



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 05:02 PM UTC

PDB ID : 4JWU / pdb_00004jwu
Title : Crystal structure of Cytochrome P450cam-putidaredoxin complex
Authors : Tripathi, S.M.; Li, H.; Poulos, T.L.
Deposited on : 2013-03-27
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

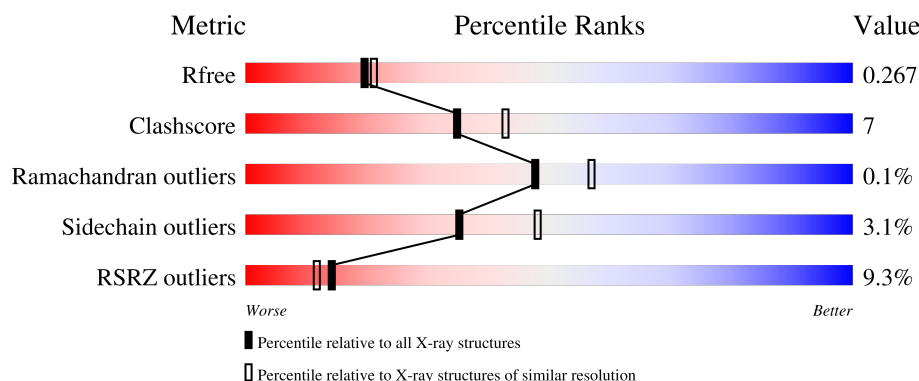
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	415	13% 80% 18% .
1	B	415	3% 81% 15% ..
2	C	113	6% 73% 19% 6%
2	D	113	18% 80% 13% 6%

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
6	FES	C	201	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8399 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 Camphor 5-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3204	2030	559	601	14			
1	B	403	Total	C	N	O	S	0	0	0
			3185	2020	554	597	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	SER	CYS	engineered mutation	UNP P00183
A	85	SER	CYS	engineered mutation	UNP P00183
A	136	SER	CYS	engineered mutation	UNP P00183
A	285	SER	CYS	engineered mutation	UNP P00183
A	334	ALA	CYS	engineered mutation	UNP P00183
A	344	CYS	LYS	engineered mutation	UNP P00183
B	58	SER	CYS	engineered mutation	UNP P00183
B	85	SER	CYS	engineered mutation	UNP P00183
B	136	SER	CYS	engineered mutation	UNP P00183
B	285	SER	CYS	engineered mutation	UNP P00183
B	334	ALA	CYS	engineered mutation	UNP P00183
B	344	CYS	LYS	engineered mutation	UNP P00183

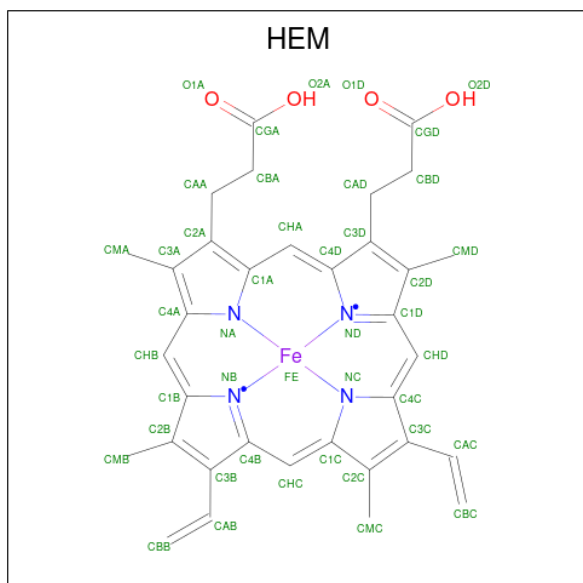
- Molecule 2 is a protein called Putidaredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	106	Total	C	N	O	S	0	0	0
			792	487	136	160	9			
2	D	106	Total	C	N	O	S	0	0	0
			792	487	136	160	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	HIS	-	expression tag	UNP P00259
C	-5	HIS	-	expression tag	UNP P00259
C	-4	HIS	-	expression tag	UNP P00259
C	-3	HIS	-	expression tag	UNP P00259
C	-2	HIS	-	expression tag	UNP P00259
C	-1	HIS	-	expression tag	UNP P00259
C	19	CYS	ASP	engineered mutation	UNP P00259
C	73	SER	CYS	engineered mutation	UNP P00259
D	-6	HIS	-	expression tag	UNP P00259
D	-5	HIS	-	expression tag	UNP P00259
D	-4	HIS	-	expression tag	UNP P00259
D	-3	HIS	-	expression tag	UNP P00259
D	-2	HIS	-	expression tag	UNP P00259
D	-1	HIS	-	expression tag	UNP P00259
D	19	CYS	ASP	engineered mutation	UNP P00259
D	73	SER	CYS	engineered mutation	UNP P00259

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

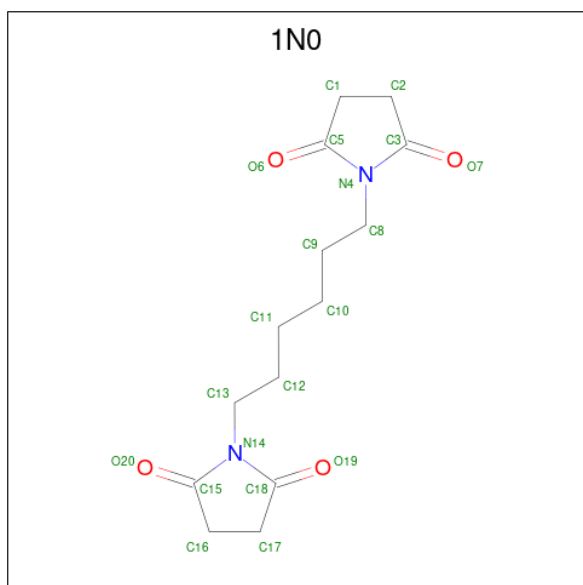


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is 1,1'-hexane-1,6-diylidipyrrolidine-2,5-dione (CCD ID: 1N0) (formula: $C_{14}H_{20}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			20	14	2	4		

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	Fe	S	0	0
			4	2	2		
6	D	1	Total	Fe	S	0	0
			4	2	2		

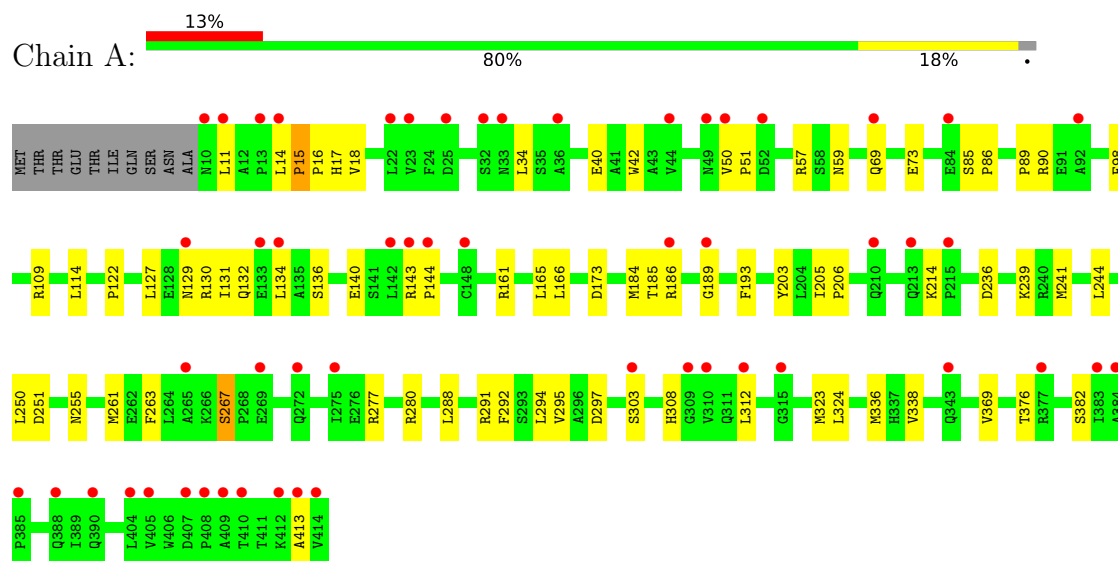
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	98	Total	O	0	0
			98	98		
7	B	155	Total	O	0	0
			155	155		
7	C	27	Total	O	0	0
			27	27		
7	D	30	Total	O	0	0
			30	30		

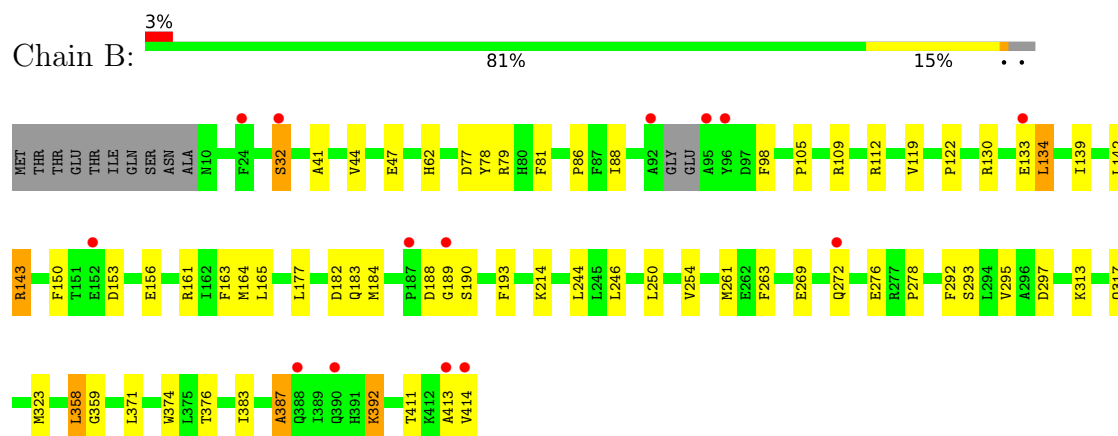
3 Residue-property plots [i](#)

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: Camphor 5-monooxygenase



• Molecule 1: Camphor 5-monooxygenase

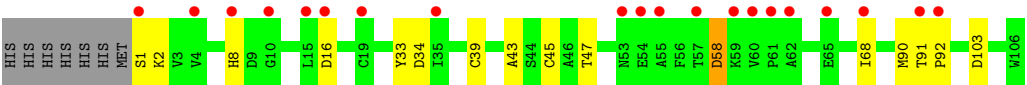
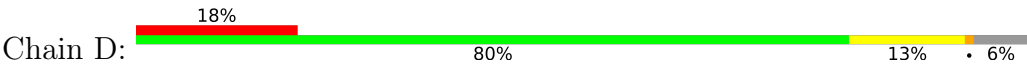


• Molecule 2: Putidaredoxin





● Molecule 2: Putidaredoxin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.68Å 110.05Å 86.50Å 90.00° 109.51° 90.00°	Depositor
Resolution (Å)	39.01 – 2.20 39.01 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (39.01-2.20) 97.8 (39.01-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	19.19 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.205 , 0.266 0.209 , 0.267	Depositor DCC
R_{free} test set	2621 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8399	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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: 1N0, CA, FES, 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	0.59	0/3283	0.94	5/4461 (0.1%)
1	B	0.64	0/3263	0.95	4/4434 (0.1%)
2	C	0.59	0/803	0.94	0/1090
2	D	0.59	0/803	0.86	0/1090
All	All	0.61	0/8152	0.93	9/11075 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	LYS	CA-C-N	6.61	126.59	119.78
1	A	214	LYS	C-N-CA	6.61	126.59	119.78
1	A	189	GLY	N-CA-C	-6.33	106.98	115.21
1	B	143	ARG	CA-C-N	-5.97	113.59	120.04
1	B	143	ARG	C-N-CA	-5.97	113.59	120.04
1	A	15	PRO	CA-C-N	5.43	126.63	119.84
1	A	15	PRO	C-N-CA	5.43	126.63	119.84
1	B	32	SER	N-CA-C	5.43	118.12	111.82
1	B	189	GLY	N-CA-C	-5.01	107.88	114.95

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	3204	0	3147	47	0
1	B	3185	0	3127	40	0
2	C	792	0	770	17	0
2	D	792	0	771	12	0
3	A	43	0	30	3	0
3	B	43	0	30	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	20	0	17	0	0
6	C	4	0	0	2	0
6	D	4	0	0	1	0
7	A	98	0	0	4	0
7	B	155	0	0	6	0
7	C	27	0	0	0	0
7	D	30	0	0	0	0
All	All	8399	0	7892	119	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 7.

All (119) 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)
3:A:501:HEM:HHD	3:A:501:HEM:HBC2	1.64	0.78
1:B:164:MET:HE1	1:B:177:LEU:HD12	1.65	0.78
1:A:42:TRP:CB	1:A:323:MET:HE1	2.19	0.73
3:B:501:HEM:HBC2	3:B:501:HEM:HHD	1.75	0.69
1:A:185:THR:HG22	1:A:186:ARG:HG3	1.74	0.69
1:B:183:GLN:NE2	1:B:190:SER:OG	2.25	0.69
1:B:47:GLU:O	7:B:693:HOH:O	2.11	0.67
1:B:392:LYS:NZ	7:B:658:HOH:O	2.29	0.66
1:B:269:GLU:OE2	7:B:656:HOH:O	2.15	0.63
1:A:98:PHE:HZ	1:A:184:MET:HE1	1.64	0.63
2:D:1:SER:HB2	2:D:90:MET:HE3	1.83	0.59
1:A:42:TRP:HB2	1:A:323:MET:HE1	1.84	0.59
1:A:129:ASN:HA	1:A:132:GLN:HG2	1.85	0.58
1:A:109:ARG:NH2	7:A:648:HOH:O	2.35	0.57
1:B:77:ASP:OD1	1:B:79:ARG:HG2	2.04	0.57
2:D:8:HIS:CD2	2:D:103:ASP:HB3	2.40	0.56
1:A:263:PHE:O	1:A:267:SER:OG	2.19	0.55
2:D:43:ALA:HA	6:D:201:FES:S1	2.46	0.55
1:A:73:GLU:CD	1:A:308:HIS:HE2	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASP:OD2	1:A:203:TYR:OH	2.21	0.55
1:A:205:ILE:HG22	1:A:206:PRO:HD3	1.87	0.55
1:A:134:LEU:HD21	1:A:161:ARG:HB3	1.88	0.55
1:B:134:LEU:HD11	1:B:161:ARG:HD2	1.89	0.55
1:B:143:ARG:HG2	1:B:143:ARG:HH11	1.72	0.55
1:A:34:LEU:O	7:A:670:HOH:O	2.18	0.54
1:B:276:GLU:O	1:B:278:PRO:HD3	2.07	0.54
1:A:98:PHE:CZ	1:A:184:MET:HE1	2.42	0.54
1:B:105:PRO:HB3	1:B:109:ARG:NH1	2.23	0.54
2:C:56:PHE:O	2:C:60:VAL:HG23	2.07	0.54
2:C:3:VAL:HG13	2:C:97:ILE:HG23	1.90	0.53
1:A:251:ASP:O	1:A:255:ASN:ND2	2.42	0.53
1:A:122:PRO:HG3	2:C:33:TYR:CD1	2.43	0.52
2:D:1:SER:OG	2:D:92:PRO:HA	2.08	0.52
2:C:39:CYS:HB3	2:C:45:CYS:HB3	1.92	0.52
1:A:109:ARG:NH1	7:A:637:HOH:O	2.42	0.51
2:C:7:SER:HB2	2:C:11:THR:CG2	2.40	0.51
1:A:11:LEU:HD13	1:A:57:ARG:HB2	1.91	0.51
1:A:143:ARG:NH2	1:A:413:ALA:HB2	2.25	0.51
2:C:43:ALA:HA	6:C:201:FES:S2	2.51	0.51
1:B:295:VAL:HG11	3:B:501:HEM:HMA3	1.92	0.50
2:D:39:CYS:HB3	2:D:45:CYS:HB3	1.92	0.50
1:B:359:GLY:HA3	3:B:501:HEM:C3C	2.46	0.50
1:A:42:TRP:HB3	1:A:323:MET:HE1	1.95	0.49
2:D:8:HIS:CG	2:D:103:ASP:HB3	2.48	0.49
1:B:150:PHE:CZ	1:B:261:MET:HG3	2.48	0.48
1:B:143:ARG:HG2	1:B:143:ARG:NH1	2.28	0.48
1:A:86:PRO:O	1:A:297:ASP:HB2	2.14	0.48
1:B:78:TYR:HA	1:B:81:PHE:O	2.14	0.48
2:C:56:PHE:CE2	2:C:97:ILE:HA	2.49	0.48
1:B:183:GLN:OE1	1:B:188:ASP:HB2	2.13	0.48
2:C:58:ASP:OD1	2:C:58:ASP:N	2.44	0.48
1:A:73:GLU:OE2	1:A:308:HIS:NE2	2.46	0.47
2:C:36:VAL:HB	2:C:47:THR:HB	1.96	0.47
1:B:163:PHE:CZ	1:B:246:LEU:HB2	2.49	0.47
1:B:313:LYS:NZ	7:B:609:HOH:O	2.47	0.47
2:C:7:SER:HB2	2:C:11:THR:HG23	1.96	0.47
1:B:156:GLU:HA	1:B:254:VAL:HG22	1.96	0.47
1:A:323:MET:HB3	1:A:323:MET:HE2	1.34	0.47
1:B:122:PRO:HG3	2:D:33:TYR:CD1	2.50	0.47
1:B:112:ARG:CZ	1:B:358:LEU:HD13	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:501:HEM:HHC	3:B:501:HEM:HBB2	1.97	0.46
1:B:134:LEU:HD21	1:B:161:ARG:HB3	1.99	0.45
1:B:184:MET:HE3	1:B:193:PHE:CE1	2.51	0.45
2:C:23:LEU:HB2	2:C:85:CYS:HB2	1.97	0.45
1:A:50:VAL:HA	1:A:51:PRO:HD2	1.76	0.45
1:B:98:PHE:HB3	1:B:244:LEU:HB2	1.99	0.45
2:C:8:HIS:ND1	2:C:103:ASP:HB3	2.31	0.45
1:B:142:LEU:HD21	1:B:153:ASP:HB3	1.99	0.45
2:C:45:CYS:C	2:C:70:MET:HE2	2.42	0.45
1:A:143:ARG:CZ	1:A:413:ALA:HB2	2.47	0.45
1:B:143:ARG:HD2	1:B:411:THR:HB	1.99	0.45
3:B:501:HEM:HBC2	3:B:501:HEM:CHD	2.44	0.44
1:B:182:ASP:OD1	7:B:751:HOH:O	2.21	0.44
1:A:11:LEU:HB3	1:A:57:ARG:HB2	2.00	0.44
2:D:34:ASP:OD1	2:D:34:ASP:N	2.47	0.44
1:B:263:PHE:HB2	1:B:292:PHE:CZ	2.52	0.44
1:A:184:MET:HE2	1:A:193:PHE:CE1	2.54	0.43
1:A:98:PHE:HB3	1:A:244:LEU:HB2	1.99	0.43
1:B:86:PRO:O	1:B:297:ASP:HB2	2.18	0.43
1:B:163:PHE:CD2	1:B:246:LEU:HD13	2.54	0.43
1:A:59:ASN:O	1:A:89:PRO:HB3	2.19	0.43
1:A:277:ARG:HB3	1:A:280:ARG:HG2	2.01	0.43
1:B:62:HIS:CD2	1:B:88:ILE:HG21	2.54	0.43
1:A:236:ASP:HA	1:A:239:LYS:HD3	2.01	0.42
1:A:40:GLU:HG3	1:A:336:MET:HE3	2.01	0.42
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.70	0.42
1:A:14:LEU:HA	1:A:15:PRO:HD3	1.79	0.42
1:A:85:SER:OG	1:A:90:ARG:HG3	2.19	0.42
1:A:291:ARG:HG2	1:A:338:VAL:HG22	2.01	0.42
1:B:387:ALA:N	7:B:743:HOH:O	2.53	0.42
1:B:41:ALA:O	1:B:44:VAL:HG22	2.20	0.42
1:B:293:SER:O	1:B:323:MET:HG3	2.19	0.42
1:B:371:LEU:HD23	1:B:371:LEU:HA	1.87	0.42
1:A:114:LEU:HD23	1:A:241:MET:HE1	2.00	0.42
1:A:17:HIS:CE1	1:A:18:VAL:HG23	2.55	0.42
1:A:130:ARG:HE	1:A:165:LEU:HD11	1.84	0.42
1:A:15:PRO:HA	1:A:16:PRO:HD2	1.81	0.41
1:A:143:ARG:HB3	1:A:144:PRO:HD3	2.02	0.41
2:D:58:ASP:OD1	2:D:58:ASP:N	2.38	0.41
1:A:69:GLN:O	1:A:73:GLU:HG3	2.20	0.41
1:A:263:PHE:HB2	1:A:292:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:64:ASN:O	2:C:68:ILE:HD12	2.20	0.41
2:C:34:ASP:OD1	2:C:34:ASP:N	2.44	0.41
2:C:13:ARG:NH1	2:C:30:ASN:O	2.53	0.41
1:A:132:GLN:HA	1:A:369:VAL:HG11	2.02	0.41
1:A:132:GLN:O	1:A:136:SER:OG	2.32	0.41
1:B:130:ARG:NE	1:B:165:LEU:HD11	2.36	0.41
2:D:91:THR:HB	2:D:92:PRO:HD2	2.03	0.41
1:A:127:LEU:O	1:A:131:ILE:HG13	2.21	0.41
1:B:183:GLN:OE1	1:B:183:GLN:HA	2.20	0.41
2:D:45:CYS:SG	2:D:47:THR:OG1	2.75	0.41
1:B:139:ILE:HD13	1:B:374:TRP:HA	2.02	0.40
2:D:2:LYS:HG2	2:D:16:ASP:OD1	2.20	0.40
1:B:143:ARG:NH2	1:B:413:ALA:HB2	2.36	0.40
1:B:246:LEU:O	1:B:250:LEU:HG	2.22	0.40
1:A:109:ARG:NE	7:A:648:HOH:O	2.54	0.40
2:C:84:LEU:HD13	6:C:201:FES:S2	2.62	0.40
1:A:295:VAL:HG21	3:A:501:HEM:HBB	2.04	0.40
3:A:501:HEM:HBD1	3:A:501:HEM:HHA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	403/415 (97%)	375 (93%)	28 (7%)	0	100	100
1	B	399/415 (96%)	382 (96%)	16 (4%)	1 (0%)	36	42
2	C	104/113 (92%)	102 (98%)	2 (2%)	0	100	100
2	D	104/113 (92%)	102 (98%)	2 (2%)	0	100	100
All	All	1010/1056 (96%)	961 (95%)	48 (5%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	387	ALA

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	349/358 (98%)	338 (97%)	11 (3%)	34	47
1	B	347/358 (97%)	335 (96%)	12 (4%)	32	43
2	C	89/96 (93%)	87 (98%)	2 (2%)	45	61
2	D	89/96 (93%)	87 (98%)	2 (2%)	45	61
All	All	874/908 (96%)	847 (97%)	27 (3%)	35	48

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	GLU
1	A	166	LEU
1	A	250	LEU
1	A	261	MET
1	A	267	SER
1	A	288	LEU
1	A	294	LEU
1	A	303	SER
1	A	312	LEU
1	A	376	THR
1	A	382	SER
1	B	32	SER
1	B	119	VAL
1	B	133	GLU
1	B	134	LEU
1	B	214	LYS
1	B	272	GLN
1	B	317	GLN
1	B	358	LEU
1	B	376	THR
1	B	383	ILE

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Mol	Chain	Res	Type
1	B	392	LYS
1	B	414	VAL
2	C	58	ASP
2	C	68	ILE
2	D	58	ASP
2	D	68	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	225	ASN
1	A	255	ASN
1	A	311	GLN
1	B	117	GLN
1	B	145	GLN
1	B	225	ASN
2	D	8	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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	HEM	A	501	1,7	50,50,50	2.10	9 (18%)	67,82,82	1.59	14 (20%)
6	FES	D	201	2	0,4,4	-	-	-		
6	FES	C	201	2	0,4,4	-	-	-		
5	1N0	A	503	1,2	21,21,21	1.49	4 (19%)	28,28,28	2.56	8 (28%)
3	HEM	B	501	1,7	50,50,50	2.17	8 (16%)	67,82,82	1.75	13 (19%)

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	HEM	A	501	1,7	-	4/14/54/54	-
6	FES	D	201	2	-	-	0/1/1/1
6	FES	C	201	2	-	-	0/1/1/1
5	1N0	A	503	1,2	-	4/9/35/35	0/2/2/2
3	HEM	B	501	1,7	-	2/14/54/54	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	HEM	C3D-C2D	8.11	1.54	1.36
3	B	501	HEM	C3D-C2D	8.01	1.54	1.36
3	B	501	HEM	FE-NB	7.04	2.16	1.94
3	A	501	HEM	FE-NB	6.25	2.14	1.94
3	A	501	HEM	FE-ND	6.19	2.14	1.94
3	B	501	HEM	FE-NC	6.08	2.15	1.95
5	A	503	1N0	C15-N14	-4.18	1.32	1.38
3	B	501	HEM	FE-ND	3.75	2.06	1.94
3	A	501	HEM	FE-NC	3.54	2.06	1.95
3	A	501	HEM	CAC-C3C	3.41	1.56	1.47
5	A	503	1N0	C17-C16	-3.14	1.44	1.52
3	B	501	HEM	CAB-C3B	3.02	1.55	1.47
3	B	501	HEM	CAC-C3C	2.90	1.55	1.47
3	A	501	HEM	CAB-C3B	2.79	1.54	1.47
3	A	501	HEM	CMD-C2D	2.55	1.56	1.50
3	A	501	HEM	CAA-C2A	2.33	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	HEM	CMB-C2B	2.26	1.55	1.50
3	B	501	HEM	CMC-C2C	2.25	1.55	1.50
5	A	503	1N0	C1-C2	-2.13	1.47	1.52
3	B	501	HEM	CMD-C2D	2.11	1.55	1.50
5	A	503	1N0	C3-N4	-2.08	1.35	1.38

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	503	1N0	C5-N4-C3	7.96	116.41	112.94
5	A	503	1N0	C18-N14-C15	7.59	116.25	112.94
3	B	501	HEM	C4D-ND-C1D	6.11	112.45	105.21
3	A	501	HEM	C4D-ND-C1D	5.81	112.09	105.21
3	B	501	HEM	C3B-C2B-C1B	4.44	109.75	106.41
3	B	501	HEM	CHB-C1B-NB	4.19	129.55	124.37
3	A	501	HEM	C1B-NB-C4B	3.29	109.11	105.21
5	A	503	1N0	C16-C15-N14	-3.21	105.24	108.03
5	A	503	1N0	O6-C5-N4	3.17	127.34	123.94
3	B	501	HEM	C1B-NB-C4B	3.15	108.94	105.21
3	A	501	HEM	CHD-C1D-ND	2.97	127.61	124.42
5	A	503	1N0	O19-C18-N14	2.96	127.12	123.94
3	B	501	HEM	CHC-C4B-C3B	2.88	130.82	125.07
3	B	501	HEM	C3B-C4B-NB	-2.88	107.40	109.47
3	A	501	HEM	C4A-C3A-C2A	2.75	109.96	106.82
3	A	501	HEM	CHB-C4A-NA	2.68	128.71	123.86
3	A	501	HEM	C3B-C4B-NB	-2.65	107.56	109.47
3	B	501	HEM	CHD-C4C-NC	2.55	127.23	124.45
3	A	501	HEM	O2D-CGD-CBD	2.48	121.84	114.00
3	B	501	HEM	CHC-C4B-NB	-2.46	121.77	124.42
3	B	501	HEM	CAB-C3B-C2B	-2.45	120.46	128.43
5	A	503	1N0	C1-C5-N4	-2.37	105.97	108.03
3	A	501	HEM	CBD-CAD-C3D	-2.35	106.04	112.53
3	A	501	HEM	O1D-CGD-CBD	-2.34	115.66	123.09
3	B	501	HEM	CMC-C2C-C3C	-2.32	122.82	128.43
3	A	501	HEM	C3A-C4A-NA	-2.30	106.46	110.14
5	A	503	1N0	O7-C3-N4	2.27	126.38	123.94
3	A	501	HEM	C2B-C1B-NB	-2.25	107.26	109.84
3	B	501	HEM	C2B-C1B-NB	-2.21	107.30	109.84
3	B	501	HEM	CAD-CBD-CGD	-2.21	107.80	113.67
5	A	503	1N0	C2-C3-N4	-2.20	106.12	108.03
3	A	501	HEM	C3B-C2B-C1B	2.11	108.00	106.41
3	A	501	HEM	C1D-C2D-C3D	-2.10	104.77	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	HEM	C3D-C4D-ND	-2.04	107.93	110.17
3	B	501	HEM	CMC-C2C-C1C	2.03	128.31	124.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

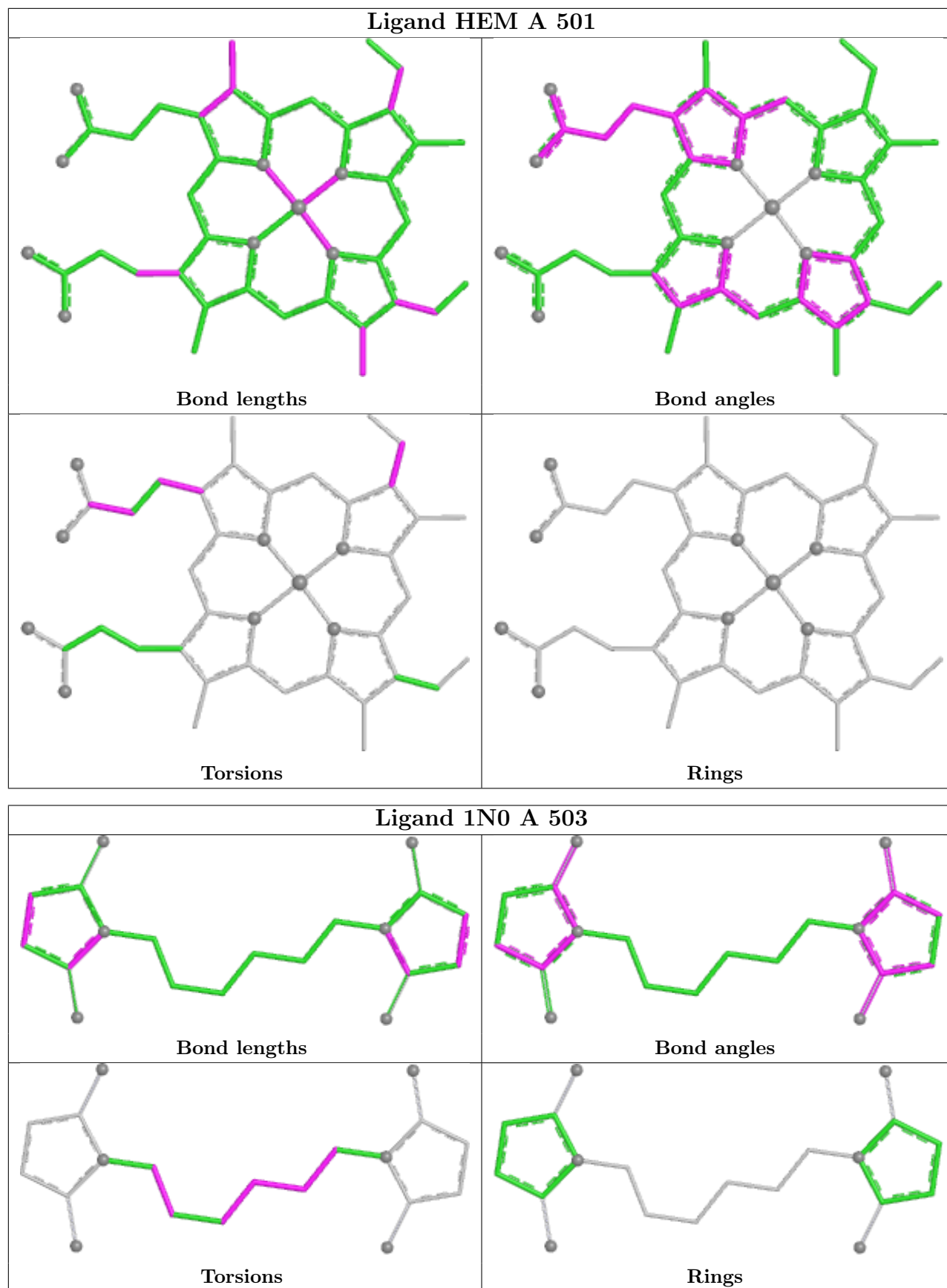
Mol	Chain	Res	Type	Atoms
5	A	503	1N0	N4-C8-C9-C10
5	A	503	1N0	C11-C12-C13-N14
5	A	503	1N0	C9-C10-C11-C12
5	A	503	1N0	C11-C10-C9-C8
3	A	501	HEM	C4C-C3C-CAC-CBC
3	B	501	HEM	C4B-C3B-CAB-CBB
3	B	501	HEM	C4C-C3C-CAC-CBC
3	A	501	HEM	CAD-CBD-CGD-O1D
3	A	501	HEM	CAD-CBD-CGD-O2D
3	A	501	HEM	C4D-C3D-CAD-CBD

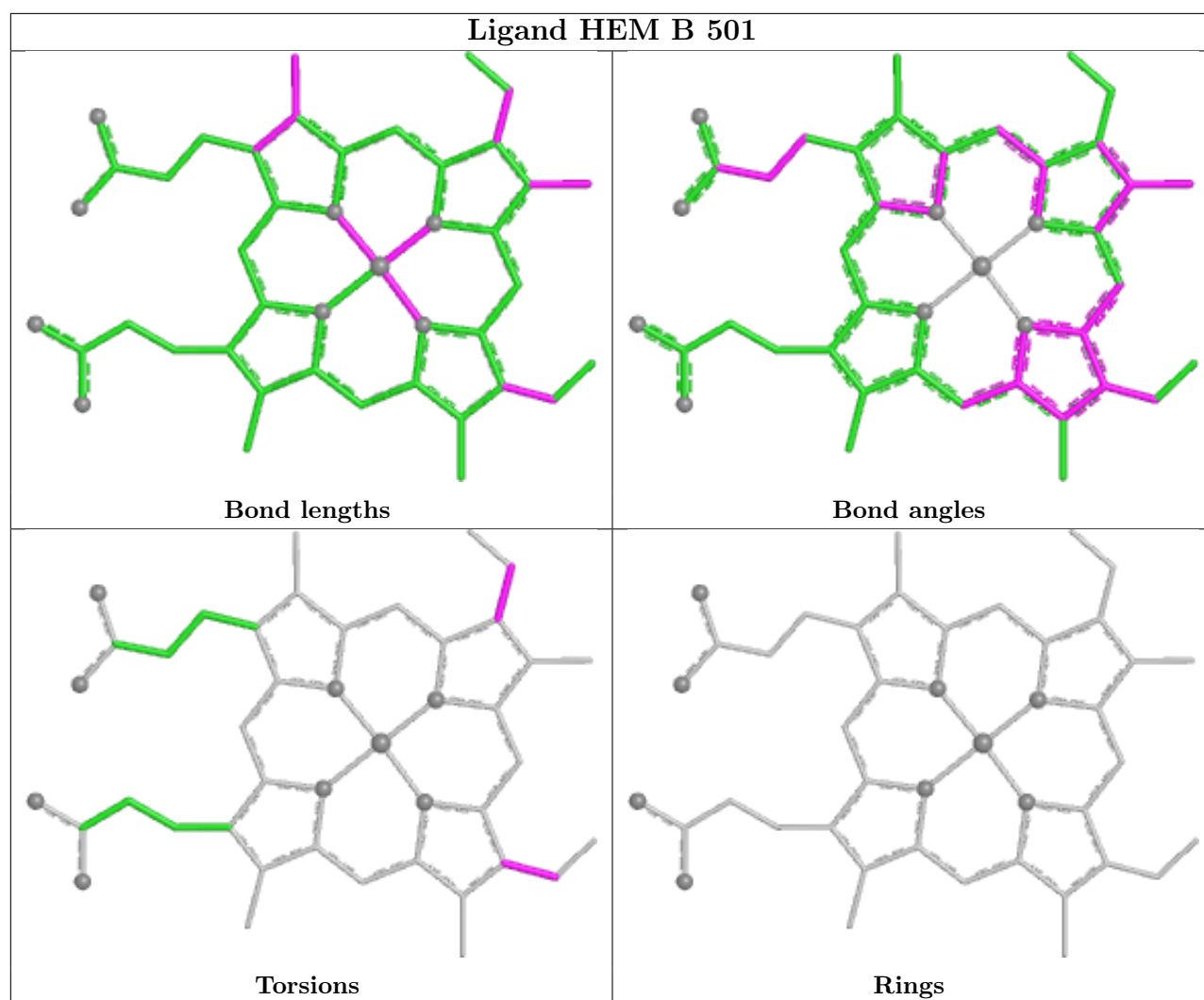
There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	HEM	3	0
6	D	201	FES	1	0
6	C	201	FES	2	0
3	B	501	HEM	5	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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	405/415 (97%)	0.99	54 (13%) 7 5	28, 54, 92, 126	0
1	B	403/415 (97%)	0.64	14 (3%) 47 44	25, 43, 70, 99	0
2	C	106/113 (93%)	0.95	7 (6%) 24 21	33, 56, 85, 98	0
2	D	106/113 (93%)	1.33	20 (18%) 3 2	31, 67, 97, 111	0
All	All	1020/1056 (96%)	0.88	95 (9%) 14 12	25, 50, 90, 126	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	409	ALA	5.0
1	B	95	ALA	5.0
1	B	414	VAL	4.9
1	B	187	PRO	4.4
1	A	414	VAL	4.0
1	A	413	ALA	3.8
1	B	96	TYR	3.6
2	D	60	VAL	3.6
1	A	388	GLN	3.4
2	D	59	LYS	3.4
1	B	413	ALA	3.3
1	A	384	ALA	3.2
1	A	186	ARG	3.2
2	D	62	ALA	3.1
1	A	408	PRO	3.0
1	A	49	ASN	3.0
2	D	10	GLY	2.9
2	D	68	ILE	2.9
1	A	383	ILE	2.9
1	A	13	PRO	2.8
1	A	269	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	36	ALA	2.8
1	A	50	VAL	2.8
1	A	10	ASN	2.7
2	D	65	GLU	2.7
2	D	19	CYS	2.7
2	D	4	VAL	2.7
2	D	1	SER	2.7
2	D	92	PRO	2.7
1	A	142	LEU	2.6
1	A	315	GLY	2.6
1	B	152	GLU	2.6
1	B	32	SER	2.6
1	A	44	VAL	2.6
1	A	385	PRO	2.6
1	A	275	ILE	2.6
1	A	11	LEU	2.5
1	A	134	LEU	2.5
1	A	407	ASP	2.5
1	A	405	VAL	2.5
1	A	143	ARG	2.5
1	B	92	ALA	2.5
1	A	215	PRO	2.5
2	D	57	THR	2.5
1	A	92	ALA	2.5
2	D	16	ASP	2.5
1	A	144	PRO	2.5
1	A	84	GLU	2.4
1	A	310	VAL	2.4
1	B	24	PHE	2.4
2	D	8	HIS	2.4
1	A	210	GLN	2.4
1	A	343	GLN	2.4
1	B	388	GLN	2.4
1	B	189	GLY	2.3
2	C	10	GLY	2.3
1	A	22	LEU	2.3
1	A	25	ASP	2.3
2	D	54	GLU	2.3
2	D	35	ILE	2.3
2	C	14	GLU	2.3
2	C	77	GLU	2.3
2	C	98	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	133	GLU	2.2
1	A	309	GLY	2.2
1	B	272	GLN	2.2
1	A	377	ARG	2.2
1	A	272	GLN	2.2
1	A	390	GLN	2.2
1	A	410	THR	2.2
2	D	55	ALA	2.2
2	D	91	THR	2.2
2	D	53	ASN	2.1
1	A	412	LYS	2.1
1	A	14	LEU	2.1
2	C	65	GLU	2.1
2	D	61	PRO	2.1
1	A	148	CYS	2.1
1	A	32	SER	2.1
1	A	33	ASN	2.1
1	A	69	GLN	2.1
2	C	19	CYS	2.1
1	A	52	ASP	2.1
1	A	129	ASN	2.1
1	A	213	GLN	2.1
1	A	312	LEU	2.1
1	B	390	GLN	2.1
1	A	23	VAL	2.1
1	A	133	GLU	2.0
1	A	404	LEU	2.0
2	D	15	LEU	2.0
2	C	92	PRO	2.0
1	A	189	GLY	2.0
1	A	303	SER	2.0
1	A	265	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

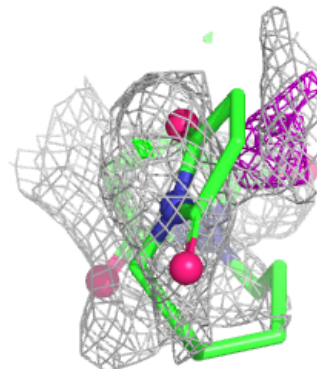
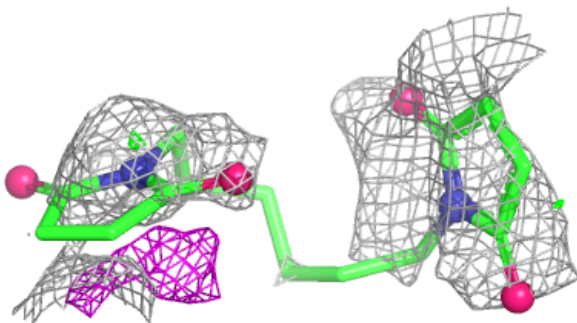
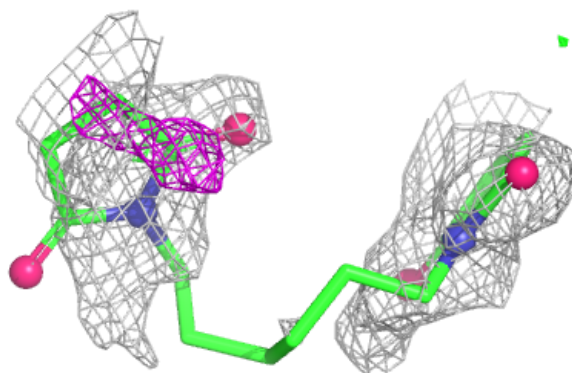
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	1N0	A	503	20/20	0.66	0.26	84,113,120,120	0
4	CA	A	502	1/1	0.97	0.06	30,30,30,30	0
4	CA	B	502	1/1	0.97	0.15	30,30,30,30	0
3	HEM	A	501	43/43	0.97	0.07	15,28,40,46	0
3	HEM	B	501	43/43	0.98	0.07	19,28,39,52	0
6	FES	C	201	4/4	0.98	0.03	30,33,33,34	0
6	FES	D	201	4/4	0.98	0.06	35,40,40,47	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.

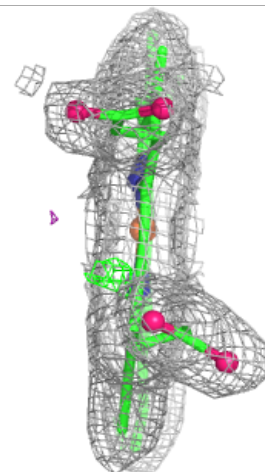
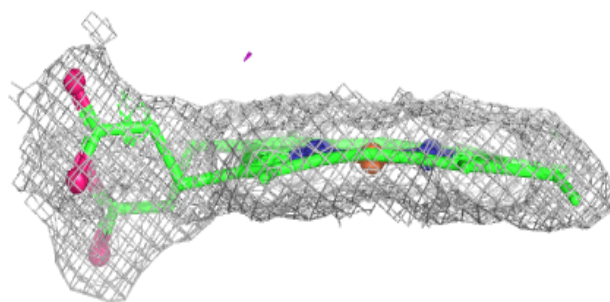
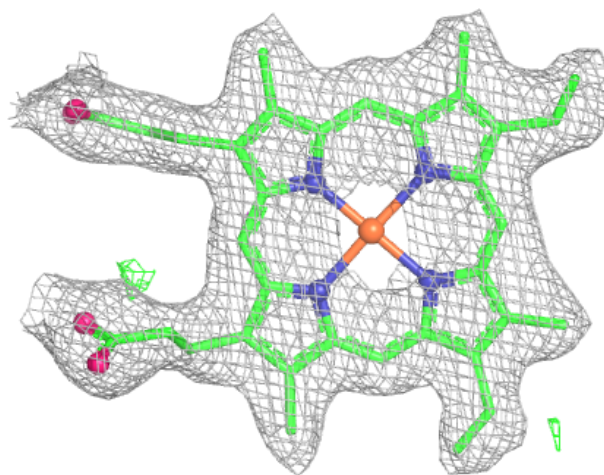
Electron density around 1N0 A 503:

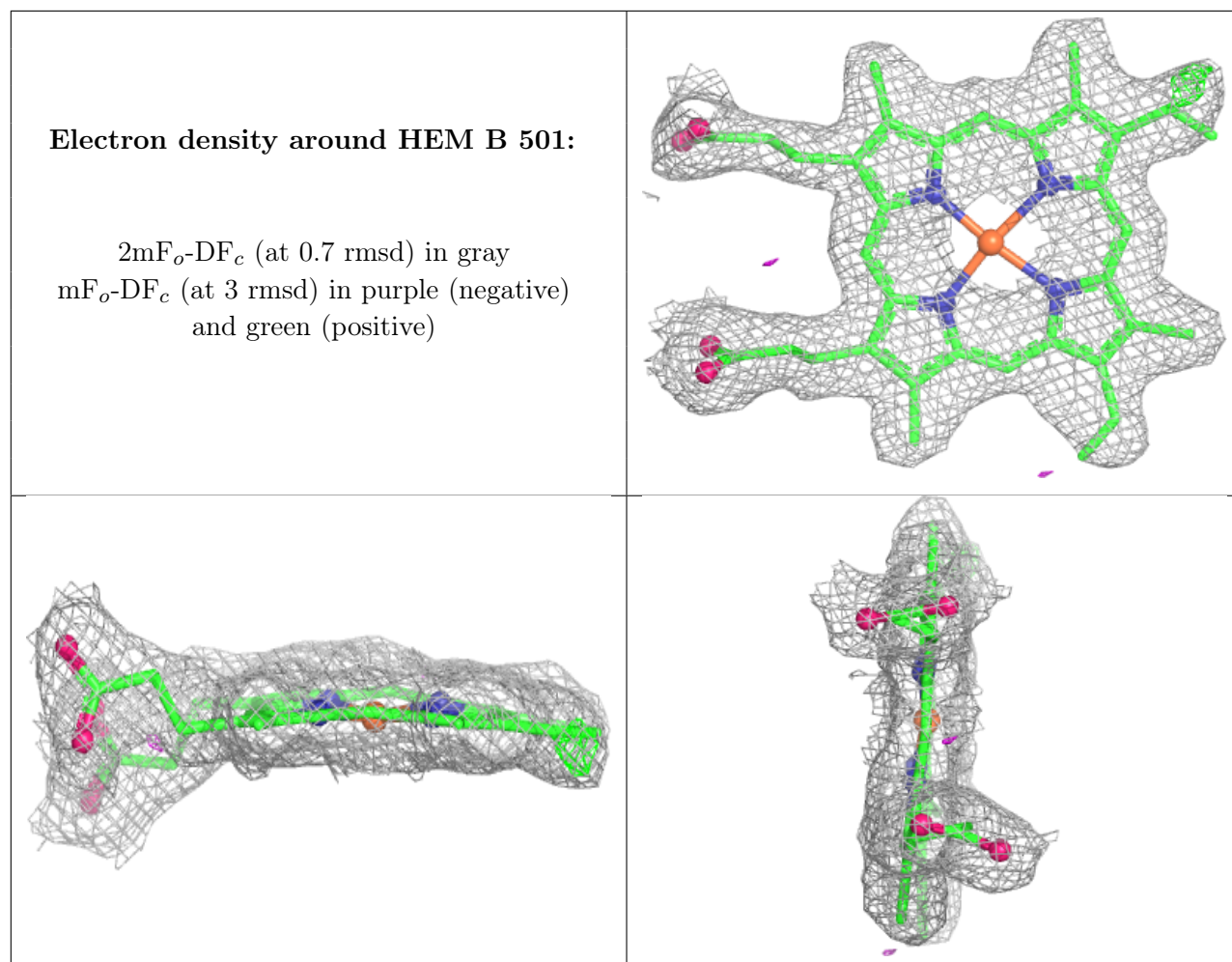
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.