Full wwPDB X-ray Structure Validation Report (i)

Aug 25, 2026 – 07:04 am BST

PDB ID	:	6ZI2 / pdb_00006zi2
Title	:	OleP-oleandolide(DEO) in low salt crystallization conditions
Authors	:	Savino, C.; Montemiglio, L.C.; Vallone, B.; Parisi, G.; Cecchetti, C.
Deposited on	:	2020-06-24
Resolution	:	2.93 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

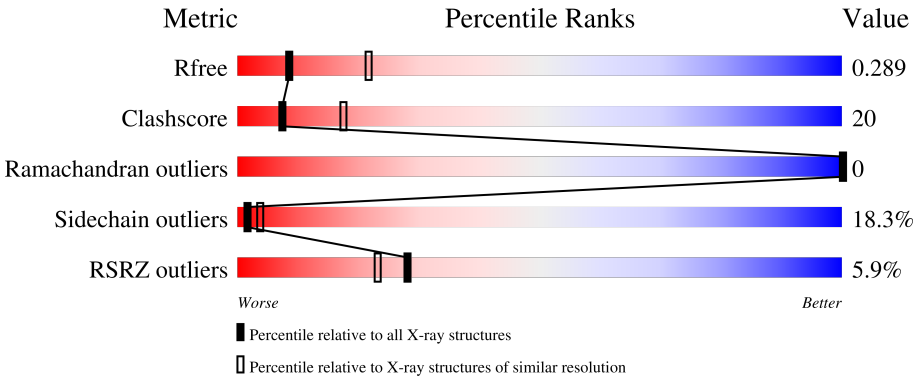
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.93 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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

Mol	Chain	Length	Quality of chain
1	A	407	59% 32% 5% ·
1	B	407	3% 54% 32% 11% ·
1	C	407	54% 36% 7% ·
1	D	407	2% 62% 30% 5% ·
1	E	407	2% 58% 30% 7% 5%

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Mol	Chain	Length	Quality of chain
1	F	407	3% 61% 29% 7%
1	G	407	10% 58% 29% 7% 6%
1	H	407	3% 59% 31% 7%
1	I	407	26% 30% 24% 7% 39%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	QR8	E	502	X	X	-	-

2 Entry composition (i)

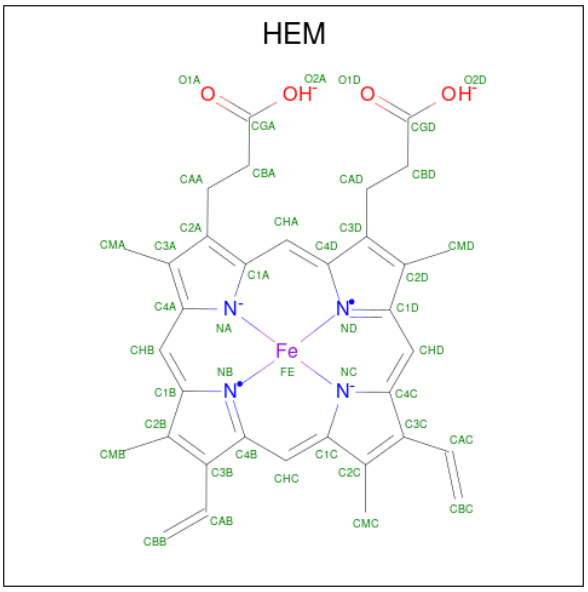
There are 4 unique types of molecules in this entry. The entry contains 27067 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cytochrome P-450.

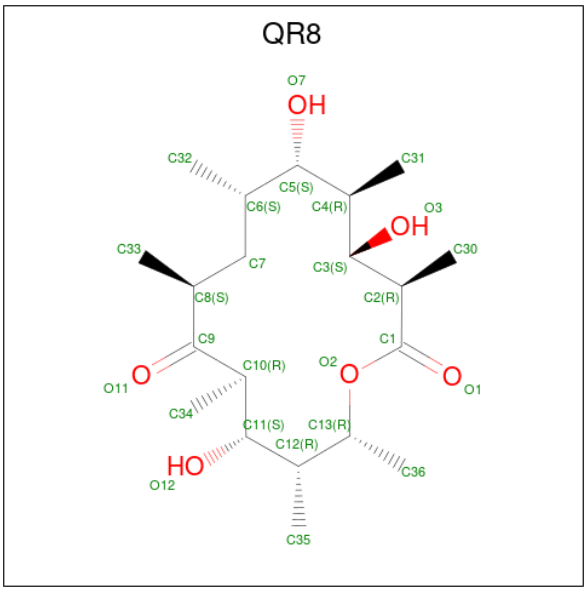
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3073	1934	551	575	13			
1	B	395	Total	C	N	O	S	0	0	0
			3078	1937	552	576	13			
1	C	395	Total	C	N	O	S	0	0	0
			3078	1937	552	576	13			
1	D	394	Total	C	N	O	S	0	0	0
			3067	1931	548	575	13			
1	E	386	Total	C	N	O	S	0	0	0
			3012	1897	540	563	12			
1	F	394	Total	C	N	O	S	0	0	0
			3073	1934	551	575	13			
1	G	381	Total	C	N	O	S	0	0	0
			2976	1879	534	550	13			
1	H	395	Total	C	N	O	S	0	0	0
			3078	1937	552	576	13			
1	I	248	Total	C	N	O	S	0	0	0
			1915	1214	344	346	11			

- 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	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is (3 {R},4 {S},5 {R},6 {S},7 {S},9 {S},11 {R},12 {S},13 {R},14 {R})-3,5,7,9,11,13,14-heptamethyl-4,6,12-tris(oxidanyl)-1-oxacyclotetradecane-2,10-dione (CCD ID: QR8) (formula: $C_{20}H_{36}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 26 20 6	0	0
3	B	1	Total C O 26 20 6	0	0
3	C	1	Total C O 26 20 6	0	0
3	D	1	Total C O 26 20 6	0	0
3	E	1	Total C O 26 20 6	0	0
3	F	1	Total C O 26 20 6	0	0
3	G	1	Total C O 26 20 6	0	0
3	H	1	Total C O 26 20 6	0	0
3	I	1	Total C O 26 20 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	19	Total O 19 19	0	0
4	B	7	Total O 7 7	0	0
4	C	14	Total O 14 14	0	0

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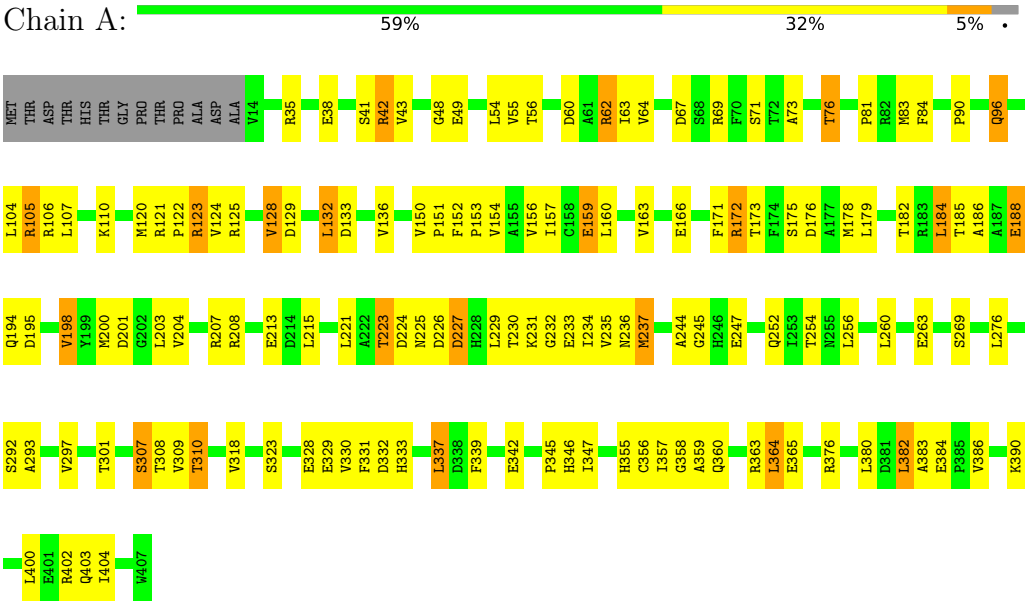
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	25	Total O 25 25	0	0
4	E	6	Total O 6 6	0	0
4	F	7	Total O 7 7	0	0
4	G	9	Total O 9 9	0	0
4	H	4	Total O 4 4	0	0
4	I	5	Total O 5 5	0	0

3 Residue-property plots (i)

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

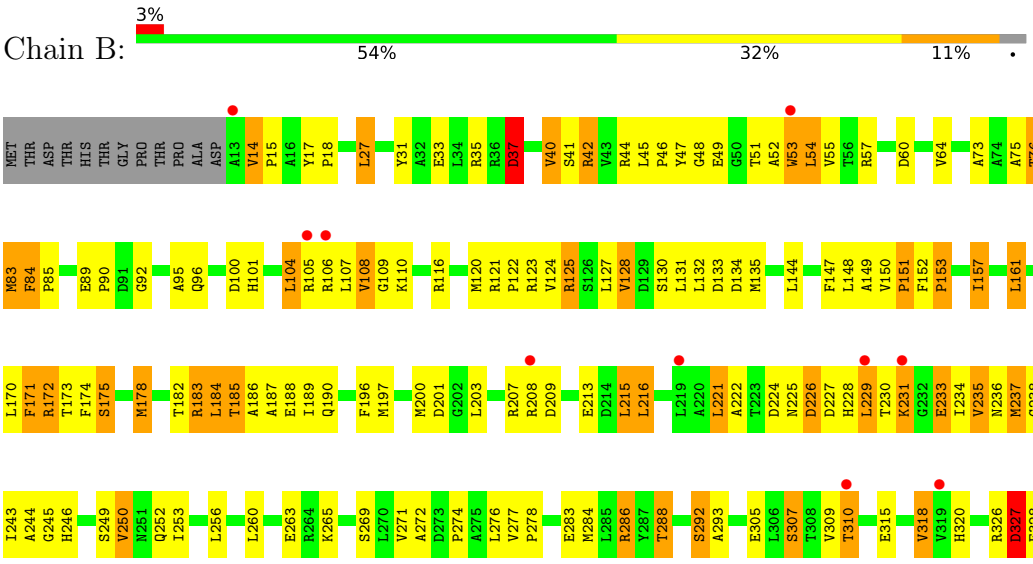
• Molecule 1: Cytochrome P-450

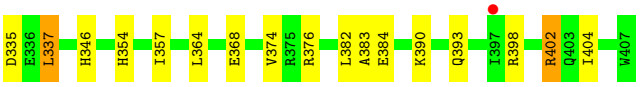
Chain A:



• Molecule 1: Cytochrome P-450

Chain B:

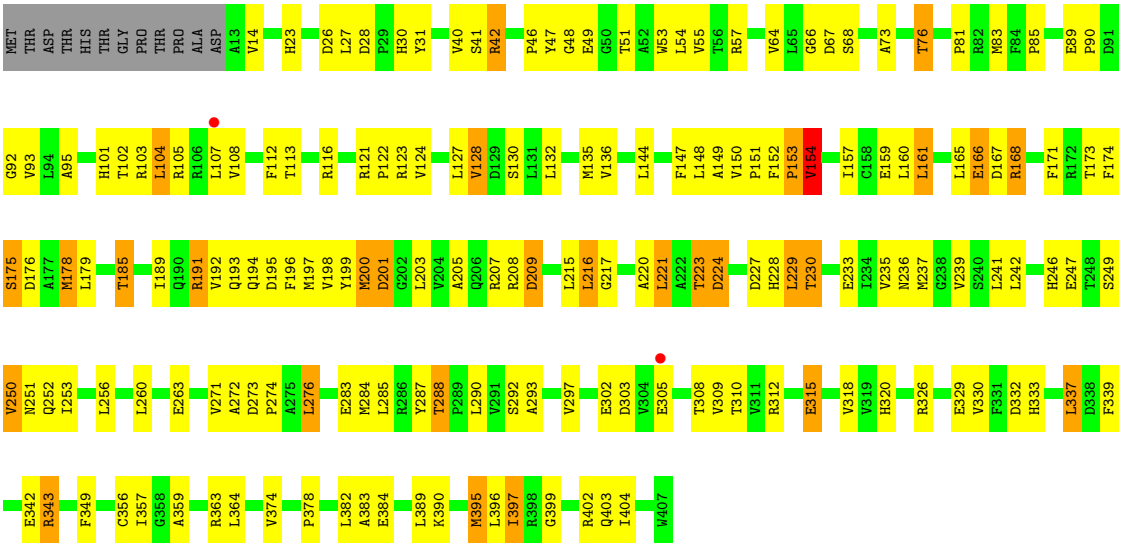




• Molecule 1: Cytochrome P-450

Chain C:

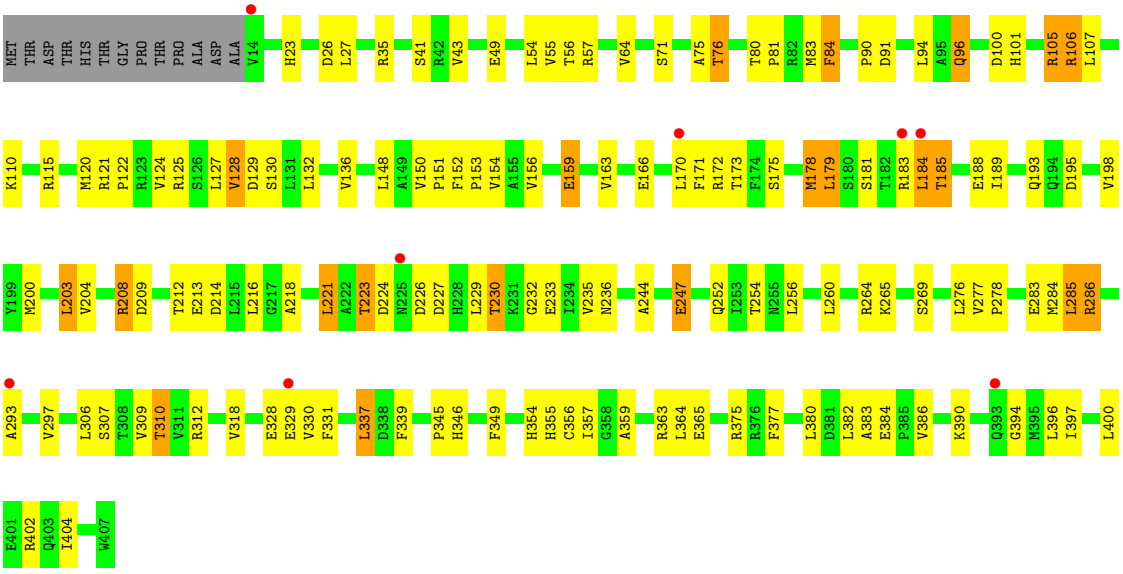




• Molecule 1: Cytochrome P-450

Chain D:

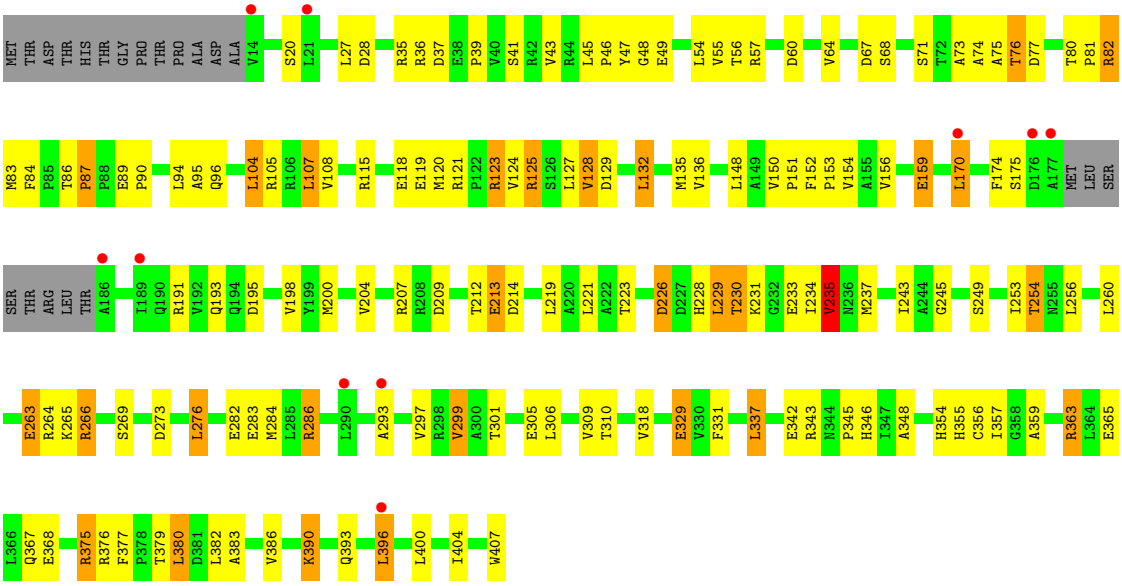




• Molecule 1: Cytochrome P-450

Chain E:

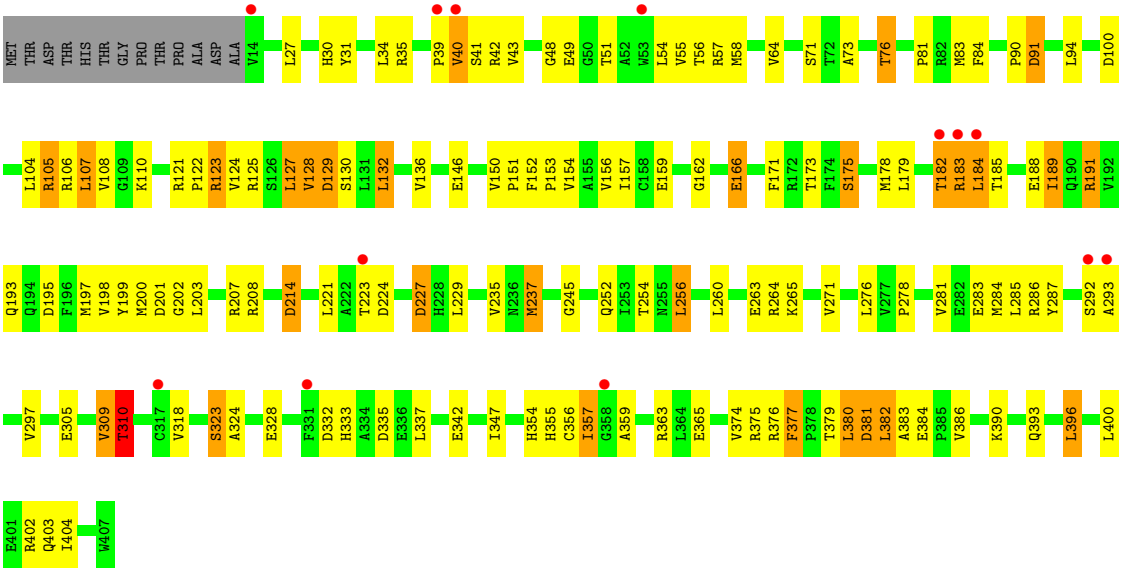




• Molecule 1: Cytochrome P-450

Chain F:

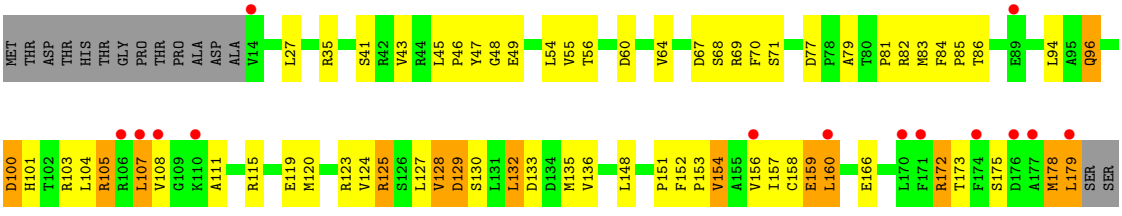


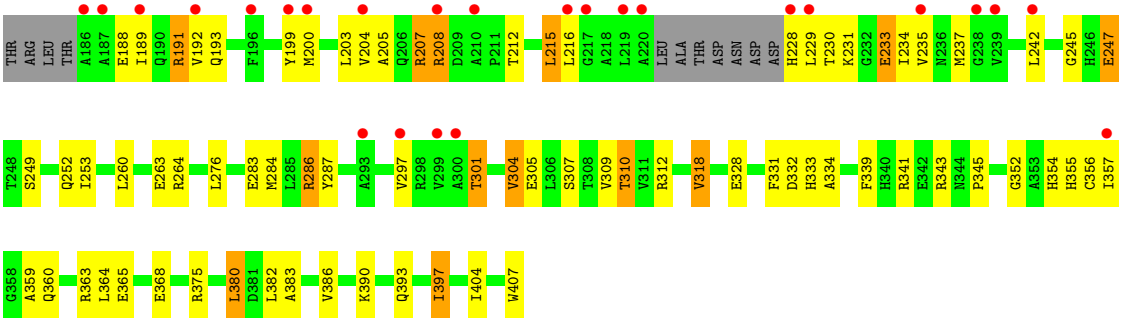


• Molecule 1: Cytochrome P-450

Chain G:



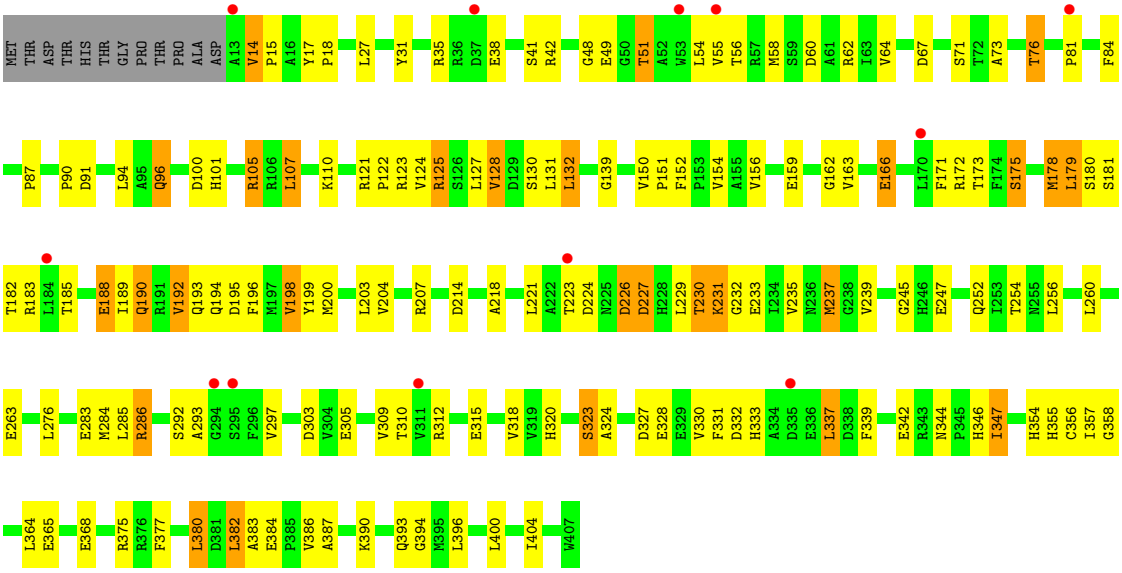




• Molecule 1: Cytochrome P-450

Chain H:

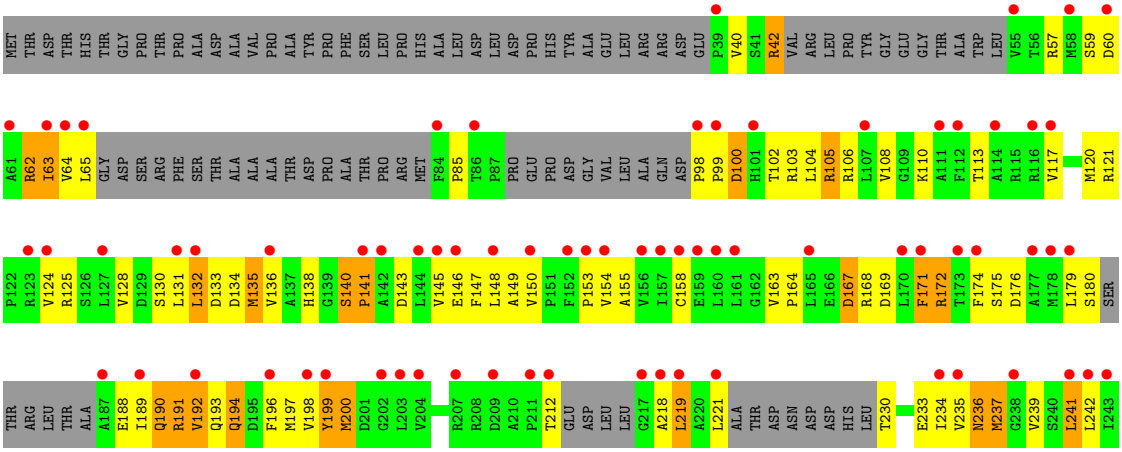


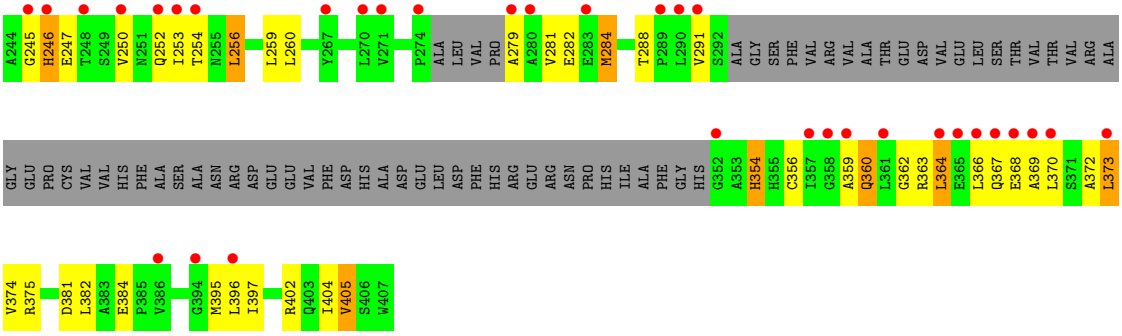


• Molecule 1: Cytochrome P-450

Chain I:






A244 G245 H246 E247 T248 S249 V250 N251 Q252 I253 T254 N255 L256 L259 L260 Y267 L270 V271 P274 ALA LEU VAL PRO A279 A280 V281 E282 E283 M284 T288 P289 L290 V291 S292 ALA GLY SER PHE VAL ARG VAL ALA THR GLU ASP VAL GLU LEU SER THR VAL THR VAL ARG ALA
GLY GLU PRO CYS VAL VAL HIS PHE ALA SER ALA ASN ARG ASP GLU GLU VAL PHE ASP HIS ALA ASP GLU LEU ASP PHE HIS ARG GLU ARG ASN PRO HIS ILE ALA PHE GLY HIS G352 A353 H354 H355 C356 I357 G358 A359 Q360 L361 G362 R363 L364 E365 L366 Q367 E368 A369 L370 S371 A372 L373
V374 R375 D381 L382 A383 E384 P385 V386 G394 M395 L396 I397 R402 Q403 I404 V405 S406 W407

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	112.07Å 116.64Å 125.17Å 104.43° 104.25° 113.91°	Depositor
Resolution (Å)	39.89 – 2.93 39.89 – 2.93	Depositor EDS
% Data completeness (in resolution range)	84.2 (39.89-2.93) 84.1 (39.89-2.93)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.239 , 0.291 0.240 , 0.289	Depositor DCC
R_{free} test set	4684 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	44.1	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 39.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.015 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	27067	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QR8, 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	1.06	0/3140	1.42	4/4277 (0.1%)
1	B	1.02	0/3145	1.43	8/4284 (0.2%)
1	C	1.03	1/3145 (0.0%)	1.43	6/4284 (0.1%)
1	D	1.05	1/3134 (0.0%)	1.41	3/4270 (0.1%)
1	E	0.97	1/3078 (0.0%)	1.41	4/4192 (0.1%)
1	F	0.97	0/3140	1.37	4/4277 (0.1%)
1	G	0.99	0/3041	1.41	6/4138 (0.1%)
1	H	0.98	0/3145	1.40	6/4284 (0.1%)
1	I	1.16	2/1942 (0.1%)	1.61	6/2622 (0.2%)
All	All	1.02	5/26910 (0.0%)	1.43	47/36628 (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	D	0	1
1	H	0	1
1	I	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	141	PRO	C-O	-17.84	0.87	1.23
1	D	285	LEU	C-O	6.19	1.31	1.24
1	C	285	LEU	C-O	5.44	1.30	1.24
1	I	212	THR	C-O	5.23	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	390	LYS	C-O	5.10	1.29	1.23

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	141	PRO	O-C-N	13.72	147.17	121.10
1	I	141	PRO	CA-C-O	-9.18	98.17	120.20
1	A	225	ASN	N-CA-C	-8.64	100.75	112.94
1	C	201	ASP	CA-CB-CG	-7.87	104.73	112.60
1	C	154	VAL	N-CA-C	-6.99	103.71	110.42
1	B	153	PRO	CB-CA-C	-6.95	101.36	112.21
1	G	159	GLU	CB-CG-CD	6.83	124.20	112.60
1	H	139	GLY	CA-C-O	-6.82	117.53	122.23
1	B	327	ASP	CA-CB-CG	6.53	119.13	112.60
1	F	310	THR	CB-CA-C	6.43	120.84	109.72
1	B	151	PRO	CB-CA-C	-6.11	103.38	112.55
1	A	224	ASP	CA-CB-CG	6.08	118.68	112.60
1	H	87	PRO	N-CA-CB	6.04	106.57	103.19
1	E	87	PRO	N-CA-CB	6.00	106.55	103.19
1	E	379	THR	CA-CB-OG1	-5.95	100.67	109.60
1	C	112	PHE	CB-CA-C	-5.86	101.27	110.94
1	B	171	PHE	CA-CB-CG	5.85	119.65	113.80
1	C	159	GLU	CB-CA-C	5.80	119.99	110.88
1	A	310	THR	CB-CA-C	5.76	119.69	109.72
1	E	363	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	I	218	ALA	CA-C-N	5.67	127.88	120.28
1	I	218	ALA	C-N-CA	5.67	127.88	120.28
1	B	224	ASP	CA-C-N	5.58	128.22	120.29
1	B	224	ASP	C-N-CA	5.58	128.22	120.29
1	B	310	THR	CB-CA-C	5.49	119.19	110.19
1	F	335	ASP	CA-CB-CG	-5.46	107.14	112.60
1	B	37	ASP	CA-CB-CG	5.36	117.96	112.60
1	C	153	PRO	CB-CA-C	-5.36	104.28	112.11
1	H	67	ASP	CA-CB-CG	5.33	117.94	112.60
1	C	399	GLY	CA-C-O	-5.29	116.43	121.62
1	F	223	THR	N-CA-C	-5.29	106.96	113.41
1	D	306	LEU	CA-C-N	5.27	128.11	120.79
1	D	306	LEU	C-N-CA	5.27	128.11	120.79
1	F	227	ASP	N-CA-C	-5.25	103.10	110.50
1	I	194	GLN	CA-C-N	5.20	127.51	120.44
1	I	194	GLN	C-N-CA	5.20	127.51	120.44
1	A	364	LEU	N-CA-C	-5.19	105.51	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	387	ALA	CA-C-N	5.14	126.56	120.14
1	H	387	ALA	C-N-CA	5.14	126.56	120.14
1	H	110	LYS	CB-CA-C	-5.12	102.15	110.85
1	G	352	GLY	CA-C-N	5.10	127.63	120.28
1	G	352	GLY	C-N-CA	5.10	127.63	120.28
1	D	310	THR	CB-CA-C	5.09	118.52	109.72
1	G	133	ASP	CA-CB-CG	5.08	117.68	112.60
1	E	235	VAL	N-CA-C	-5.02	105.60	110.42
1	G	158	CYS	CA-C-N	5.01	127.31	120.54
1	G	158	CYS	C-N-CA	5.01	127.31	120.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	394	GLY	Peptide
1	B	402	ARG	Sidechain
1	D	394	GLY	Peptide
1	H	394	GLY	Peptide
1	I	140	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3073	0	3051	108	0
1	B	3078	0	3056	166	0
1	C	3078	0	3057	123	0
1	D	3067	0	3041	84	0
1	E	3012	0	2983	118	0
1	F	3073	0	3052	98	0
1	G	2976	0	2961	100	0
1	H	3078	0	3057	127	0
1	I	1915	0	1945	133	0
2	A	43	0	30	12	0
2	B	43	0	30	5	0
2	C	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	43	0	30	8	0
2	E	43	0	30	15	0
2	F	43	0	30	10	0
2	G	43	0	30	8	0
2	H	43	0	30	12	0
2	I	43	0	30	7	0
3	A	26	0	0	10	0
3	B	26	0	0	2	0
3	C	26	0	0	1	0
3	D	26	0	0	4	0
3	E	26	0	0	5	0
3	F	26	0	0	4	0
3	G	26	0	0	4	0
3	H	26	0	0	4	0
3	I	26	0	0	5	0
4	A	19	0	0	2	0
4	B	7	0	0	1	0
4	C	14	0	0	1	0
4	D	25	0	0	1	0
4	E	6	0	0	1	0
4	F	7	0	0	2	0
4	G	9	0	0	0	0
4	H	4	0	0	0	0
4	I	5	0	0	1	0
All	All	27067	0	26473	1085	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 20.

All (1085) 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:B:197:MET:HE1	1:B:235:VAL:CG1	1.70	1.21
1:I:135:MET:CE	1:I:147:PHE:HB2	1.71	1.20
1:B:185:THR:HG21	1:H:166:GLU:OE1	0.99	1.16
1:F:185:THR:O	1:F:189:ILE:HG22	1.45	1.16
1:D:185:THR:HB	1:D:188:GLU:HB2	1.18	1.14
1:B:185:THR:CG2	1:H:166:GLU:OE1	1.94	1.14
1:H:218:ALA:O	1:H:221:LEU:CD2	1.96	1.13
1:E:74:ALA:HB3	1:E:299:VAL:CG2	1.87	1.05
1:B:197:MET:HE1	1:B:235:VAL:HG12	1.34	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LEU:O	1:B:107:LEU:HB3	1.58	1.04
1:I:135:MET:HE3	1:I:147:PHE:HB2	1.40	1.03
1:F:198:VAL:O	1:F:201:ASP:OD1	1.76	1.02
1:D:185:THR:CB	1:D:188:GLU:HB2	1.89	1.02
1:C:40:VAL:HG21	1:C:309:VAL:HG12	1.40	1.01
1:A:42:ARG:HG2	1:A:42:ARG:HH11	1.22	1.00
1:H:185:THR:HG21	1:H:188:GLU:HB2	1.42	0.99
1:D:384:GLU:CD	1:D:402:ARG:HH22	1.71	0.98
1:H:218:ALA:O	1:H:221:LEU:HD23	1.63	0.96
1:I:200:MET:HA	1:I:200:MET:HE2	1.47	0.96
1:F:83:MET:HE2	1:F:293:ALA:HB1	1.48	0.95
1:B:41:SER:HB3	1:B:54:LEU:CD2	1.96	0.95
1:E:356:CYS:SG	2:E:501:HEM:NC	2.40	0.95
1:B:108:VAL:CG1	1:B:215:LEU:HD23	1.96	0.95
1:B:40:VAL:HG21	1:B:309:VAL:HG12	1.46	0.94
1:I:196:PHE:CE1	1:I:239:VAL:HG13	2.02	0.94
1:A:182:THR:O	1:A:185:THR:HG23	1.68	0.93
1:A:223:THR:HG23	1:A:226:ASP:HB2	1.50	0.92
1:B:197:MET:HE1	1:B:235:VAL:HG11	1.48	0.91
1:B:221:LEU:O	1:B:225:ASN:HB3	1.71	0.90
1:E:74:ALA:HB3	1:E:299:VAL:HG21	1.51	0.90
1:H:224:ASP:O	1:H:226:ASP:OD1	1.89	0.90
1:B:108:VAL:HG11	1:B:215:LEU:HD23	1.55	0.88
1:B:172:ARG:HG2	1:B:172:ARG:HH11	1.37	0.88
1:E:263:GLU:HB3	1:E:266:ARG:HD2	1.54	0.88
1:C:260:LEU:HG	1:C:284:MET:HE1	1.53	0.88
1:E:260:LEU:HG	1:E:284:MET:HE1	1.56	0.87
1:H:185:THR:CG2	1:H:188:GLU:HB2	2.06	0.86
1:B:237:MET:HE3	1:B:237:MET:O	1.76	0.86
1:H:218:ALA:O	1:H:221:LEU:HD21	1.74	0.86
1:A:105:ARG:NH2	1:A:355:HIS:O	2.09	0.86
1:B:40:VAL:HG21	1:B:309:VAL:CG1	2.05	0.85
1:C:200:MET:HE2	1:C:200:MET:HA	1.59	0.85
1:G:157:ILE:HD12	1:G:242:LEU:CD1	2.07	0.84
1:E:356:CYS:SG	2:E:501:HEM:ND	2.49	0.84
1:H:356:CYS:SG	2:H:501:HEM:NC	2.51	0.84
1:E:74:ALA:CB	1:E:299:VAL:HG21	2.09	0.83
1:B:330:VAL:HG13	1:B:331:PHE:CD2	2.13	0.83
1:I:260:LEU:HD13	1:I:284:MET:HE1	1.60	0.82
1:G:260:LEU:HG	1:G:284:MET:HE1	1.59	0.82
1:B:107:LEU:O	1:B:107:LEU:HD12	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LEU:HD23	1:B:54:LEU:O	1.78	0.82
1:E:231:LYS:O	1:E:234:ILE:HG22	1.80	0.82
1:E:356:CYS:SG	2:E:501:HEM:FE	1.69	0.82
1:B:197:MET:CE	1:B:235:VAL:CG1	2.57	0.82
1:I:135:MET:HE3	1:I:147:PHE:CB	2.09	0.81
1:I:369:ALA:O	1:I:373:LEU:HB2	1.79	0.81
1:H:185:THR:HG21	1:H:188:GLU:CB	2.10	0.81
2:E:501:HEM:HBA2	3:E:502:QR8:C32	2.10	0.81
1:B:183:ARG:C	1:B:184:LEU:HD23	2.05	0.81
1:G:231:LYS:O	1:G:234:ILE:HG22	1.81	0.81
1:F:356:CYS:SG	2:F:501:HEM:NC	2.53	0.81
1:D:179:LEU:HD11	1:D:247:GLU:HG3	1.62	0.81
1:D:260:LEU:HG	1:D:284:MET:HE1	1.63	0.81
1:B:260:LEU:HG	1:B:284:MET:HE1	1.63	0.80
1:B:354:HIS:HA	2:B:501:HEM:O2D	1.81	0.80
1:I:190:GLN:O	1:I:194:GLN:HG3	1.81	0.80
1:I:59:SER:O	1:I:63:ILE:HD13	1.81	0.80
1:I:197:MET:HE1	1:I:236:ASN:HA	1.64	0.80
1:B:48:GLY:HA3	1:B:81:PRO:HA	1.61	0.80
1:C:42:ARG:NH1	1:C:53:TRP:CZ2	2.50	0.80
2:E:501:HEM:HBB2	2:E:501:HEM:HMB2	1.65	0.79
1:C:92:GLY:HA2	1:C:236:ASN:ND2	1.98	0.79
1:G:356:CYS:SG	2:G:501:HEM:NB	2.54	0.79
1:B:197:MET:CE	1:B:235:VAL:HG11	2.11	0.79
1:A:48:GLY:HA3	1:A:81:PRO:HA	1.64	0.78
2:H:501:HEM:HBB2	2:H:501:HEM:HMB1	1.66	0.78
1:I:155:ALA:HA	1:I:158:CYS:SG	2.23	0.78
1:I:171:PHE:HZ	1:I:242:LEU:HD13	1.47	0.78
1:G:105:ARG:NH1	1:G:355:HIS:O	2.16	0.78
1:F:396:LEU:HD23	3:F:502:QR8:C34	2.14	0.77
1:B:41:SER:HB3	1:B:54:LEU:HD21	1.66	0.77
1:C:284:MET:O	1:C:288:THR:CG2	2.32	0.77
1:B:85:PRO:HG2	1:B:189:ILE:HD12	1.65	0.77
1:A:184:LEU:HD12	1:A:186:ALA:H	1.49	0.77
2:F:501:HEM:HMB2	2:F:501:HEM:HBB2	1.68	0.76
1:B:221:LEU:O	1:B:225:ASN:CB	2.33	0.76
1:F:396:LEU:CD2	3:F:502:QR8:C34	2.64	0.76
1:I:135:MET:CE	1:I:147:PHE:CB	2.59	0.76
1:I:197:MET:HE2	1:I:239:VAL:HG21	1.68	0.76
1:A:99:PRO:O	1:A:102:THR:HG22	1.86	0.75
1:B:166:GLU:N	1:B:166:GLU:OE2	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LEU:O	1:B:107:LEU:CB	2.34	0.75
1:E:82:ARG:HG3	1:E:82:ARG:HH11	1.52	0.75
1:F:40:VAL:HG21	1:F:309:VAL:HB	1.68	0.74
1:A:356:CYS:HB2	2:A:501:HEM:NA	2.02	0.74
1:C:40:VAL:HG21	1:C:309:VAL:CG1	2.18	0.74
1:A:244:ALA:CB	3:A:502:QR8:C31	2.66	0.74
1:F:185:THR:O	1:F:189:ILE:CG2	2.32	0.74
1:E:74:ALA:HB3	1:E:299:VAL:HG23	1.70	0.74
1:A:42:ARG:HH11	1:A:42:ARG:CG	2.01	0.74
1:E:119:GLU:HB2	4:E:602:HOH:O	1.87	0.74
1:B:96:GLN:NE2	1:B:233:GLU:OE1	2.21	0.74
1:H:194:GLN:O	1:H:198:VAL:HG13	1.88	0.74
1:D:384:GLU:CD	1:D:402:ARG:NH2	2.46	0.73
1:A:62:ARG:HG3	1:A:62:ARG:HH11	1.53	0.73
3:G:502:QR8:O1	3:G:502:QR8:O12	2.05	0.73
1:E:204:VAL:HG11	1:E:234:ILE:HG23	1.69	0.73
1:A:237:MET:HE3	1:A:237:MET:HA	1.71	0.73
1:A:260:LEU:HG	1:A:284:MET:HE1	1.68	0.73
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.71	0.73
1:C:203:LEU:O	1:C:207:ARG:HD2	1.89	0.73
1:E:107:LEU:HD23	1:E:229:LEU:HD23	1.69	0.73
1:H:328:GLU:OE2	1:H:328:GLU:N	2.22	0.73
1:H:185:THR:CG2	1:H:188:GLU:CB	2.66	0.72
1:I:85:PRO:HA	4:I:603:HOH:O	1.87	0.72
1:B:149:ALA:O	1:B:250:VAL:HG23	1.89	0.72
1:D:100:ASP:OD1	1:F:208:ARG:NH2	2.21	0.72
1:G:305:GLU:HG2	1:G:310:THR:HB	1.70	0.72
1:E:47:TYR:HB3	1:E:82:ARG:HH12	1.54	0.72
1:F:260:LEU:HG	1:F:284:MET:HE1	1.71	0.72
1:G:157:ILE:HD12	1:G:242:LEU:HD13	1.70	0.72
1:H:237:MET:HE3	1:H:237:MET:HA	1.71	0.72
1:C:384:GLU:OE2	1:C:402:ARG:NH1	2.22	0.71
1:A:182:THR:O	1:A:185:THR:CG2	2.38	0.71
1:A:191:ARG:O	1:A:195:ASP:OD1	2.06	0.71
1:C:85:PRO:HG2	1:C:189:ILE:HD12	1.72	0.71
1:D:356:CYS:SG	2:D:501:HEM:NC	2.64	0.71
1:A:244:ALA:HB1	3:A:502:QR8:C31	2.21	0.71
1:C:302:GLU:OE2	1:I:402:ARG:NH2	2.24	0.70
1:B:108:VAL:HG12	1:B:215:LEU:HD23	1.71	0.70
1:C:42:ARG:NH1	1:C:53:TRP:CE2	2.58	0.70
1:G:82:ARG:NH1	1:G:85:PRO:O	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:HEM:HBA1	3:A:502:QR8:C32	2.22	0.70
1:F:105:ARG:NH2	1:F:357:ILE:HG12	2.06	0.70
1:G:157:ILE:CD1	1:G:242:LEU:CD1	2.69	0.70
1:E:174:PHE:HZ	1:E:243:ILE:HD11	1.56	0.70
1:C:284:MET:O	1:C:288:THR:HG22	1.91	0.69
1:D:183:ARG:O	1:D:189:ILE:HD11	1.91	0.69
1:E:263:GLU:O	1:E:266:ARG:HD3	1.92	0.69
1:G:356:CYS:SG	2:G:501:HEM:NC	2.65	0.69
1:B:14:VAL:HG23	1:B:15:PRO:HD2	1.74	0.69
1:B:108:VAL:CG1	1:B:215:LEU:CD2	2.70	0.69
1:E:207:ARG:NH2	1:E:214:ASP:OD2	2.19	0.69
1:E:282:GLU:OE2	1:E:363:ARG:NH2	2.25	0.69
1:I:219:LEU:C	1:I:219:LEU:HD23	2.17	0.69
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.75	0.69
1:G:204:VAL:HG11	1:G:234:ILE:CG2	2.23	0.69
1:A:184:LEU:HD12	1:A:184:LEU:C	2.17	0.69
1:I:246:HIS:O	1:I:250:VAL:HG23	1.91	0.69
1:G:157:ILE:HD12	1:G:242:LEU:HD12	1.74	0.69
1:H:58:MET:HE2	1:H:324:ALA:HB1	1.74	0.69
2:D:501:HEM:HMC1	2:D:501:HEM:HBC2	1.75	0.68
1:F:105:ARG:HH22	1:F:357:ILE:HG12	1.57	0.68
1:G:286:ARG:NH2	1:G:334:ALA:O	2.27	0.68
1:H:312:ARG:N	1:H:315:GLU:OE1	2.25	0.68
1:H:347:ILE:HG22	1:H:347:ILE:O	1.93	0.68
1:H:260:LEU:HG	1:H:284:MET:HE1	1.76	0.68
1:B:33:GLU:O	1:B:37:ASP:OD1	2.11	0.68
1:F:182:THR:O	1:F:184:LEU:HD23	1.93	0.68
1:A:96:GLN:HB3	1:A:101:HIS:HB2	1.76	0.68
1:D:83:MET:HE2	1:D:293:ALA:HB1	1.76	0.68
1:I:359:ALA:O	1:I:363:ARG:HD2	1.94	0.68
1:G:100:ASP:OD1	1:G:100:ASP:N	2.19	0.67
1:B:41:SER:HB3	1:B:54:LEU:HD22	1.75	0.67
1:G:230:THR:HB	1:G:233:GLU:HB2	1.76	0.67
1:B:213:GLU:HG3	1:B:213:GLU:O	1.95	0.67
1:C:83:MET:HE2	1:C:293:ALA:HB1	1.75	0.67
1:G:108:VAL:HG11	1:G:237:MET:HE3	1.76	0.67
1:C:343:ARG:CZ	1:C:343:ARG:HB3	2.24	0.67
1:F:195:ASP:O	1:F:198:VAL:HG12	1.95	0.67
1:A:230:THR:HG22	1:A:232:GLY:H	1.59	0.67
1:G:204:VAL:HG11	1:G:234:ILE:HG21	1.77	0.67
1:I:219:LEU:HD11	1:I:234:ILE:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ASP:OD1	1:G:355:HIS:HB3	1.95	0.67
1:A:356:CYS:HB2	2:A:501:HEM:C1A	2.31	0.66
1:B:284:MET:O	1:B:288:THR:CG2	2.43	0.66
1:E:47:TYR:HB3	1:E:82:ARG:NH1	2.09	0.66
1:I:250:VAL:O	1:I:253:ILE:HG22	1.95	0.66
1:F:58:MET:HE2	1:F:324:ALA:HB1	1.77	0.66
1:D:178:MET:HE1	1:D:193:GLN:OE1	1.96	0.66
1:I:175:SER:HB3	1:I:247:GLU:CD	2.20	0.66
1:D:356:CYS:SG	2:D:501:HEM:ND	2.68	0.66
1:B:237:MET:HE1	1:B:241:LEU:HG	1.77	0.66
1:A:186:ALA:HB3	1:A:188:GLU:HG2	1.78	0.66
1:D:283:GLU:HG3	1:D:337:LEU:CD2	2.26	0.66
1:B:168:ARG:HA	1:B:171:PHE:CE2	2.31	0.66
1:C:135:MET:HE1	1:C:144:LEU:HA	1.78	0.66
1:F:356:CYS:SG	2:F:501:HEM:ND	2.69	0.66
1:H:94:LEU:HD12	1:H:354:HIS:CD2	2.31	0.66
1:I:171:PHE:CZ	1:I:242:LEU:HD13	2.31	0.66
2:I:501:HEM:HMB1	2:I:501:HEM:HBB2	1.77	0.65
1:E:396:LEU:HD13	1:E:396:LEU:H	1.61	0.65
1:F:376:ARG:HB2	1:F:377:PHE:CD1	2.31	0.65
1:H:73:ALA:O	1:H:76:THR:OG1	2.14	0.65
1:H:105:ARG:NH2	1:H:355:HIS:O	2.29	0.65
1:H:231:LYS:HG3	1:H:232:GLY:N	2.10	0.65
1:I:200:MET:HA	1:I:200:MET:CE	2.24	0.65
1:B:108:VAL:HG11	1:B:215:LEU:CD2	2.26	0.65
1:B:150:VAL:HA	1:B:250:VAL:CG2	2.27	0.65
1:D:185:THR:HB	1:D:188:GLU:CB	2.11	0.65
1:E:148:LEU:O	1:E:151:PRO:HD2	1.97	0.65
1:I:163:VAL:HG13	1:I:199:TYR:OH	1.97	0.65
1:A:62:ARG:HH11	1:A:62:ARG:CG	2.10	0.65
1:A:62:ARG:HH12	1:A:347:ILE:CG2	2.10	0.65
1:E:223:THR:HB	1:E:226:ASP:HA	1.78	0.65
1:G:203:LEU:O	1:G:207:ARG:HG2	1.97	0.65
1:A:83:MET:HE2	1:A:293:ALA:HB1	1.78	0.65
1:H:183:ARG:CZ	1:H:183:ARG:HB3	2.27	0.65
1:H:221:LEU:HD23	1:H:221:LEU:H	1.61	0.64
1:I:153:PRO:HG2	1:I:250:VAL:HG22	1.78	0.64
1:A:232:GLY:O	1:A:236:ASN:ND2	2.30	0.64
1:B:178:MET:CE	1:B:196:PHE:HD2	2.10	0.64
1:B:222:ALA:O	1:B:226:ASP:HB3	1.97	0.64
1:D:212:THR:HB	1:D:214:ASP:OD1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:189:ILE:HG22	1:I:193:GLN:OE1	1.98	0.64
1:H:356:CYS:SG	2:H:501:HEM:NB	2.71	0.64
1:I:104:LEU:HD12	1:I:105:ARG:N	2.13	0.64
1:D:356:CYS:SG	2:D:501:HEM:NB	2.70	0.64
1:F:73:ALA:O	1:F:76:THR:OG1	2.15	0.64
2:H:501:HEM:HMC1	2:H:501:HEM:HBC2	1.80	0.64
1:D:94:LEU:CD2	3:D:502:QR8:C35	2.76	0.64
1:E:60:ASP:OD2	1:E:306:LEU:HB3	1.98	0.64
1:B:178:MET:HE1	1:B:196:PHE:HD2	1.63	0.64
1:B:252:GLN:OE1	1:B:252:GLN:HA	1.98	0.64
1:C:200:MET:HG3	1:C:239:VAL:CG1	2.27	0.64
1:D:383:ALA:HB3	1:D:404:ILE:HG22	1.80	0.64
1:H:183:ARG:HB3	1:H:183:ARG:NH1	2.12	0.63
1:B:135:MET:HE1	1:B:144:LEU:HA	1.79	0.63
1:C:149:ALA:O	1:C:250:VAL:HG23	1.98	0.63
1:B:31:TYR:CZ	1:B:320:HIS:ND1	2.67	0.63
1:C:23:HIS:CE1	1:D:312:ARG:HD2	2.33	0.63
1:E:200:MET:HB3	1:E:235:VAL:HG22	1.80	0.63
1:G:96:GLN:HB3	1:G:101:HIS:HB2	1.80	0.63
1:F:91:ASP:OD1	1:F:91:ASP:N	2.32	0.63
1:F:237:MET:HE3	1:F:237:MET:HA	1.79	0.63
1:G:157:ILE:CD1	1:G:242:LEU:HD13	2.28	0.63
1:C:252:GLN:HA	1:C:252:GLN:OE1	1.97	0.63
1:H:356:CYS:SG	2:H:501:HEM:ND	2.71	0.63
1:E:213:GLU:OE1	1:E:213:GLU:HA	1.99	0.63
1:B:42:ARG:H	1:B:53:TRP:HB3	1.64	0.62
1:E:329:GLU:HA	1:E:329:GLU:OE2	1.98	0.62
1:C:165:LEU:O	1:C:168:ARG:HG2	1.99	0.62
3:E:502:QR8:O11	3:E:502:QR8:O12	2.15	0.62
1:E:260:LEU:CG	1:E:284:MET:HE1	2.27	0.62
1:H:62:ARG:NH1	1:H:347:ILE:HD11	2.15	0.62
1:B:170:LEU:HD22	1:G:115:ARG:HE	1.62	0.62
1:B:172:ARG:HG2	1:B:172:ARG:NH1	2.11	0.62
1:C:55:VAL:HG21	1:C:64:VAL:HG21	1.81	0.62
1:C:200:MET:HA	1:C:200:MET:CE	2.28	0.62
1:F:328:GLU:OE2	1:F:328:GLU:N	2.33	0.62
1:D:203:LEU:CD1	1:D:216:LEU:HD12	2.30	0.62
3:F:502:QR8:O12	3:F:502:QR8:O1	2.17	0.62
1:H:347:ILE:O	1:H:347:ILE:CG2	2.47	0.62
1:B:237:MET:HE3	1:B:237:MET:C	2.24	0.62
1:C:236:ASN:O	1:C:239:VAL:HG22	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:ARG:O	1:F:127:LEU:HD23	2.00	0.62
1:C:283:GLU:HG3	1:C:337:LEU:CD2	2.30	0.62
1:E:191:ARG:C	1:E:191:ARG:HD3	2.25	0.62
1:I:104:LEU:O	1:I:108:VAL:HG12	1.99	0.62
1:B:152:PHE:HB3	1:B:153:PRO:HD3	1.81	0.62
1:G:383:ALA:HB3	1:G:404:ILE:HG22	1.81	0.62
1:H:254:THR:HG21	1:H:400:LEU:HB2	1.81	0.62
1:A:189:ILE:HD12	1:A:190:GLN:N	2.13	0.62
1:I:133:ASP:O	1:I:136:VAL:CG2	2.48	0.62
1:E:230:THR:HB	1:E:233:GLU:H	1.63	0.61
1:B:166:GLU:CD	1:B:166:GLU:H	2.08	0.61
1:C:284:MET:O	1:C:288:THR:HG23	1.98	0.61
1:I:171:PHE:CE2	1:I:242:LEU:HB3	2.35	0.61
1:C:260:LEU:CG	1:C:284:MET:HE1	2.28	0.61
1:H:14:VAL:HG12	1:H:15:PRO:HD2	1.80	0.61
1:H:252:GLN:HA	1:H:252:GLN:OE1	2.00	0.61
1:I:133:ASP:HA	1:I:136:VAL:HG22	1.80	0.61
1:E:82:ARG:HE	1:E:87:PRO:HA	1.65	0.61
1:E:107:LEU:HD23	1:E:229:LEU:CD2	2.31	0.61
1:B:213:GLU:O	1:B:213:GLU:CG	2.48	0.61
1:F:94:LEU:HD12	1:F:354:HIS:CD2	2.35	0.61
1:C:200:MET:HG3	1:C:239:VAL:HG13	1.82	0.61
1:D:254:THR:HG21	1:D:400:LEU:HB2	1.83	0.61
1:E:254:THR:HG21	1:E:400:LEU:HB2	1.82	0.61
1:B:284:MET:O	1:B:288:THR:HG22	2.01	0.61
1:C:150:VAL:HA	1:C:250:VAL:CG2	2.31	0.61
1:E:83:MET:HE2	1:E:293:ALA:HB1	1.81	0.61
1:I:402:ARG:HD2	1:I:404:ILE:HD11	1.82	0.61
1:A:160:LEU:HD11	1:A:215:LEU:HD22	1.83	0.61
1:B:231:LYS:C	1:B:231:LYS:HD2	2.25	0.61
1:A:254:THR:HG21	1:A:400:LEU:HB2	1.82	0.60
1:B:326:ARG:HH21	1:B:335:ASP:HA	1.66	0.60
1:C:160:LEU:HG	1:C:215:LEU:HD12	1.83	0.60
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.31	0.60
1:I:150:VAL:O	1:I:154:VAL:HG23	2.02	0.60
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.83	0.60
1:H:327:ASP:O	1:H:330:VAL:HG23	2.02	0.60
1:F:283:GLU:OE2	1:F:286:ARG:NE	2.30	0.60
1:H:221:LEU:CD2	1:H:221:LEU:H	2.15	0.60
1:G:69:ARG:O	1:G:301:THR:OG1	2.20	0.60
1:G:283:GLU:O	1:G:286:ARG:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:THR:HB	1:E:214:ASP:OD1	2.02	0.59
1:F:183:ARG:HD3	1:F:184:LEU:H	1.66	0.59
1:H:151:PRO:HA	1:H:172:ARG:HH12	1.68	0.59
1:B:120:MET:C	1:B:122:PRO:HD2	2.27	0.59
1:F:354:HIS:CD2	2:F:501:HEM:O1D	2.56	0.59
1:B:237:MET:CE	1:B:241:LEU:HG	2.31	0.59
1:F:30:HIS:CE1	4:F:601:HOH:O	2.56	0.59
1:H:195:ASP:O	1:H:198:VAL:HG22	2.02	0.59
1:H:327:ASP:O	1:H:330:VAL:CG2	2.50	0.59
3:H:502:QR8:O11	3:H:502:QR8:O12	2.20	0.59
1:G:77:ASP:OD1	1:G:79:ALA:HB3	2.03	0.59
1:I:98:PRO:HA	1:I:99:PRO:C	2.27	0.59
2:I:501:HEM:HMC1	2:I:501:HEM:HBC2	1.84	0.59
1:H:125:ARG:HG3	1:H:368:GLU:OE1	2.03	0.59
1:I:62:ARG:HB2	1:I:62:ARG:CZ	2.32	0.59
1:G:360:GLN:OE1	1:G:360:GLN:HA	2.02	0.59
1:B:157:ILE:HG21	1:B:245:GLY:HA3	1.84	0.59
1:F:254:THR:HG21	1:F:400:LEU:HB2	1.85	0.59
2:G:501:HEM:HMB1	2:G:501:HEM:HBB2	1.84	0.59
1:H:131:LEU:HD21	1:H:151:PRO:HB2	1.84	0.59
1:A:123:ARG:NE	1:A:159:GLU:OE1	2.31	0.58
1:C:152:PHE:HB3	1:C:153:PRO:HD3	1.84	0.58
1:G:178:MET:HE1	1:G:193:GLN:NE2	2.18	0.58
1:H:218:ALA:C	1:H:221:LEU:CD2	2.74	0.58
1:B:171:PHE:O	1:B:175:SER:OG	2.20	0.58
1:G:48:GLY:HA3	1:G:81:PRO:HA	1.86	0.58
1:E:125:ARG:HG3	1:E:368:GLU:OE2	2.04	0.58
1:A:200:MET:HB3	1:A:235:VAL:HG13	1.85	0.58
1:C:48:GLY:HA3	1:C:81:PRO:HA	1.84	0.58
1:E:207:ARG:HH21	1:E:214:ASP:CG	2.10	0.58
2:G:501:HEM:HMC2	2:G:501:HEM:HBC2	1.86	0.58
1:I:164:PRO:HG2	1:I:167:ASP:CG	2.29	0.58
1:B:283:GLU:HG3	1:B:337:LEU:CD2	2.34	0.58
1:F:354:HIS:HD2	2:F:501:HEM:O1D	1.85	0.58
1:G:125:ARG:HG3	1:G:368:GLU:OE2	2.03	0.58
1:H:127:LEU:O	1:H:131:LEU:HD13	2.03	0.58
1:A:223:THR:HG23	1:A:226:ASP:CB	2.28	0.58
1:E:396:LEU:HD13	1:E:396:LEU:N	2.19	0.58
1:F:376:ARG:HB2	1:F:377:PHE:HD1	1.68	0.58
1:G:152:PHE:HB3	1:G:153:PRO:HD3	1.85	0.58
1:C:108:VAL:HG11	1:C:241:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:PHE:CZ	1:C:242:LEU:HD23	2.39	0.57
1:D:223:THR:HB	1:D:226:ASP:HB2	1.86	0.57
1:F:48:GLY:HA3	1:F:81:PRO:HA	1.86	0.57
1:G:191:ARG:HD2	1:G:191:ARG:C	2.29	0.57
1:A:356:CYS:SG	2:A:501:HEM:C4C	2.96	0.57
1:E:36:ARG:HD3	1:E:37:ASP:OD1	2.04	0.57
1:I:106:ARG:HH21	1:I:110:LYS:HG2	1.68	0.57
1:I:196:PHE:CD1	1:I:239:VAL:HG13	2.39	0.57
1:D:94:LEU:HD12	1:D:354:HIS:CD2	2.39	0.57
1:A:133:ASP:OD1	1:A:376:ARG:NH2	2.36	0.57
1:B:383:ALA:HB3	1:B:404:ILE:HG22	1.86	0.57
1:D:230:THR:HB	1:D:233:GLU:H	1.68	0.57
1:E:356:CYS:SG	2:E:501:HEM:NB	2.77	0.57
1:H:221:LEU:HD23	1:H:221:LEU:N	2.18	0.57
1:A:330:VAL:HG22	1:C:272:ALA:HB1	1.86	0.57
2:C:501:HEM:HMC1	2:C:501:HEM:HBC2	1.86	0.57
1:C:103:ARG:O	1:C:107:LEU:HG	2.04	0.57
1:I:133:ASP:O	1:I:136:VAL:HG22	2.05	0.57
1:B:105:ARG:HD3	1:B:105:ARG:C	2.30	0.57
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.34	0.57
1:C:135:MET:HE3	1:C:147:PHE:HB2	1.85	0.57
1:C:66:GLY:O	1:I:138:HIS:CE1	2.57	0.56
1:F:124:VAL:O	1:F:128:VAL:HG23	2.05	0.56
1:G:245:GLY:HA2	2:G:501:HEM:C2C	2.40	0.56
1:A:203:LEU:O	1:A:207:ARG:HG2	2.06	0.56
1:C:93:VAL:HG11	1:C:237:MET:CE	2.35	0.56
1:D:252:GLN:OE1	1:D:252:GLN:HA	2.05	0.56
1:E:47:TYR:CB	1:E:82:ARG:NH1	2.68	0.56
1:G:104:LEU:O	1:G:108:VAL:HG13	2.04	0.56
1:G:200:MET:HB3	1:G:235:VAL:HG13	1.86	0.56
1:E:82:ARG:HH11	1:E:82:ARG:CG	2.18	0.56
2:E:501:HEM:HBB2	2:E:501:HEM:CMB	2.34	0.56
1:G:172:ARG:HH21	1:G:172:ARG:CG	2.19	0.56
1:I:256:LEU:O	1:I:284:MET:HE2	2.06	0.56
1:B:53:TRP:CD1	1:B:53:TRP:N	2.71	0.56
1:B:184:LEU:HD23	1:B:184:LEU:N	2.17	0.56
1:F:40:VAL:CG2	1:F:309:VAL:HB	2.35	0.56
1:F:252:GLN:OE1	1:F:252:GLN:HA	2.03	0.56
1:A:81:PRO:O	1:A:297:VAL:HG21	2.06	0.56
1:D:208:ARG:NH2	1:F:100:ASP:OD1	2.39	0.56
1:C:168:ARG:HA	1:C:171:PHE:CE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:282:GLU:CD	1:E:363:ARG:HH21	2.12	0.56
1:D:35:ARG:HG3	1:D:56:THR:HG22	1.88	0.56
1:B:326:ARG:HH21	1:B:335:ASP:CB	2.19	0.56
1:D:355:HIS:O	1:D:356:CYS:C	2.49	0.56
1:E:55:VAL:HG21	1:E:64:VAL:HG21	1.87	0.56
1:I:281:VAL:HG12	1:I:281:VAL:O	2.06	0.55
1:B:284:MET:O	1:B:288:THR:HG23	2.07	0.55
1:I:359:ALA:O	1:I:363:ARG:CD	2.54	0.55
3:B:502:QR8:C32	3:B:502:QR8:C33	2.85	0.55
1:E:75:ALA:HB1	1:E:297:VAL:HG13	1.88	0.55
1:G:204:VAL:CG1	1:G:234:ILE:HG21	2.36	0.55
1:A:42:ARG:HG2	1:A:42:ARG:NH1	2.02	0.55
1:A:184:LEU:CD1	1:A:186:ALA:H	2.17	0.55
3:D:502:QR8:C30	3:D:502:QR8:C31	2.85	0.55
1:F:356:CYS:SG	2:F:501:HEM:NB	2.79	0.55
1:H:293:ALA:O	1:H:320:HIS:ND1	2.40	0.55
1:I:360:GLN:HA	1:I:360:GLN:OE1	2.07	0.55
3:I:502:QR8:C32	3:I:502:QR8:C33	2.85	0.55
2:E:501:HEM:CBA	3:E:502:QR8:C32	2.83	0.55
1:G:286:ARG:HG3	1:G:287:TYR:N	2.21	0.55
2:I:501:HEM:HBA2	3:I:502:QR8:O12	2.07	0.55
3:A:502:QR8:C34	3:A:502:QR8:C35	2.85	0.55
1:D:84:PHE:N	1:D:84:PHE:CD1	2.75	0.55
1:E:375:ARG:HG3	1:E:375:ARG:HH11	1.72	0.55
1:H:48:GLY:HA3	1:H:81:PRO:HA	1.89	0.55
1:B:272:ALA:HB1	1:D:330:VAL:HG22	1.87	0.55
1:B:327:ASP:OD1	1:B:329:GLU:HB2	2.07	0.55
1:A:73:ALA:O	1:A:76:THR:OG1	2.19	0.55
1:B:42:ARG:HA	1:B:52:ALA:O	2.07	0.55
1:C:73:ALA:O	1:C:76:THR:OG1	2.24	0.55
1:G:84:PHE:CE1	3:G:502:QR8:C34	2.90	0.55
1:C:154:VAL:O	1:C:157:ILE:HG22	2.08	0.54
2:F:501:HEM:HMC2	2:F:501:HEM:HBC2	1.89	0.54
1:G:252:GLN:OE1	1:G:252:GLN:HA	2.06	0.54
3:H:502:QR8:C11	3:H:502:QR8:C1	2.85	0.54
1:A:203:LEU:HD11	1:A:207:ARG:NH2	2.23	0.54
1:B:235:VAL:O	1:B:238:GLY:N	2.40	0.54
1:F:191:ARG:HH11	1:F:191:ARG:CG	2.19	0.54
1:G:179:LEU:HB2	1:G:247:GLU:OE1	2.07	0.54
1:G:286:ARG:HH12	1:G:341:ARG:NH2	2.04	0.54
1:A:283:GLU:HG3	1:A:337:LEU:CD2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:ARG:HE	1:C:216:LEU:HB3	1.73	0.54
3:G:502:QR8:C1	3:G:502:QR8:C11	2.85	0.54
1:H:81:PRO:O	1:H:297:VAL:HG21	2.07	0.54
1:H:124:VAL:O	1:H:128:VAL:HG23	2.07	0.54
1:B:271:VAL:HA	1:B:374:VAL:HG13	1.90	0.54
1:G:69:ARG:CZ	1:G:304:VAL:HG12	2.38	0.54
1:A:252:GLN:OE1	1:A:252:GLN:HA	2.07	0.54
1:C:178:MET:HE1	1:C:193:GLN:HG2	1.89	0.54
1:B:53:TRP:CD1	1:B:53:TRP:H	2.26	0.54
1:E:174:PHE:CZ	1:E:243:ILE:HD11	2.40	0.54
1:G:260:LEU:CG	1:G:284:MET:HE1	2.33	0.54
1:D:107:LEU:HD12	1:D:229:LEU:CD2	2.38	0.54
1:E:75:ALA:CB	1:E:297:VAL:HG13	2.38	0.54
1:G:67:ASP:OD1	1:G:68:SER:N	2.41	0.54
1:H:180:SER:O	1:H:181:SER:OG	2.24	0.54
1:G:124:VAL:O	1:G:128:VAL:HG23	2.08	0.54
1:H:107:LEU:HD23	1:H:229:LEU:HD23	1.89	0.54
3:I:502:QR8:C30	3:I:502:QR8:C31	2.86	0.54
3:E:502:QR8:C33	3:E:502:QR8:C34	2.85	0.54
1:G:179:LEU:HD12	1:G:179:LEU:C	2.32	0.54
2:A:501:HEM:CBA	3:A:502:QR8:C32	2.86	0.54
1:F:200:MET:HB3	1:F:235:VAL:HG13	1.90	0.54
1:I:175:SER:O	1:I:179:LEU:CD2	2.55	0.53
1:I:189:ILE:HA	1:I:192:VAL:CG2	2.39	0.53
1:A:99:PRO:HA	1:A:102:THR:HG22	1.89	0.53
3:A:502:QR8:C32	3:A:502:QR8:C33	2.85	0.53
1:D:152:PHE:HB3	1:D:153:PRO:HD3	1.90	0.53
1:I:256:LEU:HD11	1:I:366:LEU:HD13	1.89	0.53
1:A:328:GLU:N	1:A:328:GLU:OE2	2.40	0.53
1:C:194:GLN:O	1:C:198:VAL:HG23	2.09	0.53
1:C:200:MET:CE	1:C:203:LEU:HD12	2.38	0.53
3:H:502:QR8:C34	3:H:502:QR8:C35	2.85	0.53
1:I:179:LEU:CD1	1:I:396:LEU:HD12	2.39	0.53
3:I:502:QR8:C34	3:I:502:QR8:C35	2.85	0.53
1:A:194:GLN:O	1:A:198:VAL:HG22	2.07	0.53
1:B:237:MET:HE1	1:B:241:LEU:CG	2.39	0.53
1:E:260:LEU:CD2	1:E:284:MET:HE1	2.39	0.53
1:I:172:ARG:O	1:I:176:ASP:CG	2.52	0.53
1:I:384:GLU:OE1	1:I:402:ARG:NH1	2.40	0.53
1:A:184:LEU:HD12	1:A:186:ALA:N	2.19	0.53
1:B:83:MET:HE2	1:B:293:ALA:HB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:VAL:O	1:B:128:VAL:HG23	2.08	0.53
1:C:26:ASP:OD2	1:D:312:ARG:NH1	2.41	0.53
1:C:124:VAL:O	1:C:128:VAL:HG23	2.08	0.53
1:G:103:ARG:O	1:G:107:LEU:HG	2.07	0.53
1:G:70:PHE:CZ	1:G:304:VAL:HG21	2.44	0.53
1:B:178:MET:HE3	1:B:243:ILE:HD11	1.90	0.53
1:E:245:GLY:HA2	2:E:501:HEM:C2C	2.44	0.53
1:F:292:SER:O	1:F:293:ALA:HB3	2.09	0.53
1:A:245:GLY:HA2	2:A:501:HEM:C2C	2.43	0.53
1:E:283:GLU:HG3	1:E:337:LEU:CD2	2.39	0.53
1:F:104:LEU:O	1:F:108:VAL:HG13	2.09	0.53
1:A:152:PHE:HB3	1:A:153:PRO:HD3	1.90	0.53
1:F:383:ALA:HB3	1:F:404:ILE:HG22	1.90	0.53
1:H:151:PRO:HB3	1:H:172:ARG:HH12	1.74	0.53
1:I:135:MET:HE1	1:I:147:PHE:HB2	1.80	0.53
1:H:42:ARG:NH1	1:H:51:THR:HG23	2.24	0.52
1:F:376:ARG:CB	1:F:377:PHE:CD1	2.92	0.52
1:F:183:ARG:HD3	1:F:184:LEU:N	2.24	0.52
2:F:501:HEM:HBB2	2:F:501:HEM:CMB	2.38	0.52
1:G:94:LEU:HD12	1:G:354:HIS:CD2	2.44	0.52
1:F:162:GLY:HA3	1:F:214:ASP:CG	2.34	0.52
1:H:200:MET:HB3	1:H:235:VAL:HG13	1.92	0.52
1:I:59:SER:O	1:I:62:ARG:HG3	2.09	0.52
1:I:131:LEU:HD13	1:I:134:ASP:OD2	2.09	0.52
1:I:370:LEU:O	1:I:374:VAL:HG23	2.10	0.52
1:B:183:ARG:NH1	1:B:393:GLN:O	2.42	0.52
1:E:124:VAL:O	1:E:128:VAL:HG23	2.10	0.52
1:B:170:LEU:HD11	1:B:174:PHE:CZ	2.44	0.52
1:B:172:ARG:HH11	1:B:172:ARG:CG	2.18	0.52
1:B:230:THR:O	1:B:233:GLU:HB2	2.07	0.52
1:C:76:THR:HG21	1:C:90:PRO:HA	1.92	0.52
1:D:55:VAL:HG21	1:D:64:VAL:HG21	1.92	0.52
1:E:105:ARG:NH2	1:E:355:HIS:O	2.42	0.52
1:F:55:VAL:HG21	1:F:64:VAL:HG21	1.91	0.52
1:H:179:LEU:O	1:H:182:THR:HB	2.09	0.52
2:H:501:HEM:HBB2	2:H:501:HEM:CMB	2.36	0.52
1:B:125:ARG:HG2	1:B:368:GLU:OE2	2.10	0.52
1:C:208:ARG:HG2	1:C:209:ASP:N	2.24	0.52
1:D:247:GLU:OE2	1:D:397:ILE:HD12	2.09	0.52
1:G:123:ARG:O	1:G:127:LEU:HD13	2.08	0.52
1:H:245:GLY:HA2	2:H:501:HEM:C2C	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:286:ARG:HD3	1:H:344:ASN:HD22	1.74	0.52
1:I:65:LEU:CD2	1:I:354:HIS:H	2.23	0.52
1:C:196:PHE:HZ	1:C:242:LEU:HD23	1.75	0.52
1:D:107:LEU:HD12	1:D:229:LEU:HD23	1.91	0.52
1:H:224:ASP:C	1:H:226:ASP:OD1	2.52	0.52
1:I:121:ARG:NH1	1:I:368:GLU:OE1	2.43	0.52
1:A:213:GLU:OE1	1:A:213:GLU:HA	2.10	0.52
1:E:74:ALA:CB	1:E:299:VAL:CG2	2.70	0.52
1:I:135:MET:HE2	1:I:147:PHE:HB2	1.78	0.52
1:I:356:CYS:SG	2:I:501:HEM:C4B	3.02	0.52
1:B:121:ARG:N	1:B:122:PRO:HD2	2.24	0.52
1:C:349:PHE:CE1	1:C:359:ALA:HA	2.44	0.52
1:A:184:LEU:HD12	1:A:185:THR:N	2.26	0.51
1:B:135:MET:CE	1:B:144:LEU:HA	2.41	0.51
1:B:178:MET:HE1	1:B:196:PHE:CD2	2.43	0.51
1:C:148:LEU:O	1:C:151:PRO:HD2	2.10	0.51
1:G:207:ARG:HA	1:G:207:ARG:HH11	1.75	0.51
1:A:99:PRO:C	1:A:102:THR:HG22	2.35	0.51
1:A:186:ALA:HB3	1:A:188:GLU:CG	2.40	0.51
1:B:326:ARG:NH2	1:B:335:ASP:HB3	2.26	0.51
1:C:40:VAL:HG22	1:C:308:THR:HG23	1.92	0.51
1:E:263:GLU:CB	1:E:266:ARG:HD2	2.33	0.51
1:I:120:MET:O	1:I:124:VAL:HG23	2.09	0.51
1:E:132:LEU:O	1:E:136:VAL:HG23	2.10	0.51
1:H:35:ARG:HG3	1:H:56:THR:HG22	1.93	0.51
1:B:42:ARG:CG	1:B:53:TRP:CE3	2.93	0.51
1:H:55:VAL:HG21	1:H:64:VAL:HG21	1.92	0.51
1:H:151:PRO:HA	1:H:172:ARG:NH1	2.25	0.51
1:B:35:ARG:HD3	1:B:327:ASP:HB2	1.93	0.51
1:D:260:LEU:CG	1:D:284:MET:HE1	2.38	0.51
1:C:135:MET:CE	1:C:144:LEU:HA	2.41	0.51
1:D:132:LEU:HD22	1:D:377:PHE:HE2	1.75	0.51
1:H:31:TYR:HB3	1:H:323:SER:OG	2.10	0.51
1:G:55:VAL:HG21	1:G:64:VAL:HG21	1.93	0.51
1:G:172:ARG:HH21	1:G:172:ARG:HG2	1.75	0.51
1:H:185:THR:HG23	1:H:188:GLU:CB	2.41	0.51
1:I:132:LEU:HD11	1:I:148:LEU:HD22	1.93	0.51
1:C:104:LEU:HD13	1:C:229:LEU:CD2	2.40	0.51
1:C:396:LEU:HD13	3:C:502:QR8:C36	2.40	0.51
1:I:132:LEU:CD1	1:I:148:LEU:HD22	2.40	0.51
1:E:121:ARG:NH2	1:E:367:GLN:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:150:VAL:HB	1:H:151:PRO:HD3	1.93	0.51
1:B:42:ARG:N	1:B:53:TRP:HB3	2.27	0.50
1:B:107:LEU:HD12	1:B:107:LEU:C	2.30	0.50
1:B:235:VAL:HG12	1:B:236:ASN:N	2.26	0.50
1:C:46:PRO:HB2	1:C:47:TYR:CD1	2.47	0.50
1:D:331:PHE:CE1	1:D:345:PRO:HD2	2.47	0.50
1:E:132:LEU:HG	1:E:377:PHE:HE2	1.76	0.50
1:I:364:LEU:HD23	1:I:364:LEU:C	2.37	0.50
1:G:83:MET:CE	1:G:318:VAL:HG21	2.41	0.50
1:B:326:ARG:NH2	1:B:335:ASP:CB	2.74	0.50
1:F:376:ARG:C	1:F:377:PHE:CD1	2.90	0.50
1:I:197:MET:CE	1:I:236:ASN:HA	2.40	0.50
1:B:161:LEU:HD12	1:B:215:LEU:HB2	1.93	0.50
1:D:195:ASP:O	1:D:198:VAL:HG12	2.11	0.50
1:G:178:MET:HE1	1:G:193:GLN:HE21	1.75	0.50
1:H:382:LEU:HD22	1:H:384:GLU:O	2.11	0.50
1:I:132:LEU:O	1:I:135:MET:HB3	2.10	0.50
1:I:252:GLN:HG2	1:I:366:LEU:HD11	1.94	0.50
1:A:172:ARG:CG	1:A:172:ARG:HH21	2.23	0.50
1:I:260:LEU:HD13	1:I:284:MET:CE	2.39	0.50
1:A:99:PRO:CA	1:A:102:THR:HG22	2.41	0.50
1:B:203:LEU:O	1:B:207:ARG:HG2	2.12	0.50
1:C:271:VAL:HA	1:C:374:VAL:HG13	1.94	0.50
1:F:245:GLY:HA2	2:F:501:HEM:C2C	2.47	0.50
1:G:189:ILE:O	1:G:193:GLN:HG3	2.11	0.50
1:A:359:ALA:O	1:A:363:ARG:HG3	2.12	0.50
1:A:355:HIS:O	1:A:356:CYS:C	2.52	0.50
1:B:200:MET:HG3	1:B:239:VAL:HG22	1.94	0.50
1:E:383:ALA:HB3	1:E:404:ILE:HG22	1.94	0.50
1:H:84:PHE:CE1	3:H:502:QR8:C34	2.95	0.50
1:B:54:LEU:HA	1:B:318:VAL:O	2.12	0.49
1:C:179:LEU:CD1	1:C:247:GLU:HG3	2.42	0.49
1:D:402:ARG:HG2	1:D:402:ARG:HH21	1.77	0.49
1:G:35:ARG:HG3	1:G:56:THR:HG22	1.94	0.49
1:E:48:GLY:HA3	1:E:81:PRO:HA	1.94	0.49
1:I:174:PHE:HB3	1:I:196:PHE:HD2	1.77	0.49
3:I:502:QR8:C32	3:I:502:QR8:C9	2.90	0.49
1:B:55:VAL:HG21	1:B:64:VAL:HG21	1.93	0.49
1:B:277:VAL:HB	1:B:278:PRO:HD3	1.94	0.49
1:E:375:ARG:HH11	1:E:375:ARG:CG	2.26	0.49
1:G:154:VAL:O	1:G:157:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:327:ASP:HB3	1:H:330:VAL:HG21	1.92	0.49
1:B:200:MET:HE2	1:B:238:GLY:HA3	1.94	0.49
1:B:260:LEU:CG	1:B:284:MET:HE1	2.39	0.49
1:B:73:ALA:HA	1:B:95:ALA:O	2.12	0.49
1:B:135:MET:HE3	1:B:147:PHE:HB2	1.95	0.49
1:C:200:MET:HB3	1:C:235:VAL:HG13	1.94	0.49
1:D:185:THR:O	1:D:189:ILE:HG13	2.12	0.49
1:D:200:MET:HB3	1:D:235:VAL:HG13	1.94	0.49
1:I:245:GLY:HA2	2:I:501:HEM:HMC3	1.93	0.49
1:A:106:ARG:HH12	1:A:110:LYS:HE3	1.76	0.49
1:A:230:THR:HB	1:A:233:GLU:H	1.77	0.49
1:B:326:ARG:HH21	1:B:335:ASP:CA	2.24	0.49
1:I:98:PRO:HB2	1:I:99:PRO:HA	1.95	0.49
1:I:106:ARG:NH2	1:I:110:LYS:HA	2.28	0.49
1:F:245:GLY:HA2	2:F:501:HEM:C1C	2.48	0.49
1:G:356:CYS:SG	2:G:501:HEM:ND	2.86	0.49
1:I:133:ASP:O	1:I:136:VAL:HG23	2.12	0.49
1:A:55:VAL:HG21	1:A:64:VAL:HG21	1.95	0.49
1:B:121:ARG:N	1:B:122:PRO:CD	2.76	0.49
1:B:200:MET:HG3	1:B:239:VAL:CG2	2.42	0.49
1:B:330:VAL:CG1	1:B:331:PHE:CD2	2.91	0.49
1:C:108:VAL:HG13	1:C:215:LEU:CD2	2.43	0.49
1:H:327:ASP:HB3	1:H:330:VAL:CG2	2.43	0.49
1:A:245:GLY:HA2	2:A:501:HEM:C1C	2.47	0.49
1:C:402:ARG:HG2	1:C:403:GLN:N	2.27	0.49
1:D:96:GLN:HB3	1:D:101:HIS:HB2	1.95	0.49
1:G:332:ASP:O	1:G:333:HIS:C	2.55	0.49
1:I:99:PRO:O	1:I:102:THR:N	2.44	0.49
1:B:231:LYS:C	1:B:231:LYS:CD	2.86	0.49
2:H:501:HEM:HBC2	2:H:501:HEM:CMC	2.43	0.49
1:B:60:ASP:OD1	1:B:307:SER:HB3	2.13	0.48
1:E:229:LEU:CD1	1:E:233:GLU:HG3	2.43	0.48
1:G:172:ARG:HG2	1:G:172:ARG:NH2	2.27	0.48
1:H:283:GLU:HG3	1:H:337:LEU:CD2	2.43	0.48
1:I:189:ILE:N	1:I:189:ILE:HD12	2.27	0.48
1:I:197:MET:CE	1:I:239:VAL:HG21	2.41	0.48
1:A:332:ASP:O	1:A:333:HIS:C	2.55	0.48
1:B:200:MET:CG	1:B:239:VAL:HG22	2.43	0.48
1:C:185:THR:HG22	1:F:166:GLU:OE1	2.13	0.48
1:C:332:ASP:O	1:C:333:HIS:C	2.56	0.48
1:D:23:HIS:CD2	1:D:26:ASP:OD1	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:359:ALA:O	1:E:363:ARG:HG3	2.13	0.48
1:H:151:PRO:CA	1:H:172:ARG:HH12	2.25	0.48
1:I:190:GLN:O	1:I:194:GLN:CG	2.56	0.48
1:I:219:LEU:HD21	1:I:234:ILE:O	2.13	0.48
1:A:198:VAL:O	1:A:201:ASP:HB2	2.12	0.48
1:A:195:ASP:O	1:A:198:VAL:HG23	2.14	0.48
1:C:176:ASP:OD1	1:C:247:GLU:OE2	2.32	0.48
1:D:375:ARG:NH1	4:D:601:HOH:O	2.38	0.48
1:H:162:GLY:HA3	1:H:214:ASP:OD2	2.13	0.48
1:A:124:VAL:O	1:A:128:VAL:HG23	2.14	0.48
1:C:93:VAL:HG11	1:C:237:MET:SD	2.53	0.48
1:C:101:HIS:CE1	1:C:105:ARG:HG3	2.49	0.48
1:C:209:ASP:OD1	1:E:105:ARG:NH2	2.46	0.48
1:D:150:VAL:HB	1:D:151:PRO:HD3	1.95	0.48
1:E:94:LEU:HD12	1:E:354:HIS:CD2	2.48	0.48
1:H:283:GLU:OE2	1:H:286:ARG:NH2	2.45	0.48
1:I:100:ASP:HA	1:I:103:ARG:CD	2.43	0.48
1:I:141:PRO:HB3	1:I:405:VAL:O	2.14	0.48
1:I:197:MET:HE3	1:I:236:ASN:CG	2.38	0.48
1:A:260:LEU:CG	1:A:284:MET:HE1	2.41	0.48
1:C:66:GLY:O	1:I:138:HIS:HE1	1.96	0.48
1:E:396:LEU:HG	3:E:502:QR8:C36	2.43	0.48
1:I:65:LEU:HD23	1:I:354:HIS:H	1.78	0.48
1:I:146:GLU:HG2	1:I:147:PHE:CD1	2.47	0.48
1:B:104:LEU:HG	1:B:237:MET:HG3	1.94	0.48
1:C:287:TYR:O	1:C:326:ARG:NH1	2.46	0.48
1:E:264:ARG:NH2	1:E:380:LEU:O	2.40	0.48
1:I:279:ALA:HA	1:I:282:GLU:HG2	1.95	0.48
1:A:200:MET:O	1:A:204:VAL:HG23	2.13	0.48
1:A:284:MET:HE3	1:A:339:PHE:HZ	1.79	0.48
1:C:230:THR:HB	1:C:233:GLU:H	1.78	0.48
1:D:384:GLU:OE1	1:D:402:ARG:NH2	2.47	0.48
1:F:377:PHE:O	1:F:380:LEU:HB2	2.13	0.48
1:B:208:ARG:NH2	1:G:355:HIS:NE2	2.62	0.48
1:H:254:THR:CG2	1:H:400:LEU:HB2	2.44	0.48
1:H:330:VAL:HG23	1:H:331:PHE:CD2	2.49	0.48
1:A:62:ARG:CG	1:A:62:ARG:NH1	2.72	0.47
1:C:108:VAL:HG13	1:C:215:LEU:HD22	1.94	0.47
1:F:201:ASP:OD1	1:F:202:GLY:N	2.47	0.47
1:H:185:THR:CG2	1:H:188:GLU:HB3	2.41	0.47
1:H:196:PHE:CE1	1:H:200:MET:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:121:ARG:NH2	1:I:367:GLN:OE1	2.46	0.47
1:I:149:ALA:HA	1:I:253:ILE:HG21	1.95	0.47
1:A:150:VAL:HB	1:A:151:PRO:HD3	1.96	0.47
1:A:230:THR:O	1:A:234:ILE:HG13	2.14	0.47
1:B:236:ASN:C	1:B:236:ASN:ND2	2.73	0.47
1:D:232:GLY:O	1:D:236:ASN:ND2	2.47	0.47
1:G:45:LEU:HD22	1:G:81:PRO:HB2	1.96	0.47
1:I:143:ASP:OD1	1:I:402:ARG:HB2	2.13	0.47
1:I:188:GLU:HA	1:I:191:ARG:HD2	1.96	0.47
1:B:57:ARG:NH2	1:B:329:GLU:HG2	2.29	0.47
1:E:200:MET:HB3	1:E:235:VAL:CG2	2.44	0.47
1:F:30:HIS:HD2	1:F:34:LEU:HG	1.79	0.47
1:G:56:THR:HG22	1:G:56:THR:O	2.14	0.47
1:G:284:MET:HE3	1:G:339:PHE:HZ	1.79	0.47
3:A:502:QR8:C31	4:A:604:HOH:O	2.61	0.47
1:B:105:ARG:NH1	1:B:109:GLY:HA3	2.30	0.47
1:C:31:TYR:CZ	1:C:320:HIS:ND1	2.82	0.47
1:D:254:THR:CG2	1:D:400:LEU:HB2	2.45	0.47
1:G:356:CYS:SG	2:G:501:HEM:NA	2.87	0.47
1:I:106:ARG:NH2	1:I:110:LYS:HG2	2.28	0.47
1:D:106:ARG:NH1	1:D:110:LYS:HE3	2.30	0.47
1:F:152:PHE:HB3	1:F:153:PRO:HD3	1.97	0.47
1:I:149:ALA:CB	1:I:253:ILE:CG2	2.93	0.47
1:A:358:GLY:HA3	2:A:501:HEM:C3C	2.49	0.47
1:A:383:ALA:HB3	1:A:404:ILE:HG22	1.95	0.47
1:B:54:LEU:HD23	1:B:54:LEU:C	2.36	0.47
1:C:179:LEU:HD13	1:C:397:ILE:HD11	1.96	0.47
1:C:383:ALA:HB3	1:C:404:ILE:HG22	1.96	0.47
1:H:58:MET:CE	1:H:324:ALA:HB1	2.44	0.47
1:A:230:THR:HG22	1:A:231:LYS:N	2.29	0.47
1:B:14:VAL:HG13	1:B:44:ARG:NH2	2.30	0.47
1:B:84:PHE:CD1	1:B:84:PHE:N	2.82	0.47
1:B:135:MET:HA	1:B:147:PHE:CD2	2.50	0.47
1:B:168:ARG:HD3	1:B:172:ARG:HD3	1.95	0.47
1:B:244:ALA:HB1	2:B:501:HEM:C4C	2.50	0.47
1:C:150:VAL:HB	1:C:151:PRO:HD3	1.96	0.47
1:C:197:MET:HE1	1:C:235:VAL:CG1	2.43	0.47
1:C:260:LEU:CD2	1:C:284:MET:HE1	2.44	0.47
1:D:328:GLU:OE2	1:D:328:GLU:N	2.42	0.47
1:E:73:ALA:O	1:E:76:THR:OG1	2.28	0.47
1:F:39:PRO:HB3	1:F:57:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:ARG:HD3	1:F:159:GLU:OE1	2.15	0.47
1:I:194:GLN:O	1:I:198:VAL:HG23	2.15	0.47
1:I:260:LEU:CD1	1:I:284:MET:HE1	2.38	0.47
1:I:384:GLU:CD	1:I:402:ARG:HH12	2.22	0.47
1:B:75:ALA:HA	1:B:80:THR:HG21	1.96	0.47
1:E:45:LEU:HD22	1:E:81:PRO:HB2	1.97	0.47
1:E:356:CYS:HA	2:E:501:HEM:C4D	2.49	0.47
1:B:85:PRO:HB2	1:B:186:ALA:HB2	1.97	0.47
1:B:249:SER:O	1:B:253:ILE:HG13	2.15	0.47
1:C:81:PRO:O	1:C:297:VAL:HG21	2.15	0.47
1:C:167:ASP:HB3	1:C:199:TYR:OH	2.15	0.47
1:C:274:PRO:HD2	4:C:613:HOH:O	2.15	0.47
1:C:303:ASP:OD1	1:C:312:ARG:HA	2.15	0.47
1:E:123:ARG:O	1:E:127:LEU:HD13	2.15	0.47
1:F:107:LEU:O	1:F:110:LYS:HG2	2.15	0.47
1:F:252:GLN:HE21	1:F:285:LEU:HD23	1.79	0.47
1:I:133:ASP:CA	1:I:136:VAL:HG22	2.45	0.47
1:C:249:SER:O	1:C:253:ILE:HG13	2.16	0.46
1:F:305:GLU:HG2	1:F:310:THR:HB	1.97	0.46
1:H:203:LEU:HD21	1:H:207:ARG:NH2	2.30	0.46
1:I:219:LEU:CD1	1:I:234:ILE:O	2.63	0.46
1:A:260:LEU:CD2	1:A:284:MET:HE1	2.45	0.46
1:B:149:ALA:O	1:B:250:VAL:CG2	2.60	0.46
1:B:187:ALA:HB3	1:H:166:GLU:CG	2.45	0.46
1:B:274:PRO:O	1:B:277:VAL:HG23	2.15	0.46
1:D:329:GLU:OE2	1:D:329:GLU:HA	2.14	0.46
1:E:120:MET:CE	1:E:159:GLU:HB3	2.44	0.46
1:E:152:PHE:HB3	1:E:153:PRO:HD3	1.97	0.46
1:E:212:THR:HG22	1:E:213:GLU:N	2.30	0.46
1:A:35:ARG:HG3	1:A:56:THR:HG22	1.97	0.46
1:A:286:ARG:HB2	1:A:346:HIS:HB3	1.97	0.46
1:A:382:LEU:HD22	1:A:384:GLU:O	2.15	0.46
1:B:42:ARG:HG3	1:B:53:TRP:CE3	2.50	0.46
1:D:349:PHE:C	2:D:501:HEM:HMA3	2.40	0.46
1:F:30:HIS:ND1	4:F:601:HOH:O	2.36	0.46
1:F:150:VAL:HB	1:F:151:PRO:HD3	1.98	0.46
1:A:67:ASP:OD2	1:A:69:ARG:NE	2.44	0.46
1:B:200:MET:HA	1:B:203:LEU:HD12	1.97	0.46
1:C:356:CYS:SG	2:C:501:HEM:C1C	3.00	0.46
1:H:107:LEU:HD23	1:H:229:LEU:CD2	2.45	0.46
1:B:42:ARG:HG2	1:B:53:TRP:CE3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:VAL:HG21	1:D:171:PHE:CZ	2.50	0.46
1:G:156:VAL:HG21	1:G:365:GLU:HG2	1.98	0.46
1:H:200:MET:O	1:H:204:VAL:HG23	2.15	0.46
1:I:143:ASP:OD2	1:I:145:VAL:N	2.48	0.46
1:E:74:ALA:HB1	1:E:299:VAL:HG21	1.95	0.46
1:H:38:GLU:O	1:H:38:GLU:HG3	2.15	0.46
1:H:127:LEU:O	1:H:131:LEU:CD1	2.63	0.46
1:C:220:ALA:O	1:C:223:THR:HG22	2.14	0.46
1:E:55:VAL:HG13	1:E:60:ASP:HB3	1.97	0.46
1:E:105:ARG:HA	1:E:105:ARG:HD2	1.58	0.46
1:E:286:ARG:HB2	1:E:346:HIS:HB3	1.98	0.46
1:F:376:ARG:CB	1:F:377:PHE:CE1	2.99	0.46
1:F:377:PHE:CD1	1:F:377:PHE:N	2.84	0.46
1:I:135:MET:HE3	1:I:135:MET:HB2	1.64	0.46
1:I:143:ASP:HB3	1:I:146:GLU:HB3	1.98	0.46
1:B:200:MET:HE1	1:B:216:LEU:HD11	1.98	0.46
1:C:67:ASP:OD1	1:C:68:SER:N	2.48	0.46
1:C:200:MET:HG3	1:C:239:VAL:HG12	1.96	0.46
1:D:121:ARG:HB3	1:D:122:PRO:HD3	1.98	0.46
1:B:46:PRO:HB2	1:B:47:TYR:CD1	2.51	0.46
1:B:172:ARG:NH1	1:B:172:ARG:CG	2.78	0.46
2:B:501:HEM:HBA2	3:B:502:QR8:O12	2.16	0.46
1:C:57:ARG:NH1	1:C:329:GLU:OE2	2.49	0.46
1:C:93:VAL:HG11	1:C:237:MET:HE2	1.97	0.46
1:C:207:ARG:HE	1:C:216:LEU:CB	2.28	0.46
1:C:359:ALA:O	1:C:363:ARG:HG3	2.16	0.46
2:C:501:HEM:HBB2	2:C:501:HEM:HMB2	1.98	0.46
1:F:254:THR:CG2	1:F:400:LEU:HB2	2.46	0.46
1:G:132:LEU:O	1:G:136:VAL:HG23	2.15	0.46
1:B:272:ALA:HB1	1:D:330:VAL:CG2	2.46	0.46
1:C:200:MET:CG	1:C:239:VAL:HG12	2.45	0.46
1:C:284:MET:HE3	1:C:339:PHE:HZ	1.81	0.46
1:D:218:ALA:HA	1:D:221:LEU:HD23	1.98	0.46
1:E:356:CYS:SG	2:E:501:HEM:NA	2.89	0.46
1:I:104:LEU:HD12	1:I:105:ARG:HG2	1.98	0.46
1:I:384:GLU:CD	1:I:402:ARG:NH1	2.74	0.46
1:H:96:GLN:HB3	1:H:101:HIS:HB2	1.98	0.45
1:H:156:VAL:HG21	1:H:365:GLU:HG2	1.97	0.45
1:I:40:VAL:HB	1:I:42:ARG:HH12	1.81	0.45
1:I:199:TYR:CD1	1:I:199:TYR:C	2.94	0.45
1:A:35:ARG:HE	1:A:323:SER:HG	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:PRO:HG2	1:B:189:ILE:CD1	2.40	0.45
1:F:305:GLU:OE1	1:F:310:THR:HG21	2.16	0.45
1:G:208:ARG:HG3	1:G:231:LYS:HD3	1.99	0.45
1:G:260:LEU:CD2	1:G:284:MET:HE1	2.46	0.45
1:E:156:VAL:HG21	1:E:365:GLU:HG2	1.98	0.45
1:G:215:LEU:C	1:G:215:LEU:HD13	2.41	0.45
1:H:221:LEU:CD2	1:H:221:LEU:N	2.79	0.45
1:B:168:ARG:HA	1:B:171:PHE:CD2	2.50	0.45
1:C:402:ARG:CD	1:C:404:ILE:HG13	2.46	0.45
2:D:501:HEM:HBC2	2:D:501:HEM:CMC	2.44	0.45
2:E:501:HEM:HBC2	2:E:501:HEM:HMC2	1.97	0.45
1:I:189:ILE:O	1:I:192:VAL:HG23	2.15	0.45
1:A:120:MET:CE	1:A:159:GLU:HB3	2.47	0.45
1:B:229:LEU:HD13	1:B:229:LEU:HA	1.76	0.45
1:B:235:VAL:O	1:B:236:ASN:C	2.56	0.45
1:E:27:LEU:HD23	1:E:27:LEU:HA	1.81	0.45
1:E:75:ALA:HA	1:E:80:THR:HG21	1.98	0.45
1:E:212:THR:HG22	1:E:213:GLU:H	1.81	0.45
1:F:31:TYR:HB3	1:F:323:SER:OG	2.16	0.45
1:F:81:PRO:O	1:F:297:VAL:HG21	2.17	0.45
1:F:107:LEU:HD23	1:F:229:LEU:HD23	1.98	0.45
1:H:226:ASP:O	1:H:227:ASP:C	2.57	0.45
1:H:286:ARG:HB2	1:H:346:HIS:HB3	1.98	0.45
1:E:35:ARG:HG3	1:E:56:THR:HG22	1.97	0.45
1:E:56:THR:HG22	1:E:56:THR:O	2.17	0.45
1:G:129:ASP:OD1	1:G:375:ARG:NH2	2.46	0.45
1:B:73:ALA:O	1:B:76:THR:OG1	2.27	0.45
1:A:307:SER:OG	1:A:308:THR:HG23	2.17	0.45
1:B:236:ASN:ND2	1:B:236:ASN:O	2.50	0.45
1:G:83:MET:HE3	1:G:318:VAL:HG21	1.98	0.45
1:I:381:ASP:OD1	1:I:382:LEU:O	2.34	0.45
1:A:84:PHE:CD1	1:A:84:PHE:N	2.84	0.45
1:B:57:ARG:HH22	1:B:329:GLU:HG2	1.82	0.45
1:B:92:GLY:HA2	1:B:236:ASN:ND2	2.32	0.45
1:D:204:VAL:HG21	1:D:235:VAL:HG22	1.99	0.45
1:E:150:VAL:HB	1:E:151:PRO:HD3	1.99	0.45
1:F:121:ARG:HB3	1:F:122:PRO:HD3	1.99	0.45
1:G:286:ARG:NH2	1:G:334:ALA:HA	2.32	0.45
1:A:63:ILE:HG12	1:C:378:PRO:HB2	1.99	0.45
1:B:150:VAL:HB	1:B:151:PRO:HD3	1.99	0.45
1:C:191:ARG:NH1	1:C:195:ASP:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:376:ARG:HB2	1:F:377:PHE:CE1	2.52	0.45
1:H:189:ILE:O	1:H:192:VAL:HG13	2.16	0.45
1:E:229:LEU:HD13	1:E:233:GLU:HB3	1.99	0.44
1:F:264:ARG:NE	1:F:381:ASP:OD1	2.48	0.44
1:H:27:LEU:HD23	1:H:27:LEU:HA	1.90	0.44
1:H:355:HIS:O	1:H:356:CYS:C	2.60	0.44
1:I:219:LEU:HD11	1:I:235:VAL:HA	1.98	0.44
1:E:377:PHE:O	1:E:380:LEU:HB2	2.18	0.44
2:E:501:HEM:HMB2	2:E:501:HEM:CBB	2.40	0.44
1:G:46:PRO:HB2	1:G:47:TYR:CD1	2.51	0.44
1:G:120:MET:CE	1:G:160:LEU:HD23	2.47	0.44
1:A:172:ARG:HH21	1:A:172:ARG:HG2	1.82	0.44
1:D:244:ALA:HA	3:D:502:QR8:C30	2.47	0.44
1:D:260:LEU:CD2	1:D:284:MET:HE1	2.47	0.44
1:D:284:MET:HE3	1:D:339:PHE:HZ	1.82	0.44
1:A:208:ARG:NH2	1:H:100:ASP:OD1	2.50	0.44
1:B:101:HIS:CD2	1:B:354:HIS:CE1	3.05	0.44
1:B:148:LEU:O	1:B:151:PRO:HD2	2.18	0.44
1:B:157:ILE:HD11	1:B:246:HIS:HB3	2.00	0.44
1:D:286:ARG:HB2	1:D:346:HIS:HB3	2.00	0.44
1:E:346:HIS:HD2	1:E:348:ALA:H	1.65	0.44
1:F:58:MET:HE1	1:F:347:ILE:HG12	1.99	0.44
1:F:191:ARG:HH11	1:F:191:ARG:HG3	1.81	0.44
3:G:502:QR8:C9	3:G:502:QR8:C32	2.95	0.44
1:H:183:ARG:NH1	1:H:183:ARG:CB	2.78	0.44
1:I:188:GLU:HA	1:I:191:ARG:CD	2.47	0.44
1:A:156:VAL:HG21	1:A:365:GLU:HG2	1.98	0.44
1:E:82:ARG:NH1	1:E:82:ARG:CG	2.81	0.44
1:E:104:LEU:HD22	1:E:237:MET:HE3	1.99	0.44
1:F:191:ARG:CG	1:F:191:ARG:NH1	2.80	0.44
1:H:252:GLN:HE21	1:H:285:LEU:HD23	1.82	0.44
1:I:188:GLU:HA	1:I:191:ARG:CG	2.47	0.44
1:A:254:THR:CG2	1:A:400:LEU:HB2	2.46	0.44
1:D:120:MET:CE	1:D:159:GLU:HB3	2.48	0.44
1:D:124:VAL:O	1:D:128:VAL:HG23	2.18	0.44
1:F:382:LEU:HD22	1:F:384:GLU:O	2.17	0.44
1:G:245:GLY:HA2	2:G:501:HEM:C1C	2.52	0.44
1:G:60:ASP:OD1	1:G:307:SER:HB3	2.17	0.44
1:I:153:PRO:CG	1:I:250:VAL:HG22	2.47	0.44
1:I:362:GLY:O	1:I:366:LEU:HG	2.18	0.44
1:D:184:LEU:HA	1:D:189:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:ASP:HB3	1:E:80:THR:OG1	2.18	0.44
1:E:135:MET:HE3	1:E:407:TRP:CZ3	2.53	0.44
1:I:108:VAL:HG11	1:I:237:MET:HE1	2.00	0.44
1:I:128:VAL:HG23	1:I:148:LEU:HD11	2.00	0.44
1:I:154:VAL:O	1:I:158:CYS:SG	2.76	0.44
1:C:166:GLU:C	1:C:168:ARG:H	2.25	0.44
1:D:81:PRO:O	1:D:297:VAL:HG21	2.18	0.44
1:D:384:GLU:OE2	1:D:402:ARG:NH2	2.51	0.44
1:E:363:ARG:O	1:E:367:GLN:HG3	2.17	0.44
1:F:30:HIS:CD2	1:F:34:LEU:HG	2.53	0.44
3:A:502:QR8:O11	3:A:502:QR8:O12	2.31	0.43
1:B:286:ARG:HB2	1:B:346:HIS:HB3	1.99	0.43
1:E:67:ASP:OD1	1:E:68:SER:N	2.51	0.43
1:G:157:ILE:CD1	1:G:242:LEU:HD12	2.43	0.43
1:I:364:LEU:O	1:I:368:GLU:HG2	2.18	0.43
1:A:38:GLU:OE1	4:A:601:HOH:O	2.21	0.43
1:A:76:THR:HG21	1:A:90:PRO:HA	2.00	0.43
1:D:277:VAL:HB	1:D:278:PRO:HD3	2.00	0.43
1:H:163:VAL:HG21	1:H:171:PHE:CZ	2.53	0.43
1:C:402:ARG:HD3	1:C:404:ILE:CG1	2.48	0.43
1:E:195:ASP:O	1:E:198:VAL:HG12	2.18	0.43
1:H:151:PRO:CB	1:H:172:ARG:HH12	2.31	0.43
1:A:223:THR:CG2	1:A:226:ASP:HB2	2.36	0.43
1:C:171:PHE:O	1:C:175:SER:OG	2.36	0.43
1:G:178:MET:CE	1:G:193:GLN:HE21	2.31	0.43
1:H:284:MET:HE3	1:H:339:PHE:HZ	1.83	0.43
1:E:273:ASP:O	1:E:276:LEU:HB2	2.18	0.43
1:E:329:GLU:OE2	1:E:329:GLU:CA	2.65	0.43
1:F:359:ALA:O	1:F:363:ARG:HG3	2.18	0.43
1:G:154:VAL:HA	1:G:157:ILE:CD1	2.49	0.43
1:H:332:ASP:C	1:H:333:HIS:ND1	2.76	0.43
1:I:197:MET:HE3	1:I:236:ASN:ND2	2.34	0.43
1:B:76:THR:HG21	1:B:90:PRO:HA	2.00	0.43
1:D:106:ARG:HH12	1:D:110:LYS:HE3	1.82	0.43
1:D:148:LEU:O	1:D:151:PRO:HD2	2.18	0.43
1:A:402:ARG:HG2	1:A:403:GLN:N	2.34	0.43
1:F:256:LEU:N	1:F:256:LEU:HD23	2.34	0.43
1:H:76:THR:HG21	1:H:90:PRO:HA	2.01	0.43
1:H:190:GLN:HE21	1:H:190:GLN:HB3	1.56	0.43
1:E:118:GLU:O	1:E:118:GLU:HG3	2.19	0.43
1:E:204:VAL:HG11	1:E:234:ILE:CG2	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:PHE:CE2	1:E:345:PRO:HD2	2.54	0.43
1:F:129:ASP:OD1	1:F:375:ARG:NH2	2.46	0.43
1:F:171:PHE:O	1:F:175:SER:OG	2.35	0.43
1:I:149:ALA:CB	1:I:253:ILE:HG21	2.49	0.43
1:C:402:ARG:HD3	1:C:404:ILE:HG13	2.00	0.43
1:H:332:ASP:O	1:H:333:HIS:C	2.62	0.43
1:A:163:VAL:HG21	1:A:171:PHE:CZ	2.54	0.43
1:C:92:GLY:HA2	1:C:236:ASN:CG	2.43	0.43
1:C:113:THR:OG1	1:C:116:ARG:HG3	2.19	0.43
1:F:132:LEU:O	1:F:136:VAL:HG23	2.19	0.43
1:G:264:ARG:NH2	1:G:380:LEU:O	2.42	0.43
1:A:230:THR:HG22	1:A:232:GLY:N	2.29	0.42
1:B:45:LEU:HD22	1:B:81:PRO:HB2	2.01	0.42
1:C:27:LEU:HA	1:C:27:LEU:HD23	1.78	0.42
1:D:57:ARG:HH22	1:D:329:GLU:HB2	1.84	0.42
1:H:383:ALA:HB3	1:H:404:ILE:HG22	2.01	0.42
1:B:14:VAL:CG1	1:B:44:ARG:NH2	2.82	0.42
1:B:170:LEU:CD1	1:B:174:PHE:CZ	3.03	0.42
1:C:161:LEU:HD12	1:C:215:LEU:HB2	2.01	0.42
1:D:27:LEU:HD23	1:D:27:LEU:HA	1.86	0.42
1:D:75:ALA:HA	1:D:80:THR:HG21	2.01	0.42
1:G:205:ALA:HA	1:G:231:LYS:NZ	2.34	0.42
1:H:303:ASP:OD1	1:H:312:ARG:HA	2.19	0.42
1:B:384:GLU:OE1	1:B:402:ARG:NH2	2.52	0.42
1:E:20:SER:OG	1:E:28:ASP:OD2	2.36	0.42
1:E:170:LEU:HD12	1:E:170:LEU:O	2.19	0.42
1:G:111:ALA:HB1	1:G:215:LEU:HD22	2.00	0.42
1:H:178:MET:HE1	1:H:193:GLN:OE1	2.19	0.42
1:E:286:ARG:HB2	1:E:346:HIS:CB	2.49	0.42
1:F:287:TYR:CG	1:F:337:LEU:HD13	2.54	0.42
1:G:148:LEU:O	1:G:151:PRO:HD2	2.19	0.42
1:H:94:LEU:HD12	1:H:94:LEU:HA	1.87	0.42
1:H:180:SER:O	1:H:181:SER:CB	2.66	0.42
1:F:76:THR:HG21	1:F:90:PRO:HA	2.01	0.42
1:H:152:PHE:O	1:H:156:VAL:HG23	2.19	0.42
1:H:358:GLY:HA3	2:H:501:HEM:C3C	2.54	0.42
1:I:179:LEU:HD13	1:I:396:LEU:HD12	2.02	0.42
1:C:343:ARG:CZ	1:C:343:ARG:CB	2.96	0.42
1:F:355:HIS:O	1:F:356:CYS:C	2.62	0.42
1:G:286:ARG:HH12	1:G:341:ARG:CZ	2.32	0.42
1:H:84:PHE:N	1:H:84:PHE:CD1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASP:OD2	1:A:307:SER:HB3	2.20	0.42
1:C:252:GLN:OE1	1:C:290:LEU:HD13	2.20	0.42
1:D:356:CYS:SG	2:D:501:HEM:NA	2.92	0.42
1:D:359:ALA:O	1:D:363:ARG:HG3	2.19	0.42
1:H:55:VAL:HG13	1:H:60:ASP:HB3	2.01	0.42
1:H:171:PHE:O	1:H:175:SER:OG	2.38	0.42
1:A:356:CYS:HA	2:A:501:HEM:C4D	2.55	0.42
1:E:73:ALA:HA	1:E:95:ALA:O	2.19	0.42
1:E:148:LEU:C	1:E:151:PRO:HD2	2.43	0.42
1:E:254:THR:CG2	1:E:400:LEU:HB2	2.49	0.42
1:H:132:LEU:HG	1:H:377:PHE:HE2	1.85	0.42
1:I:237:MET:HE2	1:I:241:LEU:HD21	2.01	0.42
1:I:384:GLU:OE2	1:I:404:ILE:HG12	2.20	0.42
2:I:501:HEM:HBB2	2:I:501:HEM:CMB	2.47	0.42
1:A:227:ASP:OD1	1:A:227:ASP:N	2.42	0.42
1:A:360:GLN:OE1	1:A:363:ARG:NH1	2.53	0.42
1:B:208:ARG:NH2	1:G:355:HIS:CE1	2.88	0.42
1:H:121:ARG:HB3	1:H:122:PRO:HD3	2.00	0.42
1:E:46:PRO:HB2	1:E:47:TYR:CD1	2.54	0.42
1:F:156:VAL:HG21	1:F:365:GLU:HG2	2.01	0.42
1:F:203:LEU:HD11	1:F:207:ARG:NH2	2.35	0.42
1:G:247:GLU:HG2	1:G:397:ILE:CD1	2.50	0.42
1:H:245:GLY:HA2	2:H:501:HEM:C1C	2.55	0.42
1:I:155:ALA:CA	1:I:158:CYS:SG	3.03	0.42
1:B:17:TYR:HA	1:B:18:PRO:C	2.45	0.41
1:B:131:LEU:O	1:B:134:ASP:HB2	2.20	0.41
1:B:230:THR:HB	1:B:233:GLU:OE2	2.20	0.41
1:C:207:ARG:NE	1:C:216:LEU:HB3	2.34	0.41
1:C:273:ASP:O	1:C:276:LEU:HB2	2.19	0.41
1:G:135:MET:HE3	1:G:407:TRP:CZ3	2.55	0.41
1:G:199:TYR:O	1:G:199:TYR:CD1	2.73	0.41
1:H:354:HIS:CD2	2:H:501:HEM:O1D	2.72	0.41
1:D:56:THR:HG22	1:D:56:THR:O	2.19	0.41
1:F:197:MET:HE1	1:F:235:VAL:HG12	2.02	0.41
1:F:271:VAL:HA	1:F:374:VAL:HG13	2.00	0.41
1:F:376:ARG:HB3	1:F:377:PHE:CE1	2.55	0.41
1:G:81:PRO:O	1:G:297:VAL:HG21	2.21	0.41
1:I:98:PRO:CA	1:I:99:PRO:C	2.92	0.41
1:B:150:VAL:HA	1:B:250:VAL:HG21	2.02	0.41
1:C:395:MET:HE2	1:C:395:MET:HB3	1.86	0.41
1:D:252:GLN:HE21	1:D:285:LEU:HD23	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:LEU:HD12	1:E:94:LEU:HA	1.92	0.41
1:F:84:PHE:CD1	1:F:84:PHE:N	2.89	0.41
1:I:113:THR:O	1:I:117:VAL:HG23	2.20	0.41
1:I:133:ASP:HA	1:I:136:VAL:CG2	2.48	0.41
1:I:153:PRO:HB2	1:I:246:HIS:HA	2.02	0.41
1:I:219:LEU:CG	1:I:234:ILE:O	2.68	0.41
1:A:42:ARG:CG	1:A:42:ARG:NH1	2.69	0.41
1:A:107:LEU:HD12	1:A:229:LEU:HD23	2.01	0.41
1:C:290:LEU:O	1:C:397:ILE:HG22	2.20	0.41
1:E:39:PRO:HB3	1:E:57:ARG:HD2	2.02	0.41
1:G:27:LEU:HD23	1:G:27:LEU:HA	1.83	0.41
1:H:230:THR:HB	1:H:233:GLU:H	1.86	0.41
1:I:176:ASP:OD1	1:I:247:GLU:OE2	2.38	0.41
1:C:205:ALA:HA	1:C:208:ARG:HD2	2.02	0.41
1:E:219:LEU:HB2	1:E:234:ILE:HD11	2.02	0.41
1:F:396:LEU:HG	3:F:502:QR8:C34	2.50	0.41
1:H:199:TYR:CE2	1:H:203:LEU:HD12	2.54	0.41
1:C:223:THR:HG22	1:C:224:ASP:OD1	2.21	0.41
1:D:94:LEU:HD21	3:D:502:QR8:C35	2.50	0.41
1:D:227:ASP:HB3	1:F:227:ASP:HB2	2.03	0.41
1:F:402:ARG:HG2	1:F:403:GLN:N	2.34	0.41
1:I:108:VAL:HG11	1:I:237:MET:SD	2.61	0.41
1:I:219:LEU:C	1:I:219:LEU:CD2	2.88	0.41
1:C:217:GLY:O	1:C:221:LEU:HD12	2.21	0.41
1:E:356:CYS:SG	2:E:501:HEM:C4C	3.13	0.41
1:H:356:CYS:HA	2:H:501:HEM:C4D	2.56	0.41
1:I:175:SER:O	1:I:179:LEU:HD23	2.20	0.41
1:A:227:ASP:HB3	1:H:227:ASP:HB2	2.02	0.41
1:B:31:TYR:CZ	1:B:320:HIS:CE1	3.09	0.41
1:C:28:ASP:OD1	1:C:30:HIS:HB2	2.20	0.41
1:C:150:VAL:HA	1:C:250:VAL:HG21	2.02	0.41
1:C:290:LEU:HG	1:C:397:ILE:HG22	2.03	0.41
1:D:156:VAL:HG21	1:D:365:GLU:HG2	2.02	0.41
1:G:247:GLU:HG2	1:G:397:ILE:HD11	2.02	0.41
1:H:35:ARG:HH11	1:H:328:GLU:CD	2.29	0.41
1:H:94:LEU:HD12	1:H:354:HIS:HD2	1.79	0.41
1:A:176:ASP:O	1:A:182:THR:HB	2.21	0.41
1:A:204:VAL:HG21	1:A:235:VAL:HG22	2.03	0.41
1:A:244:ALA:HB2	3:A:502:QR8:C31	2.51	0.41
3:A:502:QR8:C32	3:A:502:QR8:O11	2.69	0.41
1:B:133:ASP:OD1	1:B:376:ARG:NH2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:SER:HB2	1:B:398:ARG:HG2	2.03	0.41
1:C:121:ARG:HB3	1:C:122:PRO:HD3	2.02	0.41
1:E:354:HIS:HA	2:E:501:HEM:O2D	2.21	0.41
1:F:278:PRO:O	1:F:281:VAL:HG22	2.20	0.41
1:F:332:ASP:O	1:F:333:HIS:C	2.64	0.41
1:G:249:SER:O	1:G:253:ILE:HG13	2.20	0.41
1:G:331:PHE:CE2	1:G:345:PRO:HD2	2.55	0.41
1:H:55:VAL:HG13	1:H:60:ASP:CB	2.51	0.41
1:H:125:ARG:HG2	1:H:375:ARG:HH22	1.85	0.41
1:H:377:PHE:O	1:H:380:LEU:HB2	2.21	0.41
1:I:117:VAL:HG21	1:I:360:GLN:HB3	2.01	0.41
1:B:27:LEU:HD13	4:B:604:HOH:O	2.21	0.41
1:B:237:MET:HE2	1:B:237:MET:HB3	1.58	0.41
1:C:42:ARG:NH2	1:C:315:GLU:OE1	2.54	0.41
1:D:94:LEU:HD12	1:D:94:LEU:HA	1.93	0.41
1:E:76:THR:HG21	1:E:90:PRO:HA	2.02	0.41
1:E:104:LEU:O	1:E:108:VAL:HG13	2.20	0.41
1:F:27:LEU:HD23	1:F:27:LEU:HA	1.93	0.41
1:F:260:LEU:CG	1:F:284:MET:HE1	2.45	0.41
1:H:31:TYR:CE2	1:H:320:HIS:CD2	3.09	0.41
1:H:189:ILE:HG23	1:H:190:GLN:N	2.36	0.41
1:H:218:ALA:HA	1:H:221:LEU:HD22	2.03	0.41
1:I:179:LEU:HD12	1:I:396:LEU:HD12	2.01	0.41
1:A:331:PHE:CE1	1:A:345:PRO:HD2	2.56	0.40
1:B:105:ARG:HD3	1:B:105:ARG:O	2.21	0.40
1:G:154:VAL:HA	1:G:157:ILE:HD11	2.03	0.40
1:H:17:TYR:HA	1:H:18:PRO:C	2.46	0.40
1:B:327:ASP:O	1:B:330:VAL:HG12	2.21	0.40
1:C:73:ALA:HA	1:C:95:ALA:O	2.21	0.40
1:F:35:ARG:HG3	1:F:56:THR:HG22	2.03	0.40
1:A:107:LEU:HD12	1:A:229:LEU:CD2	2.51	0.40
1:A:121:ARG:HB3	1:A:122:PRO:HD3	2.02	0.40
1:A:132:LEU:O	1:A:136:VAL:HG23	2.22	0.40
1:D:76:THR:HG21	1:D:90:PRO:HA	2.02	0.40
1:D:105:ARG:NH1	2:D:501:HEM:O2D	2.54	0.40
1:F:199:TYR:CE1	1:F:203:LEU:HD22	2.56	0.40
1:G:200:MET:HE1	1:G:216:LEU:HD11	2.03	0.40
1:G:359:ALA:O	1:G:363:ARG:HG3	2.22	0.40
1:H:127:LEU:HD23	1:H:127:LEU:HA	1.85	0.40
1:H:235:VAL:O	1:H:239:VAL:HG23	2.21	0.40
1:I:241:LEU:CD2	2:I:501:HEM:HMD2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:372:ALA:HA	1:I:375:ARG:NH2	2.35	0.40
1:B:178:MET:CE	1:B:196:PHE:CD2	2.97	0.40
1:C:384:GLU:OE1	1:C:389:LEU:HD23	2.21	0.40
1:E:249:SER:O	1:E:253:ILE:HG13	2.21	0.40
1:E:263:GLU:O	1:E:266:ARG:CD	2.65	0.40
1:I:148:LEU:HD12	1:I:148:LEU:HA	1.78	0.40
1:A:172:ARG:HG2	1:A:172:ARG:NH2	2.37	0.40
1:C:174:PHE:HA	1:C:192:VAL:CG1	2.51	0.40
1:C:250:VAL:CG1	1:C:251:ASN:N	2.83	0.40
1:G:69:ARG:HD2	1:G:304:VAL:HG13	2.04	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	392/407 (96%)	380 (97%)	12 (3%)	0	100	100
1	B	393/407 (97%)	374 (95%)	19 (5%)	0	100	100
1	C	393/407 (97%)	382 (97%)	11 (3%)	0	100	100
1	D	392/407 (96%)	381 (97%)	11 (3%)	0	100	100
1	E	382/407 (94%)	370 (97%)	12 (3%)	0	100	100
1	F	392/407 (96%)	374 (95%)	18 (5%)	0	100	100
1	G	375/407 (92%)	365 (97%)	10 (3%)	0	100	100
1	H	393/407 (97%)	379 (96%)	14 (4%)	0	100	100
1	I	230/407 (56%)	219 (95%)	11 (5%)	0	100	100
All	All	3342/3663 (91%)	3224 (96%)	118 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/341 (97%)	275 (83%)	56 (17%)	2	5
1	B	331/341 (97%)	256 (77%)	75 (23%)	1	1
1	C	331/341 (97%)	274 (83%)	57 (17%)	2	5
1	D	330/341 (97%)	273 (83%)	57 (17%)	2	5
1	E	323/341 (95%)	264 (82%)	59 (18%)	2	4
1	F	331/341 (97%)	273 (82%)	58 (18%)	2	4
1	G	319/341 (94%)	264 (83%)	55 (17%)	2	5
1	H	331/341 (97%)	276 (83%)	55 (17%)	2	6
1	I	205/341 (60%)	160 (78%)	45 (22%)	1	2
All	All	2832/3069 (92%)	2315 (82%)	517 (18%)	2	4

All (517) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	SER
1	A	42	ARG
1	A	43	VAL
1	A	49	GLU
1	A	54	LEU
1	A	62	ARG
1	A	71	SER
1	A	76	THR
1	A	96	GLN
1	A	104	LEU
1	A	105	ARG
1	A	123	ARG
1	A	125	ARG
1	A	128	VAL
1	A	129	ASP
1	A	132	LEU
1	A	154	VAL
1	A	157	ILE

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Mol	Chain	Res	Type
1	A	159	GLU
1	A	166	GLU
1	A	172	ARG
1	A	173	THR
1	A	175	SER
1	A	178	MET
1	A	179	LEU
1	A	184	LEU
1	A	188	GLU
1	A	193	GLN
1	A	198	VAL
1	A	221	LEU
1	A	223	THR
1	A	227	ASP
1	A	237	MET
1	A	247	GLU
1	A	256	LEU
1	A	263	GLU
1	A	269	SER
1	A	276	LEU
1	A	286	ARG
1	A	292	SER
1	A	301	THR
1	A	307	SER
1	A	309	VAL
1	A	310	THR
1	A	318	VAL
1	A	329	GLU
1	A	337	LEU
1	A	342	GLU
1	A	357	ILE
1	A	364	LEU
1	A	380	LEU
1	A	382	LEU
1	A	386	VAL
1	A	390	LYS
1	A	393	GLN
1	A	396	LEU
1	B	14	VAL
1	B	27	LEU
1	B	37	ASP
1	B	40	VAL

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Mol	Chain	Res	Type
1	B	42	ARG
1	B	49	GLU
1	B	51	THR
1	B	53	TRP
1	B	54	LEU
1	B	76	THR
1	B	83	MET
1	B	84	PHE
1	B	89	GLU
1	B	100	ASP
1	B	104	LEU
1	B	106	ARG
1	B	108	VAL
1	B	110	LYS
1	B	116	ARG
1	B	123	ARG
1	B	125	ARG
1	B	127	LEU
1	B	128	VAL
1	B	130	SER
1	B	132	LEU
1	B	157	ILE
1	B	161	LEU
1	B	166	GLU
1	B	168	ARG
1	B	172	ARG
1	B	173	THR
1	B	175	SER
1	B	178	MET
1	B	182	THR
1	B	183	ARG
1	B	184	LEU
1	B	185	THR
1	B	188	GLU
1	B	190	GLN
1	B	201	ASP
1	B	215	LEU
1	B	216	LEU
1	B	221	LEU
1	B	226	ASP
1	B	227	ASP
1	B	228	HIS

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Mol	Chain	Res	Type
1	B	229	LEU
1	B	231	LYS
1	B	233	GLU
1	B	234	ILE
1	B	235	VAL
1	B	237	MET
1	B	242	LEU
1	B	250	VAL
1	B	256	LEU
1	B	263	GLU
1	B	265	LYS
1	B	269	SER
1	B	276	LEU
1	B	286	ARG
1	B	288	THR
1	B	292	SER
1	B	305	GLU
1	B	307	SER
1	B	310	THR
1	B	315	GLU
1	B	318	VAL
1	B	327	ASP
1	B	328	GLU
1	B	329	GLU
1	B	337	LEU
1	B	357	ILE
1	B	364	LEU
1	B	382	LEU
1	B	390	LYS
1	C	14	VAL
1	C	41	SER
1	C	42	ARG
1	C	49	GLU
1	C	51	THR
1	C	54	LEU
1	C	76	THR
1	C	89	GLU
1	C	102	THR
1	C	104	LEU
1	C	123	ARG
1	C	127	LEU
1	C	128	VAL

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Mol	Chain	Res	Type
1	C	130	SER
1	C	132	LEU
1	C	136	VAL
1	C	154	VAL
1	C	161	LEU
1	C	166	GLU
1	C	168	ARG
1	C	173	THR
1	C	175	SER
1	C	178	MET
1	C	185	THR
1	C	191	ARG
1	C	200	MET
1	C	201	ASP
1	C	209	ASP
1	C	216	LEU
1	C	221	LEU
1	C	223	THR
1	C	224	ASP
1	C	227	ASP
1	C	228	HIS
1	C	229	LEU
1	C	230	THR
1	C	246	HIS
1	C	250	VAL
1	C	256	LEU
1	C	263	GLU
1	C	276	LEU
1	C	288	THR
1	C	292	SER
1	C	305	GLU
1	C	310	THR
1	C	315	GLU
1	C	318	VAL
1	C	330	VAL
1	C	337	LEU
1	C	342	GLU
1	C	343	ARG
1	C	357	ILE
1	C	364	LEU
1	C	382	LEU
1	C	390	LYS

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Mol	Chain	Res	Type
1	C	395	MET
1	C	397	ILE
1	D	41	SER
1	D	43	VAL
1	D	49	GLU
1	D	54	LEU
1	D	71	SER
1	D	76	THR
1	D	84	PHE
1	D	91	ASP
1	D	96	GLN
1	D	105	ARG
1	D	106	ARG
1	D	115	ARG
1	D	125	ARG
1	D	127	LEU
1	D	128	VAL
1	D	129	ASP
1	D	130	SER
1	D	136	VAL
1	D	154	VAL
1	D	159	GLU
1	D	166	GLU
1	D	170	LEU
1	D	172	ARG
1	D	173	THR
1	D	175	SER
1	D	178	MET
1	D	179	LEU
1	D	181	SER
1	D	184	LEU
1	D	185	THR
1	D	203	LEU
1	D	208	ARG
1	D	209	ASP
1	D	213	GLU
1	D	221	LEU
1	D	223	THR
1	D	224	ASP
1	D	230	THR
1	D	247	GLU
1	D	256	LEU

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Mol	Chain	Res	Type
1	D	264	ARG
1	D	265	LYS
1	D	269	SER
1	D	276	LEU
1	D	286	ARG
1	D	307	SER
1	D	309	VAL
1	D	310	THR
1	D	318	VAL
1	D	337	LEU
1	D	357	ILE
1	D	364	LEU
1	D	380	LEU
1	D	382	LEU
1	D	386	VAL
1	D	390	LYS
1	D	396	LEU
1	E	41	SER
1	E	43	VAL
1	E	49	GLU
1	E	54	LEU
1	E	71	SER
1	E	76	THR
1	E	82	ARG
1	E	84	PHE
1	E	86	THR
1	E	89	GLU
1	E	96	GLN
1	E	104	LEU
1	E	107	LEU
1	E	115	ARG
1	E	123	ARG
1	E	125	ARG
1	E	128	VAL
1	E	129	ASP
1	E	132	LEU
1	E	154	VAL
1	E	159	GLU
1	E	170	LEU
1	E	175	SER
1	E	193	GLN
1	E	209	ASP

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Mol	Chain	Res	Type
1	E	213	GLU
1	E	221	LEU
1	E	226	ASP
1	E	228	HIS
1	E	229	LEU
1	E	230	THR
1	E	235	VAL
1	E	254	THR
1	E	256	LEU
1	E	263	GLU
1	E	265	LYS
1	E	266	ARG
1	E	269	SER
1	E	276	LEU
1	E	286	ARG
1	E	299	VAL
1	E	301	THR
1	E	305	GLU
1	E	309	VAL
1	E	310	THR
1	E	318	VAL
1	E	329	GLU
1	E	337	LEU
1	E	342	GLU
1	E	343	ARG
1	E	357	ILE
1	E	375	ARG
1	E	376	ARG
1	E	380	LEU
1	E	382	LEU
1	E	386	VAL
1	E	390	LYS
1	E	393	GLN
1	E	396	LEU
1	F	40	VAL
1	F	41	SER
1	F	42	ARG
1	F	43	VAL
1	F	49	GLU
1	F	51	THR
1	F	54	LEU
1	F	71	SER

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Mol	Chain	Res	Type
1	F	76	THR
1	F	91	ASP
1	F	105	ARG
1	F	106	ARG
1	F	107	LEU
1	F	123	ARG
1	F	125	ARG
1	F	127	LEU
1	F	128	VAL
1	F	129	ASP
1	F	130	SER
1	F	132	LEU
1	F	146	GLU
1	F	154	VAL
1	F	157	ILE
1	F	166	GLU
1	F	173	THR
1	F	175	SER
1	F	178	MET
1	F	179	LEU
1	F	182	THR
1	F	183	ARG
1	F	184	LEU
1	F	188	GLU
1	F	189	ILE
1	F	191	ARG
1	F	193	GLN
1	F	214	ASP
1	F	221	LEU
1	F	224	ASP
1	F	237	MET
1	F	256	LEU
1	F	263	GLU
1	F	265	LYS
1	F	276	LEU
1	F	309	VAL
1	F	310	THR
1	F	318	VAL
1	F	323	SER
1	F	342	GLU
1	F	357	ILE
1	F	377	PHE

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Mol	Chain	Res	Type
1	F	379	THR
1	F	380	LEU
1	F	381	ASP
1	F	382	LEU
1	F	386	VAL
1	F	390	LYS
1	F	393	GLN
1	F	396	LEU
1	G	41	SER
1	G	43	VAL
1	G	49	GLU
1	G	54	LEU
1	G	71	SER
1	G	86	THR
1	G	96	GLN
1	G	100	ASP
1	G	105	ARG
1	G	107	LEU
1	G	119	GLU
1	G	125	ARG
1	G	128	VAL
1	G	129	ASP
1	G	130	SER
1	G	132	LEU
1	G	154	VAL
1	G	159	GLU
1	G	160	LEU
1	G	166	GLU
1	G	172	ARG
1	G	173	THR
1	G	175	SER
1	G	178	MET
1	G	179	LEU
1	G	188	GLU
1	G	191	ARG
1	G	192	VAL
1	G	207	ARG
1	G	208	ARG
1	G	212	THR
1	G	215	LEU
1	G	228	HIS
1	G	229	LEU

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Mol	Chain	Res	Type
1	G	233	GLU
1	G	247	GLU
1	G	263	GLU
1	G	276	LEU
1	G	286	ARG
1	G	301	THR
1	G	304	VAL
1	G	309	VAL
1	G	310	THR
1	G	312	ARG
1	G	318	VAL
1	G	328	GLU
1	G	343	ARG
1	G	357	ILE
1	G	364	LEU
1	G	380	LEU
1	G	382	LEU
1	G	386	VAL
1	G	390	LYS
1	G	393	GLN
1	G	397	ILE
1	H	14	VAL
1	H	41	SER
1	H	49	GLU
1	H	51	THR
1	H	54	LEU
1	H	71	SER
1	H	76	THR
1	H	91	ASP
1	H	96	GLN
1	H	105	ARG
1	H	107	LEU
1	H	123	ARG
1	H	125	ARG
1	H	128	VAL
1	H	130	SER
1	H	132	LEU
1	H	154	VAL
1	H	159	GLU
1	H	166	GLU
1	H	173	THR
1	H	175	SER

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Mol	Chain	Res	Type
1	H	178	MET
1	H	179	LEU
1	H	188	GLU
1	H	190	GLN
1	H	192	VAL
1	H	198	VAL
1	H	223	THR
1	H	226	ASP
1	H	227	ASP
1	H	230	THR
1	H	231	LYS
1	H	237	MET
1	H	247	GLU
1	H	256	LEU
1	H	263	GLU
1	H	276	LEU
1	H	286	ARG
1	H	292	SER
1	H	305	GLU
1	H	309	VAL
1	H	310	THR
1	H	318	VAL
1	H	323	SER
1	H	337	LEU
1	H	342	GLU
1	H	347	ILE
1	H	357	ILE
1	H	364	LEU
1	H	380	LEU
1	H	382	LEU
1	H	386	VAL
1	H	390	LYS
1	H	393	GLN
1	H	396	LEU
1	I	42	ARG
1	I	57	ARG
1	I	60	ASP
1	I	62	ARG
1	I	63	ILE
1	I	64	VAL
1	I	100	ASP
1	I	105	ARG

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Mol	Chain	Res	Type
1	I	125	ARG
1	I	130	SER
1	I	132	LEU
1	I	135	MET
1	I	140	SER
1	I	167	ASP
1	I	168	ARG
1	I	169	ASP
1	I	171	PHE
1	I	172	ARG
1	I	180	SER
1	I	190	GLN
1	I	191	ARG
1	I	192	VAL
1	I	199	TYR
1	I	200	MET
1	I	219	LEU
1	I	221	LEU
1	I	230	THR
1	I	233	GLU
1	I	236	ASN
1	I	237	MET
1	I	241	LEU
1	I	246	HIS
1	I	254	THR
1	I	256	LEU
1	I	259	LEU
1	I	284	MET
1	I	288	THR
1	I	291	VAL
1	I	354	HIS
1	I	360	GLN
1	I	364	LEU
1	I	373	LEU
1	I	395	MET
1	I	397	ILE
1	I	405	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	GLN

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Mol	Chain	Res	Type
1	A	228	HIS
1	A	340	HIS
1	B	30	HIS
1	B	193	GLN
1	B	206	GLN
1	B	236	ASN
1	B	351	HIS
1	C	194	GLN
1	C	236	ASN
1	C	258	HIS
1	C	403	GLN
1	D	228	HIS
1	D	236	ASN
1	D	354	HIS
1	E	194	GLN
1	E	340	HIS
1	E	346	HIS
1	E	354	HIS
1	E	403	GLN
1	F	96	GLN
1	F	194	GLN
1	F	225	ASN
1	F	228	HIS
1	F	236	ASN
1	F	354	HIS
1	F	355	HIS
1	F	403	GLN
1	G	190	GLN
1	G	194	GLN
1	G	354	HIS
1	H	190	GLN
1	H	194	GLN
1	H	236	ASN
1	H	344	ASN
1	H	351	HIS
1	H	354	HIS
1	H	403	GLN
1	I	138	HIS
1	I	236	ASN
1	I	246	HIS
1	I	251	ASN
1	I	258	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

18 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	E	501	-	50,50,50	1.69	9 (18%)	66,82,82	1.74	16 (24%)
2	HEM	G	501	1	50,50,50	1.66	9 (18%)	66,82,82	1.71	10 (15%)
3	QR8	D	502	-	26,26,26	1.70	5 (19%)	35,38,38	2.45	11 (31%)
3	QR8	H	502	-	26,26,26	1.60	4 (15%)	35,38,38	2.40	12 (34%)
2	HEM	F	501	4,1	50,50,50	1.56	7 (14%)	66,82,82	1.46	11 (16%)
2	HEM	C	501	1	50,50,50	1.80	13 (26%)	66,82,82	1.90	15 (22%)
2	HEM	A	501	4,1	50,50,50	1.71	10 (20%)	66,82,82	1.72	13 (19%)
2	HEM	D	501	4,1	50,50,50	1.69	11 (22%)	66,82,82	1.63	9 (13%)
3	QR8	B	502	-	26,26,26	2.01	7 (26%)	35,38,38	1.82	6 (17%)
3	QR8	G	502	-	26,26,26	1.59	5 (19%)	35,38,38	1.77	9 (25%)
3	QR8	F	502	-	26,26,26	1.59	5 (19%)	35,38,38	1.94	12 (34%)
3	QR8	E	502	-	26,26,26	1.51	2 (7%)	35,38,38	2.52	15 (42%)
2	HEM	B	501	1	50,50,50	1.97	12 (24%)	66,82,82	1.94	17 (25%)
2	HEM	I	501	1	50,50,50	1.60	5 (10%)	66,82,82	1.67	14 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	QR8	I	502	1	26,26,26	1.32	3 (11%)	35,38,38	2.12	9 (25%)
3	QR8	C	502	-	26,26,26	1.71	6 (23%)	35,38,38	2.23	9 (25%)
3	QR8	A	502	-	26,26,26	1.79	7 (26%)	35,38,38	2.22	12 (34%)
2	HEM	H	501	4,1	50,50,50	1.73	10 (20%)	66,82,82	1.41	10 (15%)

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	E	501	-	-	0/14/54/54	-
2	HEM	G	501	1	-	0/14/54/54	-
3	QR8	D	502	-	-	25/48/48/48	0/1/1/1
3	QR8	H	502	-	-	20/48/48/48	0/1/1/1
2	HEM	F	501	4,1	-	2/14/54/54	-
2	HEM	C	501	1	-	4/14/54/54	-
2	HEM	A	501	4,1	-	3/14/54/54	-
2	HEM	D	501	4,1	-	0/14/54/54	-
3	QR8	B	502	-	-	24/48/48/48	0/1/1/1
3	QR8	G	502	-	-	19/48/48/48	0/1/1/1
3	QR8	F	502	-	-	27/48/48/48	0/1/1/1
3	QR8	E	502	-	2/2/12/12	29/48/48/48	1/1/1/1
2	HEM	B	501	1	-	0/14/54/54	-
2	HEM	I	501	1	-	6/14/54/54	-
3	QR8	I	502	1	-	16/48/48/48	0/1/1/1
3	QR8	C	502	-	-	23/48/48/48	0/1/1/1
3	QR8	A	502	-	-	18/48/48/48	0/1/1/1
2	HEM	H	501	4,1	-	0/14/54/54	-

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	HEM	FE-NB	6.02	2.13	1.94
2	B	501	HEM	C1B-NB	-5.85	1.30	1.40
2	I	501	HEM	FE-NB	5.78	2.12	1.94
2	H	501	HEM	FE-NB	5.55	2.12	1.94
2	G	501	HEM	FE-NB	5.45	2.11	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C1B-NB	-5.41	1.31	1.40
3	E	502	QR8	O2-C1	-5.26	1.22	1.34
2	B	501	HEM	FE-NC	5.21	2.12	1.95
2	I	501	HEM	FE-NC	5.06	2.12	1.95
2	E	501	HEM	FE-NB	4.98	2.10	1.94
2	C	501	HEM	FE-NB	4.92	2.10	1.94
3	B	502	QR8	O2-C13	-4.84	1.38	1.46
3	G	502	QR8	O2-C1	4.68	1.45	1.34
2	E	501	HEM	C1B-NB	-4.61	1.32	1.40
2	H	501	HEM	FE-NC	4.58	2.10	1.95
3	A	502	QR8	C10-C9	-4.57	1.45	1.52
3	D	502	QR8	O2-C13	-4.52	1.39	1.46
2	F	501	HEM	FE-NC	4.45	2.10	1.95
3	I	502	QR8	O2-C1	4.45	1.44	1.34
2	D	501	HEM	FE-NC	4.43	2.10	1.95
2	B	501	HEM	C1C-C2C	-4.34	1.36	1.45
3	B	502	QR8	C10-C9	-4.33	1.46	1.52
2	B	501	HEM	FE-NB	4.31	2.08	1.94
2	C	501	HEM	C1B-NB	-4.26	1.33	1.40
2	D	501	HEM	C1B-NB	-4.22	1.33	1.40
3	A	502	QR8	O2-C1	4.16	1.44	1.34
3	H	502	QR8	O2-C1	4.14	1.44	1.34
2	D	501	HEM	FE-NB	4.09	2.07	1.94
2	B	501	HEM	C4A-NA	-3.99	1.32	1.39
2	A	501	HEM	FE-NC	3.95	2.08	1.95
3	C	502	QR8	O2-C13	-3.91	1.40	1.46
2	A	501	HEM	C4A-NA	-3.87	1.32	1.39
3	F	502	QR8	C10-C9	-3.86	1.46	1.52
2	G	501	HEM	C1D-ND	-3.84	1.30	1.38
2	C	501	HEM	FE-NC	3.82	2.08	1.95
3	F	502	QR8	O2-C1	3.81	1.43	1.34
2	H	501	HEM	C1B-NB	-3.71	1.33	1.40
2	E	501	HEM	C4D-ND	-3.57	1.34	1.40
3	E	502	QR8	C10-C9	-3.55	1.47	1.52
2	I	501	HEM	C1B-NB	-3.51	1.34	1.40
3	D	502	QR8	C10-C9	-3.50	1.47	1.52
2	D	501	HEM	C4D-C3D	3.48	1.51	1.45
2	C	501	HEM	C4B-NB	-3.46	1.31	1.38
2	E	501	HEM	FE-NC	3.46	2.06	1.95
3	B	502	QR8	O2-C1	3.42	1.42	1.34
3	C	502	QR8	O2-C1	3.35	1.42	1.34
2	C	501	HEM	C1C-C2C	-3.32	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C4D-C3D	3.29	1.50	1.45
2	E	501	HEM	C4B-NB	-3.27	1.32	1.38
3	H	502	QR8	O2-C13	-3.20	1.41	1.46
2	A	501	HEM	FE-NB	3.18	2.04	1.94
2	A	501	HEM	C4B-NB	-3.07	1.32	1.38
2	G	501	HEM	FE-NC	3.06	2.05	1.95
3	F	502	QR8	O2-C13	-3.02	1.41	1.46
2	D	501	HEM	C4B-NB	-3.02	1.32	1.38
2	G	501	HEM	C4D-ND	-3.00	1.35	1.40
2	G	501	HEM	C1B-NB	-2.96	1.35	1.40
2	B	501	HEM	C4D-C3D	2.92	1.50	1.45
2	I	501	HEM	C4D-ND	-2.91	1.35	1.40
2	C	501	HEM	C1C-NC	-2.89	1.34	1.39
2	H	501	HEM	C4D-ND	-2.89	1.35	1.40
2	H	501	HEM	C4C-NC	-2.89	1.34	1.39
2	E	501	HEM	C1D-ND	-2.88	1.32	1.38
2	E	501	HEM	C3D-C2D	-2.86	1.30	1.36
2	D	501	HEM	C3C-C4C	-2.84	1.41	1.46
3	G	502	QR8	O2-C13	-2.81	1.42	1.46
2	G	501	HEM	FE-ND	-2.80	1.86	1.94
3	C	502	QR8	C7-C6	-2.79	1.49	1.54
2	C	501	HEM	C3C-C4C	-2.77	1.41	1.46
3	H	502	QR8	C2-C1	-2.73	1.45	1.51
2	C	501	HEM	C1A-C2A	-2.70	1.39	1.44
2	B	501	HEM	C1D-C2D	2.69	1.49	1.44
2	D	501	HEM	C1C-C2C	-2.68	1.40	1.45
2	H	501	HEM	C3C-C4C	-2.67	1.41	1.46
3	B	502	QR8	O11-C9	-2.66	1.17	1.21
3	G	502	QR8	C7-C6	-2.66	1.49	1.54
3	A	502	QR8	O2-C13	-2.66	1.42	1.46
3	D	502	QR8	O2-C1	2.65	1.40	1.34
3	H	502	QR8	C10-C9	-2.64	1.48	1.52
2	B	501	HEM	C3C-C4C	-2.58	1.41	1.46
2	F	501	HEM	C1B-NB	-2.58	1.35	1.40
3	A	502	QR8	O11-C9	-2.57	1.17	1.21
2	D	501	HEM	C4D-ND	-2.54	1.35	1.40
3	I	502	QR8	O2-C13	-2.54	1.42	1.46
2	D	501	HEM	C1C-NC	-2.47	1.35	1.39
3	A	502	QR8	C10-C11	-2.42	1.49	1.53
3	D	502	QR8	C7-C6	-2.42	1.50	1.54
2	G	501	HEM	C4C-NC	-2.40	1.35	1.39
2	C	501	HEM	C4D-C3D	2.40	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C1A-NA	-2.38	1.35	1.39
2	H	501	HEM	C4B-NB	-2.36	1.33	1.38
2	D	501	HEM	C1D-C2D	2.36	1.49	1.44
2	D	501	HEM	C4A-NA	-2.34	1.35	1.39
2	H	501	HEM	C1C-C2C	-2.33	1.40	1.45
2	G	501	HEM	C1C-C2C	-2.31	1.40	1.45
2	B	501	HEM	CBD-CGD	2.30	1.55	1.50
3	C	502	QR8	O11-C9	-2.30	1.17	1.21
3	G	502	QR8	C10-C9	-2.29	1.49	1.52
3	C	502	QR8	C10-C9	-2.29	1.49	1.52
2	A	501	HEM	C1A-C2A	-2.27	1.40	1.44
2	H	501	HEM	FE-ND	-2.27	1.87	1.94
2	F	501	HEM	C1D-C2D	2.27	1.48	1.44
3	F	502	QR8	C2-C1	-2.26	1.46	1.51
2	G	501	HEM	C4B-NB	-2.26	1.34	1.38
2	F	501	HEM	C4D-C3D	2.25	1.48	1.45
2	C	501	HEM	C4C-NC	-2.23	1.35	1.39
3	B	502	QR8	C2-C1	-2.23	1.46	1.51
2	I	501	HEM	CHB-C1B	2.22	1.43	1.38
3	F	502	QR8	C10-C11	-2.21	1.49	1.53
2	F	501	HEM	C4D-ND	-2.21	1.36	1.40
2	A	501	HEM	C1D-ND	-2.17	1.34	1.38
2	E	501	HEM	C3B-C2B	-2.15	1.32	1.37
2	B	501	HEM	O1D-CGD	2.14	1.29	1.22
2	A	501	HEM	C3D-C2D	-2.13	1.32	1.36
3	D	502	QR8	O11-C9	-2.10	1.18	1.21
2	E	501	HEM	C1C-C2C	-2.10	1.41	1.45
3	I	502	QR8	C2-C1	-2.08	1.47	1.51
2	A	501	HEM	CHC-C1C	-2.08	1.34	1.38
2	H	501	HEM	C3B-C4B	2.08	1.49	1.44
3	B	502	QR8	C2-C3	-2.07	1.49	1.53
3	A	502	QR8	C2-C1	-2.06	1.47	1.51
3	A	502	QR8	C7-C6	-2.06	1.50	1.54
3	B	502	QR8	C7-C6	-2.06	1.50	1.54
2	B	501	HEM	C4D-ND	-2.04	1.36	1.40
2	C	501	HEM	C3C-C2C	2.04	1.41	1.37
3	G	502	QR8	C10-C11	-2.03	1.49	1.53
3	C	502	QR8	C12-C13	-2.02	1.48	1.53
2	F	501	HEM	FE-ND	-2.02	1.88	1.94
2	C	501	HEM	C4D-ND	-2.02	1.36	1.40
2	C	501	HEM	C1D-ND	-2.00	1.34	1.38

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	502	QR8	C13-O2-C1	-8.04	105.86	117.51
2	B	501	HEM	CHC-C4B-NB	7.12	132.15	124.42
2	A	501	HEM	CHC-C4B-NB	6.44	131.41	124.42
2	B	501	HEM	C1B-NB-C4B	6.43	111.72	105.07
3	H	502	QR8	C35-C12-C13	-6.25	104.10	112.18
3	H	502	QR8	C6-C5-C4	-5.97	107.02	116.27
3	E	502	QR8	O2-C1-C2	5.70	124.08	111.56
2	I	501	HEM	CHC-C4B-NB	5.69	130.60	124.42
2	A	501	HEM	C1B-NB-C4B	5.68	110.94	105.07
2	G	501	HEM	CHC-C4B-NB	5.65	130.56	124.42
2	C	501	HEM	C1B-NB-C4B	5.50	110.76	105.07
3	I	502	QR8	C13-O2-C1	-5.37	109.73	117.51
3	C	502	QR8	C36-C13-C12	-5.37	106.62	114.39
3	E	502	QR8	C34-C10-C9	-5.32	98.82	108.08
2	C	501	HEM	CAA-CBA-CGA	-5.24	102.33	113.60
3	A	502	QR8	C13-O2-C1	-5.20	109.98	117.51
3	A	502	QR8	O2-C1-C2	5.16	122.89	111.56
3	C	502	QR8	O2-C1-C2	5.11	122.77	111.56
3	D	502	QR8	C6-C5-C4	-5.01	108.51	116.27
2	C	501	HEM	CHC-C4B-NB	4.97	129.82	124.42
2	E	501	HEM	CHC-C4B-NB	4.96	129.81	124.42
3	B	502	QR8	C36-C13-C12	-4.87	107.34	114.39
2	D	501	HEM	C1B-NB-C4B	4.84	110.08	105.07
3	G	502	QR8	C6-C5-C4	-4.69	109.00	116.27
3	C	502	QR8	O2-C1-O1	-4.64	115.28	123.94
2	D	501	HEM	CHC-C4B-NB	4.63	129.45	124.42
3	I	502	QR8	O2-C1-C2	4.60	121.67	111.56
3	C	502	QR8	C6-C5-C4	-4.56	109.21	116.27
3	H	502	QR8	C30-C2-C3	4.53	119.92	112.37
3	I	502	QR8	C3-C2-C1	-4.52	100.33	110.02
2	D	501	HEM	CHD-C1D-ND	4.49	129.30	124.42
3	I	502	QR8	C36-C13-C12	-4.42	107.98	114.39
3	B	502	QR8	C3-C2-C1	-4.42	100.55	110.02
3	F	502	QR8	O2-C1-C2	4.31	121.02	111.56
2	I	501	HEM	CHD-C1D-ND	4.29	129.08	124.42
3	D	502	QR8	O2-C1-O1	-4.28	115.95	123.94
3	D	502	QR8	O2-C1-C2	4.26	120.92	111.56
2	B	501	HEM	CHD-C1D-ND	4.21	128.99	124.42
2	I	501	HEM	C1B-NB-C4B	4.21	109.42	105.07
3	H	502	QR8	C3-C4-C5	-4.20	104.10	112.54
2	G	501	HEM	C1B-NB-C4B	4.20	109.41	105.07
2	A	501	HEM	C4B-C3B-C2B	-4.16	103.81	107.11
2	H	501	HEM	CHD-C1D-ND	4.14	128.91	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	HEM	C4C-NC-C1C	4.11	109.38	105.35
3	C	502	QR8	O12-C11-C12	-4.09	100.38	109.49
3	E	502	QR8	C6-C5-C4	-4.06	109.98	116.27
2	G	501	HEM	CHA-C4D-ND	4.05	129.37	124.37
2	E	501	HEM	C4C-NC-C1C	4.01	109.28	105.35
3	B	502	QR8	C6-C5-C4	-3.95	110.15	116.27
3	D	502	QR8	C11-C10-C9	-3.88	103.33	110.36
2	F	501	HEM	CHC-C4B-NB	3.87	128.62	124.42
2	D	501	HEM	CHD-C1D-C2D	-3.87	118.93	124.98
3	A	502	QR8	C11-C10-C9	-3.87	103.36	110.36
2	F	501	HEM	CHD-C1D-ND	3.83	128.58	124.42
3	E	502	QR8	C36-C13-C12	-3.82	108.85	114.39
2	G	501	HEM	C4C-NC-C1C	3.78	109.05	105.35
3	G	502	QR8	C32-C6-C7	-3.74	105.09	110.69
2	G	501	HEM	CHD-C1D-ND	3.67	128.41	124.42
2	E	501	HEM	C1B-NB-C4B	3.63	108.82	105.07
3	G	502	QR8	O2-C1-C2	3.61	119.47	111.56
3	F	502	QR8	C11-C10-C9	-3.56	103.90	110.36
3	I	502	QR8	C6-C5-C4	-3.56	110.76	116.27
2	A	501	HEM	CAD-C3D-C4D	3.55	130.86	124.66
2	I	501	HEM	CHA-C4D-ND	3.52	128.72	124.37
2	F	501	HEM	C1B-NB-C4B	3.52	108.71	105.07
3	E	502	QR8	O2-C13-C12	3.52	115.40	106.30
3	C	502	QR8	C35-C12-C13	-3.50	107.65	112.18
3	G	502	QR8	C13-O2-C1	-3.50	112.44	117.51
2	D	501	HEM	CAD-C3D-C4D	3.49	130.76	124.66
2	H	501	HEM	C3C-C2C-C1C	-3.46	103.77	107.08
3	A	502	QR8	C33-C8-C9	-3.45	101.15	109.44
3	F	502	QR8	C30-C2-C1	-3.43	101.26	109.02
3	D	502	QR8	C36-C13-C12	-3.43	109.42	114.39
2	B	501	HEM	CAD-C3D-C4D	3.42	130.63	124.66
3	E	502	QR8	C35-C12-C13	-3.31	107.89	112.18
3	E	502	QR8	C30-C2-C3	-3.31	106.85	112.37
3	E	502	QR8	C31-C4-C5	-3.30	104.71	111.39
2	E	501	HEM	CHD-C1D-C2D	-3.29	119.84	124.98
3	H	502	QR8	O2-C1-C2	3.26	118.72	111.56
3	C	502	QR8	C32-C6-C7	-3.24	105.83	110.69
3	A	502	QR8	C35-C12-C13	-3.24	107.99	112.18
3	F	502	QR8	C36-C13-C12	-3.22	109.73	114.39
2	H	501	HEM	CHD-C1D-C2D	-3.22	119.95	124.98
3	E	502	QR8	C35-C12-C11	-3.22	104.89	111.39
3	E	502	QR8	O11-C9-C10	-3.21	116.04	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	502	QR8	O3-C3-C2	-3.15	101.48	108.82
3	F	502	QR8	C34-C10-C11	-3.14	107.13	112.37
2	F	501	HEM	CAD-C3D-C4D	3.14	130.14	124.66
2	E	501	HEM	CAD-C3D-C4D	3.13	130.13	124.66
3	F	502	QR8	C35-C12-C11	-3.12	105.09	111.39
3	B	502	QR8	O2-C1-C2	3.11	118.39	111.56
2	E	501	HEM	CHD-C1D-ND	3.11	127.80	124.42
2	E	501	HEM	CMD-C2D-C1D	3.10	129.76	125.04
2	H	501	HEM	CHC-C4B-NB	3.06	127.74	124.42
2	G	501	HEM	CHA-C4D-C3D	-3.05	119.59	125.33
3	F	502	QR8	C10-C11-C12	-3.05	108.13	114.41
2	E	501	HEM	CHD-C4C-NC	3.01	127.69	124.44
3	A	502	QR8	O11-C9-C10	-3.01	116.33	120.60
3	B	502	QR8	C34-C10-C9	-3.00	102.87	108.08
3	E	502	QR8	O1-C1-C2	-2.99	116.09	124.08
2	C	501	HEM	O2D-CGD-CBD	2.98	123.61	114.03
2	I	501	HEM	CAA-C2A-C1A	2.97	130.73	124.89
3	H	502	QR8	C3-C2-C1	-2.96	103.66	110.02
3	A	502	QR8	O1-C1-C2	-2.96	116.16	124.08
3	H	502	QR8	O11-C9-C10	-2.96	116.39	120.60
2	C	501	HEM	C4B-C3B-C2B	-2.95	104.77	107.11
3	D	502	QR8	C32-C6-C7	-2.94	106.29	110.69
2	I	501	HEM	CHD-C1D-C2D	-2.91	120.43	124.98
2	F	501	HEM	CHA-C4D-ND	2.91	127.96	124.37
3	A	502	QR8	C34-C10-C9	-2.90	103.03	108.08
2	E	501	HEM	CMB-C2B-C1B	2.89	129.43	125.04
3	H	502	QR8	C8-C9-C10	2.88	124.11	119.10
3	A	502	QR8	C36-C13-C12	-2.82	110.31	114.39
3	I	502	QR8	O2-C13-C12	2.79	113.51	106.30
2	F	501	HEM	CMD-C2D-C1D	2.78	129.28	125.04
3	H	502	QR8	C13-O2-C1	-2.76	113.52	117.51
3	A	502	QR8	C32-C6-C7	-2.71	106.62	110.69
2	C	501	HEM	C4A-NA-C1A	2.69	107.98	105.35
2	C	501	HEM	CHD-C4C-NC	2.66	127.32	124.44
2	G	501	HEM	CAD-C3D-C4D	2.66	129.31	124.66
2	H	501	HEM	C1B-NB-C4B	2.66	107.82	105.07
2	C	501	HEM	CHA-C1A-NA	2.66	128.73	123.85
2	A	501	HEM	CHD-C1D-C2D	-2.65	120.84	124.98
3	C	502	QR8	C3-C2-C1	2.64	115.69	110.02
2	H	501	HEM	C4B-C3B-C2B	-2.64	105.02	107.11
2	E	501	HEM	C4A-NA-C1A	2.64	107.93	105.35
3	H	502	QR8	C30-C2-C1	-2.64	103.06	109.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	501	HEM	CHD-C1D-C2D	-2.63	120.87	124.98
2	E	501	HEM	CHA-C4D-ND	2.63	127.61	124.37
2	B	501	HEM	CAA-C2A-C1A	2.62	130.04	124.89
3	I	502	QR8	C35-C12-C13	-2.61	108.80	112.18
3	D	502	QR8	C2-C3-C4	-2.61	109.03	114.41
2	I	501	HEM	O2A-CGA-CBA	2.60	122.37	114.03
2	C	501	HEM	CHD-C1D-ND	2.58	127.22	124.42
2	F	501	HEM	CHD-C1D-C2D	-2.58	120.95	124.98
2	C	501	HEM	CBA-CAA-C2A	2.57	119.76	112.63
2	D	501	HEM	CAD-C3D-C2D	-2.55	123.13	127.88
3	G	502	QR8	C33-C8-C7	-2.54	106.21	111.55
2	B	501	HEM	C4B-C3B-C2B	-2.51	105.12	107.11
2	G	501	HEM	C1A-CHA-C4D	-2.49	120.43	126.34
2	C	501	HEM	CHD-C1D-C2D	-2.49	121.09	124.98
2	I	501	HEM	O2A-CGA-O1A	-2.48	117.12	123.30
2	A	501	HEM	CHC-C4B-C3B	-2.45	119.85	125.13
3	E	502	QR8	C3-C4-C5	2.45	117.46	112.54
2	B	501	HEM	O2D-CGD-O1D	-2.44	117.22	123.30
2	G	501	HEM	CHB-C1B-NB	2.44	127.38	124.37
2	I	501	HEM	CBA-CAA-C2A	2.44	119.40	112.63
2	F	501	HEM	CHA-C4D-C3D	-2.43	120.77	125.33
2	B	501	HEM	CMA-C3A-C4A	2.42	129.06	125.37
3	I	502	QR8	O1-C1-C2	-2.42	117.62	124.08
2	D	501	HEM	O1D-CGD-CBD	-2.41	115.35	123.08
3	B	502	QR8	O2-C1-O1	-2.40	119.46	123.94
3	D	502	QR8	C33-C8-C7	-2.37	106.58	111.55
2	H	501	HEM	CMB-C2B-C1B	2.36	128.64	125.04
2	F	501	HEM	C4C-NC-C1C	2.35	107.65	105.35
2	A	501	HEM	C1A-CHA-C4D	-2.33	120.81	126.34
2	C	501	HEM	CAD-CBD-CGD	2.32	118.61	113.60
2	H	501	HEM	CAA-C2A-C1A	2.32	129.45	124.89
2	E	501	HEM	O2D-CGD-CBD	2.29	121.37	114.03
2	D	501	HEM	C4C-CHD-C1D	-2.28	121.13	126.06
3	G	502	QR8	C30-C2-C1	-2.28	103.87	109.02
2	H	501	HEM	CMA-C3A-C4A	2.27	128.82	125.37
3	H	502	QR8	C34-C10-C9	-2.26	104.14	108.08
3	C	502	QR8	C2-C3-C4	-2.26	109.75	114.41
3	F	502	QR8	C13-O2-C1	-2.25	114.24	117.51
2	I	501	HEM	C4B-C3B-C2B	-2.25	105.33	107.11
2	A	501	HEM	CHC-C1C-NC	-2.25	122.01	124.44
2	A	501	HEM	CHA-C1A-NA	2.24	127.97	123.85
2	I	501	HEM	C4C-NC-C1C	2.23	107.53	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	HEM	O2D-CGD-O1D	-2.22	117.76	123.30
2	B	501	HEM	C4D-C3D-C2D	-2.22	103.67	106.90
3	A	502	QR8	C8-C9-C10	2.20	122.93	119.10
3	E	502	QR8	O2-C1-O1	-2.20	119.83	123.94
2	B	501	HEM	C4C-NC-C1C	2.19	107.49	105.35
2	A	501	HEM	CHD-C1D-ND	2.19	126.79	124.42
3	F	502	QR8	O2-C13-C36	2.18	112.55	108.21
3	F	502	QR8	C32-C6-C7	-2.17	107.44	110.69
3	I	502	QR8	C30-C2-C3	-2.15	108.78	112.37
2	B	501	HEM	C1D-C2D-C3D	2.15	109.22	106.96
3	E	502	QR8	C32-C6-C5	-2.15	107.56	111.54
2	F	501	HEM	C4A-C3A-C2A	2.14	109.34	106.83
3	F	502	QR8	O2-C1-O1	-2.14	119.94	123.94
2	I	501	HEM	CHC-C4B-C3B	-2.13	120.54	125.13
3	G	502	QR8	C32-C6-C5	2.13	115.48	111.54
2	I	501	HEM	C4A-C3A-C2A	2.12	109.32	106.83
2	D	501	HEM	CHA-C1A-NA	2.12	127.75	123.85
2	I	501	HEM	CHA-C4D-C3D	-2.12	121.34	125.33
2	B	501	HEM	CHD-C4C-NC	2.11	126.72	124.44
2	B	501	HEM	CAB-C3B-C2B	2.11	135.54	128.60
3	F	502	QR8	C8-C9-C10	-2.10	115.45	119.10
2	B	501	HEM	C4C-CHD-C1D	-2.10	121.53	126.06
2	E	501	HEM	C1A-CHA-C4D	-2.09	121.38	126.34
3	G	502	QR8	O2-C1-O1	-2.08	120.05	123.94
2	A	501	HEM	CHB-C1B-NB	2.08	126.94	124.37
2	F	501	HEM	C1A-CHA-C4D	-2.08	121.41	126.34
2	A	501	HEM	C4D-C3D-C2D	-2.07	103.88	106.90
2	E	501	HEM	CAD-C3D-C2D	-2.07	124.03	127.88
3	D	502	QR8	O11-C9-C8	-2.06	117.44	121.26
2	A	501	HEM	C2D-C1D-ND	2.06	112.35	109.88
2	E	501	HEM	C2D-C1D-ND	2.06	112.34	109.88
2	B	501	HEM	CBA-CAA-C2A	2.05	118.33	112.63
3	G	502	QR8	C35-C12-C11	-2.04	107.26	111.39
3	D	502	QR8	O3-C3-C2	2.04	113.55	108.82
2	B	501	HEM	O2A-CGA-O1A	-2.03	118.23	123.30
3	H	502	QR8	C36-C13-C12	-2.03	111.45	114.39
2	H	501	HEM	CHA-C4D-ND	2.03	126.88	124.37
3	A	502	QR8	C30-C2-C1	-2.02	104.45	109.02
2	C	501	HEM	CMA-C3A-C4A	2.02	128.44	125.37
2	E	501	HEM	CHA-C1A-NA	2.01	127.55	123.85
2	B	501	HEM	CHC-C4B-C3B	-2.01	120.81	125.13

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	502	QR8	C11
3	E	502	QR8	C8

All (216) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	501	HEM	C1A-C2A-CAA-CBA
3	A	502	QR8	C10-C11-C12-C35
3	A	502	QR8	C10-C11-C12-C13
3	A	502	QR8	O12-C11-C12-C13
3	A	502	QR8	C11-C12-C13-O2
3	A	502	QR8	C35-C12-C13-O2
3	A	502	QR8	C3-C4-C5-C6
3	A	502	QR8	C3-C4-C5-O7
3	A	502	QR8	O3-C3-C4-C5
3	A	502	QR8	C2-C3-C4-C5
3	A	502	QR8	O3-C3-C4-C31
3	A	502	QR8	C2-C3-C4-C31
3	B	502	QR8	C9-C10-C11-O12
3	B	502	QR8	C10-C11-C12-C35
3	B	502	QR8	C10-C11-C12-C13
3	B	502	QR8	O12-C11-C12-C35
3	B	502	QR8	O12-C11-C12-C13
3	B	502	QR8	C12-C13-O2-C1
3	B	502	QR8	C1-C2-C3-C4
3	C	502	QR8	C9-C10-C11-O12
3	C	502	QR8	O12-C11-C12-C13
3	C	502	QR8	C5-C6-C7-C8
3	C	502	QR8	O7-C5-C6-C7
3	C	502	QR8	O7-C5-C6-C32
3	C	502	QR8	C4-C5-C6-C32
3	D	502	QR8	C9-C10-C11-O12
3	D	502	QR8	C9-C10-C11-C12
3	D	502	QR8	C34-C10-C11-C12
3	D	502	QR8	C11-C12-C13-C36
3	D	502	QR8	C11-C12-C13-O2
3	D	502	QR8	C35-C12-C13-C36
3	D	502	QR8	C35-C12-C13-O2
3	D	502	QR8	C2-C1-O2-C13
3	D	502	QR8	O1-C1-O2-C13
3	D	502	QR8	C4-C5-C6-C7
3	D	502	QR8	O7-C5-C6-C32
3	D	502	QR8	C31-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	D	502	QR8	C3-C4-C5-C6
3	D	502	QR8	C31-C4-C5-O7
3	D	502	QR8	C3-C4-C5-O7
3	E	502	QR8	C33-C8-C9-O11
3	E	502	QR8	C33-C8-C9-C10
3	E	502	QR8	C9-C10-C11-O12
3	E	502	QR8	C9-C10-C11-C12
3	E	502	QR8	C34-C10-C11-O12
3	E	502	QR8	C10-C11-C12-C13
3	E	502	QR8	C12-C13-O2-C1
3	E	502	QR8	C36-C13-O2-C1
3	E	502	QR8	C6-C7-C8-C9
3	E	502	QR8	C6-C7-C8-C33
3	E	502	QR8	O7-C5-C6-C7
3	E	502	QR8	O7-C5-C6-C32
3	E	502	QR8	C3-C4-C5-C6
3	F	502	QR8	C4-C5-C6-C7
3	F	502	QR8	C4-C5-C6-C32
3	F	502	QR8	C3-C4-C5-O7
3	F	502	QR8	O3-C3-C4-C5
3	F	502	QR8	C1-C2-C3-C4
3	H	502	QR8	C10-C11-C12-C35
3	H	502	QR8	C10-C11-C12-C13
3	H	502	QR8	O12-C11-C12-C35
3	H	502	QR8	O12-C11-C12-C13
3	H	502	QR8	C6-C7-C8-C33
3	H	502	QR8	C5-C6-C7-C8
3	H	502	QR8	C31-C4-C5-C6
3	H	502	QR8	C3-C4-C5-C6
3	H	502	QR8	C31-C4-C5-O7
3	H	502	QR8	C3-C4-C5-O7
3	I	502	QR8	O12-C11-C12-C35
3	I	502	QR8	C32-C6-C7-C8
3	I	502	QR8	C4-C5-C6-C7
3	I	502	QR8	O7-C5-C6-C32
3	I	502	QR8	C4-C5-C6-C32
3	I	502	QR8	C3-C4-C5-C6
3	E	502	QR8	C2-C1-O2-C13
3	I	502	QR8	C2-C1-O2-C13
3	E	502	QR8	O1-C1-O2-C13
3	A	502	QR8	O12-C11-C12-C35
3	C	502	QR8	O12-C11-C12-C35

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Mol	Chain	Res	Type	Atoms
3	F	502	QR8	C31-C4-C5-O7
3	E	502	QR8	O12-C11-C12-C13
3	E	502	QR8	O3-C3-C4-C5
3	I	502	QR8	O12-C11-C12-C13
3	I	502	QR8	C3-C4-C5-O7
3	C	502	QR8	C10-C11-C12-C35
3	I	502	QR8	C10-C11-C12-C35
3	C	502	QR8	C10-C11-C12-C13
3	A	502	QR8	C2-C1-O2-C13
3	I	502	QR8	O1-C1-O2-C13
3	C	502	QR8	C36-C13-O2-C1
3	F	502	QR8	O3-C3-C4-C31
3	G	502	QR8	O3-C3-C4-C31
3	C	502	QR8	C3-C4-C5-O7
3	G	502	QR8	O3-C3-C4-C5
3	F	502	QR8	C10-C11-C12-C35
2	C	501	HEM	C1A-C2A-CAA-CBA
3	B	502	QR8	C30-C2-C3-O3
3	C	502	QR8	C30-C2-C3-O3
3	D	502	QR8	C34-C10-C11-O12
3	B	502	QR8	C34-C10-C11-C12
3	C	502	QR8	C34-C10-C11-C12
3	C	502	QR8	C30-C2-C3-C4
3	D	502	QR8	C30-C2-C3-C4
3	E	502	QR8	C34-C10-C11-C12
3	E	502	QR8	C3-C4-C5-O7
2	I	501	HEM	C3A-C2A-CAA-CBA
3	F	502	QR8	C31-C4-C5-C6
3	F	502	QR8	C10-C11-C12-C13
3	F	502	QR8	C2-C3-C4-C5
3	G	502	QR8	C2-C3-C4-C5
3	F	502	QR8	O7-C5-C6-C32
3	C	502	QR8	C31-C4-C5-O7
3	E	502	QR8	C31-C4-C5-O7
3	F	502	QR8	O12-C11-C12-C35
3	F	502	QR8	C2-C3-C4-C31
3	G	502	QR8	C2-C3-C4-C31
3	F	502	QR8	C3-C4-C5-C6
3	I	502	QR8	C10-C11-C12-C13
3	A	502	QR8	O1-C1-O2-C13
3	D	502	QR8	O7-C5-C6-C7
3	F	502	QR8	O7-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	B	502	QR8	C9-C10-C11-C12
3	C	502	QR8	C9-C10-C11-C12
3	E	502	QR8	C4-C5-C6-C32
3	F	502	QR8	O12-C11-C12-C13
3	A	502	QR8	C31-C4-C5-C6
3	C	502	QR8	C34-C10-C11-O12
3	E	502	QR8	C2-C3-C4-C5
3	C	502	QR8	C32-C6-C7-C8
3	B	502	QR8	O3-C3-C4-C31
3	B	502	QR8	C30-C2-C3-C4
3	G	502	QR8	C30-C2-C3-C4
3	B	502	QR8	O3-C3-C4-C5
3	G	502	QR8	C3-C4-C5-O7
2	C	501	HEM	C3A-C2A-CAA-CBA
3	B	502	QR8	C4-C5-C6-C7
3	C	502	QR8	C4-C5-C6-C7
3	E	502	QR8	C4-C5-C6-C7
3	H	502	QR8	C4-C5-C6-C7
3	H	502	QR8	C6-C7-C8-C9
3	F	502	QR8	C11-C10-C9-O11
3	E	502	QR8	C31-C4-C5-C6
3	A	502	QR8	C31-C4-C5-O7
3	B	502	QR8	C34-C10-C11-O12
3	G	502	QR8	C30-C2-C3-O3
3	F	502	QR8	C11-C10-C9-C8
3	E	502	QR8	O3-C3-C4-C31
3	I	502	QR8	O7-C5-C6-C7
3	C	502	QR8	C31-C4-C5-C6
3	E	502	QR8	C10-C11-C12-C35
3	E	502	QR8	C2-C3-C4-C31
3	I	502	QR8	C31-C4-C5-C6
3	B	502	QR8	C2-C3-C4-C5
3	I	502	QR8	C31-C4-C5-O7
3	F	502	QR8	C34-C10-C9-C8
3	C	502	QR8	C3-C4-C5-C6
3	D	502	QR8	C32-C6-C7-C8
3	F	502	QR8	C32-C6-C7-C8
3	G	502	QR8	C32-C6-C7-C8
3	H	502	QR8	C32-C6-C7-C8
3	G	502	QR8	C31-C4-C5-O7
3	B	502	QR8	C2-C3-C4-C31
3	F	502	QR8	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	G	502	QR8	O2-C1-C2-C3
3	F	502	QR8	O1-C1-C2-C3
3	H	502	QR8	C2-C3-C4-C31
3	A	502	QR8	C6-C7-C8-C9
3	B	502	QR8	C1-C2-C3-O3
3	C	502	QR8	C1-C2-C3-C4
3	C	502	QR8	C1-C2-C3-O3
3	G	502	QR8	C1-C2-C3-O3
3	G	502	QR8	O7-C5-C6-C7
3	H	502	QR8	O7-C5-C6-C7
3	E	502	QR8	O12-C11-C12-C35
3	G	502	QR8	C11-C10-C9-O11
3	G	502	QR8	C9-C10-C11-O12
3	G	502	QR8	O1-C1-C2-C3
3	B	502	QR8	C3-C4-C5-O7
3	H	502	QR8	C30-C2-C3-C4
3	D	502	QR8	C5-C6-C7-C8
3	F	502	QR8	C5-C6-C7-C8
3	G	502	QR8	C3-C4-C5-C6
3	F	502	QR8	C34-C10-C9-O11
3	G	502	QR8	C31-C4-C5-C6
3	D	502	QR8	C7-C8-C9-C10
3	F	502	QR8	C7-C8-C9-C10
3	G	502	QR8	C7-C8-C9-C10
3	H	502	QR8	C7-C8-C9-C10
3	E	502	QR8	C11-C12-C13-C36
2	A	501	HEM	C3D-CAD-CBD-CGD
3	B	502	QR8	O7-C5-C6-C7
2	I	501	HEM	CAA-CBA-CGA-O2A
3	B	502	QR8	C33-C8-C9-O11
3	A	502	QR8	C35-C12-C13-C36
3	H	502	QR8	O7-C5-C6-C32
2	I	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAD-CBD-CGD-O2D
2	I	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O1D
3	I	502	QR8	O3-C3-C4-C31
3	H	502	QR8	C4-C5-C6-C32
2	I	501	HEM	CAD-CBD-CGD-O1D
2	C	501	HEM	CAA-CBA-CGA-O2A
3	B	502	QR8	O7-C5-C6-C32
3	B	502	QR8	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	502	QR8	C33-C8-C9-C10
3	D	502	QR8	C33-C8-C9-C10
3	D	502	QR8	C30-C2-C3-O3
3	F	502	QR8	C33-C8-C9-C10
3	D	502	QR8	C11-C10-C9-C8
3	G	502	QR8	C11-C10-C9-C8
2	F	501	HEM	CAD-CBD-CGD-O2D
3	D	502	QR8	C34-C10-C9-C8
3	H	502	QR8	C7-C8-C9-O11
2	F	501	HEM	CAD-CBD-CGD-O1D
2	C	501	HEM	CAA-CBA-CGA-O1A

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	502	QR8	C1-C10-C11-C12-C13-C2-C3-C4-C5-C6-C7-C8-C9-O2

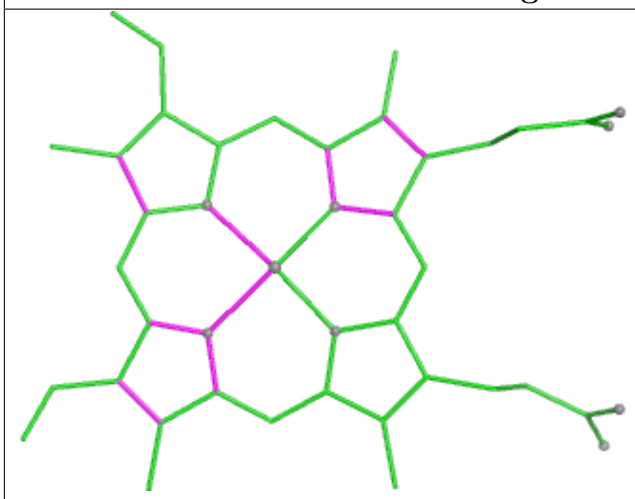
18 monomers are involved in 113 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	HEM	15	0
2	G	501	HEM	8	0
3	D	502	QR8	4	0
3	H	502	QR8	4	0
2	F	501	HEM	10	0
2	C	501	HEM	3	0
2	A	501	HEM	12	0
2	D	501	HEM	8	0
3	B	502	QR8	2	0
3	G	502	QR8	4	0
3	F	502	QR8	4	0
3	E	502	QR8	5	0
2	B	501	HEM	5	0
2	I	501	HEM	7	0
3	I	502	QR8	5	0
3	C	502	QR8	1	0
3	A	502	QR8	10	0
2	H	501	HEM	12	0

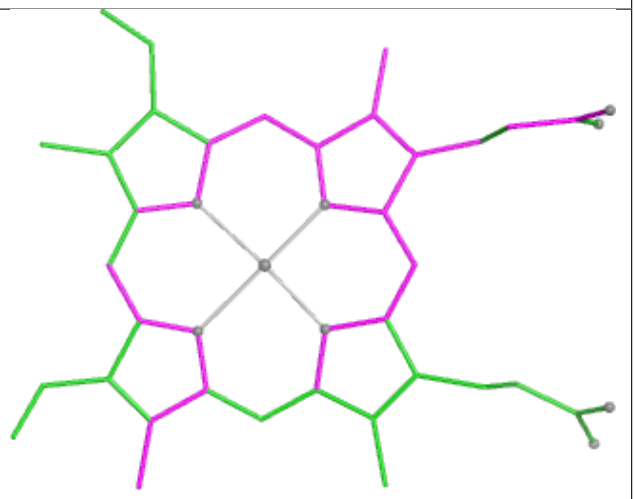
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

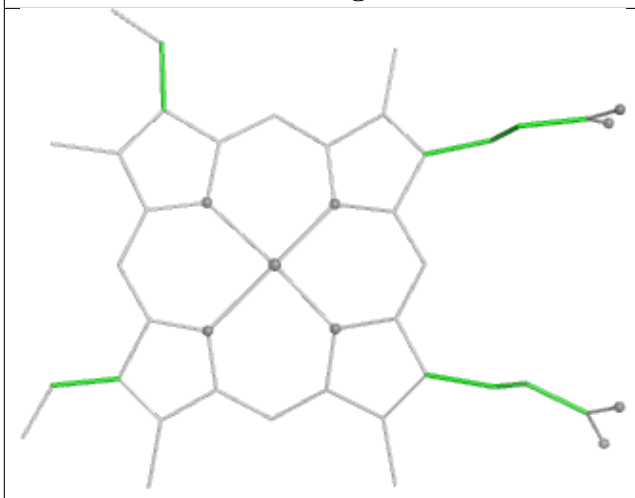
Ligand HEM E 501



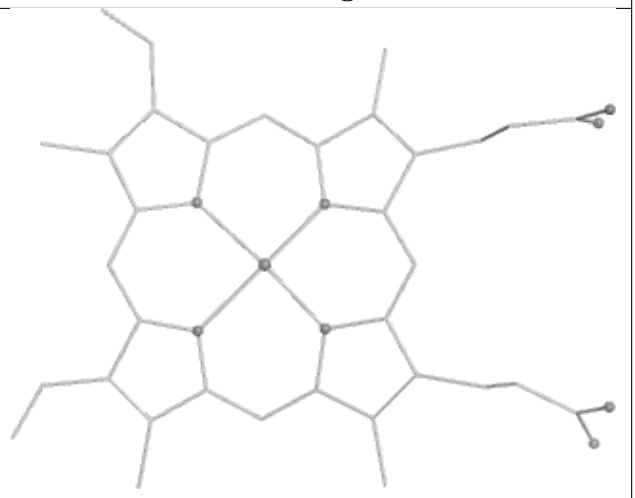
Bond lengths



Bond angles

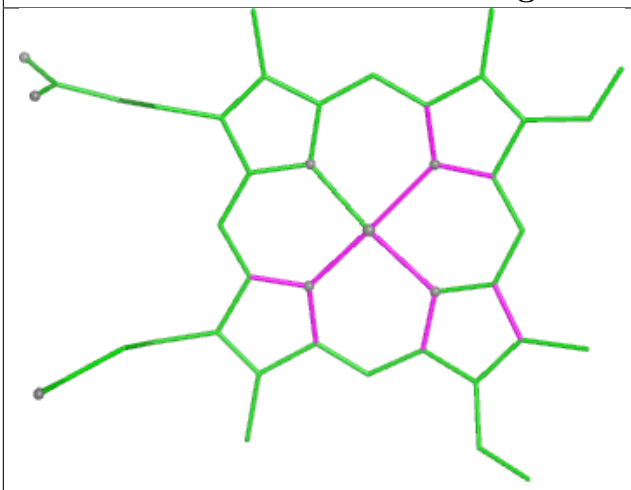


Torsions

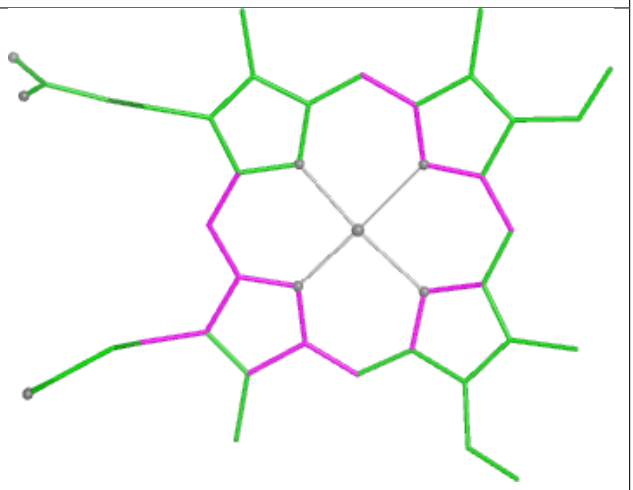


Rings

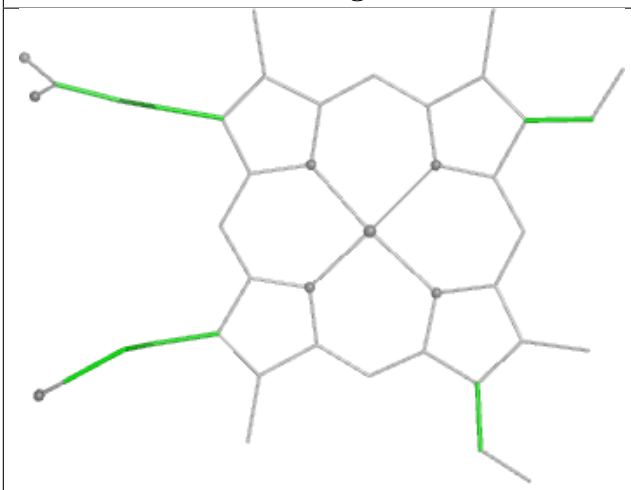
Ligand HEM G 501



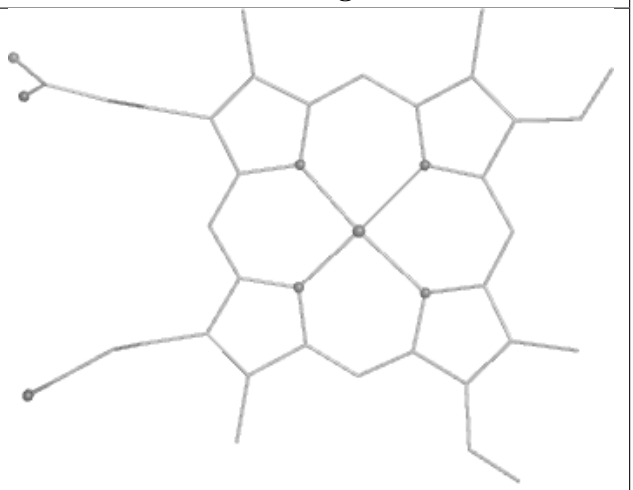
Bond lengths



Bond angles

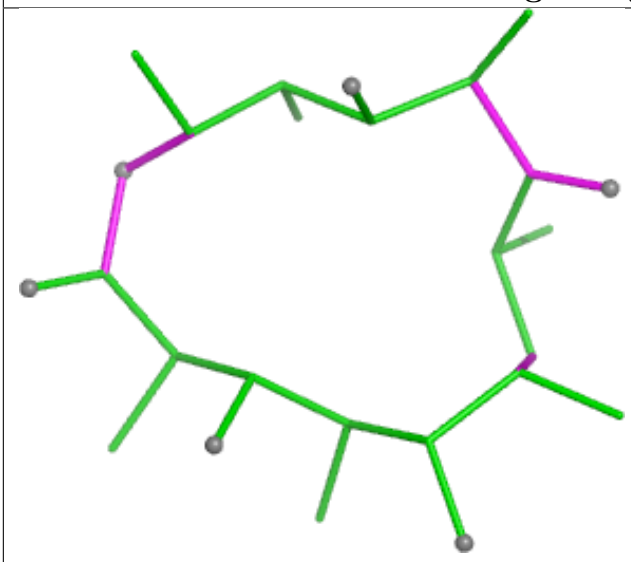


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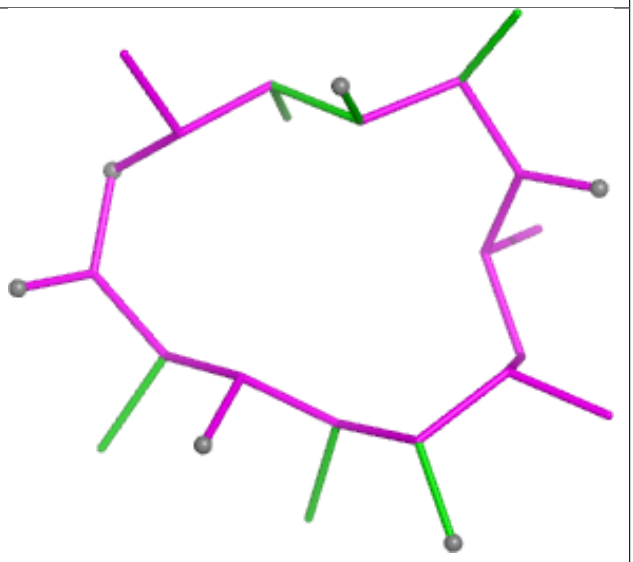


Rings

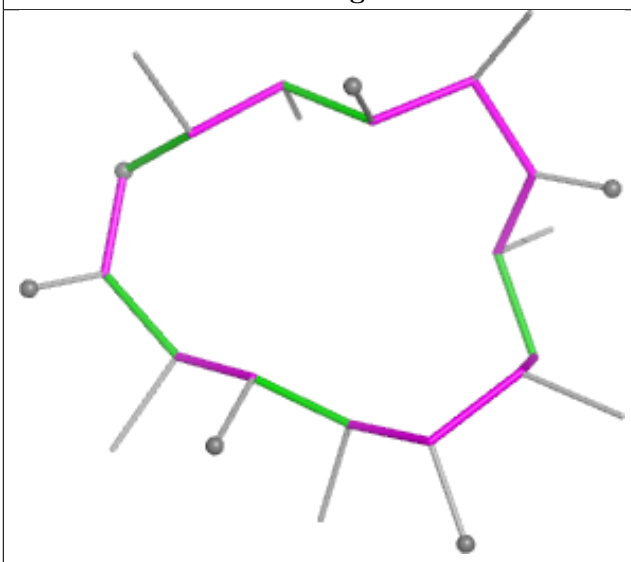
Ligand QR8 D 502



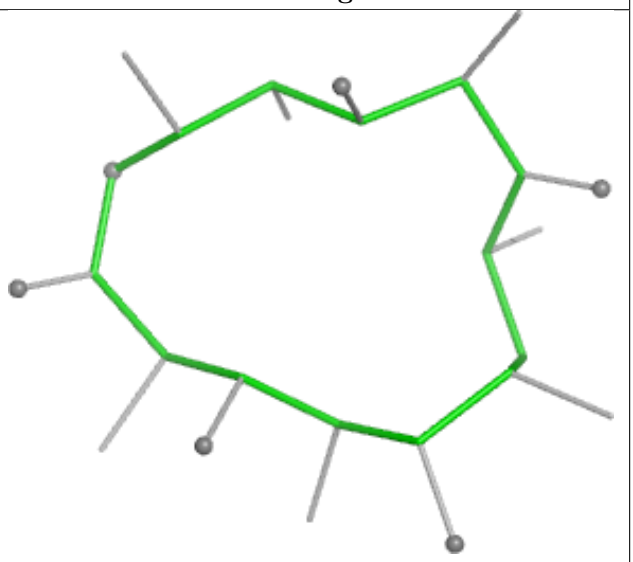
Bond lengths



Bond angles

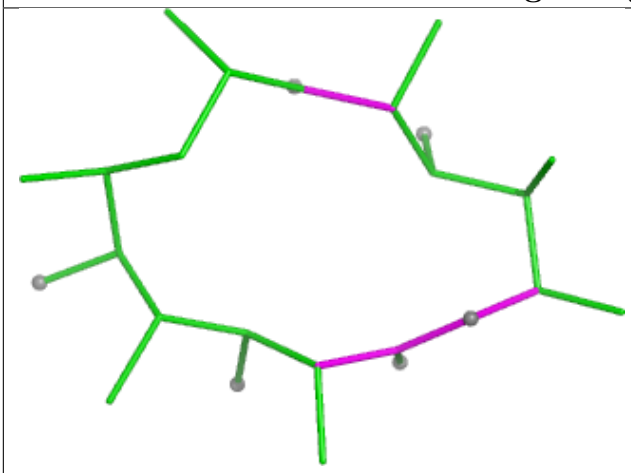


Torsions

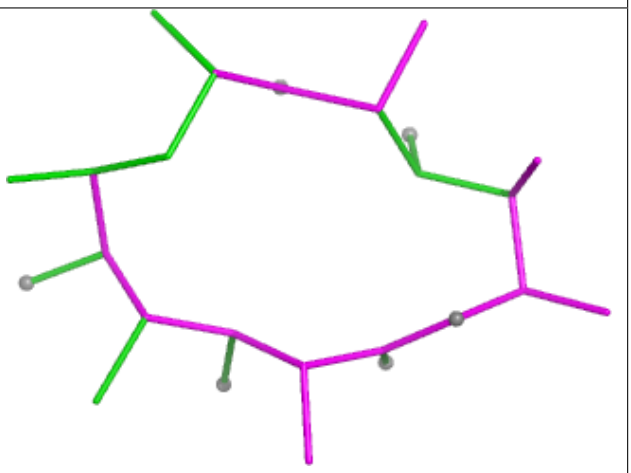


Rings

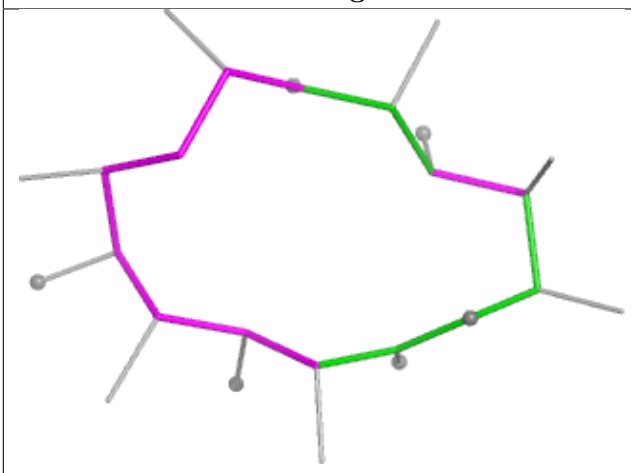
Ligand QR8 H 502



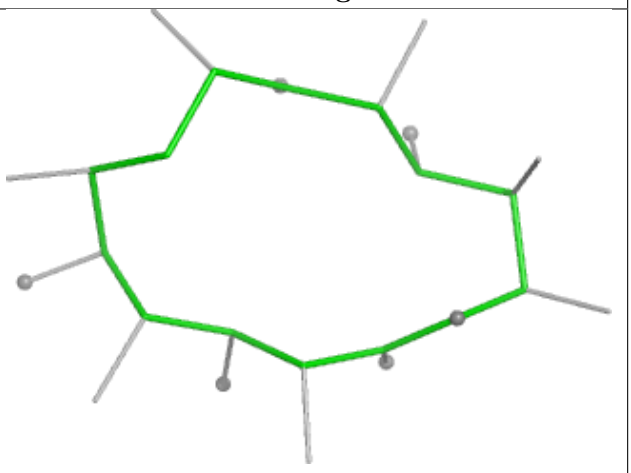
Bond lengths



Bond angles

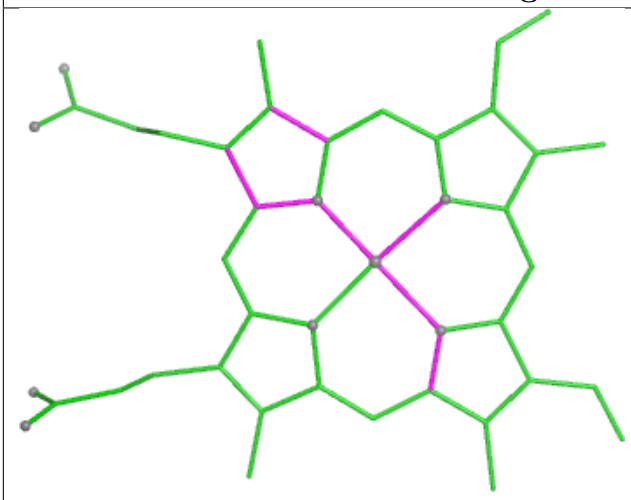


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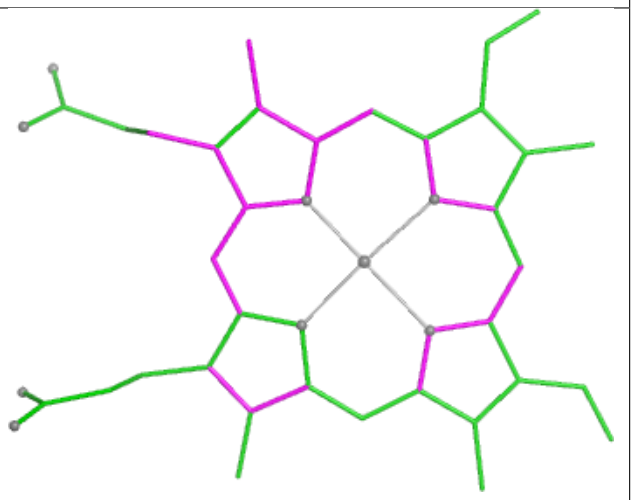


Rings

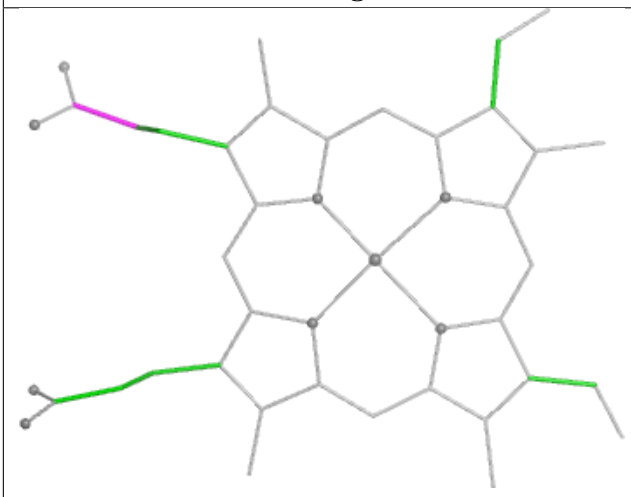
Ligand HEM F 501



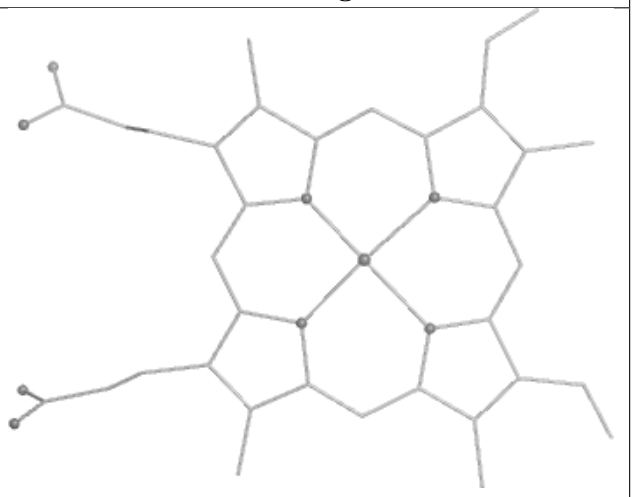
Bond lengths



Bond angles

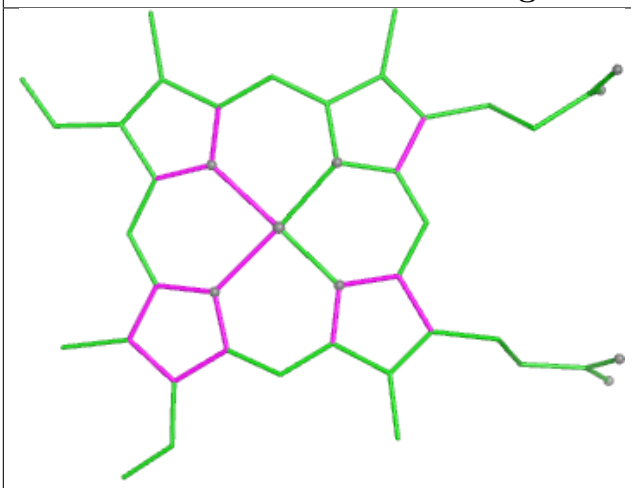


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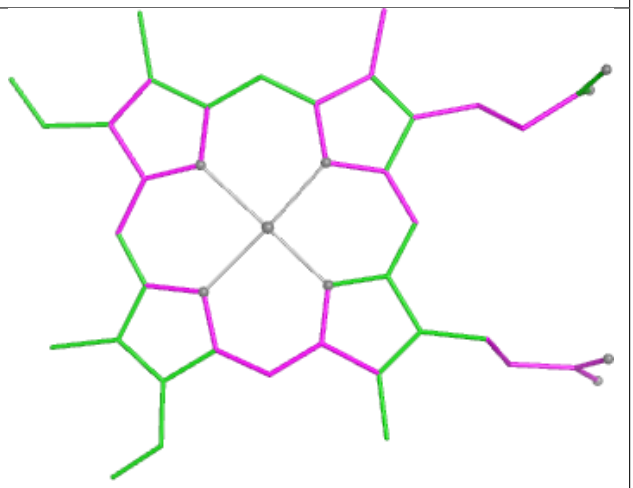


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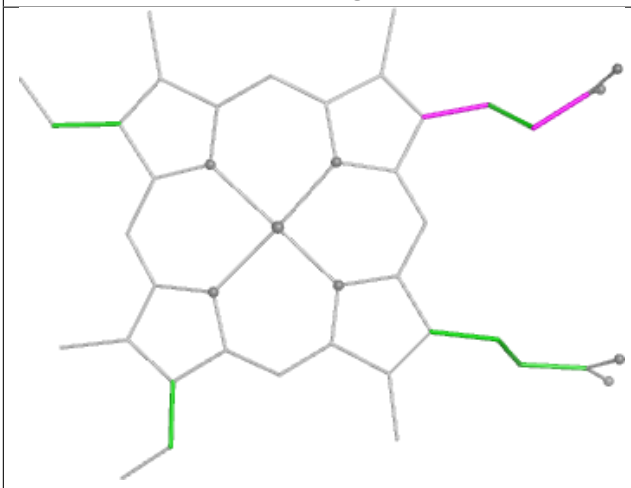
Ligand HEM C 501



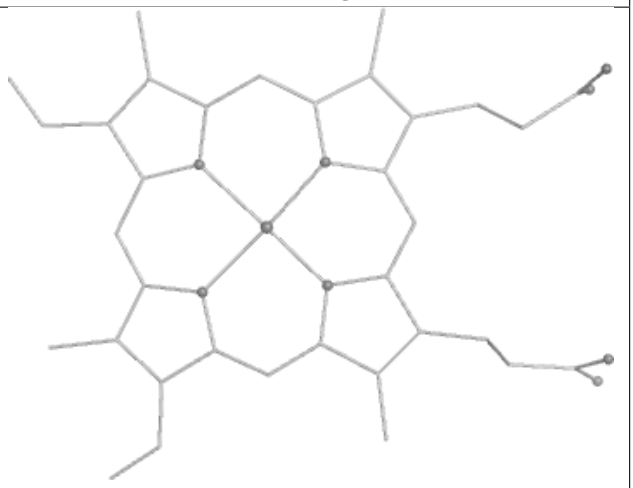
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Bond angles

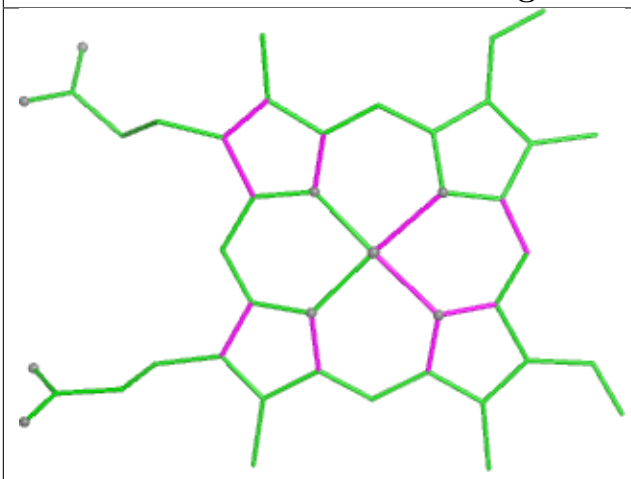


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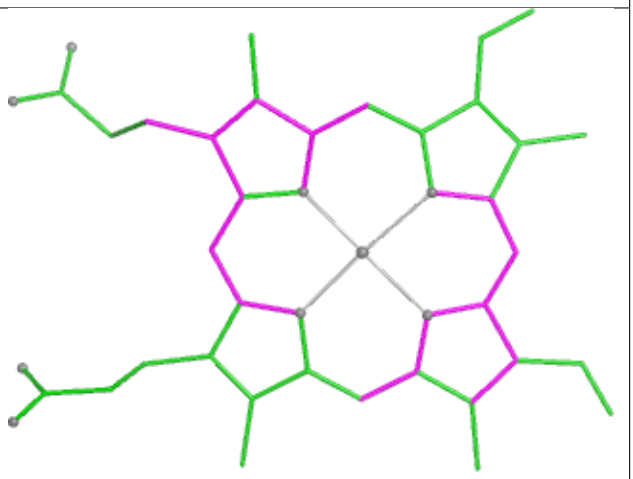


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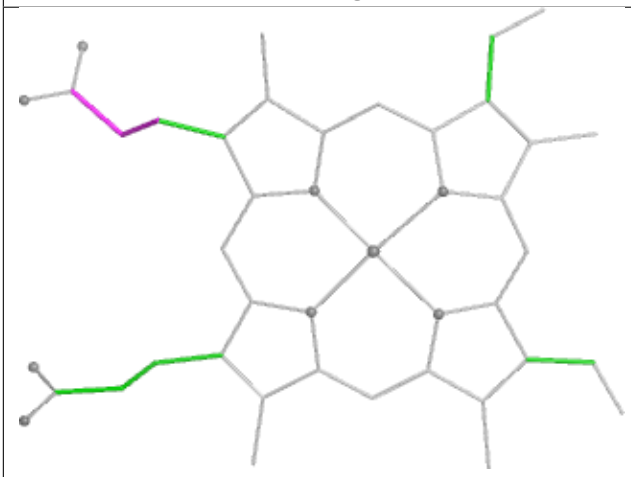
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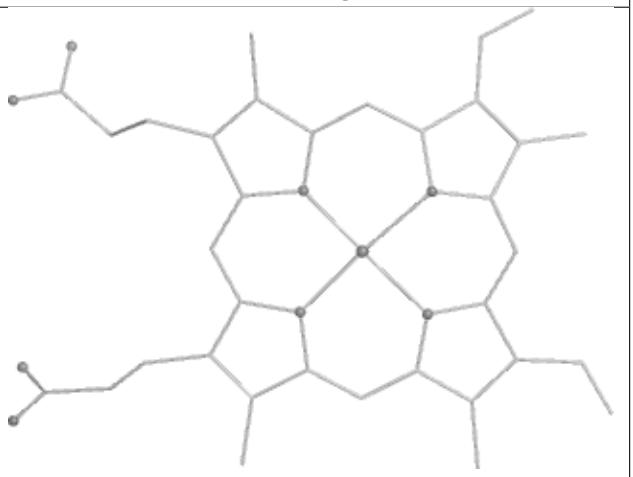
Bond lengths



Bond angles

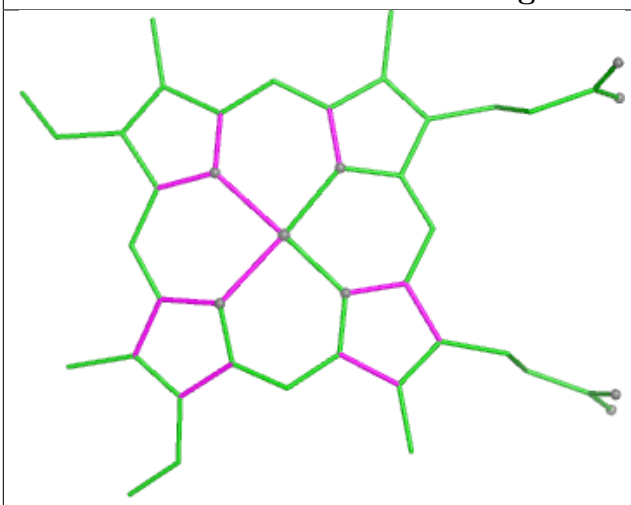


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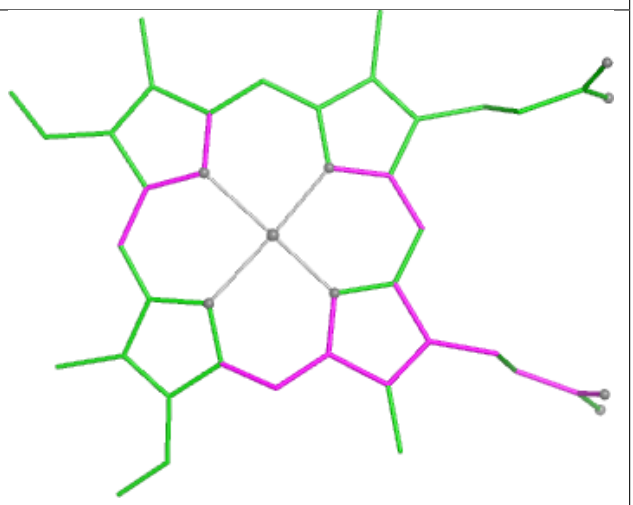


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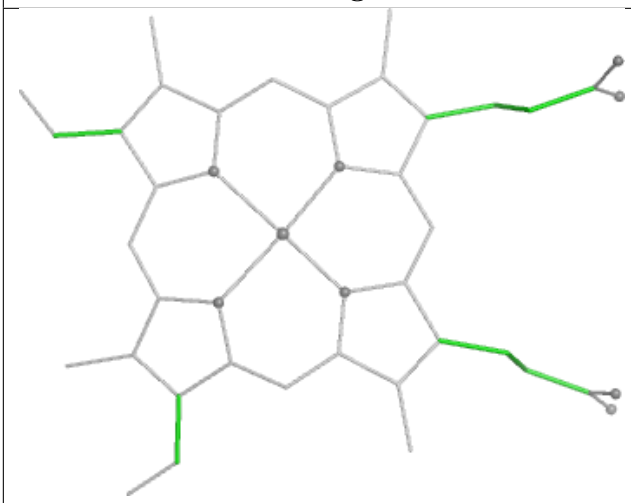
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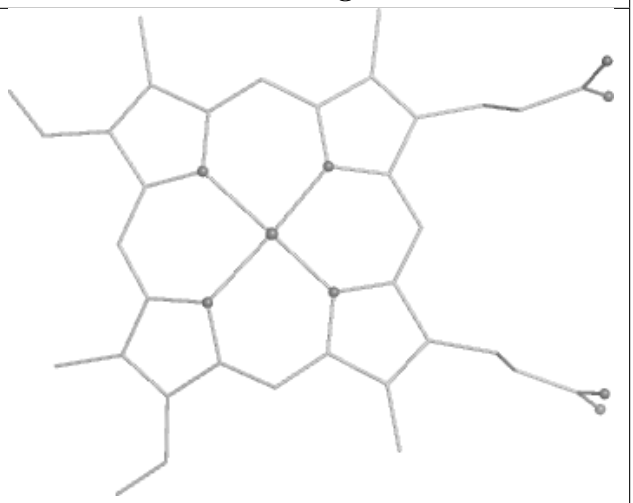
Bond lengths



Bond angles

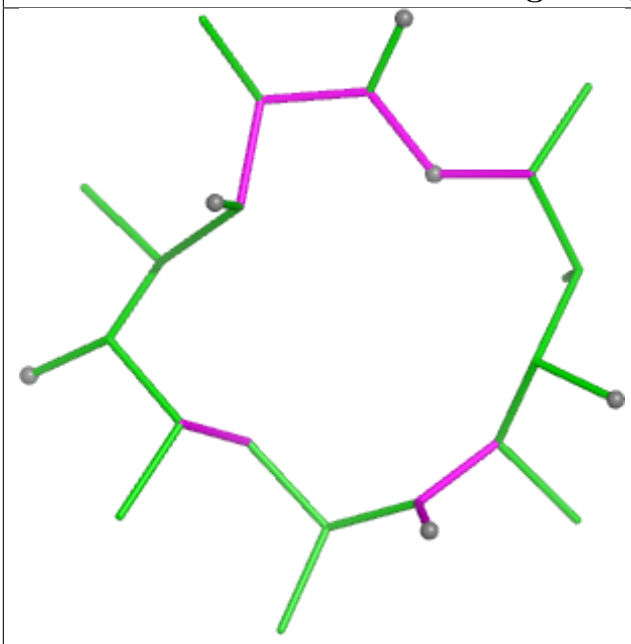


Torsions

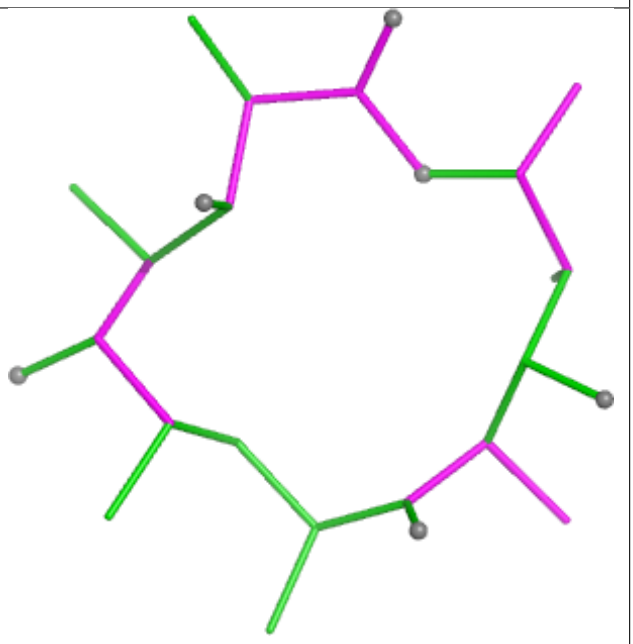


Rings

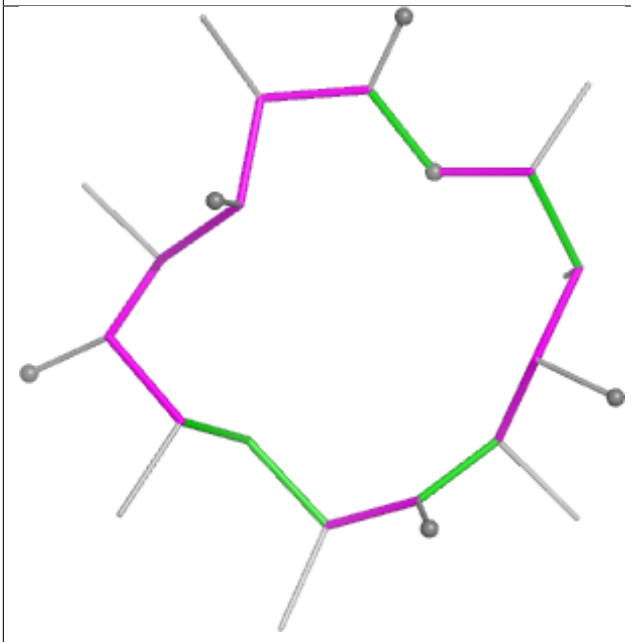
Ligand QR8 B 502



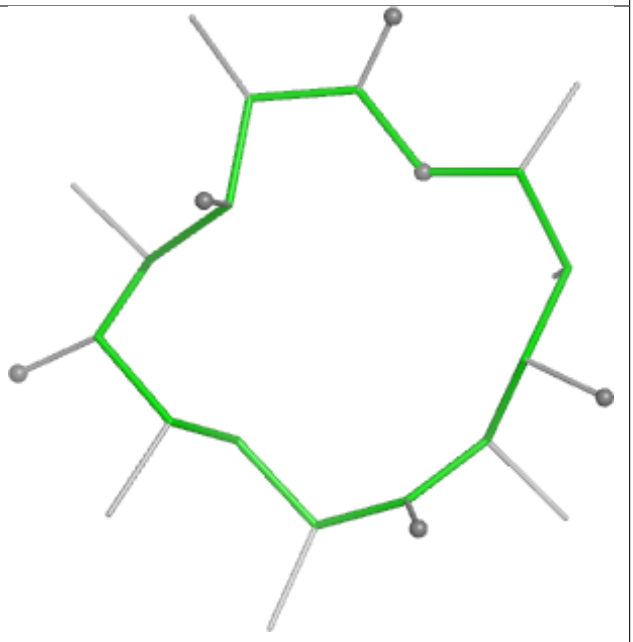
Bond lengths



Bond angles

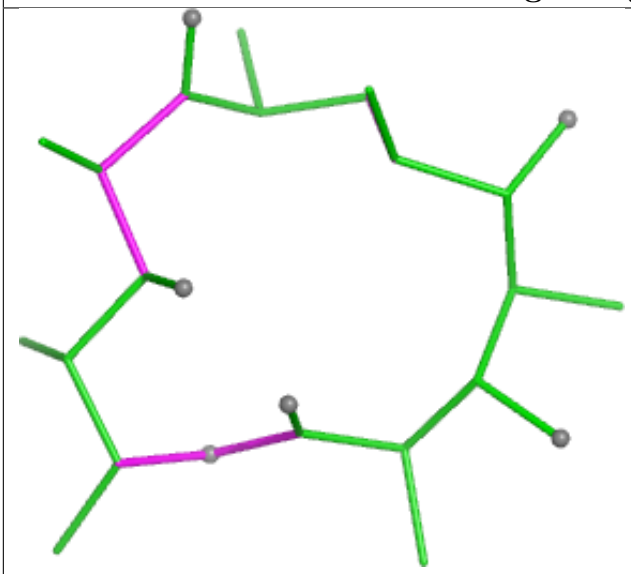


Torsions

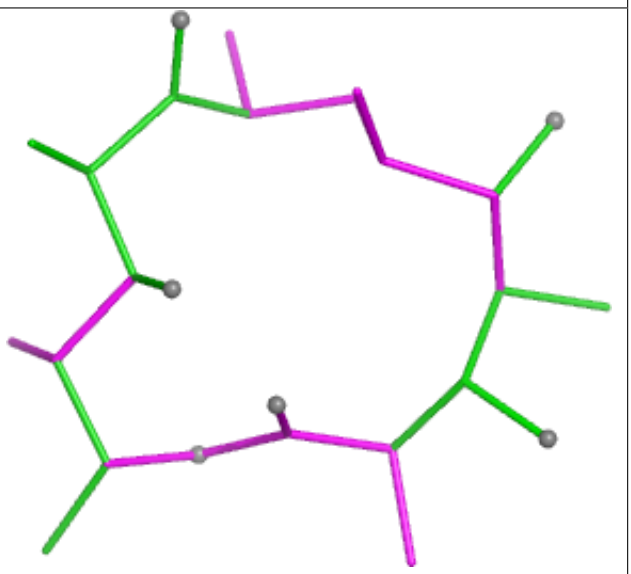


Rings

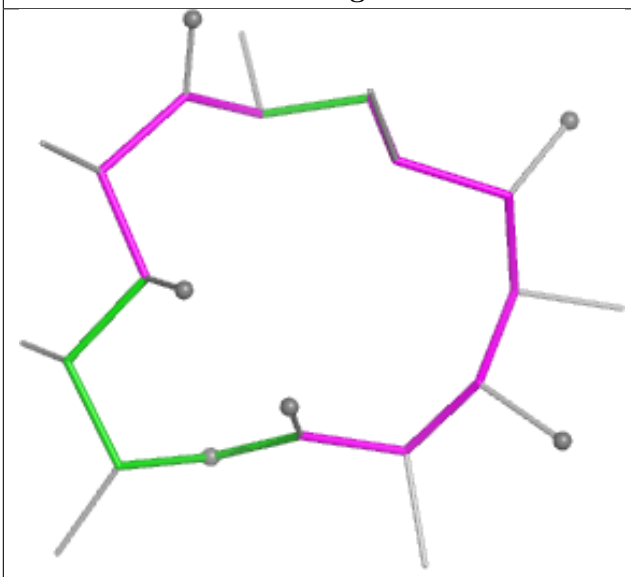
Ligand QR8 G 502



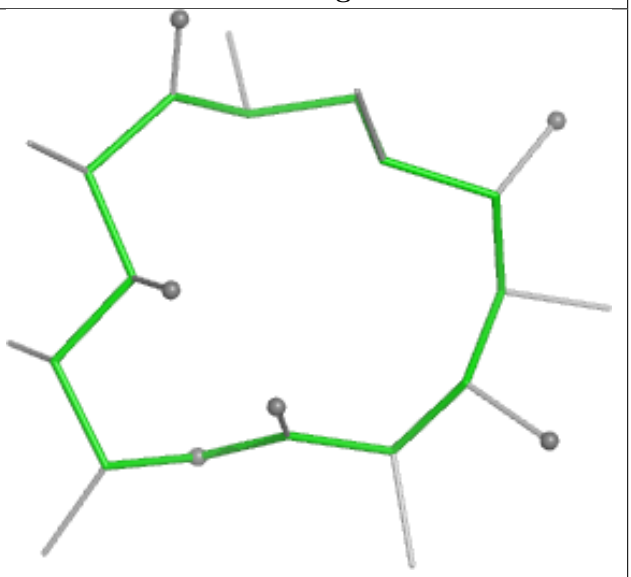
Bond lengths



Bond angles

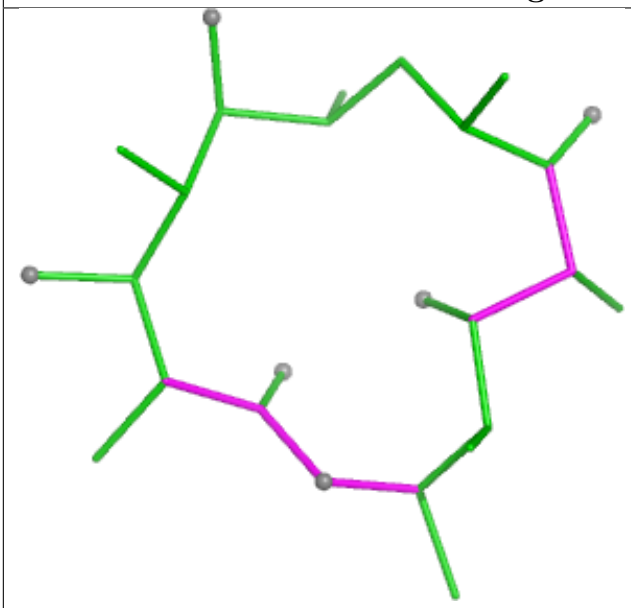


Torsions

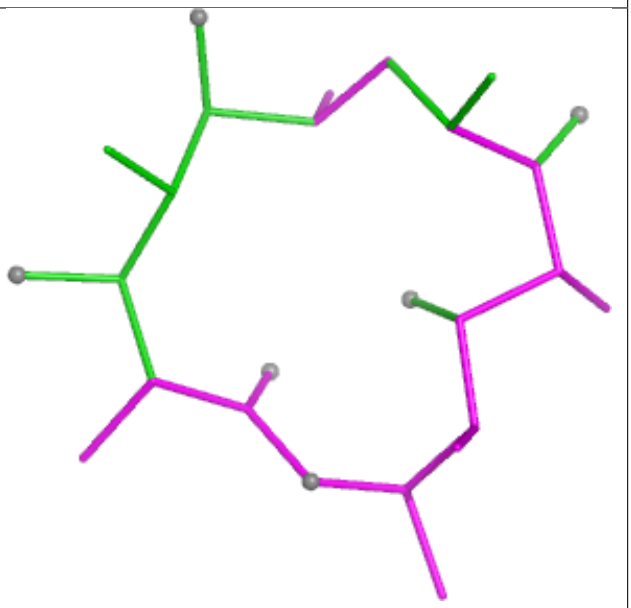


Rings

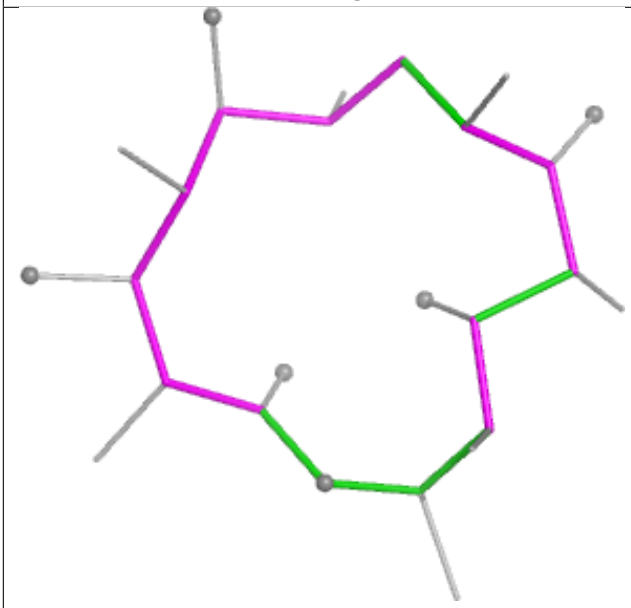
Ligand QR8 F 502



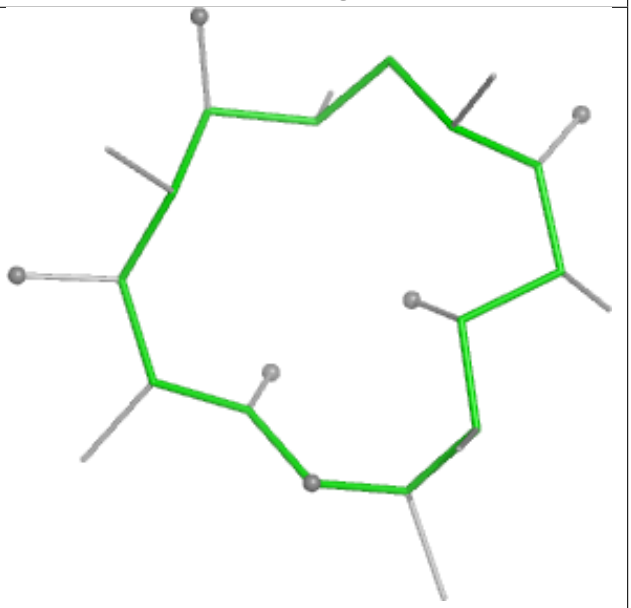
Bond lengths



Bond angles

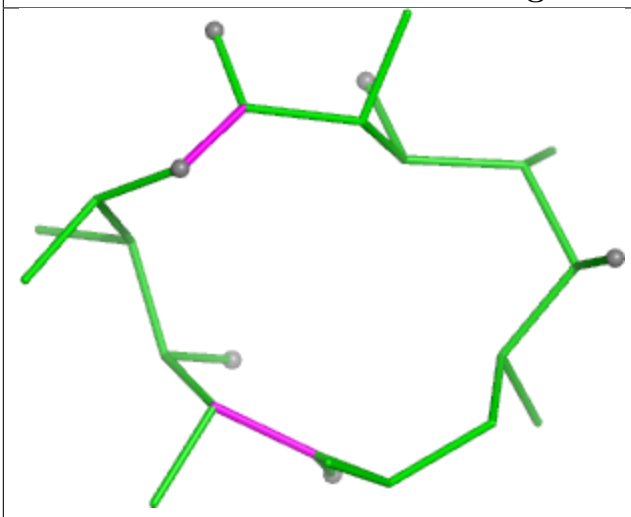


Torsions

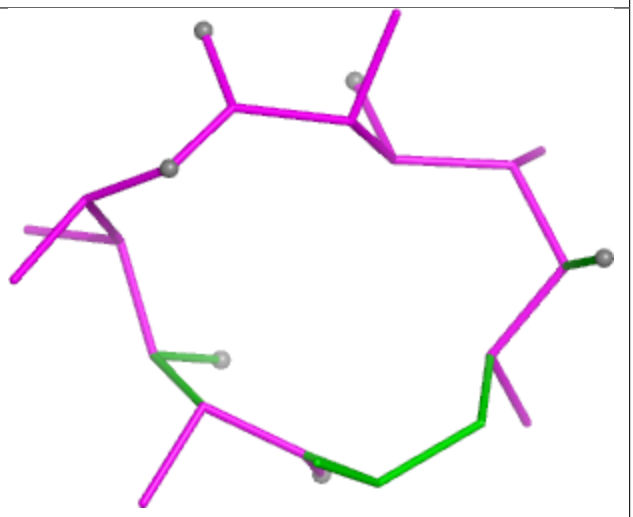


Rings

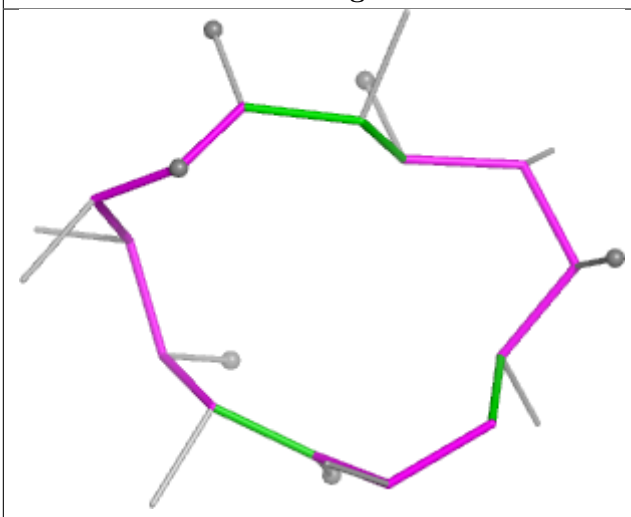
Ligand QR8 E 502



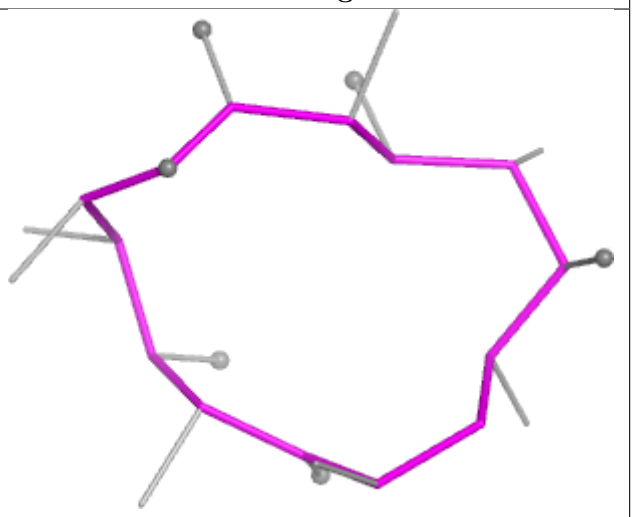
Bond lengths



Bond angles

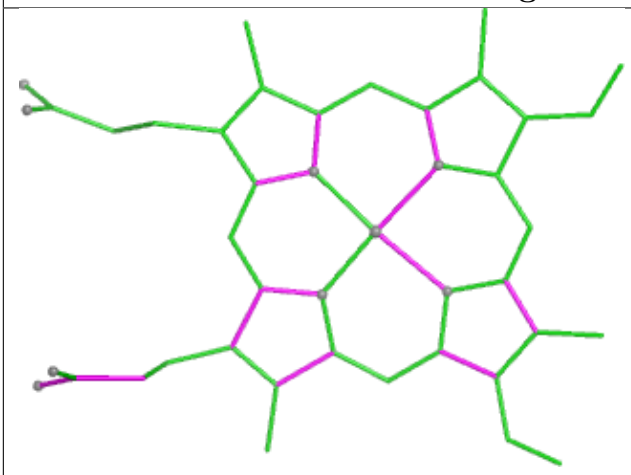


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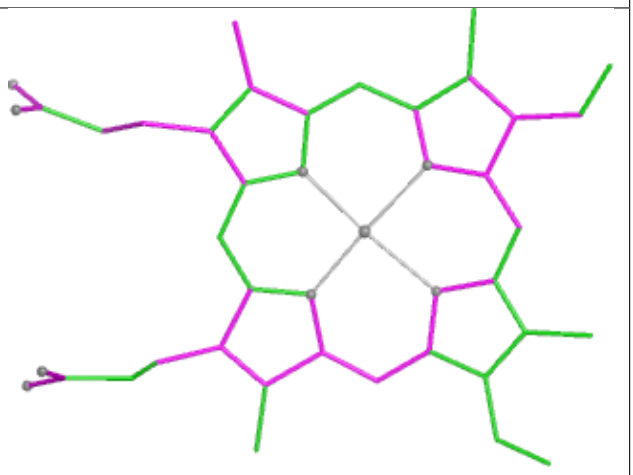


Rings

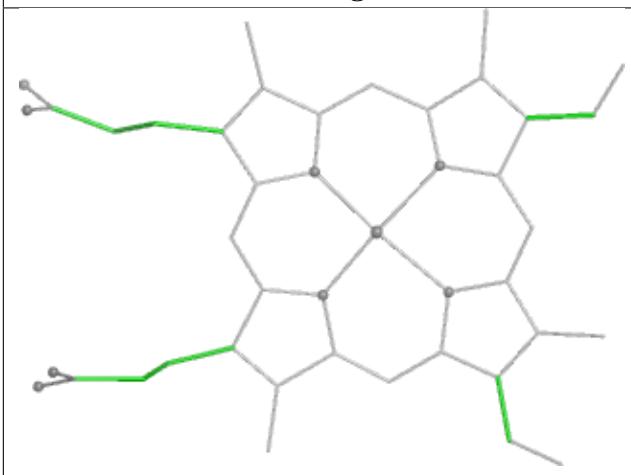
Ligand HEM B 501



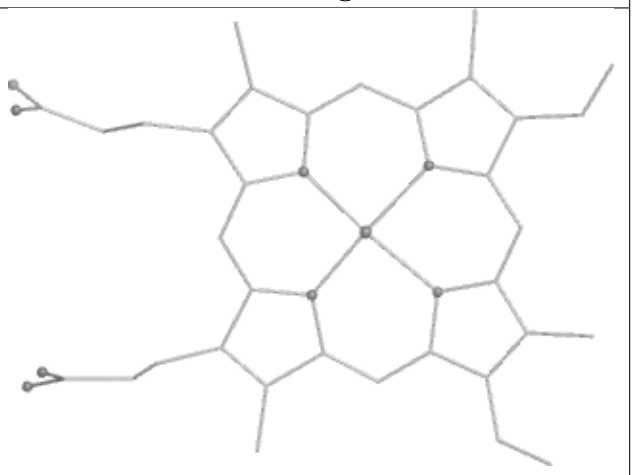
Bond lengths



Bond angles

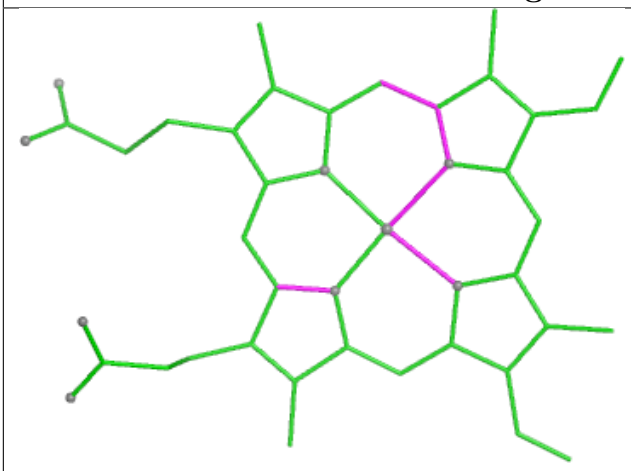


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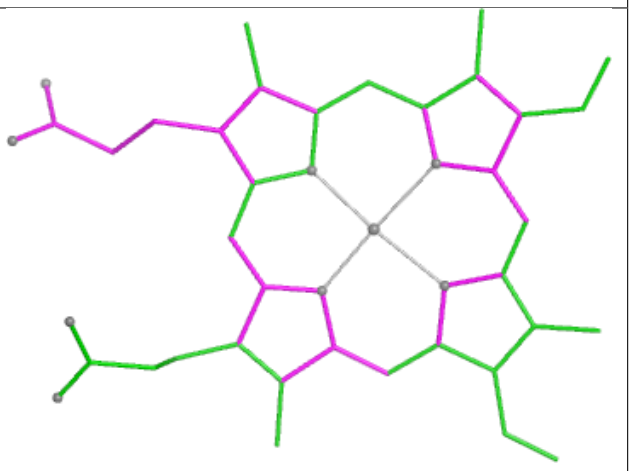


Rings

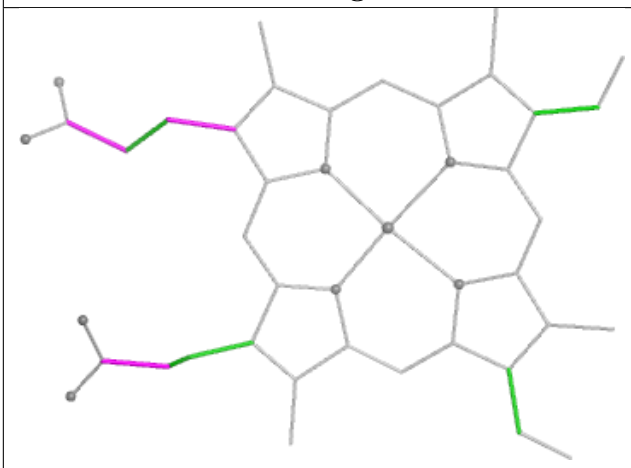
Ligand HEM I 501



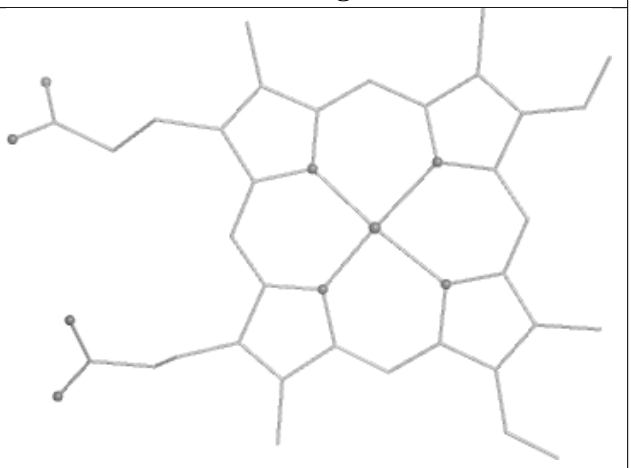
Bond lengths



Bond angles

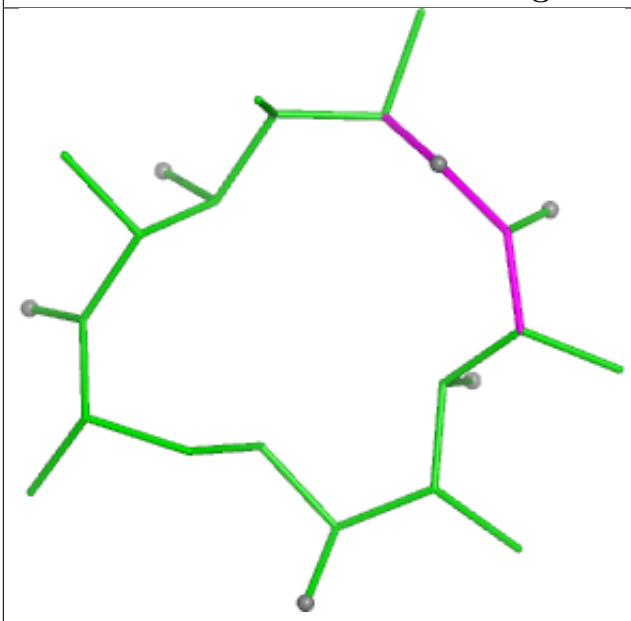


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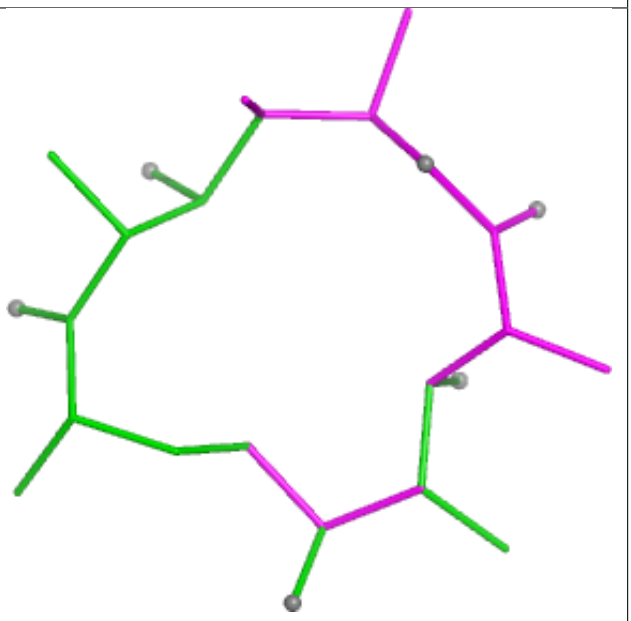


Rings

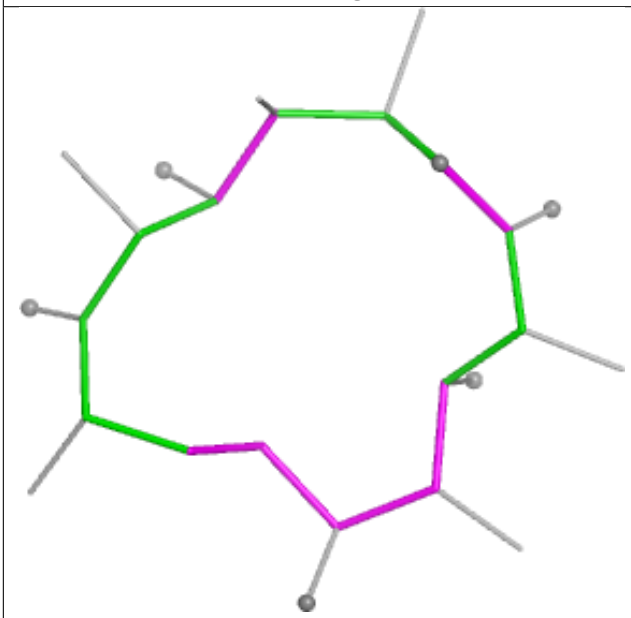
Ligand QR8 I 502



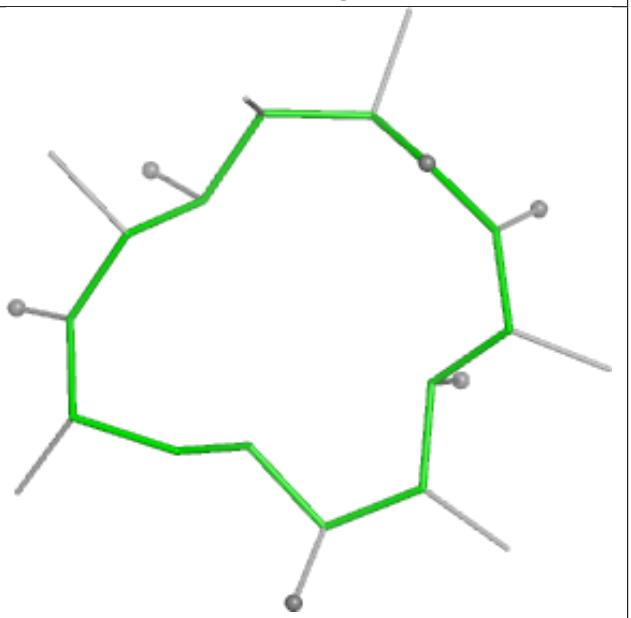
Bond lengths



Bond angles

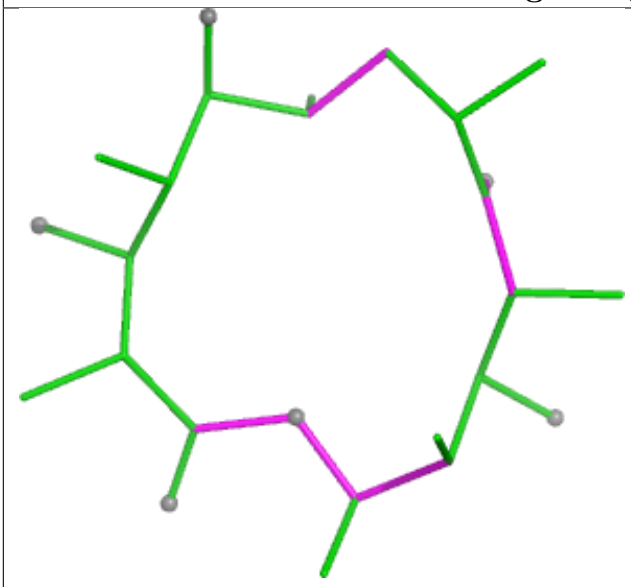


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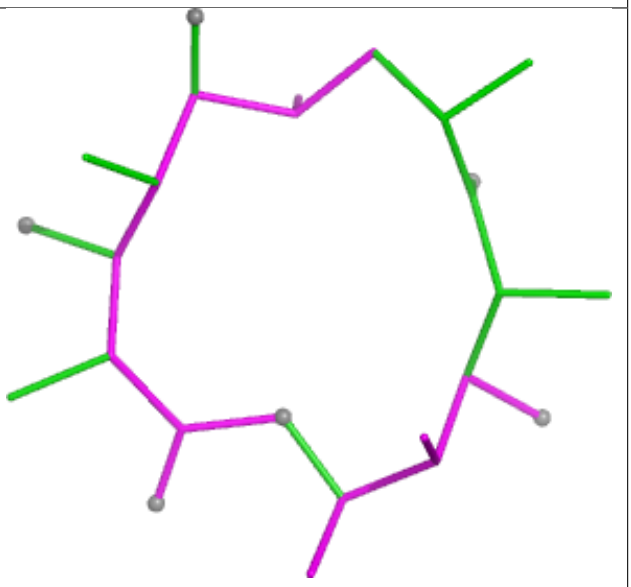


Rings

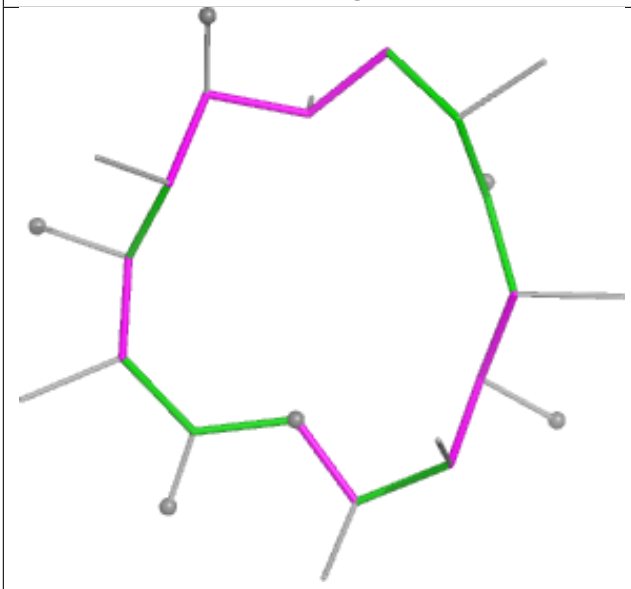
Ligand QR8 C 502



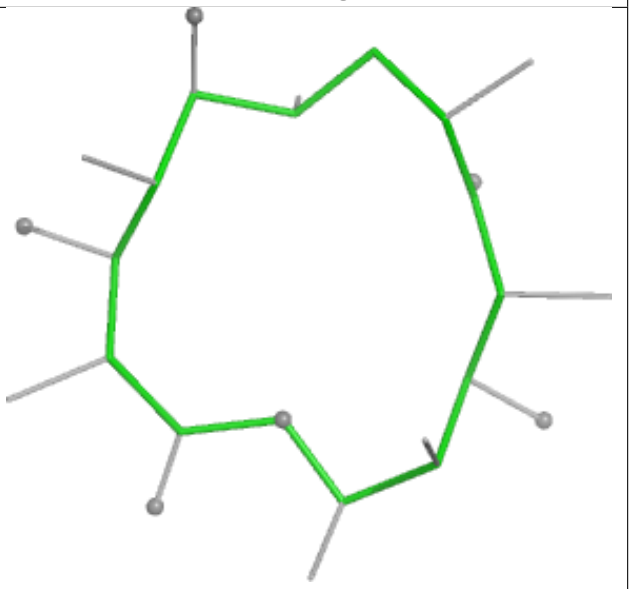
Bond lengths



Bond angles

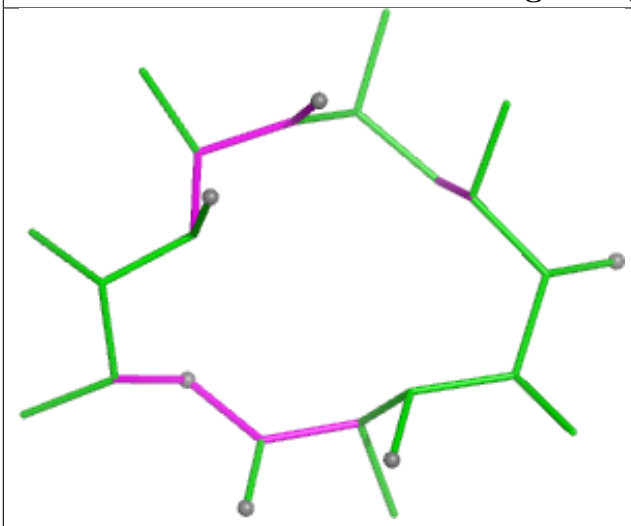


Torsions

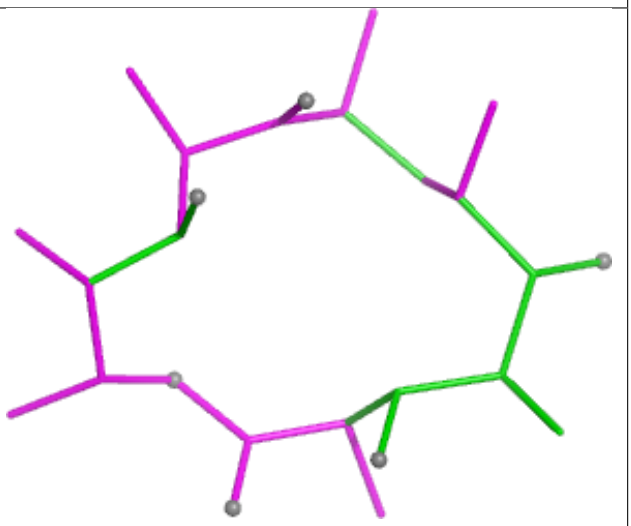


Rings

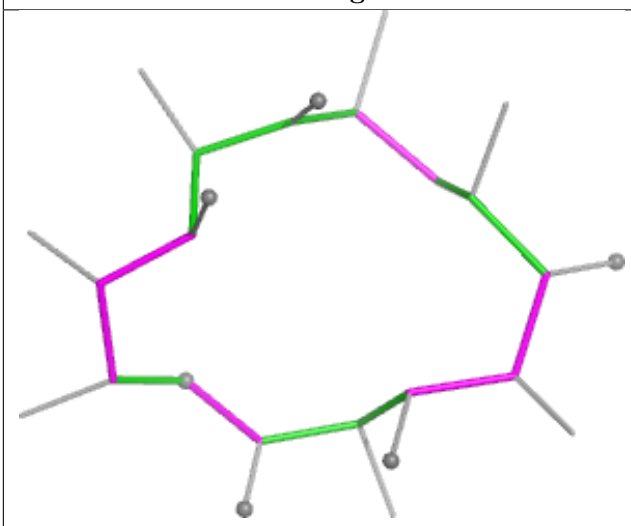
Ligand QR8 A 502



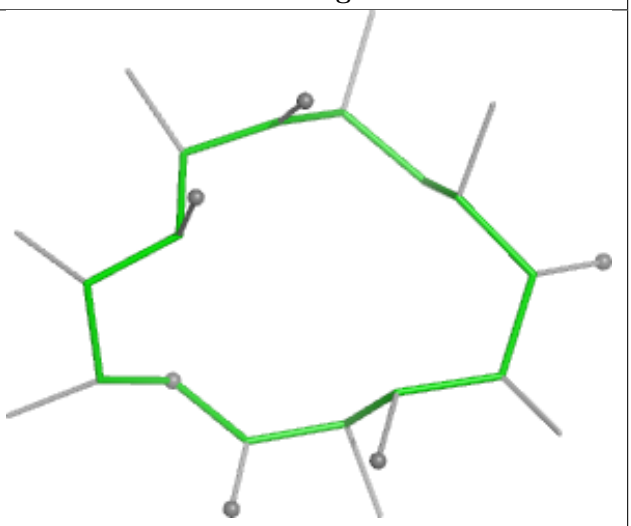
Bond lengths



Bond angles

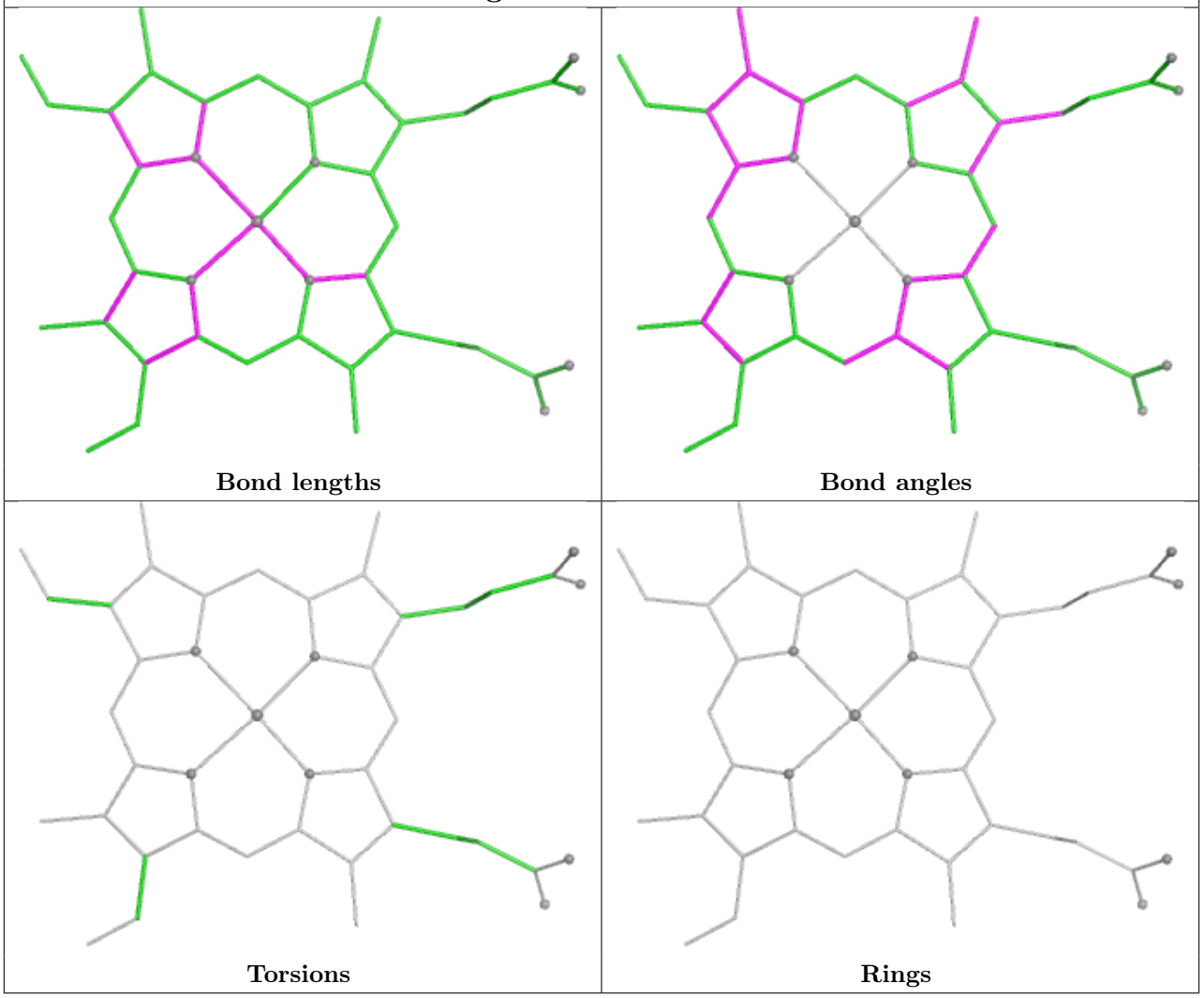


Torsions



Rings

Ligand HEM H 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	394/407 (96%)	-0.08	1 (0%) 90 88	9, 28, 77, 129	0
1	B	395/407 (97%)	0.24	11 (2%) 55 46	16, 46, 84, 116	0
1	C	395/407 (97%)	0.01	2 (0%) 87 83	13, 40, 69, 107	0
1	D	394/407 (96%)	0.01	8 (2%) 65 56	15, 33, 80, 128	0
1	E	386/407 (94%)	0.47	10 (2%) 57 48	18, 58, 101, 167	0
1	F	394/407 (96%)	0.38	13 (3%) 49 41	16, 49, 85, 147	0
1	G	381/407 (93%)	0.78	39 (10%) 12 11	22, 65, 129, 172	0
1	H	395/407 (97%)	0.40	12 (3%) 52 44	21, 50, 86, 126	0
1	I	248/407 (60%)	1.84	105 (42%) 0 0	69, 109, 148, 182	0
All	All	3382/3663 (92%)	0.39	201 (5%) 28 23	9, 48, 112, 182	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	293	ALA	5.6
1	I	171	PHE	5.5
1	I	64	VAL	5.0
1	E	293	ALA	4.9
1	G	14	VAL	4.8
1	I	369	ALA	4.6
1	I	84	PHE	4.5
1	I	253	ILE	4.5
1	I	274	PRO	4.4
1	I	212	THR	4.3
1	G	238	GLY	4.3
1	G	187	ALA	4.2
1	I	189	ILE	4.2
1	I	161	LEU	4.2
1	G	174	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	184	LEU	4.0
1	I	65	LEU	3.9
1	I	242	LEU	3.9
1	I	279	ALA	3.9
1	F	14	VAL	3.9
1	I	217	GLY	3.9
1	I	157	ILE	3.9
1	F	53	TRP	3.8
1	I	136	VAL	3.7
1	I	170	LEU	3.7
1	G	300	ALA	3.6
1	G	199	TYR	3.6
1	I	361	LEU	3.6
1	G	177	ALA	3.6
1	I	123	ARG	3.6
1	G	171	PHE	3.6
1	B	231	LYS	3.5
1	G	216	LEU	3.5
1	I	365	GLU	3.5
1	I	144	LEU	3.5
1	E	189	ILE	3.5
1	C	107	LEU	3.5
1	I	241	LEU	3.5
1	F	223	THR	3.5
1	I	127	LEU	3.4
1	G	160	LEU	3.4
1	E	186	ALA	3.4
1	I	107	LEU	3.3
1	I	173	THR	3.3
1	I	101	HIS	3.3
1	I	177	ALA	3.3
1	I	367	GLN	3.3
1	I	246	HIS	3.3
1	G	229	LEU	3.2
1	G	239	VAL	3.2
1	I	235	VAL	3.2
1	I	198	VAL	3.2
1	G	110	LYS	3.2
1	I	145	VAL	3.2
1	I	124	VAL	3.2
1	G	189	ILE	3.2
1	F	184	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	154	VAL	3.1
1	I	204	VAL	3.1
1	I	165	LEU	3.1
1	I	370	LEU	3.1
1	G	186	ALA	3.1
1	I	111	ALA	3.0
1	G	108	VAL	3.0
1	D	184	LEU	3.0
1	I	196	PHE	3.0
1	B	310	THR	2.9
1	G	297	VAL	2.9
1	H	294	GLY	2.9
1	G	235	VAL	2.9
1	I	153	PRO	2.9
1	H	81	PRO	2.9
1	I	187	ALA	2.8
1	I	211	PRO	2.8
1	I	156	VAL	2.8
1	H	335	ASP	2.8
1	I	114	ALA	2.8
1	D	225	ASN	2.8
1	F	292	SER	2.8
1	I	245	GLY	2.8
1	F	40	VAL	2.7
1	G	210	ALA	2.7
1	I	131	LEU	2.7
1	I	219	LEU	2.7
1	H	295	SER	2.7
1	I	98	PRO	2.7
1	I	386	VAL	2.7
1	I	112	PHE	2.7
1	I	357	ILE	2.7
1	I	290	LEU	2.7
1	I	373	LEU	2.7
1	I	394	GLY	2.7
1	C	305	GLU	2.7
1	I	234	ILE	2.6
1	I	174	PHE	2.6
1	E	21	LEU	2.6
1	G	170	LEU	2.6
1	G	192	VAL	2.6
1	I	150	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	243	ILE	2.6
1	I	271	VAL	2.6
1	G	293	ALA	2.6
1	I	218	ALA	2.6
1	B	53	TRP	2.5
1	G	200	MET	2.5
1	I	364	LEU	2.5
1	I	368	GLU	2.5
1	F	183	ARG	2.5
1	I	158	CYS	2.5
1	I	192	VAL	2.5
1	F	182	THR	2.5
1	H	37	ASP	2.5
1	I	209	ASP	2.5
1	I	160	LEU	2.5
1	F	358	GLY	2.5
1	D	293	ALA	2.5
1	I	142	ALA	2.5
1	I	254	THR	2.5
1	B	105	ARG	2.4
1	B	229	LEU	2.4
1	D	170	LEU	2.4
1	E	396	LEU	2.4
1	I	99	PRO	2.4
1	I	159	GLU	2.4
1	H	13	ALA	2.4
1	I	359	ALA	2.4
1	I	39	PRO	2.4
1	I	141	PRO	2.4
1	G	156	VAL	2.4
1	D	329	GLU	2.4
1	H	53	TRP	2.4
1	I	86	THR	2.4
1	E	14	VAL	2.4
1	B	219	LEU	2.4
1	I	132	LEU	2.4
1	I	179	LEU	2.4
1	I	55	VAL	2.3
1	I	117	VAL	2.3
1	I	221	LEU	2.3
1	D	183	ARG	2.3
1	E	176	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	217	GLY	2.3
1	I	352	GLY	2.3
1	E	177	ALA	2.3
1	I	146	GLU	2.3
1	E	170	LEU	2.3
1	I	202	GLY	2.3
1	I	178	MET	2.2
1	B	13	ALA	2.2
1	G	242	LEU	2.2
1	I	270	LEU	2.2
1	I	252	GLN	2.2
1	B	208	ARG	2.2
1	F	39	PRO	2.2
1	I	280	ALA	2.2
1	I	58	MET	2.2
1	G	196	PHE	2.2
1	G	89	GLU	2.2
1	I	61	ALA	2.2
1	B	106	ARG	2.2
1	G	228	HIS	2.2
1	D	14	VAL	2.2
1	H	55	VAL	2.2
1	H	311	VAL	2.2
1	I	199	TYR	2.2
1	I	366	LEU	2.2
1	G	106	ARG	2.2
1	G	176	ASP	2.2
1	G	299	VAL	2.2
1	I	289	PRO	2.2
1	F	331	PHE	2.2
1	I	396	LEU	2.2
1	I	283	GLU	2.2
1	B	397	ILE	2.1
1	I	291	VAL	2.1
1	I	60	ASP	2.1
1	H	223	THR	2.1
1	E	290	LEU	2.1
1	I	148	LEU	2.1
1	D	393	GLN	2.1
1	G	204	VAL	2.1
1	I	238	GLY	2.1
1	G	107	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	179	LEU	2.1
1	H	170	LEU	2.1
1	I	152	PHE	2.1
1	I	207	ARG	2.1
1	F	317	CYS	2.1
1	B	319	VAL	2.1
1	I	248	THR	2.1
1	G	220	ALA	2.1
1	G	357	ILE	2.1
1	G	219	LEU	2.1
1	I	203	LEU	2.1
1	I	358	GLY	2.1
1	G	208	ARG	2.1
1	I	63	ILE	2.1
1	I	267	TYR	2.1
1	I	250	VAL	2.0
1	A	393	GLN	2.0
1	I	116	ARG	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 (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	QR8	I	502	26/26	0.64	0.22	82,110,131,138	0
3	QR8	E	502	26/26	0.80	0.21	44,74,99,102	0
3	QR8	A	502	26/26	0.80	0.18	27,33,39,44	0
3	QR8	H	502	26/26	0.82	0.16	38,45,52,56	0
2	HEM	I	501	43/43	0.82	0.21	88,152,169,172	0

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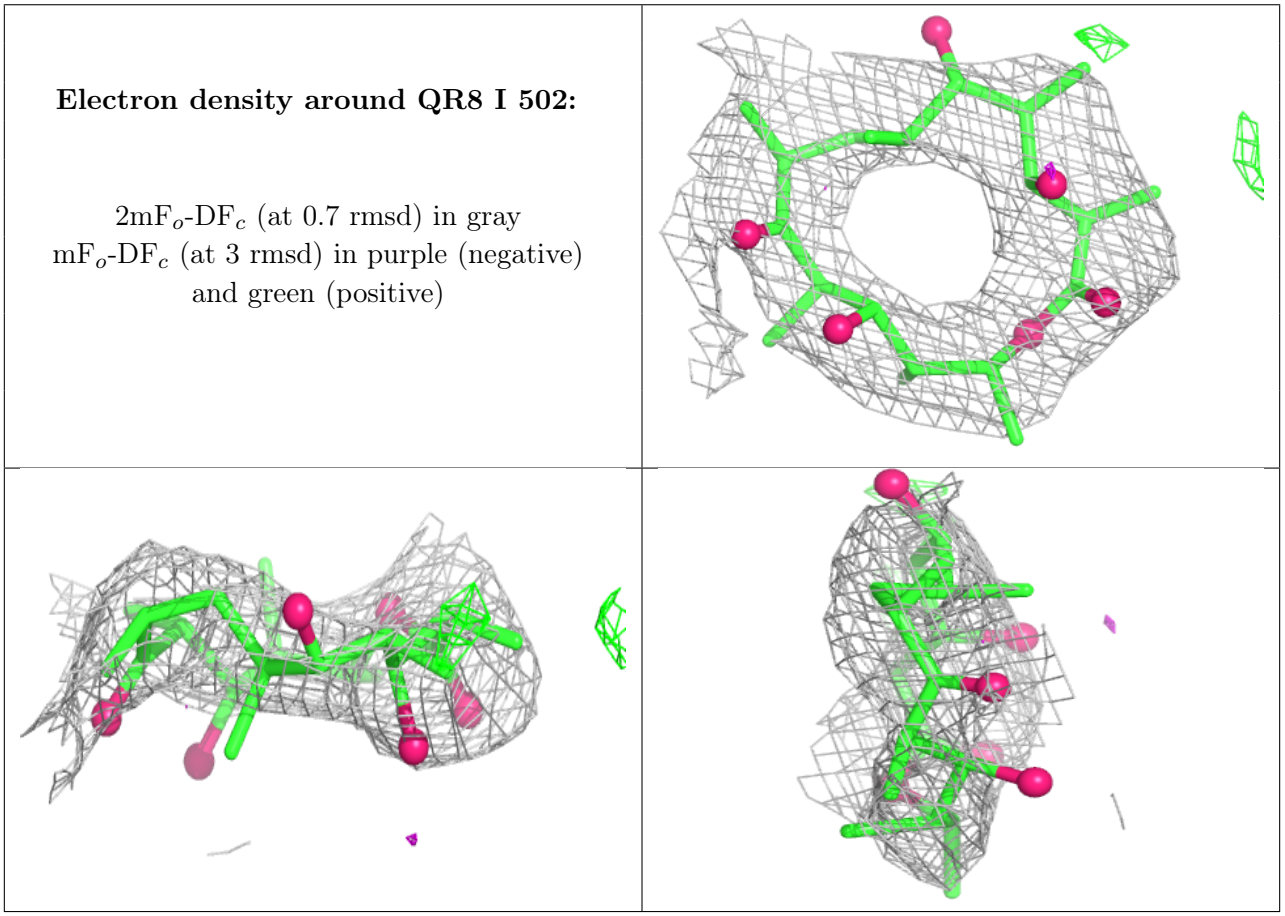
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	QR8	G	502	26/26	0.84	0.18	46,57,78,85	0
3	QR8	F	502	26/26	0.85	0.17	49,53,61,67	0
3	QR8	D	502	26/26	0.89	0.13	36,46,52,52	0
3	QR8	B	502	26/26	0.93	0.11	28,31,36,42	0
2	HEM	F	501	43/43	0.94	0.14	35,68,79,81	0
3	QR8	C	502	26/26	0.94	0.10	16,18,19,21	0
2	HEM	B	501	43/43	0.95	0.11	28,33,42,46	0
2	HEM	H	501	43/43	0.95	0.12	26,57,69,75	0
2	HEM	G	501	43/43	0.96	0.10	47,53,67,70	0
2	HEM	E	501	43/43	0.97	0.08	34,39,48,54	0
2	HEM	D	501	43/43	0.98	0.07	19,24,40,48	0
2	HEM	A	501	43/43	0.98	0.06	7,8,9,10	0
2	HEM	C	501	43/43	0.98	0.07	21,23,28,33	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.

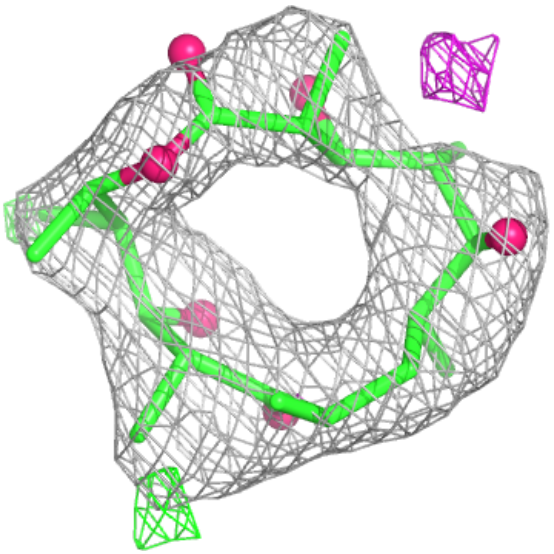
Electron density around QR8 I 502:

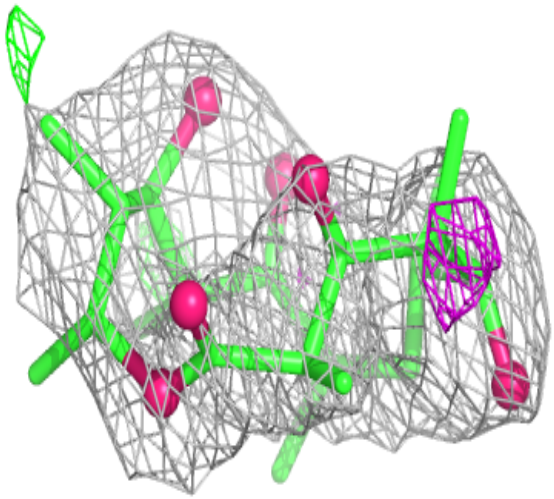
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

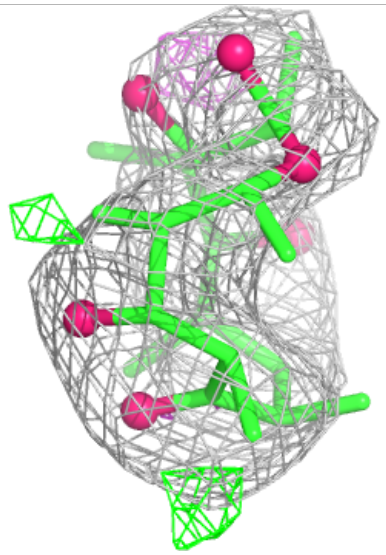


Electron density around QR8 E 502:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

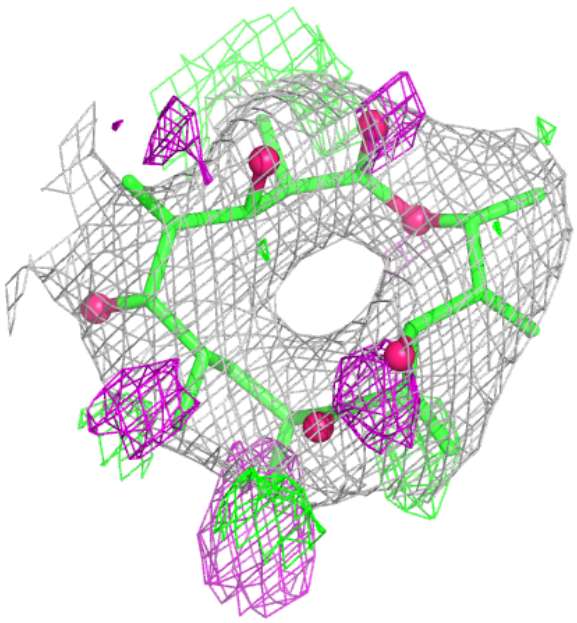


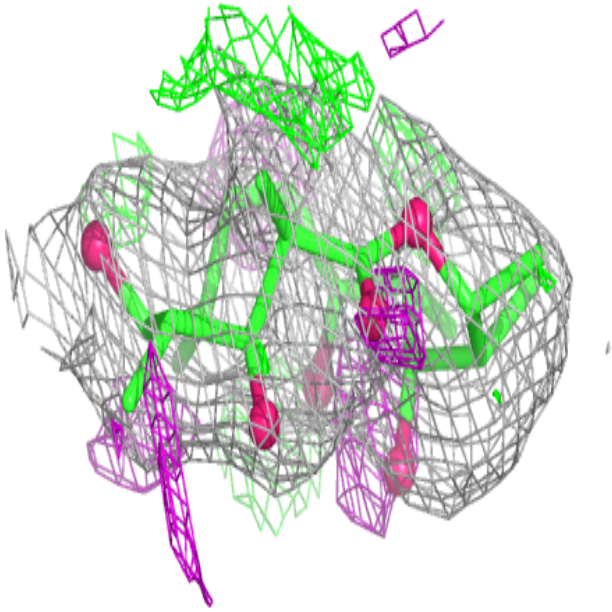




Electron density around QR8 A 502:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

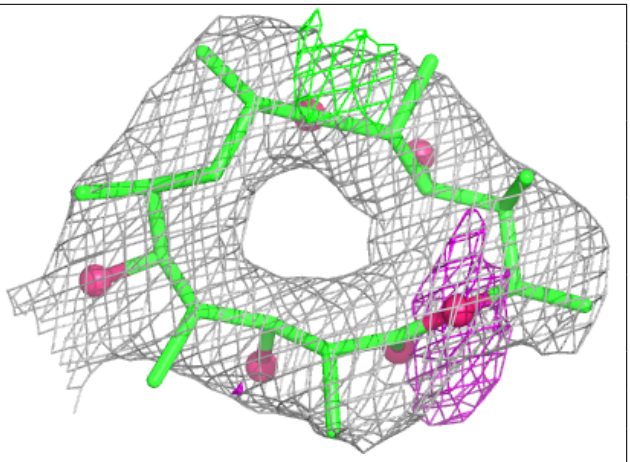


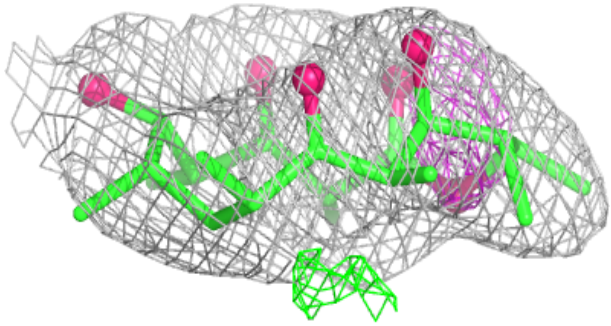


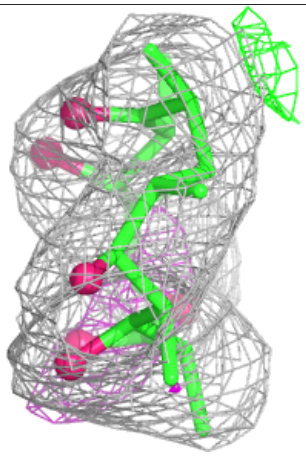


Electron density around QR8 H 502:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

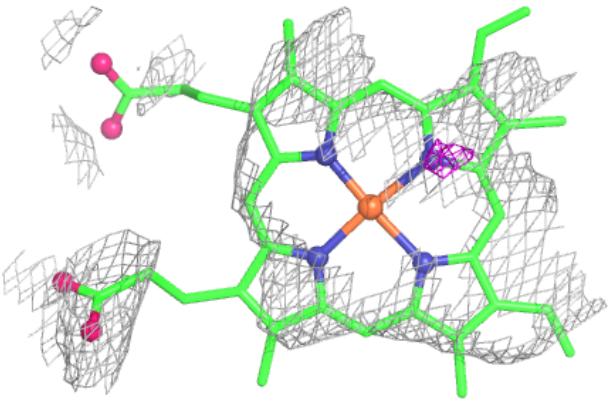


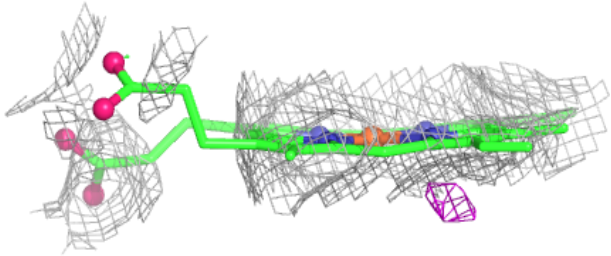


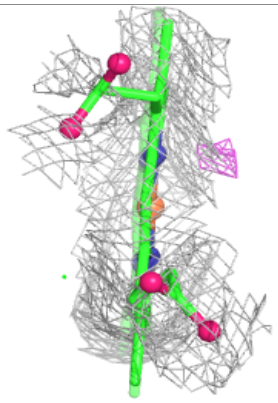


Electron density around HEM I 501:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

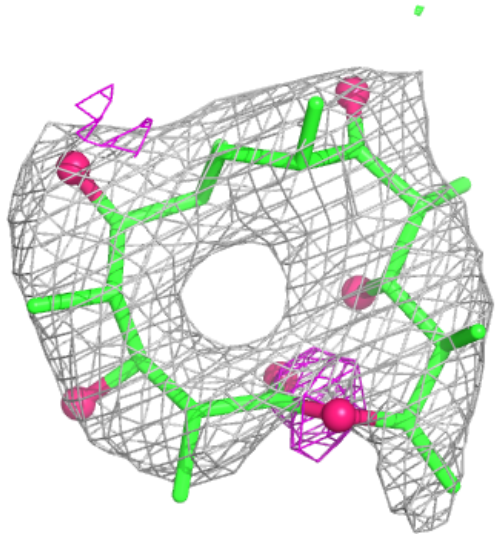


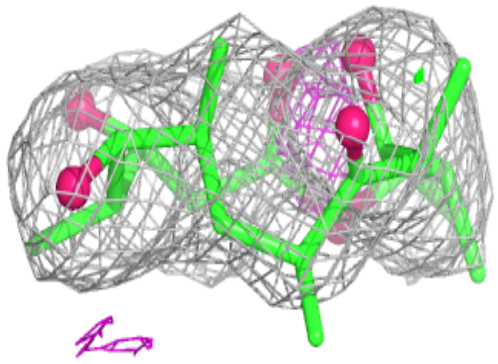


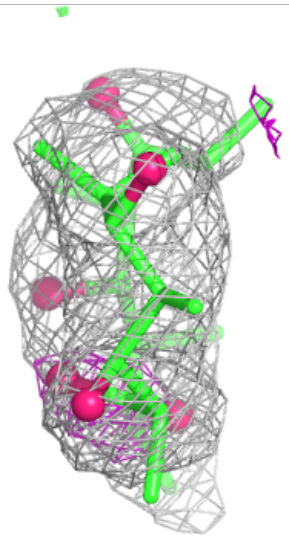


Electron density around QR8 G 502:

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

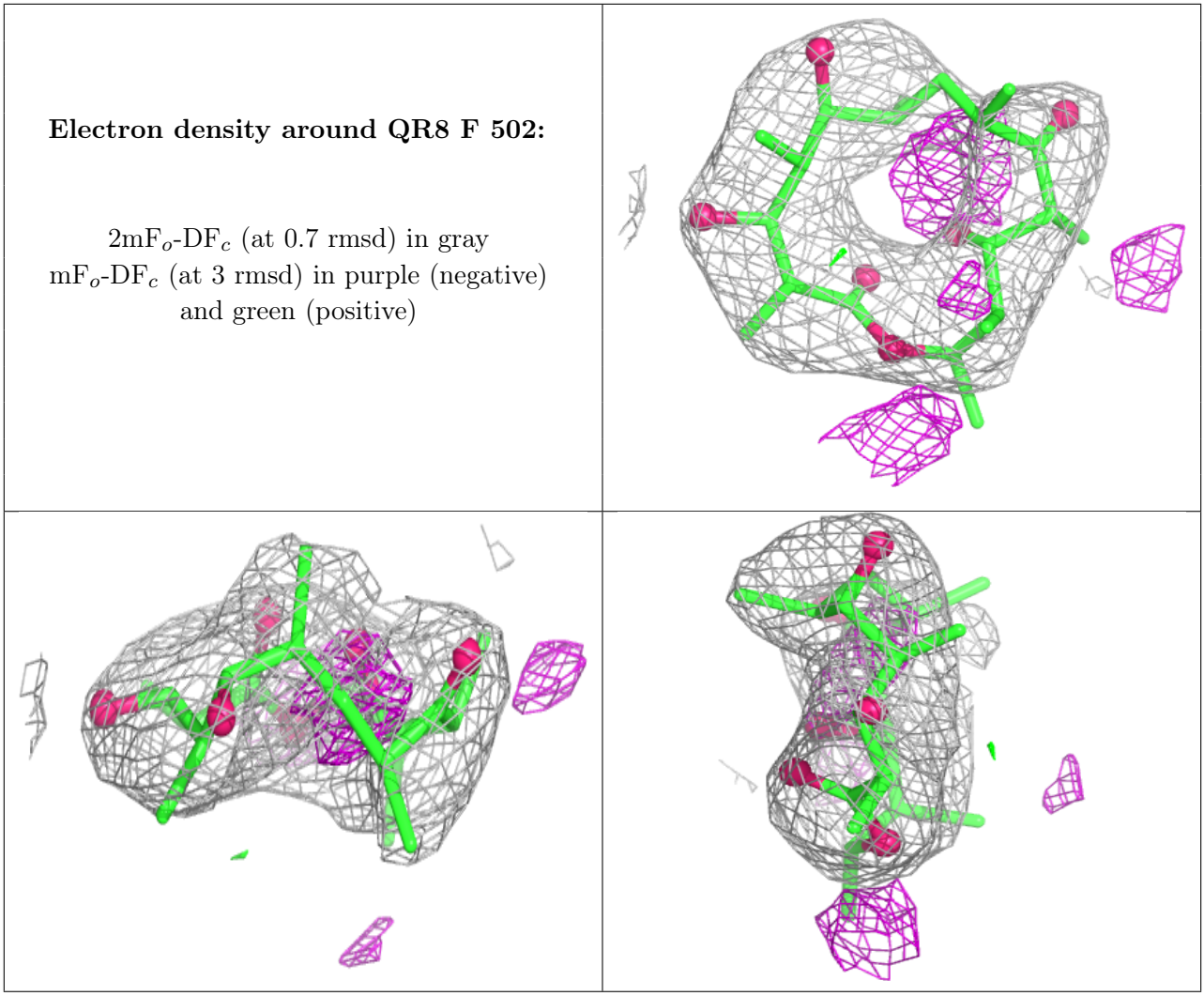






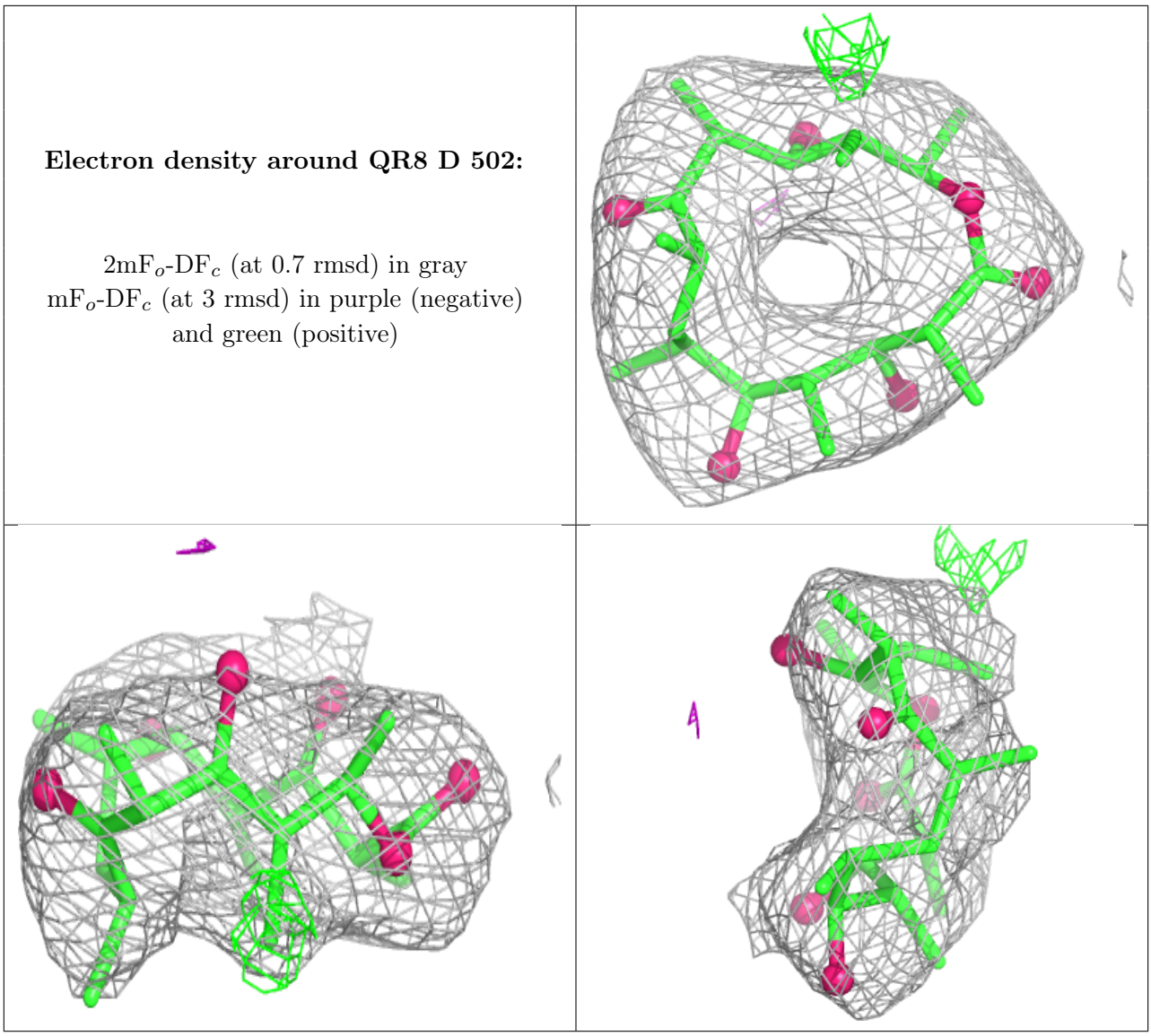
Electron density around QR8 F 502:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



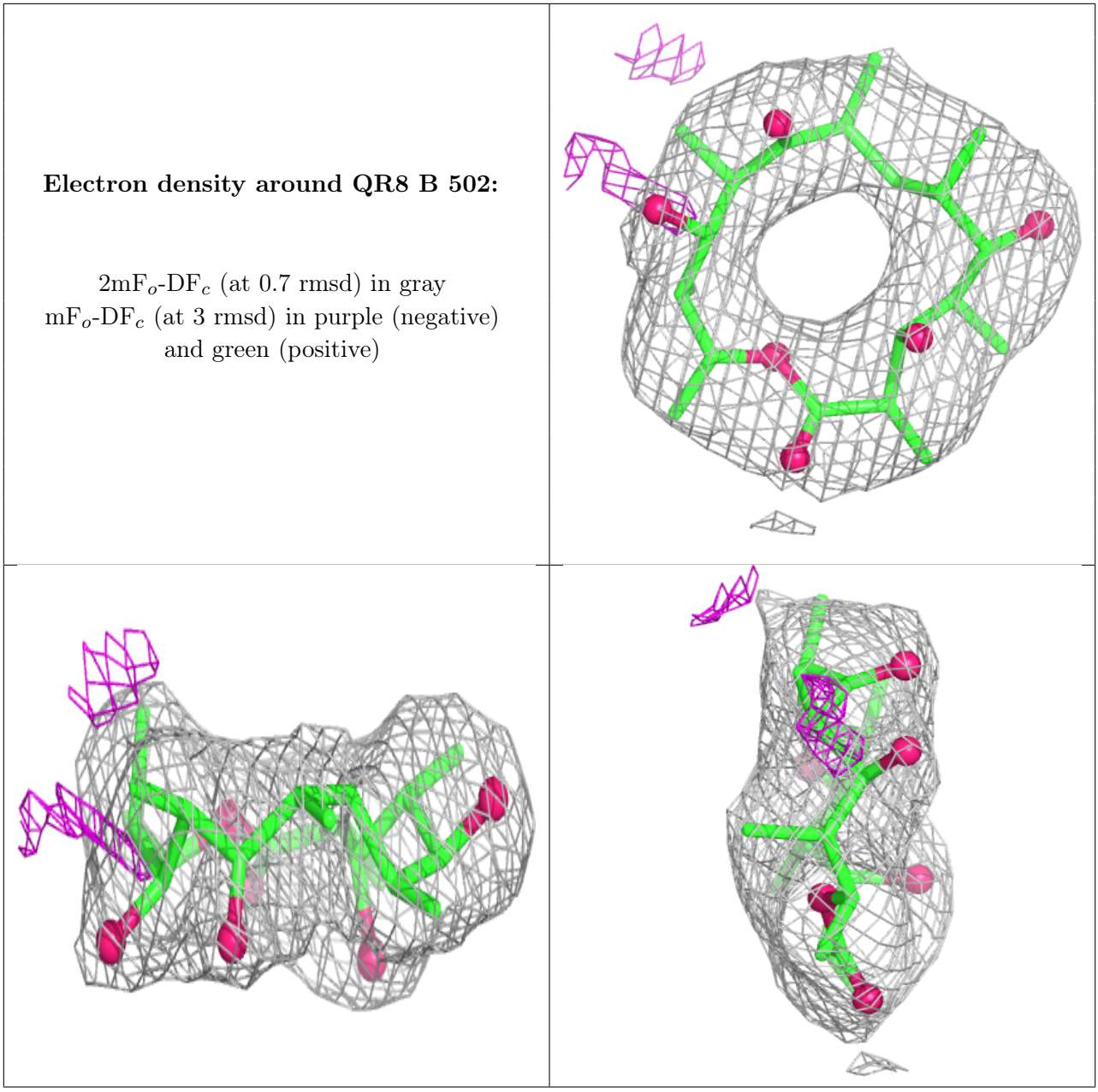
Electron density around QR8 D 502:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



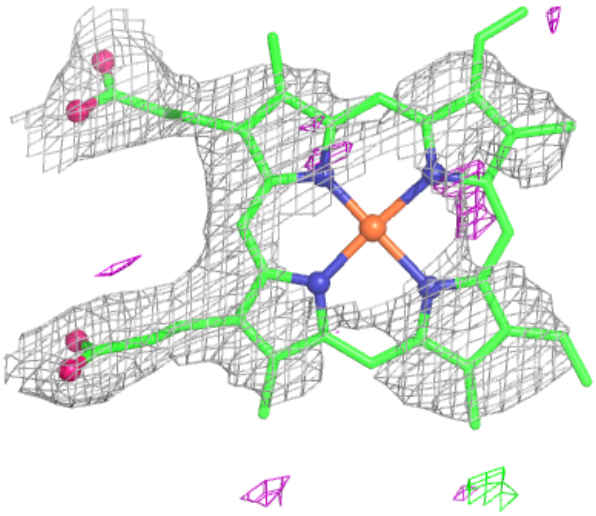
Electron density around QR8 B 502:

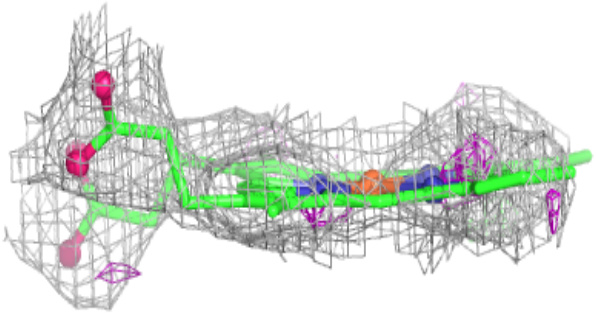
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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

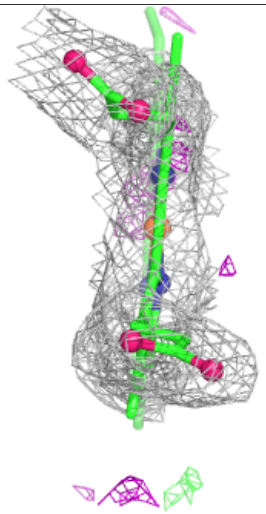


Electron density around HEM F 501:

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

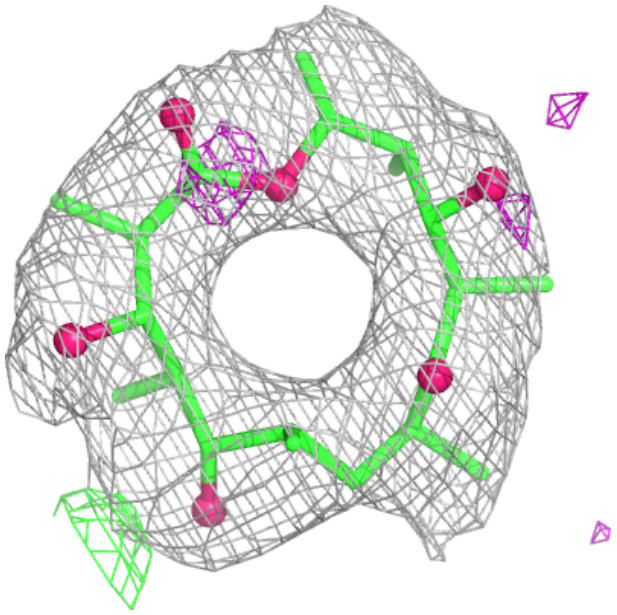


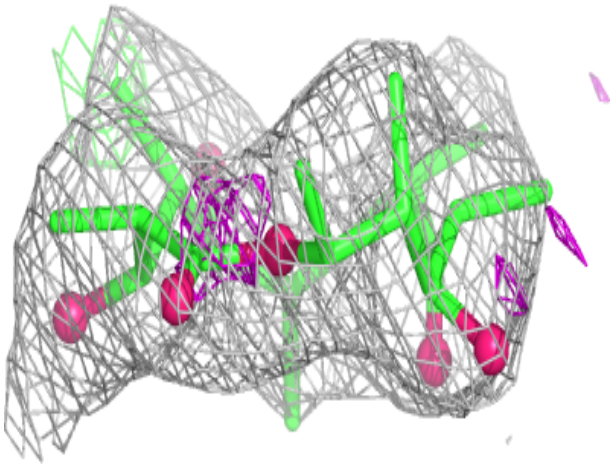


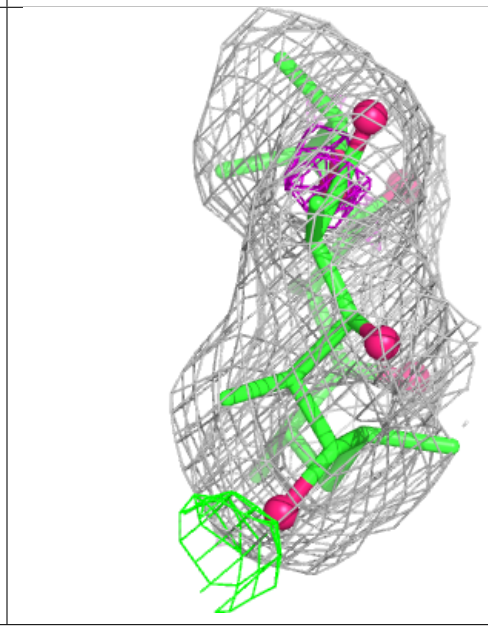


Electron density around QR8 C 502:

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

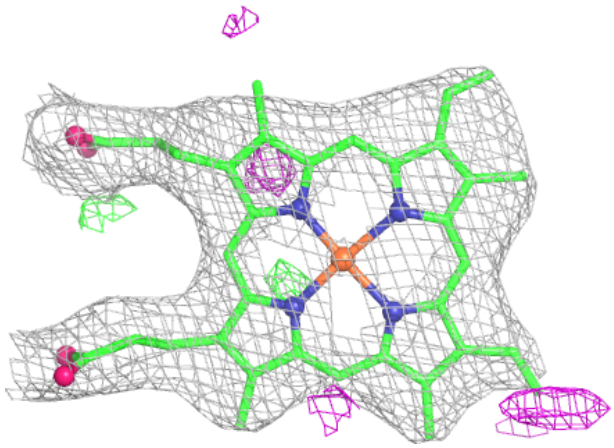


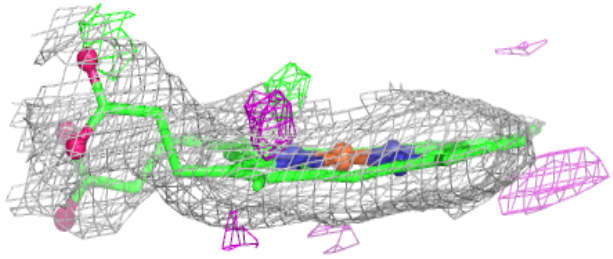


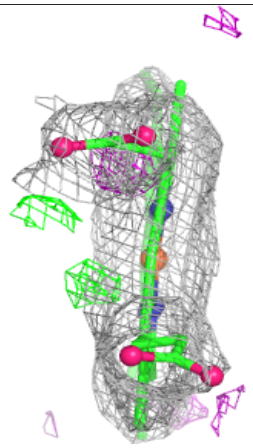


Electron density around HEM B 501:

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

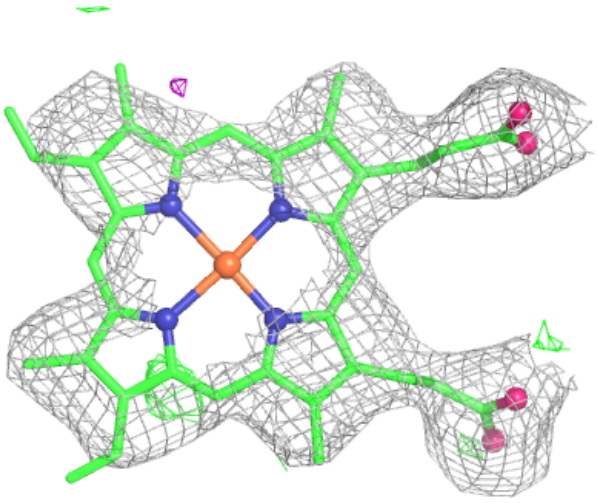


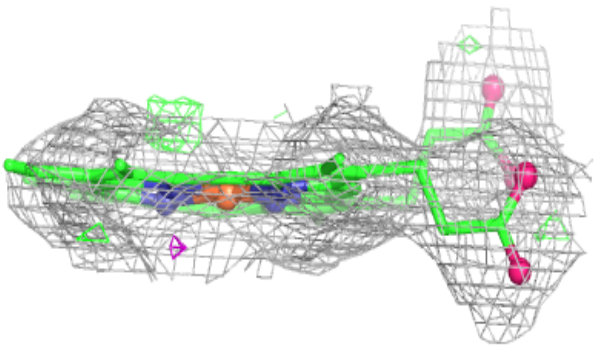




Electron density around HEM H 501:

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

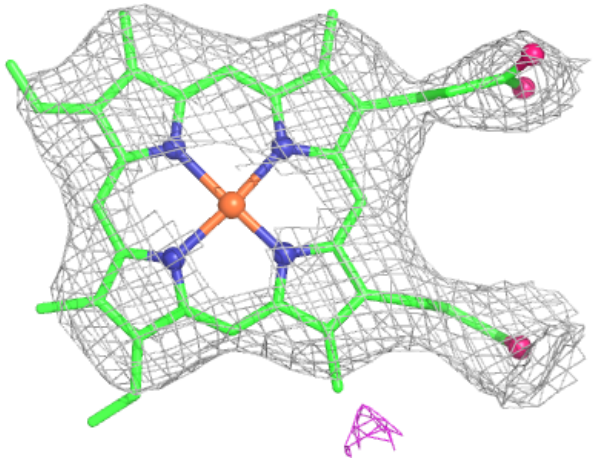


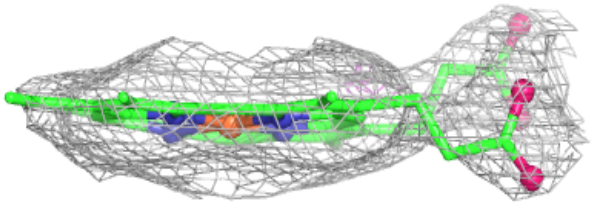


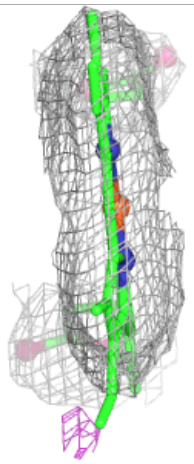


Electron density around HEM G 501:

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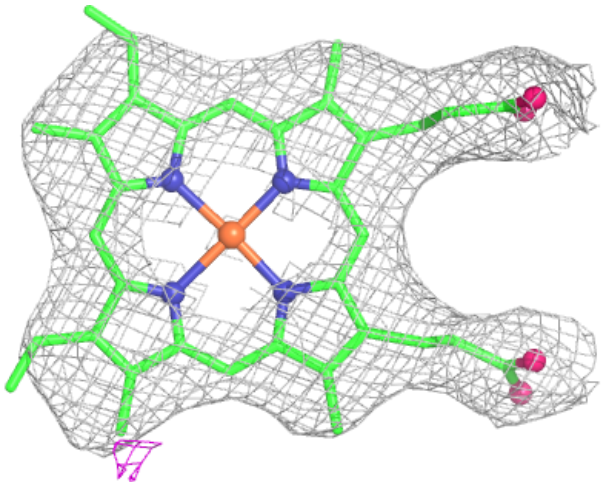


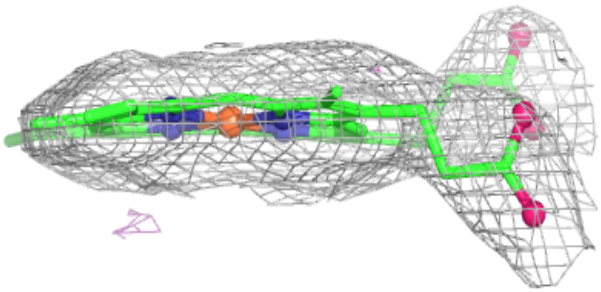


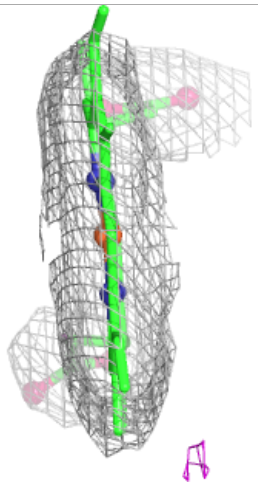


Electron density around HEM E 501:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

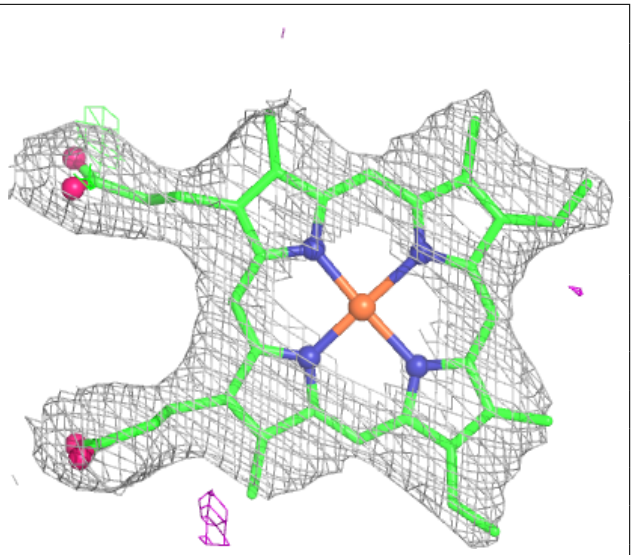


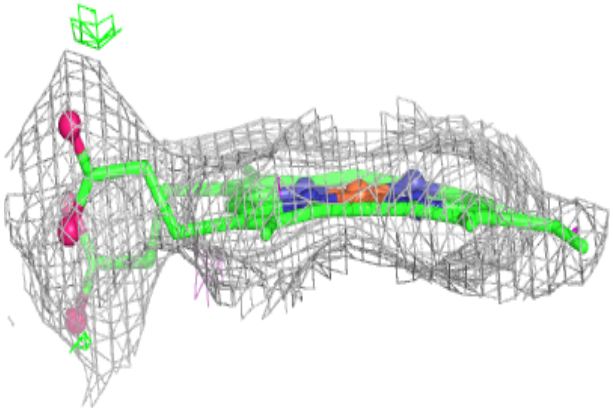


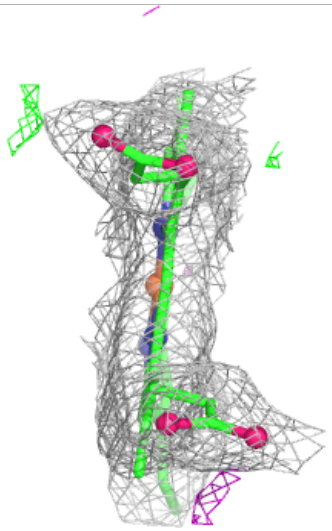


Electron density around HEM D 501:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

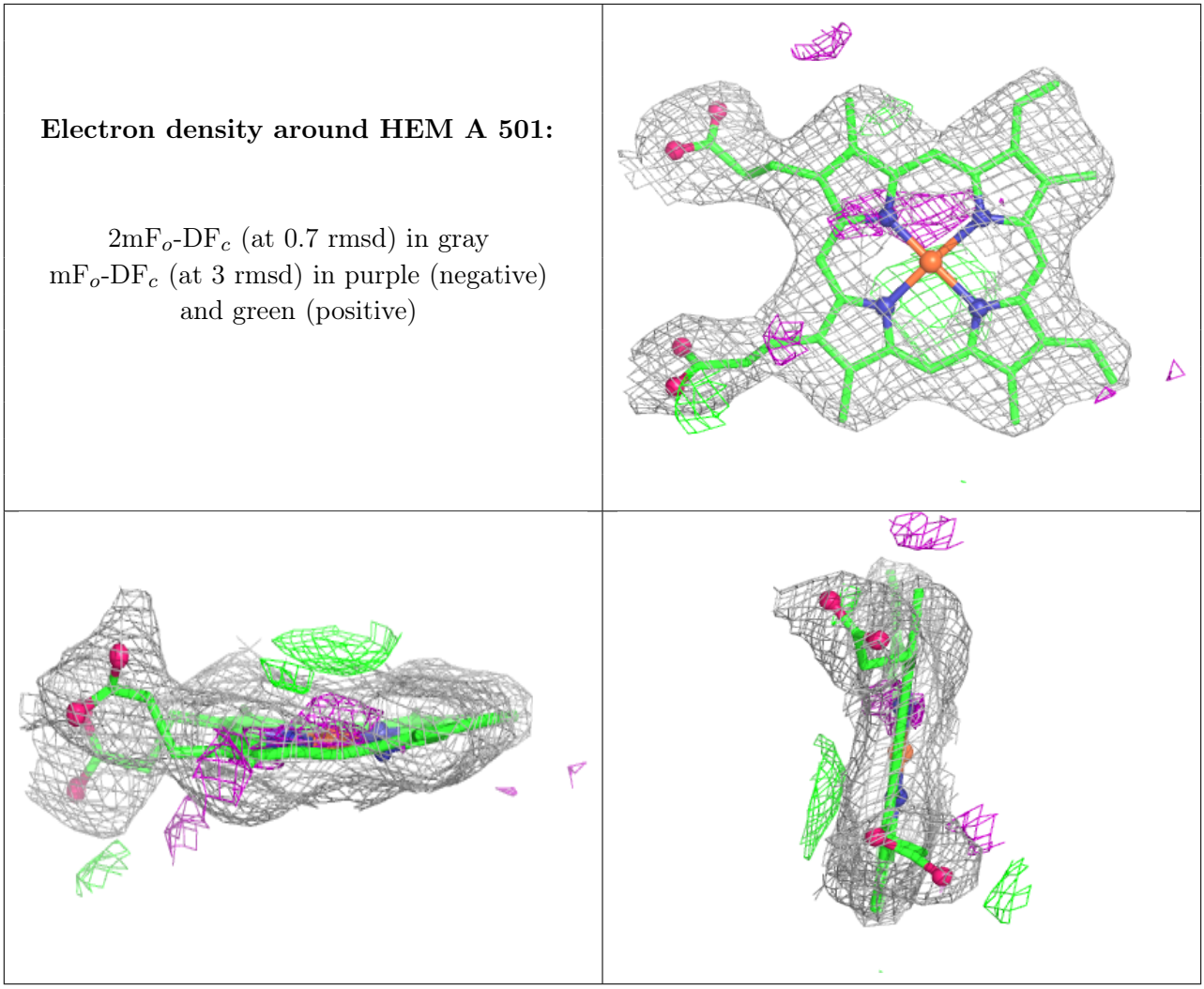






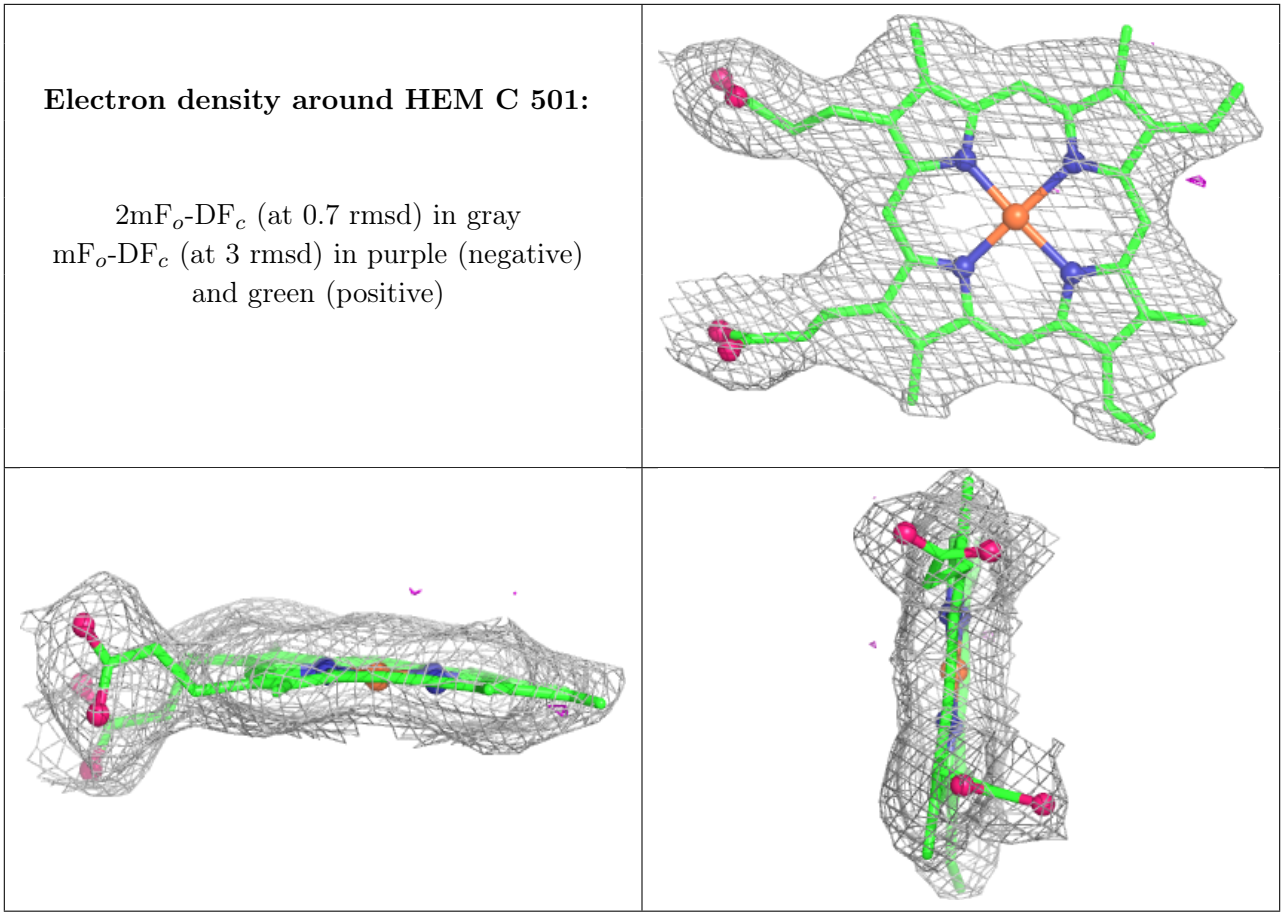
Electron density around HEM A 501:

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



Electron density around HEM C 501:

$2mF_o$-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

There are no such residues in this entry.