



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:59 pm BST

PDB ID : 1DZ9
Title : Putative oxo complex of P450cam from *Pseudomonas putida*
Authors : Schlichting, I.; Berendzen, J.; Chu, K.; Stock, A.M.; Maves, S.A.; Benson, D.E.; Sweet, R.M.; Ringe, D.; Petsko, G.A.; Sligar, S.G.
Deposited on : 2000-02-18
Resolution : 1.90 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 : 2.11
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) : 2.11

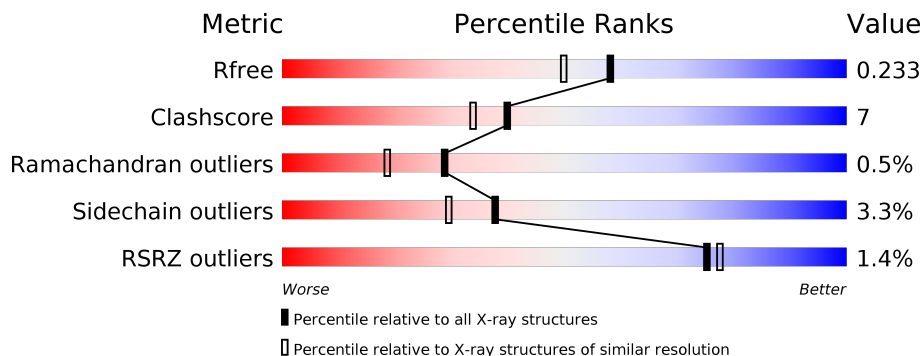
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	414	 2% 72% 22% . .
1	B	414	 75% 18% . .

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7243 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-CAM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	404	Total 3203	C 2031	N 559	O 595	S 18	0	1	0
1	B	405	Total 3211	C 2035	N 561	O 597	S 18	0	1	0

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

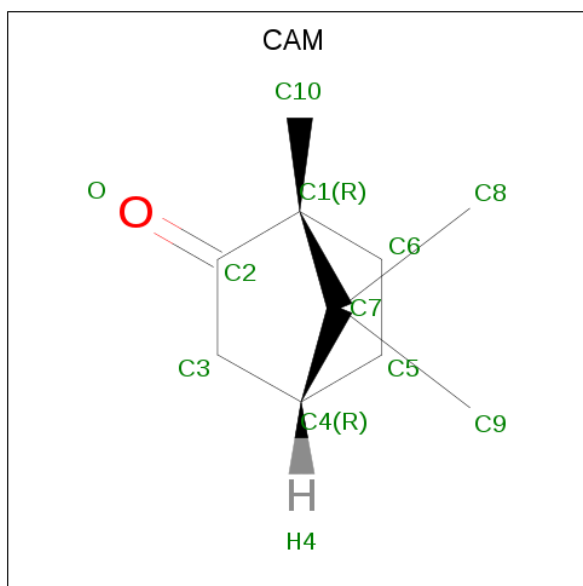


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0

- Molecule 4 is CAMPHOR (three-letter code: CAM) (formula: $C_{10}H_{16}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 10 1	0	0
4	B	1	Total C O 11 10 1	0	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	8	4	1	3	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
6	B	2	2	2	0	0
6	A	1	1	1	0	0

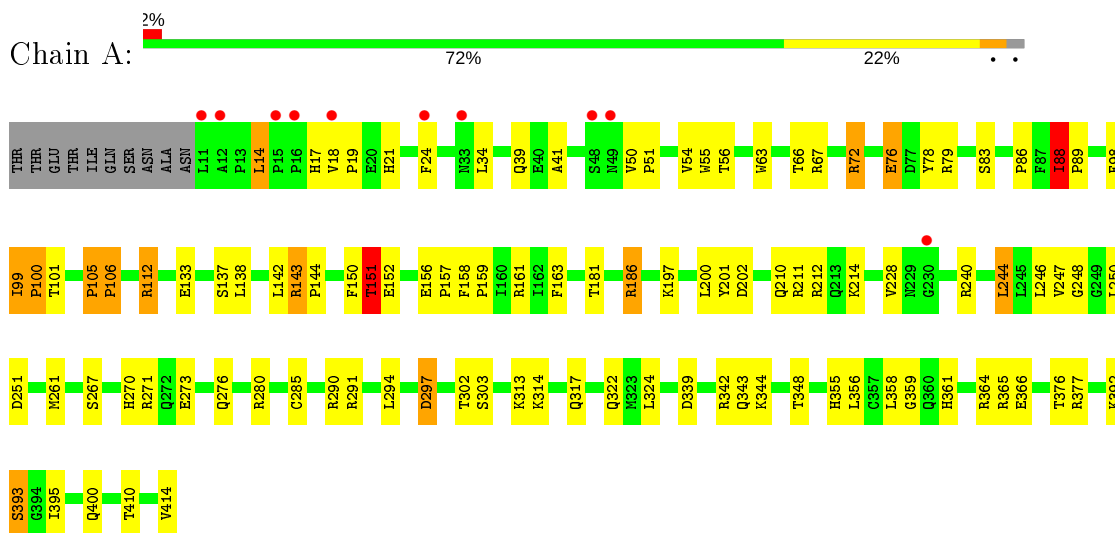
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	317	317	317	0	0
7	B	392	392	392	0	0

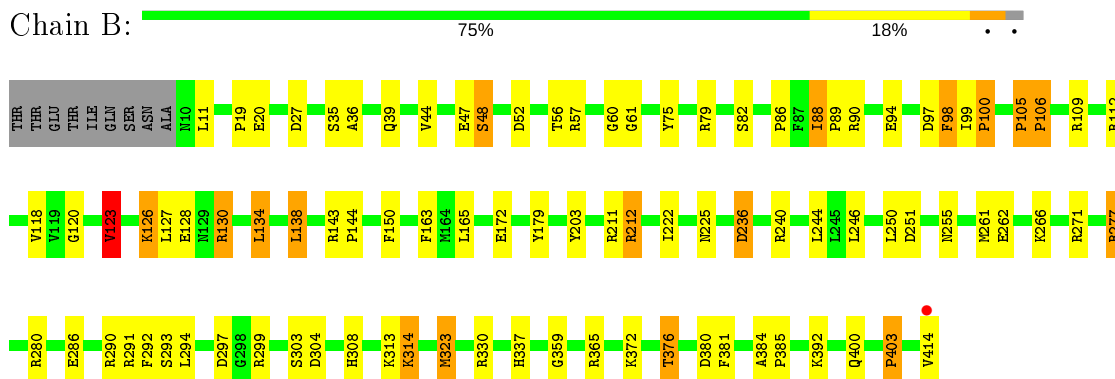
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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-CAM



- Molecule 1: CYTOCHROME P450-CAM



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.90Å 61.70Å 94.60Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	19.00 – 1.90 29.41 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (19.00-1.90) 92.8 (29.41-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.80Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.177 , 0.248 0.166 , 0.233	Depositor DCC
R_{free} test set	4550 reflections (6.85%)	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtrriage
Anisotropy	0.273	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7243	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, HEM, K, CAM, O

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	0.79	0/3286	1.68	58/4464 (1.3%)
1	B	0.88	1/3294 (0.0%)	1.77	65/4475 (1.5%)
All	All	0.83	1/6580 (0.0%)	1.73	123/8939 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	SER	CA-CB	7.16	1.63	1.52

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	ARG	NE-CZ-NH2	-17.89	111.36	120.30
1	A	291	ARG	NE-CZ-NH1	17.57	129.09	120.30
1	B	112	ARG	NE-CZ-NH2	-17.51	111.55	120.30
1	B	271	ARG	NE-CZ-NH1	16.10	128.35	120.30
1	B	212	ARG	NE-CZ-NH2	-14.82	112.89	120.30
1	A	112	ARG	NE-CZ-NH2	-14.32	113.14	120.30
1	B	291	ARG	NE-CZ-NH1	14.07	127.34	120.30
1	B	212	ARG	NE-CZ-NH1	13.10	126.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	ARG	NE-CZ-NH2	-12.25	114.18	120.30
1	B	304	ASP	CB-CG-OD1	11.94	129.05	118.30
1	A	339	ASP	CB-CG-OD1	11.74	128.87	118.30
1	A	291	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	A	280	ARG	NE-CZ-NH2	-10.68	114.96	120.30
1	B	90	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	B	79	ARG	NE-CZ-NH1	-10.30	115.15	120.30
1	A	291	ARG	CD-NE-CZ	10.27	137.97	123.60
1	A	365	ARG	NE-CZ-NH2	-9.55	115.52	120.30
1	B	297	ASP	CB-CG-OD1	9.52	126.87	118.30
1	B	330	ARG	NE-CZ-NH2	9.19	124.89	120.30
1	A	100	PRO	N-CA-CB	8.84	113.90	103.30
1	A	88	ILE	CA-C-O	-8.82	101.57	120.10
1	A	297	ASP	CB-CG-OD1	8.70	126.13	118.30
1	A	366	GLU	OE1-CD-OE2	-8.68	112.89	123.30
1	A	377	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	B	90	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	A	339	ASP	CB-CG-OD2	-8.54	110.61	118.30
1	B	203	TYR	CB-CG-CD2	-8.53	115.88	121.00
1	B	100	PRO	N-CA-CB	8.40	113.38	103.30
1	A	186	ARG	NE-CZ-NH1	-8.38	116.11	120.30
1	B	179	TYR	CB-CG-CD2	-8.18	116.09	121.00
1	A	106	PRO	CA-N-CD	-8.16	100.07	111.50
1	B	52	ASP	CB-CG-OD1	8.12	125.61	118.30
1	A	280	ARG	NH1-CZ-NH2	8.04	128.25	119.40
1	A	342	ARG	CG-CD-NE	8.04	128.68	111.80
1	A	365	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	A	89	PRO	CA-N-CD	-7.87	100.48	111.50
1	A	271	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	A	100	PRO	CA-N-CD	-7.82	100.55	111.50
1	B	106	PRO	N-CA-CB	7.72	112.57	103.30
1	B	211	ARG	NE-CZ-NH1	-7.72	116.44	120.30
1	A	105	PRO	CA-C-O	-7.70	101.72	120.20
1	A	151	THR	N-CA-CB	-7.69	95.69	110.30
1	B	277	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	B	88	ILE	CA-C-O	-7.64	104.05	120.10
1	B	89	PRO	CA-N-CD	-7.51	100.98	111.50
1	A	100	PRO	N-CD-CG	7.50	114.45	103.20
1	B	291	ARG	CD-NE-CZ	7.46	134.04	123.60
1	B	89	PRO	N-CA-CB	7.36	112.13	103.30
1	A	290	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	B	52	ASP	CB-CG-OD2	-7.34	111.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	VAL	CG1-CB-CG2	-7.20	99.39	110.90
1	B	94	GLU	OE1-CD-OE2	-7.10	114.78	123.30
1	A	251	ASP	CB-CG-OD1	7.04	124.64	118.30
1	A	364	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	280	ARG	NE-CZ-NH1	-7.01	116.80	120.30
1	A	14	LEU	CA-CB-CG	6.95	131.28	115.30
1	B	35	SER	O-C-N	-6.92	111.62	122.70
1	A	89	PRO	N-CA-CB	6.89	111.56	103.30
1	A	106	PRO	N-CA-CB	6.88	111.55	103.30
1	B	271	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	393	SER	CB-CA-C	-6.87	97.05	110.10
1	B	57	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	B	380	ASP	CB-CG-OD1	6.84	124.46	118.30
1	B	299	ARG	NE-CZ-NH1	-6.83	116.89	120.30
1	B	100	PRO	CA-N-CD	-6.73	102.08	111.50
1	B	286	GLU	OE1-CD-OE2	-6.70	115.26	123.30
1	B	57	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	67	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	151	THR	OG1-CB-CG2	6.62	125.24	110.00
1	A	143	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	A	240	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	A	211	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	B	179	TYR	CB-CG-CD1	6.42	124.85	121.00
1	B	292	PHE	CB-CG-CD1	-6.42	116.31	120.80
1	A	99	ILE	CA-C-O	-6.42	106.63	120.10
1	B	251	ASP	CB-CG-OD1	6.37	124.04	118.30
1	A	78	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	B	271	ARG	CD-NE-CZ	6.30	132.42	123.60
1	A	342	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	A	76	GLU	OE1-CD-OE2	-6.21	115.85	123.30
1	B	314	LYS	N-CA-CB	-6.19	99.45	110.60
1	B	212	ARG	CD-NE-CZ	6.09	132.13	123.60
1	B	109	ARG	NH1-CZ-NH2	6.08	126.09	119.40
1	B	314	LYS	O-C-N	-6.08	112.87	123.20
1	B	304	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	B	106	PRO	CA-N-CD	-6.05	103.03	111.50
1	B	97	ASP	CB-CG-OD1	5.95	123.66	118.30
1	B	277	ARG	CD-NE-CZ	5.88	131.83	123.60
1	B	27	ASP	CB-CG-OD1	5.86	123.58	118.30
1	A	112	ARG	NH1-CZ-NH2	5.84	125.83	119.40
1	A	212	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	B	236	ASP	CB-CG-OD1	-5.76	113.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	PRO	CA-C-O	-5.74	106.44	120.20
1	B	130	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	297	ASP	N-CA-CB	5.70	120.85	110.60
1	B	112	ARG	NH1-CZ-NH2	5.68	125.65	119.40
1	A	366	GLU	CG-CD-OE1	5.59	129.48	118.30
1	B	280	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	72	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	A	142	LEU	CB-CG-CD1	-5.48	101.69	111.00
1	A	342	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	A	395	ILE	C-N-CA	-5.43	108.12	121.70
1	A	361	HIS	CA-CB-CG	-5.43	104.37	113.60
1	B	98	PHE	CB-CG-CD2	5.43	124.60	120.80
1	A	56	THR	N-CA-CB	5.41	120.57	110.30
1	A	161	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	75	TYR	CG-CD2-CE2	-5.34	117.03	121.30
1	B	290	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	323	MET	CG-SD-CE	5.31	108.70	100.20
1	B	308	HIS	CA-CB-CG	-5.30	104.58	113.60
1	B	255	ASN	CA-CB-CG	-5.28	101.79	113.40
1	A	143	ARG	CD-NE-CZ	5.22	130.91	123.60
1	B	36	ALA	CB-CA-C	-5.19	102.31	110.10
1	B	60	GLY	C-N-CA	5.19	133.19	122.30
1	A	202	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	B	381	PHE	O-C-N	5.14	130.92	122.70
1	A	89	PRO	N-CD-CG	5.12	110.87	103.20
1	A	410	THR	CA-CB-CG2	-5.11	105.25	112.40
1	B	48	SER	C-N-CA	-5.10	108.94	121.70
1	A	302	THR	CA-CB-CG2	-5.09	105.28	112.40
1	A	186	ARG	CA-CB-CG	5.05	124.52	113.40
1	B	20	GLU	OE1-CD-OE2	5.03	129.34	123.30
1	B	250	LEU	O-C-N	-5.03	114.65	122.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	PRO	Mainchain,Peptide
1	A	88	ILE	Mainchain,Peptide
1	A	99	ILE	Mainchain,Peptide
1	B	105	PRO	Mainchain,Peptide
1	B	88	ILE	Mainchain,Peptide
1	B	99	ILE	Mainchain,Peptide

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3203	0	3155	51	0
1	B	3211	0	3161	41	0
2	A	43	0	30	7	0
2	B	43	0	30	1	0
3	A	1	0	0	1	0
4	A	11	0	16	1	0
4	B	11	0	16	2	0
5	A	8	0	12	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
7	A	317	0	0	7	0
7	B	392	0	0	8	0
All	All	7243	0	6420	95	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 (95) 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:163:PHE:HE2	1:A:246:LEU:HD23	1.42	0.85
4:B:502:CAM:H52	7:B:653:HOH:O	1.77	0.84
1:B:130:ARG:HD2	1:B:165:LEU:HD21	1.61	0.82
1:B:134:LEU:HD22	1:B:138:LEU:HD22	1.65	0.79
1:A:163:PHE:CE2	1:A:246:LEU:HD23	2.20	0.76
1:A:210:GLN:HE22	1:A:214:LYS:HD2	1.54	0.72
1:A:181[A]:THR:HG22	1:A:247:VAL:HG22	1.72	0.71
1:B:126:LYS:HD3	1:B:130:ARG:HH22	1.57	0.68
1:B:163:PHE:HE2	1:B:246:LEU:HD23	1.66	0.60
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.85	0.58
1:B:143:ARG:HB3	1:B:144:PRO:HD3	1.85	0.58
1:B:128:GLU:HB2	1:B:365:ARG:HH12	1.68	0.58
1:A:14:LEU:HB2	7:A:837:HOH:O	2.02	0.58
1:B:130:ARG:HD2	1:B:165:LEU:CD2	2.32	0.58
1:B:376:THR:HG23	1:B:414:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ASP:HB3	7:B:678:HOH:O	2.04	0.57
1:A:303:SER:HA	1:A:314:LYS:HB2	1.85	0.57
1:A:19:PRO:HB2	1:A:21:HIS:CE1	2.40	0.56
1:B:303:SER:HA	1:B:314:LYS:HB2	1.86	0.56
1:B:127:LEU:HA	1:B:130:ARG:HH21	1.71	0.56
1:A:267:SER:OG	1:A:270:HIS:ND1	2.37	0.55
1:B:127:LEU:HD23	1:B:130:ARG:NH2	2.22	0.55
1:A:24:PHE:HB3	1:A:54:VAL:HG21	1.88	0.55
1:A:143:ARG:HB3	1:A:144:PRO:HD3	1.88	0.55
1:A:276:GLN:HE21	1:B:172:GLU:H	1.55	0.55
1:A:151:THR:HG23	7:A:645:HOH:O	2.07	0.54
1:A:197:LYS:HE3	1:A:201:TYR:CE2	2.43	0.54
1:B:56:THR:O	1:B:61:GLY:HA2	2.09	0.53
3:A:502:O:O	4:A:503:CAM:H52	2.08	0.53
1:B:163:PHE:CE2	1:B:246:LEU:HD23	2.44	0.52
1:A:112:ARG:HG3	1:A:358:LEU:HD11	1.91	0.52
1:A:313:LYS:HE3	7:A:834:HOH:O	2.09	0.52
1:A:197:LYS:HE3	1:A:201:TYR:HE2	1.73	0.51
1:A:17:HIS:CD2	1:A:313:LYS:HB2	2.46	0.51
1:A:210:GLN:NE2	1:A:214:LYS:HD2	2.25	0.51
1:B:337:HIS:HB3	7:B:934:HOH:O	2.11	0.50
1:B:126:LYS:CD	1:B:130:ARG:HH22	2.25	0.50
1:B:120:GLY:O	1:B:123:VAL:HG12	2.12	0.50
1:B:277:ARG:HH11	1:B:277:ARG:HG3	1.78	0.49
1:B:262:GLU:CG	1:B:266:LYS:HE3	2.43	0.49
1:B:372:LYS:NZ	1:B:372:LYS:HB3	2.29	0.48
1:A:273:GLU:HG3	7:A:757:HOH:O	2.12	0.48
1:B:392:LYS:HD3	1:B:400:GLN:OE1	2.14	0.48
1:A:133:GLU:O	1:A:137:SER:HB2	2.14	0.47
1:A:356:LEU:HB2	7:A:728:HOH:O	2.15	0.47
1:B:212:ARG:HA	1:B:225:ASN:HD21	1.80	0.46
1:A:83:SER:HB3	1:A:101:THR:O	2.15	0.46
1:B:98:PHE:HB3	1:B:244:LEU:HB2	1.97	0.46
1:A:151:THR:CG2	1:A:152:GLU:N	2.79	0.46
1:A:19:PRO:HB2	1:A:21:HIS:ND1	2.31	0.45
2:A:501:HEM:HMB2	2:A:501:HEM:HBB2	1.97	0.45
1:B:262:GLU:HG2	1:B:266:LYS:HE3	1.98	0.45
1:A:88:ILE:HD11	1:A:317:GLN:HB3	1.99	0.45
1:B:392:LYS:NZ	7:B:612:HOH:O	2.50	0.45
2:A:501:HEM:CMB	2:A:501:HEM:HBB2	2.47	0.45
1:B:293:SER:OG	1:B:323:MET:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HD23	1:A:294:LEU:H	1.83	0.44
1:A:322:GLN:HB3	1:A:348:THR:O	2.17	0.44
1:B:376:THR:CG2	1:B:414:VAL:HG21	2.48	0.44
1:A:18:VAL:HG22	1:A:63:TRP:CZ2	2.53	0.44
1:A:276:GLN:HE21	1:B:172:GLU:N	2.16	0.43
1:A:156:GLU:N	1:A:157:PRO:HD2	2.33	0.43
1:A:55:TRP:HB2	1:A:63:TRP:CZ3	2.53	0.43
1:A:244:LEU:CD1	2:A:501:HEM:HMD2	2.49	0.43
1:A:376:THR:HG22	1:A:414:VAL:HG21	2.01	0.43
1:B:313:LYS:O	1:B:314:LYS:C	2.55	0.43
1:A:186:ARG:HD2	1:A:392:LYS:HG3	2.00	0.43
1:A:72:ARG:O	1:A:76:GLU:HG3	2.18	0.43
1:B:372:LYS:HZ1	1:B:372:LYS:HB3	1.83	0.43
1:A:297:ASP:OD2	2:A:501:HEM:O2A	2.36	0.43
1:A:150:PHE:CZ	1:A:261:MET:HG3	2.53	0.42
1:B:44:VAL:HA	1:B:47:GLU:HG3	2.01	0.42
1:A:151:THR:HG22	1:A:152:GLU:H	1.83	0.42
1:B:403:PRO:HB3	7:B:727:HOH:O	2.19	0.42
1:B:19:PRO:HD3	7:B:636:HOH:O	2.18	0.42
1:B:236:ASP:CB	7:B:678:HOH:O	2.67	0.42
4:B:502:CAM:H93	7:B:653:HOH:O	2.20	0.42
1:A:98:PHE:HB3	1:A:244:LEU:HG	2.02	0.42
1:A:244:LEU:HD13	2:A:501:HEM:HMD2	2.02	0.41
1:A:414:VAL:O	1:A:414:VAL:HG12	2.20	0.41
1:A:151:THR:HG22	1:A:152:GLU:N	2.35	0.41
1:A:66:THR:HA	1:A:324:LEU:HD23	2.02	0.41
1:B:150:PHE:CZ	1:B:261:MET:HG3	2.55	0.41
1:A:355:HIS:HD1	2:A:501:HEM:CGD	2.32	0.41
1:A:248:GLY:HA2	7:A:609:HOH:O	2.20	0.41
1:A:34:LEU:HA	1:A:41:ALA:HB2	2.02	0.41
1:A:359:GLY:HA3	2:A:501:HEM:C3C	2.56	0.41
1:B:118:VAL:HG12	1:B:222:ILE:HG21	2.02	0.40
1:B:236:ASP:O	1:B:240:ARG:HG3	2.21	0.40
1:B:294:LEU:H	1:B:294:LEU:HD23	1.86	0.40
1:B:359:GLY:HA3	2:B:501:HEM:C3C	2.57	0.40
1:A:138:LEU:HA	1:A:138:LEU:HD23	1.92	0.40
1:B:384:ALA:HA	1:B:385:PRO:HD3	1.99	0.40
1:A:50:VAL:HA	1:A:51:PRO:HD3	1.96	0.40
1:A:79:ARG:HG3	7:A:801:HOH:O	2.21	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	403/414 (97%)	383 (95%)	18 (4%)	2 (0%)	29	18
1	B	404/414 (98%)	391 (97%)	11 (3%)	2 (0%)	29	18
All	All	807/828 (98%)	774 (96%)	29 (4%)	4 (0%)	29	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	PRO
1	A	100	PRO
1	B	106	PRO
1	B	100	PRO

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	350/358 (98%)	337 (96%)	13 (4%)	34	25
1	B	351/358 (98%)	341 (97%)	10 (3%)	43	36
All	All	701/716 (98%)	678 (97%)	23 (3%)	38	29

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	86	PRO

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Mol	Chain	Res	Type
1	A	88	ILE
1	A	151	THR
1	A	200	LEU
1	A	228	VAL
1	A	244	LEU
1	A	250	LEU
1	A	285	CYS
1	A	343	GLN
1	A	344	LYS
1	A	393	SER
1	A	400	GLN
1	B	11	LEU
1	B	39	GLN
1	B	48	SER
1	B	86	PRO
1	B	123	VAL
1	B	126	LYS
1	B	134	LEU
1	B	138	LEU
1	B	376	THR
1	B	403	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	39	GLN
1	A	46	GLN
1	A	210	GLN
1	A	225	ASN
1	A	272	GLN
1	A	276	GLN
1	A	311	GLN
1	A	400	GLN
1	B	30	ASN
1	B	33	ASN
1	B	39	GLN
1	B	46	GLN
1	B	69	GLN
1	B	132	GLN
1	B	210	GLN
1	B	225	ASN

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Mol	Chain	Res	Type
1	B	400	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 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$
4	CAM	A	503	-	12,12,12	1.10	1 (8%)	20,21,21	2.87	9 (45%)
2	HEM	B	501	1,7	27,50,50	2.05	6 (22%)	17,82,82	2.65	9 (52%)
2	HEM	A	501	1	27,50,50	1.91	6 (22%)	17,82,82	2.78	8 (47%)
5	TRS	A	504	-	7,7,7	1.84	3 (42%)	9,9,9	1.48	1 (11%)
4	CAM	B	502	-	12,12,12	1.34	1 (8%)	20,21,21	2.80	11 (55%)

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	-
4	CAM	B	502	-	-	-	0/3/2/2
5	TRS	A	504	-	-	3/9/9/9	-
2	HEM	B	501	1,7	-	0/6/54/54	-
4	CAM	A	503	-	-	-	0/3/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3B-C2B	-5.15	1.33	1.40
2	A	501	HEM	C3B-C2B	-4.68	1.33	1.40
2	A	501	HEM	C3C-C2C	-4.35	1.34	1.40
2	B	501	HEM	C3C-C2C	-4.26	1.34	1.40
4	B	502	CAM	C1-C2	3.94	1.58	1.52
2	B	501	HEM	CAA-C2A	3.64	1.57	1.52
2	B	501	HEM	C3C-CAC	3.56	1.55	1.47
4	A	503	CAM	C1-C2	3.23	1.57	1.52
2	A	501	HEM	C3B-CAB	3.18	1.54	1.47
2	A	501	HEM	C3C-CAC	3.15	1.54	1.47
2	B	501	HEM	C3B-CAB	2.96	1.54	1.47
2	A	501	HEM	CAA-C2A	2.79	1.56	1.52
5	A	504	TRS	O2-C2	2.78	1.51	1.42
5	A	504	TRS	O1-C1	2.40	1.50	1.42
5	A	504	TRS	O3-C3	2.27	1.49	1.42
2	B	501	HEM	C1A-NA	2.26	1.40	1.36
2	A	501	HEM	CAD-C3D	2.04	1.55	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	CAM	C3-C2-C1	-6.20	95.04	107.34
2	A	501	HEM	CMA-C3A-C4A	-6.09	119.10	128.46
4	B	502	CAM	C5-C4-C3	-5.66	90.80	106.40
4	A	503	CAM	C5-C4-C3	-5.43	91.44	106.40
4	B	502	CAM	C3-C2-C1	-5.34	96.75	107.34
2	B	501	HEM	CMD-C2D-C1D	-5.10	120.62	128.46
2	B	501	HEM	CBD-CAD-C3D	4.55	120.87	112.48
4	A	503	CAM	C4-C3-C2	4.55	109.81	102.03
4	A	503	CAM	O-C2-C3	4.46	135.74	126.47
2	A	501	HEM	CBD-CAD-C3D	4.44	120.65	112.48
2	B	501	HEM	CMA-C3A-C4A	-4.41	121.68	128.46
4	B	502	CAM	O-C2-C3	4.34	135.48	126.47
2	A	501	HEM	CMA-C3A-C2A	4.29	133.03	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	CAM	O-C2-C1	-4.09	120.42	125.39
2	A	501	HEM	CMD-C2D-C1D	-4.08	122.19	128.46
4	A	503	CAM	C7-C1-C2	3.93	106.98	100.30
2	B	501	HEM	CMD-C2D-C3D	3.60	131.72	124.94
4	B	502	CAM	C9-C7-C8	3.59	116.67	107.62
4	B	502	CAM	C7-C1-C2	3.36	106.02	100.30
4	B	502	CAM	C6-C1-C7	3.35	108.69	101.53
2	A	501	HEM	CMC-C2C-C3C	3.02	130.32	124.68
5	A	504	TRS	C3-C-C2	-2.99	101.54	110.81
2	B	501	HEM	CBA-CAA-C2A	2.96	117.95	112.49
4	B	502	CAM	C4-C3-C2	2.93	107.03	102.03
2	B	501	HEM	CMA-C3A-C2A	2.87	130.34	124.94
4	B	502	CAM	C5-C6-C1	-2.83	99.08	104.79
2	A	501	HEM	CBA-CAA-C2A	2.82	117.70	112.49
2	B	501	HEM	CAA-CBA-CGA	2.82	117.40	112.67
2	A	501	HEM	CMD-C2D-C3D	2.53	129.71	124.94
4	A	503	CAM	C9-C7-C8	2.48	113.88	107.62
2	A	501	HEM	CMB-C2B-C3B	2.46	129.28	124.68
2	B	501	HEM	CMB-C2B-C3B	2.37	129.11	124.68
4	B	502	CAM	C5-C4-C7	2.22	107.02	102.88
4	A	503	CAM	C9-C7-C4	-2.20	108.22	113.50
4	B	502	CAM	C6-C5-C4	2.16	106.53	103.15
2	B	501	HEM	CMC-C2C-C3C	2.15	128.71	124.68
4	A	503	CAM	C6-C1-C7	2.08	105.98	101.53
4	B	502	CAM	C9-C7-C4	-2.04	108.59	113.50

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	TRS	C1-C-C3-O3
5	A	504	TRS	N-C-C3-O3
5	A	504	TRS	C2-C-C3-O3

There are no ring outliers.

4 monomers are involved in 11 short contacts:

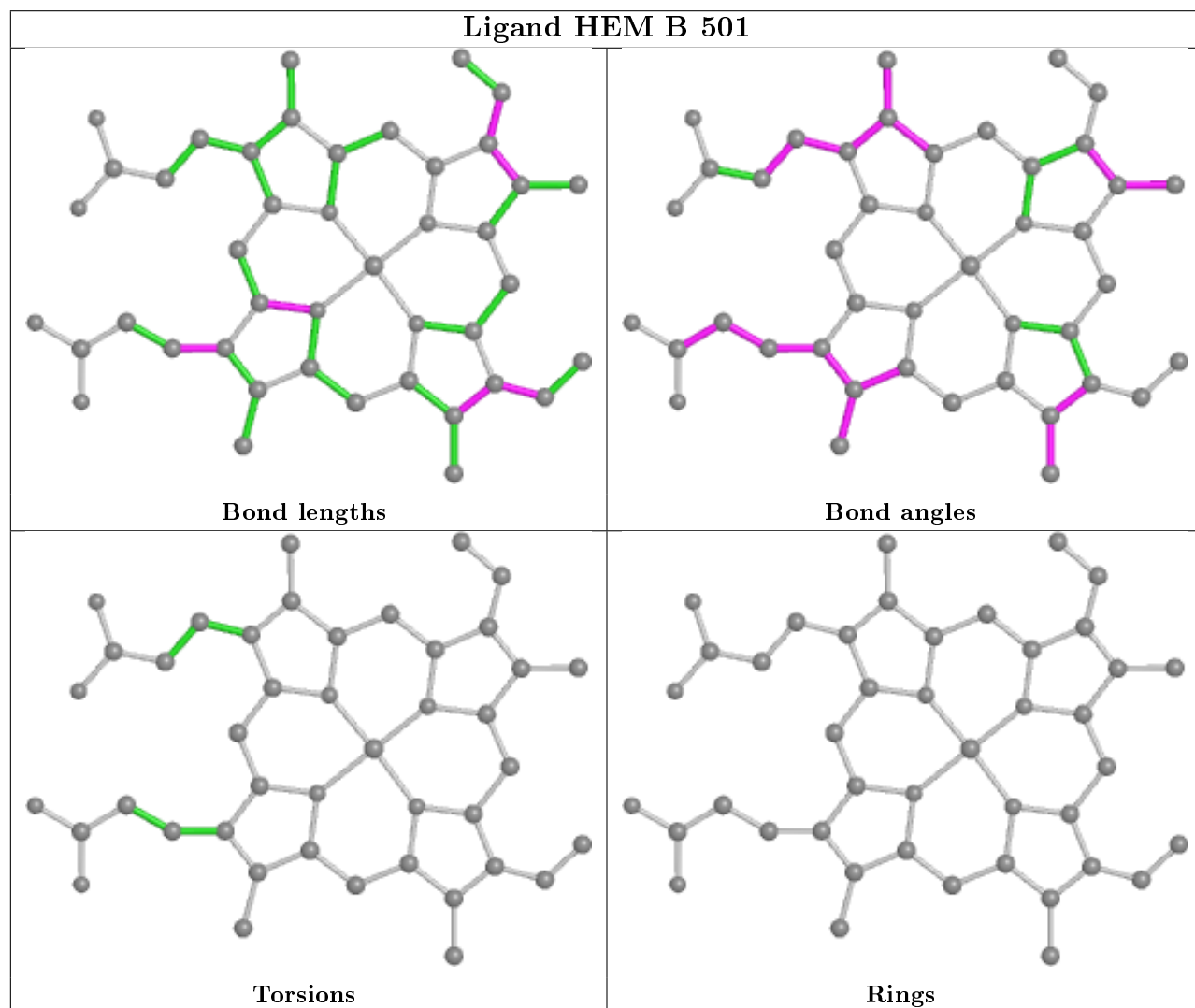
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	CAM	1	0
2	B	501	HEM	1	0
2	A	501	HEM	7	0

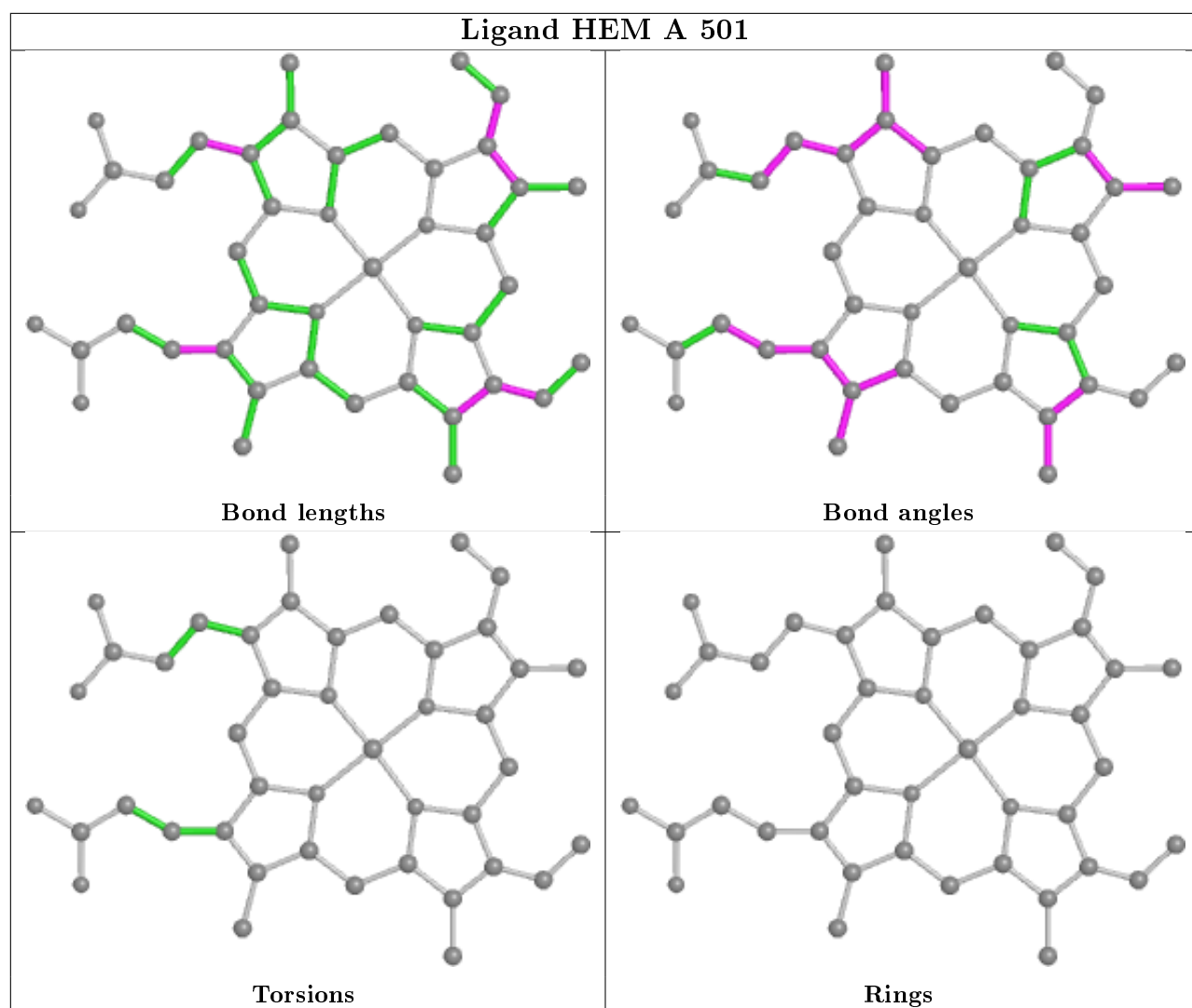
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	502	CAM	2	0

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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	404/414 (97%)	-0.11	10 (2%) 57 60	10, 22, 46, 75	1 (0%)
1	B	405/414 (97%)	-0.43	1 (0%) 95 95	8, 17, 38, 58	0
All	All	809/828 (97%)	-0.27	11 (1%) 75 77	8, 19, 42, 75	1 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	ASN	3.8
1	A	11	LEU	3.3
1	A	48	SER	3.1
1	A	16	PRO	2.5
1	A	18	VAL	2.5
1	A	12	ALA	2.5
1	B	414	VAL	2.5
1	A	24	PHE	2.5
1	A	230	GLY	2.1
1	A	15	PRO	2.0
1	A	33	ASN	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 carbohydrates in this entry.

6.4 Ligands

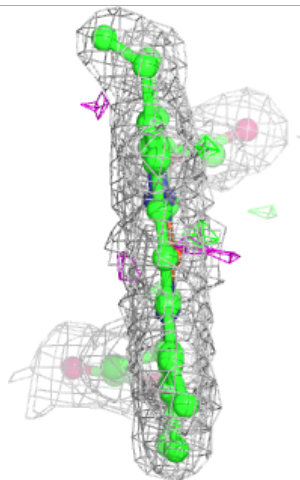
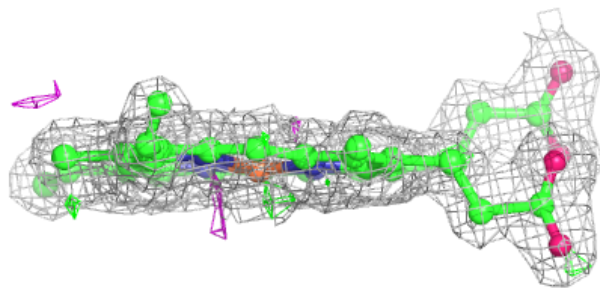
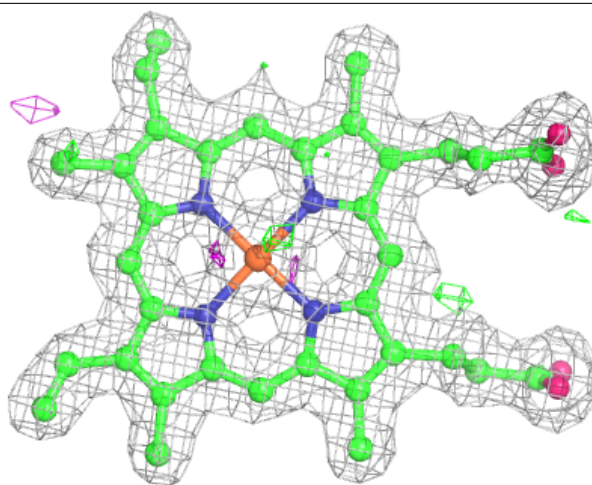
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

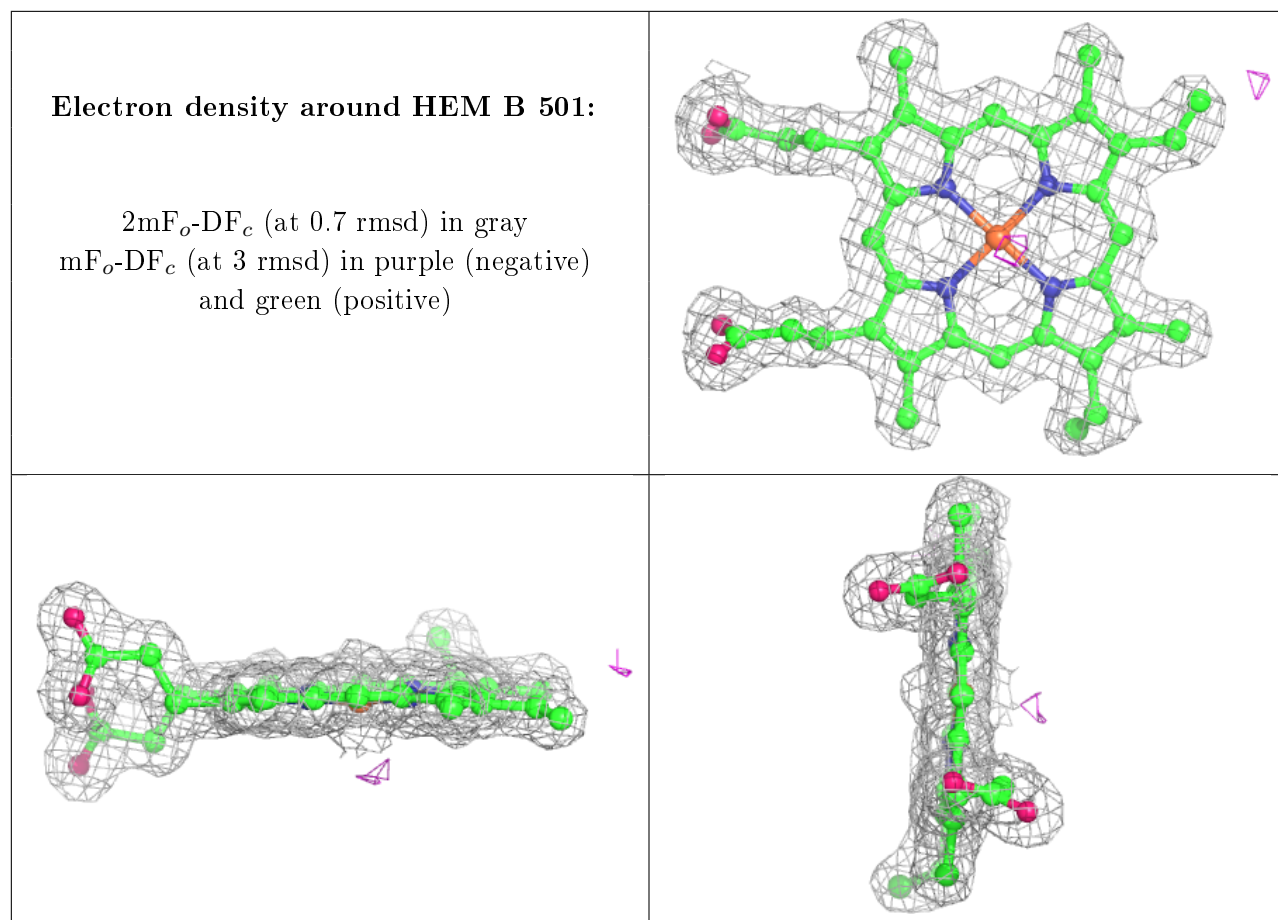
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CAM	A	503	11/11	0.96	0.23	17,20,23,23	0
4	CAM	B	502	11/11	0.96	0.16	8,12,19,20	0
5	TRS	A	504	8/8	0.97	0.07	9,15,22,30	0
2	HEM	A	501	43/43	0.98	0.14	7,16,22,24	0
6	K	B	504	1/1	0.99	0.04	17,17,17,17	0
6	K	A	505	1/1	0.99	0.04	19,19,19,19	0
2	HEM	B	501	43/43	0.99	0.13	5,13,18,24	0
3	O	A	502	1/1	0.99	0.10	18,18,18,18	1
6	K	B	503	1/1	1.00	0.05	12,12,12,12	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 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 [\(i\)](#)

There are no such residues in this entry.