Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 09:12 AM EDT

PDB ID	:	3ME6
Title	:	Crystal structure of cytochrome 2B4 in complex with the anti-platelet drug clopidogrel
Authors	:	Gay, S.C.; Roberts, A.G.; Maekawa, K.; Talakad, J.C.; Hong, W.X.; Zhang, Q.; Stout, C.D.; Halpert, J.R.
Deposited on	:	2010-03-31
Resolution	:	3.10 Å(reported)

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

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

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

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

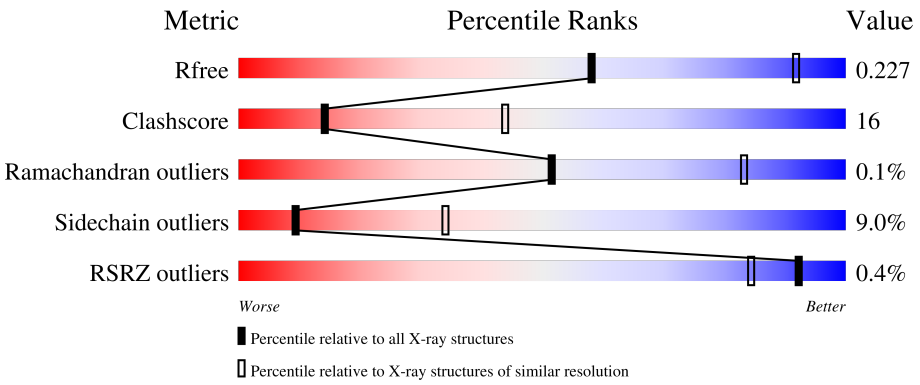
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	476	67% 26% • •
1	B	476	66% 28% • •
1	C	476	67% 28% • •
1	D	476	68% 25% 5% •

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	CGE	B	501	-	-	X	-
3	CGE	C	501	-	-	X	-
3	CGE	D	501	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15302 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 P450 2B4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	465	3723	2402	643	667	11	0	1	0
1	B	465	3729	2405	646	667	11	0	1	0
1	C	465	3729	2405	646	667	11	0	1	0
1	D	465	3733	2407	646	669	11	0	1	0

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ALA	GLU	engineered mutation	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	SER	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	ALA	deletion	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	ALA	deletion	UNP P00178
A	?	-	GLY	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	ARG	deletion	UNP P00178
A	22	LYS	GLY	engineered mutation	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LYS	HIS	engineered mutation	UNP P00178
A	24	THR	PRO	engineered mutation	UNP P00178
A	25	SER	LYS	engineered mutation	UNP P00178
A	26	SER	ALA	engineered mutation	UNP P00178
A	27	LYS	HIS	engineered mutation	UNP P00178
A	29	LYS	ARG	engineered mutation	UNP P00178
A	221	SER	PRO	SEE REMARK 999	UNP P00178
A	226	TYR	HIS	engineered mutation	UNP P00178
A	492	HIS	-	expression tag	UNP P00178
A	493	HIS	-	expression tag	UNP P00178
A	494	HIS	-	expression tag	UNP P00178
A	495	HIS	-	expression tag	UNP P00178
B	21	ALA	GLU	engineered mutation	UNP P00178
B	?	-	PHE	deletion	UNP P00178
B	?	-	SER	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	ALA	deletion	UNP P00178
B	?	-	PHE	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	ALA	deletion	UNP P00178
B	?	-	GLY	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	PHE	deletion	UNP P00178
B	?	-	ARG	deletion	UNP P00178
B	22	LYS	GLY	engineered mutation	UNP P00178
B	23	LYS	HIS	engineered mutation	UNP P00178
B	24	THR	PRO	engineered mutation	UNP P00178
B	25	SER	LYS	engineered mutation	UNP P00178
B	26	SER	ALA	engineered mutation	UNP P00178
B	27	LYS	HIS	engineered mutation	UNP P00178
B	29	LYS	ARG	engineered mutation	UNP P00178
B	221	SER	PRO	SEE REMARK 999	UNP P00178
B	226	TYR	HIS	engineered mutation	UNP P00178
B	492	HIS	-	expression tag	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
B	493	HIS	-	expression tag	UNP P00178
B	494	HIS	-	expression tag	UNP P00178
B	495	HIS	-	expression tag	UNP P00178
C	21	ALA	GLU	engineered mutation	UNP P00178
C	?	-	PHE	deletion	UNP P00178
C	?	-	SER	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	ALA	deletion	UNP P00178
C	?	-	PHE	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	ALA	deletion	UNP P00178
C	?	-	GLY	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	PHE	deletion	UNP P00178
C	?	-	ARG	deletion	UNP P00178
C	22	LYS	GLY	engineered mutation	UNP P00178
C	23	LYS	HIS	engineered mutation	UNP P00178
C	24	THR	PRO	engineered mutation	UNP P00178
C	25	SER	LYS	engineered mutation	UNP P00178
C	26	SER	ALA	engineered mutation	UNP P00178
C	27	LYS	HIS	engineered mutation	UNP P00178
C	29	LYS	ARG	engineered mutation	UNP P00178
C	221	SER	PRO	SEE REMARK 999	UNP P00178
C	226	TYR	HIS	engineered mutation	UNP P00178
C	492	HIS	-	expression tag	UNP P00178
C	493	HIS	-	expression tag	UNP P00178
C	494	HIS	-	expression tag	UNP P00178
C	495	HIS	-	expression tag	UNP P00178
D	21	ALA	GLU	engineered mutation	UNP P00178
D	?	-	PHE	deletion	UNP P00178
D	?	-	SER	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178

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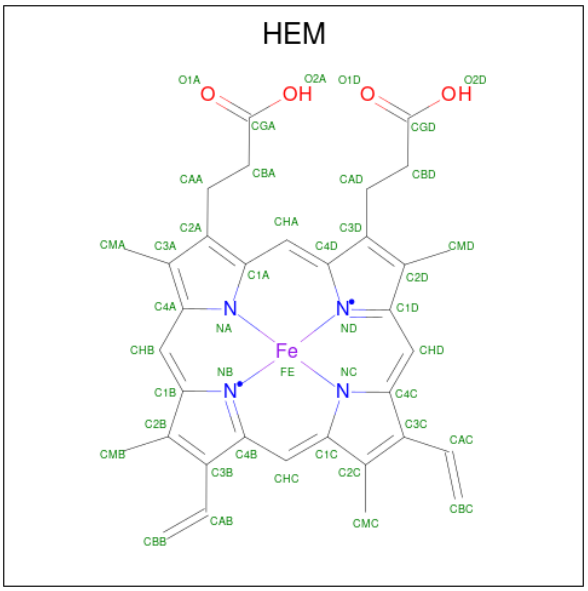
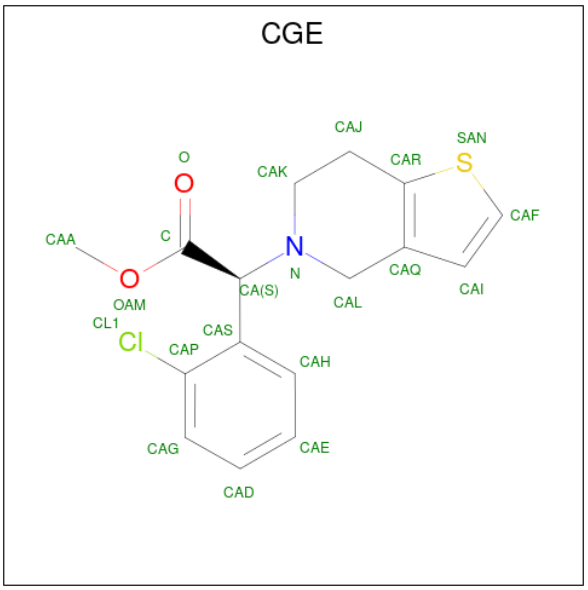
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	ALA	deletion	UNP P00178
D	?	-	PHE	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	ALA	deletion	UNP P00178
D	?	-	GLY	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	PHE	deletion	UNP P00178
D	?	-	ARG	deletion	UNP P00178
D	22	LYS	GLY	engineered mutation	UNP P00178
D	23	LYS	HIS	engineered mutation	UNP P00178
D	24	THR	PRO	engineered mutation	UNP P00178
D	25	SER	LYS	engineered mutation	UNP P00178
D	26	SER	ALA	engineered mutation	UNP P00178
D	27	LYS	HIS	engineered mutation	UNP P00178
D	29	LYS	ARG	engineered mutation	UNP P00178
D	221	SER	PRO	SEE REMARK 999	UNP P00178
D	226	TYR	HIS	engineered mutation	UNP P00178
D	492	HIS	-	expression tag	UNP P00178
D	493	HIS	-	expression tag	UNP P00178
D	494	HIS	-	expression tag	UNP P00178
D	495	HIS	-	expression tag	UNP P00178

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



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

- Molecule 3 is Clopidogrel (three-letter code: CGE) (formula: $C_{16}H_{16}ClNO_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
3	A	1	21	16	1	1	2	1	0	0
3	B	1	21	16	1	1	2	1	0	0
3	C	1	21	16	1	1	2	1	0	0
3	D	1	21	16	1	1	2	1	0	0

- Molecule 4 is water.

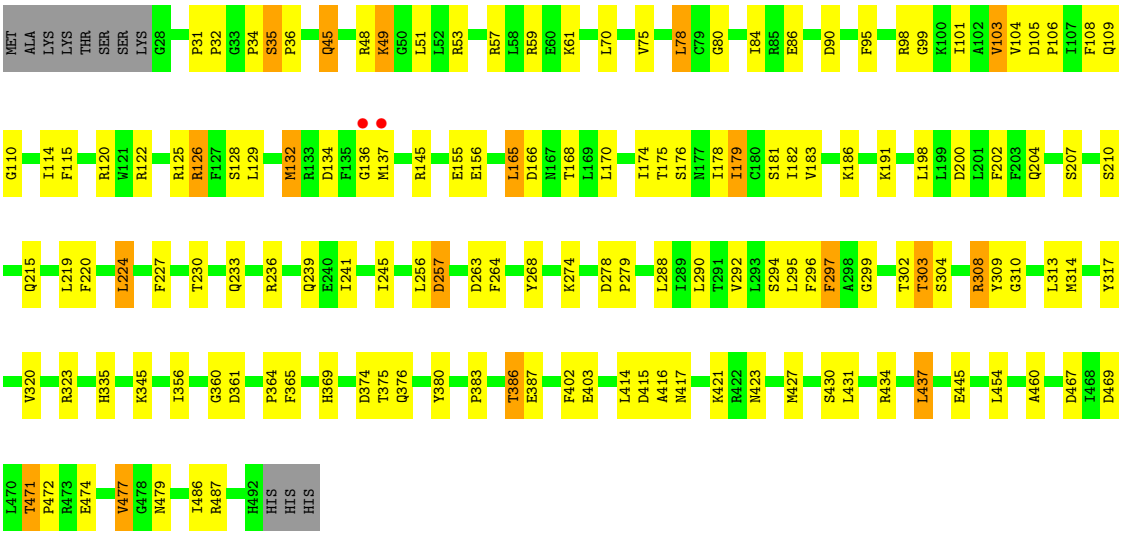
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	30	30	30	0	0
4	B	35	35	35	0	0
4	C	32	32	32	0	0
4	D	35	35	35	0	0

3 Residue-property plots (i)

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

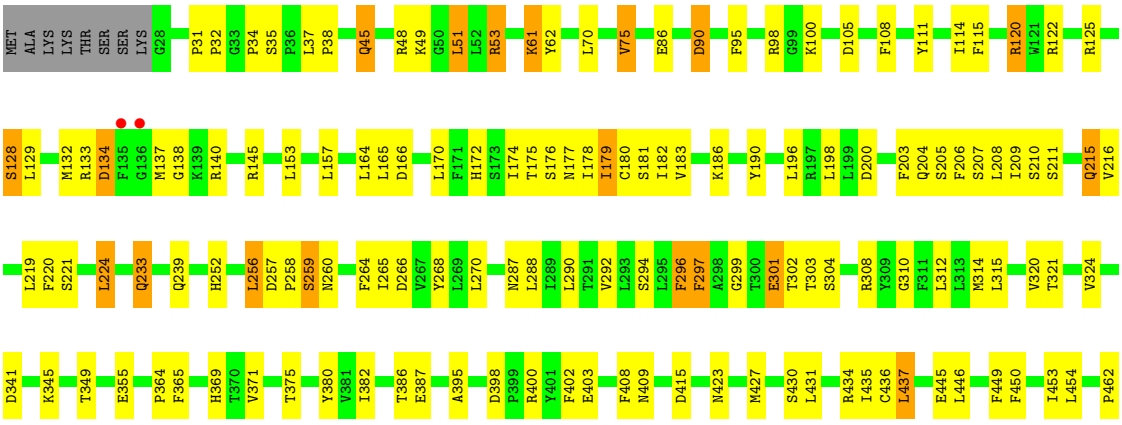
• Molecule 1: Cytochrome P450 2B4

Chain A:



• Molecule 1: Cytochrome P450 2B4

Chain B:



V463 P464 D469 L470 T471 P472 R473 E474 V477 G478 N479 I486 L489 H492 HIS HIS HIS

• Molecule 1: Cytochrome P450 2B4

Chain C: 67% 28% • •

MET ALA LYS LYS THR SER SER LYS G28 P31 P32 G33 P34 S35 P36 L37 P38 V39 L40 G41 N42 L43 L44 Q45 M46 D47 R48 K49 G50 L51 F55 L56 R57 L58 R59 L70 R73 P74 V75 E86 D90 Q91 A94 F95 R98 G99 K100 I101 A102 V103 V104 D105

P106 I107 F108 I114 E119 R122 R125 R126 F127 S128 L129 M132 R133 D134 F135 G136 M137 R140 R145 L164 L165 D166 N167 F171 T175 I179 C180 S181 I182 V183 K186 R187 F188 D189 Y190 K191 D192 L198 S205 F206 S207 L208 I209 S210 S214

L219 F220 S221 G222 F223 L224 K225 T230 Q239 E240 I241 I245 L256 D257 P258 S259 N260 F264 I265 D266 V267 Y268 L269 M272 F283 L288 I289 L290 T291 V292 L293 S294 L295 F296 F297 A298 G299 T302 T303 S304 T305 T306 L307 R308 Y309 G310 F311 L312 L313 M314

R323 P338 D341 K345 Y348 E355 I356 G360 D361 P364 P368 H369 T375 Y380 V381 K384 N385 T386 E387 H397 F402 E403 F408 N423 R434 I435 C436 L437 R443 T444 E445 L446 F450 L454 Q455 D469 L470 T471

E474 S475 G476 V477 G478 N479 Y484 Q485 I486 R487 H492 HIS HIS HIS

• Molecule 1: Cytochrome P450 2B4

Chain D: 68% 25% 5% •

MET ALA LYS LYS THR SER SER LYS G28 P31 P32 G33 P34 S35 P36 L37 P38 V39 L40 G41 N42 Q45 R48 K49 G50 L51 L52 R53 R57 L58 R59 E60 V68 Y69 V75 R85 E86 D90 F95 R98 I101 A102 V103 V104 I107 F108 I114

F115 R125 R126 R133 D134 F135 G136 M137 R140 S141 E144 R145 L153 L164 T168 L169 I174 I179 C180 S181 I182 V183 K186 D189 Y190 K191 L196 R197 L198 F202 S205 F206 S207 L208 S211 F212 S213 S214 Q215 F220 S221 G222 F223 L224

K225 Y226 F227 Q233 T234 Y235 L238 Q239 Q247 E250 L256 D257 P258 S259 N260 P261 Y268 L269 L270 S277 D278 P279 H285 Q286 N287 L288 I289 L290 T291 V292 L293 S294 L295 F296 F297 A298 G299 T302 T303 S304 T305 T306 L307 R308 Y309 L313 M314 R323

K345 Y348 V352 L359 G360 P364 F365 H369 T375 Q376 F377 R378 G379 Y380 V381 E387 V388 F389 P390 F402 F408 H412 N423 E424 M427 L431 L437 G438 E439 A442 R443 L446 F450 I468 D469 L470 T471 E474 V477 G478

N479 S483 R487 H492 HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	234.49Å 234.49Å 57.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	76.75 – 3.10 76.75 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (76.75-3.10) 97.7 (76.75-3.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 3.13Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.178 , 0.234 0.178 , 0.227	Depositor DCC
R_{free} test set	3169 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 19.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.459 for -h,-k,l 0.467 for h,-h-k,-l 0.460 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15302	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.91	0/3820	0.96	8/5173 (0.2%)
1	B	0.91	0/3826	0.97	8/5180 (0.2%)
1	C	0.94	1/3826 (0.0%)	0.96	7/5180 (0.1%)
1	D	0.95	2/3830 (0.1%)	0.96	6/5185 (0.1%)
All	All	0.93	3/15302 (0.0%)	0.96	29/20718 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	38	PRO	N-CD	5.31	1.55	1.47
1	D	258	PRO	N-CD	5.22	1.55	1.47
1	C	119	GLU	CG-CD	5.09	1.59	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	445	GLU	OE1-CD-OE2	-5.95	116.16	123.30
1	D	134	ASP	N-CA-C	5.88	126.88	111.00
1	B	400	ARG	CB-CA-C	5.87	122.15	110.40
1	C	259	SER	CB-CA-C	5.86	121.23	110.10
1	D	164	LEU	CB-CG-CD1	-5.83	101.09	111.00
1	B	259	SER	CB-CA-C	5.76	121.05	110.10
1	C	323	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	313	LEU	CB-CG-CD1	-5.68	101.34	111.00
1	B	260	ASN	N-CA-CB	-5.65	100.43	110.60
1	D	443	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	D	323	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	443	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	120	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	134	ASP	N-CA-C	5.50	125.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	260	ASN	N-CA-CB	-5.46	100.77	110.60
1	A	263	ASP	N-CA-CB	-5.41	100.87	110.60
1	D	323	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	257	ASP	CB-CA-C	5.33	121.06	110.40
1	A	78	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	165	LEU	CB-CG-CD1	-5.27	102.04	111.00
1	A	308	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	90	ASP	CB-CA-C	-5.18	100.03	110.40
1	C	58	LEU	CA-CB-CG	5.17	127.19	115.30
1	D	133	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	256	LEU	CB-CA-C	-5.15	100.42	110.20
1	A	134	ASP	N-CA-C	5.10	124.76	111.00
1	A	323	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	308	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	256	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3723	0	3722	113	0
1	B	3729	0	3733	109	0
1	C	3729	0	3733	117	0
1	D	3733	0	3737	121	0
2	A	43	0	30	6	0
2	B	43	0	30	9	0
2	C	43	0	30	5	0
2	D	43	0	30	7	0
3	A	21	0	16	6	0
3	B	21	0	16	8	0
3	C	21	0	16	8	0
3	D	21	0	16	8	0
4	A	30	0	0	2	0
4	B	35	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	32	0	0	1	0
4	D	35	0	0	5	0
All	All	15302	0	15109	472	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (472) 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:D:307:LEU:HD23	1:D:450[A]:PHE:CE2	1.52	1.45
1:C:307:LEU:HD23	1:C:450[A]:PHE:CE1	1.59	1.38
1:C:122:ARG:HD2	4:C:1160:HOH:O	1.35	1.27
1:D:75:VAL:HG12	1:D:387:GLU:HB3	1.16	1.14
1:A:297:PHE:HB3	3:A:501:CGE:HAJA	1.30	1.11
1:B:297:PHE:HB3	3:B:501:CGE:HAJA	1.33	1.10
1:B:75:VAL:HG12	1:B:387:GLU:HB3	1.28	1.08
1:D:125:ARG:HG3	1:D:437:LEU:HD11	1.39	1.03
1:A:137:MET:N	1:A:145:ARG:HH12	1.56	1.03
1:C:307:LEU:HD23	1:C:450[A]:PHE:CD1	1.91	1.03
1:D:126:ARG:HG3	1:D:126:ARG:HH11	1.20	1.02
1:D:307:LEU:CD2	1:D:450[A]:PHE:CE2	2.44	1.01
1:D:220:PHE:HB2	1:D:224:LEU:HD12	1.44	0.99
1:C:220:PHE:HB2	1:C:224:LEU:HD12	1.44	0.97
1:D:137:MET:H	1:D:145:ARG:HH12	1.06	0.96
1:A:31:PRO:HA	1:A:380:TYR:CE1	2.01	0.96
1:C:297:PHE:HB3	3:C:501:CGE:HAJA	1.47	0.95
1:B:31:PRO:HA	1:B:380:TYR:CE1	2.02	0.94
1:A:256:LEU:HD12	1:A:257:ASP:H	1.33	0.94
1:C:256:LEU:HD12	1:C:257:ASP:H	1.29	0.94
1:D:137:MET:N	1:D:145:ARG:HH12	1.67	0.93
1:B:137:MET:N	1:B:145:ARG:HH12	1.67	0.93
1:A:75:VAL:HG12	1:A:387:GLU:HB3	1.50	0.92
1:D:305:THR:HG22	4:D:1095:HOH:O	1.68	0.92
1:C:307:LEU:CD2	1:C:450[A]:PHE:CE1	2.53	0.90
1:A:183:VAL:HG11	1:A:292:VAL:HG13	1.52	0.90
2:D:500:HEM:HMB1	2:D:500:HEM:HBB2	1.52	0.90
1:D:31:PRO:HA	1:D:380:TYR:CE1	2.06	0.90
1:D:86:GLU:HA	1:D:90:ASP:OD2	1.71	0.90
1:B:220:PHE:HB2	1:B:224:LEU:HD12	1.52	0.89
1:C:75:VAL:HG12	1:C:387:GLU:HB3	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:LEU:HD23	1:D:450[A]:PHE:CD2	2.05	0.88
1:C:307:LEU:CD2	1:C:450[A]:PHE:CD1	2.57	0.88
1:A:220:PHE:HB2	1:A:224:LEU:HD12	1.53	0.87
1:D:297:PHE:HB3	3:D:501:CGE:HAJA	1.56	0.87
1:C:307:LEU:HD23	1:C:450[A]:PHE:HE1	1.04	0.86
1:D:220:PHE:HB2	1:D:224:LEU:CD1	2.03	0.86
1:B:210:SER:HA	4:B:1078:HOH:O	1.74	0.86
1:A:137:MET:H	1:A:145:ARG:HH12	1.18	0.85
1:A:210:SER:HA	4:A:1071:HOH:O	1.74	0.85
1:D:49:LYS:HE2	1:D:53:ARG:HD2	1.58	0.85
1:B:75:VAL:CG1	1:B:387:GLU:HB3	2.07	0.84
1:D:125:ARG:HG3	1:D:437:LEU:CD1	2.08	0.84
1:D:286:GLN:HG3	4:D:1168:HOH:O	1.76	0.83
1:C:179:ILE:HG21	1:C:296:PHE:HA	1.59	0.83
1:D:75:VAL:HG12	1:D:387:GLU:CB	2.04	0.83
1:B:86:GLU:HA	1:B:90:ASP:OD2	1.78	0.83
1:C:314:MET:HE2	1:C:314:MET:HA	1.59	0.83
1:D:307:LEU:HD23	1:D:450[A]:PHE:HE2	0.99	0.83
1:C:31:PRO:HA	1:C:380:TYR:CE1	2.15	0.82
1:A:477:VAL:HG13	3:A:501:CGE:HAA	1.63	0.81
1:C:137:MET:N	1:C:145:ARG:HH12	1.78	0.80
1:D:256:LEU:HD12	1:D:257:ASP:H	1.45	0.80
1:A:145:ARG:HD3	1:A:181:SER:OG	1.82	0.79
1:A:86:GLU:O	1:A:90:ASP:HB2	1.83	0.79
1:D:307:LEU:CD2	1:D:450[A]:PHE:CD2	2.64	0.79
1:C:86:GLU:HA	1:C:90:ASP:OD2	1.81	0.79
1:D:51:LEU:HD12	1:D:215:GLN:HG2	1.63	0.78
1:C:477:VAL:HG13	3:C:501:CGE:HAA	1.62	0.78
2:C:500:HEM:ND	3:C:501:CGE:HAD	1.99	0.78
1:D:307:LEU:CD2	1:D:450[A]:PHE:HE2	1.89	0.78
1:B:125:ARG:HG3	1:B:437:LEU:HD11	1.64	0.77
1:B:120:ARG:HD3	1:B:287:ASN:HD21	1.49	0.77
1:A:86:GLU:HA	1:A:90:ASP:OD2	1.85	0.76
1:D:179:ILE:HG21	1:D:296:PHE:HA	1.67	0.76
1:C:314:MET:HA	1:C:314:MET:CE	2.16	0.76
1:B:206:PHE:CD2	1:B:301:GLU:HG2	2.20	0.76
1:A:125:ARG:CZ	1:A:437:LEU:HD12	2.17	0.74
1:A:122:ARG:HD2	4:A:1130:HOH:O	1.88	0.74
1:D:126:ARG:HG3	1:D:126:ARG:NH1	1.98	0.73
1:D:227:PHE:N	1:D:227:PHE:HD1	1.85	0.73
2:D:500:HEM:HBB2	2:D:500:HEM:CMB	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:LEU:O	1:C:450[A]:PHE:HB2	1.89	0.72
1:A:137:MET:N	1:A:145:ARG:NH1	2.33	0.72
1:D:220:PHE:CB	1:D:224:LEU:HD12	2.18	0.72
2:B:500:HEM:C4D	3:B:501:CGE:HAD	2.24	0.72
1:B:402:PHE:CE1	1:B:423:ASN:ND2	2.58	0.71
3:D:501:CGE:CAH	3:D:501:CGE:HAK	2.20	0.71
1:C:268:TYR:CE1	1:C:288:LEU:HB2	2.26	0.71
1:B:449:PHE:O	1:B:453:ILE:HG13	1.91	0.71
1:D:137:MET:H	1:D:145:ARG:NH1	1.84	0.71
1:A:80:GLY:O	1:A:84:ILE:HD12	1.91	0.70
1:D:126:ARG:HH11	1:D:126:ARG:CG	2.01	0.70
1:B:125:ARG:CZ	1:B:437:LEU:HD12	2.22	0.70
1:A:70:LEU:HB3	1:A:219:LEU:HD12	1.72	0.70
1:D:268:TYR:CE1	1:D:288:LEU:HB2	2.27	0.70
1:D:227:PHE:N	1:D:227:PHE:CD1	2.58	0.69
1:B:137:MET:H	1:B:145:ARG:HH12	1.38	0.69
1:B:114:ILE:HD12	1:B:294:SER:HB3	1.73	0.69
1:D:125:ARG:CG	1:D:437:LEU:HD11	2.21	0.69
1:A:125:ARG:HG3	1:A:437:LEU:HD11	1.75	0.69
1:B:469:ASP:OD2	1:B:471:THR:HB	1.93	0.69
1:A:125:ARG:HG3	1:A:437:LEU:CD1	2.24	0.68
1:A:402:PHE:CE1	1:A:423:ASN:ND2	2.61	0.68
1:C:86:GLU:O	1:C:90:ASP:HB2	1.94	0.68
1:C:70:LEU:HD22	1:C:219:LEU:HD11	1.76	0.68
1:C:469:ASP:OD2	1:C:471:THR:HB	1.94	0.68
2:A:500:HEM:ND	3:A:501:CGE:HAD	2.09	0.67
1:B:49:LYS:HB3	1:B:53:ARG:HG2	1.76	0.67
1:A:469:ASP:OD2	1:A:471:THR:HB	1.95	0.67
1:B:86:GLU:O	1:B:90:ASP:HB2	1.94	0.67
1:D:57:ARG:O	1:D:60:GLU:HG2	1.95	0.67
1:C:307:LEU:CD2	1:C:450[A]:PHE:HD1	2.08	0.66
2:C:500:HEM:C4D	3:C:501:CGE:HAD	2.29	0.66
1:D:75:VAL:CG1	1:D:387:GLU:HB3	2.10	0.66
1:D:31:PRO:HA	1:D:380:TYR:CD1	2.31	0.66
1:A:80:GLY:O	1:A:84:ILE:CD1	2.44	0.66
1:B:98:ARG:HG2	1:B:115:PHE:HA	1.77	0.66
1:B:369:HIS:HE1	2:B:500:HEM:O2A	1.78	0.65
1:C:136:GLY:C	1:C:145:ARG:HH12	1.99	0.65
1:D:32:PRO:HD3	1:D:380:TYR:CE1	2.31	0.65
1:A:137:MET:H	1:A:145:ARG:NH1	1.92	0.65
1:B:233:GLN:OE1	1:B:233:GLN:HA	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:MET:N	1:C:145:ARG:NH1	2.45	0.64
1:D:183:VAL:HG11	1:D:292:VAL:HG13	1.80	0.63
1:B:239:GLN:OE1	1:B:239:GLN:HA	1.96	0.63
1:A:374:ASP:OD1	1:A:383:PRO:HA	1.99	0.63
1:B:427:MET:HE2	1:B:431:LEU:HD11	1.80	0.63
1:C:220:PHE:HB2	1:C:224:LEU:CD1	2.23	0.63
1:D:250:GLU:HA	1:D:250:GLU:OE2	1.99	0.63
1:A:132:MET:HG2	1:A:182:ILE:HG21	1.79	0.62
1:D:137:MET:N	1:D:145:ARG:NH1	2.43	0.62
3:C:501:CGE:CAH	3:C:501:CGE:HAK	2.29	0.62
1:C:179:ILE:HG13	1:C:299:GLY:HA3	1.81	0.62
1:B:129:LEU:HD23	1:B:437:LEU:HG	1.80	0.62
1:D:134:ASP:OD1	1:D:134:ASP:C	2.38	0.61
1:C:32:PRO:HD3	1:C:380:TYR:CE1	2.35	0.61
1:D:169:LEU:HB2	4:D:1055:HOH:O	2.01	0.61
1:A:268:TYR:CE1	1:A:288:LEU:HB2	2.36	0.61
1:A:314:MET:HA	1:A:314:MET:HE2	1.83	0.60
1:B:179:ILE:HG21	1:B:296:PHE:HA	1.82	0.60
1:B:114:ILE:HD12	1:B:294:SER:CB	2.31	0.60
1:B:128:SER:HB3	1:B:437:LEU:HD21	1.82	0.60
1:B:183:VAL:HG11	1:B:292:VAL:HG13	1.83	0.60
1:C:114:ILE:HD12	1:C:294:SER:HB3	1.83	0.60
1:B:179:ILE:HG22	1:B:180:CYS:N	2.16	0.60
1:C:222:GLY:HA2	1:C:225:LYS:HE3	1.84	0.59
1:A:101:ILE:HG22	1:A:103:VAL:HG23	1.85	0.59
1:D:427:MET:HE2	1:D:431:LEU:HD11	1.84	0.59
1:D:95:PHE:O	1:D:369:HIS:HD2	1.86	0.59
1:D:314:MET:HE2	1:D:450[B]:PHE:HZ	1.67	0.59
1:A:175:THR:HG22	1:A:445:GLU:OE1	2.03	0.58
1:D:323:ARG:HB2	1:D:348:TYR:CE2	2.37	0.58
1:A:314:MET:HA	1:A:314:MET:CE	2.33	0.58
1:D:164:LEU:HD23	1:D:487:ARG:HB3	1.86	0.58
2:B:500:HEM:ND	3:B:501:CGE:HAD	2.19	0.58
1:D:446:LEU:O	1:D:450[A]:PHE:HB2	2.04	0.58
1:B:61:LYS:HB3	1:B:62:TYR:CD2	2.39	0.58
1:C:132:MET:HG2	1:C:182:ILE:HG21	1.85	0.58
1:D:369:HIS:HE1	2:D:500:HEM:O2A	1.86	0.58
1:C:183:VAL:HG11	1:C:292:VAL:HG13	1.84	0.58
1:D:34:PRO:HB2	1:D:45:GLN:OE1	2.04	0.58
1:C:108:PHE:HA	1:C:290:LEU:HD13	1.85	0.57
1:C:256:LEU:HD12	1:C:257:ASP:N	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:ASP:OD2	1:D:471:THR:HB	2.03	0.57
2:D:500:HEM:ND	3:D:501:CGE:HAD	2.18	0.57
1:C:36:PRO:HA	1:C:41:GLY:O	2.05	0.57
1:C:114:ILE:CD1	1:C:294:SER:HB3	2.34	0.57
1:C:205:SER:O	1:C:209:ILE:HG13	2.04	0.57
1:C:34:PRO:HG2	1:C:42:ASN:ND2	2.20	0.57
3:A:501:CGE:CAH	3:A:501:CGE:HAK	2.35	0.57
1:D:126:ARG:NH1	1:D:126:ARG:CG	2.62	0.57
1:D:309:TYR:CE2	1:D:360:GLY:HA2	2.39	0.57
1:A:256:LEU:HD12	1:A:257:ASP:N	2.13	0.57
1:B:98:ARG:NH2	2:B:500:HEM:O2D	2.32	0.57
1:D:297:PHE:HD1	3:D:501:CGE:HAKA	1.69	0.57
1:C:95:PHE:O	1:C:369:HIS:HD2	1.87	0.57
1:B:205:SER:O	1:B:209:ILE:HG13	2.05	0.56
1:A:309:TYR:CE2	1:A:360:GLY:HA2	2.40	0.56
1:C:164:LEU:HD23	1:C:487:ARG:HB3	1.87	0.56
1:B:31:PRO:HA	1:B:380:TYR:CD1	2.41	0.56
1:B:175:THR:HG22	1:B:445:GLU:OE1	2.04	0.56
1:A:49:LYS:HE3	1:A:53:ARG:HG2	1.88	0.56
1:A:434:ARG:HB3	2:A:500:HEM:O1A	2.06	0.56
3:B:501:CGE:CAH	3:B:501:CGE:HAK	2.36	0.56
1:B:111:TYR:HB2	1:B:290:LEU:HD12	1.88	0.56
1:D:36:PRO:HA	1:D:41:GLY:O	2.05	0.56
1:D:140:ARG:NH2	1:D:145:ARG:HG2	2.20	0.56
1:A:179:ILE:HG21	1:A:296:PHE:HA	1.88	0.56
1:C:114:ILE:HD12	1:C:294:SER:CB	2.35	0.56
1:B:125:ARG:HG3	1:B:437:LEU:CD1	2.35	0.55
1:C:314:MET:CE	1:C:314:MET:CA	2.85	0.55
1:B:355:GLU:HG3	1:B:408:PHE:CE1	2.41	0.55
1:A:32:PRO:HD3	1:A:380:TYR:OH	2.07	0.55
1:C:38:PRO:O	1:C:39:VAL:HB	2.06	0.55
1:B:220:PHE:HB2	1:B:224:LEU:CD1	2.31	0.55
1:C:307:LEU:HA	1:C:450[A]:PHE:HE1	1.70	0.55
1:D:86:GLU:O	1:D:90:ASP:HB2	2.07	0.55
1:D:98:ARG:HG2	1:D:115:PHE:HA	1.87	0.55
1:A:51:LEU:HD12	1:A:215:GLN:HG2	1.89	0.55
1:B:446:LEU:O	1:B:450[A]:PHE:HD2	1.90	0.55
1:D:314:MET:HE1	1:D:352:VAL:HG11	1.89	0.55
1:D:258:PRO:HA	1:D:270:LEU:HD21	1.89	0.54
1:A:125:ARG:CG	1:A:437:LEU:HD11	2.37	0.54
1:C:31:PRO:HA	1:C:380:TYR:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:PHE:CE1	1:C:423:ASN:ND2	2.76	0.54
1:C:136:GLY:CA	1:C:145:ARG:HH12	2.21	0.54
1:C:103:VAL:HG21	1:C:214:SER:HB3	1.88	0.54
1:C:477:VAL:CG1	3:C:501:CGE:HAA	2.35	0.53
1:D:37:LEU:O	1:D:38:PRO:C	2.47	0.53
1:C:73:ARG:HG3	1:C:73:ARG:HH11	1.72	0.53
1:C:297:PHE:HD2	1:C:297:PHE:O	1.92	0.53
1:C:384:LYS:HG2	1:C:385:ASN:HD22	1.74	0.53
1:D:107:ILE:HD12	1:D:238:LEU:HB2	1.90	0.53
1:A:34:PRO:HB2	1:A:45:GLN:OE1	2.09	0.53
1:A:361:ASP:O	1:A:361:ASP:CG	2.46	0.53
1:D:323:ARG:HD3	4:D:1112:HOH:O	2.09	0.53
1:A:297:PHE:CB	3:A:501:CGE:HAJA	2.21	0.53
1:B:145:ARG:HD3	1:B:181:SER:OG	2.08	0.53
1:A:178:ILE:O	1:A:182:ILE:HG13	2.09	0.53
1:A:403:GLU:HG3	1:B:403:GLU:HG3	1.91	0.53
1:A:241:ILE:O	1:A:245:ILE:HG13	2.09	0.53
1:A:460:ALA:HB3	1:A:487:ARG:HG2	1.92	0.52
1:C:297:PHE:CB	3:C:501:CGE:HAJA	2.29	0.52
1:A:31:PRO:HA	1:A:380:TYR:HE1	1.71	0.52
1:A:70:LEU:HB3	1:A:219:LEU:CD1	2.38	0.52
1:C:125:ARG:HG3	1:C:437:LEU:CD1	2.39	0.52
1:A:32:PRO:HD3	1:A:380:TYR:CE1	2.45	0.52
1:A:220:PHE:HB2	1:A:224:LEU:CD1	2.32	0.52
1:C:136:GLY:HA3	1:C:145:ARG:HH12	1.74	0.52
1:B:98:ARG:HB2	1:B:434:ARG:NH1	2.24	0.52
1:C:140:ARG:HH21	1:C:145:ARG:HG2	1.74	0.52
1:B:427:MET:CE	1:B:431:LEU:HD11	2.39	0.52
1:A:98:ARG:HG3	1:A:99:GLY:O	2.09	0.52
1:B:172:HIS:HE1	1:B:203:PHE:CD1	2.27	0.52
1:C:129:LEU:HD23	1:C:437:LEU:HG	1.92	0.52
1:D:314:MET:CE	1:D:352:VAL:HG11	2.41	0.51
1:D:314:MET:CE	1:D:450[B]:PHE:HZ	2.22	0.51
1:A:98:ARG:HG2	1:A:115:PHE:HA	1.92	0.51
1:B:51:LEU:HB2	1:B:215:GLN:HG2	1.93	0.50
1:B:114:ILE:CD1	1:B:294:SER:HB3	2.40	0.50
1:A:129:LEU:CD2	1:A:437:LEU:HG	2.40	0.50
1:C:51:LEU:HD22	1:C:55:PHE:CZ	2.46	0.50
1:D:168:THR:HA	1:D:308:ARG:HD2	1.94	0.50
1:D:314:MET:HE2	1:D:450[B]:PHE:CZ	2.45	0.50
1:A:200:ASP:OD1	1:A:204:GLN:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:SER:CB	2:A:500:HEM:HBA1	2.42	0.50
1:A:239:GLN:HA	1:A:239:GLN:OE1	2.11	0.50
1:D:285:HIS:O	1:D:289:ILE:HG12	2.12	0.50
1:D:314:MET:HE1	1:D:352:VAL:CG1	2.42	0.50
1:B:430:SER:HB3	2:B:500:HEM:HBA1	1.94	0.50
1:D:477:VAL:HG13	3:D:501:CGE:HAA	1.94	0.50
1:D:298:ALA:HA	3:D:501:CGE:HAK	1.92	0.49
1:C:256:LEU:CD1	1:C:257:ASP:H	2.14	0.49
1:B:268:TYR:CZ	1:B:288:LEU:HB2	2.47	0.49
1:A:98:ARG:HB2	1:A:434:ARG:NH1	2.27	0.49
1:D:101:ILE:HB	1:D:104:VAL:HG22	1.94	0.49
1:D:107:ILE:HD11	1:D:235:TYR:HA	1.95	0.49
1:B:268:TYR:CE1	1:B:288:LEU:HB2	2.48	0.49
1:A:233:GLN:HA	1:A:233:GLN:OE1	2.12	0.49
1:A:415:ASP:O	1:A:416:ALA:C	2.51	0.49
1:C:310:GLY:O	1:C:314:MET:HG2	2.13	0.49
1:A:95:PHE:O	1:A:369:HIS:HD2	1.96	0.49
1:B:100:LYS:HD2	1:B:105:ASP:CG	2.32	0.49
1:C:32:PRO:HD3	1:C:380:TYR:CZ	2.48	0.49
1:A:125:ARG:CZ	1:A:437:LEU:CD1	2.90	0.48
1:C:98:ARG:HG3	1:C:99:GLY:O	2.13	0.48
1:B:132:MET:HG2	1:B:182:ILE:HG21	1.94	0.48
1:B:206:PHE:CD2	1:B:301:GLU:CG	2.94	0.48
2:D:500:HEM:HMB1	2:D:500:HEM:CBB	2.35	0.48
1:A:430:SER:HB3	2:A:500:HEM:HBA1	1.94	0.48
1:C:208:LEU:HD22	1:C:230:THR:HB	1.95	0.48
1:C:361:ASP:CG	1:C:361:ASP:O	2.51	0.48
1:C:307:LEU:HD21	1:C:450[A]:PHE:HD1	1.79	0.48
1:A:168:THR:HA	1:A:308:ARG:HD2	1.95	0.48
1:A:299:GLY:HA2	2:A:500:HEM:HMC3	1.96	0.48
1:A:376:GLN:HA	1:A:380:TYR:O	2.12	0.48
1:D:402:PHE:CE1	1:D:423:ASN:ND2	2.82	0.48
1:B:364:PRO:HG3	1:B:479:ASN:ND2	2.28	0.48
1:A:183:VAL:HA	1:A:264:PHE:HB3	1.96	0.48
1:A:317:TYR:HB3	1:A:320:VAL:HG23	1.96	0.48
1:B:34:PRO:HB2	1:B:45:GLN:OE1	2.14	0.48
1:B:179:ILE:HG21	1:B:296:PHE:CD1	2.49	0.48
1:A:310:GLY:O	1:A:314:MET:HG2	2.15	0.47
1:A:471:THR:HA	1:A:472:PRO:HD3	1.72	0.47
1:D:299:GLY:HA2	2:D:500:HEM:HMC3	1.96	0.47
1:C:183:VAL:HA	1:C:264:PHE:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ASN:ND2	1:C:171:PHE:CE2	2.80	0.47
1:D:134:ASP:OD1	1:D:134:ASP:O	2.33	0.47
1:C:91:GLN:HB3	1:C:94:ALA:HB3	1.96	0.47
1:A:114:ILE:CD1	1:A:294:SER:HB3	2.44	0.47
1:B:95:PHE:O	1:B:369:HIS:HD2	1.97	0.47
1:B:108:PHE:HA	1:B:290:LEU:HD13	1.96	0.47
1:B:128:SER:HB3	1:B:437:LEU:CD2	2.44	0.47
1:C:299:GLY:HA2	2:C:500:HEM:HMC2	1.95	0.47
1:D:38:PRO:O	1:D:39:VAL:HB	2.14	0.47
1:D:239:GLN:HA	1:D:239:GLN:OE1	2.14	0.47
1:D:313:LEU:HD13	1:D:408:PHE:CD1	2.50	0.47
1:B:355:GLU:CD	1:B:409:ASN:O	2.54	0.47
1:B:45:GLN:HE21	1:B:45:GLN:N	2.13	0.47
1:C:128:SER:HB2	1:C:437:LEU:HD21	1.96	0.47
1:A:174:ILE:O	1:A:178:ILE:HG12	2.15	0.46
1:A:335:HIS:HB2	1:C:341:ASP:OD2	2.15	0.46
1:A:364:PRO:HG3	1:A:479:ASN:ND2	2.31	0.46
1:B:137:MET:HB3	1:B:145:ARG:NH1	2.30	0.46
1:D:49:LYS:CE	1:D:53:ARG:HD2	2.38	0.46
1:D:45:GLN:HE21	1:D:45:GLN:N	2.13	0.46
1:D:364:PRO:HG3	1:D:479:ASN:ND2	2.30	0.46
1:C:283:PHE:CD1	1:C:283:PHE:N	2.83	0.46
1:B:190:TYR:O	1:B:196:LEU:HD21	2.15	0.46
2:B:500:HEM:CHA	3:B:501:CGE:HAD	2.46	0.46
1:C:323:ARG:HB2	1:C:348:TYR:CE2	2.51	0.46
1:D:85:ARG:NH2	1:D:424:GLU:O	2.46	0.46
1:D:114:ILE:HD12	1:D:294:SER:HB3	1.97	0.46
1:B:153:LEU:HD22	1:B:174:ILE:HD13	1.98	0.46
1:B:200:ASP:CG	1:B:204:GLN:HE21	2.19	0.46
1:B:209:ILE:HD13	3:B:501:CGE:HAI	1.98	0.46
1:B:454:LEU:HA	1:B:454:LEU:HD23	1.70	0.46
1:A:129:LEU:HD23	1:A:437:LEU:HG	1.97	0.46
1:A:179:ILE:HG21	1:A:296:PHE:HD1	1.80	0.46
1:C:338:PRO:HD3	1:C:455:GLN:OE1	2.16	0.46
1:B:164:LEU:HD21	1:B:462:PRO:HD3	1.98	0.46
1:C:47:ASP:OD2	1:C:57:ARG:HD3	2.16	0.46
1:A:136:GLY:HA3	1:A:145:ARG:HH22	1.81	0.46
1:B:320:VAL:O	1:B:321:THR:C	2.52	0.46
1:D:365:PHE:CE1	1:D:477:VAL:HG23	2.51	0.46
1:A:108:PHE:HA	1:A:290:LEU:HD13	1.97	0.46
1:B:415:ASP:OD1	1:B:415:ASP:C	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:PHE:CZ	1:C:267:VAL:HG12	2.51	0.46
1:C:132:MET:HE1	1:C:437:LEU:HD23	1.98	0.46
1:D:323:ARG:CD	4:D:1112:HOH:O	2.63	0.46
1:C:189:ASP:OD2	1:C:189:ASP:C	2.54	0.45
1:B:175:THR:OG1	1:B:304:SER:HB3	2.17	0.45
1:C:210:SER:HB2	1:C:476:GLY:HA3	1.97	0.45
1:D:307:LEU:HD21	1:D:450[A]:PHE:CD2	2.48	0.45
1:C:137:MET:H	1:C:145:ARG:HH12	1.63	0.45
1:D:205:SER:HA	1:D:208:LEU:HD12	1.97	0.45
2:A:500:HEM:C4D	3:A:501:CGE:HAD	2.51	0.45
1:D:423:ASN:OD1	1:D:423:ASN:C	2.55	0.45
1:A:49:LYS:HE3	1:A:49:LYS:HB2	1.64	0.45
1:C:355:GLU:HG3	1:C:408:PHE:CD1	2.52	0.45
1:D:108:PHE:HA	1:D:290:LEU:HD13	1.99	0.45
1:A:423:ASN:C	1:A:423:ASN:OD1	2.55	0.45
1:B:134:ASP:OD2	1:B:134:ASP:C	2.55	0.45
1:B:435:ILE:O	1:B:436:CYS:C	2.54	0.45
1:C:186:LYS:HG2	1:C:187:ARG:N	2.32	0.45
1:D:179:ILE:HD12	1:D:179:ILE:HG23	1.81	0.45
1:D:179:ILE:HG13	1:D:299:GLY:HA3	1.98	0.45
1:D:256:LEU:CD1	1:D:257:ASP:H	2.21	0.45
1:A:156:GLU:HG2	1:A:170:LEU:HD21	1.98	0.45
1:B:395:ALA:HA	1:B:398:ASP:HB2	1.98	0.45
1:C:241:ILE:O	1:C:245:ILE:HG13	2.17	0.45
1:D:359:LEU:HD12	1:D:359:LEU:HA	1.80	0.45
1:B:310:GLY:O	1:B:314:MET:HG2	2.17	0.45
1:B:324:VAL:HG13	1:B:349:THR:OG1	2.17	0.45
1:C:309:TYR:CE2	1:C:360:GLY:HA2	2.52	0.45
1:C:486:ILE:HG23	1:C:486:ILE:O	2.17	0.45
1:B:32:PRO:HD3	1:B:380:TYR:OH	2.17	0.44
1:C:179:ILE:HD12	1:C:179:ILE:HG23	1.71	0.44
1:B:252:HIS:CB	1:B:265:ILE:HG21	2.47	0.44
1:B:365:PHE:CE1	1:B:477:VAL:HG23	2.52	0.44
1:B:477:VAL:HG13	3:B:501:CGE:HAA	1.99	0.44
1:C:101:ILE:HD11	1:C:368:PRO:HD3	1.99	0.44
1:C:477:VAL:HG13	3:C:501:CGE:CAA	2.40	0.44
1:D:202:PHE:CE1	1:D:297:PHE:CD2	3.05	0.44
1:D:277:SER:O	1:D:279:PRO:HD3	2.18	0.44
1:A:101:ILE:HB	1:A:104:VAL:HG22	1.99	0.44
1:A:114:ILE:HD12	1:A:294:SER:CB	2.47	0.44
1:B:174:ILE:O	1:B:178:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ILE:O	1:B:182:ILE:HG13	2.17	0.44
1:D:260:ASN:HA	1:D:261:PRO:HD2	1.69	0.44
1:A:427:MET:HE2	1:A:431:LEU:HD11	2.00	0.44
1:B:371:VAL:HG21	1:B:382:ILE:HG22	1.98	0.44
1:A:126:ARG:HG3	1:A:126:ARG:HH11	1.81	0.44
1:C:105:ASP:N	1:C:106:PRO:HD2	2.32	0.44
1:C:133:ARG:H	1:C:133:ARG:HG3	1.52	0.44
1:D:268:TYR:CZ	1:D:288:LEU:HB2	2.52	0.44
1:D:297:PHE:CD1	3:D:501:CGE:HAKA	2.52	0.44
1:D:307:LEU:HA	1:D:450[A]:PHE:HE2	1.83	0.44
1:D:31:PRO:HA	1:D:380:TYR:HE1	1.73	0.44
1:B:170:LEU:HD23	1:B:170:LEU:HA	1.84	0.44
1:B:183:VAL:HA	1:B:264:PHE:HB3	2.00	0.44
1:B:204:GLN:O	1:B:208:LEU:HG	2.18	0.44
1:C:239:GLN:OE1	1:C:239:GLN:HA	2.18	0.43
1:A:114:ILE:HD12	1:A:294:SER:HB3	2.00	0.43
1:B:471:THR:HA	1:B:472:PRO:HD3	1.83	0.43
1:C:140:ARG:HH21	1:C:145:ARG:CG	2.31	0.43
1:C:364:PRO:HG3	1:C:479:ASN:ND2	2.33	0.43
1:A:365:PHE:CE1	1:A:477:VAL:HG23	2.52	0.43
1:C:310:GLY:HA3	1:C:450[A]:PHE:HZ	1.84	0.43
1:B:179:ILE:HG21	1:B:296:PHE:HD1	1.84	0.43
1:A:268:TYR:CG	1:A:288:LEU:HD13	2.53	0.43
1:C:45:GLN:N	1:C:45:GLN:HE21	2.16	0.43
1:B:256:LEU:HG	1:B:257:ASP:N	2.33	0.43
1:C:192:ASP:OD1	1:C:192:ASP:C	2.56	0.43
1:D:222:GLY:HA2	1:D:225:LYS:HE3	2.01	0.43
1:A:132:MET:HE2	1:A:132:MET:HB2	1.59	0.43
1:A:179:ILE:CG2	1:A:296:PHE:HD1	2.31	0.43
1:B:37:LEU:O	1:B:38:PRO:C	2.57	0.43
1:B:297:PHE:CB	3:B:501:CGE:HAJA	2.24	0.43
1:C:356:ILE:O	1:C:360:GLY:N	2.52	0.43
1:D:190:TYR:O	1:D:196:LEU:HD21	2.18	0.43
2:D:500:HEM:C4D	3:D:501:CGE:HAD	2.54	0.43
1:D:268:TYR:CG	1:D:288:LEU:HD13	2.54	0.43
1:A:278:ASP:HA	1:A:279:PRO:HD2	1.85	0.42
1:B:172:HIS:HD2	1:B:304:SER:OG	2.02	0.42
1:D:68:VAL:HG22	1:D:69:TYR:H	1.83	0.42
1:B:53:ARG:HE	1:B:53:ARG:HB2	1.65	0.42
1:D:95:PHE:HE1	1:D:388:VAL:HG21	1.83	0.42
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:SER:OG	1:D:144:GLU:HB2	2.20	0.42
1:A:179:ILE:HD13	1:A:179:ILE:HA	1.48	0.42
1:A:35:SER:HA	1:A:36:PRO:HD3	1.93	0.42
1:C:125:ARG:HG3	1:C:437:LEU:HD13	2.00	0.42
1:B:70:LEU:HB3	1:B:219:LEU:HD12	2.02	0.42
1:B:265:ILE:HG22	1:B:266:ASP:N	2.35	0.42
1:B:341:ASP:OD1	1:B:341:ASP:C	2.58	0.42
1:C:269:LEU:O	1:C:272:MET:HB2	2.19	0.42
1:B:312:LEU:O	1:B:315:LEU:HB2	2.19	0.42
1:D:32:PRO:HD3	1:D:380:TYR:HE1	1.78	0.42
1:A:310:GLY:HA2	1:A:356:ILE:HD13	2.01	0.42
1:A:415:ASP:O	1:A:417:ASN:N	2.53	0.42
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.79	0.42
1:B:125:ARG:CZ	1:B:437:LEU:CD1	2.94	0.42
1:B:299:GLY:HA2	2:B:500:HEM:HMC3	2.02	0.42
1:A:70:LEU:HD22	1:A:219:LEU:HD11	2.01	0.42
1:B:434:ARG:HB3	2:B:500:HEM:O1A	2.20	0.42
1:C:403:GLU:OE2	1:D:412:HIS:HD2	2.03	0.42
1:A:200:ASP:O	1:A:204:GLN:HB2	2.19	0.41
1:A:314:MET:CE	1:A:314:MET:CA	2.98	0.41
1:C:183:VAL:O	1:C:265:ILE:HG12	2.20	0.41
1:A:403:GLU:N	1:B:403:GLU:OE2	2.47	0.41
1:C:70:LEU:HB3	1:C:219:LEU:HD12	2.02	0.41
1:C:434:ARG:HB3	2:C:500:HEM:O1A	2.20	0.41
1:A:32:PRO:HD3	1:A:380:TYR:CZ	2.55	0.41
1:A:365:PHE:HE1	1:A:477:VAL:HG23	1.85	0.41
1:B:355:GLU:HG3	1:B:408:PHE:CD1	2.55	0.41
1:C:220:PHE:O	1:C:224:LEU:HD12	2.20	0.41
1:D:307:LEU:HD21	1:D:450[A]:PHE:HD2	1.84	0.41
1:B:369:HIS:CE1	2:B:500:HEM:O2A	2.67	0.41
1:A:295:LEU:HD23	1:A:295:LEU:HA	1.90	0.41
1:B:138:GLY:O	1:B:140:ARG:HG3	2.20	0.41
1:D:439:GLU:HG3	1:D:443:ARG:HD3	2.03	0.41
1:A:175:THR:OG1	1:A:304:SER:HB3	2.20	0.41
1:A:268:TYR:CZ	1:A:288:LEU:HB2	2.54	0.41
1:C:297:PHE:C	1:C:297:PHE:CD2	2.94	0.41
1:C:454:LEU:HA	1:C:454:LEU:HD23	1.56	0.41
1:D:95:PHE:CE1	1:D:388:VAL:HG21	2.56	0.41
1:D:153:LEU:HD22	1:D:174:ILE:HD13	2.02	0.41
1:D:307:LEU:HA	1:D:450[A]:PHE:CE2	2.56	0.41
1:A:125:ARG:HG3	1:A:437:LEU:HD13	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:THR:HG21	1:A:445:GLU:CD	2.41	0.41
1:C:313:LEU:HD23	1:C:313:LEU:HA	1.87	0.41
1:C:175:THR:HG22	1:C:445:GLU:OE1	2.19	0.41
1:D:37:LEU:O	1:D:38:PRO:O	2.39	0.41
1:C:136:GLY:HA3	1:C:145:ARG:NH1	2.35	0.41
1:C:180:CYS:SG	1:C:296:PHE:CE1	3.14	0.41
1:C:313:LEU:HD13	1:C:408:PHE:CD1	2.56	0.41
1:D:179:ILE:HA	1:D:179:ILE:HD13	1.65	0.41
1:D:202:PHE:HE1	1:D:297:PHE:CD2	2.38	0.41
1:A:179:ILE:CG2	1:A:296:PHE:CD1	3.04	0.41
1:A:414:LEU:O	1:A:421:LYS:HE2	2.20	0.41
1:C:44:LEU:C	1:C:45:GLN:HE21	2.25	0.41
1:C:295:LEU:HD23	1:C:295:LEU:HA	1.81	0.41
1:A:80:GLY:O	1:A:84:ILE:HD13	2.18	0.40
1:A:427:MET:HG3	1:A:427:MET:O	2.22	0.40
1:D:377:PHE:O	1:D:378:ARG:HB2	2.21	0.40
1:B:463:VAL:HA	1:B:464:PRO:HD3	1.92	0.40
1:C:105:ASP:O	1:C:106:PRO:C	2.60	0.40
1:C:436:CYS:HB2	2:C:500:HEM:NA	2.35	0.40
1:D:140:ARG:NH2	1:D:145:ARG:CG	2.84	0.40
1:D:145:ARG:HD3	1:D:181:SER:OG	2.21	0.40
1:A:383:PRO:HG2	1:A:386:THR:OG1	2.21	0.40
1:B:216:VAL:O	1:B:219:LEU:HB2	2.21	0.40
1:B:258:PRO:HA	1:B:270:LEU:HD21	2.02	0.40
1:C:312:LEU:HD13	1:C:484:TYR:CD1	2.56	0.40
1:D:136:GLY:HA3	1:D:145:ARG:HH22	1.86	0.40
1:B:176:SER:O	1:B:177:ASN:C	2.58	0.40
1:C:355:GLU:HG3	1:C:408:PHE:CE1	2.56	0.40
1:A:105:ASP:N	1:A:106:PRO:HD2	2.37	0.40
1:A:110:GLY:O	1:A:120:ARG:NH1	2.54	0.40
1:D:442:ALA:O	1:D:446:LEU:HG	2.22	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	464/476 (98%)	434 (94%)	30 (6%)	0	100	100
1	B	464/476 (98%)	430 (93%)	34 (7%)	0	100	100
1	C	464/476 (98%)	432 (93%)	31 (7%)	1 (0%)	47	79
1	D	464/476 (98%)	431 (93%)	33 (7%)	0	100	100
All	All	1856/1904 (98%)	1727 (93%)	128 (7%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	43	LEU

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	408/421 (97%)	368 (90%)	40 (10%)	8	29
1	B	409/421 (97%)	374 (91%)	35 (9%)	10	37
1	C	409/421 (97%)	379 (93%)	30 (7%)	14	43
1	D	410/421 (97%)	368 (90%)	42 (10%)	7	27
All	All	1636/1684 (97%)	1489 (91%)	147 (9%)	9	34

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	45	GLN
1	A	48	ARG
1	A	49	LYS
1	A	57	ARG
1	A	59	ARG
1	A	61	LYS

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Mol	Chain	Res	Type
1	A	78	LEU
1	A	103	VAL
1	A	109	GLN
1	A	126	ARG
1	A	128	SER
1	A	132	MET
1	A	155	GLU
1	A	165	LEU
1	A	166	ASP
1	A	176	SER
1	A	179	ILE
1	A	186	LYS
1	A	191	LYS
1	A	198	LEU
1	A	202	PHE
1	A	207	SER
1	A	224	LEU
1	A	227	PHE
1	A	230	THR
1	A	236	ARG
1	A	274	LYS
1	A	297	PHE
1	A	302	THR
1	A	303	THR
1	A	345	LYS
1	A	375	THR
1	A	386	THR
1	A	437	LEU
1	A	467	ASP
1	A	471	THR
1	A	474	GLU
1	A	477	VAL
1	A	486	ILE
1	B	35	SER
1	B	45	GLN
1	B	48	ARG
1	B	51	LEU
1	B	53	ARG
1	B	61	LYS
1	B	75	VAL
1	B	122	ARG
1	B	128	SER

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Mol	Chain	Res	Type
1	B	133	ARG
1	B	165	LEU
1	B	166	ASP
1	B	179	ILE
1	B	186	LYS
1	B	198	LEU
1	B	207	SER
1	B	211	SER
1	B	215	GLN
1	B	221	SER
1	B	224	LEU
1	B	233	GLN
1	B	259	SER
1	B	296	PHE
1	B	297	PHE
1	B	301	GLU
1	B	302	THR
1	B	303	THR
1	B	345	LYS
1	B	375	THR
1	B	386	THR
1	B	437	LEU
1	B	474	GLU
1	B	477	VAL
1	B	486	ILE
1	B	489	LEU
1	C	45	GLN
1	C	48	ARG
1	C	49	LYS
1	C	59	ARG
1	C	73	ARG
1	C	98	ARG
1	C	103	VAL
1	C	145	ARG
1	C	166	ASP
1	C	186	LYS
1	C	189	ASP
1	C	191	LYS
1	C	198	LEU
1	C	207	SER
1	C	219	LEU
1	C	221	SER

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Mol	Chain	Res	Type
1	C	224	LEU
1	C	296	PHE
1	C	297	PHE
1	C	302	THR
1	C	303	THR
1	C	305	THR
1	C	345	LYS
1	C	375	THR
1	C	381	VAL
1	C	386	THR
1	C	397	HIS
1	C	437	LEU
1	C	474	GLU
1	C	477	VAL
1	D	38	PRO
1	D	42	ASN
1	D	45	GLN
1	D	48	ARG
1	D	49	LYS
1	D	53	ARG
1	D	59	ARG
1	D	103	VAL
1	D	107	ILE
1	D	126	ARG
1	D	144	GLU
1	D	145	ARG
1	D	169	LEU
1	D	186	LYS
1	D	189	ASP
1	D	191	LYS
1	D	198	LEU
1	D	207	SER
1	D	208	LEU
1	D	211	SER
1	D	213	SER
1	D	221	SER
1	D	224	LEU
1	D	227	PHE
1	D	233	GLN
1	D	247	GLN
1	D	250	GLU
1	D	257	ASP

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Mol	Chain	Res	Type
1	D	260	ASN
1	D	296	PHE
1	D	302	THR
1	D	303	THR
1	D	304	SER
1	D	345	LYS
1	D	375	THR
1	D	381	VAL
1	D	390	PRO
1	D	437	LEU
1	D	468	ILE
1	D	474	GLU
1	D	477	VAL
1	D	483	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	369	HIS
1	B	172	HIS
1	B	204	GLN
1	B	260	ASN
1	B	369	HIS
1	C	369	HIS
1	C	385	ASN
1	D	172	HIS
1	D	260	ASN
1	D	369	HIS
1	D	385	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	C	500	1	41,50,50	1.90	6 (14%)	45,82,82	1.60	7 (15%)
3	CGE	D	501	-	20,23,23	1.73	3 (15%)	22,32,32	4.36	13 (59%)
2	HEM	D	500	1	41,50,50	1.82	5 (12%)	45,82,82	1.72	10 (22%)
2	HEM	B	500	1	41,50,50	1.91	8 (19%)	45,82,82	1.71	8 (17%)
3	CGE	C	501	-	20,23,23	1.75	3 (15%)	22,32,32	4.12	10 (45%)
3	CGE	A	501	-	20,23,23	1.79	3 (15%)	22,32,32	4.13	13 (59%)
3	CGE	B	501	-	20,23,23	1.77	4 (20%)	22,32,32	4.06	13 (59%)
2	HEM	A	500	1	41,50,50	1.88	6 (14%)	45,82,82	1.68	7 (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	C	500	1	-	4/12/54/54	-
3	CGE	D	501	-	-	5/14/23/23	0/3/3/3
2	HEM	D	500	1	-	4/12/54/54	-
2	HEM	B	500	1	-	6/12/54/54	-
3	CGE	C	501	-	-	5/14/23/23	0/3/3/3
3	CGE	A	501	-	-	9/14/23/23	0/3/3/3
3	CGE	B	501	-	-	7/14/23/23	0/3/3/3
2	HEM	A	500	1	-	5/12/54/54	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HEM	C3D-C2D	7.49	1.52	1.36
2	C	500	HEM	C3D-C2D	7.26	1.52	1.36
2	A	500	HEM	C3D-C2D	7.08	1.51	1.36
2	B	500	HEM	C3D-C2D	6.85	1.51	1.36
3	A	501	CGE	OAM-C	6.07	1.48	1.33
3	B	501	CGE	OAM-C	6.04	1.47	1.33
3	C	501	CGE	OAM-C	5.76	1.47	1.33
3	D	501	CGE	OAM-C	5.71	1.47	1.33
2	A	500	HEM	C3C-C2C	-5.63	1.32	1.40
2	C	500	HEM	C3C-C2C	-5.47	1.32	1.40
2	B	500	HEM	C3C-C2C	-4.85	1.33	1.40
2	D	500	HEM	C3C-C2C	-4.28	1.34	1.40
3	D	501	CGE	CAS-CA	-3.58	1.48	1.52
3	C	501	CGE	CAS-CA	-3.25	1.48	1.52
2	C	500	HEM	CAA-C2A	3.00	1.56	1.52
2	B	500	HEM	CAA-C2A	3.00	1.56	1.52
2	B	500	HEM	FE-ND	2.93	2.11	1.96
2	D	500	HEM	CAB-C3B	2.84	1.55	1.47
2	B	500	HEM	FE-NB	2.82	2.10	1.96
2	C	500	HEM	CAB-C3B	2.79	1.55	1.47
3	C	501	CGE	CAP-CL1	2.78	1.80	1.73
3	A	501	CGE	CAS-CA	-2.75	1.49	1.52
3	A	501	CGE	CAP-CL1	2.71	1.80	1.73
2	B	500	HEM	C3C-CAC	2.70	1.53	1.47
3	D	501	CGE	CAP-CL1	2.70	1.80	1.73
2	A	500	HEM	C3C-CAC	2.68	1.53	1.47
3	B	501	CGE	CAP-CL1	2.65	1.79	1.73
2	C	500	HEM	C3C-CAC	2.64	1.53	1.47
2	C	500	HEM	C3B-C2B	-2.61	1.32	1.37
2	D	500	HEM	C3C-CAC	2.61	1.53	1.47
2	A	500	HEM	CAB-C3B	2.58	1.54	1.47
2	A	500	HEM	FE-ND	2.53	2.09	1.96
2	B	500	HEM	CAB-C3B	2.51	1.54	1.47
2	B	500	HEM	C3B-C2B	-2.50	1.32	1.37
2	A	500	HEM	C3B-C2B	-2.39	1.32	1.37
2	D	500	HEM	CAA-C2A	2.36	1.55	1.52
3	B	501	CGE	CAJ-CAR	2.33	1.52	1.50
3	B	501	CGE	CAS-CA	-2.26	1.49	1.52

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	CGE	CAL-N-CAK	12.92	125.40	109.43
3	C	501	CGE	CAL-N-CAK	11.54	123.68	109.43
3	A	501	CGE	CAL-N-CAK	11.42	123.54	109.43
3	B	501	CGE	CAL-N-CAK	11.12	123.17	109.43
3	B	501	CGE	OAM-C-CA	9.55	120.81	110.58
3	A	501	CGE	OAM-C-CA	8.89	120.11	110.58
3	D	501	CGE	OAM-C-CA	8.84	120.05	110.58
3	C	501	CGE	OAM-C-CA	8.47	119.65	110.58
3	C	501	CGE	CAQ-CAL-N	-7.70	100.62	113.37
3	D	501	CGE	CAQ-CAL-N	-7.05	101.70	113.37
3	B	501	CGE	CAQ-CAL-N	-6.98	101.81	113.37
3	A	501	CGE	CAQ-CAL-N	-6.70	102.29	113.37
2	D	500	HEM	C4D-ND-C1D	6.49	111.78	105.07
2	B	500	HEM	C4D-ND-C1D	6.24	111.52	105.07
2	A	500	HEM	C4D-ND-C1D	5.57	110.83	105.07
3	C	501	CGE	CAH-CAS-CAP	5.41	122.20	116.81
3	D	501	CGE	CAH-CAS-CAP	5.15	121.94	116.81
2	C	500	HEM	C4D-ND-C1D	4.96	110.19	105.07
3	A	501	CGE	CAH-CAS-CAP	4.88	121.67	116.81
2	A	500	HEM	CAD-CBD-CGD	-4.59	103.72	113.60
2	C	500	HEM	CAD-CBD-CGD	-4.30	104.36	113.60
2	B	500	HEM	C4C-CHD-C1D	4.02	127.86	122.56
3	D	501	CGE	CAS-CAP-CL1	-3.97	116.31	120.41
3	B	501	CGE	CAH-CAS-CAP	3.96	120.75	116.81
3	D	501	CGE	CAP-CAS-CA	-3.80	113.78	121.80
3	A	501	CGE	CAP-CAS-CA	-3.69	114.02	121.80
3	B	501	CGE	CAA-OAM-C	3.65	124.19	115.94
3	A	501	CGE	CAK-N-CA	3.64	122.22	112.06
2	C	500	HEM	CBA-CAA-C2A	-3.58	106.51	112.62
3	A	501	CGE	CAA-OAM-C	3.53	123.91	115.94
3	C	501	CGE	CAK-N-CA	3.44	121.67	112.06
3	A	501	CGE	OAM-C-O	-3.39	117.22	123.84
3	B	501	CGE	CAK-N-CA	3.32	121.35	112.06
3	B	501	CGE	CAS-CAP-CL1	-3.29	117.01	120.41
3	B	501	CGE	CAP-CAS-CA	-3.28	114.88	121.80
2	B	500	HEM	CAD-CBD-CGD	-3.27	106.56	113.60
3	C	501	CGE	CAA-OAM-C	3.23	123.24	115.94
3	A	501	CGE	CAS-CAP-CL1	-3.22	117.08	120.41
3	D	501	CGE	CAA-OAM-C	3.22	123.22	115.94
3	C	501	CGE	CAP-CAS-CA	-3.21	115.04	121.80
2	B	500	HEM	CMA-C3A-C4A	-3.18	123.58	128.46
3	C	501	CGE	OAM-C-O	-3.16	117.66	123.84
3	D	501	CGE	CAK-CAJ-CAR	-3.03	106.48	111.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	HEM	CHD-C1D-ND	3.02	127.72	124.43
2	A	500	HEM	CBA-CAA-C2A	-2.96	107.57	112.62
3	B	501	CGE	OAM-C-O	-2.95	118.07	123.84
3	D	501	CGE	OAM-C-O	-2.93	118.11	123.84
3	D	501	CGE	CAK-N-CA	2.89	120.14	112.06
3	A	501	CGE	CAK-CAJ-CAR	-2.89	106.70	111.32
2	A	500	HEM	CMA-C3A-C4A	-2.80	124.15	128.46
2	C	500	HEM	CHD-C1D-ND	2.79	127.47	124.43
2	C	500	HEM	C4C-CHD-C1D	2.78	126.23	122.56
3	D	501	CGE	CAG-CAP-CL1	2.77	123.96	118.41
2	A	500	HEM	C4C-CHD-C1D	2.75	126.19	122.56
3	C	501	CGE	CAG-CAP-CAS	-2.73	119.51	121.99
2	D	500	HEM	C4C-CHD-C1D	2.73	126.16	122.56
2	C	500	HEM	O1A-CGA-CBA	-2.70	114.42	123.08
2	B	500	HEM	CBA-CAA-C2A	-2.54	108.28	112.62
2	D	500	HEM	CAD-CBD-CGD	-2.53	108.15	113.60
2	B	500	HEM	C4A-C3A-C2A	2.50	108.73	107.00
3	D	501	CGE	CAG-CAP-CAS	-2.49	119.73	121.99
2	D	500	HEM	CMC-C2C-C3C	2.44	129.24	124.68
3	C	501	CGE	CAK-CAJ-CAR	-2.40	107.49	111.32
2	A	500	HEM	CHD-C1D-ND	2.34	126.97	124.43
2	D	500	HEM	O2D-CGD-CBD	2.33	121.51	114.03
3	A	501	CGE	CAG-CAP-CAS	-2.32	119.88	121.99
3	A	501	CGE	CAG-CAP-CL1	2.31	123.03	118.41
2	B	500	HEM	CHC-C4B-C3B	2.27	128.04	124.57
2	D	500	HEM	C2D-C1D-ND	-2.21	107.23	109.88
2	C	500	HEM	O2A-CGA-CBA	2.21	121.12	114.03
2	D	500	HEM	C3B-C2B-C1B	2.19	108.11	106.49
2	D	500	HEM	O1D-CGD-CBD	-2.19	116.04	123.08
2	D	500	HEM	CBD-CAD-C3D	-2.19	106.54	112.63
3	B	501	CGE	O-C-CA	-2.16	121.12	125.11
3	B	501	CGE	CAH-CAS-CA	2.11	124.35	120.61
3	A	501	CGE	CAH-CAS-CA	2.08	124.29	120.61
3	B	501	CGE	CAS-CA-C	2.08	116.13	110.71
2	A	500	HEM	C4B-CHC-C1C	2.08	125.30	122.56
3	B	501	CGE	CAG-CAP-CL1	2.08	122.57	118.41
3	D	501	CGE	CAH-CAS-CA	2.07	124.27	120.61
2	B	500	HEM	C3D-C4D-ND	-2.02	107.92	110.17

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	HEM	C2B-C3B-CAB-CBB
2	C	500	HEM	C2B-C3B-CAB-CBB
3	A	501	CGE	C-CA-N-CAK
3	A	501	CGE	CAS-CA-N-CAK
3	B	501	CGE	OAM-C-CA-N
3	B	501	CGE	C-CA-N-CAK
3	B	501	CGE	CAS-CA-N-CAK
3	B	501	CGE	C-CA-CAS-CAP
3	C	501	CGE	O-C-OAM-CAA
3	C	501	CGE	C-CA-N-CAK
3	C	501	CGE	CAS-CA-N-CAK
3	D	501	CGE	O-C-OAM-CAA
3	D	501	CGE	C-CA-N-CAK
3	D	501	CGE	CAS-CA-N-CAK
3	B	501	CGE	O-C-OAM-CAA
3	A	501	CGE	O-C-OAM-CAA
3	C	501	CGE	CA-C-OAM-CAA
3	D	501	CGE	CA-C-OAM-CAA
3	A	501	CGE	CA-C-OAM-CAA
3	B	501	CGE	CA-C-OAM-CAA
2	B	500	HEM	C4B-C3B-CAB-CBB
2	C	500	HEM	C4B-C3B-CAB-CBB
3	A	501	CGE	OAM-C-CA-N
3	B	501	CGE	O-C-CA-N
2	A	500	HEM	C2B-C3B-CAB-CBB
3	A	501	CGE	OAM-C-CA-CAS
3	D	501	CGE	C-CA-CAS-CAP
2	D	500	HEM	CAA-CBA-CGA-O1A
2	D	500	HEM	CAA-CBA-CGA-O2A
3	A	501	CGE	O-C-CA-N
2	B	500	HEM	CAA-CBA-CGA-O2A
2	B	500	HEM	CAA-CBA-CGA-O1A
2	A	500	HEM	C4B-C3B-CAB-CBB
2	A	500	HEM	CAD-CBD-CGD-O1D
2	B	500	HEM	CAD-CBD-CGD-O1D
3	A	501	CGE	O-C-CA-CAS
2	A	500	HEM	CAD-CBD-CGD-O2D
2	C	500	HEM	CAD-CBD-CGD-O2D
2	D	500	HEM	CAD-CBD-CGD-O2D
2	D	500	HEM	CAD-CBD-CGD-O1D
2	B	500	HEM	CAD-CBD-CGD-O2D
3	A	501	CGE	C-CA-CAS-CAP
3	C	501	CGE	C-CA-CAS-CAP

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Mol	Chain	Res	Type	Atoms
2	A	500	HEM	CAA-CBA-CGA-O1A
2	C	500	HEM	CAA-CBA-CGA-O2A

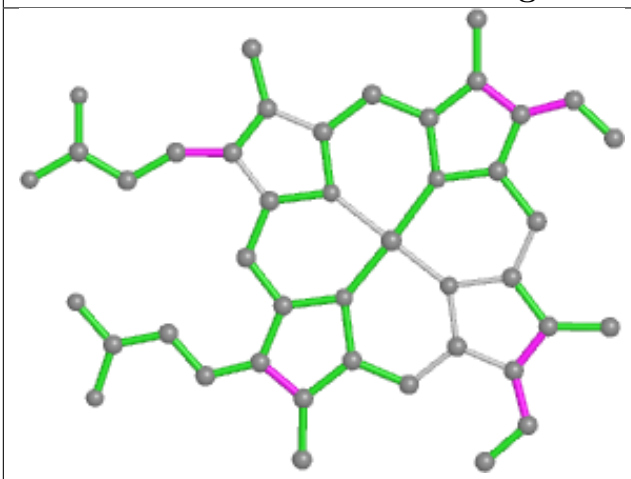
There are no ring outliers.

8 monomers are involved in 48 short contacts:

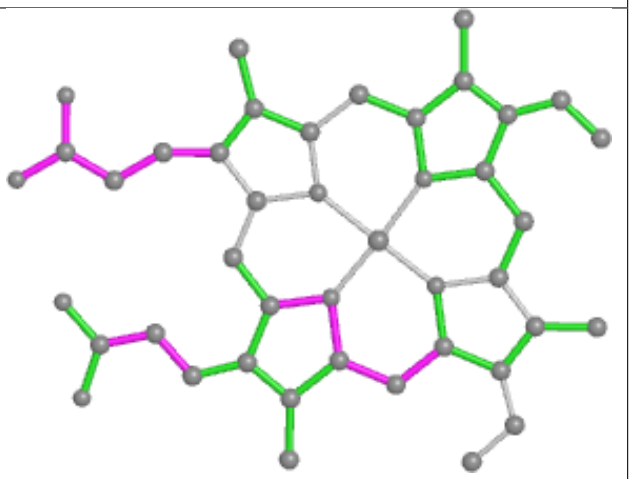
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	HEM	5	0
3	D	501	CGE	8	0
2	D	500	HEM	7	0
2	B	500	HEM	9	0
3	C	501	CGE	8	0
3	A	501	CGE	6	0
3	B	501	CGE	8	0
2	A	500	HEM	6	0

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.

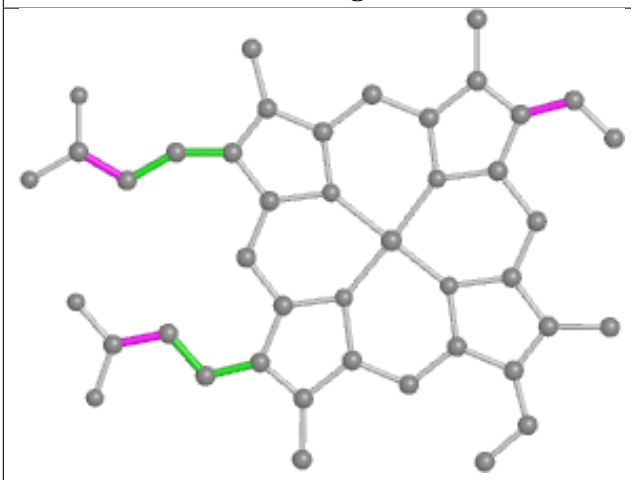
Ligand HEM C 500



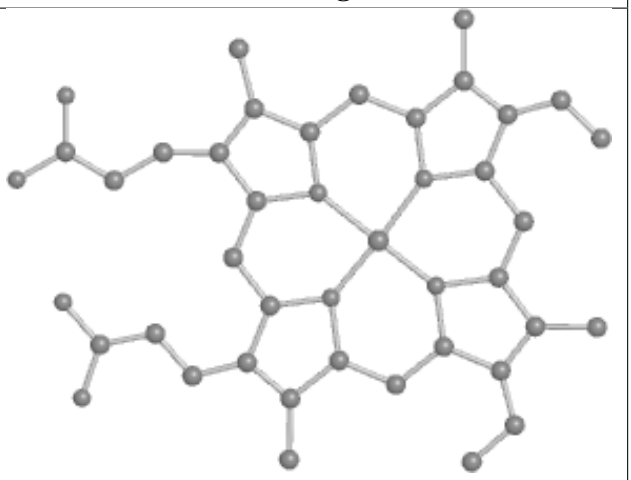
Bond lengths



Bond angles

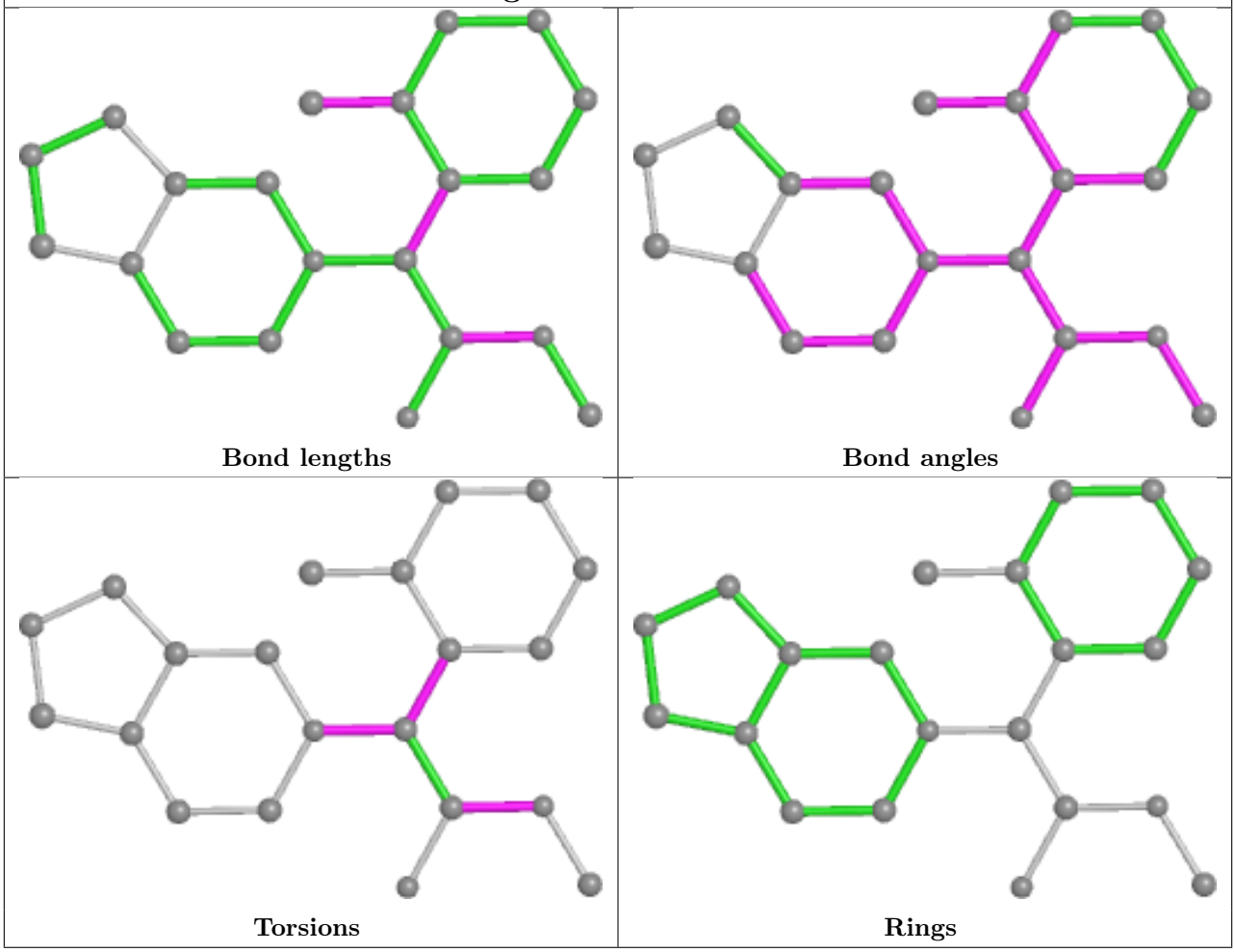


Torsions

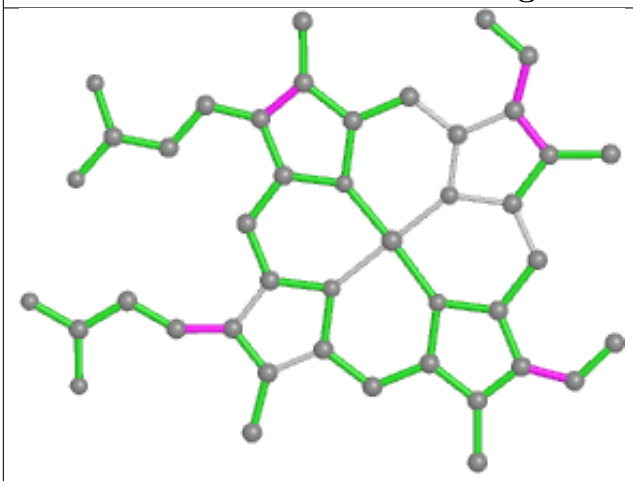


Rings

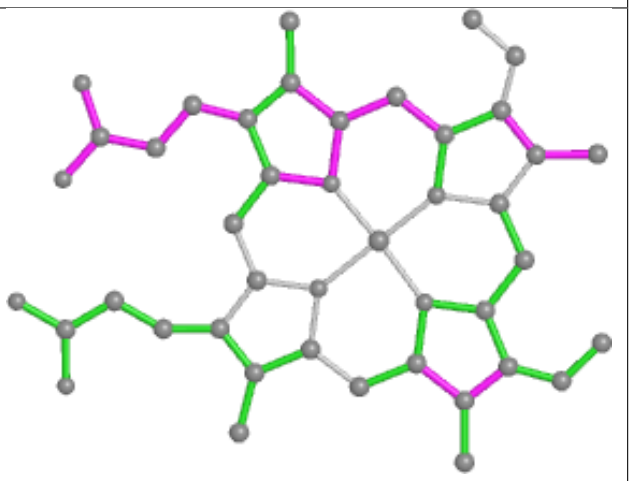
Ligand CGE D 501



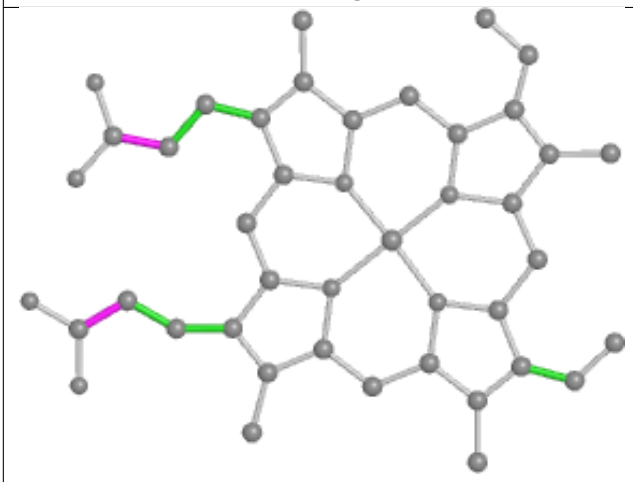
Ligand HEM D 500



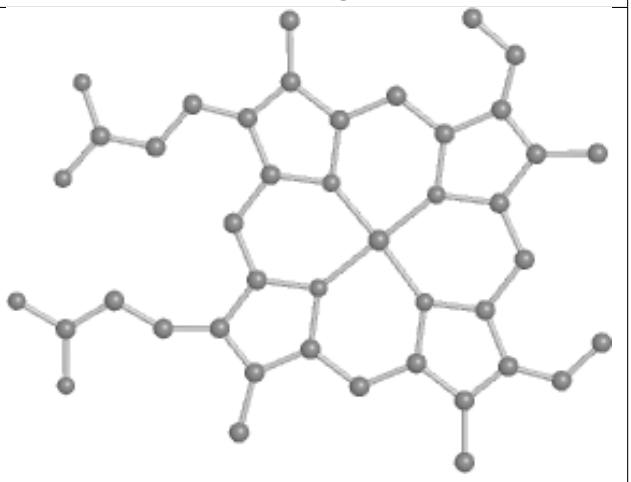
Bond lengths



Bond angles

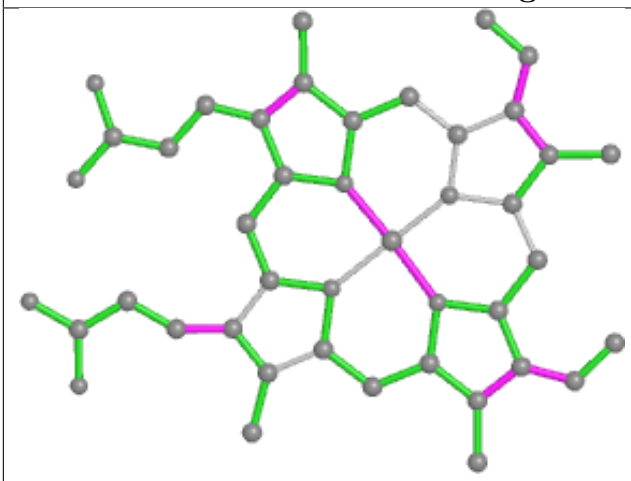


Torsions

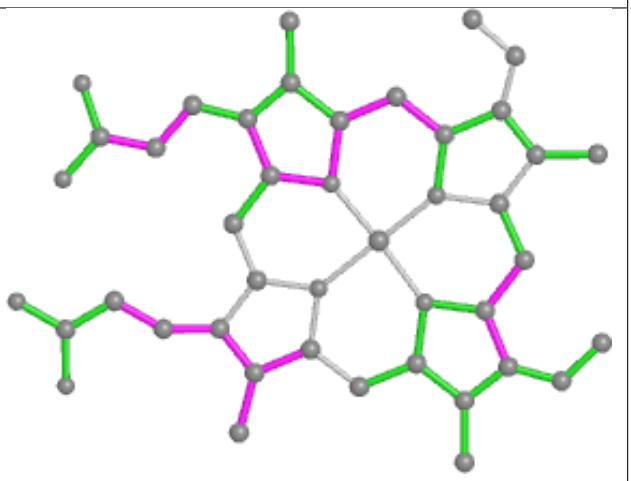


Rings

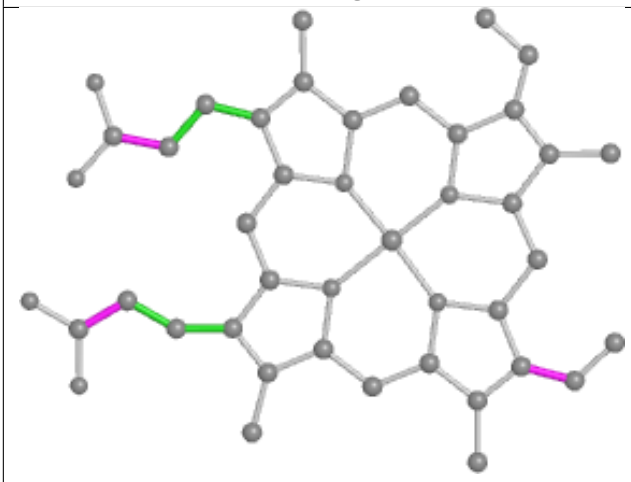
Ligand HEM B 500



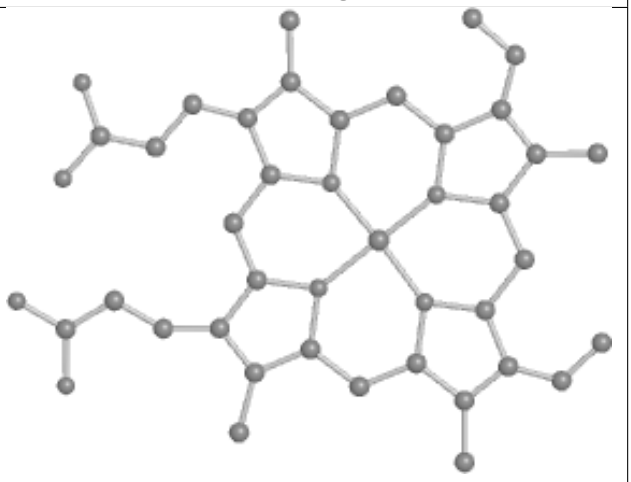
Bond lengths



Bond angles

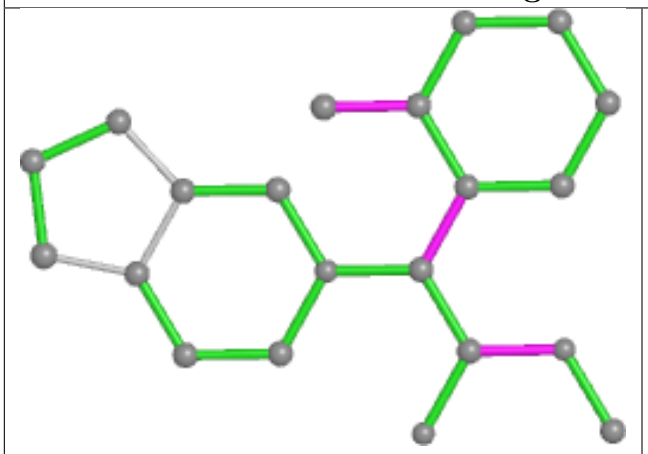


Torsions

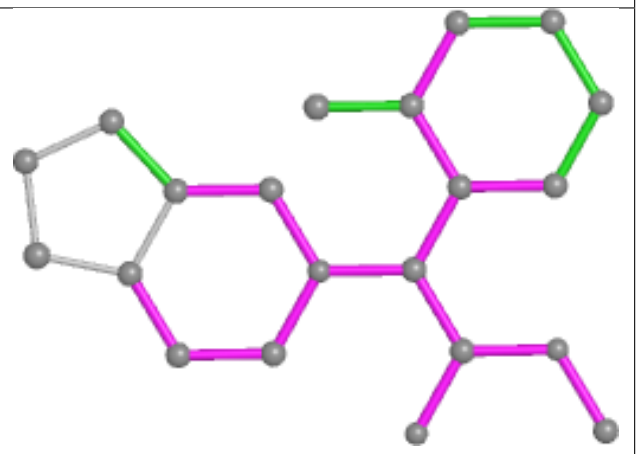


Rings

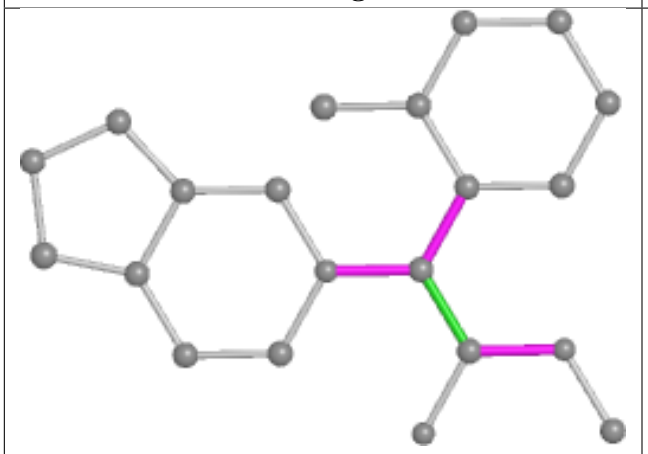
Ligand CGE C 501



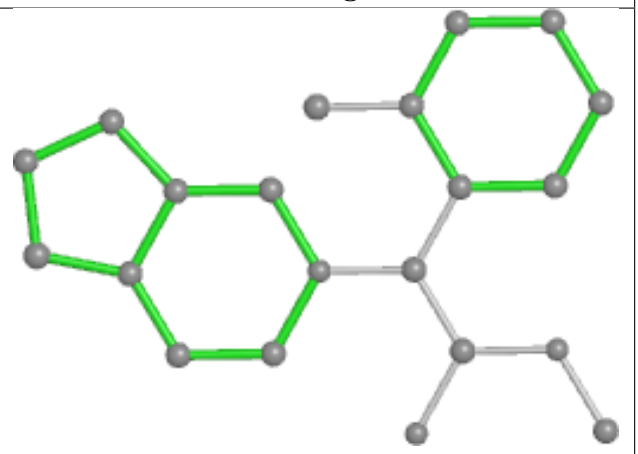
Bond lengths



Bond angles

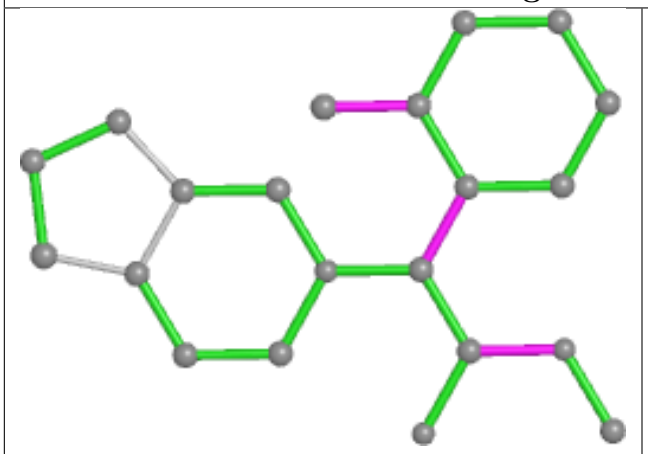


Torsions

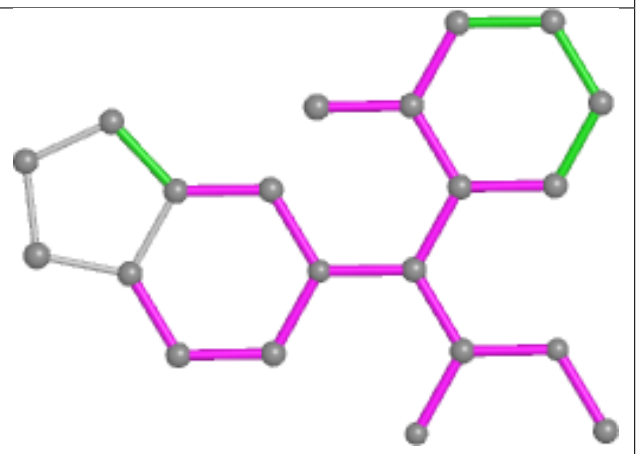


Rings

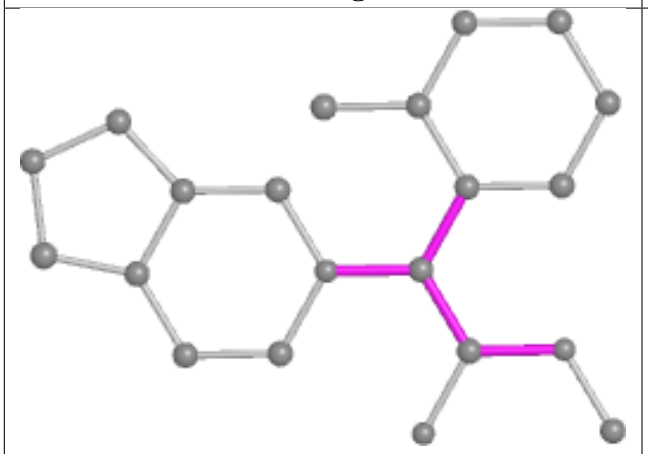
Ligand CGE A 501



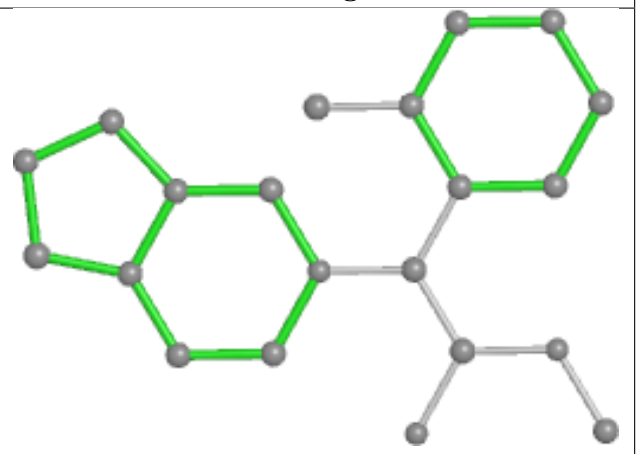
Bond lengths



Bond angles

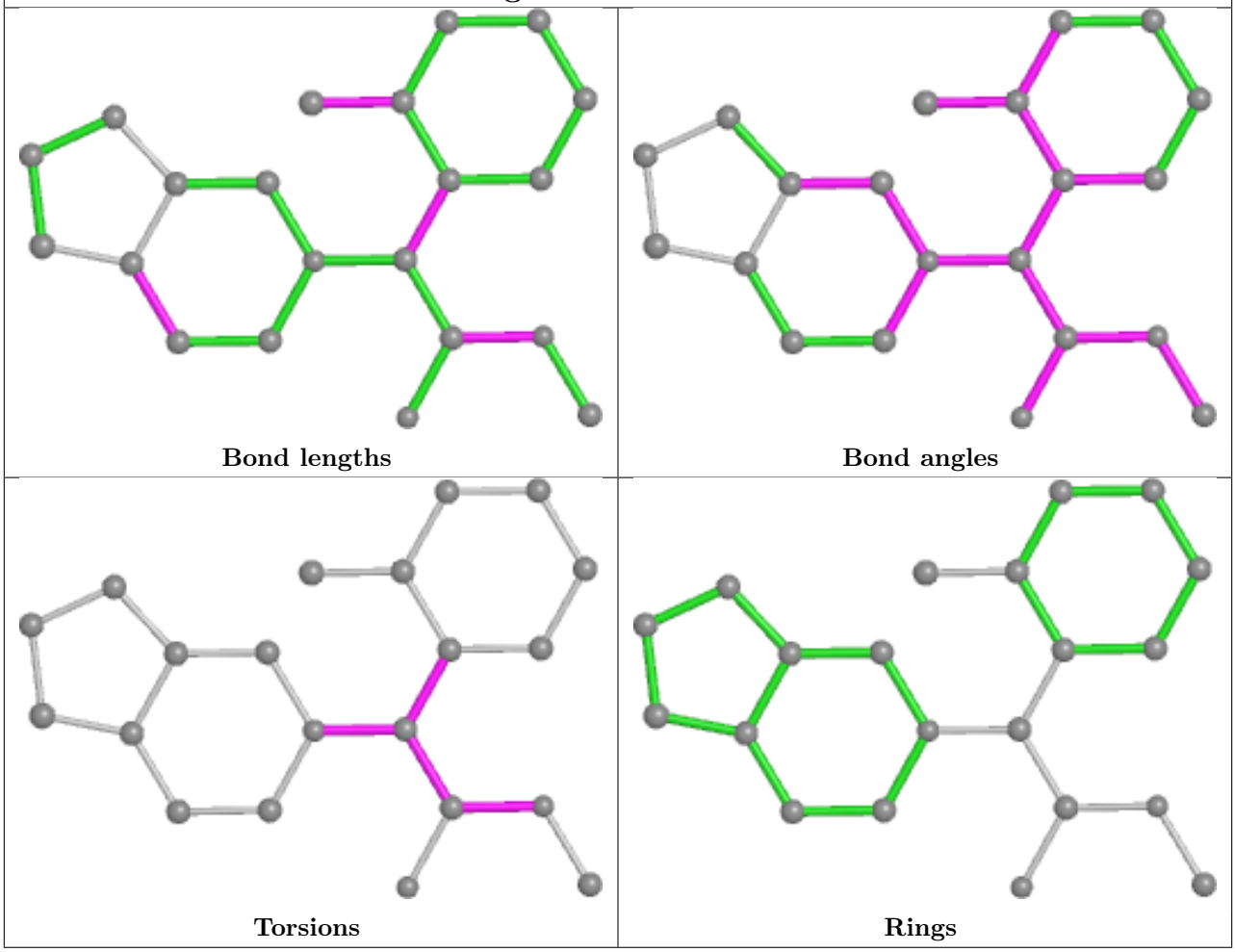


Torsions

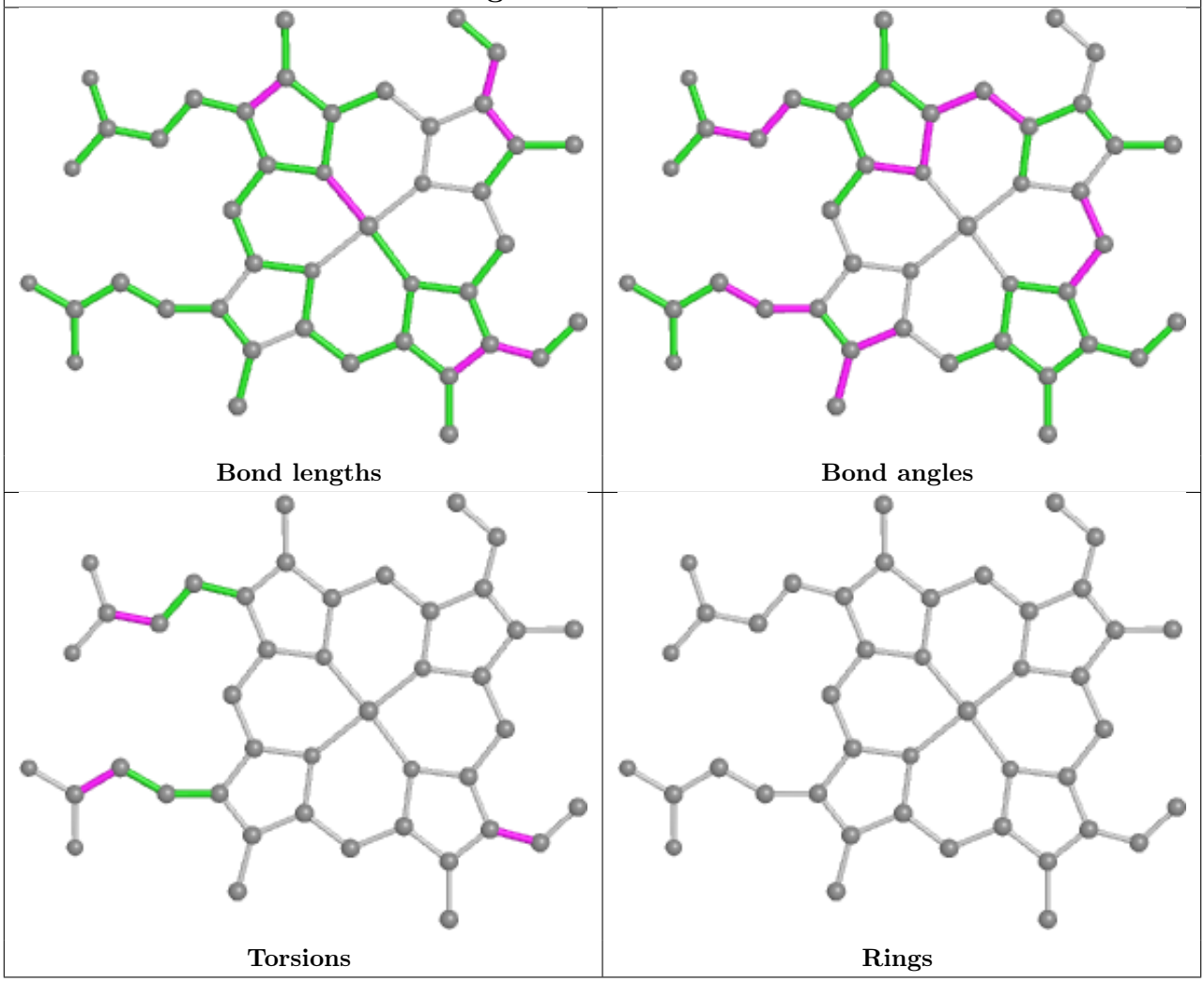


Rings

Ligand CGE B 501



Ligand HEM A 500



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	465/476 (97%)	0.05	2 (0%)	92	84	10, 41, 72, 87	7 (1%)
1	B	465/476 (97%)	0.05	2 (0%)	92	84	9, 41, 72, 86	2 (0%)
1	C	465/476 (97%)	0.07	2 (0%)	92	84	10, 41, 72, 84	2 (0%)
1	D	465/476 (97%)	0.04	2 (0%)	92	84	9, 41, 72, 84	2 (0%)
All	All	1860/1904 (97%)	0.05	8 (0%)	92	84	9, 41, 72, 87	13 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	136	GLY	4.7
1	A	136	GLY	4.5
1	C	136	GLY	4.4
1	B	136	GLY	3.6
1	C	135	PHE	2.2
1	B	135	PHE	2.2
1	A	137	MET	2.2
1	D	135	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

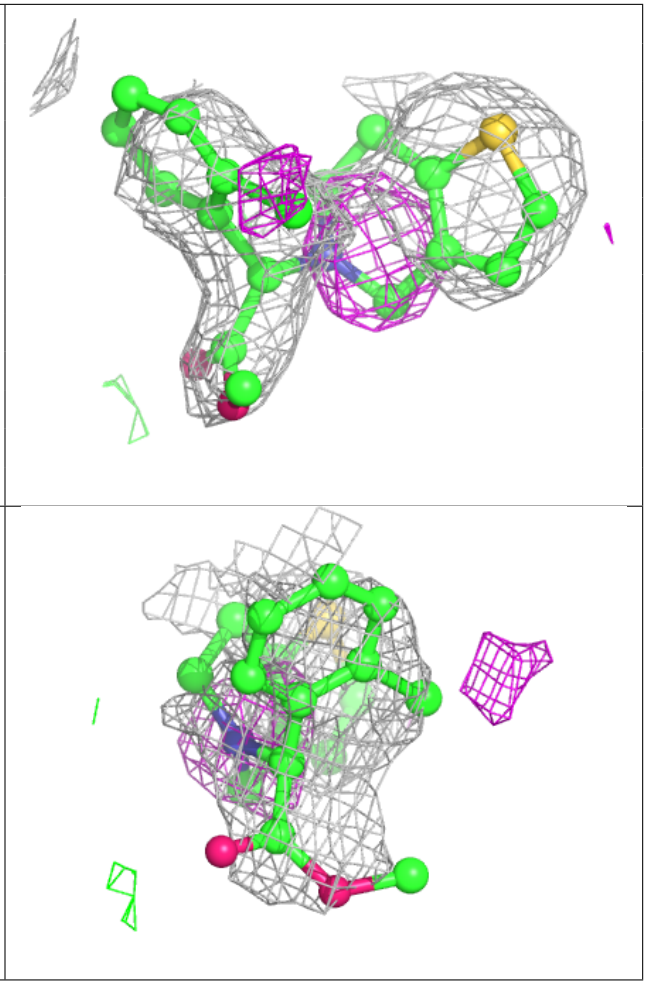
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CGE	B	501	21/21	0.90	0.53	96,101,102,103	0
3	CGE	C	501	21/21	0.92	0.49	96,101,101,103	0
3	CGE	D	501	21/21	0.92	0.58	108,111,111,111	0
3	CGE	A	501	21/21	0.93	0.53	93,97,98,99	0
2	HEM	A	500	43/43	0.99	0.25	24,31,34,41	0
2	HEM	B	500	43/43	0.99	0.27	24,28,32,40	0
2	HEM	C	500	43/43	0.99	0.25	20,26,37,42	0
2	HEM	D	500	43/43	0.99	0.25	11,26,33,37	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.

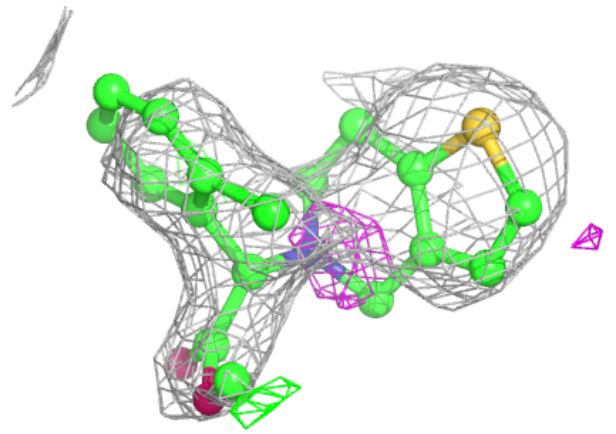
Electron density around CGE B 501:

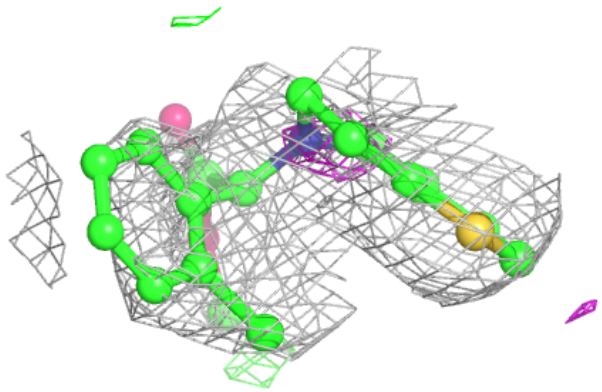
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

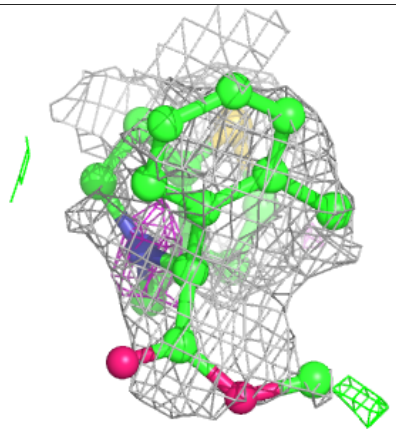


Electron density around CGE C 501:

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

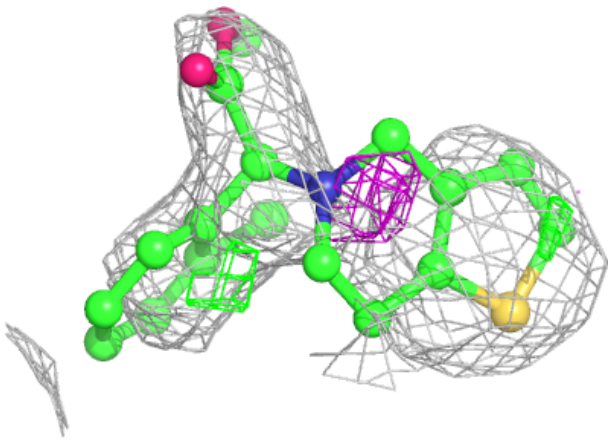


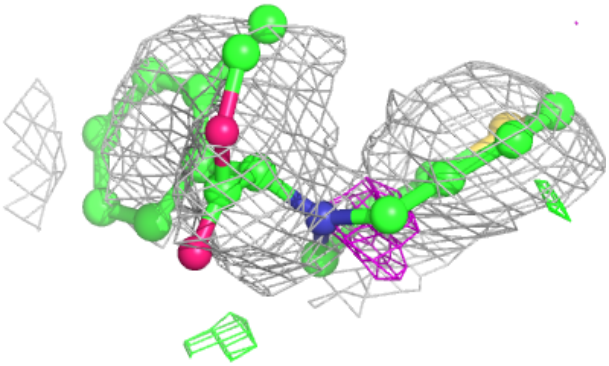


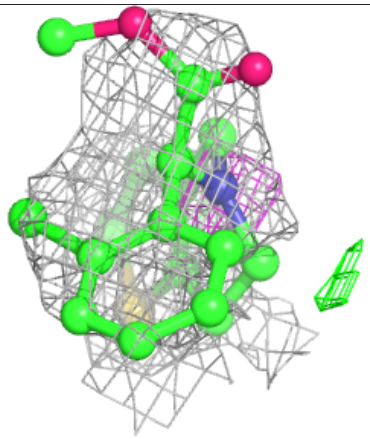


Electron density around CGE D 501:

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

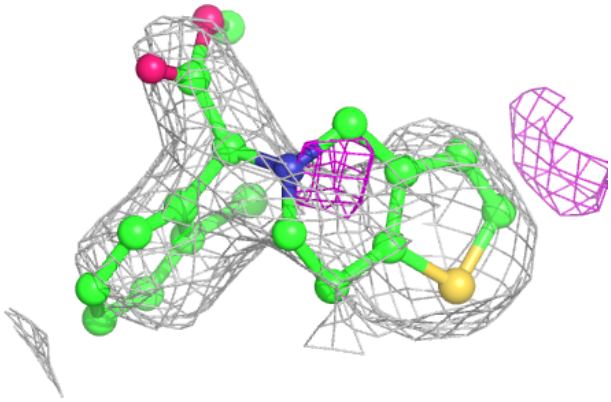


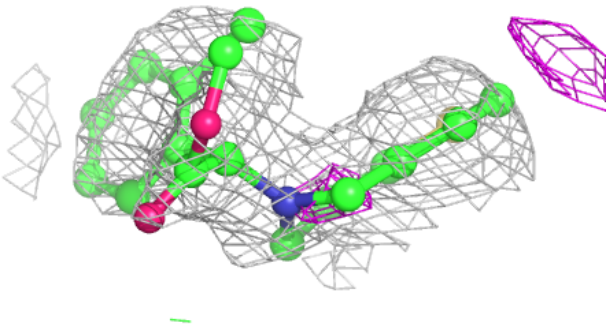


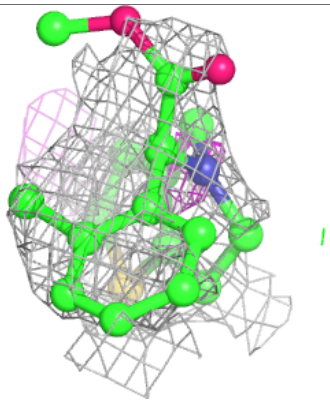


Electron density around CGE A 501:

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

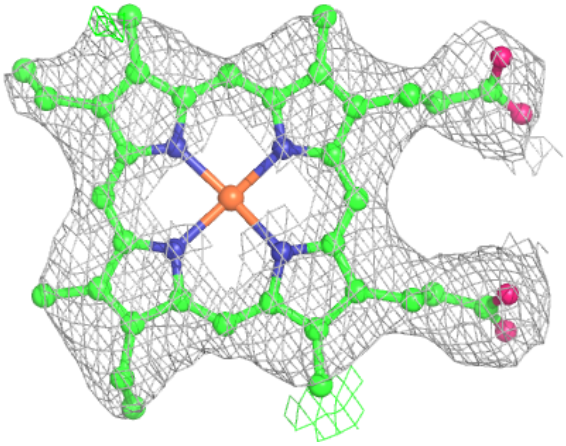


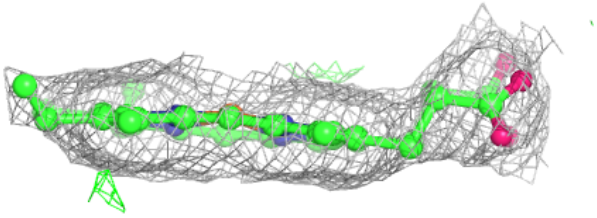


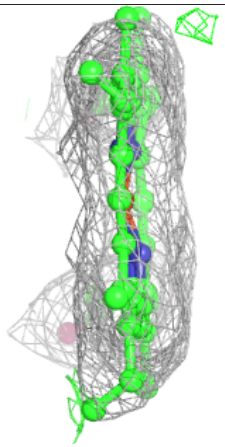


Electron density around HEM A 500:

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

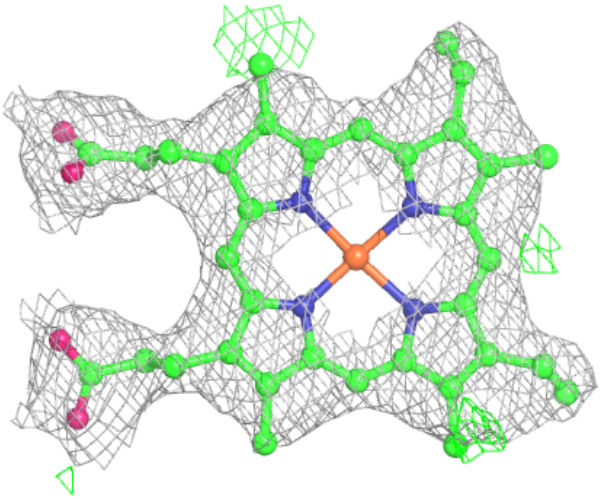


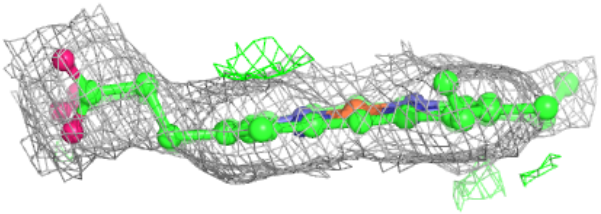


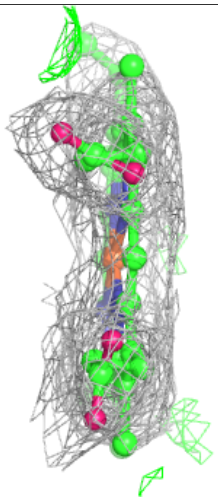


Electron density around HEM B 500:

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

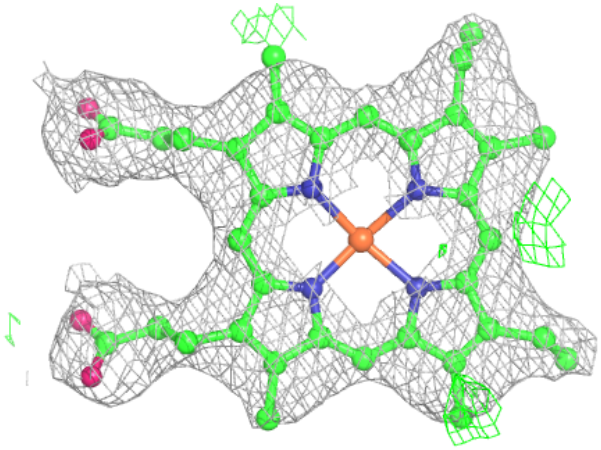


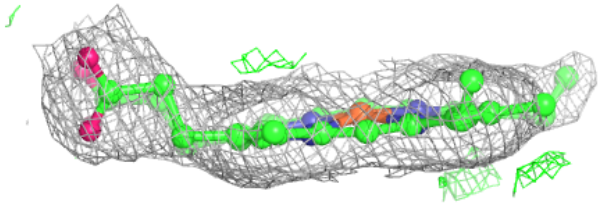


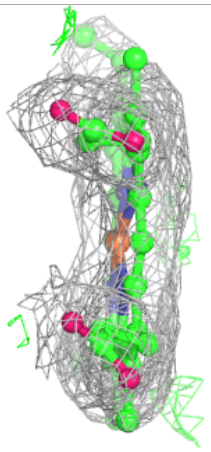


Electron density around HEM C 500:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

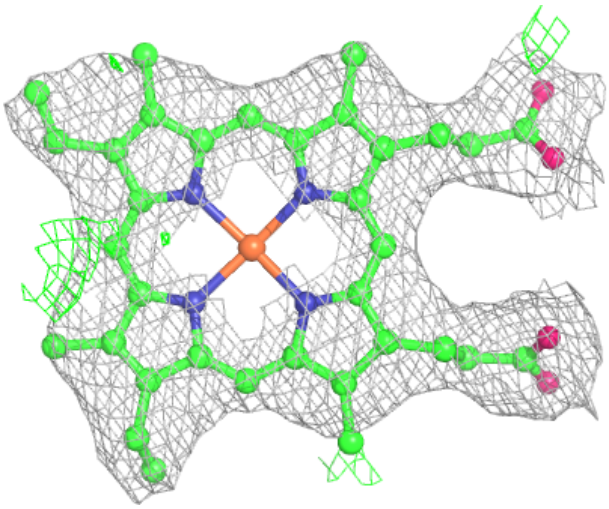


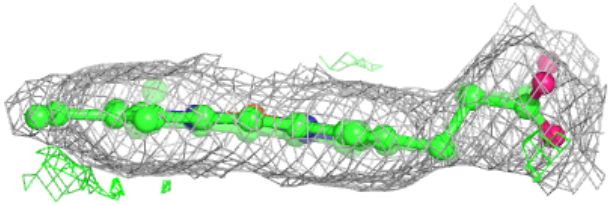


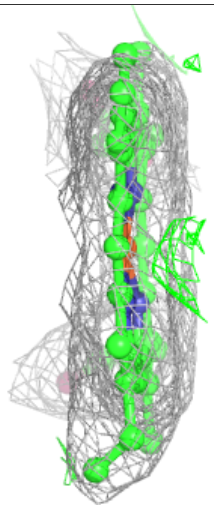


Electron density around HEM D 500:

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







6.5 Other polymers (i)

There are no such residues in this entry.