



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2L8M / pdb_00002l8m
BMRB ID : 17415
Title : Reduced and CO-bound cytochrome P450cam (CYP101A1)
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Deposited on : 2011-01-19

This is a Full wwPDB NMR 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/NMRValidationReportHelp>

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)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

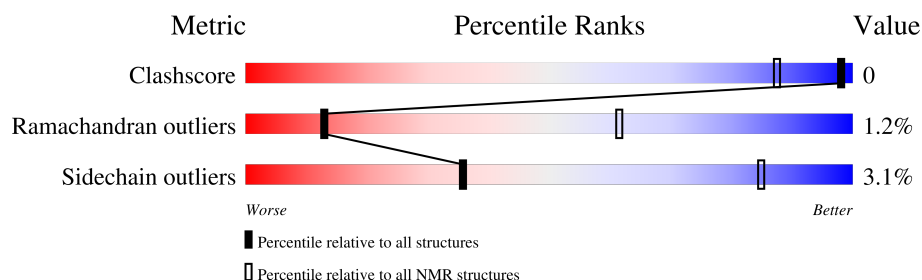
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 21%.

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)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	415	

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

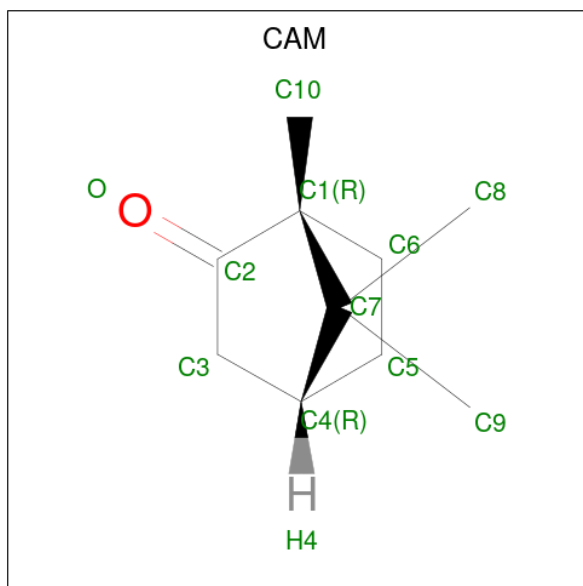
3 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16111 atoms, of which 9627 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Camphor 5-monooxygenase.

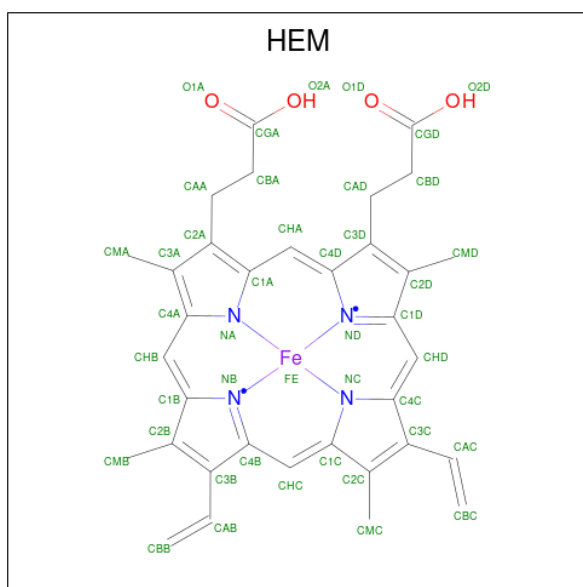
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	405	6365	2033	3157	560	597	18	0

- Molecule 2 is CAMPHOR (CCD ID: CAM) (formula: $C_{10}H_{16}O$).



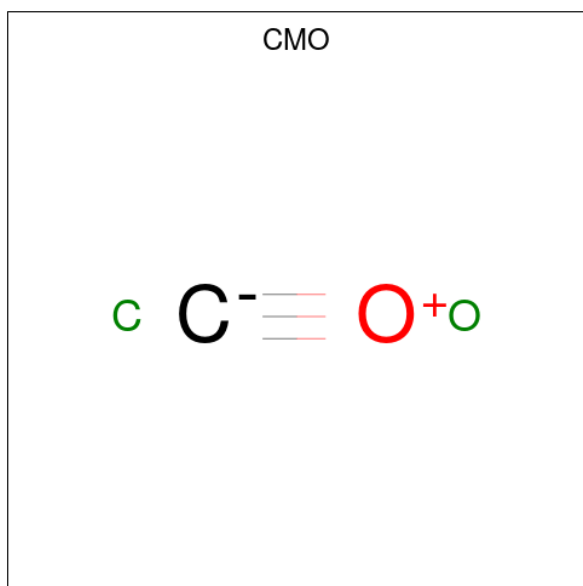
Mol	Chain	Residues	Atoms			
			Total	C	H	O
2	A	1	27	10	16	1

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



Mol	Chain	Residues	Atoms					
3	A	1	Total	C	Fe	H	N	O
			73	34	1	30	4	4

- Molecule 4 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



Mol	Chain	Residues	Atoms		
4	A	1	Total	C	O
			2	1	1

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	
5	A	4	Total	K
			4	4

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	
6	A	3	Total	Cl
			3	3

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		
7	A	3213	Total	H	O
			9637	6424	3213

- Molecule 1: Camphor 5-monooxygenase



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 18 calculated structures, 1 were deposited, based on the following criterion: *structures with the least restraint violations*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
Amber	refinement	10

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1189
Number of shifts mapped to atoms	1157
Number of unparsed shifts	0
Number of shifts with mapping errors	32
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	21%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, CL, HEM, CMO, 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 (average) 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	1.99	67/3287 (2.0%)	2.31	177/4465 (4.0%)
All	All	1.99	67/3287 (2.0%)	2.31	177/4465 (4.0%)

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	Planarity
1	A	0	11
All	All	0	11

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	GLU	CA-C	10.20	1.62	1.53
1	A	399	VAL	N-CA	9.89	1.56	1.46
1	A	403	PRO	C-O	-9.35	1.16	1.24
1	A	281	ILE	CA-CB	-9.23	1.49	1.54
1	A	121	MET	CA-C	7.67	1.60	1.52
1	A	51	PRO	CA-C	7.30	1.61	1.52
1	A	355	HIS	CD2-NE2	7.11	1.45	1.37
1	A	402	LEU	N-CA	7.02	1.54	1.46
1	A	317	GLN	CA-C	6.92	1.60	1.52
1	A	302	THR	CB-OG1	-6.82	1.32	1.43
1	A	62	HIS	CG-CD2	6.77	1.43	1.35
1	A	38	VAL	CA-C	6.74	1.61	1.52
1	A	391	HIS	CA-CB	6.70	1.63	1.53
1	A	364	ARG	CA-C	6.62	1.62	1.52
1	A	266	LYS	N-CA	-6.62	1.37	1.46
1	A	195	GLU	CA-C	6.54	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	251	ASP	CA-C	6.52	1.58	1.52
1	A	214	LYS	CA-CB	6.51	1.59	1.53
1	A	205	ILE	N-CA	6.47	1.54	1.46
1	A	290	ARG	N-CA	6.46	1.54	1.46
1	A	337	HIS	ND1-CE1	6.39	1.39	1.32
1	A	19	PRO	CA-C	6.33	1.59	1.52
1	A	214	LYS	CA-C	6.16	1.60	1.52
1	A	216	GLY	CA-C	6.16	1.58	1.51
1	A	100	PRO	N-CD	-6.15	1.39	1.47
1	A	361	HIS	CE1-NE2	6.12	1.38	1.32
1	A	290	ARG	CD-NE	6.00	1.54	1.46
1	A	186	ARG	CD-NE	5.98	1.54	1.46
1	A	243	GLY	N-CA	5.97	1.53	1.45
1	A	381	PHE	CA-C	5.94	1.59	1.52
1	A	31	PRO	CA-CB	-5.94	1.45	1.53
1	A	44	VAL	CA-CB	5.91	1.63	1.54
1	A	299	ARG	CD-NE	-5.87	1.38	1.46
1	A	342	ARG	NE-CZ	5.84	1.39	1.33
1	A	69	GLN	CA-C	-5.72	1.45	1.52
1	A	165	LEU	CA-C	5.70	1.60	1.52
1	A	114	LEU	N-CA	5.68	1.53	1.46
1	A	335	PRO	N-CD	-5.67	1.39	1.47
1	A	139	ILE	CB-CG1	5.58	1.64	1.53
1	A	32	SER	CA-CB	-5.58	1.44	1.53
1	A	205	ILE	C-N	5.57	1.40	1.33
1	A	30	ASN	CA-C	5.53	1.58	1.52
1	A	205	ILE	CA-C	5.50	1.58	1.52
1	A	143	ARG	C-N	5.47	1.38	1.33
1	A	354	SER	CA-CB	5.45	1.61	1.53
1	A	216	GLY	N-CA	5.41	1.51	1.45
1	A	389	ILE	C-N	-5.39	1.26	1.33
1	A	91	GLU	N-CA	5.38	1.53	1.46
1	A	178	LYS	N-CA	-5.36	1.39	1.46
1	A	120	GLY	CA-C	5.33	1.57	1.51
1	A	191	MET	CA-C	-5.32	1.46	1.52
1	A	154	TYR	CA-CB	5.30	1.62	1.53
1	A	228	VAL	C-O	-5.28	1.18	1.24
1	A	330	ARG	CA-C	5.28	1.60	1.52
1	A	50	VAL	N-CA	5.28	1.53	1.46
1	A	395	ILE	CA-C	5.22	1.59	1.52
1	A	400	GLN	C-N	5.22	1.40	1.33
1	A	151	THR	N-CA	5.20	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	SER	CA-CB	5.19	1.61	1.53
1	A	311	GLN	CA-C	5.18	1.59	1.52
1	A	210	GLN	N-CA	5.17	1.52	1.46
1	A	90	ARG	N-CA	5.13	1.52	1.46
1	A	405	VAL	N-CA	5.13	1.51	1.46
1	A	303	SER	N-CA	5.11	1.52	1.45
1	A	161	ARG	CZ-NH2	-5.10	1.26	1.33
1	A	360	GLN	CA-C	5.02	1.59	1.52
1	A	229	ASN	N-CA	5.01	1.54	1.46

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	GLN	OE1-CD-NE2	-11.07	111.53	122.60
1	A	360	GLN	OE1-CD-NE2	-10.53	112.07	122.60
1	A	307	PHE	CA-CB-CG	10.52	124.32	113.80
1	A	181	THR	O-C-N	9.54	131.95	122.03
1	A	24	PHE	CA-CB-CG	9.45	123.25	113.80
1	A	381	PHE	O-C-N	-9.30	114.25	123.46
1	A	362	LEU	N-CA-C	-9.03	101.00	111.03
1	A	17	HIS	CB-CG-CD2	-9.02	119.48	131.20
1	A	181	THR	CA-C-O	-8.83	111.73	121.00
1	A	403	PRO	N-CA-CB	8.76	107.82	102.92
1	A	116	ASN	OD1-CG-ND2	-8.31	114.29	122.60
1	A	384	ALA	CA-C-N	8.06	127.82	119.76
1	A	384	ALA	C-N-CA	8.06	127.82	119.76
1	A	306	GLU	CA-C-O	-7.93	111.87	120.36
1	A	116	ASN	CA-CB-CG	7.89	120.49	112.60
1	A	388	GLN	O-C-N	-7.74	114.15	123.29
1	A	270	HIS	CB-CG-CD2	-7.70	121.20	131.20
1	A	407	ASP	CA-CB-CG	7.62	120.22	112.60
1	A	352	HIS	N-CA-C	7.58	119.91	108.46
1	A	39	GLN	N-CA-C	-7.37	104.27	113.55
1	A	80	HIS	ND1-CG-CD2	7.33	113.43	106.10
1	A	232	PRO	O-C-N	-7.33	113.90	123.13
1	A	400	GLN	O-C-N	-7.27	114.17	122.03
1	A	291	ARG	NE-CZ-NH1	7.27	128.77	121.50
1	A	21	HIS	CB-CG-CD2	-7.20	121.84	131.20
1	A	14	LEU	N-CA-CB	-7.17	99.70	110.32
1	A	170	PRO	CA-C-N	7.16	130.59	120.28
1	A	170	PRO	C-N-CA	7.16	130.59	120.28
1	A	153	ASP	N-CA-CB	-7.13	99.53	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	GLN	CA-C-O	-7.03	113.04	120.63
1	A	130	ARG	NH1-CZ-NH2	-7.00	110.20	119.30
1	A	277	ARG	CA-C-N	6.90	127.47	119.47
1	A	277	ARG	C-N-CA	6.90	127.47	119.47
1	A	347	HIS	CA-CB-CG	-6.86	106.94	113.80
1	A	188	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	222	ILE	CA-C-O	-6.83	113.40	120.71
1	A	83	SER	N-CA-C	6.80	121.24	113.15
1	A	291	ARG	NE-CZ-NH2	-6.79	113.08	119.20
1	A	23	VAL	CA-C-N	6.79	132.43	122.39
1	A	23	VAL	C-N-CA	6.79	132.43	122.39
1	A	176	HIS	CB-CG-CD2	-6.74	122.44	131.20
1	A	32	SER	CA-C-O	-6.71	112.25	119.97
1	A	98	PHE	CA-CB-CG	6.70	120.50	113.80
1	A	294	LEU	O-C-N	-6.57	113.85	122.59
1	A	293	SER	CA-C-N	6.57	134.09	121.54
1	A	293	SER	C-N-CA	6.57	134.09	121.54
1	A	300	ILE	CB-CA-C	6.56	120.23	110.98
1	A	210	GLN	OE1-CD-NE2	-6.55	116.05	122.60
1	A	69	GLN	CA-C-N	6.54	129.34	120.38
1	A	69	GLN	C-N-CA	6.54	129.34	120.38
1	A	264	LEU	CA-C-O	-6.52	112.73	120.10
1	A	363	ALA	CA-C-O	-6.51	113.94	120.90
1	A	69	GLN	OE1-CD-NE2	-6.50	116.10	122.60
1	A	399	VAL	CA-C-O	-6.50	114.85	121.67
1	A	361	HIS	ND1-CG-CD2	6.43	112.53	106.10
1	A	90	ARG	NH1-CZ-NH2	-6.39	110.99	119.30
1	A	280	ARG	NE-CZ-NH1	6.39	127.89	121.50
1	A	361	HIS	CB-CG-CD2	-6.36	122.94	131.20
1	A	130	ARG	NE-CZ-NH2	6.32	124.89	119.20
1	A	390	GLN	CA-C-O	6.31	127.26	120.38
1	A	307	PHE	O-C-N	-6.30	115.67	123.36
1	A	88	ILE	O-C-N	-6.29	113.93	121.10
1	A	161	ARG	CA-C-N	6.29	129.13	122.97
1	A	161	ARG	C-N-CA	6.29	129.13	122.97
1	A	205	ILE	CA-C-O	-6.24	111.58	119.95
1	A	361	HIS	CA-C-N	6.24	129.12	120.63
1	A	361	HIS	C-N-CA	6.24	129.12	120.63
1	A	163	PHE	CA-C-N	6.24	128.55	120.44
1	A	163	PHE	C-N-CA	6.24	128.55	120.44
1	A	322	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	A	185	THR	N-CA-C	6.22	118.06	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ASN	OD1-CG-ND2	-6.20	116.40	122.60
1	A	321	PRO	CB-CA-C	6.14	119.38	111.64
1	A	145	GLN	OE1-CD-NE2	-6.12	116.48	122.60
1	A	359	GLY	O-C-N	-6.11	114.76	122.70
1	A	223	VAL	O-C-N	6.08	127.87	121.91
1	A	318	ILE	N-CA-C	6.07	116.61	108.11
1	A	149	ASN	CA-CB-CG	6.05	118.65	112.60
1	A	413	ALA	CA-C-O	-6.04	113.58	120.58
1	A	316	ASP	CA-C-O	6.01	127.92	121.55
1	A	402	LEU	N-CA-C	6.01	120.23	108.21
1	A	14	LEU	CB-CA-C	5.99	118.01	109.08
1	A	80	HIS	ND1-CE1-NE2	5.99	114.39	108.40
1	A	169	LEU	CA-C-O	-5.97	113.31	120.41
1	A	268	PRO	N-CA-C	5.93	121.78	113.53
1	A	362	LEU	CA-C-N	5.92	128.53	120.54
1	A	362	LEU	C-N-CA	5.92	128.53	120.54
1	A	313	LYS	N-CA-CB	-5.87	101.69	111.20
1	A	352	HIS	ND1-CE1-NE2	5.85	114.25	108.40
1	A	258	SER	O-C-N	-5.84	116.05	122.07
1	A	281	ILE	CA-C-O	-5.84	114.78	118.69
1	A	15	PRO	CA-C-N	5.82	125.36	119.19
1	A	15	PRO	C-N-CA	5.82	125.36	119.19
1	A	315	GLY	CA-C-N	5.81	129.53	120.75
1	A	315	GLY	C-N-CA	5.81	129.53	120.75
1	A	229	ASN	CA-CB-CG	5.75	118.35	112.60
1	A	316	ASP	O-C-N	-5.71	115.78	122.81
1	A	183	GLN	N-CA-CB	5.69	118.49	110.12
1	A	325	SER	CA-C-N	5.65	126.25	119.98
1	A	325	SER	C-N-CA	5.65	126.25	119.98
1	A	236	ASP	CB-CA-C	5.62	121.60	110.42
1	A	339	ASP	N-CA-C	5.60	117.78	108.99
1	A	161	ARG	CD-NE-CZ	5.57	132.20	124.40
1	A	395	ILE	N-CA-CB	5.57	117.43	110.47
1	A	340	PHE	N-CA-C	5.56	119.69	113.02
1	A	228	VAL	CA-CB-CG2	5.56	119.85	110.40
1	A	411	THR	CA-C-O	-5.56	114.72	121.28
1	A	375	LEU	CA-C-N	5.55	129.22	120.89
1	A	375	LEU	C-N-CA	5.55	129.22	120.89
1	A	188	ASP	CA-C-N	5.53	132.26	121.41
1	A	188	ASP	C-N-CA	5.53	132.26	121.41
1	A	179	TYR	CA-C-N	5.52	127.67	120.28
1	A	179	TYR	C-N-CA	5.52	127.67	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	TRP	N-CA-C	5.52	117.10	111.14
1	A	52	ASP	N-CA-C	5.50	117.99	111.33
1	A	368	ILE	CA-CB-CG2	5.48	119.81	110.50
1	A	360	GLN	N-CA-C	5.47	122.45	110.80
1	A	163	PHE	N-CA-C	5.46	117.94	111.33
1	A	342	ARG	N-CA-CB	5.42	118.08	109.51
1	A	292	PHE	CA-CB-CG	-5.42	108.38	113.80
1	A	270	HIS	CA-C-N	-5.37	113.45	120.44
1	A	270	HIS	C-N-CA	-5.37	113.45	120.44
1	A	16	PRO	N-CA-CB	5.37	109.21	103.52
1	A	231	ARG	NE-CZ-NH2	-5.36	114.38	119.20
1	A	92	ALA	N-CA-CB	5.35	118.28	110.47
1	A	381	PHE	CA-C-N	5.33	130.61	121.87
1	A	381	PHE	C-N-CA	5.33	130.61	121.87
1	A	104	ASP	N-CA-C	5.32	117.29	109.42
1	A	131	ILE	O-C-N	5.32	129.21	122.57
1	A	67	ARG	CA-C-N	5.31	125.87	119.98
1	A	67	ARG	C-N-CA	5.31	125.87	119.98
1	A	42	TRP	O-C-N	5.29	129.71	122.46
1	A	223	VAL	CA-C-O	-5.29	115.57	121.17
1	A	17	HIS	CB-CG-ND1	5.28	130.62	122.70
1	A	148	CYS	CA-C-O	-5.25	115.33	121.10
1	A	128	GLU	N-CA-C	5.24	117.40	111.11
1	A	130	ARG	CA-CB-CG	5.24	124.58	114.10
1	A	255	ASN	CA-CB-CG	-5.24	107.36	112.60
1	A	323	MET	O-C-N	-5.21	115.50	122.43
1	A	402	LEU	N-CA-CB	-5.21	102.65	111.30
1	A	296	ALA	CB-CA-C	5.21	119.51	111.85
1	A	342	ARG	CA-C-N	5.20	129.48	120.58
1	A	342	ARG	C-N-CA	5.20	129.48	120.58
1	A	129	ASN	O-C-N	-5.19	116.23	122.15
1	A	276	GLU	N-CA-C	5.19	117.67	111.71
1	A	182	ASP	O-C-N	-5.18	116.70	122.09
1	A	363	ALA	N-CA-CB	-5.16	102.25	109.94
1	A	137	SER	CA-C-N	-5.16	113.84	120.65
1	A	137	SER	C-N-CA	-5.16	113.84	120.65
1	A	288	LEU	CA-C-N	5.16	128.15	120.31
1	A	288	LEU	C-N-CA	5.16	128.15	120.31
1	A	264	LEU	O-C-N	5.15	128.25	122.22
1	A	125	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	208	ILE	N-CA-C	5.14	115.86	110.62
1	A	272	GLN	OE1-CD-NE2	-5.13	117.47	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	VAL	N-CA-C	5.13	116.99	108.99
1	A	136	CYS	O-C-N	-5.13	116.21	122.11
1	A	92	ALA	CA-C-N	5.13	126.73	120.22
1	A	92	ALA	C-N-CA	5.13	126.73	120.22
1	A	54	VAL	CA-C-O	-5.12	115.70	121.75
1	A	349	THR	CA-C-N	5.12	131.32	121.54
1	A	349	THR	C-N-CA	5.12	131.32	121.54
1	A	18	VAL	O-C-N	5.11	125.88	121.12
1	A	80	HIS	CB-CG-CD2	-5.10	124.56	131.20
1	A	80	HIS	CG-ND1-CE1	-5.10	100.63	109.30
1	A	112	ARG	CA-C-O	-5.09	115.02	120.42
1	A	337	HIS	N-CA-CB	-5.08	101.79	109.92
1	A	80	HIS	CE1-NE2-CD2	-5.08	103.92	109.00
1	A	315	GLY	O-C-N	-5.08	115.98	122.43
1	A	106	PRO	N-CD-CG	5.07	109.88	103.80
1	A	105	PRO	N-CA-CB	5.04	107.97	103.08
1	A	116	ASN	CB-CG-ND2	5.03	123.95	116.40
1	A	358	LEU	O-C-N	-5.02	116.17	122.24
1	A	220	ILE	CA-CB-CG1	5.01	118.92	110.40
1	A	79	ARG	CB-CA-C	5.00	120.77	110.31
1	A	294	LEU	N-CA-C	5.00	121.46	110.80
1	A	227	GLN	OE1-CD-NE2	-5.00	117.60	122.60

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	12	ALA	Peptide
1	A	75	TYR	Sidechain
1	A	88	ILE	Mainchain
1	A	96	TYR	Sidechain
1	A	130	ARG	Sidechain
1	A	201	TYR	Sidechain
1	A	203	TYR	Sidechain
1	A	240	ARG	Sidechain
1	A	292	PHE	Sidechain
1	A	324	LEU	Peptide
1	A	342	ARG	Peptide

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	3208	3157	3156	4
All	All	6484	9627	3202	4

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 0.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:103:MET:HE1	1:A:111:PHE:CE1	0.47	2.44
1:A:79:ARG:HH12	1:A:104:ASP:CG	0.44	2.21
1:A:38:VAL:HB	1:A:391:HIS:HB3	0.42	1.92
1:A:223:VAL:O	1:A:233:ILE:HG21	0.42	2.15

6.3 Torsion angles

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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%)	362 (90%)	36 (9%)	5 (1%)	13	61
All	All	403/415 (97%)	362 (90%)	36 (9%)	5 (1%)	13	61

All 5 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	97	ASP
1	A	217	THR
1	A	293	SER
1	A	294	LEU
1	A	379	PRO

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	350/359 (97%)	339 (97%)	11 (3%)	36	85
All	All	350/359 (97%)	339 (97%)	11 (3%)	36	85

All 11 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	52	ASP
1	A	119	VAL
1	A	123	VAL
1	A	151	THR
1	A	178	LYS
1	A	188	ASP
1	A	229	ASN
1	A	250	LEU
1	A	323	MET
1	A	349	THR
1	A	360	GLN

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	CAM	A	415	-	12,12,12	1.26	1 (8%)
3	HEM	A	416	1,4	50,50,50	1.52	12 (24%)
4	CMO	A	417	3	0,1,1	0.00	-

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	CAM	A	415	-	20,21,21	0.99	1 (5%)
3	HEM	A	416	1,4	67,82,82	1.46	12 (17%)
4	CMO	A	417	3	-	-	-

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	CAM	A	415	-	-	-	0,3,2,2
3	HEM	A	416	1,4	-	0,14,54,54	-

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	416	HEM	FE-NC	3.79	2.07	1.95
3	A	416	HEM	C1B-NB	3.62	1.34	1.40
2	A	415	CAM	O-C2	3.29	1.26	1.21
3	A	416	HEM	C4A-C3A	2.97	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	416	HEM	FE-NB	2.96	2.04	1.94
3	A	416	HEM	C1C-NC	2.42	1.35	1.39
3	A	416	HEM	C1C-C2C	2.40	1.40	1.45
3	A	416	HEM	CAB-C3B	2.28	1.53	1.47
3	A	416	HEM	CBD-CAD	2.19	1.59	1.51
3	A	416	HEM	CAC-C3C	2.14	1.53	1.47
3	A	416	HEM	CHA-C4D	2.04	1.34	1.38
3	A	416	HEM	C4D-ND	2.03	1.36	1.40
3	A	416	HEM	C3D-C2D	2.01	1.41	1.36

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	416	HEM	C1D-C2D-C3D	4.14	102.62	106.98
3	A	416	HEM	CMA-C3A-C2A	3.18	132.37	125.62
3	A	416	HEM	CMB-C2B-C1B	3.12	129.90	125.03
3	A	416	HEM	CHD-C4C-NC	3.06	127.78	124.45
3	A	416	HEM	O2A-CGA-CBA	2.94	123.30	114.00
3	A	416	HEM	CMA-C3A-C4A	2.75	121.23	125.42
3	A	416	HEM	CMB-C2B-C3B	2.57	122.21	128.43
3	A	416	HEM	C4C-C3C-C2C	2.23	104.88	106.81
3	A	416	HEM	CMD-C2D-C3D	2.17	132.01	126.15
2	A	415	CAM	C8-C7-C4	2.17	118.69	113.44
3	A	416	HEM	O2A-CGA-O1A	2.16	117.78	123.33
3	A	416	HEM	C4B-C3B-C2B	2.03	105.41	107.28
3	A	416	HEM	C4C-CHD-C1D	2.00	121.76	126.02

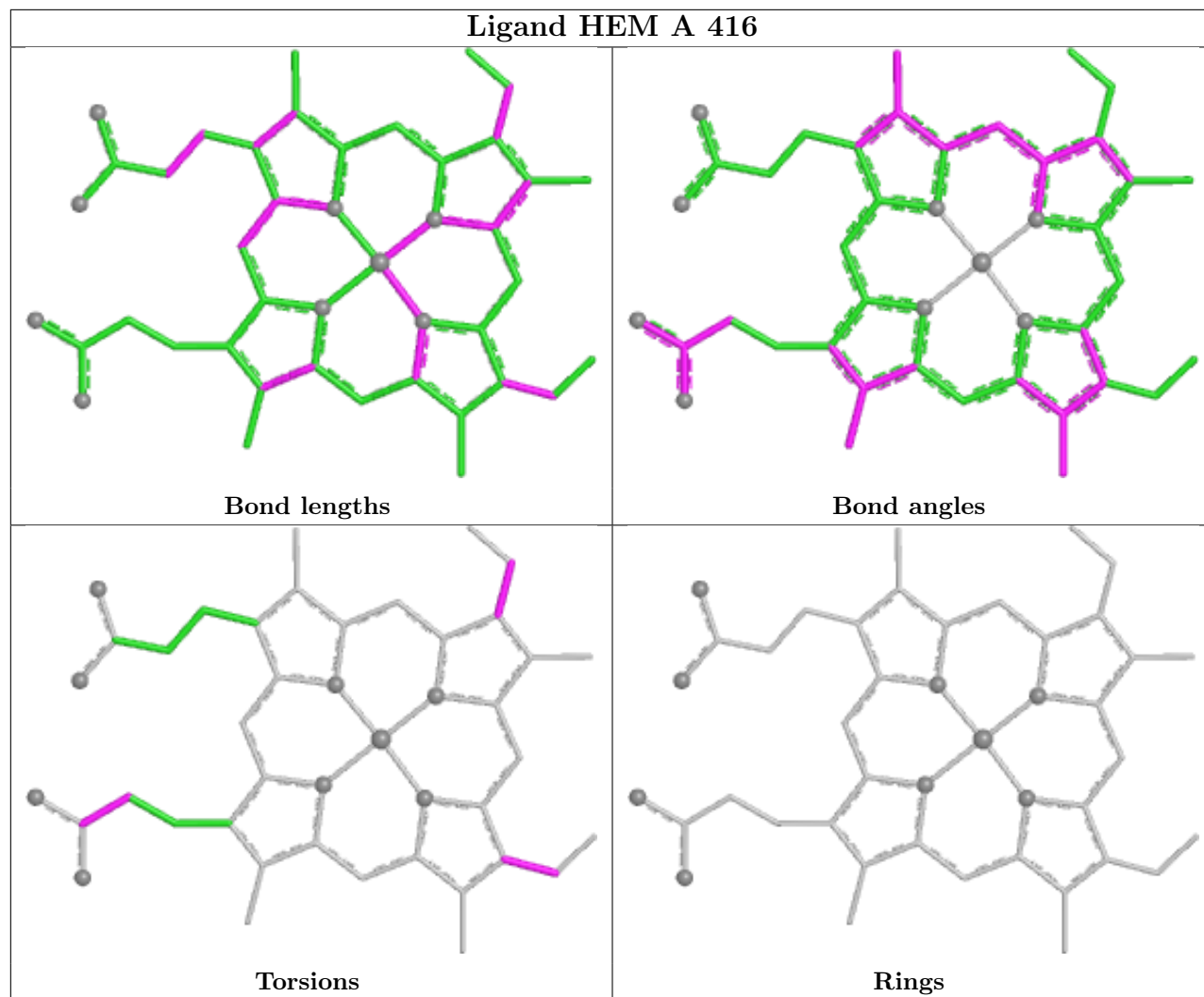
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 21% for the well-defined parts and 21% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *upload-req-shifts*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1189
Number of shifts mapped to atoms	1157
Number of unparsed shifts	0
Number of shifts with mapping errors	32
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 32 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	THR	H	8.2	0.02	1
1	A	2	THR	CA	60.7	0.1	1
1	A	2	THR	CB	68.4	0.1	1
1	A	2	THR	N	117.1	0.1	1
1	A	3	GLU	H	8.16	0.02	1
1	A	3	GLU	CA	55.2	0.1	1
1	A	3	GLU	CB	28.6	0.1	1
1	A	3	GLU	N	116.9	0.1	1
1	A	4	THR	H	8.12	0.02	1
1	A	4	THR	CA	60.7	0.1	1
1	A	4	THR	CB	68.4	0.1	1
1	A	4	THR	N	120.5	0.1	1
1	A	5	ILE	H	8.15	0.02	1
1	A	5	ILE	CA	60.2	0.1	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	ILE	CB	36.8	0.1	1
1	A	5	ILE	N	124.9	0.1	1
1	A	6	GLN	H	8.39	0.02	1
1	A	6	GLN	CA	54.5	0.1	1
1	A	6	GLN	CB	28.0	0.1	1
1	A	6	GLN	N	125.5	0.1	1
1	A	7	SER	H	8.29	0.02	1
1	A	7	SER	CA	57.2	0.1	1
1	A	7	SER	CB	62.7	0.1	1
1	A	7	SER	N	118.4	0.1	1
1	A	8	ASN	H	8.35	0.02	1
1	A	8	ASN	CA	51.9	0.1	1
1	A	8	ASN	CB	37.3	0.1	1
1	A	8	ASN	N	121.7	0.1	1
1	A	9	ALA	H	8.1	0.02	1
1	A	9	ALA	CA	51.1	0.1	1
1	A	9	ALA	CB	17.1	0.1	1
1	A	9	ALA	N	124.3	0.1	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	330	0.98 ± 0.10	Should be checked
$^{13}\text{C}_\beta$	266	1.98 ± 0.10	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	292	0.34 ± 0.14	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 21%, i.e. 1157 atoms were assigned a chemical shift out of a possible 5573. 0 out of 66 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	893/1990 (45%)	287/805 (36%)	322/810 (40%)	284/375 (76%)
Sidechain	258/3171 (8%)	0/2065 (0%)	258/982 (26%)	0/124 (0%)
Aromatic	6/412 (1%)	3/208 (1%)	0/186 (0%)	3/18 (17%)
Overall	1157/5573 (21%)	290/3078 (9%)	580/1978 (29%)	287/517 (56%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 21%, i.e. 1157 atoms were assigned a chemical shift out of a possible 5573. 0 out of 66 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	893/1990 (45%)	287/805 (36%)	322/810 (40%)	284/375 (76%)
Sidechain	258/3171 (8%)	0/2065 (0%)	258/982 (26%)	0/124 (0%)
Aromatic	6/412 (1%)	3/208 (1%)	0/186 (0%)	3/18 (17%)
Overall	1157/5573 (21%)	290/3078 (9%)	580/1978 (29%)	287/517 (56%)

7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	358	LEU	H	2.74	5.09 – 11.34	-8.8
1	A	357	CYS	H	4.04	5.02 – 11.74	-6.5
1	A	349	THR	H	11.82	5.19 – 11.27	5.9

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

