Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2022 – 04:04 PM EDT

PDB ID	:	5VBU
Title	:	Crystal Structure of Human Cytochrome P450 21A2 Hydroxyprogesterone Complex
Authors	:	Pallan, P.S.; Egli, M.
Deposited on	:	2017-03-30
Resolution	:	3.31 Å(reported)

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

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

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

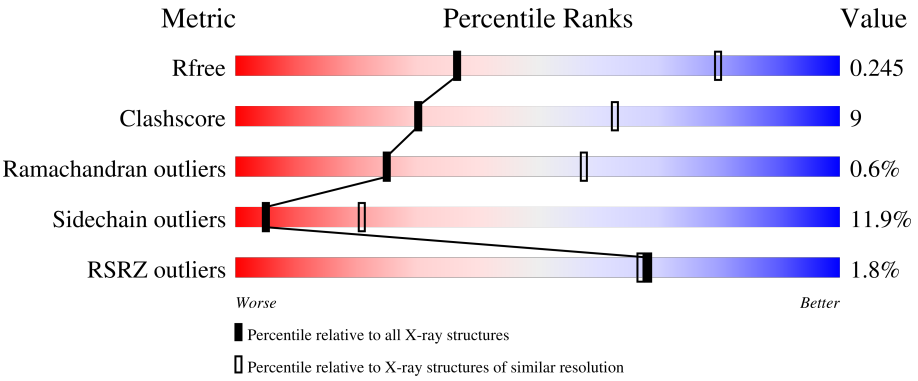
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 3.31 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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	69% 20% · 7%
1	B	476	70% 19% · 7%
1	C	476	67% 22% · 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10795 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 21-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	159	0	0
			3531	2279	617	618	17			
1	B	441	Total	C	N	O	S	116	0	0
			3527	2277	616	617	17			
1	C	442	Total	C	N	O	S	82	0	0
			3531	2279	617	618	17			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP Q16874
A	21	ALA	-	expression tag	UNP Q16874
A	22	LYS	-	expression tag	UNP Q16874
A	23	LYS	-	expression tag	UNP Q16874
A	24	THR	-	expression tag	UNP Q16874
A	25	SER	-	expression tag	UNP Q16874
A	26	SER	-	expression tag	UNP Q16874
A	27	LYS	-	expression tag	UNP Q16874
A	28	GLY	-	expression tag	UNP Q16874
A	29	LYS	-	expression tag	UNP Q16874
B	20	MET	-	initiating methionine	UNP Q16874
B	21	ALA	-	expression tag	UNP Q16874
B	22	LYS	-	expression tag	UNP Q16874
B	23	LYS	-	expression tag	UNP Q16874
B	24	THR	-	expression tag	UNP Q16874
B	25	SER	-	expression tag	UNP Q16874
B	26	SER	-	expression tag	UNP Q16874
B	27	LYS	-	expression tag	UNP Q16874
B	28	GLY	-	expression tag	UNP Q16874
B	29	LYS	-	expression tag	UNP Q16874
C	20	MET	-	initiating methionine	UNP Q16874
C	21	ALA	-	expression tag	UNP Q16874
C	22	LYS	-	expression tag	UNP Q16874

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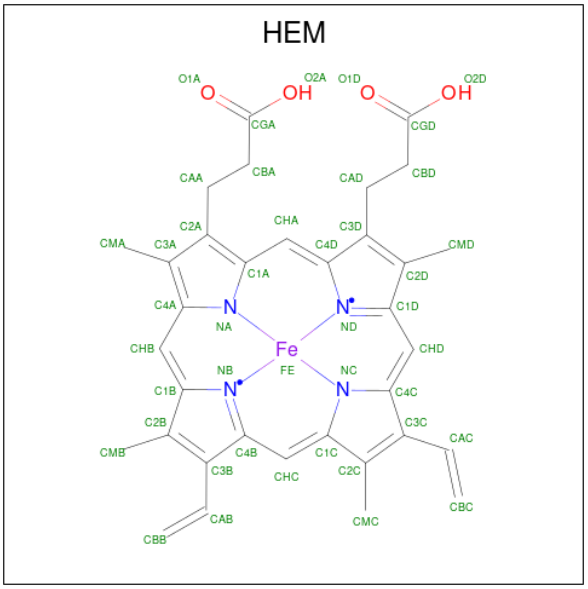
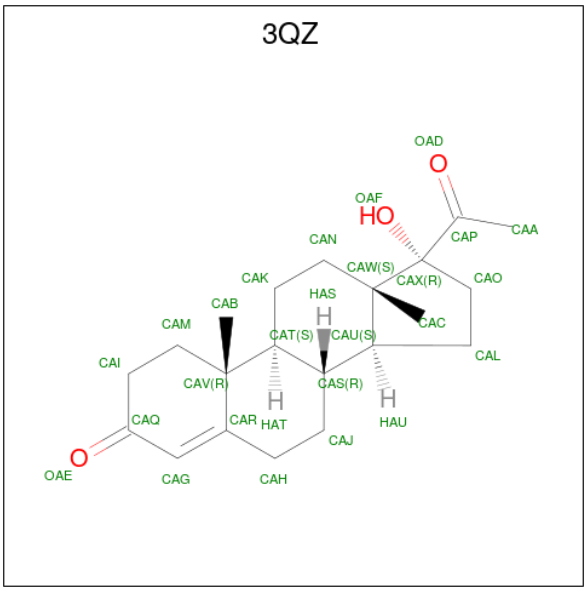
Chain	Residue	Modelled	Actual	Comment	Reference
C	23	LYS	-	expression tag	UNP Q16874
C	24	THR	-	expression tag	UNP Q16874
C	25	SER	-	expression tag	UNP Q16874
C	26	SER	-	expression tag	UNP Q16874
C	27	LYS	-	expression tag	UNP Q16874
C	28	GLY	-	expression tag	UNP Q16874
C	29	LYS	-	expression tag	UNP Q16874

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	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		

- Molecule 3 is (9beta)-17-hydroxypregn-4-ene-3,20-dione (three-letter code: 3QZ) (formula: $C_{21}H_{30}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 24 21 3	0	0
3	B	1	Total C O 24 21 3	0	0
3	C	1	Total C O 24 21 3	0	0

- Molecule 4 is water.

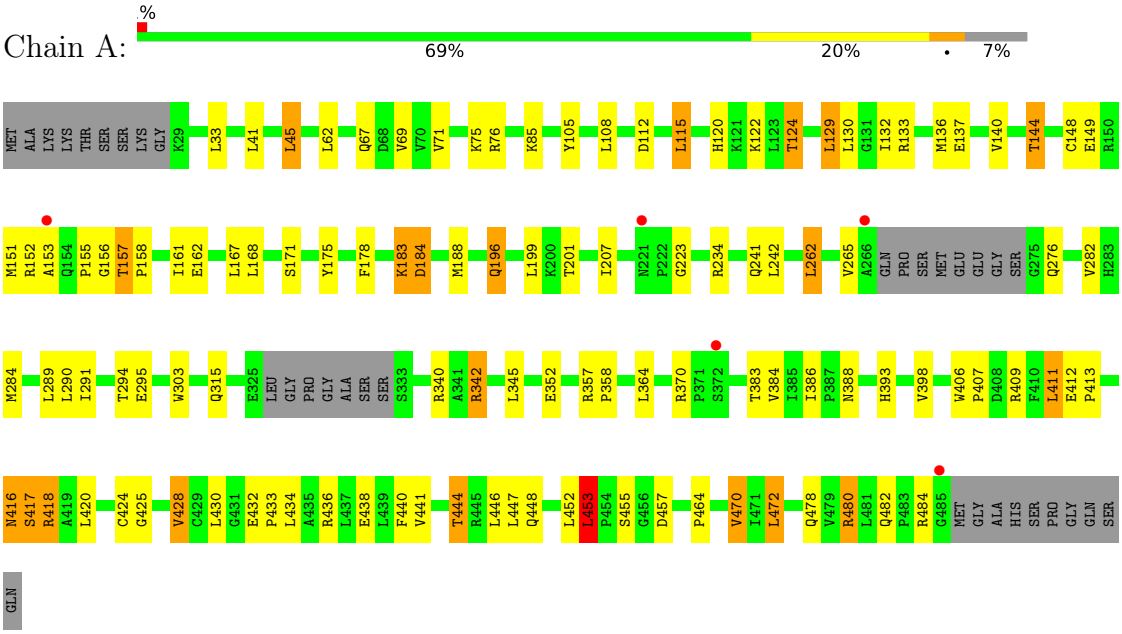
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	4	Total O 4 4	0	0

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.

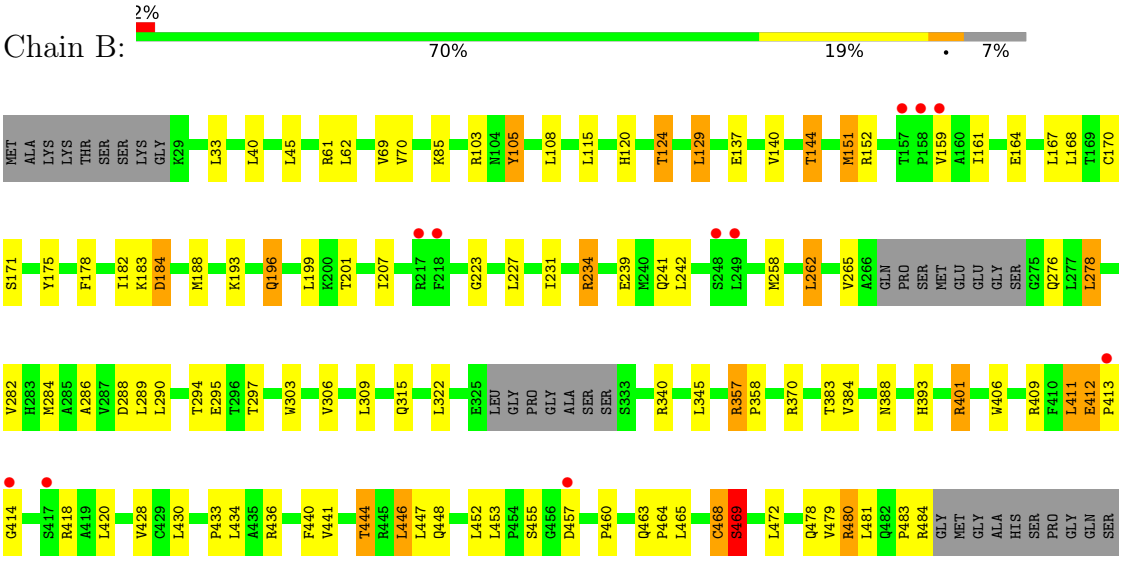
• Molecule 1: Cytochrome P450 21-hydroxylase

Chain A:



• Molecule 1: Cytochrome P450 21-hydroxylase

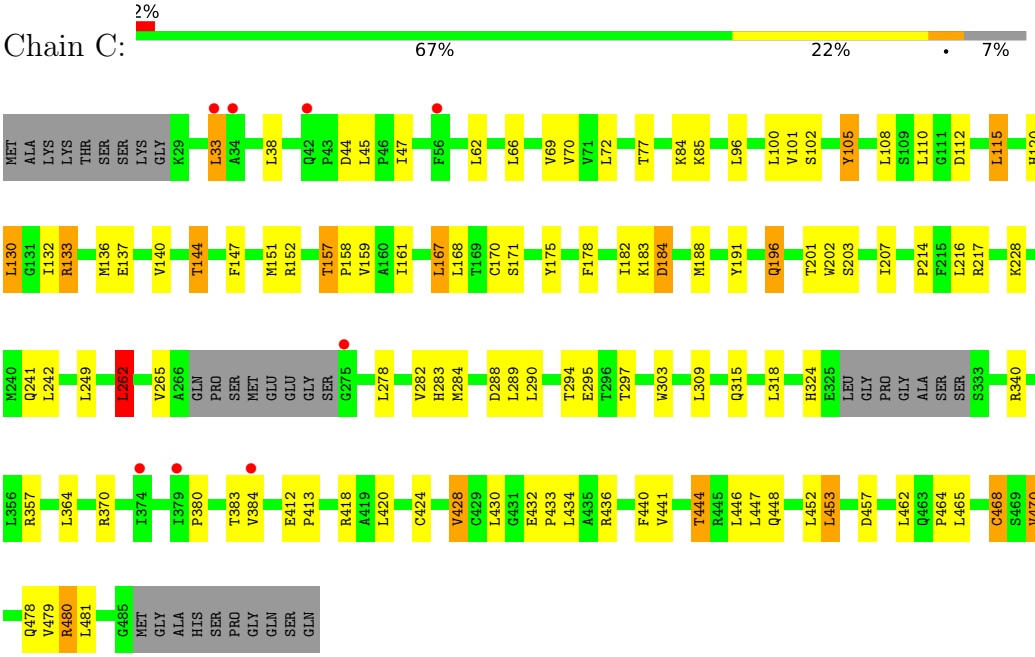
Chain B:



GLN

• Molecule 1: Cytochrome P450 21-hydroxylase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.43Å 88.39Å 111.42Å 90.00° 102.37° 90.00°	Depositor
Resolution (Å)	108.83 – 3.31 43.27 – 3.31	Depositor EDS
% Data completeness (in resolution range)	91.2 (108.83-3.31) 91.3 (43.27-3.31)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.191 , 0.241 0.200 , 0.245	Depositor DCC
R_{free} test set	1549 reflections (7.82%)	wwPDB-VP
Wilson B-factor (Å^2)	91.2	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 63.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10795	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: HEM, 3QZ

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	0.76	0/3621	1.02	11/4927 (0.2%)
1	B	0.67	0/3617	0.95	9/4922 (0.2%)
1	C	0.75	0/3621	1.03	14/4927 (0.3%)
All	All	0.72	0/10859	1.00	34/14776 (0.2%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	112	ASP	CB-CG-OD1	7.88	125.39	118.30
1	A	430	LEU	CA-CB-CG	7.69	132.99	115.30
1	C	112	ASP	CB-CG-OD1	7.37	124.93	118.30
1	C	430	LEU	CA-CB-CG	7.08	131.58	115.30
1	A	453	LEU	CA-CB-CG	6.91	131.19	115.30
1	B	278	LEU	CA-CB-CG	6.56	130.39	115.30
1	C	130	LEU	CB-CG-CD1	-6.11	100.61	111.00
1	B	430	LEU	CA-CB-CG	6.07	129.26	115.30
1	C	38	LEU	CA-CB-CG	6.03	129.18	115.30
1	A	412	GLU	N-CA-C	5.92	126.99	111.00
1	A	438	GLU	OE1-CD-OE2	-5.88	116.24	123.30
1	C	453	LEU	CA-CB-CG	5.86	128.78	115.30
1	B	103	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	115	LEU	CA-CB-CG	5.84	128.74	115.30
1	A	470	VAL	N-CA-C	-5.82	95.30	111.00
1	A	45	LEU	CB-CG-CD2	5.76	120.79	111.00
1	B	412	GLU	C-N-CD	5.71	140.40	128.40
1	A	133	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	401	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	C	262	LEU	CA-CB-CG	5.54	128.05	115.30
1	C	462	LEU	CB-CG-CD2	-5.44	101.75	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	411	LEU	CA-CB-CG	-5.42	102.84	115.30
1	C	167	LEU	CA-CB-CG	5.39	127.69	115.30
1	B	234	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	96	LEU	CB-CG-CD1	5.25	119.92	111.00
1	C	412	GLU	N-CA-C	5.23	125.13	111.00
1	A	411	LEU	CA-CB-CG	-5.21	103.32	115.30
1	C	84	LYS	CD-CE-NZ	5.15	123.54	111.70
1	B	446	LEU	CA-CB-CG	5.13	127.09	115.30
1	B	40	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	C	115	LEU	CA-CB-CG	5.10	127.03	115.30
1	C	33	LEU	CA-CB-CG	5.07	126.97	115.30
1	A	291	ILE	CG1-CB-CG2	-5.06	100.26	111.40
1	C	355	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	3531	0	3586	67	0
1	B	3527	0	3583	56	0
1	C	3531	0	3586	74	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
2	C	43	0	30	1	0
3	A	24	0	30	3	0
3	B	24	0	30	0	0
3	C	24	0	30	1	0
4	A	1	0	0	0	0
4	B	4	0	0	0	0
All	All	10795	0	10935	194	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 9.

All (194) 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:A:413:PRO:HG2	1:B:340:ARG:NH1	1.63	1.13
1:C:239:GLU:OE2	1:C:283:HIS:CE1	2.01	1.13
1:A:418:ARG:H	1:A:418:ARG:HD3	1.13	1.11
1:A:413:PRO:CG	1:B:340:ARG:HH11	1.66	1.09
1:C:129:LEU:O	1:C:133:ARG:HG2	1.56	1.03
1:C:239:GLU:OE2	1:C:283:HIS:ND1	1.96	0.99
1:A:413:PRO:HG2	1:B:340:ARG:HH11	1.22	0.97
1:A:413:PRO:CG	1:B:340:ARG:NH1	2.24	0.96
1:A:315:GLN:HE22	1:A:452:LEU:H	1.13	0.95
1:C:151:MET:HE1	1:C:159:VAL:HG11	1.52	0.92
1:C:315:GLN:HE22	1:C:452:LEU:H	1.23	0.85
1:B:61:ARG:HG2	1:B:70:VAL:HG12	1.59	0.84
1:A:75:LYS:HZ2	1:A:417:SER:HB2	1.43	0.83
1:C:157:THR:HG22	1:C:158:PRO:HD2	1.62	0.81
1:B:315:GLN:HE22	1:B:452:LEU:H	1.28	0.81
1:A:75:LYS:NZ	1:A:417:SER:HB2	1.96	0.80
1:B:413:PRO:HG2	1:C:340:ARG:HD2	1.63	0.80
1:A:178:PHE:CD1	1:A:241:GLN:HG2	2.17	0.78
1:A:196:GLN:HA	1:A:196:GLN:HE21	1.50	0.77
1:A:152:ARG:HH11	1:A:152:ARG:HA	1.49	0.76
1:A:188:MET:HE2	1:A:188:MET:HA	1.67	0.76
1:C:235:ASP:O	1:C:239:GLU:HG2	1.85	0.76
1:B:178:PHE:CD1	1:B:241:GLN:HG2	2.21	0.75
1:A:152:ARG:HH11	1:A:152:ARG:CA	1.99	0.75
1:A:140:VAL:O	1:A:144:THR:HG22	1.85	0.75
1:C:178:PHE:CD1	1:C:241:GLN:HG2	2.22	0.73
1:A:152:ARG:NH1	1:A:152:ARG:O	2.21	0.73
1:A:156:GLY:O	1:A:480:ARG:HD2	1.89	0.73
1:A:440:PHE:O	1:A:444:THR:HB	1.89	0.72
1:C:203:SER:O	1:C:468:CYS:SG	2.46	0.72
1:C:157:THR:CG2	1:C:158:PRO:HD2	2.20	0.71
1:C:130:LEU:HA	1:C:133:ARG:HG2	1.73	0.71
1:A:413:PRO:CD	1:B:340:ARG:NH1	2.55	0.70
1:A:418:ARG:H	1:A:418:ARG:CD	1.93	0.69
1:A:425:GLY:O	1:A:428:VAL:HG22	1.94	0.68
1:C:140:VAL:O	1:C:144:THR:HG22	1.94	0.67
1:B:129:LEU:HD11	1:B:433:PRO:HG2	1.76	0.67
1:C:380:PRO:HD2	1:C:383:THR:HG21	1.76	0.66
1:C:290:LEU:O	1:C:294:THR:HG23	1.95	0.65
1:B:140:VAL:O	1:B:144:THR:HG22	1.97	0.65
1:C:129:LEU:O	1:C:133:ARG:CG	2.40	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TRP:CE3	1:A:409:ARG:HB2	2.32	0.64
1:A:418:ARG:HD3	1:A:418:ARG:N	1.98	0.64
1:C:158:PRO:HB2	1:C:478:GLN:OE1	1.97	0.63
1:C:440:PHE:O	1:C:444:THR:HB	1.98	0.63
1:B:412:GLU:OE1	1:B:412:GLU:N	2.23	0.63
1:B:412:GLU:H	1:B:412:GLU:CD	1.98	0.61
1:B:196:GLN:HE21	1:B:196:GLN:HA	1.65	0.61
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.83	0.61
1:A:364:LEU:HD21	3:A:502:3QZ:OAD	2.02	0.59
1:A:188:MET:HA	1:A:188:MET:CE	2.30	0.59
1:C:191:TYR:OH	1:C:241:GLN:NE2	2.36	0.58
1:B:440:PHE:O	1:B:444:THR:HB	2.04	0.58
1:A:157:THR:CG2	1:A:158:PRO:HD2	2.34	0.57
1:A:432:GLU:O	1:A:436:ARG:HG3	2.03	0.57
1:A:175:TYR:OH	1:A:183:LYS:HB2	2.05	0.57
1:C:239:GLU:CD	1:C:283:HIS:CE1	2.76	0.56
1:B:201:THR:O	1:B:207:ILE:HD12	2.05	0.56
1:C:130:LEU:HA	1:C:133:ARG:CG	2.36	0.56
1:C:157:THR:HG22	1:C:158:PRO:CD	2.34	0.56
1:A:340:ARG:HH11	1:C:413:PRO:CD	2.18	0.56
1:B:290:LEU:O	1:B:294:THR:HG23	2.06	0.56
1:C:424:CYS:HA	1:C:428:VAL:CG1	2.36	0.55
1:B:414:GLY:H	1:C:418:ARG:HH22	1.53	0.55
1:C:157:THR:CG2	1:C:158:PRO:CD	2.84	0.55
1:A:69:VAL:HG22	1:A:384:VAL:HB	1.87	0.55
1:C:108:LEU:HD22	1:C:124:THR:HG21	1.88	0.55
1:A:406:TRP:O	1:A:409:ARG:HB3	2.06	0.55
2:B:501:HEM:HMB2	2:B:501:HEM:HBB2	1.87	0.55
1:A:424:CYS:HA	1:A:428:VAL:HG13	1.89	0.54
1:C:196:GLN:HE21	1:C:196:GLN:HA	1.72	0.54
1:C:69:VAL:HG22	1:C:384:VAL:HB	1.89	0.54
1:C:101:VAL:HG21	1:C:110:LEU:HD12	1.89	0.54
1:A:453:LEU:HB2	1:A:480:ARG:HB3	1.89	0.54
1:A:398:VAL:HG13	1:A:417:SER:OG	2.07	0.54
1:C:44:ASP:HB3	1:C:47:ILE:HB	1.88	0.54
1:C:452:LEU:HD23	1:C:481:LEU:HD22	1.87	0.54
1:A:413:PRO:HG3	1:B:340:ARG:HH11	1.66	0.53
1:C:424:CYS:HA	1:C:428:VAL:HG13	1.88	0.53
1:A:129:LEU:HD11	1:A:433:PRO:HG2	1.91	0.53
1:B:406:TRP:O	1:B:409:ARG:HB3	2.09	0.53
1:A:149:GLU:O	1:A:152:ARG:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LEU:HD13	1:B:282:VAL:HG11	1.91	0.53
1:B:151:MET:HE3	1:B:159:VAL:HG11	1.90	0.52
1:B:452:LEU:HD23	1:B:481:LEU:HD22	1.91	0.52
1:C:129:LEU:HD11	1:C:433:PRO:HG2	1.91	0.52
1:A:120:HIS:O	1:A:124:THR:HG22	2.10	0.52
1:C:309:LEU:HD11	1:C:479:VAL:HG23	1.91	0.52
1:C:465:LEU:HD13	1:C:473:LYS:O	2.10	0.51
1:A:171:SER:O	1:A:175:TYR:HD1	1.92	0.51
1:C:105:TYR:HB2	1:C:284:MET:HG2	1.93	0.51
1:B:69:VAL:HG22	1:B:384:VAL:HB	1.92	0.50
1:B:171:SER:O	1:B:175:TYR:HD1	1.94	0.50
1:A:144:THR:HG21	1:A:441:VAL:HG12	1.94	0.50
1:A:132:ILE:HD12	1:A:136:MET:HB2	1.92	0.50
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.92	0.50
1:C:178:PHE:HB2	1:C:182:ILE:HD13	1.94	0.50
1:C:188:MET:HA	1:C:188:MET:HE2	1.94	0.50
1:A:201:THR:O	1:A:207:ILE:HD12	2.12	0.50
1:B:108:LEU:HB3	1:B:288:ASP:OD2	2.13	0.49
1:A:157:THR:HG22	1:A:158:PRO:HD2	1.93	0.49
1:A:262:LEU:HD13	1:A:282:VAL:HG11	1.95	0.49
1:B:303:TRP:CD2	1:B:357:ARG:HG2	2.48	0.49
1:B:306:VAL:HG13	1:B:460:PRO:HB2	1.95	0.49
1:C:470:VAL:O	1:C:470:VAL:HG12	2.13	0.49
1:A:290:LEU:O	1:A:294:THR:HG23	2.13	0.48
1:B:309:LEU:HD11	1:B:479:VAL:HG23	1.94	0.48
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.96	0.48
1:A:398:VAL:CG1	1:A:417:SER:OG	2.61	0.48
1:C:453:LEU:HB2	1:C:480:ARG:HB3	1.94	0.48
1:A:71:VAL:HG22	1:A:386:ILE:HB	1.96	0.48
1:B:207:ILE:HD11	1:B:223:GLY:O	2.14	0.47
1:C:100:LEU:HD22	1:C:228:LYS:HE2	1.96	0.47
1:C:120:HIS:O	1:C:124:THR:HG22	2.15	0.47
1:C:171:SER:O	1:C:175:TYR:HD1	1.97	0.47
1:C:239:GLU:HG2	1:C:283:HIS:HE1	1.77	0.47
1:B:188:MET:HA	1:B:188:MET:HE2	1.97	0.47
1:A:315:GLN:NE2	1:A:452:LEU:H	1.96	0.47
1:A:413:PRO:CD	1:B:340:ARG:HH12	2.26	0.47
1:A:161:ILE:CG2	1:A:162:GLU:N	2.78	0.46
1:C:201:THR:O	1:C:207:ILE:HD12	2.15	0.46
1:C:102:SER:HB2	1:C:105:TYR:O	2.15	0.46
1:A:358:PRO:HG3	1:A:393:HIS:HD1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:LEU:CD2	1:C:124:THR:HG21	2.45	0.46
1:B:144:THR:HG21	1:B:441:VAL:HG12	1.97	0.46
1:A:411:LEU:HD23	1:A:411:LEU:HA	1.44	0.45
1:B:171:SER:HA	1:B:188:MET:SD	2.56	0.45
1:B:108:LEU:HD22	1:B:124:THR:HG21	1.99	0.45
1:C:202:TRP:HZ3	1:C:470:VAL:HG11	1.82	0.45
1:B:411:LEU:HD23	1:B:411:LEU:HA	1.59	0.45
1:C:214:PRO:O	1:C:217:ARG:HG2	2.15	0.45
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.46	0.45
1:B:227:LEU:O	1:B:231:ILE:HG12	2.16	0.45
1:B:453:LEU:HB2	1:B:480:ARG:HB3	1.98	0.45
1:C:432:GLU:O	1:C:436:ARG:HG3	2.16	0.45
1:A:352:GLU:HG3	1:A:407:PRO:HA	1.99	0.45
1:C:303:TRP:CD2	1:C:357:ARG:HG2	2.52	0.45
1:C:157:THR:HA	1:C:158:PRO:HD3	1.73	0.44
1:C:178:PHE:CG	1:C:241:GLN:HG2	2.53	0.44
1:B:120:HIS:O	1:B:124:THR:HG22	2.17	0.44
1:B:286:ALA:O	1:B:290:LEU:HG	2.17	0.44
1:A:409:ARG:HG3	1:A:416:ASN:HD21	1.82	0.44
1:C:196:GLN:HE22	1:C:295:GLU:CG	2.31	0.44
3:A:502:3QZ:OAD	3:A:502:3QZ:HACB	2.17	0.44
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.48	0.44
1:C:147:PHE:O	1:C:151:MET:HG2	2.17	0.44
1:C:364:LEU:HD21	3:C:502:3QZ:OAD	2.17	0.44
1:B:258:MET:HG2	1:B:262:LEU:HD22	1.99	0.44
1:C:262:LEU:HD13	1:C:282:VAL:HG11	2.00	0.44
1:A:153:ALA:O	1:A:155:PRO:HD3	2.17	0.44
1:B:178:PHE:HB2	1:B:182:ILE:HD13	1.99	0.43
1:B:468:CYS:HB2	1:B:469:SER:H	1.50	0.43
1:B:178:PHE:CG	1:B:241:GLN:HG2	2.53	0.43
1:A:342:ARG:HH22	1:C:324:HIS:CE1	2.36	0.43
3:A:502:3QZ:OAD	3:A:502:3QZ:CAC	2.66	0.43
1:A:148:CYS:O	1:A:152:ARG:HG2	2.19	0.43
1:B:105:TYR:HB2	1:B:284:MET:HG2	2.00	0.43
1:A:207:ILE:HD11	1:A:223:GLY:O	2.18	0.43
1:A:105:TYR:HB2	1:A:284:MET:HG2	2.00	0.43
1:C:452:LEU:HD23	1:C:481:LEU:CD2	2.49	0.43
1:B:413:PRO:HD2	1:C:340:ARG:NH1	2.34	0.42
1:A:178:PHE:CG	1:A:241:GLN:HG2	2.54	0.42
1:A:455:SER:HB2	1:A:478:GLN:O	2.20	0.42
1:B:406:TRP:CE3	1:B:409:ARG:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ARG:HG3	1:A:342:ARG:HH11	1.85	0.42
1:C:144:THR:HG21	1:C:441:VAL:HG12	2.01	0.42
1:C:465:LEU:HD11	1:C:474:MET:C	2.40	0.42
1:A:424:CYS:HA	1:A:428:VAL:CG1	2.49	0.42
1:B:483:PRO:HA	1:B:484:ARG:HA	1.77	0.42
1:C:464:PRO:HB3	1:C:472:LEU:CD2	2.50	0.42
1:A:303:TRP:CD2	1:A:357:ARG:HG2	2.55	0.41
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	2.02	0.41
1:C:132:ILE:HD12	1:C:136:MET:HB2	2.01	0.41
1:C:188:MET:HA	1:C:188:MET:CE	2.49	0.41
1:C:465:LEU:HD12	1:C:465:LEU:N	2.36	0.41
1:B:358:PRO:HG3	1:B:393:HIS:HD1	1.86	0.41
1:C:108:LEU:HB3	1:C:288:ASP:OD2	2.21	0.41
1:A:464:PRO:HB3	1:A:472:LEU:HD22	2.02	0.41
1:C:105:TYR:HB2	1:C:284:MET:CG	2.50	0.41
1:B:170:CYS:HA	1:B:294:THR:HG22	2.03	0.41
1:C:465:LEU:CD1	1:C:474:MET:C	2.88	0.41
1:B:199:LEU:HD23	1:B:295:GLU:HG3	2.02	0.41
1:C:318:LEU:CD2	1:C:346:LEU:HA	2.50	0.41
1:B:436:ARG:HH11	1:B:436:ARG:HD2	1.70	0.41
1:B:455:SER:HB2	1:B:478:GLN:O	2.21	0.41
1:C:72:LEU:HD22	1:C:77:THR:HB	2.02	0.41
1:A:108:LEU:HD22	1:A:124:THR:HG21	2.03	0.41
1:A:161:ILE:O	1:A:162:GLU:C	2.59	0.40
1:A:199:LEU:HD23	1:A:295:GLU:HG3	2.03	0.40
1:B:412:GLU:N	1:B:412:GLU:CD	2.72	0.40
1:C:170:CYS:HA	1:C:294:THR:HG22	2.03	0.40
1:C:239:GLU:HG2	1:C:283:HIS:CE1	2.55	0.40
1:B:151:MET:HE1	1:B:164:GLU:HG3	2.04	0.40
1:B:463:GLN:HA	1:B:464:PRO:HD3	1.94	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	436/476 (92%)	421 (97%)	13 (3%)	2 (0%)	29	61
1	B	435/476 (91%)	416 (96%)	17 (4%)	2 (0%)	29	61
1	C	436/476 (92%)	420 (96%)	12 (3%)	4 (1%)	17	49
All	All	1307/1428 (92%)	1257 (96%)	42 (3%)	8 (1%)	25	57

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	470	VAL
1	B	469	SER
1	C	470	VAL
1	A	184	ASP
1	B	184	ASP
1	C	184	ASP
1	C	468	CYS
1	C	157	THR

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	386/415 (93%)	338 (88%)	48 (12%)	4	19
1	B	386/415 (93%)	337 (87%)	49 (13%)	4	19
1	C	386/415 (93%)	345 (89%)	41 (11%)	6	25
All	All	1158/1245 (93%)	1020 (88%)	138 (12%)	5	21

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	41	LEU

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Mol	Chain	Res	Type
1	A	45	LEU
1	A	62	LEU
1	A	67	GLN
1	A	76	ARG
1	A	85	LYS
1	A	115	LEU
1	A	122	LYS
1	A	124	THR
1	A	129	LEU
1	A	130	LEU
1	A	137	GLU
1	A	144	THR
1	A	151	MET
1	A	157	THR
1	A	167	LEU
1	A	168	LEU
1	A	183	LYS
1	A	184	ASP
1	A	196	GLN
1	A	234	ARG
1	A	242	LEU
1	A	262	LEU
1	A	265	VAL
1	A	276	GLN
1	A	289	LEU
1	A	342	ARG
1	A	345	LEU
1	A	370	ARG
1	A	383	THR
1	A	388	ASN
1	A	416	ASN
1	A	417	SER
1	A	418	ARG
1	A	420	LEU
1	A	428	VAL
1	A	434	LEU
1	A	444	THR
1	A	446	LEU
1	A	447	LEU
1	A	448	GLN
1	A	453	LEU
1	A	457	ASP

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Mol	Chain	Res	Type
1	A	472	LEU
1	A	480	ARG
1	A	482	GLN
1	A	484	ARG
1	B	33	LEU
1	B	45	LEU
1	B	62	LEU
1	B	85	LYS
1	B	105	TYR
1	B	115	LEU
1	B	124	THR
1	B	129	LEU
1	B	137	GLU
1	B	144	THR
1	B	151	MET
1	B	152	ARG
1	B	161	ILE
1	B	167	LEU
1	B	168	LEU
1	B	183	LYS
1	B	184	ASP
1	B	193	LYS
1	B	196	GLN
1	B	234	ARG
1	B	239	GLU
1	B	242	LEU
1	B	262	LEU
1	B	265	VAL
1	B	276	GLN
1	B	278	LEU
1	B	289	LEU
1	B	297	THR
1	B	322	LEU
1	B	345	LEU
1	B	357	ARG
1	B	370	ARG
1	B	383	THR
1	B	388	ASN
1	B	401	ARG
1	B	418	ARG
1	B	420	LEU
1	B	428	VAL

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Mol	Chain	Res	Type
1	B	434	LEU
1	B	444	THR
1	B	446	LEU
1	B	447	LEU
1	B	448	GLN
1	B	457	ASP
1	B	465	LEU
1	B	468	CYS
1	B	469	SER
1	B	472	LEU
1	B	480	ARG
1	C	33	LEU
1	C	45	LEU
1	C	62	LEU
1	C	66	LEU
1	C	70	VAL
1	C	85	LYS
1	C	105	TYR
1	C	115	LEU
1	C	124	THR
1	C	129	LEU
1	C	133	ARG
1	C	137	GLU
1	C	144	THR
1	C	152	ARG
1	C	161	ILE
1	C	167	LEU
1	C	168	LEU
1	C	183	LYS
1	C	184	ASP
1	C	196	GLN
1	C	216	LEU
1	C	234	ARG
1	C	242	LEU
1	C	249	LEU
1	C	262	LEU
1	C	265	VAL
1	C	278	LEU
1	C	289	LEU
1	C	297	THR
1	C	345	LEU
1	C	370	ARG

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Mol	Chain	Res	Type
1	C	420	LEU
1	C	428	VAL
1	C	434	LEU
1	C	444	THR
1	C	446	LEU
1	C	447	LEU
1	C	448	GLN
1	C	457	ASP
1	C	472	LEU
1	C	480	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	196	GLN
1	A	241	GLN
1	A	263	GLN
1	A	315	GLN
1	A	319	GLN
1	A	347	ASN
1	A	388	ASN
1	A	448	GLN
1	B	196	GLN
1	B	241	GLN
1	B	263	GLN
1	B	315	GLN
1	B	319	GLN
1	B	388	ASN
1	B	448	GLN
1	C	196	GLN
1	C	241	GLN
1	C	263	GLN
1	C	283	HIS
1	C	315	GLN
1	C	319	GLN
1	C	388	ASN
1	C	416	ASN
1	C	448	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	A	501	1	27,50,50	1.26	3 (11%)	17,82,82	2.64	7 (41%)
2	HEM	C	501	1	27,50,50	1.30	3 (11%)	17,82,82	2.41	4 (23%)
3	3QZ	C	502	-	26,27,27	1.53	2 (7%)	41,45,45	2.04	12 (29%)
3	3QZ	B	502	-	26,27,27	1.32	1 (3%)	41,45,45	2.03	11 (26%)
3	3QZ	A	502	-	26,27,27	1.38	1 (3%)	41,45,45	1.96	11 (26%)
2	HEM	B	501	1	27,50,50	1.19	2 (7%)	17,82,82	2.69	5 (29%)

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	A	501	1	-	0/6/54/54	-
2	HEM	C	501	1	-	0/6/54/54	-
3	3QZ	C	502	-	-	2/6/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3QZ	B	502	-	-	5/6/68/68	0/4/4/4
3	3QZ	A	502	-	-	4/6/68/68	0/4/4/4
2	HEM	B	501	1	-	0/6/54/54	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	3QZ	CAA-CAP	-5.60	1.35	1.50
3	C	502	3QZ	CAA-CAP	-5.49	1.36	1.50
3	B	502	3QZ	CAA-CAP	-5.22	1.36	1.50
2	C	501	HEM	C3D-C2D	2.81	1.46	1.37
2	A	501	HEM	C4A-CHB	2.80	1.48	1.41
2	A	501	HEM	C1D-ND	-2.66	1.30	1.36
2	C	501	HEM	C4A-CHB	2.63	1.48	1.41
2	B	501	HEM	C3D-C2D	2.56	1.45	1.37
3	C	502	3QZ	CAX-CAW	-2.45	1.52	1.56
2	C	501	HEM	C1C-C2C	-2.44	1.37	1.42
2	B	501	HEM	C4A-CHB	2.36	1.47	1.41
2	A	501	HEM	C3D-C2D	2.22	1.44	1.37

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEM	C1D-C2D-C3D	-8.00	101.43	107.00
2	B	501	HEM	C1D-C2D-C3D	-7.79	101.57	107.00
3	C	502	3QZ	CAW-CAX-CAP	7.69	121.03	112.89
2	C	501	HEM	C1D-C2D-C3D	-6.72	102.32	107.00
3	B	502	3QZ	CAW-CAX-CAP	6.30	119.56	112.89
3	A	502	3QZ	CAW-CAX-CAP	4.61	117.77	112.89
2	C	501	HEM	CMC-C2C-C3C	4.55	133.20	124.68
3	A	502	3QZ	CAC-CAW-CAX	4.26	114.22	109.14
3	B	502	3QZ	CAC-CAW-CAX	4.10	114.03	109.14
3	A	502	3QZ	CAO-CAX-CAW	4.06	107.01	103.20
2	B	501	HEM	CMC-C2C-C3C	3.97	132.10	124.68
3	A	502	3QZ	CAH-CAR-CAG	-3.86	114.42	120.87
2	B	501	HEM	C4A-C3A-C2A	-3.85	104.32	107.00
3	A	502	3QZ	CAH-CAR-CAV	3.68	123.56	116.77
3	B	502	3QZ	CAN-CAK-CAT	3.63	119.40	113.11
2	A	501	HEM	CMC-C2C-C3C	3.53	131.28	124.68
3	A	502	3QZ	CAI-CAQ-CAG	3.45	122.06	116.74
3	B	502	3QZ	CAI-CAQ-CAG	3.43	122.03	116.74
3	C	502	3QZ	CAO-CAX-CAW	3.40	106.39	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	HEM	CMB-C2B-C3B	3.30	130.85	124.68
3	B	502	3QZ	CAK-CAT-CAS	3.29	116.49	111.75
3	C	502	3QZ	CAK-CAT-CAS	3.00	116.07	111.75
2	B	501	HEM	CMB-C2B-C3B	3.00	130.28	124.68
3	A	502	3QZ	CAK-CAT-CAS	2.99	116.06	111.75
3	C	502	3QZ	CAI-CAQ-CAG	2.98	121.33	116.74
3	B	502	3QZ	CAH-CAR-CAV	2.96	122.24	116.77
3	C	502	3QZ	CAH-CAR-CAG	-2.96	115.93	120.87
3	C	502	3QZ	CAH-CAR-CAV	2.84	122.00	116.77
3	A	502	3QZ	CAN-CAK-CAT	2.78	117.93	113.11
2	A	501	HEM	C2C-C3C-C4C	-2.73	104.99	106.90
3	C	502	3QZ	CAL-CAU-CAW	2.67	107.31	103.73
3	C	502	3QZ	OAF-CAX-CAO	-2.64	104.28	110.34
3	B	502	3QZ	CAN-CAW-CAX	-2.57	112.68	116.79
2	B	501	HEM	CMA-C3A-C2A	2.55	129.75	124.94
3	A	502	3QZ	CAJ-CAH-CAR	2.52	116.67	111.93
3	C	502	3QZ	CAN-CAK-CAT	2.49	117.43	113.11
2	A	501	HEM	CMA-C3A-C2A	2.45	129.55	124.94
3	A	502	3QZ	CAL-CAU-CAW	2.45	107.01	103.73
2	A	501	HEM	C4A-C3A-C2A	-2.42	105.31	107.00
3	B	502	3QZ	CAB-CAV-CAM	-2.40	105.64	109.43
3	C	502	3QZ	CAB-CAV-CAR	2.39	112.22	108.34
3	B	502	3QZ	CAH-CAR-CAG	-2.27	117.06	120.87
3	C	502	3QZ	CAJ-CAS-CAT	2.23	113.25	110.49
3	A	502	3QZ	CAR-CAG-CAQ	-2.18	120.15	123.67
2	A	501	HEM	CMA-C3A-C4A	-2.16	125.14	128.46
2	C	501	HEM	CMA-C3A-C4A	-2.13	125.19	128.46
3	B	502	3QZ	CAB-CAV-CAT	2.12	114.21	111.68
3	B	502	3QZ	CAM-CAI-CAQ	-2.10	107.14	111.62
2	A	501	HEM	CMD-C2D-C3D	2.09	128.88	124.94
3	C	502	3QZ	CAC-CAW-CAX	2.07	111.60	109.14

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	3QZ	CAA-CAP-CAX-CAO
3	A	502	3QZ	OAD-CAP-CAX-CAO
3	C	502	3QZ	CAA-CAP-CAX-CAO
3	B	502	3QZ	OAD-CAP-CAX-OAF
3	A	502	3QZ	CAA-CAP-CAX-CAW
3	A	502	3QZ	OAD-CAP-CAX-CAW

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Mol	Chain	Res	Type	Atoms
3	B	502	3QZ	CAA-CAP-CAX-CAW
3	B	502	3QZ	OAD-CAP-CAX-CAW
3	B	502	3QZ	CAA-CAP-CAX-OAF
3	B	502	3QZ	OAD-CAP-CAX-CAO
3	C	502	3QZ	OAD-CAP-CAX-CAO

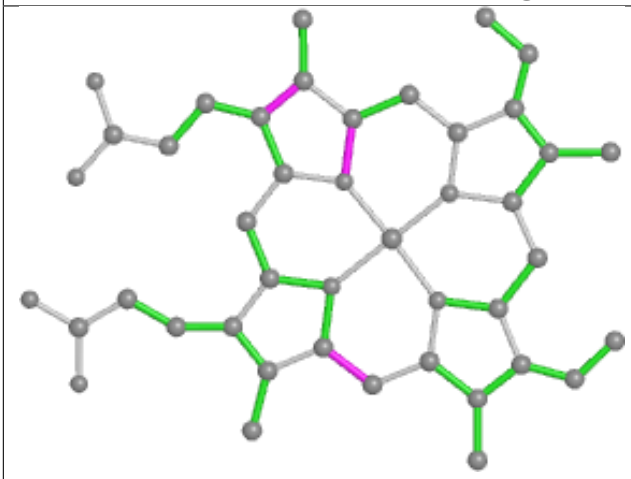
There are no ring outliers.

5 monomers are involved in 11 short contacts:

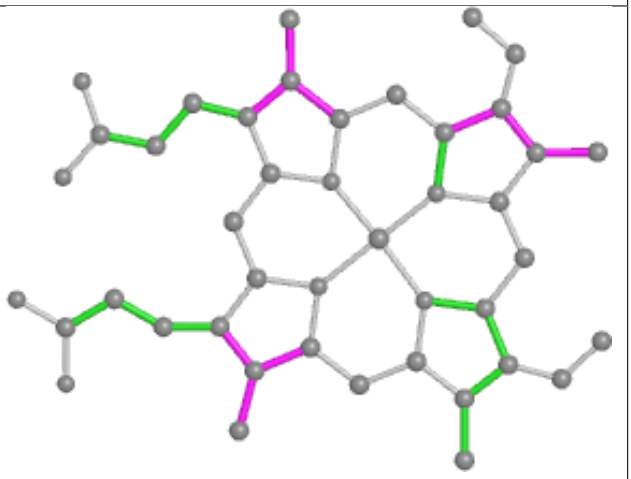
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	2	0
2	C	501	HEM	1	0
3	C	502	3QZ	1	0
3	A	502	3QZ	3	0
2	B	501	HEM	4	0

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.

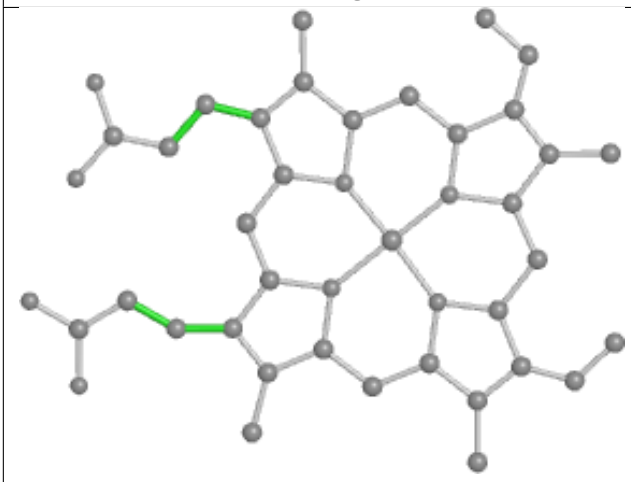
Ligand HEM A 501



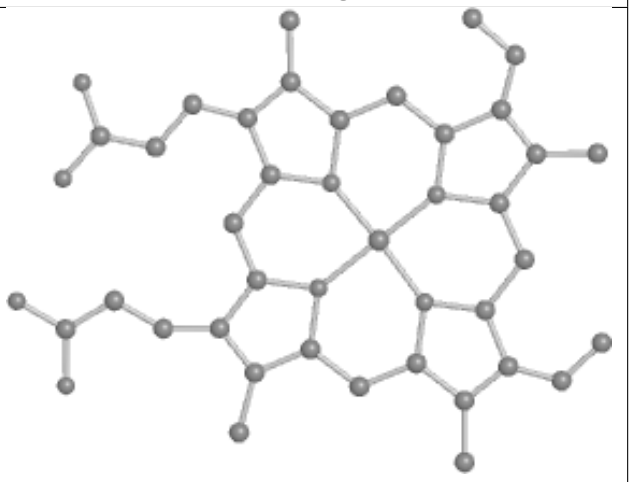
Bond lengths



Bond angles

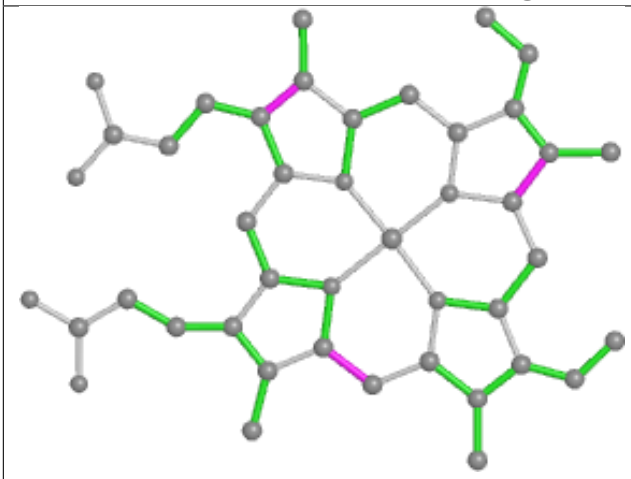


Torsions

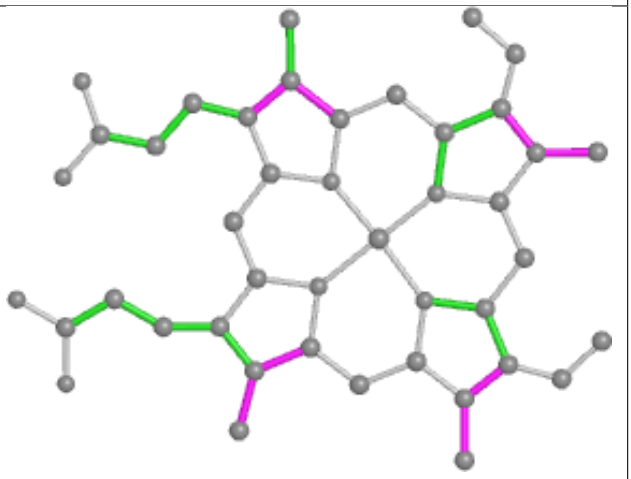


Rings

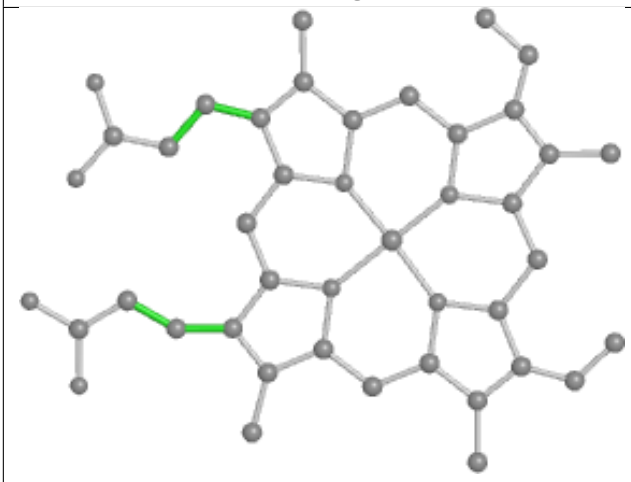
Ligand HEM C 501



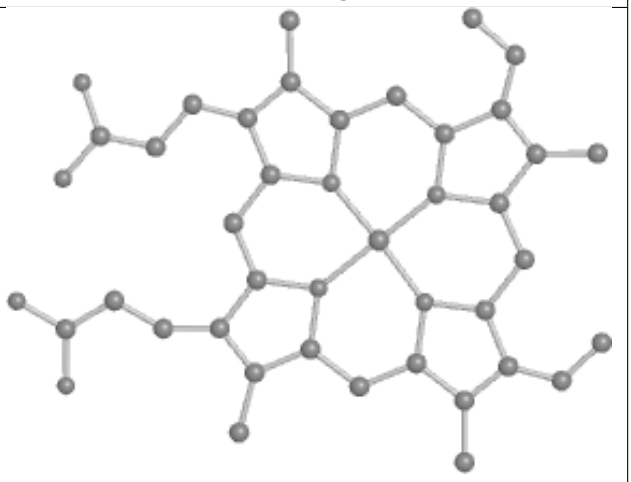
Bond lengths



Bond angles

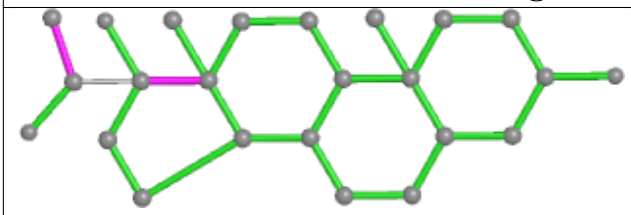


Torsions

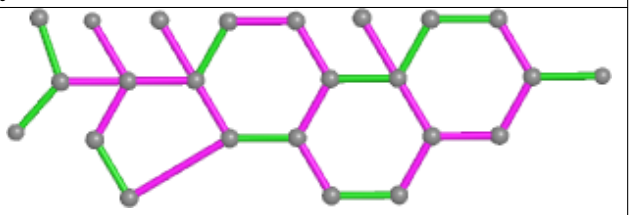


Rings

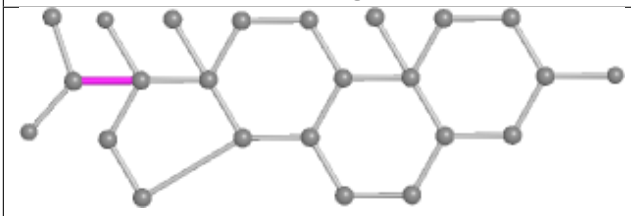
Ligand 3QZ C 502



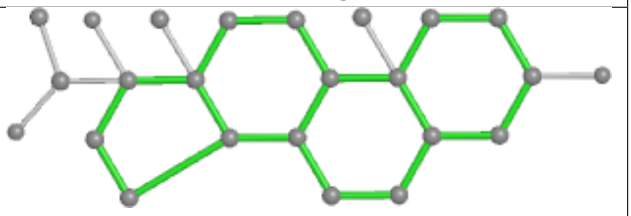
Bond lengths



Bond angles

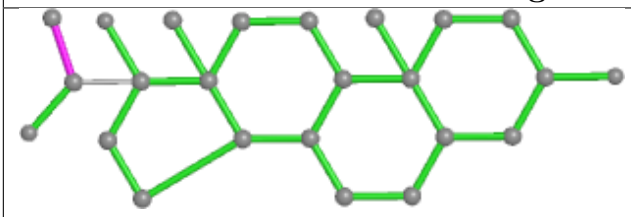


Torsions

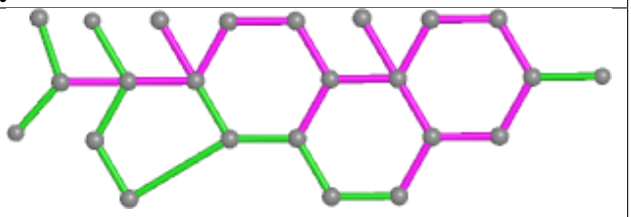


Rings

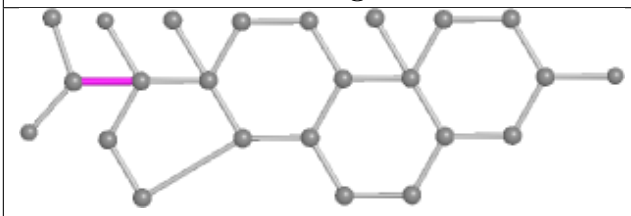
Ligand 3QZ B 502



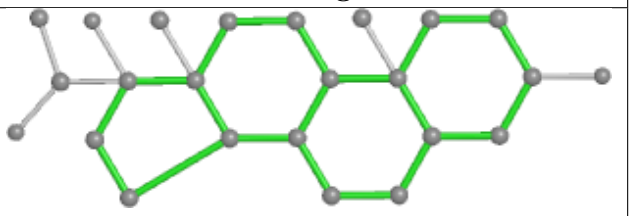
Bond lengths



Bond angles

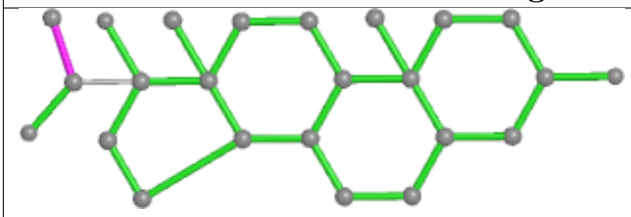


Torsions

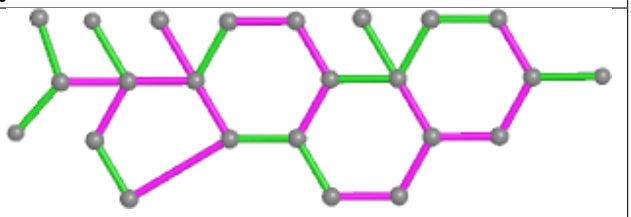


Rings

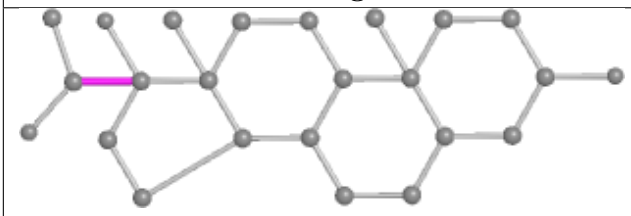
Ligand 3QZ A 502



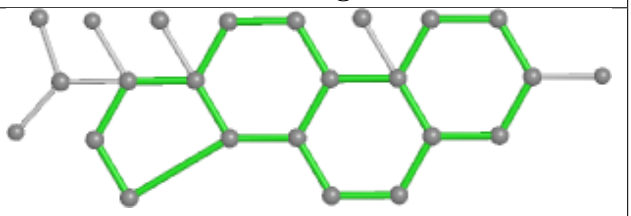
Bond lengths



Bond angles

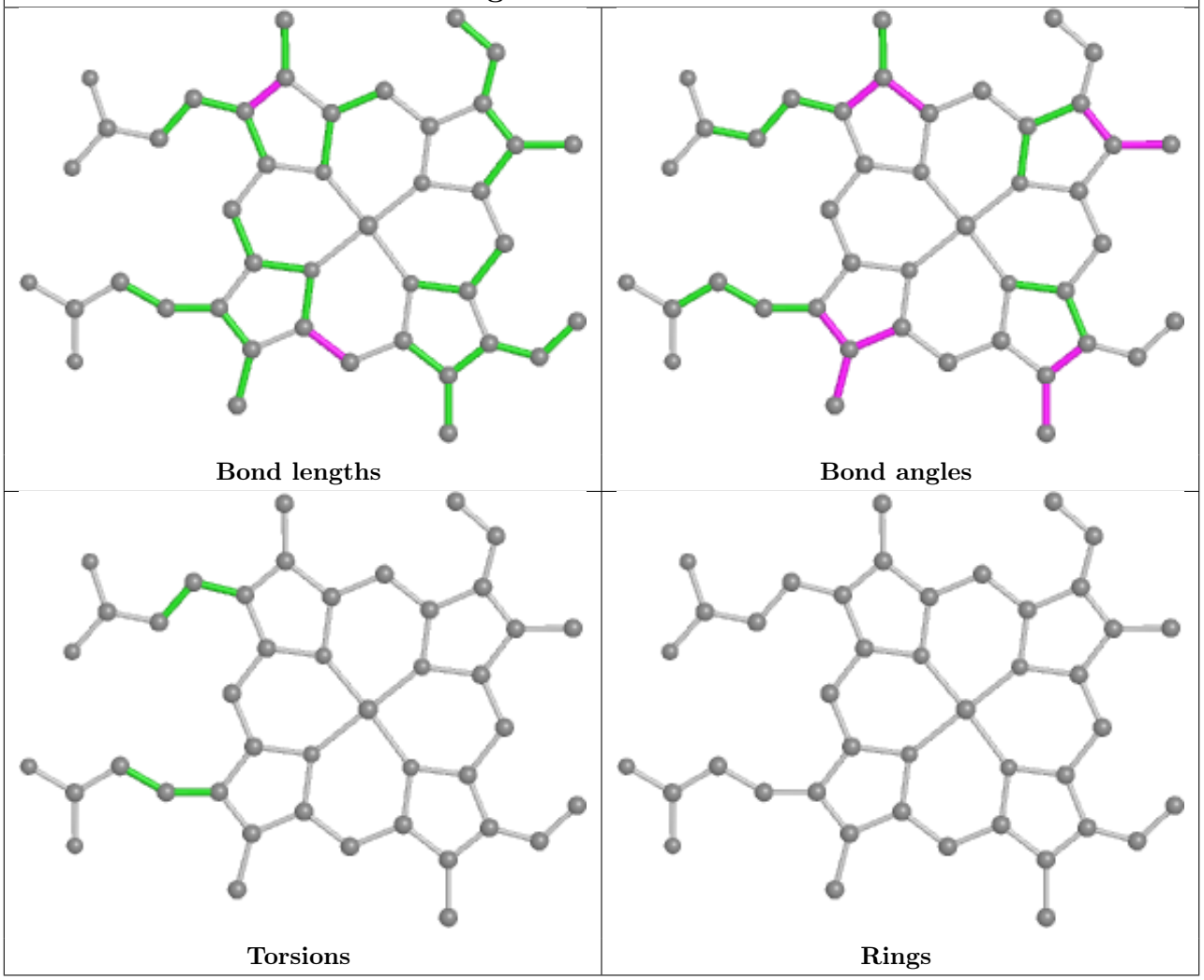


Torsions



Rings

Ligand HEM B 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	442/476 (92%)	-0.12	5 (1%)	80	81	62, 91, 129, 176	38 (8%)
1	B	441/476 (92%)	0.01	11 (2%)	57	55	63, 92, 134, 177	27 (6%)
1	C	442/476 (92%)	0.06	8 (1%)	68	67	61, 92, 125, 159	19 (4%)
All	All	1325/1428 (92%)	-0.02	24 (1%)	68	67	61, 92, 130, 177	84 (6%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	ALA	4.3
1	C	275	GLY	4.0
1	C	56	PHE	4.0
1	C	34	ALA	3.8
1	C	374	ILE	3.8
1	B	413	PRO	3.3
1	B	417	SER	3.3
1	B	157	THR	3.3
1	B	414	GLY	3.1
1	C	384	VAL	3.1
1	B	159	VAL	2.7
1	C	33	LEU	2.4
1	B	249	LEU	2.4
1	C	379	ILE	2.4
1	B	217	ARG	2.3
1	B	457	ASP	2.3
1	A	485	GLY	2.3
1	A	372	SER	2.3
1	A	221	ASN	2.2
1	B	158	PRO	2.2
1	C	42	GLN	2.2
1	B	248	SER	2.2
1	B	218	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	153	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

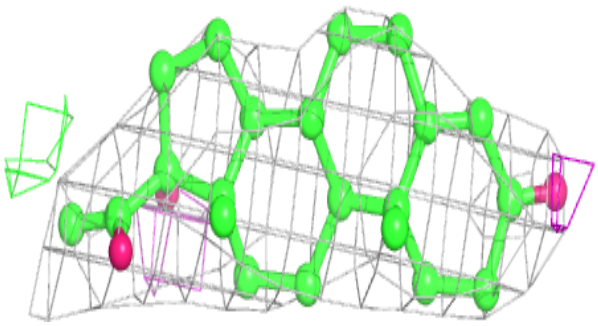
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

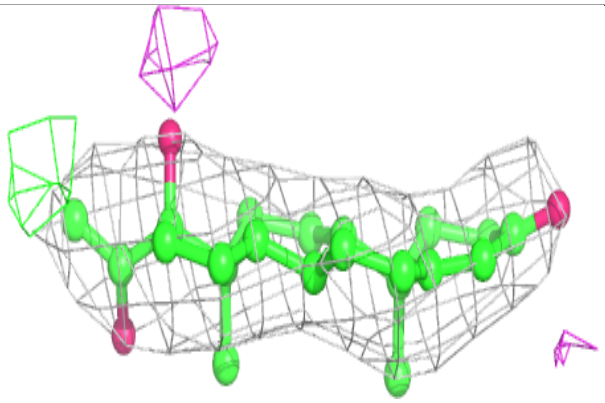
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	3QZ	A	502	24/24	0.93	0.35	77,78,86,93	0
3	3QZ	B	502	24/24	0.96	0.26	77,80,85,91	0
3	3QZ	C	502	24/24	0.96	0.27	80,86,95,103	0
2	HEM	C	501	43/43	0.97	0.24	84,98,102,104	0
2	HEM	A	501	43/43	0.97	0.25	77,91,97,99	0
2	HEM	B	501	43/43	0.98	0.22	85,100,104,116	0

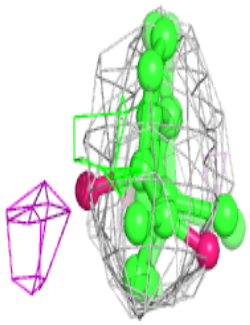
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3QZ A 502:

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

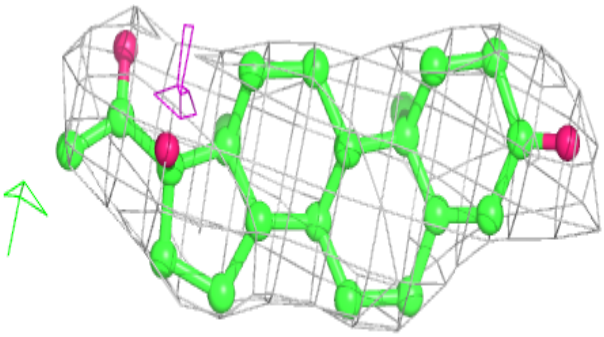


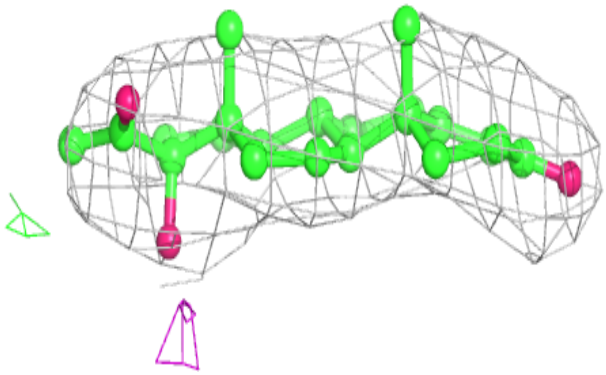


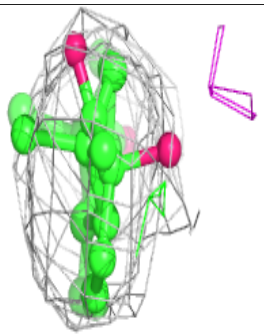


Electron density around 3QZ B 502:

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

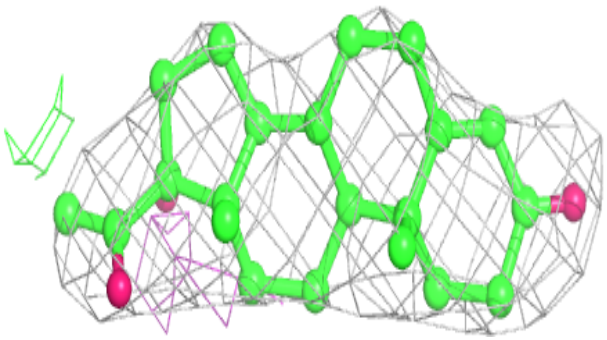


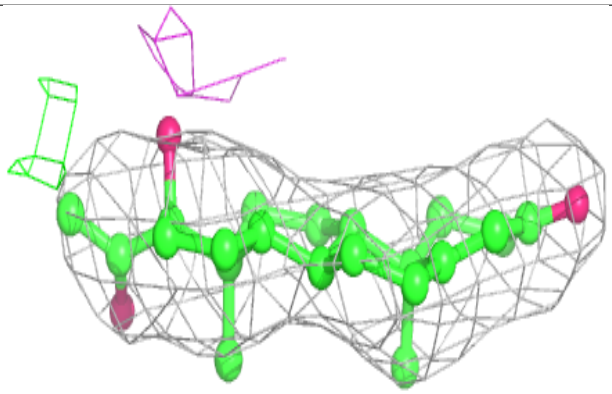


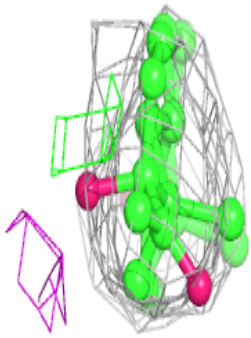


Electron density around 3QZ C 502:

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

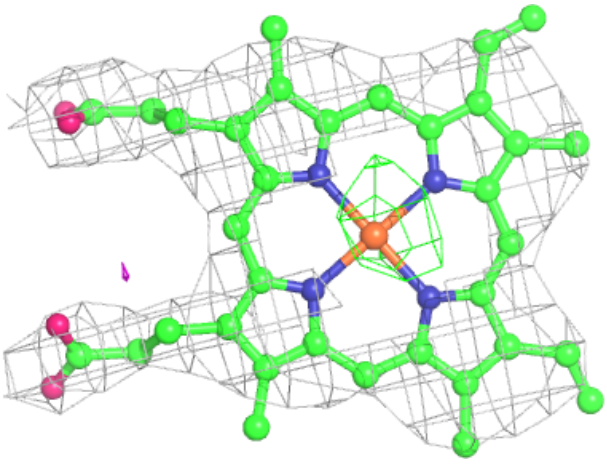


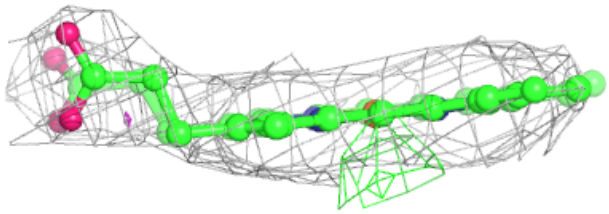


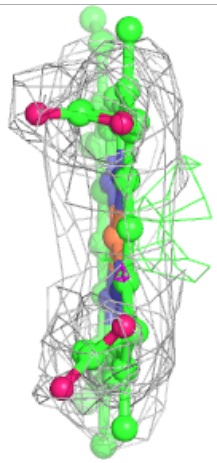


Electron density around HEM C 501:

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

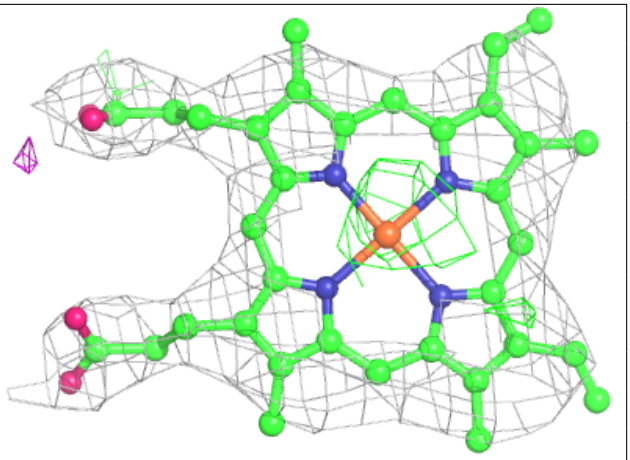


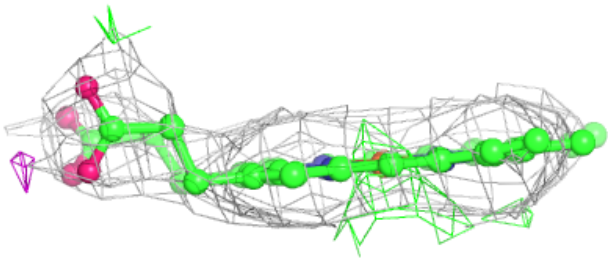


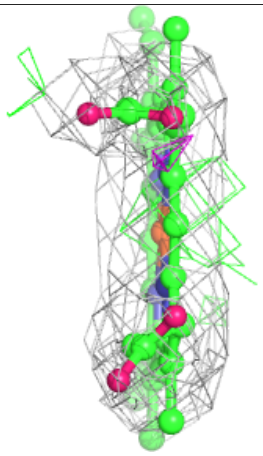


Electron density around HEM A 501:

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

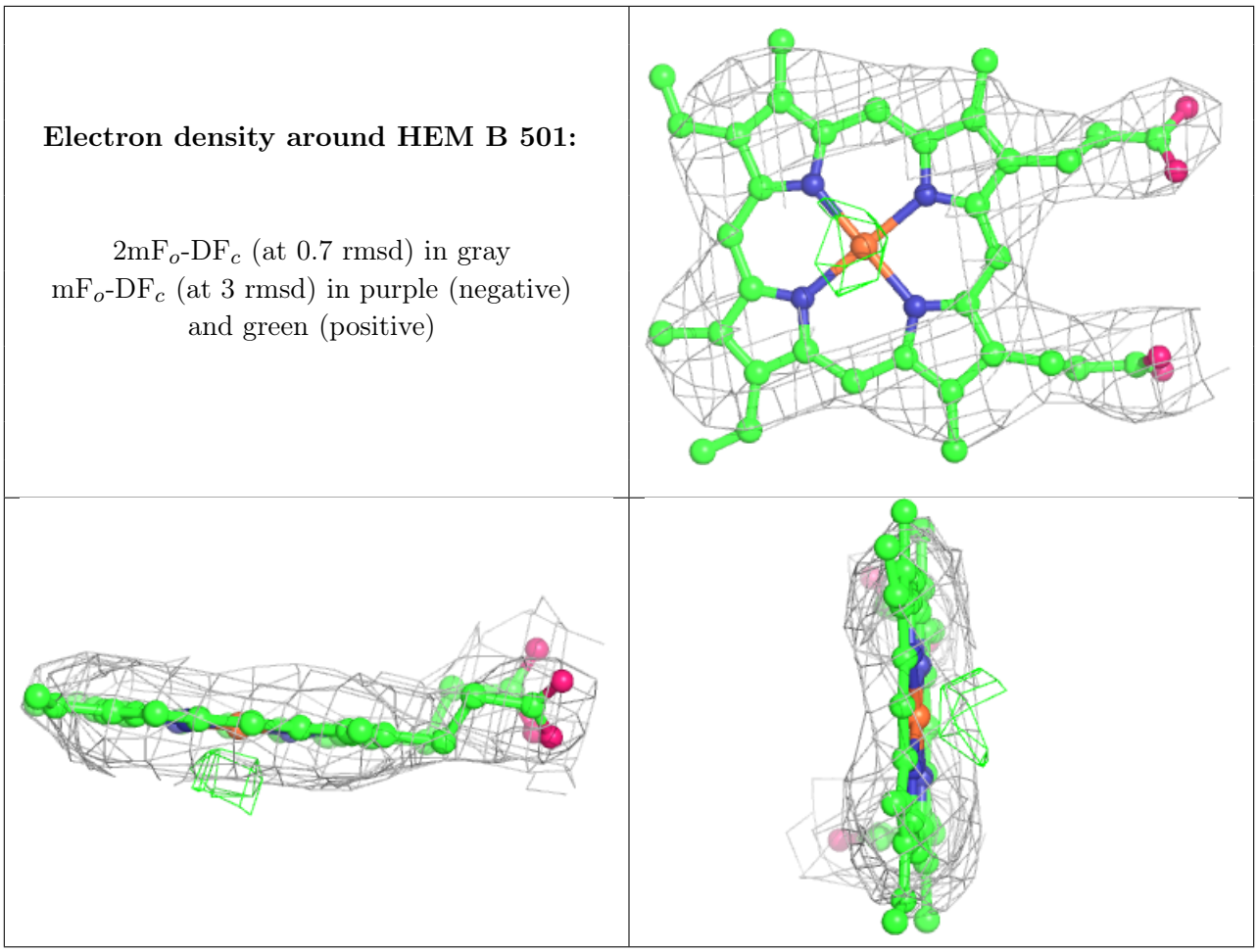






Electron density around HEM B 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.