



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:59 PM UTC

PDB ID : 2XQ1 / pdb_00002xq1
Title : Crystal structure of peroxisomal catalase from the yeast *Hansenula polymorpha*
Authors : Penya-Soler, E.; Vega, M.C.; Wilmanns, M.; Williams, C.P.
Deposited on : 2010-08-31
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

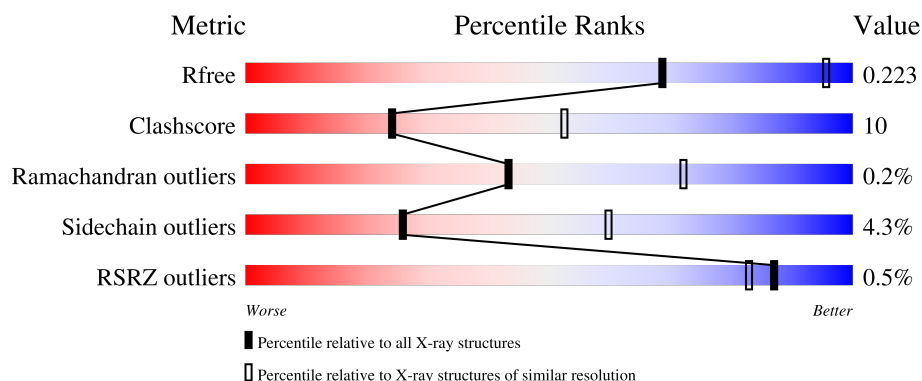
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 $\leq 5\%$. 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	509	
1	B	509	
1	C	509	
1	D	509	
1	E	509	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	509	2% 72% 24% ..
1	G	509	72% 23% ..
1	H	509	74% 21% ..
1	I	509	% 73% 22% ..
1	J	509	% 71% 25% ..
1	K	509	% 75% 20% ..
1	L	509	73% 21% ..
1	M	509	73% 22% ..
1	N	509	71% 24% ..
1	O	509	79% 17% ..
1	P	509	% 73% 21% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 63839 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

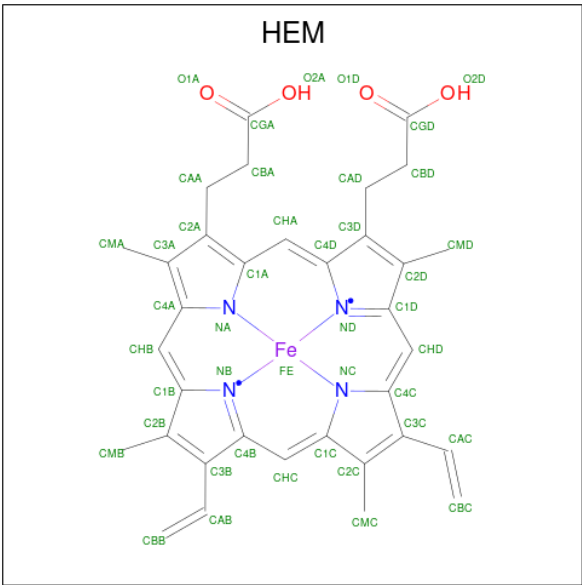
- Molecule 1 is a protein called PEROXISOMAL CATALASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3925	2517	664	731	13			
1	B	494	Total	C	N	O	S	0	0	0
			3953	2532	671	737	13			
1	C	492	Total	C	N	O	S	0	0	0
			3960	2536	672	739	13			
1	D	494	Total	C	N	O	S	0	0	0
			3959	2534	673	739	13			
1	E	490	Total	C	N	O	S	0	0	0
			3947	2527	670	737	13			
1	F	494	Total	C	N	O	S	0	0	0
			3950	2529	671	737	13			
1	G	491	Total	C	N	O	S	0	0	0
			3951	2531	671	736	13			
1	H	487	Total	C	N	O	S	0	0	0
			3922	2511	666	732	13			
1	I	491	Total	C	N	O	S	0	0	0
			3959	2534	672	740	13			
1	J	491	Total	C	N	O	S	0	0	0
			3943	2525	670	735	13			
1	K	490	Total	C	N	O	S	0	0	0
			3949	2529	670	737	13			
1	L	489	Total	C	N	O	S	0	0	0
			3933	2519	669	732	13			
1	M	491	Total	C	N	O	S	0	0	0
			3945	2526	671	735	13			
1	N	491	Total	C	N	O	S	0	0	0
			3945	2522	669	741	13			
1	O	493	Total	C	N	O	S	0	0	0
			3957	2534	673	737	13			
1	P	491	Total	C	N	O	S	0	0	0
			3931	2518	668	732	13			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P30263
A	0	ALA	-	expression tag	UNP P30263
B	-1	GLY	-	expression tag	UNP P30263
B	0	ALA	-	expression tag	UNP P30263
C	-1	GLY	-	expression tag	UNP P30263
C	0	ALA	-	expression tag	UNP P30263
D	-1	GLY	-	expression tag	UNP P30263
D	0	ALA	-	expression tag	UNP P30263
E	-1	GLY	-	expression tag	UNP P30263
E	0	ALA	-	expression tag	UNP P30263
F	-1	GLY	-	expression tag	UNP P30263
F	0	ALA	-	expression tag	UNP P30263
G	-1	GLY	-	expression tag	UNP P30263
G	0	ALA	-	expression tag	UNP P30263
H	-1	GLY	-	expression tag	UNP P30263
H	0	ALA	-	expression tag	UNP P30263
I	-1	GLY	-	expression tag	UNP P30263
I	0	ALA	-	expression tag	UNP P30263
J	-1	GLY	-	expression tag	UNP P30263
J	0	ALA	-	expression tag	UNP P30263
K	-1	GLY	-	expression tag	UNP P30263
K	0	ALA	-	expression tag	UNP P30263
L	-1	GLY	-	expression tag	UNP P30263
L	0	ALA	-	expression tag	UNP P30263
M	-1	GLY	-	expression tag	UNP P30263
M	0	ALA	-	expression tag	UNP P30263
N	-1	GLY	-	expression tag	UNP P30263
N	0	ALA	-	expression tag	UNP P30263
O	-1	GLY	-	expression tag	UNP P30263
O	0	ALA	-	expression tag	UNP P30263
P	-1	GLY	-	expression tag	UNP P30263
P	0	ALA	-	expression tag	UNP P30263

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

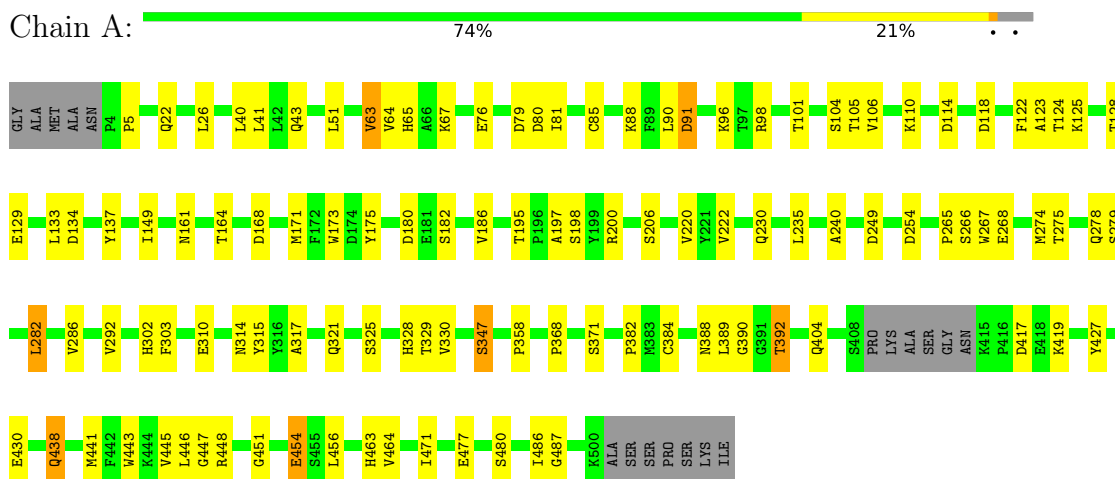
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O		
			5	5	0	0
3	B	7	Total	O		
			7	7	0	0
3	C	4	Total	O		
			4	4	0	0
3	D	6	Total	O		
			6	6	0	0
3	E	3	Total	O		
			3	3	0	0
3	F	6	Total	O		
			6	6	0	0
3	G	3	Total	O		
			3	3	0	0
3	H	2	Total	O		
			2	2	0	0
3	I	4	Total	O		
			4	4	0	0
3	J	6	Total	O		
			6	6	0	0
3	K	1	Total	O		
			1	1	0	0
3	L	6	Total	O		
			6	6	0	0
3	M	2	Total	O		
			2	2	0	0
3	N	1	Total	O		
			1	1	0	0
3	O	6	Total	O		
			6	6	0	0
3	P	3	Total	O		
			3	3	0	0

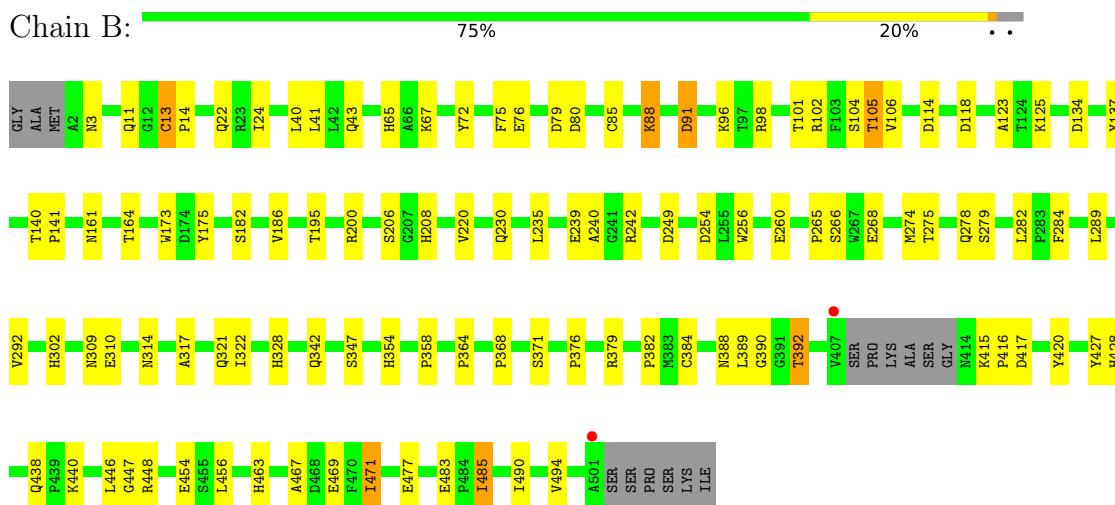
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: PEROXISOMAL CATALASE

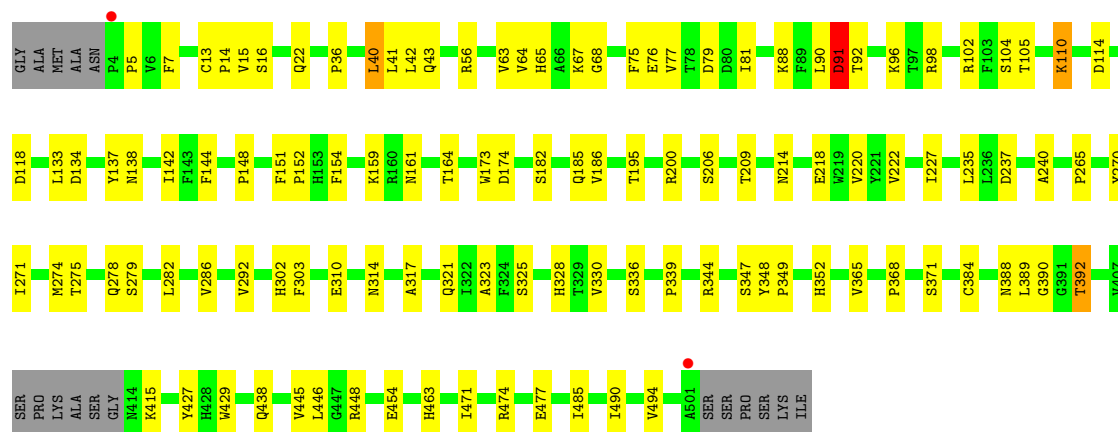


• Molecule 1: PEROXISOMAL CATALASE



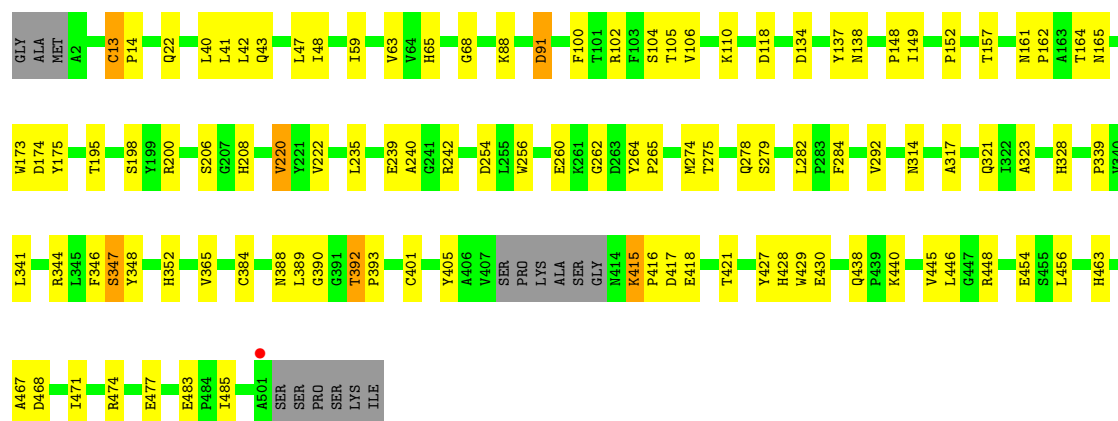
• Molecule 1: PEROXISOMAL CATALASE





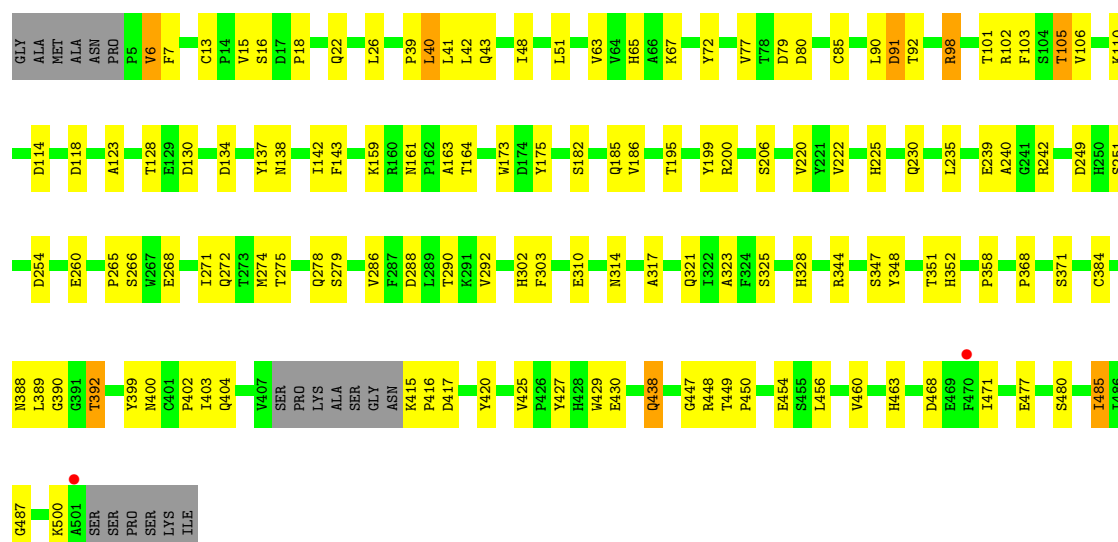
• Molecule 1: PEROXISOMAL CATALASE

Chain D: 76% 19%

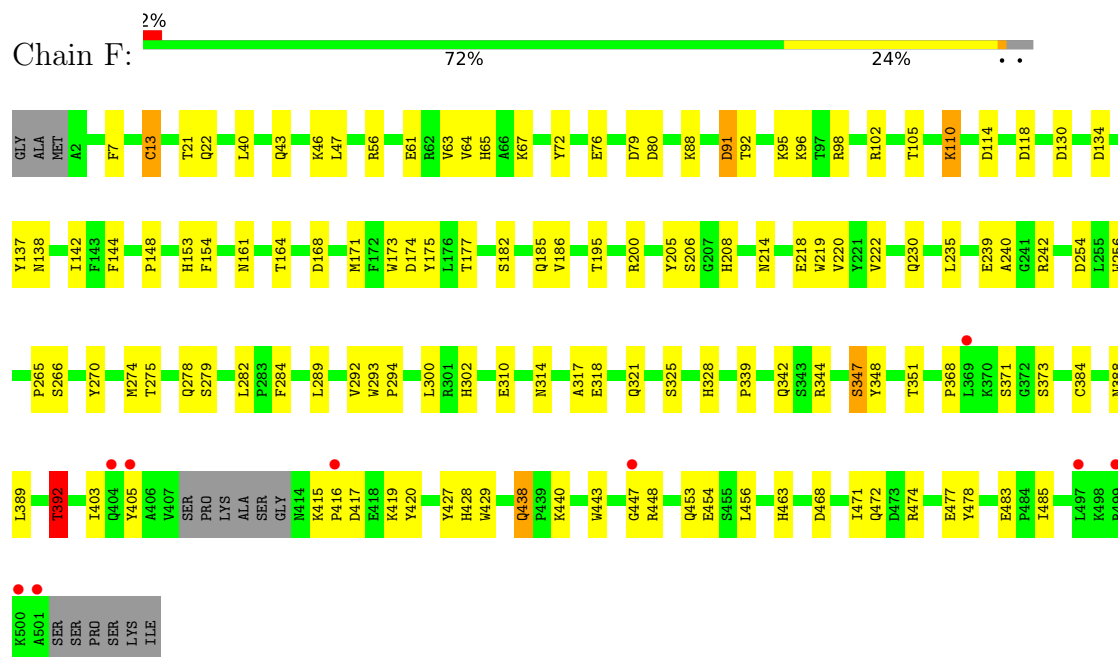


• Molecule 1: PEROXISOMAL CATALASE

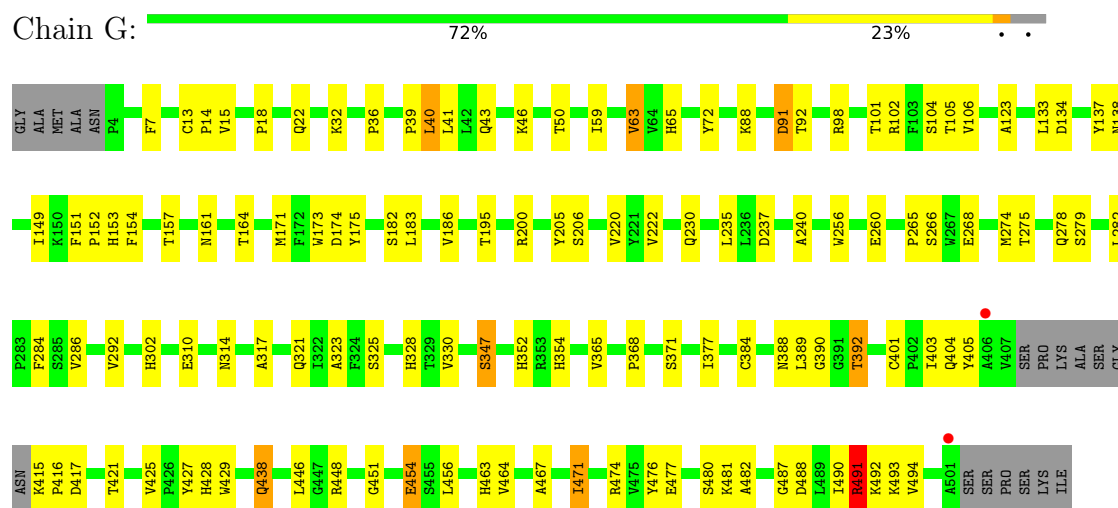
Chain E: 70% 24%



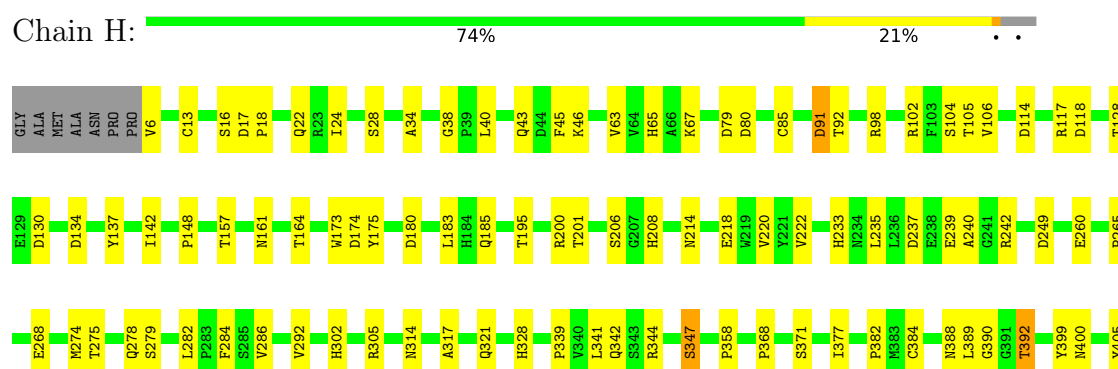
• Molecule 1: PEROXISOMAL CATALASE



• Molecule 1: PEROXISOMAL CATALASE

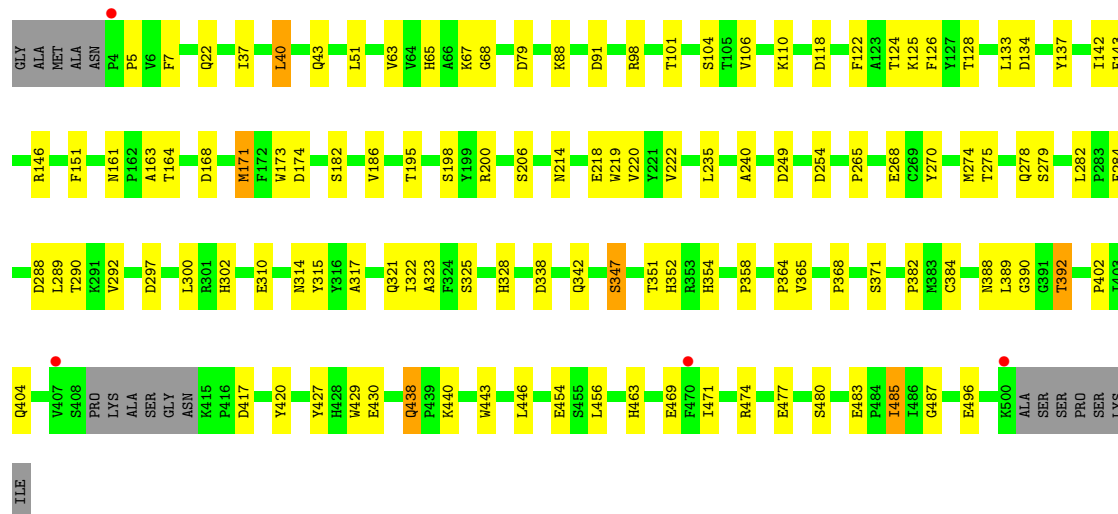


• Molecule 1: PEROXISOMAL CATALASE

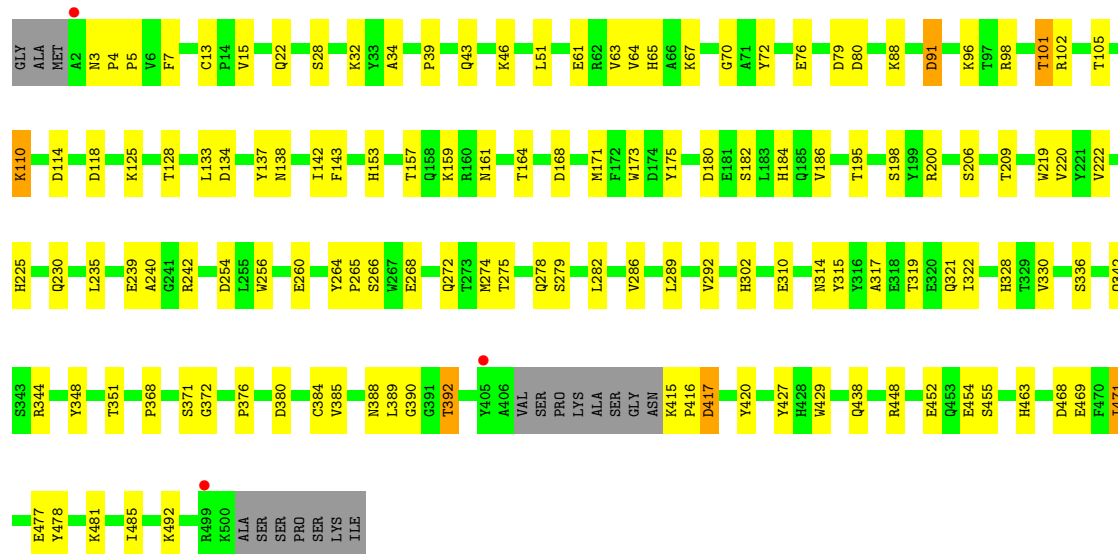




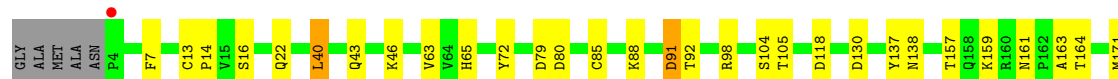
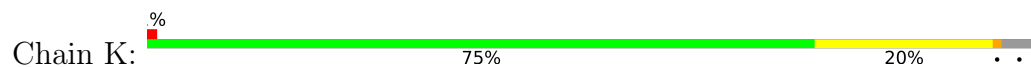
• Molecule 1: PEROXISOMAL CATALASE



• Molecule 1: PEROXISOMAL CATALASE



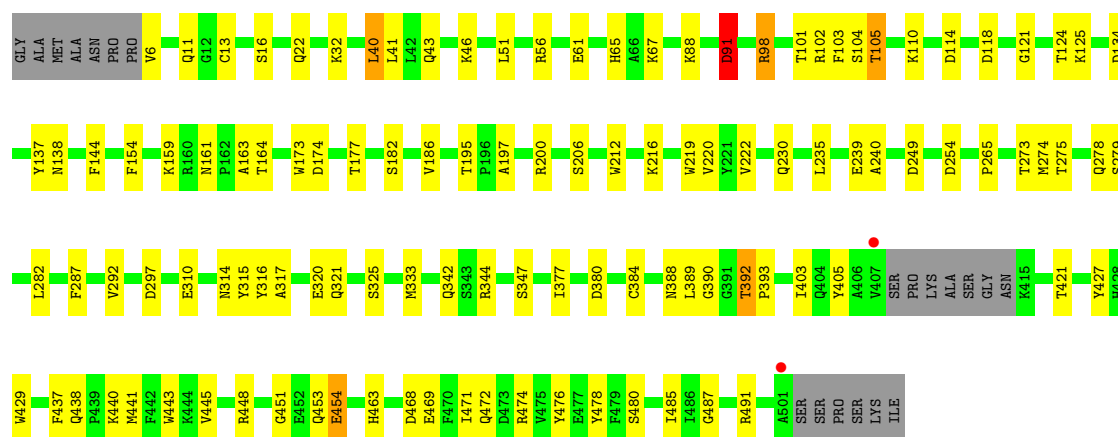
• Molecule 1: PEROXISOMAL CATALASE





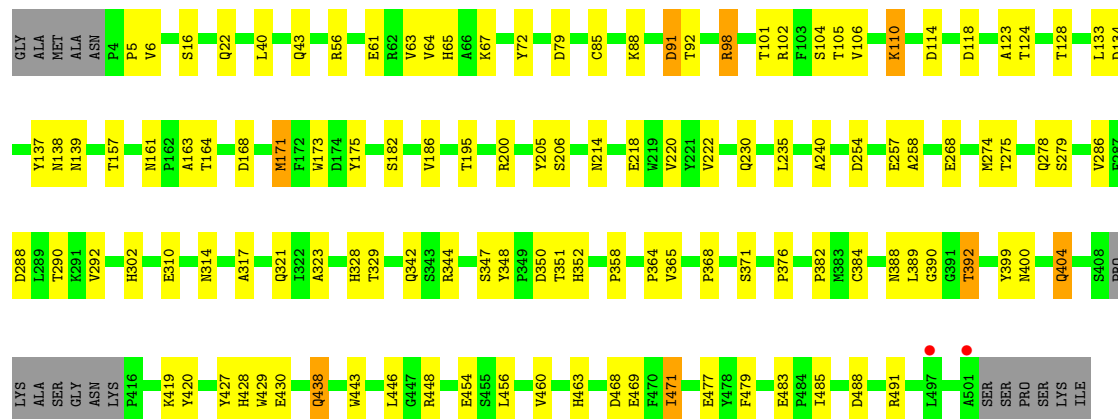
- Molecule 1: PEROXISOMAL CATALASE

Chain L: 73% 21% ..



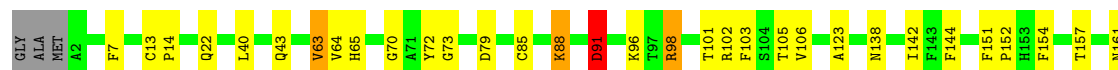
- Molecule 1: PEROXISOMAL CATALASE

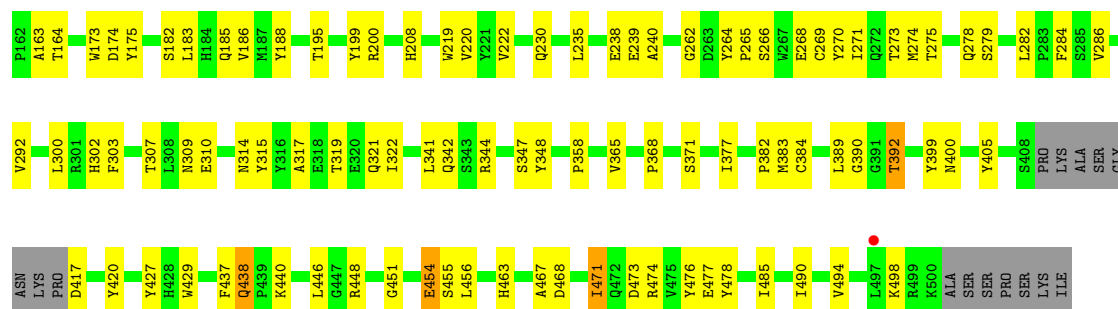
Chain M:  73% 22% . .



- Molecule 1: PEROXISOMAL CATALASE

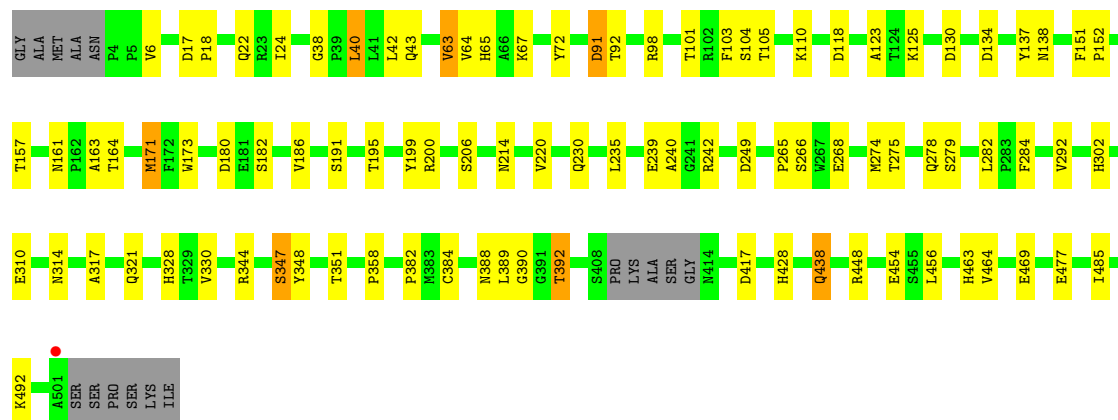
Chain N: 71% 24% ..





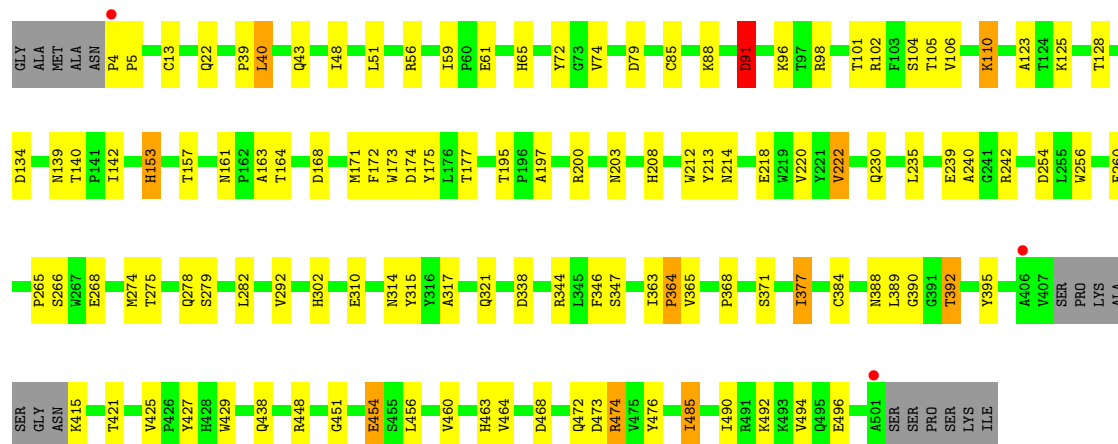
• Molecule 1: PEROXISOMAL CATALASE

Chain O: 79% 17% . .



• Molecule 1: PEROXISOMAL CATALASE

Chain P: 73% 21% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.52Å 196.68Å 170.85Å 90.00° 92.85° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.90) 99.7 (20.00-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.191 , 0.223 0.193 , 0.223	Depositor DCC
R_{free} test set	976 reflections (0.51%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	63839	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	0.84	0/4052	1.03	9/5523 (0.2%)
1	B	0.84	0/4080	1.02	10/5562 (0.2%)
1	C	0.85	0/4087	0.99	9/5566 (0.2%)
1	D	0.82	0/4086	1.05	13/5568 (0.2%)
1	E	0.84	1/4073 (0.0%)	1.02	9/5545 (0.2%)
1	F	0.85	0/4077	0.99	7/5557 (0.1%)
1	G	0.87	2/4078 (0.0%)	1.03	11/5553 (0.2%)
1	H	0.85	0/4047	1.02	6/5511 (0.1%)
1	I	0.85	0/4086	1.03	8/5563 (0.1%)
1	J	0.85	0/4070	1.04	5/5545 (0.1%)
1	K	0.81	1/4076 (0.0%)	0.98	7/5550 (0.1%)
1	L	0.84	0/4058	1.02	7/5525 (0.1%)
1	M	0.79	0/4072	0.98	6/5545 (0.1%)
1	N	0.82	0/4071	1.00	3/5547 (0.1%)
1	O	0.79	0/4084	0.99	6/5562 (0.1%)
1	P	0.81	0/4058	0.99	6/5529 (0.1%)
All	All	0.83	4/65155 (0.0%)	1.01	122/88751 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	E	0	1
1	F	0	1
1	G	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	491	ARG	CZ-NH1	9.57	1.46	1.32
1	G	491	ARG	CD-NE	6.39	1.55	1.46
1	K	403	ILE	CA-CB	6.25	1.62	1.54
1	E	242	ARG	CZ-NH1	5.56	1.40	1.32

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	491	ARG	NE-CZ-NH2	11.79	129.82	119.20
1	G	491	ARG	NH1-CZ-NH2	-8.24	108.59	119.30
1	A	448	ARG	N-CA-C	-7.88	103.39	113.16
1	B	13	CYS	CA-C-N	7.51	127.50	119.76
1	B	13	CYS	C-N-CA	7.51	127.50	119.76
1	P	448	ARG	N-CA-C	-7.00	104.72	113.18
1	B	85	CYS	N-CA-C	6.97	119.82	108.26
1	M	448	ARG	N-CA-C	-6.89	104.88	113.28
1	H	347	SER	N-CA-C	6.82	119.29	111.11
1	L	448	ARG	N-CA-C	-6.68	105.11	113.20
1	L	347	SER	N-CA-C	6.60	118.13	111.07
1	H	13	CYS	CA-C-N	6.57	126.53	119.76
1	H	13	CYS	C-N-CA	6.57	126.53	119.76
1	N	63	VAL	CB-CA-C	-6.57	103.27	112.14
1	G	63	VAL	CB-CA-C	-6.38	103.53	112.14
1	B	448	ARG	N-CA-C	-6.37	105.26	113.16
1	M	365	VAL	CB-CA-C	-6.25	102.48	112.16
1	I	347	SER	N-CA-C	6.24	118.60	111.11
1	J	448	ARG	N-CA-C	-6.22	105.66	113.18
1	P	59	ILE	CA-C-N	-6.19	113.57	119.76
1	P	59	ILE	C-N-CA	-6.19	113.57	119.76
1	D	347	SER	CB-CA-C	-6.03	101.16	110.81
1	P	153	HIS	N-CA-C	-5.99	104.44	110.97
1	K	448	ARG	N-CA-C	-5.97	105.76	113.16
1	G	448	ARG	N-CA-C	-5.97	105.76	113.16
1	K	159	LYS	N-CA-C	5.95	114.46	108.75
1	A	110	LYS	N-CA-C	5.91	117.72	111.28
1	O	191	SER	N-CA-C	-5.88	102.90	110.19
1	C	347	SER	CB-CA-C	-5.87	101.41	110.81
1	D	13	CYS	CA-C-N	5.87	125.78	119.85
1	D	13	CYS	C-N-CA	5.87	125.78	119.85
1	M	347	SER	N-CA-C	5.85	118.13	111.11
1	G	446	LEU	N-CA-C	-5.84	103.22	110.41
1	I	365	VAL	CB-CA-C	-5.84	100.64	111.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	330	VAL	N-CA-C	5.81	114.28	107.84
1	A	63	VAL	CB-CA-C	-5.79	103.60	112.05
1	L	105	THR	CA-C-N	-5.78	117.31	122.97
1	L	105	THR	C-N-CA	-5.78	117.31	122.97
1	D	68	GLY	N-CA-C	5.77	122.04	110.97
1	C	415	LYS	CA-C-N	5.76	127.04	119.84
1	C	415	LYS	C-N-CA	5.76	127.04	119.84
1	F	392	THR	CA-C-N	5.74	125.75	119.89
1	F	392	THR	C-N-CA	5.74	125.75	119.89
1	M	85	CYS	N-CA-C	5.73	117.77	108.26
1	F	448	ARG	N-CA-C	-5.72	106.07	113.16
1	E	105	THR	CA-C-N	-5.67	117.41	122.97
1	E	105	THR	C-N-CA	-5.67	117.41	122.97
1	A	85	CYS	N-CA-C	5.66	117.66	108.26
1	H	63	VAL	CB-CA-C	-5.65	104.51	112.14
1	O	347	SER	N-CA-C	5.63	117.09	111.07
1	B	105	THR	CA-C-N	-5.61	117.47	122.97
1	B	105	THR	C-N-CA	-5.61	117.47	122.97
1	C	110	LYS	N-CA-C	5.59	118.14	111.71
1	D	365	VAL	CB-CA-C	-5.59	101.11	111.79
1	N	85	CYS	N-CA-C	5.59	117.54	108.26
1	G	171	MET	CB-CA-C	-5.58	102.05	110.92
1	P	347	SER	N-CA-C	5.58	117.81	111.11
1	O	171	MET	CB-CA-C	-5.58	101.89	110.81
1	G	59	ILE	CA-C-N	-5.57	114.22	119.85
1	G	59	ILE	C-N-CA	-5.57	114.22	119.85
1	G	347	SER	N-CA-C	5.55	117.77	111.11
1	G	365	VAL	CB-CA-C	-5.54	103.96	112.05
1	K	63	VAL	CB-CA-C	-5.54	103.58	112.16
1	E	63	VAL	CB-CA-C	-5.53	104.80	112.04
1	I	446	LEU	N-CA-C	-5.53	103.24	110.53
1	D	347	SER	N-CA-C	5.51	117.72	111.11
1	J	13	CYS	CA-C-N	5.48	125.43	119.78
1	J	13	CYS	C-N-CA	5.48	125.43	119.78
1	C	159	LYS	N-CA-C	5.47	114.00	108.75
1	J	159	LYS	N-CA-C	5.47	114.00	108.75
1	C	365	VAL	CB-CA-C	-5.44	101.40	111.79
1	D	48	ILE	CB-CA-C	-5.44	105.01	111.97
1	E	85	CYS	N-CA-C	5.44	117.29	108.26
1	I	68	GLY	N-CA-C	5.44	119.47	110.55
1	E	347	SER	N-CA-C	5.43	116.88	111.07
1	K	85	CYS	N-CA-C	5.42	117.26	108.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	237	ASP	N-CA-C	5.41	116.86	111.07
1	E	159	LYS	N-CA-C	5.41	113.22	108.78
1	E	448	ARG	N-CA-C	-5.39	106.71	113.28
1	I	63	VAL	CB-CA-C	-5.38	103.83	112.16
1	O	63	VAL	CB-CA-C	-5.37	103.84	112.16
1	C	347	SER	N-CA-C	5.36	117.54	111.11
1	L	219	TRP	N-CA-C	5.36	118.32	109.85
1	K	471	ILE	CB-CA-C	5.34	117.69	111.55
1	M	446	LEU	N-CA-C	-5.34	103.84	110.41
1	A	91	ASP	N-CA-C	5.34	122.17	110.80
1	K	365	VAL	CB-CA-C	-5.33	101.61	111.79
1	K	171	MET	CB-CA-C	-5.28	102.08	110.84
1	F	13	CYS	CA-C-N	5.27	125.21	119.78
1	F	13	CYS	C-N-CA	5.27	125.21	119.78
1	N	365	VAL	CB-CA-C	-5.26	101.74	111.79
1	J	385	VAL	N-CA-C	5.26	117.95	112.90
1	H	347	SER	CB-CA-C	-5.25	102.41	110.81
1	F	403	ILE	N-CA-C	5.24	115.67	108.12
1	C	68	GLY	N-CA-C	5.24	120.84	110.83
1	D	63	VAL	CB-CA-C	-5.22	105.09	112.14
1	O	448	ARG	N-CA-C	-5.22	106.69	113.16
1	B	446	LEU	N-CA-C	-5.20	103.67	110.53
1	D	41	LEU	N-CA-C	5.20	118.28	109.76
1	B	24	ILE	N-CA-C	-5.19	101.96	107.77
1	A	446	LEU	N-CA-C	-5.18	103.69	110.53
1	B	41	LEU	N-CA-C	5.16	117.90	109.59
1	L	380	ASP	CB-CA-C	-5.16	109.65	115.79
1	H	85	CYS	N-CA-C	5.16	117.81	108.69
1	E	48	ILE	CB-CA-C	-5.14	105.20	112.14
1	G	237	ASP	N-CA-C	5.12	116.86	111.28
1	D	415	LYS	CA-C-N	5.09	125.38	119.93
1	D	415	LYS	C-N-CA	5.09	125.38	119.93
1	P	365	VAL	CB-CA-C	-5.09	104.27	112.16
1	F	347	SER	N-CA-C	5.08	117.21	111.11
1	B	3	ASN	N-CA-C	5.08	118.14	108.12
1	M	171	MET	CB-CA-C	-5.06	102.87	110.92
1	A	282	LEU	CA-C-N	5.06	125.13	119.87
1	A	282	LEU	C-N-CA	5.06	125.13	119.87
1	I	171	MET	CB-CA-C	-5.04	102.74	110.81
1	I	151	PHE	CA-C-N	-5.04	113.85	119.19
1	I	151	PHE	C-N-CA	-5.04	113.85	119.19
1	L	159	LYS	N-CA-C	5.04	113.58	108.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	SER	CB-CA-C	-5.02	103.00	110.88
1	E	6	VAL	N-CA-C	5.02	115.92	108.23
1	D	59	ILE	CA-C-N	-5.01	114.60	119.76
1	D	59	ILE	C-N-CA	-5.01	114.60	119.76

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	447	GLY	Peptide
1	B	447	GLY	Peptide
1	E	447	GLY	Peptide
1	F	447	GLY	Peptide
1	G	491	ARG	Sidechain

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	3925	0	3662	80	0
1	B	3953	0	3696	75	0
1	C	3960	0	3734	84	0
1	D	3959	0	3716	80	0
1	E	3947	0	3720	100	0
1	F	3950	0	3693	95	0
1	G	3951	0	3725	90	0
1	H	3922	0	3690	72	0
1	I	3959	0	3735	85	0
1	J	3943	0	3703	92	0
1	K	3949	0	3725	78	0
1	L	3933	0	3706	83	0
1	M	3945	0	3719	88	0
1	N	3945	0	3691	95	0
1	O	3957	0	3726	65	0
1	P	3931	0	3687	91	0
2	B	43	0	30	6	0
2	C	43	0	30	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	43	0	30	4	0
2	E	43	0	30	5	0
2	F	43	0	30	3	0
2	G	43	0	30	3	0
2	H	43	0	30	5	0
2	I	43	0	30	1	0
2	J	43	0	30	6	0
2	K	43	0	30	7	0
2	L	43	0	30	6	0
2	M	43	0	30	3	0
2	N	43	0	30	5	0
2	O	43	0	30	5	0
2	P	43	0	30	3	0
3	A	5	0	0	0	0
3	B	7	0	0	2	0
3	C	4	0	0	1	0
3	D	6	0	0	0	0
3	E	3	0	0	0	0
3	F	6	0	0	0	0
3	G	3	0	0	0	0
3	H	2	0	0	0	0
3	I	4	0	0	1	0
3	J	6	0	0	3	0
3	K	1	0	0	1	0
3	L	6	0	0	0	0
3	M	2	0	0	0	0
3	N	1	0	0	0	0
3	O	6	0	0	0	0
3	P	3	0	0	1	0
All	All	63839	0	59778	1235	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 10.

All (1235) 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:M:292:VAL:H	1:M:438:GLN:HE22	1.07	1.02
1:H:292:VAL:H	1:H:438:GLN:HE22	1.11	0.95
1:D:274:MET:CE	1:D:279:SER:HA	1.96	0.95
1:H:314:ASN:HD22	1:H:317:ALA:H	1.15	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:292:VAL:H	1:L:438:GLN:HE22	1.07	0.94
1:P:292:VAL:H	1:P:438:GLN:HE22	1.15	0.94
1:A:314:ASN:HD22	1:A:317:ALA:H	1.12	0.94
1:I:274:MET:CE	1:I:279:SER:HA	1.98	0.93
1:G:314:ASN:HD22	1:G:317:ALA:H	1.17	0.93
1:N:314:ASN:HD22	1:N:317:ALA:H	1.16	0.92
1:I:314:ASN:HD22	1:I:317:ALA:H	1.13	0.92
1:F:274:MET:CE	1:F:279:SER:HA	2.00	0.91
1:P:274:MET:HE3	1:P:279:SER:HA	1.53	0.91
1:F:274:MET:HE3	1:F:279:SER:HA	1.50	0.90
1:E:274:MET:HE3	1:E:279:SER:HA	1.53	0.90
1:M:274:MET:HE3	1:M:279:SER:HA	1.53	0.90
1:C:292:VAL:H	1:C:438:GLN:HE22	1.19	0.90
1:K:292:VAL:H	1:K:438:GLN:HE22	1.18	0.90
1:E:195:THR:HG21	1:E:240:ALA:HB2	1.54	0.89
1:J:274:MET:CE	1:J:279:SER:HA	2.02	0.89
1:N:102:ARG:HD3	2:N:1503:HEM:O1D	1.73	0.89
1:I:292:VAL:H	1:I:438:GLN:HE22	1.19	0.88
1:G:292:VAL:H	1:G:438:GLN:HE22	1.16	0.88
1:M:292:VAL:H	1:M:438:GLN:NE2	1.71	0.88
1:A:22:GLN:NE2	1:A:43:GLN:HE21	1.72	0.88
1:D:292:VAL:H	1:D:438:GLN:HE22	1.22	0.87
1:E:274:MET:CE	1:E:279:SER:HA	2.04	0.87
1:K:138:ASN:ND2	2:K:1503:HEM:HAC	1.90	0.87
1:O:200:ARG:HG2	1:O:265:PRO:HB3	1.57	0.86
1:B:314:ASN:HD22	1:B:317:ALA:H	1.17	0.86
1:E:314:ASN:HD22	1:E:317:ALA:H	1.17	0.86
1:J:314:ASN:HD22	1:J:317:ALA:H	1.23	0.86
1:K:195:THR:HG21	1:K:240:ALA:HB2	1.56	0.86
1:N:292:VAL:H	1:N:438:GLN:HE22	1.24	0.86
1:H:195:THR:HG21	1:H:240:ALA:HB2	1.56	0.85
1:F:314:ASN:HD22	1:F:317:ALA:H	1.25	0.85
1:C:275:THR:OG1	1:C:278:GLN:HG3	1.76	0.85
1:J:292:VAL:H	1:J:438:GLN:HE22	1.25	0.85
1:K:274:MET:CE	1:K:279:SER:HA	2.06	0.84
1:L:161:ASN:HD22	1:L:164:THR:H	1.24	0.84
1:I:161:ASN:HD22	1:I:164:THR:H	1.23	0.83
1:P:314:ASN:HD22	1:P:317:ALA:H	1.22	0.83
1:O:314:ASN:HD22	1:O:317:ALA:H	1.26	0.83
1:G:22:GLN:NE2	1:G:43:GLN:HE21	1.77	0.83
1:K:314:ASN:HD22	1:K:317:ALA:H	1.26	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:274:MET:CE	1:N:279:SER:HA	2.09	0.82
1:L:22:GLN:NE2	1:L:43:GLN:HE21	1.77	0.82
1:G:161:ASN:HD22	1:G:164:THR:H	1.27	0.82
1:B:292:VAL:H	1:B:438:GLN:HE22	1.28	0.82
1:M:274:MET:CE	1:M:279:SER:HA	2.09	0.82
1:L:292:VAL:H	1:L:438:GLN:NE2	1.78	0.82
1:K:274:MET:HE3	1:K:279:SER:HA	1.62	0.81
1:O:274:MET:CE	1:O:279:SER:HA	2.11	0.81
1:O:292:VAL:H	1:O:438:GLN:HE22	1.26	0.81
1:A:389:LEU:O	1:A:392:THR:OG1	1.97	0.81
1:P:102:ARG:HD3	2:P:1503:HEM:O1D	1.80	0.81
1:I:274:MET:HE3	1:I:279:SER:HA	1.62	0.81
1:B:195:THR:HG21	1:B:240:ALA:HB2	1.62	0.81
1:C:274:MET:CE	1:C:279:SER:HA	2.11	0.81
1:I:314:ASN:HD21	1:J:388:ASN:HD22	1.30	0.80
1:O:195:THR:HG21	1:O:240:ALA:HB2	1.63	0.80
1:J:274:MET:HE3	1:J:279:SER:HA	1.62	0.80
1:H:275:THR:OG1	1:H:278:GLN:HG3	1.82	0.80
1:H:292:VAL:H	1:H:438:GLN:NE2	1.79	0.80
1:N:195:THR:HG22	1:N:235:LEU:HB2	1.63	0.80
1:E:292:VAL:H	1:E:438:GLN:HE22	1.29	0.79
1:D:314:ASN:HD22	1:D:317:ALA:H	1.30	0.79
1:G:274:MET:CE	1:G:279:SER:HA	2.12	0.79
1:K:292:VAL:H	1:K:438:GLN:NE2	1.79	0.79
1:L:314:ASN:HD22	1:L:317:ALA:H	1.29	0.79
1:P:22:GLN:NE2	1:P:43:GLN:HE21	1.81	0.79
1:A:292:VAL:H	1:A:438:GLN:HE22	1.29	0.79
1:D:195:THR:HG21	1:D:240:ALA:HB2	1.63	0.78
1:I:292:VAL:HG22	1:I:438:GLN:NE2	1.98	0.78
1:A:314:ASN:ND2	1:A:317:ALA:H	1.80	0.78
1:G:292:VAL:H	1:G:438:GLN:NE2	1.82	0.78
1:E:22:GLN:HE22	1:E:43:GLN:HE21	1.32	0.77
1:A:161:ASN:HD22	1:A:164:THR:H	1.32	0.77
1:H:344:ARG:NH1	2:H:1503:HEM:HBC2	1.99	0.77
1:B:22:GLN:NE2	1:B:43:GLN:HE21	1.83	0.77
1:H:274:MET:HE3	1:H:279:SER:HA	1.65	0.77
1:F:292:VAL:H	1:F:438:GLN:HE22	1.31	0.77
1:H:200:ARG:HG2	1:H:265:PRO:HB3	1.66	0.77
1:C:22:GLN:NE2	1:C:43:GLN:HE21	1.83	0.76
1:C:200:ARG:HG2	1:C:265:PRO:HB3	1.68	0.76
1:L:195:THR:HG21	1:L:240:ALA:HB2	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:THR:HG21	1:A:240:ALA:HB2	1.67	0.76
1:P:161:ASN:HD22	1:P:164:THR:H	1.32	0.76
1:M:102:ARG:HD3	2:M:1503:HEM:O1D	1.85	0.75
1:M:161:ASN:HD22	1:M:164:THR:H	1.34	0.75
1:C:321:GLN:HE22	1:D:384:CYS:H	1.32	0.75
1:G:314:ASN:ND2	1:G:317:ALA:H	1.83	0.75
2:L:1503:HEM:HMB1	2:L:1503:HEM:HBB2	1.66	0.75
1:M:195:THR:HG21	1:M:240:ALA:HB2	1.66	0.75
1:O:274:MET:HE3	1:O:279:SER:HA	1.68	0.75
1:H:161:ASN:HD22	1:H:164:THR:H	1.31	0.75
1:E:22:GLN:NE2	1:E:43:GLN:HE21	1.83	0.75
1:H:274:MET:CE	1:H:279:SER:HA	2.16	0.75
1:K:314:ASN:HD21	1:L:388:ASN:HD22	1.32	0.75
1:M:22:GLN:NE2	1:M:43:GLN:HE21	1.85	0.75
1:C:292:VAL:H	1:C:438:GLN:NE2	1.85	0.74
1:I:292:VAL:H	1:I:438:GLN:NE2	1.85	0.74
1:B:161:ASN:HD22	1:B:164:THR:H	1.35	0.74
1:P:195:THR:HG22	1:P:235:LEU:HB2	1.69	0.74
1:A:274:MET:CE	1:A:279:SER:HA	2.18	0.74
1:D:274:MET:HE3	1:D:279:SER:HA	1.70	0.74
1:B:274:MET:HE3	1:B:279:SER:HA	1.70	0.74
1:N:161:ASN:HD22	1:N:164:THR:H	1.36	0.74
1:P:344:ARG:NH1	2:P:1503:HEM:HBC2	2.02	0.74
1:K:384:CYS:H	1:L:321:GLN:HE22	1.36	0.74
1:O:22:GLN:NE2	1:O:43:GLN:HE21	1.85	0.73
1:L:274:MET:HE3	1:L:279:SER:HA	1.68	0.73
1:N:195:THR:HG21	1:N:240:ALA:HB2	1.70	0.73
1:E:314:ASN:ND2	1:E:317:ALA:H	1.85	0.73
2:D:1503:HEM:HMB1	2:D:1503:HEM:HBB2	1.70	0.73
1:M:195:THR:HG22	1:M:235:LEU:HB2	1.69	0.73
1:K:161:ASN:HD22	1:K:164:THR:H	1.35	0.73
1:H:274:MET:HE1	1:H:282:LEU:HD22	1.69	0.72
1:I:22:GLN:NE2	1:I:43:GLN:HE21	1.87	0.72
1:C:195:THR:HG21	1:C:240:ALA:HB2	1.70	0.72
1:E:161:ASN:HD22	1:E:164:THR:H	1.35	0.72
1:M:314:ASN:HD22	1:M:317:ALA:H	1.35	0.72
1:N:292:VAL:H	1:N:438:GLN:NE2	1.87	0.72
1:B:274:MET:CE	1:B:279:SER:HA	2.20	0.72
2:C:1503:HEM:HMB2	2:C:1503:HEM:HBB2	1.71	0.72
1:M:389:LEU:O	1:M:392:THR:OG1	2.08	0.72
1:B:96:LYS:H	1:E:404:GLN:NE2	1.88	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:79:ASP:OD2	1:K:302:HIS:HD2	1.72	0.72
1:I:314:ASN:ND2	1:I:317:ALA:H	1.85	0.71
1:N:88:LYS:O	1:N:91:ASP:HB2	1.90	0.71
1:A:274:MET:HE3	1:A:279:SER:HA	1.72	0.71
1:E:384:CYS:H	1:F:321:GLN:HE22	1.38	0.71
1:C:274:MET:HE1	1:C:282:LEU:HD22	1.70	0.71
1:C:314:ASN:HD22	1:C:317:ALA:H	1.37	0.71
1:B:274:MET:HE1	1:B:282:LEU:HD22	1.71	0.71
1:N:314:ASN:ND2	1:N:317:ALA:H	1.88	0.71
1:L:138:ASN:ND2	2:L:1503:HEM:HAC	2.05	0.71
1:P:274:MET:CE	1:P:279:SER:HA	2.20	0.71
1:I:200:ARG:HG2	1:I:265:PRO:HB3	1.71	0.70
1:H:314:ASN:ND2	1:H:317:ALA:H	1.88	0.70
1:I:22:GLN:HE22	1:I:43:GLN:HE21	1.39	0.70
1:O:388:ASN:HD22	1:P:314:ASN:HD21	1.39	0.70
1:F:214:ASN:HD21	1:F:218:GLU:HB2	1.56	0.70
1:N:368:PRO:O	1:N:371:SER:O	2.10	0.70
1:J:161:ASN:HD22	1:J:164:THR:H	1.39	0.70
1:N:200:ARG:HG2	1:N:265:PRO:HB3	1.73	0.70
1:P:235:LEU:HD22	1:P:239:GLU:HG2	1.73	0.70
1:D:292:VAL:H	1:D:438:GLN:NE2	1.89	0.70
1:G:389:LEU:O	1:G:392:THR:OG1	2.09	0.70
3:I:2001:HOH:O	1:J:125:LYS:HE3	1.91	0.70
1:K:200:ARG:HG2	1:K:265:PRO:HB3	1.74	0.70
1:J:195:THR:HG21	1:J:240:ALA:HB2	1.74	0.69
1:J:368:PRO:O	1:J:371:SER:O	2.09	0.69
1:J:389:LEU:O	1:J:392:THR:OG1	2.10	0.69
1:M:200:ARG:HD3	1:M:254:ASP:OD2	1.92	0.69
1:C:274:MET:HE3	1:C:279:SER:HA	1.72	0.69
1:P:292:VAL:H	1:P:438:GLN:NE2	1.87	0.69
1:I:389:LEU:O	1:I:392:THR:OG1	2.10	0.69
1:D:389:LEU:O	1:D:392:THR:OG1	2.11	0.69
1:E:389:LEU:O	1:E:392:THR:OG1	2.10	0.69
1:J:195:THR:HG22	1:J:235:LEU:HB2	1.74	0.69
1:O:161:ASN:HD22	1:O:164:THR:H	1.37	0.69
1:A:388:ASN:HD22	1:B:314:ASN:HD21	1.40	0.69
1:F:22:GLN:NE2	1:F:43:GLN:HE21	1.91	0.69
1:J:292:VAL:H	1:J:438:GLN:NE2	1.90	0.69
1:L:22:GLN:HE22	1:L:43:GLN:HE21	1.38	0.69
1:L:173:TRP:HE1	1:L:463:HIS:HD2	1.38	0.69
1:G:195:THR:HG21	1:G:240:ALA:HB2	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:274:MET:HE3	1:N:279:SER:HA	1.72	0.69
1:O:358:PRO:HG2	1:O:382:PRO:HG2	1.74	0.69
1:E:195:THR:HG22	1:E:235:LEU:HB2	1.74	0.68
1:N:22:GLN:NE2	1:N:43:GLN:HE21	1.90	0.68
1:A:275:THR:OG1	1:A:278:GLN:HG3	1.92	0.68
1:O:292:VAL:H	1:O:438:GLN:NE2	1.91	0.68
1:B:292:VAL:H	1:B:438:GLN:NE2	1.91	0.68
1:C:138:ASN:ND2	2:C:1503:HEM:HAC	2.08	0.68
1:I:314:ASN:ND2	1:J:388:ASN:HD22	1.90	0.68
1:G:200:ARG:HG2	1:G:265:PRO:HB3	1.76	0.68
1:N:389:LEU:O	1:N:392:THR:OG1	2.10	0.68
1:E:292:VAL:H	1:E:438:GLN:NE2	1.91	0.68
1:A:182:SER:O	1:A:186:VAL:HG23	1.93	0.67
1:B:11:GLN:OE1	3:B:2001:HOH:O	2.11	0.67
1:J:67:LYS:HE2	1:J:114:ASP:OD1	1.94	0.67
1:K:314:ASN:ND2	1:K:317:ALA:H	1.93	0.67
1:B:389:LEU:O	1:B:392:THR:OG1	2.12	0.67
1:E:235:LEU:HD22	1:E:239:GLU:HG2	1.76	0.67
1:C:314:ASN:HD21	1:D:388:ASN:HD22	1.43	0.67
1:L:102:ARG:HD3	2:L:1503:HEM:O1D	1.94	0.67
1:G:138:ASN:ND2	2:G:1503:HEM:HAC	2.11	0.66
1:I:195:THR:HG21	1:I:240:ALA:HB2	1.77	0.66
1:I:275:THR:OG1	1:I:278:GLN:HG3	1.95	0.66
1:J:102:ARG:HD3	2:J:1503:HEM:O1D	1.96	0.66
1:P:490:ILE:O	1:P:494:VAL:HG23	1.95	0.66
1:M:376:PRO:HD2	1:N:7:PHE:CE1	2.30	0.66
1:B:368:PRO:O	1:B:371:SER:O	2.13	0.66
1:C:384:CYS:H	1:D:321:GLN:HE22	1.42	0.66
1:B:173:TRP:HE1	1:B:463:HIS:HD2	1.44	0.66
1:C:344:ARG:NH1	2:C:1503:HEM:HBC2	2.11	0.66
1:F:102:ARG:HD3	2:F:1503:HEM:O1D	1.95	0.66
1:B:102:ARG:HD3	2:B:1503:HEM:O1D	1.96	0.66
1:I:274:MET:HE2	1:I:279:SER:CB	2.26	0.66
1:K:22:GLN:NE2	1:K:43:GLN:HE21	1.92	0.66
1:M:275:THR:OG1	1:M:278:GLN:HG3	1.96	0.66
1:D:274:MET:HE2	1:D:279:SER:HA	1.76	0.66
1:G:476:TYR:CE2	1:G:491:ARG:HG3	2.31	0.66
1:G:321:GLN:HE22	1:H:384:CYS:H	1.42	0.65
1:O:314:ASN:ND2	1:O:317:ALA:H	1.92	0.65
1:F:88:LYS:O	1:F:91:ASP:HB2	1.96	0.65
1:J:200:ARG:HD3	1:J:254:ASP:OD2	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:274:MET:HE3	1:G:279:SER:HA	1.79	0.65
1:C:388:ASN:HD22	1:D:314:ASN:HD21	1.45	0.65
1:L:314:ASN:ND2	1:L:317:ALA:H	1.95	0.65
1:I:388:ASN:HD22	1:J:314:ASN:HD21	1.44	0.64
1:E:200:ARG:HG2	1:E:265:PRO:HB3	1.79	0.64
1:F:468:ASP:O	1:F:472:GLN:HG3	1.97	0.64
1:M:368:PRO:O	1:M:371:SER:O	2.15	0.64
1:B:22:GLN:HE22	1:B:43:GLN:HE21	1.45	0.64
1:B:195:THR:HG22	1:B:235:LEU:HB2	1.78	0.64
1:E:275:THR:OG1	1:E:278:GLN:HG3	1.97	0.64
1:F:292:VAL:H	1:F:438:GLN:NE2	1.96	0.64
1:A:22:GLN:HB3	1:A:41:LEU:HD12	1.79	0.64
1:H:22:GLN:NE2	1:H:43:GLN:HE21	1.96	0.64
1:F:274:MET:HE1	1:F:282:LEU:HD22	1.79	0.64
1:A:388:ASN:HD22	1:B:314:ASN:ND2	1.96	0.64
1:C:389:LEU:O	1:C:392:THR:OG1	2.16	0.64
1:D:427:TYR:OH	1:D:430:GLU:HG2	1.98	0.64
1:P:314:ASN:ND2	1:P:317:ALA:H	1.94	0.64
1:D:22:GLN:NE2	1:D:43:GLN:HE21	1.95	0.64
1:D:275:THR:OG1	1:D:278:GLN:HG3	1.97	0.64
1:J:314:ASN:ND2	1:J:317:ALA:H	1.94	0.64
1:N:275:THR:OG1	1:N:278:GLN:HG3	1.99	0.63
1:P:292:VAL:HG22	1:P:438:GLN:NE2	2.12	0.63
1:D:161:ASN:HD22	1:D:164:THR:H	1.45	0.63
1:F:314:ASN:ND2	1:F:317:ALA:H	1.97	0.63
1:M:314:ASN:ND2	1:M:317:ALA:H	1.95	0.63
1:A:195:THR:HG22	1:A:235:LEU:HB2	1.79	0.63
1:I:351:THR:HG21	2:I:1503:HEM:HBA1	1.80	0.63
1:F:389:LEU:O	1:F:392:THR:OG1	2.15	0.63
1:A:314:ASN:ND2	1:B:388:ASN:HD22	1.97	0.63
1:M:65:HIS:HA	1:M:105:THR:O	1.98	0.63
1:O:275:THR:OG1	1:O:278:GLN:HG3	1.99	0.63
1:I:314:ASN:HB2	1:J:390:GLY:HA2	1.80	0.63
1:K:161:ASN:ND2	1:K:163:ALA:H	1.97	0.63
1:M:214:ASN:HD21	1:M:218:GLU:HB2	1.64	0.63
1:O:384:CYS:H	1:P:321:GLN:HE22	1.45	0.63
1:F:144:PHE:CD2	1:F:154:PHE:CZ	2.87	0.63
1:F:214:ASN:ND2	1:F:218:GLU:HB2	2.13	0.63
1:G:314:ASN:HD21	1:H:388:ASN:HD22	1.47	0.63
1:L:274:MET:CE	1:L:279:SER:HA	2.29	0.63
1:O:125:LYS:HE3	3:P:2001:HOH:O	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:HIS:HA	1:B:105:THR:O	1.97	0.63
1:G:182:SER:O	1:G:186:VAL:HG23	1.99	0.63
1:I:195:THR:HG22	1:I:235:LEU:HB2	1.80	0.63
1:J:478:TYR:O	1:J:481:LYS:HB2	1.99	0.62
1:E:321:GLN:HE22	1:F:384:CYS:H	1.47	0.62
1:F:195:THR:HG22	1:F:235:LEU:HB2	1.81	0.62
1:K:314:ASN:ND2	1:L:388:ASN:HD22	1.97	0.62
1:K:321:GLN:HE22	1:L:384:CYS:H	1.47	0.62
1:P:344:ARG:HH12	2:P:1503:HEM:HBC2	1.63	0.62
1:J:98:ARG:NH2	1:J:310:GLU:OE1	2.33	0.62
1:G:274:MET:HE1	1:G:282:LEU:HD22	1.80	0.62
1:N:230:GLN:HE22	1:N:266:SER:H	1.45	0.62
2:B:1503:HEM:HBC2	2:B:1503:HEM:CMC	2.29	0.62
1:D:344:ARG:HG2	1:D:348:TYR:HE1	1.64	0.62
1:H:214:ASN:HD21	1:H:218:GLU:HB2	1.64	0.62
1:M:292:VAL:N	1:M:438:GLN:HE22	1.89	0.62
1:F:239:GLU:OE1	1:F:242:ARG:NH1	2.30	0.62
1:G:174:ASP:OD1	1:G:474:ARG:NH2	2.32	0.62
1:K:22:GLN:HE22	1:K:43:GLN:HE21	1.47	0.62
1:A:22:GLN:HE22	1:A:43:GLN:HE21	1.45	0.62
1:C:195:THR:CG2	1:C:240:ALA:HB2	2.29	0.62
1:I:67:LYS:NZ	1:I:249:ASP:OD1	2.33	0.62
1:E:98:ARG:NH2	1:E:310:GLU:OE1	2.33	0.62
1:P:389:LEU:O	1:P:392:THR:OG1	2.17	0.61
1:E:138:ASN:ND2	2:E:1503:HEM:HAC	2.15	0.61
1:N:173:TRP:HE1	1:N:463:HIS:HD2	1.48	0.61
1:L:468:ASP:O	1:L:472:GLN:HG3	2.00	0.61
1:P:65:HIS:CE1	1:P:106:VAL:HG22	2.35	0.61
1:I:182:SER:O	1:I:186:VAL:HG23	1.99	0.61
1:F:200:ARG:HG2	1:F:265:PRO:HB3	1.83	0.61
1:G:384:CYS:H	1:H:321:GLN:HE22	1.46	0.61
1:D:274:MET:CE	1:D:279:SER:CA	2.77	0.61
1:C:161:ASN:HD22	1:C:164:THR:H	1.46	0.61
1:F:173:TRP:HE1	1:F:463:HIS:HD2	1.47	0.61
1:L:195:THR:HG22	1:L:235:LEU:HB2	1.82	0.61
1:N:65:HIS:HA	1:N:105:THR:O	2.01	0.61
1:C:314:ASN:ND2	1:D:388:ASN:HD22	1.99	0.60
1:C:368:PRO:O	1:C:371:SER:O	2.19	0.60
1:E:314:ASN:HD21	1:F:388:ASN:HD22	1.47	0.60
1:D:200:ARG:HG2	1:D:265:PRO:HB3	1.83	0.60
1:E:134:ASP:OD2	1:E:328:HIS:HD2	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:79:ASP:OD2	1:N:302:HIS:HD2	1.83	0.60
1:O:388:ASN:HD22	1:P:314:ASN:ND2	1.98	0.60
1:H:79:ASP:OD2	1:H:302:HIS:HD2	1.84	0.60
1:L:441:MET:O	1:L:445:VAL:HG23	2.01	0.60
1:N:235:LEU:HD22	1:N:239:GLU:HG2	1.84	0.60
1:N:274:MET:HE1	1:N:282:LEU:HD22	1.83	0.60
1:J:138:ASN:ND2	2:J:1503:HEM:HAC	2.16	0.60
1:H:358:PRO:HG2	1:H:382:PRO:HG2	1.82	0.60
1:C:274:MET:HE2	1:C:279:SER:CB	2.31	0.60
1:D:195:THR:HG22	1:D:235:LEU:HB2	1.82	0.60
1:M:399:TYR:CE1	1:M:400:ASN:HB3	2.36	0.60
1:N:65:HIS:CE1	1:N:106:VAL:HG22	2.36	0.60
1:J:79:ASP:OD2	1:J:302:HIS:HD2	1.84	0.60
1:B:314:ASN:ND2	1:B:317:ALA:H	1.97	0.60
1:E:102:ARG:HD3	2:E:1503:HEM:O1D	2.01	0.60
1:J:427:TYR:CE2	1:J:429:TRP:HA	2.36	0.60
1:N:138:ASN:ND2	2:N:1503:HEM:HAC	2.17	0.60
1:E:79:ASP:OD1	1:E:302:HIS:HD2	1.85	0.60
1:I:388:ASN:HD22	1:J:314:ASN:ND2	2.00	0.59
2:J:1503:HEM:HMB1	2:J:1503:HEM:HBB2	1.83	0.59
1:C:173:TRP:HE1	1:C:463:HIS:HD2	1.48	0.59
1:D:88:LYS:O	1:D:91:ASP:HB2	2.02	0.59
1:D:274:MET:HE1	1:D:282:LEU:HD22	1.84	0.59
1:E:195:THR:CG2	1:E:240:ALA:HB2	2.30	0.59
1:H:67:LYS:NZ	1:H:249:ASP:OD1	2.36	0.59
1:J:96:LYS:H	1:M:404:GLN:HE22	1.50	0.59
1:K:389:LEU:O	1:K:392:THR:OG1	2.20	0.59
1:C:79:ASP:OD1	1:C:302:HIS:HD2	1.86	0.59
1:K:138:ASN:ND2	2:K:1503:HEM:CAC	2.62	0.59
1:K:415:LYS:HD3	1:K:416:PRO:HD2	1.85	0.59
1:A:314:ASN:HD21	1:B:388:ASN:HD22	1.48	0.59
1:L:200:ARG:HG2	1:L:265:PRO:HB3	1.84	0.59
1:F:161:ASN:HD22	1:F:164:THR:H	1.48	0.59
1:G:195:THR:O	1:G:195:THR:HG22	2.00	0.59
1:N:230:GLN:NE2	1:N:266:SER:H	2.01	0.59
1:H:389:LEU:O	1:H:392:THR:OG1	2.20	0.59
1:C:446:LEU:C	1:C:448:ARG:H	2.11	0.58
1:H:195:THR:HG22	1:H:235:LEU:HB2	1.85	0.58
1:K:368:PRO:O	1:K:371:SER:O	2.20	0.58
1:H:28:SER:HB2	1:H:34:ALA:HB1	1.85	0.58
1:N:490:ILE:O	1:N:494:VAL:HG23	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:98:ARG:NH2	1:P:310:GLU:OE1	2.36	0.58
1:F:79:ASP:OD2	1:F:302:HIS:HD2	1.85	0.58
1:K:65:HIS:HA	1:K:105:THR:O	2.03	0.58
1:B:275:THR:OG1	1:B:278:GLN:HG3	2.03	0.58
1:D:138:ASN:ND2	2:D:1503:HEM:HAC	2.19	0.58
1:D:314:ASN:ND2	1:D:317:ALA:H	1.99	0.58
1:P:195:THR:HG21	1:P:240:ALA:HB2	1.84	0.58
1:A:26:LEU:CD2	1:D:418:GLU:HB3	2.34	0.58
1:G:282:LEU:HD23	1:G:284:PHE:CZ	2.39	0.58
1:P:456:LEU:O	1:P:460:VAL:HG23	2.03	0.58
1:E:271:ILE:HG23	1:E:303:PHE:CE1	2.39	0.58
1:F:134:ASP:OD2	1:F:328:HIS:HD2	1.87	0.58
1:F:195:THR:HG21	1:F:240:ALA:HB2	1.86	0.58
1:G:134:ASP:OD2	1:G:328:HIS:HD2	1.87	0.58
1:M:173:TRP:HE1	1:M:463:HIS:HD2	1.52	0.58
1:M:182:SER:O	1:M:186:VAL:HG23	2.03	0.58
1:B:490:ILE:O	1:B:494:VAL:HG23	2.03	0.58
1:I:274:MET:HE2	1:I:279:SER:HA	1.84	0.58
1:K:323:ALA:HB1	1:K:352:HIS:CE1	2.39	0.58
1:A:321:GLN:HE22	1:B:384:CYS:H	1.52	0.57
2:E:1503:HEM:HMB1	2:E:1503:HEM:HBB2	1.86	0.57
1:G:137:TYR:CD1	1:G:206:SER:HA	2.39	0.57
1:M:314:ASN:HB2	1:N:390:GLY:HA2	1.86	0.57
1:O:65:HIS:HA	1:O:105:THR:O	2.03	0.57
1:O:389:LEU:O	1:O:392:THR:OG1	2.22	0.57
1:P:368:PRO:O	1:P:371:SER:O	2.21	0.57
1:C:195:THR:HG22	1:C:235:LEU:HB2	1.86	0.57
1:J:256:TRP:CE2	1:K:164:THR:HG22	2.38	0.57
1:L:443:TRP:CE2	1:L:453:GLN:NE2	2.73	0.57
1:D:220:VAL:HG22	1:D:274:MET:O	2.03	0.57
1:J:22:GLN:NE2	1:J:43:GLN:HE21	2.03	0.57
1:M:195:THR:CG2	1:M:240:ALA:HB2	2.32	0.57
1:A:456:LEU:C	1:A:456:LEU:HD23	2.30	0.57
1:F:368:PRO:O	1:F:371:SER:O	2.21	0.57
1:A:22:GLN:HE21	1:A:43:GLN:HE21	1.52	0.57
1:C:388:ASN:HD22	1:D:314:ASN:ND2	2.02	0.57
1:N:262:GLY:HA2	1:N:264:TYR:CE1	2.39	0.57
1:I:274:MET:CE	1:I:279:SER:CA	2.77	0.57
1:D:274:MET:HE2	1:D:279:SER:CA	2.34	0.57
1:D:456:LEU:HD23	1:D:456:LEU:C	2.30	0.57
1:K:468:ASP:O	1:K:471:ILE:HG22	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1503:HEM:HMB2	2:B:1503:HEM:HBB2	1.87	0.57
1:J:275:THR:OG1	1:J:278:GLN:HG3	2.05	0.57
1:L:61:GLU:OE1	1:L:110:LYS:HB2	2.05	0.57
1:F:274:MET:HE3	1:F:279:SER:CA	2.28	0.56
1:D:274:MET:HE2	1:D:279:SER:CB	2.34	0.56
1:G:292:VAL:N	1:G:438:GLN:HE22	1.96	0.56
1:J:389:LEU:HB3	1:J:392:THR:OG1	2.05	0.56
1:N:195:THR:HG22	1:N:195:THR:O	2.05	0.56
1:B:239:GLU:OE1	1:B:242:ARG:NH1	2.32	0.56
1:B:389:LEU:O	1:B:390:GLY:C	2.49	0.56
1:E:173:TRP:HE1	1:E:463:HIS:HD2	1.53	0.56
1:O:230:GLN:HE22	1:O:266:SER:H	1.52	0.56
1:D:446:LEU:C	1:D:448:ARG:H	2.11	0.56
1:I:321:GLN:HE22	1:J:384:CYS:H	1.52	0.56
1:A:137:TYR:CD1	1:A:206:SER:HA	2.40	0.56
1:C:151:PHE:HB3	1:C:152:PRO:HD3	1.88	0.56
1:P:274:MET:HE1	1:P:282:LEU:HD22	1.88	0.56
1:D:274:MET:HE2	1:D:279:SER:HB3	1.88	0.56
1:D:157:THR:HG21	1:D:175:TYR:HB2	1.88	0.55
1:L:174:ASP:OD1	1:L:474:ARG:NH2	2.39	0.55
1:O:282:LEU:HD23	1:O:284:PHE:CZ	2.41	0.55
1:A:292:VAL:H	1:A:438:GLN:NE2	2.02	0.55
1:E:468:ASP:O	1:E:471:ILE:HG22	2.05	0.55
1:A:98:ARG:NH2	1:A:310:GLU:OE1	2.40	0.55
1:H:456:LEU:C	1:H:456:LEU:HD23	2.31	0.55
1:K:137:TYR:CD1	1:K:206:SER:HA	2.41	0.55
1:L:200:ARG:HD3	1:L:254:ASP:OD2	2.05	0.55
1:M:195:THR:HG22	1:M:195:THR:O	2.05	0.55
1:A:404:GLN:NE2	1:F:96:LYS:H	2.04	0.55
1:B:256:TRP:CE2	1:C:164:THR:HG22	2.41	0.55
1:E:456:LEU:C	1:E:456:LEU:HD23	2.32	0.55
1:G:275:THR:OG1	1:G:278:GLN:HG3	2.05	0.55
1:M:16:SER:O	1:N:405:TYR:HB3	2.06	0.55
2:B:1503:HEM:HBC2	2:B:1503:HEM:HMC2	1.88	0.55
1:F:134:ASP:OD2	1:F:328:HIS:CD2	2.60	0.55
1:J:182:SER:O	1:J:186:VAL:HG23	2.07	0.55
1:J:274:MET:HE2	1:J:279:SER:CB	2.36	0.55
1:J:344:ARG:HG2	1:J:348:TYR:HE1	1.72	0.55
1:O:389:LEU:O	1:O:390:GLY:C	2.50	0.55
1:I:137:TYR:CD1	1:I:206:SER:HA	2.42	0.55
1:H:292:VAL:N	1:H:438:GLN:HE22	1.93	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:274:MET:HE1	1:L:282:LEU:HD22	1.89	0.55
1:A:274:MET:HE1	1:A:282:LEU:HD22	1.88	0.55
1:L:65:HIS:HA	1:L:105:THR:O	2.07	0.55
1:O:22:GLN:HE22	1:O:43:GLN:HE21	1.52	0.55
1:A:200:ARG:HG2	1:A:265:PRO:HB3	1.89	0.54
1:D:389:LEU:O	1:D:390:GLY:C	2.47	0.54
1:F:65:HIS:HA	1:F:105:THR:O	2.07	0.54
1:G:195:THR:HG22	1:G:235:LEU:HB2	1.87	0.54
1:M:134:ASP:OD2	1:M:328:HIS:HD2	1.89	0.54
1:A:390:GLY:HA2	1:B:314:ASN:HB2	1.88	0.54
1:C:134:ASP:OD2	1:C:328:HIS:HD2	1.90	0.54
1:F:275:THR:OG1	1:F:278:GLN:HG3	2.06	0.54
1:G:22:GLN:HE22	1:G:43:GLN:HE21	1.53	0.54
1:N:473:ASP:HA	1:N:476:TYR:CD2	2.41	0.54
1:P:195:THR:HG22	1:P:195:THR:O	2.05	0.54
1:A:173:TRP:HE1	1:A:463:HIS:HD2	1.55	0.54
1:A:451:GLY:HA2	1:A:454:GLU:HG2	1.89	0.54
1:D:427:TYR:CE2	1:D:429:TRP:HA	2.42	0.54
1:F:200:ARG:HD3	1:F:254:ASP:OD1	2.08	0.54
1:F:440:LYS:NZ	1:F:483:GLU:OE2	2.41	0.54
1:J:264:TYR:HE2	1:M:400:ASN:HA	1.71	0.54
1:K:490:ILE:O	1:K:494:VAL:HG23	2.06	0.54
1:E:134:ASP:OD2	1:E:328:HIS:CD2	2.60	0.54
1:I:198:SER:HB2	1:I:254:ASP:OD2	2.07	0.54
1:M:138:ASN:ND2	2:M:1503:HEM:HAC	2.22	0.54
1:M:390:GLY:HA2	1:N:314:ASN:HB2	1.90	0.54
1:N:274:MET:HE2	1:N:279:SER:HA	1.89	0.54
1:F:415:LYS:HB3	1:F:416:PRO:CD	2.38	0.54
1:J:342:GLN:HB2	1:K:40:LEU:HD22	1.89	0.54
1:L:389:LEU:O	1:L:392:THR:OG1	2.25	0.54
1:I:404:GLN:NE2	1:N:96:LYS:H	2.05	0.54
1:L:292:VAL:N	1:L:438:GLN:HE22	1.90	0.54
1:G:389:LEU:HB3	1:G:392:THR:OG1	2.07	0.54
1:H:22:GLN:HE22	1:H:43:GLN:HE21	1.54	0.54
1:J:173:TRP:HE1	1:J:463:HIS:HD2	1.56	0.54
2:N:1503:HEM:HBB2	2:N:1503:HEM:HMB2	1.90	0.54
1:I:274:MET:HE2	1:I:279:SER:CA	2.38	0.54
1:O:138:ASN:ND2	2:O:1503:HEM:HAC	2.23	0.54
1:A:67:LYS:HE2	1:A:114:ASP:OD1	2.08	0.54
2:C:1503:HEM:HBB2	2:C:1503:HEM:CMB	2.36	0.54
1:I:173:TRP:HE1	1:I:463:HIS:HD2	1.53	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:420:TYR:O	1:P:421:THR:HA	2.08	0.54
1:B:161:ASN:HB3	1:B:164:THR:OG1	2.08	0.54
1:I:368:PRO:O	1:I:371:SER:O	2.25	0.54
1:L:195:THR:CG2	1:L:240:ALA:HB2	2.38	0.54
1:F:274:MET:CE	1:F:279:SER:CA	2.81	0.53
1:G:173:TRP:HE1	1:G:463:HIS:HD2	1.56	0.53
1:P:274:MET:HE3	1:P:279:SER:CA	2.31	0.53
1:A:292:VAL:HG22	1:A:438:GLN:NE2	2.23	0.53
1:G:22:GLN:HE21	1:G:43:GLN:HE21	1.53	0.53
1:G:88:LYS:O	1:G:91:ASP:HB2	2.07	0.53
1:A:368:PRO:O	1:A:371:SER:O	2.25	0.53
1:B:140:THR:OG1	1:B:141:PRO:HD2	2.08	0.53
1:O:173:TRP:HE1	1:O:463:HIS:HD2	1.55	0.53
1:E:388:ASN:HD22	1:F:314:ASN:HD21	1.56	0.53
1:O:230:GLN:NE2	1:O:266:SER:H	2.06	0.53
1:B:195:THR:HG22	1:B:195:THR:O	2.08	0.53
1:D:134:ASP:OD2	1:D:328:HIS:HD2	1.92	0.53
1:G:388:ASN:HD22	1:H:314:ASN:ND2	2.05	0.53
1:G:415:LYS:HB3	1:G:416:PRO:HD3	1.90	0.53
1:P:275:THR:OG1	1:P:278:GLN:HG3	2.08	0.53
1:E:415:LYS:HB3	1:E:416:PRO:HD2	1.90	0.53
1:I:384:CYS:H	1:J:321:GLN:HE22	1.55	0.53
1:M:321:GLN:HE22	1:N:384:CYS:H	1.57	0.53
1:N:238:GLU:CD	1:N:238:GLU:H	2.17	0.53
1:P:22:GLN:HE21	1:P:43:GLN:HE21	1.55	0.53
1:I:134:ASP:OD2	1:I:328:HIS:HD2	1.92	0.53
1:B:420:TYR:O	1:D:421:THR:HA	2.09	0.53
3:C:2002:HOH:O	1:D:43:GLN:HG2	2.09	0.53
1:G:490:ILE:O	1:G:494:VAL:HG23	2.08	0.53
1:I:427:TYR:OH	1:I:430:GLU:HG2	2.09	0.53
1:H:91:ASP:HB3	1:H:92:THR:HG23	1.91	0.53
1:H:157:THR:HG21	1:H:175:TYR:HB2	1.91	0.53
1:L:137:TYR:CD1	1:L:206:SER:HA	2.44	0.53
1:E:230:GLN:HE22	1:E:266:SER:H	1.55	0.53
1:E:274:MET:CE	1:E:279:SER:CA	2.84	0.53
1:I:342:GLN:HB2	1:L:40:LEU:HD22	1.90	0.53
1:I:456:LEU:HD23	1:I:456:LEU:C	2.34	0.53
1:O:235:LEU:HD22	1:O:239:GLU:HG2	1.91	0.53
1:C:67:LYS:CE	1:C:114:ASP:OD1	2.58	0.52
1:F:427:TYR:CE2	1:F:429:TRP:HA	2.45	0.52
1:G:427:TYR:CE2	1:G:429:TRP:HA	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:292:VAL:HG22	1:I:438:GLN:HE21	1.70	0.52
1:J:137:TYR:CD1	1:J:206:SER:HA	2.43	0.52
1:K:173:TRP:HE1	1:K:463:HIS:HD2	1.57	0.52
1:P:65:HIS:HA	1:P:105:THR:O	2.09	0.52
1:F:415:LYS:HB3	1:F:416:PRO:HD2	1.92	0.52
1:G:102:ARG:HD3	2:G:1503:HEM:O1D	2.09	0.52
1:I:274:MET:HE1	1:I:282:LEU:HD22	1.92	0.52
1:J:157:THR:HG21	1:J:175:TYR:HB2	1.90	0.52
1:M:274:MET:HE3	1:M:279:SER:CA	2.34	0.52
1:G:22:GLN:HB3	1:G:41:LEU:HD12	1.90	0.52
1:N:219:TRP:HE1	1:N:417:ASP:HA	1.74	0.52
1:F:80:ASP:OD1	1:F:80:ASP:C	2.52	0.52
1:F:134:ASP:HB2	1:F:325:SER:O	2.09	0.52
1:I:358:PRO:HG2	1:I:382:PRO:HG2	1.92	0.52
1:P:157:THR:HG21	1:P:175:TYR:HB2	1.92	0.52
1:C:182:SER:O	1:C:186:VAL:HG23	2.10	0.52
1:E:274:MET:HE3	1:E:279:SER:CA	2.35	0.52
1:H:282:LEU:HD23	1:H:284:PHE:CZ	2.45	0.52
1:B:200:ARG:HG2	1:B:265:PRO:HB3	1.92	0.52
1:C:209:THR:O	1:C:336:SER:OG	2.27	0.52
1:F:195:THR:HG22	1:F:195:THR:O	2.09	0.52
1:H:389:LEU:O	1:H:390:GLY:C	2.50	0.52
1:L:274:MET:HE2	1:L:279:SER:CB	2.40	0.52
1:O:314:ASN:HB2	1:P:390:GLY:HA2	1.92	0.52
1:O:321:GLN:HE22	1:P:384:CYS:H	1.58	0.52
1:I:195:THR:HG22	1:I:195:THR:O	2.09	0.52
2:N:1503:HEM:HBB2	2:N:1503:HEM:CMB	2.41	0.52
1:L:443:TRP:CH2	1:L:453:GLN:HB3	2.45	0.51
1:A:358:PRO:HG2	1:A:382:PRO:HG2	1.91	0.51
1:B:230:GLN:HE22	1:B:266:SER:H	1.57	0.51
1:F:274:MET:HE2	1:F:279:SER:CB	2.40	0.51
1:A:101:THR:HA	1:A:123:ALA:O	2.10	0.51
1:F:137:TYR:CD1	1:F:206:SER:HA	2.45	0.51
1:J:389:LEU:O	1:J:390:GLY:C	2.52	0.51
1:N:389:LEU:O	1:N:390:GLY:C	2.53	0.51
1:B:134:ASP:OD2	1:B:328:HIS:HD2	1.93	0.51
1:D:262:GLY:HA2	1:D:264:TYR:CE1	2.46	0.51
1:F:148:PRO:HD3	1:F:339:PRO:HB2	1.92	0.51
1:H:174:ASP:OD1	1:H:474:ARG:NH2	2.44	0.51
1:K:91:ASP:HB3	1:K:92:THR:HG23	1.93	0.51
1:P:173:TRP:HE1	1:P:463:HIS:HD2	1.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:HIS:HA	1:C:105:THR:O	2.09	0.51
1:C:314:ASN:ND2	1:C:317:ALA:H	2.07	0.51
1:E:195:THR:HG21	1:E:240:ALA:CB	2.33	0.51
1:H:102:ARG:HD3	2:H:1503:HEM:O1D	2.10	0.51
1:A:195:THR:CG2	1:A:240:ALA:HB2	2.38	0.51
1:E:388:ASN:HD22	1:F:314:ASN:ND2	2.09	0.51
1:J:198:SER:OG	1:J:200:ARG:HB2	2.11	0.51
1:L:67:LYS:HE2	1:L:114:ASP:OD1	2.11	0.51
1:N:138:ASN:CG	2:N:1503:HEM:HAC	2.36	0.51
1:B:65:HIS:CE1	1:B:106:VAL:HG22	2.46	0.51
1:L:316:TYR:O	1:L:320:GLU:HB3	2.11	0.51
1:L:344:ARG:NH1	2:L:1503:HEM:HBC2	2.26	0.51
2:O:1503:HEM:CMB	2:O:1503:HEM:HBB2	2.40	0.51
1:B:76:GLU:HG3	1:B:96:LYS:HG2	1.93	0.51
1:D:134:ASP:OD2	1:D:328:HIS:CD2	2.64	0.51
1:E:101:THR:HA	1:E:123:ALA:O	2.10	0.51
1:K:292:VAL:N	1:K:438:GLN:HE22	1.98	0.51
1:L:222:VAL:HG12	1:L:273:THR:HG22	1.92	0.51
1:M:292:VAL:HG22	1:M:438:GLN:NE2	2.24	0.51
1:N:182:SER:O	1:N:186:VAL:HG23	2.11	0.51
1:N:467:ALA:HB1	1:N:471:ILE:HG23	1.93	0.51
2:B:1503:HEM:HBB2	2:B:1503:HEM:CMB	2.41	0.50
1:H:183:LEU:HD21	1:H:482:ALA:HB2	1.93	0.50
1:J:268:GLU:OE1	1:J:302:HIS:HE1	1.94	0.50
1:L:182:SER:O	1:L:186:VAL:HG23	2.11	0.50
1:N:195:THR:CG2	1:N:240:ALA:HB2	2.41	0.50
1:M:468:ASP:O	1:M:471:ILE:HG22	2.11	0.50
1:N:399:TYR:CE1	1:N:400:ASN:HB3	2.46	0.50
1:B:427:TYR:CZ	1:C:36:PRO:HD2	2.47	0.50
1:F:138:ASN:ND2	2:F:1503:HEM:HAC	2.26	0.50
1:J:372:GLY:N	3:J:2006:HOH:O	2.44	0.50
1:L:177:THR:HA	1:L:478:TYR:CD1	2.46	0.50
1:O:195:THR:HG22	1:O:235:LEU:HB2	1.92	0.50
1:O:274:MET:HE2	1:O:279:SER:CB	2.42	0.50
1:P:22:GLN:HE22	1:P:43:GLN:HE21	1.58	0.50
1:F:282:LEU:HD23	1:F:284:PHE:CZ	2.46	0.50
1:G:65:HIS:HA	1:G:105:THR:O	2.11	0.50
1:K:274:MET:CE	1:K:279:SER:CA	2.87	0.50
1:M:98:ARG:NH2	1:M:310:GLU:OE1	2.44	0.50
1:O:134:ASP:OD2	1:O:328:HIS:HD2	1.94	0.50
1:B:75:PHE:O	1:B:96:LYS:HA	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ASP:OD1	1:C:474:ARG:NH2	2.45	0.50
1:G:389:LEU:O	1:G:390:GLY:C	2.53	0.50
1:J:292:VAL:N	1:J:438:GLN:HE22	2.03	0.50
1:K:456:LEU:C	1:K:456:LEU:HD23	2.36	0.50
1:C:91:ASP:HB3	1:C:92:THR:HG23	1.93	0.50
1:D:323:ALA:HB1	1:D:352:HIS:CE1	2.47	0.50
1:E:40:LEU:HD22	1:H:342:GLN:CB	2.41	0.50
1:J:225:HIS:HE1	1:J:272:GLN:OE1	1.95	0.50
1:P:492:LYS:O	1:P:496:GLU:HG3	2.12	0.50
1:B:208:HIS:ND1	1:B:289:LEU:HD13	2.26	0.50
1:C:42:LEU:HD22	1:D:346:PHE:HB2	1.94	0.50
1:L:476:TYR:CE1	1:L:491:ARG:HA	2.46	0.50
1:O:103:PHE:HB3	1:O:199:TYR:CD1	2.47	0.50
1:G:98:ARG:NH2	1:G:310:GLU:OE1	2.45	0.50
1:J:242:ARG:NE	3:J:2003:HOH:O	2.27	0.50
1:N:292:VAL:N	1:N:438:GLN:HE22	2.02	0.50
1:P:200:ARG:HG2	1:P:265:PRO:HB3	1.94	0.50
1:P:268:GLU:OE1	1:P:302:HIS:HE1	1.94	0.50
1:B:195:THR:CG2	1:B:240:ALA:HB2	2.37	0.49
1:I:282:LEU:HD23	1:I:284:PHE:CZ	2.47	0.49
1:E:67:LYS:NZ	1:E:249:ASP:OD1	2.43	0.49
1:J:63:VAL:HG23	1:J:64:VAL:HG22	1.95	0.49
1:C:314:ASN:HB2	1:D:390:GLY:HA2	1.92	0.49
1:D:282:LEU:HD23	1:D:284:PHE:CZ	2.48	0.49
1:K:138:ASN:HD22	2:K:1503:HEM:HAC	1.74	0.49
1:M:91:ASP:HB3	1:M:92:THR:HG23	1.94	0.49
1:G:456:LEU:C	1:G:456:LEU:HD23	2.37	0.49
1:I:65:HIS:CE1	1:I:106:VAL:HG22	2.47	0.49
1:I:98:ARG:NH2	1:I:310:GLU:OE1	2.45	0.49
1:I:174:ASP:OD1	1:I:474:ARG:NH2	2.45	0.49
1:J:65:HIS:HA	1:J:105:THR:O	2.11	0.49
1:E:65:HIS:CE1	1:E:106:VAL:HG22	2.47	0.49
1:G:388:ASN:HD22	1:H:314:ASN:HD21	1.59	0.49
1:M:214:ASN:ND2	1:M:218:GLU:HB2	2.25	0.49
1:A:195:THR:HG22	1:A:195:THR:O	2.12	0.49
1:G:368:PRO:O	1:G:371:SER:O	2.30	0.49
1:O:98:ARG:NH2	1:O:310:GLU:OE1	2.45	0.49
1:A:404:GLN:HE21	1:F:96:LYS:H	1.60	0.49
1:C:427:TYR:CE2	1:C:429:TRP:HA	2.47	0.49
1:E:161:ASN:ND2	1:E:163:ALA:H	2.11	0.49
1:G:314:ASN:ND2	1:H:388:ASN:HD22	2.09	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:451:GLY:HA2	1:G:454:GLU:HG2	1.93	0.49
1:M:22:GLN:HE22	1:M:43:GLN:HE21	1.60	0.49
1:M:376:PRO:HD2	1:N:7:PHE:HE1	1.74	0.49
1:A:134:ASP:OD2	1:A:328:HIS:HD2	1.95	0.49
1:F:61:GLU:OE1	1:F:110:LYS:HB2	2.11	0.49
1:J:209:THR:O	1:J:336:SER:OG	2.13	0.49
1:K:268:GLU:OE1	1:K:302:HIS:HE1	1.95	0.49
1:K:388:ASN:HD22	1:L:314:ASN:ND2	2.10	0.49
1:B:200:ARG:HD3	1:B:254:ASP:OD2	2.12	0.49
1:D:446:LEU:C	1:D:448:ARG:N	2.71	0.49
1:E:77:VAL:HG21	1:E:90:LEU:HA	1.94	0.49
1:J:468:ASP:O	1:J:471:ILE:HG22	2.13	0.49
1:A:389:LEU:HB3	1:A:392:THR:OG1	2.12	0.49
1:E:16:SER:O	1:F:405:TYR:HB3	2.13	0.49
1:E:40:LEU:HD22	1:H:342:GLN:HB2	1.93	0.49
1:G:274:MET:HE2	1:G:279:SER:CB	2.42	0.49
1:H:137:TYR:CD1	1:H:206:SER:HA	2.48	0.49
1:J:125:LYS:HD2	1:J:322:ILE:HD11	1.94	0.49
1:K:480:SER:OG	1:K:487:GLY:HA3	2.13	0.49
1:N:144:PHE:CD2	1:N:154:PHE:CZ	3.00	0.49
1:O:137:TYR:CD1	1:O:206:SER:HA	2.48	0.49
1:A:65:HIS:CE1	1:A:106:VAL:HG22	2.48	0.48
1:H:142:ILE:HG13	1:H:185:GLN:NE2	2.28	0.48
1:I:440:LYS:NZ	1:I:483:GLU:OE2	2.45	0.48
1:E:91:ASP:HB3	1:E:92:THR:HG23	1.95	0.48
1:E:427:TYR:CE2	1:E:429:TRP:HA	2.48	0.48
1:M:195:THR:CG2	1:M:235:LEU:HB2	2.42	0.48
1:C:81:ILE:HD11	1:C:90:LEU:HD13	1.95	0.48
1:M:168:ASP:OD2	1:M:171:MET:HG3	2.14	0.48
1:B:79:ASP:OD2	1:B:302:HIS:HD2	1.96	0.48
1:D:174:ASP:OD1	1:D:474:ARG:NH2	2.47	0.48
1:E:323:ALA:HB1	1:E:352:HIS:CD2	2.48	0.48
1:J:133:LEU:HD13	1:J:330:VAL:HG22	1.96	0.48
1:J:274:MET:CE	1:J:279:SER:CA	2.84	0.48
1:N:22:GLN:HE22	1:N:43:GLN:HE21	1.59	0.48
1:N:454:GLU:H	1:N:454:GLU:CD	2.22	0.48
1:B:72:TYR:HB2	1:B:310:GLU:HB3	1.96	0.48
1:D:148:PRO:HD3	1:D:339:PRO:HB2	1.95	0.48
1:E:274:MET:HE2	1:E:279:SER:CB	2.43	0.48
1:E:420:TYR:O	1:G:421:THR:HA	2.14	0.48
1:G:65:HIS:CE1	1:G:106:VAL:HG22	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:323:ALA:HB1	1:G:352:HIS:CE1	2.48	0.48
1:P:125:LYS:HG3	1:P:134:ASP:OD1	2.13	0.48
1:A:443:TRP:CD2	1:A:486:ILE:HD11	2.48	0.48
1:C:274:MET:HE2	1:C:279:SER:HB3	1.94	0.48
1:E:130:ASP:O	1:F:13:CYS:HA	2.13	0.48
1:I:125:LYS:HD2	1:I:322:ILE:HD11	1.94	0.48
1:M:65:HIS:CE1	1:M:106:VAL:HG22	2.49	0.48
1:A:101:THR:OG1	1:A:124:THR:HG23	2.14	0.48
1:D:65:HIS:HA	1:D:105:THR:O	2.13	0.48
1:E:358:PRO:HG3	1:F:56:ARG:HD3	1.95	0.48
1:F:63:VAL:HG23	1:F:64:VAL:HG22	1.96	0.48
1:F:270:TYR:HB3	1:F:300:LEU:HB3	1.95	0.48
1:H:67:LYS:HE2	1:H:114:ASP:OD1	2.13	0.48
1:P:79:ASP:OD2	1:P:302:HIS:HD2	1.96	0.48
1:P:214:ASN:HD21	1:P:218:GLU:HB2	1.78	0.48
1:K:79:ASP:HB2	1:K:303:PHE:HA	1.96	0.48
1:K:275:THR:OG1	1:K:278:GLN:HG3	2.13	0.48
1:O:344:ARG:NH1	2:O:1503:HEM:HBC2	2.29	0.48
1:I:274:MET:HE3	1:I:279:SER:CA	2.40	0.48
1:C:7:PHE:HD2	1:C:15:VAL:HB	1.78	0.48
1:K:274:MET:HE2	1:K:279:SER:CB	2.44	0.48
1:K:388:ASN:HD22	1:L:314:ASN:HD21	1.61	0.48
1:M:67:LYS:HE2	1:M:114:ASP:OD1	2.14	0.48
1:O:161:ASN:ND2	1:O:163:ALA:H	2.12	0.48
1:B:309:ASN:ND2	1:E:402:PRO:HG3	2.30	0.47
1:E:314:ASN:ND2	1:F:388:ASN:HD22	2.11	0.47
1:J:153:HIS:CE1	1:L:377:ILE:HD12	2.49	0.47
1:A:65:HIS:HA	1:A:105:THR:O	2.13	0.47
1:D:137:TYR:CD1	1:D:206:SER:HA	2.48	0.47
1:J:242:ARG:NH2	3:J:2003:HOH:O	2.39	0.47
1:P:239:GLU:OE1	1:P:242:ARG:NH1	2.46	0.47
1:P:389:LEU:HB3	1:P:392:THR:OG1	2.14	0.47
1:B:67:LYS:HE2	1:B:114:ASP:OD1	2.14	0.47
1:C:67:LYS:HE2	1:C:114:ASP:OD1	2.14	0.47
1:F:91:ASP:HB2	1:F:95:LYS:HZ3	1.79	0.47
1:G:134:ASP:OD2	1:G:328:HIS:CD2	2.67	0.47
1:M:157:THR:HG21	1:M:175:TYR:HB2	1.97	0.47
1:N:377:ILE:CD1	1:P:153:HIS:CE1	2.98	0.47
1:O:91:ASP:HB3	1:O:92:THR:HG23	1.97	0.47
1:A:427:TYR:OH	1:A:430:GLU:HG2	2.14	0.47
1:D:389:LEU:HB3	1:D:392:THR:OG1	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:THR:CG2	1:G:240:ALA:HB2	2.43	0.47
1:J:235:LEU:HD22	1:J:239:GLU:HG2	1.95	0.47
1:K:180:ASP:OD1	1:K:481:LYS:NZ	2.34	0.47
1:N:271:ILE:HD12	1:N:273:THR:CG2	2.44	0.47
1:N:437:PHE:O	1:N:440:LYS:HB3	2.14	0.47
1:B:134:ASP:OD2	1:B:328:HIS:CD2	2.68	0.47
1:C:274:MET:CE	1:C:279:SER:CA	2.89	0.47
1:D:393:PRO:HG2	1:D:401:CYS:HB2	1.96	0.47
1:E:427:TYR:OH	1:E:430:GLU:HG2	2.14	0.47
1:H:24:ILE:O	1:H:38:GLY:HA3	2.15	0.47
1:J:315:TYR:CE1	1:J:319:THR:HG21	2.49	0.47
1:K:197:ALA:HA	1:K:235:LEU:HG	1.97	0.47
1:M:164:THR:HG22	1:P:256:TRP:CE2	2.48	0.47
1:N:456:LEU:HD23	1:N:456:LEU:C	2.39	0.47
1:O:274:MET:CE	1:O:279:SER:CA	2.89	0.47
1:A:161:ASN:HB3	1:A:164:THR:OG1	2.13	0.47
1:A:175:TYR:C	1:A:175:TYR:CD2	2.93	0.47
1:A:384:CYS:H	1:B:321:GLN:HE22	1.62	0.47
1:F:182:SER:O	1:F:186:VAL:HG23	2.14	0.47
1:G:46:LYS:O	1:G:50:THR:HG23	2.15	0.47
1:K:451:GLY:HA2	1:K:454:GLU:HG2	1.97	0.47
1:N:72:TYR:HB2	1:N:310:GLU:HB3	1.95	0.47
1:N:235:LEU:HD22	1:N:239:GLU:CG	2.44	0.47
1:A:67:LYS:NZ	1:A:249:ASP:OD1	2.46	0.47
1:A:133:LEU:HD13	1:A:330:VAL:HG22	1.95	0.47
1:C:22:GLN:HE21	1:C:43:GLN:HE21	1.57	0.47
1:C:134:ASP:OD2	1:C:328:HIS:CD2	2.67	0.47
1:C:446:LEU:C	1:C:448:ARG:N	2.73	0.47
1:D:415:LYS:HB3	1:D:416:PRO:HD2	1.96	0.47
1:H:65:HIS:HA	1:H:105:THR:O	2.14	0.47
2:H:1503:HEM:CMB	2:H:1503:HEM:HBB2	2.45	0.47
1:I:40:LEU:HD22	1:L:342:GLN:CB	2.45	0.47
1:M:61:GLU:OE1	1:M:110:LYS:HB2	2.15	0.47
1:O:138:ASN:CG	2:O:1503:HEM:HAC	2.39	0.47
1:P:74:VAL:HG11	1:P:96:LYS:HD3	1.97	0.47
1:P:214:ASN:OD1	1:P:214:ASN:C	2.57	0.47
1:P:377:ILE:HD13	1:P:377:ILE:N	2.29	0.47
1:P:451:GLY:HA2	1:P:454:GLU:HG2	1.96	0.47
1:E:480:SER:OG	1:E:487:GLY:HA3	2.15	0.47
1:G:274:MET:HE2	1:G:279:SER:HA	1.92	0.47
2:H:1503:HEM:HBB2	2:H:1503:HEM:HMB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:161:ASN:ND2	1:M:163:ALA:H	2.13	0.47
1:N:427:TYR:CE2	1:N:429:TRP:HA	2.49	0.47
1:E:348:TYR:O	1:E:351:THR:HG22	2.15	0.47
1:J:420:TYR:O	1:L:421:THR:HA	2.14	0.47
1:M:389:LEU:O	1:M:390:GLY:C	2.57	0.47
1:N:468:ASP:O	1:N:471:ILE:HG22	2.15	0.47
1:O:390:GLY:HA2	1:P:314:ASN:HB2	1.96	0.47
1:C:274:MET:HE2	1:C:279:SER:HA	1.93	0.47
1:E:18:PRO:HD3	1:F:405:TYR:CE2	2.50	0.47
1:F:168:ASP:HB3	1:F:171:MET:HE2	1.96	0.47
1:J:134:ASP:OD2	1:J:328:HIS:HD2	1.97	0.47
1:G:157:THR:HG21	1:G:175:TYR:HB2	1.96	0.46
1:H:195:THR:HG22	1:H:195:THR:O	2.14	0.46
1:H:214:ASN:ND2	1:H:218:GLU:HB2	2.30	0.46
1:E:51:LEU:HD23	1:E:51:LEU:HA	1.77	0.46
1:H:28:SER:HB2	1:H:34:ALA:CB	2.44	0.46
1:I:168:ASP:HB3	1:I:171:MET:HE2	1.97	0.46
1:M:79:ASP:OD2	1:M:302:HIS:HD2	1.98	0.46
1:N:269:CYS:HB3	1:N:303:PHE:CZ	2.50	0.46
1:O:456:LEU:C	1:O:456:LEU:HD23	2.40	0.46
1:P:61:GLU:OE1	1:P:110:LYS:HB2	2.15	0.46
1:B:440:LYS:NZ	1:B:483:GLU:OE2	2.49	0.46
1:C:292:VAL:N	1:C:438:GLN:HE22	1.98	0.46
1:M:137:TYR:CD1	1:M:206:SER:HA	2.50	0.46
1:O:348:TYR:O	1:O:351:THR:HG22	2.15	0.46
1:C:67:LYS:HE3	1:C:114:ASP:OD1	2.15	0.46
1:P:51:LEU:HD23	1:P:51:LEU:HA	1.73	0.46
1:C:98:ARG:NH2	1:C:310:GLU:OE1	2.47	0.46
1:D:65:HIS:CE1	1:D:106:VAL:HG22	2.51	0.46
1:G:467:ALA:HB1	1:G:471:ILE:HG23	1.96	0.46
1:L:88:LYS:O	1:L:91:ASP:HB2	2.15	0.46
1:M:175:TYR:CD1	1:M:175:TYR:C	2.94	0.46
1:F:420:TYR:O	1:H:421:THR:HA	2.15	0.46
1:K:344:ARG:NH1	2:K:1503:HEM:HBC2	2.30	0.46
1:C:271:ILE:HG23	1:C:303:PHE:CE2	2.50	0.46
1:F:344:ARG:NH1	2:F:1503:HEM:HBC2	2.31	0.46
1:I:389:LEU:O	1:I:390:GLY:C	2.58	0.46
1:M:134:ASP:OD2	1:M:328:HIS:CD2	2.68	0.46
1:O:130:ASP:O	1:P:13:CYS:HA	2.15	0.46
1:A:480:SER:OG	1:A:487:GLY:HA3	2.15	0.46
1:E:22:GLN:HB3	1:E:41:LEU:HD12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:292:VAL:HG22	1:L:438:GLN:NE2	2.31	0.46
1:M:101:THR:HA	1:M:123:ALA:O	2.16	0.46
1:P:72:TYR:HB2	1:P:310:GLU:HB3	1.96	0.46
1:P:197:ALA:HA	1:P:235:LEU:HG	1.96	0.46
1:A:125:LYS:NZ	1:A:134:ASP:OD1	2.49	0.46
1:B:80:ASP:OD1	1:B:80:ASP:C	2.59	0.46
1:B:88:LYS:O	1:B:91:ASP:HB2	2.16	0.46
1:B:274:MET:HE2	1:B:279:SER:CB	2.46	0.46
1:E:137:TYR:CD1	1:E:206:SER:HA	2.51	0.46
1:H:344:ARG:HH12	2:H:1503:HEM:HBC2	1.75	0.46
1:N:195:THR:CG2	1:N:235:LEU:HB2	2.41	0.46
1:D:467:ALA:HB1	1:D:471:ILE:HG23	1.97	0.46
1:K:80:ASP:OD1	1:K:80:ASP:C	2.59	0.46
1:B:292:VAL:N	1:B:438:GLN:HE22	2.05	0.45
2:B:1503:HEM:HMC2	2:B:1503:HEM:CB	2.46	0.45
1:C:274:MET:HE2	1:C:279:SER:CA	2.46	0.45
1:F:22:GLN:HE21	1:F:43:GLN:HE21	1.58	0.45
1:F:91:ASP:HB3	1:F:92:THR:HG23	1.97	0.45
1:I:443:TRP:CD1	1:I:483:GLU:HG3	2.51	0.45
1:J:351:THR:HG21	2:J:1503:HEM:HBA1	1.98	0.45
1:K:16:SER:O	1:L:405:TYR:HB3	2.16	0.45
1:L:451:GLY:HA2	1:L:454:GLU:HG2	1.97	0.45
1:O:182:SER:O	1:O:186:VAL:HG23	2.17	0.45
1:O:195:THR:CG2	1:O:240:ALA:HB2	2.40	0.45
1:P:4:PRO:HA	1:P:5:PRO:HD3	1.82	0.45
1:A:76:GLU:HG3	1:A:96:LYS:HG2	1.98	0.45
1:C:148:PRO:HD3	1:C:339:PRO:HB2	1.98	0.45
1:C:200:ARG:HG2	1:C:265:PRO:CB	2.44	0.45
1:J:7:PHE:HD1	1:J:15:VAL:HB	1.80	0.45
1:J:142:ILE:HD13	1:J:184:HIS:CG	2.51	0.45
1:K:208:HIS:CG	1:K:341:LEU:HB2	2.51	0.45
1:L:98:ARG:NH2	1:L:310:GLU:OE1	2.48	0.45
1:L:144:PHE:CD1	1:L:154:PHE:CZ	3.03	0.45
1:O:63:VAL:HG23	1:O:64:VAL:HG22	1.98	0.45
1:C:22:GLN:HB3	1:C:41:LEU:HD12	1.98	0.45
1:F:177:THR:HA	1:F:478:TYR:CD1	2.52	0.45
1:O:200:ARG:HG2	1:O:265:PRO:CB	2.38	0.45
1:P:389:LEU:O	1:P:390:GLY:C	2.58	0.45
1:A:80:ASP:OD1	1:A:80:ASP:C	2.60	0.45
1:B:342:GLN:HB2	1:C:40:LEU:HD22	1.97	0.45
1:C:75:PHE:CD1	1:C:75:PHE:C	2.94	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:VAL:O	1:C:448:ARG:HB2	2.17	0.45
1:D:239:GLU:OE1	1:D:242:ARG:NH1	2.48	0.45
1:E:468:ASP:O	1:E:471:ILE:CG2	2.65	0.45
1:F:67:LYS:HE2	1:F:114:ASP:OD1	2.17	0.45
1:G:405:TYR:HB3	1:H:16:SER:O	2.16	0.45
1:I:338:ASP:OD1	1:I:338:ASP:C	2.60	0.45
1:J:274:MET:HE2	1:J:279:SER:HB3	1.97	0.45
1:L:134:ASP:HB2	1:L:325:SER:O	2.16	0.45
1:M:274:MET:HE2	1:M:279:SER:CB	2.47	0.45
1:N:151:PHE:HB3	1:N:152:PRO:HD3	1.98	0.45
1:N:161:ASN:ND2	1:N:163:ALA:H	2.14	0.45
1:P:177:THR:OG1	1:P:474:ARG:NH1	2.49	0.45
1:E:200:ARG:HD3	1:E:254:ASP:OD2	2.17	0.45
1:E:399:TYR:CE2	1:E:400:ASN:HB3	2.52	0.45
1:F:208:HIS:ND1	1:F:289:LEU:HD13	2.31	0.45
1:H:117:ARG:NH1	1:H:237:ASP:OD1	2.46	0.45
1:I:79:ASP:OD1	1:I:302:HIS:HD2	2.00	0.45
1:E:134:ASP:HB2	1:E:325:SER:O	2.16	0.45
1:E:199:TYR:CE2	1:E:251:SER:HB3	2.51	0.45
1:M:342:GLN:HB2	1:P:40:LEU:HD22	1.98	0.45
1:P:195:THR:CG2	1:P:240:ALA:HB2	2.47	0.45
1:B:415:LYS:HB3	1:B:416:PRO:CD	2.46	0.45
1:C:137:TYR:CD1	1:C:206:SER:HA	2.52	0.45
1:C:490:ILE:O	1:C:494:VAL:HG23	2.16	0.45
1:E:182:SER:O	1:E:186:VAL:HG23	2.17	0.45
1:E:368:PRO:O	1:E:371:SER:O	2.35	0.45
1:J:348:TYR:O	1:J:351:THR:HG22	2.16	0.45
1:K:235:LEU:HD22	1:K:239:GLU:HG2	1.99	0.45
1:O:24:ILE:O	1:O:38:GLY:HA3	2.17	0.45
1:O:72:TYR:HB2	1:O:310:GLU:HB3	1.98	0.45
1:P:88:LYS:O	1:P:91:ASP:HB2	2.16	0.45
1:A:88:LYS:HD3	1:A:129:GLU:OE1	2.16	0.45
1:B:456:LEU:HD23	1:B:456:LEU:C	2.41	0.45
1:C:76:GLU:HG3	1:C:96:LYS:HG2	1.99	0.45
1:F:72:TYR:HB2	1:F:310:GLU:HB3	1.99	0.45
1:G:183:LEU:HD21	1:G:482:ALA:HB2	1.99	0.45
1:P:427:TYR:CE2	1:P:429:TRP:HA	2.52	0.45
1:B:282:LEU:HD23	1:B:284:PHE:CZ	2.52	0.45
1:C:389:LEU:O	1:C:390:GLY:C	2.59	0.45
1:E:268:GLU:OE1	1:E:302:HIS:HE1	2.00	0.45
1:F:76:GLU:HG3	1:F:96:LYS:HG2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:LEU:HD22	1:F:239:GLU:HG2	1.99	0.45
2:K:1503:HEM:HMB2	2:K:1503:HEM:HBB2	1.99	0.45
1:M:214:ASN:OD1	1:M:214:ASN:C	2.60	0.45
1:P:168:ASP:HB3	1:P:171:MET:HE2	1.98	0.45
1:B:376:PRO:O	1:B:379:ARG:HD3	2.16	0.45
1:A:43:GLN:HG2	3:B:2007:HOH:O	2.17	0.44
1:A:134:ASP:HB2	1:A:325:SER:O	2.16	0.44
1:D:42:LEU:HD23	1:D:42:LEU:HA	1.87	0.44
1:G:91:ASP:HB3	1:G:92:THR:HG23	1.99	0.44
1:I:7:PHE:CD1	1:J:376:PRO:HD2	2.52	0.44
1:J:200:ARG:HG2	1:J:265:PRO:HB3	1.99	0.44
1:M:274:MET:CE	1:M:279:SER:CA	2.89	0.44
1:O:268:GLU:HB3	1:O:302:HIS:HE1	1.83	0.44
1:P:85:CYS:HA	1:P:213:TYR:O	2.17	0.44
1:B:67:LYS:NZ	1:B:249:ASP:OD1	2.50	0.44
1:B:358:PRO:HG2	1:B:382:PRO:HG2	1.99	0.44
1:H:80:ASP:OD1	1:H:80:ASP:C	2.61	0.44
1:I:325:SER:HB3	1:I:328:HIS:CD2	2.52	0.44
1:J:72:TYR:HB2	1:J:310:GLU:HB3	1.98	0.44
1:K:195:THR:HG21	1:K:240:ALA:CB	2.38	0.44
1:A:51:LEU:HA	1:A:51:LEU:HD23	1.60	0.44
1:A:134:ASP:OD2	1:A:328:HIS:CD2	2.70	0.44
1:B:467:ALA:HB1	1:B:471:ILE:HG23	1.98	0.44
1:I:420:TYR:HE2	1:K:424:VAL:HG23	1.81	0.44
1:J:230:GLN:HE22	1:J:266:SER:H	1.64	0.44
1:K:389:LEU:O	1:K:390:GLY:C	2.56	0.44
1:L:212:TRP:CZ2	1:L:333:MET:HE2	2.52	0.44
1:L:427:TYR:CE2	1:L:429:TRP:HA	2.53	0.44
1:F:219:TRP:HE1	1:F:417:ASP:HA	1.82	0.44
1:F:256:TRP:CE2	1:G:164:THR:HG22	2.53	0.44
1:J:168:ASP:HB3	1:J:171:MET:HE2	1.98	0.44
1:L:275:THR:OG1	1:L:278:GLN:HG3	2.18	0.44
1:M:56:ARG:HD3	1:N:358:PRO:HG3	1.98	0.44
1:M:72:TYR:HB2	1:M:310:GLU:HB3	1.98	0.44
1:M:344:ARG:NH1	2:M:1503:HEM:HBC2	2.32	0.44
1:N:157:THR:HG21	1:N:175:TYR:HB2	1.99	0.44
1:A:149:ILE:HD12	1:D:47:LEU:HA	2.00	0.44
1:P:456:LEU:HD23	1:P:456:LEU:C	2.42	0.44
1:B:208:HIS:CE1	1:B:289:LEU:HD13	2.53	0.44
1:C:133:LEU:HD13	1:C:330:VAL:HG22	2.00	0.44
1:E:72:TYR:HB2	1:E:310:GLU:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:405:TYR:CE1	1:H:18:PRO:HD3	2.53	0.44
1:I:146:ARG:HD2	1:I:429:TRP:CD2	2.53	0.44
1:K:157:THR:HG21	1:K:175:TYR:HB2	1.99	0.44
1:M:427:TYR:CE2	1:M:429:TRP:HA	2.53	0.44
1:N:101:THR:HA	1:N:123:ALA:O	2.17	0.44
1:P:363:ILE:O	1:P:364:PRO:C	2.60	0.44
1:A:198:SER:HB2	1:A:254:ASP:OD2	2.17	0.44
1:C:325:SER:HB3	1:C:328:HIS:CD2	2.52	0.44
1:G:13:CYS:HA	1:H:130:ASP:O	2.18	0.44
1:I:40:LEU:HD22	1:L:342:GLN:HB2	2.00	0.44
1:I:268:GLU:OE1	1:I:302:HIS:HE1	2.01	0.44
1:K:138:ASN:CG	2:K:1503:HEM:HAC	2.41	0.44
1:P:140:THR:HG23	1:P:142:ILE:O	2.17	0.44
1:C:214:ASN:HD21	1:C:218:GLU:HB2	1.83	0.44
1:I:270:TYR:HB3	1:I:300:LEU:HB3	1.99	0.44
1:I:389:LEU:HB3	1:I:392:THR:OG1	2.18	0.44
1:I:485:ILE:H	1:I:485:ILE:HG13	1.32	0.44
1:M:173:TRP:NE1	1:M:463:HIS:HD2	2.14	0.44
1:D:440:LYS:NZ	1:D:483:GLU:OE2	2.49	0.44
1:D:445:VAL:O	1:D:448:ARG:HB2	2.18	0.44
1:L:200:ARG:O	1:L:230:GLN:HB2	2.17	0.44
1:O:67:LYS:NZ	1:O:249:ASP:OD1	2.48	0.44
1:C:22:GLN:HE22	1:C:43:GLN:HE21	1.61	0.43
1:E:142:ILE:HG13	1:E:185:GLN:NE2	2.33	0.43
1:H:45:PHE:O	1:H:46:LYS:C	2.58	0.43
1:K:195:THR:HG22	1:K:235:LEU:HB2	1.99	0.43
1:K:274:MET:HE1	1:K:282:LEU:HD22	1.99	0.43
1:M:388:ASN:HD22	1:N:314:ASN:ND2	2.16	0.43
1:A:315:TYR:CG	1:D:165:ASN:HB2	2.52	0.43
1:B:125:LYS:HD2	1:B:322:ILE:HD11	2.00	0.43
1:F:153:HIS:CE1	1:H:377:ILE:HD12	2.53	0.43
1:F:342:GLN:CB	1:G:40:LEU:HD22	2.48	0.43
1:J:46:LYS:HB3	1:J:46:LYS:HE2	1.78	0.43
1:J:342:GLN:CB	1:K:40:LEU:HD22	2.48	0.43
1:P:200:ARG:HD3	1:P:254:ASP:OD2	2.18	0.43
1:A:200:ARG:HD3	1:A:254:ASP:OD2	2.19	0.43
1:A:230:GLN:HE22	1:A:266:SER:H	1.66	0.43
1:I:51:LEU:HD23	1:I:51:LEU:HA	1.82	0.43
1:I:195:THR:CG2	1:I:240:ALA:HB2	2.47	0.43
1:J:80:ASP:C	1:J:80:ASP:OD1	2.61	0.43
1:K:467:ALA:HB1	1:K:471:ILE:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:163:ALA:O	1:P:315:TYR:HB2	2.19	0.43
1:O:17:ASP:OD1	1:O:18:PRO:HD2	2.18	0.43
1:D:292:VAL:HG22	1:D:438:GLN:NE2	2.33	0.43
1:E:26:LEU:HD21	1:H:418:GLU:HB3	2.01	0.43
1:E:314:ASN:HD22	1:E:317:ALA:N	2.00	0.43
1:I:161:ASN:HD22	1:I:164:THR:N	2.04	0.43
1:M:348:TYR:O	1:M:351:THR:HG22	2.18	0.43
1:E:65:HIS:HA	1:E:105:THR:O	2.18	0.43
1:G:151:PHE:HB3	1:G:152:PRO:HD3	2.00	0.43
1:G:480:SER:OG	1:G:487:GLY:HA3	2.17	0.43
1:J:61:GLU:OE1	1:J:110:LYS:HB2	2.19	0.43
1:L:46:LYS:HB3	1:L:46:LYS:HE2	1.85	0.43
1:L:443:TRP:CZ2	1:L:453:GLN:CD	2.96	0.43
1:L:480:SER:OG	1:L:487:GLY:HA3	2.18	0.43
1:M:101:THR:OG1	1:M:124:THR:HG23	2.18	0.43
1:M:427:TYR:OH	1:M:430:GLU:HG2	2.18	0.43
1:N:268:GLU:OE1	1:N:302:HIS:HE1	2.00	0.43
1:O:157:THR:HA	1:O:171:MET:SD	2.58	0.43
1:C:102:ARG:HD3	2:C:1503:HEM:O1D	2.18	0.43
1:G:491:ARG:HH11	1:G:491:ARG:HB3	1.82	0.43
1:J:51:LEU:HD23	1:J:51:LEU:HA	1.85	0.43
1:K:389:LEU:HB3	1:K:392:THR:OG1	2.19	0.43
1:M:88:LYS:O	1:M:91:ASP:HB2	2.18	0.43
1:N:103:PHE:HB3	1:N:199:TYR:CD1	2.54	0.43
1:P:139:ASN:HA	1:P:203:ASN:O	2.19	0.43
1:C:142:ILE:HG13	1:C:185:GLN:HE21	1.84	0.43
1:E:161:ASN:HB3	1:E:164:THR:OG1	2.18	0.43
1:G:101:THR:HA	1:G:123:ALA:O	2.18	0.43
1:G:268:GLU:OE1	1:G:302:HIS:HE1	2.02	0.43
1:J:143:PHE:HB3	1:J:289:LEU:CD2	2.49	0.43
1:B:101:THR:HA	1:B:123:ALA:O	2.18	0.43
1:D:468:ASP:O	1:D:471:ILE:HG22	2.19	0.43
1:H:65:HIS:CE1	1:H:106:VAL:HG22	2.54	0.43
1:H:292:VAL:HG22	1:H:438:GLN:NE2	2.33	0.43
1:I:219:TRP:HE1	1:I:417:ASP:HA	1.83	0.43
1:N:98:ARG:NH2	1:N:310:GLU:OE1	2.52	0.43
1:N:315:TYR:HB2	1:O:163:ALA:O	2.18	0.43
1:O:239:GLU:OE1	1:O:242:ARG:NH1	2.49	0.43
1:P:214:ASN:ND2	1:P:218:GLU:HB2	2.34	0.43
1:E:288:ASP:OD1	1:E:290:THR:OG1	2.31	0.43
1:E:344:ARG:NH1	2:E:1503:HEM:HBC2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:348:TYR:O	1:F:351:THR:HG22	2.19	0.43
1:G:138:ASN:ND2	2:G:1503:HEM:CAC	2.82	0.43
1:I:390:GLY:HA2	1:J:314:ASN:HB2	1.99	0.43
1:I:402:PRO:HG3	1:N:309:ASN:ND2	2.34	0.43
1:K:7:PHE:HB2	1:L:403:ILE:CG2	2.49	0.43
1:K:130:ASP:O	1:L:13:CYS:HA	2.19	0.43
1:K:314:ASN:O	1:K:318:GLU:HG3	2.19	0.43
1:M:139:ASN:OD1	1:M:139:ASN:C	2.62	0.43
1:P:485:ILE:H	1:P:485:ILE:HG13	1.45	0.43
1:E:230:GLN:NE2	1:E:266:SER:H	2.17	0.43
1:G:488:ASP:HA	1:G:491:ARG:NH1	2.34	0.43
1:M:358:PRO:HG2	1:M:382:PRO:HG2	2.00	0.43
1:N:161:ASN:HB3	1:N:164:THR:OG1	2.19	0.43
1:A:79:ASP:HB2	1:A:303:PHE:HA	2.01	0.42
1:B:230:GLN:NE2	1:B:266:SER:H	2.17	0.42
1:E:7:PHE:HD2	1:E:15:VAL:HB	1.84	0.42
1:F:389:LEU:HB3	1:F:392:THR:OG1	2.19	0.42
1:H:134:ASP:OD2	1:H:328:HIS:HD2	2.01	0.42
1:K:328:HIS:CE1	1:L:11:GLN:HG3	2.54	0.42
1:C:13:CYS:HA	1:C:14:PRO:HD3	1.88	0.42
1:G:7:PHE:HD2	1:G:15:VAL:HB	1.83	0.42
1:M:323:ALA:HB1	1:M:352:HIS:CD2	2.54	0.42
1:M:384:CYS:H	1:N:321:GLN:HE22	1.65	0.42
1:A:88:LYS:O	1:A:91:ASP:HB2	2.19	0.42
1:E:13:CYS:HA	1:F:130:ASP:O	2.18	0.42
1:I:161:ASN:ND2	1:I:163:ALA:H	2.17	0.42
1:K:174:ASP:OD1	1:K:474:ARG:NH2	2.52	0.42
3:K:2001:HOH:O	1:L:125:LYS:HE3	2.20	0.42
1:L:103:PHE:HA	1:L:121:GLY:O	2.19	0.42
1:M:63:VAL:HG23	1:M:64:VAL:N	2.35	0.42
1:N:377:ILE:HD12	1:P:153:HIS:CE1	2.54	0.42
1:O:344:ARG:HG2	1:O:348:TYR:HE1	1.85	0.42
1:P:230:GLN:HE22	1:P:266:SER:H	1.66	0.42
1:P:274:MET:HE2	1:P:279:SER:CB	2.49	0.42
1:P:473:ASP:HA	1:P:476:TYR:CD2	2.54	0.42
1:B:175:TYR:CD1	1:B:175:TYR:C	2.96	0.42
1:D:22:GLN:HE22	1:D:43:GLN:HE21	1.63	0.42
1:D:195:THR:CG2	1:D:240:ALA:HB2	2.42	0.42
1:D:208:HIS:CD2	1:D:341:LEU:HD13	2.54	0.42
1:F:427:TYR:CZ	1:G:36:PRO:HD2	2.55	0.42
1:M:350:ASP:OD2	1:P:56:ARG:NH1	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:70:GLY:HA2	1:N:101:THR:O	2.19	0.42
1:N:174:ASP:OD1	1:N:474:ARG:NH2	2.52	0.42
1:P:208:HIS:HD1	1:P:338:ASP:CG	2.26	0.42
1:A:63:VAL:HG23	1:A:64:VAL:N	2.34	0.42
1:A:81:ILE:HD11	1:A:90:LEU:HD13	2.02	0.42
1:A:164:THR:HG22	1:D:256:TRP:CE2	2.53	0.42
1:B:485:ILE:H	1:B:485:ILE:HG13	1.64	0.42
1:D:208:HIS:CG	1:D:341:LEU:HB2	2.54	0.42
1:E:175:TYR:CD2	1:E:175:TYR:C	2.98	0.42
1:E:389:LEU:O	1:E:390:GLY:C	2.60	0.42
1:G:153:HIS:O	1:G:154:PHE:C	2.62	0.42
1:I:37:ILE:HG21	1:L:287:PHE:CD2	2.55	0.42
1:J:278:GLN:O	1:J:282:LEU:CD1	2.67	0.42
1:K:72:TYR:HB2	1:K:310:GLU:HB3	2.02	0.42
1:K:405:TYR:HB3	1:L:16:SER:O	2.18	0.42
1:L:235:LEU:HD22	1:L:239:GLU:HG2	2.01	0.42
1:M:257:GLU:O	1:M:258:ALA:C	2.63	0.42
1:O:274:MET:HE2	1:O:279:SER:HB3	2.02	0.42
1:O:292:VAL:N	1:O:438:GLN:HE22	2.06	0.42
2:O:1503:HEM:HBB2	2:O:1503:HEM:HMB2	2.00	0.42
1:A:268:GLU:HB3	1:A:302:HIS:HE1	1.84	0.42
1:C:173:TRP:NE1	1:C:463:HIS:HD2	2.13	0.42
1:I:101:THR:OG1	1:I:124:THR:HG23	2.18	0.42
1:I:420:TYR:CE2	1:K:424:VAL:HG23	2.55	0.42
1:C:63:VAL:HG23	1:C:64:VAL:HG22	2.01	0.42
1:E:403:ILE:HG21	1:F:7:PHE:HB2	2.01	0.42
1:F:56:ARG:HG2	1:G:354:HIS:CG	2.55	0.42
1:G:46:LYS:HE2	1:G:46:LYS:HB3	1.77	0.42
1:N:269:CYS:HB3	1:N:303:PHE:CE1	2.55	0.42
1:N:271:ILE:HD12	1:N:273:THR:HG23	2.00	0.42
1:N:342:GLN:CB	1:O:40:LEU:HD22	2.49	0.42
1:O:314:ASN:HD21	1:P:388:ASN:HD22	1.68	0.42
1:A:133:LEU:HD12	1:A:329:THR:HA	2.02	0.42
1:F:443:TRP:O	1:F:453:GLN:NE2	2.52	0.42
1:G:377:ILE:HD13	1:G:377:ILE:N	2.35	0.42
1:G:477:GLU:O	1:G:481:LYS:HG3	2.20	0.42
1:L:315:TYR:CD1	1:L:315:TYR:C	2.98	0.42
1:M:342:GLN:CB	1:P:40:LEU:HD22	2.50	0.42
1:P:174:ASP:OD1	1:P:474:ARG:NH2	2.53	0.42
1:B:354:HIS:CG	1:C:56:ARG:HG2	2.54	0.42
1:D:100:PHE:CD1	1:D:100:PHE:C	2.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ASN:HB3	1:D:164:THR:OG1	2.20	0.42
1:E:26:LEU:CD2	1:H:418:GLU:HB3	2.49	0.42
1:G:488:ASP:HA	1:G:491:ARG:HH12	1.85	0.42
1:H:368:PRO:O	1:H:371:SER:O	2.37	0.42
1:J:292:VAL:HG22	1:J:438:GLN:NE2	2.34	0.42
1:K:46:LYS:HE2	1:K:46:LYS:HB3	1.89	0.42
2:L:1503:HEM:HBB2	2:L:1503:HEM:CMB	2.42	0.42
1:A:168:ASP:OD2	1:A:171:MET:HG3	2.20	0.42
1:I:354:HIS:CG	1:L:56:ARG:HG2	2.55	0.42
1:J:4:PRO:HA	1:J:5:PRO:HD3	1.92	0.42
1:M:268:GLU:OE1	1:M:302:HIS:HE1	2.03	0.42
1:M:456:LEU:HD23	1:M:456:LEU:C	2.45	0.42
1:N:185:GLN:O	1:N:188:TYR:HB2	2.20	0.42
1:A:389:LEU:O	1:A:390:GLY:C	2.61	0.41
1:E:67:LYS:HE2	1:E:114:ASP:OD1	2.20	0.41
1:F:195:THR:CG2	1:F:240:ALA:HB2	2.50	0.41
1:G:175:TYR:CD2	1:G:175:TYR:C	2.99	0.41
1:I:137:TYR:CE1	1:I:206:SER:HA	2.55	0.41
1:I:480:SER:OG	1:I:487:GLY:HA3	2.19	0.41
1:J:28:SER:HB2	1:J:34:ALA:HB1	2.02	0.41
1:K:65:HIS:CD2	2:K:1503:HEM:C4D	3.08	0.41
1:L:101:THR:OG1	1:L:124:THR:HG23	2.20	0.41
1:L:197:ALA:HA	1:L:235:LEU:HG	2.02	0.41
1:M:230:GLN:N	1:M:230:GLN:CD	2.78	0.41
1:B:137:TYR:CD1	1:B:206:SER:HA	2.54	0.41
1:B:389:LEU:HB3	1:B:392:THR:OG1	2.20	0.41
1:D:102:ARG:HD3	2:D:1503:HEM:O1D	2.20	0.41
1:E:143:PHE:HA	1:E:185:GLN:HG2	2.02	0.41
1:E:403:ILE:HG22	1:E:404:GLN:N	2.35	0.41
1:F:137:TYR:HB3	1:F:205:TYR:O	2.19	0.41
1:H:268:GLU:HB3	1:H:302:HIS:HE1	1.85	0.41
1:J:70:GLY:HA2	1:J:101:THR:O	2.20	0.41
1:J:76:GLU:HG3	1:J:96:LYS:HG2	2.02	0.41
1:K:214:ASN:OD1	1:K:214:ASN:C	2.63	0.41
1:O:214:ASN:C	1:O:214:ASN:OD1	2.63	0.41
1:F:175:TYR:CD1	1:F:175:TYR:C	2.98	0.41
1:I:126:PHE:HB2	1:I:133:LEU:HB3	2.02	0.41
1:I:315:TYR:HB2	1:L:163:ALA:O	2.20	0.41
1:J:138:ASN:ND2	2:J:1503:HEM:CAC	2.83	0.41
1:K:13:CYS:HA	1:K:14:PRO:HD3	1.93	0.41
1:N:63:VAL:HG23	1:N:64:VAL:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:451:GLY:HA2	1:N:454:GLU:HG2	2.03	0.41
1:E:142:ILE:HG13	1:E:185:GLN:HE21	1.86	0.41
1:F:153:HIS:CE1	1:H:377:ILE:CD1	3.04	0.41
1:H:399:TYR:CE1	1:H:400:ASN:HB3	2.55	0.41
1:I:214:ASN:HD21	1:I:218:GLU:HB2	1.85	0.41
1:J:184:HIS:HE1	1:J:438:GLN:HE21	1.68	0.41
1:J:415:LYS:HA	1:J:416:PRO:HD3	1.86	0.41
1:N:274:MET:HE2	1:N:279:SER:CB	2.50	0.41
1:N:344:ARG:HG2	1:N:348:TYR:HE1	1.85	0.41
1:N:455:SER:O	1:N:456:LEU:C	2.64	0.41
1:D:13:CYS:HA	1:D:14:PRO:HD3	1.78	0.41
1:E:103:PHE:HB3	1:E:199:TYR:CD1	2.54	0.41
1:E:195:THR:HG22	1:E:195:THR:O	2.20	0.41
1:H:17:ASP:OD1	1:H:18:PRO:HD2	2.20	0.41
1:N:270:TYR:HB3	1:N:300:LEU:HB3	2.01	0.41
1:D:198:SER:HB2	1:D:254:ASP:OD2	2.21	0.41
1:D:292:VAL:N	1:D:438:GLN:HE22	2.02	0.41
1:E:460:VAL:O	1:E:460:VAL:HG12	2.20	0.41
1:H:201:THR:HB	1:H:233:HIS:H	1.85	0.41
1:H:208:HIS:CG	1:H:341:LEU:HB2	2.56	0.41
1:J:452:GLU:O	1:J:455:SER:HB2	2.19	0.41
1:M:133:LEU:HD12	1:M:329:THR:HA	2.03	0.41
1:A:441:MET:O	1:A:445:VAL:HG23	2.20	0.41
1:E:80:ASP:OD1	1:E:80:ASP:C	2.64	0.41
1:F:47:LEU:HA	1:G:149:ILE:HD12	2.02	0.41
1:F:293:TRP:HA	1:F:294:PRO:HD2	1.95	0.41
1:G:134:ASP:HB2	1:G:325:SER:O	2.21	0.41
1:J:274:MET:HE2	1:J:279:SER:CA	2.50	0.41
1:L:389:LEU:O	1:L:390:GLY:C	2.61	0.41
1:P:161:ASN:ND2	1:P:163:ALA:H	2.18	0.41
1:D:149:ILE:O	1:D:152:PRO:HD2	2.21	0.41
1:D:173:TRP:HE1	1:D:463:HIS:HD2	1.67	0.41
1:E:39:PRO:HB2	1:G:41:LEU:HD22	2.02	0.41
1:F:230:GLN:HE22	1:F:266:SER:H	1.69	0.41
1:F:456:LEU:HD23	1:F:456:LEU:C	2.46	0.41
1:G:72:TYR:HB2	1:G:310:GLU:HB3	2.03	0.41
1:J:198:SER:HB2	1:J:254:ASP:OD2	2.21	0.41
1:J:219:TRP:HE1	1:J:417:ASP:HA	1.86	0.41
1:K:214:ASN:HD21	1:K:218:GLU:HB2	1.85	0.41
1:L:392:THR:HA	1:L:393:PRO:HD3	1.93	0.41
1:M:443:TRP:CD1	1:M:483:GLU:HG3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:319:THR:O	1:N:322:ILE:HG22	2.20	0.41
1:O:314:ASN:ND2	1:P:388:ASN:HD22	2.19	0.41
1:A:79:ASP:OD2	1:A:302:HIS:HD2	2.04	0.41
1:A:265:PRO:HB2	1:A:267:TRP:CZ3	2.56	0.41
1:C:323:ALA:HB1	1:C:352:HIS:CE1	2.56	0.41
1:C:348:TYR:HB2	1:C:349:PRO:HD3	2.03	0.41
1:D:138:ASN:CG	2:D:1503:HEM:HAC	2.45	0.41
1:E:485:ILE:H	1:E:485:ILE:HG13	1.64	0.41
1:F:72:TYR:OH	1:F:318:GLU:OE1	2.32	0.41
1:F:174:ASP:OD1	1:F:474:ARG:NH2	2.53	0.41
1:G:230:GLN:HE22	1:G:266:SER:H	1.69	0.41
1:G:274:MET:HE2	1:G:279:SER:CA	2.51	0.41
1:H:415:LYS:HA	1:H:416:PRO:HD3	1.92	0.41
1:I:342:GLN:CB	1:L:40:LEU:HD22	2.51	0.41
1:K:88:LYS:O	1:K:91:ASP:HB2	2.20	0.41
1:L:437:PHE:O	1:L:440:LYS:HB3	2.21	0.41
1:M:288:ASP:OD1	1:M:290:THR:OG1	2.33	0.41
1:N:183:LEU:HA	1:N:478:TYR:OH	2.20	0.41
1:P:395:TYR:N	1:P:395:TYR:CD1	2.89	0.41
1:C:16:SER:O	1:D:405:TYR:HB3	2.21	0.41
1:E:138:ASN:ND2	2:E:1503:HEM:CAC	2.82	0.41
1:F:46:LYS:HE2	1:F:46:LYS:HB3	1.86	0.41
1:G:137:TYR:HB3	1:G:205:TYR:O	2.21	0.41
1:I:288:ASP:OD1	1:I:290:THR:OG1	2.34	0.41
1:J:138:ASN:CG	2:J:1503:HEM:HAC	2.46	0.41
1:M:420:TYR:CE2	1:P:39:PRO:HD3	2.56	0.41
1:N:382:PRO:O	1:N:383:MET:C	2.64	0.41
1:O:42:LEU:HD22	1:P:346:PHE:HB2	2.02	0.41
1:O:101:THR:HA	1:O:123:ALA:O	2.21	0.41
1:C:79:ASP:HB2	1:C:303:PHE:HA	2.03	0.40
1:C:142:ILE:HG13	1:C:185:GLN:NE2	2.36	0.40
1:E:42:LEU:HD23	1:E:42:LEU:HA	1.87	0.40
1:G:18:PRO:HD3	1:H:405:TYR:CE2	2.56	0.40
1:M:460:VAL:HG11	1:M:479:PHE:CE2	2.56	0.40
1:M:488:ASP:OD1	1:M:491:ARG:NH2	2.55	0.40
1:N:13:CYS:HA	1:N:14:PRO:HD3	1.90	0.40
1:N:274:MET:CE	1:N:279:SER:CA	2.91	0.40
1:O:151:PHE:HB3	1:O:152:PRO:HD3	2.02	0.40
1:P:468:ASP:O	1:P:472:GLN:HG3	2.20	0.40
1:C:344:ARG:HH12	2:C:1503:HEM:HBC2	1.86	0.40
1:E:225:HIS:HE1	1:E:272:GLN:OE1	2.05	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:ARG:NH2	1:F:310:GLU:OE1	2.53	0.40
1:G:13:CYS:HA	1:G:14:PRO:HD3	1.95	0.40
1:J:39:PRO:HB2	1:L:41:LEU:HD22	2.03	0.40
1:K:227:ILE:HD12	1:K:270:TYR:CE1	2.56	0.40
1:K:390:GLY:HA2	1:L:314:ASN:HB2	2.02	0.40
1:N:208:HIS:CG	1:N:341:LEU:HB2	2.57	0.40
1:P:171:MET:O	1:P:172:PHE:C	2.63	0.40
1:A:197:ALA:HA	1:A:235:LEU:HG	2.04	0.40
1:B:182:SER:O	1:B:186:VAL:HG23	2.21	0.40
1:C:227:ILE:HD12	1:C:270:TYR:CE1	2.56	0.40
1:D:161:ASN:HA	1:D:162:PRO:HD3	1.98	0.40
1:D:195:THR:HG22	1:D:195:THR:O	2.21	0.40
1:E:41:LEU:HD22	1:G:39:PRO:HB2	2.03	0.40
1:E:323:ALA:HB1	1:E:352:HIS:NE2	2.37	0.40
1:G:133:LEU:HD13	1:G:330:VAL:HG22	2.02	0.40
1:H:148:PRO:HD3	1:H:339:PRO:HB2	2.03	0.40
1:I:323:ALA:HB1	1:I:352:HIS:CD2	2.56	0.40
1:K:282:LEU:HD23	1:K:284:PHE:CZ	2.56	0.40
1:L:51:LEU:HD23	1:L:51:LEU:HA	1.83	0.40
1:M:389:LEU:HB3	1:M:392:THR:OG1	2.21	0.40
1:N:73:GLY:HA3	1:N:307:THR:O	2.21	0.40
1:P:101:THR:HA	1:P:123:ALA:O	2.21	0.40
1:B:268:GLU:OE1	1:B:302:HIS:HE1	2.05	0.40
1:C:77:VAL:HG21	1:C:90:LEU:HA	2.03	0.40
1:C:144:PHE:CD2	1:C:154:PHE:CZ	3.10	0.40
1:F:142:ILE:HG13	1:F:185:GLN:HE21	1.86	0.40
1:F:164:THR:HG22	1:G:256:TRP:CE2	2.56	0.40
1:I:143:PHE:HB3	1:I:289:LEU:CD2	2.51	0.40
1:I:173:TRP:NE1	1:I:463:HIS:HD2	2.19	0.40
1:L:67:LYS:NZ	1:L:249:ASP:OD1	2.52	0.40
1:M:137:TYR:HB3	1:M:205:TYR:O	2.21	0.40
1:N:282:LEU:HD23	1:N:284:PHE:CZ	2.56	0.40
1:N:446:LEU:C	1:N:448:ARG:H	2.29	0.40
1:P:212:TRP:CE2	1:P:222:VAL:HG21	2.56	0.40
1:A:230:GLN:CD	1:A:230:GLN:N	2.79	0.40
1:A:314:ASN:HD22	1:A:317:ALA:N	1.96	0.40
1:B:13:CYS:HA	1:B:14:PRO:HD3	1.83	0.40
1:E:449:THR:HA	1:E:450:PRO:HD2	1.83	0.40
1:H:173:TRP:HE1	1:H:463:HIS:HD2	1.69	0.40
1:H:239:GLU:OE1	1:H:242:ARG:NH1	2.50	0.40
1:K:183:LEU:HD21	1:K:482:ALA:HB2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:344:ARG:HH12	2:L:1503:HEM:HBC2	1.87	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	487/509 (96%)	464 (95%)	21 (4%)	2 (0%)	30	59
1	B	490/509 (96%)	471 (96%)	19 (4%)	0	100	100
1	C	488/509 (96%)	464 (95%)	22 (4%)	2 (0%)	30	59
1	D	490/509 (96%)	473 (96%)	17 (4%)	0	100	100
1	E	486/509 (96%)	463 (95%)	21 (4%)	2 (0%)	30	59
1	F	490/509 (96%)	467 (95%)	23 (5%)	0	100	100
1	G	487/509 (96%)	468 (96%)	19 (4%)	0	100	100
1	H	483/509 (95%)	456 (94%)	25 (5%)	2 (0%)	30	59
1	I	487/509 (96%)	467 (96%)	18 (4%)	2 (0%)	30	59
1	J	487/509 (96%)	466 (96%)	18 (4%)	3 (1%)	21	51
1	K	486/509 (96%)	462 (95%)	23 (5%)	1 (0%)	43	72
1	L	485/509 (95%)	464 (96%)	20 (4%)	1 (0%)	43	72
1	M	487/509 (96%)	458 (94%)	28 (6%)	1 (0%)	43	72
1	N	487/509 (96%)	466 (96%)	20 (4%)	1 (0%)	43	72
1	O	489/509 (96%)	464 (95%)	24 (5%)	1 (0%)	43	72
1	P	487/509 (96%)	473 (97%)	13 (3%)	1 (0%)	43	72
All	All	7796/8144 (96%)	7446 (96%)	331 (4%)	19 (0%)	43	72

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	ASP
1	J	91	ASP
1	N	91	ASP
1	P	91	ASP
1	E	91	ASP
1	H	180	ASP
1	O	180	ASP
1	C	91	ASP
1	E	500	LYS
1	I	5	PRO
1	I	91	ASP
1	J	180	ASP
1	L	91	ASP
1	A	5	PRO
1	H	91	ASP
1	M	5	PRO
1	K	91	ASP
1	J	3	ASN
1	C	5	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	412/447 (92%)	395 (96%)	17 (4%)	27	61
1	B	417/447 (93%)	399 (96%)	18 (4%)	26	60
1	C	424/447 (95%)	410 (97%)	14 (3%)	33	67
1	D	421/447 (94%)	406 (96%)	15 (4%)	31	65
1	E	422/447 (94%)	405 (96%)	17 (4%)	28	62
1	F	417/447 (93%)	400 (96%)	17 (4%)	27	61
1	G	422/447 (94%)	399 (94%)	23 (6%)	19	50
1	H	419/447 (94%)	398 (95%)	21 (5%)	22	53
1	I	425/447 (95%)	404 (95%)	21 (5%)	22	54
1	J	419/447 (94%)	399 (95%)	20 (5%)	23	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	423/447 (95%)	405 (96%)	18 (4%)	26	60
1	L	419/447 (94%)	404 (96%)	15 (4%)	31	65
1	M	422/447 (94%)	400 (95%)	22 (5%)	21	52
1	N	420/447 (94%)	404 (96%)	16 (4%)	29	64
1	O	422/447 (94%)	404 (96%)	18 (4%)	26	60
1	P	417/447 (93%)	399 (96%)	18 (4%)	26	60
All	All	6721/7152 (94%)	6431 (96%)	290 (4%)	26	60

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	104	SER
1	A	118	ASP
1	A	122	PHE
1	A	128	THR
1	A	220	VAL
1	A	222	VAL
1	A	286	VAL
1	A	347	SER
1	A	392	THR
1	A	417	ASP
1	A	419	LYS
1	A	438	GLN
1	A	454	GLU
1	A	464	VAL
1	A	471	ILE
1	A	477	GLU
1	B	40	LEU
1	B	88	LYS
1	B	91	ASP
1	B	98	ARG
1	B	104	SER
1	B	118	ASP
1	B	220	VAL
1	B	260	GLU
1	B	347	SER
1	B	364	PRO
1	B	392	THR
1	B	417	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	428	HIS
1	B	454	GLU
1	B	469	GLU
1	B	471	ILE
1	B	477	GLU
1	B	485	ILE
1	C	40	LEU
1	C	88	LYS
1	C	91	ASP
1	C	104	SER
1	C	110	LYS
1	C	118	ASP
1	C	220	VAL
1	C	222	VAL
1	C	286	VAL
1	C	392	THR
1	C	454	GLU
1	C	471	ILE
1	C	477	GLU
1	C	485	ILE
1	D	40	LEU
1	D	91	ASP
1	D	104	SER
1	D	110	LYS
1	D	118	ASP
1	D	220	VAL
1	D	222	VAL
1	D	260	GLU
1	D	347	SER
1	D	392	THR
1	D	417	ASP
1	D	428	HIS
1	D	454	GLU
1	D	477	GLU
1	D	485	ILE
1	E	6	VAL
1	E	40	LEU
1	E	98	ARG
1	E	110	LYS
1	E	118	ASP
1	E	128	THR
1	E	220	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	222	VAL
1	E	260	GLU
1	E	286	VAL
1	E	392	THR
1	E	417	ASP
1	E	425	VAL
1	E	438	GLN
1	E	454	GLU
1	E	477	GLU
1	E	485	ILE
1	F	21	THR
1	F	40	LEU
1	F	91	ASP
1	F	110	LYS
1	F	118	ASP
1	F	220	VAL
1	F	222	VAL
1	F	347	SER
1	F	373	SER
1	F	392	THR
1	F	419	LYS
1	F	428	HIS
1	F	438	GLN
1	F	454	GLU
1	F	471	ILE
1	F	477	GLU
1	F	485	ILE
1	G	32	LYS
1	G	40	LEU
1	G	63	VAL
1	G	91	ASP
1	G	104	SER
1	G	220	VAL
1	G	222	VAL
1	G	260	GLU
1	G	286	VAL
1	G	347	SER
1	G	392	THR
1	G	401	CYS
1	G	403	ILE
1	G	404	GLN
1	G	417	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	425	VAL
1	G	428	HIS
1	G	438	GLN
1	G	454	GLU
1	G	464	VAL
1	G	471	ILE
1	G	492	LYS
1	G	493	LYS
1	H	6	VAL
1	H	40	LEU
1	H	98	ARG
1	H	104	SER
1	H	118	ASP
1	H	128	THR
1	H	220	VAL
1	H	222	VAL
1	H	260	GLU
1	H	286	VAL
1	H	305	ARG
1	H	347	SER
1	H	392	THR
1	H	417	ASP
1	H	419	LYS
1	H	428	HIS
1	H	438	GLN
1	H	454	GLU
1	H	471	ILE
1	H	477	GLU
1	H	485	ILE
1	I	40	LEU
1	I	88	LYS
1	I	104	SER
1	I	110	LYS
1	I	118	ASP
1	I	122	PHE
1	I	128	THR
1	I	142	ILE
1	I	220	VAL
1	I	222	VAL
1	I	297	ASP
1	I	347	SER
1	I	364	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	392	THR
1	I	438	GLN
1	I	454	GLU
1	I	469	GLU
1	I	471	ILE
1	I	477	GLU
1	I	485	ILE
1	I	496	GLU
1	J	32	LYS
1	J	88	LYS
1	J	91	ASP
1	J	101	THR
1	J	110	LYS
1	J	118	ASP
1	J	128	THR
1	J	220	VAL
1	J	222	VAL
1	J	260	GLU
1	J	286	VAL
1	J	380	ASP
1	J	392	THR
1	J	417	ASP
1	J	454	GLU
1	J	469	GLU
1	J	471	ILE
1	J	477	GLU
1	J	485	ILE
1	J	492	LYS
1	K	40	LEU
1	K	98	ARG
1	K	104	SER
1	K	118	ASP
1	K	220	VAL
1	K	222	VAL
1	K	260	GLU
1	K	347	SER
1	K	392	THR
1	K	419	LYS
1	K	425	VAL
1	K	428	HIS
1	K	438	GLN
1	K	440	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	454	GLU
1	K	469	GLU
1	K	477	GLU
1	K	485	ILE
1	L	6	VAL
1	L	32	LYS
1	L	40	LEU
1	L	91	ASP
1	L	98	ARG
1	L	104	SER
1	L	118	ASP
1	L	216	LYS
1	L	220	VAL
1	L	297	ASP
1	L	392	THR
1	L	454	GLU
1	L	469	GLU
1	L	471	ILE
1	L	485	ILE
1	M	6	VAL
1	M	40	LEU
1	M	91	ASP
1	M	98	ARG
1	M	104	SER
1	M	110	LYS
1	M	118	ASP
1	M	128	THR
1	M	220	VAL
1	M	222	VAL
1	M	286	VAL
1	M	364	PRO
1	M	392	THR
1	M	404	GLN
1	M	419	LYS
1	M	428	HIS
1	M	438	GLN
1	M	454	GLU
1	M	469	GLU
1	M	471	ILE
1	M	477	GLU
1	M	485	ILE
1	N	40	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	88	LYS
1	N	91	ASP
1	N	98	ARG
1	N	142	ILE
1	N	220	VAL
1	N	222	VAL
1	N	286	VAL
1	N	347	SER
1	N	392	THR
1	N	438	GLN
1	N	454	GLU
1	N	471	ILE
1	N	477	GLU
1	N	485	ILE
1	N	498	LYS
1	O	6	VAL
1	O	40	LEU
1	O	91	ASP
1	O	104	SER
1	O	110	LYS
1	O	118	ASP
1	O	220	VAL
1	O	347	SER
1	O	392	THR
1	O	417	ASP
1	O	428	HIS
1	O	438	GLN
1	O	454	GLU
1	O	464	VAL
1	O	469	GLU
1	O	477	GLU
1	O	485	ILE
1	O	492	LYS
1	P	40	LEU
1	P	48	ILE
1	P	91	ASP
1	P	104	SER
1	P	110	LYS
1	P	128	THR
1	P	220	VAL
1	P	222	VAL
1	P	260	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	364	PRO
1	P	377	ILE
1	P	392	THR
1	P	415	LYS
1	P	425	VAL
1	P	454	GLU
1	P	464	VAL
1	P	474	ARG
1	P	485	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (233) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	65	HIS
1	A	158	GLN
1	A	161	ASN
1	A	165	ASN
1	A	230	GLN
1	A	302	HIS
1	A	314	ASN
1	A	321	GLN
1	A	328	HIS
1	A	354	HIS
1	A	397	ASN
1	A	404	GLN
1	A	438	GLN
1	A	463	HIS
1	B	11	GLN
1	B	22	GLN
1	B	158	GLN
1	B	161	ASN
1	B	165	ASN
1	B	185	GLN
1	B	225	HIS
1	B	230	GLN
1	B	302	HIS
1	B	314	ASN
1	B	321	GLN
1	B	328	HIS
1	B	404	GLN
1	B	438	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	463	HIS
1	C	11	GLN
1	C	22	GLN
1	C	65	HIS
1	C	138	ASN
1	C	158	GLN
1	C	161	ASN
1	C	165	ASN
1	C	185	GLN
1	C	230	GLN
1	C	302	HIS
1	C	314	ASN
1	C	321	GLN
1	C	328	HIS
1	C	438	GLN
1	C	463	HIS
1	C	495	GLN
1	D	11	GLN
1	D	22	GLN
1	D	65	HIS
1	D	158	GLN
1	D	161	ASN
1	D	185	GLN
1	D	230	GLN
1	D	278	GLN
1	D	302	HIS
1	D	314	ASN
1	D	321	GLN
1	D	328	HIS
1	D	378	ASN
1	D	438	GLN
1	D	463	HIS
1	E	22	GLN
1	E	65	HIS
1	E	161	ASN
1	E	165	ASN
1	E	185	GLN
1	E	225	HIS
1	E	230	GLN
1	E	302	HIS
1	E	314	ASN
1	E	321	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	328	HIS
1	E	354	HIS
1	E	378	ASN
1	E	404	GLN
1	E	428	HIS
1	E	438	GLN
1	E	463	HIS
1	F	22	GLN
1	F	158	GLN
1	F	161	ASN
1	F	185	GLN
1	F	225	HIS
1	F	230	GLN
1	F	302	HIS
1	F	314	ASN
1	F	321	GLN
1	F	328	HIS
1	F	438	GLN
1	F	463	HIS
1	G	22	GLN
1	G	65	HIS
1	G	158	GLN
1	G	161	ASN
1	G	185	GLN
1	G	230	GLN
1	G	302	HIS
1	G	314	ASN
1	G	321	GLN
1	G	328	HIS
1	G	397	ASN
1	G	438	GLN
1	G	463	HIS
1	H	11	GLN
1	H	22	GLN
1	H	65	HIS
1	H	158	GLN
1	H	161	ASN
1	H	230	GLN
1	H	302	HIS
1	H	314	ASN
1	H	321	GLN
1	H	328	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	342	GLN
1	H	354	HIS
1	H	438	GLN
1	H	463	HIS
1	I	22	GLN
1	I	65	HIS
1	I	161	ASN
1	I	185	GLN
1	I	278	GLN
1	I	302	HIS
1	I	314	ASN
1	I	321	GLN
1	I	328	HIS
1	I	354	HIS
1	I	404	GLN
1	I	438	GLN
1	I	463	HIS
1	J	22	GLN
1	J	65	HIS
1	J	161	ASN
1	J	165	ASN
1	J	185	GLN
1	J	225	HIS
1	J	230	GLN
1	J	302	HIS
1	J	314	ASN
1	J	321	GLN
1	J	328	HIS
1	J	354	HIS
1	J	378	ASN
1	J	438	GLN
1	J	463	HIS
1	K	22	GLN
1	K	65	HIS
1	K	161	ASN
1	K	165	ASN
1	K	185	GLN
1	K	225	HIS
1	K	230	GLN
1	K	302	HIS
1	K	314	ASN
1	K	321	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	328	HIS
1	K	354	HIS
1	K	438	GLN
1	K	463	HIS
1	L	22	GLN
1	L	65	HIS
1	L	158	GLN
1	L	161	ASN
1	L	179	ASN
1	L	230	GLN
1	L	314	ASN
1	L	321	GLN
1	L	328	HIS
1	L	354	HIS
1	L	438	GLN
1	L	453	GLN
1	L	463	HIS
1	M	22	GLN
1	M	65	HIS
1	M	158	GLN
1	M	161	ASN
1	M	165	ASN
1	M	185	GLN
1	M	230	GLN
1	M	234	ASN
1	M	302	HIS
1	M	314	ASN
1	M	321	GLN
1	M	328	HIS
1	M	378	ASN
1	M	404	GLN
1	M	438	GLN
1	M	463	HIS
1	N	11	GLN
1	N	22	GLN
1	N	65	HIS
1	N	158	GLN
1	N	161	ASN
1	N	165	ASN
1	N	230	GLN
1	N	234	ASN
1	N	302	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	314	ASN
1	N	321	GLN
1	N	328	HIS
1	N	337	ASN
1	N	397	ASN
1	N	404	GLN
1	N	438	GLN
1	N	463	HIS
1	O	11	GLN
1	O	22	GLN
1	O	65	HIS
1	O	161	ASN
1	O	165	ASN
1	O	185	GLN
1	O	230	GLN
1	O	302	HIS
1	O	314	ASN
1	O	321	GLN
1	O	328	HIS
1	O	438	GLN
1	O	462	ASN
1	O	463	HIS
1	P	22	GLN
1	P	65	HIS
1	P	158	GLN
1	P	161	ASN
1	P	165	ASN
1	P	185	GLN
1	P	230	GLN
1	P	302	HIS
1	P	314	ASN
1	P	321	GLN
1	P	397	ASN
1	P	428	HIS
1	P	438	GLN
1	P	463	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

15 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	B	1503	1	50,50,50	1.99	10 (20%)	67,82,82	1.60	8 (11%)
2	HEM	O	1503	1	50,50,50	1.92	8 (16%)	67,82,82	1.54	13 (19%)
2	HEM	D	1503	1	50,50,50	2.03	9 (18%)	67,82,82	1.79	18 (26%)
2	HEM	P	1503	1	50,50,50	1.88	10 (20%)	67,82,82	1.51	9 (13%)
2	HEM	I	1503	1	50,50,50	1.95	7 (14%)	67,82,82	1.56	9 (13%)
2	HEM	H	1503	1	50,50,50	2.07	10 (20%)	67,82,82	1.57	11 (16%)
2	HEM	J	1503	1	50,50,50	2.06	9 (18%)	67,82,82	1.44	7 (10%)
2	HEM	E	1503	1	50,50,50	1.93	10 (20%)	67,82,82	1.71	14 (20%)
2	HEM	K	1503	1	50,50,50	1.92	8 (16%)	67,82,82	1.67	11 (16%)
2	HEM	M	1503	1	50,50,50	2.00	10 (20%)	67,82,82	1.70	13 (19%)
2	HEM	G	1503	1	50,50,50	2.04	8 (16%)	67,82,82	1.76	15 (22%)
2	HEM	C	1503	1	50,50,50	1.77	8 (16%)	67,82,82	1.55	9 (13%)
2	HEM	N	1503	1	50,50,50	2.01	7 (14%)	67,82,82	1.61	13 (19%)
2	HEM	L	1503	1	50,50,50	1.91	7 (14%)	67,82,82	1.64	10 (14%)
2	HEM	F	1503	1	50,50,50	1.98	9 (18%)	67,82,82	1.63	12 (17%)

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	B	1503	1	-	2/14/54/54	-
2	HEM	O	1503	1	-	4/14/54/54	-
2	HEM	D	1503	1	-	4/14/54/54	-
2	HEM	P	1503	1	-	4/14/54/54	-
2	HEM	I	1503	1	-	2/14/54/54	-
2	HEM	H	1503	1	-	4/14/54/54	-
2	HEM	J	1503	1	-	4/14/54/54	-
2	HEM	E	1503	1	-	4/14/54/54	-
2	HEM	K	1503	1	-	6/14/54/54	-
2	HEM	M	1503	1	-	4/14/54/54	-
2	HEM	G	1503	1	-	4/14/54/54	-
2	HEM	C	1503	1	-	4/14/54/54	-
2	HEM	N	1503	1	-	4/14/54/54	-
2	HEM	L	1503	1	-	4/14/54/54	-
2	HEM	F	1503	1	-	4/14/54/54	-

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1503	HEM	C3D-C2D	8.40	1.54	1.36
2	F	1503	HEM	C3D-C2D	8.01	1.54	1.36
2	H	1503	HEM	C3D-C2D	7.97	1.54	1.36
2	J	1503	HEM	C3D-C2D	7.86	1.53	1.36
2	K	1503	HEM	C3D-C2D	7.83	1.53	1.36
2	N	1503	HEM	C3D-C2D	7.69	1.53	1.36
2	M	1503	HEM	C3D-C2D	7.69	1.53	1.36
2	P	1503	HEM	C3D-C2D	7.67	1.53	1.36
2	I	1503	HEM	C3D-C2D	7.62	1.53	1.36
2	C	1503	HEM	C3D-C2D	7.42	1.52	1.36
2	O	1503	HEM	C3D-C2D	7.40	1.52	1.36
2	D	1503	HEM	C3D-C2D	7.23	1.52	1.36
2	G	1503	HEM	C3D-C2D	7.19	1.52	1.36
2	L	1503	HEM	C3D-C2D	6.99	1.51	1.36
2	E	1503	HEM	C3D-C2D	6.93	1.51	1.36
2	D	1503	HEM	FE-NB	6.54	2.15	1.94
2	J	1503	HEM	FE-NB	6.22	2.14	1.94
2	G	1503	HEM	FE-NB	6.13	2.13	1.94
2	E	1503	HEM	FE-NC	6.12	2.15	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1503	HEM	FE-NC	5.91	2.14	1.95
2	F	1503	HEM	FE-NB	5.87	2.13	1.94
2	L	1503	HEM	FE-NC	5.86	2.14	1.95
2	I	1503	HEM	FE-NA	5.77	2.14	1.95
2	E	1503	HEM	FE-NB	5.60	2.12	1.94
2	N	1503	HEM	FE-NB	5.35	2.11	1.94
2	L	1503	HEM	FE-NB	5.29	2.11	1.94
2	G	1503	HEM	FE-NA	5.20	2.12	1.95
2	O	1503	HEM	FE-ND	5.12	2.10	1.94
2	P	1503	HEM	FE-NB	5.11	2.10	1.94
2	I	1503	HEM	FE-NB	5.02	2.10	1.94
2	M	1503	HEM	FE-NA	5.02	2.11	1.95
2	N	1503	HEM	FE-NA	5.00	2.11	1.95
2	H	1503	HEM	FE-NA	4.93	2.11	1.95
2	H	1503	HEM	FE-NB	4.88	2.09	1.94
2	B	1503	HEM	FE-NB	4.70	2.09	1.94
2	M	1503	HEM	FE-NB	4.65	2.09	1.94
2	M	1503	HEM	FE-NC	4.62	2.10	1.95
2	B	1503	HEM	FE-NA	4.60	2.10	1.95
2	J	1503	HEM	FE-NC	4.57	2.10	1.95
2	K	1503	HEM	FE-NC	4.55	2.10	1.95
2	C	1503	HEM	FE-NB	4.50	2.08	1.94
2	H	1503	HEM	FE-NC	4.49	2.10	1.95
2	O	1503	HEM	FE-NB	4.28	2.08	1.94
2	H	1503	HEM	FE-ND	4.19	2.07	1.94
2	N	1503	HEM	FE-NC	4.12	2.08	1.95
2	F	1503	HEM	FE-ND	3.82	2.06	1.94
2	M	1503	HEM	FE-ND	3.80	2.06	1.94
2	B	1503	HEM	FE-NC	3.76	2.07	1.95
2	O	1503	HEM	FE-NA	3.70	2.07	1.95
2	K	1503	HEM	FE-NA	3.63	2.07	1.95
2	G	1503	HEM	FE-NC	3.61	2.07	1.95
2	K	1503	HEM	FE-NB	3.43	2.05	1.94
2	K	1503	HEM	FE-ND	3.42	2.05	1.94
2	J	1503	HEM	FE-NA	3.38	2.06	1.95
2	K	1503	HEM	CAB-C3B	3.29	1.56	1.47
2	I	1503	HEM	CAB-C3B	3.23	1.56	1.47
2	J	1503	HEM	CAB-C3B	3.20	1.55	1.47
2	F	1503	HEM	FE-NA	3.17	2.05	1.95
2	P	1503	HEM	FE-NC	3.16	2.05	1.95
2	P	1503	HEM	FE-NA	3.16	2.05	1.95
2	J	1503	HEM	CAC-C3C	3.15	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1503	HEM	FE-NC	3.07	2.05	1.95
2	E	1503	HEM	CAB-C3B	3.04	1.55	1.47
2	C	1503	HEM	FE-NC	3.02	2.05	1.95
2	G	1503	HEM	FE-ND	2.98	2.04	1.94
2	C	1503	HEM	CMB-C2B	2.90	1.56	1.50
2	P	1503	HEM	CAB-C3B	2.87	1.55	1.47
2	F	1503	HEM	FE-NC	2.86	2.04	1.95
2	B	1503	HEM	CAB-C3B	2.85	1.55	1.47
2	G	1503	HEM	CAC-C3C	2.82	1.54	1.47
2	H	1503	HEM	CAB-C3B	2.80	1.54	1.47
2	M	1503	HEM	CAB-C3B	2.77	1.54	1.47
2	H	1503	HEM	CAC-C3C	2.76	1.54	1.47
2	D	1503	HEM	CAB-C3B	2.76	1.54	1.47
2	N	1503	HEM	CAC-C3C	2.75	1.54	1.47
2	F	1503	HEM	CMB-C2B	2.72	1.56	1.50
2	B	1503	HEM	CAC-C3C	2.70	1.54	1.47
2	G	1503	HEM	CAB-C3B	2.66	1.54	1.47
2	F	1503	HEM	CAB-C3B	2.65	1.54	1.47
2	B	1503	HEM	CMB-C2B	2.64	1.56	1.50
2	D	1503	HEM	FE-ND	2.58	2.02	1.94
2	B	1503	HEM	CMC-C2C	2.58	1.56	1.50
2	E	1503	HEM	CAC-C3C	2.56	1.54	1.47
2	I	1503	HEM	FE-ND	2.55	2.02	1.94
2	D	1503	HEM	CAC-C3C	2.54	1.54	1.47
2	P	1503	HEM	CAC-C3C	2.52	1.54	1.47
2	N	1503	HEM	FE-ND	2.47	2.02	1.94
2	N	1503	HEM	CAB-C3B	2.46	1.53	1.47
2	C	1503	HEM	CAB-C3B	2.44	1.53	1.47
2	L	1503	HEM	CAB-C3B	2.42	1.53	1.47
2	F	1503	HEM	CAC-C3C	2.39	1.53	1.47
2	M	1503	HEM	CAC-C3C	2.39	1.53	1.47
2	K	1503	HEM	CAC-C3C	2.38	1.53	1.47
2	C	1503	HEM	FE-NA	2.34	2.02	1.95
2	E	1503	HEM	C2A-C3A	-2.34	1.32	1.38
2	K	1503	HEM	CMD-C2D	2.28	1.55	1.50
2	L	1503	HEM	CAC-C3C	2.28	1.53	1.47
2	O	1503	HEM	CAA-C2A	2.26	1.57	1.51
2	O	1503	HEM	CAB-C3B	2.25	1.53	1.47
2	I	1503	HEM	CAC-C3C	2.25	1.53	1.47
2	I	1503	HEM	CMA-C3A	2.25	1.55	1.50
2	C	1503	HEM	CAC-C3C	2.24	1.53	1.47
2	H	1503	HEM	CMB-C2B	2.21	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	1503	HEM	CMD-C2D	2.21	1.55	1.50
2	E	1503	HEM	CMB-C2B	2.20	1.55	1.50
2	J	1503	HEM	CMB-C2B	2.19	1.55	1.50
2	M	1503	HEM	CMC-C2C	2.19	1.55	1.50
2	E	1503	HEM	FE-NA	2.19	2.02	1.95
2	C	1503	HEM	CAA-C2A	2.18	1.57	1.51
2	E	1503	HEM	CMC-C2C	2.18	1.55	1.50
2	M	1503	HEM	CMA-C3A	2.18	1.55	1.50
2	D	1503	HEM	FE-NA	2.17	2.02	1.95
2	B	1503	HEM	CMD-C2D	2.16	1.55	1.50
2	D	1503	HEM	CMC-C2C	2.15	1.55	1.50
2	B	1503	HEM	O1D-CGD	2.14	1.29	1.22
2	L	1503	HEM	C1B-NB	-2.13	1.36	1.40
2	D	1503	HEM	CMD-C2D	2.12	1.55	1.50
2	P	1503	HEM	C3C-C2C	-2.12	1.32	1.37
2	J	1503	HEM	CMD-C2D	2.11	1.55	1.50
2	L	1503	HEM	CMA-C3A	2.11	1.55	1.50
2	G	1503	HEM	CMA-C3A	2.09	1.55	1.50
2	H	1503	HEM	CMA-C3A	2.08	1.55	1.50
2	J	1503	HEM	O1D-CGD	2.08	1.28	1.22
2	E	1503	HEM	FE-ND	2.08	2.01	1.94
2	F	1503	HEM	C1B-NB	-2.04	1.36	1.40
2	P	1503	HEM	CMA-C3A	2.04	1.55	1.50
2	H	1503	HEM	CMD-C2D	2.04	1.55	1.50
2	O	1503	HEM	CMD-C2D	2.03	1.54	1.50
2	P	1503	HEM	O1A-CGA	2.03	1.28	1.22
2	M	1503	HEM	CAA-C2A	2.03	1.56	1.51

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1503	HEM	C4D-ND-C1D	6.91	113.39	105.21
2	M	1503	HEM	C4D-ND-C1D	6.80	113.26	105.21
2	E	1503	HEM	C4D-ND-C1D	6.61	113.03	105.21
2	I	1503	HEM	C4D-ND-C1D	6.48	112.88	105.21
2	D	1503	HEM	C4D-ND-C1D	6.34	112.71	105.21
2	H	1503	HEM	C4D-ND-C1D	6.21	112.56	105.21
2	F	1503	HEM	C4D-ND-C1D	6.07	112.40	105.21
2	P	1503	HEM	C4D-ND-C1D	5.87	112.16	105.21
2	K	1503	HEM	C4D-ND-C1D	5.80	112.07	105.21
2	C	1503	HEM	C4D-ND-C1D	5.68	111.94	105.21
2	B	1503	HEM	C4D-ND-C1D	5.62	111.86	105.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1503	HEM	C4D-ND-C1D	5.62	111.86	105.21
2	O	1503	HEM	C4D-ND-C1D	5.57	111.80	105.21
2	L	1503	HEM	C4D-ND-C1D	5.57	111.80	105.21
2	J	1503	HEM	C4D-ND-C1D	5.55	111.78	105.21
2	C	1503	HEM	CAD-CBD-CGD	-4.50	101.74	113.67
2	B	1503	HEM	CBD-CAD-C3D	-4.46	100.19	112.53
2	L	1503	HEM	CAD-C3D-C4D	4.36	132.30	124.70
2	K	1503	HEM	CAD-CBD-CGD	-4.23	102.45	113.67
2	B	1503	HEM	C3B-C4B-NB	-4.12	106.51	109.47
2	B	1503	HEM	C1B-NB-C4B	4.06	110.01	105.21
2	P	1503	HEM	CAD-CBD-CGD	-4.05	102.91	113.67
2	M	1503	HEM	C3B-C4B-NB	-3.94	106.64	109.47
2	D	1503	HEM	C1B-NB-C4B	3.91	109.84	105.21
2	L	1503	HEM	CHD-C1D-ND	3.84	128.55	124.42
2	K	1503	HEM	CHA-C4D-ND	3.75	129.01	124.37
2	H	1503	HEM	C1B-NB-C4B	3.73	109.62	105.21
2	G	1503	HEM	CHA-C4D-ND	3.63	128.86	124.37
2	N	1503	HEM	C1B-NB-C4B	3.62	109.49	105.21
2	F	1503	HEM	CHC-C1C-NC	3.55	128.32	124.45
2	D	1503	HEM	CAD-CBD-CGD	-3.55	104.26	113.67
2	O	1503	HEM	C1B-NB-C4B	3.47	109.31	105.21
2	I	1503	HEM	CHA-C4D-ND	3.47	128.66	124.37
2	N	1503	HEM	CHA-C4D-ND	3.44	128.62	124.37
2	M	1503	HEM	C1B-NB-C4B	3.41	109.25	105.21
2	H	1503	HEM	C3B-C4B-NB	-3.39	107.03	109.47
2	D	1503	HEM	C3B-C4B-NB	-3.33	107.08	109.47
2	N	1503	HEM	C2B-C1B-NB	-3.28	106.06	109.84
2	C	1503	HEM	O1A-CGA-CBA	-3.28	112.69	123.09
2	G	1503	HEM	C1B-NB-C4B	3.27	109.08	105.21
2	E	1503	HEM	CAD-CBD-CGD	-3.24	105.06	113.67
2	E	1503	HEM	CHD-C4C-C3C	3.19	130.59	125.21
2	F	1503	HEM	CHA-C4D-ND	3.19	128.31	124.37
2	K	1503	HEM	CBA-CAA-C2A	-3.09	103.99	112.53
2	G	1503	HEM	C2D-C1D-ND	-3.08	106.34	109.90
2	K	1503	HEM	C3B-C4B-NB	-3.07	107.26	109.47
2	L	1503	HEM	C3B-C4B-NB	-3.07	107.27	109.47
2	K	1503	HEM	C1B-NB-C4B	3.06	108.83	105.21
2	E	1503	HEM	CHA-C4D-ND	3.04	128.13	124.37
2	J	1503	HEM	C1B-NB-C4B	3.03	108.79	105.21
2	K	1503	HEM	C4C-C3C-C2C	3.01	109.43	106.81
2	E	1503	HEM	C3B-C4B-NB	-3.00	107.32	109.47
2	C	1503	HEM	CHD-C1D-ND	2.99	127.64	124.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1503	HEM	CAD-C3D-C2D	-2.93	122.39	127.87
2	G	1503	HEM	C2B-C1B-NB	-2.91	106.49	109.84
2	D	1503	HEM	C4A-NA-C1A	2.91	110.56	105.82
2	M	1503	HEM	CHD-C1D-ND	2.90	127.54	124.42
2	J	1503	HEM	CHA-C4D-ND	2.89	127.94	124.37
2	F	1503	HEM	C1B-NB-C4B	2.87	108.61	105.21
2	G	1503	HEM	CHD-C4C-C3C	2.87	130.04	125.21
2	D	1503	HEM	C2A-C1A-NA	-2.86	106.98	110.15
2	J	1503	HEM	CAD-CBD-CGD	-2.86	106.09	113.67
2	P	1503	HEM	CHD-C1D-ND	2.85	127.49	124.42
2	K	1503	HEM	CMD-C2D-C1D	2.82	129.44	125.03
2	O	1503	HEM	C3B-C4B-NB	-2.81	107.45	109.47
2	E	1503	HEM	CBA-CAA-C2A	-2.80	104.78	112.53
2	O	1503	HEM	C2B-C1B-NB	-2.80	106.62	109.84
2	G	1503	HEM	CHC-C1C-NC	2.79	127.50	124.45
2	E	1503	HEM	C1B-NB-C4B	2.79	108.51	105.21
2	E	1503	HEM	C2A-C1A-NA	-2.78	107.06	110.15
2	D	1503	HEM	C3A-C4A-NA	-2.78	105.68	110.14
2	C	1503	HEM	O2A-CGA-CBA	2.76	122.73	114.00
2	L	1503	HEM	C1B-NB-C4B	2.76	108.48	105.21
2	I	1503	HEM	CHC-C1C-NC	2.75	127.45	124.45
2	C	1503	HEM	CHA-C4D-ND	2.74	127.76	124.37
2	M	1503	HEM	CHA-C4D-ND	2.71	127.72	124.37
2	D	1503	HEM	C2B-C1B-NB	-2.70	106.74	109.84
2	F	1503	HEM	CAD-CBD-CGD	-2.69	106.54	113.67
2	E	1503	HEM	CHD-C1D-ND	2.66	127.29	124.42
2	E	1503	HEM	C2D-C1D-ND	-2.66	106.83	109.90
2	J	1503	HEM	C3B-C4B-NB	-2.66	107.56	109.47
2	O	1503	HEM	C3B-C2B-C1B	2.66	108.41	106.41
2	G	1503	HEM	CMD-C2D-C1D	2.66	129.19	125.03
2	F	1503	HEM	C4C-C3C-C2C	2.63	109.10	106.81
2	L	1503	HEM	CHC-C4B-NB	2.63	127.25	124.42
2	H	1503	HEM	C2B-C1B-NB	-2.62	106.83	109.84
2	G	1503	HEM	C3A-C4A-NA	-2.62	105.95	110.14
2	I	1503	HEM	C2A-C1A-NA	-2.61	107.25	110.15
2	L	1503	HEM	C2A-C1A-NA	-2.60	107.26	110.15
2	M	1503	HEM	C3D-C4D-ND	-2.60	107.33	110.17
2	N	1503	HEM	C3B-C4B-NB	-2.59	107.61	109.47
2	F	1503	HEM	C2A-C1A-NA	-2.58	107.29	110.15
2	H	1503	HEM	C2A-C1A-NA	-2.55	107.32	110.15
2	L	1503	HEM	CHB-C4A-NA	2.55	128.48	123.86
2	F	1503	HEM	C4C-NC-C1C	2.54	109.96	105.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1503	HEM	C2D-C1D-ND	-2.53	106.97	109.90
2	O	1503	HEM	CBC-CAC-C3C	-2.53	114.90	127.53
2	D	1503	HEM	C4A-C3A-C2A	2.52	109.70	106.82
2	N	1503	HEM	C3B-C2B-C1B	2.50	108.29	106.41
2	D	1503	HEM	C3D-C4D-ND	-2.49	107.44	110.17
2	O	1503	HEM	CMD-C2D-C1D	2.45	128.87	125.03
2	N	1503	HEM	CMD-C2D-C1D	2.45	128.86	125.03
2	D	1503	HEM	CHC-C4B-NB	2.44	127.05	124.42
2	M	1503	HEM	C4C-NC-C1C	2.43	109.79	105.82
2	G	1503	HEM	C4A-NA-C1A	2.43	109.78	105.82
2	K	1503	HEM	CBC-CAC-C3C	-2.42	115.42	127.53
2	P	1503	HEM	CHA-C4D-ND	2.42	127.36	124.37
2	B	1503	HEM	CHA-C4D-ND	2.41	127.35	124.37
2	B	1503	HEM	C1D-C2D-C3D	-2.40	104.46	106.98
2	M	1503	HEM	CAD-C3D-C4D	2.38	128.85	124.70
2	E	1503	HEM	C4C-NC-C1C	2.38	109.70	105.82
2	D	1503	HEM	CBD-CAD-C3D	-2.36	106.00	112.53
2	B	1503	HEM	C2B-C1B-NB	-2.36	107.13	109.84
2	N	1503	HEM	C3A-C4A-NA	-2.36	106.36	110.14
2	O	1503	HEM	O1D-CGD-CBD	-2.35	115.64	123.09
2	D	1503	HEM	CHD-C4C-C3C	2.34	129.16	125.21
2	I	1503	HEM	CAD-CBD-CGD	-2.34	107.45	113.67
2	F	1503	HEM	C4A-NA-C1A	2.33	109.62	105.82
2	C	1503	HEM	CMA-C3A-C4A	-2.32	121.88	125.42
2	D	1503	HEM	CHD-C1D-ND	2.31	126.91	124.42
2	F	1503	HEM	CBC-CAC-C3C	-2.30	116.02	127.53
2	O	1503	HEM	CAD-CBD-CGD	-2.30	107.56	113.67
2	N	1503	HEM	C4C-NC-C1C	2.30	109.57	105.82
2	C	1503	HEM	O1D-CGD-CBD	-2.30	115.80	123.09
2	F	1503	HEM	CBD-CAD-C3D	-2.29	106.21	112.53
2	D	1503	HEM	C1D-C2D-C3D	-2.29	104.58	106.98
2	N	1503	HEM	C3C-C2C-C1C	2.28	109.21	107.05
2	H	1503	HEM	CAD-CBD-CGD	-2.28	107.61	113.67
2	I	1503	HEM	C3D-C4D-ND	-2.28	107.67	110.17
2	M	1503	HEM	CBC-CAC-C3C	-2.28	116.14	127.53
2	J	1503	HEM	C3C-C2C-C1C	2.28	109.20	107.05
2	P	1503	HEM	C2A-C1A-NA	-2.27	107.63	110.15
2	H	1503	HEM	C3A-C4A-NA	-2.27	106.50	110.14
2	G	1503	HEM	CAD-CBD-CGD	-2.27	107.64	113.67
2	N	1503	HEM	CHC-C1C-NC	2.27	126.92	124.45
2	M	1503	HEM	C4A-NA-C1A	2.25	109.50	105.82
2	M	1503	HEM	C2A-C1A-NA	-2.25	107.66	110.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1503	HEM	CBA-CAA-C2A	-2.25	106.32	112.53
2	C	1503	HEM	C1B-NB-C4B	2.24	107.86	105.21
2	D	1503	HEM	CBA-CAA-C2A	-2.24	106.34	112.53
2	N	1503	HEM	CHD-C4C-C3C	2.24	128.98	125.21
2	P	1503	HEM	CBC-CAC-C3C	-2.23	116.36	127.53
2	G	1503	HEM	C4C-NC-C1C	2.23	109.46	105.82
2	N	1503	HEM	O1A-CGA-CBA	-2.23	116.03	123.09
2	H	1503	HEM	C4A-NA-C1A	2.22	109.44	105.82
2	H	1503	HEM	C4C-NC-C1C	2.22	109.44	105.82
2	I	1503	HEM	CHC-C4B-NB	-2.19	122.06	124.42
2	I	1503	HEM	C2D-C1D-ND	-2.19	107.37	109.90
2	K	1503	HEM	C4C-NC-C1C	2.18	109.38	105.82
2	K	1503	HEM	C1D-C2D-C3D	-2.18	104.69	106.98
2	P	1503	HEM	C1B-NB-C4B	2.18	107.78	105.21
2	O	1503	HEM	C3A-C4A-NA	-2.17	106.66	110.14
2	E	1503	HEM	C3D-C4D-ND	-2.16	107.81	110.17
2	O	1503	HEM	CAD-C3D-C4D	2.15	128.44	124.70
2	D	1503	HEM	C4C-NC-C1C	2.15	109.32	105.82
2	H	1503	HEM	C2D-C1D-ND	-2.13	107.44	109.90
2	P	1503	HEM	C3B-C2B-C1B	2.12	108.00	106.41
2	P	1503	HEM	C3D-C4D-ND	-2.12	107.85	110.17
2	O	1503	HEM	C4A-C3A-C2A	2.11	109.24	106.82
2	G	1503	HEM	C3B-C2B-C1B	2.11	108.00	106.41
2	E	1503	HEM	CMD-C2D-C1D	2.11	128.33	125.03
2	H	1503	HEM	CHD-C4C-C3C	2.09	128.73	125.21
2	J	1503	HEM	CAA-CBA-CGA	-2.08	108.16	113.67
2	D	1503	HEM	O1D-CGD-CBD	-2.07	116.52	123.09
2	O	1503	HEM	C4C-C3C-C2C	2.06	108.60	106.81
2	G	1503	HEM	C4A-C3A-C2A	2.05	109.17	106.82
2	E	1503	HEM	CHC-C1C-NC	2.04	126.67	124.45
2	F	1503	HEM	C3A-C4A-NA	-2.02	106.90	110.14
2	M	1503	HEM	CHC-C4B-NB	2.01	126.59	124.42
2	G	1503	HEM	CHD-C1D-ND	2.01	126.59	124.42
2	L	1503	HEM	CBA-CAA-C2A	-2.01	106.98	112.53
2	I	1503	HEM	CHA-C1A-C2A	2.00	129.68	125.30

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1503	HEM	C2C-C3C-CAC-CBC
2	C	1503	HEM	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	1503	HEM	C2C-C3C-CAC-CBC
2	D	1503	HEM	C4C-C3C-CAC-CBC
2	E	1503	HEM	C2C-C3C-CAC-CBC
2	E	1503	HEM	C4C-C3C-CAC-CBC
2	F	1503	HEM	C2C-C3C-CAC-CBC
2	G	1503	HEM	C2C-C3C-CAC-CBC
2	G	1503	HEM	C4C-C3C-CAC-CBC
2	H	1503	HEM	C2C-C3C-CAC-CBC
2	K	1503	HEM	C2C-C3C-CAC-CBC
2	K	1503	HEM	C4C-C3C-CAC-CBC
2	L	1503	HEM	C2C-C3C-CAC-CBC
2	L	1503	HEM	C4C-C3C-CAC-CBC
2	M	1503	HEM	C2C-C3C-CAC-CBC
2	M	1503	HEM	C4C-C3C-CAC-CBC
2	O	1503	HEM	C2C-C3C-CAC-CBC
2	P	1503	HEM	C2C-C3C-CAC-CBC
2	J	1503	HEM	C2C-C3C-CAC-CBC
2	N	1503	HEM	C2C-C3C-CAC-CBC
2	F	1503	HEM	C4C-C3C-CAC-CBC
2	H	1503	HEM	C4C-C3C-CAC-CBC
2	N	1503	HEM	C4C-C3C-CAC-CBC
2	O	1503	HEM	C4C-C3C-CAC-CBC
2	P	1503	HEM	C4C-C3C-CAC-CBC
2	J	1503	HEM	C4C-C3C-CAC-CBC
2	K	1503	HEM	C4D-C3D-CAD-CBD
2	K	1503	HEM	C2D-C3D-CAD-CBD
2	N	1503	HEM	CAD-CBD-CGD-O2D
2	P	1503	HEM	CAD-CBD-CGD-O2D
2	C	1503	HEM	CAD-CBD-CGD-O2D
2	P	1503	HEM	CAD-CBD-CGD-O1D
2	N	1503	HEM	CAD-CBD-CGD-O1D
2	J	1503	HEM	CAD-CBD-CGD-O2D
2	O	1503	HEM	CAD-CBD-CGD-O1D
2	K	1503	HEM	CAD-CBD-CGD-O1D
2	K	1503	HEM	CAD-CBD-CGD-O2D
2	E	1503	HEM	CAD-CBD-CGD-O2D
2	F	1503	HEM	CAD-CBD-CGD-O2D
2	O	1503	HEM	CAD-CBD-CGD-O2D
2	C	1503	HEM	CAD-CBD-CGD-O1D
2	J	1503	HEM	CAD-CBD-CGD-O1D
2	D	1503	HEM	CAD-CBD-CGD-O2D
2	E	1503	HEM	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	1503	HEM	CAD-CBD-CGD-O1D
2	B	1503	HEM	CAD-CBD-CGD-O2D
2	G	1503	HEM	CAD-CBD-CGD-O2D
2	H	1503	HEM	CAD-CBD-CGD-O2D
2	B	1503	HEM	CAD-CBD-CGD-O1D
2	L	1503	HEM	CAD-CBD-CGD-O2D
2	D	1503	HEM	CAD-CBD-CGD-O1D
2	I	1503	HEM	CAD-CBD-CGD-O2D
2	H	1503	HEM	CAD-CBD-CGD-O1D
2	L	1503	HEM	CAD-CBD-CGD-O1D
2	M	1503	HEM	CAD-CBD-CGD-O2D
2	G	1503	HEM	CAD-CBD-CGD-O1D
2	I	1503	HEM	CAD-CBD-CGD-O1D
2	M	1503	HEM	CAD-CBD-CGD-O1D

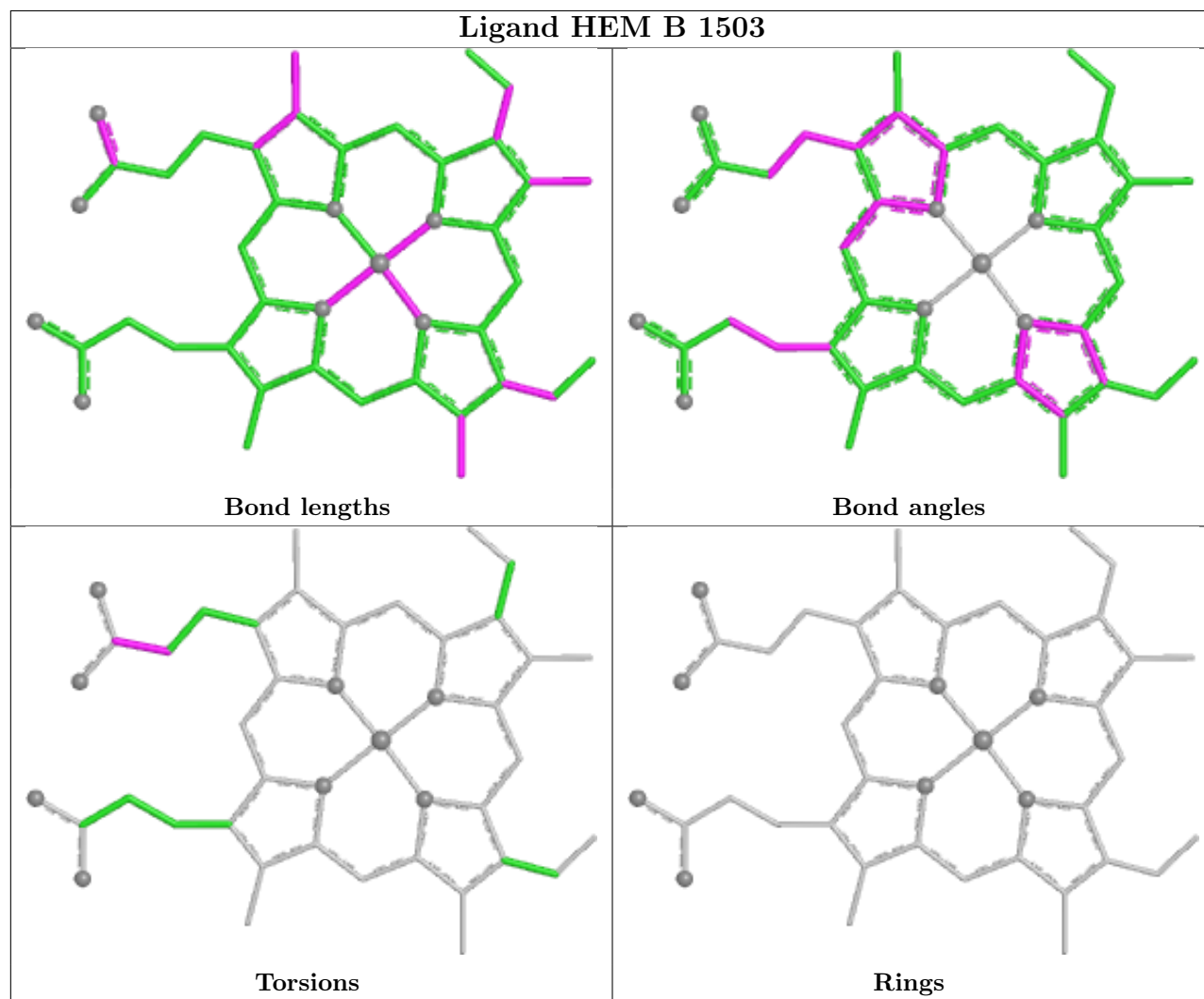
There are no ring outliers.

15 monomers are involved in 68 short contacts:

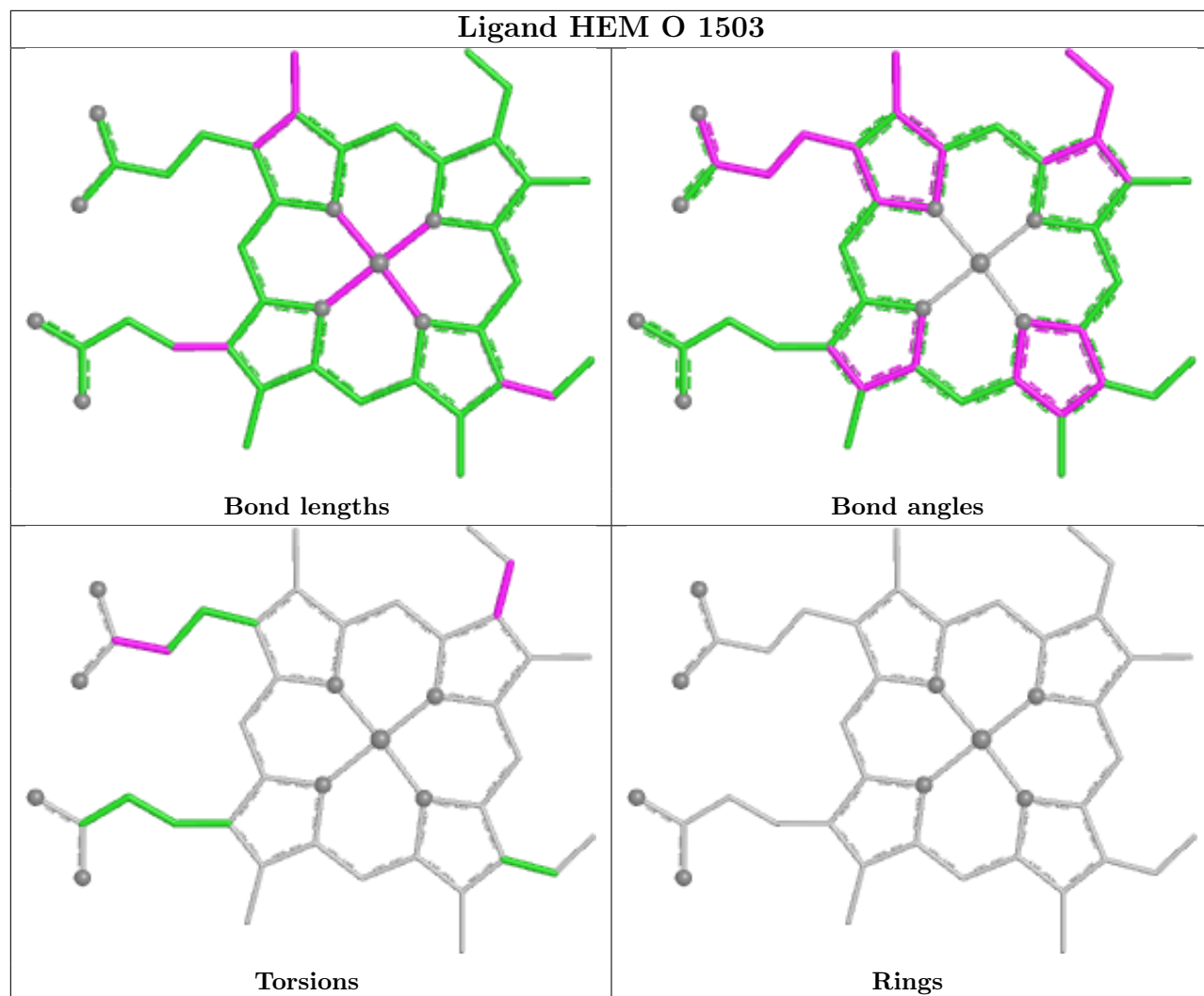
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1503	HEM	6	0
2	O	1503	HEM	5	0
2	D	1503	HEM	4	0
2	P	1503	HEM	3	0
2	I	1503	HEM	1	0
2	H	1503	HEM	5	0
2	J	1503	HEM	6	0
2	E	1503	HEM	5	0
2	K	1503	HEM	7	0
2	M	1503	HEM	3	0
2	G	1503	HEM	3	0
2	C	1503	HEM	6	0
2	N	1503	HEM	5	0
2	L	1503	HEM	6	0
2	F	1503	HEM	3	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

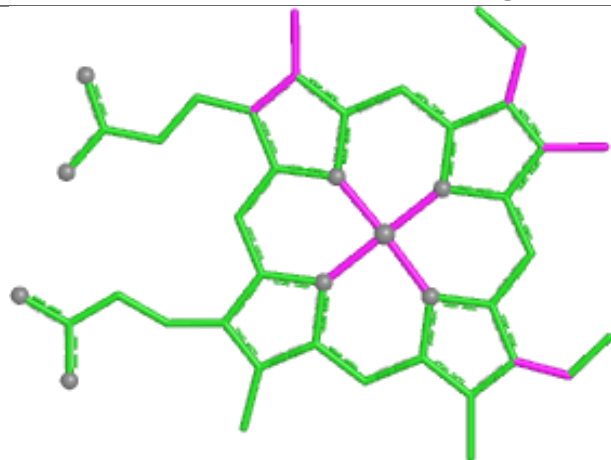
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



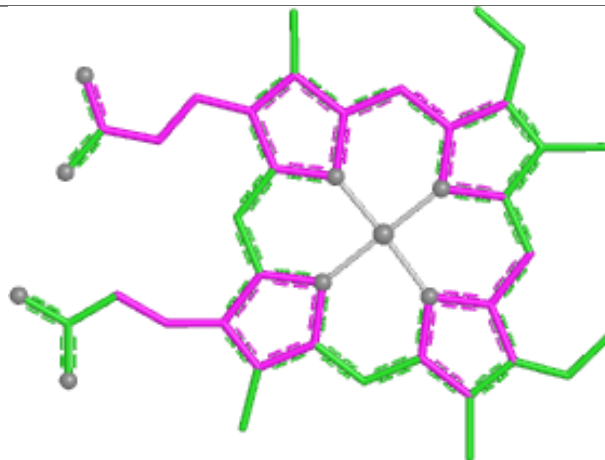
Ligand HEM O 1503



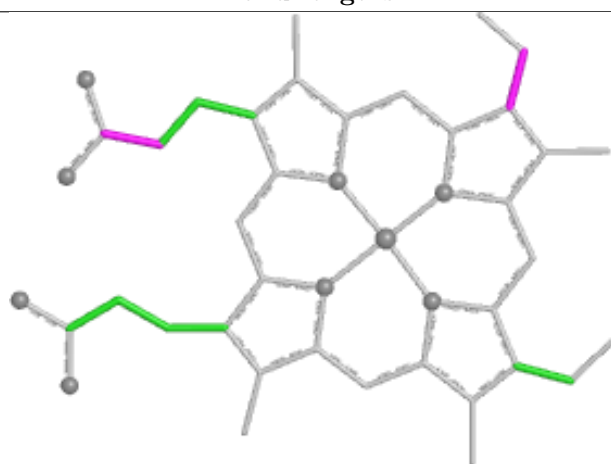
Ligand HEM D 1503



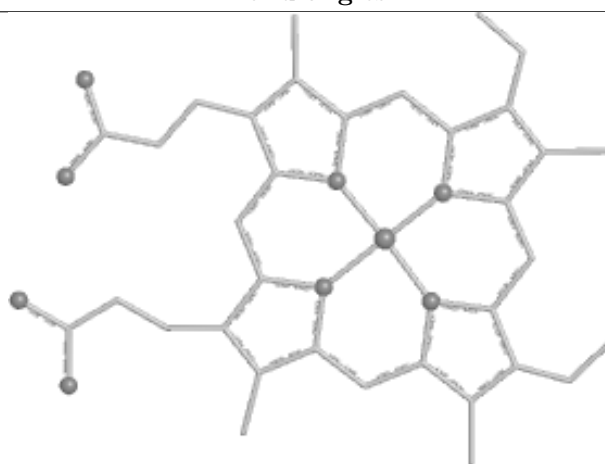
Bond lengths



Bond angles

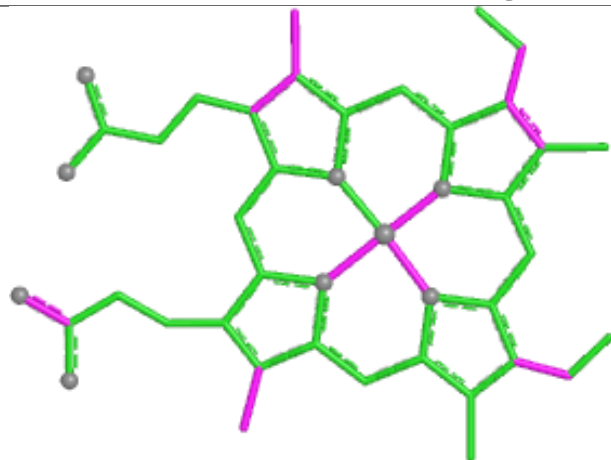


Torsions

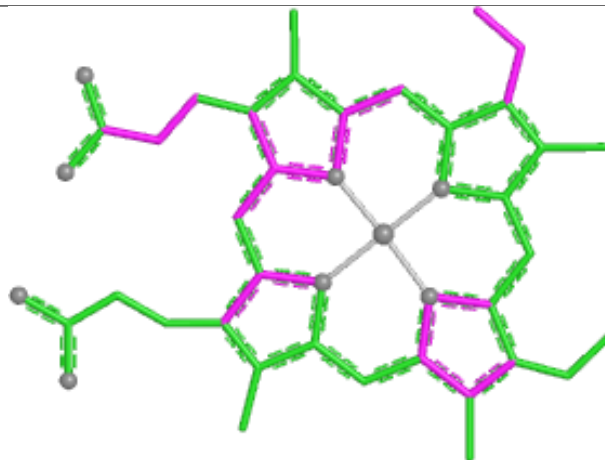


Rings

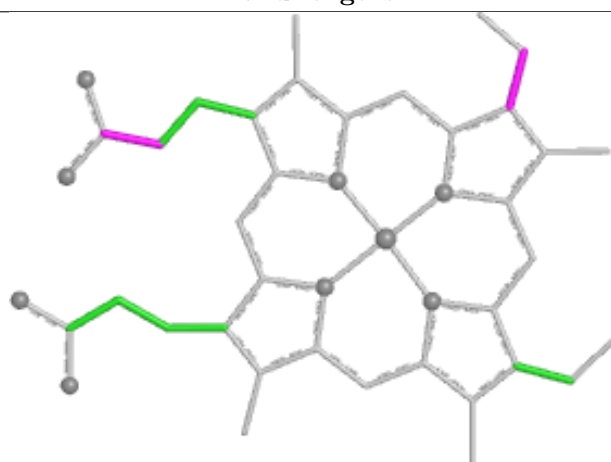
Ligand HEM P 1503



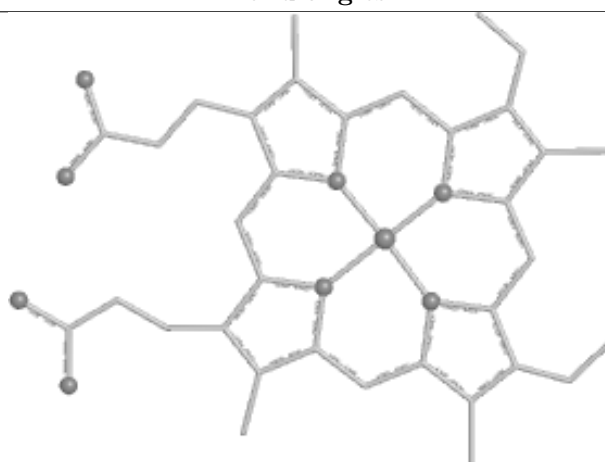
Bond lengths



Bond angles

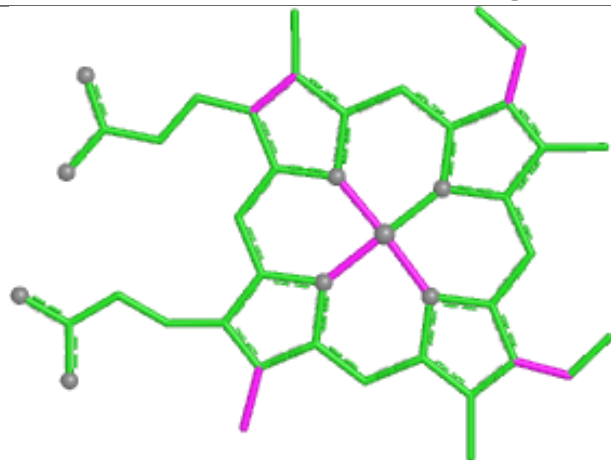


Torsions

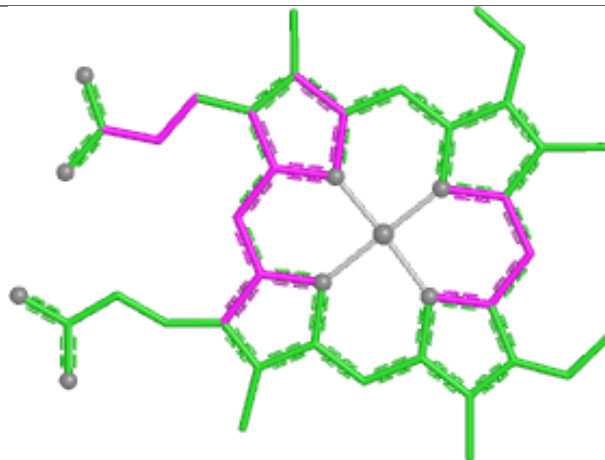


Rings

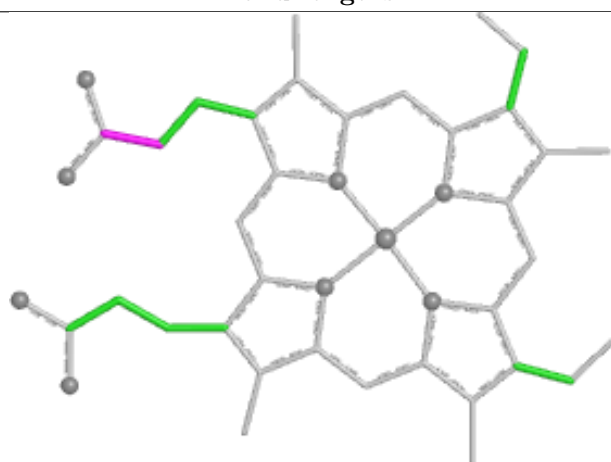
Ligand HEM I 1503



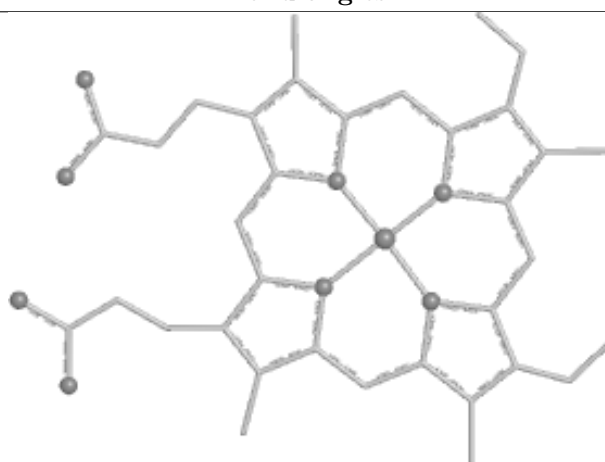
Bond lengths



Bond angles

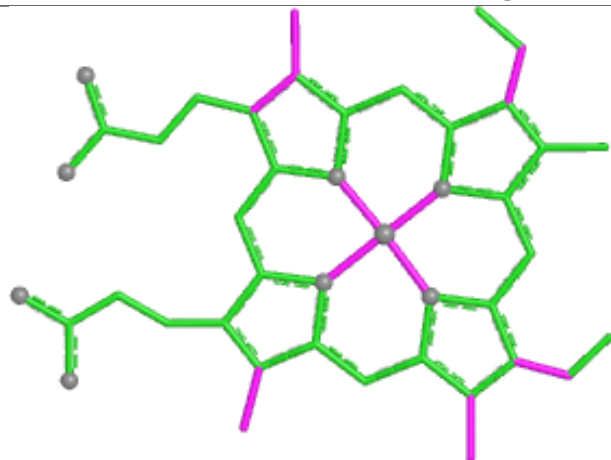


Torsions

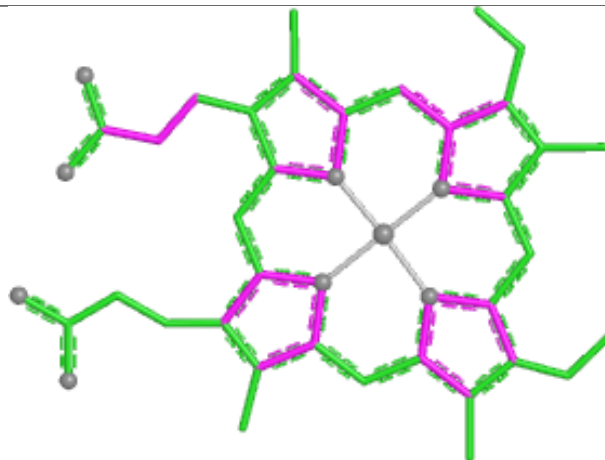


Rings

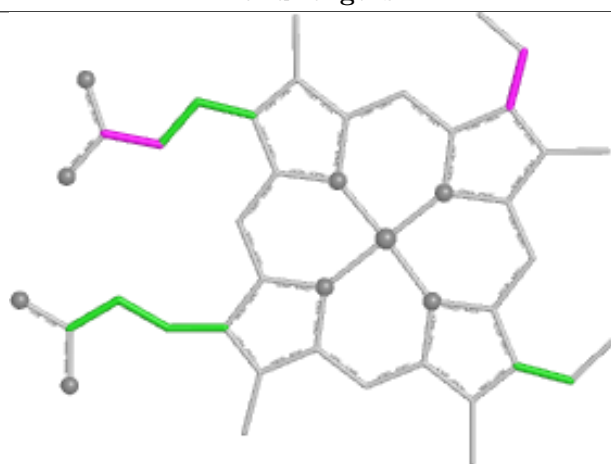
Ligand HEM H 1503



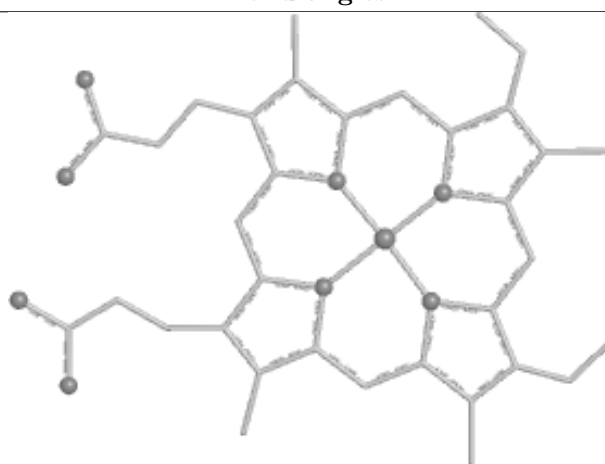
Bond lengths



Bond angles

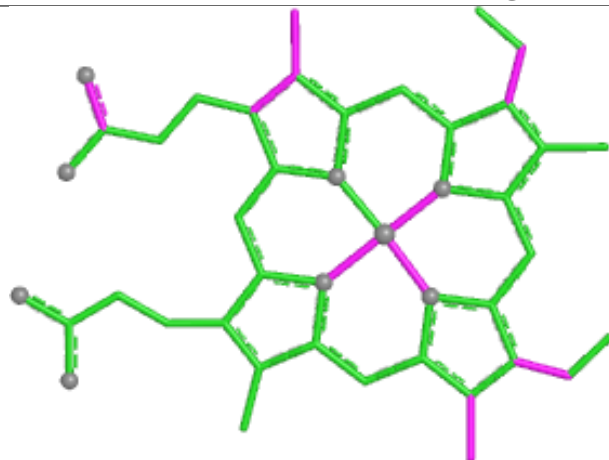


Torsions

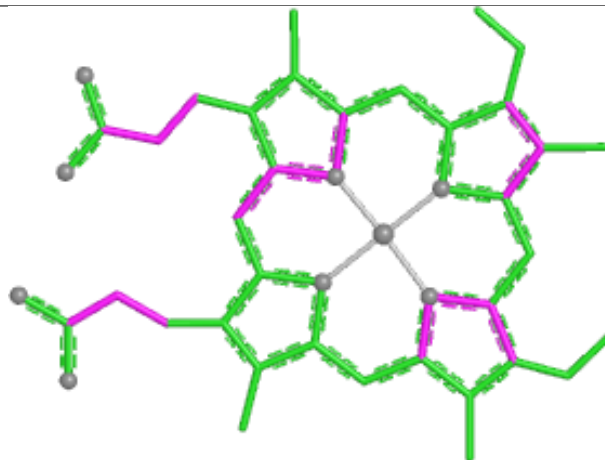


Rings

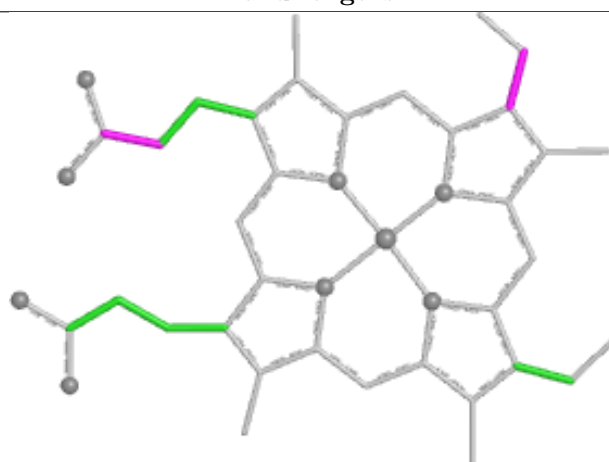
Ligand HEM J 1503



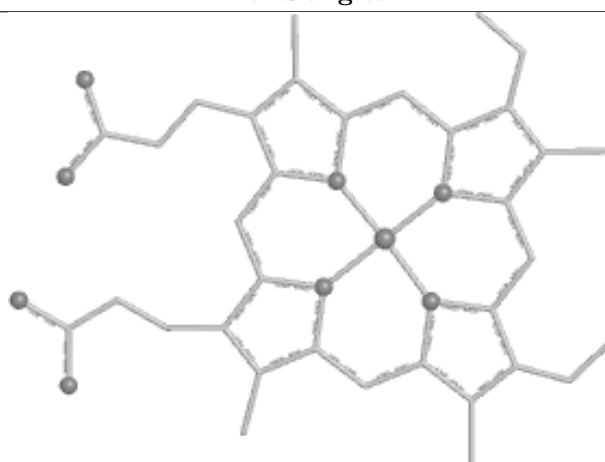
Bond lengths



Bond angles

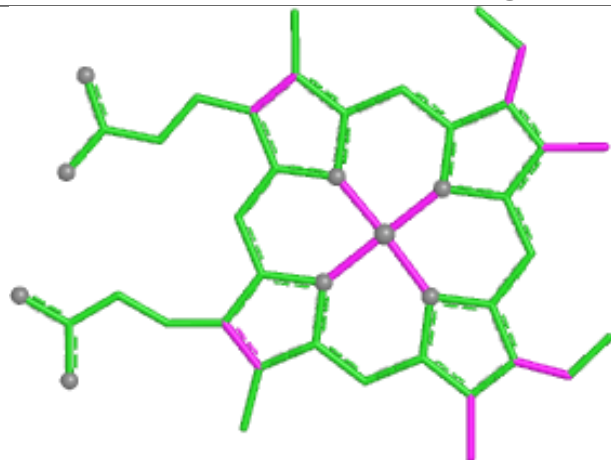


Torsions

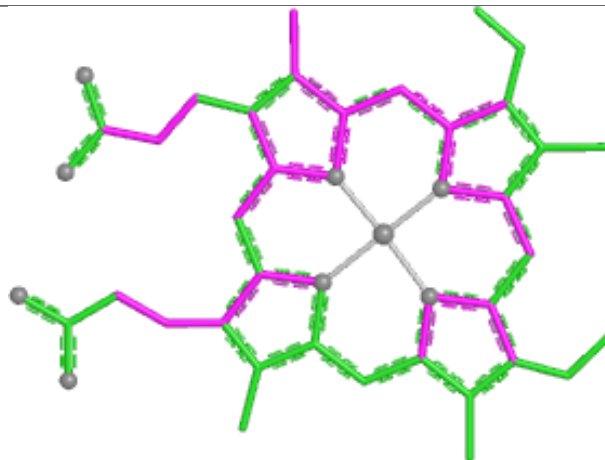


Rings

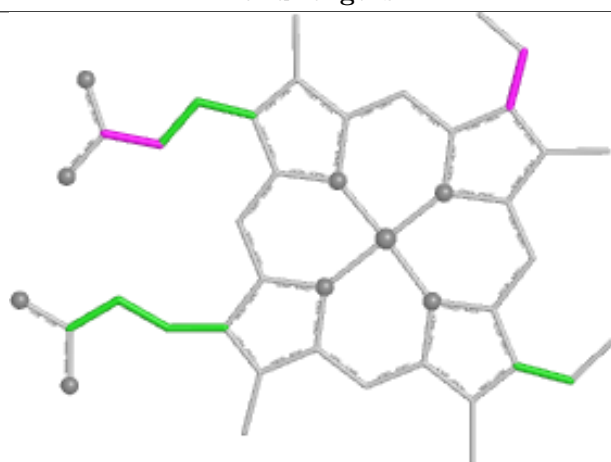
Ligand HEM E 1503



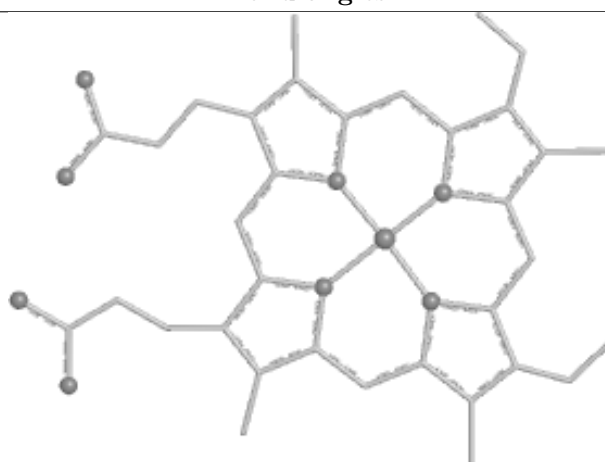
Bond lengths



Bond angles

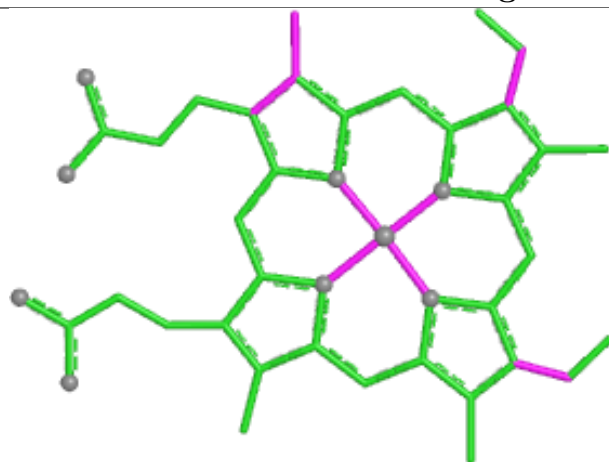


Torsions

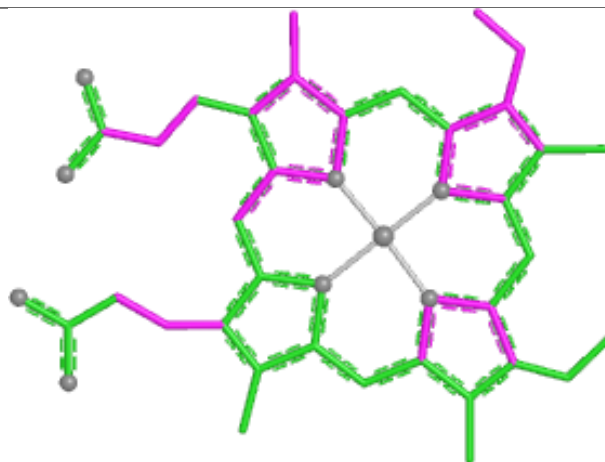


Rings

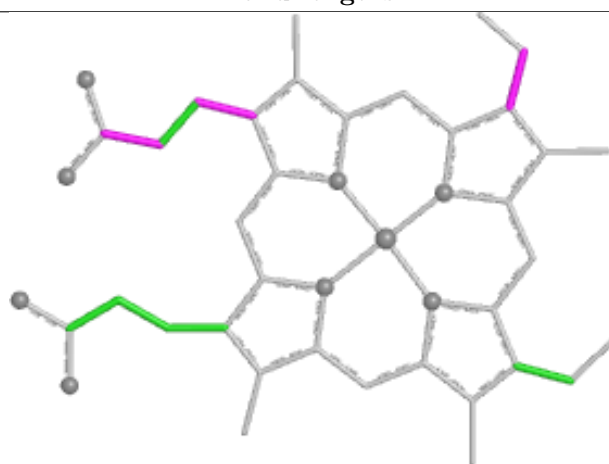
Ligand HEM K 1503



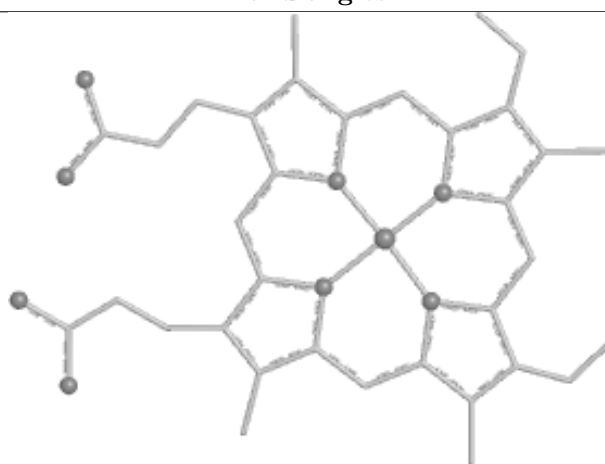
Bond lengths



Bond angles

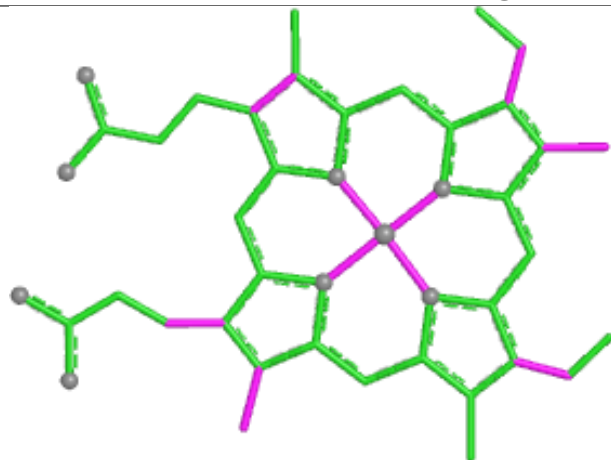


Torsions

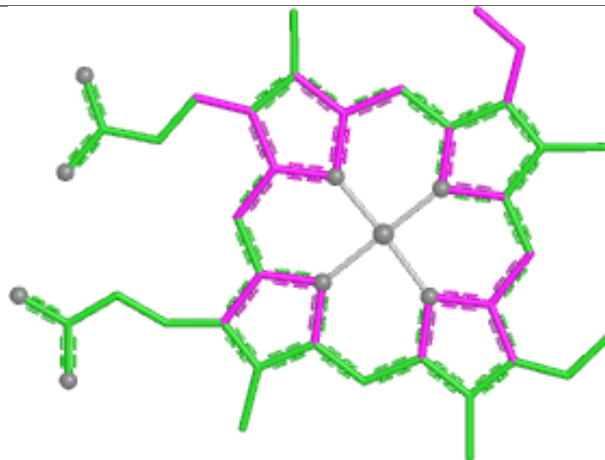


Rings

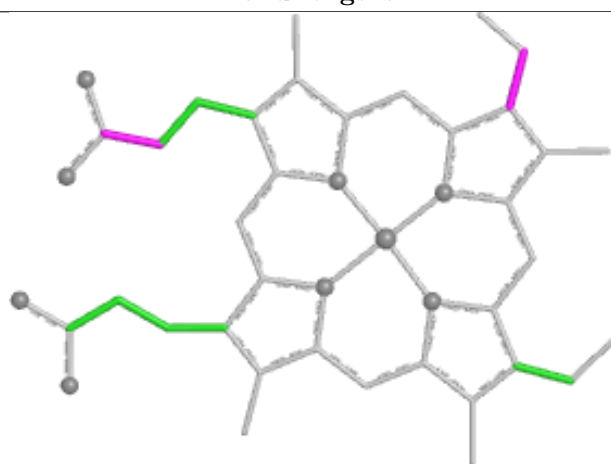
Ligand HEM M 1503



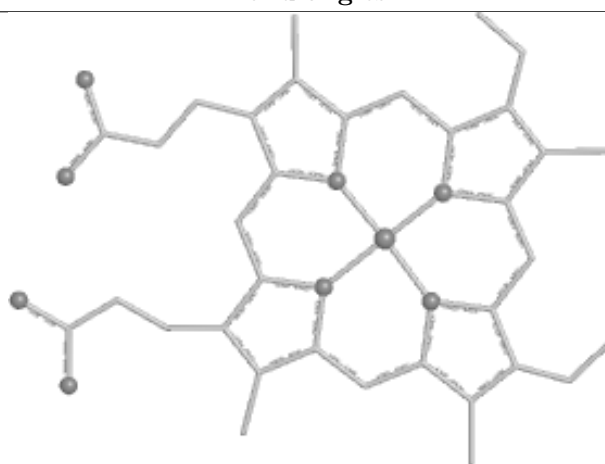
Bond lengths



Bond angles

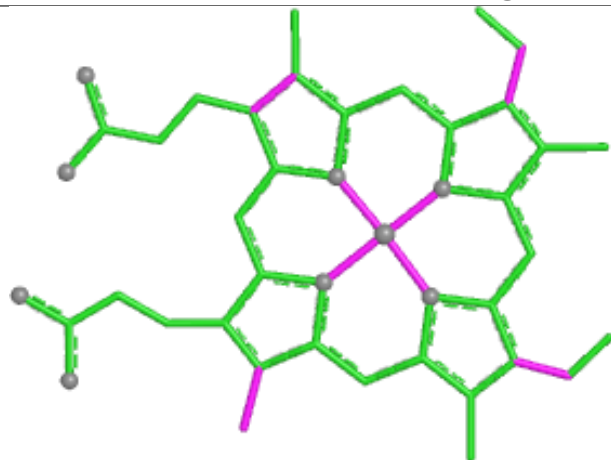


Torsions

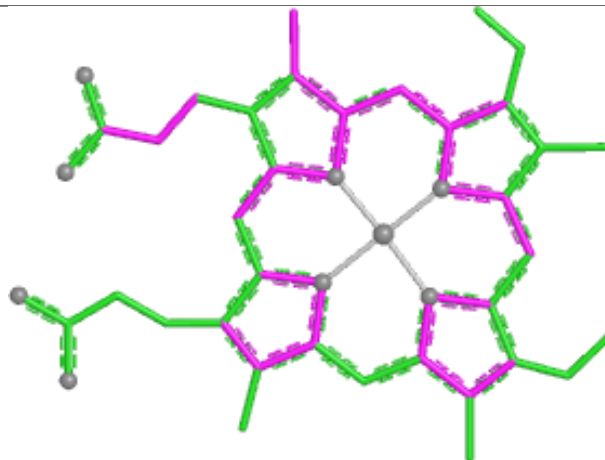


Rings

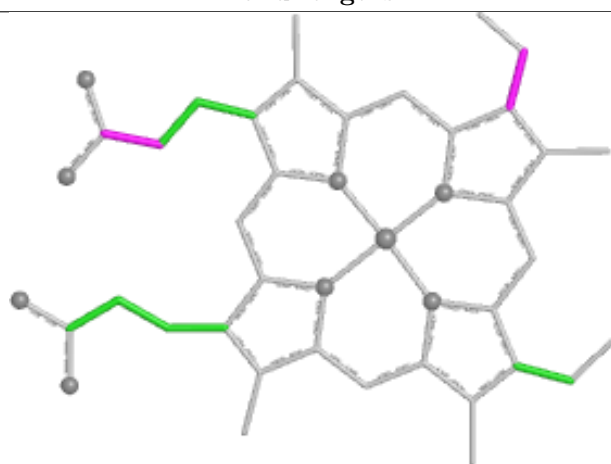
Ligand HEM G 1503



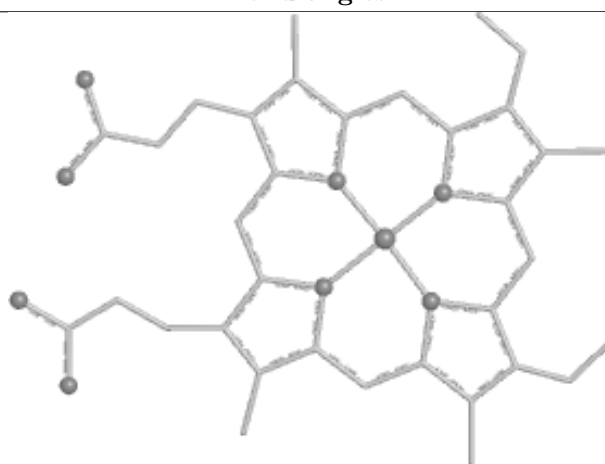
Bond lengths



Bond angles

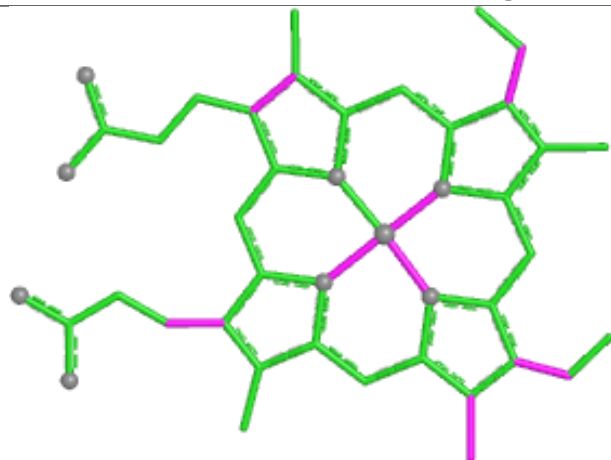


Torsions

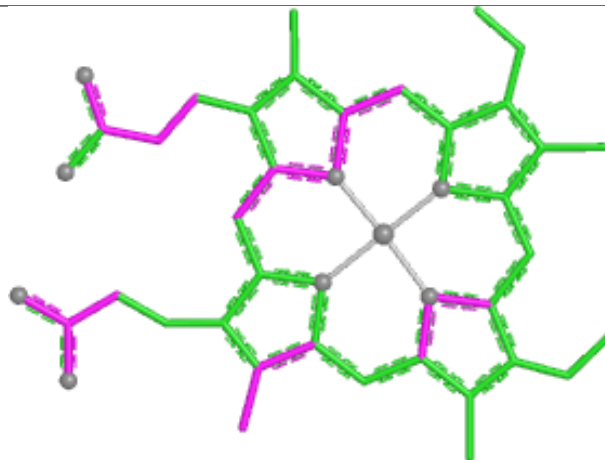


Rings

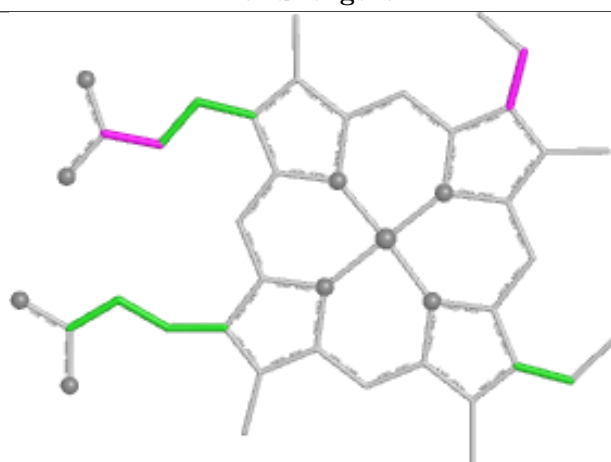
Ligand HEM C 1503



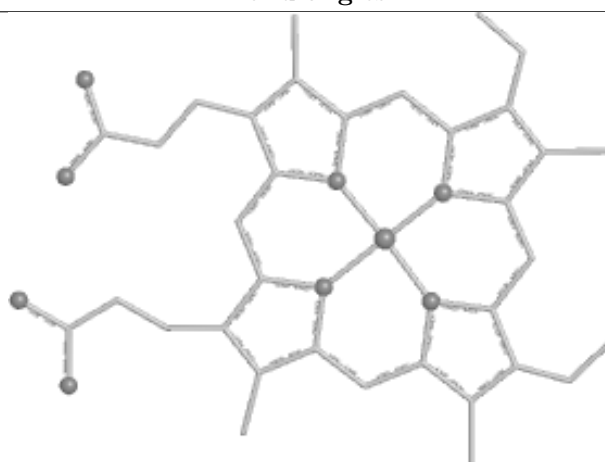
Bond lengths



Bond angles

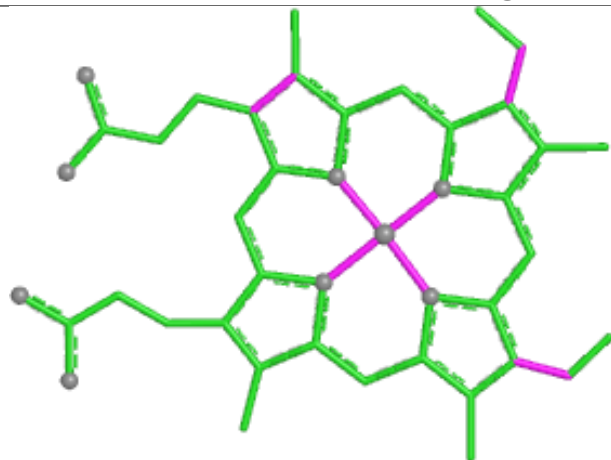


Torsions

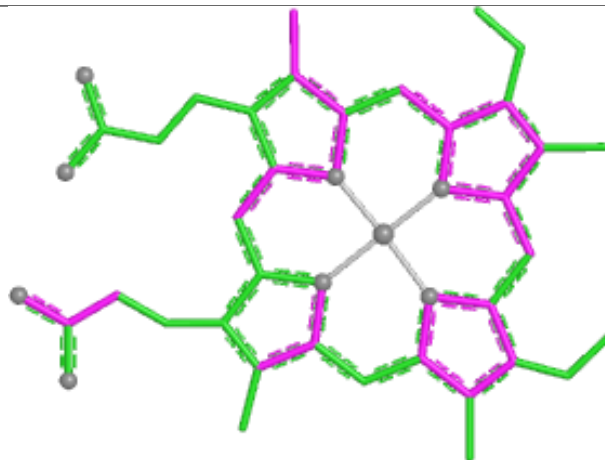


Rings

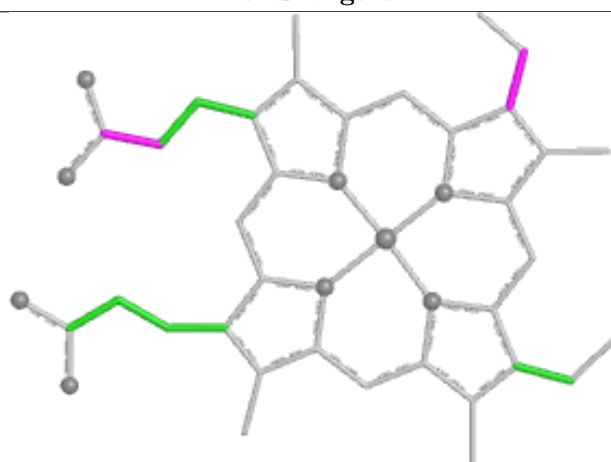
Ligand HEM N 1503



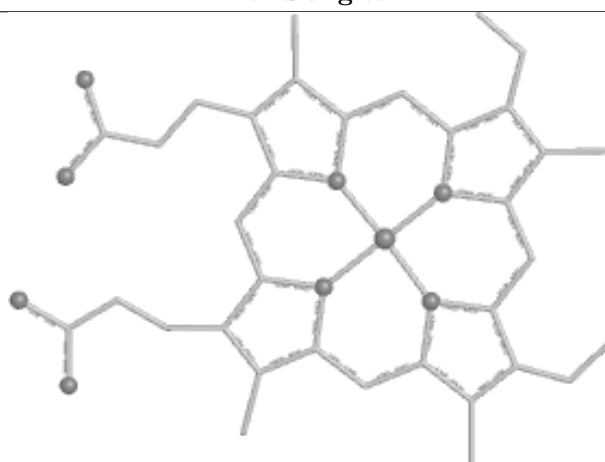
Bond lengths



Bond angles

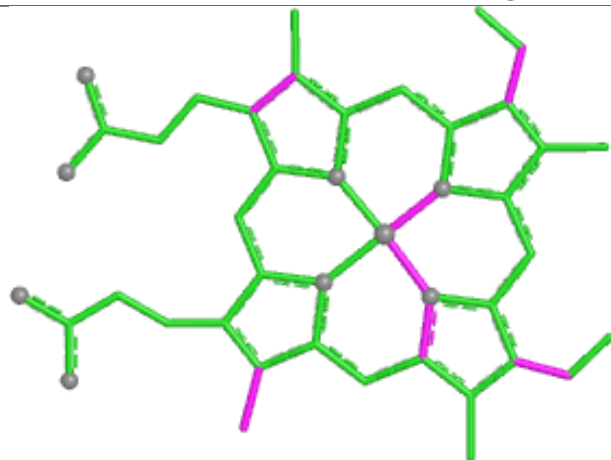


Torsions

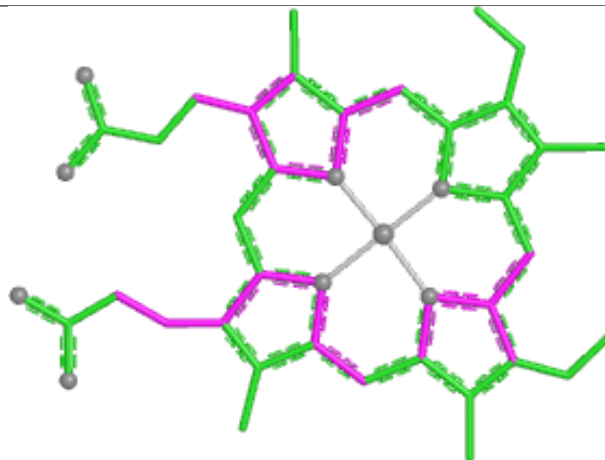


Rings

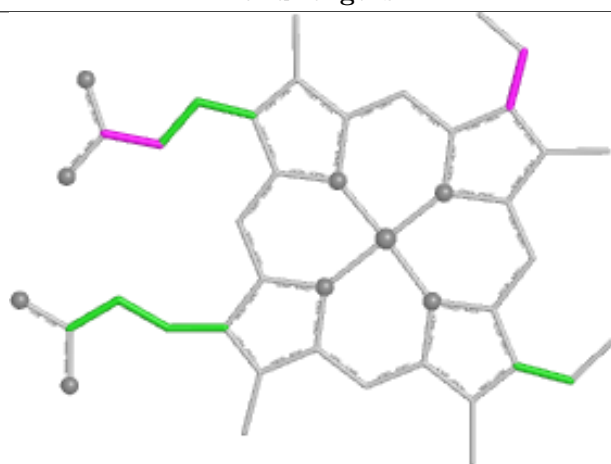
Ligand HEM L 1503



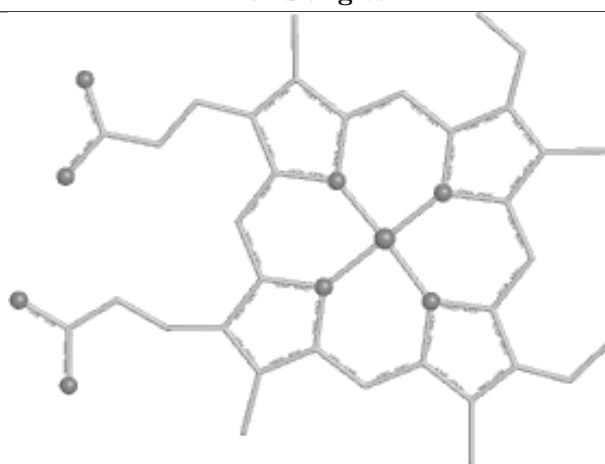
Bond lengths



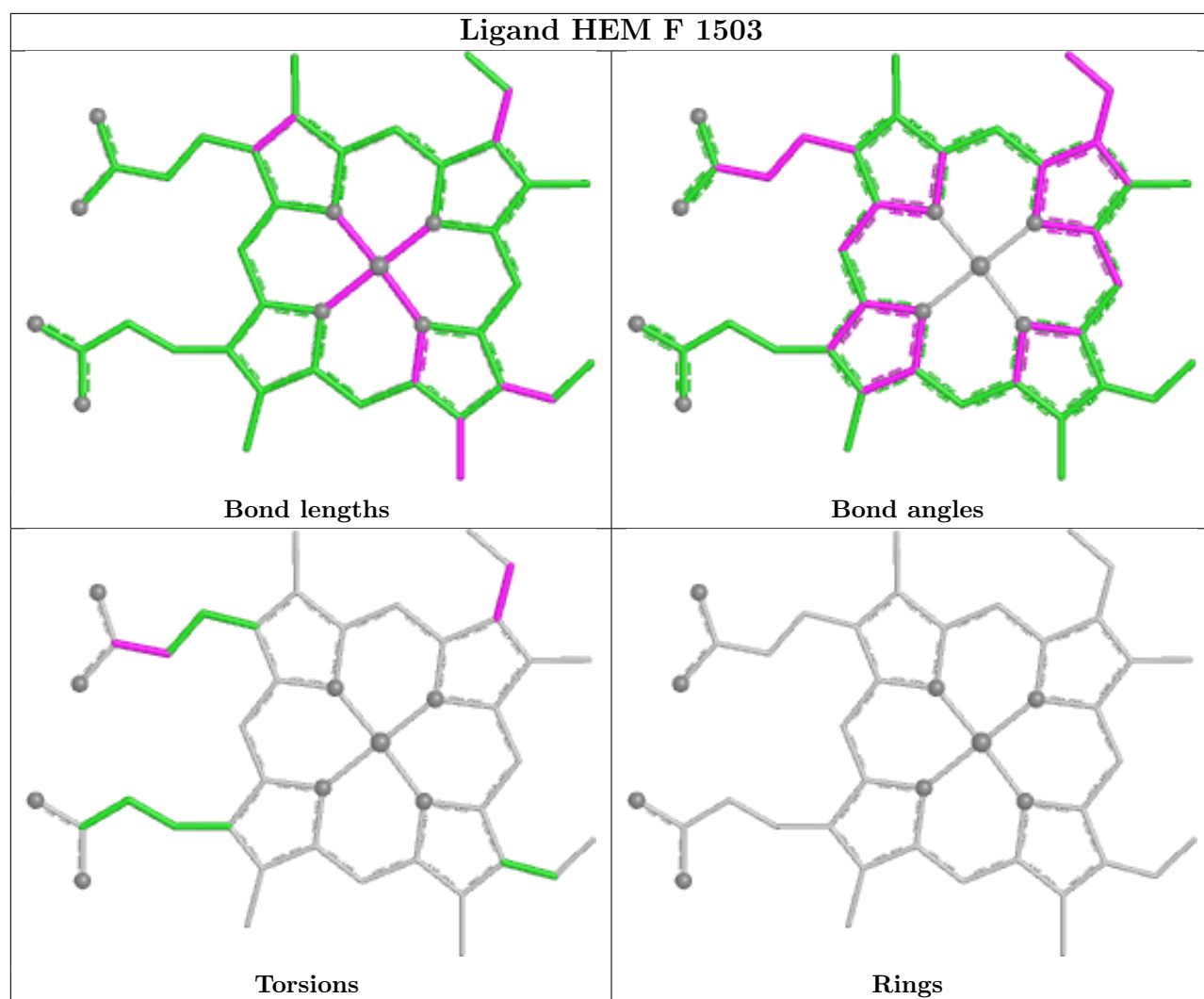
Bond angles



Torsions



Rings



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, 95th 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	491/509 (96%)	-0.37	0 100 100	21, 41, 67, 105	0
1	B	494/509 (97%)	-0.30	2 (0%) 88 85	20, 41, 68, 105	0
1	C	492/509 (96%)	-0.31	2 (0%) 88 85	20, 41, 68, 122	0
1	D	494/509 (97%)	-0.40	1 (0%) 91 89	20, 42, 69, 105	0
1	E	490/509 (96%)	-0.36	2 (0%) 88 85	20, 41, 68, 105	0
1	F	494/509 (97%)	-0.34	9 (1%) 67 59	20, 40, 69, 151	0
1	G	491/509 (96%)	-0.31	2 (0%) 88 85	20, 41, 68, 105	0
1	H	487/509 (95%)	-0.38	1 (0%) 91 89	21, 41, 68, 109	0
1	I	491/509 (96%)	-0.31	4 (0%) 82 77	20, 41, 69, 105	0
1	J	491/509 (96%)	-0.30	3 (0%) 85 81	21, 41, 68, 105	0
1	K	490/509 (96%)	-0.39	3 (0%) 85 81	20, 41, 69, 105	0
1	L	489/509 (96%)	-0.37	2 (0%) 88 85	21, 41, 69, 104	0
1	M	491/509 (96%)	-0.37	2 (0%) 88 85	22, 42, 69, 105	0
1	N	491/509 (96%)	-0.32	1 (0%) 91 89	22, 42, 69, 105	0
1	O	493/509 (96%)	-0.44	1 (0%) 91 89	21, 42, 70, 105	0
1	P	491/509 (96%)	-0.31	3 (0%) 85 81	21, 42, 70, 105	0
All	All	7860/8144 (96%)	-0.35	38 (0%) 87 83	20, 41, 69, 151	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	501	ALA	6.6
1	L	501	ALA	6.2
1	M	501	ALA	6.1
1	K	501	ALA	6.0
1	E	501	ALA	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	P	501	ALA	5.7
1	O	501	ALA	5.7
1	D	501	ALA	5.5
1	C	501	ALA	5.0
1	B	501	ALA	4.8
1	H	501	ALA	4.1
1	G	501	ALA	3.4
1	B	407	VAL	3.2
1	C	4	PRO	3.2
1	F	500	LYS	2.9
1	G	406	ALA	2.9
1	J	2	ALA	2.5
1	F	416	PRO	2.5
1	F	404	GLN	2.5
1	J	499	ARG	2.4
1	I	4	PRO	2.4
1	I	470	PHE	2.4
1	F	405	TYR	2.3
1	L	407	VAL	2.2
1	I	500	LYS	2.2
1	M	497	LEU	2.2
1	K	404	GLN	2.2
1	P	406	ALA	2.1
1	F	499	ARG	2.1
1	P	4	PRO	2.1
1	E	470	PHE	2.1
1	N	497	LEU	2.1
1	K	4	PRO	2.1
1	J	405	TYR	2.1
1	F	497	LEU	2.0
1	F	447	GLY	2.0
1	F	369	LEU	2.0
1	I	407	VAL	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 oligosaccharides in this entry.

6.4 Ligands

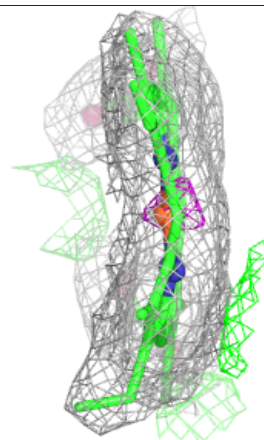
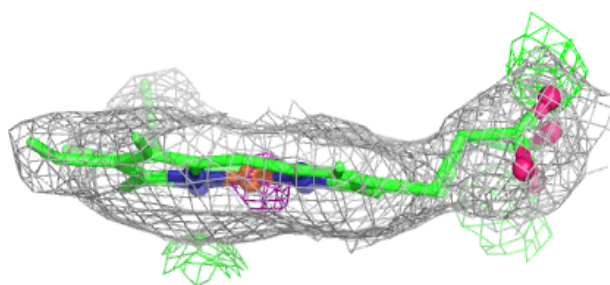
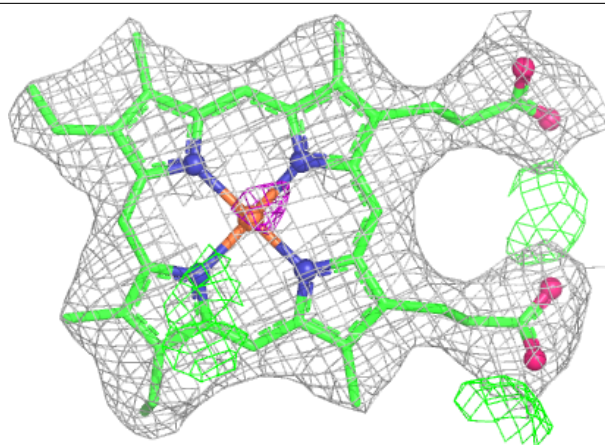
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	C	1503	43/43	0.96	0.07	19,25,31,34	0
2	HEM	D	1503	43/43	0.96	0.07	21,32,36,40	0
2	HEM	E	1503	43/43	0.96	0.08	22,30,35,38	0
2	HEM	H	1503	43/43	0.96	0.07	22,41,45,47	0
2	HEM	N	1503	43/43	0.96	0.08	28,37,39,41	0
2	HEM	O	1503	43/43	0.96	0.08	20,32,35,39	0
2	HEM	B	1503	43/43	0.97	0.06	16,26,31,34	0
2	HEM	I	1503	43/43	0.97	0.07	25,34,39,43	0
2	HEM	J	1503	43/43	0.97	0.07	24,34,39,41	0
2	HEM	K	1503	43/43	0.97	0.07	20,30,35,38	0
2	HEM	L	1503	43/43	0.97	0.07	22,27,31,35	0
2	HEM	M	1503	43/43	0.97	0.07	27,33,37,39	0
2	HEM	F	1503	43/43	0.97	0.07	17,25,29,34	0
2	HEM	G	1503	43/43	0.97	0.07	19,24,29,32	0
2	HEM	P	1503	43/43	0.97	0.07	31,41,44,46	0

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.

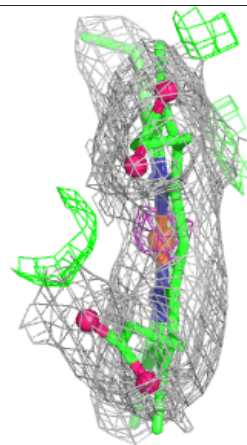
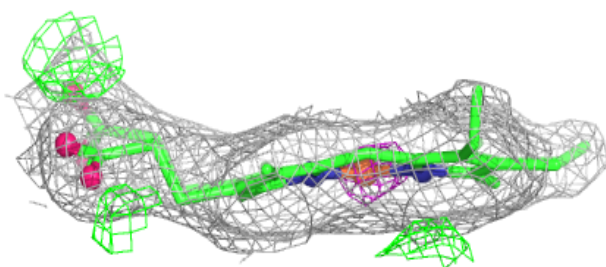
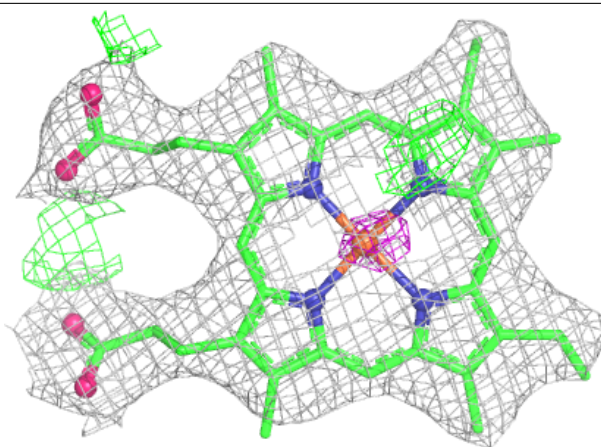
Electron density around HEM C 1503:

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



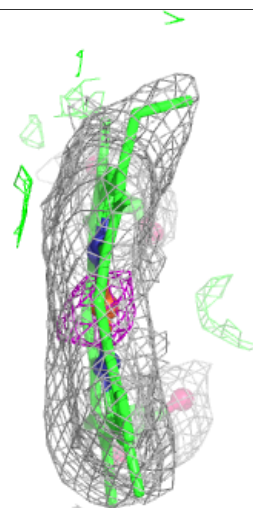
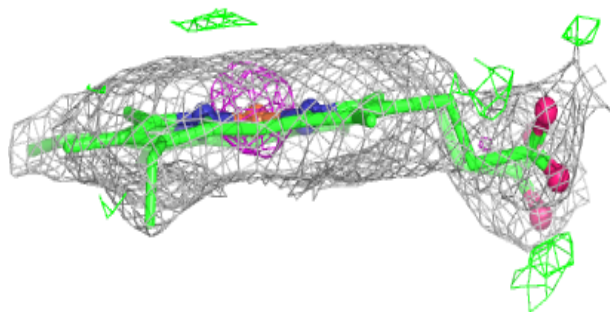
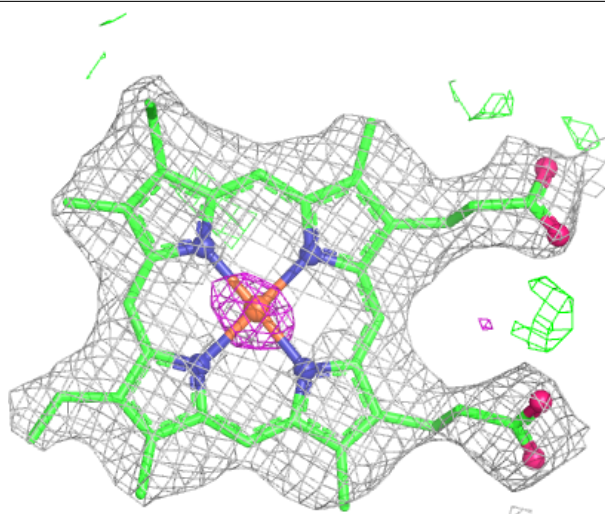
Electron density around HEM D 1503:

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



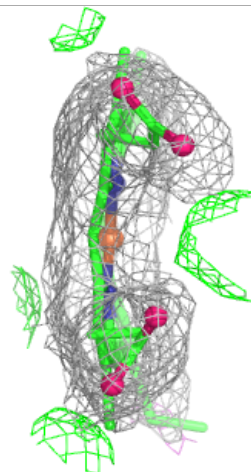
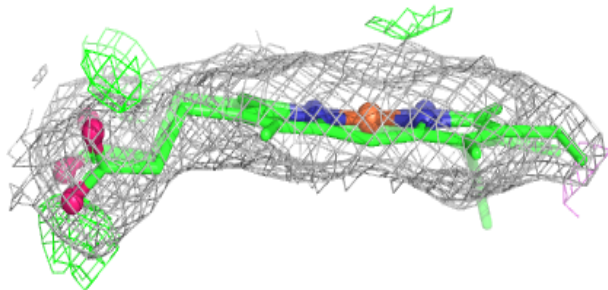
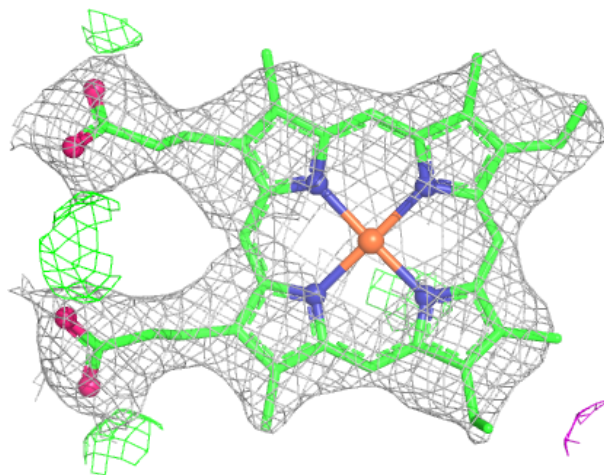
Electron density around HEM E 1503:

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



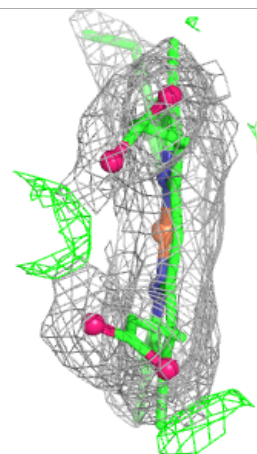
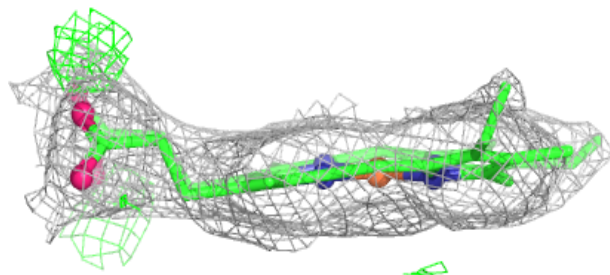
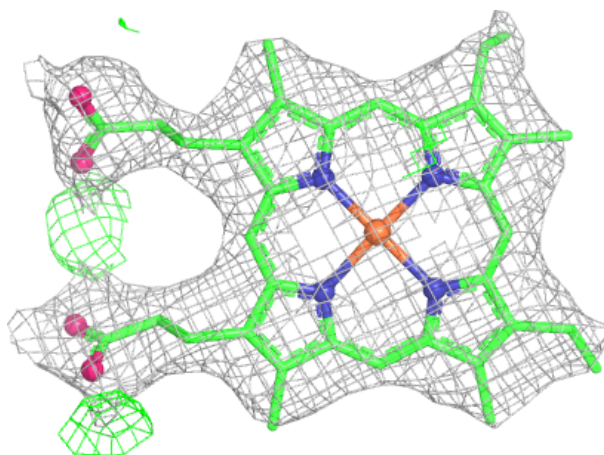
Electron density around HEM H 1503:

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



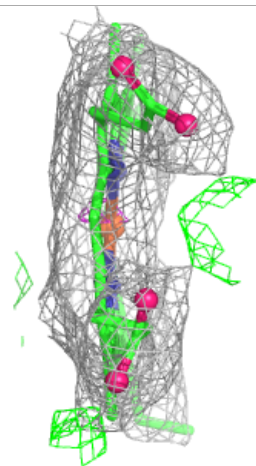
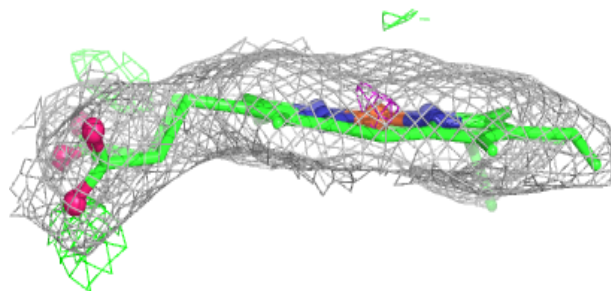
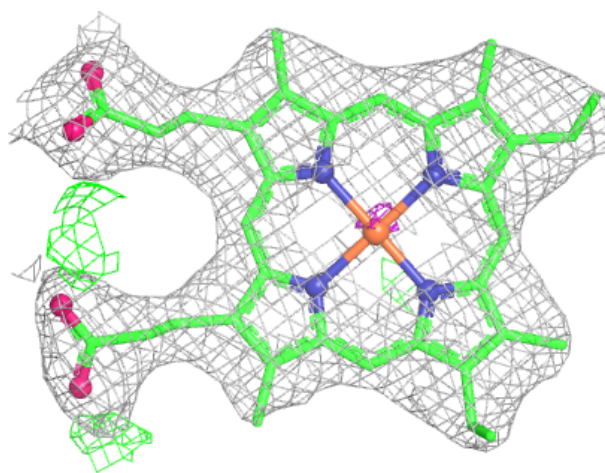
Electron density around HEM N 1503:

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



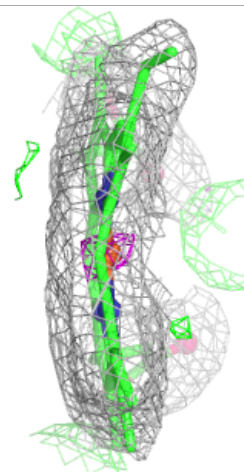
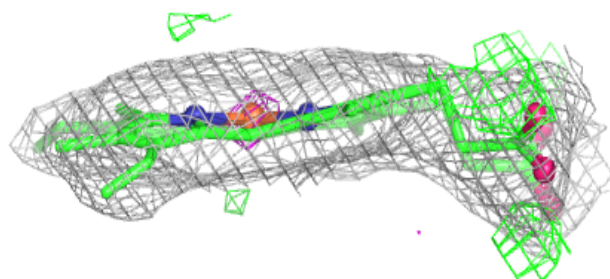
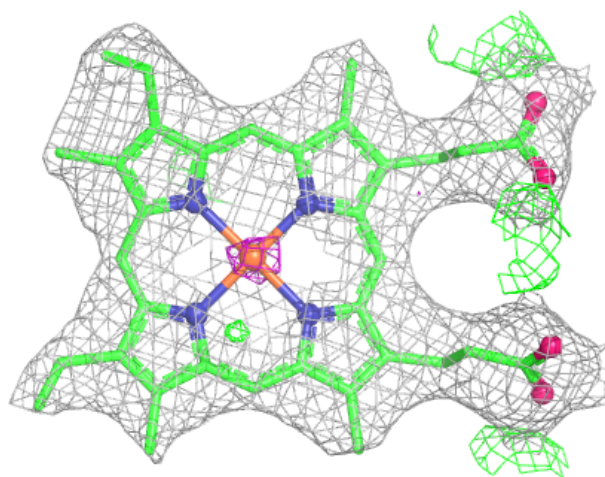
Electron density around HEM O 1503:

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



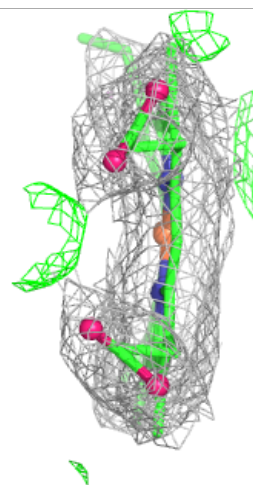
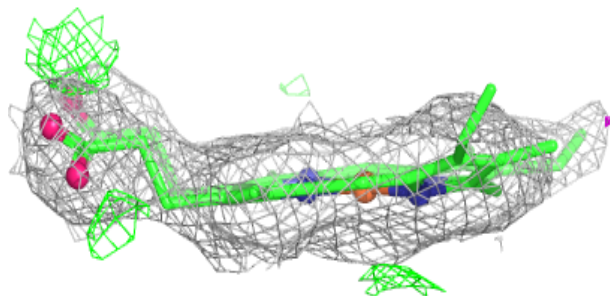
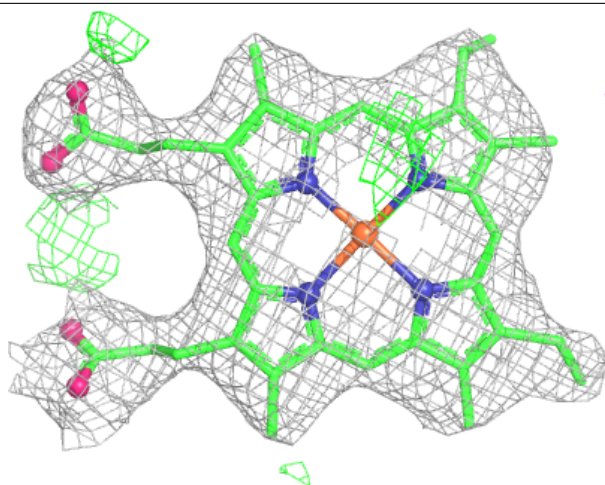
Electron density around HEM B 1503:

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



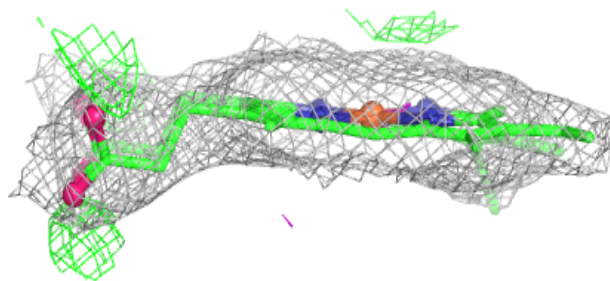
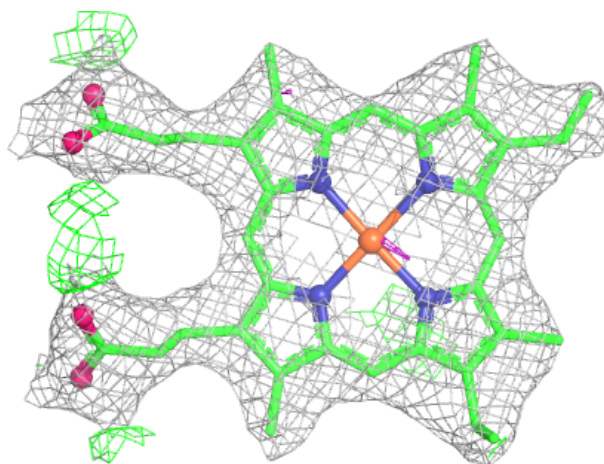
Electron density around HEM I 1503:

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



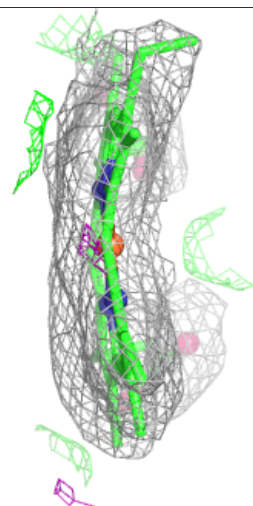
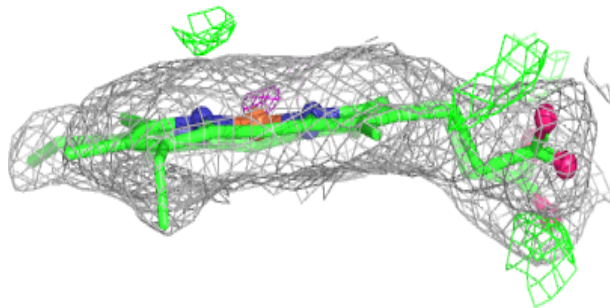
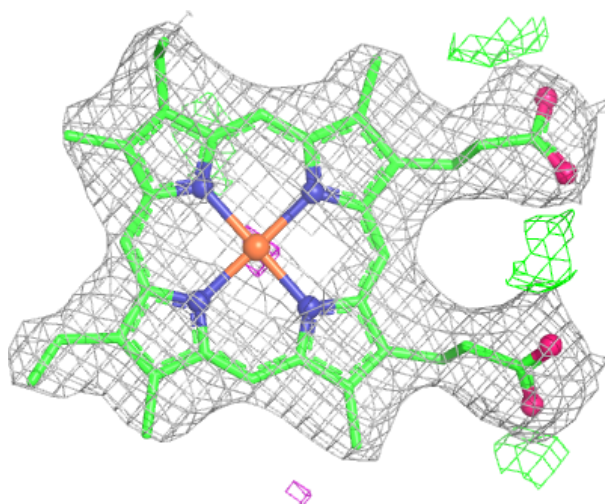
Electron density around HEM J 1503:

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



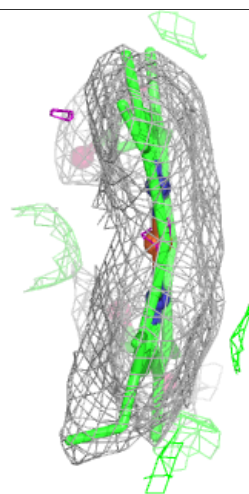
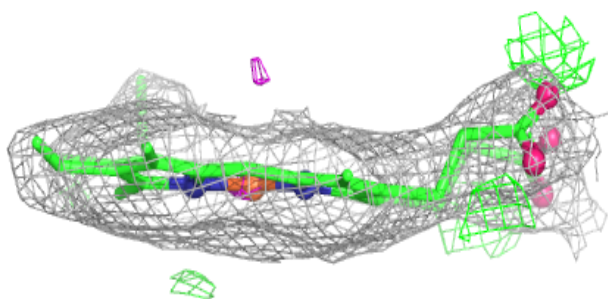
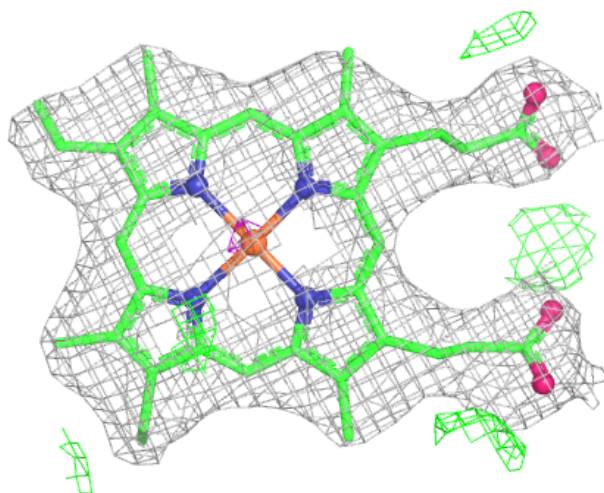
Electron density around HEM K 1503:

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



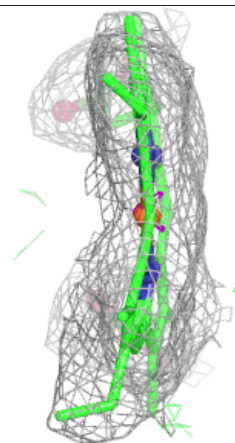
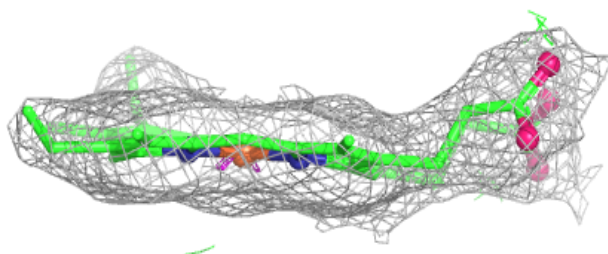
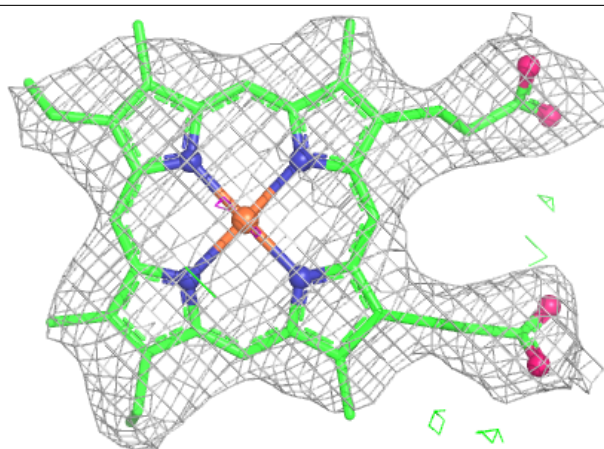
Electron density around HEM L 1503:

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



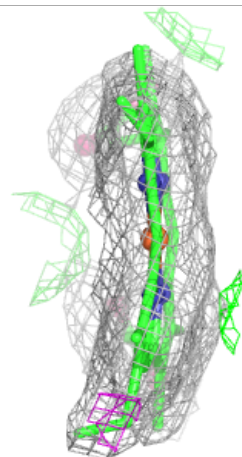
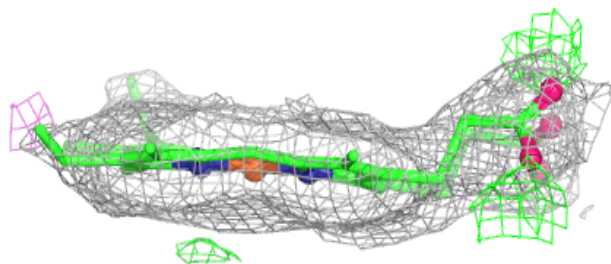
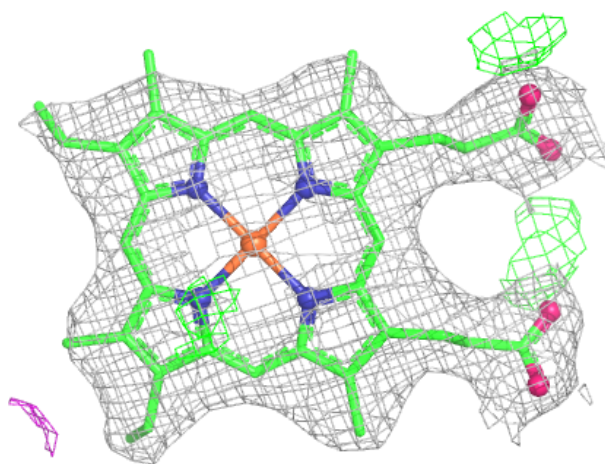
Electron density around HEM M 1503:

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



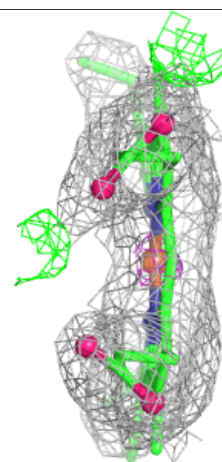
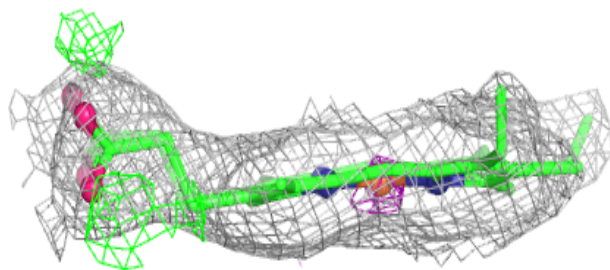
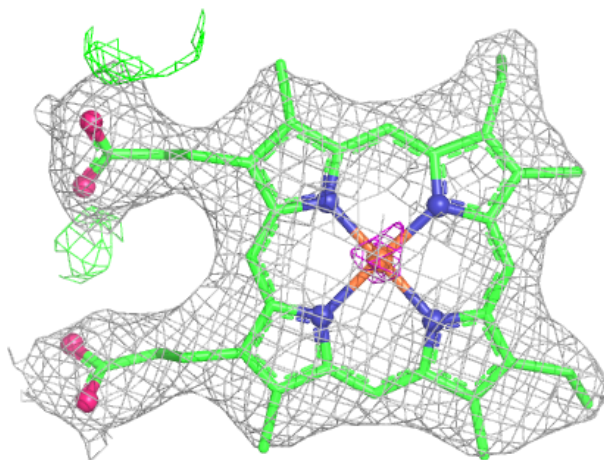
Electron density around HEM F 1503:

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



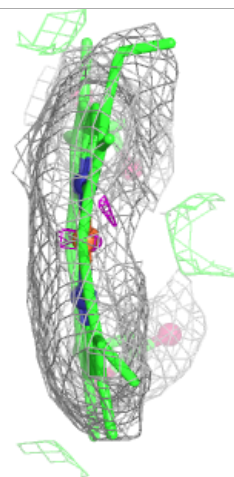
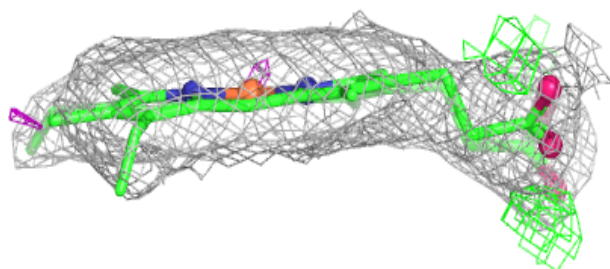
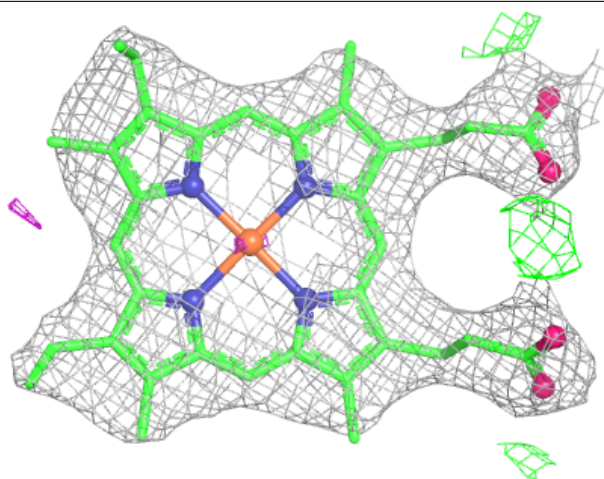
Electron density around HEM G 1503:

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



Electron density around HEM P 1503:

$2mF_o-DF_c$ (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.