Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 12:27 PM EDT

PDB ID	:	8GK3
Title	:	Cytochrome P450 3A7 in complex with Dehydroepiandrosterone sulfate
Authors	:	Liu, J.; Scott, E.E.
Deposited on	:	2023-03-16
Resolution	:	2.60 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

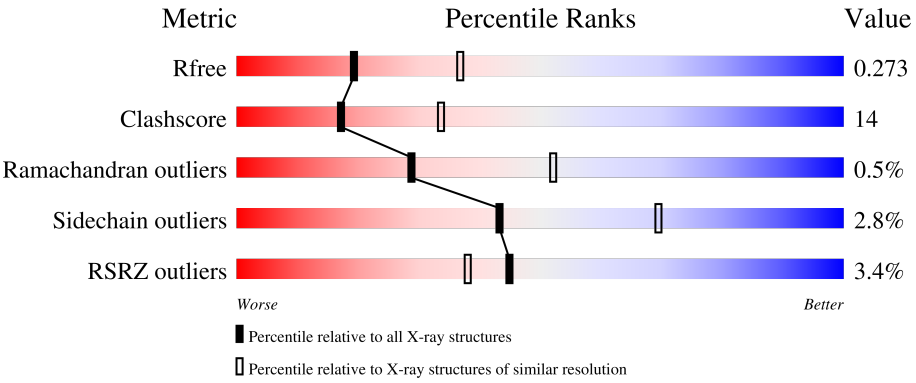
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.60 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))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 of 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	486	76% 21%
1	B	486	72% 23% 5%
1	C	486	70% 23% 5%
1	D	486	71% 22% 6%
1	E	486	68% 25% 5%

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Mol	Chain	Length	Quality of chain
1	F	486	2% 64% 28% 5%
1	G	486	3% 69% 26% 5%
1	H	486	3% 68% 25% 6%
1	I	486	6% 68% 26% 5%
1	J	486	3% 66% 26% 6%
1	K	486	3% 67% 26% 5%
1	L	486	12% 50% 37% 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 91794 atoms, of which 46378 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 Cytochrome P450 3A7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	473	Total	C	H	N	O	S	0	0	0
			7690	2470	3892	628	681	19			
1	B	462	Total	C	H	N	O	S	0	0	0
			7501	2417	3796	609	660	19			
1	C	463	Total	C	H	N	O	S	0	0	0
			7507	2417	3798	608	665	19			
1	D	459	Total	C	H	N	O	S	0	0	0
			7453	2402	3771	606	655	19			
1	E	460	Total	C	H	N	O	S	0	0	0
			7469	2404	3783	604	659	19			
1	F	461	Total	C	H	N	O	S	0	0	0
			7496	2413	3799	608	657	19			
1	G	462	Total	C	H	N	O	S	0	0	0
			7503	2417	3798	609	660	19			
1	H	458	Total	C	H	N	O	S	0	0	0
			7434	2396	3763	602	654	19			
1	I	463	Total	C	H	N	O	S	0	0	0
			7508	2417	3799	608	665	19			
1	J	458	Total	C	H	N	O	S	0	0	0
			7441	2395	3771	602	654	19			
1	K	462	Total	C	H	N	O	S	0	0	0
			7503	2417	3798	609	660	19			
1	L	440	Total	C	H	N	O	S	0	0	0
			7133	2307	3602	580	626	18			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	initiating methionine	UNP P24462
A	23	ALA	-	expression tag	UNP P24462
A	69	GLY	ARG	conflict	UNP P24462
A	77	GLY	CYS	conflict	UNP P24462
A	244	GLU	LYS	conflict	UNP P24462

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Chain	Residue	Modelled	Actual	Comment	Reference
A	421	ALA	LYS	conflict	UNP P24462
A	422	ALA	LYS	conflict	UNP P24462
A	424	ALA	LYS	conflict	UNP P24462
A	504	HIS	-	expression tag	UNP P24462
A	505	HIS	-	expression tag	UNP P24462
A	506	HIS	-	expression tag	UNP P24462
A	507	HIS	-	expression tag	UNP P24462
B	22	MET	-	initiating methionine	UNP P24462
B	23	ALA	-	expression tag	UNP P24462
B	69	GLY	ARG	conflict	UNP P24462
B	77	GLY	CYS	conflict	UNP P24462
B	244	GLU	LYS	conflict	UNP P24462
B	421	ALA	LYS	conflict	UNP P24462
B	422	ALA	LYS	conflict	UNP P24462
B	424	ALA	LYS	conflict	UNP P24462
B	504	HIS	-	expression tag	UNP P24462
B	505	HIS	-	expression tag	UNP P24462
B	506	HIS	-	expression tag	UNP P24462
B	507	HIS	-	expression tag	UNP P24462
C	22	MET	-	initiating methionine	UNP P24462
C	23	ALA	-	expression tag	UNP P24462
C	69	GLY	ARG	conflict	UNP P24462
C	77	GLY	CYS	conflict	UNP P24462
C	244	GLU	LYS	conflict	UNP P24462
C	421	ALA	LYS	conflict	UNP P24462
C	422	ALA	LYS	conflict	UNP P24462
C	424	ALA	LYS	conflict	UNP P24462
C	504	HIS	-	expression tag	UNP P24462
C	505	HIS	-	expression tag	UNP P24462
C	506	HIS	-	expression tag	UNP P24462
C	507	HIS	-	expression tag	UNP P24462
D	22	MET	-	initiating methionine	UNP P24462
D	23	ALA	-	expression tag	UNP P24462
D	69	GLY	ARG	conflict	UNP P24462
D	77	GLY	CYS	conflict	UNP P24462
D	244	GLU	LYS	conflict	UNP P24462
D	421	ALA	LYS	conflict	UNP P24462
D	422	ALA	LYS	conflict	UNP P24462
D	424	ALA	LYS	conflict	UNP P24462
D	504	HIS	-	expression tag	UNP P24462
D	505	HIS	-	expression tag	UNP P24462
D	506	HIS	-	expression tag	UNP P24462

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Chain	Residue	Modelled	Actual	Comment	Reference
D	507	HIS	-	expression tag	UNP P24462
E	22	MET	-	initiating methionine	UNP P24462
E	23	ALA	-	expression tag	UNP P24462
E	69	GLY	ARG	conflict	UNP P24462
E	77	GLY	CYS	conflict	UNP P24462
E	244	GLU	LYS	conflict	UNP P24462
E	421	ALA	LYS	conflict	UNP P24462
E	422	ALA	LYS	conflict	UNP P24462
E	424	ALA	LYS	conflict	UNP P24462
E	504	HIS	-	expression tag	UNP P24462
E	505	HIS	-	expression tag	UNP P24462
E	506	HIS	-	expression tag	UNP P24462
E	507	HIS	-	expression tag	UNP P24462
F	22	MET	-	initiating methionine	UNP P24462
F	23	ALA	-	expression tag	UNP P24462
F	69	GLY	ARG	conflict	UNP P24462
F	77	GLY	CYS	conflict	UNP P24462
F	244	GLU	LYS	conflict	UNP P24462
F	421	ALA	LYS	conflict	UNP P24462
F	422	ALA	LYS	conflict	UNP P24462
F	424	ALA	LYS	conflict	UNP P24462
F	504	HIS	-	expression tag	UNP P24462
F	505	HIS	-	expression tag	UNP P24462
F	506	HIS	-	expression tag	UNP P24462
F	507	HIS	-	expression tag	UNP P24462
G	22	MET	-	initiating methionine	UNP P24462
G	23	ALA	-	expression tag	UNP P24462
G	69	GLY	ARG	conflict	UNP P24462
G	77	GLY	CYS	conflict	UNP P24462
G	244	GLU	LYS	conflict	UNP P24462
G	421	ALA	LYS	conflict	UNP P24462
G	422	ALA	LYS	conflict	UNP P24462
G	424	ALA	LYS	conflict	UNP P24462
G	504	HIS	-	expression tag	UNP P24462
G	505	HIS	-	expression tag	UNP P24462
G	506	HIS	-	expression tag	UNP P24462
G	507	HIS	-	expression tag	UNP P24462
H	22	MET	-	initiating methionine	UNP P24462
H	23	ALA	-	expression tag	UNP P24462
H	69	GLY	ARG	conflict	UNP P24462
H	77	GLY	CYS	conflict	UNP P24462
H	244	GLU	LYS	conflict	UNP P24462

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Chain	Residue	Modelled	Actual	Comment	Reference
H	421	ALA	LYS	conflict	UNP P24462
H	422	ALA	LYS	conflict	UNP P24462
H	424	ALA	LYS	conflict	UNP P24462
H	504	HIS	-	expression tag	UNP P24462
H	505	HIS	-	expression tag	UNP P24462
H	506	HIS	-	expression tag	UNP P24462
H	507	HIS	-	expression tag	UNP P24462
I	22	MET	-	initiating methionine	UNP P24462
I	23	ALA	-	expression tag	UNP P24462
I	69	GLY	ARG	conflict	UNP P24462
I	77	GLY	CYS	conflict	UNP P24462
I	244	GLU	LYS	conflict	UNP P24462
I	421	ALA	LYS	conflict	UNP P24462
I	422	ALA	LYS	conflict	UNP P24462
I	424	ALA	LYS	conflict	UNP P24462
I	504	HIS	-	expression tag	UNP P24462
I	505	HIS	-	expression tag	UNP P24462
I	506	HIS	-	expression tag	UNP P24462
I	507	HIS	-	expression tag	UNP P24462
J	22	MET	-	initiating methionine	UNP P24462
J	23	ALA	-	expression tag	UNP P24462
J	69	GLY	ARG	conflict	UNP P24462
J	77	GLY	CYS	conflict	UNP P24462
J	244	GLU	LYS	conflict	UNP P24462
J	421	ALA	LYS	conflict	UNP P24462
J	422	ALA	LYS	conflict	UNP P24462
J	424	ALA	LYS	conflict	UNP P24462
J	504	HIS	-	expression tag	UNP P24462
J	505	HIS	-	expression tag	UNP P24462
J	506	HIS	-	expression tag	UNP P24462
J	507	HIS	-	expression tag	UNP P24462
K	22	MET	-	initiating methionine	UNP P24462
K	23	ALA	-	expression tag	UNP P24462
K	69	GLY	ARG	conflict	UNP P24462
K	77	GLY	CYS	conflict	UNP P24462
K	244	GLU	LYS	conflict	UNP P24462
K	421	ALA	LYS	conflict	UNP P24462
K	422	ALA	LYS	conflict	UNP P24462
K	424	ALA	LYS	conflict	UNP P24462
K	504	HIS	-	expression tag	UNP P24462
K	505	HIS	-	expression tag	UNP P24462
K	506	HIS	-	expression tag	UNP P24462

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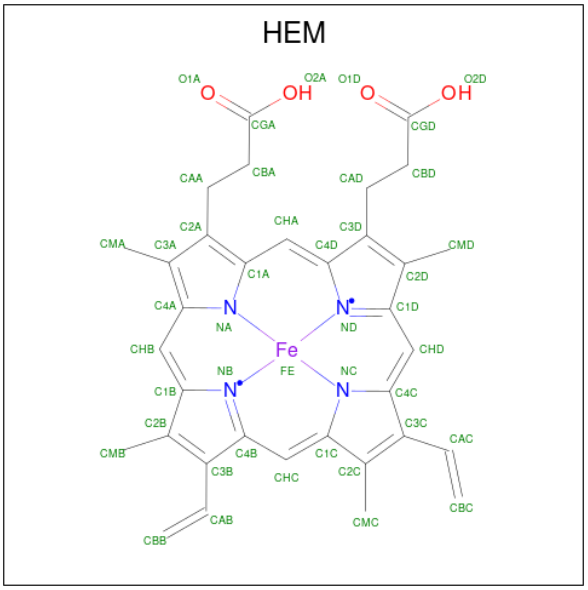
Chain	Residue	Modelled	Actual	Comment	Reference
K	507	HIS	-	expression tag	UNP P24462
L	22	MET	-	initiating methionine	UNP P24462
L	23	ALA	-	expression tag	UNP P24462
L	69	GLY	ARG	conflict	UNP P24462
L	77	GLY	CYS	conflict	UNP P24462
L	244	GLU	LYS	conflict	UNP P24462
L	421	ALA	LYS	conflict	UNP P24462
L	422	ALA	LYS	conflict	UNP P24462
L	424	ALA	LYS	conflict	UNP P24462
L	504	HIS	-	expression tag	UNP P24462
L	505	HIS	-	expression tag	UNP P24462
L	506	HIS	-	expression tag	UNP P24462
L	507	HIS	-	expression tag	UNP P24462

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	D	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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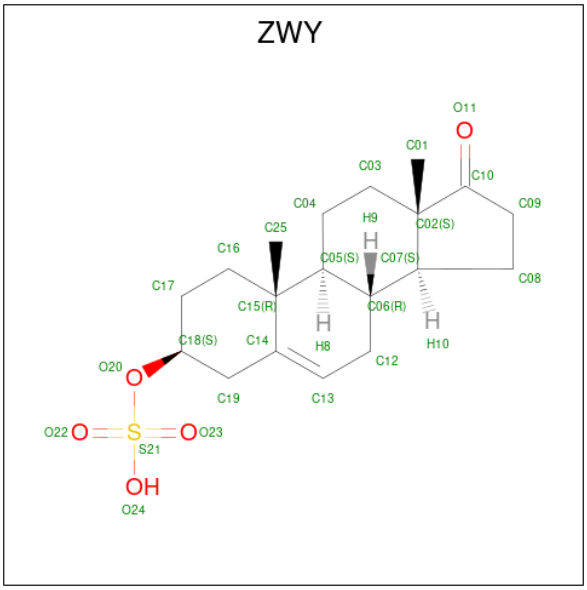
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	G	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	H	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	I	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	J	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	K	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	L	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 3 is 17-oxoandrost-5-en-3beta-yl hydrogen sulfate (three-letter code: ZWY) (formula: $C_{19}H_{28}O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	A	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	B	1	Total	C	H	O	S	0	0
			52	19	27	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	C	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	C	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	C	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	C	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	D	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	D	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	D	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	D	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	D	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	E	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	E	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	E	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	E	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	H	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	H	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	H	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	I	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	I	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	J	1	Total	C	H	O	S	0	0
			52	19	27	5	1		
3	J	1	Total	C	H	O	S	0	0
			52	19	27	5	1		

- Molecule 4 is water.

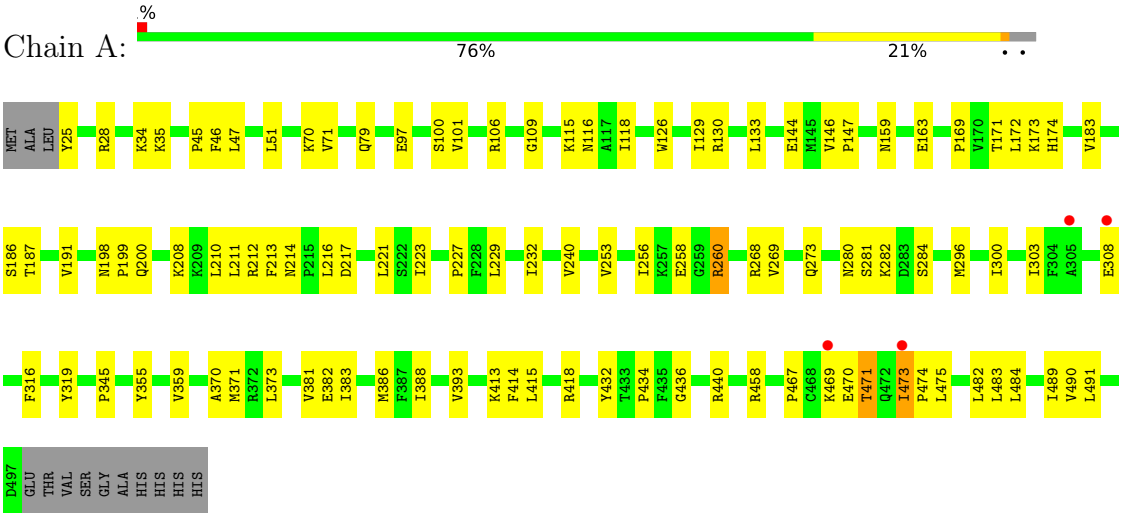
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0
4	B	7	Total O 7 7	0	0
4	E	2	Total O 2 2	0	0
4	F	4	Total O 4 4	0	0
4	G	5	Total O 5 5	0	0
4	H	2	Total O 2 2	0	0
4	I	1	Total O 1 1	0	0
4	J	1	Total O 1 1	0	0
4	K	5	Total O 5 5	0	0

3 Residue-property plots (i)

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

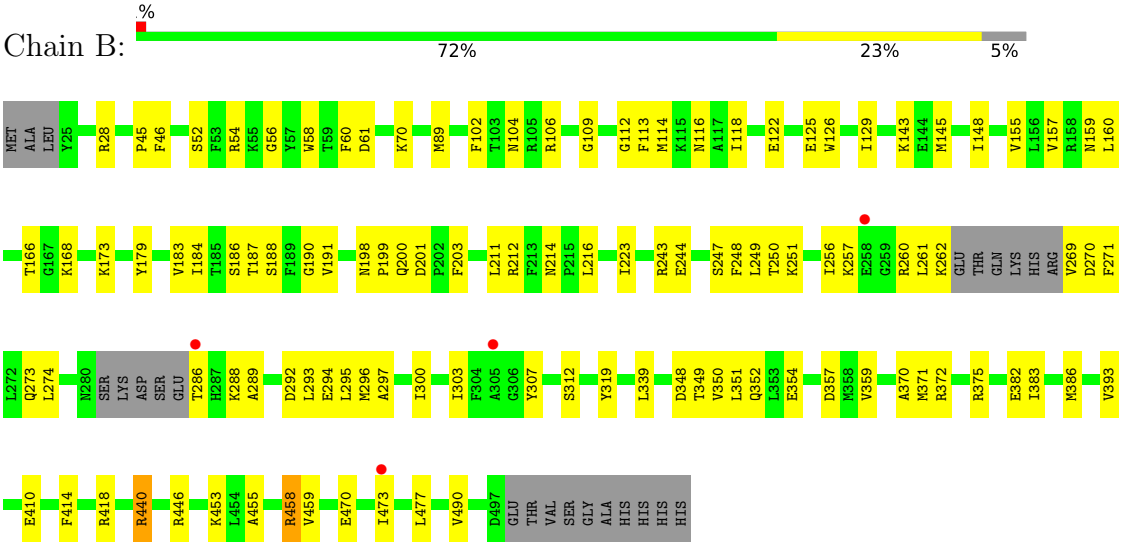
• Molecule 1: Cytochrome P450 3A7

Chain A:



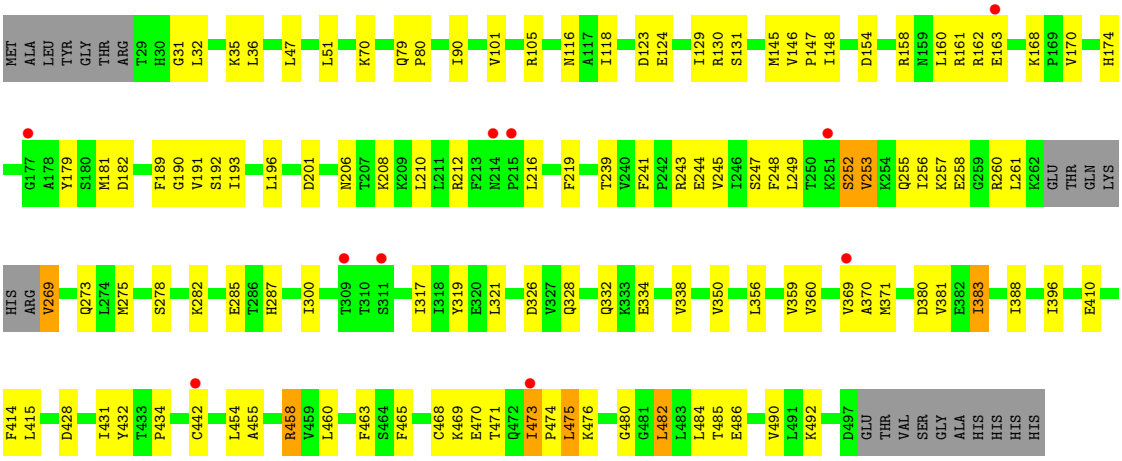
• Molecule 1: Cytochrome P450 3A7

Chain B:



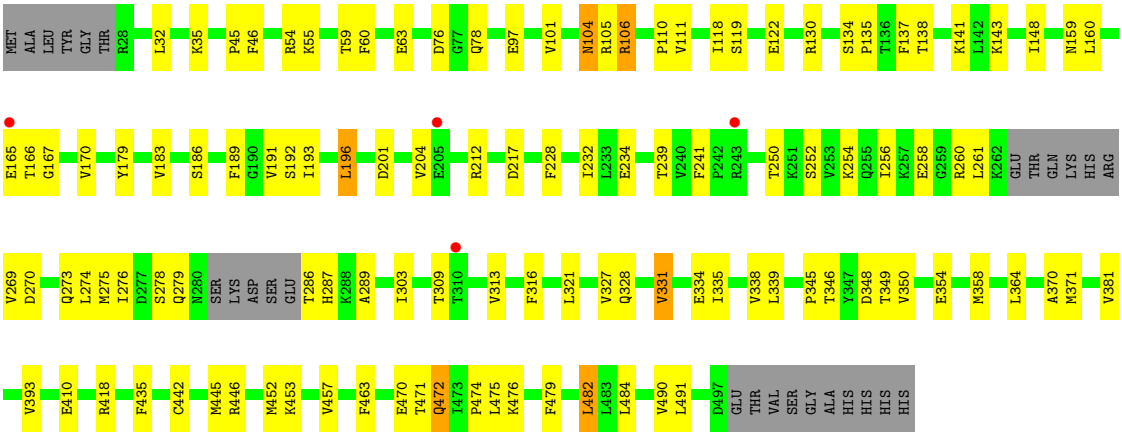
• Molecule 1: Cytochrome P450 3A7

Chain C:



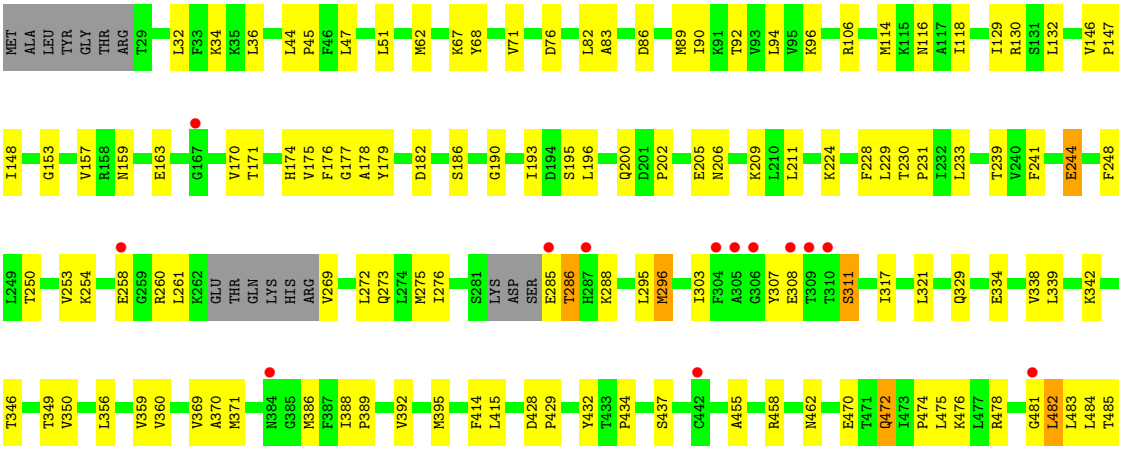
• Molecule 1: Cytochrome P450 3A7

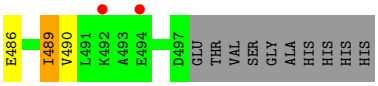
Chain D:



• Molecule 1: Cytochrome P450 3A7

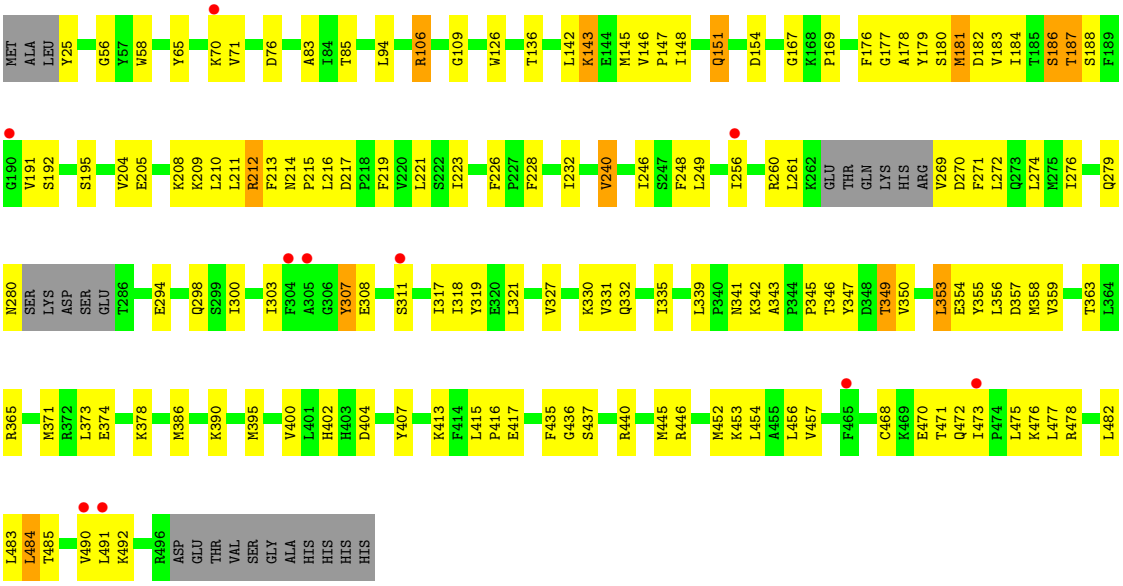
Chain E:





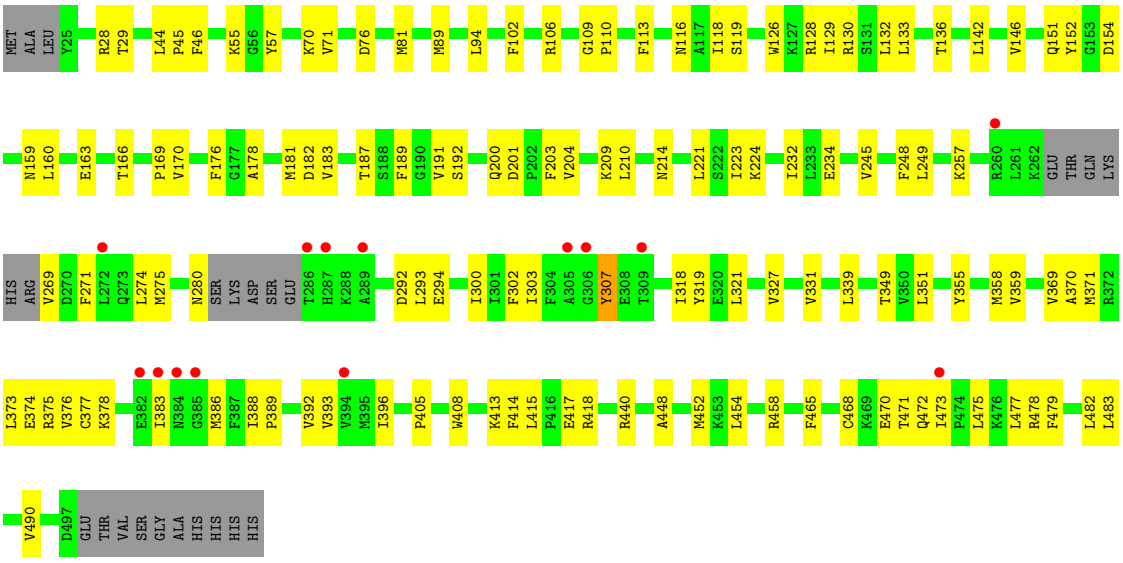
• Molecule 1: Cytochrome P450 3A7

Chain F:



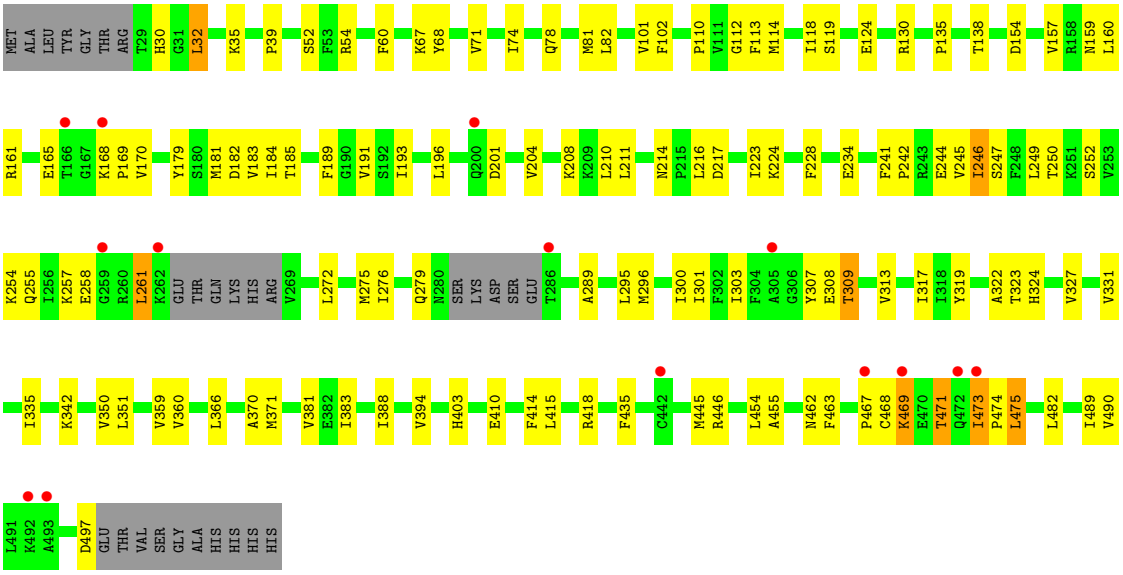
• Molecule 1: Cytochrome P450 3A7

Chain G:



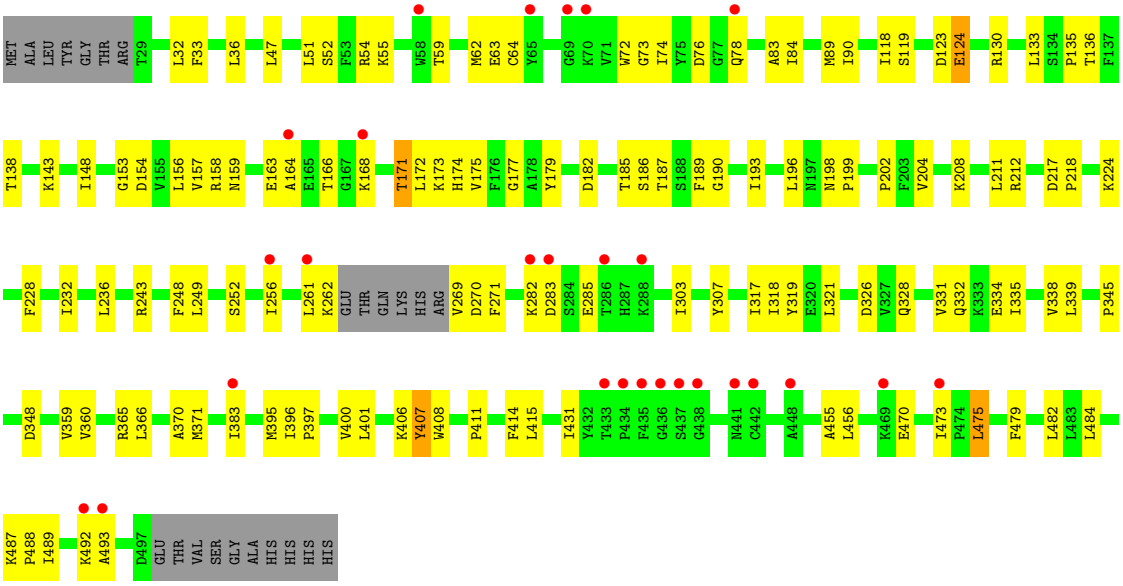
• Molecule 1: Cytochrome P450 3A7

Chain H:



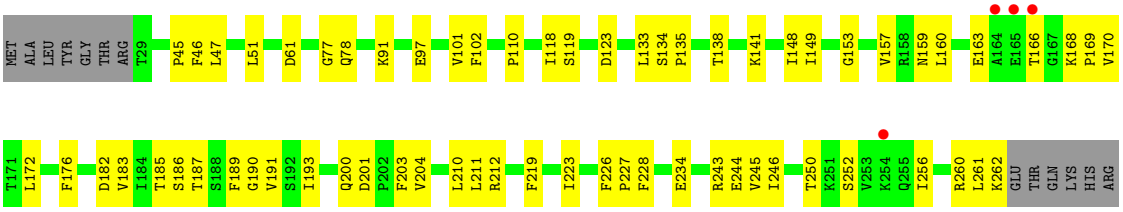
• Molecule 1: Cytochrome P450 3A7

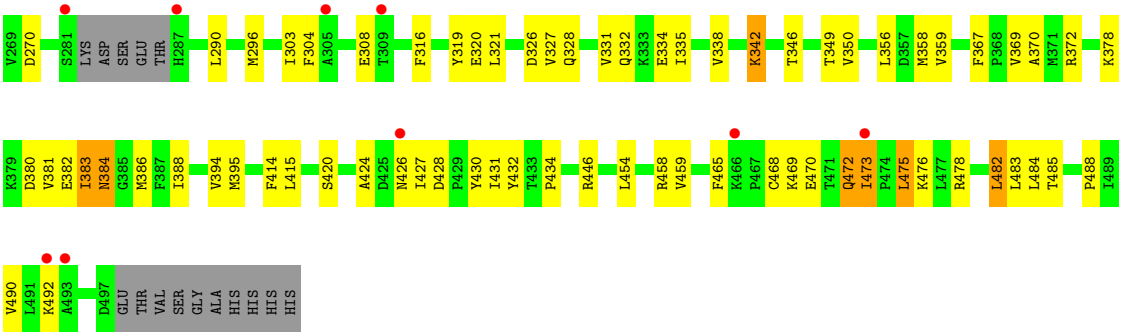
Chain I:



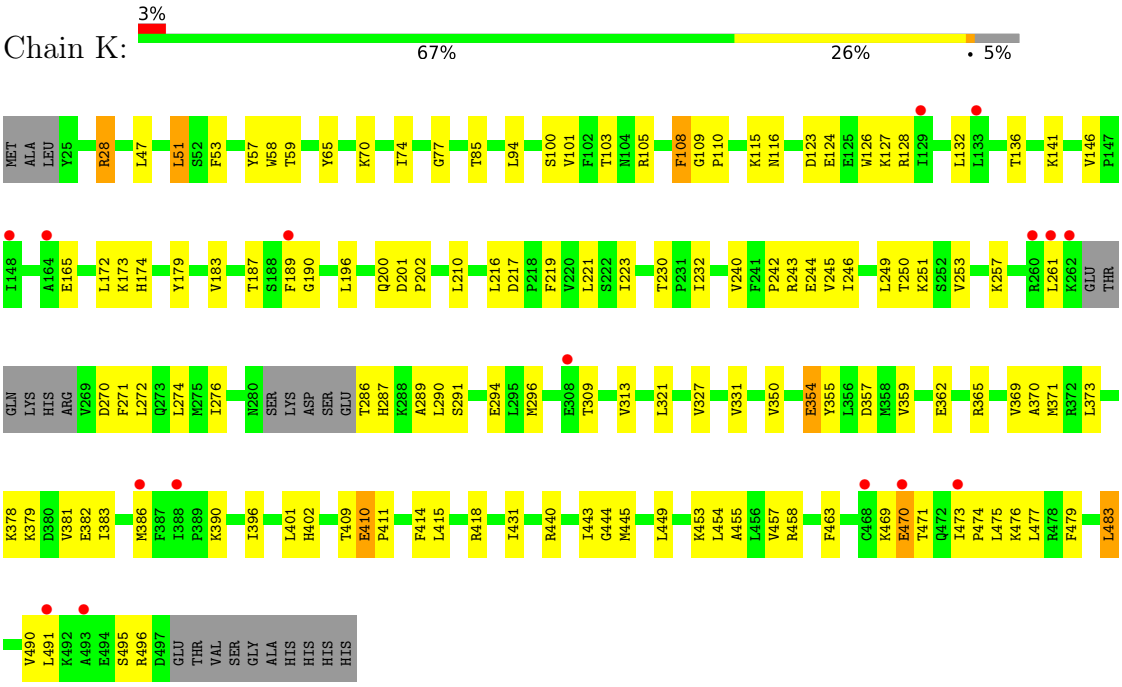
• Molecule 1: Cytochrome P450 3A7

Chain J:

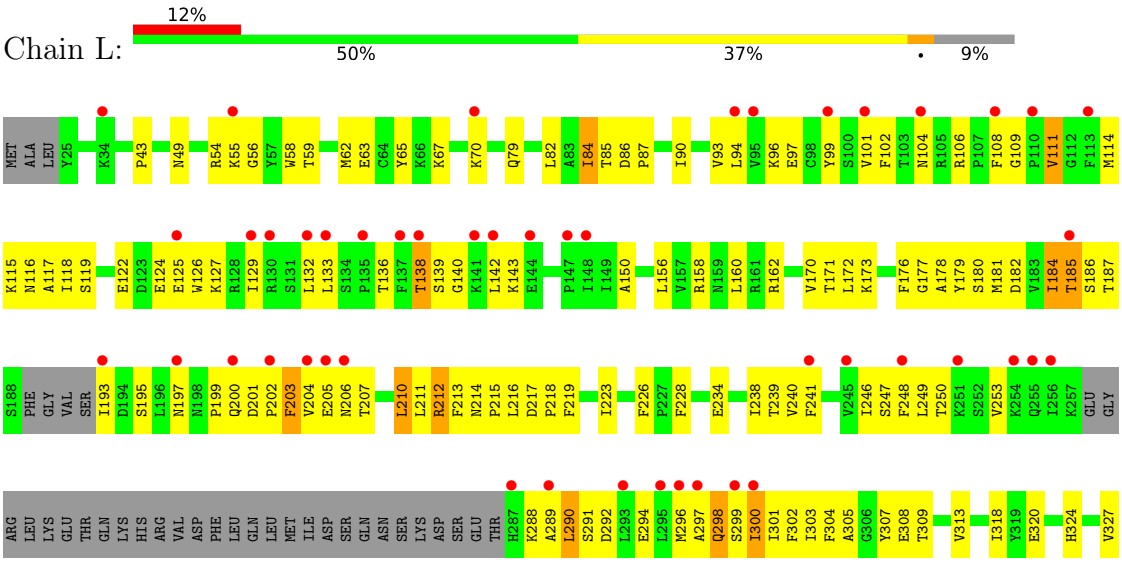


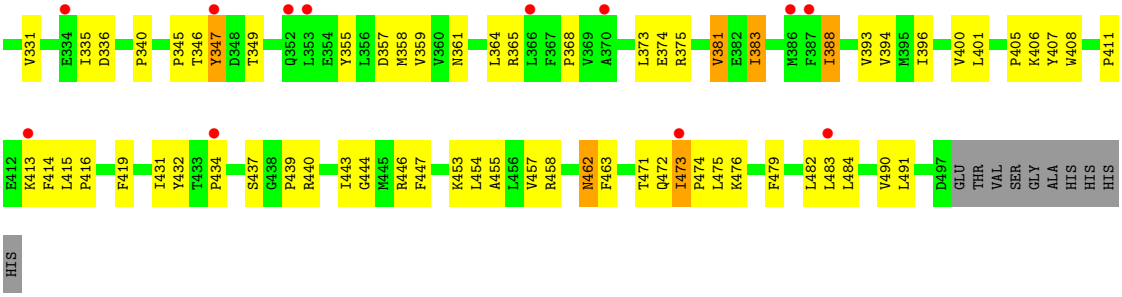


• Molecule 1: Cytochrome P450 3A7



• Molecule 1: Cytochrome P450 3A7




V331
E334
I335
D336
P340
P345
T346
Y347
D348
T349
Q352
L353
E354
Y355
L356
D357
M358
V359
V360
N361
L364
R365
L366
F367
P368
V369
A370
L373
E374
R375
V381
E382
I383
M386
F387
I388
V393
V394
M395
I396
V400
L401
P405
K406
Y407
W408
P411
E412
K413
F414
L415
P416
F419
I431
Y432
T433
P434
S437
G438
P439
R440
I443
G444
M445
R446
F447
K453
L454
A455
L456
V457
R458
N462
F463
T471
Q472
I473
P474
L475
K476
F479
L482
L483
L484
V490
L491
D497
GLU
THR
VAL
SER
GLY
ALA
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	114.52Å 219.38Å 130.45Å 90.00° 102.17° 90.00°	Depositor
Resolution (Å)	39.94 – 2.60 39.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (39.94-2.60) 98.4 (39.94-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.210 , 0.273 0.210 , 0.273	Depositor DCC
R_{free} test set	1999 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å^2)	68.5	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	91794	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZWY, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.49	0/3892	0.57	0/5274
1	B	0.50	0/3796	0.62	0/5144
1	C	0.50	0/3800	0.60	0/5150
1	D	0.57	0/3772	0.62	0/5111
1	E	0.60	0/3776	0.62	0/5117
1	F	0.55	0/3788	0.61	0/5133
1	G	0.54	0/3796	0.65	0/5144
1	H	0.48	0/3761	0.60	0/5097
1	I	0.56	0/3800	0.65	0/5150
1	J	0.53	0/3760	0.64	0/5095
1	K	0.55	0/3796	0.65	0/5144
1	L	0.65	0/3620	0.78	0/4908
All	All	0.55	0/45357	0.64	0/61467

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3798	3892	3891	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3705	3796	3802	74	0
1	C	3709	3798	3804	88	0
1	D	3682	3771	3783	86	0
1	E	3686	3783	3781	96	0
1	F	3697	3799	3798	124	0
1	G	3705	3798	3803	96	0
1	H	3671	3763	3770	87	0
1	I	3709	3799	3804	106	0
1	J	3670	3771	3768	111	0
1	K	3705	3798	3802	114	0
1	L	3531	3602	3628	200	0
2	A	43	30	30	2	0
2	B	43	30	30	3	0
2	C	43	30	30	4	0
2	D	43	30	30	6	0
2	E	43	30	30	2	0
2	F	43	30	30	4	0
2	G	43	30	30	5	0
2	H	43	30	30	3	0
2	I	43	30	30	3	0
2	J	43	30	30	3	0
2	K	43	30	30	7	0
2	L	43	30	30	5	0
3	A	50	54	0	1	0
3	B	50	54	0	0	0
3	C	100	108	0	0	0
3	D	125	135	0	2	0
3	E	100	108	0	1	0
3	H	75	81	0	1	0
3	I	50	54	0	0	0
3	J	50	54	0	0	0
4	A	5	0	0	0	0
4	B	7	0	0	0	0
4	E	2	0	0	0	0
4	F	4	0	0	0	0
4	G	5	0	0	0	0
4	H	2	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	5	0	0	0	0
All	All	45416	46378	45794	1268	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 14.

All (1268) 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)
1:E:286:THR:HG22	1:G:351:LEU:O	1.40	1.18
1:L:250:THR:HG23	1:L:296:MET:SD	1.84	1.18
1:F:232:ILE:HD11	1:G:232:ILE:HD11	1.15	1.11
1:K:183:VAL:O	1:K:187:THR:HG22	1.54	1.07
1:J:185:THR:HB	1:J:193:ILE:HD11	1.41	1.02
1:F:346:THR:O	1:F:350:VAL:HG23	1.61	1.01
1:G:106:ARG:HD2	1:G:393:VAL:HG21	1.38	0.99
1:J:183:VAL:O	1:J:187:THR:HG22	1.61	0.99
1:L:132:LEU:HD11	1:L:289:ALA:HA	1.44	0.98
1:L:133:LEU:HD11	1:L:298:GLN:HG3	1.47	0.96
1:A:473:ILE:HG22	1:A:474:PRO:HD3	1.47	0.95
1:L:413:LYS:HE2	1:L:415:LEU:HD21	1.51	0.93
1:I:211:LEU:HD21	1:I:303:ILE:HG22	1.51	0.92
1:B:250:THR:HB	1:B:296:MET:HE2	1.51	0.92
1:I:76:ASP:OD2	1:I:224:LYS:HE3	1.71	0.90
1:L:126:TRP:CZ2	1:L:440:ARG:HB2	2.06	0.90
1:L:211:LEU:HD11	1:L:303:ILE:HG22	1.54	0.89
1:L:473:ILE:HG22	1:L:474:PRO:N	1.87	0.89
1:L:290:LEU:HD13	1:L:294:GLU:HB2	1.55	0.88
1:L:127:LYS:O	1:L:127:LYS:NZ	2.07	0.87
1:H:169:PRO:HG3	1:H:468:CYS:SG	2.15	0.86
1:E:369:VAL:HB	1:E:482:LEU:HD11	1.57	0.86
1:C:470:GLU:OE1	1:C:470:GLU:N	2.07	0.85
1:B:183:VAL:O	1:B:187:THR:HG22	1.76	0.84
1:K:250:THR:HG22	1:K:296:MET:HG2	1.57	0.84
1:L:206:ASN:ND2	1:L:248:PHE:CD2	2.45	0.84
1:D:327:VAL:O	1:D:331:VAL:HG23	1.78	0.83
1:L:43:PRO:HA	1:L:49:ASN:OD1	1.77	0.83
1:F:136:THR:HG23	1:F:274:LEU:HB3	1.58	0.83
1:L:126:TRP:CD1	1:L:440:ARG:CZ	2.62	0.82
1:L:126:TRP:CE2	1:L:440:ARG:HD2	2.14	0.82
1:L:298:GLN:O	1:L:301:ILE:HG22	1.80	0.82
1:F:142:LEU:HD12	1:F:142:LEU:O	1.81	0.81
1:G:376:VAL:HG22	1:G:393:VAL:HG22	1.64	0.80
1:L:106:ARG:HE	1:L:393:VAL:HG21	1.47	0.80
1:C:206:ASN:HB3	1:C:245:VAL:HG13	1.63	0.79
1:G:106:ARG:CD	1:G:393:VAL:HG21	2.11	0.79
1:L:471:THR:O	1:L:473:ILE:CD1	2.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:248:PHE:CD2	1:L:249:LEU:HD23	2.18	0.78
1:J:61:ASP:OD2	1:J:372:ARG:CD	2.32	0.77
1:K:174:HIS:NE2	1:K:196:LEU:HD21	2.00	0.77
1:F:136:THR:HG23	1:F:274:LEU:CB	2.13	0.77
1:E:211:LEU:HD21	1:E:303:ILE:HG22	1.65	0.77
1:C:192:SER:O	1:C:193:ILE:HD13	1.86	0.75
1:I:76:ASP:OD2	1:I:224:LYS:CE	2.34	0.75
1:I:359:VAL:HG23	1:I:414:PHE:HZ	1.51	0.75
1:F:452:MET:O	1:F:456:LEU:HD12	1.86	0.75
1:F:180:SER:O	1:F:184:ILE:HG22	1.87	0.75
1:L:401:LEU:HD13	1:L:431:ILE:HA	1.69	0.74
1:L:126:TRP:NE1	1:L:440:ARG:NE	2.35	0.74
1:A:211:LEU:HD21	1:A:303:ILE:HG22	1.67	0.74
1:I:211:LEU:HD13	1:I:307:TYR:CD1	2.23	0.74
1:L:473:ILE:O	1:L:475:LEU:N	2.20	0.74
1:F:232:ILE:HD11	1:G:232:ILE:CD1	2.09	0.73
1:G:136:THR:HG23	1:G:274:LEU:HD12	1.70	0.73
1:D:334:GLU:O	1:D:338:VAL:HG23	1.88	0.73
1:F:167:GLY:O	1:F:492:LYS:HE2	1.88	0.73
1:I:232:ILE:HD13	1:I:232:ILE:N	2.03	0.73
1:I:321:LEU:HD21	1:I:359:VAL:HG21	1.71	0.73
1:G:128:ARG:O	1:G:132:LEU:HG	1.87	0.72
1:H:350:VAL:HG21	1:H:454:LEU:HD23	1.70	0.72
1:L:462:ASN:OD1	1:L:462:ASN:N	2.18	0.72
1:F:339:LEU:HB3	1:F:343:ALA:HB3	1.70	0.72
1:K:189:PHE:CZ	1:K:249:LEU:HD23	2.24	0.72
1:L:132:LEU:HD11	1:L:289:ALA:CA	2.18	0.72
2:L:601:HEM:HBC2	2:L:601:HEM:HMC2	1.70	0.72
1:J:61:ASP:OD2	1:J:372:ARG:HD3	1.90	0.72
2:F:601:HEM:HBC2	2:F:601:HEM:HMC2	1.70	0.71
1:F:331:VAL:HG12	1:F:335:ILE:HD11	1.72	0.71
1:K:58:TRP:NE1	1:K:59:THR:HG23	2.05	0.71
1:L:473:ILE:O	1:L:474:PRO:C	2.24	0.71
1:C:206:ASN:CB	1:C:245:VAL:HG13	2.21	0.70
1:K:179:TYR:CE2	1:K:455:ALA:HB2	2.26	0.70
1:A:473:ILE:HG22	1:A:474:PRO:CD	2.19	0.70
1:H:32:LEU:HD12	1:H:32:LEU:O	1.91	0.70
1:L:143:LYS:HD2	1:L:347:TYR:CD2	2.26	0.70
1:A:473:ILE:CG2	1:A:474:PRO:HD3	2.21	0.70
1:L:86:ASP:OD1	1:L:87:PRO:HD2	1.91	0.70
1:F:478:ARG:HH11	1:F:484:LEU:HD23	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211:LEU:HD21	1:F:303:ILE:HG22	1.73	0.70
1:F:214:ASN:HB2	1:F:215:PRO:HD2	1.74	0.70
1:L:250:THR:HG23	1:L:296:MET:CE	2.21	0.70
1:I:47:LEU:HD13	1:I:51:LEU:HD11	1.74	0.69
1:B:106:ARG:HD3	1:B:393:VAL:HG21	1.75	0.69
2:L:601:HEM:HBB2	2:L:601:HEM:HMB2	1.73	0.69
1:F:106:ARG:HD3	1:F:374:GLU:OE2	1.93	0.69
1:F:232:ILE:HD12	1:F:232:ILE:H	1.58	0.69
1:K:101:VAL:HG11	1:K:381:VAL:HG11	1.75	0.69
1:K:132:LEU:HD13	1:K:290:LEU:HD22	1.74	0.69
1:B:250:THR:CB	1:B:296:MET:HE2	2.21	0.69
1:L:99:TYR:HE2	1:L:127:LYS:HD3	1.57	0.69
1:C:369:VAL:HB	1:C:482:LEU:HD11	1.74	0.68
1:A:169:PRO:HG2	1:A:470:GLU:OE1	1.92	0.68
1:D:189:PHE:CE2	1:D:303:ILE:HD11	2.27	0.68
1:F:331:VAL:O	1:F:335:ILE:HD12	1.93	0.68
1:E:470:GLU:HB2	1:E:490:VAL:HG21	1.75	0.68
1:G:70:LYS:HG2	1:G:71:VAL:HG23	1.74	0.68
1:J:185:THR:HB	1:J:193:ILE:CD1	2.22	0.67
1:L:215:PRO:C	1:L:216:LEU:HD12	2.14	0.67
2:G:601:HEM:HBC2	2:G:601:HEM:HMC2	1.77	0.67
1:D:76:ASP:OD2	1:D:106:ARG:NH2	2.27	0.67
1:L:126:TRP:CD1	1:L:440:ARG:NE	2.62	0.67
1:L:248:PHE:CE2	1:L:249:LEU:HD23	2.29	0.67
1:B:270:ASP:O	1:B:274:LEU:HD12	1.94	0.67
1:B:350:VAL:HG13	1:B:453:LYS:HD3	1.75	0.67
1:K:51:LEU:N	1:K:51:LEU:HD23	2.09	0.67
1:I:269:VAL:O	1:I:269:VAL:HG22	1.94	0.67
1:J:61:ASP:OD2	1:J:372:ARG:HD2	1.95	0.67
1:B:250:THR:HB	1:B:296:MET:CE	2.23	0.67
1:F:371:MET:SD	1:F:483:LEU:HD13	2.35	0.66
1:L:216:LEU:HD12	1:L:216:LEU:N	2.10	0.66
1:D:286:THR:HG23	1:D:287:HIS:H	1.59	0.66
1:I:32:LEU:HD11	1:I:36:LEU:HD11	1.76	0.66
1:B:212:ARG:HD2	1:I:212:ARG:HD3	1.78	0.66
1:L:179:TYR:CZ	1:L:455:ALA:HB2	2.31	0.66
1:I:32:LEU:HD11	1:I:36:LEU:CD1	2.26	0.66
1:J:372:ARG:HD2	1:J:395:MET:SD	2.36	0.66
1:I:135:PRO:O	1:I:138:THR:HG23	1.95	0.66
1:I:401:LEU:HD13	1:I:431:ILE:HD13	1.78	0.65
1:B:350:VAL:HG13	1:B:453:LYS:CD	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:250:THR:HG22	1:K:296:MET:CG	2.27	0.65
1:J:472:GLN:O	1:J:472:GLN:HG2	1.96	0.65
1:D:165:GLU:O	1:D:167:GLY:N	2.30	0.65
1:B:269:VAL:O	1:B:269:VAL:HG22	1.97	0.65
1:E:286:THR:CG2	1:G:351:LEU:O	2.33	0.64
1:B:211:LEU:HD21	1:B:303:ILE:HG22	1.79	0.64
2:K:601:HEM:HBB2	2:K:601:HEM:HMB2	1.80	0.64
1:C:118:ILE:HD11	1:C:130:ARG:HD2	1.79	0.64
1:D:159:ASN:HB3	1:D:196:LEU:HD13	1.80	0.64
1:L:211:LEU:HD11	1:L:303:ILE:CG2	2.26	0.64
1:J:182:ASP:O	1:J:186:SER:HB2	1.97	0.64
1:D:165:GLU:C	1:D:167:GLY:H	2.01	0.64
1:J:334:GLU:O	1:J:338:VAL:HG23	1.97	0.64
1:D:453:LYS:O	1:D:457:VAL:HG23	1.97	0.64
1:H:32:LEU:HD12	1:H:32:LEU:C	2.18	0.64
1:L:359:VAL:HG13	1:L:414:PHE:HZ	1.63	0.64
1:L:43:PRO:CA	1:L:49:ASN:OD1	2.47	0.63
1:I:179:TYR:CZ	1:I:455:ALA:HB2	2.32	0.63
1:F:186:SER:HB3	1:F:191:VAL:O	1.97	0.63
1:L:210:LEU:HD21	1:L:304:PHE:CE2	2.33	0.63
1:C:105:ARG:NH2	2:C:601:HEM:O2D	2.31	0.63
1:F:353:LEU:HD23	1:F:356:LEU:HD23	1.81	0.63
1:H:169:PRO:CG	1:H:468:CYS:SG	2.87	0.63
1:J:172:LEU:HD12	1:J:176:PHE:CE2	2.34	0.63
1:A:183:VAL:O	1:A:187:THR:HG22	1.99	0.63
1:L:327:VAL:O	1:L:331:VAL:HG23	1.99	0.62
1:F:415:LEU:N	1:F:415:LEU:HD22	2.13	0.62
1:G:232:ILE:H	1:G:232:ILE:HD12	1.64	0.62
1:G:248:PHE:HD2	1:G:249:LEU:HD12	1.63	0.62
1:E:389:PRO:O	1:E:392:VAL:HG22	1.99	0.62
1:I:185:THR:HB	1:I:193:ILE:CD1	2.29	0.62
1:L:104:ASN:HD22	1:L:122:GLU:HB2	1.64	0.62
1:K:409:THR:O	1:K:409:THR:HG23	2.00	0.62
1:L:357:ASP:OD1	1:L:453:LYS:HD3	1.99	0.62
1:H:468:CYS:N	1:H:471:THR:HG21	2.13	0.62
1:G:28:ARG:HG3	1:G:29:THR:HG23	1.80	0.62
1:K:109:GLY:HA2	1:K:223:ILE:HG21	1.82	0.62
1:L:90:ILE:HG23	1:L:396:ILE:HG12	1.82	0.62
1:A:210:LEU:HD21	1:A:300:ILE:HG23	1.81	0.61
1:J:201:ASP:HB3	1:J:204:VAL:HG23	1.82	0.61
1:J:321:LEU:HD21	1:J:359:VAL:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ILE:O	1:A:260:ARG:HB2	2.01	0.61
2:D:601:HEM:HBB2	2:D:601:HEM:HMB2	1.81	0.61
1:C:475:LEU:HD21	1:C:485:THR:CG2	2.30	0.61
1:I:189:PHE:CZ	1:I:249:LEU:HD23	2.35	0.61
1:A:467:PRO:HB3	1:A:471:THR:HG21	1.82	0.61
1:C:475:LEU:HD21	1:C:485:THR:HG21	1.81	0.61
1:J:118:ILE:HG23	1:J:119:SER:N	2.15	0.61
1:L:239:THR:HG23	1:L:241:PHE:O	2.00	0.61
1:E:178:ALA:HB1	1:E:195:SER:HB2	1.81	0.61
1:G:189:PHE:CD2	1:G:203:PHE:HE2	2.18	0.61
1:L:214:ASN:OD1	1:L:215:PRO:HD2	2.00	0.61
1:H:383:ILE:HD11	1:H:388:ILE:HD11	1.83	0.61
1:J:190:GLY:HA3	1:J:260:ARG:NH2	2.16	0.61
1:L:126:TRP:CE2	1:L:440:ARG:CD	2.84	0.60
1:B:212:ARG:CD	1:I:212:ARG:HD3	2.30	0.60
2:B:601:HEM:HMC2	2:B:601:HEM:HBC2	1.81	0.60
1:H:250:THR:HG22	1:H:296:MET:HG2	1.83	0.60
1:K:53:PHE:CD2	1:K:57:TYR:HE1	2.19	0.60
1:C:206:ASN:HB3	1:C:245:VAL:CG1	2.31	0.60
1:E:71:VAL:HG21	1:E:386:MET:HE3	1.82	0.60
1:K:58:TRP:CZ2	1:K:477:LEU:HB2	2.36	0.60
1:L:94:LEU:HD13	1:L:437:SER:HB3	1.82	0.60
1:C:282:LYS:O	1:C:285:GLU:HB3	2.02	0.60
1:L:471:THR:O	1:L:473:ILE:HD12	2.00	0.60
1:F:142:LEU:HD12	1:F:142:LEU:C	2.20	0.60
1:L:102:PHE:HE2	1:L:394:VAL:HG21	1.65	0.60
1:E:478:ARG:NH1	1:E:484:LEU:HD12	2.17	0.60
1:J:191:VAL:HG23	1:J:191:VAL:O	2.01	0.60
2:J:601:HEM:HMB2	2:J:601:HEM:HBB2	1.84	0.60
1:H:210:LEU:HD21	1:H:300:ILE:HG23	1.83	0.60
1:L:143:LYS:HD2	1:L:347:TYR:CE2	2.37	0.60
1:G:136:THR:HG23	1:G:274:LEU:CD1	2.31	0.60
1:G:359:VAL:HG13	1:G:414:PHE:HZ	1.66	0.60
1:C:163:GLU:OE1	1:K:200:GLN:NE2	2.35	0.60
1:E:229:LEU:CD2	1:E:233:LEU:HD11	2.32	0.60
1:L:160:LEU:HD23	1:L:463:PHE:CE2	2.37	0.60
1:D:105:ARG:NH2	2:D:601:HEM:O2D	2.35	0.59
1:G:126:TRP:CZ2	1:G:440:ARG:HG3	2.38	0.59
1:D:232:ILE:HD12	1:D:232:ILE:H	1.67	0.59
1:J:383:ILE:HD13	1:J:388:ILE:HD12	1.84	0.59
1:L:172:LEU:HD11	1:L:491:LEU:HD12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:185:THR:CB	1:J:193:ILE:HD11	2.23	0.59
2:C:601:HEM:HBB2	2:C:601:HEM:HMB2	1.83	0.59
1:D:111:VAL:O	1:D:234:GLU:OE2	2.20	0.59
1:F:126:TRP:CZ2	1:F:440:ARG:HD2	2.37	0.59
1:L:253:VAL:HG21	1:L:296:MET:HG2	1.84	0.59
1:L:345:PRO:HD2	1:L:458:ARG:CZ	2.32	0.59
2:H:601:HEM:HMB1	2:H:601:HEM:HBB2	1.83	0.59
1:L:160:LEU:HD23	1:L:463:PHE:CD2	2.38	0.59
1:L:199:PRO:HA	1:L:204:VAL:HG11	1.85	0.59
1:F:332:GLN:HA	1:F:335:ILE:CD1	2.33	0.59
1:F:477:LEU:HA	1:F:484:LEU:O	2.03	0.59
1:I:282:LYS:O	1:I:285:GLU:HB2	2.03	0.59
1:J:211:LEU:HD21	1:J:303:ILE:HG22	1.85	0.59
1:L:313:VAL:HG11	1:L:364:LEU:HD21	1.85	0.59
1:F:269:VAL:O	1:F:269:VAL:HG22	2.03	0.59
1:F:350:VAL:HG21	1:F:454:LEU:CD2	2.33	0.59
1:J:252:SER:O	1:J:256:ILE:HD12	2.03	0.59
1:L:82:LEU:HD23	1:L:388:ILE:HD11	1.85	0.59
1:B:261:LEU:O	1:B:261:LEU:HD12	2.03	0.58
1:B:350:VAL:CG1	1:B:453:LYS:HD2	2.33	0.58
1:F:350:VAL:HG12	1:F:453:LYS:HE3	1.86	0.58
1:G:383:ILE:HD11	1:G:388:ILE:HD12	1.84	0.58
1:I:164:ALA:HB2	1:I:493:ALA:HB3	1.85	0.58
1:D:435:PHE:CG	1:D:445:MET:HG3	2.39	0.58
1:A:144:GLU:HB3	1:A:269:VAL:HG11	1.85	0.58
1:F:145:MET:CE	1:F:270:ASP:HA	2.33	0.58
1:C:31:GLY:O	1:C:35:LYS:HB3	2.03	0.58
1:G:159:ASN:O	1:G:163:GLU:HG2	2.03	0.58
1:L:401:LEU:HB3	1:L:431:ILE:HG23	1.84	0.58
1:D:106:ARG:NH2	3:D:602:ZWY:O22	2.37	0.58
1:D:118:ILE:HD11	1:D:130:ARG:HD2	1.85	0.58
1:D:316:PHE:CE2	1:D:475:LEU:HD21	2.39	0.58
2:I:601:HEM:HMB2	2:I:601:HEM:HBB2	1.84	0.58
1:J:169:PRO:HB2	1:J:490:VAL:HG12	1.86	0.58
1:K:355:TYR:O	1:K:359:VAL:HG23	2.04	0.58
1:E:269:VAL:O	1:E:269:VAL:HG12	2.02	0.58
1:J:369:VAL:HA	1:J:483:LEU:HD21	1.85	0.58
1:K:242:PRO:HB2	1:K:245:VAL:HB	1.85	0.58
1:L:471:THR:O	1:L:473:ILE:HD13	2.04	0.58
1:F:210:LEU:HD11	1:F:246:ILE:HD11	1.85	0.58
1:F:269:VAL:O	1:F:269:VAL:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:101:VAL:CG1	1:K:381:VAL:HG11	2.34	0.58
1:D:191:VAL:HG12	1:D:191:VAL:O	2.02	0.58
1:E:132:LEU:HD11	1:E:288:LYS:O	2.04	0.58
1:I:492:LYS:HD2	1:I:493:ALA:N	2.19	0.58
1:E:171:THR:HG23	1:E:490:VAL:HG12	1.86	0.57
2:K:601:HEM:HMC2	2:K:601:HEM:HBC2	1.86	0.57
1:C:468:CYS:HB3	1:C:492:LYS:HG3	1.85	0.57
1:A:469:LYS:HE2	1:A:469:LYS:HA	1.86	0.57
1:D:137:PHE:O	1:D:446:ARG:NH2	2.37	0.57
1:F:204:VAL:HG12	1:F:208:LYS:HD2	1.85	0.57
1:K:362:GLU:HG3	1:K:414:PHE:CD1	2.38	0.57
1:L:290:LEU:HD13	1:L:294:GLU:CB	2.32	0.57
1:B:109:GLY:HA2	1:B:223:ILE:HG21	1.86	0.57
1:C:334:GLU:O	1:C:338:VAL:HG23	2.03	0.57
1:D:260:ARG:NH2	1:D:270:ASP:OD2	2.36	0.57
1:E:253:VAL:HB	1:E:296:MET:HE2	1.85	0.57
1:I:148:ILE:O	1:I:148:ILE:HG22	2.03	0.57
1:L:216:LEU:N	1:L:216:LEU:CD1	2.67	0.57
1:G:142:LEU:HD23	1:G:142:LEU:O	2.04	0.57
1:J:250:THR:HG22	1:J:296:MET:HG2	1.86	0.57
1:L:361:ASN:HB3	1:L:419:PHE:CD1	2.40	0.57
1:H:468:CYS:N	1:H:471:THR:CG2	2.68	0.57
1:C:189:PHE:CE2	1:C:249:LEU:HD22	2.39	0.57
1:F:350:VAL:HG21	1:F:454:LEU:HD23	1.86	0.57
1:G:189:PHE:HD2	1:G:203:PHE:HE2	1.51	0.57
1:K:105:ARG:NH1	2:K:601:HEM:O2A	2.37	0.57
1:J:326:ASP:OD2	1:J:326:ASP:N	2.38	0.57
1:J:468:CYS:CB	1:J:492:LYS:HE2	2.34	0.57
1:L:111:VAL:O	1:L:234:GLU:OE2	2.23	0.57
1:L:211:LEU:O	1:L:213:PHE:N	2.37	0.57
1:D:111:VAL:O	1:D:234:GLU:CD	2.44	0.57
1:I:232:ILE:O	1:I:236:LEU:HD23	2.05	0.57
1:K:257:LYS:HG2	1:K:276:ILE:HD11	1.87	0.57
1:L:86:ASP:O	1:L:90:ILE:HG13	2.05	0.57
1:I:118:ILE:HD11	1:I:130:ARG:HD2	1.86	0.56
1:K:53:PHE:HZ	1:K:74:ILE:HD12	1.70	0.56
1:L:211:LEU:C	1:L:213:PHE:H	2.08	0.56
1:K:243:ARG:CG	1:K:244:GLU:OE1	2.53	0.56
1:C:239:THR:HG22	1:C:241:PHE:H	1.70	0.56
1:G:89:MET:SD	1:G:386:MET:CE	2.94	0.56
1:K:146:VAL:HG13	1:K:454:LEU:HD11	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:70:LYS:HB2	1:L:85:THR:OG1	2.05	0.56
1:L:150:ALA:HB1	1:L:458:ARG:HH11	1.69	0.56
1:L:313:VAL:HG11	1:L:364:LEU:CD2	2.35	0.56
1:D:111:VAL:O	1:D:234:GLU:OE1	2.23	0.56
1:H:181:MET:HG2	1:H:185:THR:OG1	2.05	0.56
1:I:185:THR:HB	1:I:193:ILE:HD11	1.87	0.56
1:L:388:ILE:O	1:L:388:ILE:HG22	2.04	0.56
1:F:332:GLN:HA	1:F:335:ILE:HD13	1.88	0.56
1:E:157:VAL:HG11	1:E:462:ASN:HD22	1.71	0.56
1:E:369:VAL:HB	1:E:482:LEU:CD1	2.34	0.56
1:H:275:MET:HB3	1:H:295:LEU:HD12	1.87	0.56
1:J:47:LEU:HD13	1:J:51:LEU:HD11	1.88	0.56
1:L:58:TRP:O	1:L:62:MET:HG2	2.06	0.56
1:A:413:LYS:O	1:A:418:ARG:NH2	2.38	0.56
1:F:345:PRO:HG3	1:F:457:VAL:HG11	1.88	0.56
1:J:78:GLN:HE22	1:J:227:PRO:HG2	1.70	0.56
1:J:342:LYS:HD3	1:J:342:LYS:N	2.21	0.56
1:K:475:LEU:HD12	1:K:476:LYS:N	2.19	0.56
1:L:126:TRP:CZ2	1:L:440:ARG:CB	2.85	0.56
1:L:201:ASP:OD1	1:L:203:PHE:HB2	2.06	0.56
1:C:359:VAL:HG23	1:C:414:PHE:HZ	1.70	0.55
1:E:153:GLY:O	1:E:157:VAL:HG23	2.05	0.55
1:F:216:LEU:C	1:F:221:LEU:HD11	2.26	0.55
1:A:345:PRO:HD2	1:A:458:ARG:HD3	1.88	0.55
1:C:321:LEU:HD21	1:C:359:VAL:HG21	1.88	0.55
1:D:54:ARG:HD2	1:D:479:PHE:CE2	2.42	0.55
1:D:286:THR:HG23	1:D:287:HIS:N	2.22	0.55
1:K:496:ARG:O	1:L:158:ARG:NH1	2.39	0.55
1:C:319:TYR:OH	1:C:473:ILE:O	2.24	0.55
1:K:246:ILE:O	1:K:250:THR:HG23	2.05	0.55
1:L:126:TRP:CZ2	1:L:440:ARG:HD2	2.42	0.55
1:A:345:PRO:CD	1:A:458:ARG:HD3	2.37	0.55
1:C:275:MET:O	1:C:278:SER:OG	2.23	0.55
1:E:157:VAL:HG11	1:E:462:ASN:ND2	2.22	0.55
1:G:327:VAL:O	1:G:331:VAL:HG23	2.07	0.55
1:L:99:TYR:CE2	1:L:127:LYS:HD3	2.39	0.55
1:L:132:LEU:HD11	1:L:288:LYS:O	2.07	0.55
1:D:104:ASN:OD1	1:D:122:GLU:HA	2.07	0.55
1:D:148:ILE:HD12	1:D:269:VAL:HG12	1.87	0.55
1:K:200:GLN:OE1	1:K:200:GLN:N	2.38	0.55
1:F:330:LYS:HD2	1:F:355:TYR:CZ	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:370:ALA:O	1:K:371:MET:HB2	2.07	0.55
1:C:245:VAL:HG12	1:C:245:VAL:O	2.08	0.54
1:F:186:SER:CB	1:F:191:VAL:O	2.55	0.54
1:B:70:LYS:HD2	1:B:70:LYS:N	2.21	0.54
1:D:370:ALA:O	1:D:371:MET:HB2	2.06	0.54
1:H:181:MET:O	1:H:182:ASP:C	2.45	0.54
1:H:189:PHE:CZ	1:H:249:LEU:HD22	2.43	0.54
1:K:354:GLU:N	1:K:354:GLU:OE1	2.41	0.54
1:L:473:ILE:CG2	1:L:474:PRO:N	2.59	0.54
1:I:172:LEU:HD12	1:I:489:ILE:CG2	2.37	0.54
1:C:168:LYS:HE2	1:C:168:LYS:HA	1.90	0.54
1:H:414:PHE:O	1:H:415:LEU:HD23	2.07	0.54
1:K:471:THR:OG1	1:K:490:VAL:O	2.22	0.54
1:L:84:ILE:HG12	1:L:84:ILE:O	2.06	0.54
1:B:114:MET:HE3	1:B:300:ILE:HG21	1.89	0.54
1:C:256:ILE:HD12	1:C:256:ILE:H	1.72	0.54
1:H:191:VAL:HG23	1:H:193:ILE:HG23	1.88	0.54
1:F:221:LEU:HD12	1:F:221:LEU:N	2.23	0.54
1:F:471:THR:OG1	1:F:491:LEU:HD23	2.08	0.54
1:D:130:ARG:O	1:D:134:SER:OG	2.24	0.54
1:G:113:PHE:O	1:G:116:ASN:ND2	2.41	0.54
1:J:342:LYS:N	1:J:342:LYS:CD	2.70	0.54
1:G:275:MET:CE	1:G:302:PHE:HE2	2.21	0.54
1:B:102:PHE:HB3	1:B:375:ARG:HB3	1.89	0.54
1:D:435:PHE:HB3	1:D:442:CYS:HB3	1.90	0.54
1:H:102:PHE:CE2	1:H:394:VAL:HG21	2.42	0.54
1:L:182:ASP:OD1	1:L:195:SER:HB3	2.08	0.54
1:E:163:GLU:HB3	1:E:170:VAL:HG12	1.88	0.54
1:L:241:PHE:HE2	1:L:304:PHE:CZ	2.25	0.54
1:D:338:VAL:HG12	1:D:349:THR:HG22	1.89	0.53
1:E:346:THR:O	1:E:350:VAL:HG23	2.07	0.53
1:L:62:MET:SD	1:L:400:VAL:HG22	2.48	0.53
1:J:458:ARG:HH11	1:J:458:ARG:HG2	1.73	0.53
1:L:109:GLY:HA2	1:L:223:ILE:HG21	1.91	0.53
1:L:179:TYR:O	1:L:182:ASP:N	2.41	0.53
2:A:601:HEM:HMB2	2:A:601:HEM:HBB2	1.90	0.53
1:I:370:ALA:O	1:I:371:MET:HB2	2.07	0.53
1:L:210:LEU:CD2	1:L:304:PHE:CZ	2.92	0.53
1:E:356:LEU:O	1:E:359:VAL:HG12	2.08	0.53
1:J:133:LEU:HD11	1:J:290:LEU:HD11	1.89	0.53
1:J:468:CYS:HB3	1:J:492:LYS:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:ILE:HD12	1:F:148:ILE:H	1.73	0.53
1:F:317:ILE:HG13	1:F:363:THR:HG21	1.91	0.53
1:G:106:ARG:CG	1:G:393:VAL:HG21	2.38	0.53
1:I:64:CYS:HB3	1:I:72:TRP:CD1	2.43	0.53
1:J:350:VAL:HG11	1:J:454:LEU:HD23	1.89	0.53
1:L:86:ASP:OD1	1:L:87:PRO:CD	2.56	0.53
1:L:320:GLU:O	1:L:324:HIS:HB2	2.09	0.53
1:B:200:GLN:O	1:B:201:ASP:C	2.47	0.53
1:K:371:MET:SD	1:K:483:LEU:HD13	2.48	0.53
1:I:407:TYR:CD1	1:I:407:TYR:N	2.76	0.53
1:K:243:ARG:HG2	1:K:244:GLU:OE1	2.08	0.53
2:L:601:HEM:HBB2	2:L:601:HEM:CMB	2.39	0.53
1:D:261:LEU:HD12	1:D:261:LEU:O	2.09	0.53
1:K:189:PHE:CZ	1:K:249:LEU:CD2	2.92	0.53
1:A:172:LEU:HD11	1:A:491:LEU:HD12	1.91	0.53
1:A:470:GLU:O	1:A:471:THR:C	2.45	0.53
1:D:275:MET:O	1:D:278:SER:OG	2.26	0.53
1:E:186:SER:O	1:E:190:GLY:N	2.36	0.53
1:E:470:GLU:CB	1:E:490:VAL:HG21	2.37	0.53
1:H:39:PRO:HB2	1:H:68:TYR:CD2	2.44	0.53
1:H:118:ILE:HD11	1:H:130:ARG:HD2	1.91	0.53
1:K:475:LEU:HD12	1:K:476:LYS:H	1.74	0.53
1:L:108:PHE:O	1:L:108:PHE:CD1	2.62	0.53
1:L:443:ILE:HG23	1:L:444:GLY:N	2.24	0.53
1:E:92:THR:HA	1:E:96:LYS:HD2	1.91	0.53
1:E:334:GLU:O	1:E:338:VAL:HG23	2.08	0.53
1:H:189:PHE:CE2	1:H:303:ILE:HD11	2.44	0.53
1:J:458:ARG:HG2	1:J:458:ARG:NH1	2.23	0.52
1:L:90:ILE:HG22	1:L:94:LEU:HD11	1.92	0.52
1:A:473:ILE:CG2	1:A:474:PRO:CD	2.86	0.52
1:C:31:GLY:O	1:C:35:LYS:CB	2.57	0.52
1:E:432:TYR:CZ	1:E:434:PRO:HG3	2.44	0.52
1:J:482:LEU:O	1:J:483:LEU:C	2.48	0.52
1:K:253:VAL:HB	1:K:296:MET:HE1	1.91	0.52
1:L:97:GLU:O	1:L:102:PHE:HD1	1.92	0.52
1:C:332:GLN:NE2	1:C:460:LEU:O	2.41	0.52
1:E:159:ASN:HB3	1:E:196:LEU:HD13	1.90	0.52
1:F:187:THR:HG23	1:F:271:PHE:CD2	2.44	0.52
1:G:152:TYR:OH	1:G:192:SER:CB	2.57	0.52
1:I:179:TYR:CE2	1:I:455:ALA:HB2	2.45	0.52
1:J:319:TYR:OH	1:J:473:ILE:O	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:TYR:OH	1:B:473:ILE:O	2.20	0.52
1:D:435:PHE:CD1	1:D:445:MET:HG3	2.45	0.52
1:F:109:GLY:HA2	1:F:223:ILE:HG21	1.92	0.52
1:F:210:LEU:HD21	1:F:300:ILE:HG23	1.91	0.52
1:H:169:PRO:HB3	1:H:468:CYS:SG	2.50	0.52
1:B:157:VAL:CG2	1:B:458:ARG:HG3	2.39	0.52
1:C:476:LYS:HB2	1:C:486:GLU:HG3	1.92	0.52
1:D:239:THR:HG23	1:D:241:PHE:O	2.09	0.52
1:E:174:HIS:CE1	1:E:196:LEU:HD21	2.44	0.52
1:G:169:PRO:HG3	1:G:470:GLU:OE2	2.09	0.52
1:L:473:ILE:CD1	1:L:473:ILE:N	2.72	0.52
1:E:254:LYS:O	1:E:258:GLU:HG2	2.10	0.52
1:H:319:TYR:OH	1:H:473:ILE:O	2.21	0.52
1:A:473:ILE:CB	1:A:474:PRO:CD	2.88	0.52
1:C:471:THR:OG1	1:C:490:VAL:O	2.26	0.52
1:F:319:TYR:OH	1:F:473:ILE:O	2.27	0.52
1:A:213:PHE:HE1	1:A:240:VAL:HG22	1.75	0.52
1:A:473:ILE:HB	1:A:474:PRO:HD2	1.91	0.52
1:D:170:VAL:HG12	1:D:491:LEU:O	2.10	0.52
1:H:490:VAL:HG23	1:H:490:VAL:O	2.10	0.52
1:C:160:LEU:HD21	1:C:465:PHE:HZ	1.73	0.52
2:F:601:HEM:HBB2	2:F:601:HEM:HMB2	1.90	0.52
1:J:210:LEU:HD21	1:J:304:PHE:CE2	2.45	0.52
1:B:352:GLN:HG2	1:C:474:PRO:HG3	1.92	0.52
1:F:145:MET:HE2	1:F:270:ASP:HA	1.92	0.52
1:C:476:LYS:CB	1:C:486:GLU:HG3	2.39	0.51
1:F:182:ASP:O	1:F:186:SER:OG	2.28	0.51
1:J:319:TYR:CE2	1:J:475:LEU:HD22	2.46	0.51
1:J:359:VAL:HG23	1:J:414:PHE:HZ	1.75	0.51
1:K:327:VAL:O	1:K:331:VAL:HG23	2.09	0.51
1:F:353:LEU:CD1	1:F:353:LEU:N	2.72	0.51
1:L:79:GLN:HG2	1:L:106:ARG:HD3	1.92	0.51
1:L:117:ALA:HB2	1:L:297:ALA:HB1	1.92	0.51
1:I:365:ARG:NH2	1:I:366:LEU:HD21	2.25	0.51
1:K:103:THR:O	1:K:440:ARG:NH1	2.44	0.51
1:K:132:LEU:HB3	1:K:290:LEU:HD21	1.91	0.51
1:K:286:THR:OG1	1:K:287:HIS:N	2.42	0.51
1:L:106:ARG:NE	1:L:393:VAL:HG21	2.21	0.51
1:A:208:LYS:O	1:A:212:ARG:HG3	2.10	0.51
1:E:285:GLU:O	1:E:285:GLU:HG2	2.11	0.51
2:E:601:HEM:HBB2	2:E:601:HEM:HMB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:VAL:O	1:G:187:THR:HG23	2.11	0.51
1:L:309:THR:O	1:L:313:VAL:HG23	2.09	0.51
1:B:470:GLU:HB3	1:B:490:VAL:HG21	1.93	0.51
1:H:160:LEU:HD23	1:H:463:PHE:CE2	2.45	0.51
1:I:59:THR:O	1:I:63:GLU:HG3	2.10	0.51
1:A:109:GLY:HA2	1:A:223:ILE:HG21	1.92	0.51
2:D:601:HEM:HBB2	2:D:601:HEM:CMB	2.41	0.51
1:E:260:ARG:HD3	1:E:273:GLN:OE1	2.10	0.51
1:I:84:ILE:HD12	1:I:89:MET:HG2	1.93	0.51
1:I:182:ASP:O	1:I:186:SER:OG	2.21	0.51
1:L:407:TYR:CG	1:L:431:ILE:HD13	2.46	0.51
1:A:280:ASN:O	1:A:281:SER:OG	2.29	0.51
1:B:187:THR:O	1:B:271:PHE:HB2	2.11	0.51
1:C:206:ASN:ND2	1:C:248:PHE:CG	2.79	0.51
1:C:326:ASP:OD2	1:C:326:ASP:N	2.43	0.51
1:E:308:GLU:HG2	1:E:482:LEU:HB2	1.93	0.51
1:J:163:GLU:O	1:J:168:LYS:HB2	2.10	0.51
1:B:211:LEU:HD13	1:B:307:TYR:CD1	2.45	0.51
1:G:321:LEU:HD21	1:G:359:VAL:HG11	1.91	0.51
1:H:468:CYS:O	1:H:471:THR:HG22	2.11	0.51
1:K:53:PHE:CZ	1:K:74:ILE:HD12	2.45	0.51
1:B:295:LEU:C	1:B:295:LEU:HD23	2.31	0.51
1:F:272:LEU:HG	1:F:276:ILE:HD11	1.92	0.51
1:J:356:LEU:HD12	1:J:359:VAL:CG1	2.41	0.51
1:K:172:LEU:HD11	1:K:491:LEU:HD12	1.92	0.51
1:K:210:LEU:HB2	1:K:245:VAL:HG11	1.92	0.51
1:D:273:GLN:HA	1:D:276:ILE:HG22	1.93	0.51
1:E:94:LEU:HD13	1:E:437:SER:HB3	1.93	0.51
1:I:470:GLU:OE2	1:I:470:GLU:N	2.42	0.51
1:L:58:TRP:NE1	1:L:59:THR:HG23	2.25	0.51
1:L:59:THR:O	1:L:63:GLU:HG3	2.11	0.51
1:D:250:THR:O	1:D:254:LYS:HG2	2.11	0.50
1:D:309:THR:HG22	1:D:482:LEU:HD21	1.93	0.50
1:G:116:ASN:HB3	1:G:294:GLU:HG2	1.92	0.50
1:J:169:PRO:HB2	1:J:490:VAL:CG1	2.41	0.50
1:K:261:LEU:HD12	1:K:261:LEU:O	2.10	0.50
1:B:296:MET:O	1:B:297:ALA:C	2.48	0.50
1:F:471:THR:OG1	1:F:490:VAL:O	2.24	0.50
1:G:189:PHE:CD2	1:G:203:PHE:CE2	2.98	0.50
1:J:328:GLN:O	1:J:332:GLN:HG3	2.10	0.50
1:J:367:PHE:CZ	1:J:475:LEU:HD21	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:488:PRO:O	1:J:490:VAL:HG23	2.11	0.50
1:K:116:ASN:CG	1:K:294:GLU:OE2	2.49	0.50
1:L:126:TRP:CD1	1:L:440:ARG:NH2	2.79	0.50
1:L:473:ILE:HG22	1:L:474:PRO:CD	2.39	0.50
1:D:313:VAL:HG21	1:D:364:LEU:HD21	1.93	0.50
1:G:118:ILE:HD12	1:G:133:LEU:HD12	1.93	0.50
1:H:309:THR:O	1:H:313:VAL:HG23	2.10	0.50
1:J:470:GLU:N	1:J:470:GLU:OE1	2.42	0.50
2:K:601:HEM:HBB2	2:K:601:HEM:CMB	2.41	0.50
1:L:90:ILE:HG22	1:L:94:LEU:CD1	2.41	0.50
1:I:32:LEU:HD12	1:I:32:LEU:O	2.12	0.50
1:E:200:GLN:HG2	1:L:171:THR:HG21	1.94	0.50
1:F:65:TYR:CD2	1:F:400:VAL:CG1	2.94	0.50
1:F:187:THR:CG2	1:F:188:SER:N	2.75	0.50
2:I:601:HEM:HBB2	2:I:601:HEM:CMB	2.41	0.50
1:K:136:THR:HG23	1:K:274:LEU:HB3	1.93	0.50
1:A:118:ILE:HD11	1:A:130:ARG:HD2	1.92	0.50
1:D:165:GLU:C	1:D:167:GLY:N	2.64	0.50
1:E:179:TYR:CE2	1:E:455:ALA:HB2	2.47	0.50
1:H:370:ALA:O	1:H:371:MET:HB2	2.11	0.50
1:I:148:ILE:O	1:I:148:ILE:CG2	2.60	0.50
1:H:216:LEU:HD23	1:H:216:LEU:N	2.26	0.50
1:I:171:THR:O	1:I:171:THR:HG22	2.10	0.50
1:L:248:PHE:HD2	1:L:249:LEU:HD23	1.74	0.50
2:B:601:HEM:HMB2	2:B:601:HEM:HBB2	1.94	0.50
1:C:253:VAL:HA	1:C:256:ILE:HD13	1.94	0.50
1:D:212:ARG:NH1	1:D:212:ARG:HG3	2.26	0.50
1:E:211:LEU:HD13	1:E:307:TYR:CD1	2.47	0.50
1:G:89:MET:SD	1:G:386:MET:HE1	2.52	0.50
1:H:468:CYS:SG	1:H:469:LYS:N	2.85	0.50
1:B:70:LYS:N	1:B:70:LYS:CD	2.75	0.50
1:F:106:ARG:NH1	1:F:374:GLU:OE1	2.45	0.50
1:G:142:LEU:HD23	1:G:142:LEU:C	2.32	0.50
1:H:160:LEU:HD23	1:H:463:PHE:CD2	2.47	0.50
1:K:373:LEU:HD22	2:K:601:HEM:CGA	2.42	0.50
1:A:106:ARG:HG3	1:A:393:VAL:HG21	1.94	0.49
1:B:126:TRP:CZ2	1:B:440:ARG:HG3	2.47	0.49
1:B:190:GLY:HA2	1:B:270:ASP:OD1	2.12	0.49
1:E:76:ASP:OD2	1:E:224:LYS:NZ	2.38	0.49
1:I:185:THR:CG2	1:I:193:ILE:HD13	2.42	0.49
1:J:320:GLU:HA	1:J:320:GLU:OE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:LEU:HD12	1:E:359:VAL:HG11	1.94	0.49
1:G:152:TYR:OH	1:G:192:SER:HB2	2.13	0.49
1:G:319:TYR:OH	1:G:473:ILE:O	2.29	0.49
1:H:185:THR:HB	1:H:193:ILE:CD1	2.42	0.49
1:K:189:PHE:CE2	1:K:249:LEU:HD21	2.46	0.49
1:A:25:TYR:N	3:A:602:ZWY:O22	2.45	0.49
1:E:202:PRO:O	1:E:206:ASN:ND2	2.43	0.49
1:H:211:LEU:HD13	1:H:307:TYR:CD1	2.47	0.49
1:L:116:ASN:O	1:L:117:ALA:C	2.49	0.49
1:B:410:GLU:O	1:B:418:ARG:NH2	2.40	0.49
1:C:319:TYR:CE2	1:C:475:LEU:HD12	2.47	0.49
1:L:162:ARG:NH1	1:L:197:ASN:OD1	2.45	0.49
1:D:201:ASP:HB3	1:D:204:VAL:HG23	1.94	0.49
1:E:148:ILE:N	1:E:148:ILE:HD12	2.27	0.49
1:F:205:GLU:OE1	1:F:209:LYS:NZ	2.45	0.49
1:I:397:PRO:HB2	1:I:400:VAL:CG2	2.41	0.49
1:L:119:SER:HB3	2:L:601:HEM:HAD1	1.94	0.49
1:G:415:LEU:O	1:G:418:ARG:HG3	2.13	0.49
1:H:322:ALA:O	1:H:467:PRO:HD3	2.13	0.49
1:I:189:PHE:CZ	1:I:303:ILE:CD1	2.96	0.49
1:A:213:PHE:CE1	1:A:240:VAL:HG22	2.47	0.49
1:B:382:GLU:HA	1:B:386:MET:O	2.13	0.49
1:D:148:ILE:CD1	1:D:269:VAL:HG12	2.41	0.49
1:G:210:LEU:HD21	1:G:300:ILE:HG23	1.95	0.49
1:H:468:CYS:C	1:H:471:THR:HG22	2.33	0.49
1:D:228:PHE:CD1	1:H:78:GLN:OE1	2.66	0.49
1:E:179:TYR:CZ	1:E:455:ALA:HB2	2.48	0.49
1:E:250:THR:HA	1:E:296:MET:CE	2.43	0.49
1:H:319:TYR:CZ	1:H:475:LEU:HD22	2.47	0.49
1:I:54:ARG:HD2	1:I:479:PHE:CE2	2.48	0.49
1:J:219:PHE:O	1:J:223:ILE:HG12	2.13	0.49
1:L:181:MET:O	1:L:182:ASP:C	2.51	0.49
1:A:282:LYS:O	1:L:55:LYS:HE2	2.13	0.49
1:C:255:GLN:O	1:C:258:GLU:HB2	2.13	0.49
1:E:321:LEU:HD21	1:E:359:VAL:HG21	1.95	0.49
1:E:485:THR:HG21	1:E:489:ILE:HD11	1.94	0.49
1:D:63:GLU:HA	1:D:63:GLU:OE1	2.13	0.49
1:E:67:LYS:HE2	1:E:68:TYR:CZ	2.48	0.49
2:F:601:HEM:HBB2	2:F:601:HEM:CMB	2.42	0.49
1:G:269:VAL:HG22	1:G:269:VAL:O	2.13	0.49
1:J:346:THR:O	1:J:350:VAL:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:102:PHE:CE2	1:L:394:VAL:HG21	2.46	0.49
1:L:125:GLU:O	1:L:129:ILE:HG13	2.13	0.49
1:L:241:PHE:HB3	1:L:246:ILE:HD11	1.94	0.49
1:F:358:MET:HE2	1:F:416:PRO:O	2.13	0.48
1:C:356:LEU:HD12	1:C:359:VAL:CG1	2.42	0.48
1:F:446:ARG:HH11	1:F:446:ARG:HG3	1.78	0.48
1:G:405:PRO:HA	1:G:408:TRP:O	2.13	0.48
1:I:153:GLY:O	1:I:157:VAL:HG13	2.14	0.48
1:I:319:TYR:OH	1:I:473:ILE:O	2.25	0.48
1:C:212:ARG:NH1	1:K:217:ASP:OD2	2.46	0.48
1:C:243:ARG:O	1:C:247:SER:OG	2.26	0.48
2:C:601:HEM:HBB2	2:C:601:HEM:CMB	2.44	0.48
1:E:388:ILE:HG23	1:E:392:VAL:HG21	1.95	0.48
1:G:413:LYS:HE3	1:G:415:LEU:HD21	1.96	0.48
1:K:53:PHE:HD2	1:K:57:TYR:HE1	1.61	0.48
1:K:189:PHE:CE2	1:K:249:LEU:CD2	2.96	0.48
2:G:601:HEM:HMB2	2:G:601:HEM:HBB2	1.94	0.48
1:J:356:LEU:O	1:J:359:VAL:HG12	2.12	0.48
1:K:124:GLU:OE1	1:K:127:LYS:NZ	2.46	0.48
1:L:446:ARG:O	1:L:447:PHE:C	2.49	0.48
1:F:339:LEU:CB	1:F:343:ALA:HB3	2.40	0.48
1:I:185:THR:HB	1:I:193:ILE:HD13	1.95	0.48
1:I:414:PHE:O	1:I:415:LEU:HD23	2.13	0.48
1:L:345:PRO:HD2	1:L:458:ARG:NH1	2.27	0.48
1:A:34:LYS:HD3	1:A:34:LYS:N	2.28	0.48
1:A:214:ASN:OD1	1:A:216:LEU:N	2.39	0.48
1:B:257:LYS:NZ	1:B:292:ASP:OD2	2.45	0.48
1:E:356:LEU:HD12	1:E:359:VAL:CG1	2.44	0.48
1:G:221:LEU:HD23	1:G:224:LYS:HE3	1.94	0.48
1:G:471:THR:HA	1:G:490:VAL:HG23	1.95	0.48
1:I:319:TYR:CZ	1:I:475:LEU:HG	2.49	0.48
1:J:160:LEU:HD13	1:J:170:VAL:HG11	1.96	0.48
1:E:157:VAL:CG1	1:E:462:ASN:HD22	2.25	0.48
1:E:428:ASP:OD1	1:E:429:PRO:HD2	2.14	0.48
1:G:377:CYS:SG	1:G:388:ILE:HG22	2.54	0.48
1:J:185:THR:CG2	1:J:193:ILE:CD1	2.92	0.48
1:J:189:PHE:CE1	1:J:303:ILE:HD11	2.49	0.48
1:K:108:PHE:N	1:K:108:PHE:CD2	2.80	0.48
1:L:180:SER:O	1:L:184:ILE:HB	2.14	0.48
1:A:126:TRP:CZ2	1:A:440:ARG:HD2	2.48	0.48
1:A:470:GLU:CB	1:A:490:VAL:HG21	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:GLU:O	1:B:247:SER:N	2.47	0.48
1:C:32:LEU:O	1:C:36:LEU:HD12	2.13	0.48
1:E:205:GLU:OE2	1:E:205:GLU:HA	2.14	0.48
1:F:136:THR:HG23	1:F:274:LEU:HD23	1.95	0.48
1:F:279:GLN:O	1:F:280:ASN:HB3	2.13	0.48
1:H:468:CYS:O	1:H:471:THR:CG2	2.62	0.48
1:I:190:GLY:HA2	1:I:270:ASP:OD2	2.13	0.48
1:J:134:SER:OG	1:J:135:PRO:HD3	2.14	0.48
1:J:210:LEU:HB2	1:J:245:VAL:HG11	1.96	0.48
1:J:256:ILE:HD12	1:J:256:ILE:H	1.78	0.48
1:K:359:VAL:HG13	1:K:414:PHE:HZ	1.79	0.48
1:B:212:ARG:CG	1:I:212:ARG:HD3	2.43	0.48
1:C:475:LEU:HD23	1:C:476:LYS:N	2.29	0.48
1:E:114:MET:HG3	1:E:241:PHE:CE1	2.49	0.48
1:G:146:VAL:HG13	1:G:454:LEU:HD11	1.95	0.48
1:G:355:TYR:O	1:G:359:VAL:HG23	2.14	0.48
1:I:198:ASN:N	1:I:199:PRO:HD3	2.29	0.48
1:J:383:ILE:O	1:J:384:ASN:C	2.50	0.48
1:K:469:LYS:C	1:K:471:THR:H	2.17	0.48
1:B:370:ALA:O	1:B:371:MET:HB2	2.14	0.48
1:E:275:MET:HB3	1:E:295:LEU:HD12	1.95	0.48
1:F:477:LEU:CA	1:F:484:LEU:O	2.62	0.48
2:G:601:HEM:HBC2	2:G:601:HEM:CMC	2.44	0.48
2:G:601:HEM:HBB2	2:G:601:HEM:CMB	2.44	0.48
1:H:67:LYS:HD2	1:H:68:TYR:CZ	2.49	0.48
1:I:326:ASP:OD2	1:I:326:ASP:N	2.47	0.48
1:L:102:PHE:HB3	1:L:375:ARG:HB3	1.95	0.48
1:L:132:LEU:HD13	1:L:290:LEU:HD23	1.96	0.48
1:F:248:PHE:HD2	1:F:249:LEU:HD12	1.79	0.47
1:H:185:THR:HB	1:H:193:ILE:HD11	1.95	0.47
1:E:486:GLU:OE1	1:E:486:GLU:HA	2.14	0.47
1:F:143:LYS:HA	1:F:347:TYR:CD1	2.49	0.47
1:F:341:ASN:O	1:F:342:LYS:HB2	2.14	0.47
1:G:187:THR:HG1	1:G:271:PHE:HD2	1.61	0.47
1:I:252:SER:O	1:I:256:ILE:HG12	2.14	0.47
1:K:354:GLU:O	1:K:357:ASP:HB2	2.15	0.47
1:L:473:ILE:CB	1:L:474:PRO:CD	2.91	0.47
1:B:184:ILE:O	1:B:188:SER:OG	2.22	0.47
1:C:317:ILE:HD13	1:C:360:VAL:HG22	1.96	0.47
1:H:119:SER:HB3	2:H:601:HEM:HAD1	1.97	0.47
1:J:97:GLU:OE2	1:J:97:GLU:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:362:GLU:HG3	1:K:414:PHE:CE1	2.49	0.47
1:K:469:LYS:O	1:K:471:THR:N	2.47	0.47
1:L:56:GLY:HA3	1:L:58:TRP:CZ3	2.49	0.47
1:L:90:ILE:O	1:L:93:VAL:HG22	2.13	0.47
1:L:291:SER:H	1:L:294:GLU:CG	2.28	0.47
1:L:383:ILE:HG12	1:L:383:ILE:O	2.14	0.47
1:B:179:TYR:CE2	1:B:455:ALA:HB2	2.50	0.47
1:B:260:ARG:HD3	1:B:273:GLN:OE1	2.15	0.47
1:B:339:LEU:HD21	1:B:349:THR:HG21	1.95	0.47
1:C:260:ARG:HD3	1:C:273:GLN:OE1	2.14	0.47
1:C:328:GLN:O	1:C:332:GLN:HG3	2.14	0.47
1:D:59:THR:O	1:D:63:GLU:HG2	2.13	0.47
2:J:601:HEM:HBB2	2:J:601:HEM:CMB	2.44	0.47
1:L:65:TYR:CE1	1:L:85:THR:HG21	2.50	0.47
1:A:47:LEU:HD13	1:A:51:LEU:HD21	1.97	0.47
1:F:176:PHE:CE2	1:F:318:ILE:HG13	2.49	0.47
1:I:397:PRO:HB2	1:I:400:VAL:HG23	1.96	0.47
1:J:468:CYS:HA	1:J:492:LYS:HE3	1.96	0.47
1:J:469:LYS:HG2	1:J:470:GLU:OE1	2.14	0.47
1:K:243:ARG:HG3	1:K:244:GLU:OE1	2.14	0.47
1:L:300:ILE:O	1:L:304:PHE:HD2	1.97	0.47
1:C:162:ARG:HG3	1:C:162:ARG:HH11	1.77	0.47
2:D:601:HEM:HBC2	2:D:601:HEM:HMC2	1.96	0.47
1:F:321:LEU:HD21	1:F:359:VAL:HG11	1.95	0.47
1:G:470:GLU:N	1:G:470:GLU:OE1	2.46	0.47
1:I:317:ILE:HD13	1:I:360:VAL:HG22	1.97	0.47
1:K:216:LEU:HD13	1:K:479:PHE:CE2	2.49	0.47
1:L:129:ILE:HG22	1:L:133:LEU:HD12	1.97	0.47
1:L:320:GLU:OE2	1:L:320:GLU:HA	2.15	0.47
1:B:157:VAL:HG23	1:B:458:ARG:HG3	1.96	0.47
1:C:79:GLN:NE2	1:C:80:PRO:O	2.39	0.47
1:D:346:THR:O	1:D:350:VAL:HG22	2.15	0.47
1:E:44:LEU:HB3	1:E:45:PRO:HD2	1.96	0.47
1:E:472:GLN:HG2	1:E:474:PRO:O	2.15	0.47
1:H:204:VAL:O	1:H:208:LYS:HG3	2.15	0.47
1:H:242:PRO:HB2	1:H:245:VAL:HG23	1.96	0.47
1:I:119:SER:HB3	2:I:601:HEM:HAD1	1.97	0.47
1:K:190:GLY:HA2	1:K:270:ASP:OD2	2.15	0.47
1:L:186:SER:OG	1:L:193:ILE:HG12	2.14	0.47
1:L:238:ILE:HG22	1:L:238:ILE:O	2.13	0.47
1:L:335:ILE:HG23	1:L:457:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:361:ASN:HB3	1:L:419:PHE:CE1	2.50	0.47
1:L:407:TYR:CD1	1:L:431:ILE:CD1	2.97	0.47
1:L:483:LEU:C	1:L:484:LEU:HD23	2.35	0.47
1:D:119:SER:HB3	2:D:601:HEM:HAD1	1.97	0.47
1:D:217:ASP:C	1:D:217:ASP:OD1	2.53	0.47
1:F:378:LYS:O	1:F:390:LYS:NZ	2.45	0.47
1:H:159:ASN:ND2	1:H:196:LEU:HD12	2.30	0.47
1:I:202:PRO:HB2	1:I:248:PHE:CZ	2.50	0.47
1:I:328:GLN:O	1:I:332:GLN:HG3	2.14	0.47
1:B:155:VAL:HG12	1:B:159:ASN:OD1	2.15	0.47
1:G:109:GLY:HA2	1:G:223:ILE:HG21	1.97	0.47
1:L:206:ASN:ND2	1:L:248:PHE:CE2	2.72	0.47
1:L:219:PHE:CD2	1:L:240:VAL:HG23	2.50	0.47
1:B:61:ASP:OD1	1:B:372:ARG:NH2	2.48	0.47
1:C:116:ASN:O	1:C:129:ILE:HD13	2.14	0.47
1:E:317:ILE:CD1	1:E:360:VAL:HG22	2.45	0.47
1:H:201:ASP:HB3	1:H:204:VAL:HG23	1.96	0.47
1:I:33:PHE:CD1	1:I:73:GLY:HA3	2.50	0.47
1:I:172:LEU:HD12	1:I:489:ILE:HG22	1.96	0.47
1:J:190:GLY:HA3	1:J:260:ARG:HH22	1.78	0.47
1:L:138:THR:C	1:L:140:GLY:N	2.62	0.47
1:L:407:TYR:CE1	1:L:431:ILE:CD1	2.98	0.47
1:F:274:LEU:CD1	1:F:274:LEU:N	2.78	0.46
1:H:319:TYR:O	1:H:323:THR:HG23	2.15	0.46
1:J:169:PRO:HG3	1:J:470:GLU:OE2	2.15	0.46
1:K:357:ASP:OD2	1:K:453:LYS:NZ	2.44	0.46
1:L:473:ILE:HB	1:L:474:PRO:CD	2.45	0.46
1:E:481:GLY:C	1:E:484:LEU:HD23	2.35	0.46
1:H:135:PRO:O	1:H:138:THR:HG23	2.15	0.46
1:J:465:PHE:HA	1:J:492:LYS:O	2.14	0.46
1:K:100:SER:O	1:K:379:LYS:HE3	2.15	0.46
1:C:257:LYS:O	1:C:261:LEU:HD23	2.14	0.46
1:E:163:GLU:OE2	1:L:200:GLN:NE2	2.48	0.46
1:E:329:GLN:OE1	1:E:329:GLN:N	2.49	0.46
1:F:415:LEU:O	1:F:417:GLU:N	2.48	0.46
1:J:160:LEU:CD1	1:J:170:VAL:HG11	2.45	0.46
1:J:468:CYS:CB	1:J:492:LYS:CE	2.94	0.46
1:L:106:ARG:NH2	1:L:374:GLU:CD	2.69	0.46
1:L:178:ALA:O	1:L:182:ASP:HB2	2.14	0.46
1:L:210:LEU:CD2	1:L:210:LEU:C	2.84	0.46
1:A:159:ASN:O	1:A:163:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:GLU:O	1:E:261:LEU:HD23	2.16	0.46
1:F:65:TYR:CD2	1:F:400:VAL:HG13	2.51	0.46
1:F:256:ILE:O	1:F:260:ARG:HB2	2.16	0.46
1:F:354:GLU:O	1:F:357:ASP:HB2	2.16	0.46
1:G:57:TYR:HB2	1:G:371:MET:CE	2.45	0.46
1:G:57:TYR:HB2	1:G:371:MET:HE1	1.97	0.46
1:G:468:CYS:SG	1:G:470:GLU:HG2	2.56	0.46
1:K:70:LYS:N	1:K:70:LYS:HD2	2.30	0.46
1:K:123:ASP:OD1	1:K:378:LYS:HD3	2.15	0.46
2:A:601:HEM:HBB2	2:A:601:HEM:CMB	2.45	0.46
1:B:54:ARG:NH1	1:I:243:ARG:HD3	2.30	0.46
1:C:428:ASP:HB3	1:C:431:ILE:HG12	1.97	0.46
1:G:176:PHE:HE2	1:G:318:ILE:HG13	1.80	0.46
1:L:405:PRO:O	1:L:408:TRP:O	2.33	0.46
1:C:145:MET:HG3	1:C:269:VAL:O	2.16	0.46
1:D:143:LYS:HE2	1:D:348:ASP:OD2	2.16	0.46
1:E:478:ARG:HD3	1:E:486:GLU:CD	2.36	0.46
1:H:161:ARG:O	1:H:165:GLU:HG3	2.15	0.46
1:H:317:ILE:HD13	1:H:360:VAL:HG22	1.98	0.46
1:K:47:LEU:O	1:K:77:GLY:N	2.47	0.46
1:D:78:GLN:NE2	1:H:228:PHE:CD1	2.84	0.46
1:E:86:ASP:O	1:E:90:ILE:HG13	2.16	0.46
1:F:145:MET:HE1	1:F:270:ASP:HA	1.96	0.46
1:G:176:PHE:CE2	1:G:318:ILE:HG13	2.51	0.46
1:G:369:VAL:HB	1:G:482:LEU:HD22	1.98	0.46
1:H:410:GLU:O	1:H:418:ARG:NH2	2.42	0.46
1:I:52:SER:O	1:I:55:LYS:HG2	2.15	0.46
1:L:55:LYS:HG3	1:L:55:LYS:O	2.16	0.46
1:L:67:LYS:HD3	1:L:67:LYS:HA	1.81	0.46
1:E:182:ASP:OD1	1:E:193:ILE:HG13	2.16	0.46
1:F:178:ALA:HB1	1:F:195:SER:OG	2.16	0.46
1:F:179:TYR:CZ	1:F:183:VAL:HG21	2.51	0.46
1:G:160:LEU:HD21	1:G:465:PHE:HZ	1.81	0.46
1:K:128:ARG:NH2	1:K:289:ALA:O	2.49	0.46
1:E:47:LEU:HD13	1:E:51:LEU:HD11	1.98	0.46
1:F:94:LEU:HD22	1:F:437:SER:O	2.16	0.46
1:F:308:GLU:O	1:F:308:GLU:HG3	2.15	0.46
1:G:142:LEU:C	1:G:142:LEU:CD2	2.84	0.46
1:G:275:MET:CE	1:G:302:PHE:CE2	2.99	0.46
1:H:359:VAL:HG13	1:H:414:PHE:HZ	1.81	0.46
1:C:170:VAL:O	1:C:490:VAL:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:TYR:CZ	1:C:434:PRO:HG3	2.51	0.46
1:D:345:PRO:HB3	1:D:457:VAL:HG11	1.97	0.46
1:E:177:GLY:HA2	1:E:311:SER:HB2	1.98	0.46
1:G:76:ASP:OD2	1:G:106:ARG:NH2	2.48	0.46
1:I:370:ALA:O	1:I:371:MET:CB	2.62	0.46
1:J:244:GLU:HA	1:J:244:GLU:OE1	2.16	0.46
1:L:116:ASN:O	1:L:129:ILE:CD1	2.63	0.46
1:L:447:PHE:C	1:L:447:PHE:CD1	2.89	0.46
1:A:370:ALA:O	1:A:371:MET:HB2	2.15	0.45
1:B:143:LYS:NZ	1:B:348:ASP:OD1	2.39	0.45
1:E:342:LYS:HE3	1:E:462:ASN:OD1	2.16	0.45
1:F:148:ILE:HD12	1:F:148:ILE:N	2.30	0.45
1:H:110:PRO:HB3	1:H:234:GLU:HG2	1.98	0.45
1:D:354:GLU:O	1:D:358:MET:HG3	2.16	0.45
1:F:213:PHE:CZ	1:F:240:VAL:HG13	2.51	0.45
1:H:331:VAL:O	1:H:335:ILE:HG13	2.17	0.45
1:H:366:LEU:HD23	1:H:403:HIS:CE1	2.52	0.45
1:D:313:VAL:HG11	1:D:452:MET:SD	2.56	0.45
1:E:475:LEU:HD12	1:E:476:LYS:H	1.81	0.45
1:I:159:ASN:O	1:I:163:GLU:HG2	2.16	0.45
1:J:428:ASP:HB3	1:J:431:ILE:HG12	1.98	0.45
1:A:45:PRO:O	1:A:46:PHE:HB2	2.17	0.45
1:E:482:LEU:O	1:E:483:LEU:C	2.55	0.45
1:F:180:SER:OG	1:F:307:TYR:O	2.31	0.45
1:L:173:LYS:O	1:L:177:GLY:N	2.45	0.45
1:D:97:GLU:OE2	1:D:97:GLU:HA	2.15	0.45
1:E:118:ILE:HD11	1:E:130:ARG:HD2	1.97	0.45
1:F:335:ILE:HD12	1:F:335:ILE:H	1.82	0.45
1:F:452:MET:C	1:F:456:LEU:HD12	2.37	0.45
1:G:293:LEU:HD12	1:G:293:LEU:HA	1.85	0.45
1:I:78:GLN:NE2	1:J:228:PHE:CD1	2.82	0.45
1:I:166:THR:HG23	1:I:168:LYS:H	1.81	0.45
1:J:370:ALA:O	1:J:372:ARG:N	2.42	0.45
1:J:459:VAL:HG12	1:J:465:PHE:HE1	1.81	0.45
1:K:309:THR:O	1:K:313:VAL:HG23	2.16	0.45
1:K:458:ARG:HH21	1:K:458:ARG:HG3	1.82	0.45
1:K:471:THR:HG22	1:K:473:ILE:HD13	1.98	0.45
1:B:45:PRO:O	1:B:46:PHE:HB2	2.16	0.45
1:C:252:SER:O	1:C:253:VAL:C	2.55	0.45
1:E:229:LEU:CD2	1:E:233:LEU:CD1	2.95	0.45
1:E:253:VAL:HG21	1:E:296:MET:HE1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:LEU:HG	1:F:347:TYR:HE1	1.81	0.45
1:G:471:THR:HA	1:G:490:VAL:CG2	2.46	0.45
1:K:216:LEU:HD13	1:K:479:PHE:CZ	2.52	0.45
1:L:143:LYS:CD	1:L:347:TYR:CD2	2.99	0.45
1:A:35:LYS:O	1:A:35:LYS:HG3	2.17	0.45
1:D:55:LYS:HE3	1:D:60:PHE:HB2	1.99	0.45
1:H:258:GLU:O	1:H:261:LEU:HD23	2.16	0.45
1:H:350:VAL:HG21	1:H:454:LEU:CD2	2.42	0.45
1:J:189:PHE:CD1	1:J:203:PHE:HE1	2.34	0.45
1:J:260:ARG:O	1:J:262:LYS:N	2.49	0.45
1:K:210:LEU:HD12	1:K:210:LEU:O	2.16	0.45
1:A:281:SER:OG	1:A:281:SER:O	2.32	0.45
1:C:174:HIS:NE2	1:C:196:LEU:HD21	2.32	0.45
1:C:469:LYS:HA	1:C:469:LYS:HD3	1.75	0.45
1:D:106:ARG:CZ	3:D:602:ZWY:O22	2.65	0.45
1:D:106:ARG:HD2	1:D:393:VAL:HG21	1.99	0.45
1:D:410:GLU:O	1:D:418:ARG:NH2	2.47	0.45
1:I:317:ILE:HG21	1:I:456:LEU:HD11	1.99	0.45
1:K:174:HIS:CE1	1:K:196:LEU:HD21	2.52	0.45
1:K:321:LEU:HD21	1:K:359:VAL:HG11	1.99	0.45
1:L:126:TRP:NE1	1:L:440:ARG:CD	2.80	0.45
1:L:132:LEU:CD1	1:L:288:LYS:O	2.65	0.45
1:L:336:ASP:O	1:L:340:PRO:CA	2.65	0.45
1:A:281:SER:HB2	1:L:63:GLU:OE2	2.15	0.45
1:A:383:ILE:HD11	1:A:388:ILE:HD11	1.98	0.45
1:D:279:GLN:HA	1:D:289:ALA:HB1	1.99	0.45
2:D:601:HEM:HBC2	2:D:601:HEM:CMC	2.47	0.45
1:E:359:VAL:HG23	1:E:414:PHE:HZ	1.82	0.45
1:F:435:PHE:CD1	1:F:445:MET:HG3	2.52	0.45
1:H:119:SER:OG	1:H:301:ILE:HG12	2.17	0.45
1:J:172:LEU:HD12	1:J:176:PHE:HE2	1.80	0.45
1:G:339:LEU:HD21	1:G:349:THR:HG21	1.99	0.45
1:L:407:TYR:CD2	1:L:431:ILE:HD13	2.51	0.45
1:B:186:SER:HA	1:B:191:VAL:O	2.17	0.44
1:E:239:THR:O	1:L:218:PRO:HB3	2.17	0.44
1:H:324:HIS:HB3	1:H:327:VAL:HG23	1.99	0.44
1:K:453:LYS:O	1:K:457:VAL:HG23	2.17	0.44
1:L:373:LEU:HB2	1:L:396:ILE:HB	1.98	0.44
1:C:90:ILE:HG23	1:C:396:ILE:HD13	1.99	0.44
1:G:118:ILE:HD11	1:G:130:ARG:HD2	2.00	0.44
1:H:279:GLN:HA	1:H:289:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:90:ILE:HG23	1:I:396:ILE:HD13	1.98	0.44
1:K:141:LYS:HB3	1:K:274:LEU:HD11	1.99	0.44
1:K:313:VAL:HG21	2:K:601:HEM:CBB	2.47	0.44
1:K:443:ILE:CG2	1:K:444:GLY:N	2.80	0.44
1:L:84:ILE:HD11	1:L:396:ILE:HG13	1.98	0.44
1:L:93:VAL:HG12	1:L:102:PHE:CZ	2.52	0.44
1:L:176:PHE:CE2	1:L:318:ILE:HG13	2.52	0.44
1:A:25:TYR:OH	1:A:227:PRO:HD2	2.17	0.44
1:B:350:VAL:CG1	1:B:453:LYS:CD	2.92	0.44
1:C:191:VAL:O	1:C:193:ILE:HG12	2.18	0.44
2:E:601:HEM:HBB2	2:E:601:HEM:CMB	2.47	0.44
1:F:65:TYR:HD2	1:F:400:VAL:HG13	1.82	0.44
1:F:191:VAL:O	1:F:191:VAL:HG13	2.18	0.44
1:L:118:ILE:O	1:L:440:ARG:NH2	2.50	0.44
1:L:210:LEU:HD21	1:L:304:PHE:CZ	2.52	0.44
1:L:405:PRO:HA	1:L:408:TRP:O	2.17	0.44
1:A:169:PRO:CG	1:A:470:GLU:OE1	2.62	0.44
1:A:173:LYS:HZ2	1:A:489:ILE:H	1.65	0.44
1:A:186:SER:HA	1:A:191:VAL:O	2.17	0.44
1:B:58:TRP:CZ2	1:B:477:LEU:HB2	2.53	0.44
1:B:288:LYS:HD3	1:B:288:LYS:N	2.32	0.44
2:B:601:HEM:HBB2	2:B:601:HEM:CMB	2.47	0.44
1:D:110:PRO:CB	1:D:234:GLU:HG2	2.47	0.44
1:E:272:LEU:O	1:E:276:ILE:HG13	2.16	0.44
1:F:435:PHE:CE1	1:F:445:MET:HG3	2.52	0.44
1:F:446:ARG:HG3	1:F:446:ARG:NH1	2.33	0.44
1:F:470:GLU:HG3	1:F:490:VAL:HG21	1.99	0.44
1:G:94:LEU:HD21	1:G:396:ILE:HD13	1.99	0.44
1:G:166:THR:O	1:G:166:THR:HG22	2.17	0.44
1:H:35:LYS:C	1:H:35:LYS:HD3	2.37	0.44
1:H:252:SER:O	1:H:255:GLN:N	2.50	0.44
1:H:342:LYS:HE2	1:H:462:ASN:OD1	2.16	0.44
1:I:174:HIS:NE2	1:I:196:LEU:HD21	2.32	0.44
1:I:339:LEU:HD11	1:I:345:PRO:HA	2.00	0.44
1:J:186:SER:OG	1:J:193:ILE:HG12	2.18	0.44
1:J:432:TYR:CZ	1:J:434:PRO:HG3	2.53	0.44
1:B:470:GLU:CB	1:B:490:VAL:HG21	2.47	0.44
1:D:179:TYR:O	1:D:183:VAL:HG23	2.18	0.44
1:F:353:LEU:N	1:F:353:LEU:HD13	2.32	0.44
1:H:110:PRO:HD3	1:H:223:ILE:CD1	2.47	0.44
1:I:136:THR:HG22	1:I:136:THR:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:58:TRP:CE2	1:K:59:THR:HG23	2.53	0.44
1:K:201:ASP:HA	1:K:202:PRO:HD3	1.90	0.44
1:L:170:VAL:O	1:L:490:VAL:HA	2.18	0.44
1:A:432:TYR:CZ	1:A:434:PRO:HG3	2.53	0.44
1:A:473:ILE:HB	1:A:474:PRO:CD	2.47	0.44
1:D:471:THR:OG1	1:D:490:VAL:O	2.22	0.44
1:D:474:PRO:O	1:D:476:LYS:HG3	2.18	0.44
1:G:257:LYS:NZ	1:G:292:ASP:OD1	2.50	0.44
1:L:181:MET:HG2	1:L:185:THR:OG1	2.18	0.44
1:B:446:ARG:HG3	1:B:446:ARG:HH11	1.83	0.44
1:G:189:PHE:CE2	1:G:303:ILE:HD11	2.53	0.44
1:J:118:ILE:CG2	1:J:119:SER:N	2.79	0.44
1:L:179:TYR:O	1:L:182:ASP:HB2	2.18	0.44
1:L:473:ILE:HD12	1:L:473:ILE:N	2.32	0.44
1:A:308:GLU:HG2	1:A:482:LEU:HD12	2.00	0.44
1:C:243:ARG:HE	1:C:243:ARG:HB3	1.58	0.44
1:H:112:GLY:C	1:H:114:MET:N	2.71	0.44
1:J:110:PRO:CB	1:J:234:GLU:HG2	2.48	0.44
1:L:156:LEU:HD12	1:L:156:LEU:O	2.18	0.44
1:A:229:LEU:HD22	1:J:226:PHE:CE1	2.52	0.44
1:B:198:ASN:N	1:B:199:PRO:HD3	2.33	0.44
1:C:210:LEU:HD21	1:C:300:ILE:HG23	2.00	0.44
1:E:482:LEU:CD2	3:E:605:ZWY:C16	2.96	0.44
1:F:177:GLY:HA2	1:F:311:SER:HB2	1.98	0.44
1:G:245:VAL:O	1:G:249:LEU:HD13	2.18	0.44
1:H:257:LYS:O	1:H:261:LEU:HD22	2.18	0.44
1:I:62:MET:SD	1:I:400:VAL:HG13	2.58	0.44
1:I:171:THR:HG22	1:I:174:HIS:HB3	1.99	0.44
1:I:232:ILE:O	1:I:236:LEU:CD2	2.66	0.44
1:I:487:LYS:HD2	1:I:488:PRO:HD2	2.00	0.44
1:K:28:ARG:HG3	1:K:28:ARG:HH11	1.82	0.44
1:K:28:ARG:HG3	1:K:28:ARG:NH1	2.33	0.44
1:K:126:TRP:CE2	1:K:440:ARG:HD2	2.53	0.44
1:K:383:ILE:HG13	1:K:383:ILE:O	2.17	0.44
1:L:443:ILE:CG2	1:L:444:GLY:N	2.81	0.44
1:A:383:ILE:HD11	1:A:388:ILE:CD1	2.47	0.43
1:B:359:VAL:HG13	1:B:414:PHE:HZ	1.83	0.43
1:C:219:PHE:CD1	1:K:219:PHE:HA	2.53	0.43
1:C:442:CYS:HB2	2:C:601:HEM:NA	2.33	0.43
1:F:169:PRO:HB3	1:F:468:CYS:SG	2.58	0.43
1:G:358:MET:CE	1:G:417:GLU:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:318:ILE:O	1:I:318:ILE:HG22	2.18	0.43
1:K:94:LEU:HD21	1:K:396:ILE:CD1	2.48	0.43
1:A:284:SER:OG	1:A:284:SER:O	2.36	0.43
1:I:189:PHE:CE2	1:I:249:LEU:HD23	2.52	0.43
1:K:415:LEU:O	1:K:418:ARG:HG3	2.18	0.43
1:B:104:ASN:OD1	1:B:122:GLU:HB3	2.19	0.43
1:D:110:PRO:HB3	1:D:234:GLU:HG2	2.00	0.43
1:D:258:GLU:O	1:D:261:LEU:HG	2.19	0.43
1:H:201:ASP:O	1:H:204:VAL:N	2.51	0.43
1:I:282:LYS:HE3	1:I:282:LYS:HB3	1.81	0.43
1:I:331:VAL:O	1:I:335:ILE:HG13	2.18	0.43
1:L:142:LEU:HD13	1:L:447:PHE:CD2	2.52	0.43
1:E:275:MET:HE3	1:E:295:LEU:HG	2.01	0.43
1:H:241:PHE:HB3	1:H:246:ILE:CD1	2.48	0.43
1:H:249:LEU:C	1:H:296:MET:HE1	2.39	0.43
1:I:154:ASP:O	1:I:157:VAL:HG22	2.18	0.43
1:K:365:ARG:O	1:K:402:HIS:HB3	2.18	0.43
1:L:211:LEU:C	1:L:213:PHE:N	2.71	0.43
1:A:355:TYR:O	1:A:359:VAL:HG23	2.18	0.43
1:F:83:ALA:HA	1:F:395:MET:O	2.18	0.43
1:F:208:LYS:O	1:F:212:ARG:HG3	2.19	0.43
1:F:473:ILE:O	1:F:475:LEU:N	2.51	0.43
2:F:601:HEM:HBC2	2:F:601:HEM:CMC	2.42	0.43
1:G:44:LEU:HB3	1:G:45:PRO:CD	2.48	0.43
1:I:157:VAL:CG2	1:I:158:ARG:N	2.81	0.43
1:I:189:PHE:CZ	1:I:303:ILE:HD11	2.53	0.43
1:J:138:THR:OG1	1:J:141:LYS:HG2	2.18	0.43
1:J:468:CYS:HB2	1:J:492:LYS:HE2	2.01	0.43
1:K:47:LEU:HD13	1:K:51:LEU:HD21	2.01	0.43
1:L:150:ALA:HA	1:L:454:LEU:HD21	2.01	0.43
1:L:432:TYR:CZ	1:L:434:PRO:HG3	2.53	0.43
1:B:351:LEU:HD21	1:C:473:ILE:HG21	2.00	0.43
1:D:212:ARG:HG3	1:D:212:ARG:HH11	1.84	0.43
1:F:76:ASP:OD2	1:F:106:ARG:NH2	2.49	0.43
1:F:136:THR:CG2	1:F:274:LEU:HD23	2.49	0.43
1:F:217:ASP:OD1	1:F:217:ASP:O	2.36	0.43
1:G:191:VAL:HG13	1:G:191:VAL:O	2.17	0.43
1:J:331:VAL:O	1:J:335:ILE:HG13	2.18	0.43
1:L:217:ASP:O	1:L:219:PHE:N	2.51	0.43
1:A:116:ASN:O	1:A:129:ILE:CD1	2.67	0.43
1:A:316:PHE:HE2	1:A:475:LEU:HD21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:TYR:CD2	1:A:319:TYR:C	2.92	0.43
1:A:469:LYS:HE2	1:A:469:LYS:CA	2.48	0.43
1:C:47:LEU:HD13	1:C:51:LEU:HD11	2.01	0.43
1:C:179:TYR:CZ	1:C:455:ALA:HB2	2.53	0.43
1:E:229:LEU:HD23	1:E:233:LEU:HG	2.01	0.43
1:H:224:LYS:HD2	3:H:602:ZWY:O24	2.19	0.43
1:I:204:VAL:O	1:I:208:LYS:HG3	2.18	0.43
1:I:232:ILE:HD12	1:J:45:PRO:HB3	1.99	0.43
1:J:101:VAL:HG21	1:J:381:VAL:HG11	2.00	0.43
1:J:166:THR:OG1	1:J:168:LYS:HG3	2.18	0.43
1:J:478:ARG:NE	1:J:484:LEU:HD23	2.34	0.43
1:L:307:TYR:CD2	1:L:308:GLU:HB2	2.54	0.43
1:L:308:GLU:HG2	1:L:482:LEU:HD12	2.01	0.43
1:B:173:LYS:NZ	1:B:312:SER:OG	2.52	0.43
1:C:146:VAL:N	1:C:147:PRO:HD2	2.34	0.43
1:C:206:ASN:CG	1:C:245:VAL:HG13	2.39	0.43
1:D:160:LEU:HD21	1:D:463:PHE:CD2	2.54	0.43
1:D:321:LEU:HB3	1:D:328:GLN:HG2	2.01	0.43
1:E:206:ASN:ND2	1:E:248:PHE:CE2	2.86	0.43
1:F:25:TYR:CD2	1:F:25:TYR:C	2.90	0.43
1:F:143:LYS:HE3	1:F:143:LYS:HB3	1.84	0.43
1:G:478:ARG:HG2	1:G:479:PHE:N	2.33	0.43
1:H:191:VAL:HG23	1:H:191:VAL:O	2.18	0.43
1:J:200:GLN:HA	1:J:200:GLN:OE1	2.18	0.43
1:J:478:ARG:HE	1:J:478:ARG:HB3	1.62	0.43
1:K:132:LEU:HD13	1:K:290:LEU:CD2	2.47	0.43
1:L:178:ALA:O	1:L:182:ASP:CB	2.67	0.43
1:A:382:GLU:HA	1:A:386:MET:O	2.19	0.43
1:C:317:ILE:CD1	1:C:360:VAL:HG22	2.49	0.43
1:D:472:GLN:O	1:D:472:GLN:HG2	2.18	0.43
1:F:226:PHE:HB3	1:F:228:PHE:CZ	2.54	0.43
1:G:370:ALA:HB2	2:G:601:HEM:HMA2	2.00	0.43
1:H:30:HIS:NE2	1:H:78:GLN:NE2	2.67	0.43
1:H:468:CYS:H	1:H:471:THR:HG21	1.80	0.43
1:A:79:GLN:HG2	1:A:106:ARG:HD3	2.01	0.43
1:C:101:VAL:HG21	1:C:381:VAL:HG11	2.01	0.43
1:D:252:SER:O	1:D:256:ILE:HG13	2.18	0.43
1:F:477:LEU:HA	1:F:485:THR:HA	1.99	0.43
1:G:151:GLN:O	1:G:154:ASP:HB2	2.19	0.43
1:G:471:THR:O	1:G:471:THR:HG23	2.19	0.43
1:H:435:PHE:CG	1:H:445:MET:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:156:LEU:CD1	1:I:175:VAL:HG22	2.49	0.43
1:K:253:VAL:CB	1:K:296:MET:HE1	2.49	0.43
1:K:469:LYS:C	1:K:471:THR:N	2.71	0.43
2:L:601:HEM:HBC2	2:L:601:HEM:CMC	2.45	0.43
1:C:148:ILE:HG22	1:C:148:ILE:O	2.19	0.42
1:C:216:LEU:HD11	1:C:480:GLY:HA2	2.01	0.42
1:F:56:GLY:HA3	1:F:58:TRP:CZ3	2.54	0.42
1:F:146:VAL:N	1:F:147:PRO:CD	2.82	0.42
1:G:178:ALA:O	1:G:182:ASP:HB2	2.19	0.42
1:H:179:TYR:CE2	1:H:455:ALA:HB2	2.53	0.42
1:I:317:ILE:CD1	1:I:360:VAL:HG22	2.49	0.42
1:C:148:ILE:O	1:C:148:ILE:CG2	2.68	0.42
1:C:158:ARG:O	1:C:162:ARG:HB2	2.19	0.42
1:F:71:VAL:HG21	1:F:386:MET:CE	2.49	0.42
1:K:354:GLU:O	1:K:355:TYR:C	2.58	0.42
1:L:101:VAL:HG11	1:L:381:VAL:HG21	2.01	0.42
1:B:52:SER:HB3	1:B:60:PHE:CE2	2.54	0.42
1:B:160:LEU:CD2	1:B:459:VAL:HG23	2.49	0.42
1:C:160:LEU:HD21	1:C:465:PHE:CZ	2.53	0.42
1:C:179:TYR:CE2	1:C:455:ALA:HB2	2.54	0.42
1:C:256:ILE:O	1:C:257:LYS:C	2.57	0.42
1:C:370:ALA:O	1:C:371:MET:HB2	2.19	0.42
1:E:71:VAL:HG13	1:E:82:LEU:HD11	2.00	0.42
1:E:116:ASN:O	1:E:129:ILE:HD13	2.20	0.42
1:F:151:GLN:O	1:F:154:ASP:HB2	2.19	0.42
1:F:272:LEU:HG	1:F:276:ILE:CD1	2.49	0.42
1:F:339:LEU:HD21	1:F:349:THR:HG21	2.01	0.42
1:H:189:PHE:CE2	1:H:303:ILE:CD1	3.01	0.42
1:I:261:LEU:O	1:I:262:LYS:HG3	2.18	0.42
1:K:382:GLU:HA	1:K:386:MET:O	2.18	0.42
1:A:118:ILE:HD12	1:A:133:LEU:HD12	2.01	0.42
1:D:313:VAL:CG1	1:D:452:MET:SD	3.07	0.42
1:G:110:PRO:HA	1:G:234:GLU:OE2	2.18	0.42
1:G:189:PHE:HD2	1:G:203:PHE:CE2	2.36	0.42
1:H:383:ILE:HD11	1:H:388:ILE:CD1	2.48	0.42
1:J:468:CYS:HB3	1:J:492:LYS:CE	2.49	0.42
1:K:126:TRP:CZ2	1:K:440:ARG:HD2	2.54	0.42
1:L:124:GLU:N	1:L:124:GLU:CD	2.73	0.42
1:B:116:ASN:HB3	1:B:294:GLU:HG2	2.00	0.42
1:B:166:THR:OG1	1:B:168:LYS:HE2	2.19	0.42
1:C:190:GLY:HA3	1:C:260:ARG:HH22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:VAL:HG21	1:D:381:VAL:HG11	2.01	0.42
1:G:45:PRO:O	1:G:46:PHE:HB2	2.19	0.42
1:G:170:VAL:O	1:G:490:VAL:HA	2.19	0.42
1:I:163:GLU:O	1:I:166:THR:HG22	2.20	0.42
1:I:487:LYS:CD	1:I:488:PRO:HD2	2.50	0.42
1:L:301:ILE:O	1:L:305:ALA:N	2.49	0.42
1:A:146:VAL:N	1:A:147:PRO:CD	2.82	0.42
1:B:383:ILE:O	1:B:383:ILE:HG13	2.19	0.42
1:G:81:MET:CE	1:G:106:ARG:NH1	2.82	0.42
1:H:415:LEU:O	1:H:418:ARG:HG3	2.19	0.42
1:J:46:PHE:O	1:J:77:GLY:HA2	2.19	0.42
1:J:358:MET:HE1	1:J:420:SER:HB3	2.02	0.42
1:A:415:LEU:O	1:A:418:ARG:HG3	2.20	0.42
1:B:145:MET:O	1:B:148:ILE:HG12	2.19	0.42
1:D:45:PRO:O	1:D:46:PHE:HB3	2.20	0.42
1:D:270:ASP:O	1:D:274:LEU:HG	2.20	0.42
1:E:244:GLU:OE2	1:E:244:GLU:HA	2.19	0.42
1:A:97:GLU:OE2	1:A:100:SER:OG	2.32	0.42
1:D:470:GLU:HB2	1:D:490:VAL:HG21	2.02	0.42
1:E:146:VAL:N	1:E:147:PRO:CD	2.82	0.42
1:J:380:ASP:O	1:J:381:VAL:HG13	2.20	0.42
1:K:410:GLU:N	1:K:411:PRO:CD	2.82	0.42
1:L:407:TYR:CE1	1:L:431:ILE:HD11	2.54	0.42
1:D:32:LEU:HA	1:D:35:LYS:HE3	2.01	0.42
1:D:339:LEU:HD21	1:D:349:THR:HG21	2.02	0.42
1:E:83:ALA:HA	1:E:395:MET:O	2.19	0.42
1:F:217:ASP:OD1	1:F:217:ASP:C	2.58	0.42
1:H:74:ILE:HG13	1:H:81:MET:HB2	2.02	0.42
1:I:217:ASP:HB2	1:I:218:PRO:HD2	2.00	0.42
1:J:118:ILE:HG21	2:J:601:HEM:HMD1	2.01	0.42
1:K:401:LEU:HD13	1:K:431:ILE:HD12	2.02	0.42
1:L:184:ILE:HD13	1:L:184:ILE:HA	1.85	0.42
1:L:291:SER:H	1:L:294:GLU:HG3	1.84	0.42
1:L:359:VAL:HA	1:L:416:PRO:HB3	2.02	0.42
1:L:475:LEU:O	1:L:476:LYS:HE2	2.20	0.42
1:A:258:GLU:C	1:A:260:ARG:H	2.24	0.42
1:B:89:MET:HG2	1:B:383:ILE:HD12	2.02	0.42
1:C:414:PHE:O	1:C:415:LEU:HD23	2.20	0.42
1:D:101:VAL:HG11	1:D:381:VAL:HG11	2.01	0.42
1:D:134:SER:HB2	1:D:135:PRO:HD3	2.02	0.42
1:D:138:THR:OG1	1:D:141:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:358:MET:CE	1:F:416:PRO:O	2.67	0.42
1:F:415:LEU:O	1:F:416:PRO:C	2.57	0.42
1:G:89:MET:CE	1:G:386:MET:HE2	2.50	0.42
1:I:143:LYS:NZ	1:I:348:ASP:OD1	2.52	0.42
1:J:414:PHE:O	1:J:415:LEU:HD12	2.20	0.42
1:K:65:TYR:CE1	1:K:85:THR:HG21	2.55	0.42
1:K:449:LEU:HD23	1:K:449:LEU:HA	1.87	0.42
1:A:198:ASN:N	1:A:199:PRO:CD	2.83	0.41
1:F:483:LEU:HD12	1:F:483:LEU:HA	1.92	0.41
1:K:110:PRO:HB3	1:K:230:THR:HG23	2.02	0.41
1:K:445:MET:O	1:K:449:LEU:HG	2.20	0.41
1:L:199:PRO:CA	1:L:204:VAL:HG11	2.49	0.41
1:A:373:LEU:HD11	1:A:436:GLY:HA2	2.02	0.41
1:C:161:ARG:HB2	1:C:463:PHE:HZ	1.85	0.41
1:C:181:MET:HE1	1:C:208:LYS:HG2	2.02	0.41
1:C:193:ILE:HD12	1:C:201:ASP:OD2	2.19	0.41
1:D:254:LYS:HA	1:D:254:LYS:HD3	1.77	0.41
1:D:339:LEU:CD2	1:D:349:THR:HG21	2.50	0.41
1:E:414:PHE:O	1:E:415:LEU:HD23	2.20	0.41
1:G:200:GLN:O	1:G:201:ASP:C	2.59	0.41
1:G:373:LEU:HB2	1:G:396:ILE:HB	2.01	0.41
1:G:448:ALA:O	1:G:452:MET:HG3	2.20	0.41
1:I:270:ASP:O	1:I:271:PHE:C	2.57	0.41
1:I:383:ILE:O	1:I:383:ILE:HG13	2.20	0.41
1:J:91:LYS:HD2	1:J:430:TYR:CE1	2.54	0.41
1:J:478:ARG:NH1	1:J:485:THR:O	2.53	0.41
1:L:115:LYS:HE2	1:L:234:GLU:OE2	2.20	0.41
1:L:358:MET:HB3	1:L:416:PRO:O	2.21	0.41
1:A:414:PHE:O	1:A:415:LEU:HD23	2.20	0.41
1:A:470:GLU:HB2	1:A:490:VAL:HG21	2.02	0.41
1:B:354:GLU:O	1:B:357:ASP:HB2	2.21	0.41
1:F:404:ASP:HB3	1:F:407:TYR:HD1	1.86	0.41
2:H:601:HEM:HBB2	2:H:601:HEM:CMB	2.49	0.41
1:J:123:ASP:OD1	1:J:378:LYS:NZ	2.51	0.41
1:J:148:ILE:HG13	1:J:149:ILE:HG13	2.02	0.41
1:J:338:VAL:HG12	1:J:349:THR:HG22	2.02	0.41
1:A:101:VAL:HG21	1:A:381:VAL:HG11	2.01	0.41
1:D:335:ILE:O	1:D:339:LEU:N	2.42	0.41
1:E:339:LEU:HD21	1:E:349:THR:HB	2.02	0.41
1:F:219:PHE:CD1	1:F:240:VAL:HG23	2.55	0.41
1:I:431:ILE:HD13	1:I:431:ILE:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:327:VAL:O	1:J:331:VAL:HG23	2.21	0.41
1:K:53:PHE:N	1:K:53:PHE:CD1	2.87	0.41
1:K:369:VAL:HA	1:K:483:LEU:HD23	2.01	0.41
1:L:298:GLN:HB3	1:L:302:PHE:CZ	2.55	0.41
1:D:189:PHE:CE2	1:D:303:ILE:CD1	3.00	0.41
1:E:250:THR:HA	1:E:296:MET:HE2	2.03	0.41
1:G:102:PHE:HB3	1:G:375:ARG:HB3	2.03	0.41
1:G:181:MET:HB2	1:G:307:TYR:CD2	2.56	0.41
1:I:83:ALA:HA	1:I:395:MET:O	2.19	0.41
1:L:248:PHE:CD2	1:L:249:LEU:CD2	2.96	0.41
1:A:126:TRP:CE2	1:A:440:ARG:HD2	2.56	0.41
1:A:173:LYS:HE2	1:A:173:LYS:HB2	1.86	0.41
1:A:217:ASP:O	1:A:221:LEU:HG	2.21	0.41
1:B:214:ASN:OD1	1:B:216:LEU:N	2.43	0.41
1:C:380:ASP:O	1:C:381:VAL:HG13	2.20	0.41
1:E:76:ASP:OD2	1:E:106:ARG:NH2	2.49	0.41
1:F:221:LEU:HD12	1:F:221:LEU:H	1.84	0.41
1:F:478:ARG:NH1	1:F:484:LEU:HD23	2.30	0.41
1:H:101:VAL:HG21	1:H:381:VAL:HG11	2.03	0.41
1:H:272:LEU:O	1:H:276:ILE:HG13	2.20	0.41
1:I:189:PHE:CE2	1:I:303:ILE:HD11	2.56	0.41
1:I:283:ASP:OD2	1:I:283:ASP:N	2.53	0.41
1:I:334:GLU:O	1:I:338:VAL:HG23	2.20	0.41
1:J:383:ILE:O	1:J:383:ILE:HG12	2.20	0.41
1:A:70:LYS:O	1:A:71:VAL:HG23	2.21	0.41
1:A:483:LEU:O	1:A:484:LEU:HD23	2.21	0.41
1:B:125:GLU:O	1:B:129:ILE:HG13	2.20	0.41
1:B:191:VAL:HG23	1:B:256:ILE:HD13	2.02	0.41
1:C:181:MET:HE3	1:C:208:LYS:HE2	2.03	0.41
1:D:148:ILE:HD12	1:D:269:VAL:CG1	2.51	0.41
1:F:181:MET:O	1:F:182:ASP:C	2.56	0.41
1:I:173:LYS:O	1:I:177:GLY:N	2.45	0.41
1:I:408:TRP:HB2	1:I:411:PRO:HB3	2.03	0.41
1:J:308:GLU:HB3	1:J:482:LEU:HD23	2.03	0.41
1:K:240:VAL:HG22	1:K:240:VAL:O	2.20	0.41
1:L:408:TRP:HB2	1:L:411:PRO:HB3	2.03	0.41
1:A:214:ASN:OD1	1:A:214:ASN:C	2.58	0.41
1:G:44:LEU:HB3	1:G:45:PRO:HD2	2.03	0.41
1:G:118:ILE:HG23	1:G:119:SER:N	2.35	0.41
1:I:32:LEU:HD12	1:I:32:LEU:C	2.41	0.41
1:I:118:ILE:HD12	1:I:133:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:302:PHE:O	1:L:303:ILE:C	2.59	0.41
1:A:116:ASN:O	1:A:129:ILE:HD13	2.20	0.41
1:A:212:ARG:O	1:J:212:ARG:NH2	2.54	0.41
1:B:113:PHE:HB2	1:B:293:LEU:HD21	2.03	0.41
1:B:446:ARG:HG3	1:B:446:ARG:NH1	2.36	0.41
1:C:383:ILE:HD13	1:C:388:ILE:HD12	2.02	0.41
1:C:458:ARG:HA	1:C:458:ARG:HD2	1.91	0.41
1:C:475:LEU:CD2	1:C:485:THR:HG22	2.50	0.41
1:D:193:ILE:HD12	1:D:204:VAL:HG22	2.03	0.41
1:E:230:THR:HB	1:E:231:PRO:HD3	2.03	0.41
1:E:472:GLN:OE1	1:E:475:LEU:HD12	2.21	0.41
1:F:371:MET:CG	1:F:483:LEU:HD13	2.50	0.41
1:F:373:LEU:HD11	1:F:436:GLY:HA2	2.03	0.41
1:G:189:PHE:CE2	1:G:303:ILE:CD1	3.04	0.41
1:G:201:ASP:HB3	1:G:204:VAL:HG23	2.02	0.41
1:G:389:PRO:HG2	1:G:392:VAL:CG2	2.50	0.41
1:I:187:THR:HG23	1:I:271:PHE:HD2	1.85	0.41
1:I:359:VAL:HG23	1:I:414:PHE:CZ	2.42	0.41
1:I:482:LEU:HD23	1:I:482:LEU:HA	1.92	0.41
1:J:159:ASN:O	1:J:163:GLU:HG2	2.21	0.41
1:J:316:PHE:CE2	1:J:475:LEU:HD11	2.55	0.41
1:K:105:ARG:NH2	2:K:601:HEM:HAD2	2.35	0.41
1:K:251:LYS:HE2	1:K:251:LYS:HB3	1.91	0.41
1:K:470:GLU:HB2	1:K:490:VAL:HG21	2.03	0.41
1:K:473:ILE:HB	1:K:474:PRO:CD	2.51	0.41
1:L:226:PHE:HB3	1:L:228:PHE:CZ	2.56	0.41
1:L:406:LYS:HD3	1:L:407:TYR:CZ	2.56	0.41
1:A:171:THR:O	1:A:174:HIS:HB3	2.21	0.41
1:A:268:ARG:HB2	1:A:273:GLN:HG2	2.03	0.41
1:F:70:LYS:O	1:F:85:THR:OG1	2.24	0.41
1:F:294:GLU:O	1:F:298:GLN:HG2	2.21	0.41
1:F:415:LEU:N	1:F:415:LEU:CD2	2.83	0.41
1:G:458:ARG:HA	1:G:458:ARG:HD2	1.95	0.41
1:H:473:ILE:HB	1:H:474:PRO:CD	2.51	0.41
1:J:102:PHE:CE2	1:J:394:VAL:HG21	2.56	0.41
1:J:420:SER:O	1:J:424:ALA:N	2.52	0.41
1:J:426:ASN:C	1:J:427:ILE:HD13	2.42	0.41
1:K:115:LYS:HB3	1:K:115:LYS:HE3	1.95	0.41
1:L:54:ARG:HA	1:L:479:PHE:CE1	2.56	0.41
1:L:301:ILE:CG2	1:L:302:PHE:N	2.84	0.41
1:B:458:ARG:HA	1:B:458:ARG:HD3	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:ASP:HB3	1:E:89:MET:HB2	2.02	0.40
1:H:52:SER:HB3	1:H:60:PHE:CE1	2.56	0.40
1:H:71:VAL:HG13	1:H:82:LEU:HD11	2.02	0.40
1:H:308:GLU:HB3	1:H:482:LEU:HD23	2.04	0.40
1:J:190:GLY:HA2	1:J:270:ASP:OD2	2.21	0.40
1:L:346:THR:H	1:L:349:THR:HG1	1.69	0.40
1:A:253:VAL:HA	1:A:256:ILE:HD12	2.02	0.40
1:B:56:GLY:HA3	1:B:58:TRP:CZ3	2.56	0.40
1:B:248:PHE:HD2	1:B:249:LEU:HD23	1.86	0.40
1:B:248:PHE:CD2	1:B:249:LEU:HD23	2.55	0.40
1:E:34:LYS:O	1:E:34:LYS:HD3	2.21	0.40
1:E:175:VAL:HG23	1:E:176:PHE:N	2.36	0.40
1:F:327:VAL:O	1:F:331:VAL:HG23	2.21	0.40
1:H:179:TYR:O	1:H:183:VAL:HG23	2.22	0.40
1:H:244:GLU:O	1:H:247:SER:OG	2.36	0.40
1:J:153:GLY:O	1:J:157:VAL:HG23	2.21	0.40
1:K:350:VAL:CG2	1:K:453:LYS:HB3	2.51	0.40
1:K:379:LYS:HA	1:K:390:LYS:HG3	2.03	0.40
1:L:136:THR:O	1:L:136:THR:HG22	2.21	0.40
1:C:350:VAL:HG21	1:C:454:LEU:HD23	2.02	0.40
1:E:250:THR:HA	1:E:296:MET:HE3	2.03	0.40
1:F:365:ARG:O	1:F:402:HIS:HB3	2.21	0.40
1:G:477:LEU:HD13	1:G:483:LEU:HD22	2.03	0.40
1:I:190:GLY:CA	1:I:270:ASP:OD2	2.69	0.40
1:J:382:GLU:HA	1:J:386:MET:O	2.22	0.40
1:J:468:CYS:SG	1:J:470:GLU:N	2.94	0.40
1:K:271:PHE:O	1:K:272:LEU:C	2.60	0.40
1:L:301:ILE:HD12	1:L:301:ILE:HA	1.86	0.40
1:L:336:ASP:O	1:L:340:PRO:HA	2.21	0.40
1:E:200:GLN:CG	1:L:171:THR:HG21	2.52	0.40
1:G:191:VAL:O	1:G:191:VAL:CG1	2.69	0.40
1:H:154:ASP:O	1:H:157:VAL:HG12	2.21	0.40
1:I:118:ILE:HG23	1:I:119:SER:N	2.36	0.40
1:L:210:LEU:C	1:L:210:LEU:HD23	2.42	0.40
1:C:181:MET:O	1:C:182:ASP:C	2.60	0.40
1:E:32:LEU:HD11	1:E:36:LEU:HD11	2.03	0.40
1:E:370:ALA:O	1:E:371:MET:HB2	2.21	0.40
1:K:354:GLU:OE1	1:K:354:GLU:CA	2.69	0.40
1:K:463:PHE:CD1	1:K:495:SER:HA	2.57	0.40
1:L:355:TYR:O	1:L:359:VAL:HG23	2.21	0.40
1:L:365:ARG:O	1:L:368:PRO:HD3	2.21	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	471/486 (97%)	435 (92%)	35 (7%)	1 (0%)	47	71
1	B	456/486 (94%)	423 (93%)	30 (7%)	3 (1%)	22	43
1	C	459/486 (94%)	425 (93%)	30 (6%)	4 (1%)	17	35
1	D	453/486 (93%)	421 (93%)	30 (7%)	2 (0%)	34	57
1	E	454/486 (93%)	421 (93%)	31 (7%)	2 (0%)	34	57
1	F	455/486 (94%)	425 (93%)	28 (6%)	2 (0%)	34	57
1	G	456/486 (94%)	419 (92%)	36 (8%)	1 (0%)	47	71
1	H	452/486 (93%)	412 (91%)	37 (8%)	3 (1%)	22	43
1	I	459/486 (94%)	432 (94%)	25 (5%)	2 (0%)	34	57
1	J	452/486 (93%)	418 (92%)	32 (7%)	2 (0%)	34	57
1	K	456/486 (94%)	415 (91%)	40 (9%)	1 (0%)	47	71
1	L	434/486 (89%)	376 (87%)	53 (12%)	5 (1%)	13	27
All	All	5457/5832 (94%)	5022 (92%)	407 (8%)	28 (0%)	29	52

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	473	ILE
1	D	166	THR
1	L	212	ARG
1	C	252	SER
1	C	473	ILE
1	E	228	PHE
1	F	472	GLN
1	G	307	TYR
1	I	123	ASP

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Mol	Chain	Res	Type
1	L	473	ILE
1	B	243	ARG
1	C	123	ASP
1	C	253	VAL
1	H	309	THR
1	I	124	GLU
1	J	384	ASN
1	B	289	ALA
1	E	472	GLN
1	F	307	TYR
1	H	113	PHE
1	J	261	LEU
1	K	470	GLU
1	L	347	TYR
1	B	112	GLY
1	D	331	VAL
1	L	439	PRO
1	H	473	ILE
1	L	202	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	428/438 (98%)	421 (98%)	7 (2%)	62 82
1	B	417/438 (95%)	409 (98%)	8 (2%)	57 79
1	C	419/438 (96%)	406 (97%)	13 (3%)	40 66
1	D	415/438 (95%)	407 (98%)	8 (2%)	57 79
1	E	416/438 (95%)	407 (98%)	9 (2%)	52 76
1	F	416/438 (95%)	400 (96%)	16 (4%)	33 59
1	G	417/438 (95%)	408 (98%)	9 (2%)	52 76
1	H	414/438 (94%)	396 (96%)	18 (4%)	29 54
1	I	419/438 (96%)	411 (98%)	8 (2%)	57 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	414/438 (94%)	404 (98%)	10 (2%)	49 74
1	K	417/438 (95%)	406 (97%)	11 (3%)	46 72
1	L	397/438 (91%)	372 (94%)	25 (6%)	18 36
All	All	4989/5256 (95%)	4847 (97%)	142 (3%)	43 69

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	115	LYS
1	A	200	GLN
1	A	232	ILE
1	A	260	ARG
1	A	296	MET
1	A	471	THR
1	B	28	ARG
1	B	118	ILE
1	B	203	PHE
1	B	251	LYS
1	B	262	LYS
1	B	286	THR
1	B	440	ARG
1	B	458	ARG
1	C	70	LYS
1	C	124	GLU
1	C	131	SER
1	C	154	ASP
1	C	244	GLU
1	C	269	VAL
1	C	287	HIS
1	C	383	ILE
1	C	410	GLU
1	C	458	ARG
1	C	475	LEU
1	C	482	LEU
1	C	484	LEU
1	D	104	ASN
1	D	106	ARG
1	D	186	SER
1	D	192	SER
1	D	196	LEU

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Mol	Chain	Res	Type
1	D	472	GLN
1	D	482	LEU
1	D	484	LEU
1	E	62	MET
1	E	209	LYS
1	E	244	GLU
1	E	286	THR
1	E	296	MET
1	E	311	SER
1	E	458	ARG
1	E	482	LEU
1	E	489	ILE
1	F	106	ARG
1	F	143	LYS
1	F	151	GLN
1	F	181	MET
1	F	186	SER
1	F	187	THR
1	F	192	SER
1	F	212	ARG
1	F	240	VAL
1	F	261	LEU
1	F	349	THR
1	F	353	LEU
1	F	413	LYS
1	F	476	LYS
1	F	482	LEU
1	F	484	LEU
1	G	55	LYS
1	G	129	ILE
1	G	209	LYS
1	G	214	ASN
1	G	280	ASN
1	G	374	GLU
1	G	378	LYS
1	G	472	GLN
1	G	475	LEU
1	H	32	LEU
1	H	54	ARG
1	H	124	GLU
1	H	168	LYS
1	H	170	VAL

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Mol	Chain	Res	Type
1	H	184	ILE
1	H	214	ASN
1	H	217	ASP
1	H	246	ILE
1	H	254	LYS
1	H	261	LEU
1	H	351	LEU
1	H	446	ARG
1	H	469	LYS
1	H	471	THR
1	H	475	LEU
1	H	489	ILE
1	H	497	ASP
1	I	74	ILE
1	I	124	GLU
1	I	171	THR
1	I	228	PHE
1	I	406	LYS
1	I	407	TYR
1	I	475	LEU
1	I	484	LEU
1	J	243	ARG
1	J	246	ILE
1	J	342	LYS
1	J	383	ILE
1	J	446	ARG
1	J	472	GLN
1	J	473	ILE
1	J	475	LEU
1	J	476	LYS
1	J	482	LEU
1	K	28	ARG
1	K	51	LEU
1	K	108	PHE
1	K	165	GLU
1	K	173	LYS
1	K	221	LEU
1	K	232	ILE
1	K	291	SER
1	K	354	GLU
1	K	410	GLU
1	K	483	LEU

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Mol	Chain	Res	Type
1	L	84	ILE
1	L	96	LYS
1	L	111	VAL
1	L	114	MET
1	L	138	THR
1	L	139	SER
1	L	184	ILE
1	L	185	THR
1	L	187	THR
1	L	203	PHE
1	L	205	GLU
1	L	207	THR
1	L	210	LEU
1	L	212	ARG
1	L	247	SER
1	L	290	LEU
1	L	292	ASP
1	L	298	GLN
1	L	299	SER
1	L	300	ILE
1	L	381	VAL
1	L	383	ILE
1	L	388	ILE
1	L	462	ASN
1	L	472	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	78	GLN
1	J	78	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

36 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEM	F	601	-	41,50,50	1.46	3 (7%)	45,82,82	1.29	6 (13%)
3	ZWY	D	605	-	28,28,28	2.36	9 (32%)	42,46,46	3.68	22 (52%)
3	ZWY	A	602	-	28,28,28	2.28	11 (39%)	42,46,46	3.53	18 (42%)
2	HEM	L	601	-	41,50,50	1.50	5 (12%)	45,82,82	1.38	7 (15%)
3	ZWY	C	605	-	28,28,28	2.22	8 (28%)	42,46,46	3.68	23 (54%)
3	ZWY	C	603	-	28,28,28	2.38	10 (35%)	42,46,46	3.98	20 (47%)
2	HEM	E	601	1	41,50,50	1.49	6 (14%)	45,82,82	1.35	5 (11%)
3	ZWY	H	603	-	28,28,28	2.34	9 (32%)	42,46,46	3.77	20 (47%)
3	ZWY	B	602	-	28,28,28	2.37	8 (28%)	42,46,46	4.01	21 (50%)
3	ZWY	C	602	-	28,28,28	2.19	8 (28%)	42,46,46	3.63	18 (42%)
3	ZWY	B	603	-	28,28,28	2.18	9 (32%)	42,46,46	3.61	18 (42%)
3	ZWY	D	606	-	28,28,28	2.46	11 (39%)	42,46,46	3.72	21 (50%)
3	ZWY	H	602	-	28,28,28	2.38	9 (32%)	42,46,46	3.62	20 (47%)
3	ZWY	D	604	-	28,28,28	2.36	11 (39%)	42,46,46	3.82	20 (47%)
3	ZWY	D	602	-	28,28,28	2.24	9 (32%)	42,46,46	3.60	18 (42%)
2	HEM	J	601	-	41,50,50	1.48	3 (7%)	45,82,82	1.35	5 (11%)
3	ZWY	I	602	-	28,28,28	2.23	9 (32%)	42,46,46	3.60	17 (40%)
2	HEM	B	601	1	41,50,50	1.45	4 (9%)	45,82,82	1.43	6 (13%)
3	ZWY	I	603	-	28,28,28	2.25	9 (32%)	42,46,46	3.67	23 (54%)
3	ZWY	E	605	-	28,28,28	2.28	9 (32%)	42,46,46	3.59	22 (52%)
2	HEM	G	601	-	41,50,50	1.45	3 (7%)	45,82,82	1.28	6 (13%)
3	ZWY	J	603	-	28,28,28	2.25	9 (32%)	42,46,46	3.68	23 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEM	A	601	1	41,50,50	1.49	5 (12%)	45,82,82	1.40	7 (15%)
3	ZWY	E	603	-	28,28,28	2.32	9 (32%)	42,46,46	3.56	22 (52%)
2	HEM	C	601	1	41,50,50	1.50	3 (7%)	45,82,82	1.43	6 (13%)
3	ZWY	C	604	-	28,28,28	2.16	9 (32%)	42,46,46	3.54	20 (47%)
3	ZWY	J	602	-	28,28,28	2.36	8 (28%)	42,46,46	3.60	18 (42%)
2	HEM	D	601	1	41,50,50	1.45	4 (9%)	45,82,82	1.43	6 (13%)
3	ZWY	E	602	-	28,28,28	2.37	9 (32%)	42,46,46	3.64	20 (47%)
2	HEM	H	601	1	41,50,50	1.46	3 (7%)	45,82,82	1.35	6 (13%)
3	ZWY	H	604	-	28,28,28	2.14	8 (28%)	42,46,46	3.57	22 (52%)
3	ZWY	A	603	-	28,28,28	2.44	9 (32%)	42,46,46	3.93	23 (54%)
3	ZWY	D	603	-	28,28,28	2.39	11 (39%)	42,46,46	3.87	22 (52%)
3	ZWY	E	604	-	28,28,28	2.27	8 (28%)	42,46,46	3.56	18 (42%)
2	HEM	K	601	1	41,50,50	1.47	4 (9%)	45,82,82	1.42	7 (15%)
2	HEM	I	601	1	41,50,50	1.47	4 (9%)	45,82,82	1.37	5 (11%)

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
2	HEM	F	601	-	-	2/12/54/54	-
3	ZWY	D	605	-	-	0/5/63/63	0/4/4/4
3	ZWY	A	602	-	-	0/5/63/63	0/4/4/4
2	HEM	L	601	-	-	4/12/54/54	-
3	ZWY	C	605	-	-	1/5/63/63	0/4/4/4
3	ZWY	C	603	-	-	0/5/63/63	0/4/4/4
2	HEM	E	601	1	-	2/12/54/54	-
3	ZWY	H	603	-	-	1/5/63/63	0/4/4/4
3	ZWY	B	602	-	-	0/5/63/63	0/4/4/4
3	ZWY	C	602	-	-	0/5/63/63	0/4/4/4
3	ZWY	B	603	-	-	0/5/63/63	0/4/4/4
3	ZWY	D	606	-	-	0/5/63/63	0/4/4/4
3	ZWY	H	602	-	-	0/5/63/63	0/4/4/4
3	ZWY	D	604	-	-	0/5/63/63	0/4/4/4
3	ZWY	D	602	-	-	0/5/63/63	0/4/4/4
2	HEM	J	601	-	-	2/12/54/54	-
3	ZWY	I	602	-	-	0/5/63/63	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	601	1	-	2/12/54/54	-
3	ZWY	I	603	-	-	0/5/63/63	0/4/4/4
3	ZWY	E	605	-	-	0/5/63/63	0/4/4/4
2	HEM	G	601	-	-	0/12/54/54	-
3	ZWY	J	603	-	-	0/5/63/63	0/4/4/4
2	HEM	A	601	1	-	2/12/54/54	-
3	ZWY	E	603	-	-	2/5/63/63	0/4/4/4
2	HEM	C	601	1	-	2/12/54/54	-
3	ZWY	C	604	-	-	0/5/63/63	0/4/4/4
3	ZWY	J	602	-	-	0/5/63/63	0/4/4/4
2	HEM	D	601	1	-	2/12/54/54	-
3	ZWY	E	602	-	-	3/5/63/63	0/4/4/4
2	HEM	H	601	1	-	0/12/54/54	-
3	ZWY	H	604	-	-	2/5/63/63	0/4/4/4
3	ZWY	A	603	-	-	0/5/63/63	0/4/4/4
3	ZWY	D	603	-	-	2/5/63/63	0/4/4/4
3	ZWY	E	604	-	-	0/5/63/63	0/4/4/4
2	HEM	K	601	1	-	4/12/54/54	-
2	HEM	I	601	1	-	3/12/54/54	-

All (266) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	606	ZWY	C25-C15	-7.83	1.41	1.54
3	E	603	ZWY	C25-C15	-7.59	1.41	1.54
3	A	603	ZWY	C25-C15	-7.40	1.41	1.54
3	D	603	ZWY	C25-C15	-7.34	1.42	1.54
3	C	603	ZWY	C25-C15	-7.31	1.42	1.54
3	I	603	ZWY	C25-C15	-7.28	1.42	1.54
3	J	602	ZWY	C25-C15	-7.28	1.42	1.54
3	E	604	ZWY	C25-C15	-7.24	1.42	1.54
3	H	603	ZWY	C25-C15	-7.23	1.42	1.54
3	B	602	ZWY	C25-C15	-7.19	1.42	1.54
3	C	605	ZWY	C25-C15	-7.17	1.42	1.54
3	D	605	ZWY	C25-C15	-7.11	1.42	1.54
3	D	602	ZWY	C25-C15	-7.11	1.42	1.54
3	H	602	ZWY	C25-C15	-7.07	1.42	1.54
3	H	604	ZWY	C25-C15	-7.07	1.42	1.54
3	D	604	ZWY	C25-C15	-7.05	1.42	1.54
3	J	603	ZWY	C25-C15	-7.03	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	ZWY	C25-C15	-7.01	1.42	1.54
3	B	603	ZWY	C25-C15	-7.00	1.42	1.54
3	A	602	ZWY	C25-C15	-6.99	1.42	1.54
3	I	602	ZWY	C25-C15	-6.87	1.42	1.54
3	E	605	ZWY	C25-C15	-6.87	1.42	1.54
3	C	602	ZWY	C25-C15	-6.81	1.42	1.54
3	C	604	ZWY	C25-C15	-6.58	1.43	1.54
3	D	603	ZWY	C12-C06	-5.08	1.44	1.53
2	H	601	HEM	C3C-C2C	-4.87	1.33	1.40
2	C	601	HEM	C3C-C2C	-4.87	1.33	1.40
3	C	603	ZWY	C12-C06	-4.81	1.45	1.53
3	A	603	ZWY	C12-C06	-4.62	1.45	1.53
3	H	602	ZWY	C02-C10	-4.59	1.46	1.52
2	J	601	HEM	C3C-C2C	-4.53	1.34	1.40
3	H	603	ZWY	C16-C15	-4.52	1.45	1.54
3	J	602	ZWY	C02-C10	-4.35	1.46	1.52
2	E	601	HEM	C3C-C2C	-4.35	1.34	1.40
2	I	601	HEM	C3C-C2C	-4.30	1.34	1.40
3	B	602	ZWY	C12-C06	-4.24	1.46	1.53
3	J	603	ZWY	C15-C05	-4.23	1.48	1.56
3	B	602	ZWY	C16-C15	-4.22	1.46	1.54
3	A	603	ZWY	C16-C15	-4.21	1.46	1.54
3	E	605	ZWY	C12-C06	-4.15	1.46	1.53
3	H	603	ZWY	C12-C06	-4.14	1.46	1.53
3	D	604	ZWY	C16-C15	-4.11	1.46	1.54
2	A	601	HEM	C3C-C2C	-4.10	1.34	1.40
3	E	602	ZWY	C02-C10	-4.09	1.46	1.52
2	D	601	HEM	C3C-C2C	-4.03	1.34	1.40
3	C	603	ZWY	C16-C15	-4.02	1.46	1.54
3	H	602	ZWY	C12-C06	-4.00	1.46	1.53
3	D	606	ZWY	C15-C05	-4.00	1.49	1.56
2	F	601	HEM	C3C-C2C	-3.98	1.34	1.40
3	D	605	ZWY	C12-C06	-3.97	1.46	1.53
3	E	604	ZWY	C15-C05	-3.95	1.49	1.56
3	E	604	ZWY	C02-C10	-3.93	1.47	1.52
3	I	603	ZWY	C15-C05	-3.92	1.49	1.56
3	D	603	ZWY	C16-C15	-3.92	1.46	1.54
3	D	602	ZWY	C15-C05	-3.90	1.49	1.56
2	G	601	HEM	C3C-C2C	-3.90	1.35	1.40
3	A	602	ZWY	C16-C15	-3.85	1.46	1.54
2	B	601	HEM	C3C-CAC	3.83	1.55	1.47
2	K	601	HEM	C3C-CAC	3.83	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	605	ZWY	C16-C15	-3.82	1.46	1.54
3	H	602	ZWY	C16-C15	-3.82	1.46	1.54
3	E	602	ZWY	C12-C06	-3.82	1.46	1.53
3	C	605	ZWY	C15-C05	-3.81	1.49	1.56
3	E	605	ZWY	C02-C10	-3.79	1.47	1.52
3	J	602	ZWY	C12-C06	-3.78	1.46	1.53
2	L	601	HEM	C3C-CAC	3.78	1.55	1.47
2	L	601	HEM	C3C-C2C	-3.75	1.35	1.40
3	B	602	ZWY	C15-C05	-3.75	1.49	1.56
2	K	601	HEM	C3C-C2C	-3.71	1.35	1.40
3	E	602	ZWY	C15-C05	-3.70	1.49	1.56
3	H	602	ZWY	C15-C05	-3.70	1.49	1.56
3	D	605	ZWY	C16-C15	-3.70	1.47	1.54
3	I	602	ZWY	C16-C15	-3.70	1.47	1.54
3	D	606	ZWY	O20-C18	-3.70	1.40	1.48
2	B	601	HEM	C3C-C2C	-3.69	1.35	1.40
3	E	602	ZWY	C16-C15	-3.68	1.47	1.54
3	D	605	ZWY	C15-C05	-3.68	1.49	1.56
3	D	604	ZWY	C15-C05	-3.68	1.49	1.56
3	E	603	ZWY	C16-C15	-3.68	1.47	1.54
2	A	601	HEM	C3C-CAC	3.68	1.55	1.47
3	D	605	ZWY	O20-C18	-3.67	1.40	1.48
2	F	601	HEM	C3C-CAC	3.66	1.55	1.47
2	D	601	HEM	C3C-CAC	3.65	1.55	1.47
3	B	603	ZWY	C15-C14	-3.64	1.45	1.52
3	D	606	ZWY	C16-C15	-3.63	1.47	1.54
2	G	601	HEM	C3C-CAC	3.62	1.55	1.47
3	C	604	ZWY	C15-C05	-3.60	1.50	1.56
3	D	605	ZWY	C15-C14	-3.60	1.45	1.52
3	C	602	ZWY	C02-C10	-3.60	1.47	1.52
3	B	602	ZWY	C02-C10	-3.59	1.47	1.52
3	C	602	ZWY	C15-C05	-3.59	1.50	1.56
3	H	604	ZWY	C15-C05	-3.57	1.50	1.56
3	E	603	ZWY	C15-C05	-3.56	1.50	1.56
3	J	602	ZWY	C15-C05	-3.56	1.50	1.56
3	I	602	ZWY	C12-C06	-3.55	1.47	1.53
3	D	606	ZWY	C12-C06	-3.55	1.47	1.53
3	E	603	ZWY	C12-C06	-3.55	1.47	1.53
3	J	602	ZWY	O20-C18	-3.54	1.40	1.48
3	C	602	ZWY	C16-C15	-3.54	1.47	1.54
3	D	602	ZWY	C12-C06	-3.54	1.47	1.53
3	I	602	ZWY	C02-C10	-3.54	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	604	ZWY	C16-C15	-3.53	1.47	1.54
3	D	606	ZWY	C02-C10	-3.53	1.47	1.52
3	E	603	ZWY	C02-C10	-3.53	1.47	1.52
3	I	603	ZWY	C15-C14	-3.53	1.45	1.52
3	J	603	ZWY	C15-C14	-3.52	1.45	1.52
3	C	603	ZWY	C15-C05	-3.49	1.50	1.56
3	E	602	ZWY	O20-C18	-3.49	1.41	1.48
3	A	603	ZWY	C15-C14	-3.48	1.46	1.52
3	A	603	ZWY	O20-C18	-3.48	1.41	1.48
2	I	601	HEM	C3C-CAC	3.47	1.54	1.47
3	D	604	ZWY	C15-C14	-3.46	1.46	1.52
3	D	602	ZWY	C16-C15	-3.45	1.47	1.54
2	C	601	HEM	C3C-CAC	3.45	1.54	1.47
3	D	604	ZWY	C12-C06	-3.43	1.47	1.53
3	E	605	ZWY	O20-C18	-3.43	1.41	1.48
3	A	602	ZWY	C15-C05	-3.42	1.50	1.56
3	A	602	ZWY	C02-C10	-3.42	1.47	1.52
2	J	601	HEM	C3C-CAC	3.41	1.54	1.47
2	E	601	HEM	C3C-CAC	3.40	1.54	1.47
3	D	603	ZWY	C02-C10	-3.40	1.47	1.52
3	H	603	ZWY	C15-C05	-3.39	1.50	1.56
2	H	601	HEM	C3C-CAC	3.39	1.54	1.47
3	H	602	ZWY	C15-C14	-3.37	1.46	1.52
3	D	604	ZWY	C02-C10	-3.37	1.47	1.52
3	J	603	ZWY	C12-C06	-3.36	1.47	1.53
3	E	604	ZWY	C15-C14	-3.34	1.46	1.52
3	J	602	ZWY	C16-C15	-3.33	1.47	1.54
3	J	603	ZWY	C16-C15	-3.33	1.47	1.54
3	A	603	ZWY	C15-C05	-3.33	1.50	1.56
3	I	602	ZWY	C15-C05	-3.32	1.50	1.56
3	C	605	ZWY	C15-C14	-3.32	1.46	1.52
3	D	603	ZWY	C15-C14	-3.32	1.46	1.52
3	C	602	ZWY	O20-C18	-3.32	1.41	1.48
3	E	605	ZWY	C15-C14	-3.31	1.46	1.52
3	E	602	ZWY	C15-C14	-3.31	1.46	1.52
3	A	602	ZWY	C15-C14	-3.31	1.46	1.52
3	A	603	ZWY	C02-C10	-3.31	1.47	1.52
3	C	604	ZWY	C15-C14	-3.30	1.46	1.52
3	C	603	ZWY	C02-C10	-3.30	1.47	1.52
3	C	605	ZWY	C16-C15	-3.28	1.48	1.54
3	B	602	ZWY	C15-C14	-3.27	1.46	1.52
3	I	603	ZWY	C02-C10	-3.26	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	ZWY	C15-C05	-3.26	1.50	1.56
3	D	602	ZWY	O20-C18	-3.25	1.41	1.48
3	D	604	ZWY	O20-C18	-3.24	1.41	1.48
3	C	603	ZWY	C15-C14	-3.22	1.46	1.52
3	H	603	ZWY	C15-C14	-3.21	1.46	1.52
3	B	603	ZWY	C16-C15	-3.17	1.48	1.54
3	H	604	ZWY	C15-C14	-3.14	1.46	1.52
3	E	603	ZWY	C15-C14	-3.14	1.46	1.52
3	B	603	ZWY	C02-C10	-3.13	1.48	1.52
3	C	605	ZWY	C12-C06	-3.11	1.47	1.53
3	E	604	ZWY	C16-C15	-3.11	1.48	1.54
3	H	604	ZWY	O20-C18	-3.09	1.41	1.48
3	E	604	ZWY	C12-C06	-3.07	1.47	1.53
3	H	602	ZWY	O20-C18	-3.05	1.41	1.48
3	C	602	ZWY	C12-C06	-3.04	1.48	1.53
2	L	601	HEM	CAB-C3B	3.04	1.55	1.47
3	J	603	ZWY	C02-C10	-2.99	1.48	1.52
3	J	603	ZWY	O20-C18	-2.98	1.42	1.48
3	B	603	ZWY	O20-C18	-2.98	1.42	1.48
2	E	601	HEM	CAB-C3B	2.97	1.55	1.47
2	F	601	HEM	CAB-C3B	2.97	1.55	1.47
2	K	601	HEM	CAB-C3B	2.96	1.55	1.47
2	H	601	HEM	CAB-C3B	2.96	1.55	1.47
3	H	603	ZWY	O20-C18	-2.96	1.42	1.48
2	C	601	HEM	CAB-C3B	2.95	1.55	1.47
3	I	602	ZWY	C15-C14	-2.95	1.47	1.52
2	A	601	HEM	CAB-C3B	2.95	1.55	1.47
2	B	601	HEM	CAB-C3B	2.95	1.55	1.47
3	C	604	ZWY	C12-C06	-2.94	1.48	1.53
3	C	605	ZWY	C02-C10	-2.93	1.48	1.52
2	J	601	HEM	CAB-C3B	2.93	1.55	1.47
3	C	604	ZWY	C02-C10	-2.93	1.48	1.52
3	D	602	ZWY	C15-C14	-2.93	1.47	1.52
2	G	601	HEM	CAB-C3B	2.93	1.55	1.47
2	D	601	HEM	CAB-C3B	2.91	1.55	1.47
3	I	602	ZWY	O20-C18	-2.90	1.42	1.48
2	I	601	HEM	CAB-C3B	2.89	1.55	1.47
3	H	604	ZWY	C16-C15	-2.89	1.48	1.54
3	E	603	ZWY	O20-C18	-2.88	1.42	1.48
3	H	604	ZWY	C12-C06	-2.87	1.48	1.53
3	I	603	ZWY	C16-C15	-2.87	1.48	1.54
3	D	606	ZWY	C15-C14	-2.86	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	602	ZWY	C15-C14	-2.85	1.47	1.52
3	I	603	ZWY	O20-C18	-2.84	1.42	1.48
3	D	602	ZWY	C02-C10	-2.83	1.48	1.52
3	A	602	ZWY	C12-C06	-2.83	1.48	1.53
3	I	603	ZWY	C12-C06	-2.83	1.48	1.53
3	B	602	ZWY	O20-C18	-2.80	1.42	1.48
3	D	605	ZWY	C02-C10	-2.79	1.48	1.52
3	A	602	ZWY	O20-C18	-2.78	1.42	1.48
3	E	605	ZWY	C15-C05	-2.77	1.51	1.56
3	H	603	ZWY	C02-C10	-2.74	1.48	1.52
3	C	605	ZWY	O20-C18	-2.72	1.42	1.48
3	D	603	ZWY	O20-C18	-2.69	1.42	1.48
3	D	603	ZWY	C15-C05	-2.69	1.51	1.56
3	E	604	ZWY	O20-C18	-2.68	1.42	1.48
3	D	606	ZWY	C13-C14	-2.67	1.27	1.33
3	B	603	ZWY	C12-C06	-2.64	1.48	1.53
3	H	604	ZWY	C02-C10	-2.62	1.48	1.52
3	C	603	ZWY	O20-C18	-2.56	1.42	1.48
3	D	603	ZWY	C13-C14	-2.55	1.27	1.33
3	C	602	ZWY	C15-C14	-2.51	1.47	1.52
3	D	604	ZWY	C13-C14	-2.50	1.27	1.33
3	H	604	ZWY	C13-C14	-2.48	1.27	1.33
3	H	603	ZWY	C13-C14	-2.45	1.27	1.33
3	A	602	ZWY	O20-S21	-2.44	1.50	1.57
3	D	605	ZWY	C13-C14	-2.43	1.27	1.33
2	E	601	HEM	FE-ND	2.43	2.08	1.96
3	C	604	ZWY	O20-C18	-2.41	1.43	1.48
3	E	604	ZWY	C13-C14	-2.40	1.27	1.33
3	I	602	ZWY	C03-C02	-2.37	1.49	1.54
3	E	602	ZWY	C13-C14	-2.37	1.27	1.33
3	E	605	ZWY	C13-C14	-2.37	1.27	1.33
3	J	603	ZWY	C13-C14	-2.36	1.27	1.33
3	I	602	ZWY	C13-C14	-2.35	1.27	1.33
3	C	602	ZWY	C13-C14	-2.35	1.27	1.33
3	J	602	ZWY	C13-C14	-2.31	1.27	1.33
2	K	601	HEM	FE-ND	2.28	2.08	1.96
3	C	605	ZWY	C13-C14	-2.27	1.27	1.33
3	H	602	ZWY	C19-C18	2.26	1.57	1.52
2	L	601	HEM	FE-NB	2.26	2.08	1.96
3	B	602	ZWY	C19-C18	2.26	1.57	1.52
3	C	603	ZWY	C01-C02	-2.25	1.50	1.54
2	B	601	HEM	CAA-C2A	2.24	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	603	ZWY	C13-C14	-2.23	1.28	1.33
3	D	602	ZWY	C13-C14	-2.21	1.28	1.33
3	C	604	ZWY	C13-C14	-2.21	1.28	1.33
3	A	602	ZWY	C01-C02	-2.21	1.50	1.54
3	D	606	ZWY	C19-C18	2.20	1.57	1.52
3	D	605	ZWY	C03-C02	-2.20	1.50	1.54
3	A	602	ZWY	C13-C14	-2.18	1.28	1.33
2	A	601	HEM	CAA-C2A	2.15	1.55	1.52
3	A	602	ZWY	C03-C02	-2.14	1.50	1.54
3	B	603	ZWY	C06-C07	-2.14	1.49	1.53
3	D	603	ZWY	C03-C02	-2.13	1.50	1.54
3	C	603	ZWY	C13-C14	-2.12	1.28	1.33
3	D	604	ZWY	C01-C02	-2.12	1.51	1.54
2	A	601	HEM	CMB-C2B	2.11	1.55	1.50
2	E	601	HEM	CAA-C2A	2.11	1.55	1.52
3	I	603	ZWY	C13-C14	-2.11	1.28	1.33
3	D	606	ZWY	O20-S21	-2.10	1.51	1.57
3	C	603	ZWY	C19-C18	2.10	1.57	1.52
2	L	601	HEM	CMB-C2B	2.09	1.55	1.50
3	D	604	ZWY	C19-C18	2.09	1.57	1.52
3	J	603	ZWY	C19-C18	2.08	1.57	1.52
2	D	601	HEM	CAA-C2A	2.07	1.55	1.52
3	D	603	ZWY	C19-C18	2.07	1.57	1.52
2	I	601	HEM	FE-ND	2.07	2.07	1.96
3	D	602	ZWY	C03-C02	-2.07	1.50	1.54
3	E	602	ZWY	C19-C18	2.07	1.57	1.52
3	C	604	ZWY	C03-C02	-2.06	1.50	1.54
3	E	605	ZWY	C19-C18	2.06	1.57	1.52
3	D	603	ZWY	C01-C02	-2.06	1.51	1.54
3	H	602	ZWY	C13-C14	-2.06	1.28	1.33
3	B	603	ZWY	C13-C14	-2.05	1.28	1.33
3	E	603	ZWY	C03-C02	-2.05	1.50	1.54
3	H	603	ZWY	C19-C18	2.04	1.56	1.52
3	A	603	ZWY	C03-C02	-2.04	1.50	1.54
2	E	601	HEM	CMB-C2B	2.04	1.55	1.50
3	D	604	ZWY	O20-S21	-2.04	1.51	1.57
3	A	603	ZWY	C13-C14	-2.03	1.28	1.33
3	I	603	ZWY	O20-S21	-2.03	1.51	1.57
3	D	606	ZWY	C01-C02	-2.01	1.51	1.54

All (561) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	ZWY	C25-C15-C14	-15.97	82.50	108.34
3	A	603	ZWY	C25-C15-C14	-15.81	82.77	108.34
3	C	603	ZWY	C25-C15-C14	-15.80	82.78	108.34
3	C	602	ZWY	C25-C15-C14	-15.76	82.84	108.34
3	D	604	ZWY	C25-C15-C14	-15.75	82.86	108.34
3	D	605	ZWY	C25-C15-C14	-15.61	83.08	108.34
3	E	605	ZWY	C25-C15-C14	-15.61	83.09	108.34
3	H	602	ZWY	C25-C15-C14	-15.60	83.10	108.34
3	D	602	ZWY	C25-C15-C14	-15.59	83.12	108.34
3	I	602	ZWY	C25-C15-C14	-15.57	83.16	108.34
3	H	603	ZWY	C25-C15-C14	-15.56	83.17	108.34
3	E	603	ZWY	C25-C15-C14	-15.48	83.29	108.34
3	D	603	ZWY	C25-C15-C14	-15.38	83.45	108.34
3	J	602	ZWY	C25-C15-C14	-15.37	83.47	108.34
3	A	602	ZWY	C25-C15-C14	-15.28	83.62	108.34
3	H	604	ZWY	C25-C15-C14	-15.28	83.62	108.34
3	D	606	ZWY	C25-C15-C14	-15.23	83.70	108.34
3	E	602	ZWY	C25-C15-C14	-15.19	83.77	108.34
3	B	603	ZWY	C25-C15-C14	-15.16	83.82	108.34
3	C	604	ZWY	C25-C15-C14	-15.06	83.97	108.34
3	J	603	ZWY	C25-C15-C14	-15.01	84.06	108.34
3	E	604	ZWY	C25-C15-C14	-14.94	84.17	108.34
3	I	603	ZWY	C25-C15-C14	-14.90	84.24	108.34
3	C	605	ZWY	C25-C15-C14	-14.77	84.44	108.34
3	A	603	ZWY	C25-C15-C16	9.62	124.62	109.43
3	C	603	ZWY	C25-C15-C16	9.56	124.53	109.43
3	B	602	ZWY	C25-C15-C16	9.46	124.37	109.43
3	H	603	ZWY	C25-C15-C16	8.85	123.41	109.43
3	C	605	ZWY	C25-C15-C16	8.76	123.26	109.43
3	D	603	ZWY	C25-C15-C16	8.74	123.24	109.43
3	H	602	ZWY	C25-C15-C16	8.74	123.23	109.43
3	D	605	ZWY	C25-C15-C16	8.72	123.20	109.43
3	I	603	ZWY	C25-C15-C16	8.69	123.15	109.43
3	H	604	ZWY	C25-C15-C16	8.64	123.07	109.43
3	J	603	ZWY	C25-C15-C16	8.57	122.96	109.43
3	E	605	ZWY	C25-C15-C16	8.48	122.82	109.43
3	D	606	ZWY	C25-C15-C16	8.43	122.74	109.43
3	E	602	ZWY	C25-C15-C16	8.42	122.73	109.43
3	D	604	ZWY	C25-C15-C16	8.30	122.53	109.43
3	E	604	ZWY	C25-C15-C16	8.03	122.11	109.43
3	B	603	ZWY	C25-C15-C16	7.90	121.90	109.43
3	A	602	ZWY	C25-C15-C16	7.74	121.66	109.43
3	E	603	ZWY	C25-C15-C16	7.65	121.52	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	604	ZWY	C25-C15-C16	7.61	121.46	109.43
3	C	603	ZWY	C18-O20-S21	-7.61	109.19	117.64
3	J	602	ZWY	C25-C15-C16	7.44	121.19	109.43
3	B	602	ZWY	C18-O20-S21	-7.39	109.44	117.64
3	D	602	ZWY	C25-C15-C16	7.38	121.08	109.43
3	I	602	ZWY	C25-C15-C16	7.33	121.00	109.43
3	C	602	ZWY	C25-C15-C16	7.29	120.94	109.43
3	A	603	ZWY	C18-O20-S21	-7.24	109.60	117.64
3	J	602	ZWY	C08-C07-C02	-7.15	97.67	104.08
3	E	602	ZWY	C08-C07-C02	-6.78	98.00	104.08
3	C	602	ZWY	C08-C07-C02	-6.73	98.04	104.08
3	D	602	ZWY	C08-C07-C02	-6.46	98.29	104.08
3	I	602	ZWY	C08-C07-C02	-6.45	98.29	104.08
3	B	603	ZWY	C08-C07-C02	-6.40	98.34	104.08
3	E	604	ZWY	C08-C07-C02	-6.39	98.35	104.08
3	H	602	ZWY	C08-C07-C02	-6.17	98.54	104.08
3	D	603	ZWY	C18-O20-S21	-6.17	110.79	117.64
3	B	602	ZWY	C06-C12-C13	-6.14	103.92	112.73
3	C	603	ZWY	C06-C12-C13	-6.10	103.97	112.73
3	C	604	ZWY	C08-C07-C02	-6.08	98.63	104.08
3	A	603	ZWY	C06-C12-C13	-5.95	104.18	112.73
3	D	605	ZWY	C08-C07-C02	-5.94	98.75	104.08
3	D	604	ZWY	C18-O20-S21	-5.86	111.14	117.64
3	B	602	ZWY	C08-C07-C02	-5.85	98.83	104.08
3	A	602	ZWY	C08-C07-C02	-5.85	98.83	104.08
3	D	603	ZWY	C18-C19-C14	-5.81	102.49	111.52
3	H	603	ZWY	C06-C12-C13	-5.80	104.40	112.73
3	D	603	ZWY	C08-C07-C02	-5.77	98.90	104.08
3	B	603	ZWY	C18-O20-S21	-5.76	111.25	117.64
3	C	603	ZWY	C08-C07-C02	-5.73	98.94	104.08
3	B	603	ZWY	C19-C14-C15	5.59	123.84	116.42
3	C	605	ZWY	C18-O20-S21	-5.57	111.45	117.64
3	D	604	ZWY	C18-C19-C14	-5.56	102.88	111.52
3	D	604	ZWY	C02-C07-C06	-5.54	107.19	113.12
3	H	603	ZWY	C18-O20-S21	-5.46	111.58	117.64
3	C	604	ZWY	C19-C14-C15	5.44	123.64	116.42
3	D	603	ZWY	C06-C12-C13	-5.42	104.94	112.73
3	I	603	ZWY	C08-C07-C02	-5.39	99.25	104.08
3	D	602	ZWY	C19-C14-C15	5.33	123.50	116.42
3	H	604	ZWY	C19-C14-C15	5.33	123.50	116.42
3	D	604	ZWY	C06-C12-C13	-5.33	105.08	112.73
3	A	603	ZWY	C08-C07-C02	-5.32	99.31	104.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	603	ZWY	C18-O20-S21	-5.29	111.77	117.64
3	J	603	ZWY	C08-C07-C02	-5.27	99.36	104.08
3	D	603	ZWY	C02-C07-C06	-5.25	107.50	113.12
3	J	602	ZWY	C19-C14-C15	5.24	123.39	116.42
3	I	602	ZWY	C19-C14-C15	5.17	123.28	116.42
3	D	606	ZWY	C02-C07-C06	-5.16	107.60	113.12
3	A	602	ZWY	C19-C14-C15	5.15	123.26	116.42
3	H	603	ZWY	C02-C07-C06	-5.11	107.65	113.12
3	C	602	ZWY	C19-C14-C15	5.10	123.20	116.42
3	D	606	ZWY	C18-C19-C14	-5.07	103.65	111.52
3	C	605	ZWY	C08-C07-C02	-5.04	99.56	104.08
3	E	604	ZWY	C19-C14-C15	5.00	123.06	116.42
3	D	606	ZWY	C08-C07-C02	-4.97	99.63	104.08
3	E	603	ZWY	C02-C07-C06	-4.94	107.83	113.12
3	E	603	ZWY	C19-C14-C15	4.91	122.94	116.42
3	I	603	ZWY	C19-C14-C15	4.89	122.91	116.42
3	J	603	ZWY	C19-C14-C15	4.78	122.76	116.42
3	D	604	ZWY	C17-C18-C19	-4.77	103.87	110.99
3	D	602	ZWY	C16-C15-C05	4.76	115.38	108.73
3	I	603	ZWY	C02-C07-C06	-4.75	108.03	113.12
3	C	605	ZWY	C19-C14-C15	4.74	122.72	116.42
3	H	603	ZWY	C18-C19-C14	-4.73	104.16	111.52
3	I	602	ZWY	C16-C15-C05	4.70	115.30	108.73
3	H	604	ZWY	C08-C07-C02	-4.70	99.86	104.08
3	C	602	ZWY	C16-C15-C05	4.70	115.28	108.73
3	E	603	ZWY	C06-C12-C13	-4.69	105.99	112.73
3	C	604	ZWY	C18-O20-S21	-4.68	112.44	117.64
3	D	606	ZWY	C06-C12-C13	-4.67	106.02	112.73
3	I	603	ZWY	C18-O20-S21	-4.67	112.46	117.64
3	J	603	ZWY	C02-C07-C06	-4.66	108.14	113.12
3	C	605	ZWY	C02-C07-C06	-4.65	108.14	113.12
3	D	603	ZWY	C19-C14-C15	4.64	122.58	116.42
3	D	605	ZWY	C06-C12-C13	-4.62	106.10	112.73
3	D	604	ZWY	C08-C07-C02	-4.59	99.97	104.08
3	C	603	ZWY	C18-C19-C14	-4.54	104.47	111.52
3	D	606	ZWY	C19-C14-C15	4.52	122.43	116.42
3	J	602	ZWY	C16-C15-C05	4.51	115.03	108.73
3	B	602	ZWY	C18-C19-C14	-4.47	104.58	111.52
3	D	603	ZWY	C16-C15-C05	4.45	114.95	108.73
3	D	605	ZWY	C19-C14-C15	4.45	122.33	116.42
3	E	604	ZWY	C02-C07-C06	-4.44	108.36	113.12
3	H	603	ZWY	C08-C07-C02	-4.43	100.11	104.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	603	ZWY	C02-C07-C06	-4.39	108.42	113.12
3	B	602	ZWY	C02-C07-C06	-4.36	108.45	113.12
3	H	603	ZWY	C17-C18-C19	-4.36	104.48	110.99
3	E	603	ZWY	C08-C07-C02	-4.35	100.17	104.08
3	H	604	ZWY	C16-C15-C05	4.31	114.75	108.73
3	B	602	ZWY	C19-C14-C15	4.28	122.11	116.42
3	E	605	ZWY	C19-C14-C15	4.28	122.10	116.42
3	C	603	ZWY	C02-C07-C06	-4.27	108.55	113.12
3	E	605	ZWY	C02-C07-C06	-4.26	108.56	113.12
3	D	605	ZWY	C02-C07-C06	-4.22	108.61	113.12
3	A	602	ZWY	C02-C07-C06	-4.18	108.64	113.12
3	E	605	ZWY	C18-O20-S21	-4.18	113.00	117.64
3	A	603	ZWY	C18-C19-C14	-4.18	105.03	111.52
3	H	602	ZWY	C19-C14-C15	4.17	121.96	116.42
3	B	603	ZWY	C02-C07-C06	-4.13	108.70	113.12
3	D	605	ZWY	C04-C05-C15	-4.13	107.64	113.08
3	D	604	ZWY	C19-C14-C15	4.12	121.90	116.42
3	E	602	ZWY	C19-C14-C15	4.11	121.89	116.42
3	E	605	ZWY	C06-C12-C13	-4.10	106.83	112.73
3	H	603	ZWY	C19-C14-C15	4.08	121.85	116.42
3	A	603	ZWY	C19-C14-C15	4.08	121.83	116.42
3	C	604	ZWY	C16-C15-C05	4.07	114.41	108.73
3	H	603	ZWY	C16-C15-C05	4.06	114.40	108.73
3	E	603	ZWY	C16-C15-C05	4.04	114.36	108.73
3	C	603	ZWY	C19-C14-C15	4.03	121.78	116.42
3	C	604	ZWY	C02-C07-C06	-3.99	108.85	113.12
3	A	602	ZWY	C16-C15-C05	3.99	114.30	108.73
3	D	606	ZWY	C08-C07-C06	-3.94	112.59	119.08
3	E	604	ZWY	C17-C18-C19	-3.91	105.15	110.99
3	H	602	ZWY	C06-C12-C13	-3.86	107.19	112.73
3	I	603	ZWY	C04-C05-C15	-3.82	108.04	113.08
3	E	602	ZWY	C18-O20-S21	-3.80	113.42	117.64
3	C	605	ZWY	C07-C06-C05	-3.79	104.01	109.09
3	D	606	ZWY	C17-C18-C19	-3.76	105.38	110.99
3	A	603	ZWY	C08-C07-C06	-3.74	112.92	119.08
3	B	602	ZWY	C08-C07-C06	-3.74	112.92	119.08
3	B	603	ZWY	C16-C15-C05	3.74	113.95	108.73
3	J	602	ZWY	C17-C18-C19	-3.73	105.43	110.99
3	C	603	ZWY	C08-C07-C06	-3.72	112.95	119.08
3	J	603	ZWY	C12-C13-C14	3.72	131.93	125.06
3	C	605	ZWY	C12-C13-C14	3.70	131.89	125.06
3	A	602	ZWY	C18-O20-S21	-3.68	113.55	117.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	ZWY	C16-C15-C05	3.68	113.87	108.73
3	I	603	ZWY	C07-C06-C05	-3.68	104.17	109.09
3	D	605	ZWY	C18-C19-C14	-3.67	105.81	111.52
3	I	602	ZWY	C06-C12-C13	-3.67	107.46	112.73
3	C	605	ZWY	C06-C12-C13	-3.66	107.48	112.73
3	J	603	ZWY	C06-C12-C13	-3.65	107.49	112.73
3	C	602	ZWY	C12-C13-C14	3.64	131.78	125.06
3	C	602	ZWY	C06-C12-C13	-3.64	107.50	112.73
3	C	603	ZWY	C12-C13-C14	3.63	131.75	125.06
3	E	602	ZWY	C02-C07-C06	-3.61	109.25	113.12
3	D	602	ZWY	C12-C13-C14	3.61	131.72	125.06
3	C	605	ZWY	C04-C05-C15	-3.61	108.33	113.08
3	C	604	ZWY	C12-C13-C14	3.60	131.70	125.06
3	E	604	ZWY	C12-C13-C14	3.59	131.69	125.06
3	E	604	ZWY	C18-O20-S21	-3.59	113.66	117.64
3	I	602	ZWY	C17-C18-C19	-3.59	105.64	110.99
3	I	602	ZWY	C12-C13-C14	3.58	131.66	125.06
3	J	603	ZWY	C07-C06-C05	-3.58	104.30	109.09
3	H	602	ZWY	C02-C07-C06	-3.57	109.30	113.12
3	H	604	ZWY	C02-C07-C06	-3.57	109.30	113.12
3	J	602	ZWY	C06-C12-C13	-3.57	107.60	112.73
3	E	605	ZWY	C07-C06-C05	-3.56	104.33	109.09
3	A	602	ZWY	C12-C13-C14	3.55	131.61	125.06
3	I	603	ZWY	C06-C12-C13	-3.55	107.63	112.73
3	D	606	ZWY	C12-C13-C14	3.53	131.57	125.06
3	H	602	ZWY	C12-C13-C14	3.52	131.56	125.06
3	I	603	ZWY	C12-C13-C14	3.51	131.53	125.06
3	J	603	ZWY	C04-C05-C15	-3.50	108.47	113.08
3	D	602	ZWY	C06-C12-C13	-3.49	107.71	112.73
3	A	603	ZWY	C12-C13-C14	3.48	131.49	125.06
3	E	605	ZWY	C09-C10-C02	-3.48	105.16	108.59
3	E	604	ZWY	C06-C12-C13	-3.46	107.75	112.73
3	H	602	ZWY	C18-O20-S21	-3.46	113.81	117.64
3	E	602	ZWY	C07-C06-C05	-3.44	104.48	109.09
3	B	602	ZWY	C12-C06-C07	-3.44	105.92	110.91
3	E	603	ZWY	C09-C08-C07	-3.43	97.67	103.00
3	E	604	ZWY	C16-C15-C05	3.43	113.52	108.73
3	B	602	ZWY	C12-C13-C14	3.43	131.39	125.06
3	E	603	ZWY	C12-C13-C14	3.42	131.38	125.06
3	E	602	ZWY	C18-C19-C14	-3.42	106.20	111.52
3	C	603	ZWY	C16-C15-C05	3.42	113.50	108.73
3	J	602	ZWY	C12-C13-C14	3.41	131.35	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	HEM	C4B-CHC-C1C	3.40	127.05	122.56
3	D	604	ZWY	C12-C13-C14	3.40	131.33	125.06
3	D	603	ZWY	C19-C14-C13	-3.38	115.73	120.61
3	B	603	ZWY	C12-C13-C14	3.37	131.28	125.06
3	C	602	ZWY	O23-S21-O22	3.37	125.75	112.22
3	H	604	ZWY	C12-C13-C14	3.37	131.28	125.06
3	I	602	ZWY	C02-C07-C06	-3.36	109.52	113.12
3	C	602	ZWY	C17-C18-C19	-3.36	105.98	110.99
3	E	602	ZWY	O23-S21-O22	3.35	125.68	112.22
3	I	602	ZWY	O23-S21-O22	3.34	125.63	112.22
3	E	603	ZWY	C19-C14-C13	-3.33	115.81	120.61
3	C	605	ZWY	C09-C08-C07	-3.33	97.83	103.00
3	C	602	ZWY	C02-C07-C06	-3.32	109.56	113.12
3	I	603	ZWY	C09-C08-C07	-3.32	97.84	103.00
3	D	602	ZWY	C17-C18-C19	-3.32	106.04	110.99
3	D	604	ZWY	C04-C05-C15	-3.32	108.71	113.08
3	I	602	ZWY	C08-C07-C06	-3.31	113.62	119.08
2	B	601	HEM	C1B-NB-C4B	3.31	108.49	105.07
3	B	603	ZWY	C06-C12-C13	-3.29	108.01	112.73
3	E	602	ZWY	C12-C13-C14	3.29	131.13	125.06
3	A	603	ZWY	C16-C15-C05	3.28	113.31	108.73
3	D	606	ZWY	C04-C03-C02	-3.28	105.63	112.74
2	K	601	HEM	C4C-CHD-C1D	3.28	126.89	122.56
3	E	602	ZWY	C09-C10-C02	-3.28	105.35	108.59
3	A	602	ZWY	C17-C18-C19	-3.27	106.11	110.99
3	E	605	ZWY	C12-C13-C14	3.27	131.09	125.06
3	J	603	ZWY	C09-C08-C07	-3.26	97.94	103.00
3	A	603	ZWY	C12-C06-C07	-3.25	106.19	110.91
3	C	604	ZWY	C08-C07-C06	-3.25	113.72	119.08
3	H	604	ZWY	C07-C06-C05	-3.25	104.74	109.09
3	J	602	ZWY	C08-C07-C06	-3.25	113.73	119.08
3	D	605	ZWY	C12-C13-C14	3.25	131.05	125.06
3	C	603	ZWY	C12-C06-C05	3.24	113.64	109.71
3	B	602	ZWY	O23-S21-O22	3.24	125.24	112.22
3	D	606	ZWY	C09-C10-C02	-3.24	105.39	108.59
3	H	604	ZWY	C04-C05-C06	-3.24	107.09	111.75
3	H	602	ZWY	C07-C06-C05	-3.23	104.77	109.09
3	H	604	ZWY	C25-C15-C05	-3.22	107.84	111.68
3	D	602	ZWY	C02-C07-C06	-3.21	109.69	113.12
3	E	604	ZWY	C04-C05-C15	-3.20	108.86	113.08
3	C	602	ZWY	C08-C07-C06	-3.20	113.82	119.08
3	D	604	ZWY	C16-C15-C05	3.19	113.19	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	ZWY	C08-C07-C06	-3.19	113.82	119.08
3	E	602	ZWY	C04-C05-C15	-3.19	108.88	113.08
3	J	602	ZWY	C02-C07-C06	-3.19	109.71	113.12
3	D	602	ZWY	O23-S21-O22	3.18	124.99	112.22
3	E	602	ZWY	C06-C12-C13	-3.18	108.16	112.73
2	K	601	HEM	C1B-NB-C4B	3.18	108.36	105.07
3	H	603	ZWY	C08-C07-C06	-3.17	113.86	119.08
3	A	602	ZWY	C06-C12-C13	-3.16	108.19	112.73
3	D	602	ZWY	C08-C07-C06	-3.16	113.88	119.08
3	E	605	ZWY	C16-C15-C05	3.16	113.14	108.73
3	D	606	ZWY	C18-O20-S21	-3.16	114.14	117.64
3	E	605	ZWY	C08-C07-C06	-3.15	113.89	119.08
3	H	602	ZWY	C18-C19-C14	-3.14	106.64	111.52
2	E	601	HEM	C1B-NB-C4B	3.14	108.31	105.07
3	D	606	ZWY	C04-C05-C15	-3.14	108.95	113.08
3	B	603	ZWY	C19-C14-C13	-3.13	116.10	120.61
3	J	603	ZWY	O23-S21-O22	3.13	124.78	112.22
3	C	603	ZWY	C12-C06-C07	-3.12	106.38	110.91
3	C	604	ZWY	C06-C12-C13	-3.12	108.24	112.73
3	J	602	ZWY	C19-C14-C13	-3.12	116.11	120.61
3	C	602	ZWY	C04-C05-C06	-3.11	107.27	111.75
3	D	604	ZWY	C08-C07-C06	-3.11	113.96	119.08
3	H	602	ZWY	O23-S21-O22	3.10	124.66	112.22
3	E	604	ZWY	C04-C03-C02	-3.09	106.05	112.74
3	I	603	ZWY	O23-S21-O22	3.08	124.59	112.22
3	I	602	ZWY	C19-C14-C13	-3.08	116.17	120.61
2	C	601	HEM	C4D-ND-C1D	3.07	108.25	105.07
3	E	604	ZWY	C08-C07-C06	-3.07	114.03	119.08
3	H	602	ZWY	C04-C05-C15	-3.06	109.05	113.08
3	D	605	ZWY	C16-C15-C05	3.05	112.99	108.73
3	B	603	ZWY	C08-C07-C06	-3.05	114.05	119.08
3	I	602	ZWY	C04-C05-C06	-3.04	107.37	111.75
3	E	602	ZWY	C16-C15-C05	3.04	112.97	108.73
3	E	605	ZWY	C18-C19-C14	-3.04	106.80	111.52
3	D	603	ZWY	C12-C13-C14	3.02	130.64	125.06
3	D	603	ZWY	C08-C07-C06	-3.02	114.11	119.08
3	H	603	ZWY	O23-S21-O22	3.01	124.31	112.22
2	I	601	HEM	C1B-NB-C4B	3.01	108.18	105.07
3	D	602	ZWY	C19-C14-C13	-3.01	116.28	120.61
2	A	601	HEM	C1B-NB-C4B	2.99	108.16	105.07
3	J	603	ZWY	C12-C06-C05	2.99	113.34	109.71
3	D	602	ZWY	C04-C05-C06	-2.99	107.45	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	605	ZWY	O23-S21-O22	2.98	124.20	112.22
3	H	603	ZWY	C12-C13-C14	2.98	130.56	125.06
3	H	602	ZWY	C16-C15-C05	2.97	112.88	108.73
3	J	602	ZWY	O23-S21-O22	2.96	124.11	112.22
2	D	601	HEM	C1B-NB-C4B	2.96	108.13	105.07
3	B	602	ZWY	C12-C06-C05	2.96	113.30	109.71
3	E	605	ZWY	C04-C03-C02	-2.96	106.33	112.74
3	H	602	ZWY	C04-C03-C02	-2.95	106.35	112.74
3	H	603	ZWY	C04-C05-C15	-2.95	109.20	113.08
3	A	603	ZWY	O23-S21-O22	2.94	124.02	112.22
3	B	602	ZWY	C01-C02-C10	2.93	110.58	105.18
3	D	605	ZWY	C01-C02-C10	2.93	110.58	105.18
3	E	602	ZWY	C08-C07-C06	-2.92	114.28	119.08
3	E	603	ZWY	C04-C05-C15	-2.91	109.24	113.08
3	C	603	ZWY	O23-S21-O22	2.91	123.89	112.22
3	E	603	ZWY	O23-S21-O22	2.90	123.84	112.22
3	H	604	ZWY	C08-C07-C06	-2.89	114.32	119.08
2	E	601	HEM	C4B-CHC-C1C	2.89	126.37	122.56
3	C	603	ZWY	C01-C02-C10	2.89	110.49	105.18
3	J	603	ZWY	C16-C15-C05	2.89	112.76	108.73
3	H	604	ZWY	C12-C06-C05	2.88	113.20	109.71
2	L	601	HEM	C1B-NB-C4B	2.88	108.05	105.07
3	C	602	ZWY	C19-C14-C13	-2.87	116.48	120.61
3	D	603	ZWY	O23-S21-O22	2.87	123.72	112.22
3	C	603	ZWY	C07-C06-C05	-2.86	105.26	109.09
2	J	601	HEM	C1B-NB-C4B	2.86	108.03	105.07
3	C	604	ZWY	C17-C18-C19	-2.86	106.72	110.99
3	C	605	ZWY	C16-C15-C05	2.86	112.72	108.73
3	D	603	ZWY	C04-C05-C06	-2.85	107.65	111.75
2	F	601	HEM	CBA-CAA-C2A	-2.85	107.76	112.62
3	C	605	ZWY	C12-C06-C05	2.84	113.16	109.71
3	I	603	ZWY	C16-C15-C05	2.82	112.67	108.73
3	D	604	ZWY	C04-C03-C02	-2.81	106.66	112.74
3	E	603	ZWY	C04-C03-C02	-2.80	106.67	112.74
2	D	601	HEM	C4C-CHD-C1D	2.80	126.25	122.56
3	H	604	ZWY	C09-C08-C07	-2.80	98.65	103.00
3	H	604	ZWY	C18-O20-S21	-2.80	114.54	117.64
3	B	603	ZWY	C17-C18-C19	-2.78	106.83	110.99
3	J	602	ZWY	C04-C05-C06	-2.77	107.76	111.75
3	B	602	ZWY	C04-C05-C06	-2.77	107.76	111.75
3	J	603	ZWY	C04-C03-C02	-2.77	106.73	112.74
3	D	606	ZWY	C19-C14-C13	-2.77	116.61	120.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	HEM	C4C-CHD-C1D	2.77	126.21	122.56
3	A	603	ZWY	C01-C02-C10	2.77	110.27	105.18
2	A	601	HEM	C4B-CHC-C1C	2.77	126.21	122.56
2	L	601	HEM	C4B-CHC-C1C	2.76	126.20	122.56
3	C	605	ZWY	C25-C15-C05	-2.76	108.39	111.68
2	A	601	HEM	C4D-ND-C1D	2.75	107.91	105.07
3	D	605	ZWY	O23-S21-O22	2.74	123.23	112.22
2	I	601	HEM	C4C-CHD-C1D	2.73	126.16	122.56
3	C	604	ZWY	C19-C14-C13	-2.73	116.68	120.61
3	A	603	ZWY	C04-C05-C06	-2.73	107.83	111.75
3	D	605	ZWY	C12-C06-C07	-2.73	106.95	110.91
3	D	603	ZWY	C09-C08-C07	-2.72	98.77	103.00
3	A	603	ZWY	C12-C06-C05	2.72	113.01	109.71
3	A	602	ZWY	C19-C14-C13	-2.72	116.69	120.61
2	J	601	HEM	C4B-CHC-C1C	2.72	126.14	122.56
2	H	601	HEM	C4D-ND-C1D	2.71	107.88	105.07
3	I	603	ZWY	C04-C03-C02	-2.71	106.88	112.74
3	I	603	ZWY	C12-C06-C05	2.70	112.98	109.71
3	C	603	ZWY	C04-C03-C02	-2.69	106.91	112.74
2	D	601	HEM	C4D-ND-C1D	2.68	107.84	105.07
3	H	603	ZWY	C12-C06-C07	-2.68	107.03	110.91
3	A	603	ZWY	C07-C06-C05	-2.67	105.51	109.09
3	D	603	ZWY	C12-C06-C05	2.67	112.95	109.71
3	D	606	ZWY	O23-S21-O22	2.67	122.92	112.22
3	A	603	ZWY	C04-C03-C02	-2.66	106.98	112.74
3	B	602	ZWY	C04-C03-C02	-2.66	106.98	112.74
2	H	601	HEM	CAA-CBA-CGA	-2.65	106.32	113.76
2	A	601	HEM	C4C-CHD-C1D	2.65	126.06	122.56
3	D	606	ZWY	C16-C15-C05	2.65	112.43	108.73
3	D	605	ZWY	C17-C18-C19	-2.64	107.05	110.99
3	E	604	ZWY	C19-C14-C13	-2.64	116.81	120.61
3	E	603	ZWY	C03-C02-C07	-2.63	104.83	108.99
3	D	604	ZWY	C19-C14-C13	-2.63	116.82	120.61
3	D	605	ZWY	C16-C15-C14	2.63	113.57	108.75
3	H	604	ZWY	C04-C03-C02	-2.63	107.05	112.74
3	C	605	ZWY	C04-C03-C02	-2.63	107.05	112.74
3	E	605	ZWY	O23-S21-O22	2.63	122.76	112.22
3	D	605	ZWY	C18-O20-S21	-2.62	114.74	117.64
3	H	604	ZWY	O23-S21-O22	2.61	122.70	112.22
3	D	606	ZWY	C16-C15-C14	2.60	113.51	108.75
3	B	602	ZWY	C07-C06-C05	-2.60	105.61	109.09
3	E	605	ZWY	C08-C07-C02	-2.59	101.75	104.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	ZWY	C07-C06-C05	-2.59	105.62	109.09
3	I	603	ZWY	C19-C14-C13	-2.59	116.88	120.61
2	C	601	HEM	C1B-NB-C4B	2.59	107.74	105.07
3	D	603	ZWY	C12-C06-C07	-2.58	107.16	110.91
2	L	601	HEM	CBA-CAA-C2A	-2.58	108.21	112.62
2	H	601	HEM	C4B-CHC-C1C	2.58	125.96	122.56
3	J	603	ZWY	C25-C15-C05	-2.57	108.61	111.68
3	C	603	ZWY	C04-C05-C06	-2.57	108.05	111.75
2	K	601	HEM	CBA-CAA-C2A	-2.57	108.24	112.62
3	I	603	ZWY	C25-C15-C05	-2.56	108.62	111.68
3	E	603	ZWY	C12-C06-C05	2.56	112.82	109.71
3	H	604	ZWY	C19-C14-C13	-2.56	116.92	120.61
3	B	602	ZWY	C19-C14-C13	-2.56	116.92	120.61
3	D	604	ZWY	C07-C06-C05	-2.55	105.67	109.09
3	C	604	ZWY	C07-C06-C05	-2.55	105.68	109.09
3	H	603	ZWY	C19-C14-C13	-2.54	116.94	120.61
3	A	602	ZWY	C04-C03-C02	-2.54	107.24	112.74
2	L	601	HEM	C4C-CHD-C1D	2.54	125.91	122.56
3	D	605	ZWY	C08-C07-C06	-2.54	114.90	119.08
2	L	601	HEM	C4D-ND-C1D	2.54	107.69	105.07
3	H	602	ZWY	C15-C05-C06	2.53	116.54	112.73
3	D	602	ZWY	C09-C10-C02	-2.53	106.10	108.59
3	E	605	ZWY	C01-C02-C10	2.52	109.82	105.18
3	B	603	ZWY	C07-C06-C05	-2.51	105.73	109.09
2	G	601	HEM	C4B-CHC-C1C	2.51	125.86	122.56
3	E	605	ZWY	C12-C06-C05	2.49	112.73	109.71
3	D	606	ZWY	C12-C06-C07	-2.49	107.29	110.91
3	J	602	ZWY	C12-C06-C05	2.49	112.73	109.71
3	J	603	ZWY	C16-C15-C14	2.48	113.30	108.75
2	F	601	HEM	C4B-CHC-C1C	2.48	125.83	122.56
3	B	603	ZWY	C04-C03-C02	-2.48	107.37	112.74
3	H	604	ZWY	C09-C10-C02	-2.48	106.15	108.59
3	E	604	ZWY	C07-C06-C05	-2.47	105.78	109.09
3	H	603	ZWY	C04-C03-C02	-2.47	107.39	112.74
3	C	604	ZWY	O23-S21-O22	2.47	122.12	112.22
2	J	601	HEM	C4D-ND-C1D	2.46	107.62	105.07
3	H	604	ZWY	C05-C15-C14	2.46	113.51	109.65
3	D	603	ZWY	C07-C06-C05	-2.46	105.80	109.09
3	H	604	ZWY	C06-C12-C13	-2.45	109.21	112.73
3	D	603	ZWY	C17-C18-C19	-2.45	107.33	110.99
3	J	603	ZWY	C19-C14-C13	-2.45	117.08	120.61
3	A	602	ZWY	O23-S21-O22	2.45	122.04	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	605	ZWY	C25-C15-C05	-2.45	108.77	111.68
3	C	604	ZWY	C04-C03-C02	-2.45	107.44	112.74
3	C	605	ZWY	C19-C14-C13	-2.44	117.09	120.61
3	B	602	ZWY	C04-C05-C15	-2.43	109.88	113.08
2	B	601	HEM	C3B-C2B-C1B	2.43	108.29	106.49
3	C	602	ZWY	C04-C03-C02	-2.43	107.49	112.74
2	D	601	HEM	C4B-CHC-C1C	2.42	125.76	122.56
2	B	601	HEM	C4B-CHC-C1C	2.41	125.74	122.56
3	C	602	ZWY	C09-C10-C02	-2.40	106.22	108.59
2	H	601	HEM	C1B-NB-C4B	2.40	107.56	105.07
3	C	605	ZWY	C16-C15-C14	2.40	113.15	108.75
3	B	603	ZWY	O23-S21-O22	2.39	121.81	112.22
2	K	601	HEM	C4B-CHC-C1C	2.39	125.71	122.56
3	J	602	ZWY	C04-C03-C02	-2.38	107.58	112.74
3	E	602	ZWY	C17-C18-C19	-2.38	107.43	110.99
3	E	602	ZWY	C15-C05-C06	2.37	116.29	112.73
3	I	602	ZWY	C04-C03-C02	-2.37	107.61	112.74
2	C	601	HEM	CAA-CBA-CGA	-2.37	107.12	113.76
3	E	605	ZWY	C04-C05-C15	-2.37	109.96	113.08
3	C	602	ZWY	C12-C06-C05	2.36	112.58	109.71
3	A	603	ZWY	C19-C14-C13	-2.36	117.21	120.61
3	E	602	ZWY	C04-C05-C06	-2.36	108.36	111.75
3	E	603	ZWY	C07-C06-C05	-2.36	105.93	109.09
3	E	603	ZWY	C08-C07-C06	-2.36	115.20	119.08
3	C	605	ZWY	C18-C19-C14	-2.35	107.86	111.52
2	B	601	HEM	CHD-C1D-ND	2.35	126.99	124.43
2	I	601	HEM	C4D-ND-C1D	2.34	107.49	105.07
3	I	602	ZWY	C12-C06-C05	2.34	112.55	109.71
3	D	602	ZWY	C04-C03-C02	-2.34	107.67	112.74
2	B	601	HEM	C4D-ND-C1D	2.34	107.49	105.07
2	G	601	HEM	C1B-NB-C4B	2.34	107.49	105.07
3	E	603	ZWY	C16-C15-C14	2.34	113.03	108.75
3	I	603	ZWY	C16-C15-C14	2.34	113.03	108.75
2	H	601	HEM	C4C-CHD-C1D	2.33	125.64	122.56
3	H	602	ZWY	C08-C07-C06	-2.33	115.24	119.08
3	I	603	ZWY	C18-C19-C14	-2.33	107.90	111.52
3	D	604	ZWY	C16-C15-C14	2.33	113.01	108.75
3	I	603	ZWY	C07-C02-C10	2.32	103.25	100.59
3	C	605	ZWY	C07-C02-C10	2.32	103.25	100.59
3	A	602	ZWY	C04-C05-C15	-2.31	110.03	113.08
3	C	603	ZWY	C04-C05-C15	-2.31	110.04	113.08
3	H	602	ZWY	C04-C05-C06	-2.31	108.43	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	603	ZWY	C18-C19-C14	-2.31	107.93	111.52
3	C	604	ZWY	C04-C05-C15	-2.30	110.05	113.08
3	H	602	ZWY	O20-C18-C17	-2.30	104.11	107.59
3	D	606	ZWY	C12-C06-C05	2.29	112.49	109.71
2	I	601	HEM	C4B-CHC-C1C	2.29	125.58	122.56
3	A	603	ZWY	C04-C05-C15	-2.29	110.07	113.08
2	G	601	HEM	C4C-CHD-C1D	2.29	125.57	122.56
3	C	605	ZWY	C09-C10-C02	-2.27	106.35	108.59
3	D	602	ZWY	C15-C05-C06	2.27	116.14	112.73
3	D	605	ZWY	C03-C04-C05	-2.27	109.19	113.11
2	K	601	HEM	C4D-ND-C1D	2.26	107.41	105.07
3	D	605	ZWY	C04-C03-C02	-2.25	107.86	112.74
3	J	603	ZWY	C15-C05-C06	2.25	116.10	112.73
2	F	601	HEM	CMC-C2C-C3C	2.24	128.88	124.68
3	J	603	ZWY	O20-C18-C17	-2.24	104.20	107.59
3	E	602	ZWY	C17-C16-C15	-2.24	107.88	112.74
2	C	601	HEM	C4C-CHD-C1D	2.24	125.51	122.56
2	G	601	HEM	C4D-ND-C1D	2.24	107.38	105.07
3	C	604	ZWY	C04-C05-C06	-2.24	108.53	111.75
3	E	603	ZWY	C17-C18-C19	-2.23	107.66	110.99
3	H	603	ZWY	C03-C02-C07	-2.23	105.47	108.99
3	C	605	ZWY	C15-C05-C06	2.23	116.07	112.73
3	D	602	ZWY	C12-C06-C05	2.23	112.41	109.71
3	H	602	ZWY	C15-C14-C13	-2.22	119.50	122.90
3	C	603	ZWY	C19-C14-C13	-2.21	117.42	120.61
3	A	602	ZWY	C04-C05-C06	-2.21	108.57	111.75
3	D	604	ZWY	C17-C16-C15	-2.21	107.96	112.74
2	J	601	HEM	C4C-CHD-C1D	2.20	125.47	122.56
3	H	604	ZWY	C15-C14-C13	-2.20	119.53	122.90
3	D	603	ZWY	C04-C03-C02	-2.20	107.97	112.74
2	A	601	HEM	CHD-C1D-ND	2.20	126.82	124.43
2	F	601	HEM	C1B-NB-C4B	2.20	107.34	105.07
3	C	602	ZWY	C07-C02-C10	2.20	103.11	100.59
3	D	605	ZWY	C09-C08-C07	-2.20	99.59	103.00
2	F	601	HEM	C4D-ND-C1D	2.19	107.34	105.07
3	E	604	ZWY	C12-C06-C05	2.19	112.36	109.71
3	D	606	ZWY	C07-C06-C05	-2.19	106.16	109.09
3	E	605	ZWY	C19-C14-C13	-2.19	117.46	120.61
2	K	601	HEM	C3B-C2B-C1B	2.19	108.11	106.49
3	B	603	ZWY	C07-C02-C10	2.19	103.09	100.59
2	D	601	HEM	C3D-C4D-ND	-2.19	107.73	110.17
3	E	604	ZWY	O23-S21-O22	2.18	120.98	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	ZWY	C09-C08-C07	-2.18	99.61	103.00
3	D	605	ZWY	C19-C14-C13	-2.18	117.47	120.61
3	I	603	ZWY	C15-C05-C06	2.17	116.00	112.73
3	E	603	ZWY	C17-C16-C15	-2.17	108.05	112.74
2	G	601	HEM	CMC-C2C-C3C	2.16	128.73	124.68
3	E	605	ZWY	C15-C05-C06	2.16	115.98	112.73
2	I	601	HEM	C3B-C2B-C1B	2.16	108.09	106.49
3	E	603	ZWY	C12-C06-C07	-2.15	107.79	110.91
2	A	601	HEM	C3D-C4D-ND	-2.15	107.77	110.17
2	L	601	HEM	C3B-C2B-C1B	2.15	108.08	106.49
3	D	602	ZWY	C07-C02-C10	2.15	103.05	100.59
3	J	602	ZWY	C12-C06-C07	-2.14	107.80	110.91
3	C	605	ZWY	C08-C07-C06	-2.14	115.56	119.08
3	B	603	ZWY	C04-C05-C06	-2.13	108.68	111.75
3	A	602	ZWY	C16-C15-C14	2.13	112.66	108.75
3	C	604	ZWY	C15-C14-C13	-2.13	119.64	122.90
2	F	601	HEM	C4C-CHD-C1D	2.13	125.37	122.56
3	J	602	ZWY	C03-C02-C07	-2.13	105.62	108.99
2	D	601	HEM	C3B-C2B-C1B	2.13	108.06	106.49
3	A	603	ZWY	C09-C08-C07	-2.12	99.71	103.00
3	E	602	ZWY	C04-C03-C02	-2.11	108.18	112.74
3	E	605	ZWY	C16-C15-C14	2.11	112.61	108.75
3	D	604	ZWY	O23-S21-O22	2.10	120.65	112.22
3	I	603	ZWY	C09-C10-C02	-2.10	106.52	108.59
3	H	604	ZWY	C15-C05-C06	2.09	115.87	112.73
3	C	604	ZWY	C07-C02-C10	2.09	102.99	100.59
2	H	601	HEM	CHC-C4B-NB	2.09	126.70	124.43
3	E	604	ZWY	C03-C04-C05	-2.09	109.49	113.11
3	J	603	ZWY	C09-C10-C02	-2.09	106.53	108.59
2	C	601	HEM	C2D-C1D-ND	-2.09	107.38	109.88
2	J	601	HEM	C3B-C2B-C1B	2.09	108.03	106.49
3	J	603	ZWY	C07-C02-C10	2.08	102.98	100.59
3	E	603	ZWY	C07-C02-C10	2.08	102.98	100.59
3	D	603	ZWY	C08-C09-C10	-2.08	103.61	105.70
3	H	603	ZWY	C01-C02-C10	2.07	108.99	105.18
3	D	603	ZWY	C25-C15-C05	-2.07	109.22	111.68
2	E	601	HEM	C4D-ND-C1D	2.06	107.20	105.07
3	I	603	ZWY	C03-C04-C05	-2.06	109.55	113.11
2	G	601	HEM	CBA-CAA-C2A	-2.06	109.11	112.62
2	E	601	HEM	C4C-CHD-C1D	2.05	125.27	122.56
2	K	601	HEM	CHB-C1B-NB	2.05	126.92	124.38
2	E	601	HEM	C3B-C2B-C1B	2.05	108.01	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	605	ZWY	C04-C05-C06	-2.05	108.81	111.75
3	C	604	ZWY	C09-C08-C07	-2.05	99.82	103.00
3	J	602	ZWY	C07-C02-C10	2.04	102.93	100.59
3	D	604	ZWY	C04-C05-C06	-2.04	108.81	111.75
3	H	603	ZWY	C09-C10-C02	-2.04	106.58	108.59
3	H	602	ZWY	C17-C18-C19	-2.04	107.95	110.99
2	A	601	HEM	C3B-C2B-C1B	2.03	108.00	106.49
3	A	603	ZWY	C17-C16-C15	-2.03	108.33	112.74
3	A	603	ZWY	C17-C18-C19	-2.02	107.98	110.99
3	I	602	ZWY	C12-C06-C07	-2.02	107.98	110.91
3	C	602	ZWY	C12-C06-C07	-2.01	107.99	110.91
2	L	601	HEM	CMA-C3A-C4A	-2.01	125.38	128.46
3	I	602	ZWY	C15-C05-C06	2.00	115.74	112.73
3	B	603	ZWY	C04-C05-C15	-2.00	110.44	113.08

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	603	ZWY	C18-O20-S21-O24
3	E	602	ZWY	C18-O20-S21-O24
3	H	604	ZWY	C18-O20-S21-O24
3	D	603	ZWY	C18-O20-S21-O23
3	E	602	ZWY	C18-O20-S21-O22
3	E	603	ZWY	C18-O20-S21-O24
2	K	601	HEM	C2D-C3D-CAD-CBD
2	K	601	HEM	C4D-C3D-CAD-CBD
3	E	602	ZWY	C18-O20-S21-O23
3	H	604	ZWY	C18-O20-S21-O23
2	K	601	HEM	CAD-CBD-CGD-O2D
2	L	601	HEM	CAA-CBA-CGA-O2A
2	C	601	HEM	CAA-CBA-CGA-O2A
2	C	601	HEM	CAA-CBA-CGA-O1A
2	K	601	HEM	CAD-CBD-CGD-O1D
2	B	601	HEM	CAD-CBD-CGD-O2D
2	I	601	HEM	CAA-CBA-CGA-O2A
2	L	601	HEM	CAA-CBA-CGA-O1A
2	J	601	HEM	CAA-CBA-CGA-O2A
2	B	601	HEM	CAD-CBD-CGD-O1D
3	C	605	ZWY	C18-O20-S21-O22
3	E	603	ZWY	C18-O20-S21-O23
3	H	603	ZWY	C18-O20-S21-O24

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Mol	Chain	Res	Type	Atoms
2	I	601	HEM	CAA-CBA-CGA-O1A
2	J	601	HEM	CAA-CBA-CGA-O1A
2	A	601	HEM	CAD-CBD-CGD-O1D
2	E	601	HEM	CAA-CBA-CGA-O2A
2	I	601	HEM	CAD-CBD-CGD-O2D
2	D	601	HEM	CAA-CBA-CGA-O2A
2	F	601	HEM	CAD-CBD-CGD-O2D
2	F	601	HEM	CAD-CBD-CGD-O1D
2	L	601	HEM	CAD-CBD-CGD-O2D
2	E	601	HEM	CAD-CBD-CGD-O1D
2	A	601	HEM	CAD-CBD-CGD-O2D
2	L	601	HEM	CAD-CBD-CGD-O1D
2	D	601	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

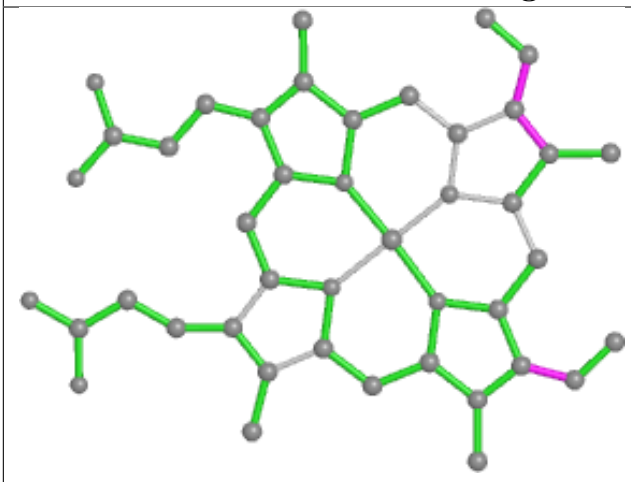
16 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	601	HEM	4	0
3	A	602	ZWY	1	0
2	L	601	HEM	5	0
2	E	601	HEM	2	0
3	H	602	ZWY	1	0
3	D	602	ZWY	2	0
2	J	601	HEM	3	0
2	B	601	HEM	3	0
3	E	605	ZWY	1	0
2	G	601	HEM	5	0
2	A	601	HEM	2	0
2	C	601	HEM	4	0
2	D	601	HEM	6	0
2	H	601	HEM	3	0
2	K	601	HEM	7	0
2	I	601	HEM	3	0

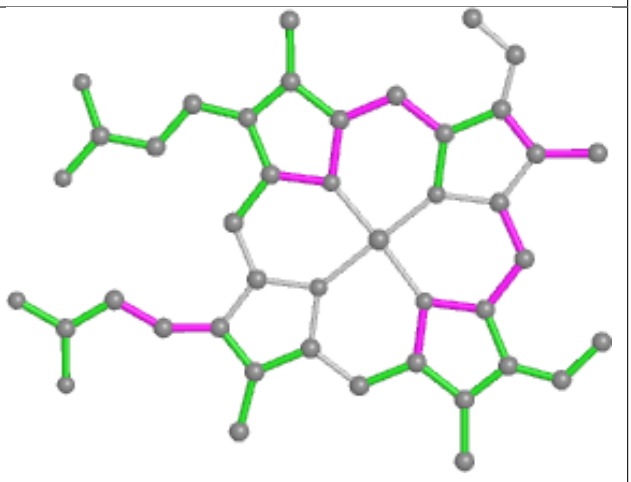
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

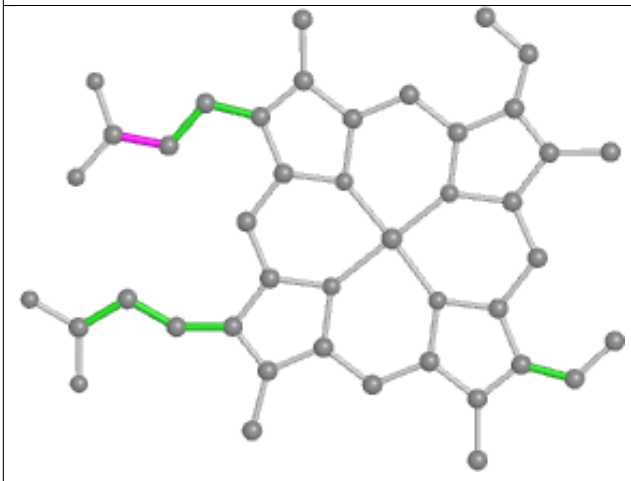
Ligand HEM F 601



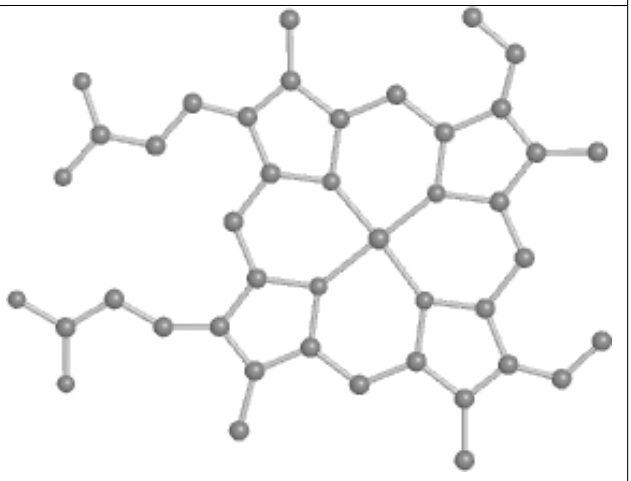
Bond lengths



Bond angles

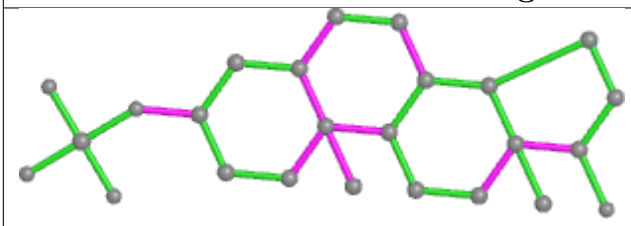


Torsions

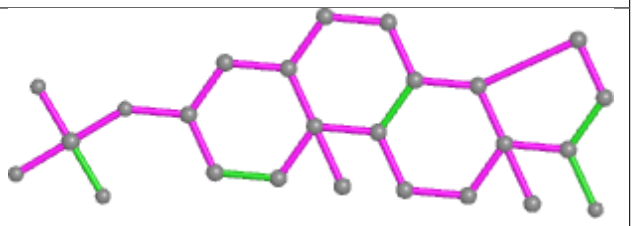


Rings

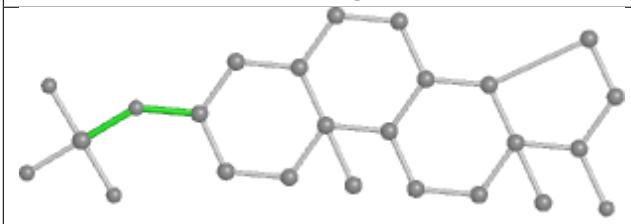
Ligand ZWY D 605



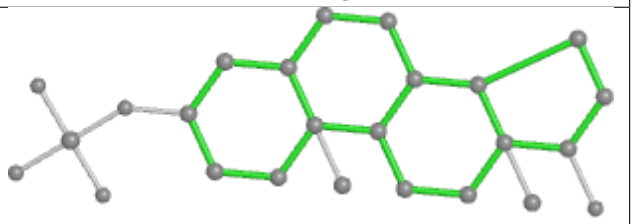
Bond lengths



Bond angles

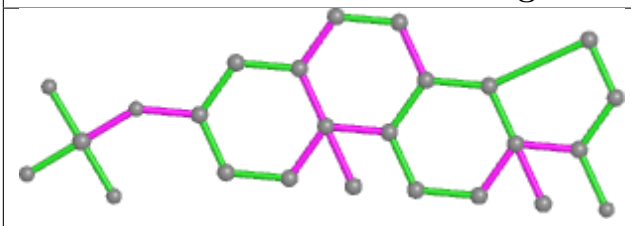


Torsions

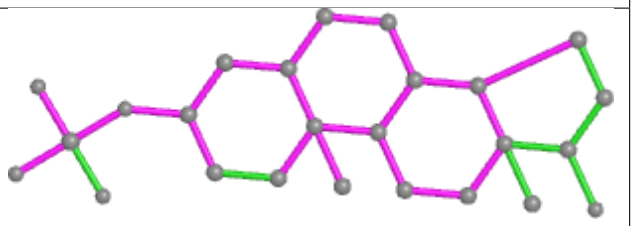


Rings

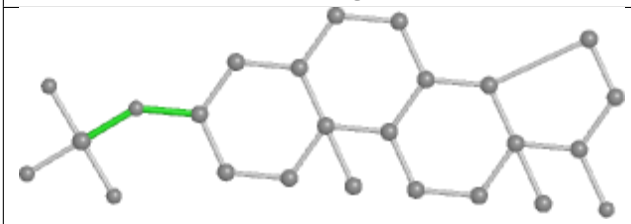
Ligand ZWY A 602



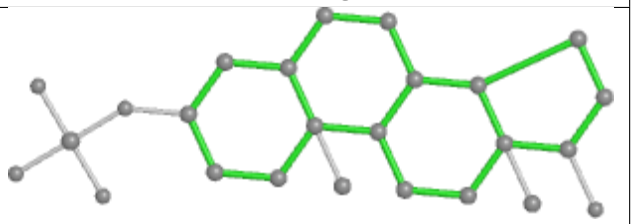
Bond lengths



Bond angles

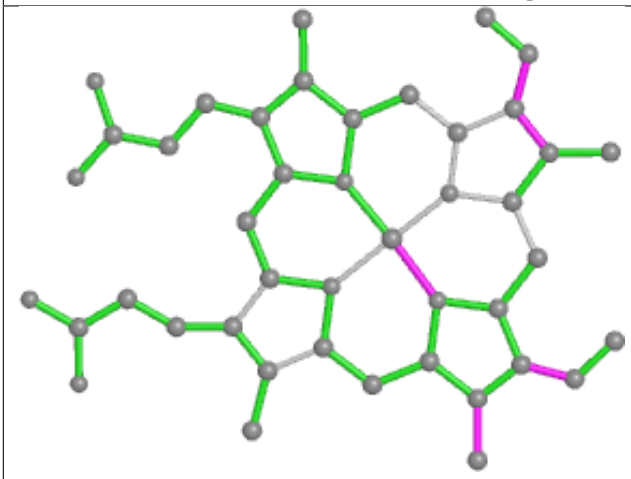


Torsions

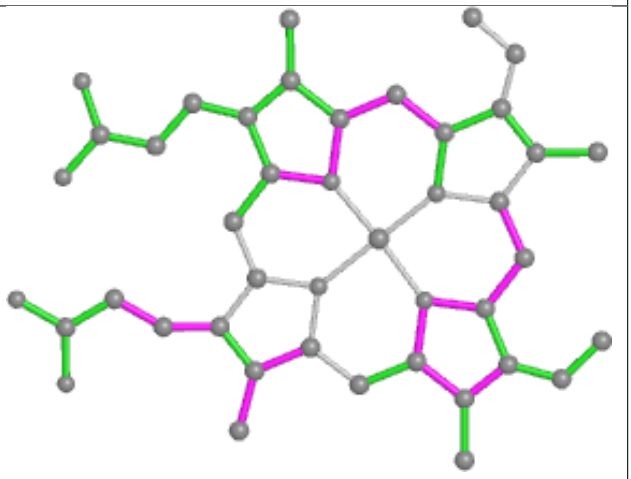


Rings

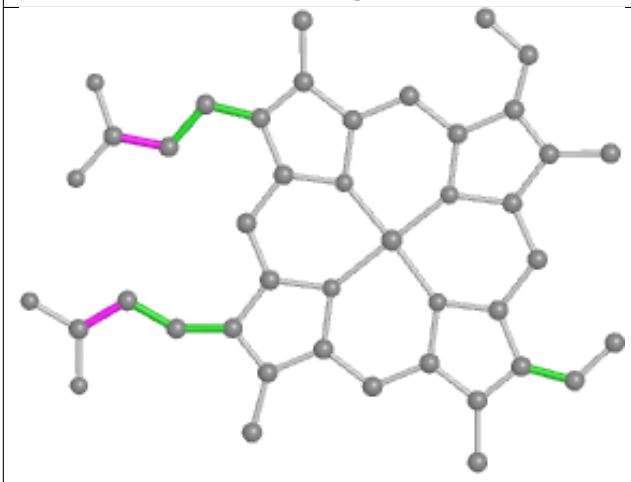
Ligand HEM L 601



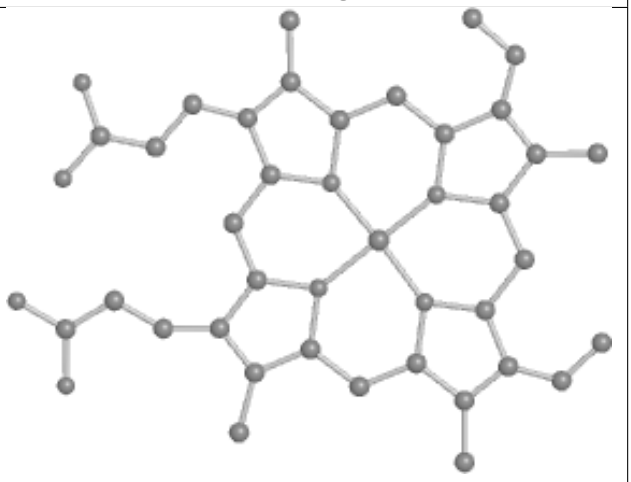
Bond lengths



Bond angles

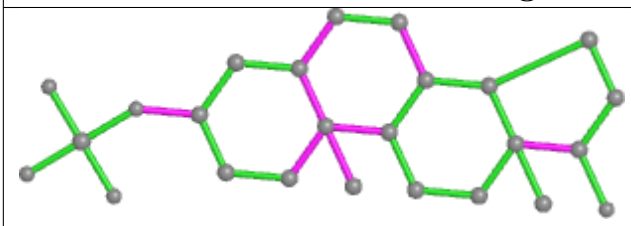


Torsions



Rings

Ligand ZWY C 605



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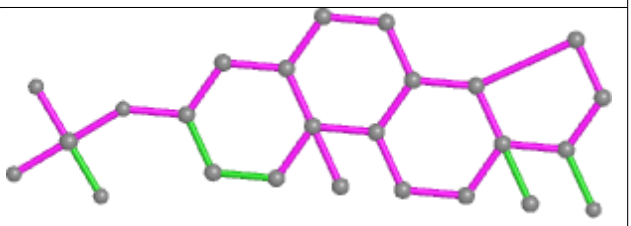
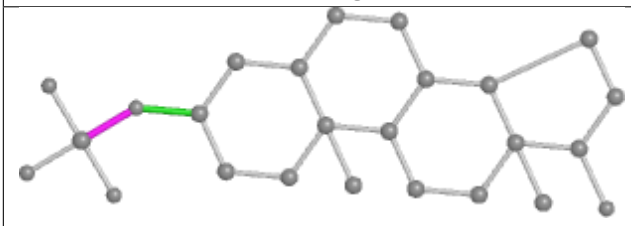
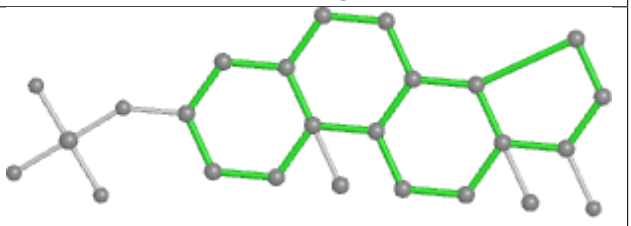


Bond angles

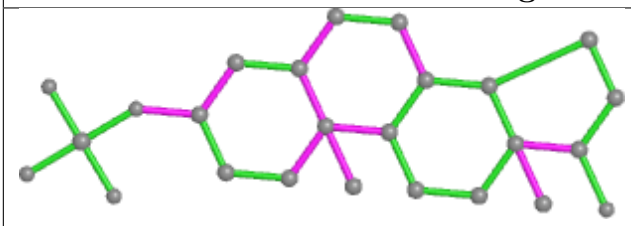


Torsions



Rings

Ligand ZWY C 603



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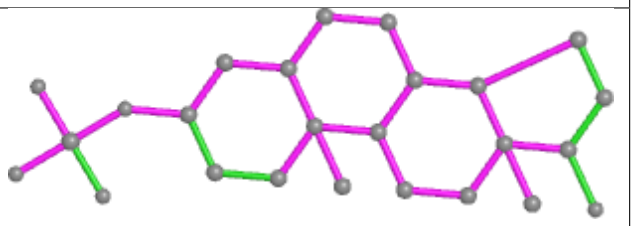
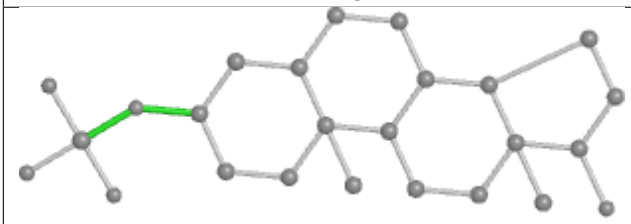


Bond angles



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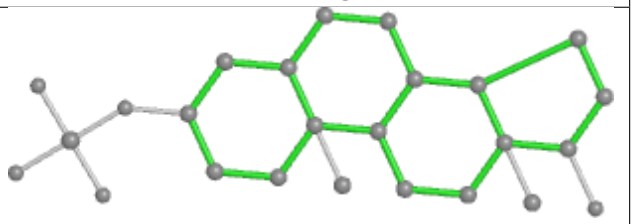
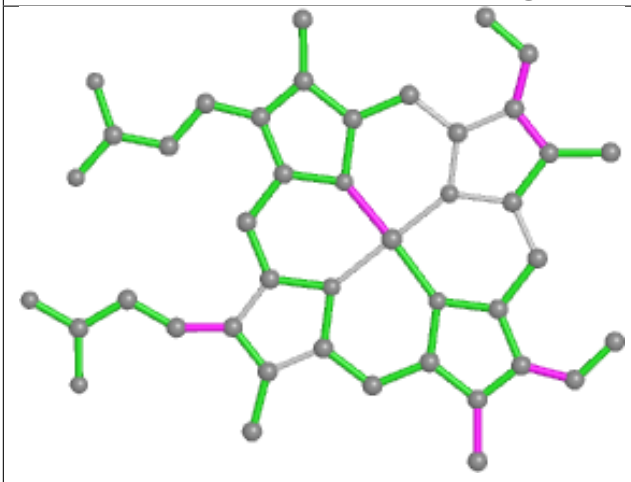


Rings

Ligand HEM E 601



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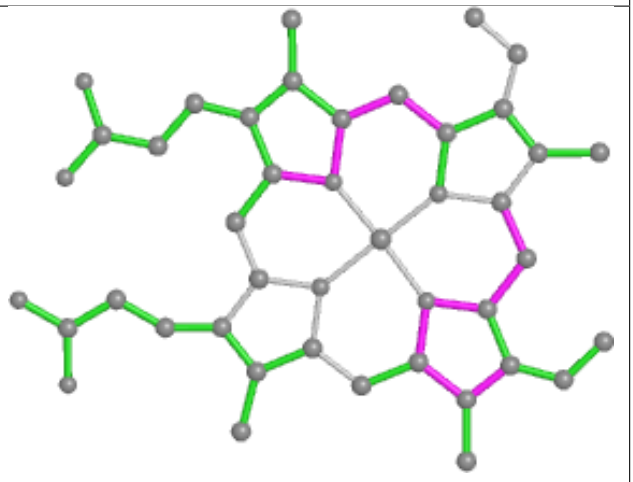
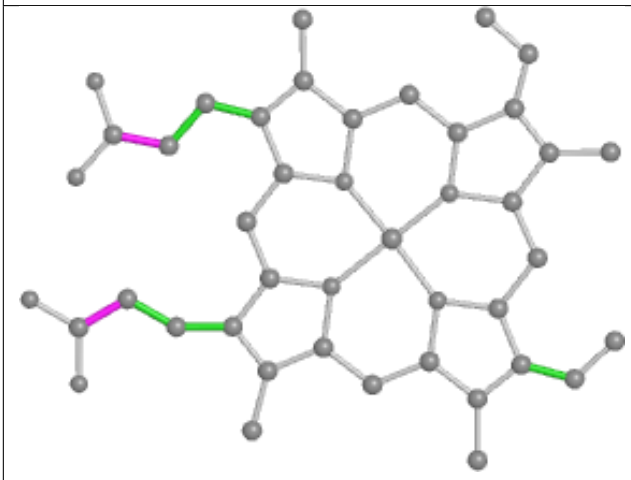


Bond angles



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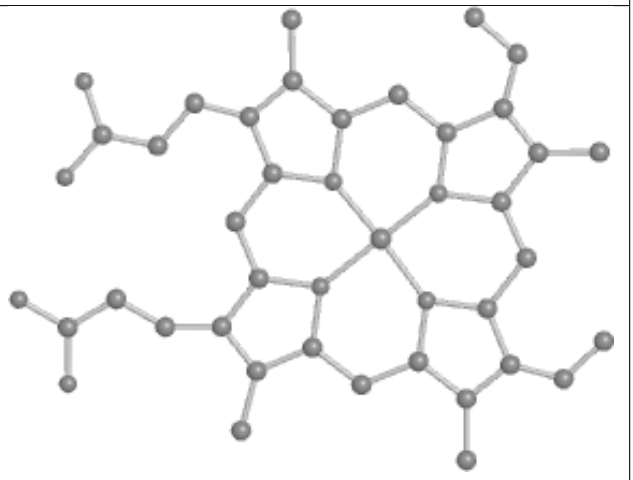
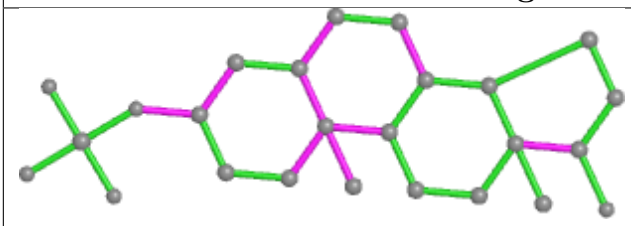


Rings

Ligand ZWY H 603



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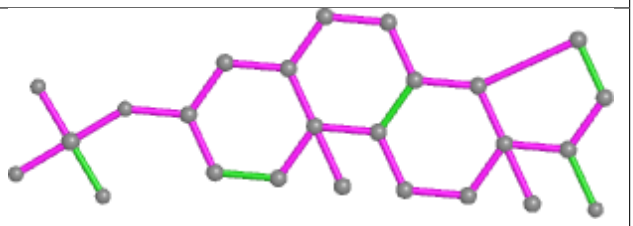
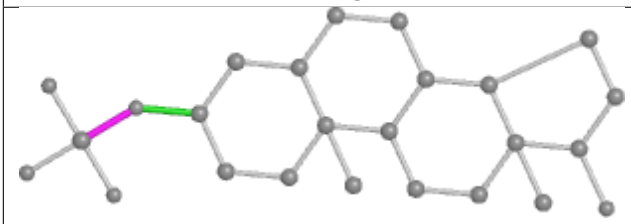


Bond angles



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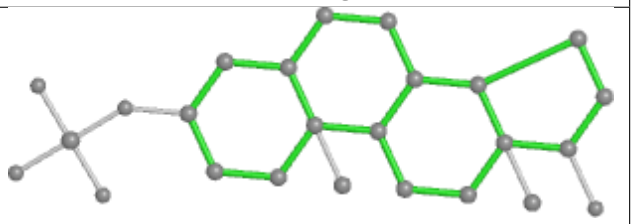
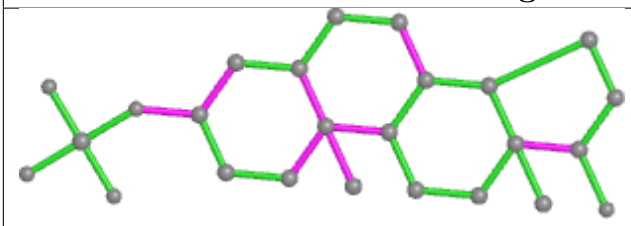


Rings

Ligand ZWY B 602



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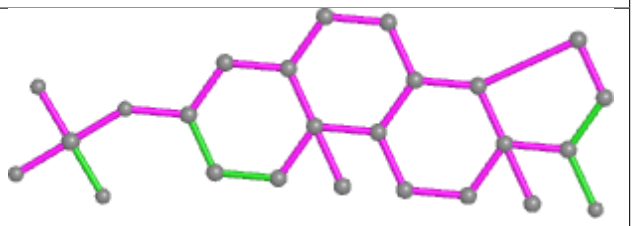

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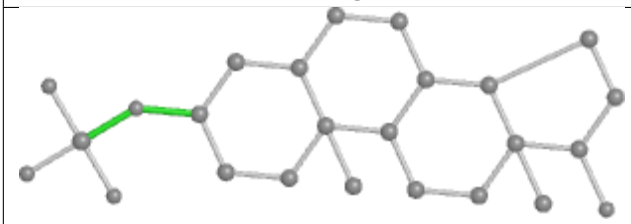

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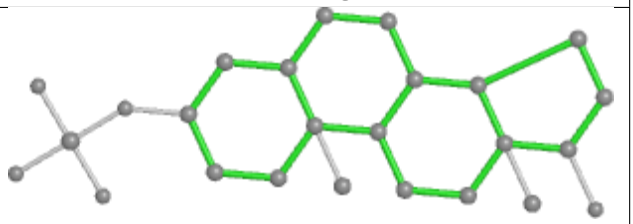
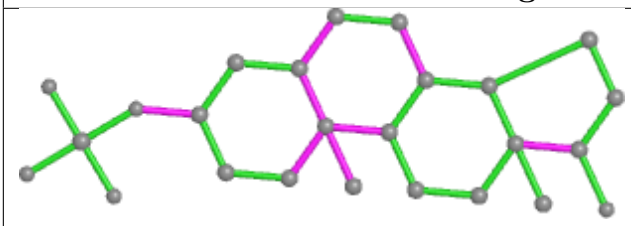


Rings

Ligand ZWY C 602



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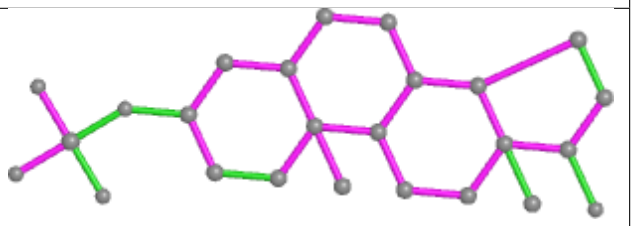
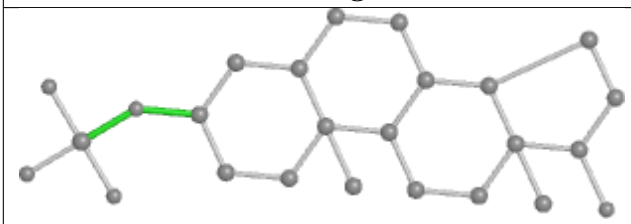


Bond angles



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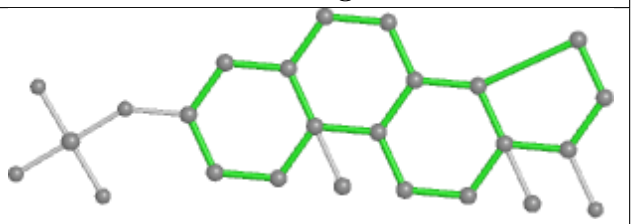
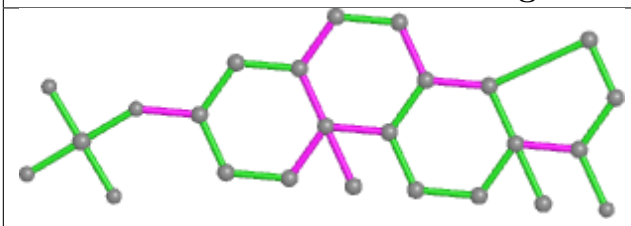


Rings

Ligand ZWY B 603



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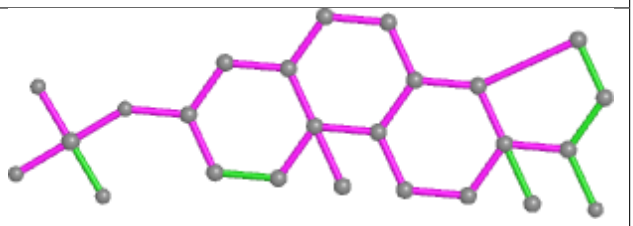
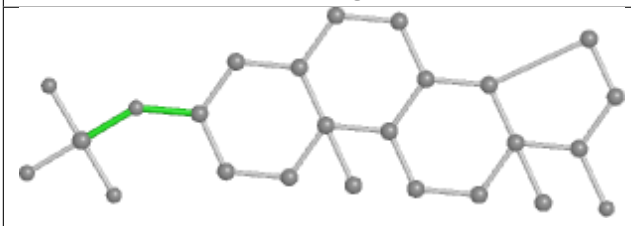


Bond angles



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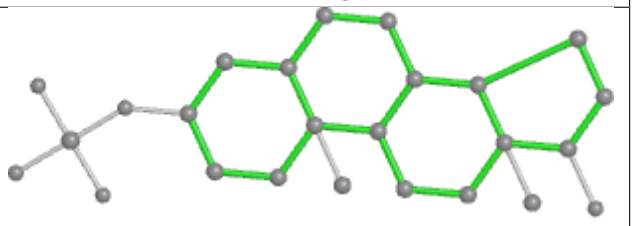
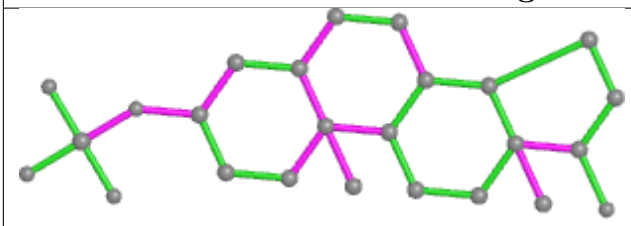


Rings

Ligand ZWY D 606



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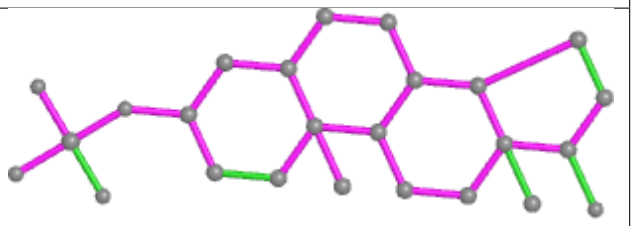
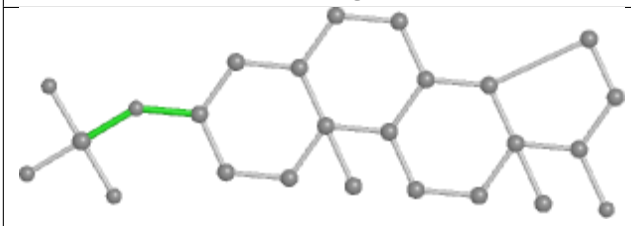


Bond angles



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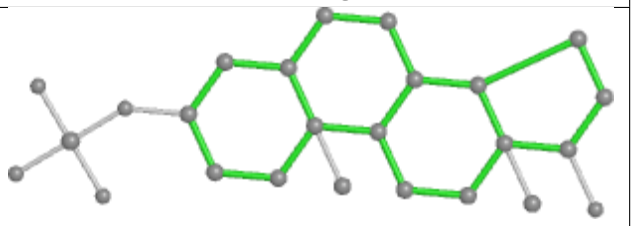
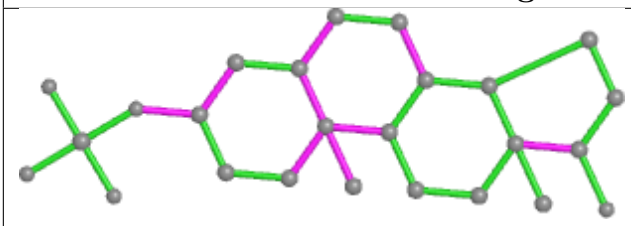


Rings

Ligand ZWY H 602



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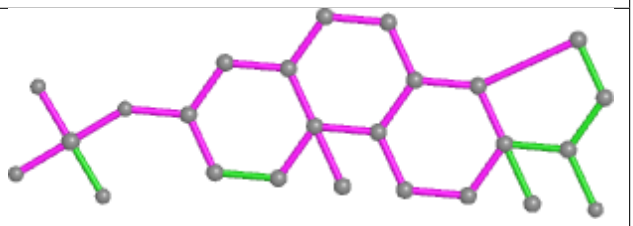
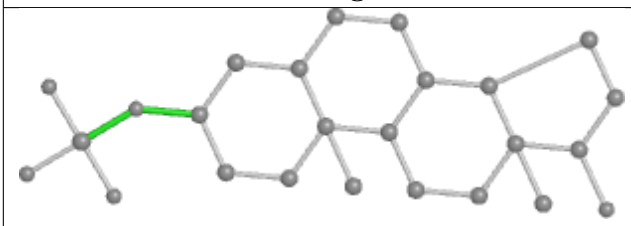


Bond angles



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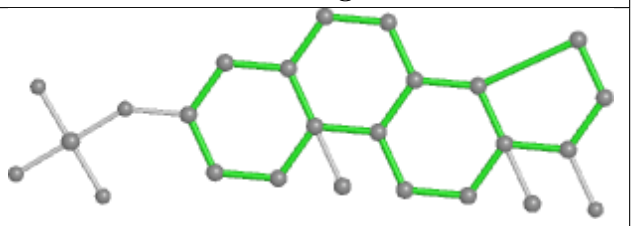
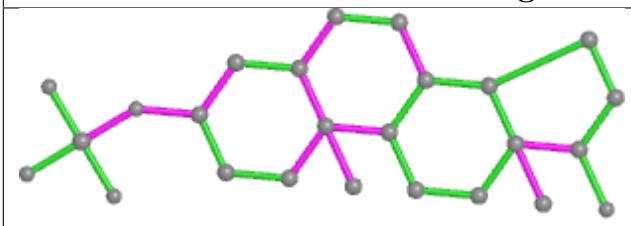


Rings

Ligand ZWY D 604



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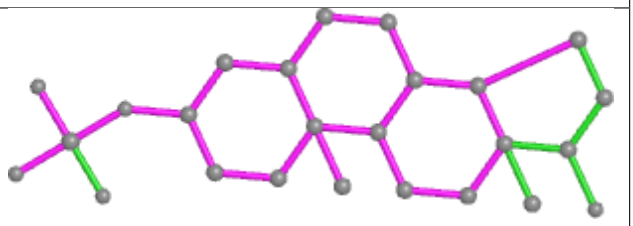
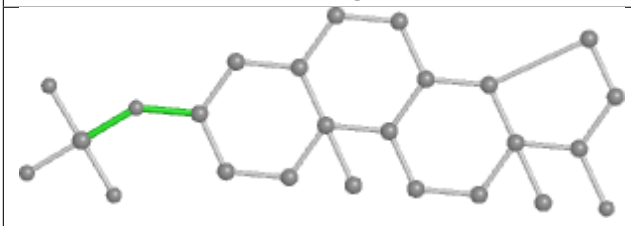


Bond angles



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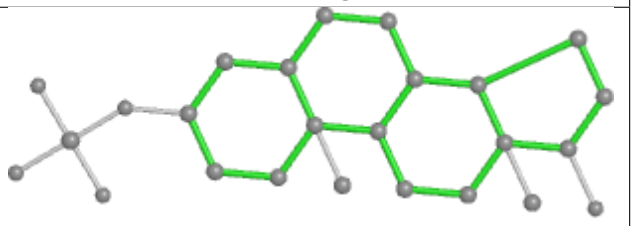
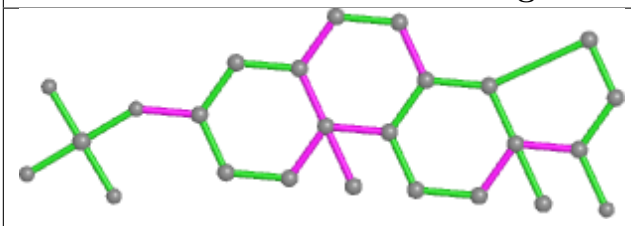


Rings

Ligand ZWY D 602



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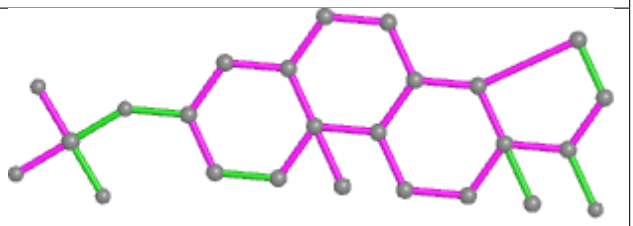

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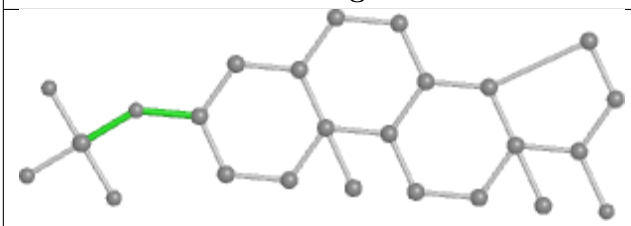

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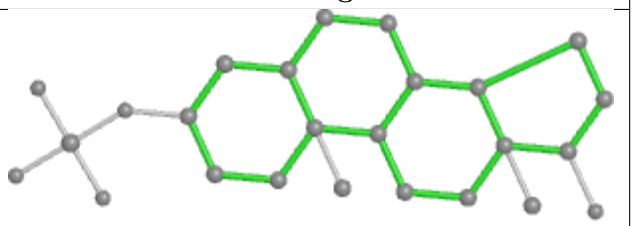
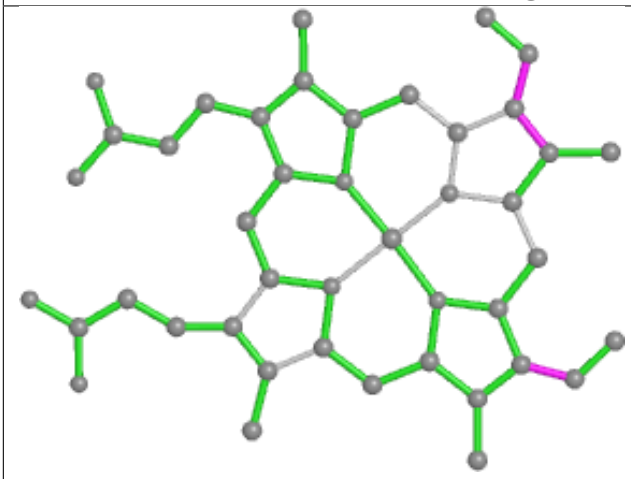


Rings

Ligand HEM J 601



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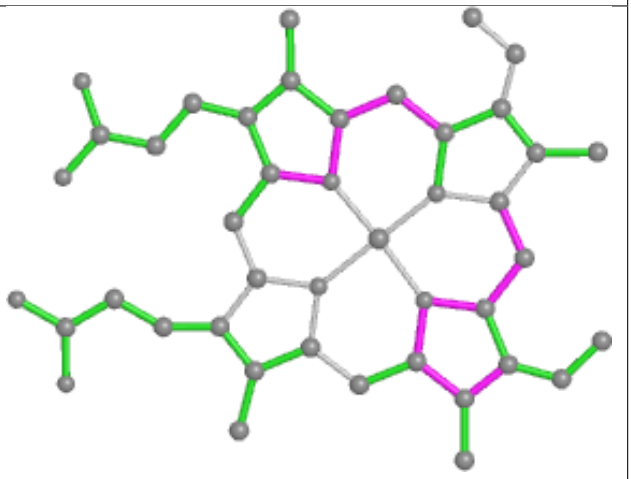
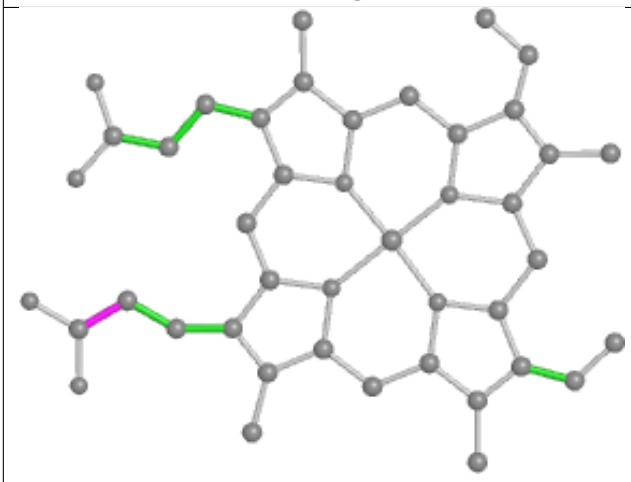


Bond angles



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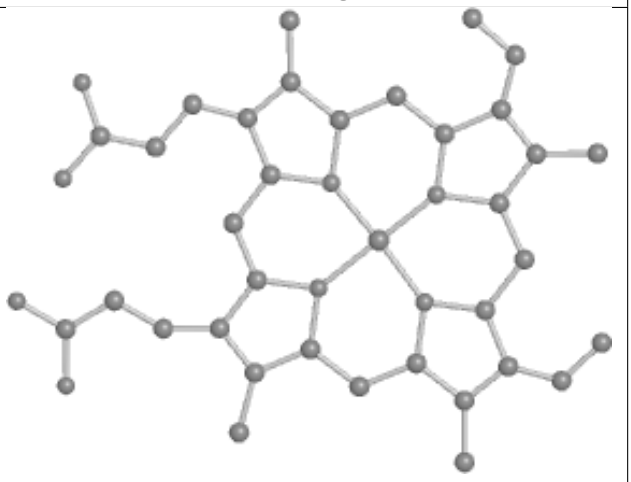
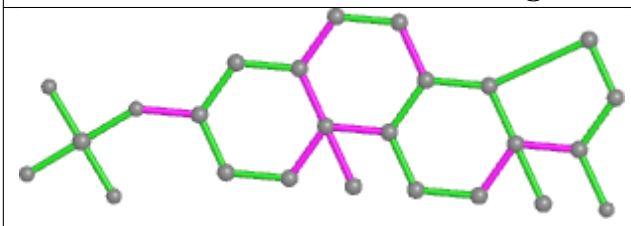


Rings

Ligand ZWY I 602



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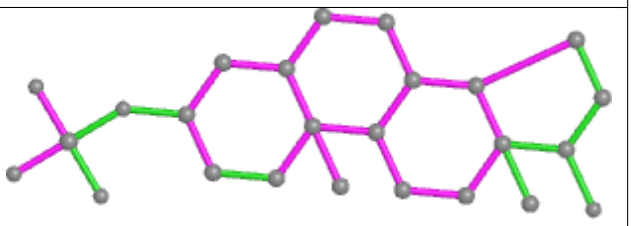
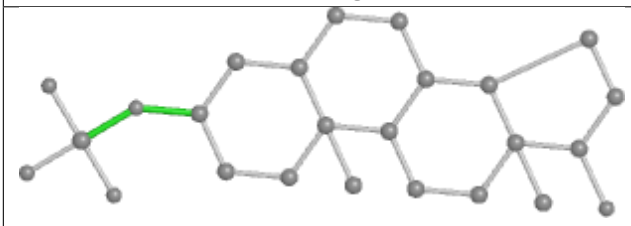


Bond angles



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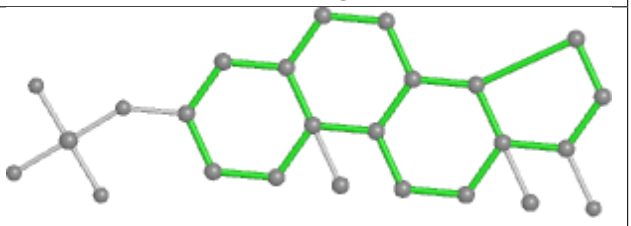
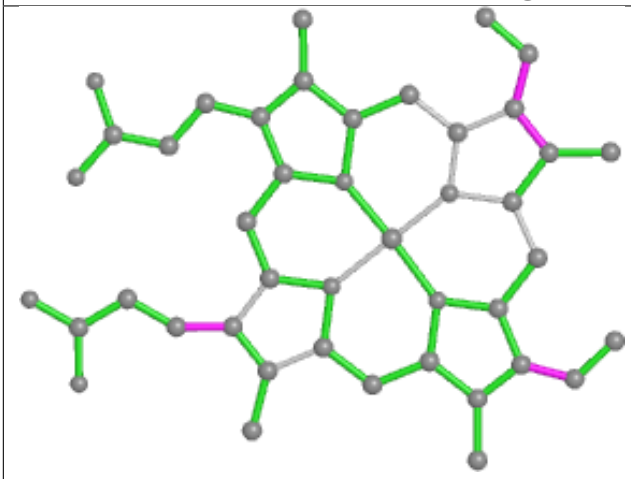


Rings

Ligand HEM B 601



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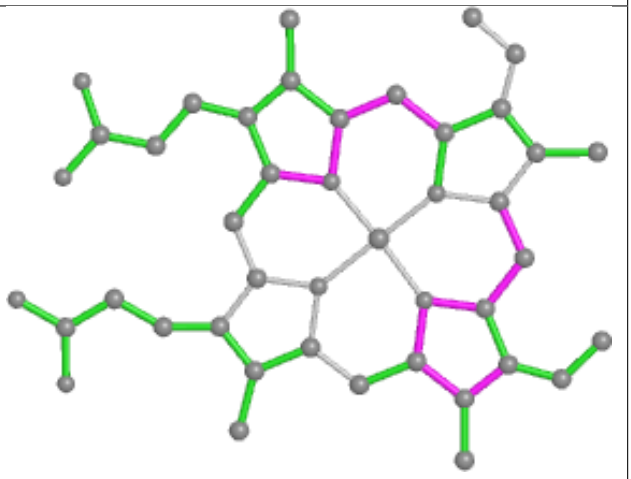
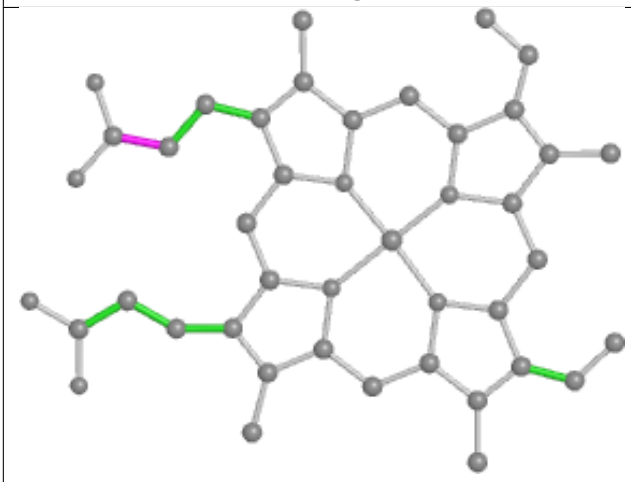
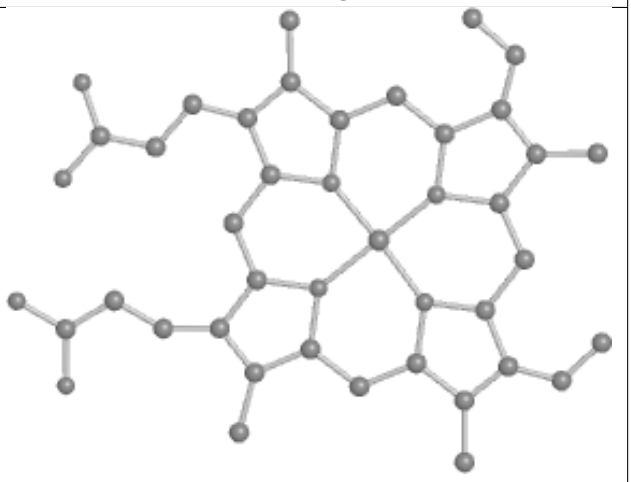


Bond angles

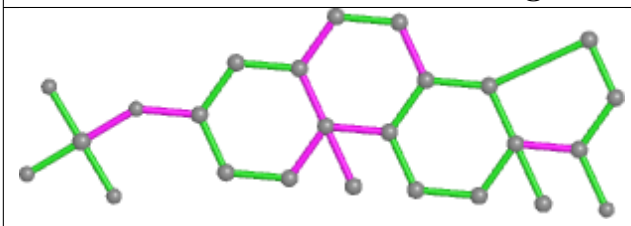


Torsions



Rings

Ligand ZWY I 603



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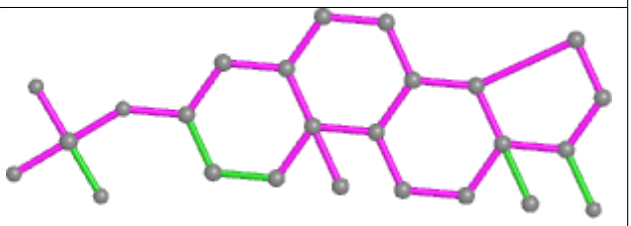
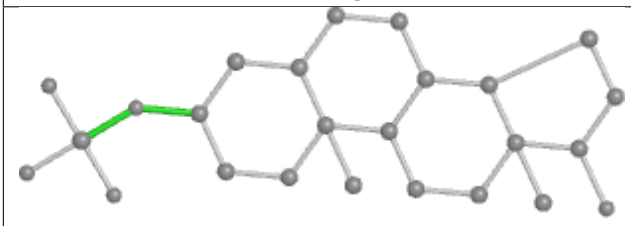
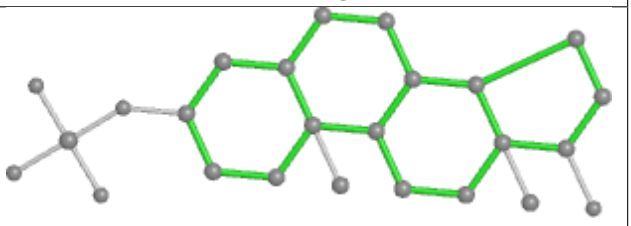


Bond angles

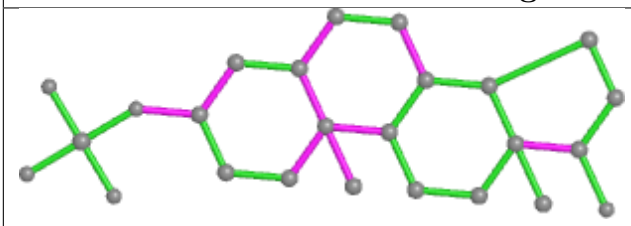


Torsions



Rings

Ligand ZWY E 605



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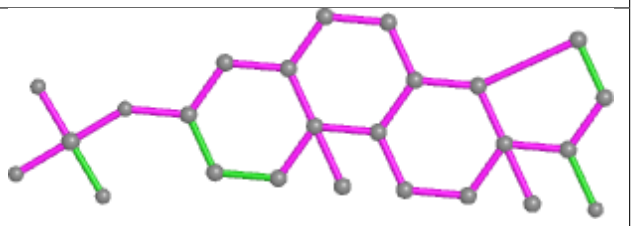

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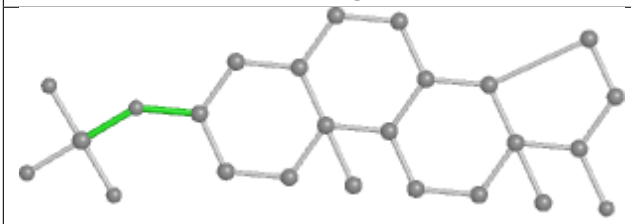

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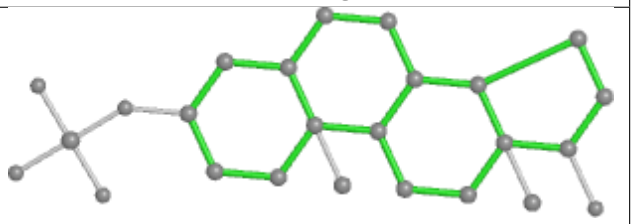
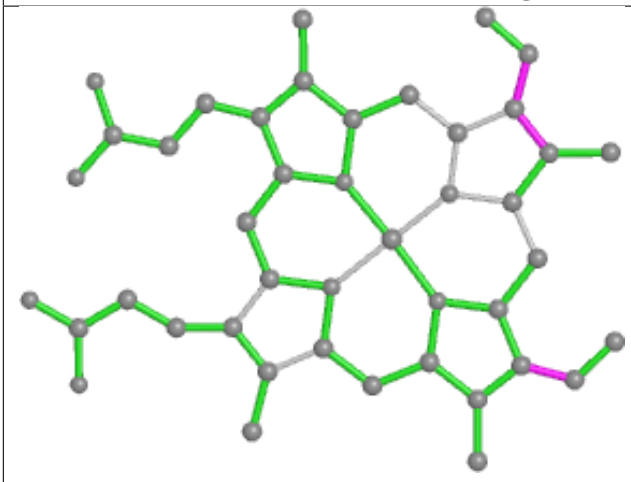


Rings

Ligand HEM G 601



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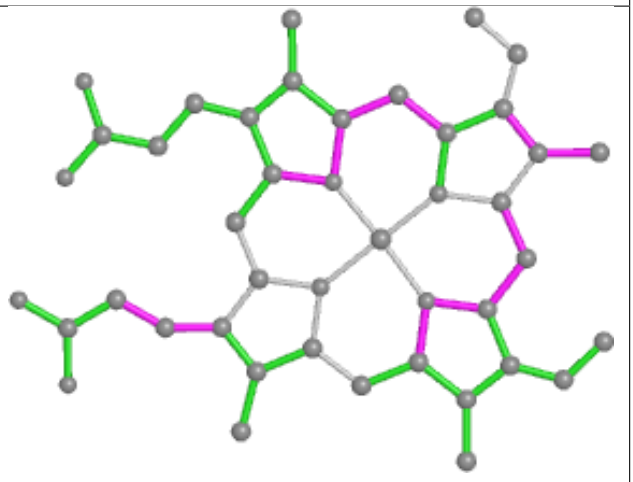

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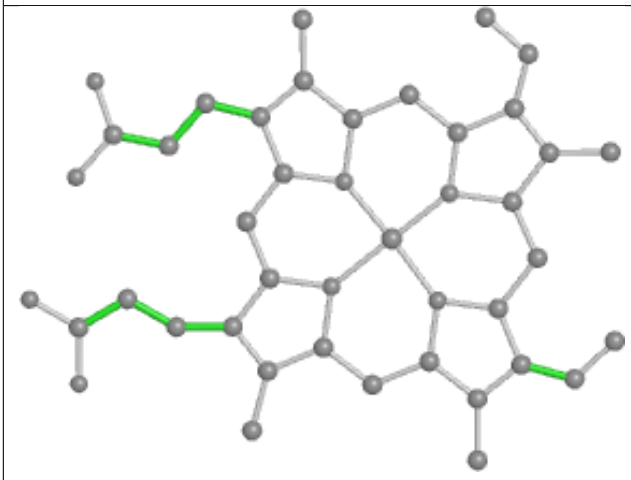

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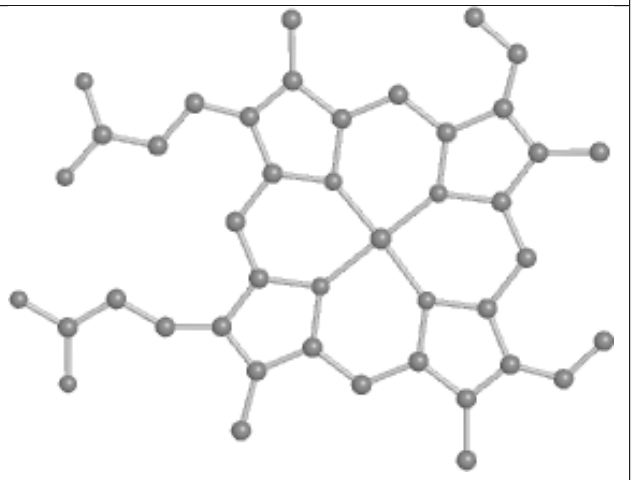
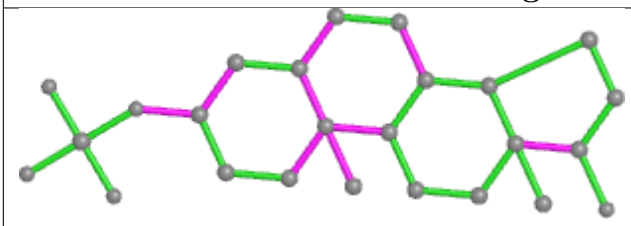


Rings

Ligand ZWY J 603



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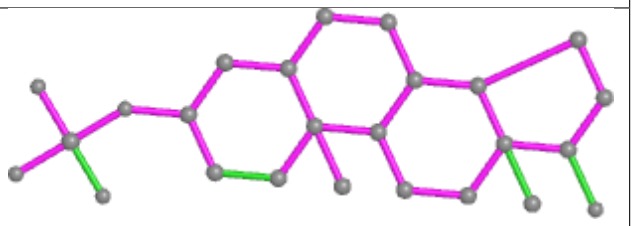

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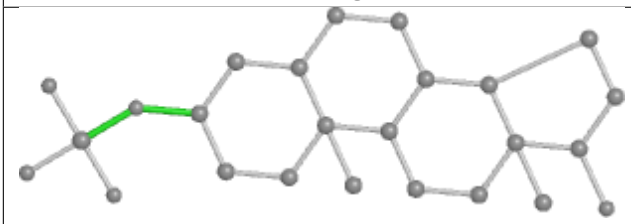

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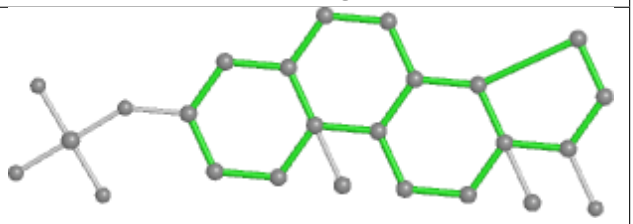
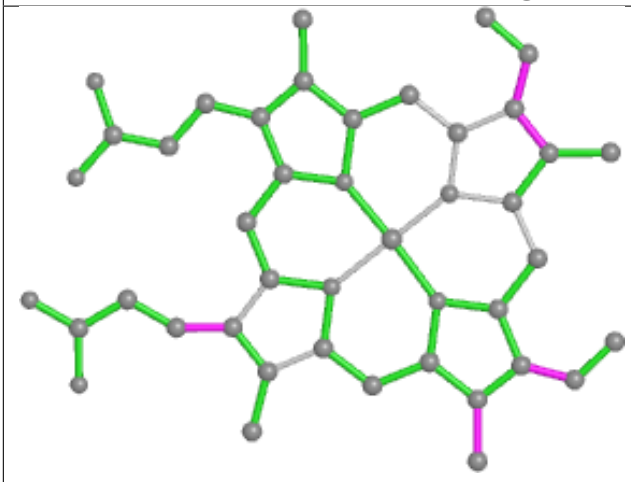


Rings

Ligand HEM A 601



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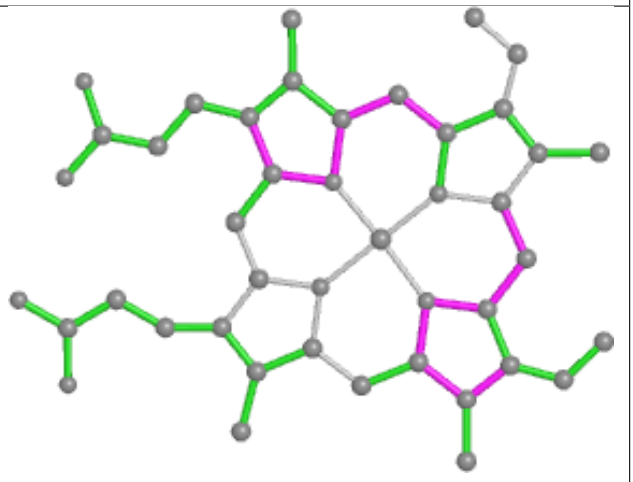

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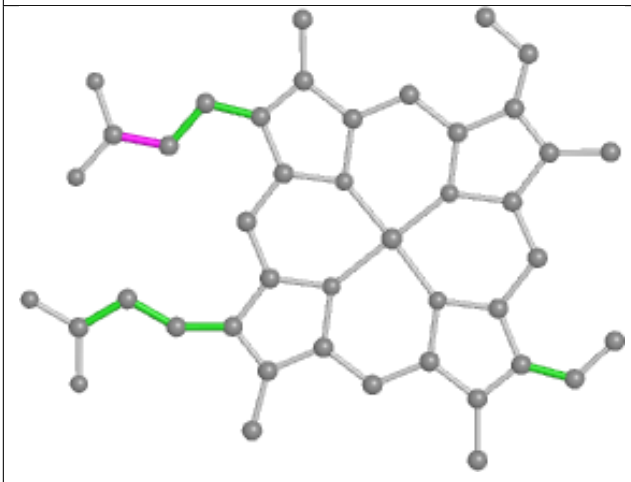

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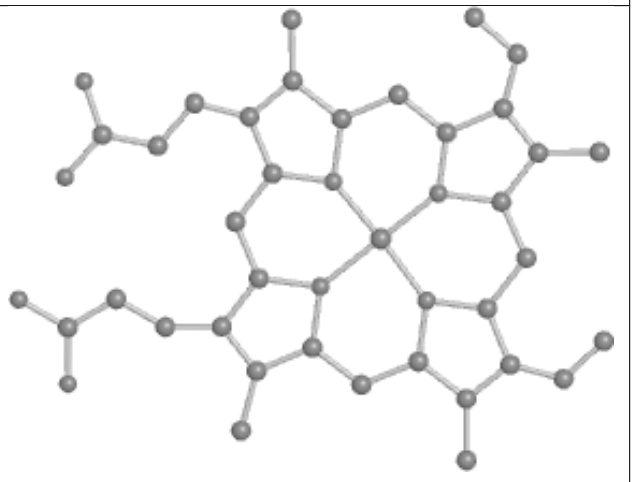
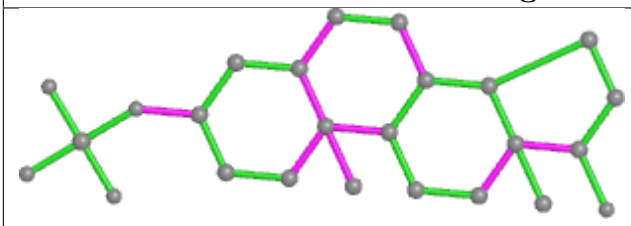


Rings

Ligand ZWY E 603



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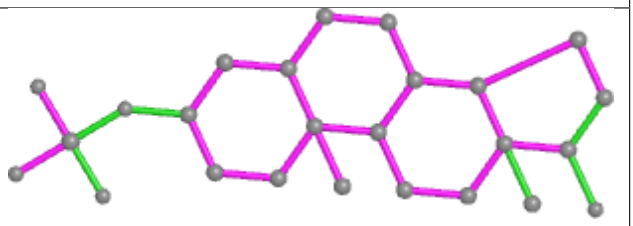

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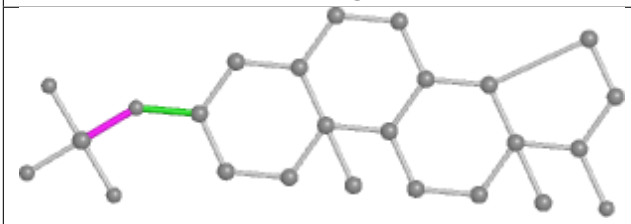

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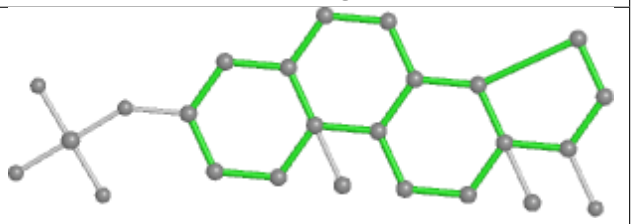
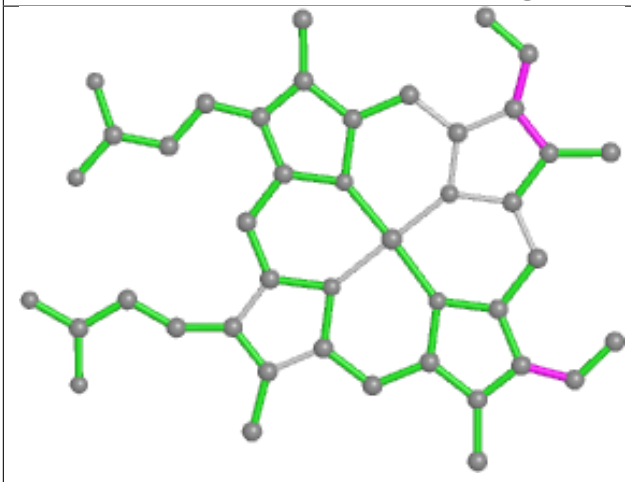


Rings

Ligand HEM C 601



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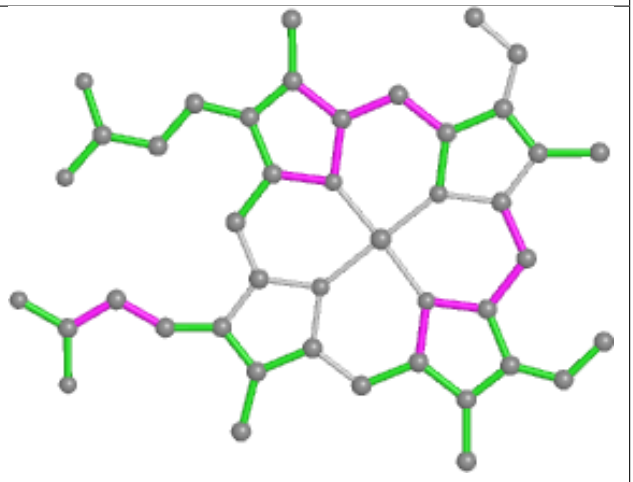

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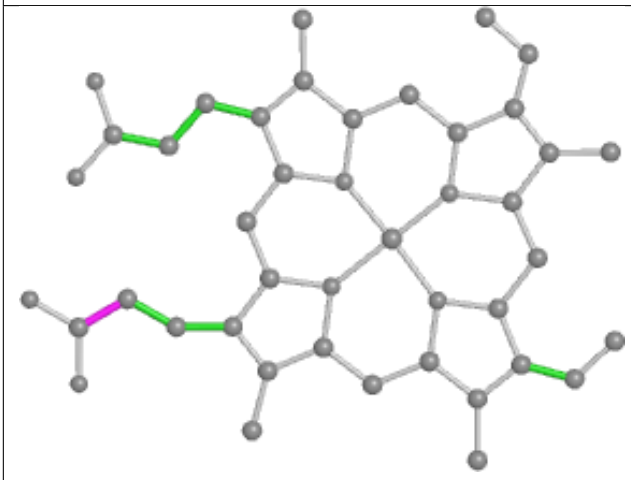

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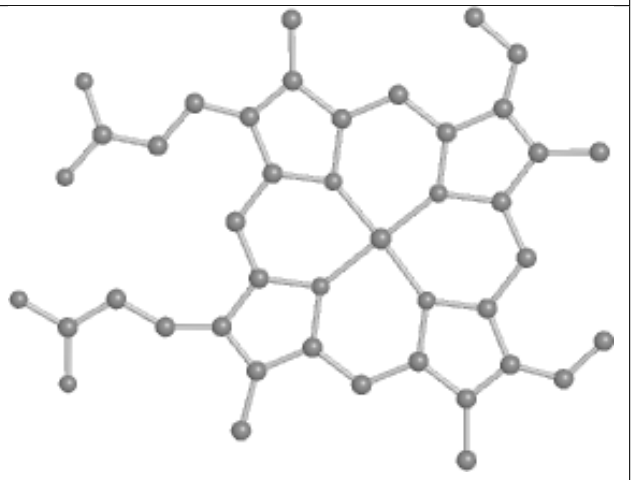

Rings

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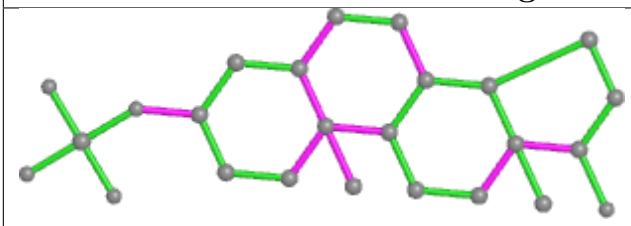

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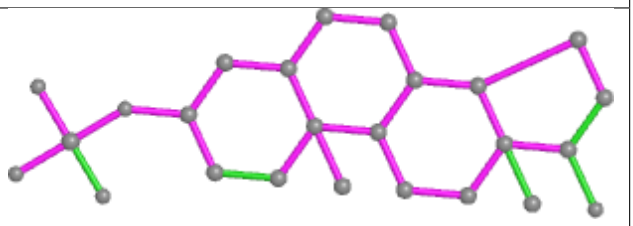

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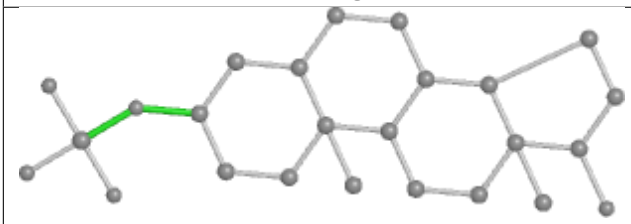

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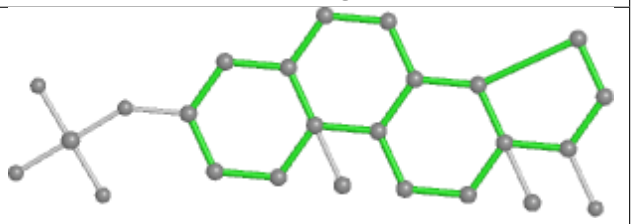

Rings

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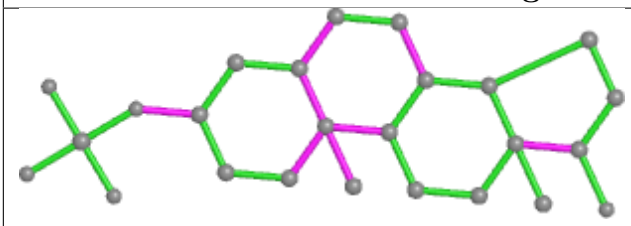

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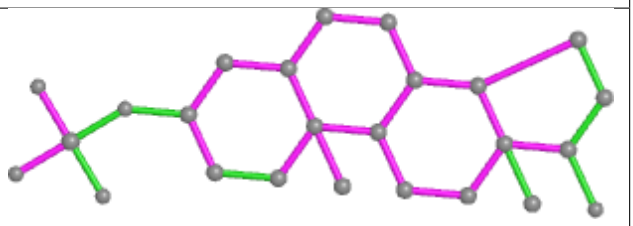

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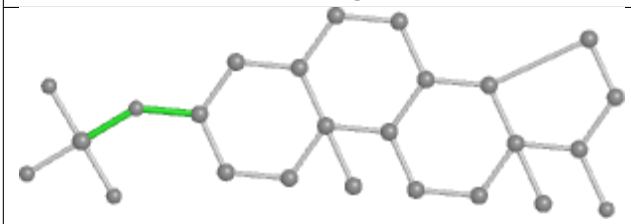

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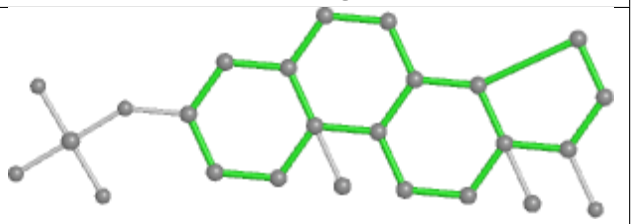

Rings

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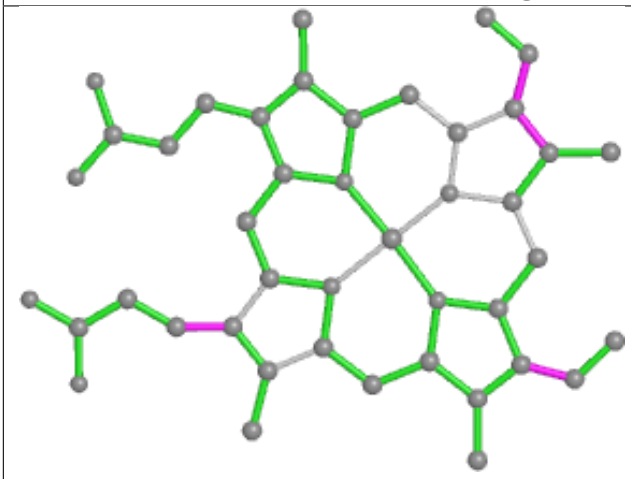

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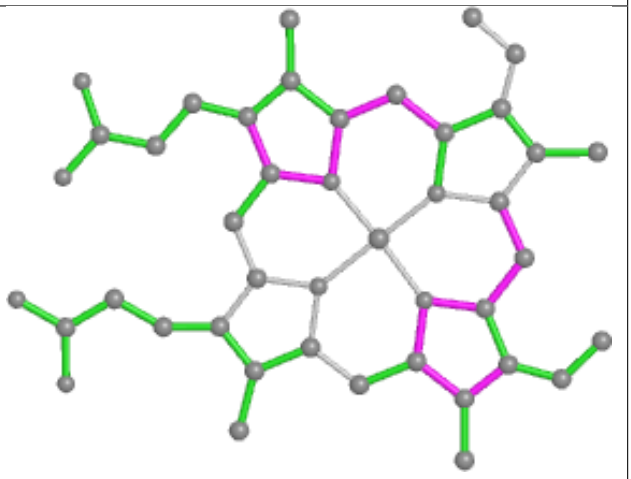

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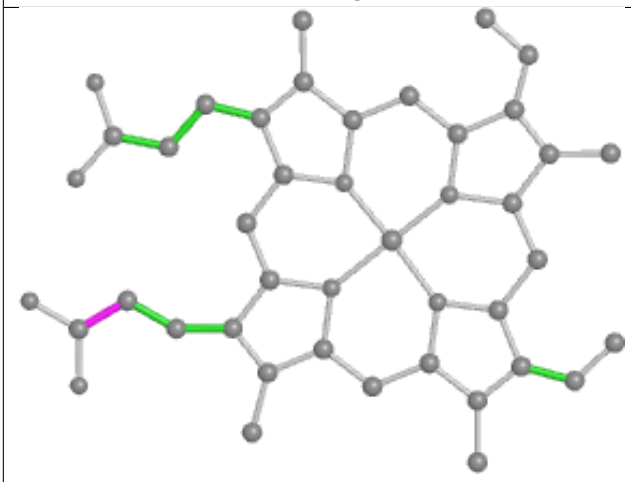

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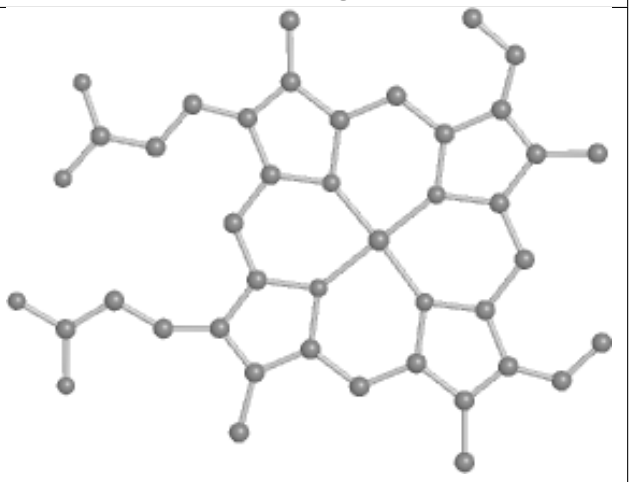
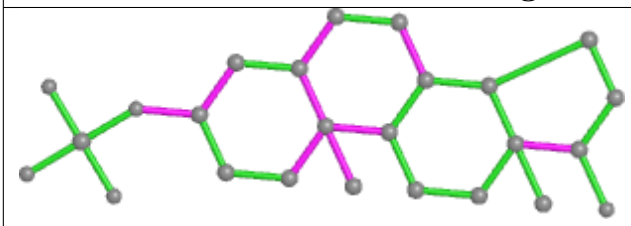


Rings

Ligand ZWY E 602



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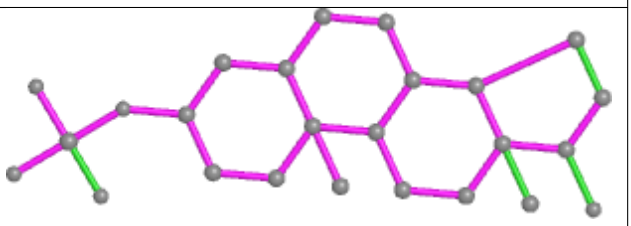

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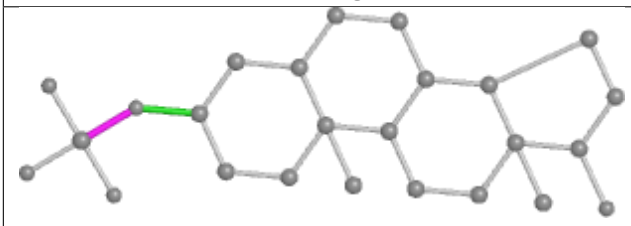

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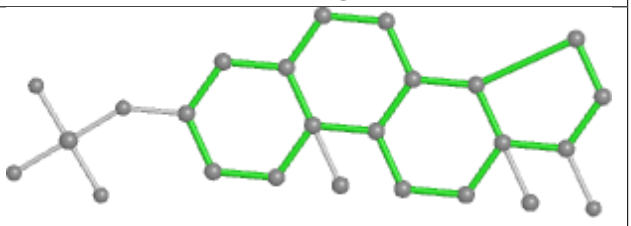
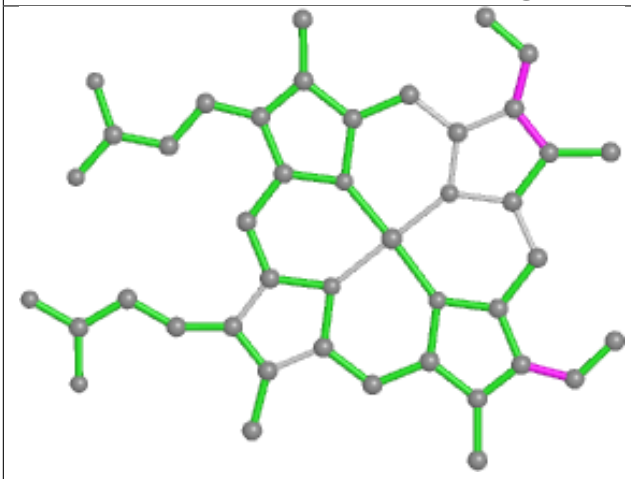


Rings

Ligand HEM H 601



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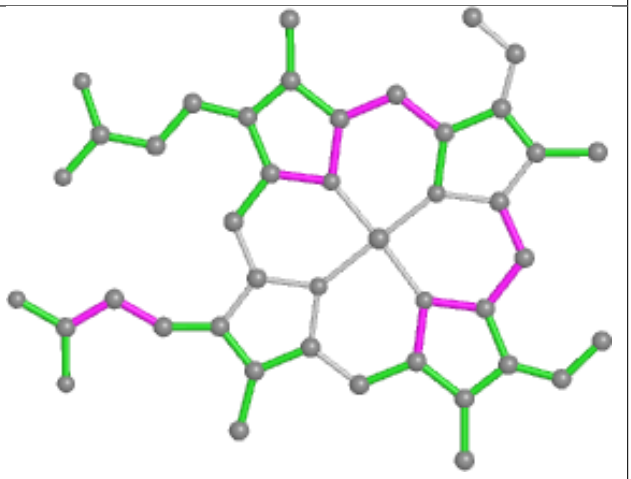

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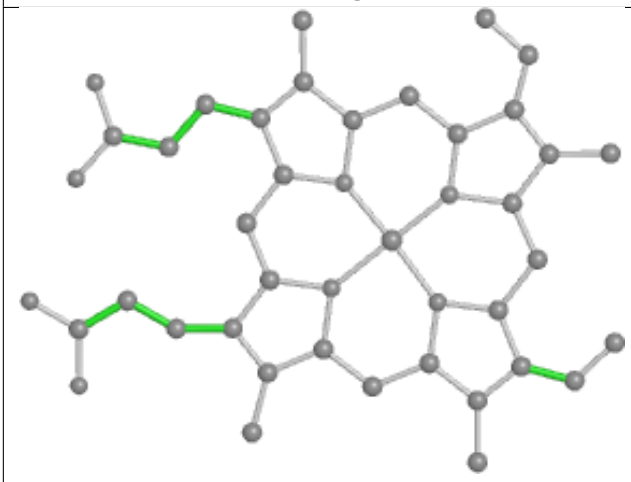

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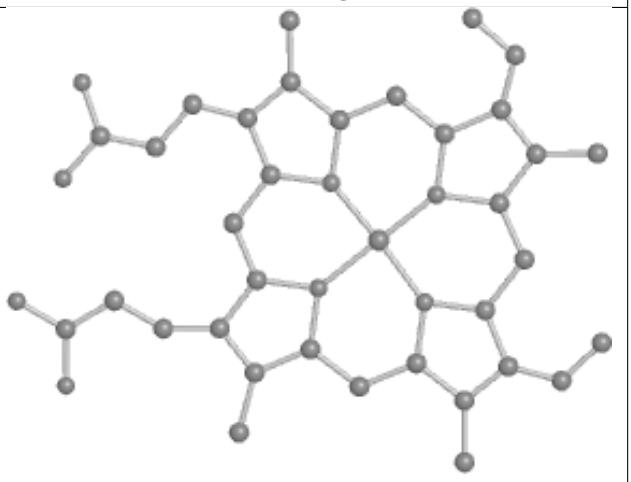
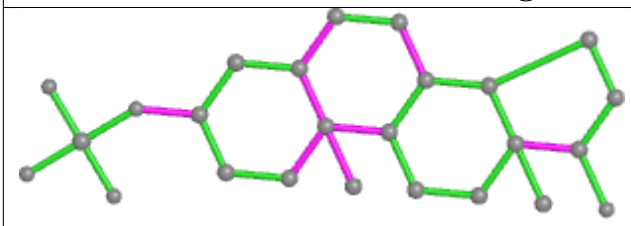


Rings

Ligand ZWY H 604



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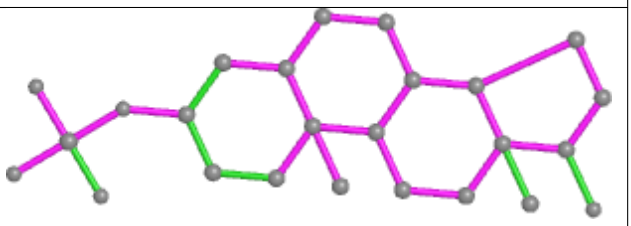

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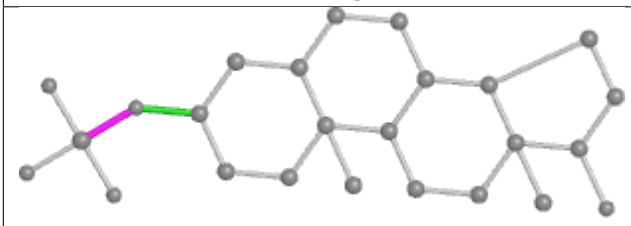

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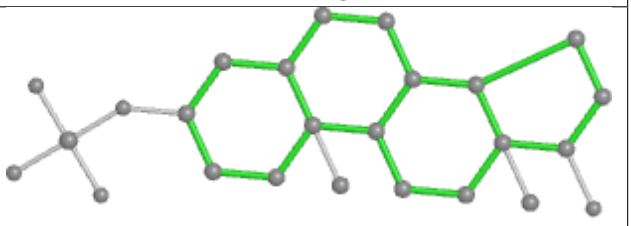
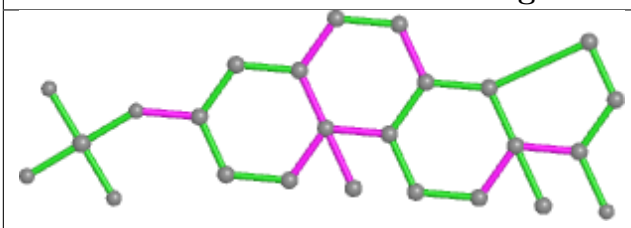


Rings

Ligand ZWY A 603



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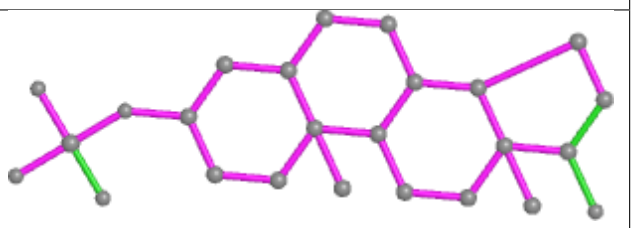
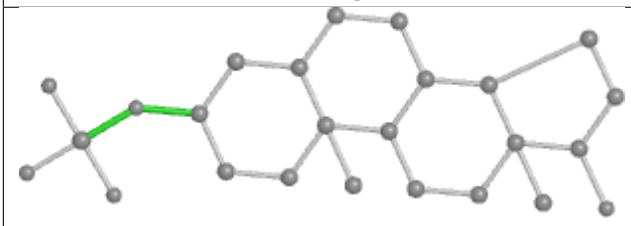


Bond angles



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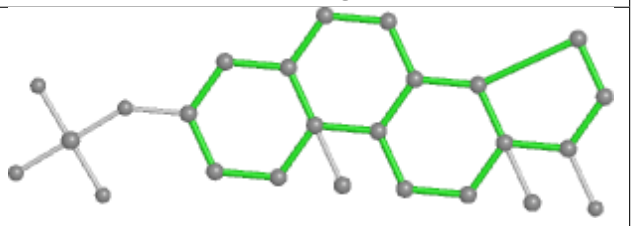
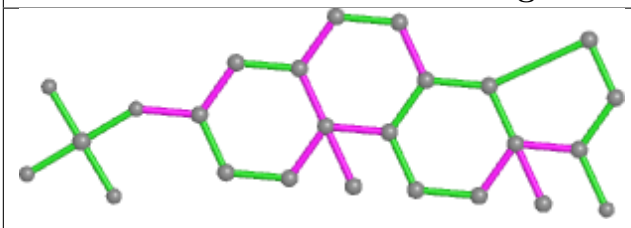
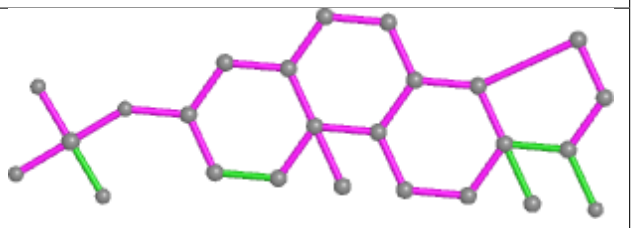


Rings

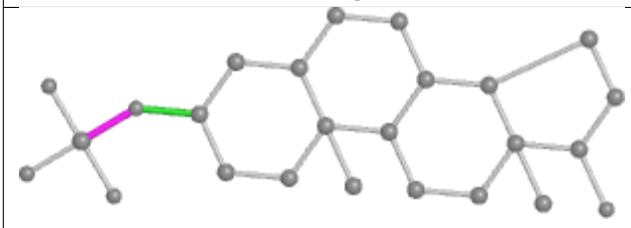
Ligand ZWY D 603



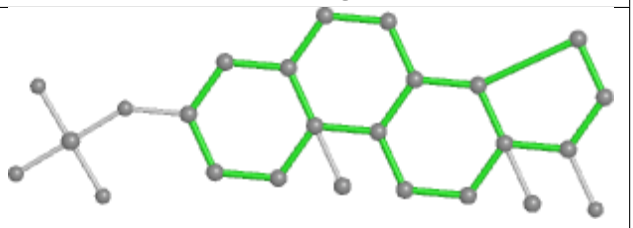
Bond lengths



Bond angles

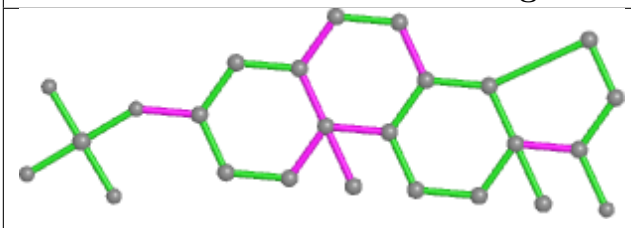


Torsions

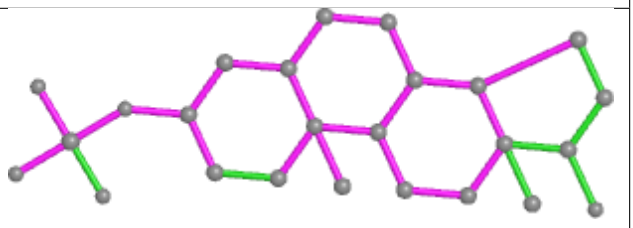


Rings

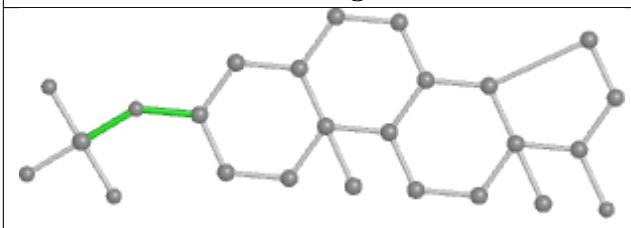
Ligand ZWY E 604



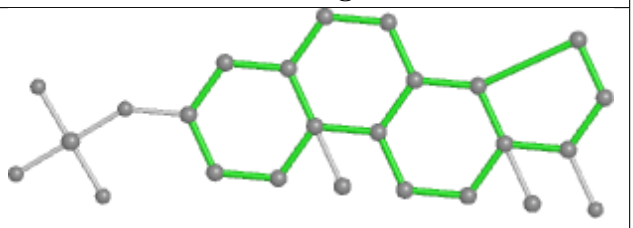
Bond lengths



Bond angles

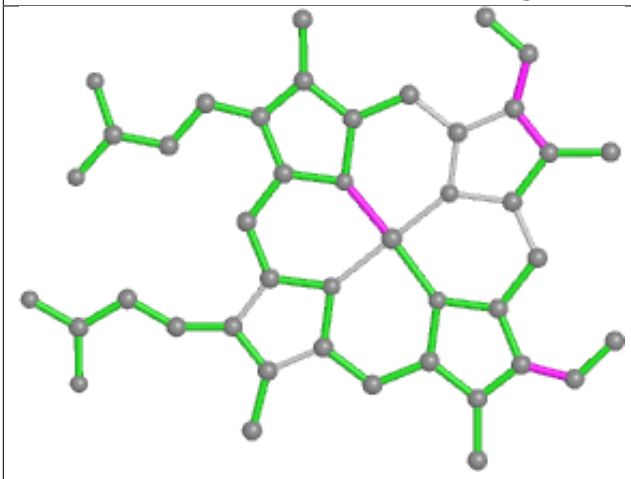


Torsions

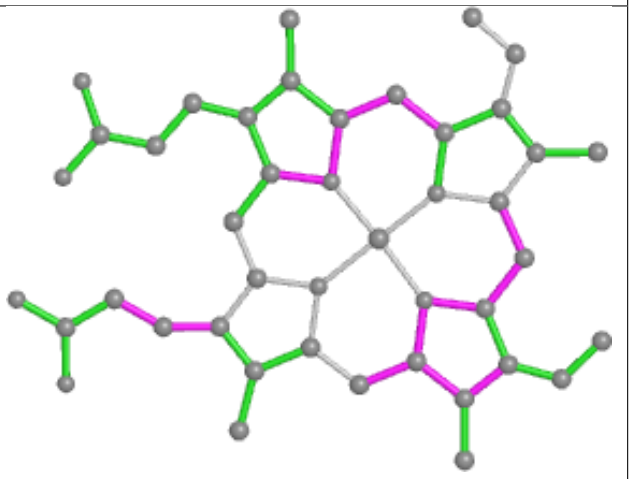


Rings

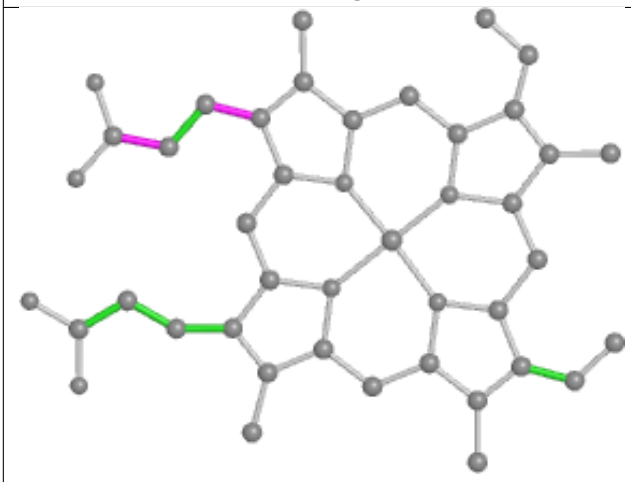
Ligand HEM K 601



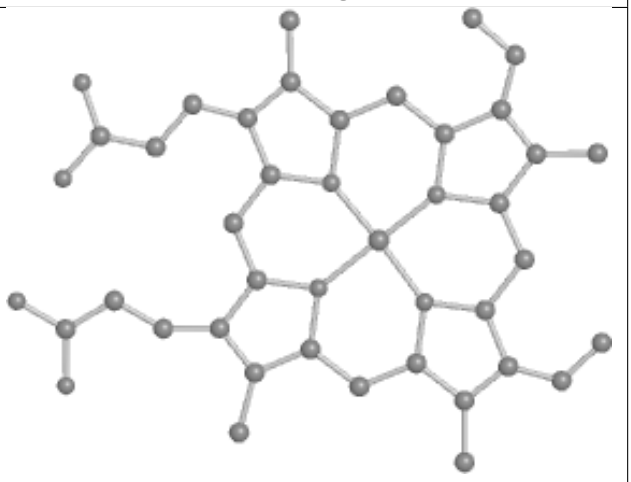
Bond lengths



Bond angles

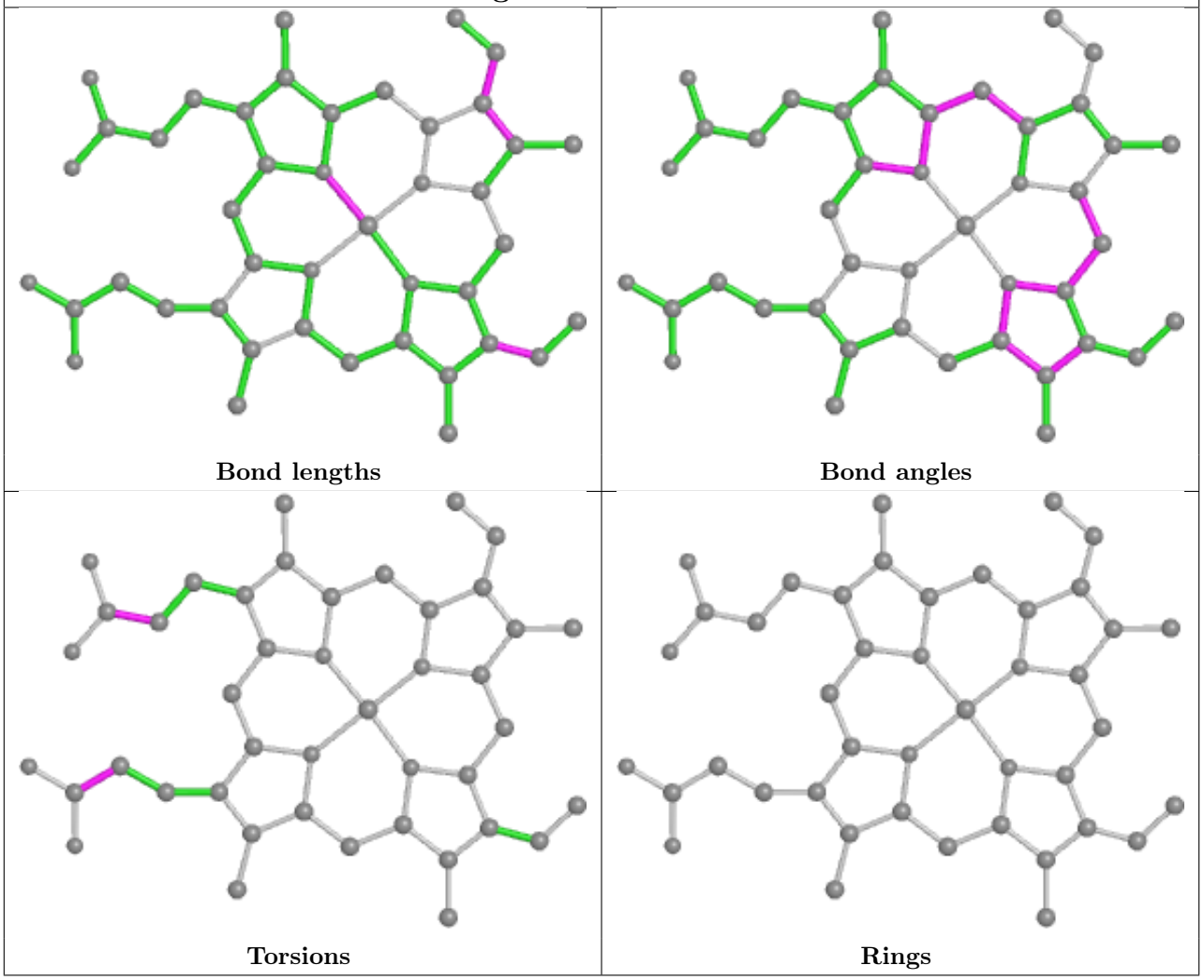


Torsions



Rings

Ligand HEM I 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	473/486 (97%)	0.03	4 (0%) 86 84	48, 68, 92, 116	0
1	B	462/486 (95%)	0.06	4 (0%) 84 82	47, 70, 89, 109	0
1	C	463/486 (95%)	0.14	10 (2%) 62 56	51, 70, 91, 113	0
1	D	459/486 (94%)	0.03	4 (0%) 84 82	53, 71, 95, 116	0
1	E	460/486 (94%)	0.23	15 (3%) 46 39	51, 75, 99, 122	0
1	F	461/486 (94%)	0.26	10 (2%) 62 56	55, 79, 98, 110	0
1	G	462/486 (95%)	0.21	14 (3%) 50 43	57, 80, 99, 116	0
1	H	458/486 (94%)	0.20	14 (3%) 49 42	58, 78, 100, 117	0
1	I	463/486 (95%)	0.36	27 (5%) 23 17	50, 81, 102, 124	0
1	J	458/486 (94%)	0.18	13 (2%) 53 46	58, 78, 101, 119	0
1	K	462/486 (95%)	0.19	16 (3%) 44 36	58, 88, 108, 122	0
1	L	440/486 (90%)	0.73	59 (13%) 3 2	56, 98, 118, 126	0
All	All	5521/5832 (94%)	0.22	190 (3%) 45 38	47, 78, 105, 126	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	256	ILE	6.3
1	L	133	LEU	6.2
1	I	282	LYS	5.2
1	G	287	HIS	5.1
1	F	491	LEU	5.1
1	F	473	ILE	5.0
1	L	204	VAL	5.0
1	H	492	LYS	4.8
1	L	130	ARG	4.7
1	B	473	ILE	4.7
1	L	135	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	L	299	SER	4.6
1	H	262	LYS	4.5
1	I	436	GLY	4.3
1	J	165	GLU	4.2
1	H	168	LYS	4.1
1	L	295	LEU	4.1
1	L	95	VAL	4.0
1	G	383	ILE	4.0
1	H	493	ALA	3.8
1	L	334	GLU	3.7
1	L	347	TYR	3.7
1	L	205	GLU	3.7
1	A	469	LYS	3.7
1	H	473	ILE	3.7
1	I	442	CYS	3.6
1	C	473	ILE	3.6
1	E	442	CYS	3.5
1	H	467	PRO	3.4
1	E	305	ALA	3.4
1	L	108	PHE	3.4
1	C	442	CYS	3.4
1	I	492	LYS	3.4
1	I	58	TRP	3.4
1	K	262	LYS	3.4
1	L	287	HIS	3.4
1	G	286	THR	3.3
1	J	281	SER	3.3
1	L	144	GLU	3.3
1	L	148	ILE	3.3
1	I	493	ALA	3.3
1	E	309	THR	3.3
1	L	245	VAL	3.3
1	E	306	GLY	3.3
1	L	473	ILE	3.3
1	L	193	ILE	3.2
1	K	491	LEU	3.2
1	H	469	LYS	3.2
1	I	473	ILE	3.2
1	E	308	GLU	3.1
1	L	141	LYS	3.1
1	I	286	THR	3.1
1	I	437	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	164	ALA	3.1
1	G	384	ASN	3.1
1	E	494	GLU	3.1
1	L	138	THR	3.0
1	J	287	HIS	3.0
1	K	470	GLU	3.0
1	G	385	GLY	3.0
1	K	260	ARG	3.0
1	K	189	PHE	3.0
1	C	163	GLU	2.9
1	J	473	ILE	2.9
1	L	137	PHE	2.9
1	J	254	LYS	2.8
1	L	248	PHE	2.8
1	L	300	ILE	2.8
1	L	147	PRO	2.8
1	I	261	LEU	2.8
1	E	492	LYS	2.8
1	D	243	ARG	2.8
1	E	285	GLU	2.7
1	L	129	ILE	2.7
1	I	164	ALA	2.7
1	A	473	ILE	2.7
1	L	289	ALA	2.7
1	J	493	ALA	2.7
1	K	133	LEU	2.7
1	K	388	ILE	2.7
1	D	165	GLU	2.7
1	L	197	ASN	2.7
1	C	311	SER	2.7
1	H	166	THR	2.7
1	L	254	LYS	2.7
1	I	435	PHE	2.6
1	B	305	ALA	2.6
1	H	259	GLY	2.6
1	F	490	VAL	2.6
1	L	255	GLN	2.6
1	A	305	ALA	2.6
1	L	70	LYS	2.6
1	I	383	ILE	2.6
1	L	185	THR	2.6
1	G	289	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	142	LEU	2.6
1	L	200	GLN	2.5
1	L	55	LYS	2.5
1	L	387	PHE	2.5
1	E	384	ASN	2.5
1	G	260	ARG	2.5
1	J	466	LYS	2.5
1	I	70	LYS	2.5
1	E	287	HIS	2.4
1	L	413	LYS	2.4
1	A	308	GLU	2.4
1	E	167	GLY	2.4
1	J	166	THR	2.4
1	F	256	ILE	2.4
1	I	283	ASP	2.4
1	J	426	ASN	2.4
1	L	99	TYR	2.4
1	I	434	PRO	2.4
1	F	190	GLY	2.4
1	G	382	GLU	2.4
1	H	305	ALA	2.4
1	I	441	ASN	2.4
1	H	472	GLN	2.4
1	C	215	PRO	2.3
1	F	305	ALA	2.3
1	I	69	GLY	2.3
1	I	65	TYR	2.3
1	L	202	PRO	2.3
1	G	272	LEU	2.3
1	L	353	LEU	2.3
1	B	286	THR	2.3
1	L	206	ASN	2.3
1	L	352	GLN	2.3
1	F	465	PHE	2.3
1	I	438	GLY	2.3
1	L	110	PRO	2.3
1	L	483	LEU	2.3
1	L	125	GLU	2.3
1	K	129	ILE	2.3
1	I	469	LYS	2.3
1	K	261	LEU	2.3
1	I	78	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	214	ASN	2.2
1	I	448	ALA	2.2
1	J	305	ALA	2.2
1	D	310	THR	2.2
1	E	258	GLU	2.2
1	E	481	GLY	2.2
1	K	386	MET	2.2
1	I	433	THR	2.2
1	L	113	PHE	2.2
1	K	473	ILE	2.2
1	L	293	LEU	2.2
1	G	309	THR	2.2
1	D	205	GLU	2.2
1	L	94	LEU	2.2
1	G	305	ALA	2.2
1	K	493	ALA	2.2
1	L	434	PRO	2.2
1	J	309	THR	2.2
1	C	177	GLY	2.1
1	L	296	MET	2.1
1	L	251	LYS	2.1
1	L	241	PHE	2.1
1	H	286	THR	2.1
1	H	200	GLN	2.1
1	E	310	THR	2.1
1	E	304	PHE	2.1
1	K	468	CYS	2.1
1	F	70	LYS	2.1
1	B	258	GLU	2.1
1	L	101	VAL	2.1
1	C	309	THR	2.1
1	F	304	PHE	2.1
1	G	306	GLY	2.1
1	G	473	ILE	2.1
1	I	168	LYS	2.1
1	K	164	ALA	2.1
1	J	492	LYS	2.1
1	F	311	SER	2.1
1	C	369	VAL	2.0
1	H	442	CYS	2.0
1	L	104	ASN	2.0
1	C	251	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	132	LEU	2.0
1	K	148	ILE	2.0
1	K	308	GLU	2.0
1	L	34	LYS	2.0
1	L	386	MET	2.0
1	I	256	ILE	2.0
1	L	297	ALA	2.0
1	L	370	ALA	2.0
1	L	366	LEU	2.0
1	G	394	VAL	2.0
1	I	288	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	E	601	43/43	0.73	0.37	47,62,77,241	0
2	HEM	C	601	43/43	0.85	0.35	45,62,83,157	0
2	HEM	A	601	43/43	0.85	0.28	44,63,92,139	0
2	HEM	G	601	43/43	0.90	0.31	60,76,94,161	0
2	HEM	F	601	43/43	0.92	0.33	61,75,93,143	0
3	ZWY	B	603	25/25	0.93	0.19	30,43,53,73	18
3	ZWY	I	602	25/25	0.93	0.23	32,44,57,78	21
3	ZWY	D	602	25/25	0.94	0.21	31,41,52,75	23
3	ZWY	D	605	25/25	0.94	0.25	33,43,51,85	22
3	ZWY	E	603	25/25	0.94	0.12	35,44,55,89	22
2	HEM	L	601	43/43	0.94	0.26	77,101,125,130	0
3	ZWY	I	603	25/25	0.94	0.24	31,45,56,76	19

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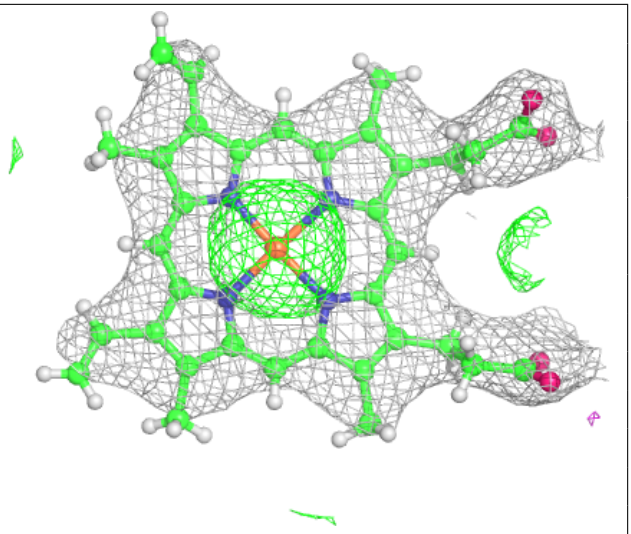
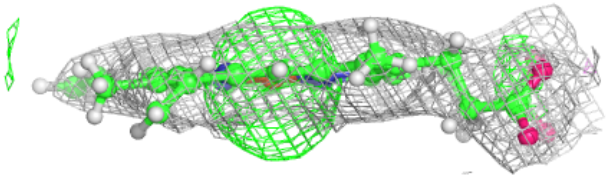
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZWY	J	602	25/25	0.94	0.31	34,45,53,72	25
3	ZWY	J	603	25/25	0.94	0.39	32,42,56,93	24
3	ZWY	E	602	25/25	0.95	0.27	34,46,52,81	25
2	HEM	D	601	43/43	0.95	0.30	44,64,83,93	0
3	ZWY	C	603	25/25	0.95	0.15	29,42,56,86	25
3	ZWY	A	602	25/25	0.95	0.15	35,45,54,62	22
3	ZWY	D	603	25/25	0.95	0.13	33,42,54,91	22
3	ZWY	A	603	25/25	0.95	0.14	30,46,59,90	25
3	ZWY	E	605	25/25	0.96	0.32	32,45,54,85	22
3	ZWY	H	603	25/25	0.96	0.12	31,41,54,78	24
2	HEM	J	601	43/43	0.96	0.30	55,75,92,96	0
3	ZWY	B	602	25/25	0.96	0.12	29,43,55,89	23
2	HEM	K	601	43/43	0.96	0.26	59,75,102,106	0
3	ZWY	E	604	25/25	0.96	0.15	30,42,51,77	20
2	HEM	B	601	43/43	0.97	0.25	47,63,83,91	0
3	ZWY	H	602	25/25	0.97	0.20	36,46,52,81	25
3	ZWY	D	604	25/25	0.97	0.17	33,45,51,62	24
3	ZWY	H	604	25/25	0.97	0.22	30,43,54,87	22
3	ZWY	C	602	25/25	0.97	0.21	32,41,50,76	22
2	HEM	H	601	43/43	0.97	0.29	51,66,86,89	0
3	ZWY	C	605	25/25	0.97	0.30	33,42,55,83	25
2	HEM	I	601	43/43	0.97	0.32	59,75,92,107	0
3	ZWY	D	606	25/25	0.98	0.12	34,42,51,62	20
3	ZWY	C	604	25/25	0.98	0.13	32,44,54,65	20

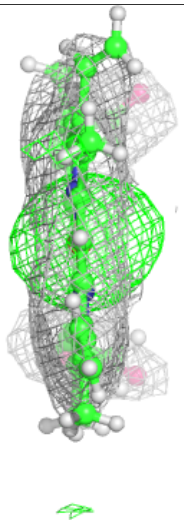
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEM E 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

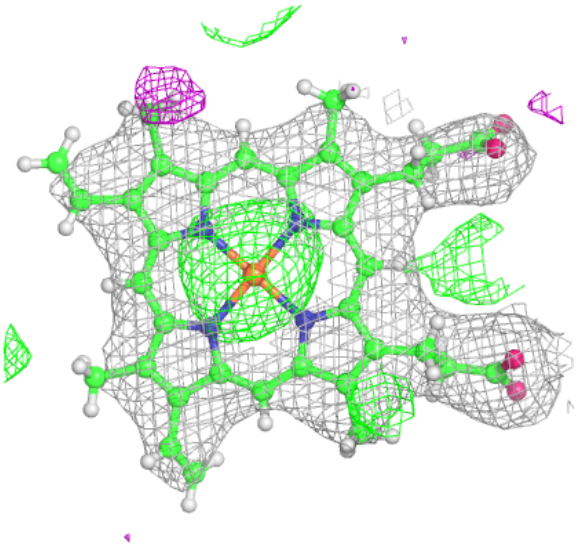


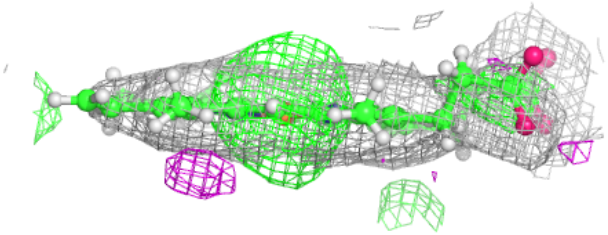


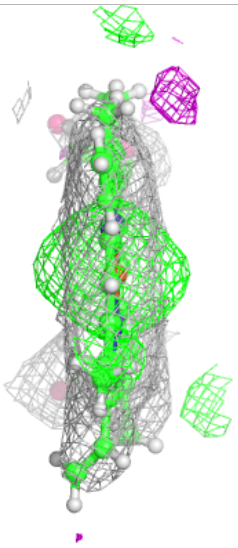


Electron density around HEM C 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

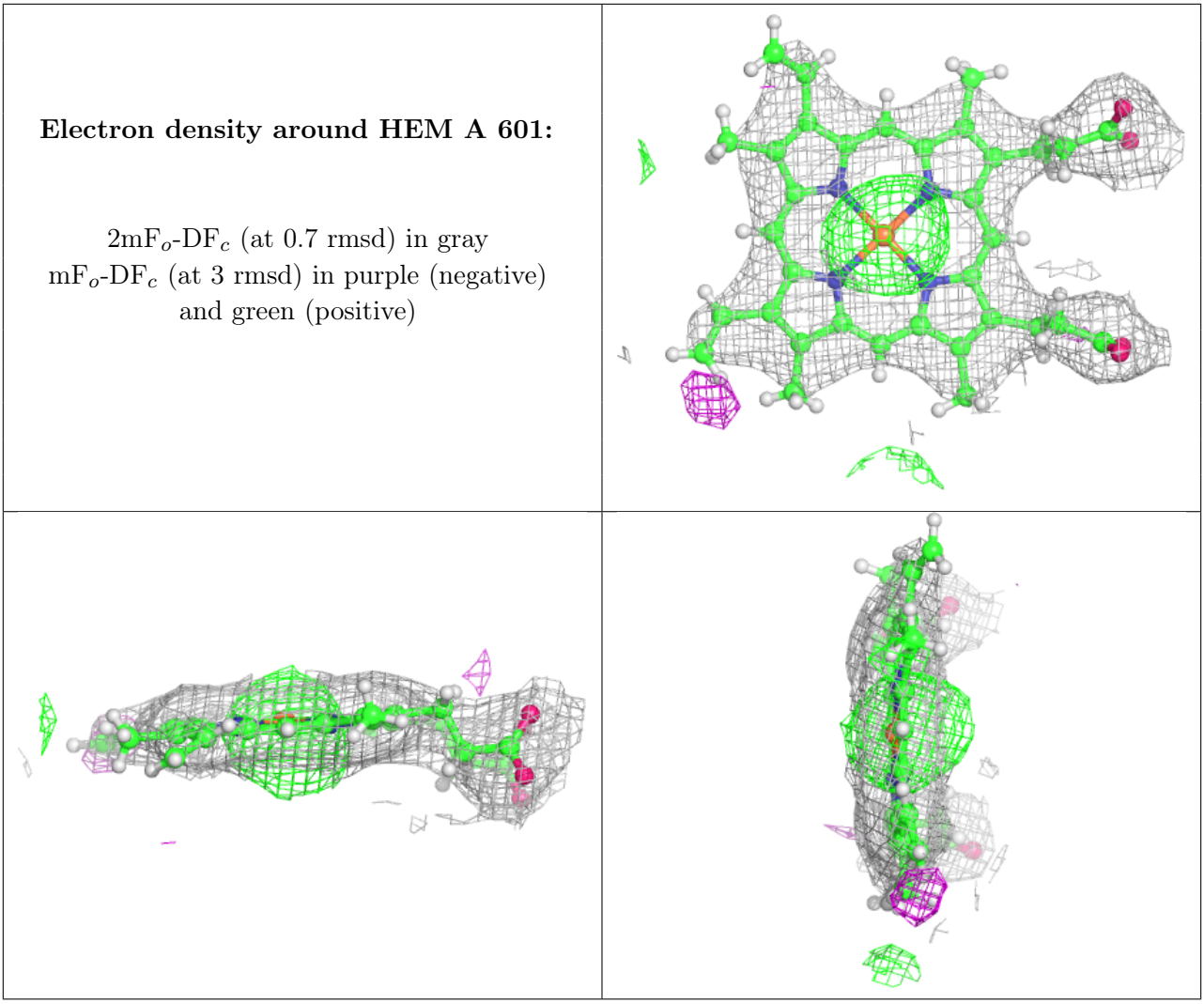






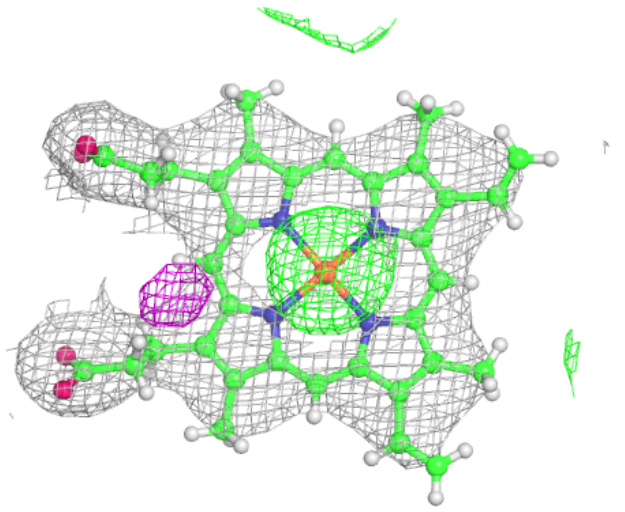
Electron density around HEM A 601:

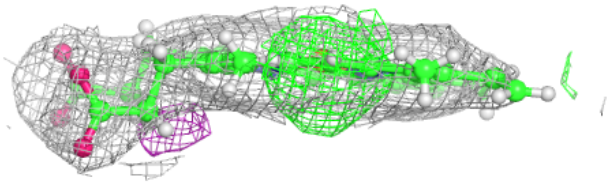
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

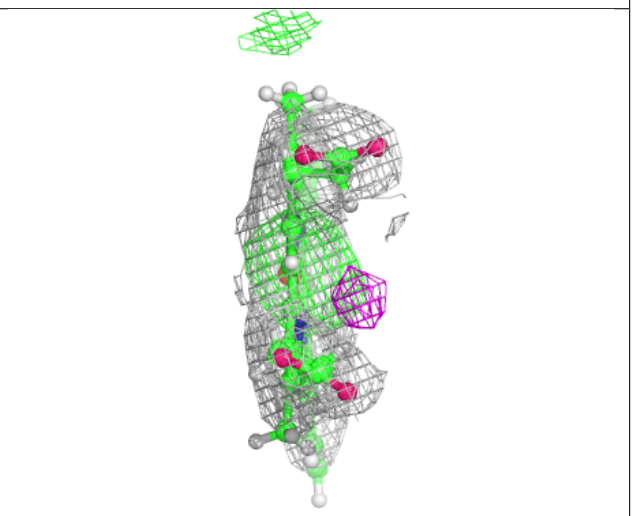


Electron density around HEM G 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

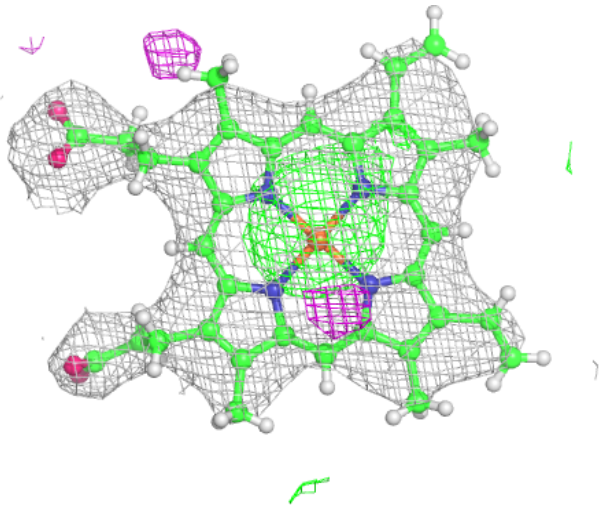


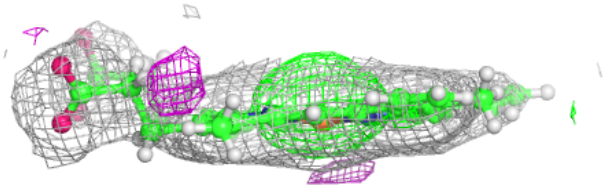


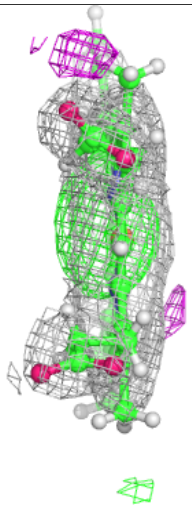


Electron density around HEM F 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

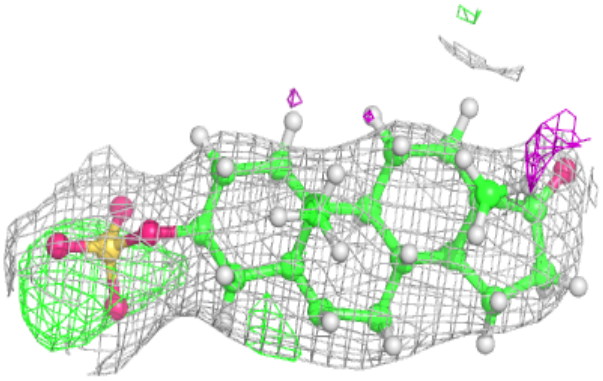


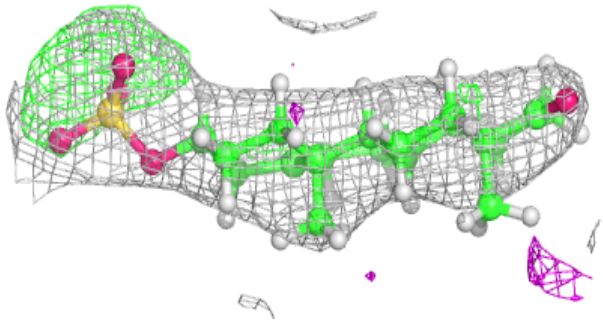


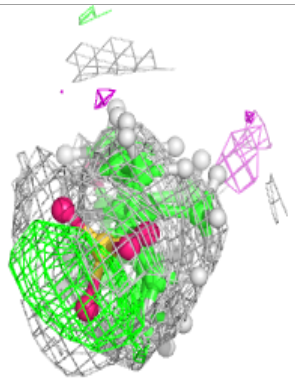


Electron density around ZWY B 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

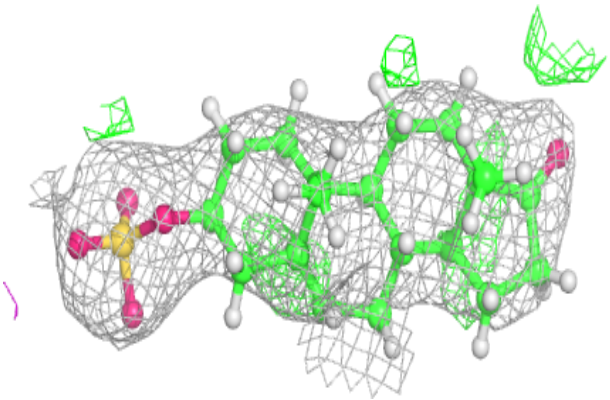


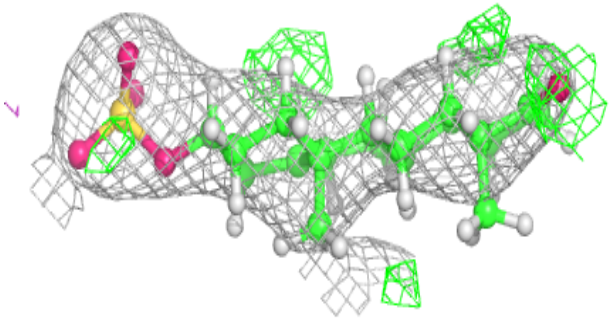


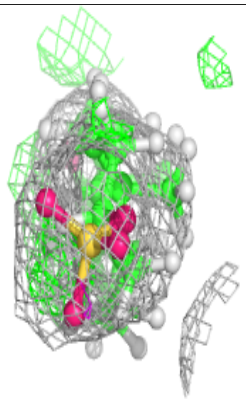


Electron density around ZWY I 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

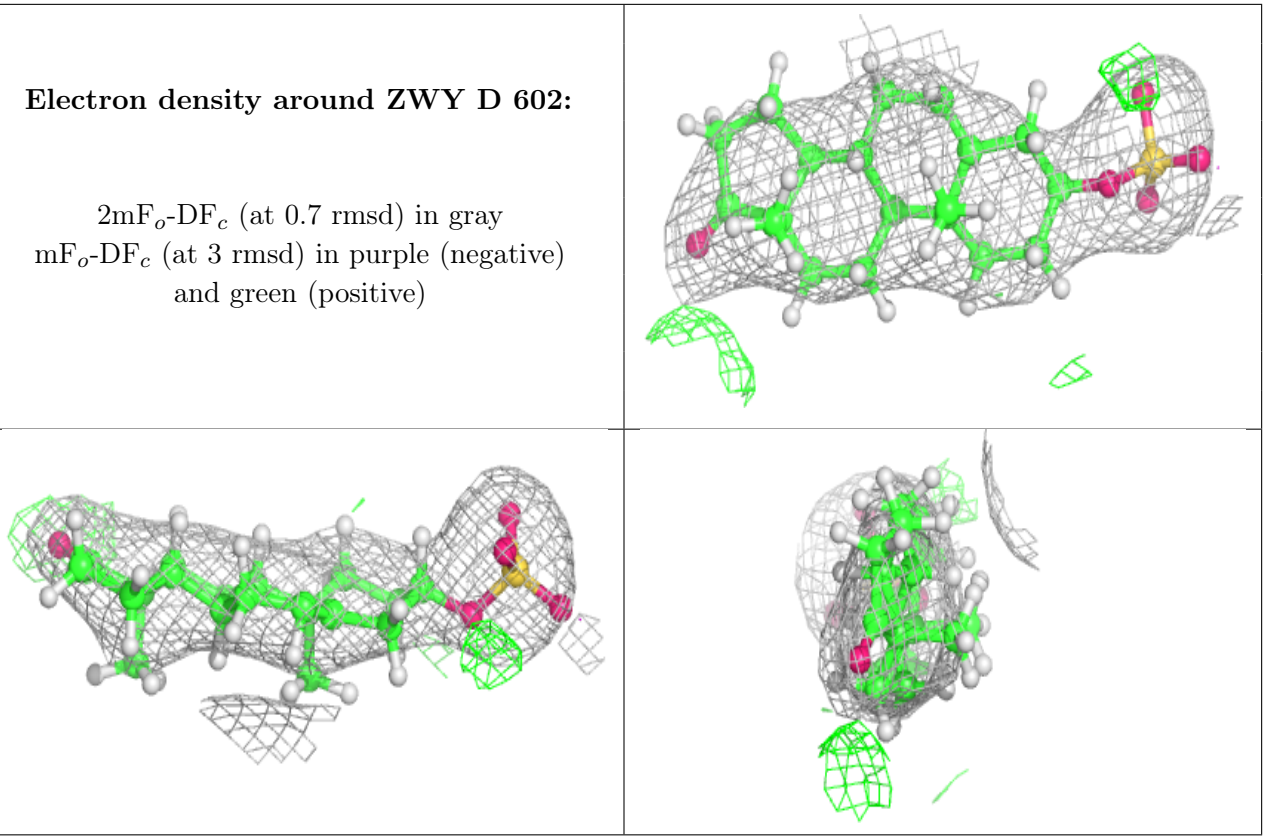






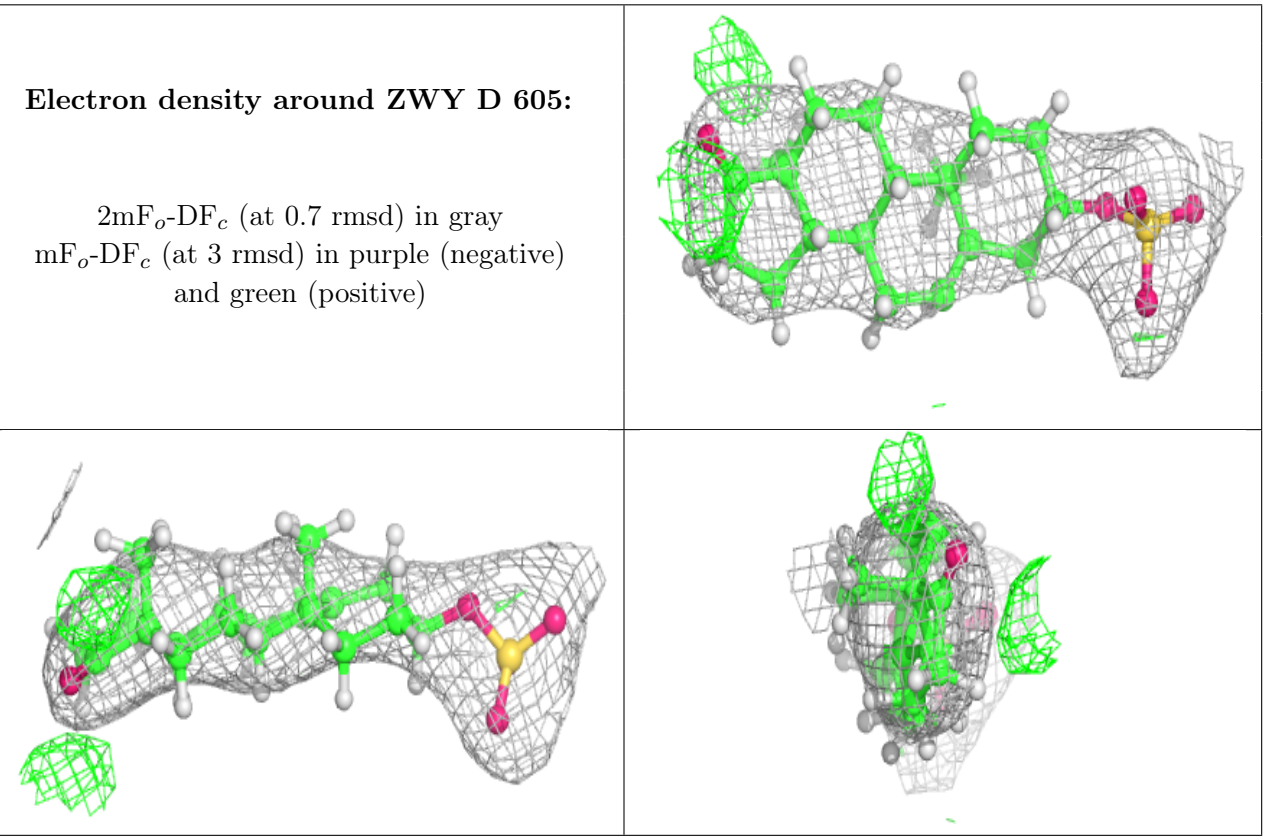
Electron density around ZWY D 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



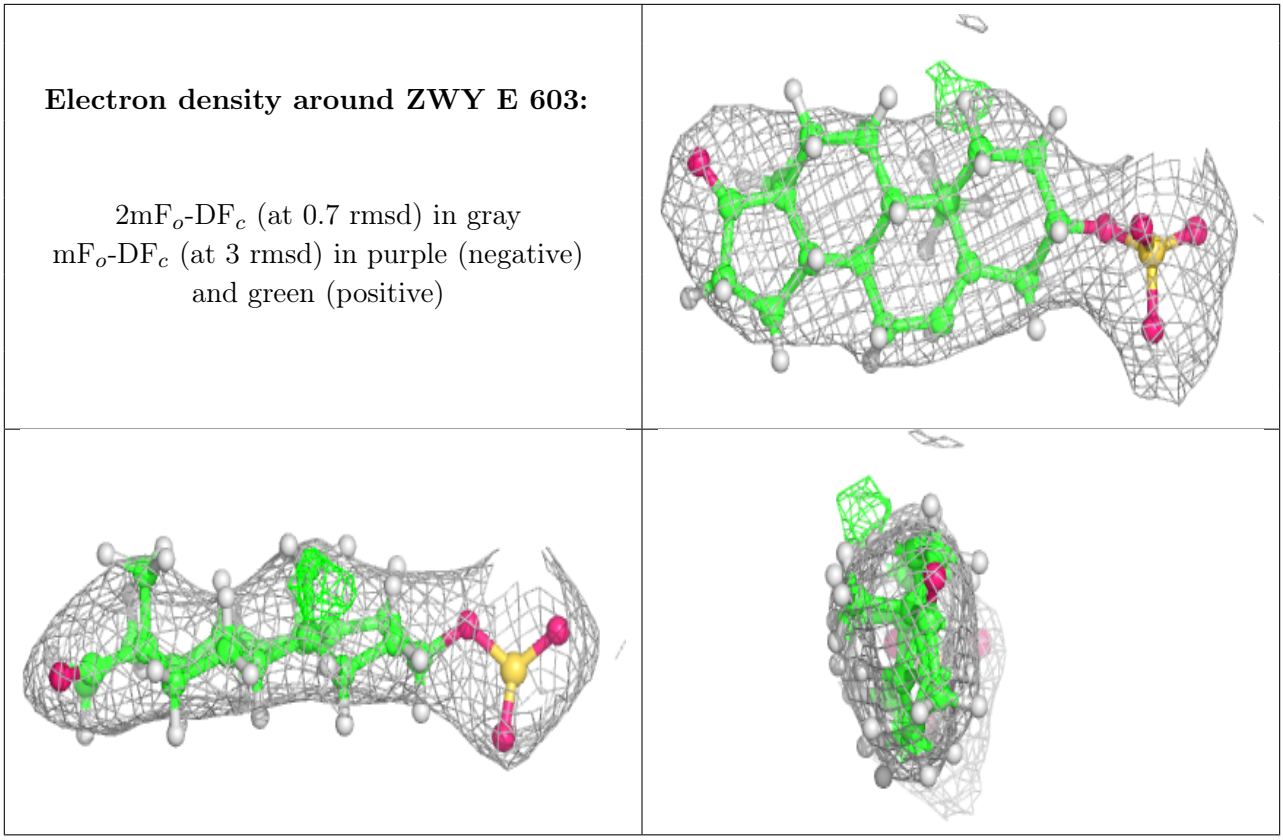
Electron density around ZWY D 605:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



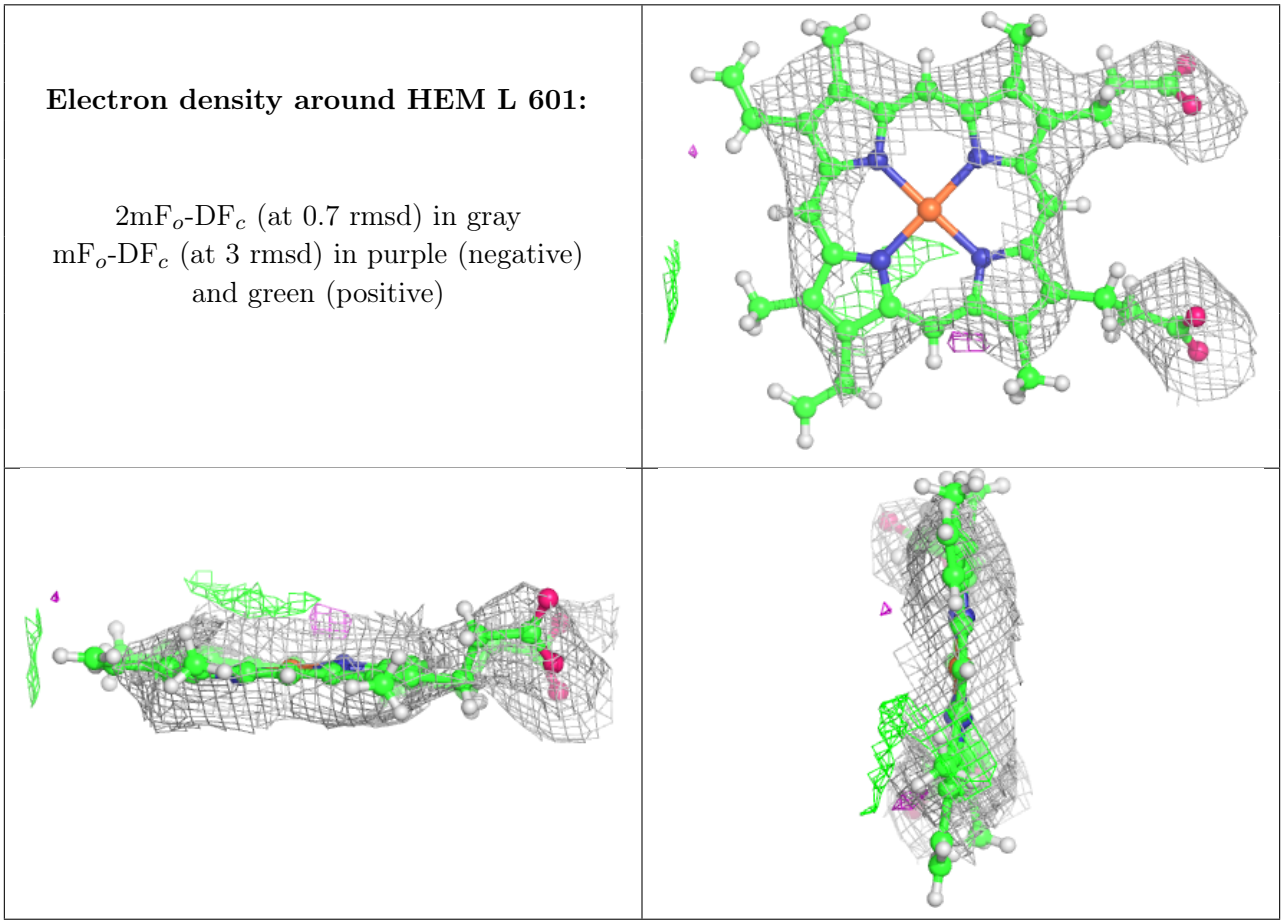
Electron density around ZWY E 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



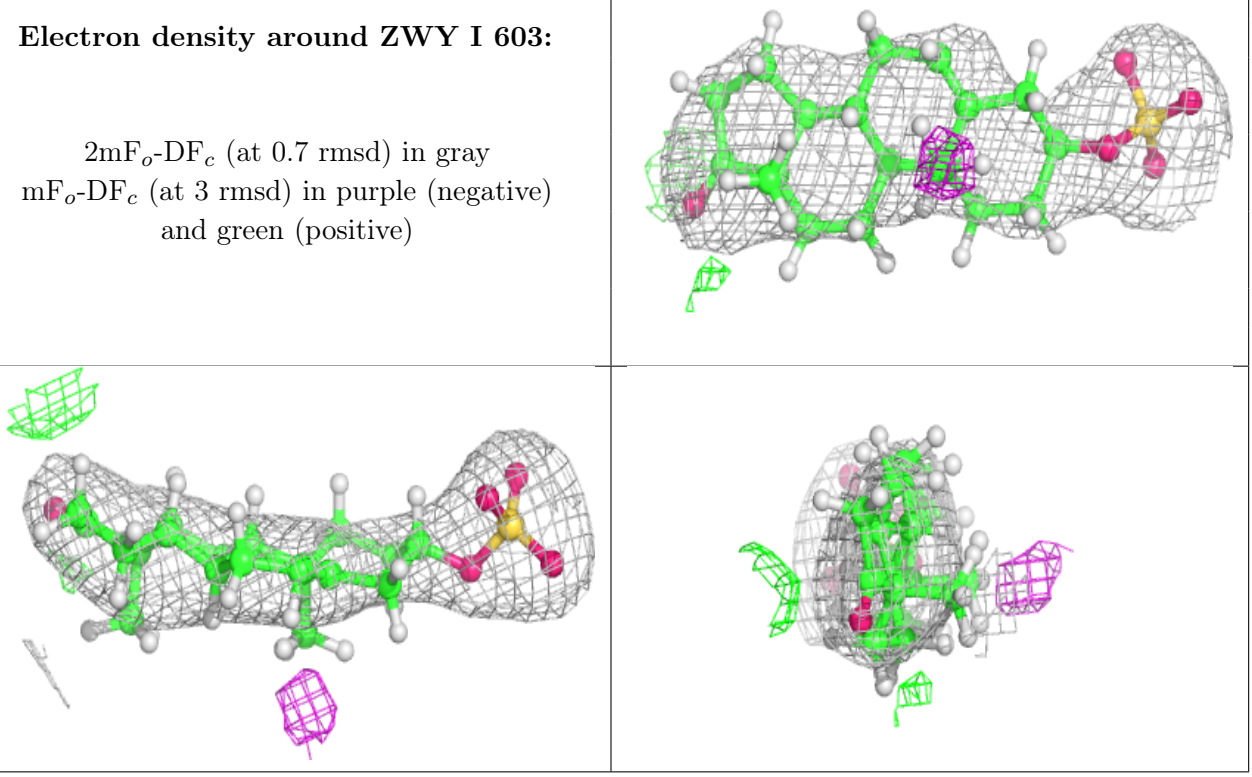
Electron density around HEM L 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



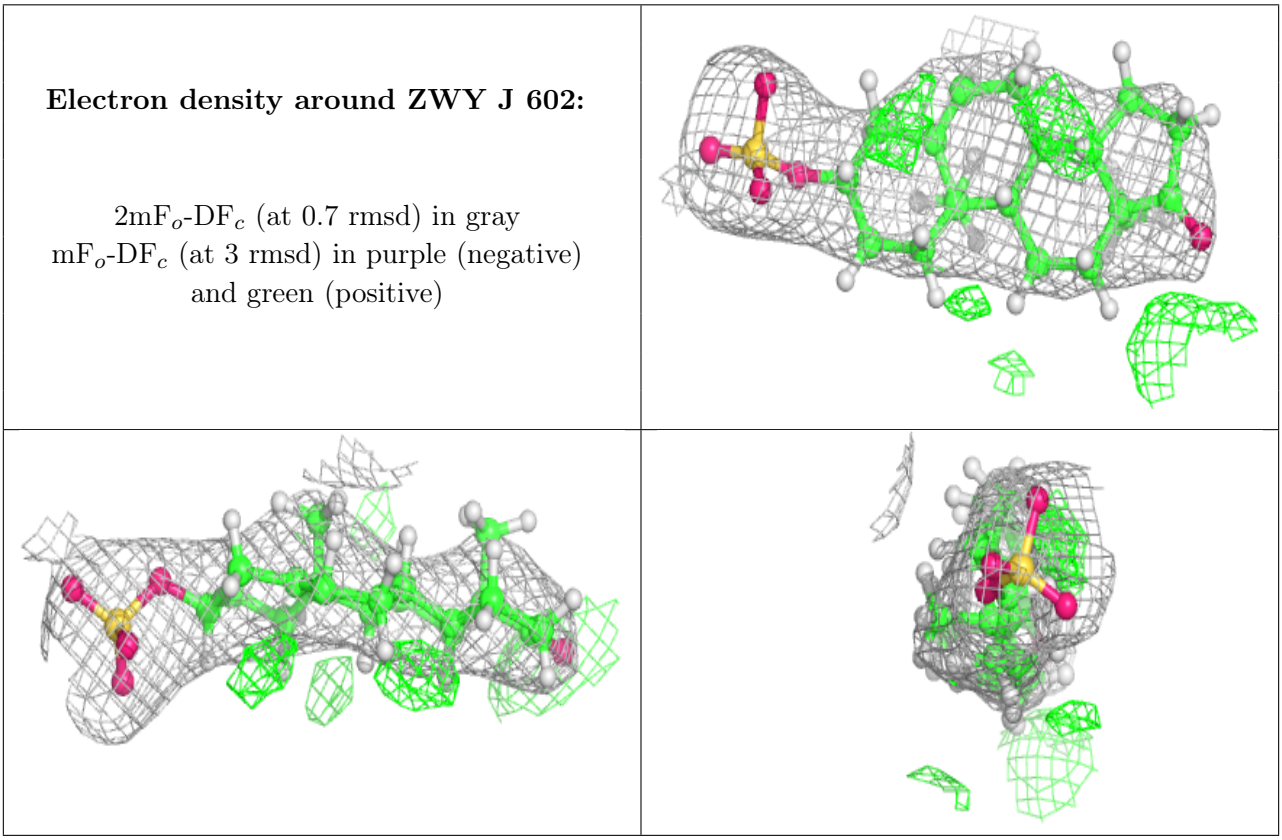
Electron density around ZWY I 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



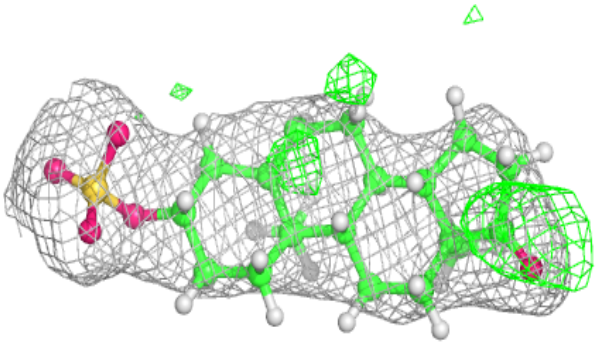
Electron density around ZWY J 602:

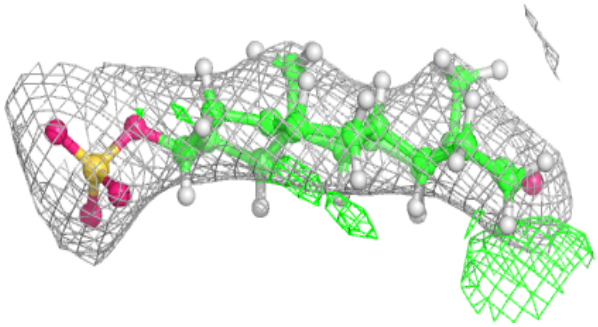
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

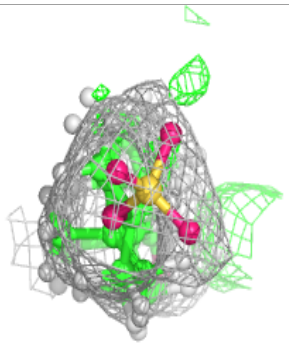


Electron density around ZWY J 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

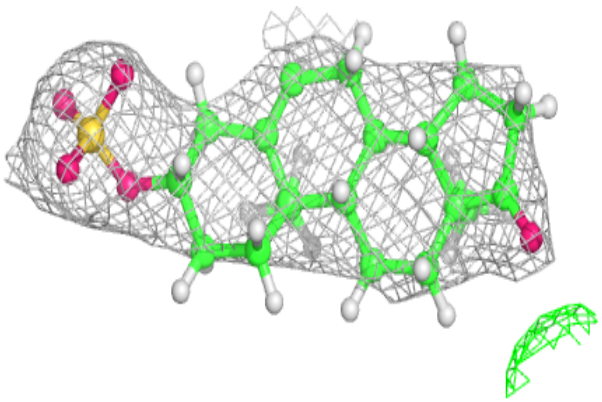


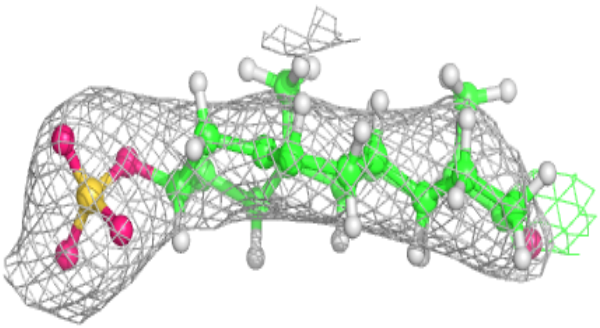


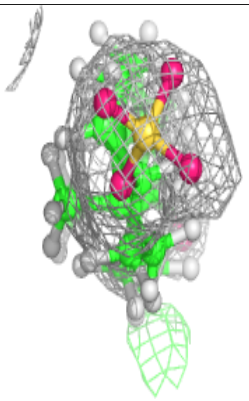


Electron density around ZWY E 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

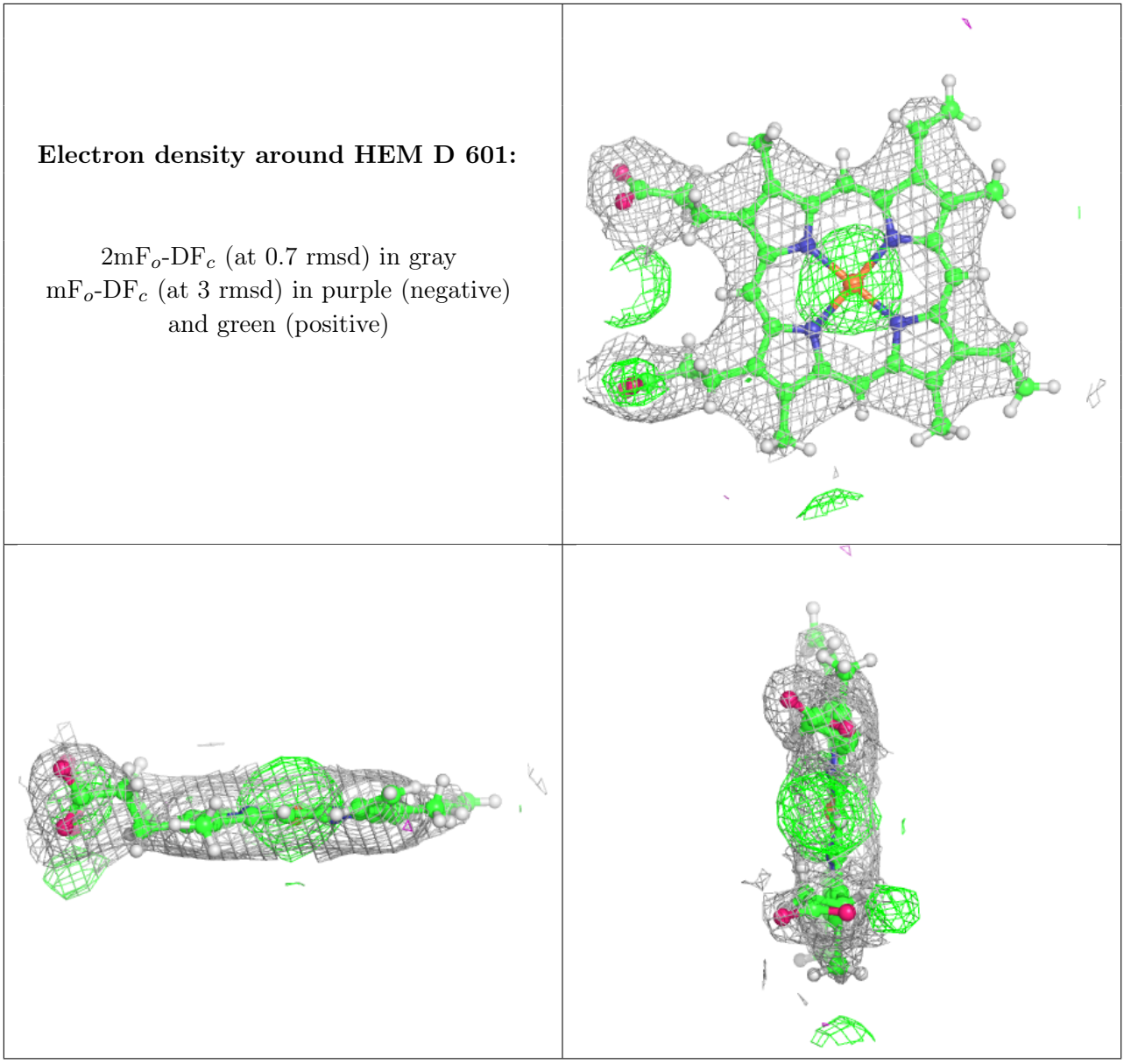






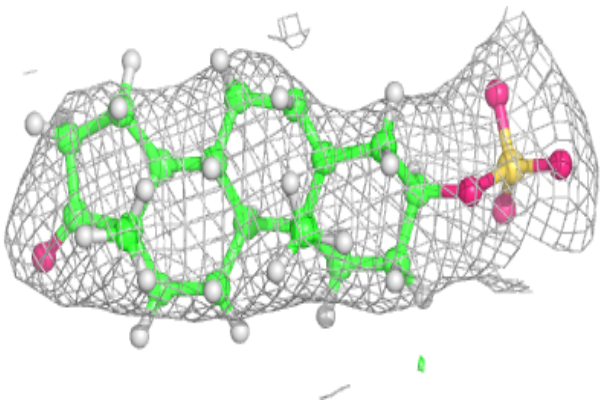
Electron density around HEM D 601:

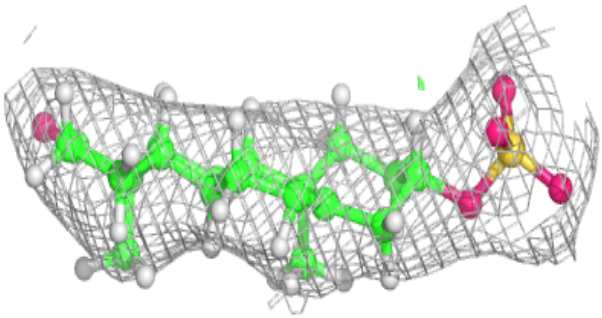
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

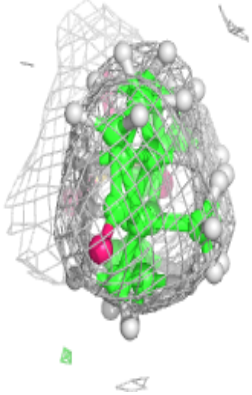


Electron density around ZWY C 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

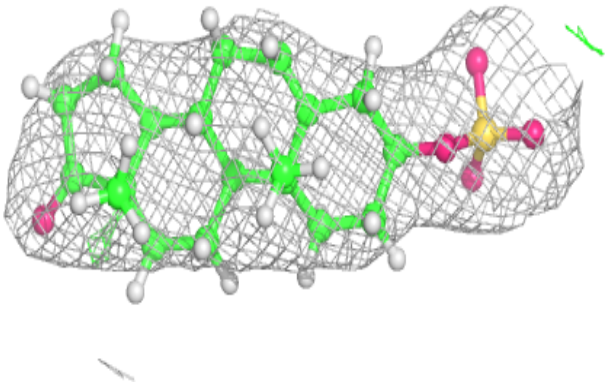


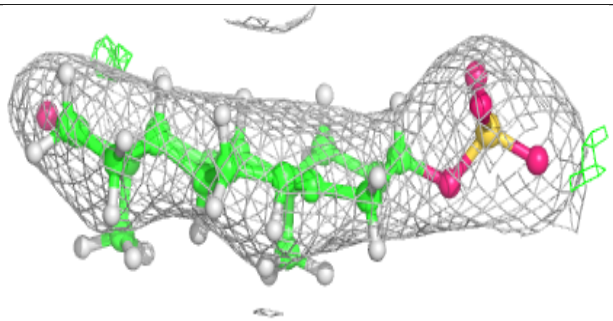


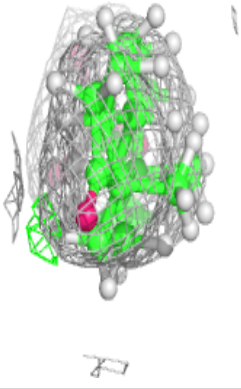


Electron density around ZWY A 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

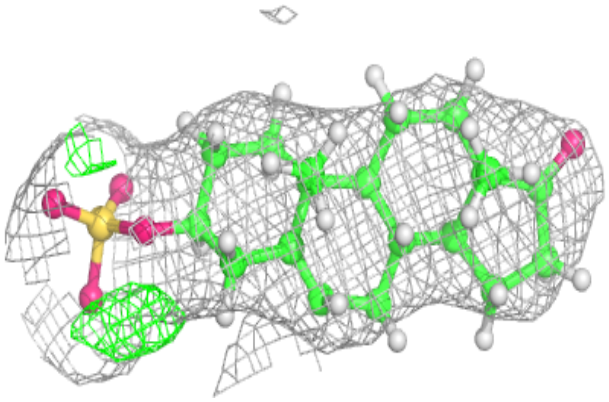


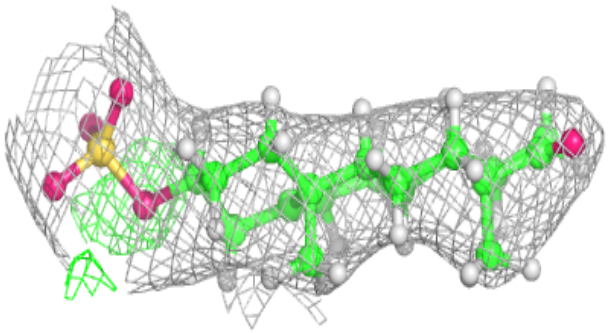


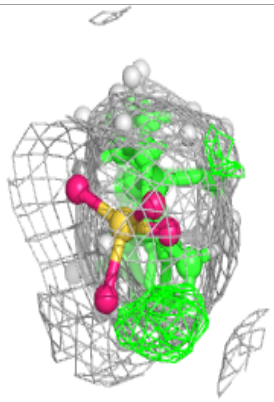


Electron density around ZWY D 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

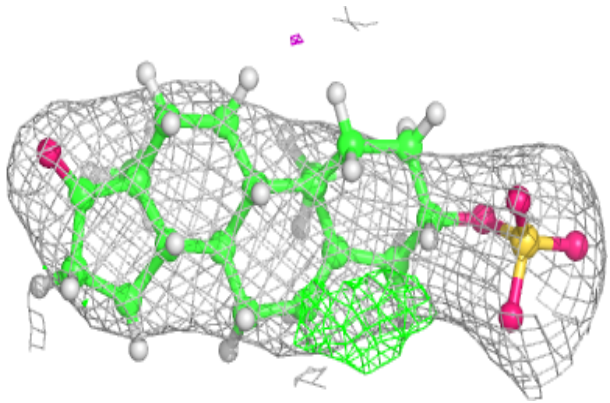


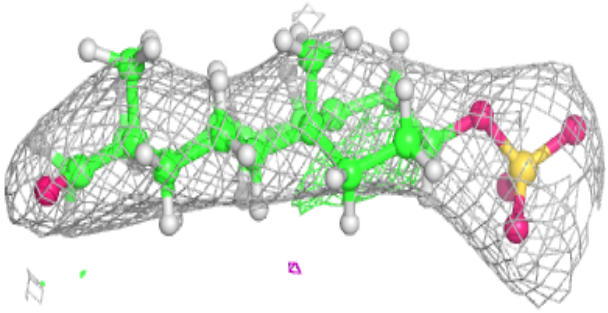


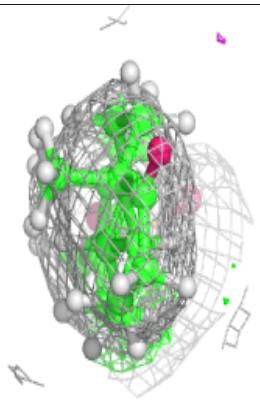


Electron density around ZWY A 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

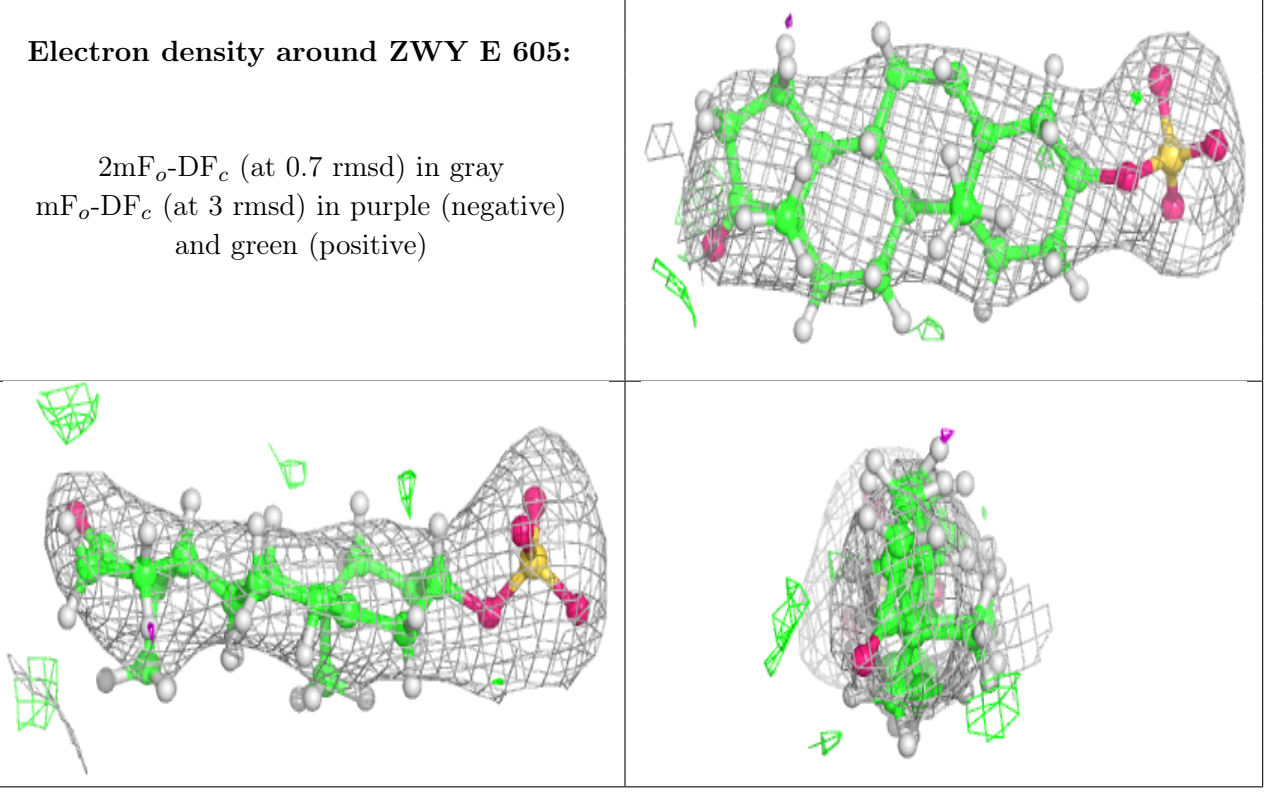






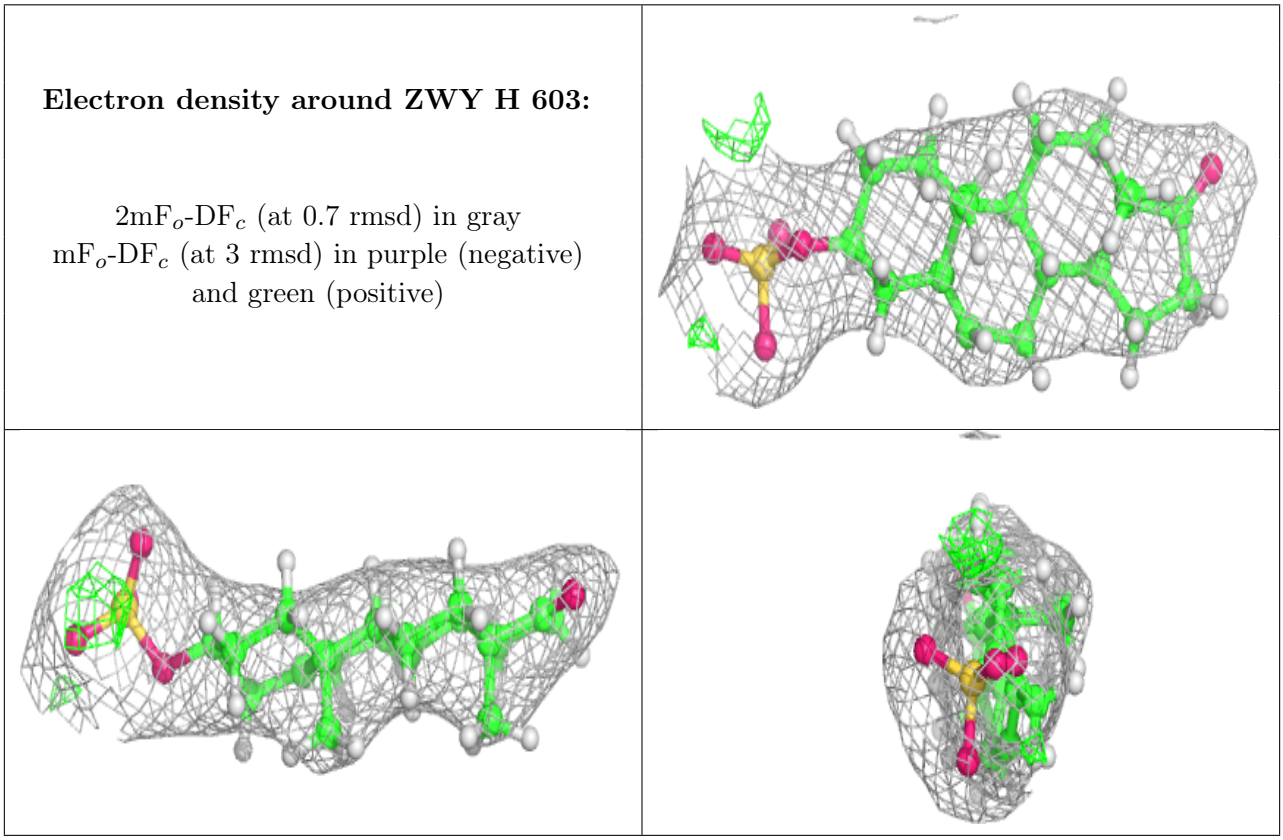
Electron density around ZWY E 605:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



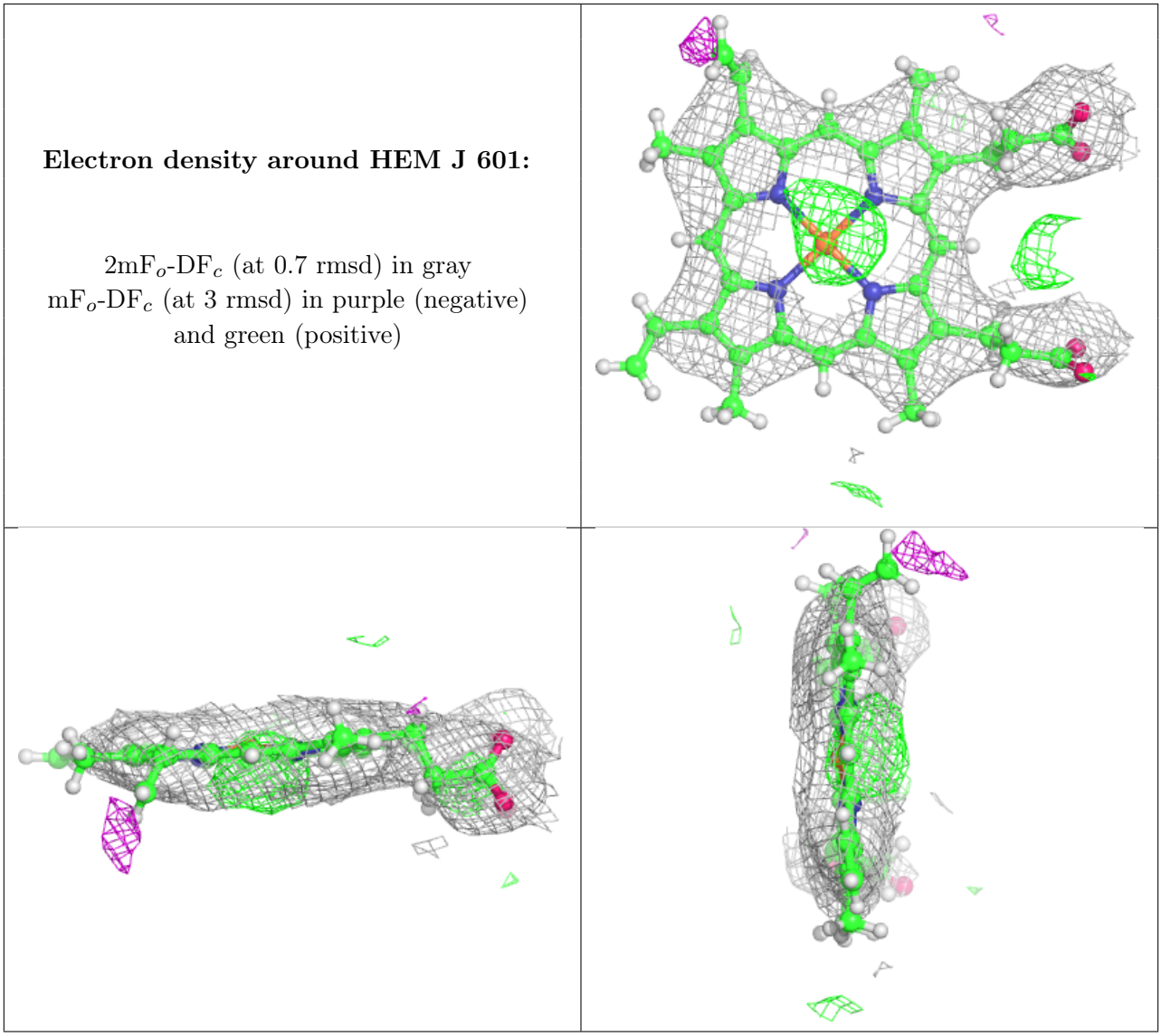
Electron density around ZWY H 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



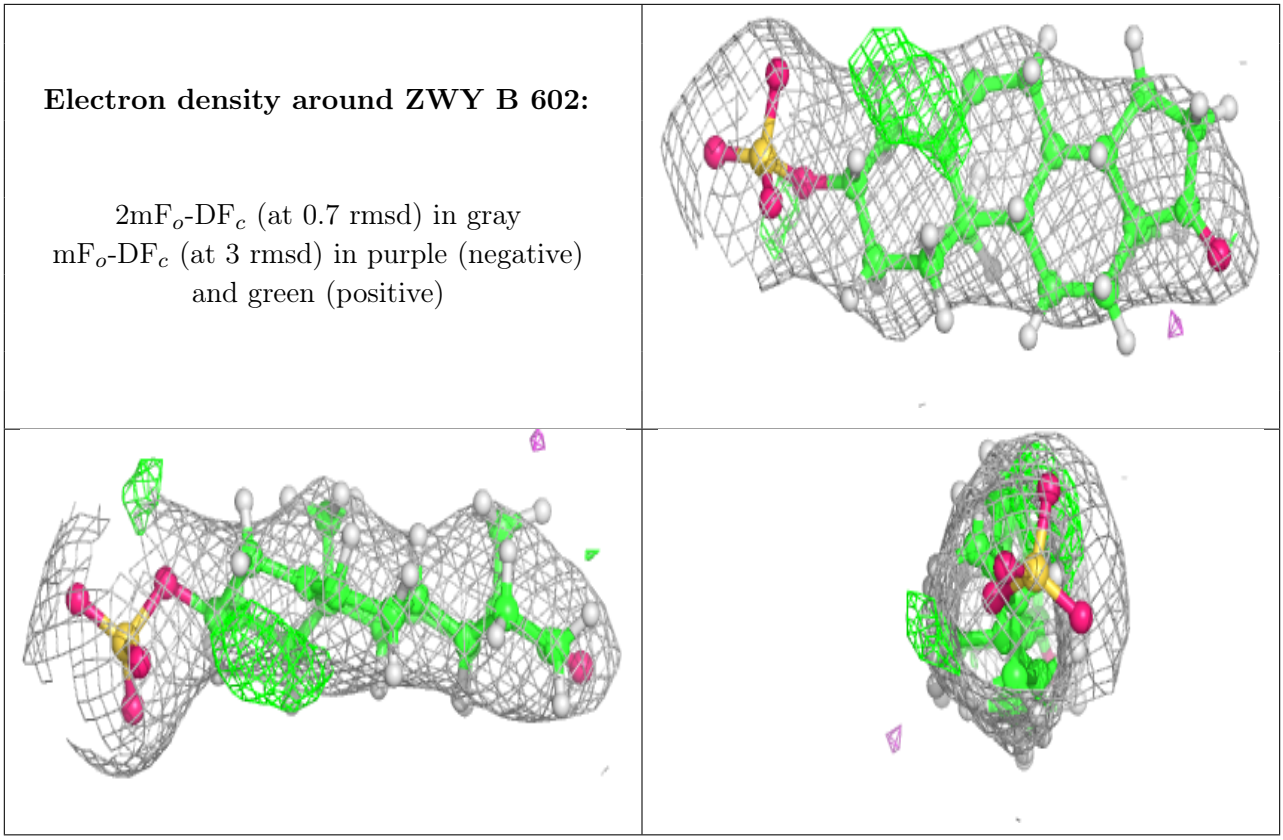
Electron density around HEM J 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



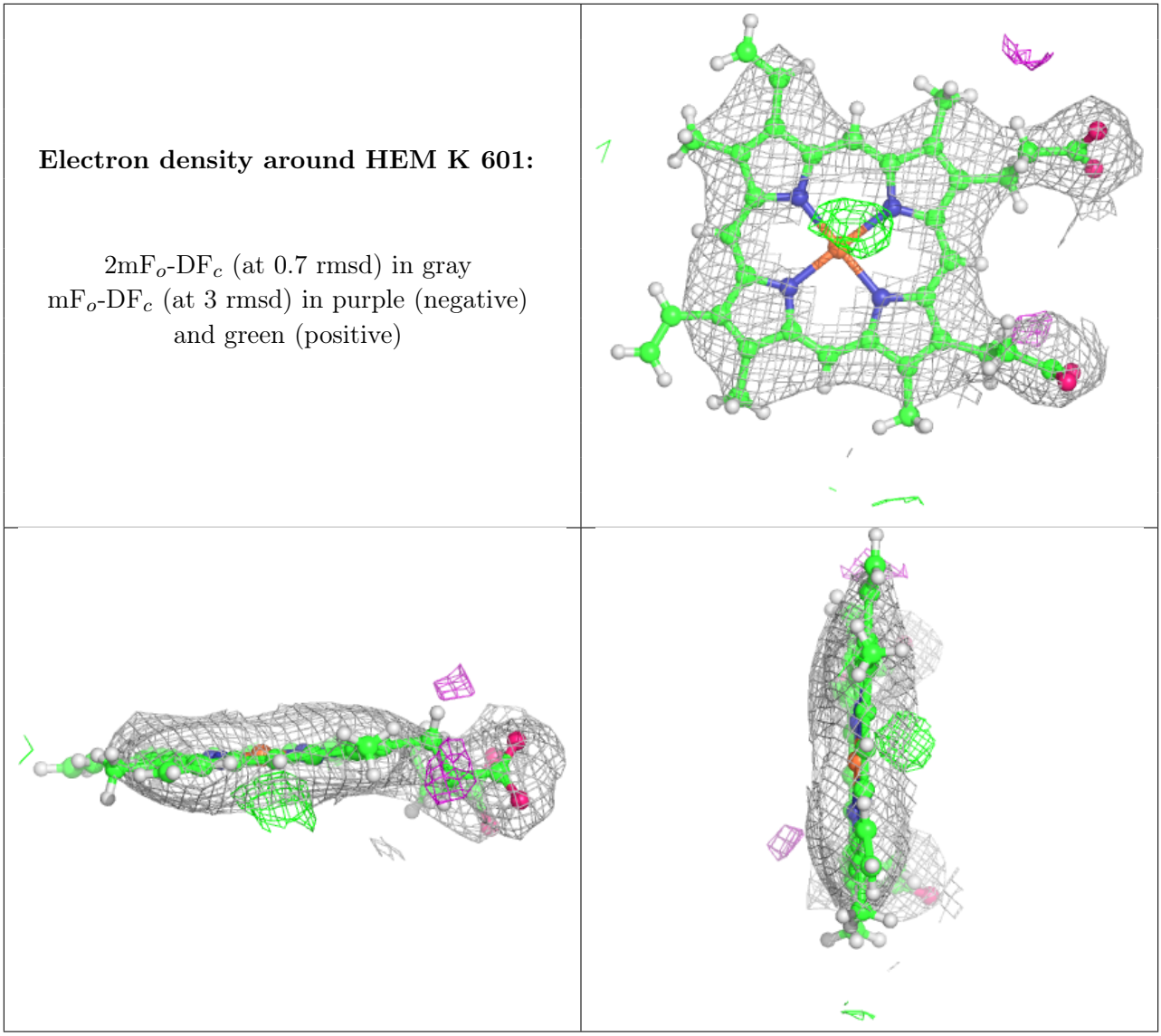
Electron density around ZWY B 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



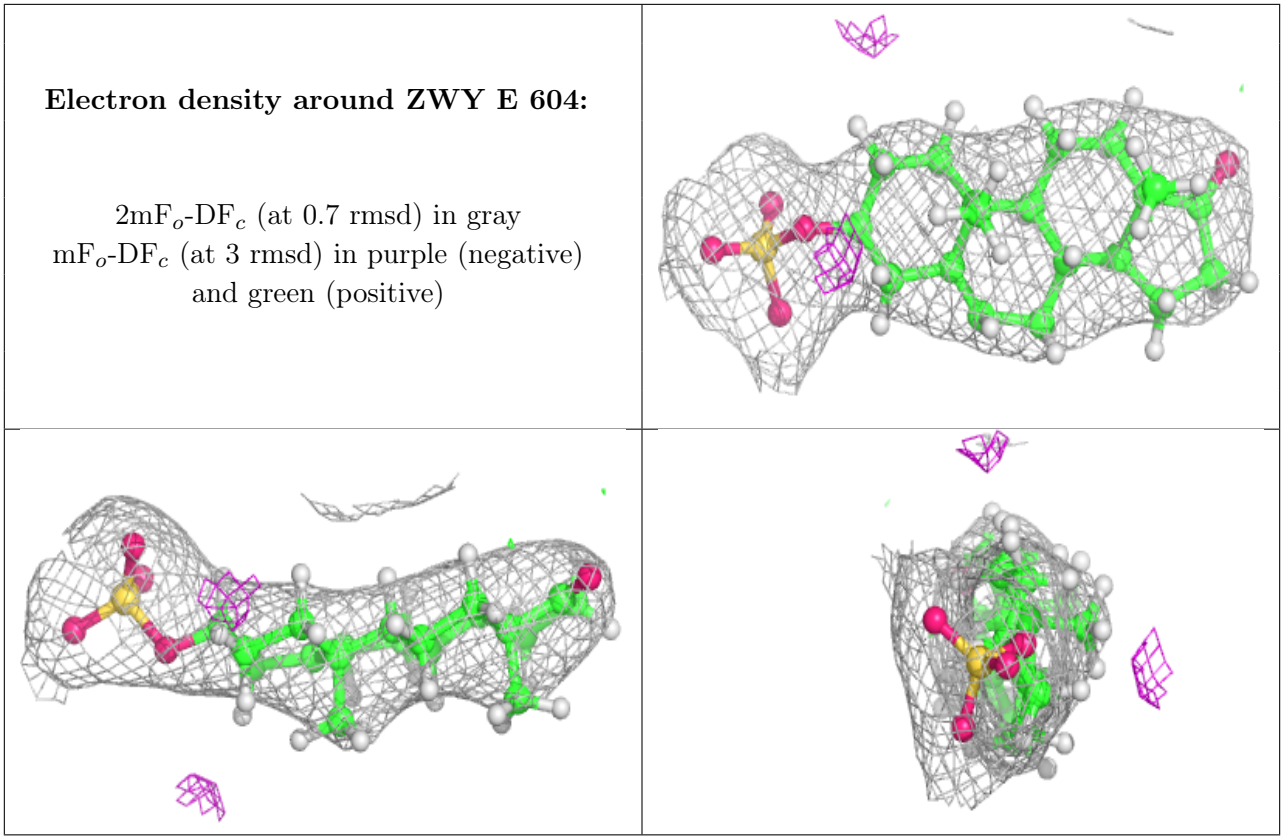
Electron density around HEM K 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



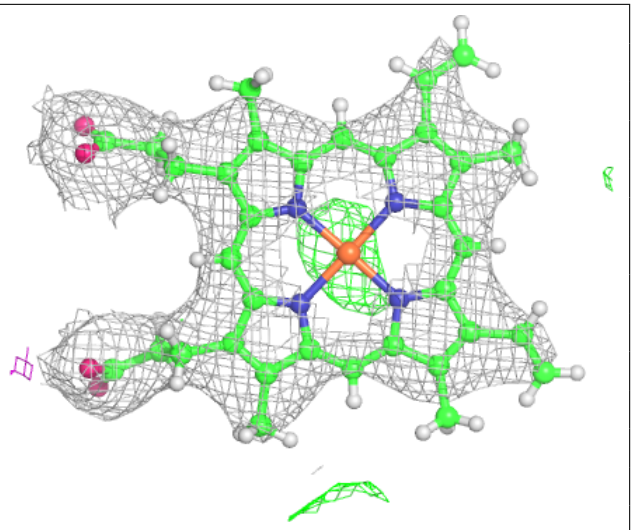
Electron density around ZWY E 604:

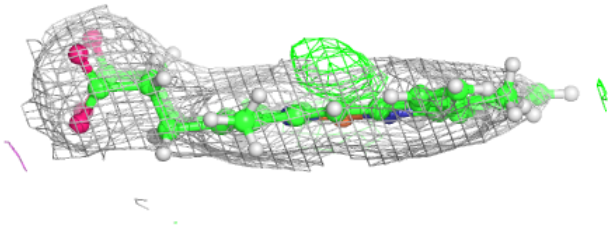
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

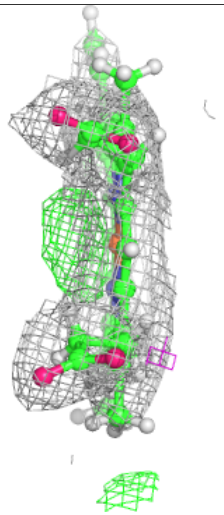


Electron density around HEM B 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

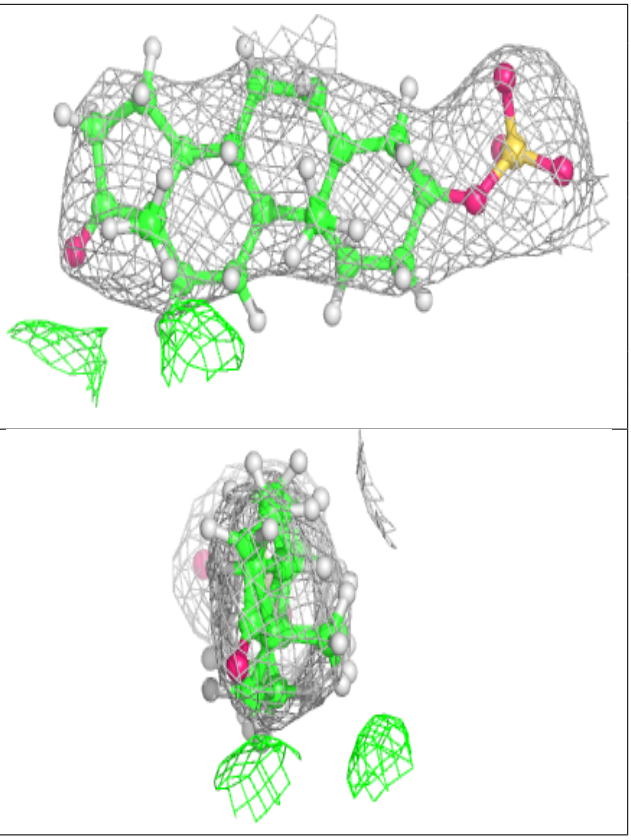






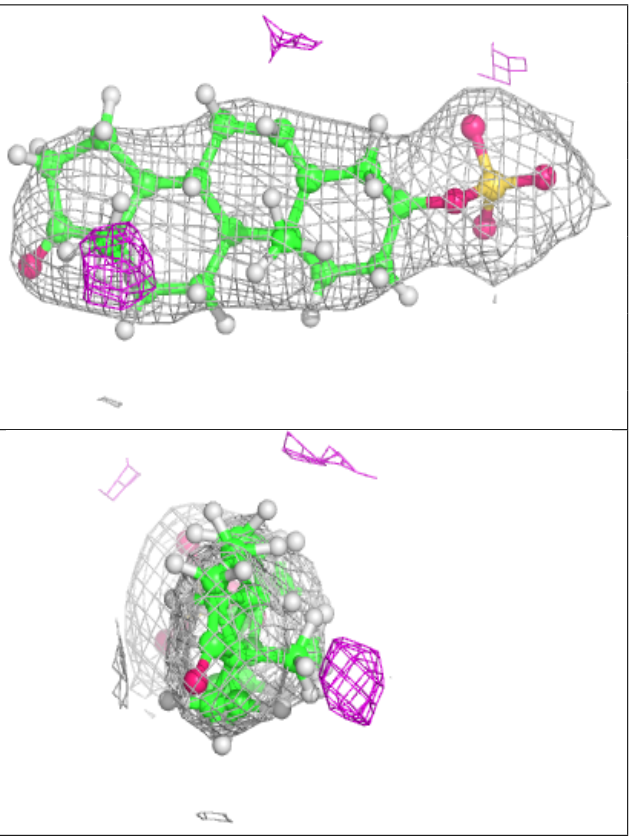
Electron density around ZWY H 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



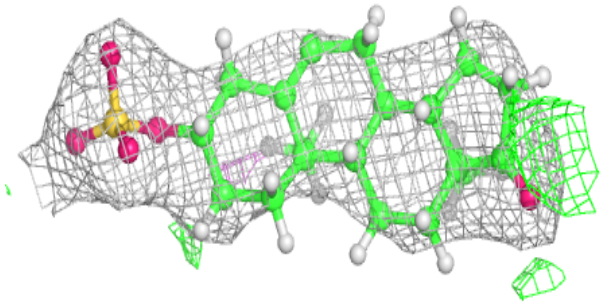
Electron density around ZWY D 604:

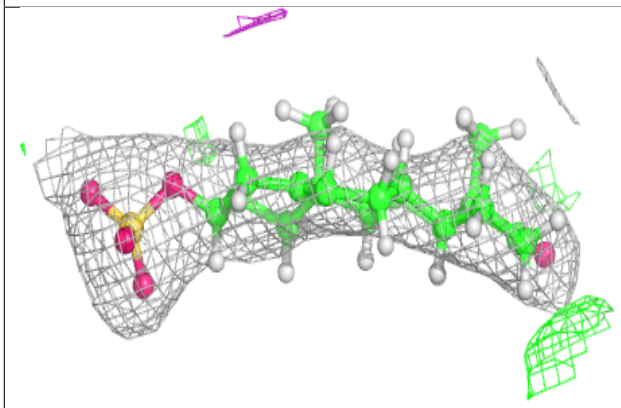
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

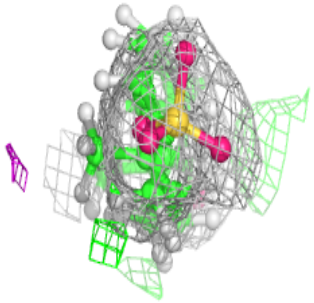


Electron density around ZWY H 604:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

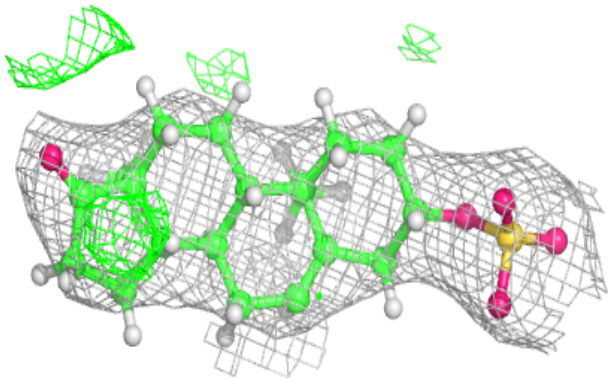


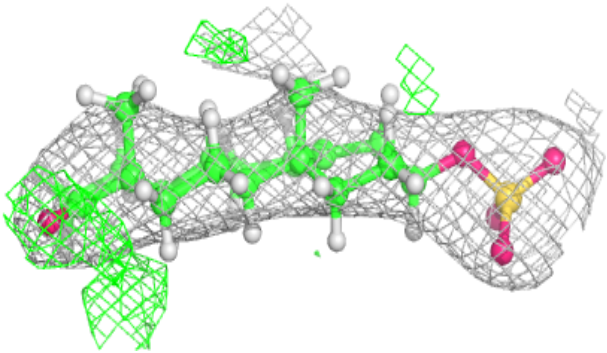


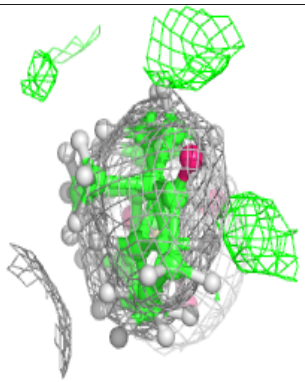


Electron density around ZWY C 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

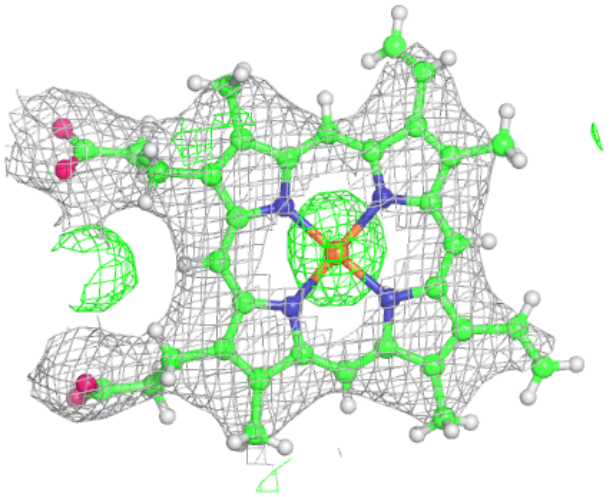


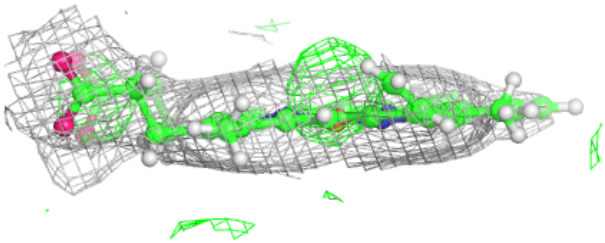


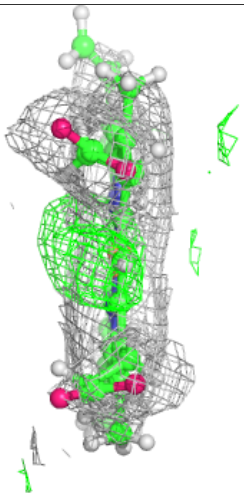


Electron density around HEM H 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

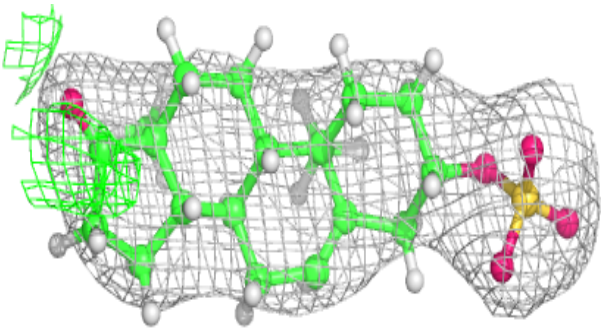


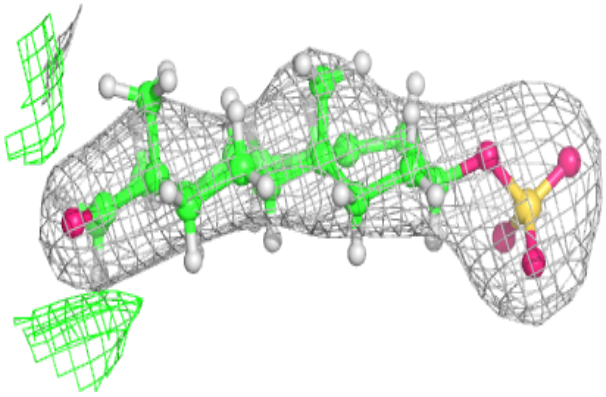


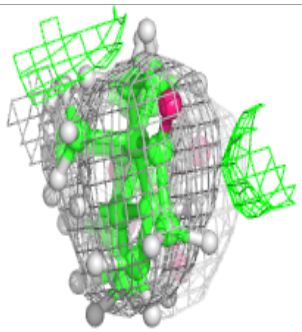


Electron density around ZWY C 605:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

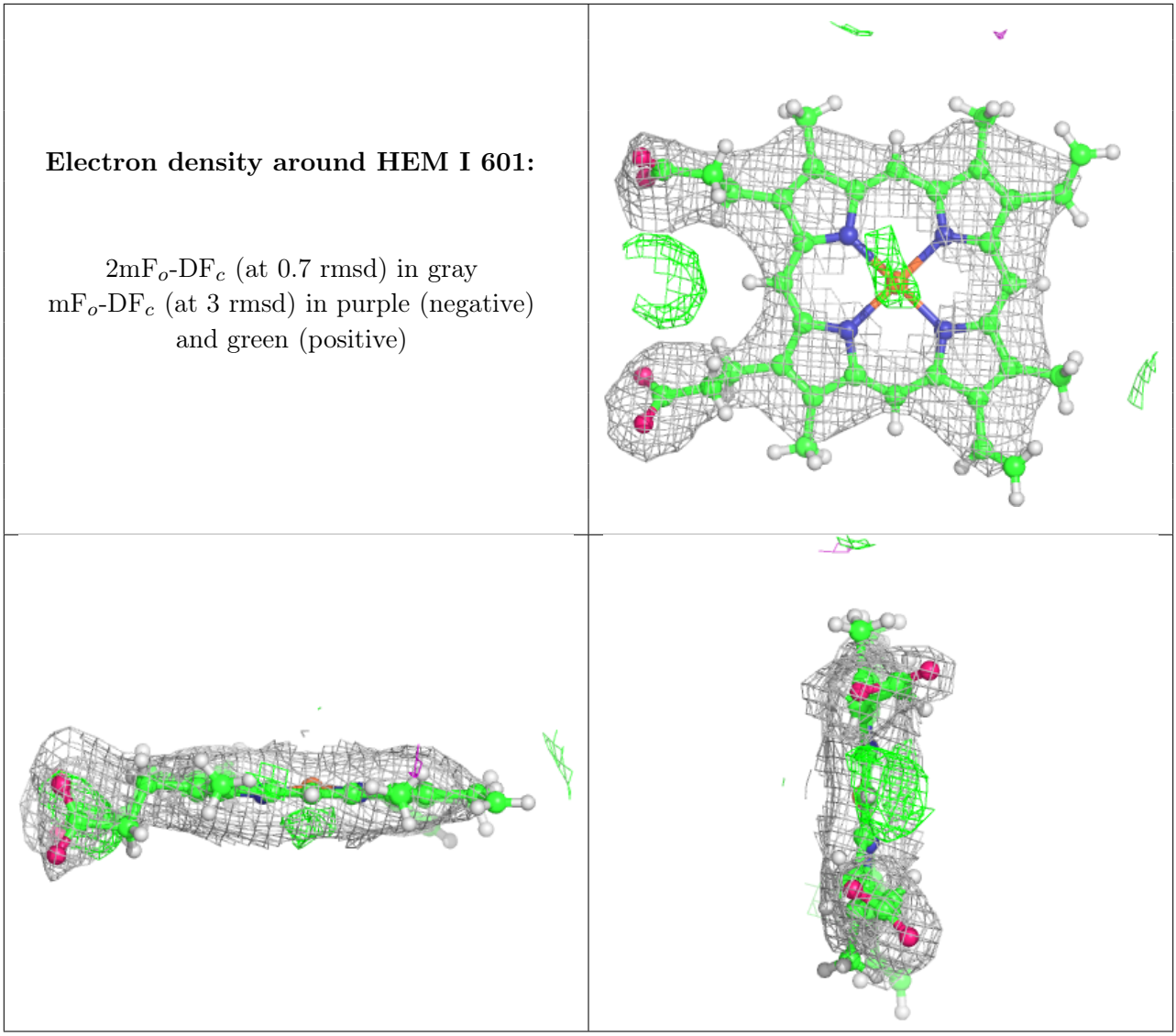






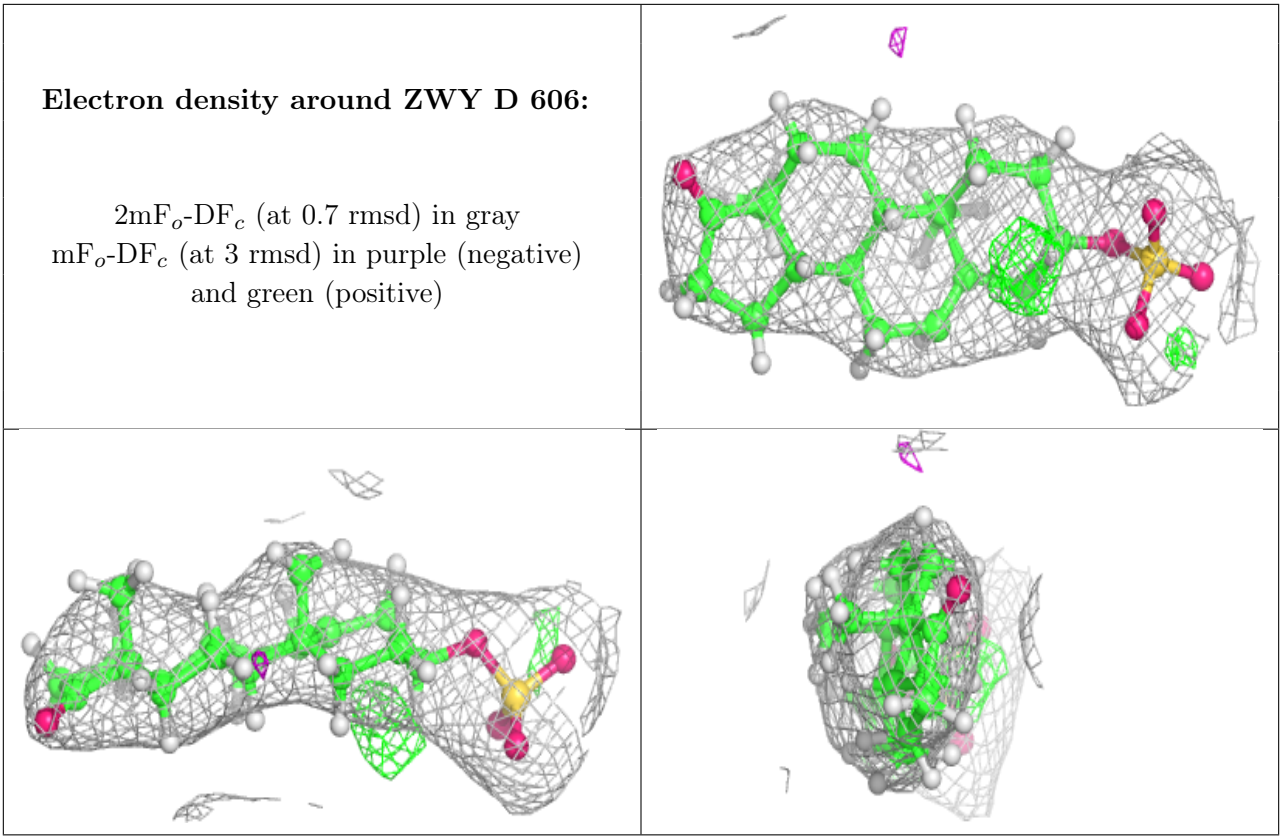
Electron density around HEM I 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



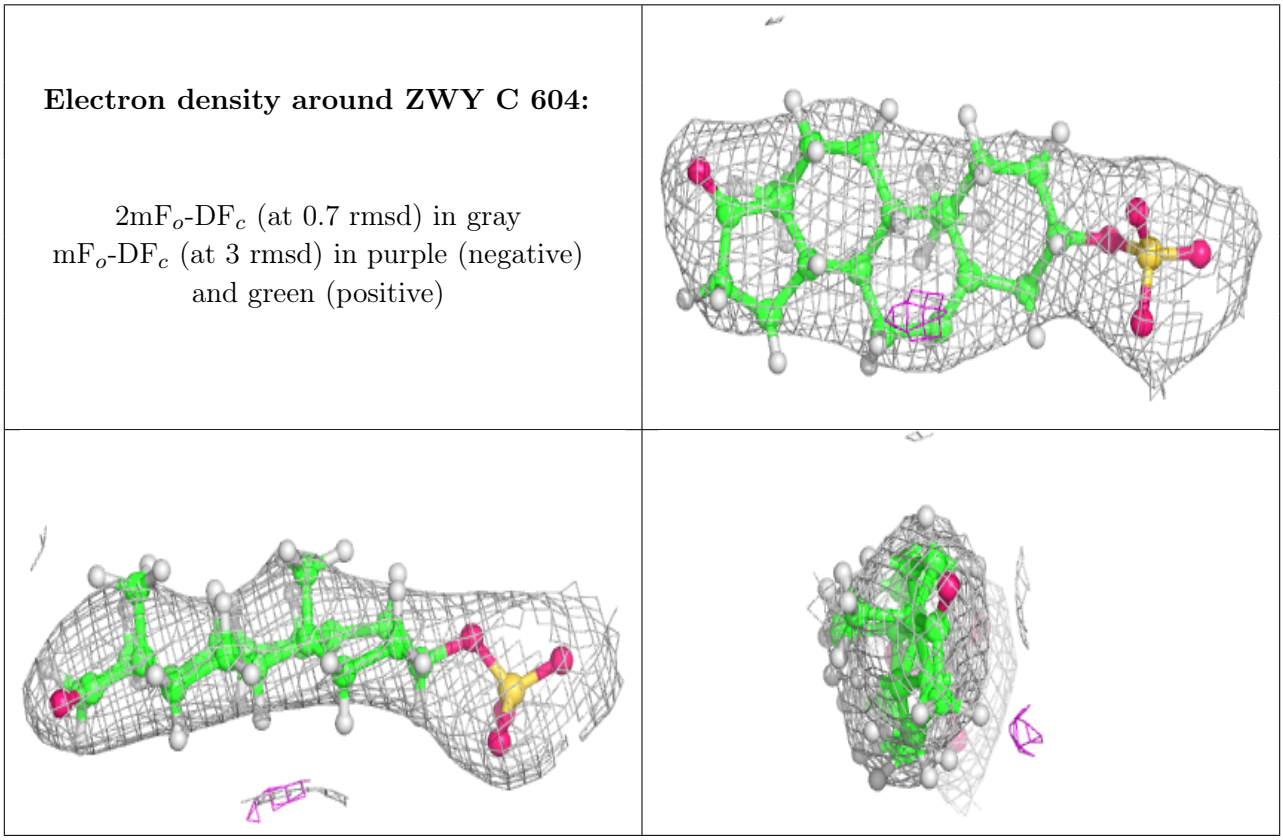
Electron density around ZWY D 606:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ZWY C 604:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.