%)
11	CLA	H	1495	-	49,63,73	1.55	9 (18%)	55,101,113	2.42	13 (23%)
11	CLA	B	1486	2	35,49,73	1.68	8 (22%)	38,84,113	2.56	11 (28%)
11	CLA	G	1346	-	45,59,73	1.78	10 (22%)	50,96,113	2.25	14 (28%)
11	CLA	C	1468	3	23,35,73	3.85	11 (47%)	26,60,113	2.92	6 (23%)
11	CLA	G	1342	1	59,73,73	1.45	9 (15%)	67,113,113	1.89	12 (17%)
11	CLA	C	1466	3	44,58,73	1.67	7 (15%)	49,95,113	2.33	12 (24%)
11	CLA	C	1469	3	35,49,73	1.68	7 (20%)	38,84,113	2.62	9 (23%)
11	CLA	I	1471	-	35,49,73	1.87	7 (20%)	38,84,113	2.52	8 (21%)
12	PHO	J	1352	-	57,59,69	1.21	5 (8%)	73,87,99	1.58	14 (19%)
12	PHO	D	1352	-	57,59,69	1.19	4 (7%)	73,87,99	1.64	13 (17%)
11	CLA	I	1461	3	23,35,73	3.78	12 (52%)	26,60,113	2.84	6 (23%)
11	CLA	B	1489	2	44,58,73	1.42	7 (15%)	49,95,113	2.33	10 (20%)
11	CLA	H	1491	-	23,35,73	3.38	13 (56%)	26,60,113	2.77	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	H	1487	-	59,73,73	1.63	9 (15%)	67,113,113	1.94	14 (20%)
11	CLA	B	1497	2	35,49,73	1.59	9 (25%)	38,84,113	2.53	11 (28%)
11	CLA	C	1464	3	50,64,73	1.49	9 (18%)	56,102,113	2.22	14 (25%)
11	CLA	H	1482	-	59,73,73	1.68	11 (18%)	67,113,113	2.19	13 (19%)
11	CLA	B	1482	-	59,73,73	1.52	11 (18%)	67,113,113	2.16	12 (17%)
11	CLA	H	1488	-	59,73,73	1.56	10 (16%)	67,113,113	1.94	10 (14%)
16	HEM	L	1046	5,6	12,32,50	2.68	7 (58%)	23,54,82	2.07	6 (26%)
11	CLA	I	1464	3	50,64,73	1.47	10 (20%)	56,102,113	2.17	12 (21%)
11	CLA	C	1461	3	23,35,73	3.87	11 (47%)	26,60,113	2.88	6 (23%)
11	CLA	H	1492	2	59,73,73	1.36	7 (11%)	67,113,113	2.16	13 (19%)
11	CLA	C	1460	3	41,55,73	1.73	7 (17%)	45,91,113	2.36	10 (22%)
11	CLA	I	1460	3	41,55,73	1.70	10 (24%)	45,91,113	2.25	8 (17%)
11	CLA	H	1493	-	36,53,73	1.67	7 (19%)	39,89,113	2.52	9 (23%)
11	CLA	H	1485	2	41,55,73	1.31	7 (17%)	45,91,113	2.09	9 (20%)
11	CLA	I	1469	3	35,49,73	1.86	6 (17%)	38,84,113	2.66	8 (21%)
11	CLA	B	1492	2	59,73,73	1.34	7 (11%)	67,113,113	2.19	14 (20%)
11	CLA	H	1484	-	36,53,73	1.40	5 (13%)	39,89,113	2.25	8 (20%)
11	CLA	C	1462	-	50,64,73	1.62	11 (22%)	56,102,113	2.10	15 (26%)
11	CLA	I	1470	-	35,49,73	1.72	6 (17%)	38,84,113	2.47	10 (26%)
11	CLA	I	1466	3	44,58,73	1.75	7 (15%)	49,95,113	2.32	11 (22%)
11	CLA	C	1467	3	41,55,73	1.67	5 (12%)	45,91,113	2.35	10 (22%)
11	CLA	I	1467	3	41,55,73	1.56	5 (12%)	45,91,113	2.34	11 (24%)
11	CLA	I	1462	-	50,64,73	1.72	11 (22%)	56,102,113	2.10	15 (26%)
11	CLA	B	1485	2	41,55,73	1.33	6 (14%)	45,91,113	2.12	8 (17%)
11	CLA	A	1344	-	36,53,73	1.76	5 (13%)	39,89,113	2.43	9 (23%)
11	CLA	B	1490	2	36,53,73	2.38	10 (27%)	39,89,113	2.38	10 (25%)
11	CLA	C	1470	-	35,49,73	1.72	7 (20%)	38,84,113	2.58	9 (23%)
11	CLA	G	1343	-	55,69,73	1.36	7 (12%)	62,108,113	2.21	12 (19%)
11	CLA	C	1465	-	59,73,73	1.25	6 (10%)	67,113,113	2.01	14 (20%)
11	CLA	B	1494	-	59,73,73	1.33	8 (13%)	67,113,113	1.97	11 (16%)
11	CLA	H	1486	2	35,49,73	1.57	6 (17%)	38,84,113	2.49	10 (26%)
16	HEM	E	1085	5,6	12,32,50	2.97	8 (66%)	23,54,82	2.06	8 (34%)
11	CLA	B	1495	-	49,63,73	1.52	10 (20%)	55,101,113	2.37	15 (27%)
11	CLA	I	1463	3	49,63,73	1.88	8 (16%)	55,101,113	2.33	13 (23%)
17	BCR	F	1046	-	41,41,41	1.70	8 (19%)	56,56,56	2.16	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	B	1491	-	23,35,73	3.18	10 (43%)	26,60,113	2.90	5 (19%)
11	CLA	H	1489	2	44,58,73	1.48	6 (13%)	49,95,113	2.47	11 (22%)
11	CLA	B	1483	2	54,68,73	1.41	5 (9%)	61,107,113	1.97	12 (19%)
11	CLA	G	1344	-	36,53,73	1.73	6 (16%)	39,89,113	2.42	11 (28%)
11	CLA	H	1490	2	36,53,73	2.29	10 (27%)	39,89,113	2.48	9 (23%)
11	CLA	H	1483	2	54,68,73	1.42	8 (14%)	61,107,113	1.90	11 (18%)
12	PHO	G	1345	-	67,69,69	0.96	3 (4%)	85,99,99	1.51	15 (17%)
11	CLA	B	1496	-	59,73,73	1.36	6 (10%)	67,113,113	2.05	15 (22%)
11	CLA	B	1493	-	36,53,73	1.69	5 (13%)	39,89,113	2.50	10 (25%)
11	CLA	D	1353	4	44,58,73	1.60	9 (20%)	49,95,113	2.27	13 (26%)
15	PL9	J	1354	-	6,6,55	2.06	2 (33%)	6,6,69	1.03	0
11	CLA	B	1484	-	36,53,73	1.51	7 (19%)	39,89,113	2.33	9 (23%)
11	CLA	A	1343	-	55,69,73	1.22	4 (7%)	62,108,113	2.13	12 (19%)
11	CLA	B	1488	-	59,73,73	1.50	10 (16%)	67,113,113	1.98	14 (20%)
11	CLA	I	1468	3	23,35,73	3.78	10 (43%)	26,60,113	2.86	6 (23%)
18	HEC	V	1138	9	26,50,50	2.18	7 (26%)	18,82,82	2.35	4 (22%)
11	CLA	C	1459	3	36,53,73	1.74	8 (22%)	39,89,113	2.27	9 (23%)
12	PHO	A	1345	-	67,69,69	0.99	3 (4%)	85,99,99	1.47	13 (15%)
11	CLA	A	1346	-	45,59,73	1.70	8 (17%)	50,96,113	2.33	14 (28%)
11	CLA	D	1351	4	59,73,73	1.63	9 (15%)	67,113,113	2.28	16 (23%)
11	CLA	I	1459	3	36,53,73	1.70	7 (19%)	39,89,113	2.42	8 (20%)
11	CLA	H	1496	-	59,73,73	1.30	9 (15%)	67,113,113	2.14	14 (20%)
11	CLA	H	1494	-	59,73,73	1.36	7 (11%)	67,113,113	2.14	13 (19%)
11	CLA	J	1351	4	59,73,73	2.19	8 (13%)	67,113,113	2.32	16 (23%)
11	CLA	H	1497	2	35,49,73	1.72	11 (31%)	38,84,113	2.61	11 (28%)

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
11	CLA	I	1465	-	3/3/20/25	13/37/135/135	-
15	PL9	D	1354	-	-	-	0/1/1/1
11	CLA	C	1471	-	3/3/15/25	5/8/106/135	-
17	BCR	L	1047	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	C	1463	3	3/3/18/25	9/25/123/135	-
18	HEC	V	1138	9	-	0/6/54/54	-
11	CLA	J	1353	4	3/3/17/25	4/19/117/135	-
18	HEC	T	1138	9	-	0/6/54/54	-
11	CLA	A	1342	1	3/3/20/25	4/37/135/135	-
11	CLA	B	1487	-	3/3/20/25	8/37/135/135	-
11	CLA	H	1495	-	3/3/18/25	9/25/123/135	-
11	CLA	B	1486	2	3/3/15/25	5/8/106/135	-
11	CLA	G	1346	-	3/3/17/25	5/21/119/135	-
12	PHO	J	1352	-	-	10/41/91/103	0/5/6/6
11	CLA	C	1468	3	3/3/8/25	-	-
11	CLA	G	1342	1	1/1/20/25	4/37/135/135	-
11	CLA	C	1466	3	3/3/17/25	7/19/117/135	-
11	CLA	C	1469	3	3/3/15/25	2/8/106/135	-
11	CLA	I	1471	-	3/3/15/25	5/8/106/135	-
11	CLA	B	1485	2	3/3/16/25	9/16/114/135	-
12	PHO	D	1352	-	-	10/41/91/103	0/5/6/6
11	CLA	I	1461	3	3/3/8/25	-	-
11	CLA	B	1489	2	3/3/17/25	4/19/117/135	-
11	CLA	H	1491	-	3/3/8/25	-	-
11	CLA	H	1487	-	3/3/20/25	8/37/135/135	-
11	CLA	B	1497	2	3/3/15/25	4/8/106/135	-
11	CLA	C	1464	3	3/3/18/25	12/27/125/135	-
11	CLA	H	1482	-	3/3/20/25	13/37/135/135	-
11	CLA	B	1482	-	3/3/20/25	12/37/135/135	-
11	CLA	C	1460	3	3/3/16/25	3/16/114/135	-
11	CLA	I	1464	3	3/3/18/25	12/27/125/135	-
11	CLA	C	1461	3	3/3/8/25	-	-
11	CLA	H	1492	2	3/3/20/25	12/37/135/135	-
11	CLA	I	1460	3	3/3/16/25	4/16/114/135	-
11	CLA	H	1493	-	3/3/16/25	5/11/111/135	-
11	CLA	H	1485	2	3/3/16/25	9/16/114/135	-
11	CLA	I	1469	3	3/3/15/25	2/8/106/135	-
11	CLA	B	1492	2	3/3/20/25	12/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	H	1484	-	3/3/16/25	3/11/111/135	-
11	CLA	C	1462	-	3/3/18/25	6/27/125/135	-
11	CLA	I	1470	-	3/3/15/25	3/8/106/135	-
11	CLA	I	1466	3	3/3/17/25	7/19/117/135	-
11	CLA	C	1467	3	3/3/16/25	7/16/114/135	-
11	CLA	I	1467	3	3/3/16/25	8/16/114/135	-
11	CLA	I	1462	-	3/3/18/25	6/27/125/135	-
11	CLA	A	1344	-	3/3/16/25	6/11/111/135	-
11	CLA	I	1463	3	3/3/18/25	7/25/123/135	-
11	CLA	B	1490	2	1/1/16/25	7/11/111/135	-
11	CLA	C	1470	-	3/3/15/25	3/8/106/135	-
11	CLA	G	1343	-	3/3/19/25	17/33/131/135	-
11	CLA	C	1465	-	3/3/20/25	14/37/135/135	-
11	CLA	B	1494	-	3/3/20/25	9/37/135/135	-
11	CLA	H	1486	2	3/3/15/25	5/8/106/135	-
11	CLA	B	1495	-	3/3/18/25	9/25/123/135	-
17	BCR	F	1046	-	-	3/29/63/63	0/2/2/2
11	CLA	B	1491	-	3/3/8/25	-	-
11	CLA	H	1489	2	3/3/17/25	4/19/117/135	-
11	CLA	B	1483	2	3/3/19/25	12/31/129/135	-
11	CLA	G	1344	-	3/3/16/25	6/11/111/135	-
11	CLA	H	1490	2	1/1/16/25	7/11/111/135	-
11	CLA	H	1483	2	3/3/19/25	12/31/129/135	-
12	PHO	G	1345	-	-	16/53/103/103	0/5/6/6
11	CLA	B	1496	-	3/3/20/25	17/37/135/135	-
11	CLA	B	1493	-	3/3/16/25	5/11/111/135	-
11	CLA	D	1353	4	3/3/17/25	4/19/117/135	-
15	PL9	J	1354	-	-	-	0/1/1/1
11	CLA	B	1484	-	3/3/16/25	3/11/111/135	-
11	CLA	A	1343	-	3/3/19/25	16/33/131/135	-
11	CLA	B	1488	-	3/3/20/25	15/37/135/135	-
11	CLA	I	1468	3	3/3/8/25	-	-
11	CLA	H	1488	-	3/3/20/25	15/37/135/135	-
11	CLA	C	1459	3	3/3/16/25	6/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PHO	A	1345	-	-	15/53/103/103	0/5/6/6
11	CLA	A	1346	-	3/3/17/25	4/21/119/135	-
11	CLA	D	1351	4	1/1/20/25	12/37/135/135	-
11	CLA	I	1459	3	3/3/16/25	5/11/111/135	-
11	CLA	H	1496	-	3/3/20/25	15/37/135/135	-
11	CLA	H	1494	-	3/3/20/25	10/37/135/135	-
11	CLA	J	1351	4	1/1/20/25	12/37/135/135	-
11	CLA	H	1497	2	3/3/15/25	4/8/106/135	-

All (634) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	J	1351	CLA	MG-NA	13.61	2.38	2.06
11	I	1468	CLA	CHB-C4A	12.51	1.44	1.34
11	C	1468	CLA	CHB-C4A	12.17	1.44	1.34
11	C	1461	CLA	CHB-C4A	10.41	1.42	1.34
11	I	1461	CLA	CHB-C4A	10.32	1.42	1.34
11	H	1490	CLA	MG-NA	9.48	2.28	2.06
11	B	1490	CLA	MG-NA	9.35	2.28	2.06
11	I	1463	CLA	MG-NA	9.33	2.28	2.06
11	C	1461	CLA	MG-NA	8.23	2.25	2.06
11	C	1463	CLA	MG-NA	7.88	2.25	2.06
11	C	1467	CLA	MG-NA	7.62	2.24	2.06
11	B	1491	CLA	CHB-C4A	7.50	1.40	1.34
11	H	1491	CLA	CHB-C4A	7.47	1.40	1.34
11	I	1461	CLA	MG-NA	7.22	2.23	2.06
11	I	1469	CLA	MG-NA	7.21	2.23	2.06
11	C	1460	CLA	MG-NA	6.91	2.22	2.06
11	G	1346	CLA	MG-NA	6.78	2.22	2.06
11	B	1493	CLA	MG-NA	6.68	2.22	2.06
11	I	1471	CLA	MG-NA	6.47	2.21	2.06
11	H	1482	CLA	MG-NA	6.44	2.21	2.06
11	C	1468	CLA	MG-NA	6.42	2.21	2.06
11	H	1491	CLA	CAD-C3D	-6.29	1.41	1.51
11	D	1351	CLA	MG-NA	6.26	2.21	2.06
11	I	1468	CLA	MG-NA	6.17	2.20	2.06
11	B	1491	CLA	CAD-C3D	-6.17	1.41	1.51
11	I	1466	CLA	MG-NA	6.12	2.20	2.06
11	H	1493	CLA	MG-NA	6.06	2.20	2.06
18	T	1138	HEC	CBB-CAB	-6.02	1.26	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1461	CLA	C4B-NB	6.02	1.40	1.35
18	V	1138	HEC	CBB-CAB	-5.95	1.27	1.49
11	I	1461	CLA	C4B-NB	5.95	1.40	1.35
11	C	1466	CLA	MG-NA	5.94	2.20	2.06
11	I	1467	CLA	MG-NA	5.94	2.20	2.06
11	C	1471	CLA	MG-NA	5.92	2.20	2.06
11	C	1468	CLA	C4B-NB	5.87	1.40	1.35
16	L	1046	HEM	C2A-C1A	5.85	1.50	1.39
11	I	1459	CLA	MG-NA	5.83	2.20	2.06
11	A	1346	CLA	MG-NA	5.81	2.20	2.06
11	H	1489	CLA	MG-NA	5.81	2.20	2.06
16	E	1085	HEM	C2A-C1A	5.76	1.50	1.39
11	I	1460	CLA	MG-NA	5.72	2.19	2.06
11	C	1470	CLA	MG-NA	5.70	2.19	2.06
11	A	1342	CLA	MG-NA	5.62	2.19	2.06
11	C	1469	CLA	MG-NA	5.55	2.19	2.06
11	A	1344	CLA	MG-NA	5.45	2.19	2.06
11	B	1491	CLA	MG-NA	5.43	2.19	2.06
11	G	1344	CLA	MG-NA	5.38	2.19	2.06
11	B	1487	CLA	MG-NA	5.33	2.18	2.06
11	C	1459	CLA	C4B-NB	5.25	1.39	1.35
11	B	1486	CLA	MG-NA	5.20	2.18	2.06
11	A	1344	CLA	CAA-C2A	5.20	1.63	1.54
11	H	1487	CLA	MG-NA	5.12	2.18	2.06
11	B	1483	CLA	MG-NA	5.08	2.18	2.06
11	H	1495	CLA	MG-NA	5.07	2.18	2.06
11	H	1491	CLA	MG-NA	5.07	2.18	2.06
11	I	1470	CLA	MG-NA	5.07	2.18	2.06
11	B	1491	CLA	C3B-C4B	5.06	1.48	1.39
11	B	1496	CLA	C4B-NB	5.04	1.39	1.35
11	H	1491	CLA	C1B-CHB	-5.03	1.33	1.43
11	C	1461	CLA	C1B-CHB	-5.02	1.33	1.43
11	H	1491	CLA	C3B-C4B	4.99	1.48	1.39
11	C	1461	CLA	C3B-C4B	4.99	1.48	1.39
11	D	1351	CLA	MG-NC	4.97	2.18	2.06
11	I	1468	CLA	CAD-C3D	-4.97	1.43	1.51
11	H	1492	CLA	C4B-NB	4.93	1.39	1.35
17	F	1046	BCR	C1-C6	4.92	1.60	1.53
11	B	1489	CLA	MG-NA	4.91	2.17	2.06
11	C	1468	CLA	C2B-C1B	4.88	1.48	1.39
11	G	1342	CLA	MG-NA	4.85	2.17	2.06
11	I	1461	CLA	C1B-CHB	-4.85	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	E	1085	HEM	C3B-C4B	4.84	1.48	1.39
11	I	1469	CLA	C1B-NB	4.82	1.39	1.35
11	B	1490	CLA	C1B-NB	4.73	1.39	1.35
11	I	1462	CLA	CAA-C2A	4.73	1.62	1.54
11	C	1464	CLA	MG-NA	4.72	2.17	2.06
11	C	1468	CLA	CAD-C3D	-4.71	1.43	1.51
11	H	1491	CLA	C4B-NB	4.71	1.39	1.35
11	H	1488	CLA	MG-NA	4.69	2.17	2.06
11	B	1495	CLA	MG-NA	4.69	2.17	2.06
11	B	1487	CLA	CAA-C2A	4.62	1.62	1.54
11	D	1351	CLA	C4B-NB	4.61	1.39	1.35
11	B	1484	CLA	C4B-NB	4.60	1.39	1.35
11	B	1491	CLA	C2B-C1B	4.59	1.48	1.39
11	C	1461	CLA	CAD-C3D	-4.59	1.44	1.51
11	H	1487	CLA	CAA-C2A	4.58	1.62	1.54
11	I	1468	CLA	C1B-CHB	-4.55	1.34	1.43
11	I	1468	CLA	C4B-NB	4.54	1.39	1.35
11	G	1343	CLA	CAA-C2A	4.53	1.62	1.54
11	H	1492	CLA	MG-NA	4.52	2.17	2.06
11	I	1461	CLA	CAD-C3D	-4.52	1.44	1.51
11	I	1470	CLA	C4B-NB	4.48	1.39	1.35
11	C	1461	CLA	C2B-C1B	4.46	1.47	1.39
11	B	1488	CLA	CAA-C2A	4.44	1.62	1.54
11	B	1482	CLA	C4B-NB	4.42	1.39	1.35
18	V	1138	HEC	C3C-C2C	-4.41	1.36	1.40
11	C	1462	CLA	CAA-C2A	4.40	1.62	1.54
11	H	1490	CLA	C1B-NB	4.39	1.39	1.35
11	I	1461	CLA	C3B-C4B	4.38	1.47	1.39
11	B	1491	CLA	C1B-CHB	-4.36	1.35	1.43
11	B	1488	CLA	MG-NA	4.34	2.16	2.06
11	C	1471	CLA	C4B-NB	4.33	1.39	1.35
11	B	1487	CLA	C1B-CHB	-4.32	1.29	1.41
16	E	1085	HEM	C3A-C4A	4.30	1.47	1.39
11	D	1353	CLA	MG-NA	4.28	2.16	2.06
11	C	1466	CLA	CAA-C2A	4.26	1.62	1.54
11	B	1482	CLA	CAA-C2A	4.24	1.62	1.54
11	C	1468	CLA	C3B-C4B	4.23	1.47	1.39
11	H	1491	CLA	C2B-C1B	4.23	1.47	1.39
11	J	1351	CLA	C4B-NB	4.22	1.39	1.35
11	H	1487	CLA	C1B-CHB	-4.21	1.29	1.41
11	B	1492	CLA	MG-NA	4.21	2.16	2.06
11	B	1486	CLA	C3A-C2A	-4.18	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1463	CLA	CAA-C2A	4.18	1.61	1.54
11	H	1482	CLA	CAA-C2A	4.18	1.61	1.54
11	C	1468	CLA	C1B-CHB	-4.17	1.35	1.43
11	I	1466	CLA	C4B-NB	4.16	1.38	1.35
11	B	1494	CLA	MG-NA	4.16	2.16	2.06
11	I	1459	CLA	C4B-NB	4.13	1.38	1.35
11	C	1470	CLA	C4B-NB	4.13	1.38	1.35
17	L	1047	BCR	C1-C6	4.12	1.59	1.53
11	H	1483	CLA	MG-NA	4.12	2.16	2.06
11	C	1459	CLA	MG-NA	4.08	2.16	2.06
11	C	1469	CLA	C4B-NB	4.07	1.38	1.35
11	I	1471	CLA	C1B-NB	4.07	1.38	1.35
11	H	1491	CLA	C1B-NB	4.06	1.38	1.35
11	I	1468	CLA	C2B-C1B	4.05	1.47	1.39
11	H	1494	CLA	MG-NA	4.04	2.15	2.06
11	I	1461	CLA	C2B-C1B	4.04	1.47	1.39
11	A	1343	CLA	CAA-C2A	4.03	1.61	1.54
11	I	1468	CLA	C3B-C4B	4.03	1.47	1.39
11	H	1488	CLA	CAA-C2A	4.01	1.61	1.54
11	B	1496	CLA	CAA-C2A	3.98	1.61	1.54
17	L	1047	BCR	C30-C25	3.95	1.59	1.53
11	I	1471	CLA	C4B-NB	3.93	1.38	1.35
17	F	1046	BCR	C2-C1	3.93	1.63	1.54
11	G	1344	CLA	C1B-NB	3.90	1.38	1.35
11	H	1497	CLA	OBD-CAD	3.89	1.27	1.22
11	I	1461	CLA	MG-NC	3.89	2.15	2.06
11	B	1490	CLA	C4B-NB	3.89	1.38	1.35
11	H	1486	CLA	C4B-NB	3.89	1.38	1.35
11	H	1496	CLA	MG-NA	3.87	2.15	2.06
11	I	1464	CLA	MG-NA	3.86	2.15	2.06
11	B	1490	CLA	CAA-C2A	3.85	1.61	1.54
16	L	1046	HEM	C3A-C4A	3.82	1.46	1.39
11	B	1482	CLA	MG-NA	3.81	2.15	2.06
11	B	1497	CLA	MG-NA	3.81	2.15	2.06
11	B	1492	CLA	C4B-NB	3.81	1.38	1.35
12	D	1352	PHO	CHB-C1B	-3.81	1.31	1.38
11	C	1465	CLA	C1B-CHB	-3.81	1.30	1.41
11	H	1484	CLA	C4B-NB	3.79	1.38	1.35
11	J	1353	CLA	MG-NA	3.79	2.15	2.06
11	I	1462	CLA	C1B-CHB	-3.77	1.30	1.41
11	A	1346	CLA	C4B-NB	3.76	1.38	1.35
11	G	1344	CLA	CAA-C2A	3.75	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	1486	CLA	C3A-C2A	-3.74	1.51	1.54
11	G	1346	CLA	C1B-NB	3.72	1.38	1.35
11	I	1462	CLA	CHC-C1C	3.71	1.44	1.35
11	C	1471	CLA	C1B-NB	3.71	1.38	1.35
11	H	1494	CLA	CHC-C1C	3.64	1.44	1.35
11	H	1484	CLA	CAA-C2A	3.64	1.60	1.54
11	B	1485	CLA	C1B-CHB	-3.63	1.30	1.41
11	I	1468	CLA	MG-NC	3.63	2.14	2.06
11	H	1486	CLA	MG-NA	3.61	2.14	2.06
11	B	1491	CLA	C1B-NB	3.61	1.38	1.35
11	B	1494	CLA	C4B-NB	3.60	1.38	1.35
17	L	1047	BCR	C29-C30	3.60	1.62	1.54
11	I	1465	CLA	C1B-CHB	-3.59	1.31	1.41
16	L	1046	HEM	C3B-C4B	3.56	1.46	1.39
11	B	1488	CLA	C1B-CHB	-3.55	1.31	1.41
17	F	1046	BCR	C29-C30	3.53	1.62	1.54
11	D	1351	CLA	CHC-C1C	3.53	1.44	1.35
12	J	1352	PHO	CHB-C1B	-3.53	1.32	1.38
11	D	1353	CLA	CAA-C2A	3.52	1.60	1.54
11	I	1460	CLA	CAA-C2A	3.51	1.60	1.54
17	L	1047	BCR	C2-C1	3.50	1.62	1.54
11	H	1496	CLA	C4B-NB	3.50	1.38	1.35
11	G	1342	CLA	C1B-CHB	-3.48	1.31	1.41
11	H	1488	CLA	CHC-C1C	3.47	1.43	1.35
11	H	1482	CLA	C1B-NB	3.47	1.38	1.35
11	B	1487	CLA	C5-C3	3.47	1.58	1.51
11	B	1488	CLA	CHC-C1C	3.46	1.43	1.35
18	V	1138	HEC	C1B-CHB	-3.46	1.31	1.41
11	B	1496	CLA	MG-NC	3.46	2.14	2.06
11	J	1351	CLA	CHC-C1C	3.45	1.43	1.35
11	H	1483	CLA	C1B-CHB	-3.42	1.31	1.41
11	A	1346	CLA	CAA-C2A	3.41	1.60	1.54
11	C	1462	CLA	CHC-C1C	3.39	1.43	1.35
11	B	1494	CLA	CHC-C1C	3.39	1.43	1.35
11	C	1460	CLA	CAA-C2A	3.39	1.60	1.54
11	G	1346	CLA	C4B-NB	3.38	1.38	1.35
11	I	1460	CLA	CHC-C1C	3.38	1.43	1.35
11	H	1493	CLA	CAA-C2A	3.37	1.60	1.54
11	B	1487	CLA	CHC-C1C	3.37	1.43	1.35
17	F	1046	BCR	C30-C25	3.37	1.58	1.53
18	T	1138	HEC	C1B-CHB	-3.35	1.31	1.41
11	D	1351	CLA	C1B-CHB	-3.35	1.31	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1471	CLA	MG-NC	3.35	2.14	2.06
11	I	1466	CLA	CAA-C2A	3.35	1.60	1.54
11	I	1462	CLA	C5-C3	3.34	1.58	1.51
11	H	1488	CLA	C1B-CHB	-3.34	1.31	1.41
11	I	1465	CLA	MG-NC	3.34	2.14	2.06
18	T	1138	HEC	CAD-C3D	-3.34	1.47	1.52
11	A	1342	CLA	C1B-CHB	-3.33	1.31	1.41
11	H	1492	CLA	C1B-CHB	-3.31	1.31	1.41
11	G	1346	CLA	C4C-C3C	3.30	1.50	1.45
11	H	1482	CLA	C4B-NB	3.30	1.38	1.35
11	C	1464	CLA	C4B-NB	3.30	1.38	1.35
11	C	1459	CLA	MG-NC	3.29	2.14	2.06
11	I	1462	CLA	C2-C3	3.29	1.40	1.33
11	I	1463	CLA	CAA-C2A	3.29	1.60	1.54
11	B	1490	CLA	MG-NC	3.28	2.14	2.06
11	I	1462	CLA	C1-C2	3.27	1.58	1.49
11	H	1490	CLA	CAA-C2A	3.27	1.60	1.54
11	H	1490	CLA	C4B-NB	3.27	1.38	1.35
11	I	1469	CLA	C4B-NB	3.26	1.38	1.35
17	F	1046	BCR	C23-C22	-3.26	1.38	1.45
11	G	1344	CLA	C1B-CHB	-3.25	1.32	1.41
15	D	1354	PL9	C3-C2	3.25	1.42	1.32
15	D	1354	PL9	C6-C5	3.24	1.42	1.32
11	H	1483	CLA	C4B-NB	3.24	1.38	1.35
11	H	1485	CLA	C1B-CHB	-3.22	1.32	1.41
11	H	1487	CLA	C4C-C3C	3.22	1.50	1.45
11	H	1482	CLA	C4-C3	3.21	1.58	1.50
11	H	1494	CLA	CAA-C2A	3.21	1.60	1.54
11	G	1343	CLA	C1B-CHB	-3.21	1.32	1.41
11	G	1342	CLA	CHC-C1C	3.21	1.43	1.35
11	C	1460	CLA	C1B-NB	3.20	1.38	1.35
11	B	1495	CLA	C1B-CHB	-3.19	1.32	1.41
11	J	1353	CLA	CAA-C2A	3.19	1.60	1.54
11	I	1462	CLA	C4B-NB	3.19	1.38	1.35
11	I	1466	CLA	C1B-NB	3.19	1.38	1.35
11	B	1484	CLA	CAA-C2A	3.19	1.60	1.54
11	H	1487	CLA	CHC-C1C	3.18	1.43	1.35
11	C	1461	CLA	C3C-C4C	3.18	1.50	1.43
11	H	1493	CLA	C1B-CHB	-3.17	1.32	1.41
11	H	1497	CLA	MG-NC	3.17	2.13	2.06
11	C	1462	CLA	C1B-CHB	-3.17	1.32	1.41
11	I	1471	CLA	MG-NC	3.16	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	1495	CLA	C1B-CHB	-3.15	1.32	1.41
18	T	1138	HEC	CAA-C2A	3.15	1.57	1.52
11	H	1496	CLA	CAA-C2A	3.15	1.60	1.54
11	A	1343	CLA	C1B-CHB	-3.15	1.32	1.41
11	I	1467	CLA	C4B-NB	3.14	1.38	1.35
11	H	1488	CLA	C5-C3	3.13	1.57	1.51
11	B	1484	CLA	C1B-CHB	-3.13	1.32	1.41
11	I	1463	CLA	C4B-NB	3.13	1.38	1.35
11	B	1489	CLA	CAA-C2A	3.12	1.59	1.54
11	C	1459	CLA	CHC-C1C	3.12	1.43	1.35
11	A	1346	CLA	MG-NC	3.12	2.13	2.06
11	A	1344	CLA	C1B-CHB	-3.09	1.32	1.41
11	I	1465	CLA	CHC-C1C	3.08	1.42	1.35
11	H	1495	CLA	C4-C3	3.08	1.58	1.50
11	H	1487	CLA	C5-C3	3.07	1.57	1.51
11	I	1464	CLA	MG-NC	3.07	2.13	2.06
11	G	1344	CLA	C4B-NB	3.07	1.37	1.35
11	I	1464	CLA	CHC-C1C	3.07	1.42	1.35
17	F	1046	BCR	C19-C18	-3.06	1.39	1.45
11	I	1470	CLA	MG-NC	3.06	2.13	2.06
17	L	1047	BCR	C23-C22	-3.06	1.39	1.45
18	T	1138	HEC	C3C-C4C	3.05	1.48	1.43
11	C	1460	CLA	C4B-NB	3.04	1.37	1.35
11	G	1343	CLA	C5-C3	3.04	1.57	1.51
11	C	1465	CLA	OBD-CAD	3.04	1.26	1.22
11	B	1483	CLA	CHC-C1C	3.03	1.42	1.35
11	C	1462	CLA	C4B-NB	3.03	1.37	1.35
11	B	1492	CLA	MG-NC	3.01	2.13	2.06
11	A	1344	CLA	CHC-C1C	3.01	1.42	1.35
11	H	1494	CLA	MG-NC	3.01	2.13	2.06
11	C	1462	CLA	C2-C3	3.01	1.40	1.33
11	H	1485	CLA	CHC-C1C	3.00	1.42	1.35
11	I	1461	CLA	C3C-C4C	3.00	1.50	1.43
11	H	1488	CLA	MG-NC	2.99	2.13	2.06
11	B	1492	CLA	C1B-CHB	-2.99	1.32	1.41
18	V	1138	HEC	CAA-C2A	2.99	1.57	1.52
11	H	1497	CLA	C1B-CHB	-2.99	1.32	1.41
11	H	1492	CLA	MG-NC	2.98	2.13	2.06
11	H	1494	CLA	C4-C3	2.98	1.58	1.50
11	C	1470	CLA	C1B-NB	2.98	1.37	1.35
11	I	1459	CLA	CHC-C1C	2.97	1.42	1.35
11	B	1485	CLA	MG-NC	2.97	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	J	1351	CLA	C1B-CHB	-2.97	1.32	1.41
11	H	1490	CLA	MG-NC	2.96	2.13	2.06
11	I	1466	CLA	C1B-CHB	-2.96	1.32	1.41
11	I	1467	CLA	C1B-NB	2.95	1.37	1.35
12	J	1352	PHO	C1D-C2D	-2.95	1.39	1.45
11	B	1486	CLA	C4B-NB	2.93	1.37	1.35
11	C	1462	CLA	C1-C2	2.92	1.57	1.49
11	C	1465	CLA	CHC-C1C	2.92	1.42	1.35
11	G	1342	CLA	MG-NC	2.92	2.13	2.06
11	B	1483	CLA	C1B-CHB	-2.92	1.32	1.41
11	C	1464	CLA	C1B-CHB	-2.91	1.32	1.41
18	T	1138	HEC	C3C-C2C	-2.91	1.37	1.40
11	H	1484	CLA	MG-NC	2.89	2.13	2.06
11	C	1463	CLA	C4-C3	2.89	1.58	1.50
11	I	1462	CLA	MG-NC	2.89	2.13	2.06
11	H	1483	CLA	CHC-C1C	2.89	1.42	1.35
11	B	1485	CLA	CHC-C1C	2.88	1.42	1.35
11	C	1471	CLA	CHC-C1C	2.88	1.42	1.35
11	J	1353	CLA	CHC-C1C	2.88	1.42	1.35
11	B	1490	CLA	C4C-C3C	2.88	1.50	1.45
11	C	1461	CLA	MG-NC	2.88	2.13	2.06
11	B	1495	CLA	C4B-NB	2.87	1.37	1.35
11	C	1464	CLA	CHC-C1C	2.87	1.42	1.35
11	H	1495	CLA	CHC-C1C	2.87	1.42	1.35
11	G	1343	CLA	CHC-C1C	2.86	1.42	1.35
11	D	1353	CLA	CHC-C1C	2.86	1.42	1.35
11	G	1342	CLA	CBA-CGA	-2.85	1.42	1.50
11	H	1497	CLA	MG-NA	2.84	2.13	2.06
11	D	1353	CLA	C4B-NB	2.84	1.37	1.35
12	D	1352	PHO	C1D-C2D	-2.84	1.39	1.45
11	B	1495	CLA	CHC-C1C	2.84	1.42	1.35
11	B	1484	CLA	MG-NA	2.84	2.13	2.06
11	C	1466	CLA	C1B-CHB	-2.83	1.33	1.41
15	J	1354	PL9	C6-C5	2.83	1.41	1.32
11	C	1470	CLA	CHC-C1C	2.82	1.42	1.35
11	I	1459	CLA	C3D-CAD	-2.82	1.38	1.46
11	B	1485	CLA	C4B-NB	2.82	1.37	1.35
11	B	1487	CLA	C1-C2	2.82	1.57	1.49
11	C	1462	CLA	MG-NA	2.82	2.13	2.06
11	B	1482	CLA	C5-C3	2.81	1.57	1.51
18	V	1138	HEC	CAD-C3D	-2.81	1.47	1.52
11	H	1488	CLA	C3D-CAD	-2.81	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	1485	CLA	C4B-NB	2.81	1.37	1.35
11	C	1462	CLA	C5-C3	2.80	1.57	1.51
11	H	1483	CLA	MG-NC	2.80	2.12	2.06
11	G	1346	CLA	CAA-C2A	2.80	1.59	1.54
11	C	1465	CLA	MG-NC	2.79	2.12	2.06
11	C	1463	CLA	CHC-C1C	2.79	1.42	1.35
11	D	1351	CLA	C1C-C2C	2.78	1.49	1.44
11	G	1343	CLA	C4B-NB	2.77	1.37	1.35
11	C	1462	CLA	C4-C3	2.77	1.57	1.50
11	I	1470	CLA	CHC-C1C	2.77	1.42	1.35
11	H	1494	CLA	C4B-NB	2.77	1.37	1.35
11	C	1466	CLA	CHC-C1C	2.76	1.42	1.35
17	L	1047	BCR	C26-C25	2.76	1.39	1.34
11	C	1470	CLA	MG-NC	2.75	2.12	2.06
11	I	1470	CLA	CAA-C2A	2.75	1.59	1.53
11	C	1468	CLA	CAD-CBD	2.74	1.57	1.54
11	I	1466	CLA	MG-NC	2.74	2.12	2.06
11	H	1482	CLA	C1-C2	2.74	1.57	1.49
11	B	1494	CLA	MG-NC	2.74	2.12	2.06
11	A	1346	CLA	C1B-CHB	-2.74	1.33	1.41
11	I	1462	CLA	C4-C3	2.73	1.57	1.50
11	I	1464	CLA	C1B-CHB	-2.73	1.33	1.41
11	C	1463	CLA	C4B-NB	2.72	1.37	1.35
11	H	1493	CLA	C4C-C3C	2.72	1.49	1.45
11	B	1482	CLA	CHC-C1C	2.72	1.41	1.35
11	B	1492	CLA	CHC-C1C	2.72	1.41	1.35
11	B	1490	CLA	C1C-C2C	2.72	1.49	1.44
11	I	1464	CLA	CAA-C2A	2.71	1.59	1.54
18	V	1138	HEC	C3C-C4C	2.71	1.48	1.43
11	I	1471	CLA	C4C-C3C	2.71	1.49	1.45
11	I	1459	CLA	C1B-CHB	-2.71	1.33	1.41
11	H	1487	CLA	C1-C2	2.70	1.57	1.49
11	B	1487	CLA	C4C-C3C	2.70	1.49	1.45
11	H	1490	CLA	CHC-C1C	2.70	1.41	1.35
11	H	1491	CLA	C3C-C4C	2.70	1.49	1.43
11	B	1488	CLA	MG-NC	2.69	2.12	2.06
11	B	1492	CLA	C4-C3	2.69	1.57	1.50
17	L	1047	BCR	C19-C18	-2.69	1.40	1.45
11	I	1461	CLA	CAD-CBD	2.69	1.57	1.54
11	I	1466	CLA	CHC-C1C	2.69	1.41	1.35
11	A	1343	CLA	CHC-C1C	2.69	1.41	1.35
11	H	1482	CLA	C5-C3	2.69	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	1489	CLA	C4-C3	2.69	1.57	1.50
11	B	1497	CLA	C1C-C2C	2.68	1.49	1.44
11	C	1464	CLA	C4-C3	2.68	1.57	1.50
11	I	1461	CLA	C2C-C1C	2.67	1.49	1.43
11	B	1483	CLA	MG-NC	2.67	2.12	2.06
11	H	1484	CLA	C1B-CHB	-2.67	1.33	1.41
12	A	1345	PHO	C3B-C4B	2.66	1.48	1.43
11	B	1497	CLA	CAA-C2A	2.66	1.58	1.53
11	D	1353	CLA	C1B-CHB	-2.66	1.33	1.41
11	B	1493	CLA	CAA-C2A	2.66	1.59	1.54
11	H	1490	CLA	C4C-C3C	2.66	1.49	1.45
11	H	1497	CLA	CBD-CGD	2.66	1.60	1.52
18	T	1138	HEC	C1A-C2A	2.65	1.48	1.42
11	J	1353	CLA	C1B-CHB	-2.65	1.33	1.41
11	J	1353	CLA	MG-NC	2.65	2.12	2.06
11	I	1460	CLA	C1B-CHB	-2.65	1.33	1.41
11	C	1468	CLA	MG-NC	2.65	2.12	2.06
11	A	1346	CLA	C4-C3	2.64	1.57	1.50
11	I	1463	CLA	CHC-C1C	2.64	1.41	1.35
11	H	1482	CLA	CHC-C1C	2.63	1.41	1.35
11	H	1486	CLA	CHC-C1C	2.63	1.41	1.35
11	I	1464	CLA	C4-C3	2.63	1.57	1.50
11	A	1342	CLA	O1D-CGD	-2.62	1.14	1.21
11	H	1489	CLA	C1B-NB	2.62	1.37	1.35
11	B	1482	CLA	MG-NC	2.62	2.12	2.06
11	C	1465	CLA	MG-NA	2.61	2.12	2.06
11	C	1464	CLA	MG-NC	2.61	2.12	2.06
11	C	1461	CLA	C2C-C1C	2.61	1.49	1.43
11	B	1496	CLA	C1B-CHB	-2.59	1.33	1.41
18	T	1138	HEC	C3B-C2B	-2.59	1.38	1.40
11	G	1342	CLA	C3B-C2B	-2.58	1.36	1.40
11	I	1465	CLA	OBD-CAD	2.58	1.25	1.22
11	C	1469	CLA	MG-NC	2.58	2.12	2.06
16	E	1085	HEM	C4B-CHC	-2.58	1.38	1.43
11	B	1494	CLA	C4-C3	2.58	1.57	1.50
11	C	1471	CLA	CAA-C2A	2.57	1.58	1.53
11	B	1488	CLA	C4B-NB	2.57	1.37	1.35
11	H	1492	CLA	CHC-C1C	2.57	1.41	1.35
11	B	1491	CLA	C4B-NB	2.56	1.37	1.35
11	A	1342	CLA	CHC-C1C	2.56	1.41	1.35
11	H	1496	CLA	MG-NC	2.55	2.12	2.06
11	B	1490	CLA	OBD-CAD	2.55	1.25	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1460	CLA	CHC-C1C	2.54	1.41	1.35
11	C	1467	CLA	CHC-C1C	2.54	1.41	1.35
11	C	1461	CLA	CAD-CBD	2.54	1.57	1.54
16	E	1085	HEM	C3A-C2A	2.54	1.52	1.39
11	C	1464	CLA	CBA-CGA	-2.54	1.43	1.50
11	C	1463	CLA	C1B-CHB	-2.53	1.33	1.41
11	C	1466	CLA	MG-NC	2.53	2.12	2.06
11	H	1488	CLA	C1C-C2C	2.53	1.49	1.44
11	C	1469	CLA	CHC-C1C	2.53	1.41	1.35
12	G	1345	PHO	CHC-C1C	2.53	1.43	1.38
11	C	1469	CLA	C1B-NB	2.53	1.37	1.35
11	C	1470	CLA	CAA-C2A	2.53	1.58	1.53
11	I	1471	CLA	OBD-CAD	2.53	1.25	1.22
11	B	1493	CLA	CHC-C1C	2.53	1.41	1.35
11	B	1493	CLA	C1B-CHB	-2.52	1.34	1.41
15	J	1354	PL9	C3-C2	2.52	1.40	1.32
11	H	1497	CLA	C1C-C2C	2.52	1.49	1.44
11	B	1482	CLA	C4C-C3C	2.52	1.49	1.45
11	B	1483	CLA	OBD-CAD	2.51	1.25	1.22
11	C	1463	CLA	C5-C3	2.51	1.56	1.51
11	B	1489	CLA	C3D-CAD	-2.51	1.39	1.46
11	J	1351	CLA	C1C-C2C	2.51	1.49	1.44
11	I	1459	CLA	MG-NC	2.51	2.12	2.06
11	B	1486	CLA	CHC-C1C	2.51	1.41	1.35
11	B	1484	CLA	CHC-C1C	2.51	1.41	1.35
11	B	1488	CLA	C1-C2	2.51	1.56	1.49
11	A	1346	CLA	CHC-C1C	2.50	1.41	1.35
11	B	1495	CLA	C4-C3	2.50	1.57	1.50
11	C	1466	CLA	C4B-NB	2.50	1.37	1.35
11	I	1468	CLA	CAD-CBD	2.50	1.57	1.54
16	E	1085	HEM	C1A-CHA	-2.49	1.38	1.43
11	H	1483	CLA	CAA-CBA	-2.49	1.45	1.52
11	B	1497	CLA	CHC-C1C	2.49	1.41	1.35
11	B	1482	CLA	C4-C3	2.49	1.57	1.50
11	B	1484	CLA	MG-NC	2.49	2.12	2.06
11	B	1494	CLA	CAA-C2A	2.48	1.58	1.54
11	B	1497	CLA	C1B-CHB	-2.47	1.34	1.41
11	I	1462	CLA	C1C-C2C	2.47	1.49	1.44
11	I	1467	CLA	C1B-CHB	-2.47	1.34	1.41
11	B	1487	CLA	MG-NC	2.47	2.12	2.06
11	H	1482	CLA	C4C-C3C	2.47	1.49	1.45
11	I	1460	CLA	C1B-NB	2.47	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	1342	CLA	CAA-CBA	-2.47	1.45	1.52
11	I	1464	CLA	C4B-NB	2.47	1.37	1.35
11	G	1342	CLA	C3D-CAD	-2.46	1.39	1.46
11	B	1497	CLA	CBD-CGD	2.46	1.60	1.52
11	B	1497	CLA	OBD-CAD	2.46	1.25	1.22
11	C	1465	CLA	CAA-C2A	2.46	1.58	1.54
11	A	1343	CLA	C4B-NB	2.46	1.37	1.35
11	B	1489	CLA	C1C-NC	-2.45	1.34	1.37
11	I	1470	CLA	C1B-NB	2.45	1.37	1.35
12	A	1345	PHO	CHB-C1B	-2.44	1.34	1.38
11	B	1497	CLA	MG-NC	2.44	2.12	2.06
11	A	1344	CLA	MG-NC	2.44	2.12	2.06
11	I	1465	CLA	CAA-C2A	2.44	1.58	1.54
11	C	1464	CLA	C3D-CAD	-2.44	1.39	1.46
11	D	1353	CLA	O2A-CGA	2.43	1.40	1.33
11	I	1460	CLA	C4B-NB	2.43	1.37	1.35
11	B	1496	CLA	C1B-NB	2.43	1.37	1.35
16	L	1046	HEM	C4B-CHC	-2.43	1.39	1.43
11	B	1487	CLA	C6-C5	2.43	1.61	1.52
11	H	1497	CLA	CAA-C2A	2.42	1.58	1.53
11	I	1463	CLA	C5-C3	2.42	1.56	1.51
11	B	1490	CLA	CHC-C1C	2.42	1.41	1.35
16	E	1085	HEM	C1D-CHD	-2.42	1.39	1.43
11	I	1463	CLA	C4-C3	2.42	1.56	1.50
11	C	1459	CLA	CAA-C2A	2.41	1.58	1.54
11	J	1353	CLA	C1-C2	2.41	1.56	1.49
11	C	1467	CLA	OBD-CAD	2.41	1.25	1.22
11	C	1463	CLA	C1C-C2C	2.40	1.49	1.44
11	H	1490	CLA	C1C-C2C	2.40	1.49	1.44
11	H	1485	CLA	C1C-C2C	2.40	1.49	1.44
11	B	1494	CLA	C3D-CAD	-2.40	1.40	1.46
11	I	1465	CLA	C4B-NB	2.39	1.37	1.35
18	T	1138	HEC	C3B-C4B	2.39	1.47	1.43
11	B	1488	CLA	C3D-CAD	-2.39	1.40	1.46
11	I	1467	CLA	CHC-C1C	2.39	1.41	1.35
11	B	1482	CLA	C1B-CHB	-2.38	1.34	1.41
11	H	1494	CLA	C1B-CHB	-2.38	1.34	1.41
11	G	1346	CLA	C4-C3	2.38	1.56	1.50
11	B	1486	CLA	C1B-CHB	-2.38	1.34	1.41
11	I	1464	CLA	C1C-C2C	2.38	1.49	1.44
11	C	1459	CLA	C4C-C3C	2.38	1.49	1.45
11	C	1469	CLA	C3D-CAD	-2.37	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1469	CLA	CAA-C2A	2.37	1.58	1.53
11	B	1494	CLA	C1B-CHB	-2.37	1.34	1.41
11	I	1462	CLA	MG-NA	2.37	2.11	2.06
11	H	1496	CLA	C3D-CAD	-2.37	1.40	1.46
11	H	1488	CLA	C4-C3	2.37	1.56	1.50
11	C	1466	CLA	C1C-NC	-2.36	1.34	1.37
11	H	1487	CLA	C6-C5	2.36	1.60	1.52
11	C	1462	CLA	MG-NC	2.36	2.11	2.06
12	A	1345	PHO	CAA-CBA	-2.36	1.45	1.52
11	H	1497	CLA	CHC-C1C	2.36	1.41	1.35
11	H	1490	CLA	CMB-C2B	2.35	1.56	1.51
11	I	1460	CLA	O2A-CGA	2.35	1.40	1.33
11	H	1496	CLA	C4-C3	2.35	1.56	1.50
11	B	1488	CLA	C1C-C2C	2.35	1.49	1.44
11	H	1496	CLA	C1B-CHB	-2.35	1.34	1.41
11	I	1460	CLA	MG-NC	2.35	2.11	2.06
11	B	1484	CLA	C3D-CAD	-2.35	1.40	1.46
12	G	1345	PHO	CHB-C1B	-2.35	1.34	1.38
11	H	1496	CLA	CHC-C1C	2.34	1.41	1.35
11	B	1495	CLA	CAA-CBA	-2.34	1.45	1.52
11	I	1463	CLA	MG-NC	2.34	2.11	2.06
11	H	1491	CLA	C2C-C1C	2.34	1.48	1.43
11	H	1497	CLA	CMA-C3A	2.34	1.58	1.53
11	H	1491	CLA	CAD-CBD	2.33	1.56	1.54
12	D	1352	PHO	C1C-NC	-2.33	1.33	1.38
11	C	1463	CLA	OBD-CAD	2.33	1.25	1.22
11	G	1346	CLA	C1B-CHB	-2.32	1.34	1.41
11	D	1353	CLA	MG-NC	2.32	2.11	2.06
11	B	1491	CLA	CAD-CBD	2.32	1.56	1.54
11	H	1492	CLA	C4-C3	2.31	1.56	1.50
11	B	1486	CLA	MG-NC	2.31	2.11	2.06
11	H	1493	CLA	CHC-C1C	2.31	1.40	1.35
12	D	1352	PHO	C4-C3	2.31	1.56	1.50
11	B	1492	CLA	C5-C3	2.30	1.56	1.51
11	H	1489	CLA	CHC-C1C	2.30	1.40	1.35
11	H	1486	CLA	C1B-CHB	-2.30	1.34	1.41
11	I	1460	CLA	C1C-C2C	2.30	1.49	1.44
11	H	1497	CLA	C3A-C2A	2.30	1.56	1.54
11	J	1351	CLA	C4-C3	2.30	1.56	1.50
11	H	1489	CLA	CAA-C2A	2.29	1.58	1.54
11	I	1469	CLA	CHC-C1C	2.29	1.40	1.35
11	H	1482	CLA	C1C-C2C	2.29	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1482	CLA	C1C-C2C	2.29	1.49	1.44
11	H	1487	CLA	C1C-C2C	2.29	1.49	1.44
11	H	1496	CLA	C5-C3	2.27	1.56	1.51
11	H	1491	CLA	MG-NC	2.27	2.11	2.06
11	D	1353	CLA	C4-C3	2.27	1.56	1.50
11	B	1489	CLA	C1B-CHB	-2.26	1.34	1.41
11	H	1486	CLA	MG-NC	2.26	2.11	2.06
11	H	1488	CLA	C1-C2	2.25	1.55	1.49
11	I	1464	CLA	C3D-CAD	-2.25	1.40	1.46
11	B	1488	CLA	C5-C3	2.25	1.56	1.51
11	G	1344	CLA	CHC-C1C	2.25	1.40	1.35
11	H	1492	CLA	C3D-CAD	-2.25	1.40	1.46
11	I	1461	CLA	C4C-NC	2.25	1.40	1.37
11	C	1471	CLA	OBD-CAD	2.24	1.25	1.22
11	B	1485	CLA	C3D-CAD	-2.24	1.40	1.46
16	L	1046	HEM	C3A-C2A	2.24	1.50	1.39
11	C	1460	CLA	C1B-CHB	-2.24	1.34	1.41
11	H	1495	CLA	O2A-CGA	2.23	1.39	1.33
16	L	1046	HEM	C4A-CHB	-2.23	1.39	1.43
11	C	1459	CLA	C1B-CHB	-2.23	1.34	1.41
11	B	1487	CLA	C1C-C2C	2.23	1.48	1.44
11	C	1468	CLA	C4B-CHC	-2.23	1.39	1.43
12	G	1345	PHO	CAA-CBA	-2.23	1.45	1.52
11	J	1351	CLA	C3D-CAD	-2.22	1.40	1.46
11	I	1465	CLA	MG-NA	2.22	2.11	2.06
11	H	1485	CLA	CAA-CBA	-2.22	1.45	1.52
11	A	1342	CLA	C3D-CAD	-2.21	1.40	1.46
11	D	1351	CLA	CAA-C2A	2.21	1.58	1.54
11	B	1482	CLA	C1-C2	2.21	1.55	1.49
11	H	1493	CLA	OBD-CAD	2.21	1.25	1.22
11	H	1495	CLA	C5-C3	2.19	1.55	1.51
11	C	1462	CLA	C1C-C2C	2.19	1.48	1.44
12	J	1352	PHO	C3B-C4B	2.19	1.47	1.43
11	B	1489	CLA	C1B-NB	2.18	1.37	1.35
11	H	1485	CLA	MG-NC	2.17	2.11	2.06
11	I	1459	CLA	CAA-C2A	2.17	1.58	1.54
11	D	1353	CLA	C2-C3	2.17	1.38	1.32
11	J	1353	CLA	C4B-NB	2.17	1.37	1.35
11	G	1346	CLA	CBD-CGD	2.17	1.59	1.52
11	H	1489	CLA	C1B-CHB	-2.16	1.35	1.41
11	B	1495	CLA	MG-NC	2.16	2.11	2.06
11	I	1469	CLA	C3D-CAD	-2.16	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1467	CLA	C4B-NB	2.16	1.37	1.35
11	I	1471	CLA	CHC-C1C	2.16	1.40	1.35
11	H	1495	CLA	CAA-CBA	-2.15	1.46	1.52
11	C	1467	CLA	C1C-NC	-2.15	1.34	1.37
11	H	1491	CLA	C4C-NC	2.15	1.40	1.37
18	T	1138	HEC	C2A-C3A	2.15	1.44	1.37
18	V	1138	HEC	C1A-C2A	2.15	1.47	1.42
11	H	1490	CLA	OBD-CAD	2.15	1.25	1.22
11	B	1490	CLA	CMB-C2B	2.15	1.56	1.51
11	B	1493	CLA	C1B-NB	2.14	1.37	1.35
11	C	1468	CLA	C2C-C1C	2.14	1.48	1.43
17	F	1046	BCR	C26-C25	2.14	1.38	1.34
16	E	1085	HEM	C4A-CHB	-2.14	1.39	1.43
11	A	1342	CLA	CAA-CBA	-2.13	1.46	1.52
11	H	1493	CLA	MG-NC	2.13	2.11	2.06
11	J	1353	CLA	C4C-C3C	2.13	1.48	1.45
11	B	1489	CLA	C4-C3	2.13	1.56	1.50
11	H	1497	CLA	C4B-NB	2.12	1.37	1.35
11	C	1464	CLA	C4C-C3C	2.12	1.48	1.45
11	I	1468	CLA	C2C-C1C	2.11	1.48	1.43
11	J	1351	CLA	CBA-CGA	-2.11	1.44	1.50
17	F	1046	BCR	C29-C28	-2.11	1.47	1.52
11	B	1497	CLA	C3B-C2B	-2.11	1.37	1.40
11	B	1495	CLA	C3D-CAD	-2.11	1.40	1.46
16	L	1046	HEM	C1D-CHD	-2.10	1.39	1.43
11	H	1483	CLA	CBA-CGA	-2.10	1.44	1.50
11	I	1463	CLA	C1B-CHB	-2.10	1.35	1.41
11	H	1483	CLA	C4C-C3C	2.10	1.48	1.45
11	B	1485	CLA	CAA-CBA	-2.09	1.46	1.52
11	C	1471	CLA	C4C-C3C	2.09	1.48	1.45
11	B	1495	CLA	CAA-C2A	2.09	1.58	1.54
11	I	1469	CLA	CAA-C2A	2.09	1.57	1.53
11	H	1495	CLA	C1C-C2C	2.09	1.48	1.44
11	G	1346	CLA	C3D-C2D	2.08	1.43	1.39
11	G	1343	CLA	C1-C2	2.08	1.55	1.49
11	B	1496	CLA	OBD-CAD	2.07	1.25	1.22
11	C	1470	CLA	C1B-CHB	-2.07	1.35	1.41
11	B	1491	CLA	C2C-C1C	2.06	1.48	1.43
11	H	1485	CLA	CAA-C2A	2.06	1.57	1.54
11	D	1351	CLA	C3B-C2B	-2.05	1.37	1.40
11	C	1459	CLA	C3D-CAD	-2.05	1.40	1.46
11	B	1486	CLA	C3D-CAD	-2.05	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1463	CLA	MG-NC	2.04	2.11	2.06
11	G	1343	CLA	MG-NC	2.04	2.11	2.06
11	A	1342	CLA	CBA-CGA	-2.04	1.44	1.50
11	H	1482	CLA	C1B-CHB	-2.04	1.35	1.41
11	H	1495	CLA	C3D-CAD	-2.03	1.40	1.46
12	J	1352	PHO	CHC-C1C	2.03	1.42	1.38
11	A	1346	CLA	C4C-C3C	2.03	1.48	1.45
11	G	1342	CLA	C1C-C2C	2.03	1.48	1.44
11	I	1460	CLA	CMB-C2B	2.03	1.55	1.51
11	D	1351	CLA	C4-C3	2.03	1.55	1.50
11	B	1486	CLA	C3B-CAB	2.02	1.52	1.47
11	H	1484	CLA	C3D-CAD	-2.02	1.41	1.46
18	T	1138	HEC	CMA-C3A	2.01	1.56	1.51
11	B	1495	CLA	O2A-CGA	2.01	1.39	1.33
11	I	1464	CLA	C1B-NB	2.01	1.37	1.35
12	J	1352	PHO	CAA-C2A	2.01	1.57	1.54
11	C	1460	CLA	MG-NC	2.01	2.11	2.06
11	G	1346	CLA	CHC-C1C	2.01	1.40	1.35

All (899) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	I	1469	CLA	C4A-NA-C1A	13.54	112.79	106.71
11	C	1469	CLA	C4A-NA-C1A	13.24	112.66	106.71
11	H	1495	CLA	C4A-NA-C1A	12.89	112.50	106.71
11	I	1463	CLA	C4A-NA-C1A	12.75	112.44	106.71
11	H	1496	CLA	C4A-NA-C1A	12.69	112.41	106.71
11	H	1489	CLA	C4A-NA-C1A	12.64	112.39	106.71
11	H	1482	CLA	C4A-NA-C1A	12.58	112.36	106.71
11	C	1470	CLA	C4A-NA-C1A	12.56	112.35	106.71
11	C	1471	CLA	C4A-NA-C1A	12.49	112.32	106.71
11	B	1492	CLA	C4A-NA-C1A	12.48	112.31	106.71
11	I	1471	CLA	C4A-NA-C1A	12.27	112.22	106.71
11	B	1482	CLA	C4A-NA-C1A	12.24	112.21	106.71
11	H	1497	CLA	C4A-NA-C1A	12.24	112.21	106.71
11	C	1463	CLA	C4A-NA-C1A	12.17	112.18	106.71
11	H	1492	CLA	C4A-NA-C1A	12.16	112.17	106.71
11	H	1494	CLA	C4A-NA-C1A	12.16	112.17	106.71
11	A	1344	CLA	C4A-NA-C1A	12.12	112.15	106.71
11	B	1495	CLA	C4A-NA-C1A	12.12	112.15	106.71
11	C	1467	CLA	C4A-NA-C1A	12.10	112.15	106.71
11	C	1460	CLA	C4A-NA-C1A	12.10	112.14	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	I	1459	CLA	C4A-NA-C1A	12.08	112.14	106.71
11	H	1490	CLA	C4A-NA-C1A	12.06	112.13	106.71
11	B	1486	CLA	C4A-NA-C1A	12.04	112.12	106.71
11	C	1466	CLA	C4A-NA-C1A	11.92	112.06	106.71
11	H	1493	CLA	C4A-NA-C1A	11.91	112.06	106.71
11	I	1467	CLA	C4A-NA-C1A	11.90	112.06	106.71
11	I	1466	CLA	C4A-NA-C1A	11.89	112.05	106.71
11	G	1344	CLA	C4A-NA-C1A	11.89	112.05	106.71
11	B	1489	CLA	C4A-NA-C1A	11.87	112.04	106.71
11	I	1460	CLA	C4A-NA-C1A	11.82	112.02	106.71
11	J	1351	CLA	C4A-NA-C1A	11.79	112.01	106.71
11	B	1493	CLA	C4A-NA-C1A	11.77	112.00	106.71
11	B	1497	CLA	C4A-NA-C1A	11.66	111.95	106.71
11	B	1491	CLA	C4A-NA-C1A	11.62	111.93	106.71
11	D	1353	CLA	C4A-NA-C1A	11.62	111.93	106.71
11	I	1470	CLA	C4A-NA-C1A	11.60	111.92	106.71
11	A	1346	CLA	C4A-NA-C1A	11.60	111.92	106.71
11	C	1468	CLA	C4A-NA-C1A	11.48	111.86	106.71
11	A	1342	CLA	C4A-NA-C1A	11.34	111.80	106.71
11	B	1484	CLA	C4A-NA-C1A	11.32	111.80	106.71
11	I	1468	CLA	C4A-NA-C1A	11.26	111.77	106.71
11	H	1488	CLA	C4A-NA-C1A	11.24	111.76	106.71
11	B	1490	CLA	C4A-NA-C1A	11.20	111.74	106.71
11	H	1486	CLA	C4A-NA-C1A	11.17	111.73	106.71
11	B	1496	CLA	C4A-NA-C1A	11.17	111.73	106.71
11	C	1461	CLA	C4A-NA-C1A	11.12	111.71	106.71
11	B	1488	CLA	C4A-NA-C1A	11.04	111.67	106.71
11	J	1353	CLA	C4A-NA-C1A	11.03	111.67	106.71
11	D	1351	CLA	C4A-NA-C1A	10.97	111.64	106.71
11	C	1464	CLA	C4A-NA-C1A	10.95	111.63	106.71
11	B	1494	CLA	C4A-NA-C1A	10.93	111.62	106.71
11	B	1483	CLA	C4A-NA-C1A	10.92	111.61	106.71
11	B	1485	CLA	C4A-NA-C1A	10.84	111.58	106.71
11	G	1346	CLA	C4A-NA-C1A	10.84	111.58	106.71
11	C	1465	CLA	C4A-NA-C1A	10.74	111.53	106.71
11	C	1459	CLA	C4A-NA-C1A	10.73	111.53	106.71
11	H	1491	CLA	C4A-NA-C1A	10.73	111.53	106.71
11	I	1464	CLA	C4A-NA-C1A	10.65	111.49	106.71
11	H	1484	CLA	C4A-NA-C1A	10.59	111.47	106.71
11	H	1485	CLA	C4A-NA-C1A	10.53	111.44	106.71
11	I	1461	CLA	C4A-NA-C1A	10.52	111.43	106.71
11	I	1465	CLA	C4A-NA-C1A	10.47	111.42	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	1342	CLA	C4A-NA-C1A	10.28	111.33	106.71
11	H	1483	CLA	C4A-NA-C1A	10.10	111.25	106.71
11	G	1343	CLA	C4A-NA-C1A	9.97	111.19	106.71
11	A	1343	CLA	C4A-NA-C1A	9.91	111.16	106.71
11	C	1462	CLA	C4A-NA-C1A	9.90	111.16	106.71
11	B	1487	CLA	C4A-NA-C1A	9.74	111.09	106.71
11	I	1462	CLA	C4A-NA-C1A	9.74	111.08	106.71
11	H	1487	CLA	C4A-NA-C1A	9.71	111.07	106.71
11	G	1343	CLA	C1-C2-C3	7.75	139.45	126.04
11	D	1351	CLA	C1-C2-C3	7.20	138.50	126.04
11	J	1351	CLA	C1-C2-C3	6.96	138.08	126.04
11	A	1343	CLA	C1-C2-C3	6.72	137.67	126.04
18	T	1138	HEC	CBD-CAD-C3D	-6.31	100.84	112.49
18	V	1138	HEC	CBD-CAD-C3D	-6.04	101.35	112.49
11	C	1461	CLA	CAD-C3D-C2D	5.56	146.21	132.79
11	I	1461	CLA	CAD-C3D-C2D	5.54	146.16	132.79
12	D	1352	PHO	C4A-NA-C1A	5.54	112.62	108.14
17	F	1046	BCR	C38-C26-C25	5.48	130.68	124.53
11	H	1491	CLA	CAD-C3D-C2D	5.40	145.82	132.79
11	I	1468	CLA	CAD-C3D-C2D	5.39	145.78	132.79
11	B	1491	CLA	CAD-C3D-C2D	5.38	145.77	132.79
11	C	1468	CLA	CAD-C3D-C2D	5.35	145.68	132.79
18	V	1138	HEC	CAD-C3D-C2D	5.33	142.56	127.25
18	T	1138	HEC	CAD-C3D-C2D	5.12	141.97	127.25
12	G	1345	PHO	C1-C2-C3	5.10	134.87	126.04
17	L	1047	BCR	C38-C26-C25	5.06	130.21	124.53
16	L	1046	HEM	C4D-CHA-C1A	-5.01	121.91	129.64
12	A	1345	PHO	C1-C2-C3	4.98	134.66	126.04
12	G	1345	PHO	C4A-NA-C1A	4.93	112.12	108.14
11	I	1461	CLA	CBD-CAD-C3D	4.92	107.86	104.34
12	J	1352	PHO	C4A-NA-C1A	4.91	112.11	108.14
11	B	1495	CLA	CAA-C2A-C3A	-4.87	99.44	112.78
12	D	1352	PHO	CBD-CHA-C4D	-4.85	103.07	108.54
16	E	1085	HEM	C4D-CHA-C1A	-4.81	122.21	129.64
11	H	1482	CLA	CAA-C2A-C3A	-4.73	99.83	112.78
11	H	1495	CLA	CAA-C2A-C3A	-4.73	99.84	112.78
11	B	1489	CLA	C1-C2-C3	4.71	134.38	126.75
11	B	1492	CLA	C7-C6-C5	-4.71	100.56	113.36
11	C	1461	CLA	CBD-CAD-C3D	4.62	107.65	104.34
11	D	1351	CLA	OBD-CAD-CBD	-4.55	119.40	125.89
11	B	1482	CLA	CAA-C2A-C3A	-4.55	100.33	112.78
12	A	1345	PHO	C4A-NA-C1A	4.54	111.81	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1346	CLA	OBD-CAD-CBD	-4.53	119.42	125.89
11	H	1489	CLA	C1-C2-C3	4.52	134.07	126.75
11	B	1486	CLA	CAA-C2A-C3A	-4.51	105.58	116.10
11	H	1491	CLA	CBD-CAD-C3D	4.49	107.55	104.34
11	B	1491	CLA	CBD-CAD-C3D	4.46	107.53	104.34
11	B	1482	CLA	CED-O2D-CGD	4.43	125.96	115.94
16	E	1085	HEM	C3A-C2A-C1A	-4.40	102.52	106.29
11	H	1492	CLA	C7-C6-C5	-4.36	101.52	113.36
11	B	1494	CLA	C1-C2-C3	4.35	133.57	126.04
12	J	1352	PHO	CBD-CHA-C4D	-4.31	103.68	108.54
11	I	1468	CLA	CBD-CAD-C3D	4.30	107.42	104.34
11	H	1492	CLA	C1-C2-C3	4.27	133.43	126.04
11	I	1465	CLA	C7-C6-C5	-4.27	101.77	113.36
17	L	1047	BCR	C7-C8-C9	4.27	132.68	126.23
11	B	1495	CLA	O2A-CGA-CBA	4.26	125.27	111.91
11	C	1465	CLA	C7-C6-C5	-4.21	101.91	113.36
11	I	1471	CLA	CAA-C2A-C3A	-4.21	106.27	116.10
11	B	1493	CLA	CAA-C2A-C3A	-4.20	101.27	112.78
11	H	1486	CLA	CAA-C2A-C3A	-4.16	106.39	116.10
18	T	1138	HEC	CAD-CBD-CGD	4.13	119.60	112.67
11	D	1351	CLA	C1D-CHD-C4C	4.12	128.00	122.56
11	H	1493	CLA	CAA-C2A-C3A	-4.12	101.50	112.78
11	H	1494	CLA	C1D-CHD-C4C	4.12	127.99	122.56
11	J	1351	CLA	C1D-CHD-C4C	4.11	127.98	122.56
11	H	1490	CLA	C1D-CHD-C4C	4.07	127.93	122.56
11	I	1464	CLA	O2A-C1-C2	4.05	119.29	108.64
12	A	1345	PHO	CBD-CHA-C4D	-4.05	103.97	108.54
11	H	1482	CLA	CED-O2D-CGD	4.04	125.07	115.94
11	H	1494	CLA	C1-C2-C3	4.02	132.99	126.04
11	I	1470	CLA	CMA-C3A-C2A	-3.99	106.79	116.10
11	H	1487	CLA	OBD-CAD-CBD	-3.97	120.22	125.89
11	G	1346	CLA	OBD-CAD-CBD	-3.96	120.23	125.89
12	G	1345	PHO	CBD-CHA-C4D	-3.96	104.08	108.54
16	L	1046	HEM	C3A-C2A-C1A	-3.95	102.91	106.29
11	H	1494	CLA	C7-C6-C5	-3.94	102.65	113.36
11	C	1468	CLA	CBD-CAD-C3D	3.94	107.16	104.34
11	H	1495	CLA	O2A-CGA-CBA	3.93	124.24	111.91
11	H	1492	CLA	C1D-CHD-C4C	3.92	127.74	122.56
11	B	1492	CLA	C1-C2-C3	3.89	132.78	126.04
11	C	1464	CLA	O2A-C1-C2	3.88	118.84	108.64
11	J	1353	CLA	OBD-CAD-CBD	-3.88	120.36	125.89
11	J	1351	CLA	O2A-C1-C2	3.88	118.82	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	I	1465	CLA	C1D-CHD-C4C	3.87	127.67	122.56
11	B	1494	CLA	C7-C6-C5	-3.86	102.86	113.36
11	B	1490	CLA	C1D-CHD-C4C	3.85	127.64	122.56
11	C	1466	CLA	CAA-C2A-C3A	-3.85	102.24	112.78
11	G	1343	CLA	OBD-CAD-CBD	-3.84	120.41	125.89
11	D	1353	CLA	OBD-CAD-CBD	-3.80	120.47	125.89
11	B	1496	CLA	C1D-CHD-C4C	3.80	127.57	122.56
11	G	1343	CLA	CED-O2D-CGD	3.79	124.52	115.94
11	C	1464	CLA	CED-O2D-CGD	3.79	124.51	115.94
11	B	1486	CLA	CMA-C3A-C2A	-3.78	107.27	116.10
17	F	1046	BCR	C7-C8-C9	3.78	131.95	126.23
17	F	1046	BCR	C38-C26-C27	-3.78	106.36	113.62
11	I	1466	CLA	CAA-C2A-C3A	-3.77	102.46	112.78
11	H	1487	CLA	O2A-CGA-CBA	3.76	123.71	111.91
11	C	1463	CLA	OBD-CAD-CBD	-3.76	120.53	125.89
11	H	1482	CLA	C1D-CHD-C4C	3.75	127.51	122.56
11	C	1462	CLA	OBD-CAD-CBD	-3.74	120.55	125.89
11	D	1351	CLA	O2A-C1-C2	3.74	118.47	108.64
11	I	1462	CLA	OBD-CAD-CBD	-3.74	120.55	125.89
11	C	1465	CLA	C1D-CHD-C4C	3.74	127.49	122.56
11	I	1459	CLA	C1D-CHD-C4C	3.73	127.48	122.56
11	J	1351	CLA	OBD-CAD-CBD	-3.72	120.57	125.89
11	C	1471	CLA	CAA-C2A-C3A	-3.72	107.41	116.10
11	C	1463	CLA	C1D-CHD-C4C	3.72	127.47	122.56
11	I	1471	CLA	CMA-C3A-C2A	-3.72	107.42	116.10
11	B	1487	CLA	OBD-CAD-CBD	-3.72	120.58	125.89
11	H	1493	CLA	C1D-CHD-C4C	3.71	127.46	122.56
11	I	1462	CLA	C1D-CHD-C4C	3.71	127.45	122.56
11	I	1469	CLA	CAA-C2A-C3A	-3.71	107.45	116.10
11	H	1496	CLA	C1D-CHD-C4C	3.70	127.45	122.56
17	L	1047	BCR	C2-C1-C6	3.70	116.18	110.48
11	H	1489	CLA	OBD-CAD-CBD	-3.70	120.61	125.89
11	B	1492	CLA	C1D-CHD-C4C	3.70	127.44	122.56
11	C	1466	CLA	C1-C2-C3	3.70	132.73	126.75
11	B	1493	CLA	OBD-CAD-CBD	-3.70	120.61	125.89
11	C	1462	CLA	C1D-CHD-C4C	3.68	127.41	122.56
11	A	1342	CLA	C7-C6-C5	-3.68	103.38	113.36
11	B	1488	CLA	O2D-CGD-CBD	3.67	117.79	111.27
17	L	1047	BCR	C33-C5-C6	3.67	128.65	124.53
11	I	1471	CLA	C1D-CHD-C4C	3.67	127.40	122.56
11	H	1486	CLA	C1D-CHD-C4C	3.66	127.38	122.56
11	B	1482	CLA	C1D-CHD-C4C	3.65	127.37	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	I	1464	CLA	CED-O2D-CGD	3.63	124.15	115.94
11	C	1466	CLA	C1D-CHD-C4C	3.63	127.34	122.56
11	H	1486	CLA	CMA-C3A-C2A	-3.63	107.64	116.10
11	B	1495	CLA	C1D-CHD-C4C	3.62	127.34	122.56
17	L	1047	BCR	C29-C30-C25	3.61	116.04	110.48
11	A	1343	CLA	CED-O2D-CGD	3.61	124.11	115.94
11	G	1342	CLA	C7-C6-C5	-3.61	103.55	113.36
11	H	1497	CLA	C1D-CHD-C4C	3.60	127.31	122.56
11	B	1482	CLA	O2A-CGA-CBA	3.60	123.20	111.91
11	I	1469	CLA	CMA-C3A-C2A	-3.60	107.70	116.10
17	F	1046	BCR	C2-C1-C6	3.59	116.01	110.48
11	C	1469	CLA	CMA-C3A-C2A	-3.58	107.73	116.10
17	L	1047	BCR	C12-C13-C14	-3.58	113.44	118.94
17	F	1046	BCR	C29-C30-C25	3.58	115.99	110.48
11	B	1495	CLA	OBD-CAD-CBD	-3.58	120.78	125.89
11	C	1470	CLA	CMA-C3A-C2A	-3.58	107.75	116.10
11	A	1346	CLA	C1D-CHD-C4C	3.57	127.28	122.56
17	L	1047	BCR	C38-C26-C27	-3.57	106.76	113.62
11	C	1469	CLA	CAA-C2A-C3A	-3.56	107.78	116.10
11	C	1459	CLA	CAA-C2A-C3A	-3.56	103.03	112.78
11	C	1468	CLA	C1C-NC-C4C	3.55	108.30	106.71
11	I	1463	CLA	C1D-CHD-C4C	3.55	127.25	122.56
11	H	1494	CLA	OBD-CAD-CBD	-3.55	120.82	125.89
11	I	1466	CLA	C1D-CHD-C4C	3.55	127.24	122.56
11	H	1482	CLA	OBD-CAD-CBD	-3.55	120.82	125.89
11	I	1467	CLA	OBD-CAD-CBD	-3.55	120.82	125.89
17	L	1047	BCR	C15-C14-C13	3.55	132.38	127.31
11	I	1463	CLA	OBD-CAD-CBD	-3.55	120.83	125.89
11	B	1487	CLA	O2A-CGA-CBA	3.54	123.00	111.91
11	C	1470	CLA	C1D-CHD-C4C	3.53	127.21	122.56
11	H	1482	CLA	C1-C2-C3	3.53	132.14	126.04
11	B	1488	CLA	OBD-CAD-CBD	-3.52	120.87	125.89
11	B	1493	CLA	C1D-CHD-C4C	3.51	127.19	122.56
11	B	1492	CLA	CED-O2D-CGD	3.51	123.88	115.94
11	G	1344	CLA	OBD-CAD-CBD	-3.50	120.89	125.89
11	C	1462	CLA	O2A-C1-C2	3.50	117.84	108.64
11	C	1471	CLA	C1D-CHD-C4C	3.50	127.18	122.56
11	B	1497	CLA	C1D-CHD-C4C	3.50	127.18	122.56
11	B	1496	CLA	OBD-CAD-CBD	-3.48	120.92	125.89
11	C	1467	CLA	C1D-CHD-C4C	3.48	127.15	122.56
11	H	1489	CLA	O2D-CGD-CBD	3.48	117.45	111.27
11	I	1463	CLA	CED-O2D-CGD	3.48	123.81	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	1490	CLA	CED-O2D-CGD	3.48	123.80	115.94
11	C	1470	CLA	CAA-C2A-C3A	-3.47	108.00	116.10
11	B	1491	CLA	C1C-NC-C4C	3.47	108.27	106.71
11	H	1495	CLA	C1D-CHD-C4C	3.47	127.13	122.56
11	I	1464	CLA	OBD-CAD-CBD	-3.46	120.95	125.89
11	B	1494	CLA	C1D-CHD-C4C	3.46	127.12	122.56
11	B	1482	CLA	C1-C2-C3	3.45	132.01	126.04
11	A	1343	CLA	OBD-CAD-CBD	-3.44	120.98	125.89
11	H	1489	CLA	C1D-CHD-C4C	3.44	127.10	122.56
11	I	1459	CLA	CAA-C2A-C3A	-3.44	103.36	112.78
11	H	1493	CLA	OBD-CAD-CBD	-3.43	120.99	125.89
12	D	1352	PHO	O2A-CGA-CBA	3.43	122.67	111.91
17	F	1046	BCR	C35-C13-C12	3.43	123.47	118.08
11	C	1460	CLA	OBD-CAD-CBD	-3.42	121.00	125.89
11	B	1496	CLA	C7-C6-C5	-3.41	104.09	113.36
17	F	1046	BCR	C33-C5-C6	3.41	128.35	124.53
11	C	1464	CLA	C7-C6-C5	-3.40	104.12	113.36
11	B	1490	CLA	CED-O2D-CGD	3.40	123.63	115.94
11	C	1469	CLA	C1D-CHD-C4C	3.40	127.04	122.56
11	C	1462	CLA	CED-O2D-CGD	3.40	123.62	115.94
11	G	1346	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
11	C	1460	CLA	C1D-CHD-C4C	3.40	127.04	122.56
11	H	1485	CLA	OBD-CAD-CBD	-3.39	121.05	125.89
11	I	1470	CLA	CAA-C2A-C3A	-3.39	108.19	116.10
11	B	1484	CLA	CAA-C2A-C3A	-3.39	103.50	112.78
11	I	1464	CLA	C7-C6-C5	-3.39	104.16	113.36
11	H	1496	CLA	C7-C6-C5	-3.38	104.19	113.36
11	H	1497	CLA	CAA-C2A-C3A	-3.38	108.22	116.10
18	V	1138	HEC	CAD-CBD-CGD	3.37	118.32	112.67
11	C	1464	CLA	C1D-CHD-C4C	3.37	127.00	122.56
11	A	1342	CLA	CED-O2D-CGD	3.36	123.54	115.94
16	L	1046	HEM	C3D-C4D-ND	3.36	110.92	108.27
12	G	1345	PHO	C7-C6-C5	-3.35	104.25	113.36
11	H	1484	CLA	CAA-C2A-C3A	-3.35	103.59	112.78
11	B	1497	CLA	CAA-C2A-C3A	-3.35	108.28	116.10
17	F	1046	BCR	C12-C13-C14	-3.34	113.81	118.94
11	C	1471	CLA	CMA-C3A-C2A	-3.34	108.30	116.10
12	D	1352	PHO	CBD-CHA-C1A	3.34	134.16	126.40
11	H	1495	CLA	O2D-CGD-CBD	3.34	117.20	111.27
11	J	1353	CLA	C1D-CHD-C4C	3.33	126.96	122.56
11	B	1489	CLA	C1D-CHD-C4C	3.33	126.95	122.56
11	A	1342	CLA	C1D-CHD-C4C	3.32	126.94	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	1492	CLA	CED-O2D-CGD	3.31	123.43	115.94
12	A	1345	PHO	CED-O2D-CGD	3.31	123.43	115.94
12	J	1352	PHO	C7-C6-C5	-3.30	104.39	113.36
11	B	1489	CLA	O2D-CGD-CBD	3.30	117.13	111.27
11	I	1469	CLA	C1D-CHD-C4C	3.30	126.91	122.56
12	D	1352	PHO	CAB-C3B-C2B	-3.30	117.74	128.60
11	B	1488	CLA	C1D-CHD-C4C	3.29	126.91	122.56
11	H	1488	CLA	O2D-CGD-CBD	3.29	117.12	111.27
11	A	1343	CLA	O2A-C1-C2	-3.29	99.98	108.64
11	G	1343	CLA	O2A-CGA-CBA	3.29	122.23	111.91
11	I	1466	CLA	C1-C2-C3	3.29	132.07	126.75
12	J	1352	PHO	CAB-C3B-C2B	-3.28	117.78	128.60
12	J	1352	PHO	CBD-CHA-C1A	3.28	134.01	126.40
11	H	1497	CLA	CED-O2D-CGD	3.28	123.35	115.94
12	G	1345	PHO	CED-O2D-CGD	3.28	123.34	115.94
17	F	1046	BCR	C23-C24-C25	3.27	136.40	127.20
11	C	1467	CLA	OBD-CAD-CBD	-3.27	121.22	125.89
17	F	1046	BCR	C15-C14-C13	3.26	131.96	127.31
11	I	1465	CLA	C1-C2-C3	3.26	131.68	126.04
11	B	1483	CLA	C1D-CHD-C4C	3.26	126.86	122.56
11	C	1460	CLA	O2A-CGA-CBA	3.26	122.12	111.91
11	B	1496	CLA	C1-C2-C3	3.25	131.66	126.04
11	B	1483	CLA	CAA-C2A-C3A	-3.25	103.89	112.78
11	G	1346	CLA	C1D-CHD-C4C	3.24	126.84	122.56
11	I	1470	CLA	C1D-CHD-C4C	3.24	126.84	122.56
11	I	1462	CLA	O2A-C1-C2	3.24	117.15	108.64
11	H	1483	CLA	C1D-CHD-C4C	3.24	126.83	122.56
11	I	1463	CLA	C7-C6-C5	-3.23	104.57	113.36
11	C	1463	CLA	C7-C6-C5	-3.23	104.58	113.36
12	D	1352	PHO	C2A-C1A-NA	-3.23	108.16	111.86
11	I	1466	CLA	CED-O2D-CGD	3.22	123.22	115.94
11	I	1462	CLA	CAA-C2A-C3A	-3.22	103.97	112.78
17	F	1046	BCR	C30-C25-C26	-3.21	118.09	122.61
12	D	1352	PHO	CAA-C2A-C3A	-3.21	103.98	112.78
11	A	1342	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
12	J	1352	PHO	CED-O2D-CGD	3.21	123.19	115.94
11	H	1483	CLA	OBD-CAD-CBD	-3.20	121.32	125.89
11	C	1464	CLA	OBD-CAD-CBD	-3.20	121.32	125.89
11	I	1464	CLA	O2D-CGD-CBD	3.20	116.95	111.27
11	C	1463	CLA	CED-O2D-CGD	3.20	123.17	115.94
11	H	1482	CLA	O2A-CGA-CBA	3.20	121.94	111.91
11	H	1485	CLA	C1D-CHD-C4C	3.20	126.78	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	1352	PHO	C7-C6-C5	-3.20	104.68	113.36
11	H	1488	CLA	OBD-CAD-CBD	-3.19	121.33	125.89
12	J	1352	PHO	C2A-C1A-NA	-3.19	108.20	111.86
11	H	1491	CLA	C1C-NC-C4C	3.19	108.14	106.71
11	G	1343	CLA	C1D-CHD-C4C	3.19	126.77	122.56
17	L	1047	BCR	C35-C13-C12	3.19	123.10	118.08
11	I	1460	CLA	CED-O2D-CGD	3.19	123.15	115.94
11	B	1487	CLA	C1-C2-C3	3.18	131.55	126.04
11	G	1342	CLA	C1D-CHD-C4C	3.17	126.74	122.56
11	I	1462	CLA	O2A-CGA-CBA	3.16	121.81	111.91
12	J	1352	PHO	CAA-C2A-C3A	-3.15	104.14	112.78
11	H	1484	CLA	CED-O2D-CGD	3.15	123.06	115.94
16	L	1046	HEM	C1B-NB-C4B	3.15	108.16	105.79
11	B	1497	CLA	C2A-C3A-C4A	3.14	105.79	101.78
12	A	1345	PHO	C7-C6-C5	-3.14	104.83	113.36
17	L	1047	BCR	C33-C5-C4	-3.13	107.60	113.62
11	I	1464	CLA	C1D-CHD-C4C	3.13	126.68	122.56
11	G	1342	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
11	B	1486	CLA	C1D-CHD-C4C	3.12	126.68	122.56
11	H	1489	CLA	O2A-CGA-CBA	3.12	121.70	111.91
16	E	1085	HEM	C3D-C4D-ND	3.12	110.73	108.27
11	H	1492	CLA	C6-C5-C3	3.12	121.64	113.45
11	H	1488	CLA	C1D-CHD-C4C	3.12	126.67	122.56
11	I	1462	CLA	CED-O2D-CGD	3.12	122.99	115.94
12	A	1345	PHO	CAB-C3B-C2B	-3.11	118.34	128.60
11	I	1460	CLA	C1D-CHD-C4C	3.11	126.66	122.56
11	A	1344	CLA	C1D-CHD-C4C	3.11	126.66	122.56
17	L	1047	BCR	C30-C25-C26	-3.11	118.24	122.61
11	C	1459	CLA	C1D-CHD-C4C	3.11	126.66	122.56
11	B	1485	CLA	C1D-CHD-C4C	3.10	126.66	122.56
11	H	1487	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
11	I	1470	CLA	OBD-CAD-CBD	-3.09	121.48	125.89
11	I	1463	CLA	O2A-CGA-CBA	3.09	121.60	111.91
11	I	1461	CLA	C1C-NC-C4C	3.09	108.09	106.71
11	H	1496	CLA	C1-C2-C3	3.08	131.38	126.04
11	C	1460	CLA	CED-O2D-CGD	3.08	122.91	115.94
11	C	1462	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
11	G	1346	CLA	C1-C2-C3	3.08	131.37	126.04
11	B	1496	CLA	C6-C5-C3	3.08	121.52	113.45
11	J	1351	CLA	O2A-CGA-CBA	3.08	121.56	111.91
12	J	1352	PHO	O2A-CGA-CBA	3.06	121.51	111.91
11	C	1465	CLA	OBD-CAD-CBD	-3.06	121.52	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	1495	CLA	C2A-C1A-CHA	3.05	129.20	123.86
11	I	1467	CLA	C4D-C3D-CAD	-3.05	106.77	108.47
11	H	1487	CLA	O2D-CGD-CBD	3.05	116.69	111.27
11	I	1460	CLA	O2A-CGA-CBA	3.05	121.47	111.91
11	H	1487	CLA	C1-C2-C3	3.05	131.31	126.04
11	B	1492	CLA	C6-C5-C3	3.05	121.44	113.45
11	H	1483	CLA	CAA-C2A-C3A	-3.04	104.44	112.78
11	B	1485	CLA	CED-O2D-CGD	3.04	122.82	115.94
17	F	1046	BCR	C33-C5-C4	-3.04	107.77	113.62
11	B	1483	CLA	OBD-CAD-CBD	-3.04	121.55	125.89
11	A	1343	CLA	O2A-CGA-CBA	3.03	121.41	111.91
11	A	1346	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
11	A	1343	CLA	C1D-CHD-C4C	3.03	126.55	122.56
11	D	1353	CLA	C1D-CHD-C4C	3.02	126.55	122.56
11	H	1495	CLA	OBD-CAD-CBD	-3.02	121.58	125.89
12	G	1345	PHO	CAB-C3B-C2B	-3.02	118.67	128.60
11	B	1487	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
11	B	1490	CLA	OBD-CAD-CBD	-3.01	121.60	125.89
11	B	1497	CLA	OBD-CAD-CBD	-3.00	121.60	125.89
11	B	1488	CLA	CAA-C2A-C3A	-3.00	104.56	112.78
11	B	1489	CLA	O2A-CGA-CBA	2.99	121.30	111.91
11	G	1344	CLA	C1D-CHD-C4C	2.99	126.51	122.56
11	C	1464	CLA	C1-C2-C3	-2.99	120.87	126.04
11	G	1344	CLA	CAA-C2A-C3A	-2.99	104.58	112.78
11	C	1468	CLA	C2A-C1A-CHA	2.99	127.34	122.71
11	C	1463	CLA	O2A-CGA-CBA	2.99	121.28	111.91
11	C	1459	CLA	OBD-CAD-CBD	-2.98	121.64	125.89
11	G	1342	CLA	O2A-CGA-CBA	2.98	121.25	111.91
11	B	1495	CLA	O2A-C1-C2	2.98	116.46	108.64
11	G	1342	CLA	CED-O2D-CGD	2.98	122.67	115.94
11	B	1495	CLA	C2A-C1A-CHA	2.97	129.06	123.86
11	A	1346	CLA	O2A-CGA-CBA	2.97	121.22	111.91
11	H	1496	CLA	CED-O2D-CGD	2.96	122.63	115.94
11	G	1346	CLA	CMB-C2B-C3B	2.95	130.21	124.68
11	C	1462	CLA	CAA-C2A-C3A	-2.95	104.69	112.78
11	H	1486	CLA	OBD-CAD-CBD	-2.95	121.68	125.89
11	G	1343	CLA	O2A-C1-C2	-2.95	100.88	108.64
11	H	1497	CLA	OBD-CAD-C3D	2.94	132.86	127.98
11	H	1484	CLA	C1D-CHD-C4C	2.93	126.43	122.56
11	B	1497	CLA	O2D-CGD-CBD	2.93	116.48	111.27
11	C	1470	CLA	CED-O2D-CGD	2.93	122.57	115.94
11	H	1490	CLA	OBD-CAD-CBD	-2.92	121.72	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	J	1351	CLA	CED-O2D-CGD	2.92	122.54	115.94
11	H	1486	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
11	C	1466	CLA	CED-O2D-CGD	2.90	122.50	115.94
11	I	1462	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
11	H	1497	CLA	OBD-CAD-CBD	-2.90	121.75	125.89
11	I	1465	CLA	OBD-CAD-CBD	-2.90	121.76	125.89
17	L	1047	BCR	C34-C9-C8	2.90	122.64	118.08
11	D	1351	CLA	O2A-CGA-CBA	2.89	120.99	111.91
11	I	1467	CLA	C1D-CHD-C4C	2.89	126.38	122.56
11	B	1482	CLA	OBD-CAD-CBD	-2.89	121.76	125.89
11	C	1461	CLA	C1C-NC-C4C	2.89	108.01	106.71
12	A	1345	PHO	CBD-CHA-C1A	2.89	133.10	126.40
11	B	1484	CLA	CED-O2D-CGD	2.89	122.47	115.94
17	L	1047	BCR	C23-C24-C25	2.89	135.31	127.20
11	C	1463	CLA	C6-C5-C3	2.88	121.02	113.45
11	I	1468	CLA	C2A-C1A-CHA	2.88	127.17	122.71
11	A	1343	CLA	CAA-C2A-C3A	-2.88	104.90	112.78
11	H	1497	CLA	C2A-C3A-C4A	2.87	105.45	101.78
11	G	1346	CLA	O2A-CGA-CBA	2.87	120.93	111.91
11	J	1353	CLA	O2A-CGA-CBA	2.87	120.92	111.91
11	I	1463	CLA	C6-C5-C3	2.87	120.98	113.45
11	B	1496	CLA	C2A-C3A-C4A	2.87	106.50	101.87
17	F	1046	BCR	C1-C6-C5	-2.86	118.58	122.61
11	J	1353	CLA	C1-C2-C3	2.86	131.38	126.75
11	C	1464	CLA	O2D-CGD-CBD	2.85	116.34	111.27
11	C	1465	CLA	O2D-CGD-CBD	2.85	116.33	111.27
11	H	1497	CLA	O2D-CGD-CBD	2.85	116.33	111.27
11	D	1353	CLA	O2A-CGA-CBA	2.85	120.86	111.91
11	B	1484	CLA	C1D-CHD-C4C	2.85	126.32	122.56
11	B	1485	CLA	OBD-CAD-CBD	-2.85	121.83	125.89
17	L	1047	BCR	C19-C18-C17	-2.84	114.58	118.94
11	B	1494	CLA	OBD-CAD-CBD	-2.84	121.83	125.89
17	L	1047	BCR	C1-C6-C5	-2.84	118.61	122.61
11	C	1462	CLA	C7-C6-C5	-2.83	105.66	113.36
11	I	1464	CLA	O2A-CGA-CBA	2.83	120.80	111.91
11	G	1346	CLA	O2D-CGD-CBD	2.83	116.30	111.27
11	A	1344	CLA	CAA-C2A-C3A	-2.83	105.04	112.78
11	I	1465	CLA	CED-O2D-CGD	2.82	122.32	115.94
12	G	1345	PHO	CBD-CHA-C1A	2.82	132.95	126.40
11	H	1493	CLA	CED-O2D-CGD	2.82	122.32	115.94
11	I	1465	CLA	O2D-CGD-CBD	2.82	116.27	111.27
11	H	1494	CLA	O2A-CGA-CBA	2.82	120.74	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	I	1461	CLA	C2A-C1A-CHA	2.81	127.07	122.71
17	L	1047	BCR	C8-C9-C10	-2.81	114.63	118.94
11	B	1487	CLA	CED-O2D-CGD	2.81	122.29	115.94
11	C	1464	CLA	O2A-CGA-CBA	2.81	120.72	111.91
11	H	1484	CLA	CMB-C2B-C1B	-2.81	124.15	128.46
11	C	1462	CLA	O2A-CGA-CBA	2.81	120.72	111.91
11	H	1483	CLA	CED-O2D-CGD	2.80	122.28	115.94
11	H	1486	CLA	CED-O2D-CGD	2.80	122.28	115.94
11	B	1482	CLA	CBA-CAA-C2A	2.80	122.14	113.86
11	B	1485	CLA	C2A-C3A-C4A	2.80	106.40	101.87
11	J	1351	CLA	C2A-C1A-CHA	2.80	128.75	123.86
11	D	1353	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
11	H	1495	CLA	O2A-C1-C2	2.79	115.97	108.64
17	F	1046	BCR	C1-C6-C7	2.79	123.67	115.78
11	A	1342	CLA	O2A-CGA-CBA	2.79	120.65	111.91
11	H	1488	CLA	CAA-C2A-C3A	-2.78	105.15	112.78
11	H	1491	CLA	C2A-C1A-CHA	2.78	127.02	122.71
11	B	1491	CLA	C2A-C1A-CHA	2.78	127.02	122.71
11	C	1461	CLA	C2A-C1A-CHA	2.77	127.00	122.71
17	L	1047	BCR	C1-C6-C7	2.76	123.58	115.78
11	C	1466	CLA	O2A-CGA-CBA	2.75	120.54	111.91
11	B	1486	CLA	C2A-C3A-C4A	2.75	105.29	101.78
11	I	1465	CLA	O2A-CGA-CBA	2.75	120.53	111.91
11	A	1346	CLA	C1-C2-C3	2.75	130.79	126.04
11	B	1494	CLA	CED-O2D-CGD	2.74	122.14	115.94
11	B	1496	CLA	O2A-CGA-CBA	2.74	120.50	111.91
11	H	1487	CLA	OBD-CAD-C3D	2.74	132.53	127.98
11	B	1488	CLA	O2A-CGA-CBA	2.74	120.50	111.91
11	H	1495	CLA	CED-O2D-CGD	2.74	122.13	115.94
11	C	1470	CLA	OBD-CAD-CBD	-2.73	121.99	125.89
17	F	1046	BCR	C19-C18-C17	-2.73	114.75	118.94
11	I	1466	CLA	CBA-CAA-C2A	2.73	121.93	113.86
11	B	1482	CLA	C2A-C3A-C4A	2.73	106.28	101.87
11	C	1467	CLA	C2A-C1A-CHA	2.72	128.62	123.86
11	B	1484	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
11	I	1459	CLA	CED-O2D-CGD	2.72	122.09	115.94
11	H	1489	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
11	I	1464	CLA	C1-C2-C3	-2.72	121.34	126.04
11	A	1343	CLA	C2A-C3A-C4A	2.72	106.25	101.87
11	A	1346	CLA	OBD-CAD-C3D	2.71	132.49	127.98
11	H	1482	CLA	CBA-CAA-C2A	2.71	121.87	113.86
11	J	1351	CLA	CAA-C2A-C3A	-2.71	105.36	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	F	1046	BCR	C36-C18-C19	2.71	122.34	118.08
11	H	1483	CLA	O2A-CGA-CBA	2.70	120.38	111.91
11	A	1346	CLA	CED-O2D-CGD	2.70	122.04	115.94
11	I	1466	CLA	O2A-CGA-CBA	2.70	120.38	111.91
11	B	1492	CLA	OBD-CAD-CBD	-2.70	122.04	125.89
11	G	1346	CLA	CAA-C2A-C3A	-2.70	105.40	112.78
11	G	1343	CLA	C2A-C3A-C4A	2.69	106.22	101.87
11	H	1492	CLA	C6-C7-C8	2.69	124.61	115.92
11	B	1497	CLA	OBD-CAD-C3D	2.69	132.44	127.98
11	I	1466	CLA	OBD-CAD-CBD	-2.69	122.05	125.89
11	H	1496	CLA	C2A-C3A-C4A	2.68	106.20	101.87
11	C	1465	CLA	C1-C2-C3	2.68	130.68	126.04
11	I	1465	CLA	C12-C11-C10	-2.68	100.93	113.24
11	C	1466	CLA	CBA-CAA-C2A	2.68	121.77	113.86
11	B	1484	CLA	OBD-CAD-CBD	-2.68	122.07	125.89
11	H	1494	CLA	CED-O2D-CGD	2.67	121.98	115.94
11	I	1469	CLA	CED-O2D-CGD	2.67	121.97	115.94
11	B	1490	CLA	CAA-C2A-C3A	-2.67	105.48	112.78
11	H	1490	CLA	CAA-C2A-C3A	-2.66	105.48	112.78
11	B	1486	CLA	CMB-C2B-C1B	-2.66	124.37	128.46
11	B	1493	CLA	OBD-CAD-C3D	2.66	132.40	127.98
11	H	1484	CLA	OBD-CAD-CBD	-2.66	122.09	125.89
11	H	1490	CLA	C2A-C1A-CHA	2.66	128.51	123.86
11	A	1343	CLA	CBA-CAA-C2A	2.66	121.72	113.86
11	I	1460	CLA	OBD-CAD-CBD	-2.66	122.09	125.89
11	H	1485	CLA	CED-O2D-CGD	2.66	121.95	115.94
11	A	1344	CLA	OBD-CAD-CBD	-2.66	122.10	125.89
11	A	1342	CLA	CAA-C2A-C3A	-2.65	105.51	112.78
11	I	1469	CLA	C2A-C3A-C4A	2.65	105.17	101.78
11	C	1465	CLA	CED-O2D-CGD	2.65	121.93	115.94
17	F	1046	BCR	C34-C9-C8	2.65	122.25	118.08
11	H	1482	CLA	OBD-CAD-C3D	2.65	132.38	127.98
11	B	1497	CLA	CED-O2D-CGD	2.65	121.92	115.94
11	B	1485	CLA	CAA-C2A-C3A	-2.64	105.56	112.78
11	H	1493	CLA	C2A-C3A-C4A	2.63	106.12	101.87
11	C	1465	CLA	O2A-CGA-CBA	2.63	120.16	111.91
11	H	1496	CLA	OBD-CAD-CBD	-2.63	122.14	125.89
11	B	1487	CLA	C1D-CHD-C4C	2.63	126.02	122.56
11	A	1346	CLA	C4D-C3D-CAD	-2.63	107.01	108.47
11	H	1494	CLA	C2A-C3A-C4A	2.62	106.11	101.87
11	I	1463	CLA	C2A-C1A-CHA	2.62	128.44	123.86
11	C	1465	CLA	C12-C11-C10	-2.62	101.21	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1487	CLA	C12-C11-C10	-2.61	101.22	113.24
11	C	1471	CLA	CED-O2D-CGD	2.61	121.83	115.94
11	B	1497	CLA	CMA-C3A-C2A	-2.61	110.02	116.10
11	J	1353	CLA	C2A-C3A-C4A	2.60	106.08	101.87
11	I	1459	CLA	C2A-C3A-C4A	2.60	106.07	101.87
11	C	1463	CLA	OBD-CAD-C3D	2.60	132.30	127.98
11	B	1483	CLA	O2D-CGD-CBD	2.60	115.89	111.27
12	D	1352	PHO	CED-O2D-CGD	2.60	121.82	115.94
11	C	1471	CLA	C2A-C3A-C4A	2.60	105.10	101.78
17	F	1046	BCR	C23-C22-C21	-2.60	114.95	118.94
11	B	1494	CLA	O2A-CGA-CBA	2.59	120.05	111.91
11	D	1351	CLA	OBD-CAD-C3D	2.59	132.28	127.98
16	L	1046	HEM	C4C-NC-C1C	2.59	107.74	105.79
11	C	1462	CLA	OBD-CAD-C3D	2.58	132.27	127.98
11	D	1351	CLA	C2A-C3A-C4A	2.58	106.04	101.87
11	B	1483	CLA	C7-C6-C5	-2.58	106.35	113.36
12	J	1352	PHO	C1-C2-C3	2.58	130.50	126.04
11	H	1496	CLA	C6-C5-C3	2.58	120.21	113.45
11	A	1346	CLA	O2D-CGD-CBD	2.57	115.84	111.27
11	G	1343	CLA	CBA-CAA-C2A	2.57	121.44	113.86
11	G	1342	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
11	I	1470	CLA	CED-O2D-CGD	2.56	121.73	115.94
11	G	1343	CLA	CAA-C2A-C3A	-2.56	105.78	112.78
11	H	1487	CLA	CMB-C2B-C3B	2.55	129.44	124.68
11	H	1482	CLA	C2A-C3A-C4A	2.54	105.98	101.87
11	C	1469	CLA	CED-O2D-CGD	2.54	121.69	115.94
11	D	1353	CLA	C2A-C3A-C4A	2.54	105.97	101.87
11	H	1487	CLA	C12-C11-C10	-2.54	101.57	113.24
11	D	1351	CLA	C12-C11-C10	-2.53	101.61	113.24
11	I	1468	CLA	C1C-NC-C4C	2.53	107.84	106.71
11	B	1483	CLA	O2A-CGA-CBA	2.53	119.84	111.91
11	A	1344	CLA	CED-O2D-CGD	2.53	121.65	115.94
11	B	1487	CLA	OBD-CAD-C3D	2.53	132.18	127.98
11	A	1344	CLA	CAA-CBA-CGA	2.52	119.02	113.59
16	E	1085	HEM	C1C-CHC-C4B	-2.52	125.75	129.64
11	H	1492	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
11	J	1353	CLA	CAA-C2A-C3A	-2.52	105.88	112.78
11	C	1469	CLA	C2A-C3A-C4A	2.52	105.00	101.78
11	H	1495	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
11	A	1344	CLA	O2D-CGD-CBD	2.52	115.74	111.27
11	B	1490	CLA	C2A-C1A-CHA	2.51	128.25	123.86
11	B	1487	CLA	O2D-CGD-CBD	2.51	115.73	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1492	CLA	O2A-CGA-CBA	2.51	119.79	111.91
11	B	1495	CLA	C2A-C3A-C4A	2.51	105.93	101.87
11	A	1346	CLA	CMB-C2B-C3B	2.51	129.38	124.68
11	G	1346	CLA	C4D-C3D-CAD	-2.51	107.07	108.47
12	G	1345	PHO	O2D-CGD-CBD	2.51	115.72	111.27
11	I	1470	CLA	C2A-C3A-C4A	2.51	104.98	101.78
11	H	1486	CLA	C2A-C3A-C4A	2.50	104.98	101.78
11	B	1493	CLA	C2A-C3A-C4A	2.50	105.91	101.87
11	I	1461	CLA	C3B-C4B-NB	-2.50	107.91	110.11
11	A	1342	CLA	OBD-CAD-CBD	-2.50	122.32	125.89
11	C	1467	CLA	CED-O2D-CGD	2.50	121.59	115.94
11	H	1487	CLA	C1D-CHD-C4C	2.50	125.86	122.56
11	H	1486	CLA	CMB-C2B-C3B	2.50	129.35	124.68
11	C	1459	CLA	CED-O2D-CGD	2.50	121.59	115.94
11	B	1489	CLA	OBD-CAD-CBD	-2.50	122.33	125.89
11	C	1462	CLA	CMB-C2B-C3B	2.49	129.34	124.68
11	D	1353	CLA	C1-C2-C3	2.49	130.78	126.75
11	I	1467	CLA	CED-O2D-CGD	2.49	121.57	115.94
11	B	1495	CLA	O2D-CGD-CBD	2.48	115.68	111.27
11	B	1488	CLA	C1-C2-C3	2.48	130.33	126.04
11	B	1496	CLA	OBD-CAD-C3D	2.48	132.09	127.98
11	J	1351	CLA	C5-C3-C2	-2.48	116.11	121.12
11	H	1492	CLA	O2A-CGA-CBA	2.48	119.68	111.91
11	H	1496	CLA	O2A-CGA-CBA	2.48	119.68	111.91
11	H	1485	CLA	C2A-C3A-C4A	2.47	105.87	101.87
12	J	1352	PHO	CAB-C3B-C4B	2.47	135.34	126.21
11	I	1462	CLA	C7-C6-C5	-2.47	106.65	113.36
12	D	1352	PHO	CAB-C3B-C4B	2.47	135.34	126.21
11	I	1471	CLA	CED-O2D-CGD	2.47	121.52	115.94
11	H	1488	CLA	O2A-CGA-CBA	2.47	119.66	111.91
11	B	1487	CLA	C4D-C3D-CAD	-2.47	107.09	108.47
11	C	1470	CLA	C2A-C3A-C4A	2.47	104.93	101.78
11	H	1485	CLA	OBD-CAD-C3D	2.46	132.07	127.98
11	A	1342	CLA	C1-C2-C3	2.46	130.30	126.04
11	I	1467	CLA	O2A-CGA-CBA	2.46	119.63	111.91
11	A	1342	CLA	CMB-C2B-C3B	2.46	129.28	124.68
11	I	1462	CLA	CMB-C2B-C3B	2.46	129.28	124.68
11	C	1463	CLA	CMB-C2B-C1B	-2.46	124.69	128.46
16	E	1085	HEM	C4C-NC-C1C	2.46	107.64	105.79
11	G	1342	CLA	C2A-C3A-C4A	2.45	105.83	101.87
11	B	1482	CLA	OBD-CAD-C3D	2.45	132.05	127.98
11	H	1487	CLA	CED-O2D-CGD	2.45	121.48	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1342	CLA	C16-C15-C13	2.45	123.85	115.92
11	H	1488	CLA	C1-O2A-CGA	2.45	122.88	116.44
11	G	1343	CLA	OBD-CAD-C3D	2.45	132.05	127.98
11	C	1466	CLA	OBD-CAD-CBD	-2.44	122.40	125.89
11	B	1496	CLA	CED-O2D-CGD	2.44	121.46	115.94
11	H	1483	CLA	O2D-CGD-CBD	2.44	115.61	111.27
11	C	1467	CLA	O2A-CGA-CBA	2.44	119.56	111.91
11	H	1485	CLA	O2A-CGA-CBA	2.44	119.56	111.91
11	B	1490	CLA	C2A-C3A-C4A	2.44	105.81	101.87
11	I	1462	CLA	OBD-CAD-C3D	2.44	132.02	127.98
11	C	1467	CLA	OBD-CAD-C3D	2.43	132.02	127.98
11	D	1351	CLA	CED-O2D-CGD	2.43	121.44	115.94
12	A	1345	PHO	CAB-C3B-C4B	2.43	135.18	126.21
11	H	1483	CLA	C7-C6-C5	-2.43	106.77	113.36
17	L	1047	BCR	C16-C17-C18	2.43	130.77	127.31
11	G	1342	CLA	C16-C15-C13	2.43	123.76	115.92
11	C	1467	CLA	CMB-C2B-C1B	-2.42	124.74	128.46
11	C	1464	CLA	C2A-C1A-CHA	2.42	128.09	123.86
11	B	1492	CLA	C6-C7-C8	2.42	123.75	115.92
11	B	1494	CLA	C6-C5-C3	2.42	119.80	113.45
11	I	1463	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
11	B	1484	CLA	C2A-C3A-C4A	2.42	105.78	101.87
11	B	1486	CLA	O2D-CGD-CBD	2.42	115.57	111.27
16	E	1085	HEM	C4D-ND-C1D	2.42	107.61	105.79
11	B	1488	CLA	CMB-C2B-C1B	-2.42	124.75	128.46
11	C	1469	CLA	O2D-CGD-CBD	2.41	115.56	111.27
11	B	1494	CLA	C2A-C1A-CHA	2.41	128.08	123.86
11	H	1496	CLA	C2A-C1A-CHA	2.41	128.08	123.86
11	B	1493	CLA	O2D-CGD-CBD	2.41	115.55	111.27
11	C	1459	CLA	C2A-C1A-CHA	2.41	128.07	123.86
12	A	1345	PHO	C5-C3-C2	-2.41	116.24	121.12
11	B	1493	CLA	CMB-C2B-C1B	-2.41	124.76	128.46
11	C	1460	CLA	C2A-C3A-C4A	2.41	105.76	101.87
11	B	1490	CLA	CMA-C3A-C2A	-2.41	104.11	113.83
11	G	1342	CLA	CMB-C2B-C3B	2.40	129.17	124.68
11	I	1467	CLA	C2A-C1A-CHA	2.40	128.06	123.86
11	I	1459	CLA	OBD-CAD-CBD	-2.40	122.47	125.89
11	C	1466	CLA	O2D-CGD-CBD	2.39	115.51	111.27
11	D	1351	CLA	CBA-CAA-C2A	2.39	120.91	113.86
11	B	1496	CLA	O2D-CGD-CBD	2.38	115.50	111.27
11	I	1464	CLA	C2A-C1A-CHA	2.38	128.03	123.86
11	D	1351	CLA	C5-C3-C2	-2.38	116.30	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	1490	CLA	C2A-C3A-C4A	2.38	105.71	101.87
11	A	1346	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
11	I	1462	CLA	C6-C7-C8	2.38	123.60	115.92
17	L	1047	BCR	C36-C18-C19	2.38	121.82	118.08
11	H	1482	CLA	C2A-C1A-CHA	2.37	128.01	123.86
11	B	1495	CLA	O1A-CGA-CBA	-2.37	114.48	123.73
11	J	1351	CLA	C12-C11-C10	-2.37	102.34	113.24
17	F	1046	BCR	C8-C9-C10	-2.37	115.30	118.94
11	C	1463	CLA	CAA-C2A-C3A	-2.37	106.29	112.78
11	H	1493	CLA	CMB-C2B-C1B	-2.37	124.83	128.46
11	G	1344	CLA	O2D-CGD-CBD	2.37	115.47	111.27
11	G	1344	CLA	OBD-CAD-C3D	2.37	131.91	127.98
17	L	1047	BCR	C23-C22-C21	-2.36	115.31	118.94
11	A	1344	CLA	C2A-C3A-C4A	2.36	105.69	101.87
12	J	1352	PHO	C2A-C3A-C4A	2.36	106.01	101.34
11	I	1471	CLA	C2A-C3A-C4A	2.36	104.79	101.78
11	H	1492	CLA	C2A-C1A-CHA	2.36	127.98	123.86
11	H	1489	CLA	CED-O2D-CGD	2.36	121.27	115.94
11	B	1489	CLA	CED-O2D-CGD	2.35	121.26	115.94
11	H	1493	CLA	OBD-CAD-C3D	2.35	131.89	127.98
11	I	1459	CLA	C2A-C1A-CHA	2.35	127.97	123.86
11	H	1494	CLA	CMB-C2B-C1B	-2.34	124.86	128.46
11	H	1494	CLA	C2A-C1A-CHA	2.34	127.96	123.86
11	A	1342	CLA	CBA-CAA-C2A	2.34	120.77	113.86
12	G	1345	PHO	CMD-C2D-C1D	2.34	128.67	125.06
11	H	1485	CLA	CMB-C2B-C1B	-2.34	124.87	128.46
16	E	1085	HEM	C1B-NB-C4B	2.34	107.55	105.79
11	I	1469	CLA	C2A-C1A-CHA	2.33	127.93	123.85
11	I	1466	CLA	O2D-CGD-CBD	2.33	115.41	111.27
11	H	1488	CLA	C1-C2-C3	2.33	130.08	126.04
16	E	1085	HEM	C2B-C1B-NB	2.33	110.11	108.27
11	D	1351	CLA	C4D-C3D-CAD	-2.33	107.17	108.47
11	B	1485	CLA	CMB-C2B-C1B	-2.33	124.88	128.46
11	H	1487	CLA	C1-O2A-CGA	2.33	122.55	116.44
11	D	1353	CLA	C4D-C3D-CAD	-2.33	107.17	108.47
12	A	1345	PHO	O2D-CGD-CBD	2.33	115.40	111.27
12	G	1345	PHO	C2A-C1A-NA	-2.32	109.20	111.86
12	G	1345	PHO	C5-C3-C2	-2.32	116.42	121.12
11	B	1497	CLA	CMB-C2B-C1B	-2.32	124.90	128.46
11	B	1486	CLA	CED-O2D-CGD	2.32	121.18	115.94
12	A	1345	PHO	O2A-CGA-CBA	2.32	119.18	111.91
11	B	1486	CLA	OBD-CAD-CBD	-2.31	122.59	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	1490	CLA	CMA-C3A-C2A	-2.31	104.49	113.83
11	J	1351	CLA	C2A-C3A-C4A	2.31	105.61	101.87
11	B	1488	CLA	C1-O2A-CGA	2.31	122.51	116.44
12	D	1352	PHO	C1-C2-C3	2.31	130.04	126.04
11	B	1495	CLA	CED-O2D-CGD	2.31	121.16	115.94
11	B	1487	CLA	C1-O2A-CGA	2.31	122.50	116.44
11	H	1497	CLA	CMA-C3A-C2A	-2.31	110.71	116.10
11	B	1492	CLA	O2D-CGD-CBD	2.31	115.37	111.27
11	I	1464	CLA	C2A-C3A-C4A	2.30	105.59	101.87
11	D	1351	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
12	A	1345	PHO	C2A-C1A-NA	-2.30	109.22	111.86
12	D	1352	PHO	C2A-C3A-C4A	2.30	105.89	101.34
11	B	1482	CLA	C1-O2A-CGA	2.30	122.48	116.44
11	I	1466	CLA	C2A-C3A-C4A	2.30	105.58	101.87
12	G	1345	PHO	CAB-C3B-C4B	2.30	134.71	126.21
11	B	1485	CLA	O2A-CGA-CBA	2.30	119.12	111.91
11	H	1489	CLA	OBD-CAD-C3D	2.30	131.79	127.98
11	C	1463	CLA	O2A-C1-C2	2.29	114.66	108.64
11	B	1494	CLA	C2A-C3A-C4A	2.29	105.57	101.87
12	D	1352	PHO	C3D-C4D-CHA	2.29	115.67	109.49
11	H	1486	CLA	O2D-CGD-CBD	2.29	115.34	111.27
11	I	1468	CLA	C2A-C3A-C4A	2.28	106.21	103.59
11	H	1484	CLA	CMB-C2B-C3B	2.28	128.95	124.68
11	C	1459	CLA	O2D-CGD-CBD	2.28	115.32	111.27
11	I	1466	CLA	C2A-C1A-CHA	2.28	127.84	123.86
11	B	1487	CLA	CMB-C2B-C3B	2.28	128.94	124.68
11	G	1344	CLA	CED-O2D-CGD	2.28	121.09	115.94
11	I	1467	CLA	OBD-CAD-C3D	2.28	131.76	127.98
18	V	1138	HEC	CBA-CAA-C2A	2.27	116.67	112.48
11	D	1351	CLA	C2A-C1A-CHA	2.27	127.83	123.86
11	H	1485	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
11	A	1343	CLA	OBD-CAD-C3D	2.27	131.74	127.98
11	A	1342	CLA	C2A-C3A-C4A	2.26	105.53	101.87
12	G	1345	PHO	O2A-CGA-CBA	2.26	119.01	111.91
11	C	1469	CLA	OBD-CAD-CBD	-2.26	122.66	125.89
11	I	1470	CLA	OBD-CAD-C3D	2.26	131.73	127.98
11	C	1463	CLA	C2A-C1A-CHA	2.26	127.81	123.86
11	C	1462	CLA	C6-C7-C8	2.25	123.21	115.92
11	B	1492	CLA	C2A-C3A-C4A	2.25	105.51	101.87
16	L	1046	HEM	C1C-CHC-C4B	-2.25	126.16	129.64
17	F	1046	BCR	C37-C22-C23	2.25	121.63	118.08
11	H	1496	CLA	O2D-CGD-CBD	2.25	115.27	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1342	CLA	C2A-C1A-CHA	2.25	127.79	123.86
11	I	1465	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
11	I	1462	CLA	C2A-C3A-C4A	2.25	105.50	101.87
11	D	1353	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
11	C	1461	CLA	C3B-C4B-NB	-2.25	108.14	110.11
11	C	1464	CLA	CMB-C2B-C1B	-2.24	125.01	128.46
11	H	1495	CLA	C2A-C3A-C4A	2.24	105.49	101.87
11	C	1471	CLA	OBD-CAD-CBD	-2.24	122.69	125.89
11	H	1488	CLA	CMB-C2B-C1B	-2.24	125.02	128.46
11	C	1470	CLA	C2A-C1A-CHA	2.24	127.76	123.85
11	J	1353	CLA	CED-O2D-CGD	2.24	121.00	115.94
11	D	1351	CLA	CMB-C2B-C1B	-2.24	125.03	128.46
11	C	1466	CLA	C2A-C3A-C4A	2.24	105.48	101.87
11	H	1496	CLA	C1-O2A-CGA	2.23	122.31	116.44
11	B	1495	CLA	CMB-C2B-C1B	-2.23	125.03	128.46
11	H	1483	CLA	C2A-C3A-C4A	2.23	105.47	101.87
11	I	1467	CLA	C2A-C3A-C4A	2.23	105.47	101.87
11	B	1482	CLA	C2A-C1A-CHA	2.23	127.76	123.86
11	H	1492	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
11	C	1466	CLA	C2A-C1A-CHA	2.22	127.74	123.86
11	B	1489	CLA	C2A-C3A-C4A	2.22	105.45	101.87
11	I	1465	CLA	C2A-C3A-C4A	2.22	105.45	101.87
11	B	1496	CLA	C2A-C1A-CHA	2.21	127.72	123.86
11	C	1462	CLA	C2A-C3A-C4A	2.21	105.44	101.87
11	I	1467	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
11	H	1492	CLA	OBD-CAD-CBD	-2.20	122.75	125.89
11	B	1486	CLA	CMB-C2B-C3B	2.20	128.79	124.68
11	G	1346	CLA	OBD-CAD-C3D	2.20	131.63	127.98
11	D	1353	CLA	CED-O2D-CGD	2.20	120.91	115.94
17	F	1046	BCR	C16-C17-C18	2.20	130.45	127.31
11	H	1483	CLA	CMB-C2B-C1B	-2.20	125.09	128.46
11	D	1353	CLA	OBD-CAD-C3D	2.20	131.63	127.98
11	G	1342	CLA	OBD-CAD-CBD	-2.20	122.76	125.89
11	I	1463	CLA	O2D-CGD-CBD	2.20	115.17	111.27
11	C	1460	CLA	O2D-CGD-CBD	2.19	115.17	111.27
11	H	1495	CLA	CMB-C2B-C3B	2.19	128.78	124.68
11	C	1468	CLA	C2A-C3A-C4A	2.19	106.10	103.59
12	A	1345	PHO	C3D-C4D-CHA	2.19	115.39	109.49
11	D	1353	CLA	CMB-C2B-C3B	2.19	128.77	124.68
11	G	1346	CLA	CMA-C3A-C2A	-2.18	105.01	113.83
11	I	1460	CLA	CBA-CAA-C2A	2.18	120.31	113.86
11	C	1465	CLA	CMB-C2B-C1B	-2.18	125.11	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	I	1471	CLA	OBD-CAD-CBD	-2.18	122.78	125.89
11	H	1497	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
11	H	1496	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
11	B	1489	CLA	C1-O2A-CGA	2.18	122.17	116.44
11	B	1492	CLA	C2A-C1A-CHA	2.18	127.67	123.86
11	B	1484	CLA	CMB-C2B-C3B	2.18	128.76	124.68
11	H	1487	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
11	J	1351	CLA	C7-C6-C5	-2.17	107.46	113.36
11	B	1496	CLA	CBA-CAA-C2A	2.17	120.28	113.86
11	H	1484	CLA	C2A-C3A-C4A	2.17	105.38	101.87
12	J	1352	PHO	C3D-C4D-CHA	2.17	115.34	109.49
11	B	1494	CLA	C1-O2A-CGA	2.17	122.14	116.44
11	I	1465	CLA	C1-O2A-CGA	2.17	122.13	116.44
11	I	1463	CLA	O2A-C1-C2	2.17	114.33	108.64
11	H	1494	CLA	C1-O2A-CGA	2.16	122.12	116.44
11	I	1470	CLA	O2D-CGD-CBD	2.16	115.11	111.27
11	B	1483	CLA	C2A-C3A-C4A	2.16	105.36	101.87
11	C	1460	CLA	CBA-CAA-C2A	2.16	120.24	113.86
11	B	1489	CLA	CMB-C2B-C1B	-2.16	125.15	128.46
11	G	1342	CLA	CBA-CAA-C2A	2.16	120.23	113.86
11	C	1464	CLA	CAA-C2A-C3A	-2.15	106.88	112.78
11	B	1493	CLA	CED-O2D-CGD	2.15	120.81	115.94
11	I	1460	CLA	C2A-C3A-C4A	2.15	105.35	101.87
11	J	1353	CLA	OBD-CAD-C3D	2.15	131.55	127.98
11	I	1469	CLA	OBD-CAD-CBD	-2.15	122.82	125.89
11	C	1466	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
11	B	1483	CLA	OBD-CAD-C3D	2.15	131.54	127.98
11	C	1469	CLA	C2A-C1A-CHA	2.15	127.60	123.85
11	C	1470	CLA	CMB-C2B-C1B	-2.15	125.17	128.46
11	H	1494	CLA	O2D-CGD-CBD	2.14	115.08	111.27
11	I	1462	CLA	C6-C5-C3	2.14	119.08	113.45
11	B	1483	CLA	CED-O2D-CGD	2.14	120.78	115.94
11	I	1459	CLA	O2D-CGD-CBD	2.14	115.07	111.27
11	B	1483	CLA	CMB-C2B-C1B	-2.14	125.17	128.46
11	H	1489	CLA	CMB-C2B-C3B	2.14	128.68	124.68
11	A	1346	CLA	C2A-C3A-C4A	2.14	105.33	101.87
11	G	1344	CLA	C2A-C3A-C4A	2.14	105.33	101.87
11	B	1492	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
11	H	1490	CLA	O2D-CGD-CBD	2.13	115.06	111.27
11	H	1494	CLA	C6-C5-C3	2.13	119.05	113.45
11	B	1488	CLA	OBD-CAD-C3D	2.13	131.51	127.98
11	H	1495	CLA	C7-C6-C5	-2.13	107.59	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	1488	CLA	CMB-C2B-C3B	2.12	128.65	124.68
11	C	1465	CLA	OBD-CAD-C3D	2.12	131.50	127.98
11	I	1471	CLA	C2A-C1A-CHA	2.12	127.56	123.85
11	G	1346	CLA	CED-O2D-CGD	2.12	120.72	115.94
11	C	1465	CLA	C2A-C3A-C4A	2.11	105.28	101.87
11	B	1483	CLA	C2A-C1A-CHA	2.11	127.56	123.86
11	D	1353	CLA	C2A-C1A-CHA	2.11	127.55	123.86
11	I	1470	CLA	C2A-C1A-CHA	2.11	127.54	123.85
11	H	1497	CLA	CMB-C2B-C3B	2.11	128.62	124.68
11	G	1344	CLA	CAA-CBA-CGA	2.11	118.12	113.59
17	F	1046	BCR	C11-C10-C9	2.11	130.32	127.31
11	B	1497	CLA	CMB-C2B-C3B	2.11	128.62	124.68
11	C	1465	CLA	CMB-C2B-C3B	2.10	128.61	124.68
12	J	1352	PHO	C6-C5-C3	2.10	118.97	113.45
12	G	1345	PHO	C3D-C4D-CHA	2.10	115.15	109.49
11	J	1351	CLA	CMB-C2B-C1B	-2.10	125.24	128.46
11	I	1465	CLA	CAA-C2A-C3A	-2.09	107.04	112.78
11	B	1488	CLA	CMB-C2B-C3B	2.09	128.59	124.68
11	C	1465	CLA	C2A-C1A-CHA	2.09	127.52	123.86
11	J	1353	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
11	I	1465	CLA	C2A-C1A-CHA	2.09	127.52	123.86
11	H	1487	CLA	CBA-CAA-C2A	2.09	120.03	113.86
11	H	1489	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
11	B	1487	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
11	J	1351	CLA	CBA-CAA-C2A	2.09	120.03	113.86
11	I	1463	CLA	OBD-CAD-C3D	2.09	131.45	127.98
11	H	1482	CLA	C1-O2A-CGA	2.09	121.92	116.44
11	G	1343	CLA	C12-C11-C10	-2.09	103.66	113.24
11	I	1462	CLA	C1-O2A-CGA	2.08	121.91	116.44
11	H	1482	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
11	H	1496	CLA	CBA-CAA-C2A	2.08	120.00	113.86
11	C	1462	CLA	C1-O2A-CGA	2.08	121.89	116.44
11	J	1353	CLA	CMB-C2B-C3B	2.08	128.56	124.68
11	B	1495	CLA	C7-C6-C5	-2.08	107.72	113.36
11	A	1343	CLA	C12-C11-C10	-2.07	103.74	113.24
11	I	1463	CLA	CMB-C2B-C1B	-2.07	125.29	128.46
11	A	1346	CLA	CMA-C3A-C2A	-2.06	105.50	113.83
11	C	1460	CLA	OBD-CAD-C3D	2.06	131.41	127.98
11	C	1467	CLA	C2A-C3A-C4A	2.06	105.20	101.87
11	H	1492	CLA	C2A-C3A-C4A	2.06	105.19	101.87
11	B	1493	CLA	CMB-C2B-C3B	2.06	128.53	124.68
11	J	1353	CLA	C4D-C3D-CAD	-2.06	107.32	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	1344	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
11	B	1496	CLA	C6-C7-C8	2.05	122.56	115.92
11	B	1495	CLA	CBA-CAA-C2A	2.05	119.92	113.86
11	B	1487	CLA	C2A-C3A-C4A	2.05	105.18	101.87
11	B	1484	CLA	C2A-C1A-CHA	2.05	127.45	123.86
11	C	1464	CLA	CBA-CAA-C2A	2.05	119.92	113.86
11	C	1464	CLA	C2A-C3A-C4A	2.05	105.18	101.87
11	B	1488	CLA	CGD-CBD-CAD	-2.05	104.09	110.73
11	G	1344	CLA	C2A-C1A-CHA	2.05	127.44	123.86
11	I	1460	CLA	C2A-C1A-CHA	2.05	127.44	123.86
11	B	1496	CLA	CMB-C2B-C1B	-2.05	125.32	128.46
11	B	1490	CLA	OBD-CAD-C3D	2.05	131.38	127.98
11	H	1483	CLA	C2A-C1A-CHA	2.04	127.43	123.86
11	C	1462	CLA	C6-C5-C3	2.04	118.81	113.45
11	H	1493	CLA	O2D-CGD-CBD	2.04	114.90	111.27
11	B	1492	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
11	B	1495	CLA	OBD-CAD-C3D	2.04	131.37	127.98
11	B	1490	CLA	CMB-C2B-C3B	2.04	128.49	124.68
17	L	1047	BCR	C32-C1-C2	-2.03	100.77	108.91
11	G	1346	CLA	C3C-C4C-NC	-2.03	108.29	110.57
11	B	1486	CLA	C2A-C1A-CHA	2.03	127.40	123.85
11	I	1467	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
11	I	1464	CLA	CBA-CAA-C2A	2.03	119.86	113.86
11	A	1342	CLA	O2D-CGD-CBD	2.03	114.88	111.27
11	A	1344	CLA	C2A-C1A-CHA	2.03	127.41	123.86
12	G	1345	PHO	C2A-C3A-C4A	2.03	105.35	101.34
17	L	1047	BCR	C37-C22-C23	2.03	121.27	118.08
11	C	1460	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
11	J	1353	CLA	C2A-C1A-CHA	2.02	127.39	123.86
11	I	1465	CLA	CMB-C2B-C3B	2.02	128.46	124.68
11	C	1467	CLA	CAA-C2A-C3A	-2.02	107.26	112.78
11	J	1351	CLA	OBD-CAD-C3D	2.02	131.33	127.98
11	C	1459	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
11	B	1488	CLA	CAA-CBA-CGA	2.01	119.13	113.25
11	B	1488	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
17	F	1046	BCR	C3-C4-C5	2.01	117.66	114.08
11	I	1465	CLA	OBD-CAD-C3D	2.00	131.31	127.98
17	F	1046	BCR	C20-C21-C22	2.00	130.16	127.31
11	C	1459	CLA	C2A-C3A-C4A	2.00	105.10	101.87

All (200) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	C	1471	CLA	NC
11	C	1471	CLA	ND
11	C	1471	CLA	NA
11	B	1487	CLA	NC
11	B	1487	CLA	ND
11	B	1487	CLA	NA
11	C	1468	CLA	NC
11	C	1468	CLA	ND
11	C	1468	CLA	NA
11	B	1489	CLA	NC
11	B	1489	CLA	ND
11	B	1489	CLA	NA
11	B	1497	CLA	NC
11	B	1497	CLA	ND
11	B	1497	CLA	NA
11	H	1482	CLA	NC
11	H	1482	CLA	ND
11	H	1482	CLA	NA
11	B	1482	CLA	NC
11	B	1482	CLA	ND
11	B	1482	CLA	NA
11	H	1492	CLA	NC
11	H	1492	CLA	ND
11	H	1492	CLA	NA
11	H	1493	CLA	NC
11	H	1493	CLA	ND
11	H	1493	CLA	NA
11	H	1485	CLA	NC
11	H	1485	CLA	ND
11	H	1485	CLA	NA
11	B	1492	CLA	NC
11	B	1492	CLA	ND
11	B	1492	CLA	NA
11	C	1462	CLA	NC
11	C	1462	CLA	ND
11	C	1462	CLA	NA
11	I	1466	CLA	NC
11	I	1466	CLA	ND
11	I	1466	CLA	NA
11	A	1344	CLA	NC
11	A	1344	CLA	ND
11	A	1344	CLA	NA
11	I	1463	CLA	C8

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Mol	Chain	Res	Type	Atom
11	I	1463	CLA	NC
11	I	1463	CLA	ND
11	H	1489	CLA	NC
11	H	1489	CLA	ND
11	H	1489	CLA	NA
11	G	1343	CLA	NC
11	G	1343	CLA	ND
11	G	1343	CLA	NA
11	C	1465	CLA	NC
11	C	1465	CLA	ND
11	C	1465	CLA	NA
11	B	1494	CLA	NC
11	B	1494	CLA	ND
11	B	1494	CLA	NA
11	H	1486	CLA	NC
11	H	1486	CLA	ND
11	H	1486	CLA	NA
11	B	1496	CLA	NC
11	B	1496	CLA	ND
11	B	1496	CLA	NA
11	B	1493	CLA	NC
11	B	1493	CLA	ND
11	B	1493	CLA	NA
11	B	1491	CLA	NC
11	B	1491	CLA	ND
11	B	1491	CLA	NA
11	H	1497	CLA	NC
11	H	1497	CLA	ND
11	H	1497	CLA	NA
11	I	1465	CLA	NC
11	I	1465	CLA	ND
11	I	1465	CLA	NA
11	A	1342	CLA	NC
11	A	1342	CLA	ND
11	A	1342	CLA	NA
11	B	1486	CLA	NC
11	B	1486	CLA	ND
11	B	1486	CLA	NA
11	G	1346	CLA	NC
11	G	1346	CLA	ND
11	G	1346	CLA	NA
11	G	1342	CLA	ND

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Mol	Chain	Res	Type	Atom
11	C	1469	CLA	NC
11	C	1469	CLA	ND
11	C	1469	CLA	NA
11	I	1461	CLA	NC
11	I	1461	CLA	ND
11	I	1461	CLA	NA
11	I	1470	CLA	NC
11	I	1470	CLA	ND
11	I	1470	CLA	NA
11	C	1467	CLA	NC
11	C	1467	CLA	ND
11	C	1467	CLA	NA
11	I	1462	CLA	NC
11	I	1462	CLA	ND
11	I	1462	CLA	NA
11	B	1485	CLA	NC
11	B	1485	CLA	ND
11	B	1485	CLA	NA
11	G	1344	CLA	NC
11	G	1344	CLA	ND
11	G	1344	CLA	NA
11	H	1491	CLA	NC
11	H	1491	CLA	ND
11	H	1491	CLA	NA
11	H	1488	CLA	NC
11	H	1488	CLA	ND
11	H	1488	CLA	NA
11	C	1463	CLA	NC
11	C	1463	CLA	ND
11	C	1463	CLA	NA
11	J	1353	CLA	NC
11	J	1353	CLA	ND
11	J	1353	CLA	NA
11	H	1495	CLA	NC
11	H	1495	CLA	ND
11	H	1495	CLA	NA
11	I	1471	CLA	NC
11	I	1471	CLA	ND
11	I	1471	CLA	NA
11	H	1487	CLA	NC
11	H	1487	CLA	ND
11	H	1487	CLA	NA

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Mol	Chain	Res	Type	Atom
11	C	1464	CLA	NC
11	C	1464	CLA	ND
11	C	1464	CLA	NA
11	C	1461	CLA	NC
11	C	1461	CLA	ND
11	C	1461	CLA	NA
11	I	1460	CLA	NC
11	I	1460	CLA	ND
11	I	1460	CLA	NA
11	I	1469	CLA	NC
11	I	1469	CLA	ND
11	I	1469	CLA	NA
11	I	1467	CLA	NC
11	I	1467	CLA	ND
11	I	1467	CLA	NA
11	D	1353	CLA	NC
11	D	1353	CLA	ND
11	D	1353	CLA	NA
11	A	1343	CLA	NC
11	A	1343	CLA	ND
11	A	1343	CLA	NA
11	B	1488	CLA	NC
11	B	1488	CLA	ND
11	B	1488	CLA	NA
11	C	1459	CLA	NC
11	C	1459	CLA	ND
11	C	1459	CLA	NA
11	A	1346	CLA	NC
11	A	1346	CLA	ND
11	A	1346	CLA	NA
11	D	1351	CLA	ND
11	J	1351	CLA	ND
11	B	1484	CLA	NC
11	B	1484	CLA	ND
11	B	1484	CLA	NA
11	B	1483	CLA	NC
11	B	1483	CLA	ND
11	B	1483	CLA	NA
11	C	1466	CLA	NC
11	C	1466	CLA	ND
11	C	1466	CLA	NA
11	H	1490	CLA	ND

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Mol	Chain	Res	Type	Atom
11	C	1460	CLA	NC
11	C	1460	CLA	ND
11	C	1460	CLA	NA
11	I	1464	CLA	NC
11	I	1464	CLA	ND
11	I	1464	CLA	NA
11	H	1484	CLA	NC
11	H	1484	CLA	ND
11	H	1484	CLA	NA
11	B	1490	CLA	ND
11	C	1470	CLA	NC
11	C	1470	CLA	ND
11	C	1470	CLA	NA
11	B	1495	CLA	NC
11	B	1495	CLA	ND
11	B	1495	CLA	NA
11	H	1483	CLA	NC
11	H	1483	CLA	ND
11	H	1483	CLA	NA
11	H	1494	CLA	NC
11	H	1494	CLA	ND
11	H	1494	CLA	NA
11	I	1468	CLA	NC
11	I	1468	CLA	ND
11	I	1468	CLA	NA
11	I	1459	CLA	NC
11	I	1459	CLA	ND
11	I	1459	CLA	NA
11	H	1496	CLA	NC
11	H	1496	CLA	ND
11	H	1496	CLA	NA

All (559) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	L	1047	BCR	C6-C7-C8-C9
17	L	1047	BCR	C23-C24-C25-C30
11	B	1487	CLA	O2A-C1-C2-C3
12	J	1352	PHO	C2B-C3B-CAB-CBB
12	J	1352	PHO	C4B-C3B-CAB-CBB
12	D	1352	PHO	C2B-C3B-CAB-CBB
12	D	1352	PHO	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	B	1489	CLA	CBD-CGD-O2D-CED
11	B	1497	CLA	CBD-CGD-O2D-CED
11	H	1482	CLA	CHA-CBD-CGD-O1D
11	H	1482	CLA	CHA-CBD-CGD-O2D
11	H	1482	CLA	C2-C3-C5-C6
11	H	1482	CLA	C4-C3-C5-C6
11	B	1482	CLA	CHA-CBD-CGD-O1D
11	B	1482	CLA	CHA-CBD-CGD-O2D
11	B	1482	CLA	C2-C3-C5-C6
11	B	1482	CLA	C4-C3-C5-C6
11	H	1492	CLA	CBD-CGD-O2D-CED
11	H	1492	CLA	C6-C7-C8-C9
11	H	1492	CLA	C11-C12-C13-C15
11	H	1485	CLA	C1A-C2A-CAA-CBA
11	H	1485	CLA	CHA-CBD-CGD-O1D
11	H	1485	CLA	CHA-CBD-CGD-O2D
11	H	1485	CLA	CBD-CGD-O2D-CED
11	B	1492	CLA	C6-C7-C8-C9
11	B	1492	CLA	C11-C12-C13-C15
11	C	1462	CLA	C1A-C2A-CAA-CBA
11	I	1466	CLA	C1A-C2A-CAA-CBA
11	I	1466	CLA	O2A-C1-C2-C3
11	A	1344	CLA	CHA-CBD-CGD-O1D
11	A	1344	CLA	CHA-CBD-CGD-O2D
11	I	1463	CLA	C2-C3-C5-C6
11	I	1463	CLA	C4-C3-C5-C6
11	H	1489	CLA	CAD-CBD-CGD-O2D
11	H	1489	CLA	CBD-CGD-O2D-CED
11	G	1343	CLA	C1A-C2A-CAA-CBA
11	G	1343	CLA	CBD-CGD-O2D-CED
11	H	1486	CLA	CBD-CGD-O2D-CED
11	H	1497	CLA	CBD-CGD-O2D-CED
11	B	1486	CLA	CBD-CGD-O2D-CED
11	G	1346	CLA	C2-C3-C5-C6
11	G	1346	CLA	C4-C3-C5-C6
11	I	1470	CLA	CBD-CGD-O2D-CED
11	C	1467	CLA	CHA-CBD-CGD-O1D
11	C	1467	CLA	CHA-CBD-CGD-O2D
11	I	1462	CLA	C1A-C2A-CAA-CBA
11	B	1485	CLA	C1A-C2A-CAA-CBA
11	B	1485	CLA	CHA-CBD-CGD-O1D
11	B	1485	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
11	B	1485	CLA	CBD-CGD-O2D-CED
11	G	1344	CLA	CHA-CBD-CGD-O1D
11	G	1344	CLA	CHA-CBD-CGD-O2D
11	C	1463	CLA	CBD-CGD-O2D-CED
11	C	1463	CLA	C2-C3-C5-C6
11	C	1463	CLA	C4-C3-C5-C6
11	H	1495	CLA	CBD-CGD-O2D-CED
11	H	1487	CLA	O2A-C1-C2-C3
11	C	1464	CLA	C1A-C2A-CAA-CBA
11	C	1464	CLA	C3A-C2A-CAA-CBA
11	I	1467	CLA	CHA-CBD-CGD-O1D
11	I	1467	CLA	CHA-CBD-CGD-O2D
12	A	1345	PHO	C2B-C3B-CAB-CBB
12	A	1345	PHO	C4B-C3B-CAB-CBB
11	A	1343	CLA	C1A-C2A-CAA-CBA
11	A	1343	CLA	CBD-CGD-O2D-CED
11	B	1488	CLA	C3A-C2A-CAA-CBA
11	C	1459	CLA	C1A-C2A-CAA-CBA
11	C	1459	CLA	C2A-CAA-CBA-CGA
11	A	1346	CLA	C2-C3-C5-C6
11	A	1346	CLA	C4-C3-C5-C6
11	D	1351	CLA	O2A-C1-C2-C3
11	B	1483	CLA	C4-C3-C5-C6
12	G	1345	PHO	C2B-C3B-CAB-CBB
12	G	1345	PHO	C4B-C3B-CAB-CBB
11	C	1466	CLA	C1A-C2A-CAA-CBA
11	C	1466	CLA	O2A-C1-C2-C3
11	H	1490	CLA	CHA-CBD-CGD-O1D
11	H	1490	CLA	CHA-CBD-CGD-O2D
11	H	1490	CLA	CBD-CGD-O2D-CED
11	I	1464	CLA	C1A-C2A-CAA-CBA
11	I	1464	CLA	C3A-C2A-CAA-CBA
11	B	1490	CLA	CHA-CBD-CGD-O1D
11	C	1470	CLA	CBD-CGD-O2D-CED
11	B	1495	CLA	CBD-CGD-O2D-CED
17	F	1046	BCR	C6-C7-C8-C9
17	F	1046	BCR	C23-C24-C25-C30
11	H	1483	CLA	CHA-CBD-CGD-O1D
11	I	1459	CLA	C1A-C2A-CAA-CBA
11	I	1459	CLA	C2A-CAA-CBA-CGA
11	H	1496	CLA	C6-C7-C8-C9
11	C	1471	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	B	1494	CLA	O1D-CGD-O2D-CED
11	C	1467	CLA	O1D-CGD-O2D-CED
11	I	1467	CLA	O1D-CGD-O2D-CED
11	H	1494	CLA	O1D-CGD-O2D-CED
11	H	1485	CLA	O1D-CGD-O2D-CED
11	A	1344	CLA	O1D-CGD-O2D-CED
11	G	1343	CLA	O1D-CGD-O2D-CED
11	G	1344	CLA	O1D-CGD-O2D-CED
11	I	1471	CLA	O1D-CGD-O2D-CED
11	A	1343	CLA	O1D-CGD-O2D-CED
11	C	1471	CLA	CBD-CGD-O2D-CED
12	J	1352	PHO	CBD-CGD-O2D-CED
12	D	1352	PHO	CBD-CGD-O2D-CED
11	H	1493	CLA	CBD-CGD-O2D-CED
11	B	1492	CLA	CBD-CGD-O2D-CED
11	I	1466	CLA	CBD-CGD-O2D-CED
11	A	1344	CLA	CBD-CGD-O2D-CED
11	I	1463	CLA	CBD-CGD-O2D-CED
11	C	1465	CLA	CBD-CGD-O2D-CED
11	B	1494	CLA	CBD-CGD-O2D-CED
11	B	1493	CLA	CBD-CGD-O2D-CED
11	I	1465	CLA	CBD-CGD-O2D-CED
11	C	1469	CLA	CBD-CGD-O2D-CED
11	C	1467	CLA	CBD-CGD-O2D-CED
11	G	1344	CLA	CBD-CGD-O2D-CED
11	I	1471	CLA	CBD-CGD-O2D-CED
11	C	1464	CLA	CBD-CGD-O2D-CED
11	I	1460	CLA	CBD-CGD-O2D-CED
11	I	1469	CLA	CBD-CGD-O2D-CED
11	I	1467	CLA	CBD-CGD-O2D-CED
11	C	1459	CLA	CBD-CGD-O2D-CED
11	B	1484	CLA	CBD-CGD-O2D-CED
11	C	1466	CLA	CBD-CGD-O2D-CED
11	C	1460	CLA	CBD-CGD-O2D-CED
11	I	1464	CLA	CBD-CGD-O2D-CED
11	H	1484	CLA	CBD-CGD-O2D-CED
11	B	1490	CLA	CBD-CGD-O2D-CED
11	H	1494	CLA	CBD-CGD-O2D-CED
11	I	1459	CLA	CBD-CGD-O2D-CED
11	C	1469	CLA	O1D-CGD-O2D-CED
11	B	1485	CLA	O1D-CGD-O2D-CED
11	C	1464	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	I	1460	CLA	O1D-CGD-O2D-CED
11	I	1469	CLA	O1D-CGD-O2D-CED
11	C	1460	CLA	O1D-CGD-O2D-CED
11	I	1464	CLA	O1D-CGD-O2D-CED
11	B	1489	CLA	O1D-CGD-O2D-CED
11	B	1497	CLA	O1D-CGD-O2D-CED
11	H	1492	CLA	O1D-CGD-O2D-CED
11	H	1489	CLA	O1D-CGD-O2D-CED
11	H	1486	CLA	O1D-CGD-O2D-CED
11	C	1462	CLA	CBD-CGD-O2D-CED
11	B	1496	CLA	CBD-CGD-O2D-CED
11	I	1462	CLA	CBD-CGD-O2D-CED
11	J	1353	CLA	CBD-CGD-O2D-CED
11	D	1353	CLA	CBD-CGD-O2D-CED
11	D	1351	CLA	CBD-CGD-O2D-CED
11	J	1351	CLA	CBD-CGD-O2D-CED
11	H	1496	CLA	CBD-CGD-O2D-CED
11	H	1497	CLA	O1D-CGD-O2D-CED
11	B	1486	CLA	O1D-CGD-O2D-CED
11	C	1463	CLA	O1D-CGD-O2D-CED
11	H	1495	CLA	O1D-CGD-O2D-CED
11	H	1490	CLA	O1D-CGD-O2D-CED
11	C	1470	CLA	O1D-CGD-O2D-CED
11	I	1465	CLA	O1D-CGD-O2D-CED
11	I	1470	CLA	O1D-CGD-O2D-CED
11	C	1459	CLA	O1D-CGD-O2D-CED
11	B	1495	CLA	O1D-CGD-O2D-CED
12	J	1352	PHO	O1D-CGD-O2D-CED
11	B	1492	CLA	O1D-CGD-O2D-CED
11	I	1463	CLA	O1D-CGD-O2D-CED
11	H	1484	CLA	O1D-CGD-O2D-CED
11	I	1459	CLA	O1D-CGD-O2D-CED
12	D	1352	PHO	C4-C3-C5-C6
11	H	1483	CLA	C4-C3-C5-C6
11	B	1483	CLA	C2-C3-C5-C6
11	B	1484	CLA	O1D-CGD-O2D-CED
12	D	1352	PHO	O1D-CGD-O2D-CED
11	C	1465	CLA	O1D-CGD-O2D-CED
11	B	1493	CLA	O1D-CGD-O2D-CED
11	H	1483	CLA	CBD-CGD-O2D-CED
11	H	1493	CLA	O1D-CGD-O2D-CED
11	I	1466	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	B	1490	CLA	O1D-CGD-O2D-CED
11	H	1490	CLA	C2A-CAA-CBA-CGA
11	B	1490	CLA	C2A-CAA-CBA-CGA
11	B	1483	CLA	CBD-CGD-O2D-CED
11	C	1466	CLA	O1D-CGD-O2D-CED
11	B	1486	CLA	C2C-C3C-CAC-CBC
11	A	1346	CLA	CBD-CGD-O2D-CED
11	B	1487	CLA	C4-C3-C5-C6
11	H	1487	CLA	C4-C3-C5-C6
11	B	1487	CLA	C2-C3-C5-C6
11	H	1487	CLA	C2-C3-C5-C6
11	H	1486	CLA	C2C-C3C-CAC-CBC
11	B	1496	CLA	O1D-CGD-O2D-CED
11	I	1462	CLA	O1D-CGD-O2D-CED
11	H	1496	CLA	O1D-CGD-O2D-CED
11	B	1496	CLA	C15-C16-C17-C18
12	A	1345	PHO	C10-C11-C12-C13
12	G	1345	PHO	C15-C16-C17-C18
12	D	1352	PHO	C2-C3-C5-C6
11	C	1462	CLA	C6-C7-C8-C9
11	G	1343	CLA	C11-C12-C13-C14
11	B	1496	CLA	C6-C7-C8-C9
11	B	1496	CLA	C14-C13-C15-C16
11	I	1462	CLA	C6-C7-C8-C9
11	H	1488	CLA	C14-C13-C15-C16
11	A	1343	CLA	C11-C12-C13-C14
11	B	1488	CLA	C14-C13-C15-C16
11	H	1496	CLA	C14-C13-C15-C16
11	C	1462	CLA	O1D-CGD-O2D-CED
11	J	1353	CLA	O1D-CGD-O2D-CED
11	D	1351	CLA	O1D-CGD-O2D-CED
11	J	1351	CLA	O1D-CGD-O2D-CED
12	A	1345	PHO	C15-C16-C17-C18
11	I	1463	CLA	C2A-CAA-CBA-CGA
11	D	1353	CLA	O1D-CGD-O2D-CED
11	B	1488	CLA	C5-C6-C7-C8
11	B	1488	CLA	C13-C15-C16-C17
11	H	1496	CLA	C15-C16-C17-C18
11	H	1488	CLA	C5-C6-C7-C8
11	H	1488	CLA	C13-C15-C16-C17
12	G	1345	PHO	C10-C11-C12-C13
11	I	1465	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
11	B	1486	CLA	C4C-C3C-CAC-CBC
11	G	1346	CLA	CBD-CGD-O2D-CED
11	C	1465	CLA	C10-C11-C12-C13
11	C	1465	CLA	C11-C10-C8-C7
11	B	1496	CLA	C6-C7-C8-C10
11	H	1492	CLA	C2A-CAA-CBA-CGA
11	B	1492	CLA	C2A-CAA-CBA-CGA
11	H	1488	CLA	C2A-CAA-CBA-CGA
11	I	1460	CLA	C2A-CAA-CBA-CGA
11	B	1488	CLA	C2A-CAA-CBA-CGA
11	C	1460	CLA	C2A-CAA-CBA-CGA
11	C	1471	CLA	C2C-C3C-CAC-CBC
11	A	1343	CLA	C10-C11-C12-C13
11	H	1483	CLA	C10-C11-C12-C13
11	I	1464	CLA	C5-C6-C7-C8
11	G	1343	CLA	C10-C11-C12-C13
11	C	1464	CLA	C5-C6-C7-C8
11	H	1486	CLA	C4C-C3C-CAC-CBC
11	H	1495	CLA	C4-C3-C5-C6
11	B	1483	CLA	C10-C11-C12-C13
11	C	1463	CLA	C2A-CAA-CBA-CGA
11	C	1464	CLA	C2A-CAA-CBA-CGA
11	B	1483	CLA	C2A-CAA-CBA-CGA
11	I	1464	CLA	C2A-CAA-CBA-CGA
11	H	1483	CLA	C2A-CAA-CBA-CGA
11	I	1471	CLA	C2C-C3C-CAC-CBC
11	B	1484	CLA	C2A-CAA-CBA-CGA
11	H	1484	CLA	C2A-CAA-CBA-CGA
11	H	1483	CLA	O1D-CGD-O2D-CED
11	G	1342	CLA	C15-C16-C17-C18
12	J	1352	PHO	C6-C7-C8-C9
11	H	1483	CLA	C2-C3-C5-C6
11	C	1465	CLA	C11-C10-C8-C9
11	I	1465	CLA	C11-C10-C8-C9
11	G	1343	CLA	C2A-CAA-CBA-CGA
11	A	1343	CLA	C2A-CAA-CBA-CGA
12	D	1352	PHO	C6-C7-C8-C9
11	B	1483	CLA	O1D-CGD-O2D-CED
11	A	1342	CLA	C15-C16-C17-C18
11	H	1493	CLA	C3A-C2A-CAA-CBA
11	H	1485	CLA	C3A-C2A-CAA-CBA
11	C	1462	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	I	1466	CLA	C3A-C2A-CAA-CBA
11	G	1343	CLA	C3A-C2A-CAA-CBA
11	B	1493	CLA	C3A-C2A-CAA-CBA
11	I	1462	CLA	C3A-C2A-CAA-CBA
11	B	1485	CLA	C3A-C2A-CAA-CBA
11	H	1488	CLA	C3A-C2A-CAA-CBA
11	A	1343	CLA	C3A-C2A-CAA-CBA
11	C	1466	CLA	C3A-C2A-CAA-CBA
11	J	1351	CLA	O2A-C1-C2-C3
12	D	1352	PHO	C6-C7-C8-C10
11	H	1496	CLA	C13-C15-C16-C17
11	B	1496	CLA	C5-C6-C7-C8
11	A	1343	CLA	C5-C6-C7-C8
11	H	1496	CLA	C5-C6-C7-C8
11	G	1343	CLA	C14-C13-C15-C16
11	A	1343	CLA	C14-C13-C15-C16
12	J	1352	PHO	C4-C3-C5-C6
11	H	1494	CLA	C4-C3-C5-C6
11	G	1343	CLA	C11-C12-C13-C15
11	I	1465	CLA	C11-C10-C8-C7
11	H	1494	CLA	C2-C3-C5-C6
11	H	1496	CLA	C6-C7-C8-C10
11	I	1465	CLA	C5-C6-C7-C8
12	J	1352	PHO	C6-C7-C8-C10
11	C	1463	CLA	C5-C6-C7-C8
11	G	1343	CLA	C5-C6-C7-C8
11	A	1346	CLA	O1D-CGD-O2D-CED
11	H	1492	CLA	C4-C3-C5-C6
11	B	1495	CLA	C4-C3-C5-C6
12	J	1352	PHO	C2-C3-C5-C6
11	B	1494	CLA	C2-C3-C5-C6
11	H	1495	CLA	C2-C3-C5-C6
11	H	1492	CLA	C11-C12-C13-C14
11	B	1492	CLA	C11-C12-C13-C14
11	D	1351	CLA	C11-C12-C13-C14
11	J	1351	CLA	C11-C12-C13-C14
12	G	1345	PHO	C14-C13-C15-C16
11	H	1494	CLA	C6-C7-C8-C9
11	A	1342	CLA	C2A-CAA-CBA-CGA
11	G	1342	CLA	C2A-CAA-CBA-CGA
11	H	1493	CLA	C1A-C2A-CAA-CBA
11	B	1493	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	H	1488	CLA	C1A-C2A-CAA-CBA
11	B	1488	CLA	C1A-C2A-CAA-CBA
11	C	1465	CLA	C5-C6-C7-C8
11	I	1463	CLA	C5-C6-C7-C8
11	G	1343	CLA	C4-C3-C5-C6
11	B	1494	CLA	C4-C3-C5-C6
11	B	1496	CLA	C13-C15-C16-C17
11	A	1343	CLA	C4-C3-C5-C6
11	B	1494	CLA	C5-C6-C7-C8
11	D	1351	CLA	C5-C6-C7-C8
11	H	1487	CLA	CAA-CBA-CGA-O2A
11	J	1351	CLA	C5-C6-C7-C8
11	B	1487	CLA	CAA-CBA-CGA-O2A
11	H	1482	CLA	C11-C10-C8-C7
11	B	1482	CLA	C11-C10-C8-C7
11	C	1462	CLA	C6-C7-C8-C10
11	G	1343	CLA	C2-C3-C5-C6
11	B	1494	CLA	C6-C7-C8-C10
11	B	1496	CLA	C11-C10-C8-C7
11	I	1462	CLA	C6-C7-C8-C10
12	A	1345	PHO	C12-C13-C15-C16
11	A	1343	CLA	C2-C3-C5-C6
11	A	1343	CLA	C11-C12-C13-C15
11	D	1351	CLA	C11-C12-C13-C15
11	J	1351	CLA	C11-C12-C13-C15
12	G	1345	PHO	C6-C7-C8-C10
12	G	1345	PHO	C12-C13-C15-C16
11	H	1494	CLA	C6-C7-C8-C10
11	H	1496	CLA	C11-C10-C8-C7
11	H	1482	CLA	C11-C10-C8-C9
11	B	1482	CLA	C11-C10-C8-C9
11	C	1465	CLA	C6-C7-C8-C9
11	B	1494	CLA	C6-C7-C8-C9
11	B	1496	CLA	C11-C10-C8-C9
11	I	1465	CLA	C6-C7-C8-C9
11	G	1342	CLA	C14-C13-C15-C16
11	H	1488	CLA	C11-C12-C13-C14
11	C	1464	CLA	C6-C7-C8-C9
12	A	1345	PHO	C14-C13-C15-C16
11	B	1488	CLA	C11-C12-C13-C14
11	H	1496	CLA	C11-C10-C8-C9
11	G	1346	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	H	1492	CLA	C2-C3-C5-C6
11	B	1487	CLA	C5-C6-C7-C8
11	D	1351	CLA	C13-C15-C16-C17
11	B	1487	CLA	C3A-C2A-CAA-CBA
11	H	1487	CLA	C3A-C2A-CAA-CBA
11	B	1492	CLA	C15-C16-C17-C18
11	J	1351	CLA	C13-C15-C16-C17
11	H	1482	CLA	CBD-CGD-O2D-CED
11	H	1492	CLA	C2-C1-O2A-CGA
11	B	1492	CLA	C2-C1-O2A-CGA
11	I	1463	CLA	C2-C1-O2A-CGA
12	G	1345	PHO	C2-C1-O2A-CGA
11	H	1482	CLA	C11-C12-C13-C14
11	B	1482	CLA	C11-C12-C13-C14
11	A	1342	CLA	C14-C13-C15-C16
12	A	1345	PHO	C6-C7-C8-C9
12	G	1345	PHO	C6-C7-C8-C9
11	I	1464	CLA	C6-C7-C8-C9
17	L	1047	BCR	C23-C24-C25-C26
17	F	1046	BCR	C23-C24-C25-C26
11	H	1487	CLA	C5-C6-C7-C8
11	H	1494	CLA	C5-C6-C7-C8
11	B	1482	CLA	C11-C12-C13-C15
11	H	1492	CLA	C6-C7-C8-C10
11	B	1492	CLA	C6-C7-C8-C10
11	C	1465	CLA	C6-C7-C8-C10
11	I	1465	CLA	C6-C7-C8-C10
11	H	1488	CLA	C11-C12-C13-C15
12	A	1345	PHO	C6-C7-C8-C10
11	B	1488	CLA	C11-C12-C13-C15
12	A	1345	PHO	C5-C6-C7-C8
11	H	1492	CLA	C15-C16-C17-C18
11	B	1489	CLA	CAD-CBD-CGD-O2D
11	I	1470	CLA	CAD-CBD-CGD-O2D
11	H	1488	CLA	CAD-CBD-CGD-O2D
11	J	1353	CLA	CAD-CBD-CGD-O2D
11	B	1488	CLA	CAD-CBD-CGD-O2D
11	D	1351	CLA	CAD-CBD-CGD-O2D
11	J	1351	CLA	CAD-CBD-CGD-O2D
11	H	1482	CLA	O1D-CGD-O2D-CED
12	G	1345	PHO	C5-C6-C7-C8
11	B	1497	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
11	B	1497	CLA	CHA-CBD-CGD-O2D
11	I	1466	CLA	CHA-CBD-CGD-O1D
11	I	1466	CLA	CHA-CBD-CGD-O2D
11	G	1343	CLA	CHA-CBD-CGD-O1D
11	H	1497	CLA	CHA-CBD-CGD-O1D
11	H	1497	CLA	CHA-CBD-CGD-O2D
11	A	1343	CLA	CHA-CBD-CGD-O1D
11	B	1483	CLA	CHA-CBD-CGD-O1D
11	C	1466	CLA	CHA-CBD-CGD-O1D
11	C	1466	CLA	CHA-CBD-CGD-O2D
11	B	1490	CLA	CHA-CBD-CGD-O2D
11	B	1495	CLA	CHA-CBD-CGD-O1D
11	H	1483	CLA	CHA-CBD-CGD-O2D
11	C	1471	CLA	C4C-C3C-CAC-CBC
11	I	1464	CLA	C11-C10-C8-C9
11	G	1344	CLA	C1A-C2A-CAA-CBA
11	B	1495	CLA	C2-C3-C5-C6
11	H	1495	CLA	C2A-CAA-CBA-CGA
11	B	1489	CLA	CAD-CBD-CGD-O1D
11	H	1492	CLA	CAD-CBD-CGD-O1D
11	B	1492	CLA	CAD-CBD-CGD-O1D
11	A	1344	CLA	CAD-CBD-CGD-O1D
11	G	1343	CLA	CAD-CBD-CGD-O1D
11	C	1467	CLA	CAD-CBD-CGD-O1D
11	G	1344	CLA	CAD-CBD-CGD-O1D
11	C	1464	CLA	CAD-CBD-CGD-O1D
11	I	1467	CLA	CAD-CBD-CGD-O1D
11	A	1343	CLA	CAD-CBD-CGD-O1D
11	H	1490	CLA	CAD-CBD-CGD-O1D
11	I	1464	CLA	CAD-CBD-CGD-O1D
11	B	1490	CLA	CAD-CBD-CGD-O1D
11	B	1492	CLA	C4-C3-C5-C6
11	H	1482	CLA	C11-C12-C13-C15
11	B	1496	CLA	C12-C13-C15-C16
11	H	1488	CLA	C12-C13-C15-C16
11	B	1488	CLA	C12-C13-C15-C16
11	H	1496	CLA	C12-C13-C15-C16
11	H	1482	CLA	CAA-CBA-CGA-O2A
11	B	1494	CLA	C13-C15-C16-C17
11	C	1465	CLA	C13-C15-C16-C17
11	B	1495	CLA	C2A-CAA-CBA-CGA
11	I	1465	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
11	I	1471	CLA	C4C-C3C-CAC-CBC
11	C	1464	CLA	C11-C10-C8-C9
11	H	1488	CLA	C6-C7-C8-C9
11	D	1353	CLA	C2A-CAA-CBA-CGA
11	J	1353	CLA	C2A-CAA-CBA-CGA
11	B	1496	CLA	C2-C1-O2A-CGA
11	C	1463	CLA	C2-C1-O2A-CGA
11	H	1496	CLA	C2-C1-O2A-CGA
11	B	1482	CLA	CAA-CBA-CGA-O2A
11	H	1494	CLA	C13-C15-C16-C17
11	C	1465	CLA	C12-C13-C15-C16
11	C	1465	CLA	C14-C13-C15-C16
11	I	1465	CLA	C14-C13-C15-C16
11	G	1343	CLA	C12-C13-C15-C16
11	A	1343	CLA	C12-C13-C15-C16
12	G	1345	PHO	O1D-CGD-O2D-CED
12	A	1345	PHO	C2-C1-O2A-CGA
11	C	1459	CLA	C3A-C2A-CAA-CBA
11	B	1488	CLA	C6-C7-C8-C9
11	B	1487	CLA	CAA-CBA-CGA-O1A
12	J	1352	PHO	O2A-C1-C2-C3
12	D	1352	PHO	O2A-C1-C2-C3
11	B	1488	CLA	O1D-CGD-O2D-CED
11	A	1344	CLA	C1A-C2A-CAA-CBA
11	H	1487	CLA	C1A-C2A-CAA-CBA
11	B	1490	CLA	C1A-C2A-CAA-CBA
11	I	1465	CLA	C12-C13-C15-C16
11	B	1483	CLA	C11-C10-C8-C7
11	H	1496	CLA	C2C-C3C-CAC-CBC
11	B	1488	CLA	CBD-CGD-O2D-CED
11	H	1487	CLA	CAA-CBA-CGA-O1A
11	B	1495	CLA	CAA-CBA-CGA-O2A
11	B	1485	CLA	C4C-C3C-CAC-CBC
11	B	1488	CLA	C15-C16-C17-C18
11	H	1488	CLA	C10-C11-C12-C13
11	H	1495	CLA	CAA-CBA-CGA-O2A
11	C	1464	CLA	C6-C7-C8-C10
12	G	1345	PHO	CBD-CGD-O2D-CED
11	B	1485	CLA	C2C-C3C-CAC-CBC
11	H	1485	CLA	C4C-C3C-CAC-CBC
11	B	1482	CLA	C5-C6-C7-C8
11	B	1485	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
11	I	1467	CLA	CAA-CBA-CGA-O2A
11	C	1465	CLA	C4-C3-C5-C6
11	B	1496	CLA	C4-C3-C5-C6
12	A	1345	PHO	C4-C3-C5-C6
11	J	1351	CLA	C4-C3-C5-C6
11	B	1492	CLA	C2-C3-C5-C6
11	H	1485	CLA	C2-C1-O2A-CGA
11	J	1351	CLA	C3A-C2A-CAA-CBA
11	B	1483	CLA	C3A-C2A-CAA-CBA
11	B	1495	CLA	C3A-C2A-CAA-CBA
11	I	1459	CLA	C3A-C2A-CAA-CBA
11	C	1467	CLA	CAA-CBA-CGA-O2A
11	C	1471	CLA	CAD-CBD-CGD-O2D
12	J	1352	PHO	CAD-CBD-CGD-O2D
12	D	1352	PHO	CAD-CBD-CGD-O2D
11	H	1493	CLA	CAD-CBD-CGD-O2D
11	B	1494	CLA	CAD-CBD-CGD-O2D
11	H	1486	CLA	CAD-CBD-CGD-O2D
11	B	1493	CLA	CAD-CBD-CGD-O2D
11	A	1342	CLA	CAD-CBD-CGD-O2D
11	G	1342	CLA	CAD-CBD-CGD-O2D
11	I	1471	CLA	CAD-CBD-CGD-O2D
12	A	1345	PHO	CAD-CBD-CGD-O2D
11	D	1353	CLA	CAD-CBD-CGD-O2D
11	C	1459	CLA	CAD-CBD-CGD-O2D
12	G	1345	PHO	CAD-CBD-CGD-O2D
11	C	1470	CLA	CAD-CBD-CGD-O2D
11	H	1494	CLA	CAD-CBD-CGD-O2D
11	H	1485	CLA	C2C-C3C-CAC-CBC
11	D	1351	CLA	C4-C3-C5-C6
12	G	1345	PHO	C4-C3-C5-C6
11	J	1351	CLA	C2-C3-C5-C6
11	I	1464	CLA	CAA-CBA-CGA-O2A
11	B	1496	CLA	O2A-C1-C2-C3
12	A	1345	PHO	O2A-C1-C2-C3
12	G	1345	PHO	O2A-C1-C2-C3
11	H	1496	CLA	O2A-C1-C2-C3
11	C	1464	CLA	CAA-CBA-CGA-O2A
11	G	1343	CLA	CHA-CBD-CGD-O2D
11	C	1465	CLA	CHA-CBD-CGD-O2D
11	I	1465	CLA	CHA-CBD-CGD-O1D
11	I	1465	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
11	H	1488	CLA	CHA-CBD-CGD-O1D
11	C	1463	CLA	CHA-CBD-CGD-O1D
11	C	1463	CLA	CHA-CBD-CGD-O2D
11	H	1495	CLA	CHA-CBD-CGD-O1D
11	H	1495	CLA	CHA-CBD-CGD-O2D
11	A	1343	CLA	CHA-CBD-CGD-O2D
11	B	1483	CLA	CHA-CBD-CGD-O2D
11	B	1495	CLA	CHA-CBD-CGD-O2D
11	D	1351	CLA	C2-C3-C5-C6
12	G	1345	PHO	C2-C3-C5-C6
11	H	1496	CLA	C4C-C3C-CAC-CBC
11	B	1496	CLA	C2C-C3C-CAC-CBC
12	A	1345	PHO	C2-C3-C5-C6
11	H	1483	CLA	C11-C10-C8-C7
11	B	1483	CLA	C11-C10-C8-C9
11	H	1483	CLA	C11-C10-C8-C9
11	C	1467	CLA	CAA-CBA-CGA-O1A
11	B	1487	CLA	C1A-C2A-CAA-CBA
11	H	1482	CLA	C1A-C2A-CAA-CBA
11	B	1482	CLA	C1A-C2A-CAA-CBA
11	C	1465	CLA	C1A-C2A-CAA-CBA
11	G	1346	CLA	C1A-C2A-CAA-CBA
11	D	1351	CLA	C1A-C2A-CAA-CBA
11	J	1351	CLA	C1A-C2A-CAA-CBA
11	B	1483	CLA	C1A-C2A-CAA-CBA
11	H	1490	CLA	C1A-C2A-CAA-CBA
11	H	1483	CLA	C1A-C2A-CAA-CBA
11	I	1467	CLA	CAA-CBA-CGA-O1A
11	I	1467	CLA	C2A-CAA-CBA-CGA
11	H	1494	CLA	C2A-CAA-CBA-CGA
11	B	1488	CLA	C10-C11-C12-C13
11	H	1488	CLA	O1D-CGD-O2D-CED
11	I	1464	CLA	CAA-CBA-CGA-O1A
11	C	1464	CLA	CAA-CBA-CGA-O1A
11	H	1489	CLA	CAD-CBD-CGD-O1D
11	B	1486	CLA	CAD-CBD-CGD-O1D
11	I	1460	CLA	CAD-CBD-CGD-O1D
11	G	1343	CLA	C6-C7-C8-C9
12	A	1345	PHO	O1D-CGD-O2D-CED
11	H	1482	CLA	C3A-C2A-CAA-CBA
11	B	1482	CLA	C3A-C2A-CAA-CBA
11	B	1496	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
11	H	1495	CLA	C3A-C2A-CAA-CBA
11	D	1351	CLA	C3A-C2A-CAA-CBA
11	I	1464	CLA	C6-C7-C8-C10
11	H	1483	CLA	C3A-C2A-CAA-CBA
11	H	1488	CLA	C15-C16-C17-C18
11	B	1496	CLA	C4C-C3C-CAC-CBC

There are no ring outliers.

78 monomers are involved in 469 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	L	1047	BCR	3	0
15	D	1354	PL9	1	0
11	C	1471	CLA	5	0
11	I	1465	CLA	9	0
11	C	1463	CLA	8	0
11	J	1353	CLA	5	0
18	T	1138	HEC	3	0
11	A	1342	CLA	18	0
11	B	1487	CLA	8	0
11	H	1495	CLA	2	0
11	B	1486	CLA	13	0
11	G	1346	CLA	6	0
11	G	1342	CLA	19	0
11	C	1466	CLA	10	0
11	C	1469	CLA	7	0
11	I	1471	CLA	5	0
12	J	1352	PHO	9	0
12	D	1352	PHO	4	0
11	B	1489	CLA	4	0
11	H	1491	CLA	2	0
11	H	1487	CLA	6	0
11	B	1497	CLA	10	0
11	C	1464	CLA	9	0
11	H	1482	CLA	2	0
11	B	1482	CLA	1	0
11	H	1488	CLA	13	0
16	L	1046	HEM	2	0
11	I	1464	CLA	11	0
11	H	1492	CLA	6	0
11	C	1460	CLA	4	0
11	I	1460	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	H	1493	CLA	2	0
11	H	1485	CLA	6	0
11	I	1469	CLA	5	0
11	B	1492	CLA	5	0
11	H	1484	CLA	8	0
11	C	1462	CLA	3	0
11	I	1470	CLA	4	0
11	I	1466	CLA	10	0
11	C	1467	CLA	8	0
11	I	1467	CLA	7	0
11	I	1462	CLA	4	0
11	B	1485	CLA	5	0
11	A	1344	CLA	6	0
11	B	1490	CLA	3	0
11	C	1470	CLA	5	0
11	G	1343	CLA	4	0
11	C	1465	CLA	5	0
11	B	1494	CLA	3	0
11	H	1486	CLA	15	0
16	E	1085	HEM	2	0
11	B	1495	CLA	3	0
11	I	1463	CLA	9	0
17	F	1046	BCR	4	0
11	B	1491	CLA	3	0
11	H	1489	CLA	4	0
11	B	1483	CLA	5	0
11	G	1344	CLA	6	0
11	H	1490	CLA	3	0
11	H	1483	CLA	4	0
12	G	1345	PHO	17	0
11	B	1496	CLA	15	0
11	B	1493	CLA	1	0
11	D	1353	CLA	6	0
15	J	1354	PL9	1	0
11	B	1484	CLA	7	0
11	A	1343	CLA	8	0
11	B	1488	CLA	7	0
18	V	1138	HEC	2	0
11	C	1459	CLA	6	0
12	A	1345	PHO	14	0
11	A	1346	CLA	7	0
11	D	1351	CLA	13	0

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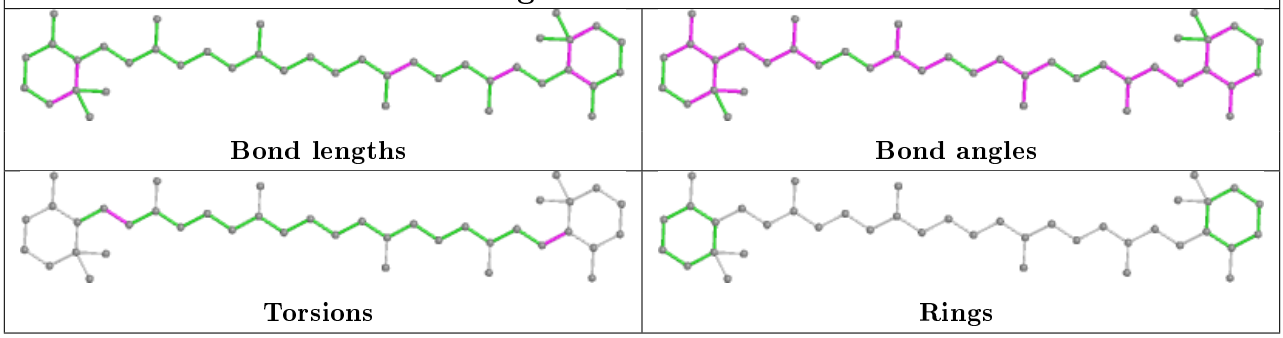
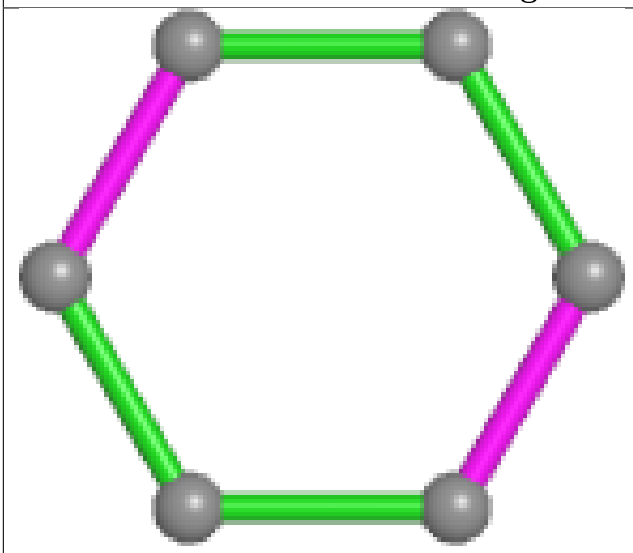
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	I	1459	CLA	5	0
11	H	1496	CLA	15	0
11	H	1494	CLA	3	0
11	J	1351	CLA	11	0
11	H	1497	CLA	10	0

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 then 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.

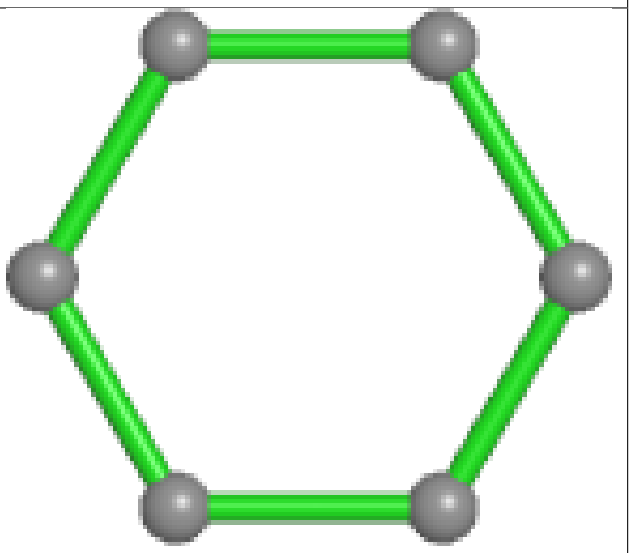
Ligand BCR L 1047



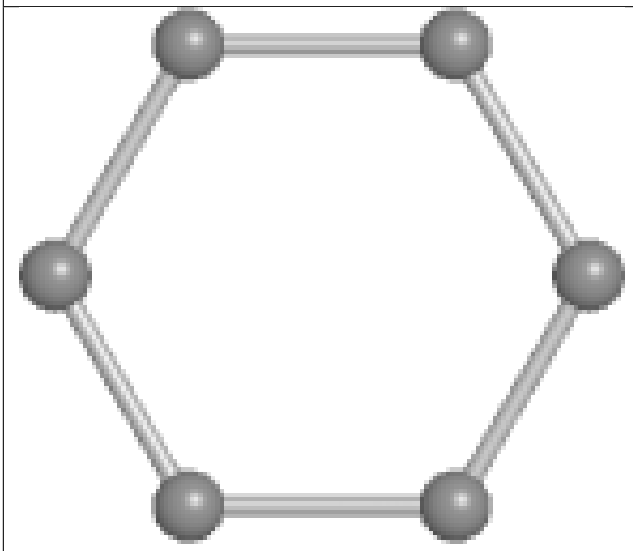
Ligand PL9 D 1354



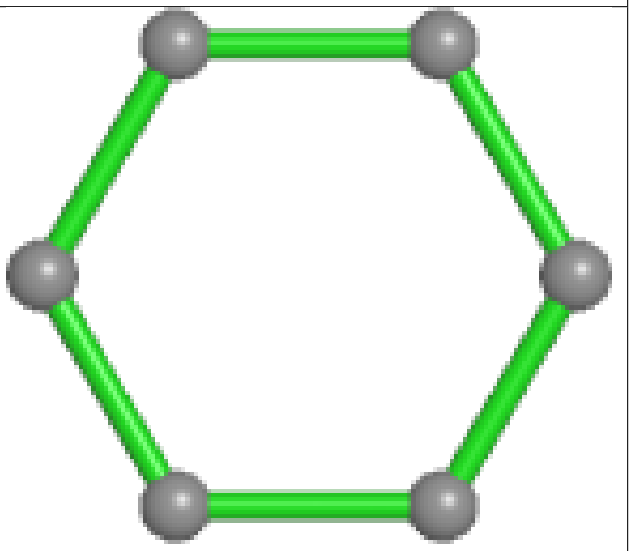
Bond lengths



Bond angles

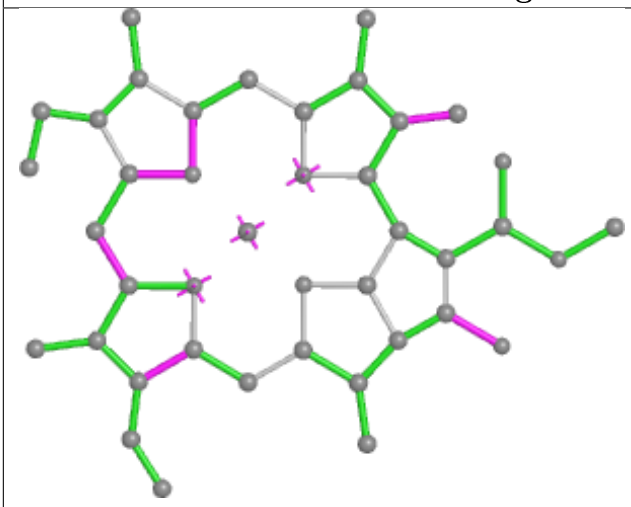


Torsions

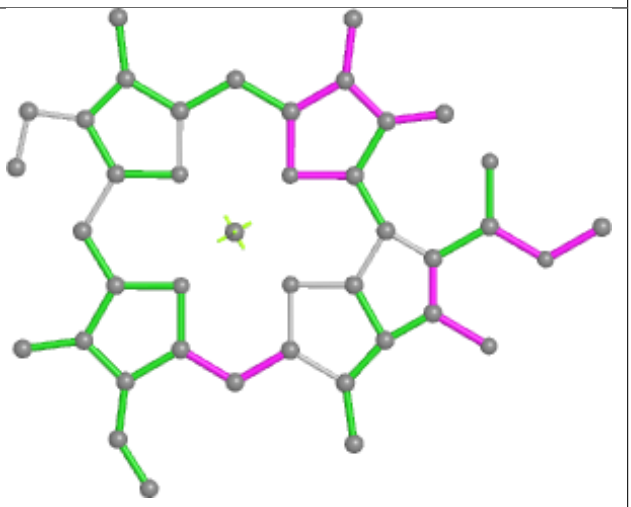


Rings

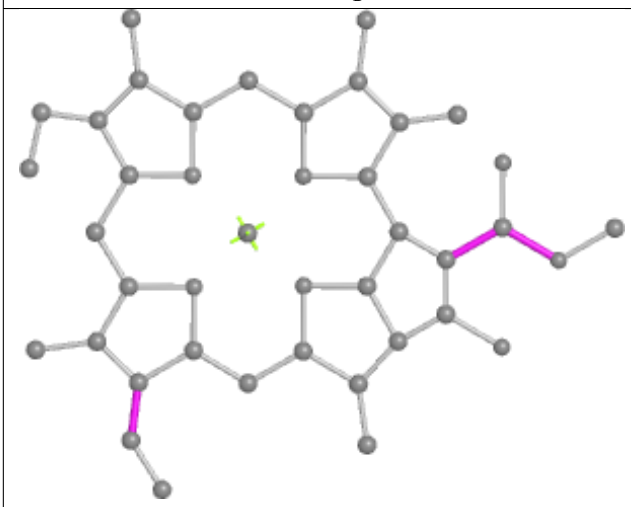
Ligand CLA C 1471



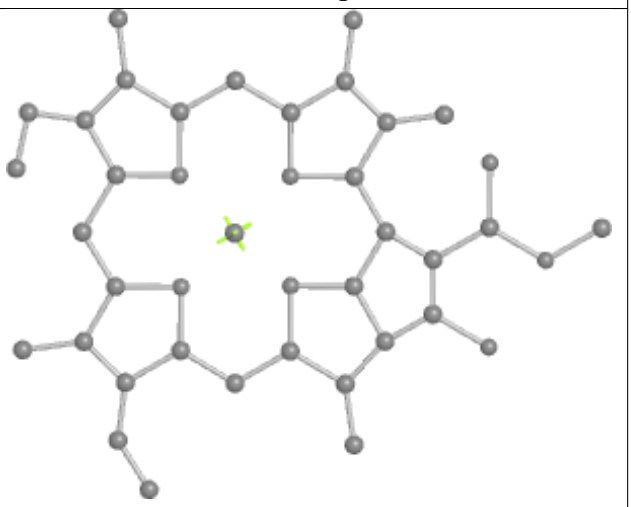
Bond lengths



Bond angles

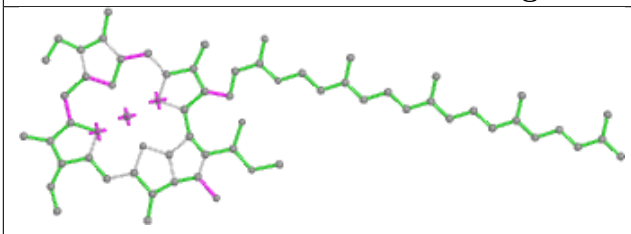


Torsions

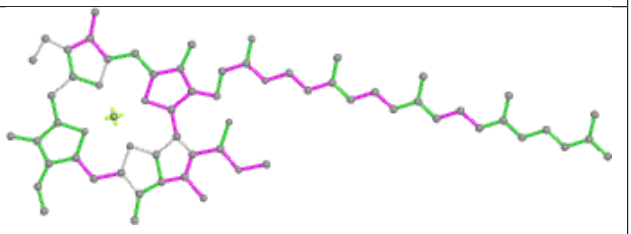


Rings

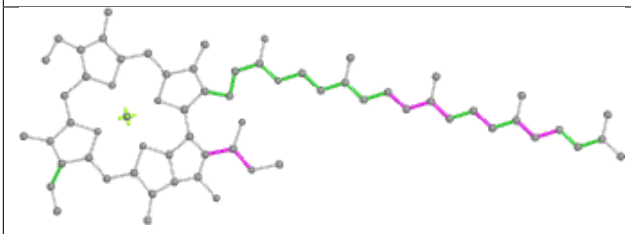
Ligand CLA I 1465



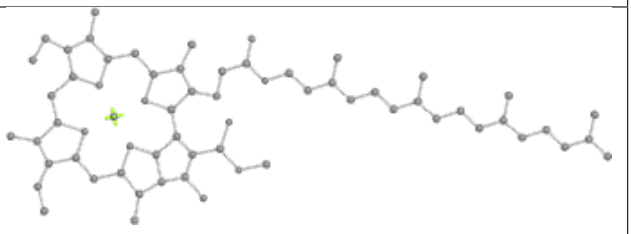
Bond lengths



Bond angles

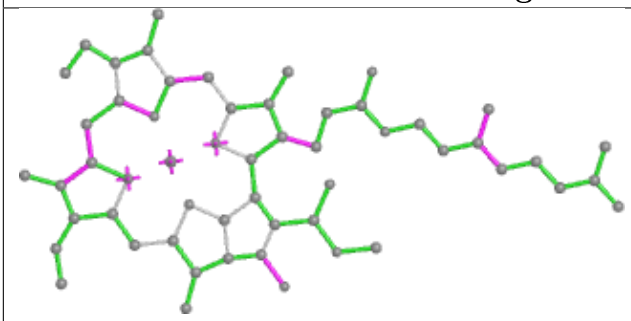


Torsions

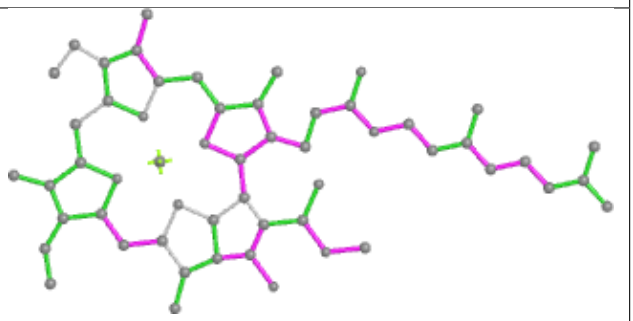


Rings

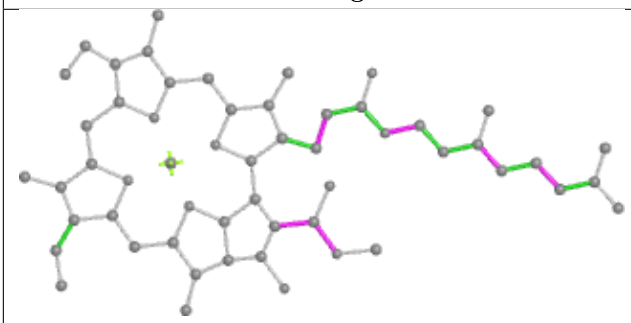
Ligand CLA C 1463



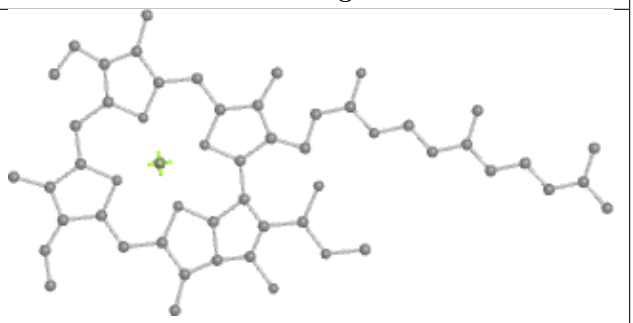
Bond lengths



Bond angles

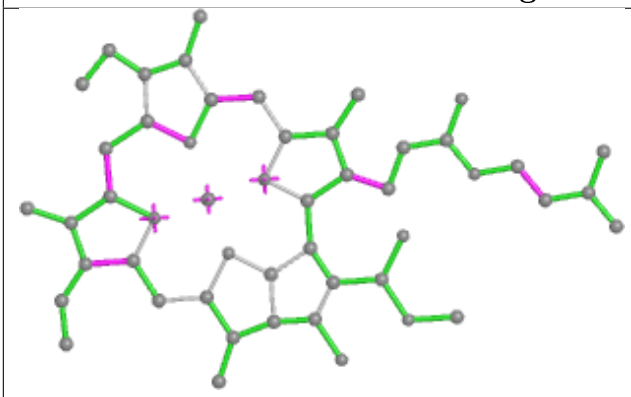


Torsions

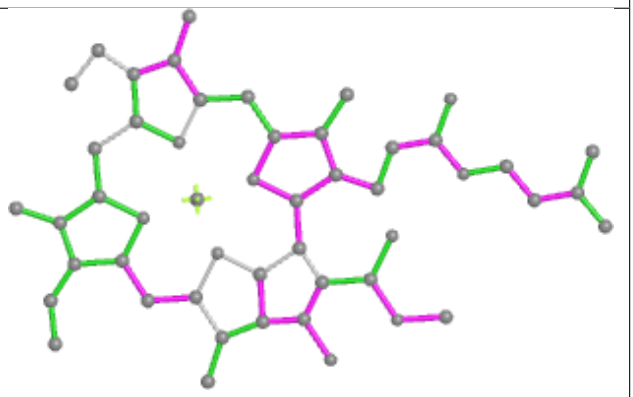


Rings

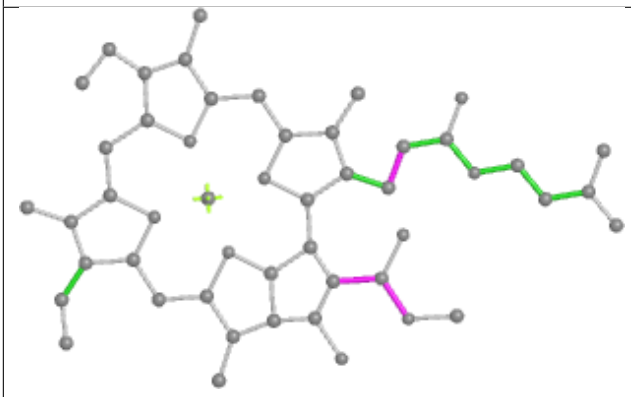
Ligand CLA J 1353



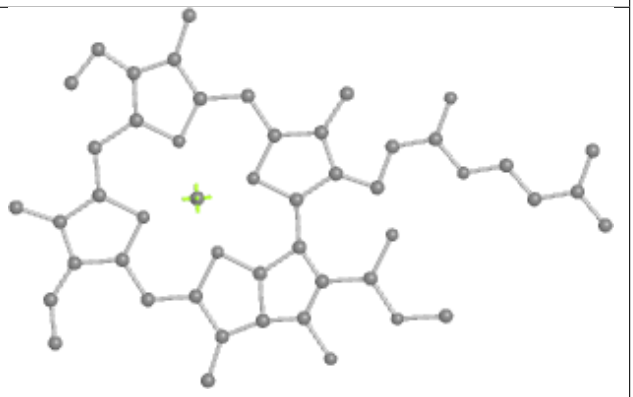
Bond lengths



Bond angles

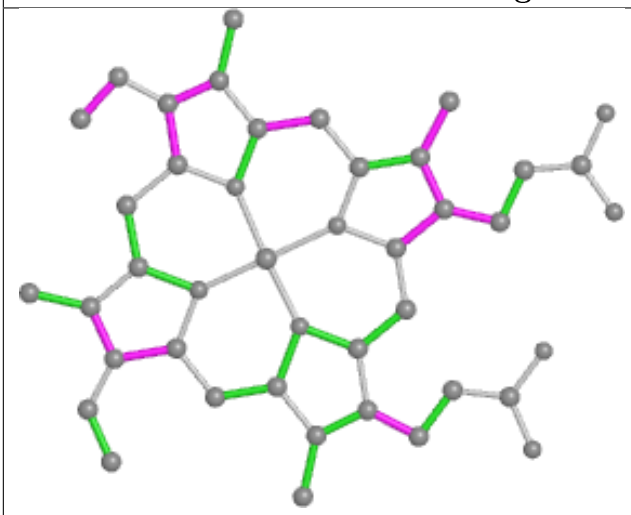


Torsions



Rings

Ligand HEC T 1138



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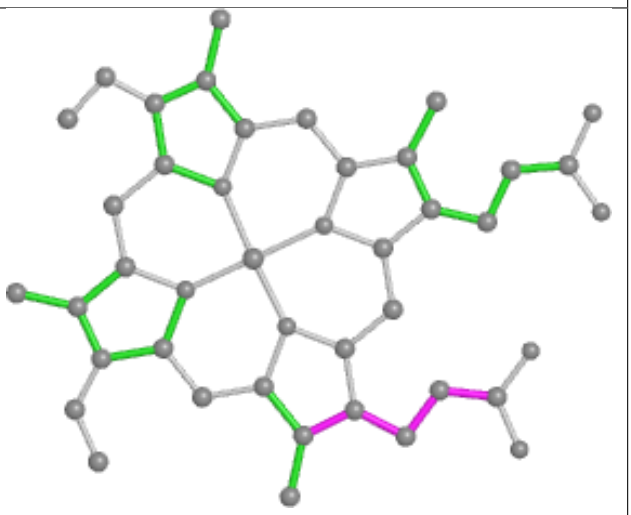
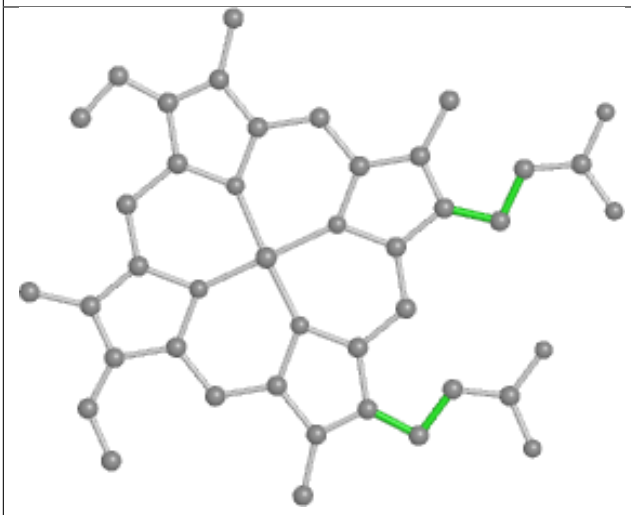
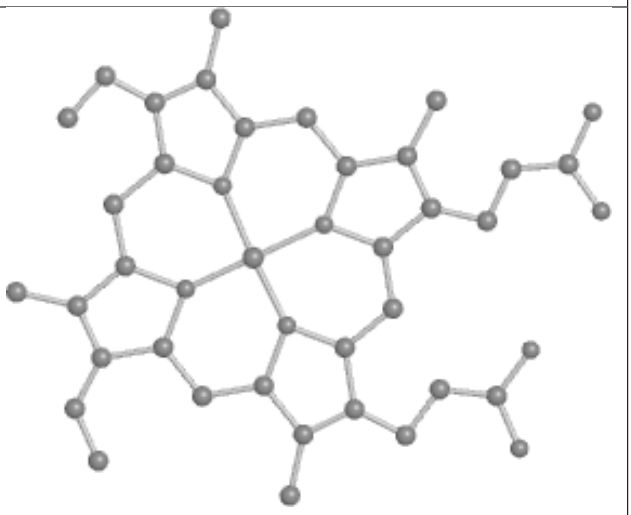


Bond angles

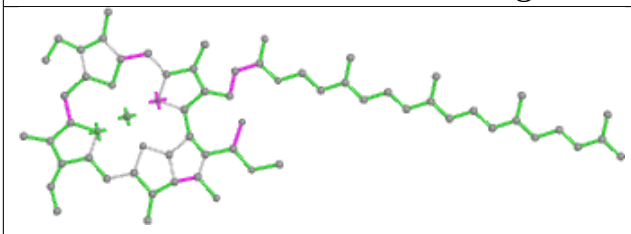


Torsions



Rings

Ligand CLA A 1342



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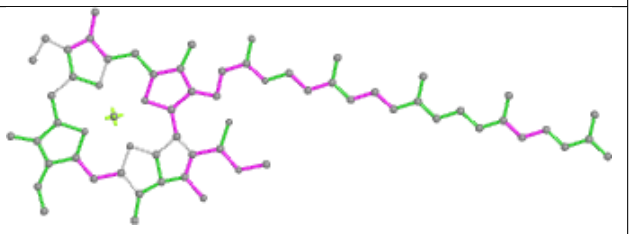
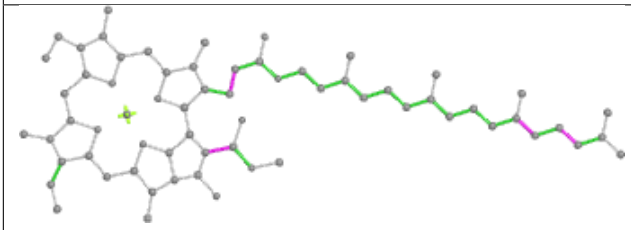
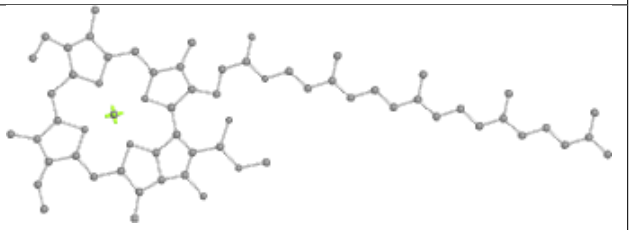


Bond angles

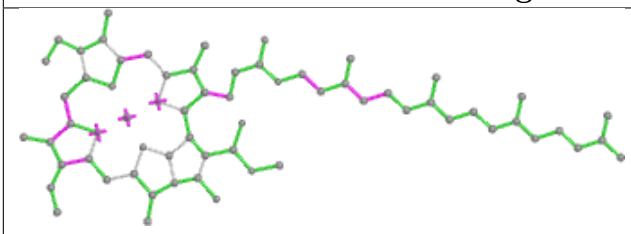


Torsions

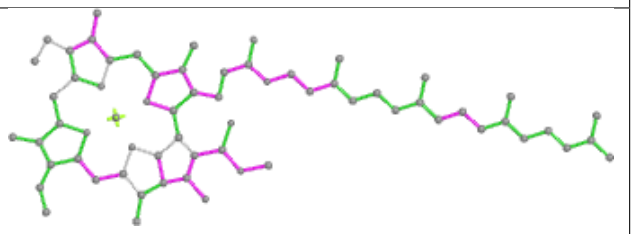


Rings

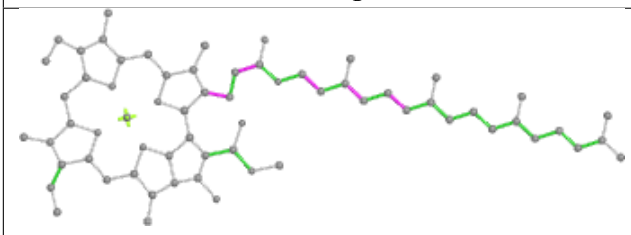
Ligand CLA B 1487



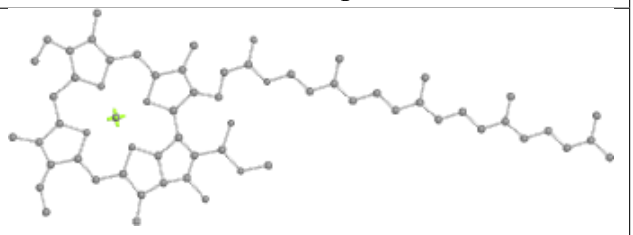
Bond lengths



Bond angles

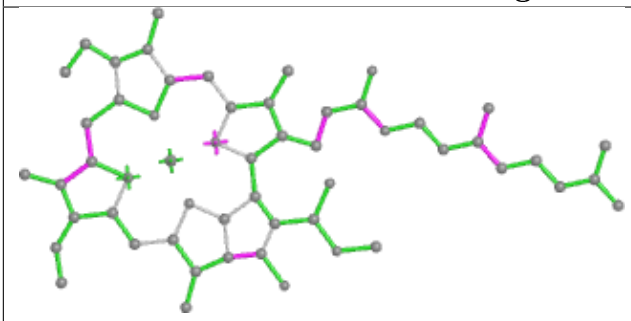


Torsions

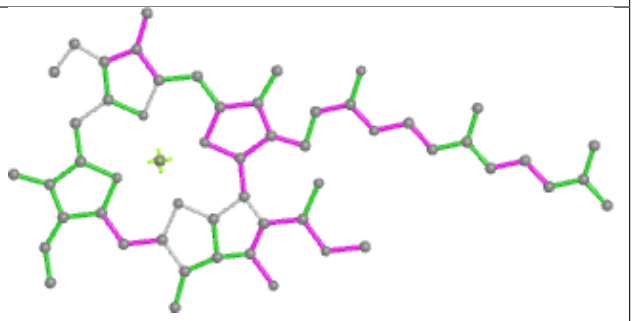


Rings

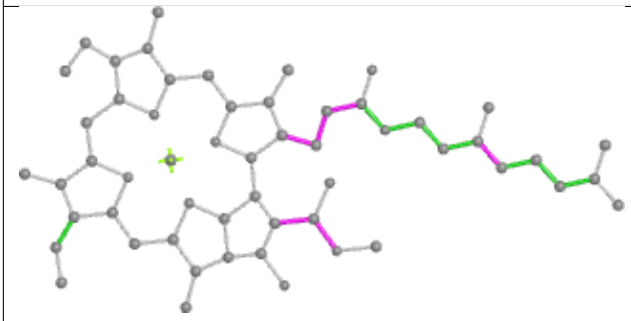
Ligand CLA H 1495



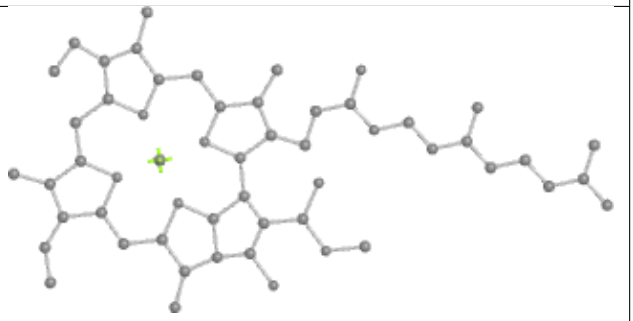
Bond lengths



Bond angles

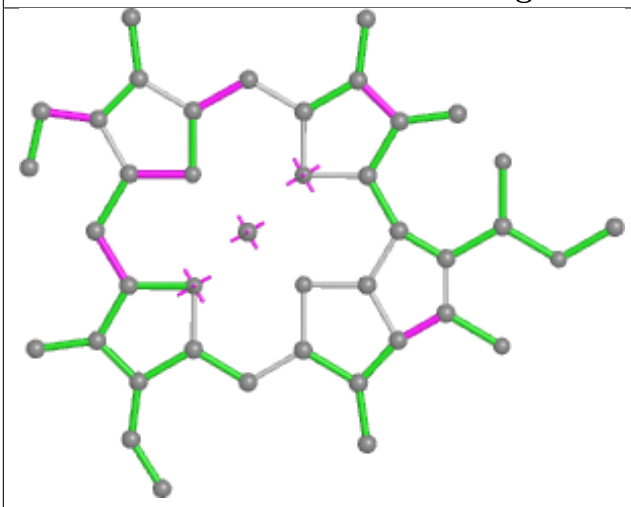


Torsions

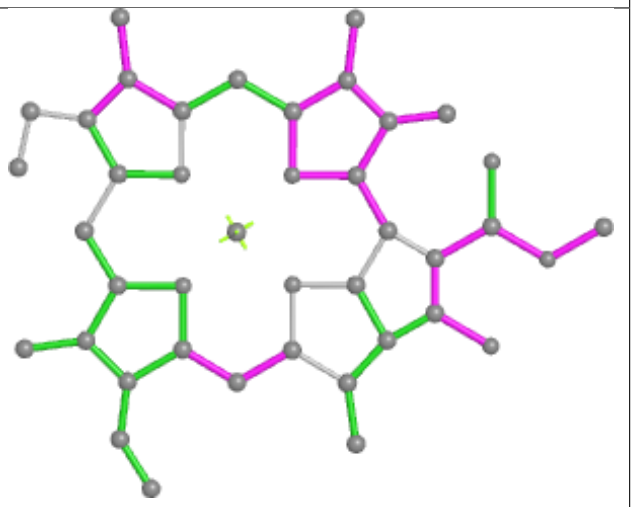


Rings

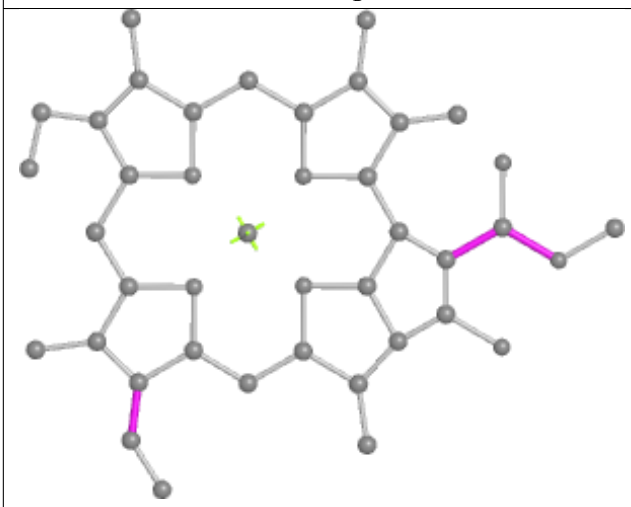
Ligand CLA B 1486



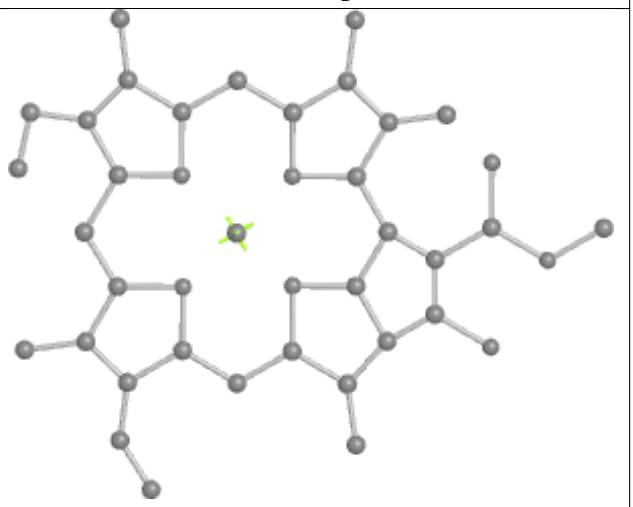
Bond lengths



Bond angles

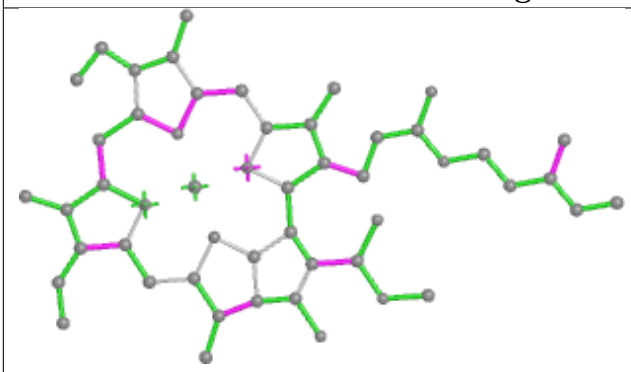


Torsions

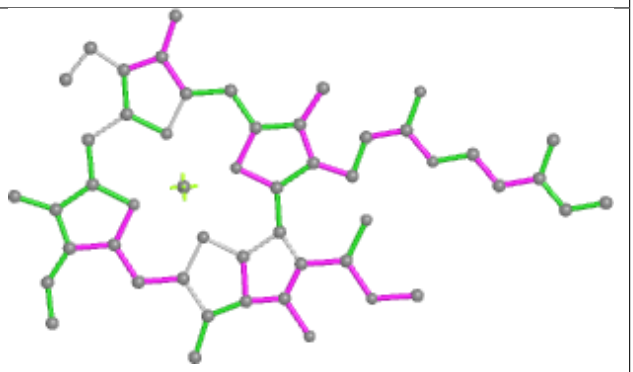


Rings

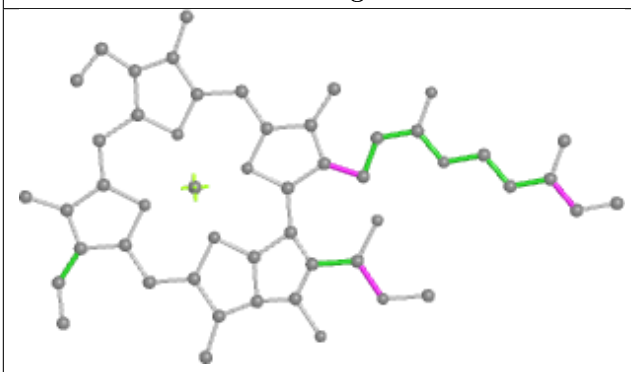
Ligand CLA G 1346



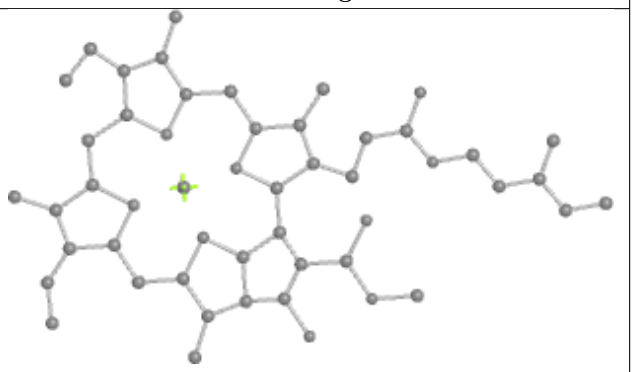
Bond lengths



Bond angles

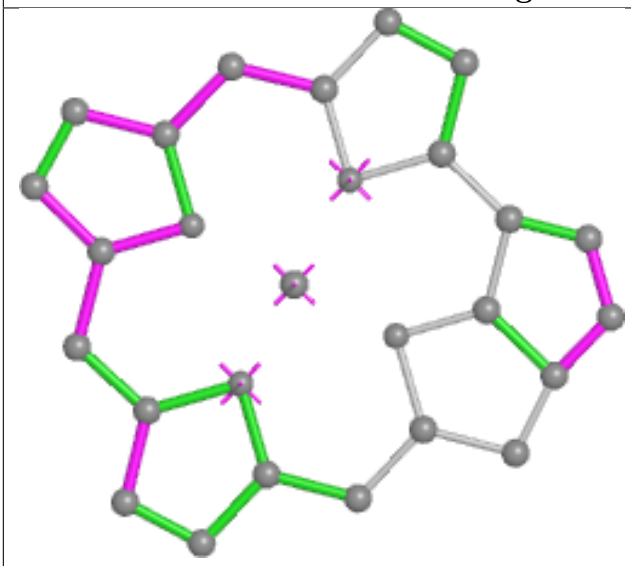


Torsions

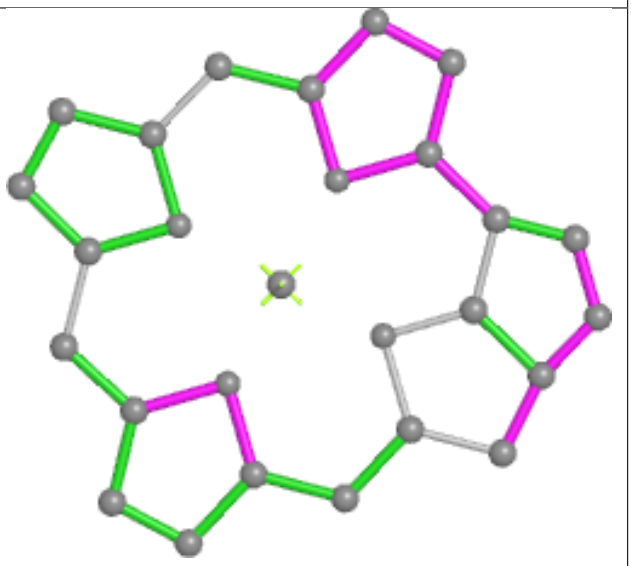


Rings

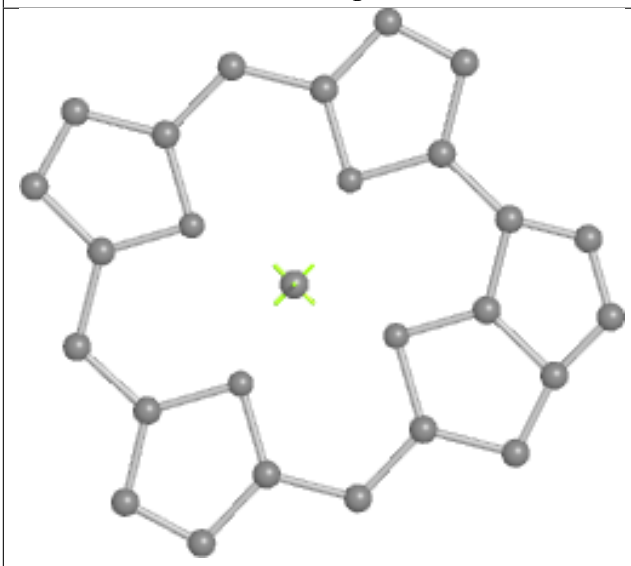
Ligand CLA C 1468



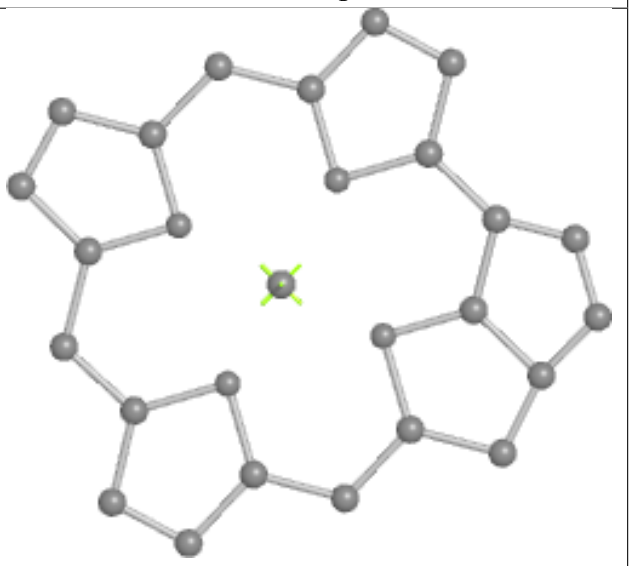
Bond lengths



Bond angles

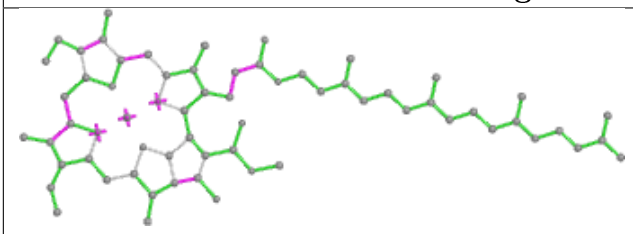


Torsions

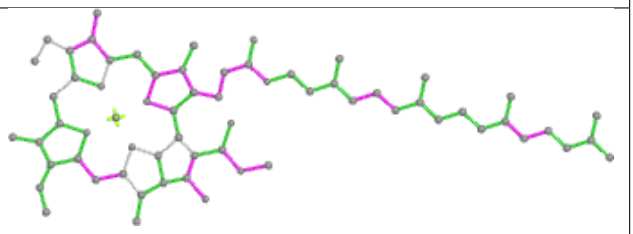


Rings

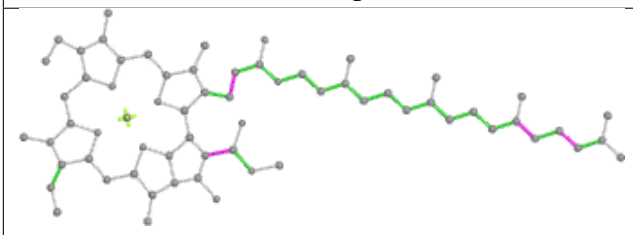
Ligand CLA G 1342



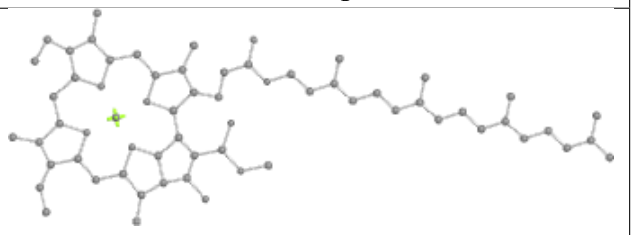
Bond lengths



Bond angles

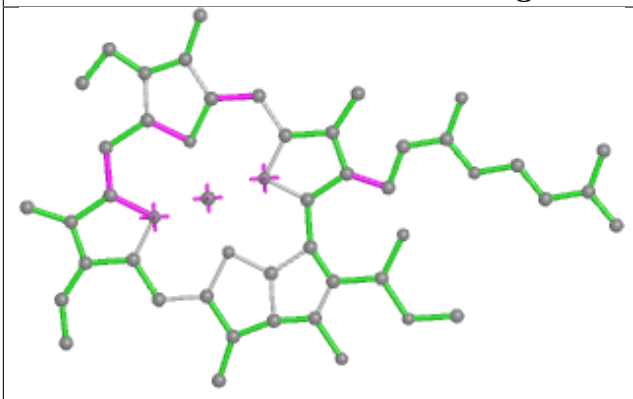


Torsions

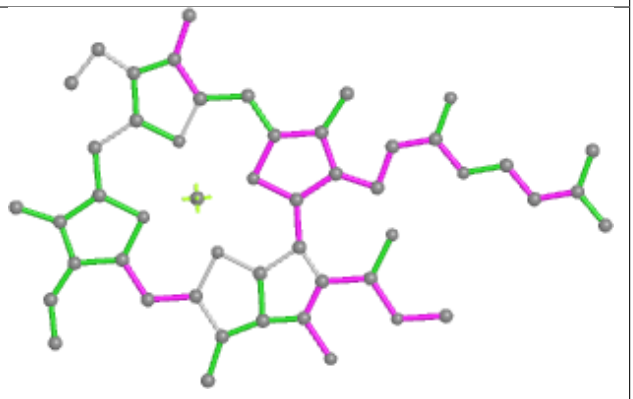


Rings

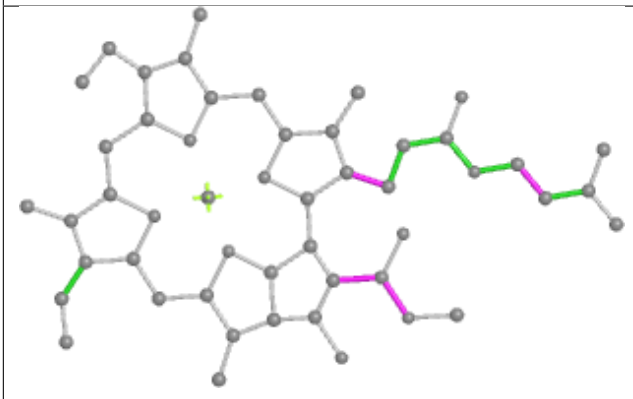
Ligand CLA C 1466



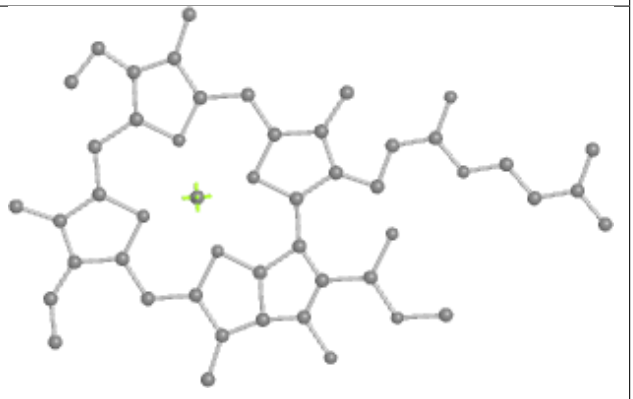
Bond lengths



Bond angles

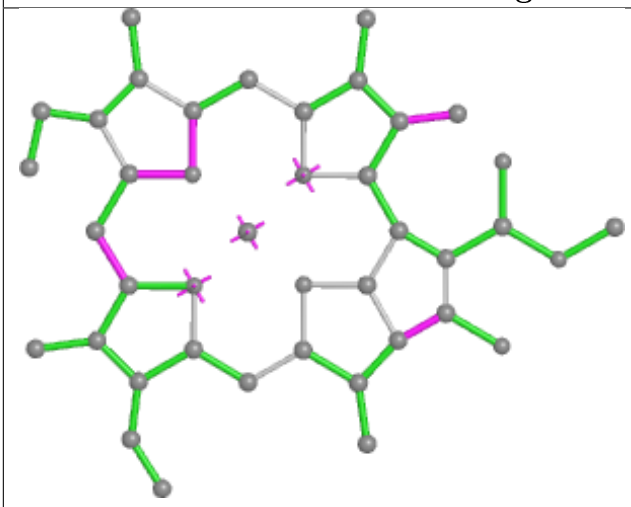


Torsions



Rings

Ligand CLA C 1469



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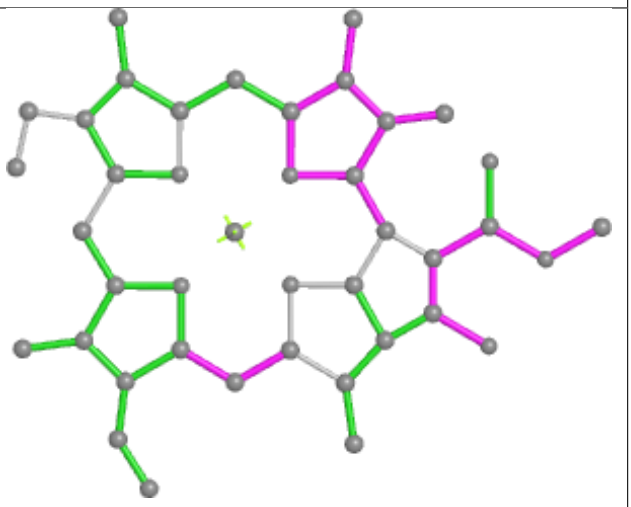
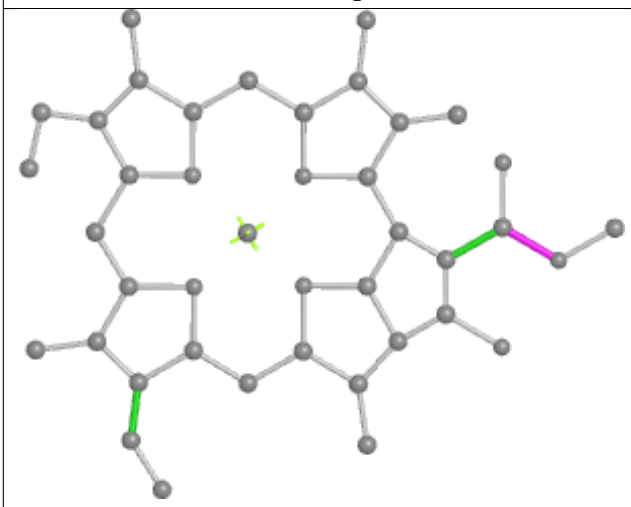
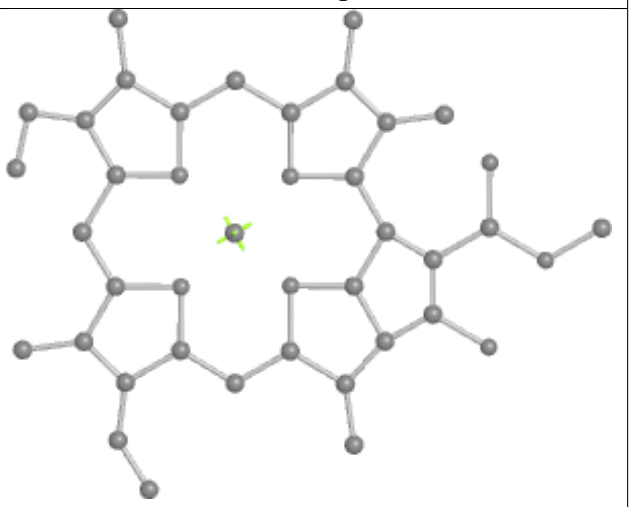


Bond angles

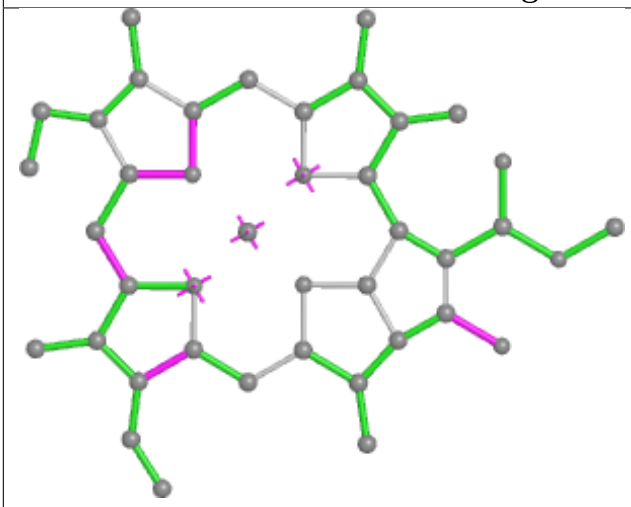


Torsions

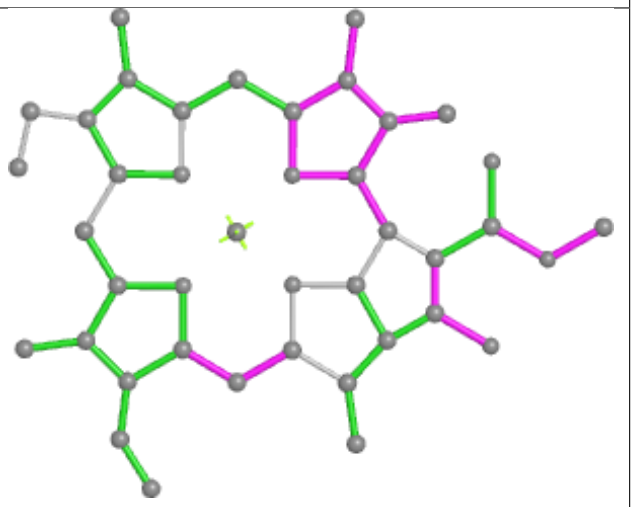


Rings

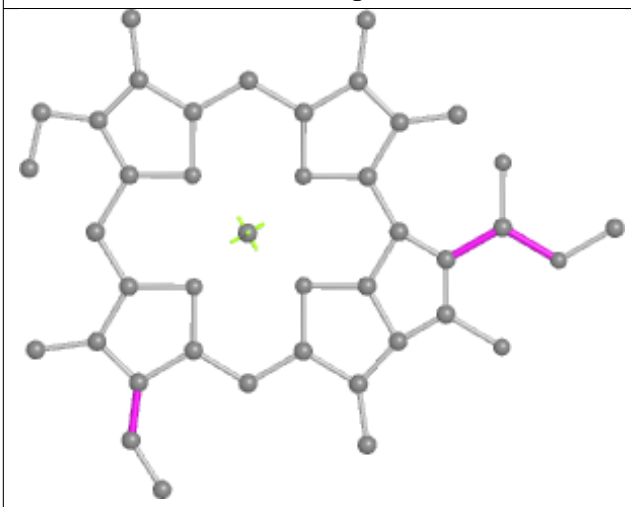
Ligand CLA I 1471



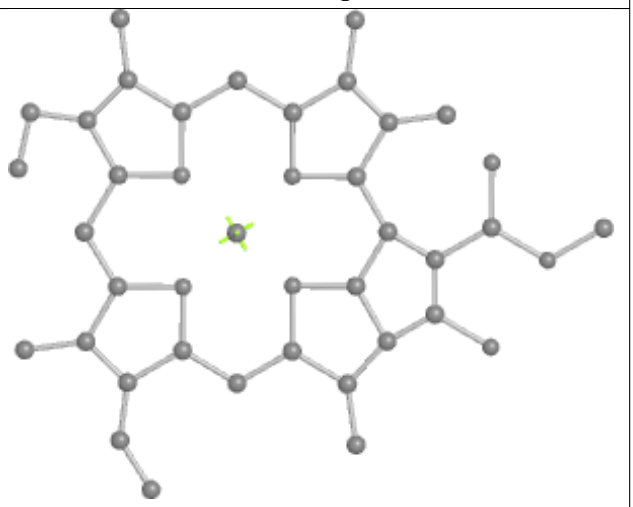
Bond lengths



Bond angles

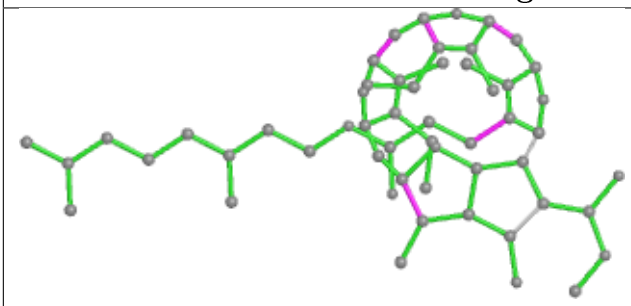


Torsions

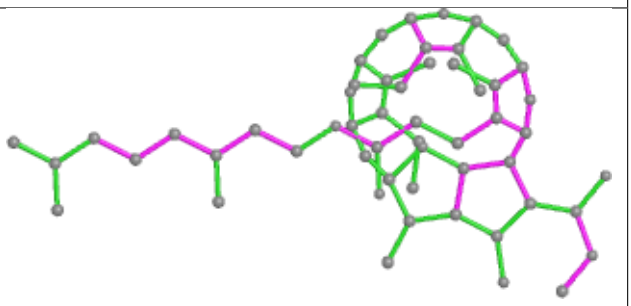


Rings

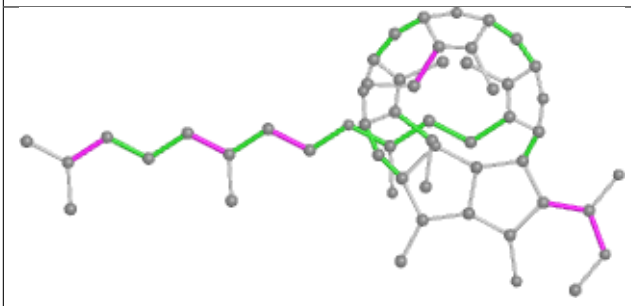
Ligand PHO J 1352



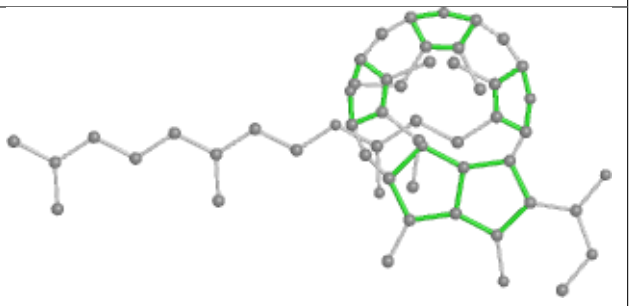
Bond lengths



Bond angles

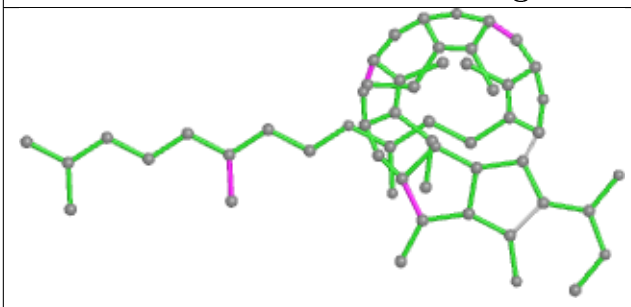


Torsions

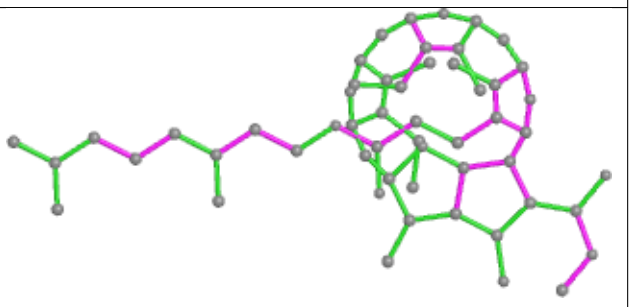


Rings

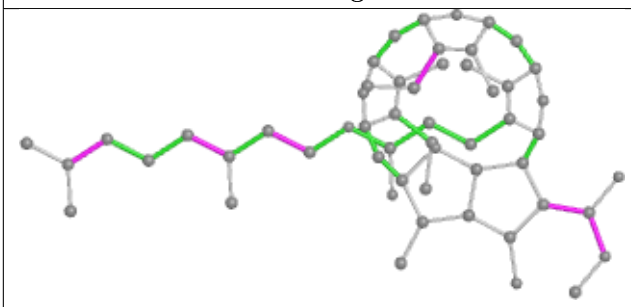
Ligand PHO D 1352



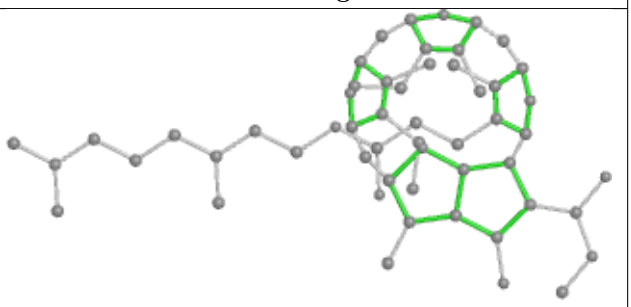
Bond lengths



Bond angles

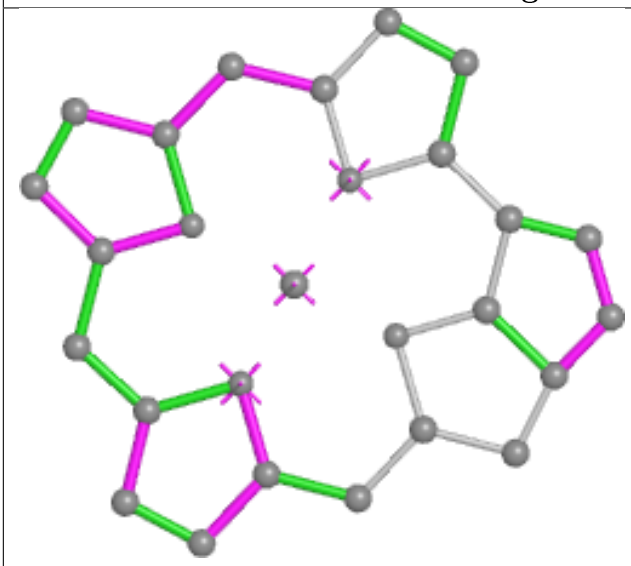


Torsions

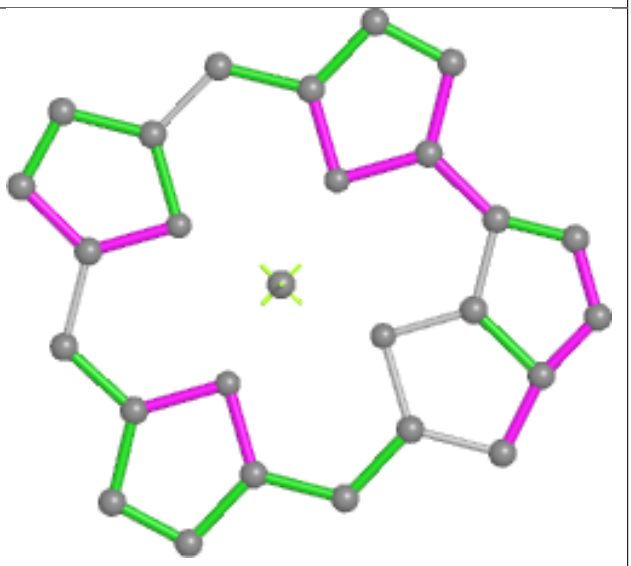


Rings

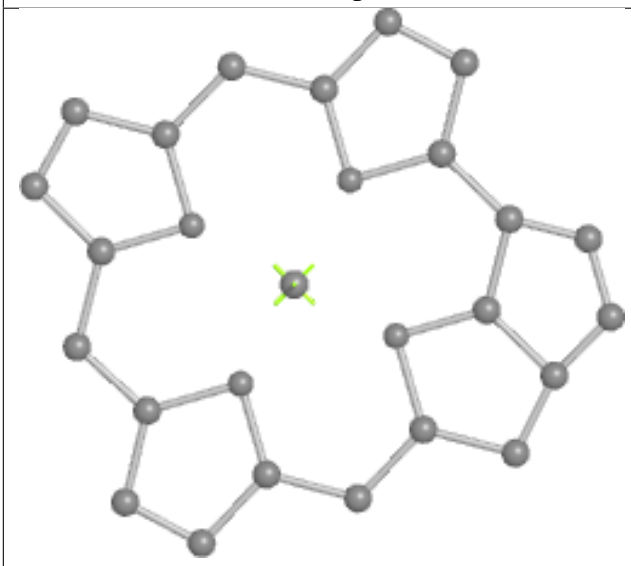
Ligand CLA I 1461



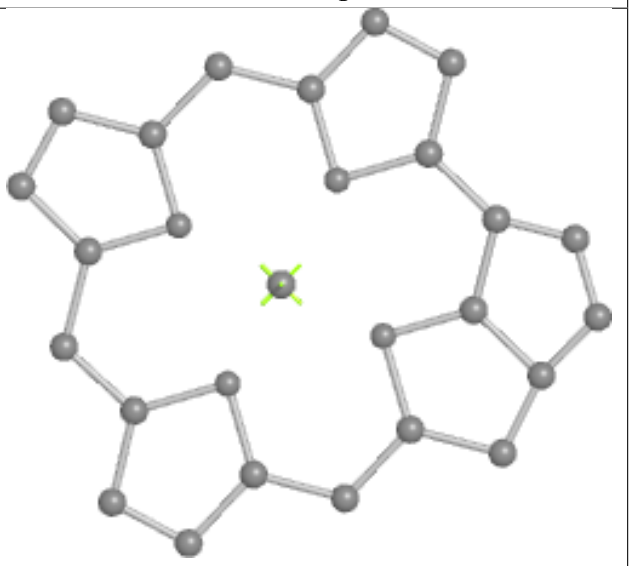
Bond lengths



Bond angles

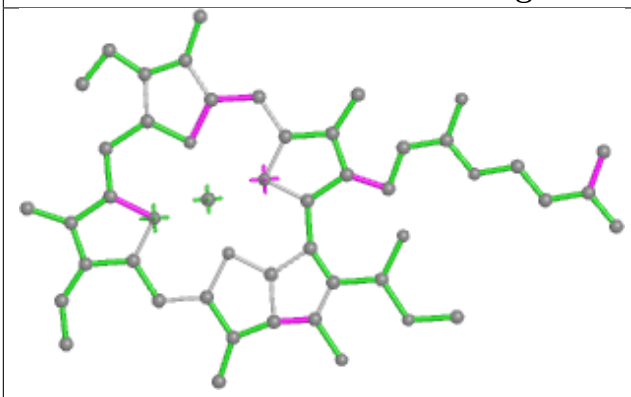


Torsions

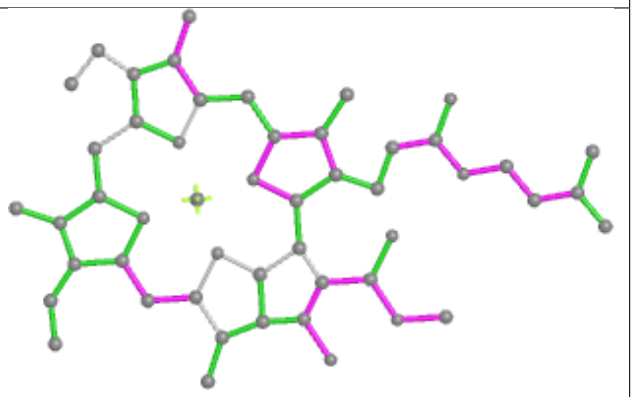


Rings

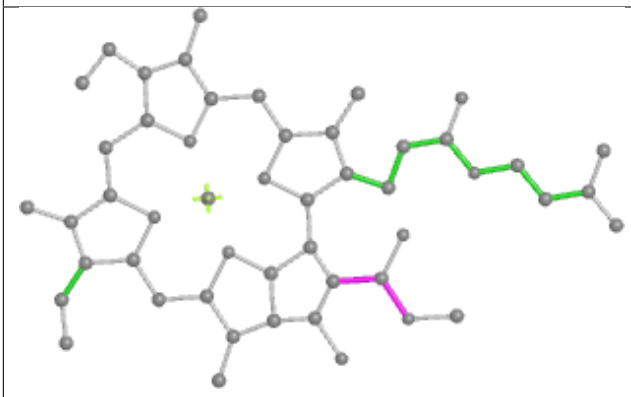
Ligand CLA B 1489



Bond lengths



Bond angles



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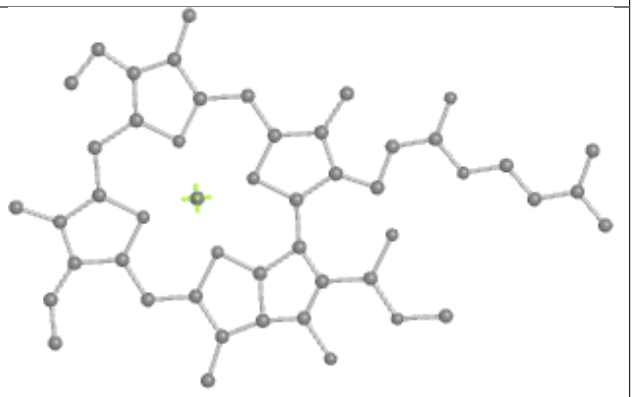
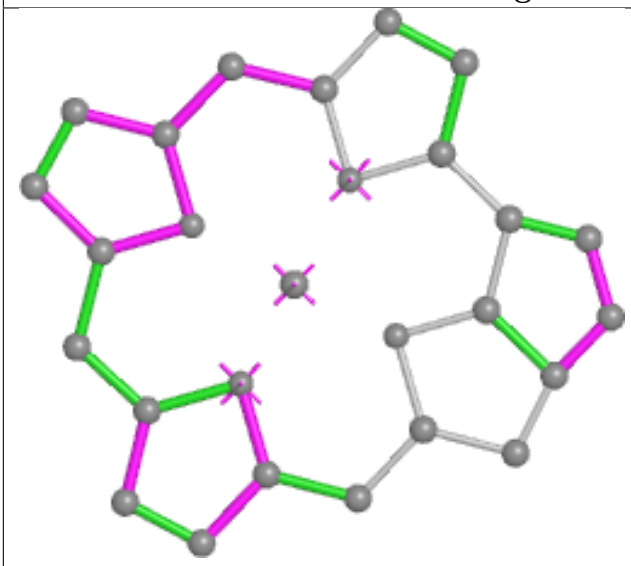


Rings

Ligand CLA H 1491



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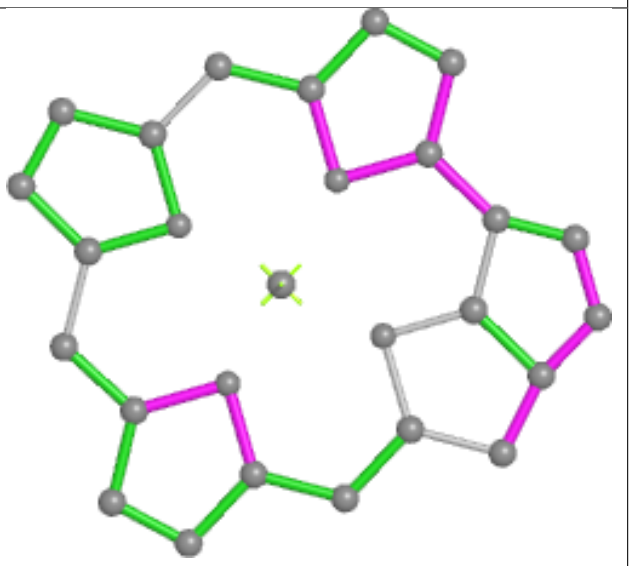
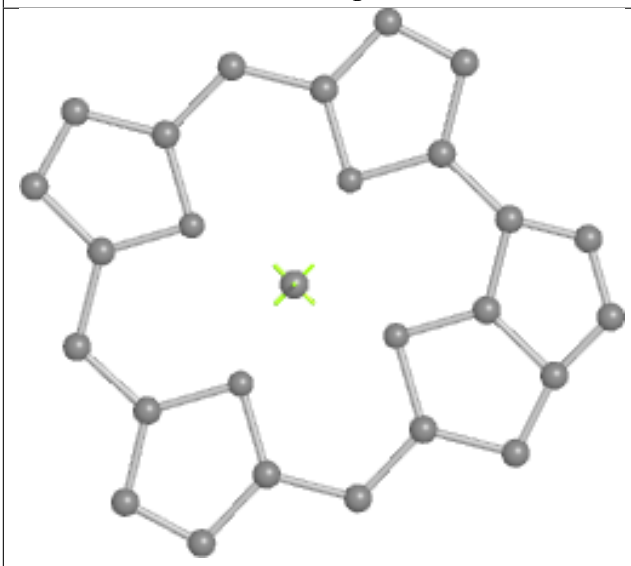


Bond angles



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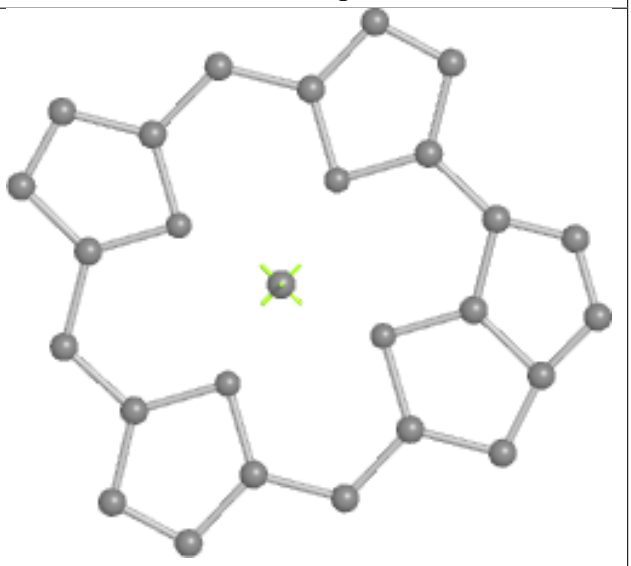
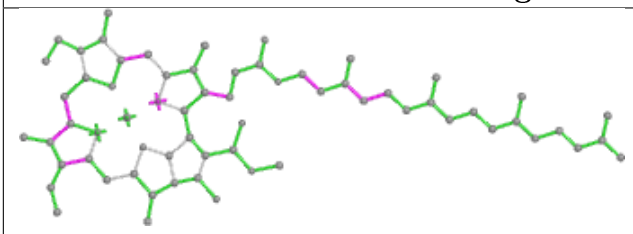
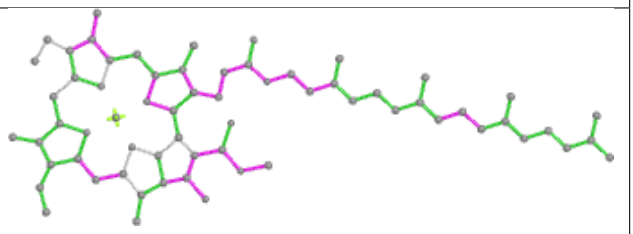


Rings

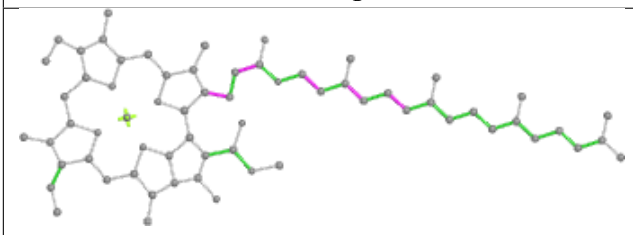
Ligand CLA H 1487



Bond lengths



Bond angles



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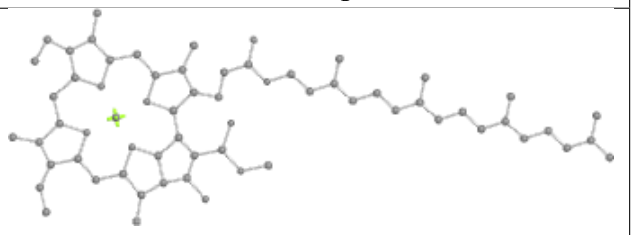
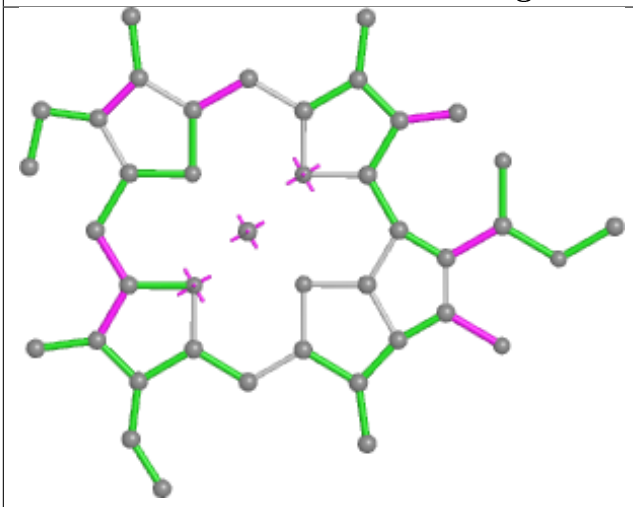


Rings

Ligand CLA B 1497



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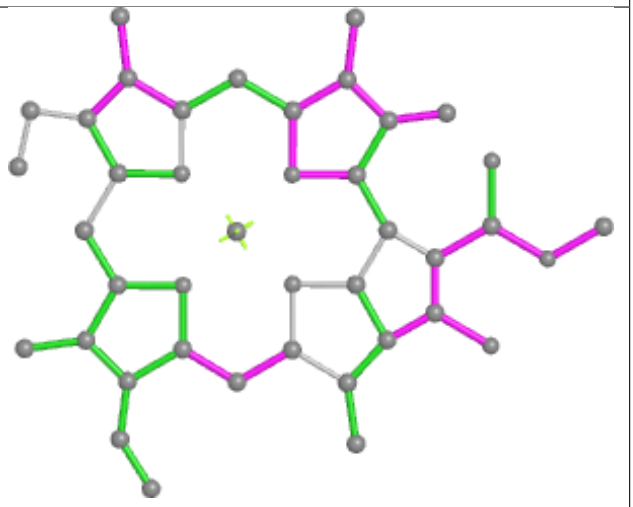
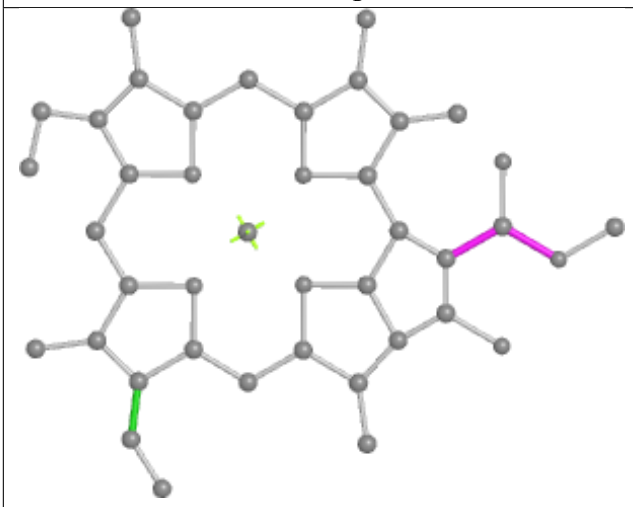


Bond angles



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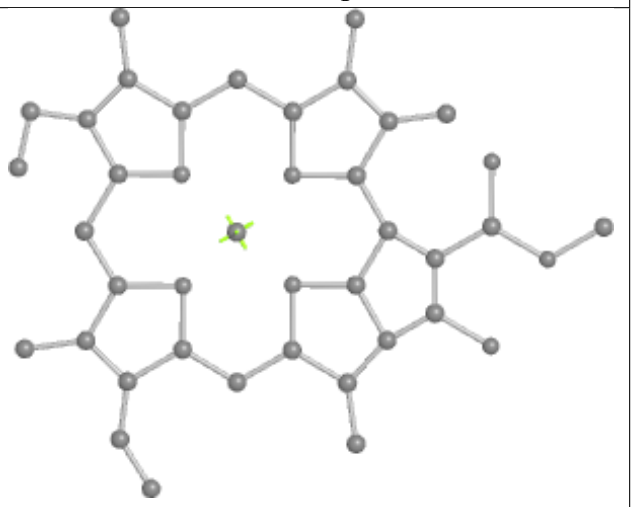
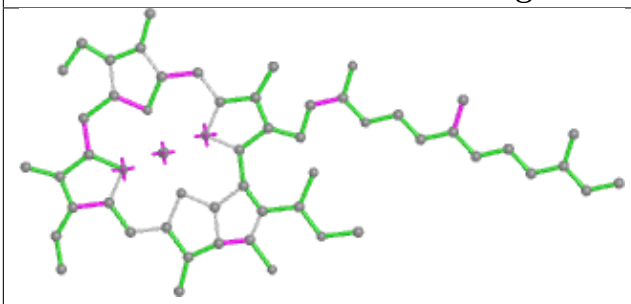
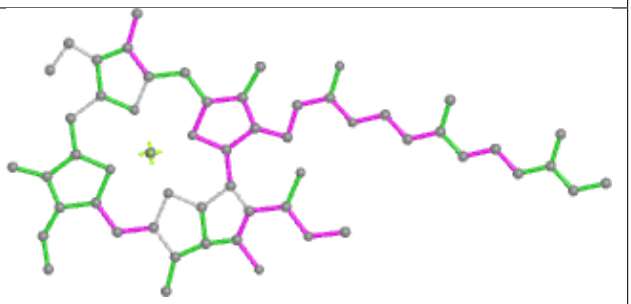


Rings

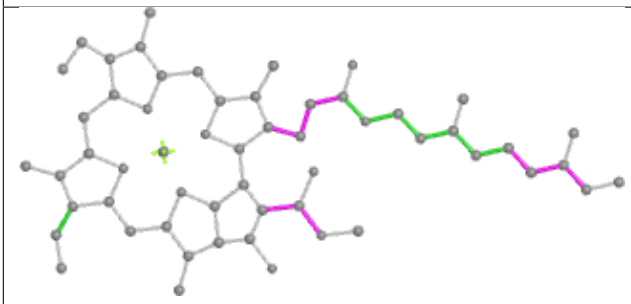
Ligand CLA C 1464



Bond lengths



Bond angles



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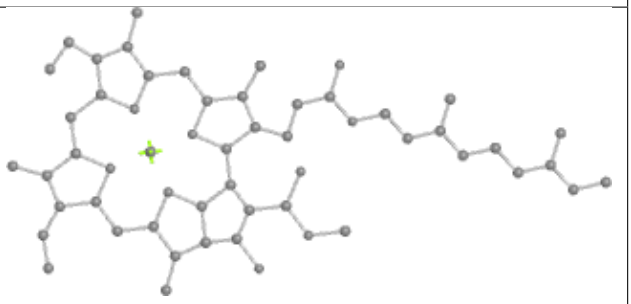
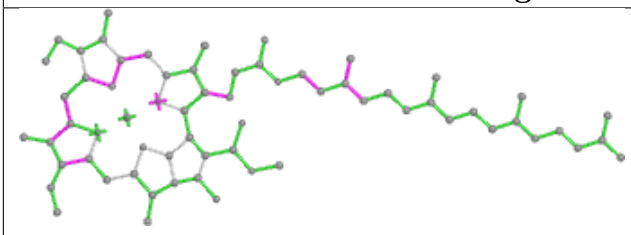


Rings

Ligand CLA H 1482



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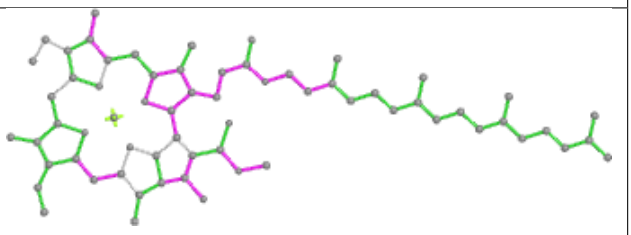
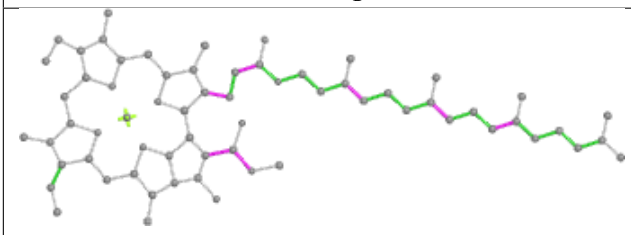


Bond angles



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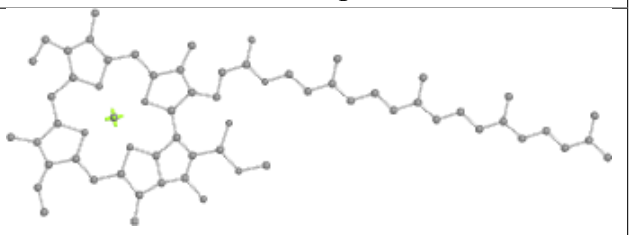
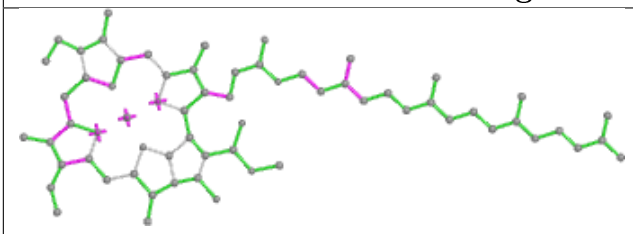


Rings

Ligand CLA B 1482



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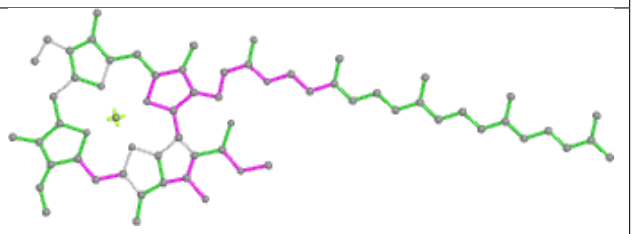
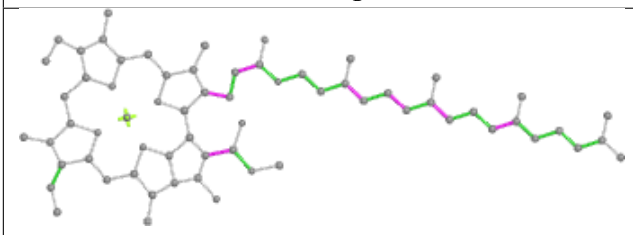


Bond angles



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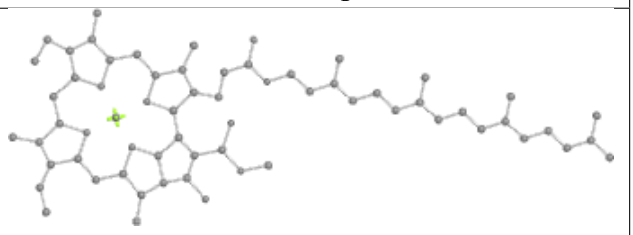
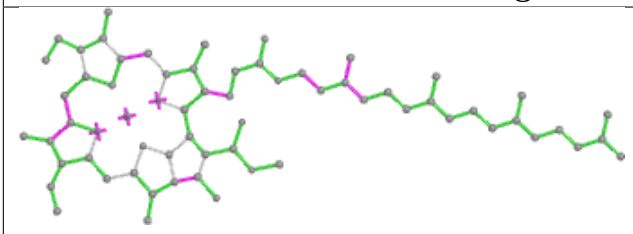
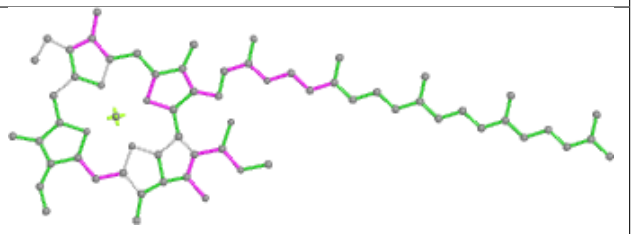


Rings

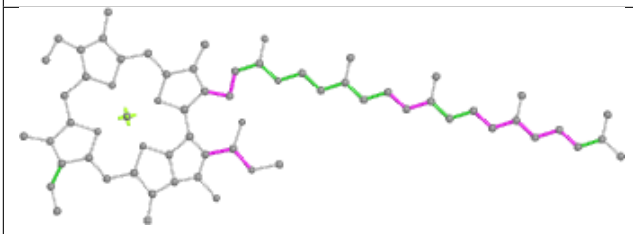
Ligand CLA H 1488



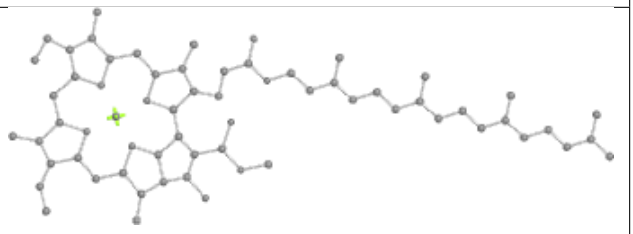
Bond lengths



Bond angles

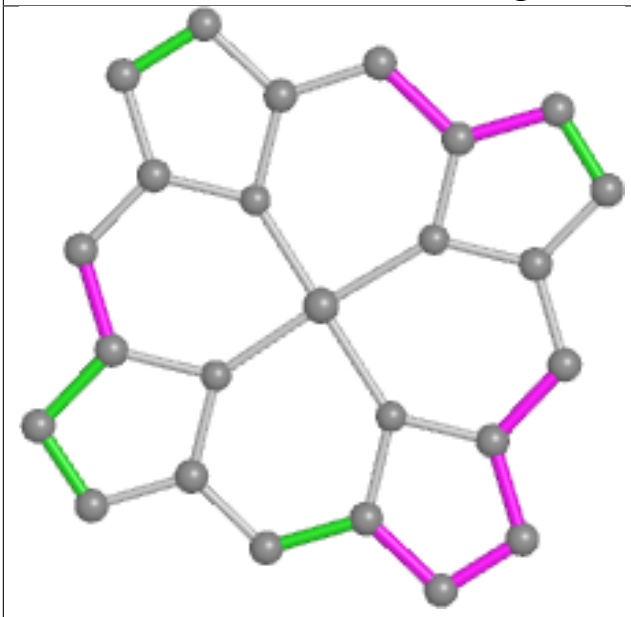


Torsions



Rings

Ligand HEM L 1046



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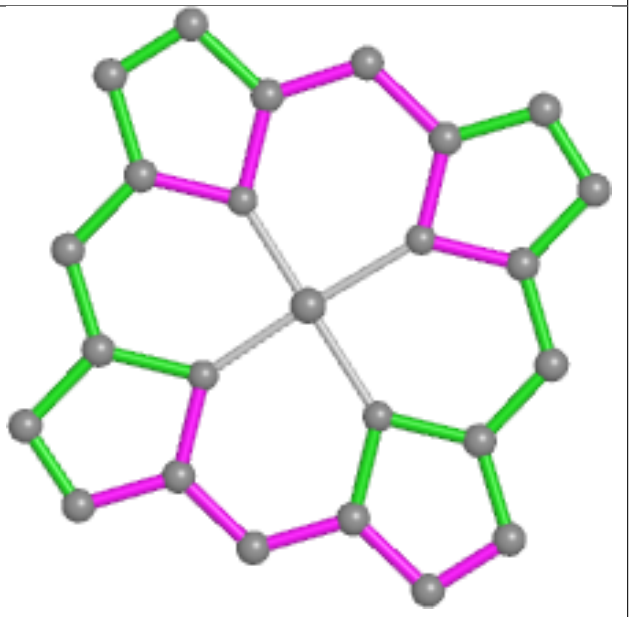
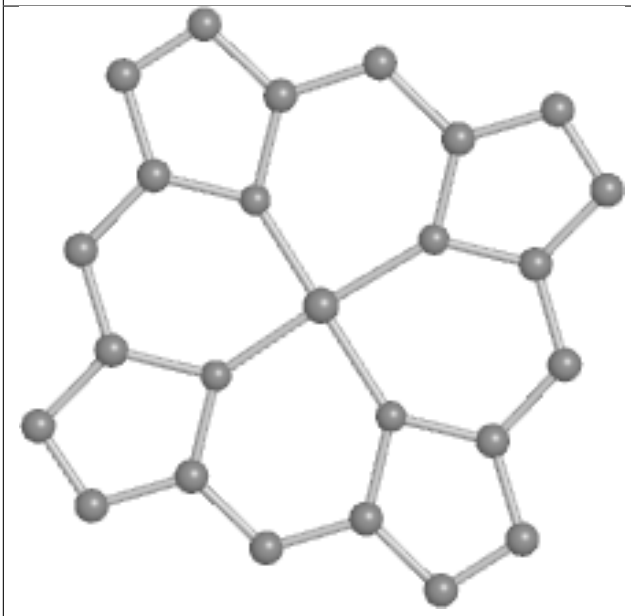
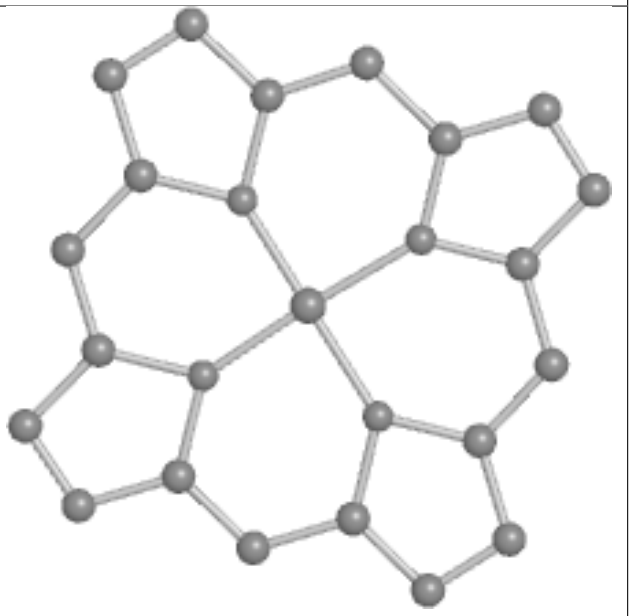


Bond angles

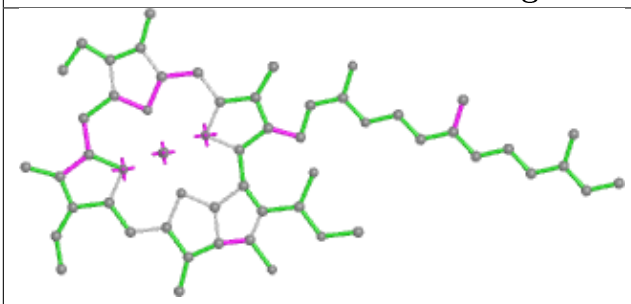


Torsions



Rings

Ligand CLA I 1464



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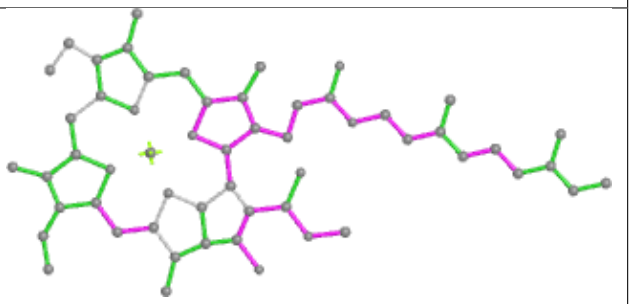
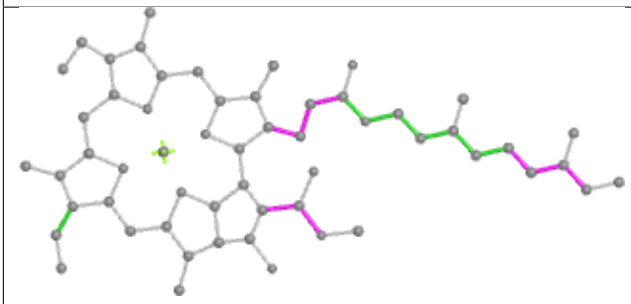


Bond angles



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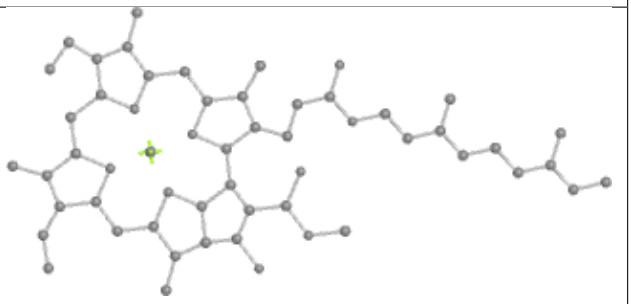
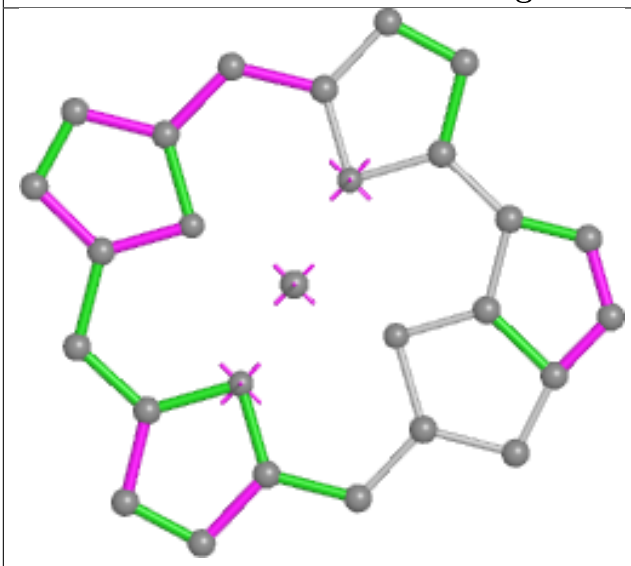
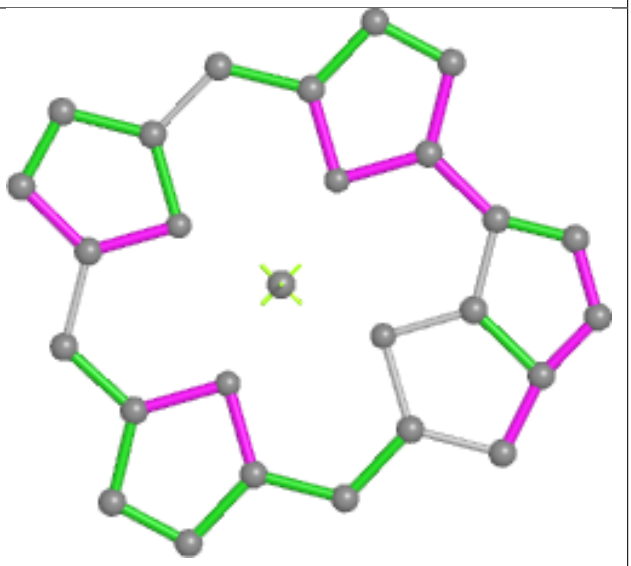


Rings

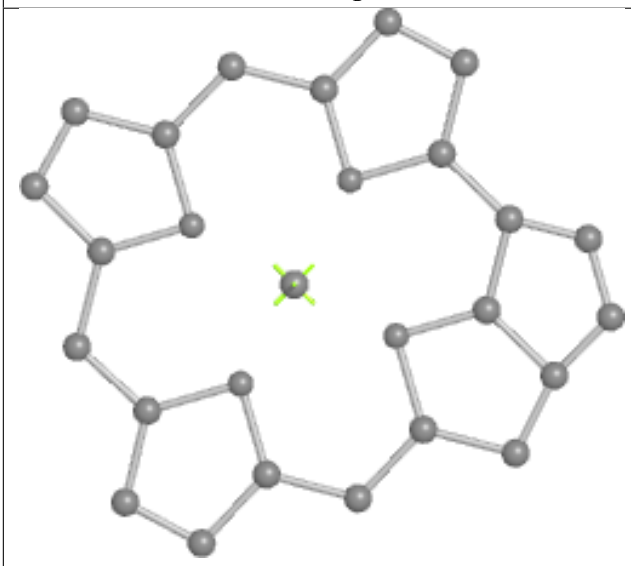
Ligand CLA C 1461



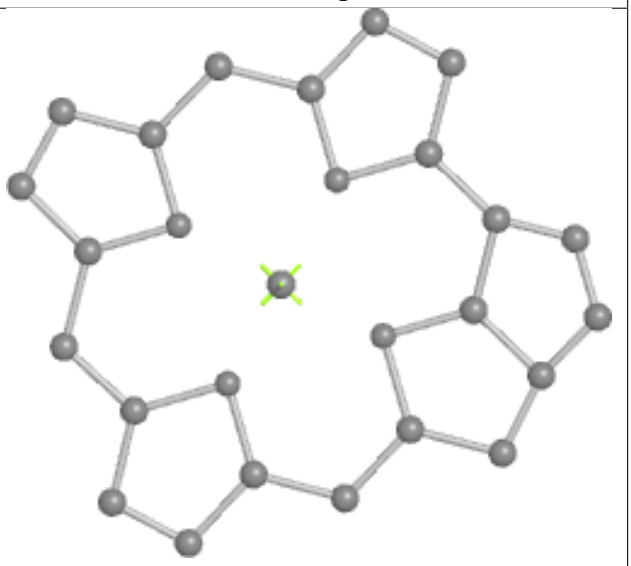
Bond lengths



Bond angles

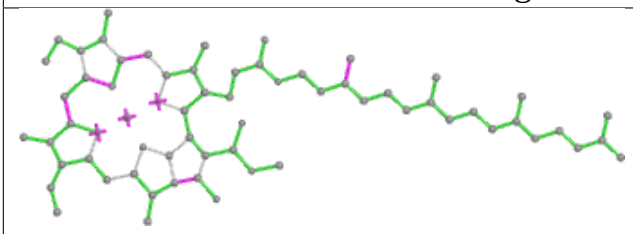


Torsions

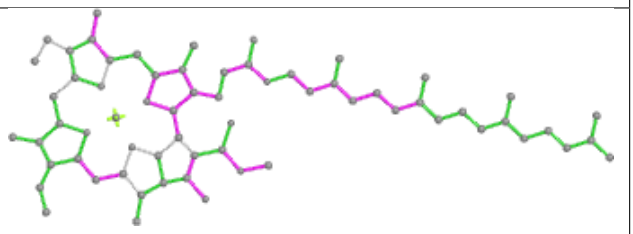


Rings

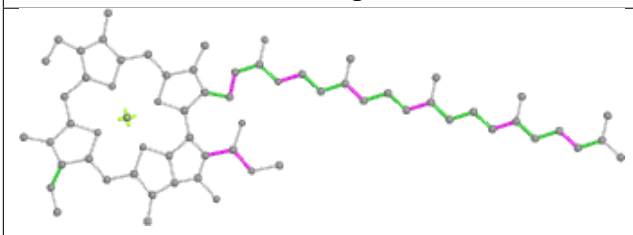
Ligand CLA H 1492



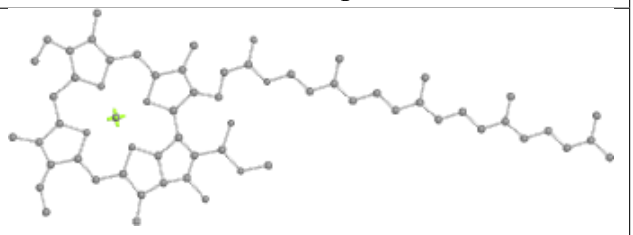
Bond lengths



Bond angles

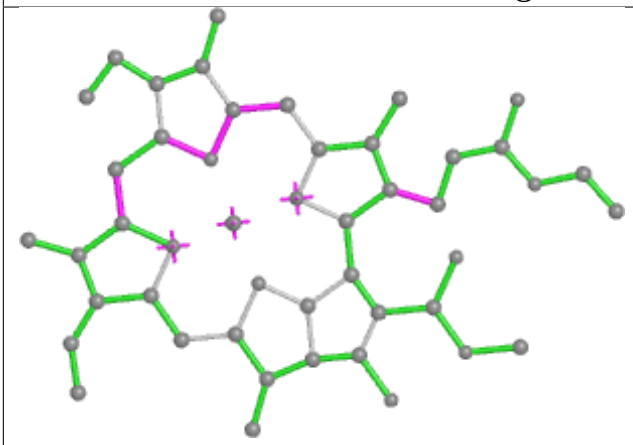


Torsions

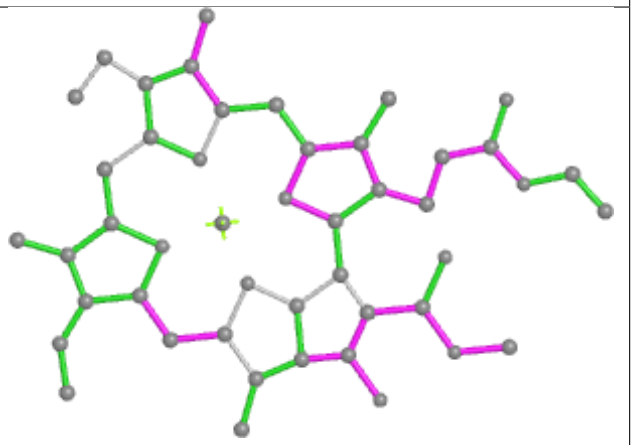


Rings

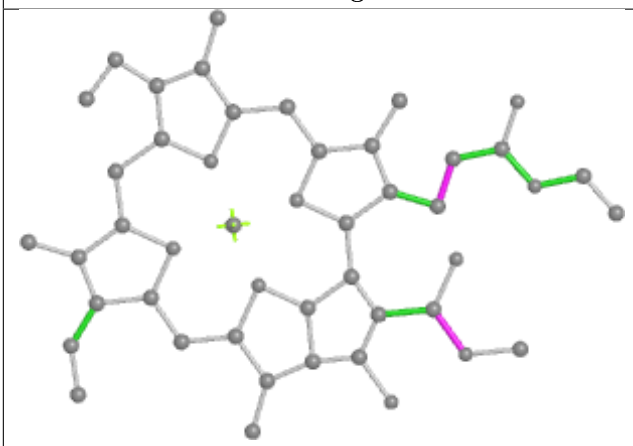
Ligand CLA C 1460



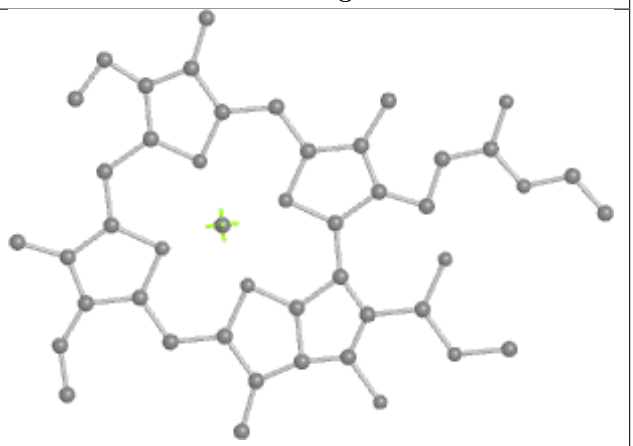
Bond lengths



Bond angles

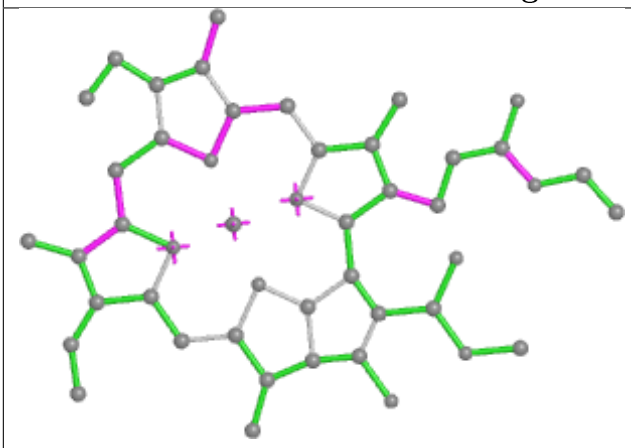


Torsions

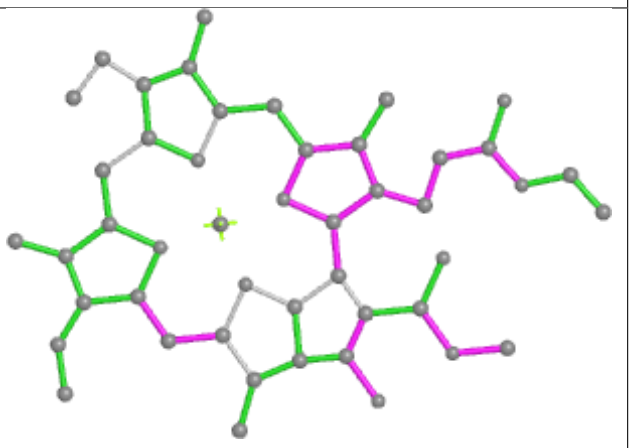


Rings

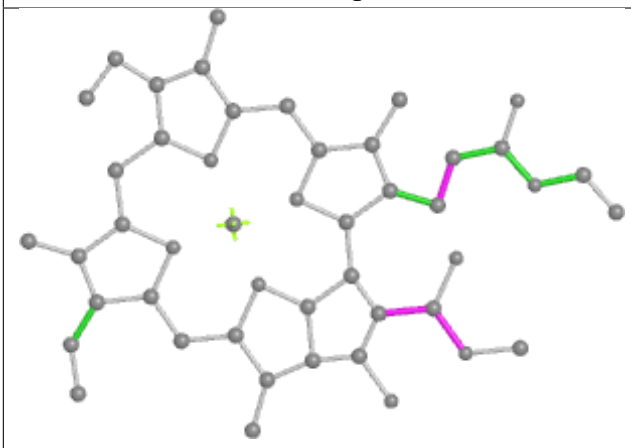
Ligand CLA I 1460



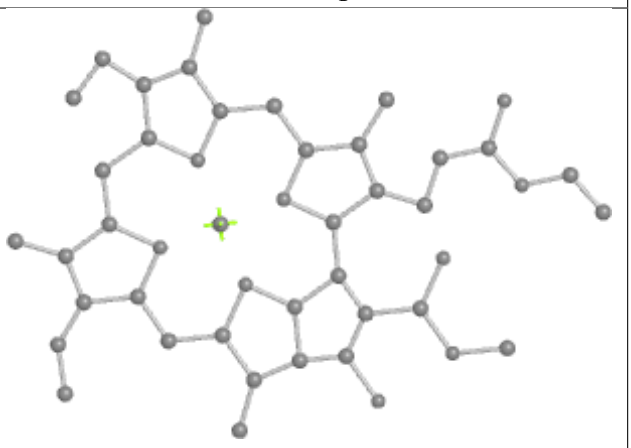
Bond lengths



Bond angles

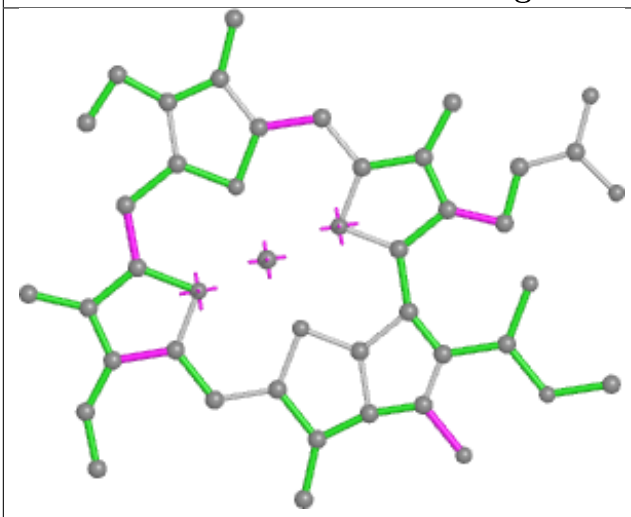


Torsions

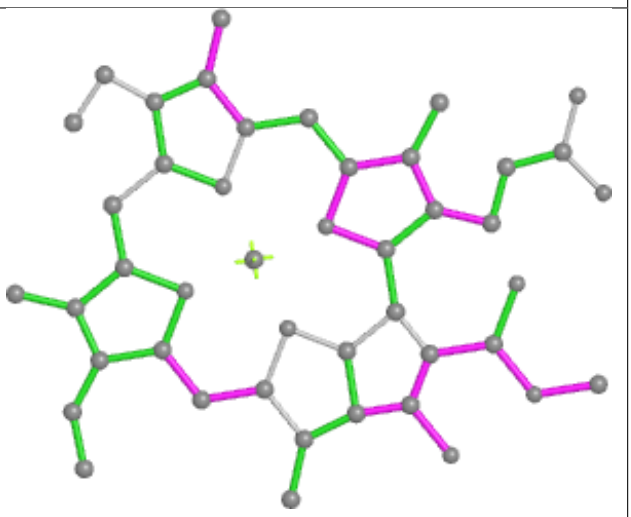


Rings

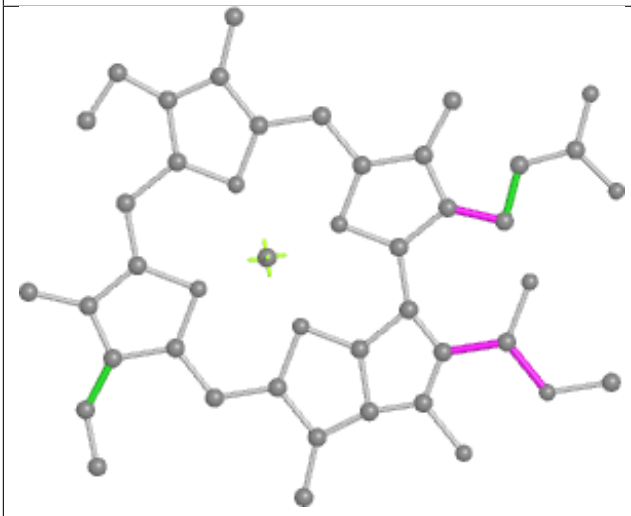
Ligand CLA H 1493



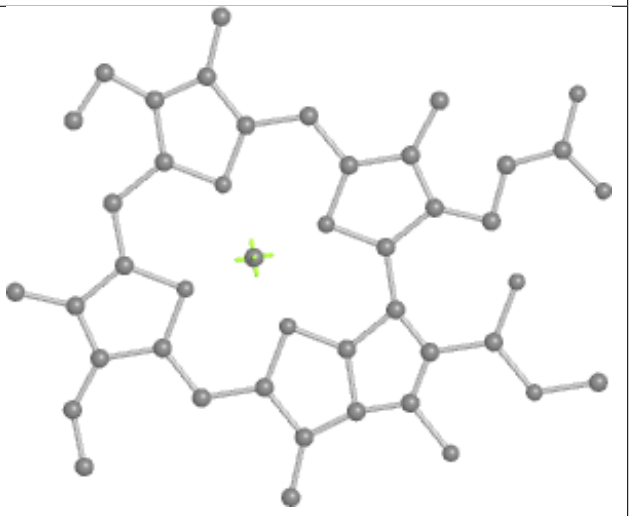
Bond lengths



Bond angles

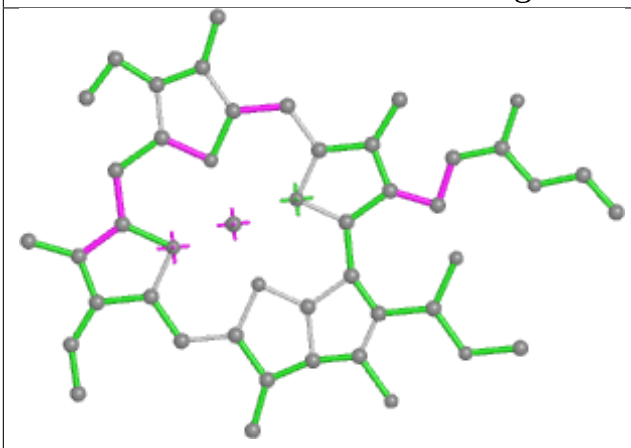


Torsions

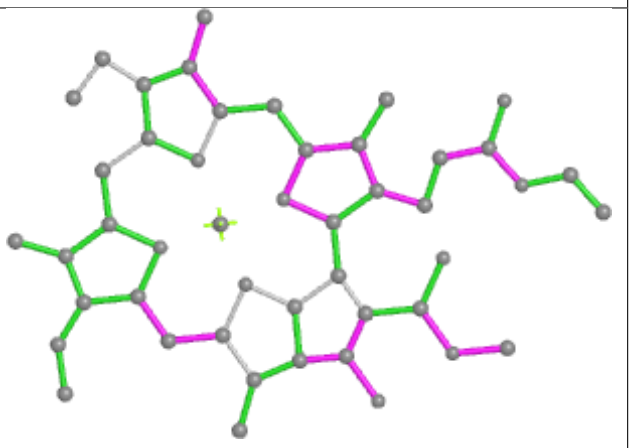


Rings

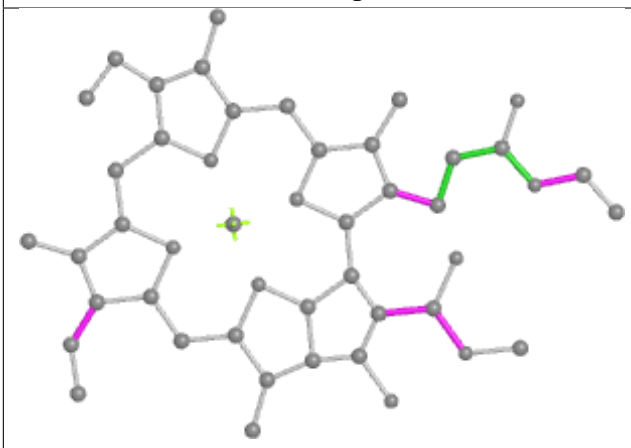
Ligand CLA H 1485



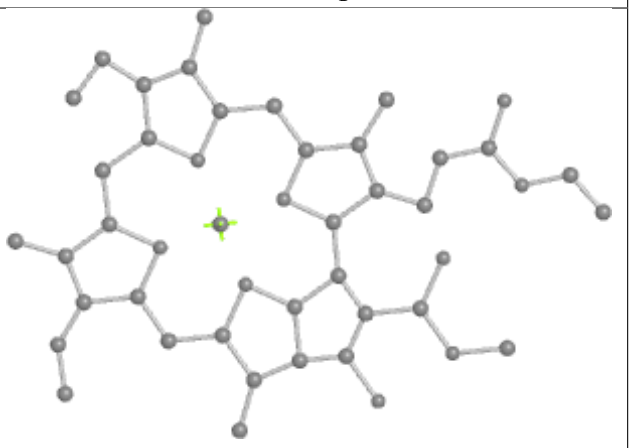
Bond lengths



Bond angles

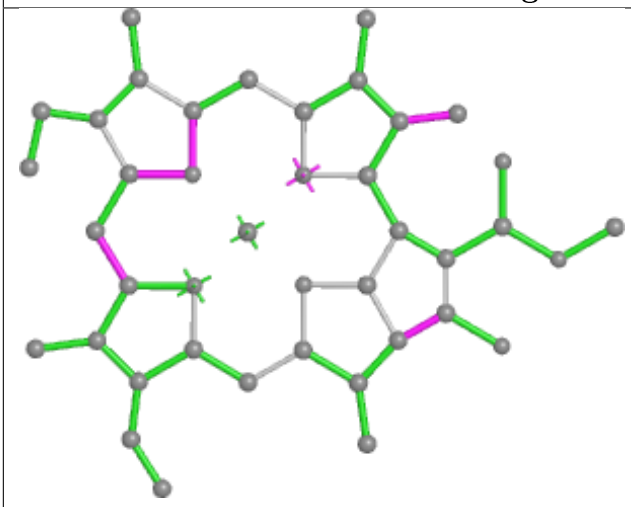


Torsions

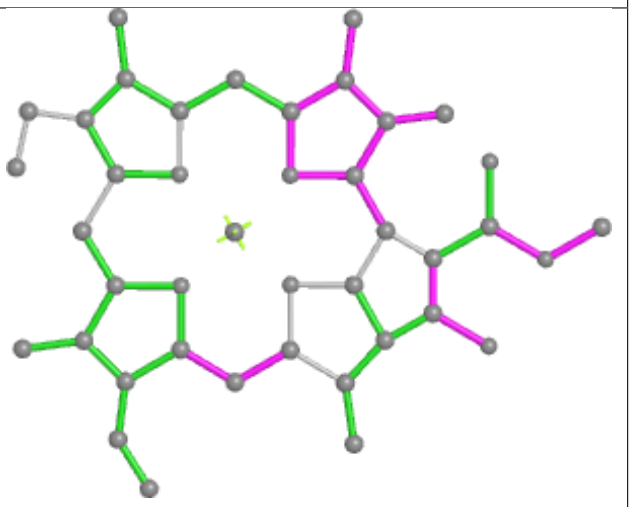


Rings

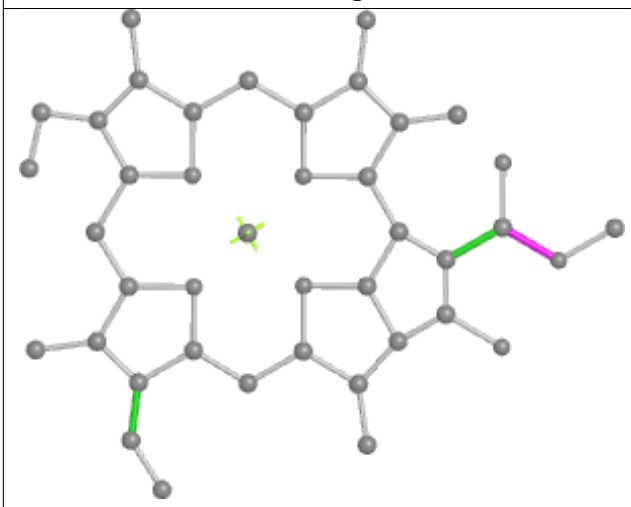
Ligand CLA I 1469



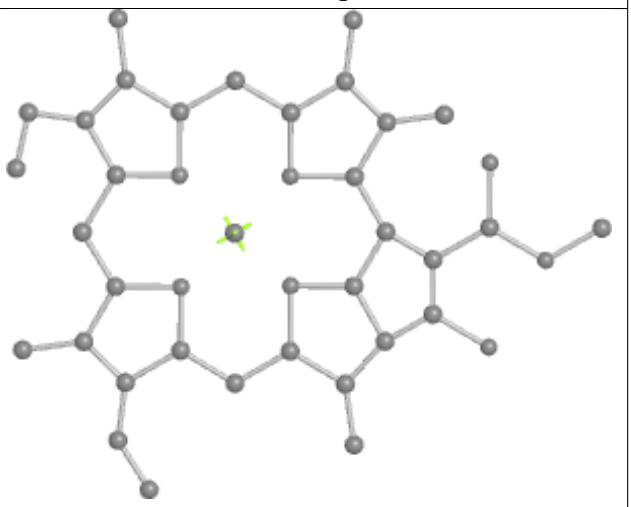
Bond lengths



Bond angles

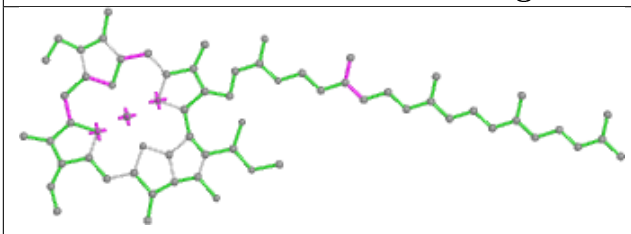


Torsions

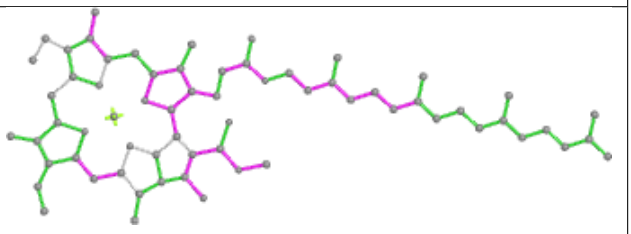


Rings

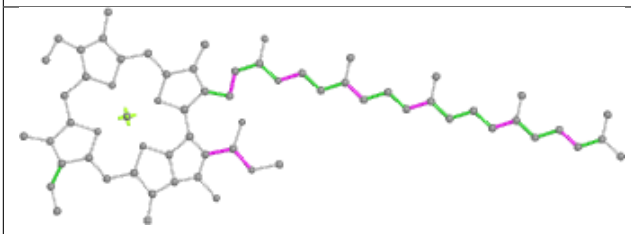
Ligand CLA B 1492



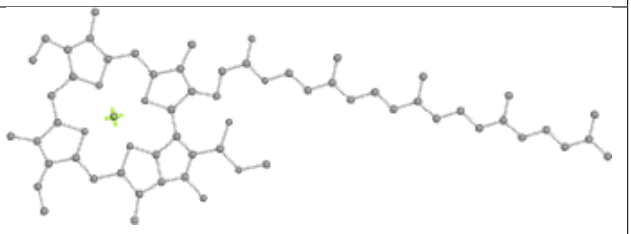
Bond lengths



Bond angles

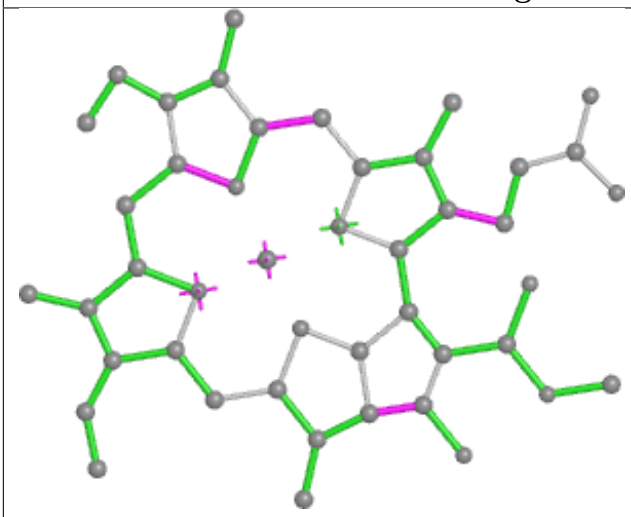


Torsions



Rings

Ligand CLA H 1484



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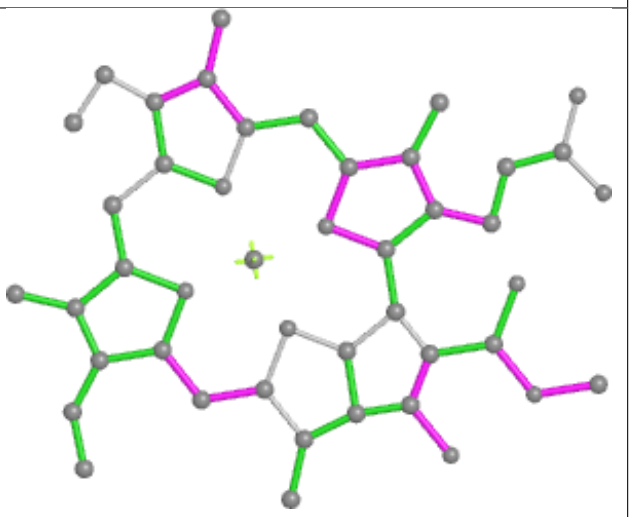
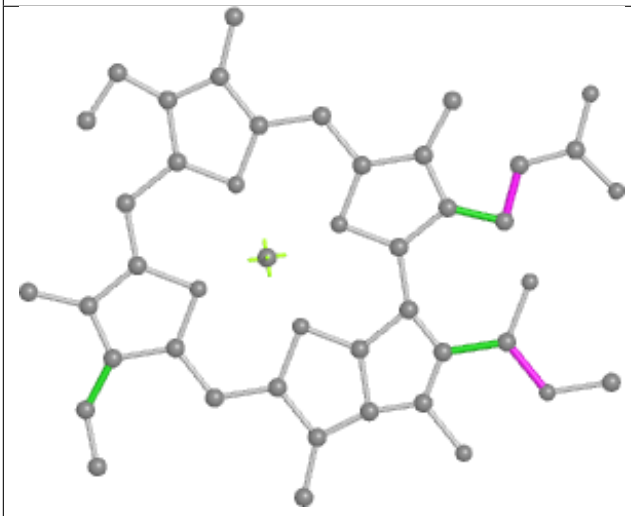
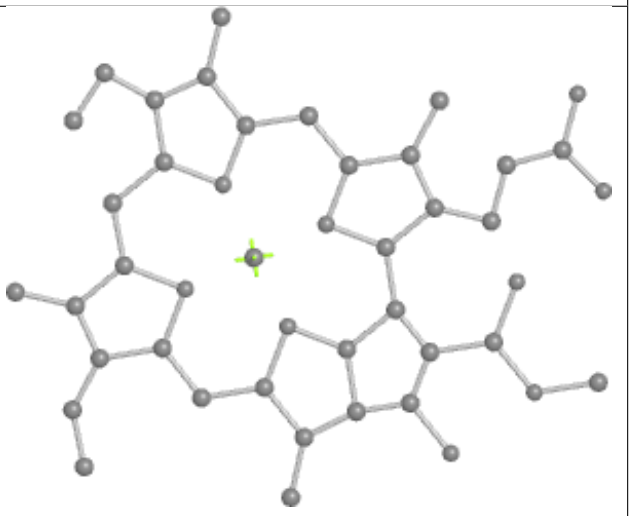


Bond angles

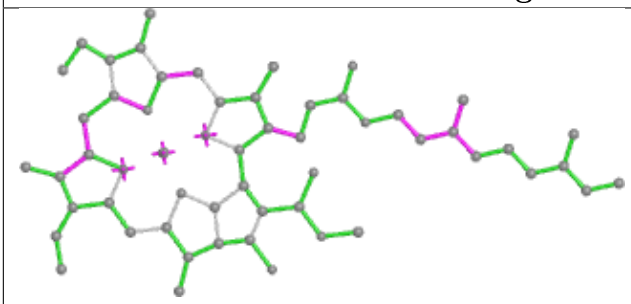


Torsions



Rings

Ligand CLA C 1462



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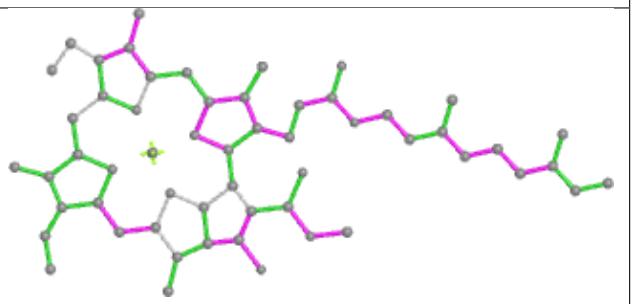
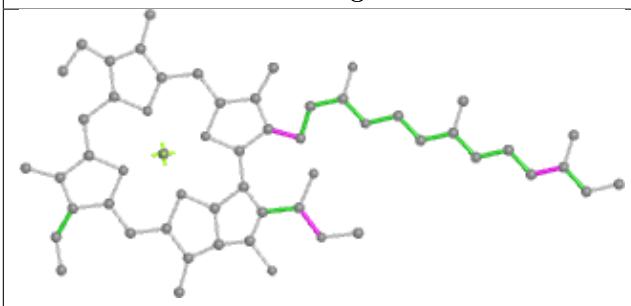


Bond angles



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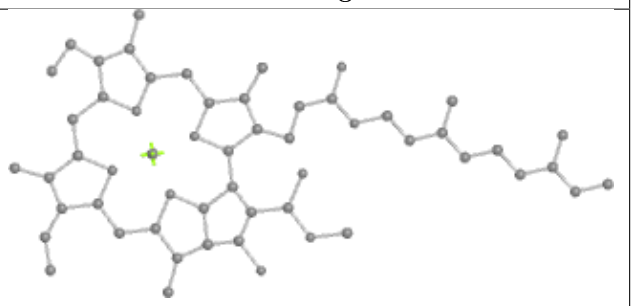
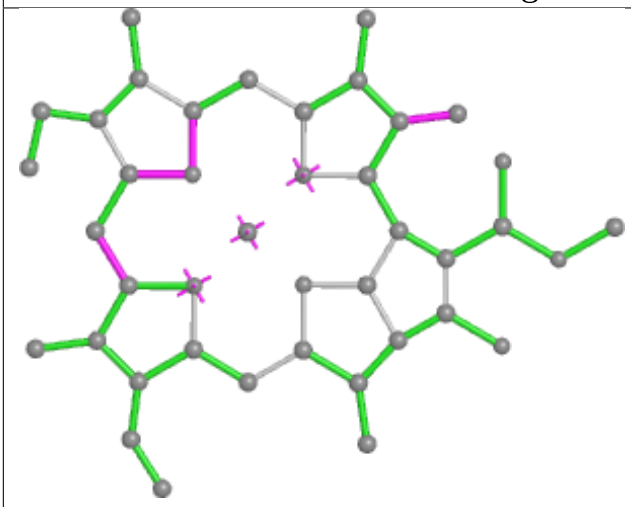
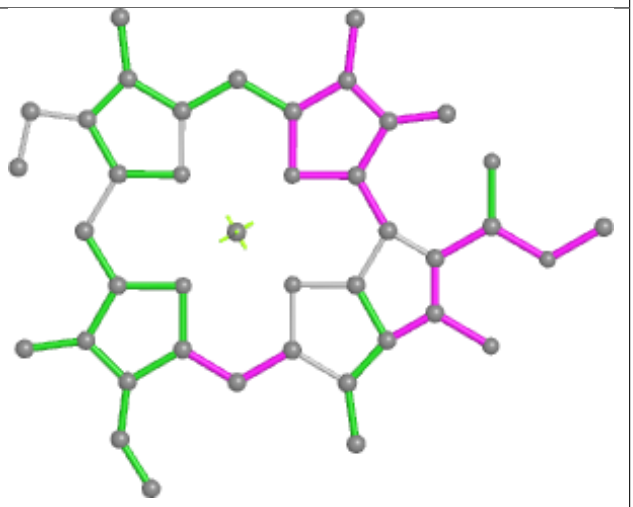


Rings

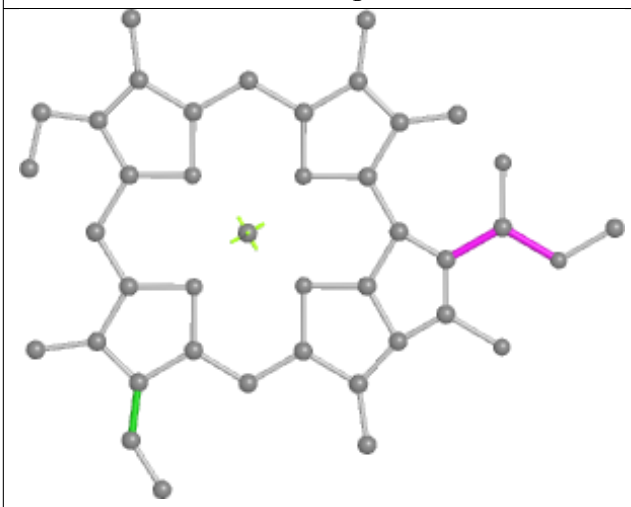
Ligand CLA I 1470



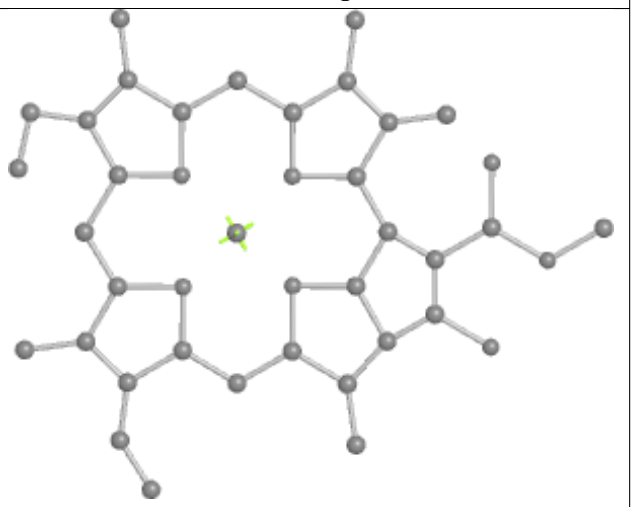
Bond lengths



Bond angles

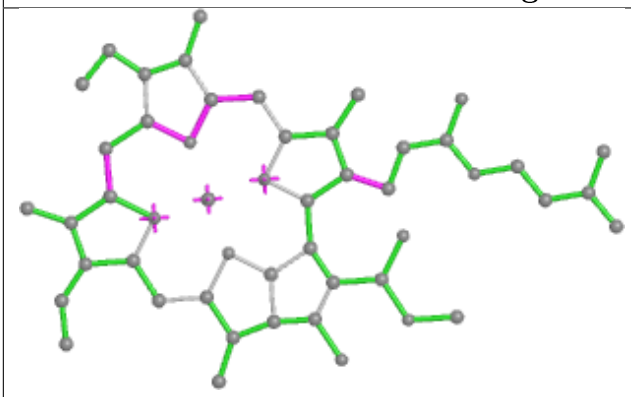


Torsions



Rings

Ligand CLA I 1466



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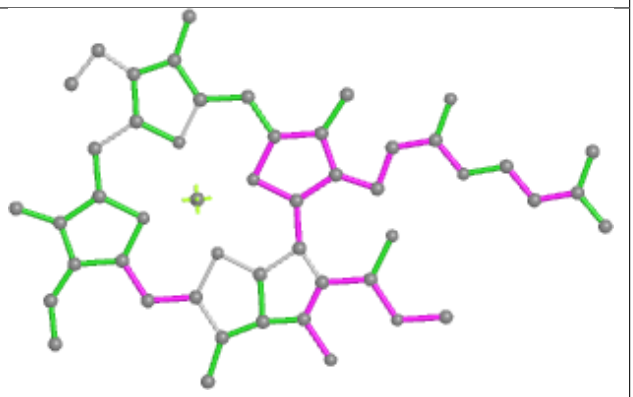
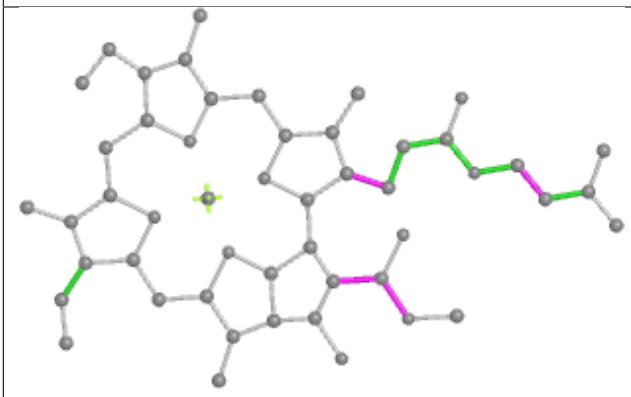
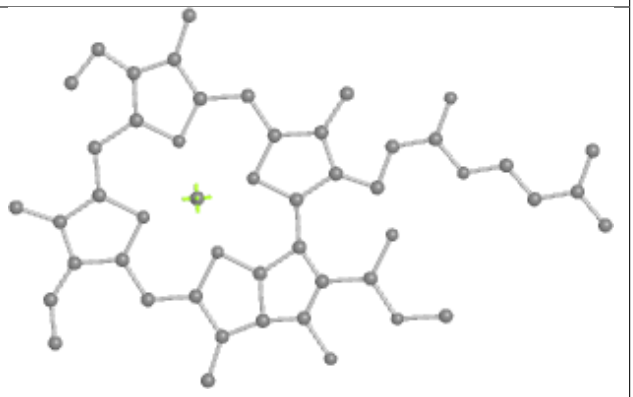


Bond angles

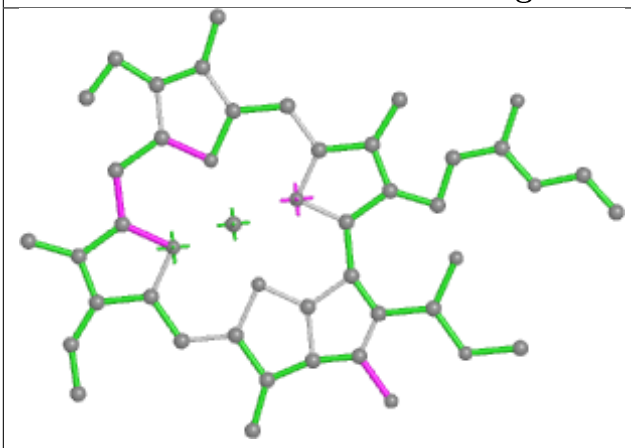


Torsions

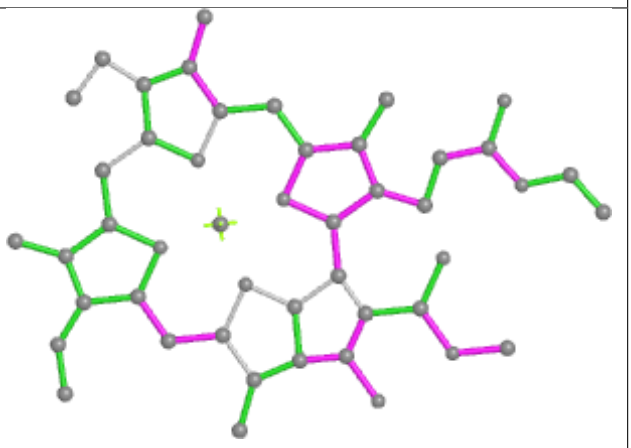


Rings

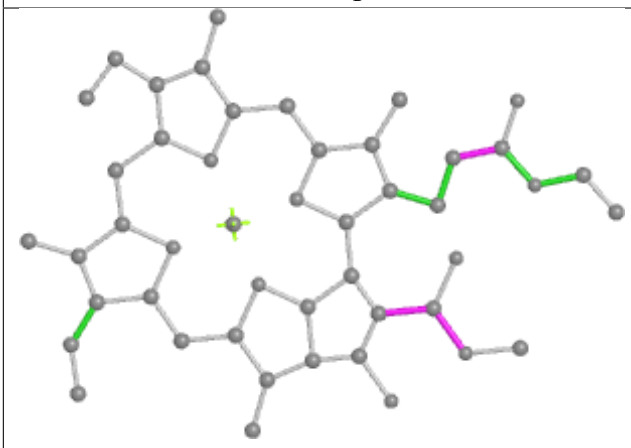
Ligand CLA C 1467



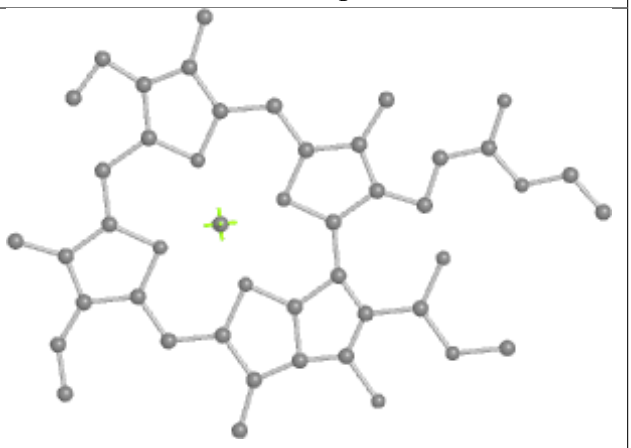
Bond lengths



Bond angles

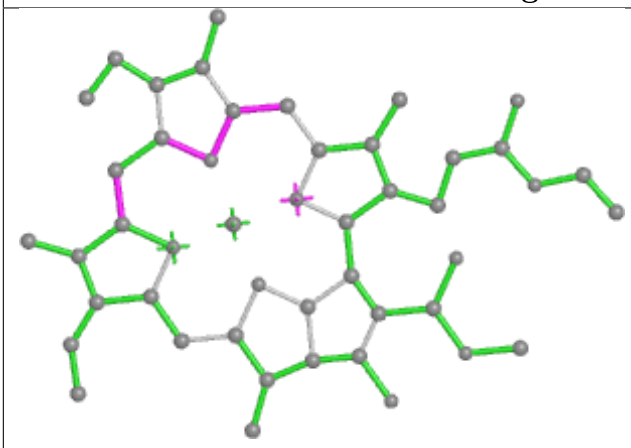


Torsions



Rings

Ligand CLA I 1467



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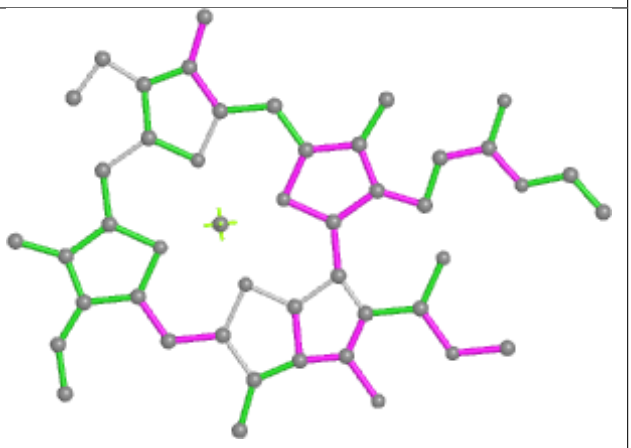
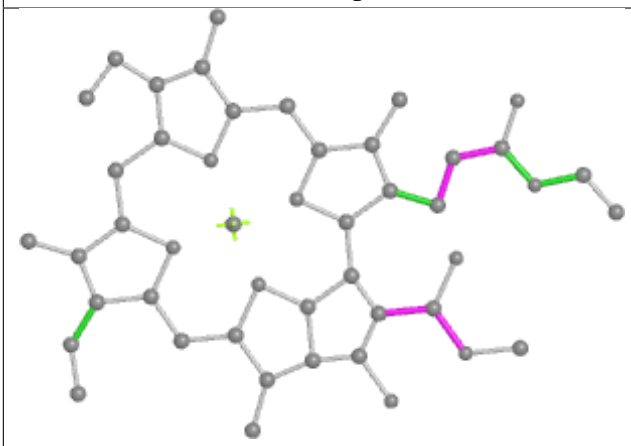
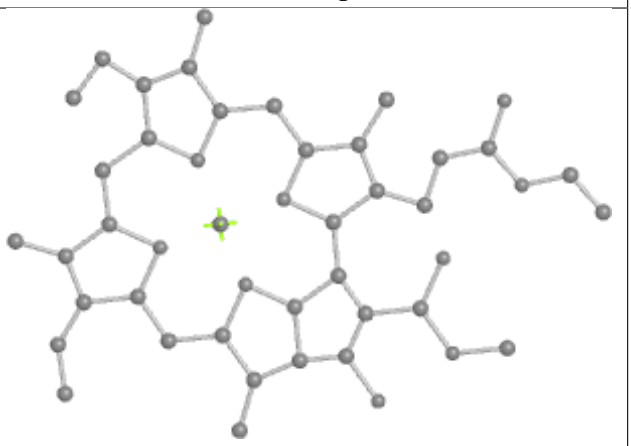


Bond angles

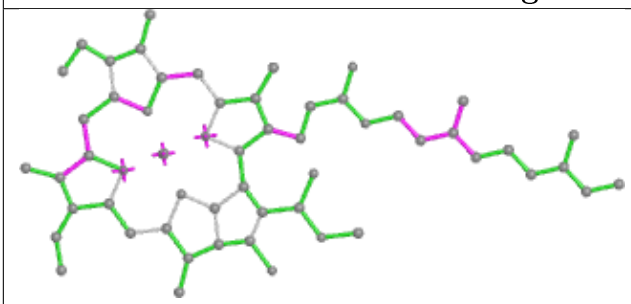


Torsions



Rings

Ligand CLA I 1462



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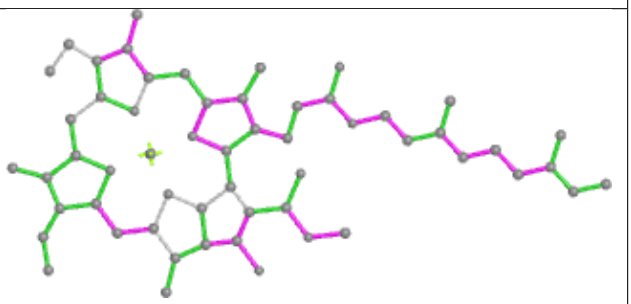
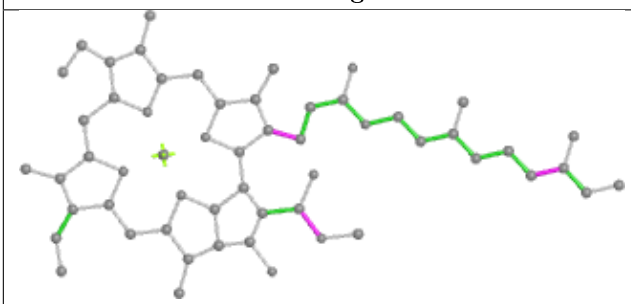
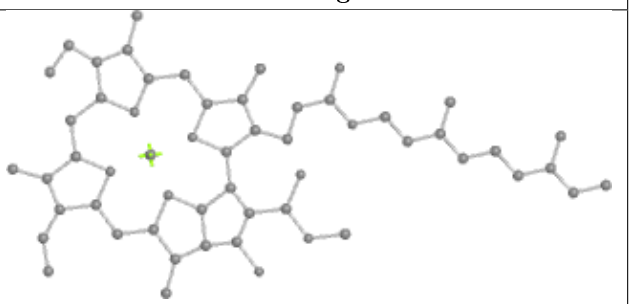


Bond angles

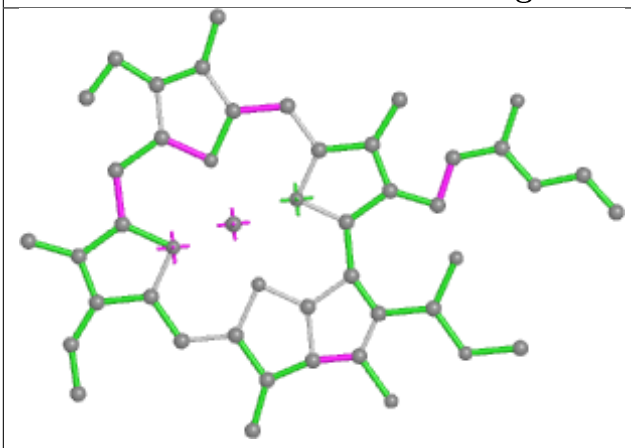


Torsions

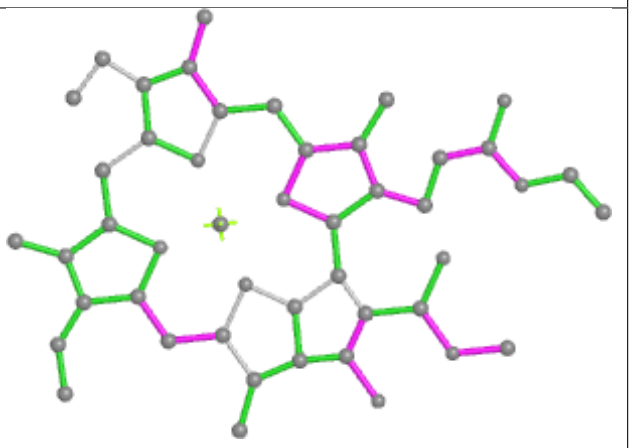


Rings

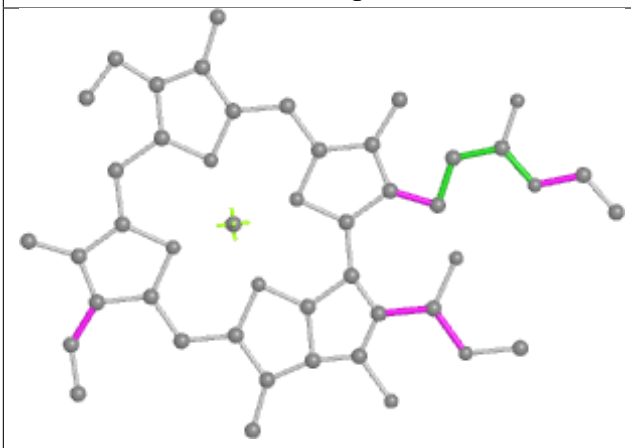
Ligand CLA B 1485



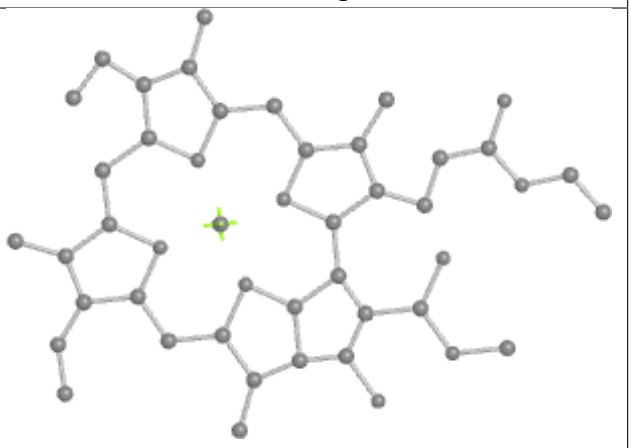
Bond lengths



Bond angles

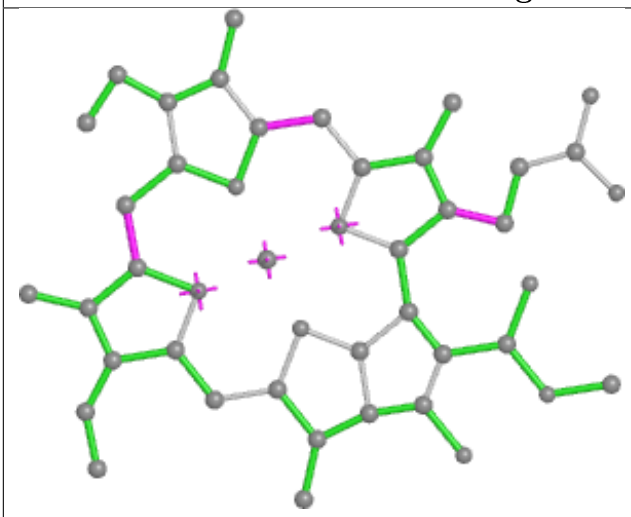


Torsions

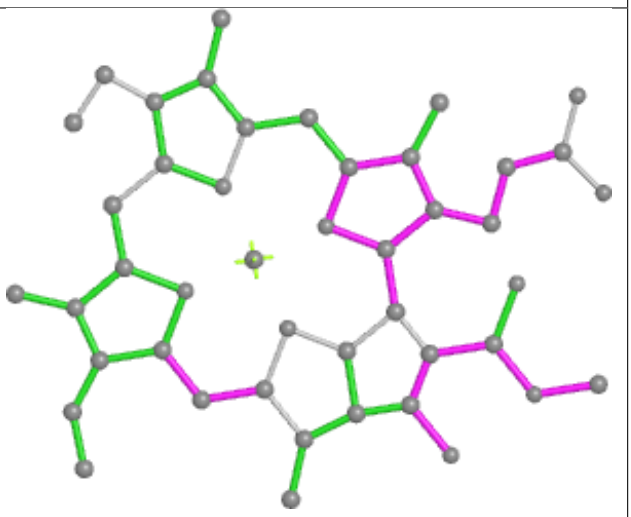


Rings

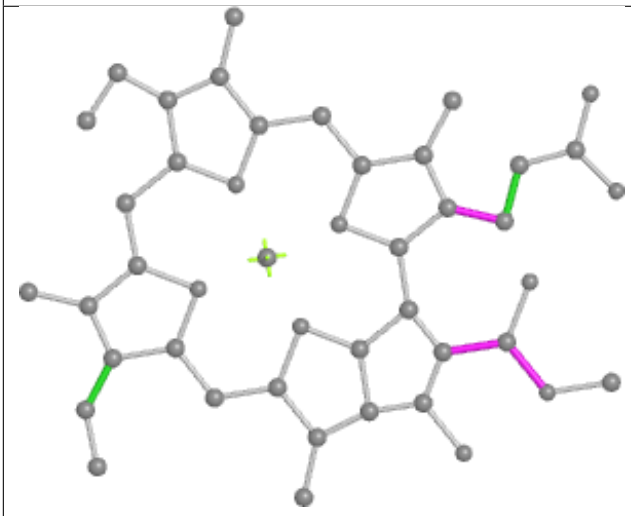
Ligand CLA A 1344



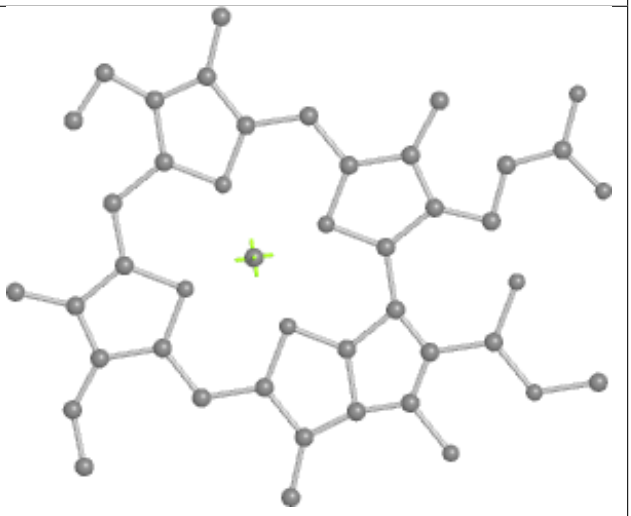
Bond lengths



Bond angles

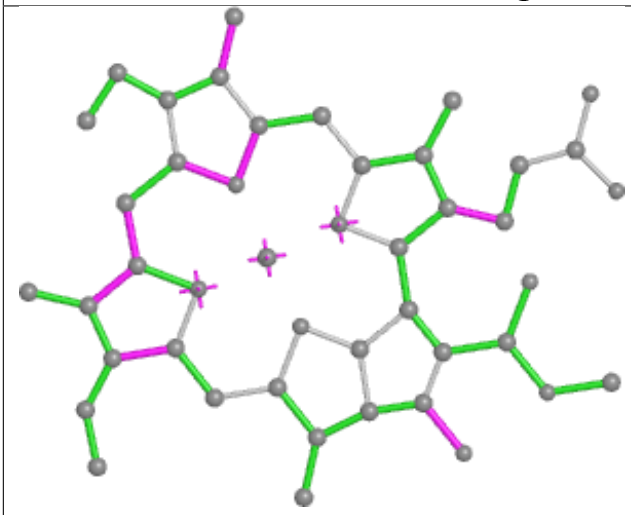


Torsions

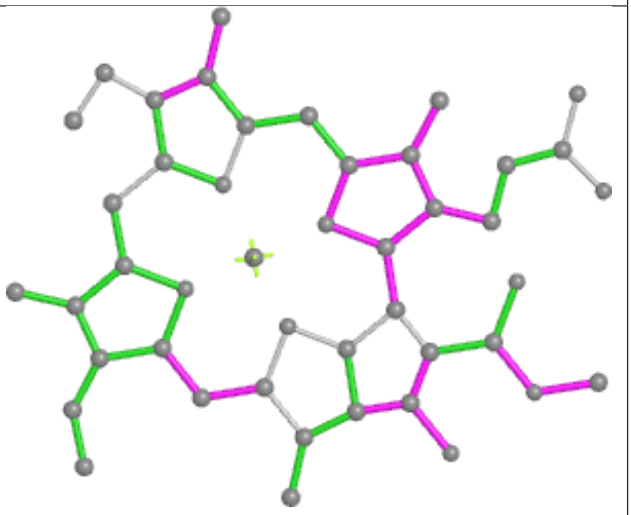


Rings

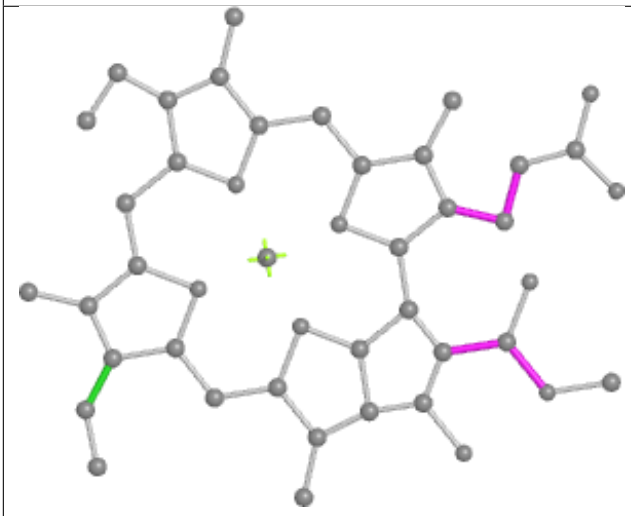
Ligand CLA B 1490



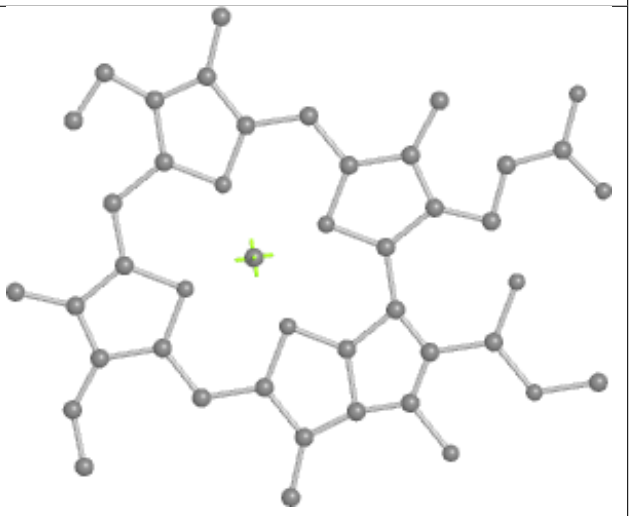
Bond lengths



Bond angles

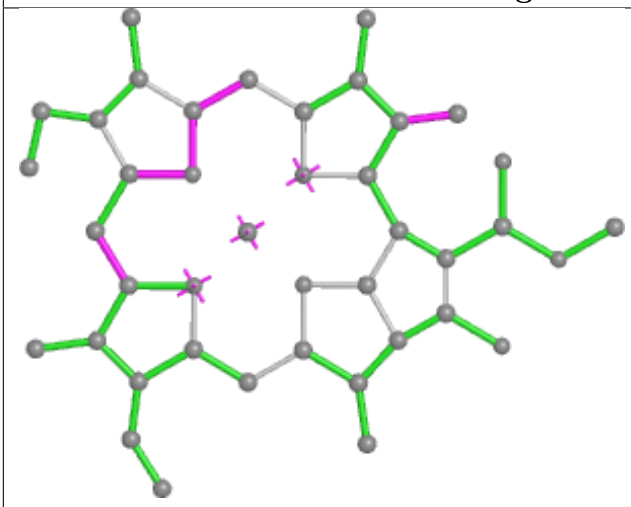


Torsions

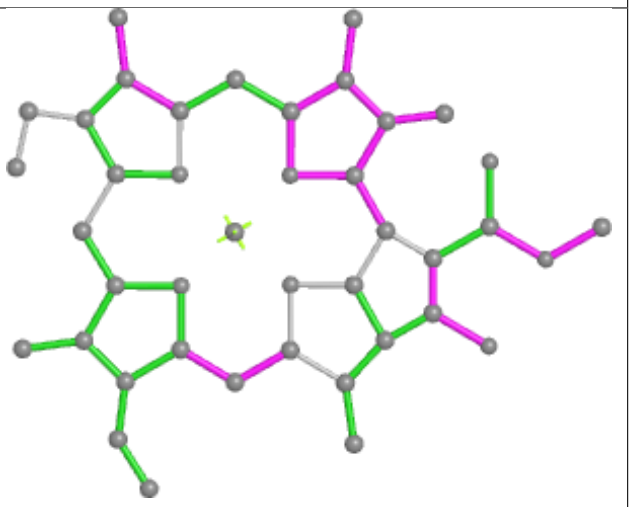


Rings

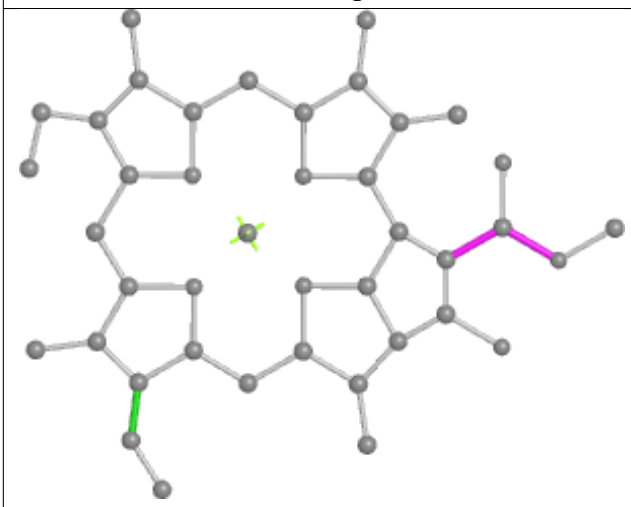
Ligand CLA C 1470



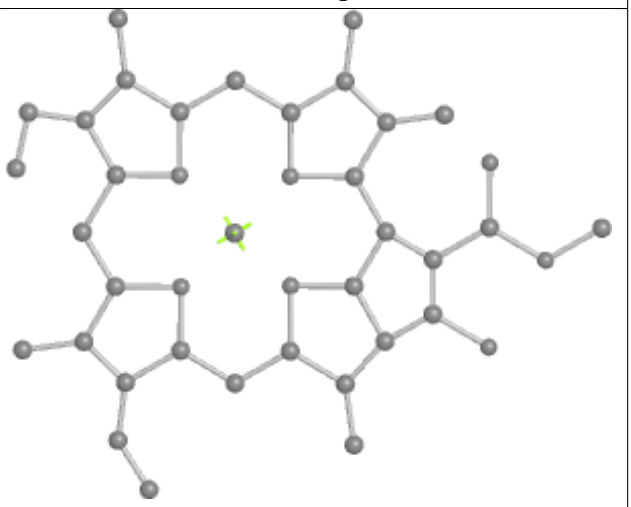
Bond lengths



Bond angles

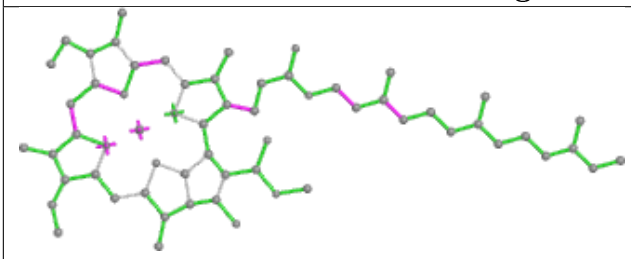


Torsions

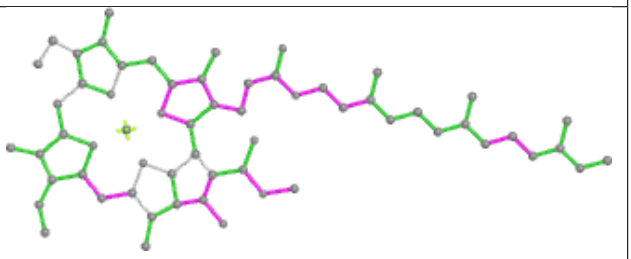


Rings

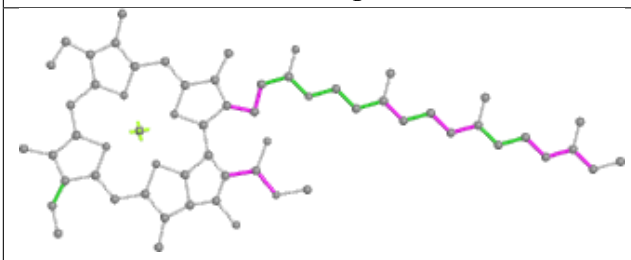
Ligand CLA G 1343



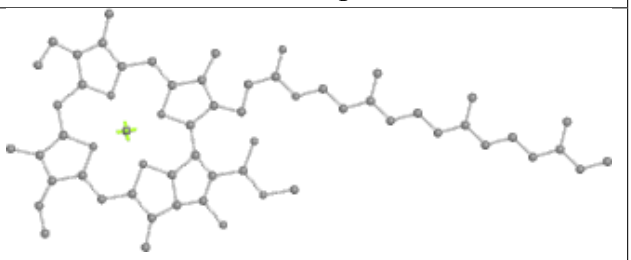
Bond lengths



Bond angles

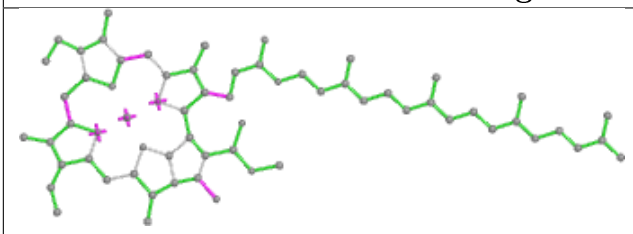


Torsions

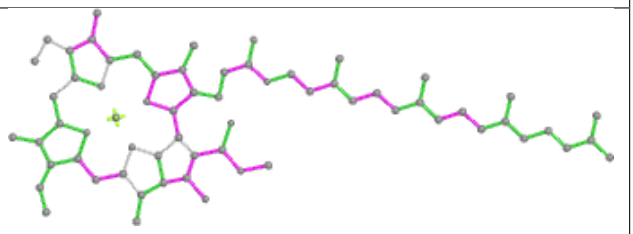


Rings

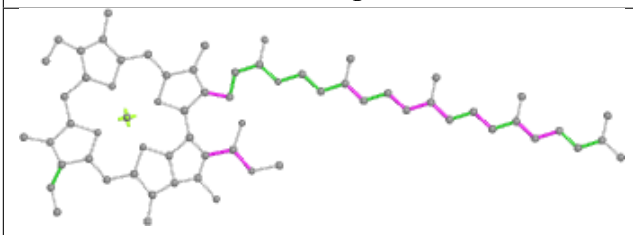
Ligand CLA C 1465



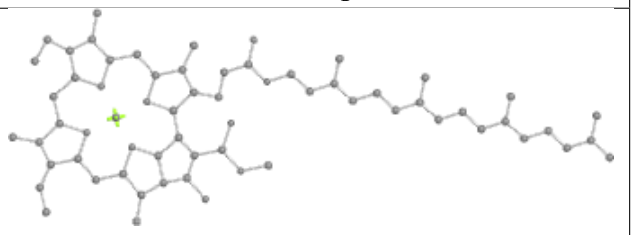
Bond lengths



Bond angles

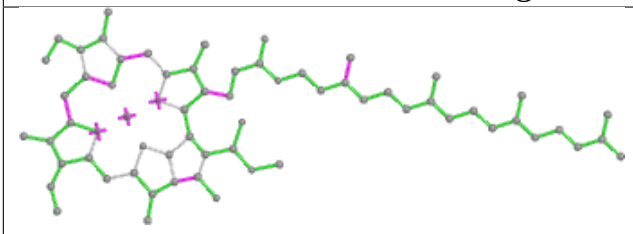


Torsions



Rings

Ligand CLA B 1494



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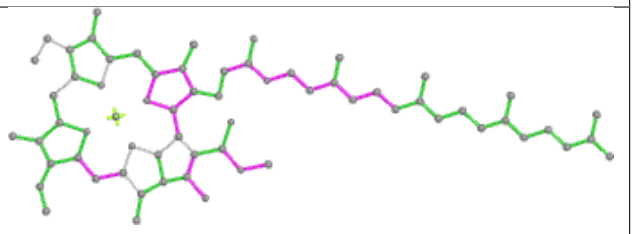
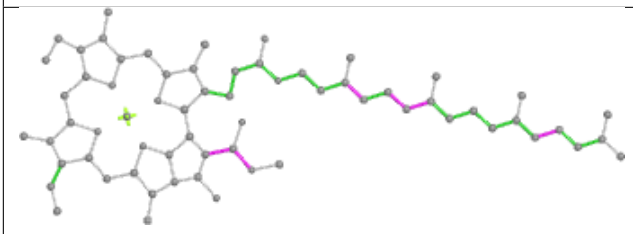
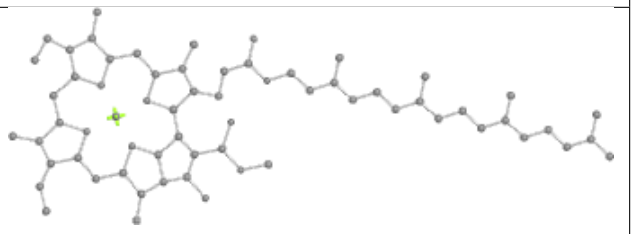


Bond angles

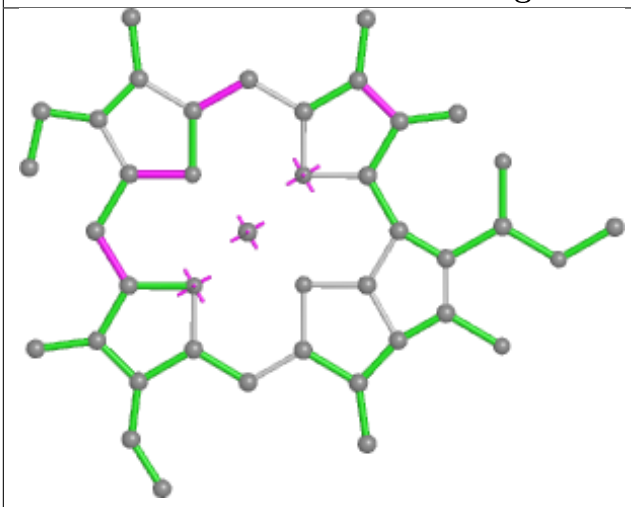


Torsions

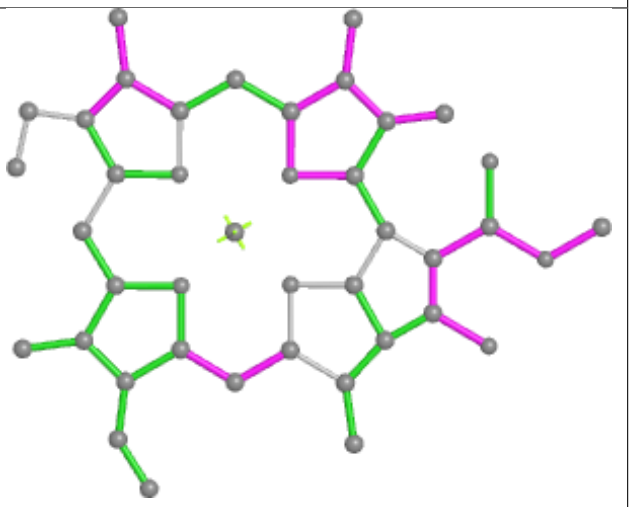


Rings

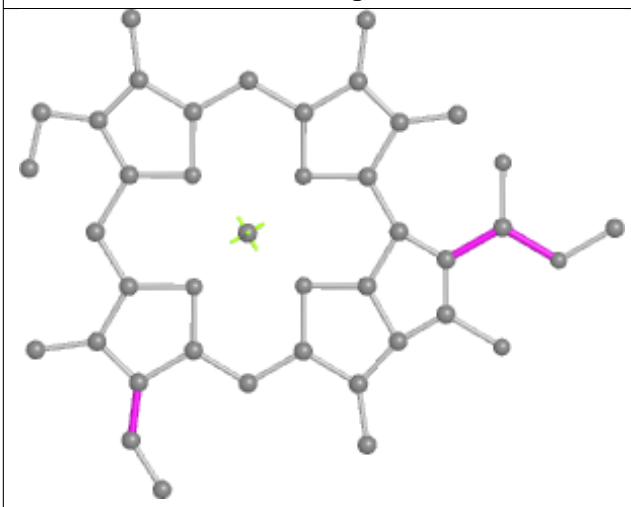
Ligand CLA H 1486



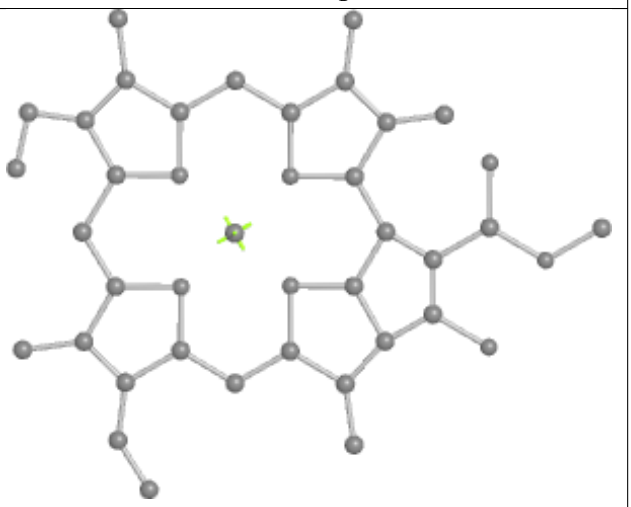
Bond lengths



Bond angles

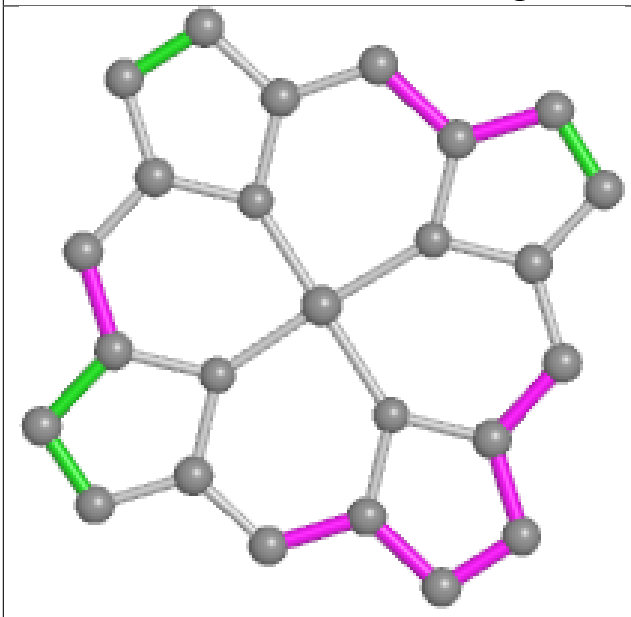


Torsions



Rings

Ligand HEM E 1085



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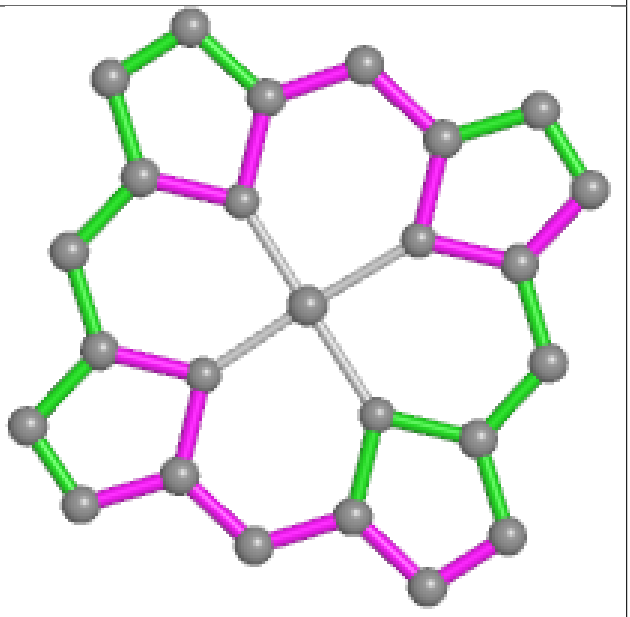
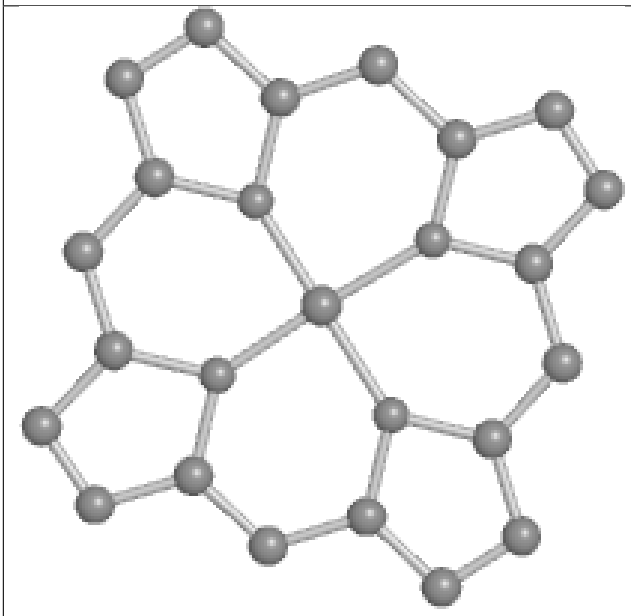
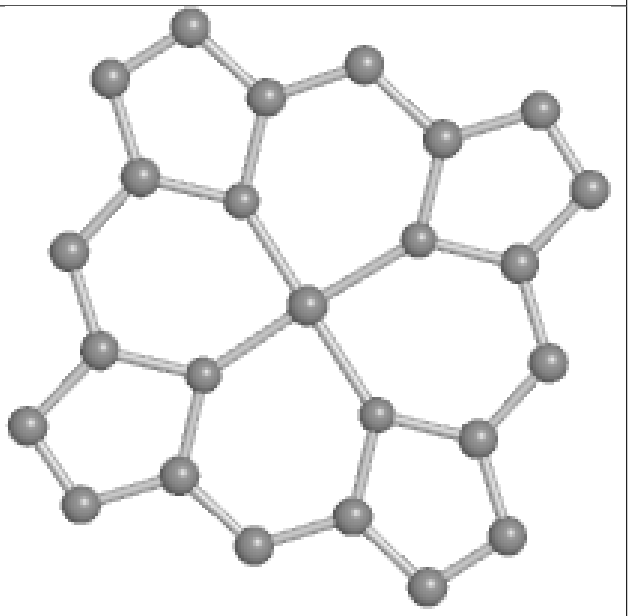


Bond angles

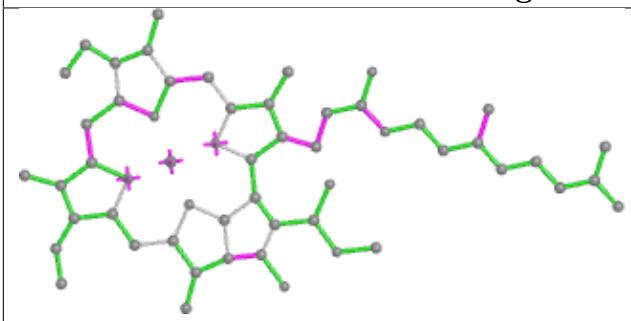


Torsions

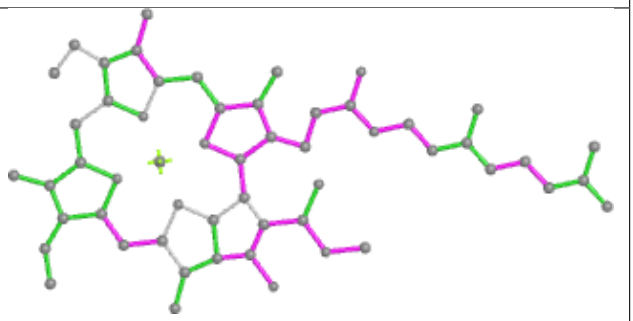


Rings

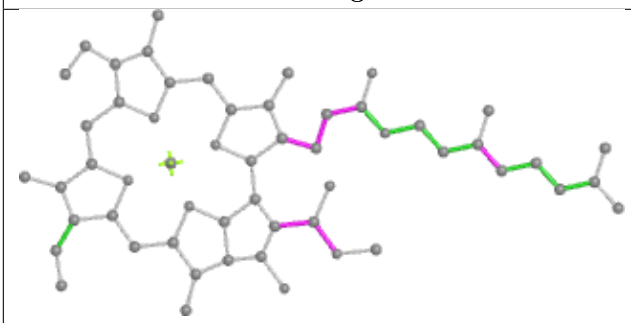
Ligand CLA B 1495



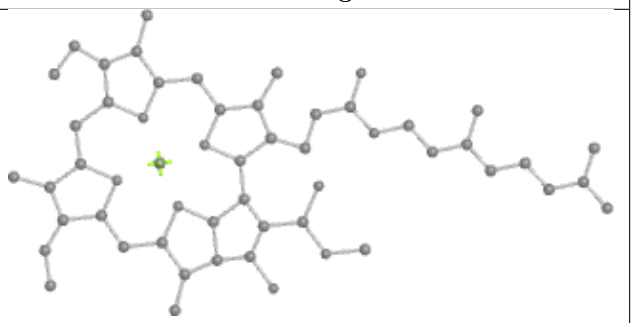
Bond lengths



Bond angles

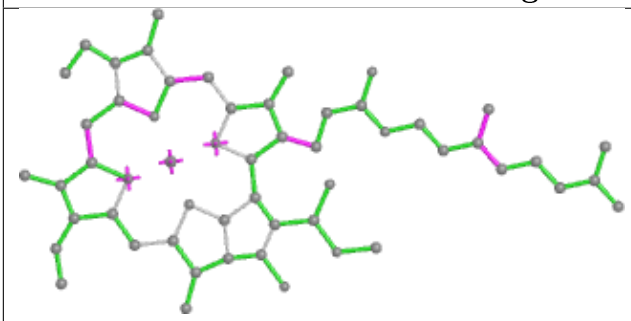


Torsions

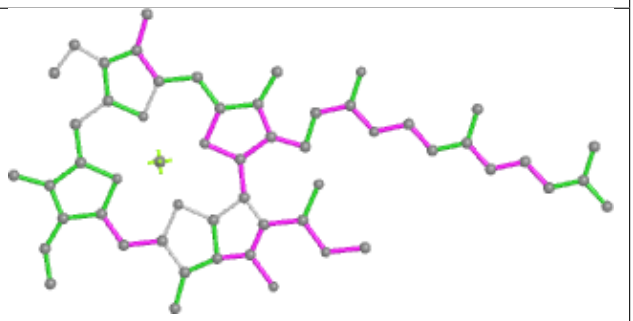


Rings

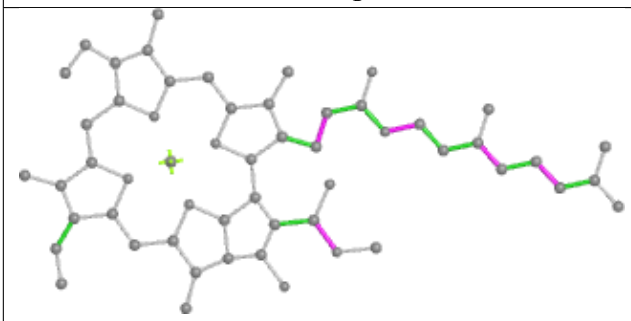
Ligand CLA I 1463



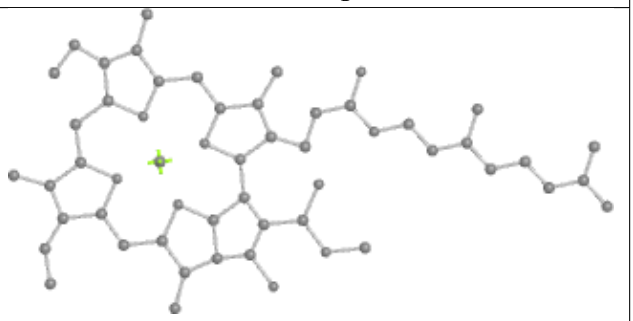
Bond lengths



Bond angles

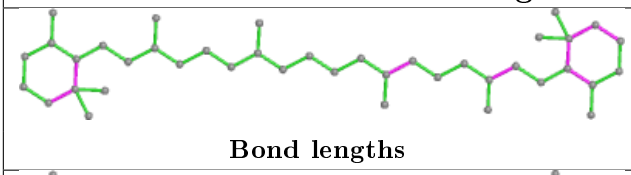


Torsions

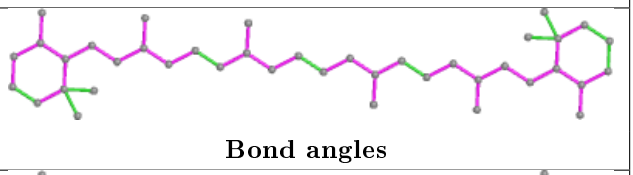


Rings

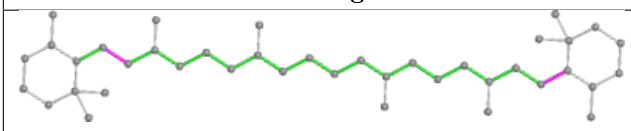
Ligand BCR F 1046



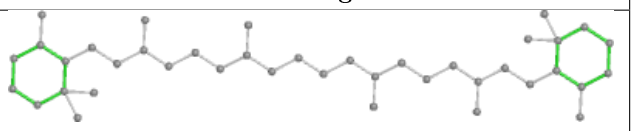
Bond lengths



Bond angles

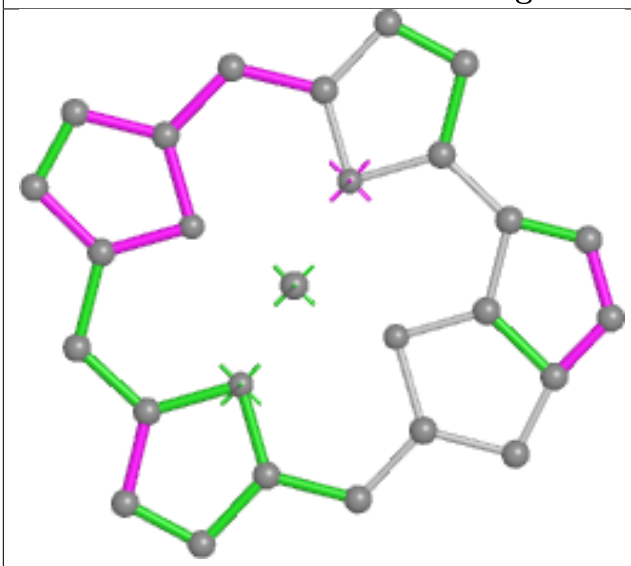


Torsions

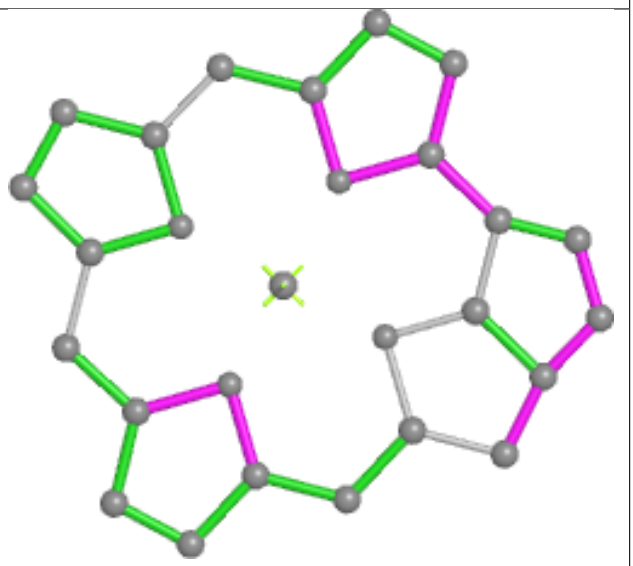


Rings

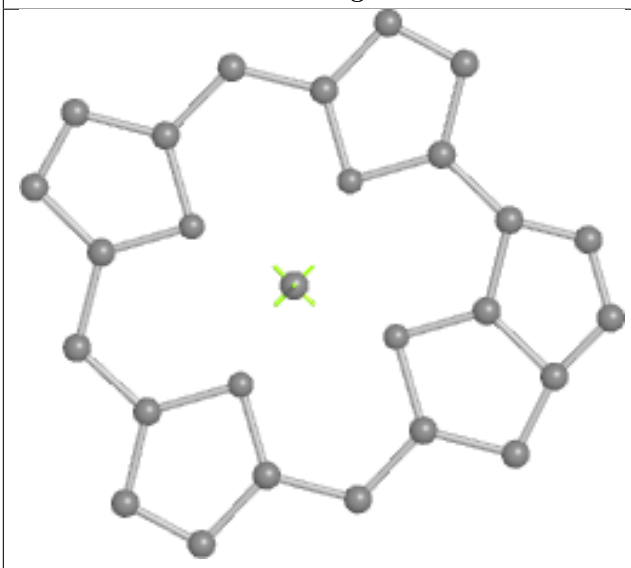
Ligand CLA B 1491



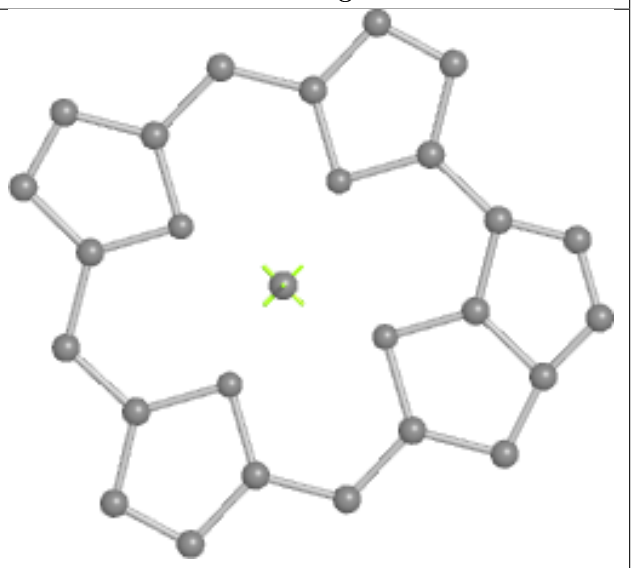
Bond lengths



Bond angles

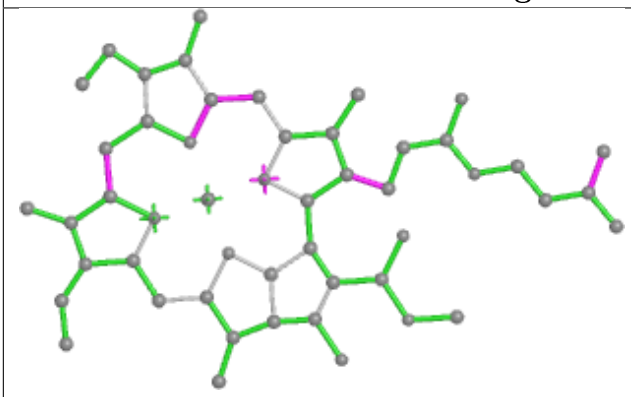


Torsions



Rings

Ligand CLA H 1489



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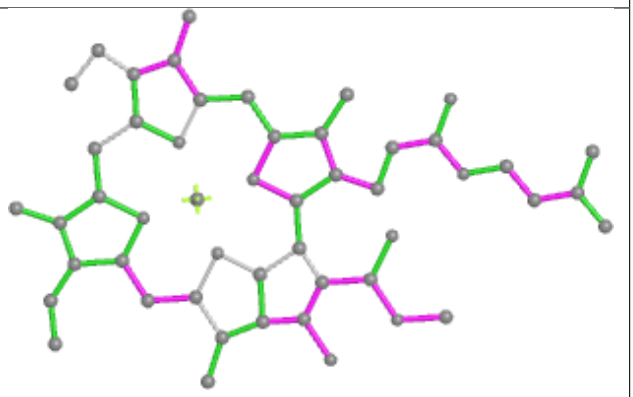
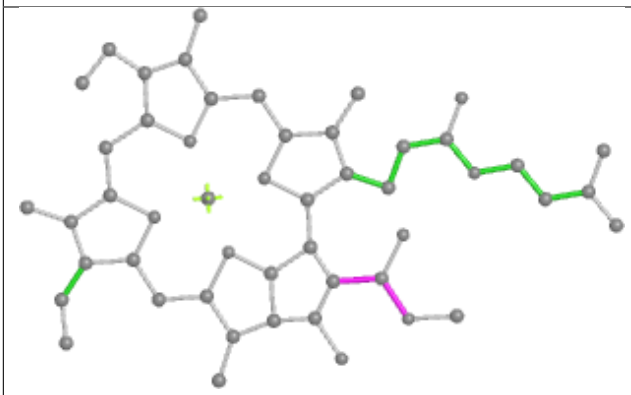
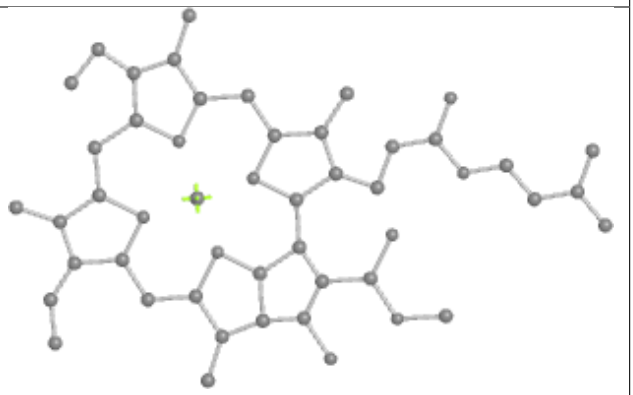


Bond angles

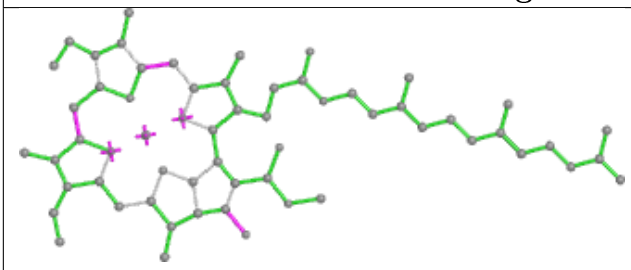


Torsions



Rings

Ligand CLA B 1483



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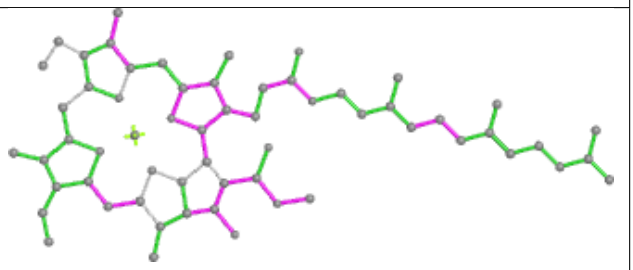
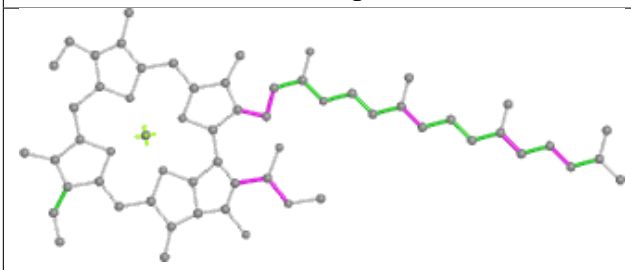
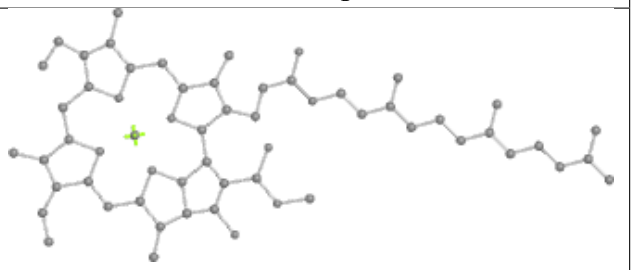


Bond angles

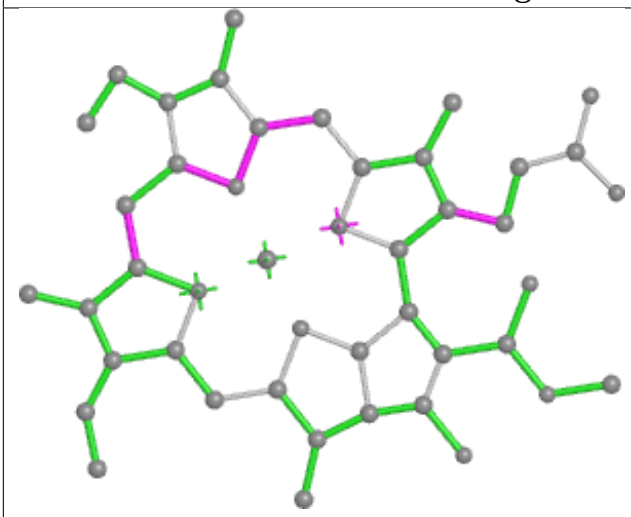


Torsions

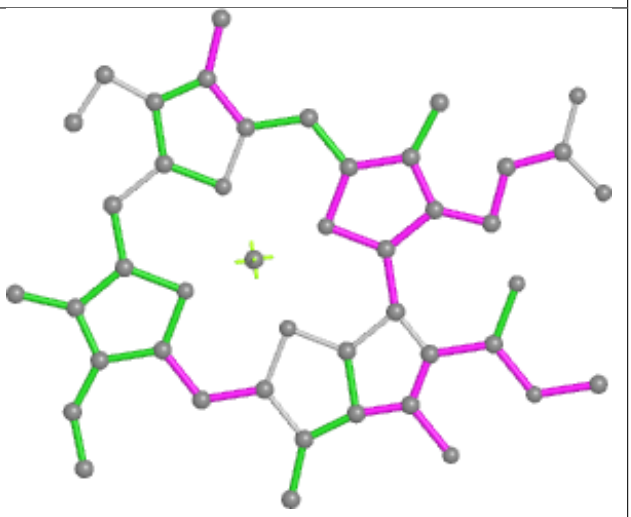


Rings

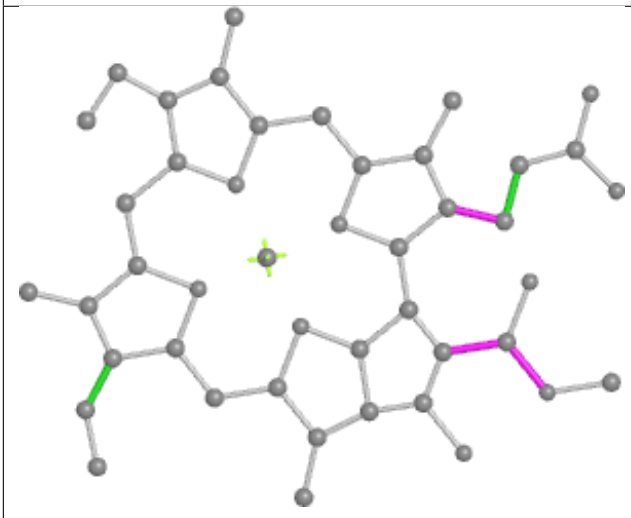
Ligand CLA G 1344



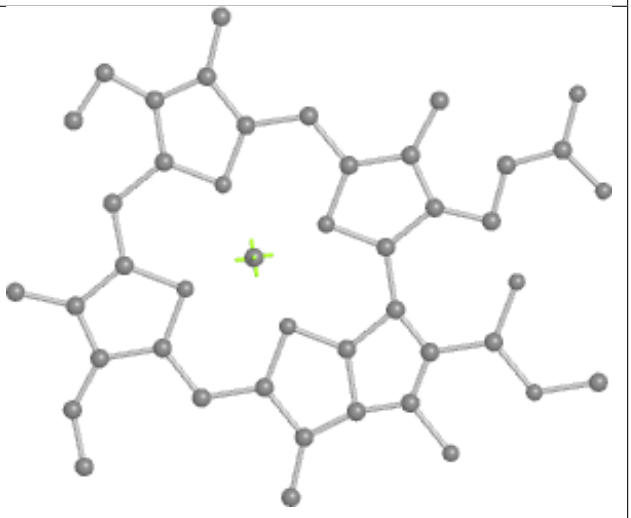
Bond lengths



Bond angles

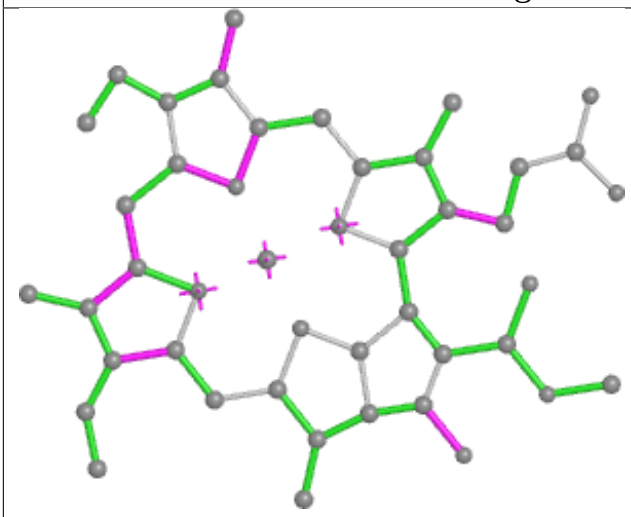


Torsions

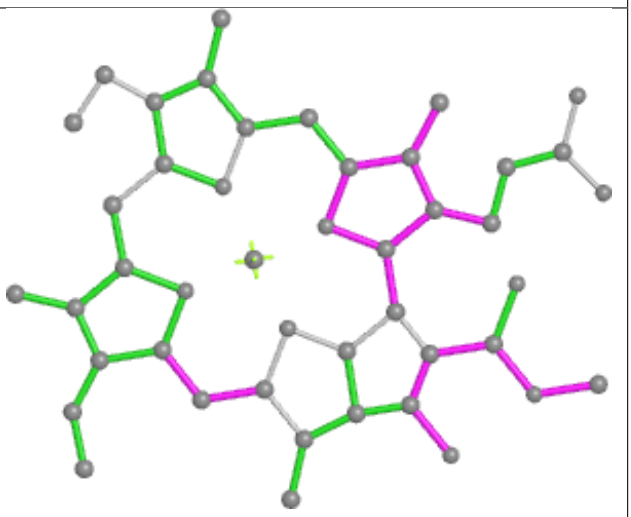


Rings

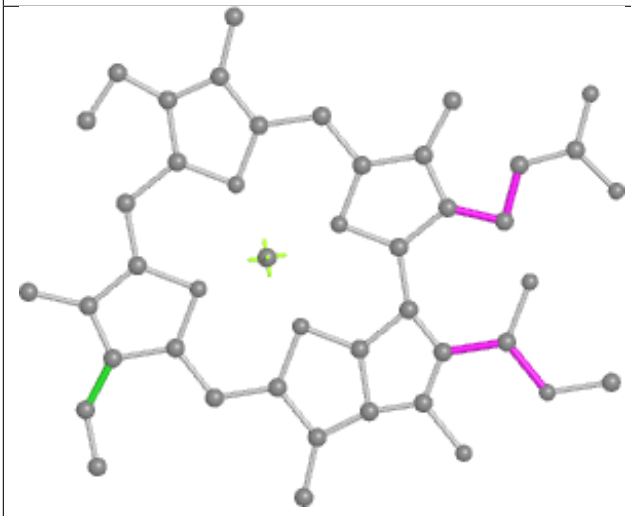
Ligand CLA H 1490



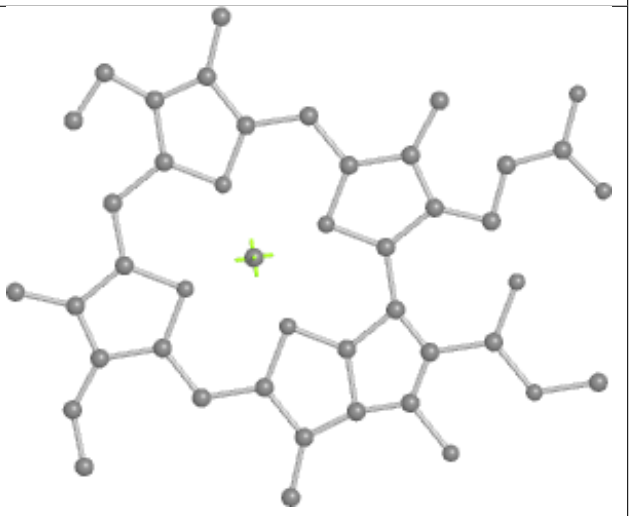
Bond lengths



Bond angles

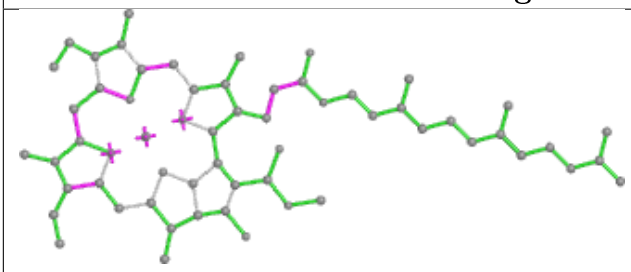


Torsions

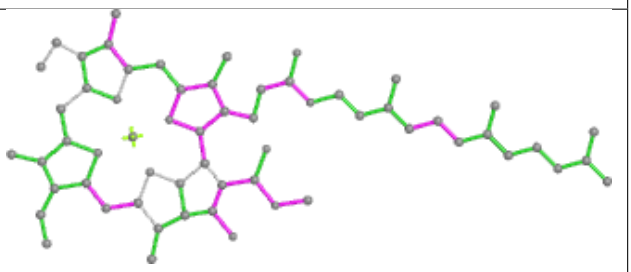


Rings

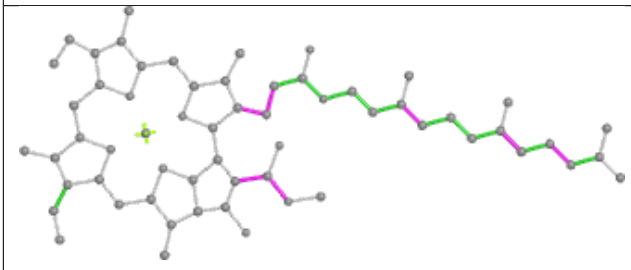
Ligand CLA H 1483



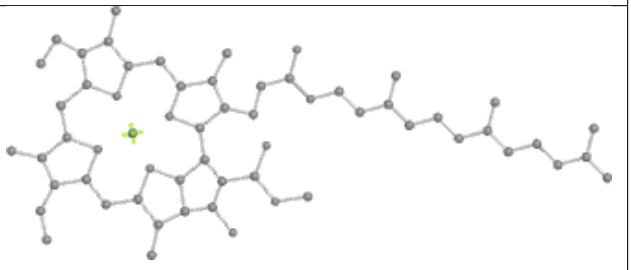
Bond lengths



Bond angles

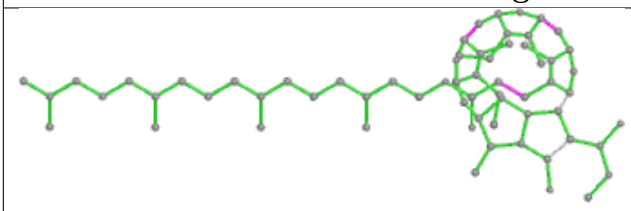


Torsions

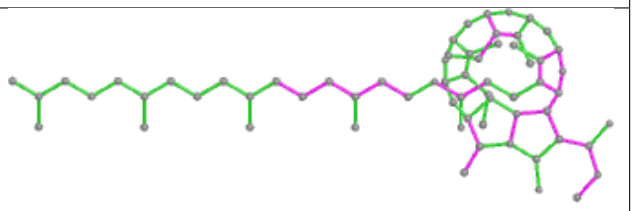


Rings

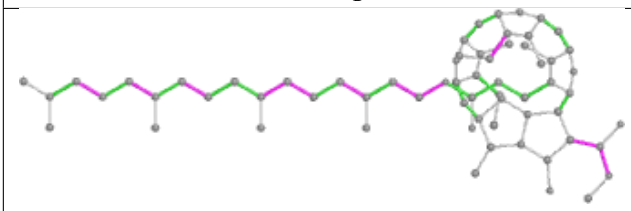
Ligand PHO G 1345



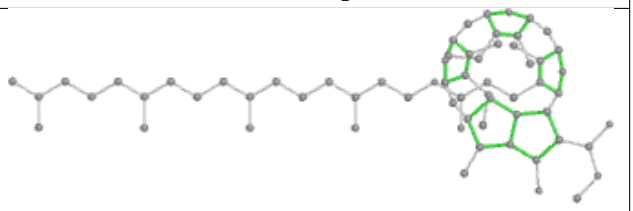
Bond lengths



Bond angles

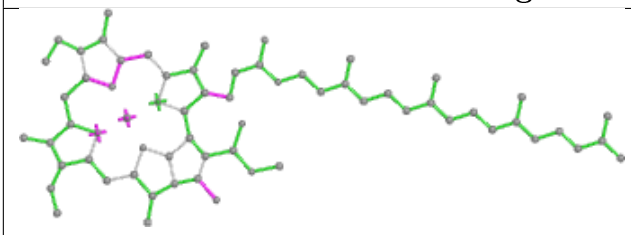


Torsions



Rings

Ligand CLA B 1496



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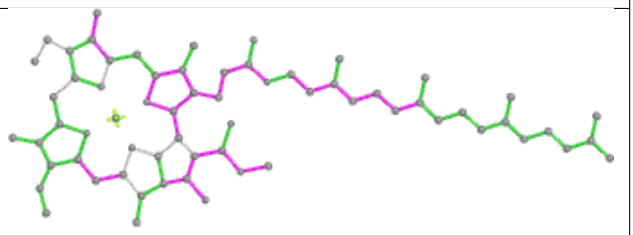
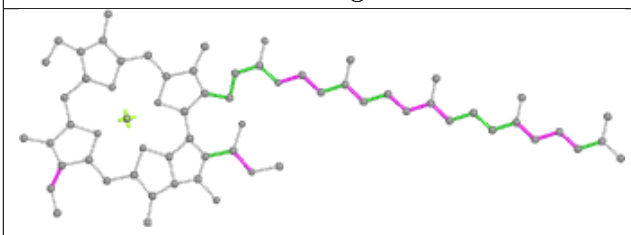
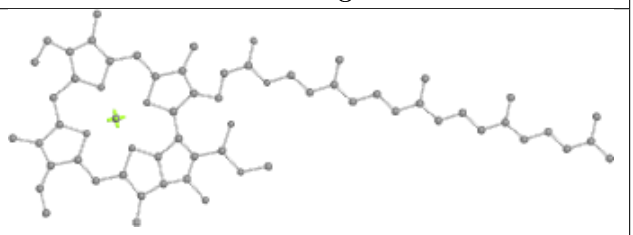


Bond angles

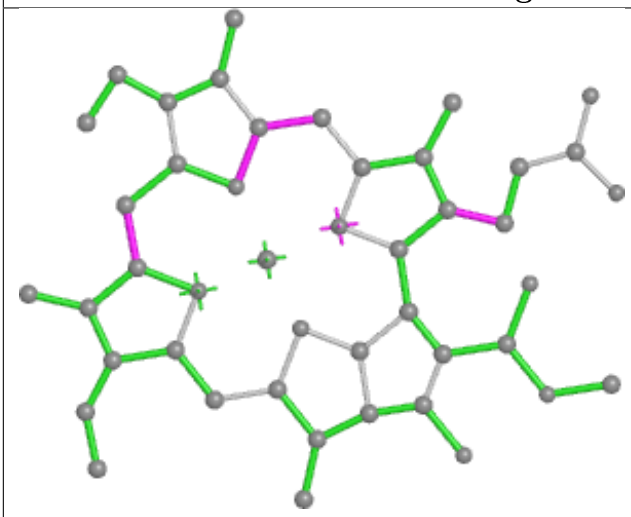


Torsions

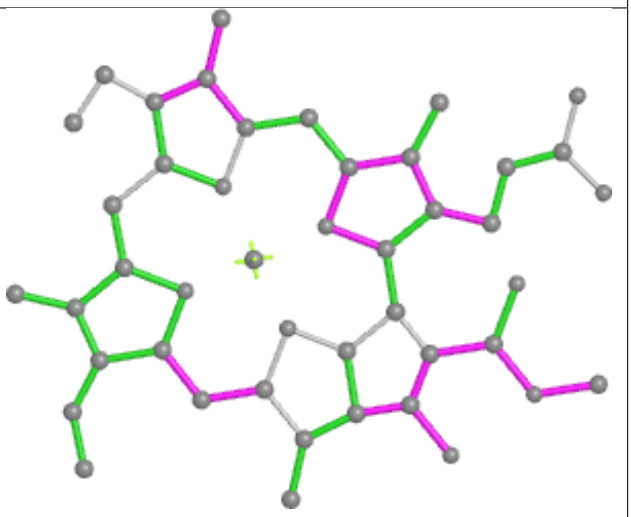


Rings

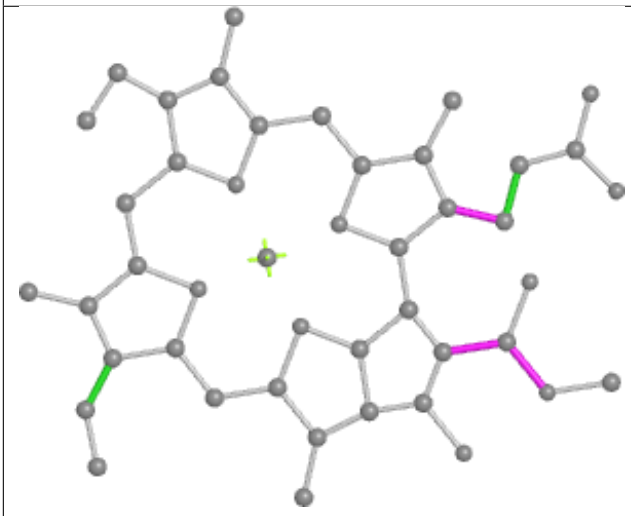
Ligand CLA B 1493



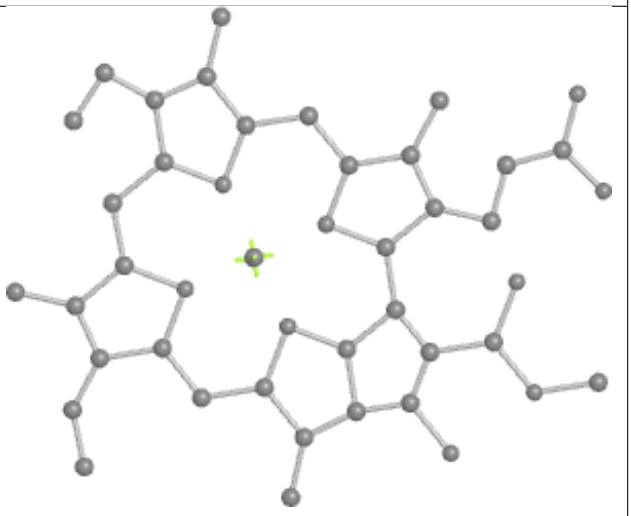
Bond lengths



Bond angles

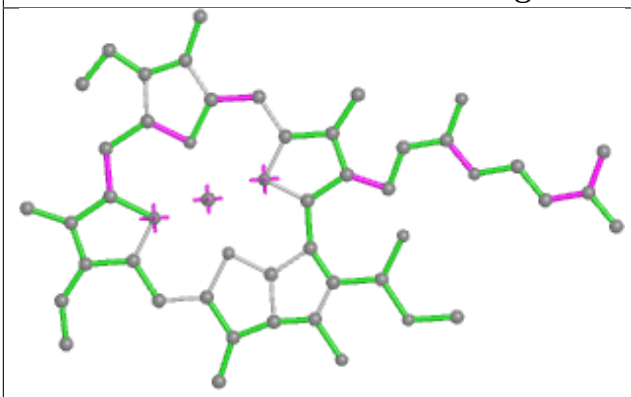


Torsions

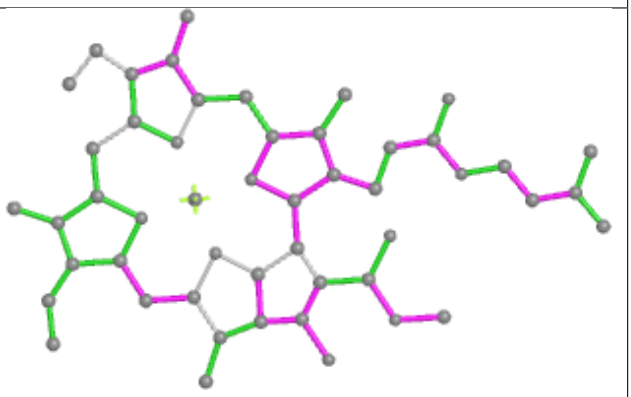


Rings

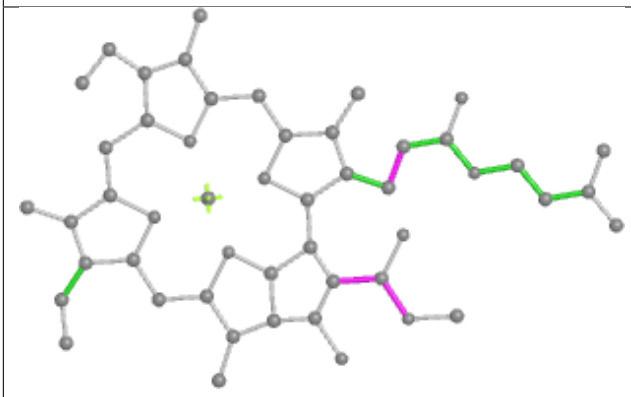
Ligand CLA D 1353



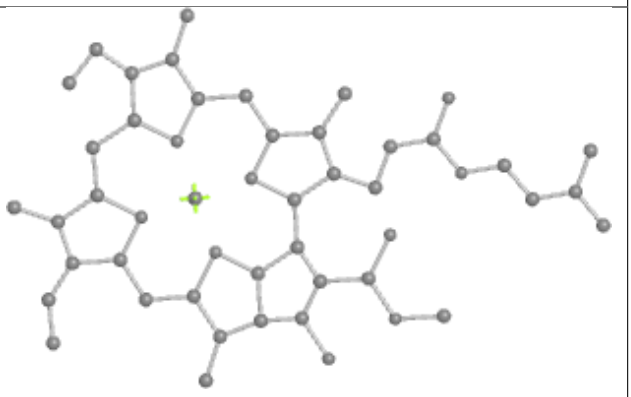
Bond lengths



Bond angles

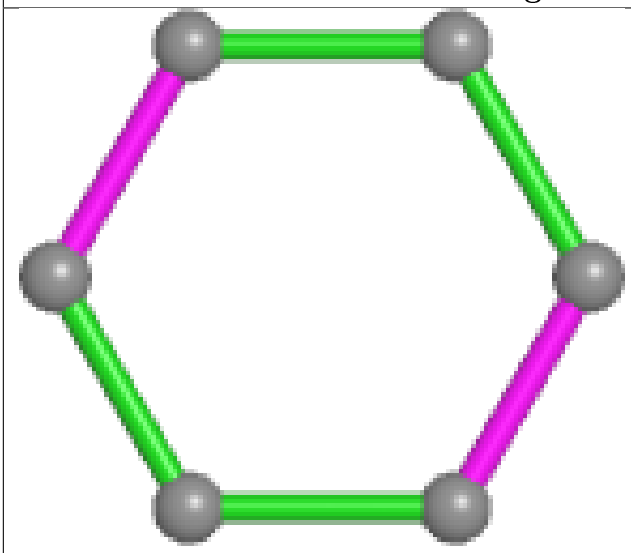


Torsions

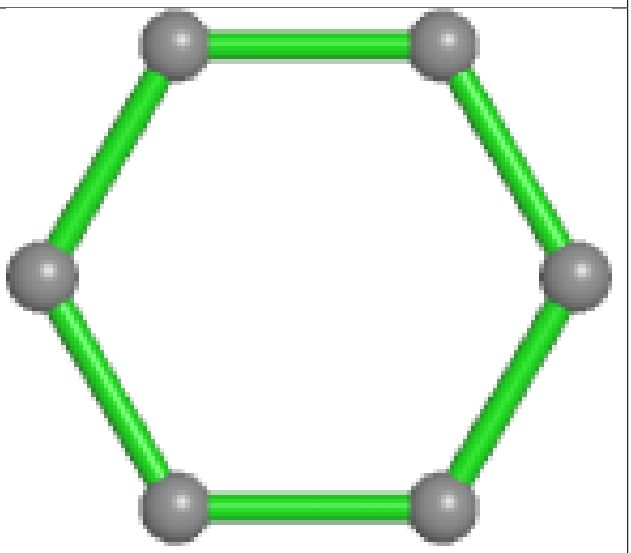


Rings

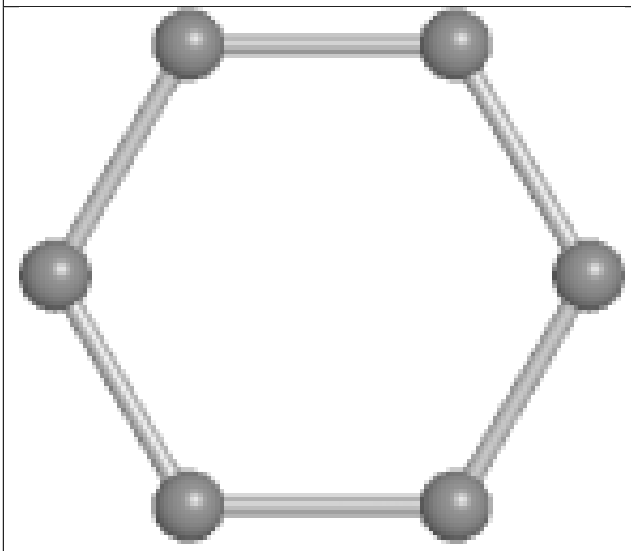
Ligand PL9 J 1354



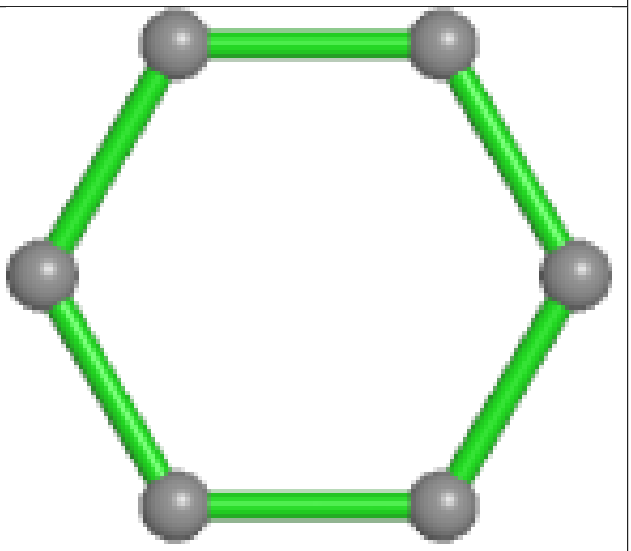
Bond lengths



Bond angles

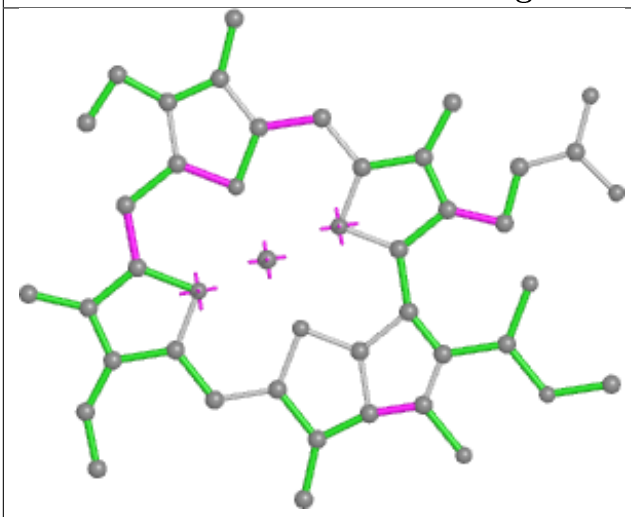


Torsions

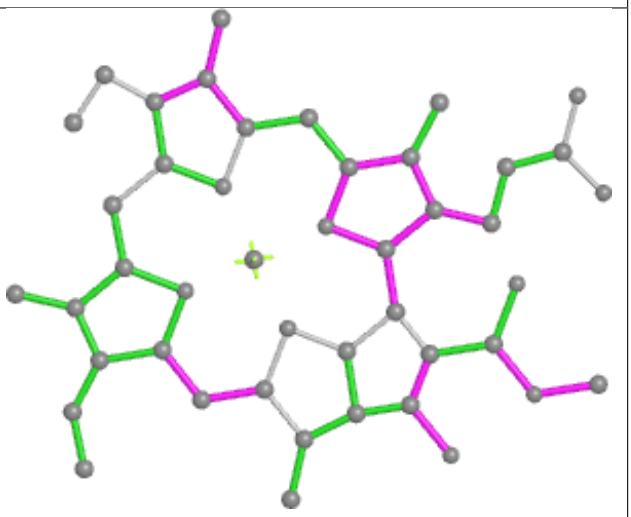


Rings

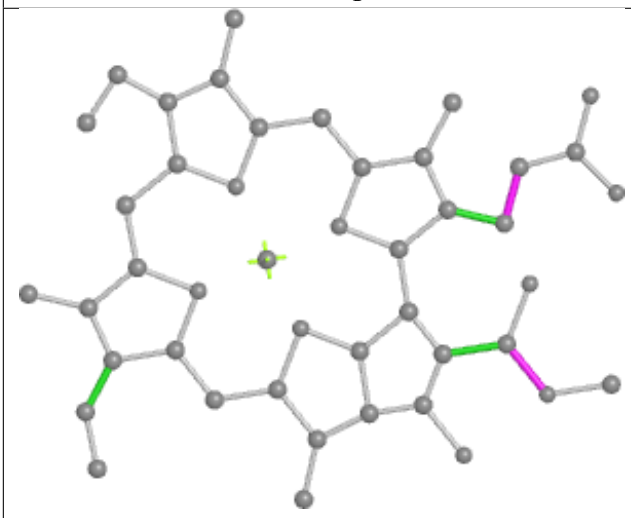
Ligand CLA B 1484



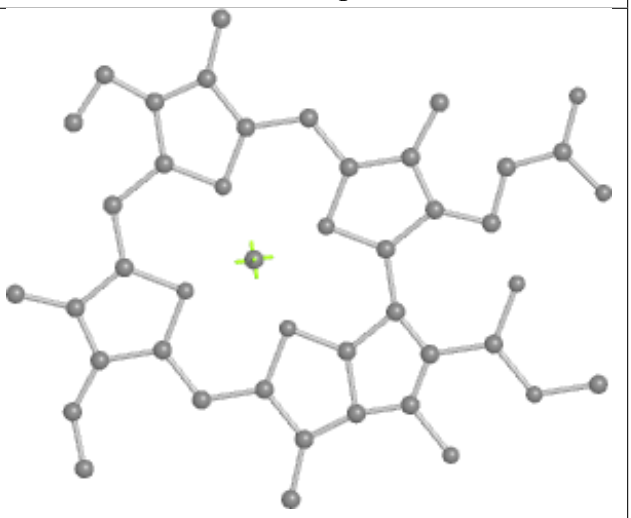
Bond lengths



Bond angles

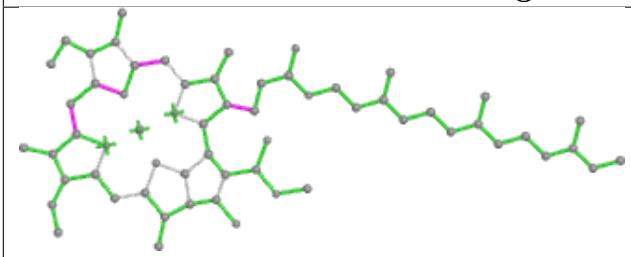


Torsions



Rings

Ligand CLA A 1343



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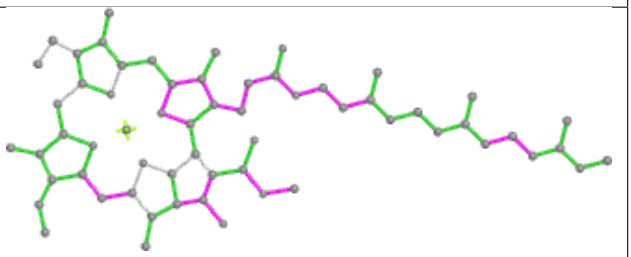
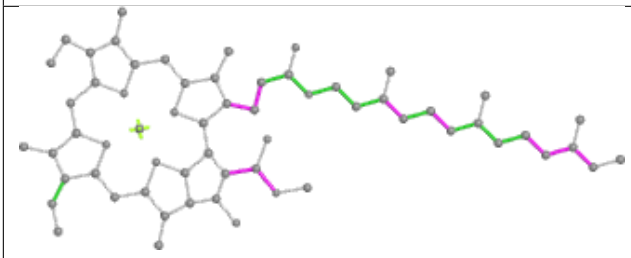
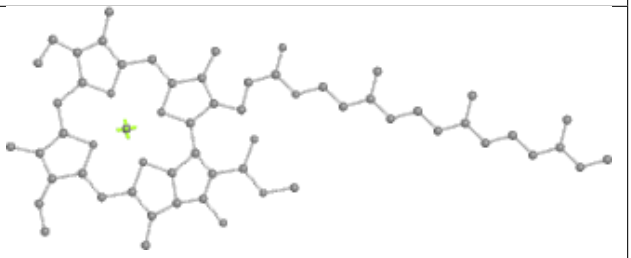


Bond angles

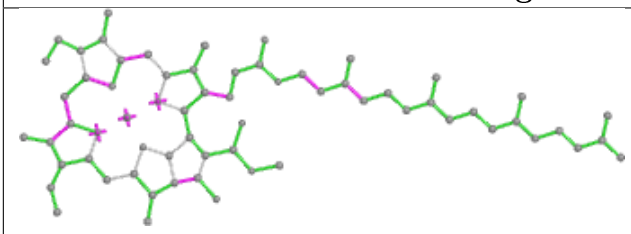


Torsions

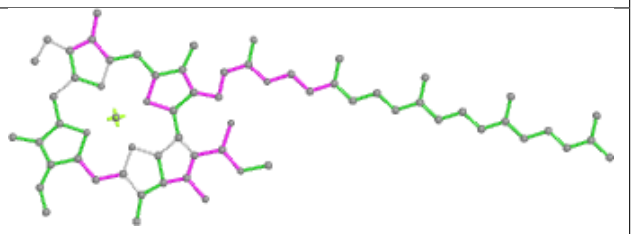


Rings

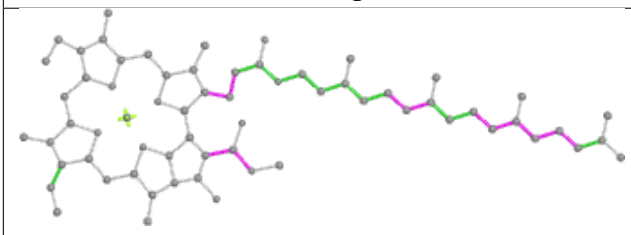
Ligand CLA B 1488



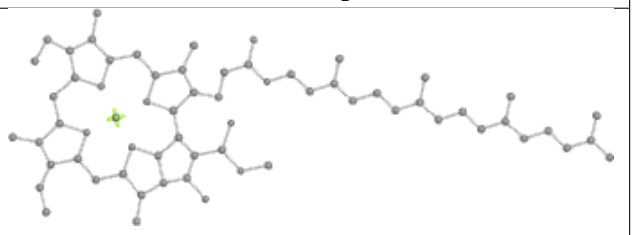
Bond lengths



Bond angles

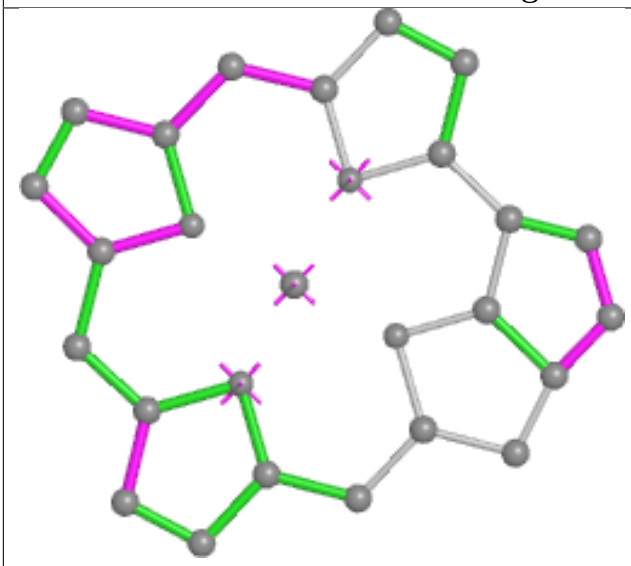


Torsions

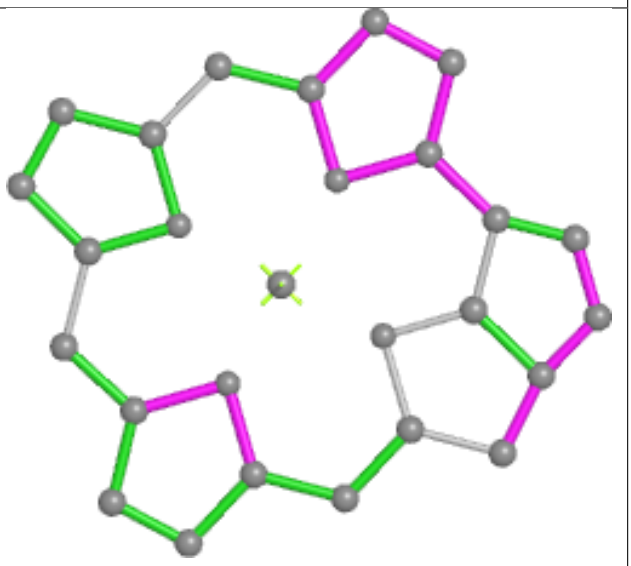


Rings

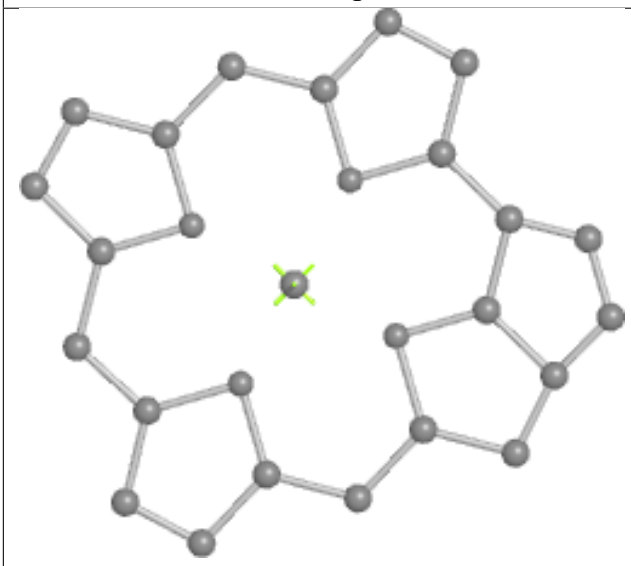
Ligand CLA I 1468



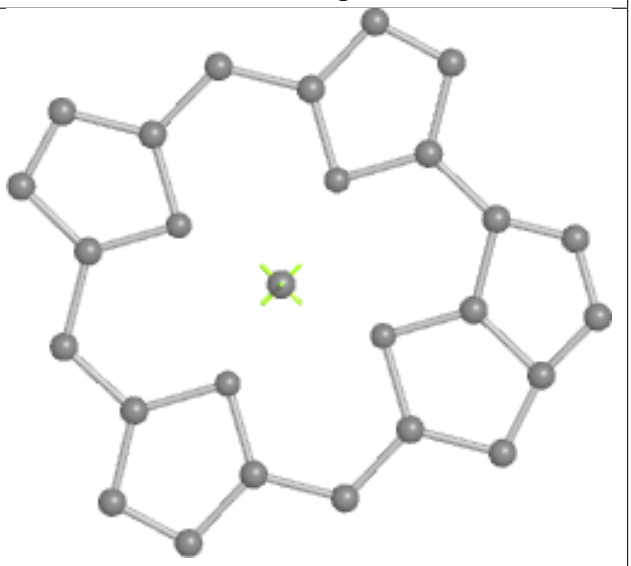
Bond lengths



Bond angles

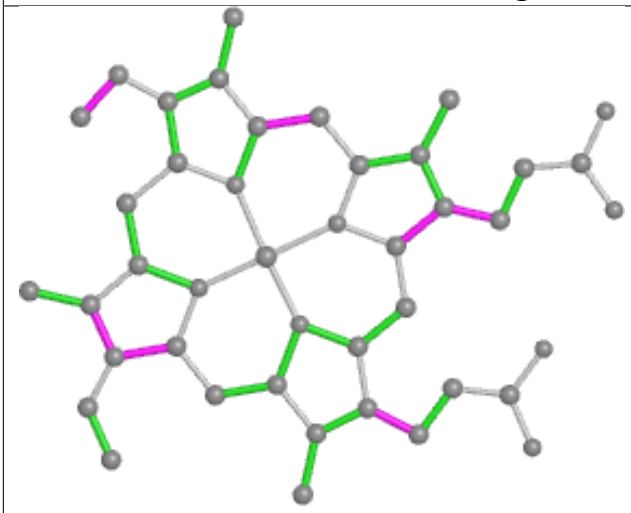


Torsions



Rings

Ligand HEC V 1138



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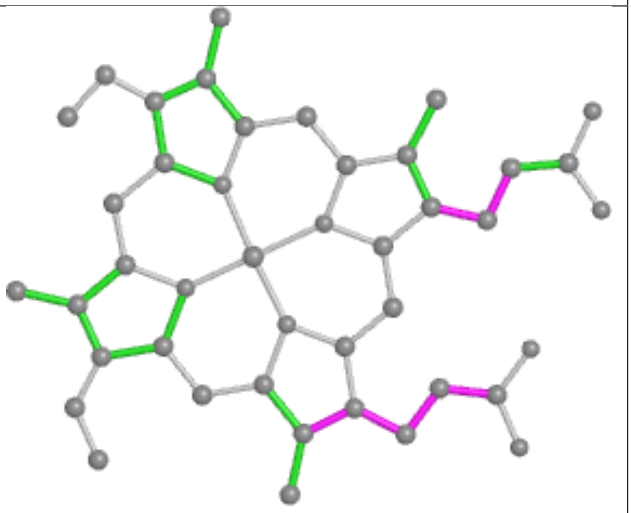
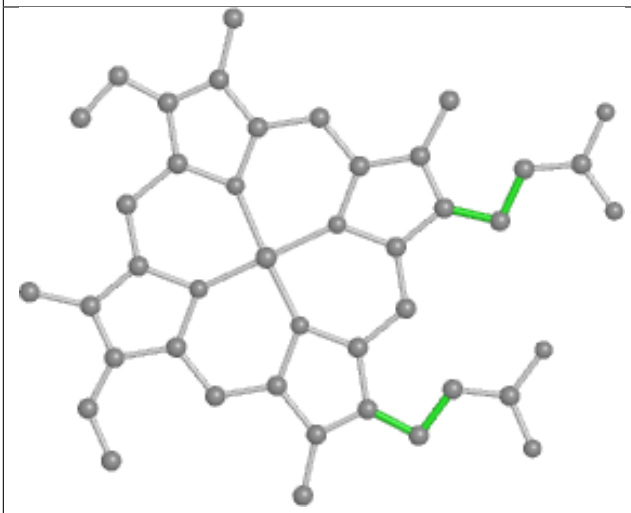
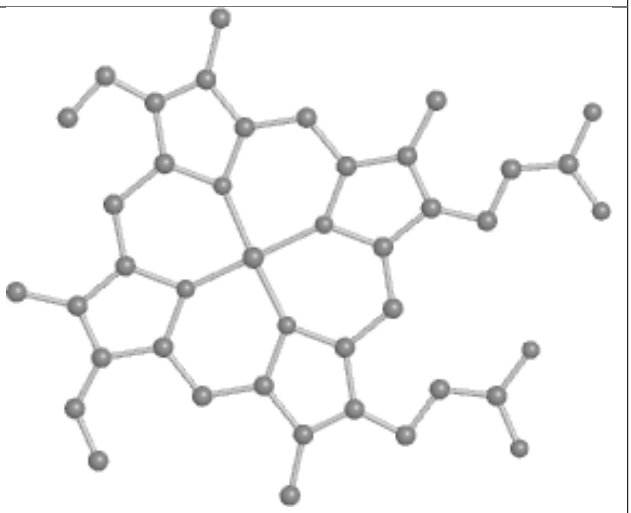


Bond angles

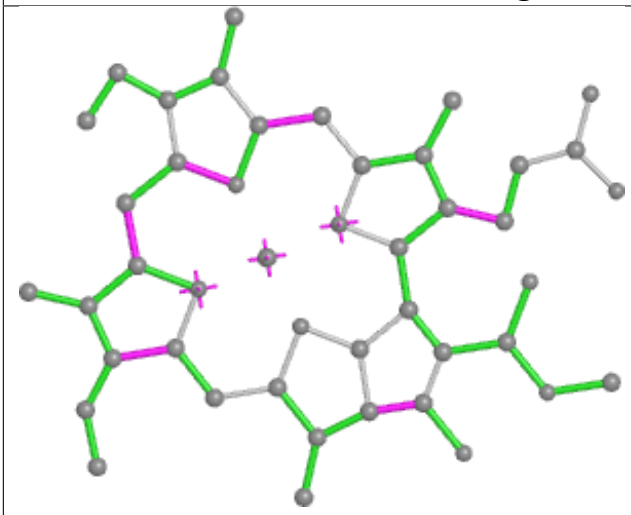


Torsions

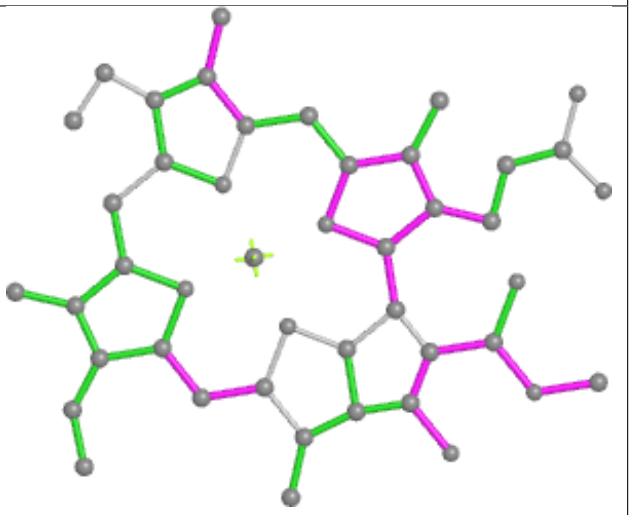


Rings

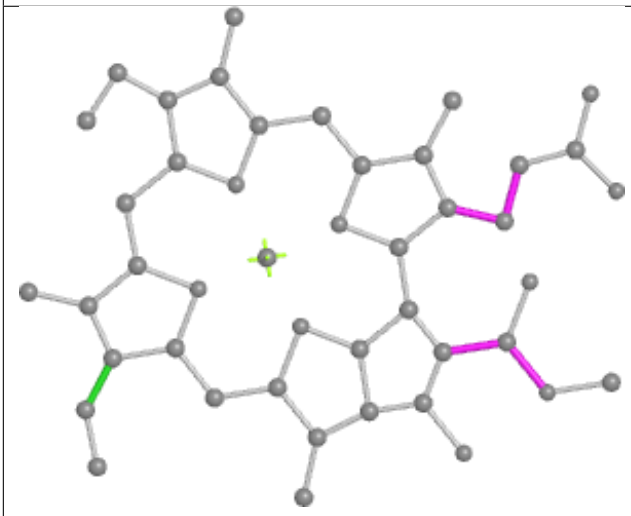
Ligand CLA C 1459



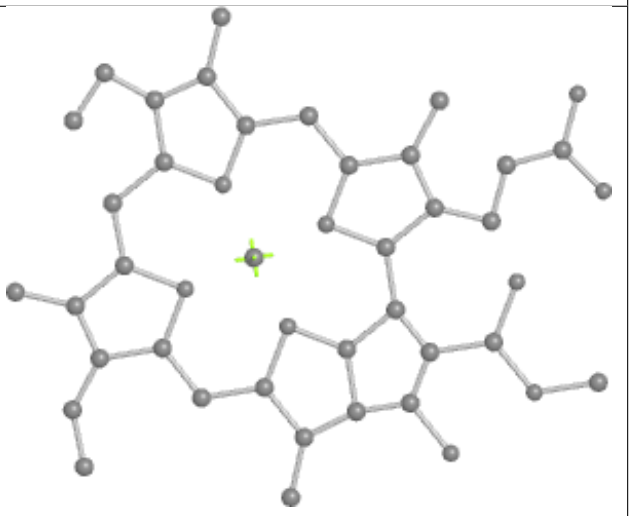
Bond lengths



Bond angles

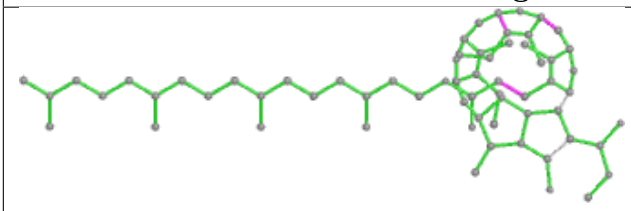


Torsions



Rings

Ligand PHO A 1345



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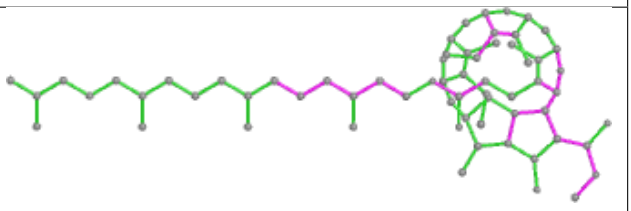
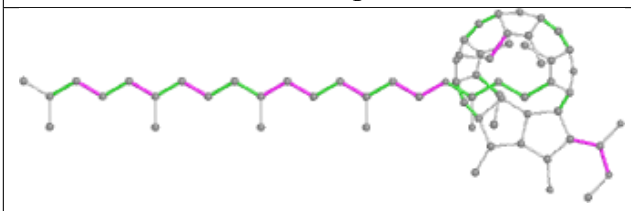
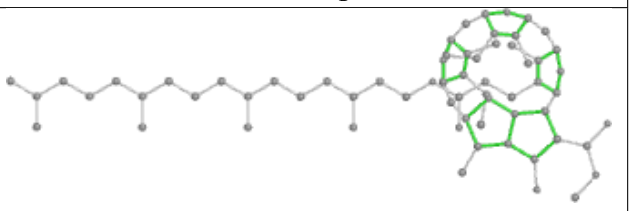


Bond angles

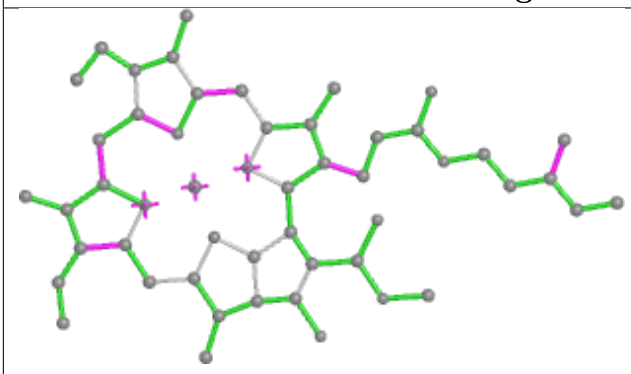


Torsions

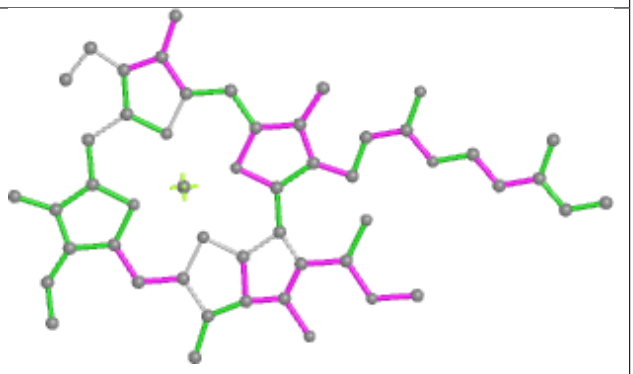


Rings

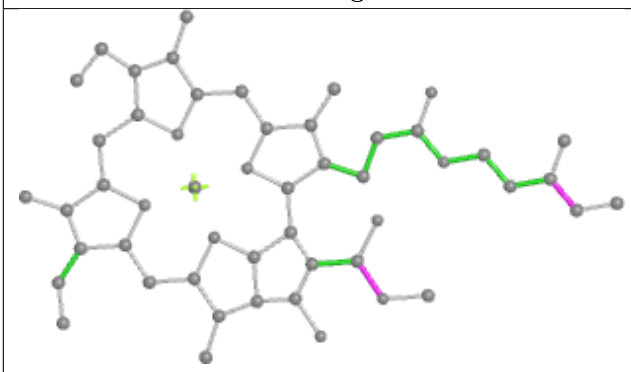
Ligand CLA A 1346



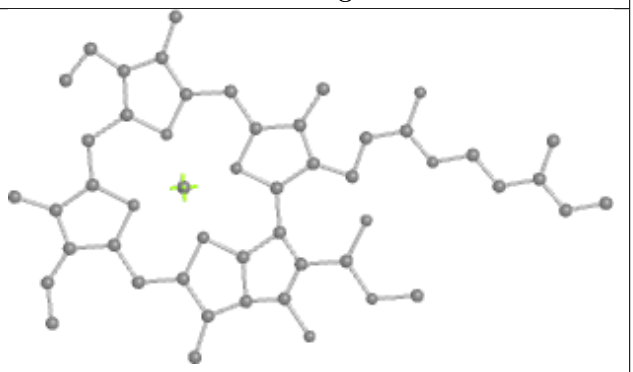
Bond lengths



Bond angles

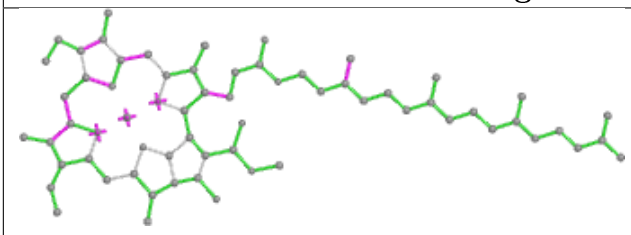


Torsions

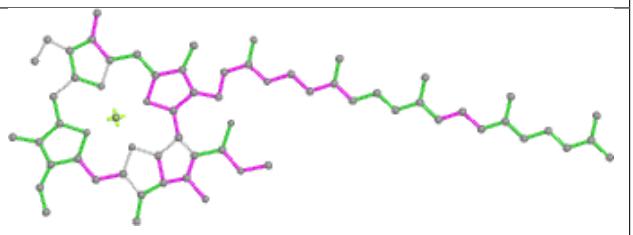


Rings

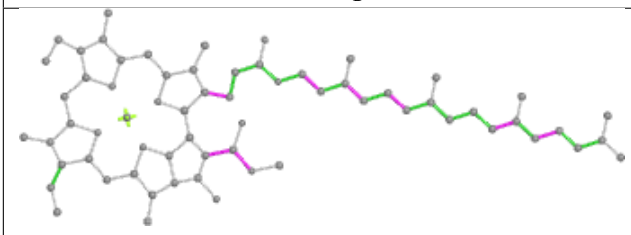
Ligand CLA D 1351



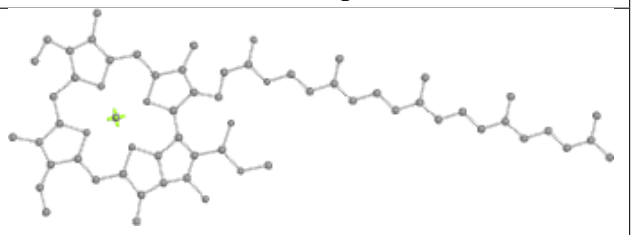
Bond lengths



Bond angles

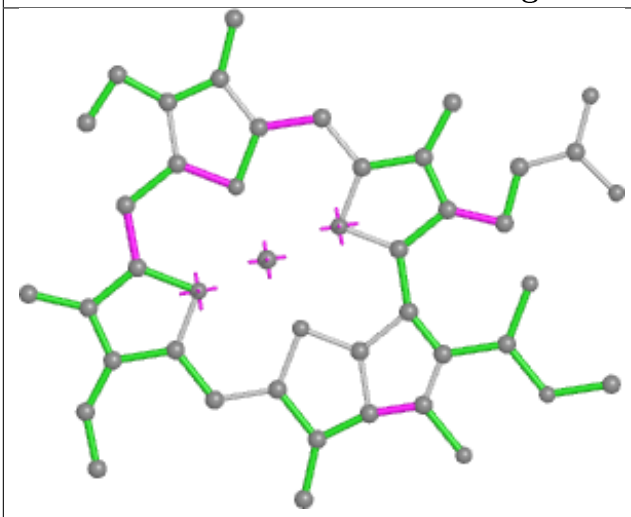


Torsions

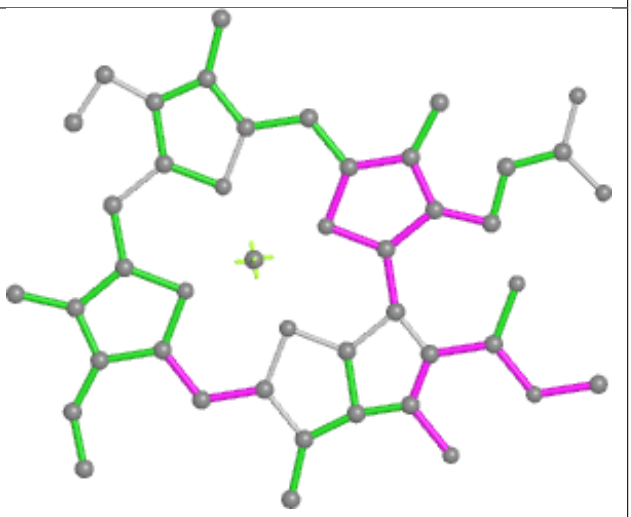


Rings

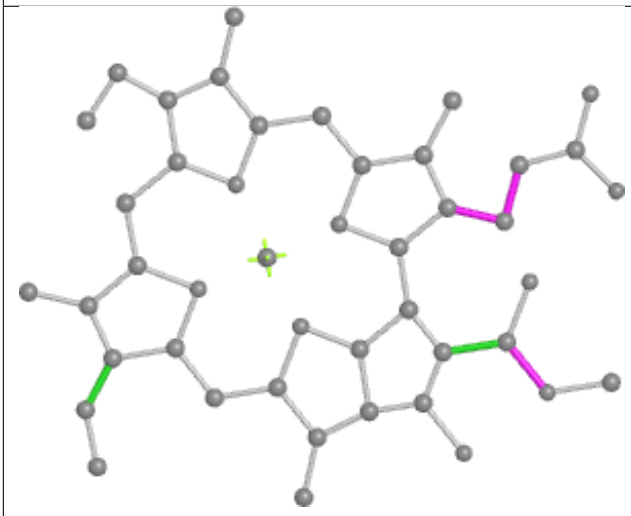
Ligand CLA I 1459



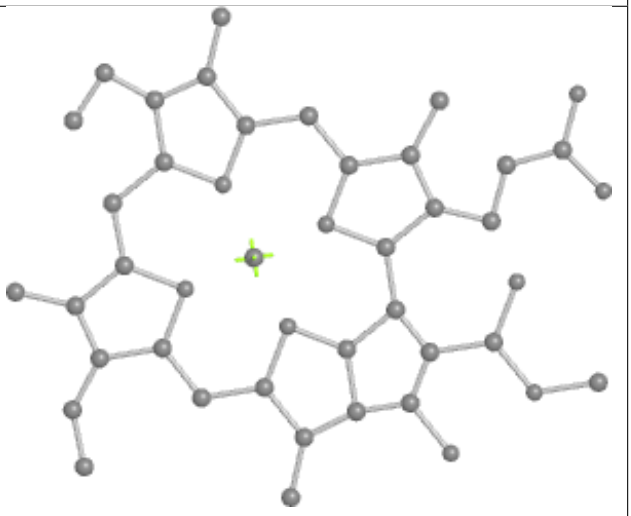
Bond lengths



Bond angles

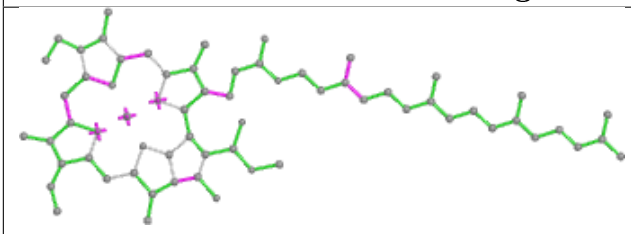


Torsions

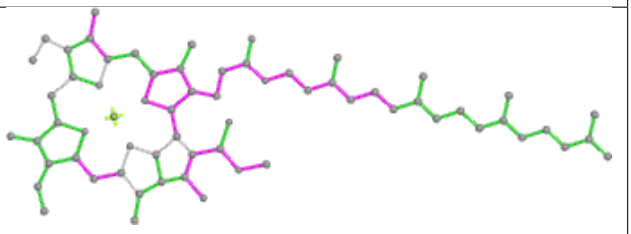


Rings

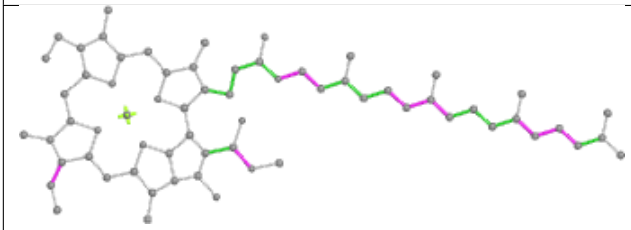
Ligand CLA H 1496



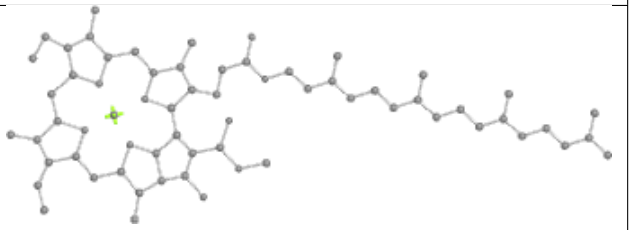
Bond lengths



Bond angles

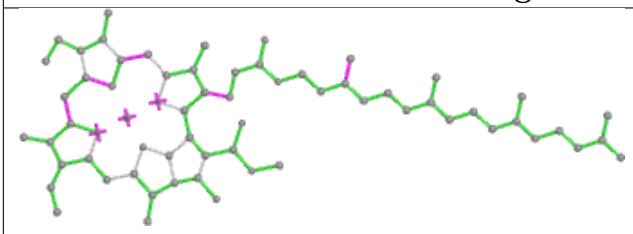


Torsions

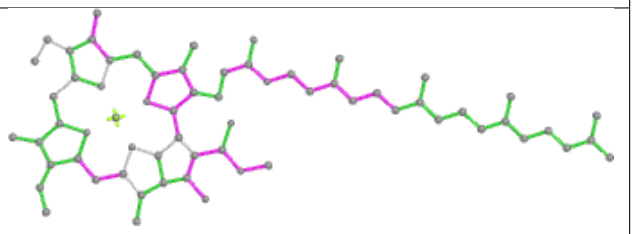


Rings

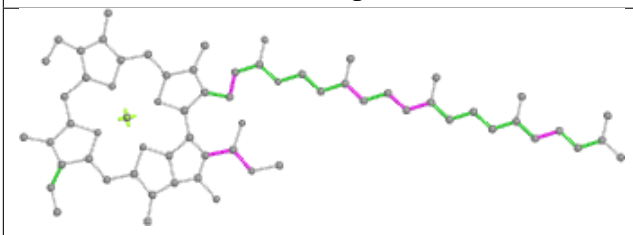
Ligand CLA H 1494



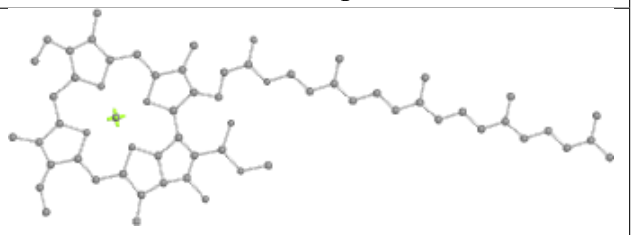
Bond lengths



Bond angles

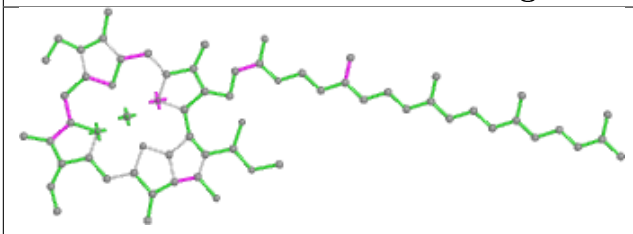


Torsions

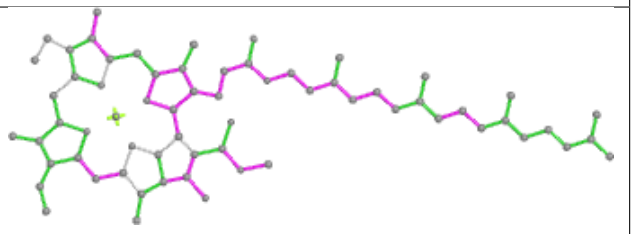


Rings

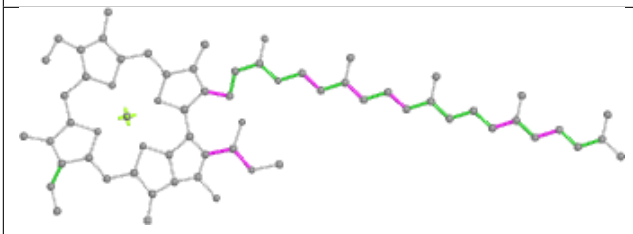
Ligand CLA J 1351



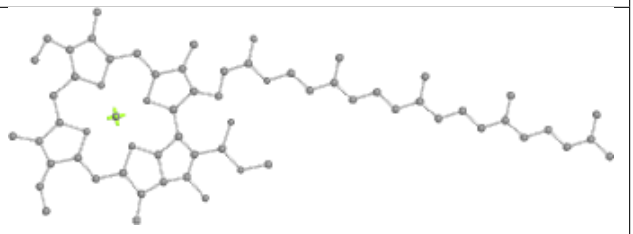
Bond lengths



Bond angles

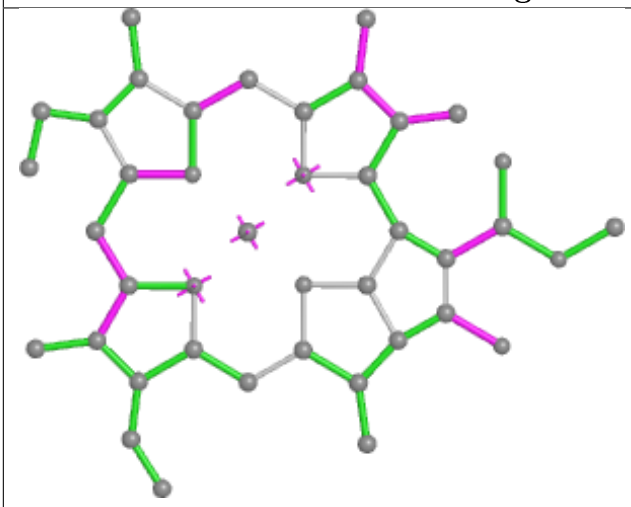


Torsions

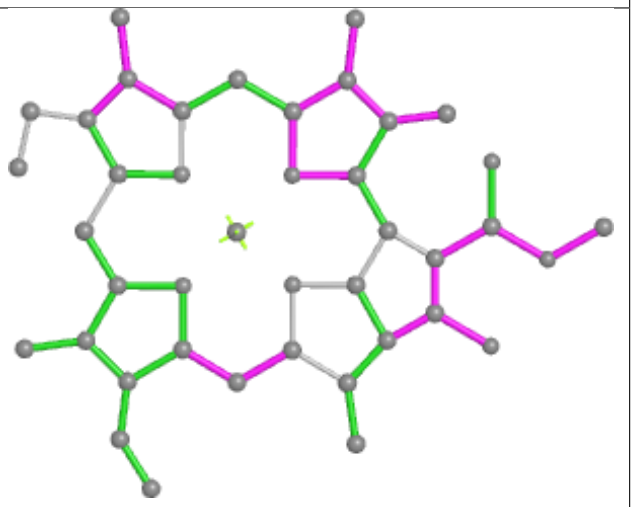


Rings

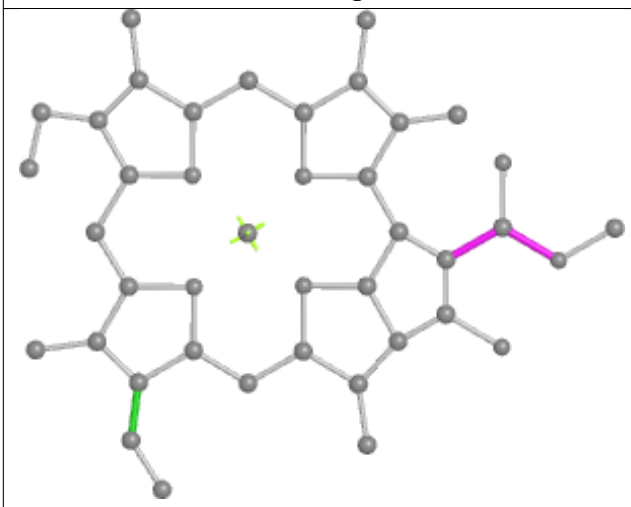
Ligand CLA H 1497



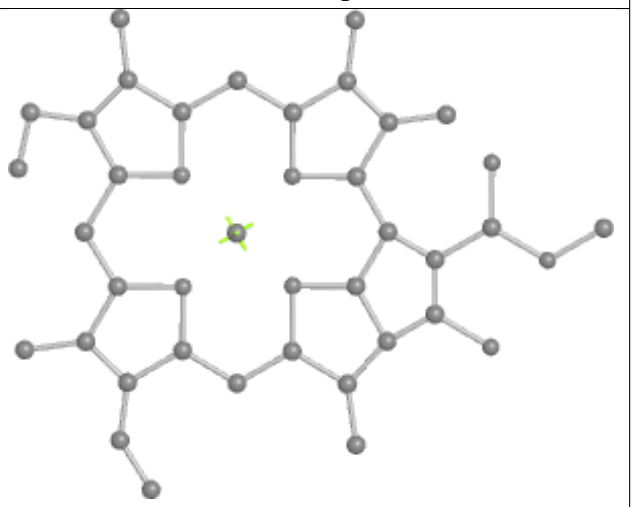
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	X	11
10	Y	11
7	O	5
7	P	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	185:UNK	C	200:UNK	N	108.56
1	X	185:UNK	C	200:UNK	N	108.51
1	X	374:UNK	C	400:UNK	N	87.82
1	Y	374:UNK	C	400:UNK	N	87.78
1	X	475:UNK	C	501:UNK	N	66.94
1	Y	475:UNK	C	501:UNK	N	66.93
1	Y	37:UNK	C	52:UNK	N	65.23
1	X	37:UNK	C	52:UNK	N	65.16
1	X	281:UNK	C	310:UNK	N	51.09
1	Y	281:UNK	C	310:UNK	N	51.09
1	X	537:UNK	C	552:UNK	N	45.76
1	Y	537:UNK	C	552:UNK	N	45.74
1	X	440:UNK	C	451:UNK	N	26.17
1	Y	440:UNK	C	451:UNK	N	26.11
1	Y	337:UNK	C	355:UNK	N	23.96
1	X	337:UNK	C	355:UNK	N	23.90
1	X	79:UNK	C	106:UNK	N	19.50
1	Y	79:UNK	C	106:UNK	N	19.46
1	O	95:UNK	C	96:UNK	N	11.66
1	P	95:UNK	C	96:UNK	N	11.66
1	P	85:UNK	C	86:UNK	N	9.75
1	O	85:UNK	C	86:UNK	N	9.73
1	P	36:UNK	C	37:UNK	N	9.25
1	O	36:UNK	C	37:UNK	N	9.24
1	Y	129:UNK	C	157:UNK	N	9.15
1	X	129:UNK	C	157:UNK	N	9.11
1	Y	227:UNK	C	252:UNK	N	8.97
1	X	227:UNK	C	252:UNK	N	8.93
1	P	146:UNK	C	147:UNK	N	5.82
1	O	146:UNK	C	147:UNK	N	5.80
1	O	47:UNK	C	48:UNK	N	4.68
1	P	47:UNK	C	48:UNK	N	4.68

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.