



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:56 AM UTC

PDB ID : 1DZ9 / pdb_00001dz9
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 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

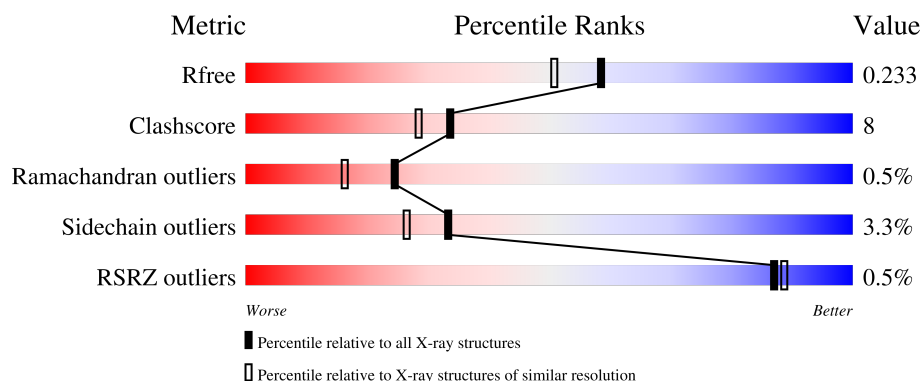
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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	414	% 64% 28% 5% ..
1	B	414	67% 25% 5% ..

2 Entry composition [i](#)

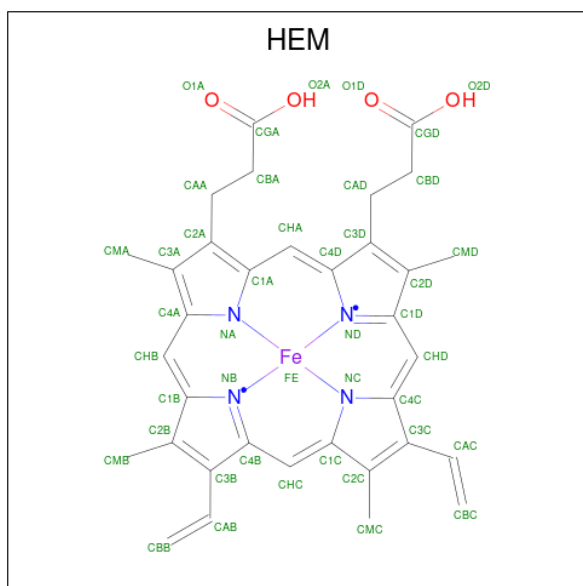
There are 7 unique types of molecules in this entry. The entry contains 7243 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	404	Total	C	N	O	S	0	1	0
			3203	2031	559	595	18			
1	B	405	Total	C	N	O	S	0	1	0
			3211	2035	561	597	18			

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

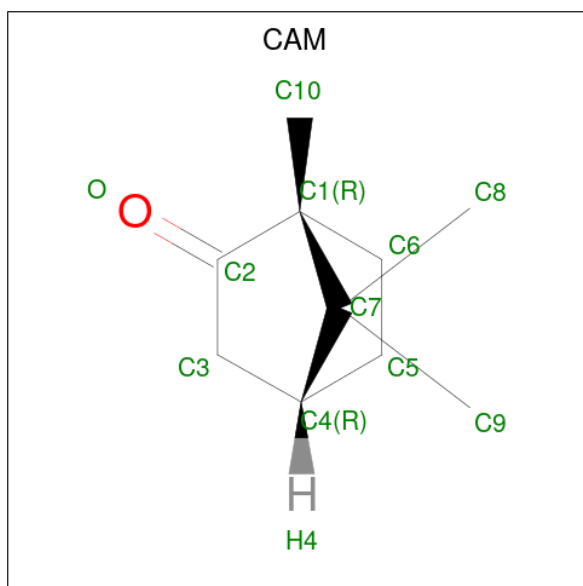


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is OXYGEN ATOM (CCD ID: O) (formula: O).

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

- Molecule 4 is CAMPHOR (CCD ID: 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 (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



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

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

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

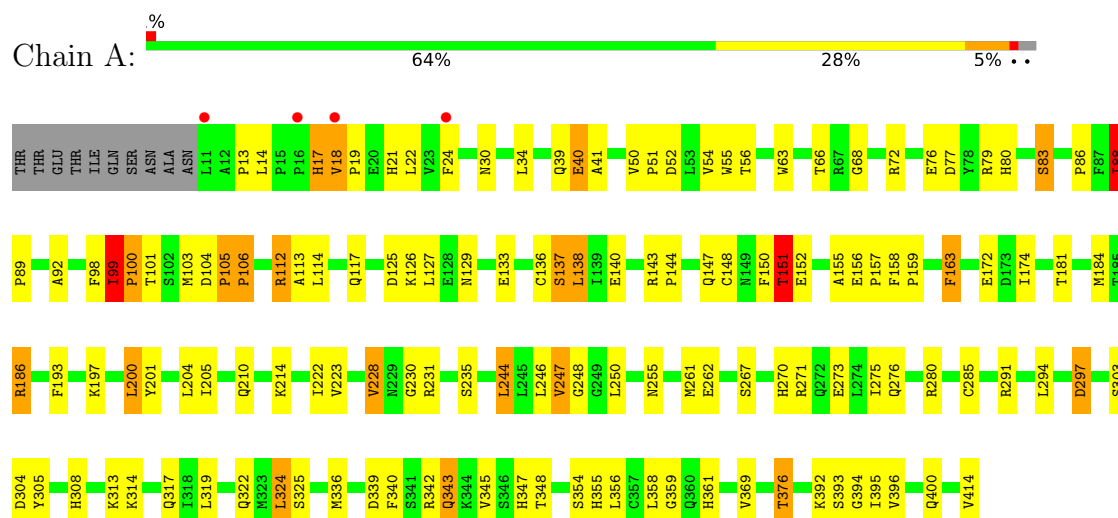
- Molecule 7 is water.

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

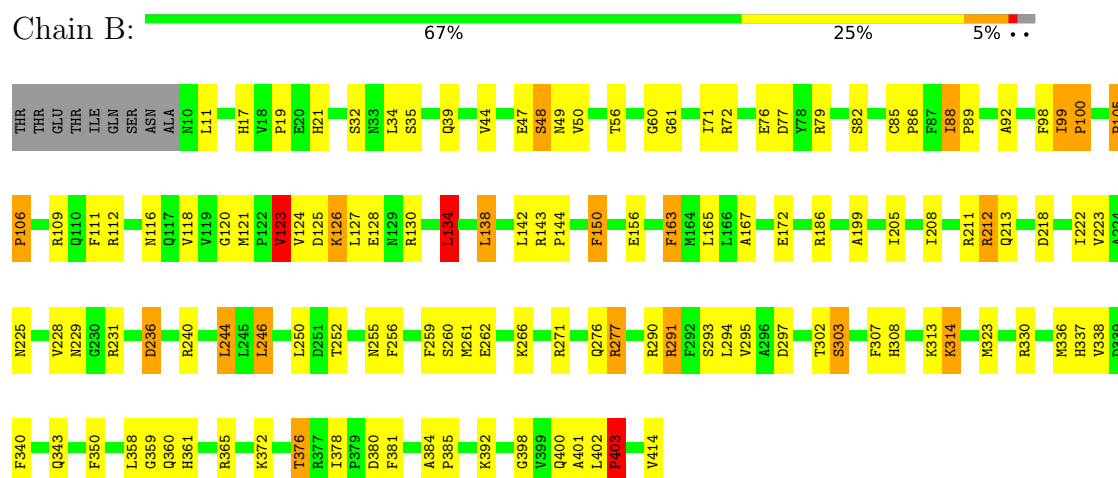
3 Residue-property plots

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-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 19.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.6 (19.00-1.90) 98.3 (19.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.80Å)	Xtriage
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	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 71.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7243	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage'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.*

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: K, TRS, O, HEM, CAM

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	1.07	1/3286 (0.0%)	2.09	119/4464 (2.7%)
1	B	1.17	5/3294 (0.2%)	2.13	120/4475 (2.7%)
All	All	1.12	6/6580 (0.1%)	2.11	239/8939 (2.7%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	SER	CA-CB	6.77	1.63	1.53
1	B	49	ASN	N-CA	6.05	1.53	1.46
1	B	205	ILE	CA-CB	5.78	1.57	1.54
1	A	174	ILE	CA-CB	5.43	1.56	1.54
1	B	99	ILE	N-CA	-5.24	1.41	1.46
1	B	71	ILE	C-N	-5.19	1.27	1.33

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	ILE	CA-C-O	-20.00	104.05	119.25
1	A	88	ILE	CA-C-O	-16.81	101.57	119.89
1	A	105	PRO	CA-C-O	-12.99	101.72	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ILE	CA-C-N	-11.47	108.12	123.14
1	A	395	ILE	C-N-CA	-11.47	108.12	123.14
1	B	99	ILE	CA-C-O	-11.09	110.44	119.98
1	B	255	ASN	CA-CB-CG	-10.81	101.79	112.60
1	B	163	PHE	CA-CB-CG	-10.50	103.30	113.80
1	A	100	PRO	N-CA-CB	10.15	113.90	103.25
1	B	50	VAL	CA-C-O	10.05	126.54	119.20
1	A	99	ILE	CA-C-O	-9.94	106.63	119.95
1	A	151	THR	N-CA-CB	-9.92	95.69	110.07
1	B	100	PRO	N-CA-CB	9.80	113.38	102.60
1	B	105	PRO	CA-C-O	-9.74	106.44	120.56
1	A	291	ARG	CD-NE-CZ	9.69	137.97	124.40
1	B	297	ASP	N-CA-CB	9.67	120.85	108.96
1	A	361	HIS	CA-CB-CG	-9.43	104.37	113.80
1	B	343	GLN	N-CA-C	9.23	121.42	111.36
1	B	308	HIS	CA-CB-CG	-9.22	104.58	113.80
1	B	48	SER	CA-C-N	-9.10	108.94	122.86
1	B	48	SER	C-N-CA	-9.10	108.94	122.86
1	B	106	PRO	N-CA-CB	9.06	112.57	102.60
1	A	396	VAL	CA-C-O	-8.86	111.08	120.39
1	B	48	SER	N-CA-C	8.83	122.01	111.33
1	B	109	ARG	NE-CZ-NH2	-8.71	111.36	119.20
1	B	403	PRO	CB-CA-C	8.69	119.31	111.40
1	B	205	ILE	N-CA-CB	-8.68	104.70	110.52
1	B	89	PRO	N-CA-CB	8.66	112.13	102.60
1	A	106	PRO	CA-N-CD	-8.52	100.07	112.00
1	B	112	ARG	NE-CZ-NH2	-8.50	111.55	119.20
1	A	255	ASN	CA-CB-CG	-8.38	104.22	112.60
1	B	35	SER	CA-C-O	8.30	129.84	119.05
1	A	89	PRO	CA-N-CD	-8.23	100.48	112.00
1	A	100	PRO	CA-N-CD	-8.18	100.55	112.00
1	B	32	SER	CA-C-N	-8.16	110.27	122.83
1	B	32	SER	C-N-CA	-8.16	110.27	122.83
1	B	116	ASN	OD1-CG-ND2	7.98	130.58	122.60
1	A	345	VAL	CA-C-N	-7.97	112.00	123.00
1	A	345	VAL	C-N-CA	-7.97	112.00	123.00
1	A	151	THR	OG1-CB-CG2	7.97	125.24	109.30
1	A	89	PRO	N-CA-CB	7.92	111.56	103.25
1	A	106	PRO	N-CA-CB	7.91	111.55	103.25
1	B	85	CYS	O-C-N	-7.88	114.27	121.37
1	B	105	PRO	CB-CA-C	-7.88	101.30	110.92
1	B	381	PHE	CA-C-O	-7.86	112.84	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	SER	O-C-N	-7.85	111.62	122.46
1	B	260	SER	O-C-N	7.80	130.11	122.07
1	B	314	LYS	O-C-N	-7.77	112.87	122.82
1	A	77	ASP	CA-CB-CG	7.71	120.31	112.60
1	A	186	ARG	O-C-N	-7.69	115.00	121.23
1	A	291	ARG	NE-CZ-NH1	7.59	129.09	121.50
1	A	342	ARG	CG-CD-NE	7.58	128.68	112.00
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	A	163	PHE	CA-CB-CG	-7.45	106.35	113.80
1	B	186	ARG	O-C-N	-7.38	115.00	121.20
1	B	314	LYS	CA-C-O	7.38	129.42	121.44
1	A	325	SER	CA-C-O	-7.15	113.31	120.82
1	A	136	CYS	CA-C-O	7.02	127.99	120.55
1	B	212	ARG	NE-CZ-NH2	-7.01	112.89	119.20
1	B	259	PHE	CA-C-N	6.97	129.50	120.44
1	B	259	PHE	C-N-CA	6.97	129.50	120.44
1	B	338	VAL	CA-C-N	6.93	132.93	122.95
1	B	338	VAL	C-N-CA	6.93	132.93	122.95
1	A	262	GLU	CA-C-O	6.91	127.74	120.42
1	B	291	ARG	CD-NE-CZ	6.89	134.04	124.40
1	B	134	LEU	O-C-N	6.88	129.53	122.09
1	A	280	ARG	NH1-CZ-NH2	6.88	128.25	119.30
1	B	271	ARG	NE-CZ-NH1	6.85	128.35	121.50
1	B	260	SER	CA-C-O	-6.83	113.65	120.82
1	B	276	GLN	CA-C-O	-6.80	113.68	120.82
1	B	99	ILE	O-C-N	6.79	128.88	120.66
1	B	255	ASN	OD1-CG-ND2	6.78	129.38	122.60
1	A	112	ARG	NE-CZ-NH2	-6.74	113.14	119.20
1	B	100	PRO	CA-N-CD	-6.73	102.08	111.50
1	B	381	PHE	O-C-N	6.73	130.92	123.25
1	B	213	GLN	CB-CG-CD	6.68	123.95	112.60
1	A	104	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	394	GLY	N-CA-C	-6.58	101.49	111.42
1	B	213	GLN	OE1-CD-NE2	-6.56	116.04	122.60
1	B	314	LYS	N-CA-CB	-6.54	99.45	109.92
1	A	172	GLU	CB-CG-CD	6.51	123.67	112.60
1	B	403	PRO	N-CA-CB	-6.51	98.87	103.23
1	A	393	SER	CB-CA-C	-6.50	97.05	109.66
1	B	229	ASN	CA-CB-CG	-6.49	106.11	112.60
1	A	308	HIS	CA-CB-CG	-6.47	107.33	113.80
1	A	151	THR	CB-CA-C	6.38	120.99	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	VAL	CA-C-N	6.37	127.05	119.98
1	A	247	VAL	C-N-CA	6.37	127.05	119.98
1	B	79	ARG	NE-CZ-NH1	-6.35	115.15	121.50
1	B	231	ARG	CA-C-O	6.34	127.63	120.46
1	B	256	PHE	CA-CB-CG	-6.33	107.47	113.80
1	B	330	ARG	NE-CZ-NH2	6.33	124.89	119.20
1	B	290	ARG	O-C-N	-6.29	115.29	122.09
1	A	155	ALA	O-C-N	6.27	128.61	122.09
1	A	324	LEU	N-CA-C	6.26	119.09	111.82
1	B	340	PHE	CA-CB-CG	6.25	120.06	113.80
1	B	252	THR	CA-CB-OG1	-6.25	100.22	109.60
1	A	354	SER	CA-CB-OG	-6.25	98.60	111.10
1	B	223	VAL	O-C-N	6.21	128.36	121.90
1	B	48	SER	CA-CB-OG	-6.20	98.70	111.10
1	A	396	VAL	O-C-N	6.16	129.91	123.26
1	A	83	SER	CA-CB-OG	-6.16	98.79	111.10
1	B	250	LEU	O-C-N	-6.15	114.65	122.34
1	B	99	ILE	N-CA-C	6.13	117.40	107.71
1	B	307	PHE	CA-CB-CG	6.13	119.93	113.80
1	A	129	ASN	CA-C-O	-6.12	114.39	120.82
1	A	395	ILE	O-C-N	6.12	127.80	121.87
1	A	205	ILE	CB-CG1-CD1	6.11	126.64	113.80
1	A	13	PRO	CA-C-N	6.11	128.96	120.65
1	A	13	PRO	C-N-CA	6.11	128.96	120.65
1	A	113	ALA	O-C-N	-6.11	115.65	122.12
1	B	360	GLN	CB-CG-CD	-6.11	102.22	112.60
1	A	155	ALA	CA-C-O	-6.09	114.38	120.90
1	A	113	ALA	CA-C-O	6.09	127.01	120.55
1	A	52	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	56	THR	N-CA-CB	6.08	120.57	110.85
1	B	111	PHE	CA-C-O	6.07	126.85	120.42
1	A	40	GLU	CA-C-O	-6.05	114.14	120.55
1	B	106	PRO	CA-N-CD	-6.05	103.03	111.50
1	A	376	THR	O-C-N	-6.01	115.74	122.12
1	B	350	PHE	CA-C-O	6.01	126.94	119.78
1	B	60	GLY	CA-C-N	6.01	133.19	121.41
1	B	60	GLY	C-N-CA	6.01	133.19	121.41
1	A	231	ARG	O-C-N	6.00	126.45	121.35
1	B	358	LEU	N-CA-C	-6.00	105.80	113.23
1	B	50	VAL	O-C-N	-5.99	116.79	121.46
1	A	204	LEU	N-CA-C	5.97	120.29	112.89
1	A	343	GLN	N-CA-C	5.93	117.41	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	LEU	CA-C-O	-5.91	113.69	120.24
1	A	88	ILE	CA-CB-CG1	5.86	120.36	110.40
1	B	291	ARG	NE-CZ-NH1	5.84	127.34	121.50
1	A	339	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	297	ASP	CA-C-N	-5.80	112.50	120.57
1	A	297	ASP	C-N-CA	-5.80	112.50	120.57
1	B	295	VAL	O-C-N	5.79	129.04	123.14
1	A	354	SER	CA-C-N	-5.77	113.44	122.73
1	A	354	SER	C-N-CA	-5.77	113.44	122.73
1	A	99	ILE	CA-C-N	5.77	127.05	119.84
1	A	99	ILE	C-N-CA	5.77	127.05	119.84
1	B	125	ASP	CA-C-N	5.77	128.58	120.28
1	B	125	ASP	C-N-CA	5.77	128.58	120.28
1	A	186	ARG	CA-C-O	5.75	127.61	121.28
1	B	271	ARG	CD-NE-CZ	5.73	132.42	124.40
1	B	100	PRO	N-CD-CG	5.71	110.65	103.80
1	B	259	PHE	O-C-N	-5.71	116.19	122.07
1	B	380	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	252	THR	CA-C-O	-5.68	115.05	120.90
1	A	394	GLY	CA-C-O	-5.68	116.55	121.04
1	A	394	GLY	O-C-N	5.62	128.47	123.80
1	B	398	GLY	N-CA-C	5.60	119.46	111.12
1	A	271	ARG	NE-CZ-NH2	-5.58	114.18	119.20
1	B	79	ARG	O-C-N	5.58	128.51	122.15
1	B	167	ALA	CA-C-O	5.58	126.03	119.28
1	B	92	ALA	CA-C-O	5.58	126.45	120.70
1	A	235	SER	CA-CB-OG	-5.57	99.96	111.10
1	B	79	ARG	CA-C-O	-5.57	114.52	120.42
1	B	92	ALA	O-C-N	-5.57	116.07	122.09
1	B	302	THR	CA-CB-OG1	-5.57	101.25	109.60
1	A	114	LEU	CB-CA-C	-5.56	101.39	110.85
1	B	156	GLU	O-C-N	-5.52	116.46	120.27
1	B	212	ARG	CD-NE-CZ	5.52	132.13	124.40
1	A	80	HIS	CA-CB-CG	-5.49	108.31	113.80
1	A	230	GLY	N-CA-C	5.45	122.61	115.36
1	A	30	ASN	CA-C-N	5.44	125.20	119.76
1	A	30	ASN	C-N-CA	5.44	125.20	119.76
1	A	228	VAL	CB-CA-C	5.43	118.59	111.53
1	A	148	CYS	O-C-N	5.43	128.96	123.26
1	A	275	ILE	N-CA-C	-5.42	105.24	110.72
1	B	21	HIS	CA-C-N	-5.42	113.99	122.65
1	B	21	HIS	C-N-CA	-5.42	113.99	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ALA	N-CA-C	-5.39	105.32	111.14
1	A	186	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	B	303	SER	CA-C-O	-5.39	115.51	121.28
1	A	163	PHE	CA-C-N	5.37	128.01	120.28
1	A	163	PHE	C-N-CA	5.37	128.01	120.28
1	B	34	LEU	N-CA-C	5.36	117.87	111.71
1	B	378	ILE	CA-C-N	5.35	125.02	119.56
1	B	378	ILE	C-N-CA	5.35	125.02	119.56
1	B	212	ARG	NE-CZ-NH1	5.35	126.85	121.50
1	A	125	ASP	CA-CB-CG	-5.33	107.27	112.60
1	A	147	GLN	CA-C-N	-5.32	112.70	121.80
1	A	147	GLN	C-N-CA	-5.32	112.70	121.80
1	B	246	LEU	O-C-N	5.32	127.55	122.07
1	B	199	ALA	CA-C-O	-5.31	114.79	120.42
1	A	126	LYS	CB-CA-C	-5.31	101.82	110.85
1	B	277	ARG	CD-NE-CZ	5.30	131.83	124.40
1	A	17	HIS	CA-C-N	-5.30	118.17	123.04
1	A	17	HIS	C-N-CA	-5.30	118.17	123.04
1	A	127	LEU	CA-C-N	5.28	128.13	120.79
1	A	127	LEU	C-N-CA	5.28	128.13	120.79
1	A	68	GLY	CA-C-O	5.26	126.09	120.30
1	B	402	LEU	O-C-N	5.26	124.91	121.23
1	A	125	ASP	CA-C-O	-5.25	114.98	120.55
1	A	340	PHE	O-C-N	-5.24	116.22	122.20
1	B	17	HIS	N-CA-C	5.24	119.53	113.18
1	A	136	CYS	O-C-N	-5.23	116.57	122.12
1	A	369	VAL	CA-C-O	-5.23	115.63	121.17
1	A	369	VAL	N-CA-C	-5.23	105.40	110.42
1	B	218	ASP	CA-CB-CG	-5.23	107.37	112.60
1	B	236	ASP	N-CA-CB	-5.23	102.44	110.12
1	B	109	ARG	NH1-CZ-NH2	5.23	126.09	119.30
1	A	186	ARG	CA-CB-CG	5.21	124.52	114.10
1	B	85	CYS	N-CA-CB	-5.20	103.56	111.21
1	B	72	ARG	CA-C-O	5.19	126.27	120.82
1	B	123	VAL	CG1-CB-CG2	-5.19	99.39	110.80
1	A	345	VAL	O-C-N	5.18	128.00	122.45
1	A	186	ARG	CB-CA-C	5.18	118.89	111.27
1	B	361	HIS	CA-CB-CG	-5.18	108.62	113.80
1	B	142	LEU	O-C-N	5.17	128.95	122.23
1	A	138	LEU	N-CA-CB	-5.17	102.51	110.16
1	B	77	ASP	O-C-N	-5.16	117.17	122.64
1	B	358	LEU	CA-C-O	-5.14	113.25	119.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	ILE	CB-CA-C	-5.14	105.21	112.14
1	B	228	VAL	N-CA-CB	5.13	118.31	111.64
1	A	89	PRO	N-CD-CG	5.12	110.87	103.20
1	B	401	ALA	CA-C-O	-5.12	115.26	120.89
1	A	18	VAL	CA-C-O	5.11	122.51	119.19
1	B	208	ILE	O-C-N	5.11	127.09	121.83
1	A	22	LEU	N-CA-C	-5.10	106.30	112.88
1	A	304	ASP	CA-C-O	-5.09	115.59	121.19
1	A	319	LEU	O-C-N	-5.09	117.08	123.04
1	B	150	PHE	CA-C-N	-5.09	113.82	120.44
1	B	150	PHE	C-N-CA	-5.09	113.82	120.44
1	A	223	VAL	CA-C-N	5.08	127.60	120.28
1	A	223	VAL	C-N-CA	5.08	127.60	120.28
1	B	76	GLU	CA-CB-CG	-5.08	103.93	114.10
1	A	106	PRO	CA-C-N	5.08	127.34	120.38
1	A	106	PRO	C-N-CA	5.08	127.34	120.38
1	A	305	TYR	CA-C-N	-5.07	116.03	122.77
1	A	305	TYR	C-N-CA	-5.07	116.03	122.77
1	B	211	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	A	89	PRO	N-CA-C	-5.06	102.06	112.47
1	A	129	ASN	CA-CB-CG	-5.05	107.55	112.60
1	A	137	SER	CA-CB-OG	-5.04	101.01	111.10
1	B	32	SER	CA-C-O	-5.04	114.41	120.10
1	A	347	HIS	O-C-N	-5.04	117.97	123.26
1	A	140	GLU	CA-C-O	5.04	125.89	120.55
1	A	112	ARG	NH1-CZ-NH2	5.02	125.83	119.30

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 ⓘ

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	56	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	7	0
All	All	7243	0	6420	100	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 8.

All (100) 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:B:121:MET:HE3	1:B:124:VAL:HB	1.88	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:184:MET:HE1	1:A:200:LEU:HD12	1.93	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:291:ARG:CZ	1:B:336:MET:HE3	2.43	0.49
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:A:99:ILE:HG12	1:A:103:MET:HE3	1.95	0.48
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:313:LYS:O	1:B:314:LYS:C	2.55	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:HBB2	2:A:501:HEM:HMB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:501:HEM:HBB2	2:A:501:HEM:CMB	2.47	0.45
1:B:293:SER:OG	1:B:323:MET:HA	2.16	0.45
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:A:313:LYS:O	1:A:314:LYS:C	2.60	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:55:TRP:HB2	1:A:63:TRP:CZ3	2.53	0.43
1:A:156:GLU:N	1:A:157:PRO:HD2	2.33	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:A:72:ARG:O	1:A:76:GLU:HG3	2.18	0.43
1:A:186:ARG:HD2	1:A:392:LYS:HG3	2.00	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:40:GLU:HG3	1:A:336:MET:HE2	2.02	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:34:LEU:HA	1:A:41:ALA:HB2	2.02	0.41
1:A:193:PHE:CD1	1:A:193:PHE:C	2.98	0.41
1:A:248:GLY:HA2	7:A:609:HOH:O	2.20	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:HD23	1:B:294:LEU:H	1.86	0.40
1:B:359:GLY:HA3	2:B:501:HEM:C3C	2.57	0.40
1:A:138:LEU:HD23	1:A:138:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	24	16
1	B	404/414 (98%)	391 (97%)	11 (3%)	2 (0%)	24	16
All	All	807/828 (98%)	774 (96%)	29 (4%)	4 (0%)	24	16

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%)	338 (97%)	12 (3%)	32	25
1	B	351/358 (98%)	340 (97%)	11 (3%)	35	29
All	All	701/716 (98%)	678 (97%)	23 (3%)	33	26

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

Mol	Chain	Res	Type
1	A	39	GLN
1	A	86	PRO
1	A	88	ILE
1	A	117	GLN
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	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	244	LEU
1	B	376	THR
1	B	403	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	39	GLN
1	A	46	GLN
1	A	59	ASN
1	A	110	GLN
1	A	210	GLN
1	A	225	ASN

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Mol	Chain	Res	Type
1	A	227	GLN
1	A	272	GLN
1	A	276	GLN
1	A	311	GLN
1	A	317	GLN
1	A	337	HIS
1	A	400	GLN
1	B	21	HIS
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	145	GLN
1	B	149	ASN
1	B	210	GLN
1	B	225	ASN
1	B	361	HIS
1	B	388	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](#)

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
5	TRS	A	504	-	7,7,7	1.95	3 (42%)	9,9,9	1.70	1 (11%)
2	HEM	B	501	1,7	50,50,50	1.42	12 (24%)	67,82,82	1.26	9 (13%)
4	CAM	B	502	-	12,12,12	1.34	1 (8%)	20,21,21	2.74	11 (55%)
4	CAM	A	503	-	12,12,12	1.09	1 (8%)	20,21,21	2.77	9 (45%)
2	HEM	A	501	1	50,50,50	1.57	11 (22%)	67,82,82	1.57	5 (7%)

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
5	TRS	A	504	-	-	3/9/9/9	-
2	HEM	B	501	1,7	-	3/14/54/54	-
4	CAM	B	502	-	-	-	0/3/2/2
4	CAM	A	503	-	-	-	0/3/2/2
2	HEM	A	501	1	-	2/14/54/54	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	CBD-CGD	4.25	1.60	1.50
4	B	502	CAM	C1-C2	3.86	1.58	1.52
4	A	503	CAM	C1-C2	3.16	1.57	1.52
2	A	501	HEM	FE-NC	3.13	2.05	1.95
2	B	501	HEM	FE-NC	2.93	2.04	1.95
2	B	501	HEM	CAC-C3C	2.89	1.55	1.47
5	A	504	TRS	O2-C2	2.89	1.51	1.42
2	A	501	HEM	FE-NB	2.79	2.03	1.94
2	A	501	HEM	FE-ND	2.79	2.03	1.94
2	A	501	HEM	CAB-C3B	2.63	1.54	1.47
2	B	501	HEM	C4C-NC	-2.58	1.34	1.39
2	A	501	HEM	CAC-C3C	2.57	1.54	1.47
5	A	504	TRS	O1-C1	2.49	1.50	1.42
2	B	501	HEM	FE-NA	2.47	2.03	1.95
2	A	501	HEM	O2D-CGD	-2.46	1.22	1.30
2	B	501	HEM	CAB-C3B	2.46	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C2A-C3A	-2.44	1.32	1.38
2	B	501	HEM	CMD-C2D	2.44	1.55	1.50
5	A	504	TRS	O3-C3	2.36	1.49	1.42
2	B	501	HEM	CMA-C3A	2.35	1.55	1.50
2	B	501	HEM	CAA-C2A	2.35	1.57	1.51
2	A	501	HEM	C1C-NC	-2.31	1.35	1.39
2	A	501	HEM	CMD-C2D	2.23	1.55	1.50
2	A	501	HEM	CMC-C2C	2.22	1.55	1.50
2	B	501	HEM	CMB-C2B	2.18	1.55	1.50
2	B	501	HEM	FE-ND	2.09	2.01	1.94
2	B	501	HEM	C4A-C3A	2.07	1.48	1.43
2	B	501	HEM	FE-NB	2.03	2.01	1.94

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	O2D-CGD-O1D	7.23	141.93	123.33
4	B	502	CAM	C5-C4-C3	-5.75	90.80	106.39
4	A	503	CAM	C5-C4-C3	-5.52	91.44	106.39
4	A	503	CAM	C3-C2-C1	-5.20	95.04	107.43
4	A	503	CAM	O-C2-C3	4.54	135.74	126.39
2	A	501	HEM	O1D-CGD-CBD	-4.53	108.72	123.09
4	B	502	CAM	C3-C2-C1	-4.48	96.75	107.43
4	A	503	CAM	C4-C3-C2	4.41	109.81	102.05
4	B	502	CAM	O-C2-C3	4.41	135.48	126.39
2	A	501	HEM	CMA-C3A-C4A	-4.15	119.10	125.42
4	A	503	CAM	O-C2-C1	-4.09	120.42	125.33
4	A	503	CAM	C7-C1-C2	3.90	106.98	100.33
2	B	501	HEM	O1D-CGD-CBD	-3.57	111.75	123.09
4	B	502	CAM	C9-C7-C8	3.55	116.67	107.67
2	A	501	HEM	CMA-C3A-C2A	3.49	133.03	125.62
5	A	504	TRS	C3-C-C2	-3.42	101.54	110.66
4	B	502	CAM	C6-C1-C7	3.40	108.69	101.52
4	B	502	CAM	C7-C1-C2	3.34	106.02	100.33
2	B	501	HEM	CBC-CAC-C3C	-3.26	111.23	127.53
2	B	501	HEM	CBD-CAD-C3D	3.01	120.87	112.53
2	A	501	HEM	CBD-CAD-C3D	2.94	120.65	112.53
4	B	502	CAM	C4-C3-C2	2.83	107.03	102.05
2	B	501	HEM	CMD-C2D-C1D	-2.83	120.62	125.03
4	B	502	CAM	C5-C6-C1	-2.80	99.08	104.73
2	B	501	HEM	O2D-CGD-O1D	2.57	129.93	123.33
2	B	501	HEM	CMA-C3A-C4A	-2.45	121.68	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	CAM	C9-C7-C8	2.45	113.88	107.67
2	B	501	HEM	CMA-C3A-C2A	2.23	130.34	125.62
4	B	502	CAM	C5-C4-C7	2.21	107.02	102.83
2	B	501	HEM	O1A-CGA-CBA	-2.16	116.23	123.09
4	B	502	CAM	C6-C5-C4	2.16	106.53	103.16
4	A	503	CAM	C9-C7-C4	-2.16	108.22	113.44
4	A	503	CAM	C6-C1-C7	2.11	105.98	101.52
2	B	501	HEM	CMD-C2D-C3D	2.06	131.72	126.15
4	B	502	CAM	C9-C7-C4	-2.00	108.59	113.44

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C2C-C3C-CAC-CBC
5	A	504	TRS	C1-C-C3-O3
2	B	501	HEM	C2C-C3C-CAC-CBC
5	A	504	TRS	N-C-C3-O3
2	A	501	HEM	C4C-C3C-CAC-CBC
5	A	504	TRS	C2-C-C3-O3
2	B	501	HEM	C4C-C3C-CAC-CBC
2	B	501	HEM	CAD-CBD-CGD-O1D

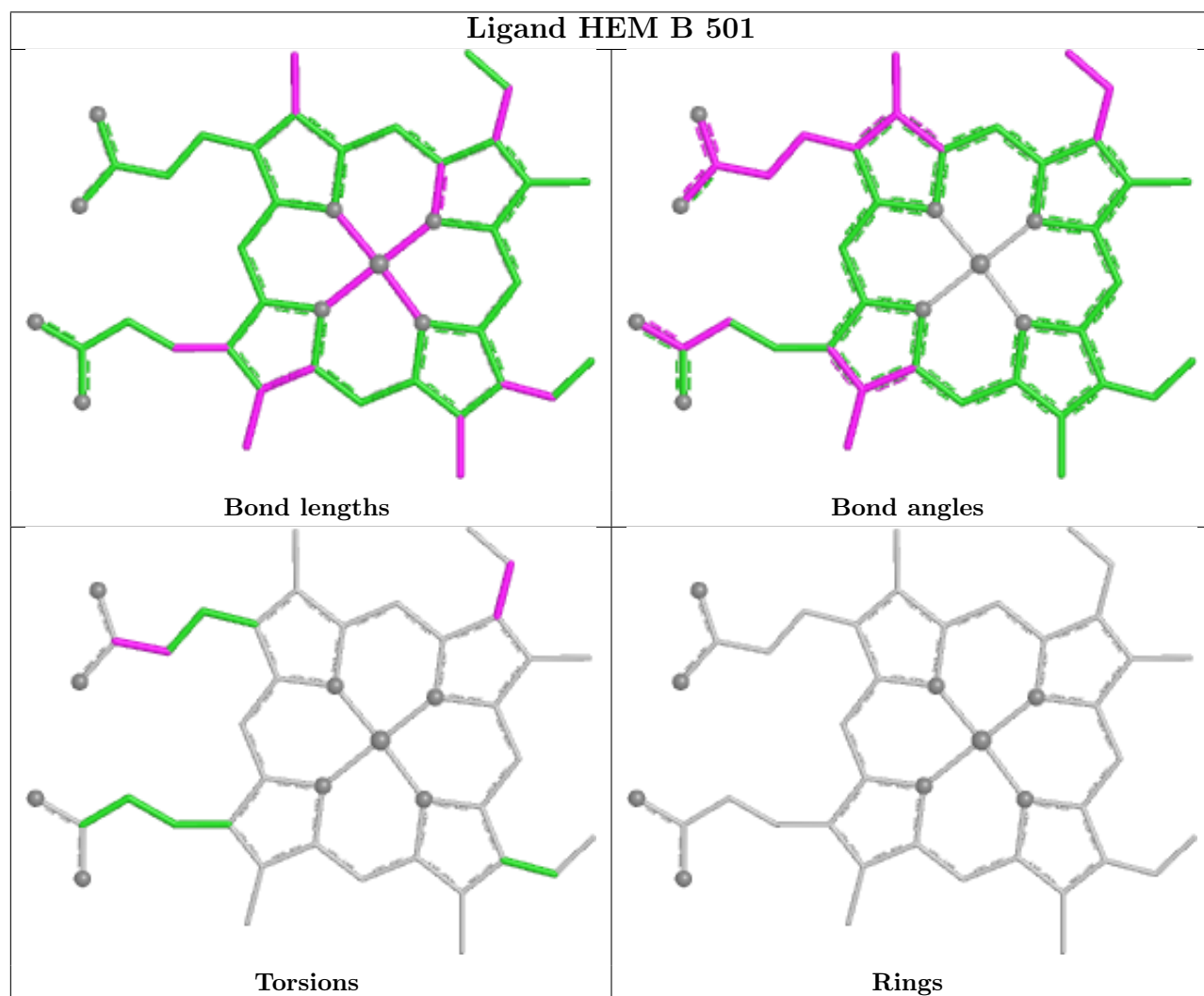
There are no ring outliers.

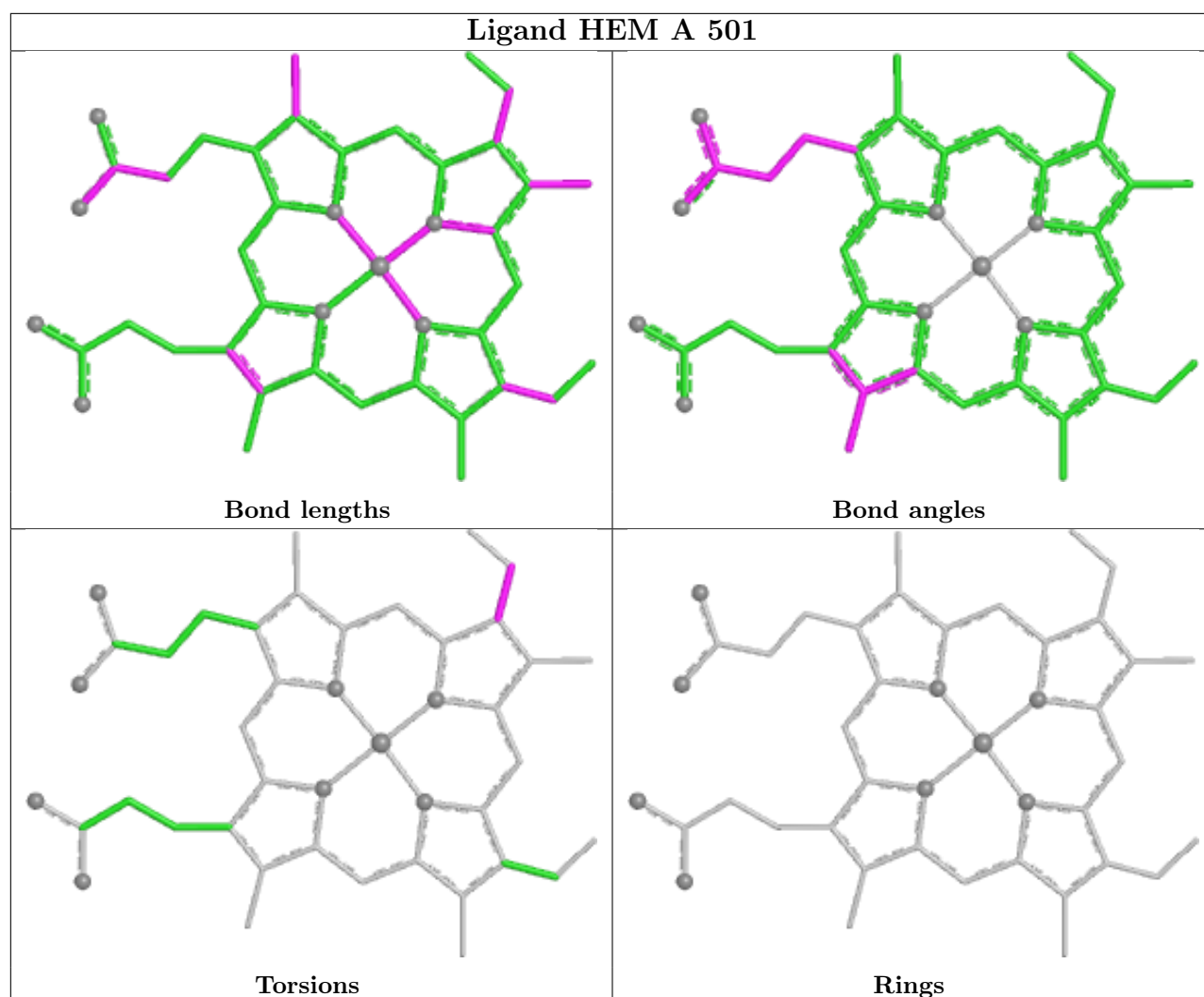
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	1	0
4	B	502	CAM	2	0
4	A	503	CAM	1	0
2	A	501	HEM	7	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%)	-0.16	4 (0%) 79 82	10, 22, 46, 75	2 (0%)
1	B	405/414 (97%)	-0.57	0 100 100	8, 17, 38, 58	1 (0%)
All	All	809/828 (97%)	-0.36	4 (0%) 87 89	8, 19, 42, 75	3 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	PRO	2.4
1	A	11	LEU	2.3
1	A	24	PHE	2.2
1	A	18	VAL	2.1

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
4	CAM	B	502	11/11	0.94	0.06	8,12,19,20	0

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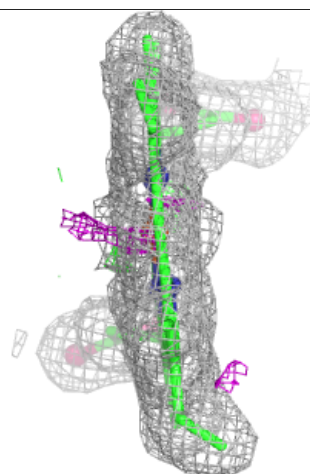
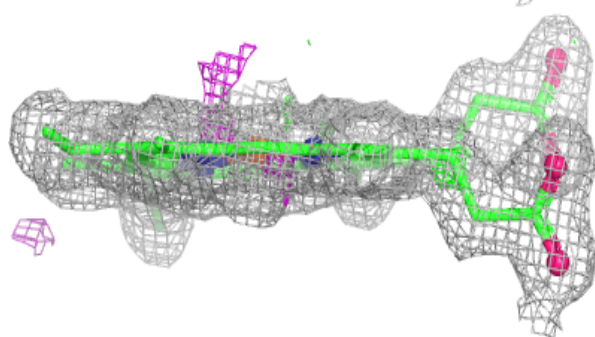
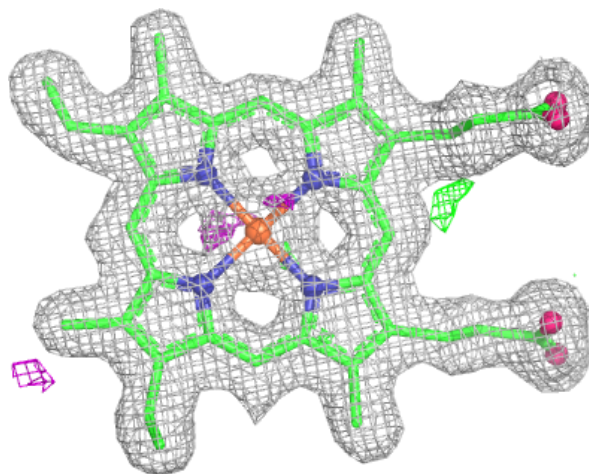
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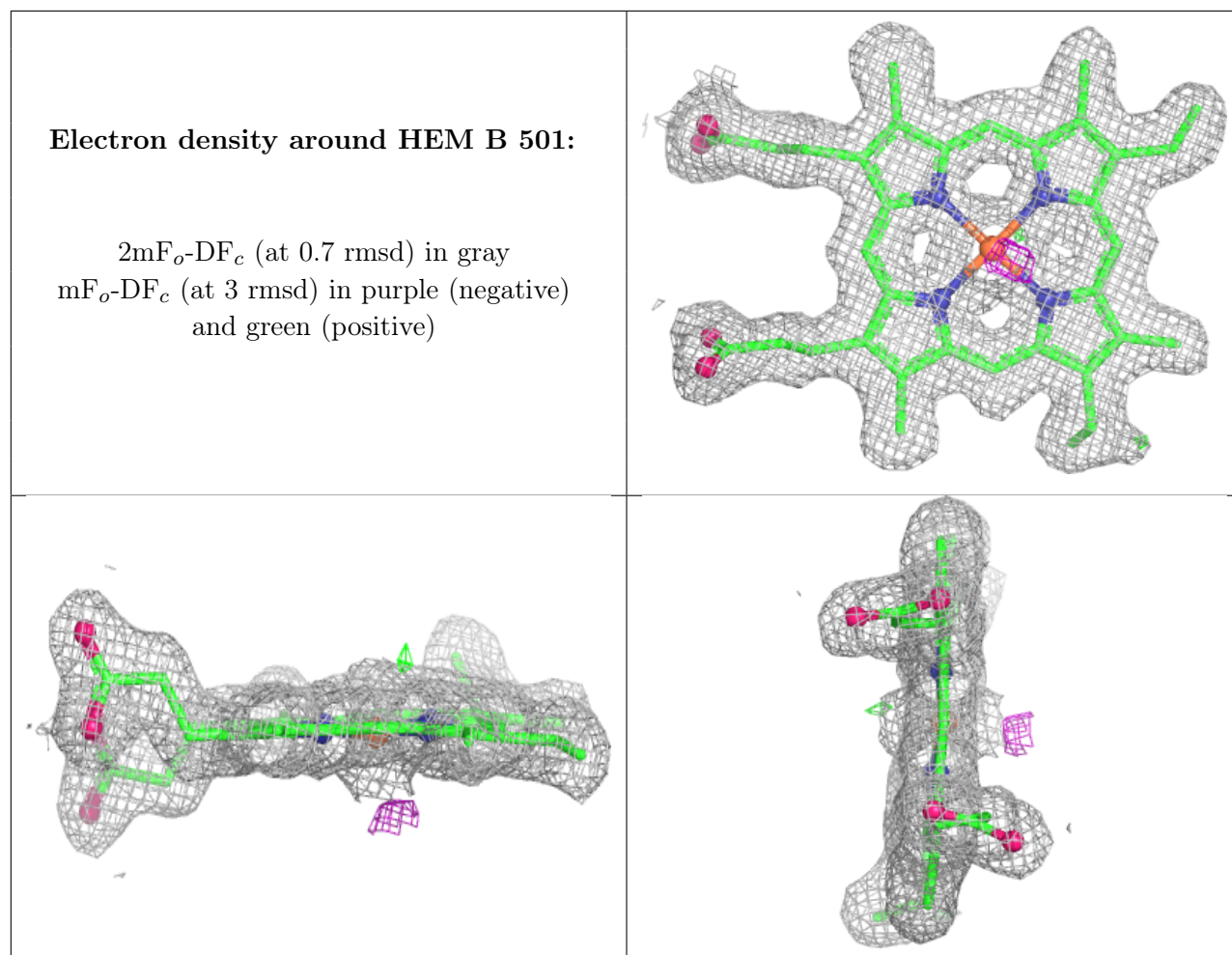
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CAM	A	503	11/11	0.95	0.05	17,20,23,23	0
5	TRS	A	504	8/8	0.96	0.06	9,15,22,30	0
3	O	A	502	1/1	0.97	0.09	18,18,18,18	1
6	K	A	505	1/1	0.97	0.04	19,19,19,19	0
2	HEM	A	501	43/43	0.98	0.05	7,16,22,24	0
6	K	B	504	1/1	0.98	0.03	17,17,17,17	0
2	HEM	B	501	43/43	0.99	0.04	5,13,18,24	0
6	K	B	503	1/1	1.00	0.01	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 ⓘ

There are no such residues in this entry.