



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:04 AM UTC

PDB ID : 5VBU / pdb_00005vbu
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 types of validation reports are described at

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

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

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

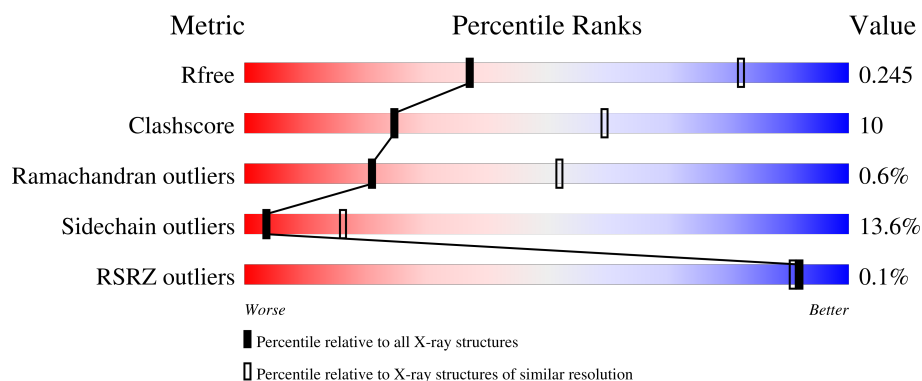
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	476	
1	B	476	
1	C	476	

2 Entry composition

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:

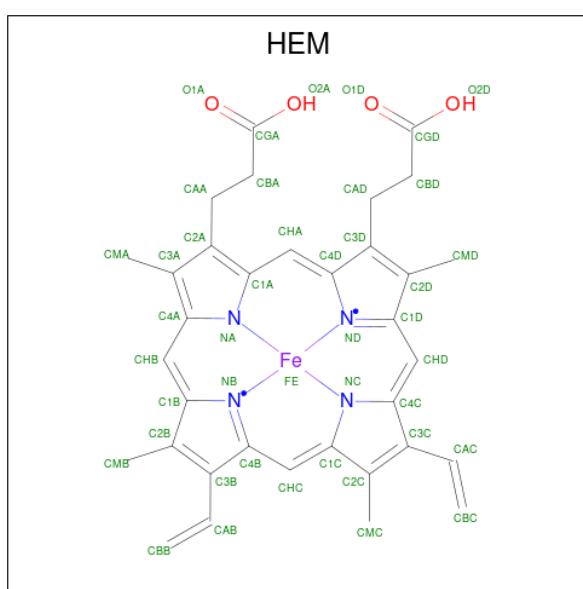
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP Q16874
A	21	ALA	-	expression tag	UNP Q16874
A	22	LYS	-	expression tag	UNP Q16874
A	23	LYS	-	expression tag	UNP Q16874
A	24	THR	-	expression tag	UNP Q16874
A	25	SER	-	expression tag	UNP Q16874
A	26	SER	-	expression tag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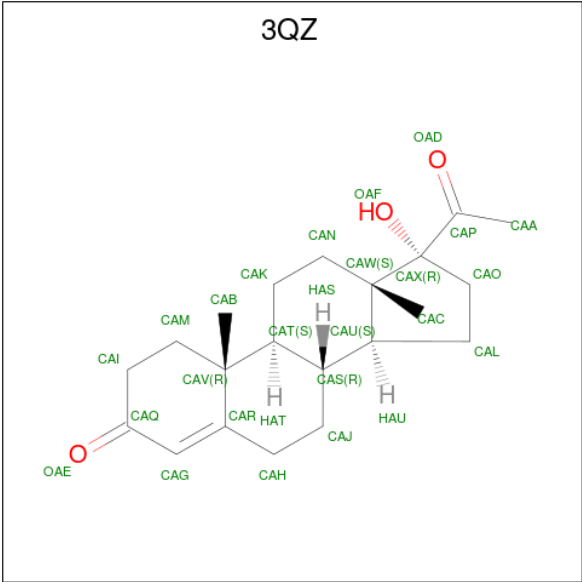
Chain	Residue	Modelled	Actual	Comment	Reference
C	23	LYS	-	expression tag	UNP Q16874
C	24	THR	-	expression tag	UNP Q16874
C	25	SER	-	expression tag	UNP Q16874
C	26	SER	-	expression tag	UNP Q16874
C	27	LYS	-	expression tag	UNP Q16874
C	28	GLY	-	expression tag	UNP Q16874
C	29	LYS	-	expression tag	UNP Q16874

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



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

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



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

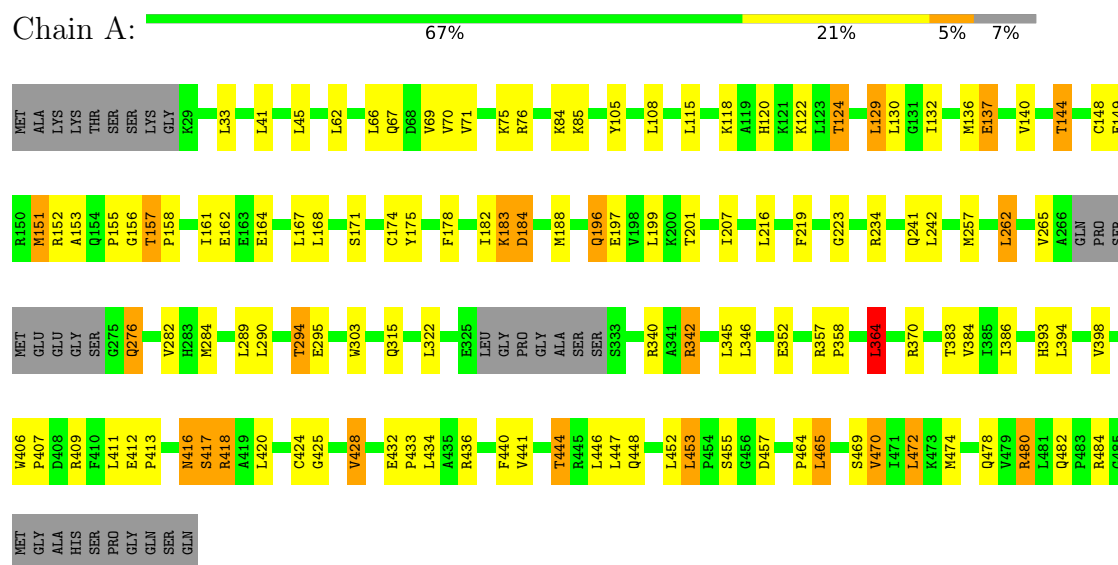
- Molecule 4 is water.

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

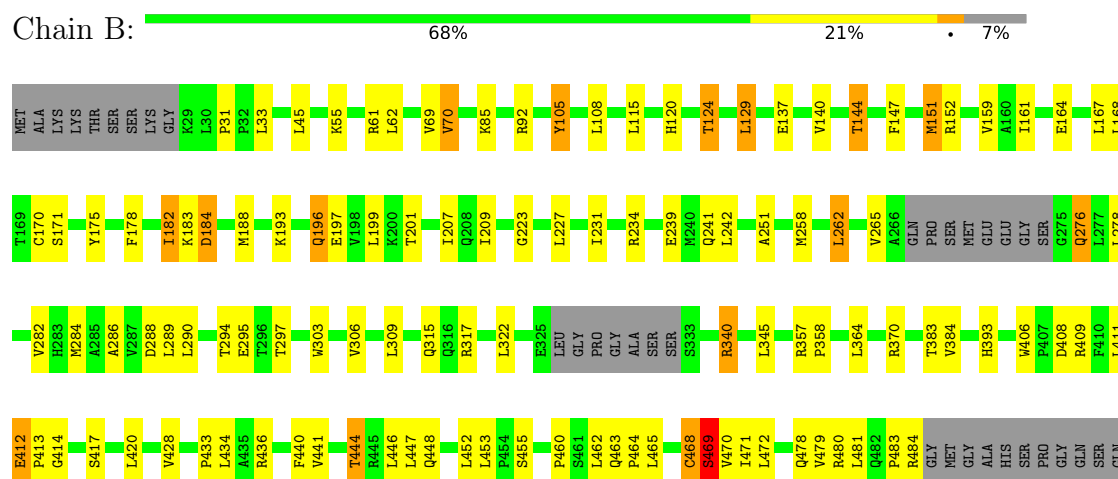
3 Residue-property plots [i](#)

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



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4 Data and refinement statistics

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 – 3.31 108.83 – 3.31	Depositor EDS
% Data completeness (in resolution range)	91.2 (108.83-3.31) 91.3 (108.83-3.31)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (7.13%)	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)	0.34 , 78.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3QZ, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.00	1/3621 (0.0%)	1.33	13/4927 (0.3%)
1	B	0.90	0/3617	1.26	14/4922 (0.3%)
1	C	0.99	2/3621 (0.1%)	1.35	13/4927 (0.3%)
All	All	0.96	3/10859 (0.0%)	1.31	40/14776 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	GLU	CA-C	5.83	1.59	1.52
1	C	406	TRP	C-O	-5.16	1.19	1.24
1	C	135	SER	N-CA	5.08	1.52	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	412	GLU	CA-C-N	-11.38	106.78	119.98
1	B	412	GLU	C-N-CA	-11.38	106.78	119.98
1	C	406	TRP	CA-C-N	11.30	131.16	119.19
1	C	406	TRP	C-N-CA	11.30	131.16	119.19
1	A	412	GLU	N-CA-C	9.74	126.99	113.16
1	C	379	ILE	CA-C-N	8.66	128.60	120.03
1	C	379	ILE	C-N-CA	8.66	128.60	120.03
1	B	412	GLU	N-CA-C	8.60	124.45	112.75
1	C	412	GLU	N-CA-C	8.43	125.13	113.16
1	C	324	HIS	N-CA-C	7.56	119.52	111.28
1	A	470	VAL	N-CA-C	-6.75	95.30	109.34
1	B	31	PRO	O-C-N	6.67	124.38	121.31
1	A	276	GLN	N-CA-C	-6.59	99.31	109.52
1	B	276	GLN	N-CA-C	-6.42	99.98	109.81
1	C	157	THR	CA-C-N	6.40	126.31	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	THR	C-N-CA	6.40	126.31	119.85
1	A	465	LEU	CA-C-N	6.21	127.61	119.84
1	A	465	LEU	C-N-CA	6.21	127.61	119.84
1	C	428	VAL	CB-CA-C	-6.20	101.96	111.08
1	A	364	LEU	CA-C-N	-5.96	113.83	119.85
1	A	364	LEU	C-N-CA	-5.96	113.83	119.85
1	B	251	ALA	N-CA-C	5.90	118.47	111.33
1	C	31	PRO	O-C-N	5.90	123.92	121.15
1	C	251	ALA	N-CA-C	5.74	119.10	111.75
1	A	257	MET	N-CA-C	5.71	117.59	111.36
1	A	412	GLU	CA-C-N	-5.71	113.91	119.90
1	A	412	GLU	C-N-CA	-5.71	113.91	119.90
1	A	219	PHE	CB-CA-C	5.45	117.20	109.08
1	A	469	SER	CA-C-N	5.41	131.70	121.97
1	A	469	SER	C-N-CA	5.41	131.70	121.97
1	C	249	LEU	N-CA-C	5.36	118.00	110.23
1	B	469	SER	N-CA-C	-5.10	99.93	110.80
1	B	340	ARG	CA-C-N	5.06	127.32	120.38
1	B	340	ARG	C-N-CA	5.06	127.32	120.38
1	C	160	ALA	N-CA-C	-5.05	98.83	108.17
1	B	92	ARG	CA-C-N	-5.02	115.61	120.98
1	B	92	ARG	C-N-CA	-5.02	115.61	120.98
1	B	370	ARG	CA-C-N	-5.01	114.42	119.83
1	B	370	ARG	C-N-CA	-5.01	114.42	119.83
1	B	417	SER	N-CA-C	5.01	117.26	110.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3531	0	3586	71	0
1	B	3527	0	3583	57	0
1	C	3531	0	3586	79	0
2	A	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	204	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (204) 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:A:188:MET:HE2	1:A:188:MET:HA	1.55	0.87
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:151:MET:HE1	1:C:159:VAL:HG11	1.72	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:C:188:MET:HA	1:C:188:MET:HE2	1.73	0.70
1:B:412:GLU:H	1:B:412:GLU:CD	1.98	0.69
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
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:239:GLU:CD	1:C:283:HIS:CE1	2.76	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:A:174:CYS:SG	1:A:188:MET:HE1	2.38	0.62
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: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:C:147:PHE:CE1	1:C:151:MET:HE2	2.39	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:B:188:MET:HA	1:B:188:MET:HE2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:262:LEU:HD13	1:B:282:VAL:HG11	1.91	0.53
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:C:107:ASP:OD1	1:C:284:MET:HE3	2.11	0.51
1:A:188:MET:HA	1:A:188:MET:CE	2.30	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:A:201:THR:O	1:A:207:ILE:HD12	2.12	0.50
1:C:151:MET:CE	1:C:159:VAL:HG11	2.42	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:174:CYS:SG	1:C:188:MET:HE1	2.54	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: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:C:465:LEU:HD11	1:C:474:MET:C	2.40	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:147:PHE:HE1	1:C:151:MET:HE2	1.78	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
1:C:108:LEU:CD2	1:C:124:THR:HG21	2.45	0.46
1:C:465:LEU:CD1	1:C:474:MET:C	2.88	0.46
1:B:144:THR:HG21	1:B:441:VAL:HG12	1.97	0.46
1:B:151:MET:HE1	1:B:164:GLU:HG3	1.98	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:412:GLU:CD	1:B:412:GLU:N	2.72	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:161:ILE:O	1:A:162:GLU:C	2.59	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:B:317:ARG:HH22	1:B:408:ASP:CG	2.25	0.44
1:C:157:THR:HA	1:C:158:PRO:HD3	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:147:PHE:CE1	1:B:151:MET:HE2	2.52	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:A:151:MET:HE1	1:A:164:GLU:HG3	2.01	0.43
1:A:152:ARG:HH11	1:A:152:ARG:C	2.26	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
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: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:412:GLU:H	1:C:412:GLU:CD	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:PRO:HB3	1:A:472:LEU:HD22	2.02	0.41
1:A:465:LEU:HD12	1:A:474:MET:C	2.44	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: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:199:LEU:HD23	1:A:295:GLU:HG3	2.03	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: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%)	24	56
1	B	435/476 (91%)	416 (96%)	17 (4%)	2 (0%)	24	56
1	C	436/476 (92%)	420 (96%)	12 (3%)	4 (1%)	14	43
All	All	1307/1428 (92%)	1257 (96%)	42 (3%)	8 (1%)	21	52

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	470	VAL
1	B	469	SER
1	C	470	VAL

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Mol	Chain	Res	Type
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 ⓘ

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%)	327 (85%)	59 (15%)	3	13
1	B	386/415 (93%)	334 (86%)	52 (14%)	4	16
1	C	386/415 (93%)	340 (88%)	46 (12%)	5	20
All	All	1158/1245 (93%)	1001 (86%)	157 (14%)	3	16

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	41	LEU
1	A	45	LEU
1	A	62	LEU
1	A	66	LEU
1	A	67	GLN
1	A	70	VAL
1	A	76	ARG
1	A	84	LYS
1	A	85	LYS
1	A	115	LEU
1	A	118	LYS
1	A	122	LYS
1	A	124	THR
1	A	129	LEU
1	A	130	LEU
1	A	137	GLU

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Mol	Chain	Res	Type
1	A	144	THR
1	A	151	MET
1	A	157	THR
1	A	167	LEU
1	A	168	LEU
1	A	182	ILE
1	A	183	LYS
1	A	184	ASP
1	A	196	GLN
1	A	197	GLU
1	A	216	LEU
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	294	THR
1	A	322	LEU
1	A	342	ARG
1	A	345	LEU
1	A	346	LEU
1	A	364	LEU
1	A	370	ARG
1	A	383	THR
1	A	394	LEU
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
1	A	472	LEU
1	A	480	ARG
1	A	482	GLN
1	A	484	ARG

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Mol	Chain	Res	Type
1	B	33	LEU
1	B	45	LEU
1	B	55	LYS
1	B	62	LEU
1	B	70	VAL
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	159	VAL
1	B	161	ILE
1	B	167	LEU
1	B	168	LEU
1	B	182	ILE
1	B	183	LYS
1	B	184	ASP
1	B	193	LYS
1	B	196	GLN
1	B	197	GLU
1	B	209	ILE
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	364	LEU
1	B	383	THR
1	B	420	LEU
1	B	428	VAL
1	B	434	LEU
1	B	444	THR

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Mol	Chain	Res	Type
1	B	446	LEU
1	B	447	LEU
1	B	448	GLN
1	B	462	LEU
1	B	465	LEU
1	B	468	CYS
1	B	469	SER
1	B	470	VAL
1	B	471	ILE
1	B	472	LEU
1	C	33	LEU
1	C	45	LEU
1	C	62	LEU
1	C	66	LEU
1	C	70	VAL
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	159	VAL
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	197	GLU
1	C	216	LEU
1	C	234	ARG
1	C	242	LEU
1	C	250	VAL
1	C	262	LEU
1	C	265	VAL
1	C	278	LEU
1	C	289	LEU
1	C	297	THR
1	C	322	LEU
1	C	345	LEU

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Mol	Chain	Res	Type
1	C	364	LEU
1	C	370	ARG
1	C	401	ARG
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	471	ILE
1	C	472	LEU
1	C	480	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	196	GLN
1	A	221	ASN
1	A	229	GLN
1	A	241	GLN
1	A	263	GLN
1	A	299	ASN
1	A	311	HIS
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	236	HIS
1	B	241	GLN
1	B	263	GLN
1	B	283	HIS
1	B	299	ASN
1	B	311	HIS
1	B	315	GLN
1	B	319	GLN
1	B	347	ASN
1	B	388	ASN

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Mol	Chain	Res	Type
1	B	390	GLN
1	B	448	GLN
1	B	478	GLN
1	C	67	GLN
1	C	196	GLN
1	C	221	ASN
1	C	229	GLN
1	C	236	HIS
1	C	241	GLN
1	C	283	HIS
1	C	299	ASN
1	C	315	GLN
1	C	319	GLN
1	C	347	ASN
1	C	388	ASN
1	C	390	GLN
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 oligosaccharides 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	$\# Z > 2$
3	3QZ	B	502	-	27,27,27	1.48	3 (11%)	44,45,45	2.05	14 (31%)
2	HEM	C	501	1	50,50,50	2.51	24 (48%)	67,82,82	2.01	17 (25%)
2	HEM	B	501	1	50,50,50	2.43	25 (50%)	67,82,82	1.97	17 (25%)
3	3QZ	A	502	-	27,27,27	1.43	1 (3%)	44,45,45	1.96	12 (27%)
3	3QZ	C	502	-	27,27,27	1.61	3 (11%)	44,45,45	1.98	14 (31%)
2	HEM	A	501	1	50,50,50	2.53	25 (50%)	67,82,82	1.93	15 (22%)

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
3	3QZ	B	502	-	-	5/6/68/68	0/4/4/4
2	HEM	C	501	1	-	0/14/54/54	-
2	HEM	B	501	1	-	0/14/54/54	-
3	3QZ	A	502	-	-	4/6/68/68	0/4/4/4
3	3QZ	C	502	-	-	2/6/68/68	0/4/4/4
2	HEM	A	501	1	-	0/14/54/54	-

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	3QZ	CAA-CAP	-5.92	1.35	1.50
3	C	502	3QZ	CAA-CAP	-5.80	1.36	1.50
3	B	502	3QZ	CAA-CAP	-5.51	1.36	1.50
2	B	501	HEM	C4D-ND	-4.99	1.31	1.40
2	A	501	HEM	CHB-C1B	4.90	1.48	1.38
2	B	501	HEM	C3C-C4C	-4.85	1.37	1.46
2	A	501	HEM	C4D-ND	-4.73	1.32	1.40
2	C	501	HEM	C3C-C4C	-4.70	1.37	1.46
2	C	501	HEM	CHB-C1B	4.62	1.47	1.38
2	A	501	HEM	FE-NB	4.58	2.09	1.94
2	B	501	HEM	CHB-C1B	4.54	1.47	1.38
2	A	501	HEM	C3C-C4C	-4.50	1.38	1.46
2	A	501	HEM	CHC-C1C	4.28	1.46	1.38
2	C	501	HEM	C4D-ND	-4.28	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C3D-C2D	4.27	1.46	1.36
2	C	501	HEM	C1C-C2C	-4.19	1.37	1.45
2	A	501	HEM	CHB-C4A	4.17	1.48	1.39
2	C	501	HEM	CHD-C4C	4.16	1.46	1.38
2	A	501	HEM	C1D-ND	-4.15	1.30	1.38
2	B	501	HEM	CHC-C1C	4.13	1.46	1.38
2	C	501	HEM	FE-NB	4.08	2.07	1.94
2	C	501	HEM	CHB-C4A	3.97	1.48	1.39
2	B	501	HEM	C3D-C2D	3.93	1.45	1.36
2	B	501	HEM	CHD-C4C	3.93	1.46	1.38
2	C	501	HEM	C1C-NC	-3.84	1.32	1.39
2	C	501	HEM	CHC-C1C	3.73	1.45	1.38
2	B	501	HEM	FE-NB	3.71	2.06	1.94
2	A	501	HEM	C1C-NC	-3.63	1.32	1.39
2	B	501	HEM	CHB-C4A	3.63	1.47	1.39
2	A	501	HEM	FE-NA	3.56	2.06	1.95
2	B	501	HEM	FE-NC	3.55	2.06	1.95
2	A	501	HEM	C4C-NC	-3.51	1.33	1.39
2	A	501	HEM	C3D-C2D	3.47	1.44	1.36
2	A	501	HEM	C1A-NA	-3.45	1.33	1.39
2	A	501	HEM	CHD-C4C	3.45	1.45	1.38
2	C	501	HEM	FE-ND	3.40	2.05	1.94
2	A	501	HEM	C1A-C2A	-3.22	1.38	1.44
2	B	501	HEM	C1A-NA	-3.22	1.33	1.39
2	B	501	HEM	C1C-C2C	-3.21	1.39	1.45
2	C	501	HEM	FE-NC	3.19	2.05	1.95
2	C	501	HEM	C4C-NC	-3.13	1.33	1.39
2	B	501	HEM	FE-NA	3.12	2.05	1.95
3	B	502	3QZ	CAX-CAP	-3.10	1.51	1.53
2	A	501	HEM	CHA-C4D	3.07	1.44	1.38
2	C	501	HEM	C4A-NA	-3.06	1.33	1.39
2	A	501	HEM	C1C-C2C	-3.06	1.39	1.45
2	C	501	HEM	CHD-C1D	2.97	1.46	1.39
2	C	501	HEM	C4B-NB	-2.92	1.33	1.38
2	B	501	HEM	C1D-ND	-2.90	1.33	1.38
2	B	501	HEM	CHC-C4B	2.87	1.45	1.39
2	C	501	HEM	FE-NA	2.87	2.04	1.95
2	B	501	HEM	C4C-NC	-2.76	1.34	1.39
2	C	501	HEM	CHC-C4B	2.72	1.45	1.39
2	B	501	HEM	C4B-NB	-2.71	1.33	1.38
2	B	501	HEM	C1B-C2B	-2.70	1.39	1.44
2	A	501	HEM	C4B-NB	-2.70	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	CHC-C4B	2.69	1.45	1.39
2	B	501	HEM	CHD-C1D	2.68	1.45	1.39
2	C	501	HEM	CHA-C1A	2.67	1.45	1.39
2	B	501	HEM	C1C-NC	-2.67	1.34	1.39
2	A	501	HEM	FE-ND	2.67	2.03	1.94
2	A	501	HEM	C4A-NA	-2.67	1.34	1.39
2	C	501	HEM	C1A-NA	-2.67	1.34	1.39
2	A	501	HEM	FE-NC	2.67	2.04	1.95
2	B	501	HEM	FE-ND	2.66	2.03	1.94
2	C	501	HEM	C1D-ND	-2.64	1.33	1.38
2	B	501	HEM	CHA-C4D	2.58	1.43	1.38
2	C	501	HEM	C1A-C2A	-2.55	1.39	1.44
2	C	501	HEM	C1B-NB	-2.50	1.35	1.40
2	B	501	HEM	C1A-C2A	-2.50	1.39	1.44
3	C	502	3QZ	CAX-CAW	-2.50	1.52	1.56
2	A	501	HEM	CHA-C1A	2.48	1.45	1.39
2	A	501	HEM	C1B-C2B	-2.38	1.39	1.44
2	C	501	HEM	C1B-C2B	-2.37	1.39	1.44
2	B	501	HEM	C1B-NB	-2.20	1.36	1.40
2	A	501	HEM	C4A-C3A	-2.14	1.38	1.43
2	A	501	HEM	O2D-CGD	-2.08	1.23	1.30
2	B	501	HEM	C4A-NA	-2.05	1.35	1.39
3	B	502	3QZ	OAD-CAP	2.04	1.25	1.21
3	C	502	3QZ	OAE-CAQ	-2.04	1.19	1.23
2	B	501	HEM	O2D-CGD	-2.04	1.24	1.30

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	3QZ	CAW-CAX-CAP	6.78	121.03	112.93
2	A	501	HEM	C2D-C1D-ND	5.88	116.70	109.90
2	C	501	HEM	C3D-C4D-ND	5.87	116.61	110.17
3	B	502	3QZ	CAW-CAX-CAP	5.55	119.56	112.93
2	A	501	HEM	C1D-C2D-C3D	-5.28	101.43	106.98
2	B	501	HEM	C1D-C2D-C3D	-5.14	101.57	106.98
2	B	501	HEM	C3C-C2C-C1C	-5.07	102.25	107.05
2	B	501	HEM	C2D-C1D-ND	4.63	115.26	109.90
2	C	501	HEM	C2D-C1D-ND	4.58	115.19	109.90
2	C	501	HEM	C2B-C1B-NB	4.50	115.01	109.84
2	C	501	HEM	C1D-C2D-C3D	-4.43	102.32	106.98
2	A	501	HEM	CHD-C1D-C2D	-4.42	118.05	125.03
3	B	502	3QZ	OAF-CAX-CAP	-4.23	97.13	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C2B-C1B-NB	4.13	114.59	109.84
3	A	502	3QZ	CAO-CAX-CAW	4.12	107.01	103.24
3	A	502	3QZ	CAC-CAW-CAX	4.10	114.22	109.11
2	B	501	HEM	CHD-C1D-C2D	-4.08	118.58	125.03
3	A	502	3QZ	CAW-CAX-CAP	4.05	117.77	112.93
3	A	502	3QZ	CAH-CAR-CAG	-4.03	114.42	120.86
2	C	501	HEM	CHA-C4D-C3D	-4.00	117.84	125.23
2	A	501	HEM	C3D-C4D-ND	3.98	114.54	110.17
3	B	502	3QZ	CAC-CAW-CAX	3.95	114.03	109.11
2	B	501	HEM	C3D-C4D-ND	3.89	114.43	110.17
3	A	502	3QZ	CAH-CAR-CAV	3.85	123.56	116.76
2	B	501	HEM	C2B-C1B-NB	3.85	114.27	109.84
2	A	501	HEM	C2A-C1A-NA	3.81	114.38	110.15
2	C	501	HEM	C3C-C2C-C1C	-3.74	103.51	107.05
3	B	502	3QZ	CAN-CAK-CAT	3.69	119.40	113.14
2	B	501	HEM	C2A-C1A-NA	3.68	114.23	110.15
2	B	501	HEM	CHA-C4D-C3D	-3.66	118.48	125.23
2	C	501	HEM	C2A-C1A-NA	3.54	114.08	110.15
3	A	502	3QZ	CAI-CAQ-CAG	3.51	122.06	116.73
3	B	502	3QZ	CAI-CAQ-CAG	3.48	122.03	116.73
3	C	502	3QZ	CAO-CAX-CAW	3.44	106.39	103.24
3	B	502	3QZ	CAK-CAT-CAS	3.38	116.49	111.78
2	B	501	HEM	CMD-C2D-C1D	3.37	130.30	125.03
3	B	502	3QZ	CAH-CAR-CAV	3.10	122.24	116.76
2	A	501	HEM	CHA-C4D-C3D	-3.09	119.52	125.23
3	C	502	3QZ	CAH-CAR-CAG	-3.09	115.93	120.86
3	C	502	3QZ	CAK-CAT-CAS	3.08	116.07	111.78
3	A	502	3QZ	CAK-CAT-CAS	3.07	116.06	111.78
2	A	501	HEM	C3C-C2C-C1C	-3.06	104.15	107.05
2	C	501	HEM	C4D-C3D-C2D	-3.04	102.47	106.89
3	C	502	3QZ	CAI-CAQ-CAG	3.02	121.33	116.73
3	C	502	3QZ	OAF-CAX-CAP	-3.01	100.06	107.26
2	C	501	HEM	CHD-C1D-C2D	-3.01	120.28	125.03
3	C	502	3QZ	CAH-CAR-CAV	2.97	122.00	116.76
2	A	501	HEM	CMD-C2D-C1D	2.95	129.65	125.03
2	C	501	HEM	CMD-C2D-C1D	2.92	129.59	125.03
2	C	501	HEM	C3B-C2B-C1B	-2.89	104.24	106.41
2	C	501	HEM	C3B-C4B-NB	2.88	111.53	109.47
2	C	501	HEM	O2D-CGD-CBD	2.84	122.98	114.00
3	A	502	3QZ	CAN-CAK-CAT	2.82	117.93	113.14
3	C	502	3QZ	CAL-CAU-CAW	2.81	107.31	103.70
2	A	501	HEM	C3B-C2B-C1B	-2.74	104.36	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	C4B-C3B-C2B	-2.63	104.86	107.28
3	B	502	3QZ	CAN-CAW-CAX	-2.61	112.68	116.77
3	A	502	3QZ	CAJ-CAH-CAR	2.59	116.67	111.93
3	A	502	3QZ	CAL-CAU-CAW	2.57	107.01	103.70
2	B	501	HEM	C3B-C2B-C1B	-2.57	104.48	106.41
3	C	502	3QZ	CAN-CAK-CAT	2.53	117.43	113.14
2	B	501	HEM	C2C-C1C-NC	2.52	114.29	109.64
3	C	502	3QZ	CAB-CAV-CAR	2.51	112.22	108.38
3	B	502	3QZ	CAB-CAV-CAM	-2.49	105.64	109.43
3	C	502	3QZ	OAF-CAX-CAO	-2.45	104.28	110.26
2	A	501	HEM	CAD-C3D-C4D	2.41	128.90	124.70
2	C	501	HEM	C1A-C2A-C3A	-2.40	103.15	106.87
2	A	501	HEM	C4D-C3D-C2D	-2.40	103.41	106.89
2	C	501	HEM	C2C-C1C-NC	2.39	114.06	109.64
3	B	502	3QZ	CAH-CAR-CAG	-2.37	117.06	120.86
2	B	501	HEM	C3A-C4A-NA	2.37	113.93	110.14
3	C	502	3QZ	CAJ-CAS-CAT	2.28	113.25	110.52
3	A	502	3QZ	CAR-CAG-CAQ	-2.28	120.15	123.67
3	B	502	3QZ	CAB-CAV-CAT	2.27	114.21	111.66
3	B	502	3QZ	CAM-CAI-CAQ	-2.19	107.14	111.60
3	A	502	3QZ	CAA-CAP-CAX	2.19	122.81	118.57
2	B	501	HEM	C4A-C3A-C2A	-2.18	104.32	106.82
2	B	501	HEM	CHB-C4A-C3A	-2.16	121.15	127.43
2	A	501	HEM	CHD-C4C-C3C	-2.16	121.56	125.21
2	B	501	HEM	CHA-C4D-ND	2.16	127.03	124.37
2	A	501	HEM	C4C-C3C-C2C	-2.10	104.99	106.81
2	A	501	HEM	C3B-C4B-NB	2.10	110.97	109.47
2	B	501	HEM	CHB-C1B-C2B	-2.09	121.01	126.95
2	B	501	HEM	C4D-C3D-C2D	-2.06	103.89	106.89
2	C	501	HEM	O1D-CGD-CBD	-2.06	116.55	123.09
3	C	502	3QZ	CAR-CAG-CAQ	-2.06	120.48	123.67
3	B	502	3QZ	CAJ-CAH-CAR	2.02	115.63	111.93
3	B	502	3QZ	CAL-CAU-CAW	2.01	106.28	103.70
3	C	502	3QZ	CAC-CAW-CAX	2.00	111.60	109.11

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

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

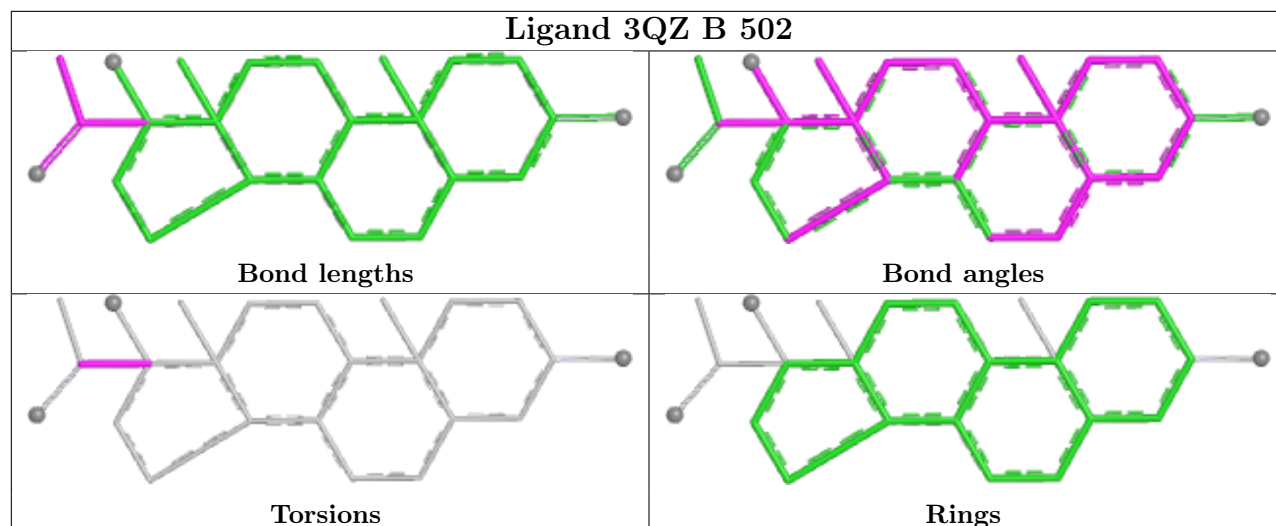
There are no ring outliers.

5 monomers are involved in 11 short contacts:

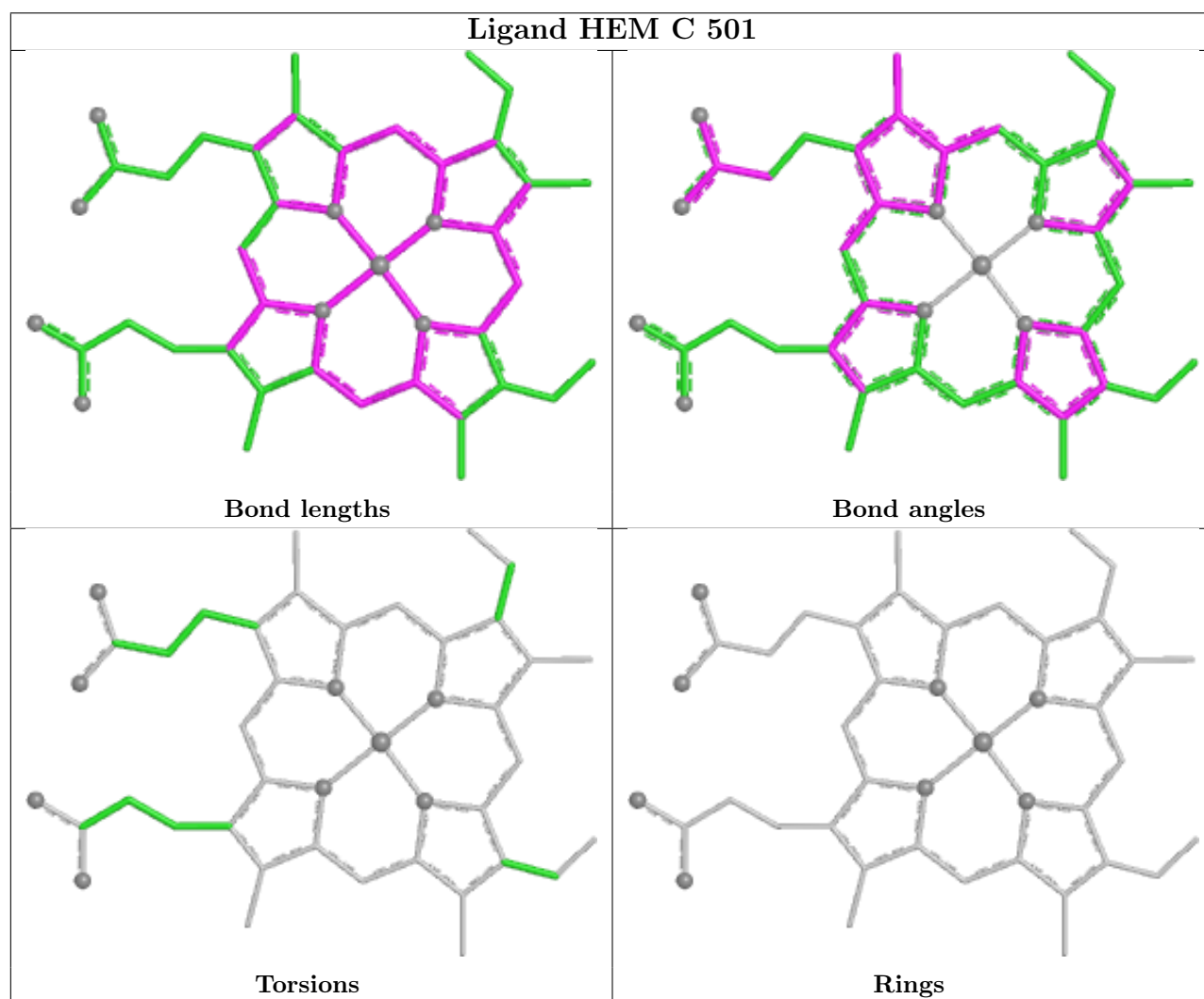
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	HEM	1	0
2	B	501	HEM	4	0
3	A	502	3QZ	3	0
3	C	502	3QZ	1	0
2	A	501	HEM	2	0

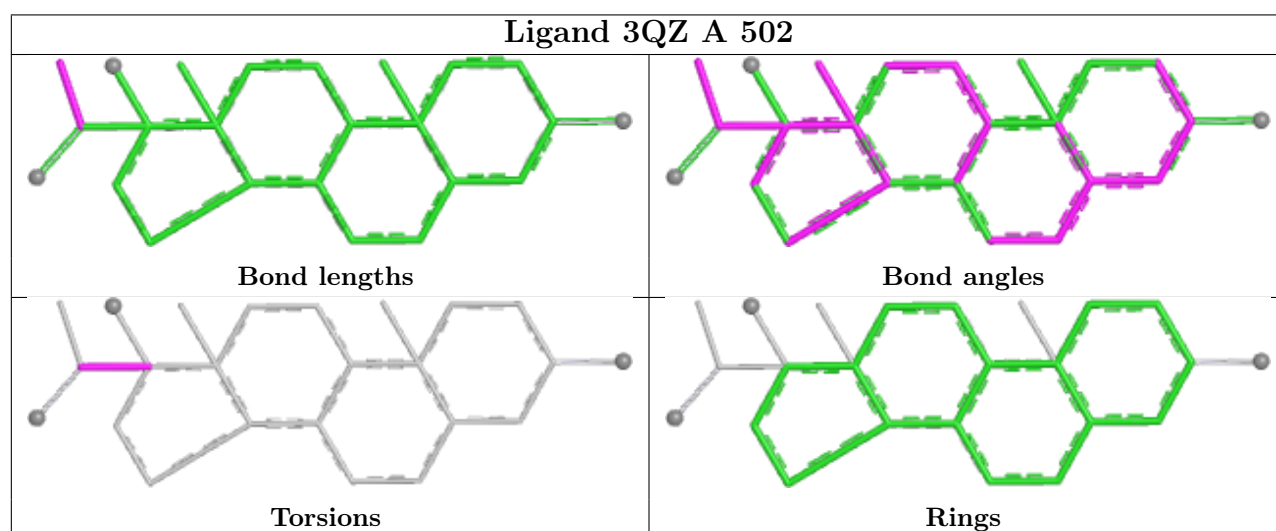
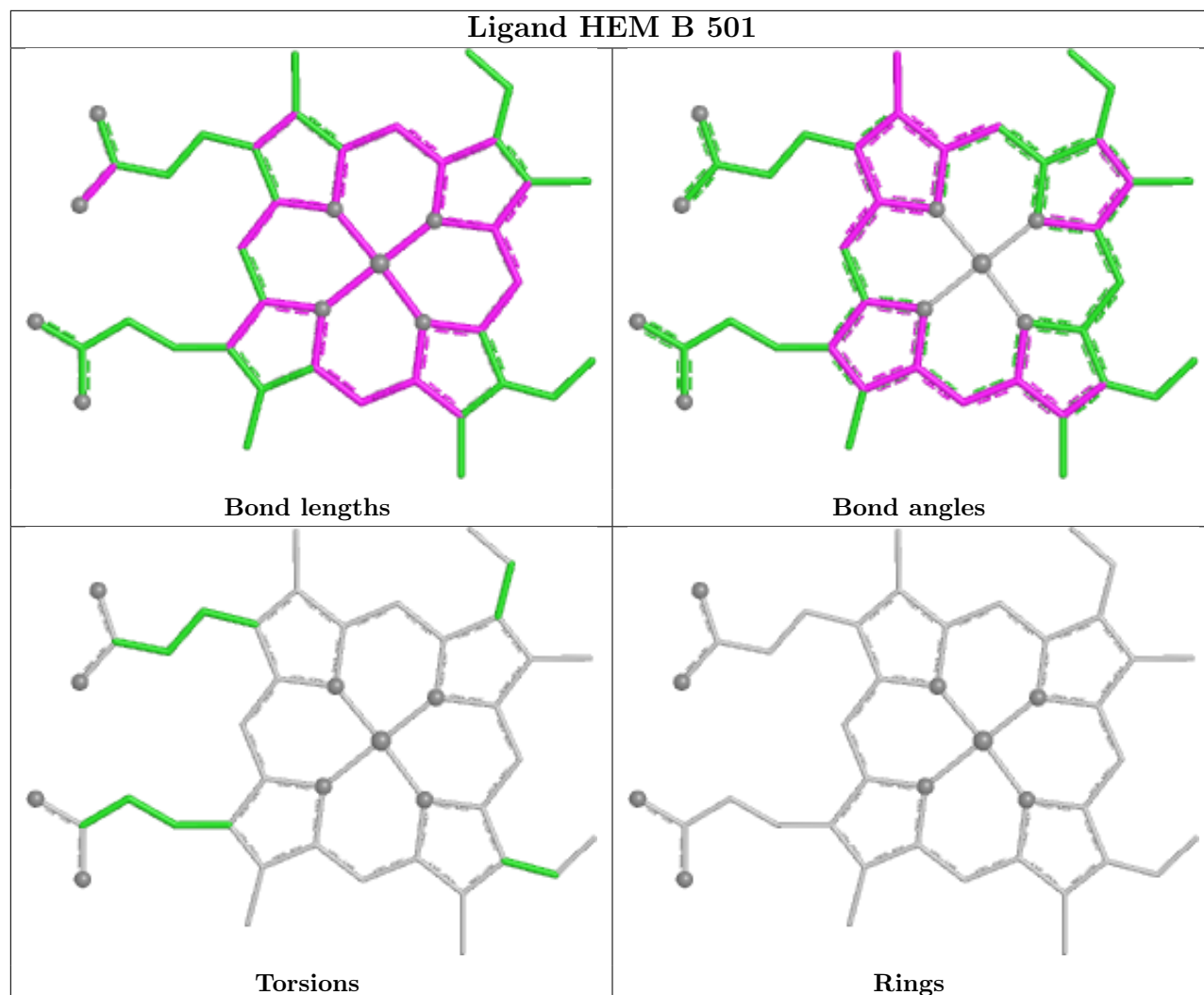
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

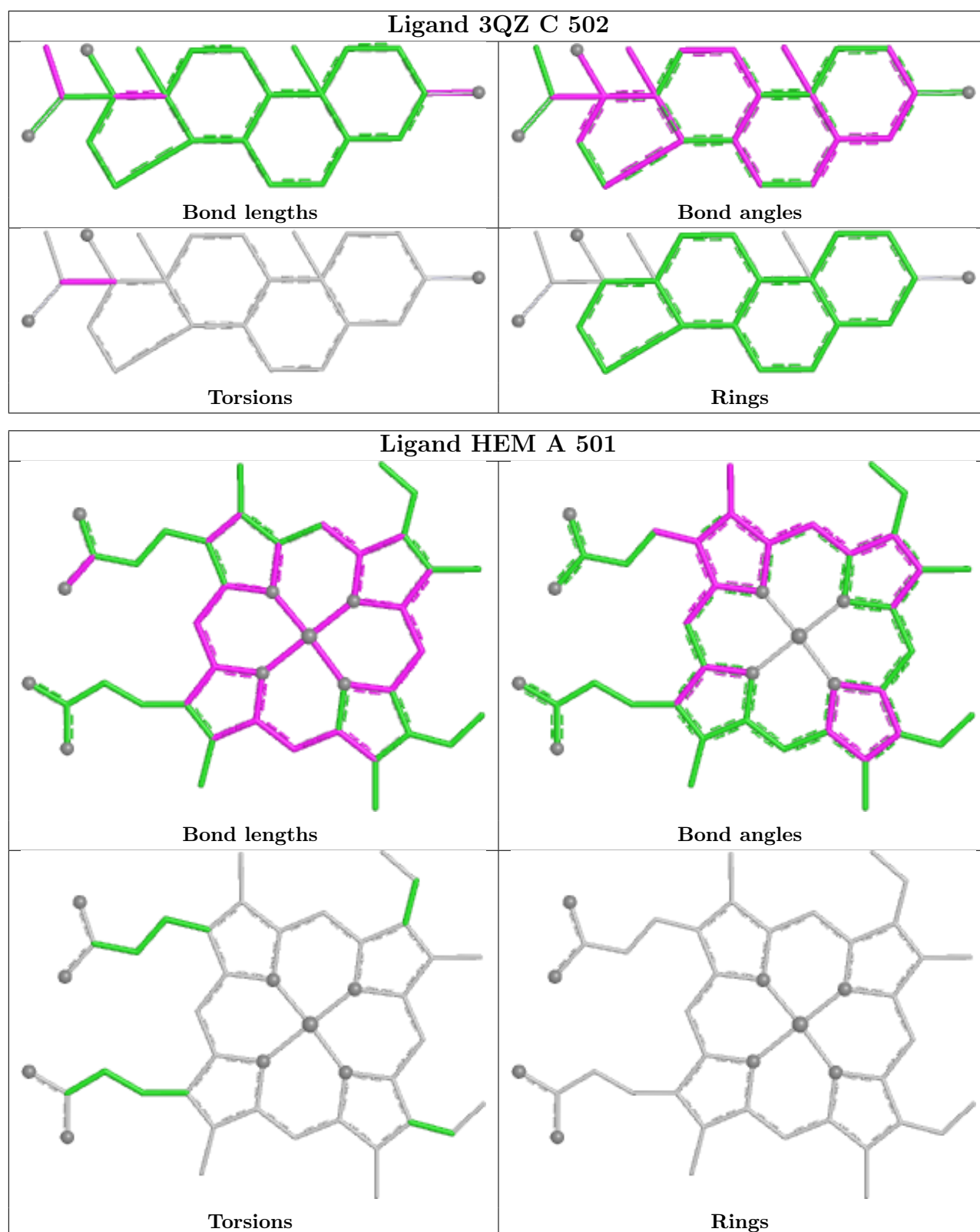
Ligand 3QZ B 502



Ligand HEM C 501







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	442/476 (92%)	-0.51	0	100 100	45, 88, 122, 165	38 (8%)
1	B	441/476 (92%)	-0.43	0	100 100	49, 89, 131, 177	27 (6%)
1	C	442/476 (92%)	-0.46	1 (0%)	91 86	44, 91, 122, 148	19 (4%)
All	All	1325/1428 (92%)	-0.47	1 (0%)	92 91	44, 89, 124, 177	84 (6%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	384	VAL	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	3QZ	A	502	24/24	0.88	0.11	77,78,86,93	0
3	3QZ	C	502	24/24	0.92	0.12	80,86,95,103	0

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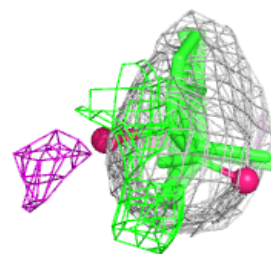
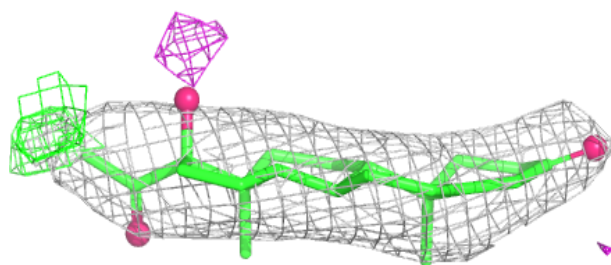
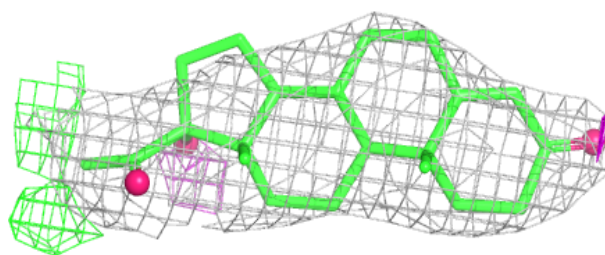
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	3QZ	B	502	24/24	0.94	0.10	77,80,85,91	0
2	HEM	C	501	43/43	0.96	0.09	84,98,102,104	0
2	HEM	A	501	43/43	0.96	0.10	77,91,97,99	0
2	HEM	B	501	43/43	0.97	0.08	85,100,104,116	0

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.

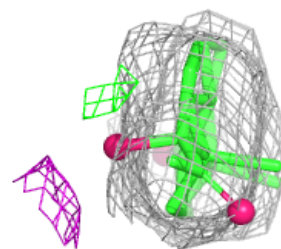
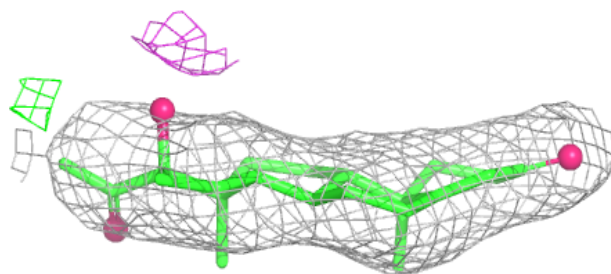
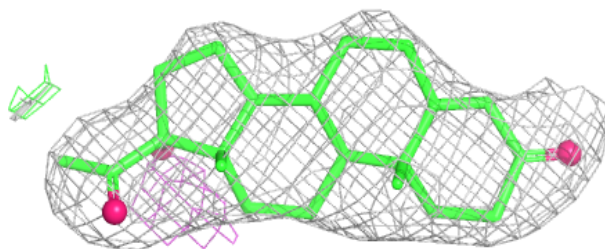
Electron density around 3QZ A 502:

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

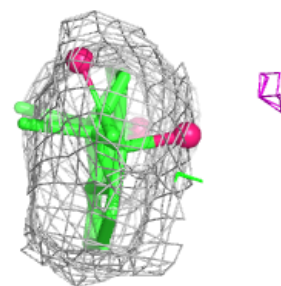
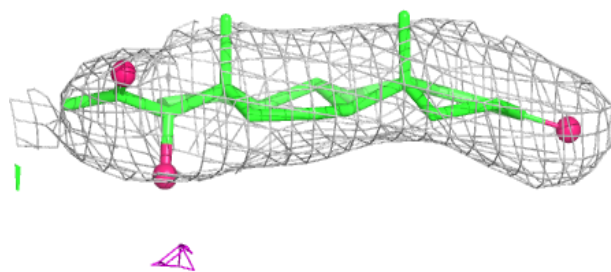
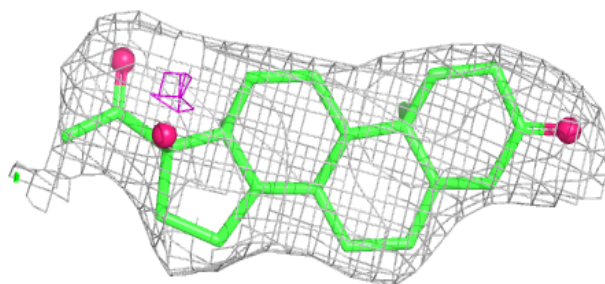


Electron density around 3QZ C 502:

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

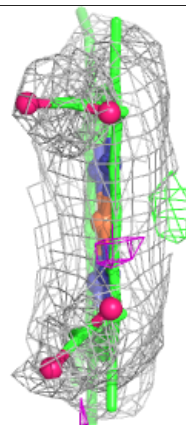
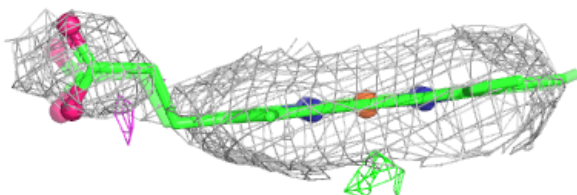
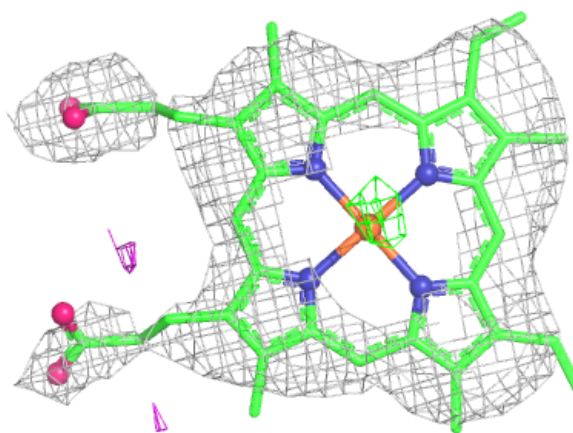
**Electron density around 3QZ B 502:**

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



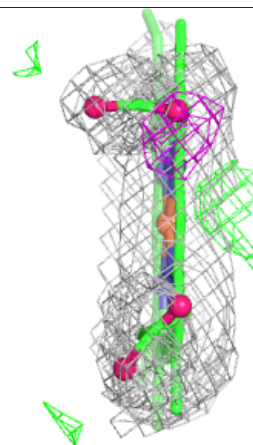
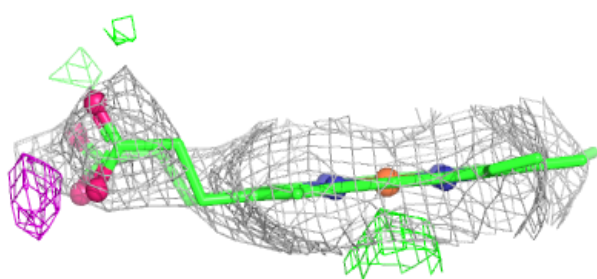
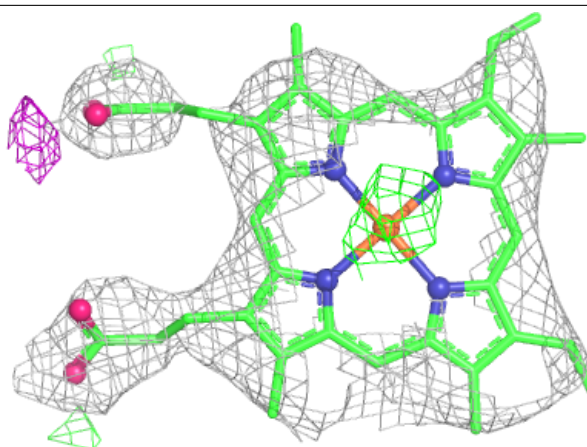
Electron density around HEM C 501:

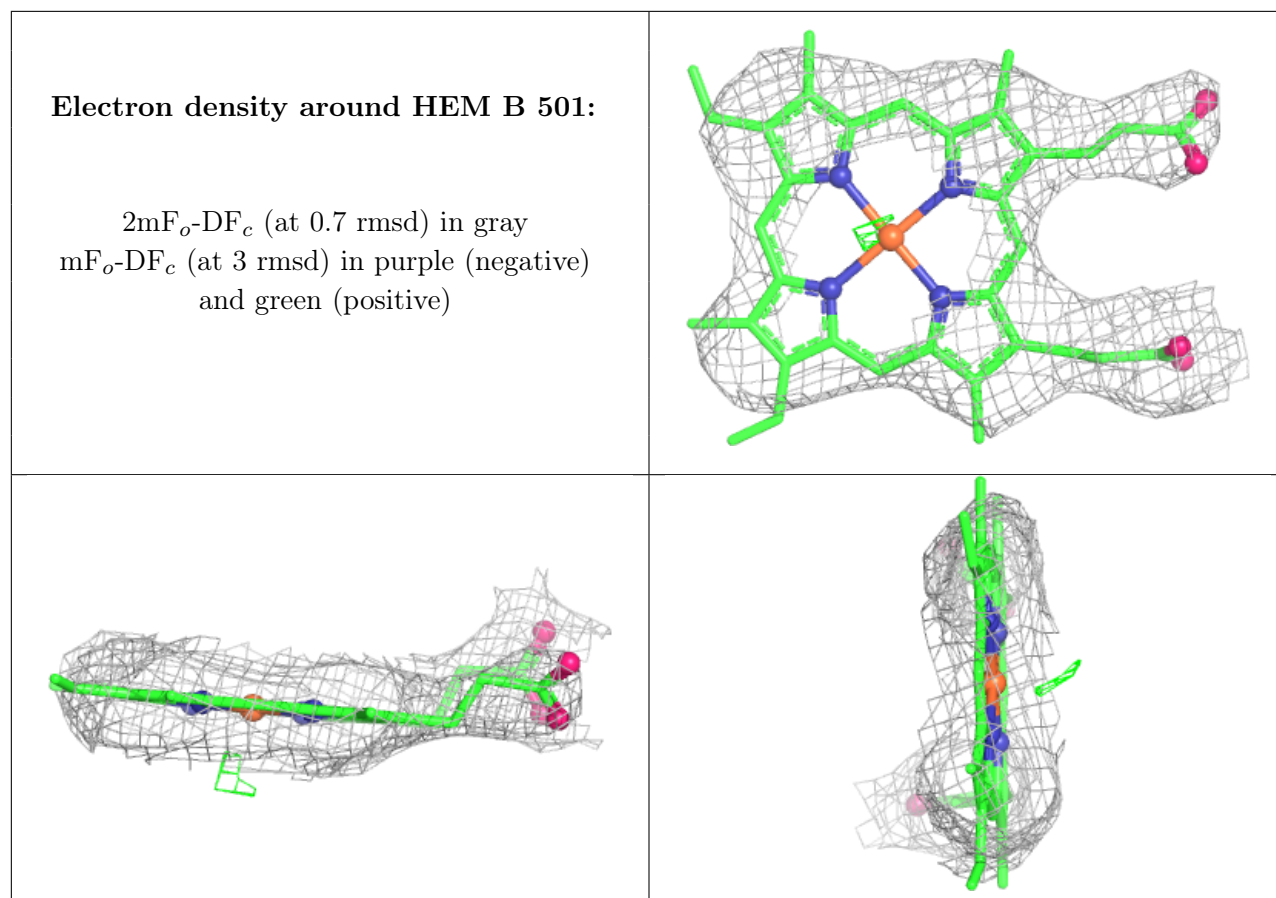
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.