



Full wwPDB NMR Structure Validation Report ⓘ

Mar 10, 2026 – 01:25 PM UTC

PDB ID : 2LQD / pdb_00002lqd
BMRB ID : 17415
Title : Reduced and CO-bound cytochrome P450cam (CYP101A1)
Authors : Pochapsky, T.C.; Pochapsky, S.S.; Ascitutto, E.; Madura, J.; Young, M.J.
Deposited on : 2012-03-02

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

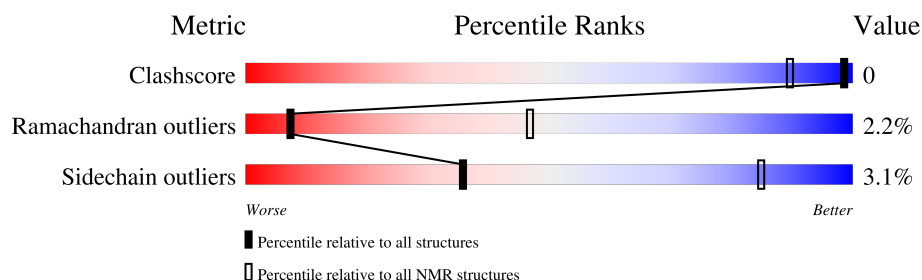
1 Overall quality at a glance

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	413	

2 Ensemble composition and analysis ⓘ

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

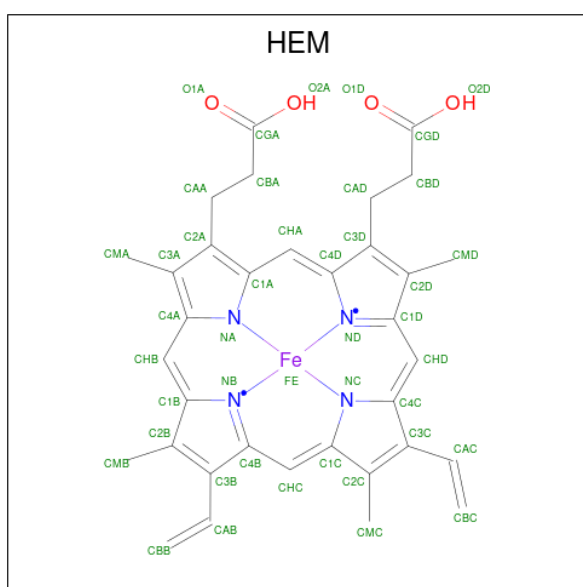
3 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6522 atoms, of which 3241 are hydrogens and 0 are deuteriums.

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

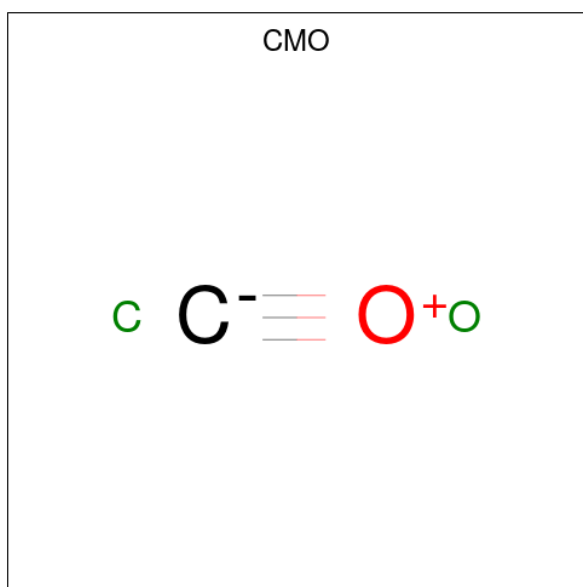
Mol	Chain	Residues	Atoms						Trace
1	A	405	Total	C	H	N	O	S	0
			6365	2033	3157	560	597	18	

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



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

- Molecule 3 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



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

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	
4	A	1	Total	K
			1	1

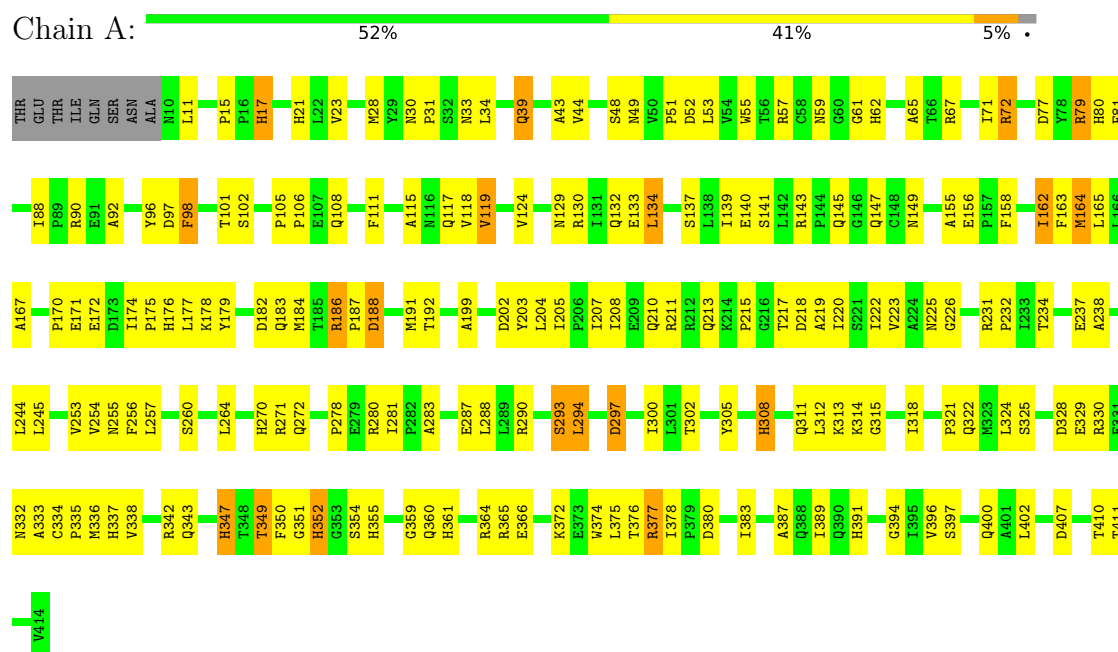
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		
5	A	27	Total	H	O
			81	54	27

4 Residue-property plots

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Camphor 5-monooxygenase



5 Refinement protocol and experimental data overview

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

Of the 100 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: CMO, K, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (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	2.07	85/3287 (2.6%)	2.37	195/4465 (4.4%)
All	All	2.07	85/3287 (2.6%)	2.37	195/4465 (4.4%)

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	Planarity
1	A	0	12
All	All	0	12

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	281	ILE	CA-C	10.56	1.64	1.52
1	A	226	GLY	CA-C	-10.32	1.43	1.52
1	A	215	PRO	CA-C	9.03	1.64	1.52
1	A	314	LYS	CA-C	8.01	1.62	1.52
1	A	48	SER	N-CA	7.93	1.56	1.46
1	A	163	PHE	CA-C	7.81	1.63	1.52
1	A	174	ILE	CA-CB	7.79	1.59	1.53
1	A	118	VAL	N-CA	7.76	1.55	1.46
1	A	374	TRP	N-CA	7.42	1.55	1.46
1	A	383	ILE	CA-CB	7.31	1.62	1.54
1	A	217	THR	CA-CB	7.27	1.62	1.52
1	A	143	ARG	C-N	7.22	1.42	1.34
1	A	411	THR	N-CA	7.11	1.55	1.45
1	A	215	PRO	N-CD	-7.07	1.37	1.47
1	A	176	HIS	CG-ND1	7.05	1.46	1.38
1	A	182	ASP	CA-C	7.00	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	HIS	CE1-NE2	6.97	1.39	1.32
1	A	376	THR	N-CA	6.88	1.54	1.46
1	A	271	ARG	CA-C	6.79	1.61	1.52
1	A	162	ILE	C-O	-6.78	1.16	1.24
1	A	30	ASN	CA-C	6.62	1.59	1.52
1	A	372	LYS	CA-C	6.58	1.58	1.52
1	A	119	VAL	N-CA	-6.53	1.38	1.46
1	A	62	HIS	CG-ND1	6.43	1.45	1.38
1	A	11	LEU	N-CA	6.27	1.53	1.46
1	A	176	HIS	ND1-CE1	6.23	1.38	1.32
1	A	186	ARG	CA-C	6.21	1.60	1.52
1	A	347	HIS	CE1-NE2	6.20	1.38	1.32
1	A	394	GLY	N-CA	6.20	1.50	1.45
1	A	378	ILE	CA-CB	6.19	1.62	1.54
1	A	336	MET	C-O	-6.18	1.16	1.24
1	A	102	SER	N-CA	6.17	1.54	1.46
1	A	184	MET	N-CA	6.14	1.53	1.46
1	A	391	HIS	ND1-CE1	6.09	1.38	1.32
1	A	155	ALA	CA-C	6.08	1.60	1.52
1	A	288	LEU	C-N	6.05	1.41	1.33
1	A	199	ALA	CA-C	5.97	1.60	1.52
1	A	170	PRO	N-CD	-5.96	1.39	1.47
1	A	264	LEU	N-CA	5.96	1.53	1.46
1	A	213	GLN	C-O	-5.96	1.16	1.24
1	A	232	PRO	C-N	-5.95	1.27	1.33
1	A	15	PRO	CA-C	5.95	1.57	1.52
1	A	21	HIS	CA-C	5.94	1.61	1.52
1	A	231	ARG	N-CA	5.93	1.54	1.46
1	A	355	HIS	CD2-NE2	5.89	1.44	1.37
1	A	278	PRO	N-CD	-5.87	1.39	1.47
1	A	389	ILE	CA-C	5.87	1.59	1.52
1	A	342	ARG	N-CA	5.86	1.53	1.45
1	A	171	GLU	N-CA	5.72	1.53	1.46
1	A	351	GLY	N-CA	5.68	1.51	1.45
1	A	80	HIS	CE1-NE2	5.62	1.38	1.32
1	A	97	ASP	N-CA	5.55	1.53	1.46
1	A	174	ILE	CA-C	5.54	1.57	1.52
1	A	177	LEU	C-N	5.48	1.41	1.33
1	A	219	ALA	CA-C	5.47	1.60	1.52
1	A	302	THR	C-N	-5.47	1.26	1.33
1	A	325	SER	C-O	5.47	1.30	1.24
1	A	61	GLY	C-N	-5.46	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	GLY	CA-C	5.41	1.59	1.51
1	A	342	ARG	CA-C	5.41	1.60	1.52
1	A	39	GLN	CA-C	5.40	1.59	1.52
1	A	80	HIS	CG-CD2	5.40	1.41	1.35
1	A	330	ARG	N-CA	5.40	1.53	1.46
1	A	80	HIS	CB-CG	5.39	1.57	1.50
1	A	211	ARG	NE-CZ	-5.39	1.27	1.33
1	A	179	TYR	CA-C	5.36	1.59	1.52
1	A	202	ASP	CA-C	5.32	1.60	1.52
1	A	179	TYR	N-CA	5.30	1.52	1.46
1	A	172	GLU	CA-C	5.29	1.59	1.52
1	A	321	PRO	N-CD	-5.29	1.40	1.47
1	A	72	ARG	CZ-NH1	-5.28	1.25	1.32
1	A	81	PHE	N-CA	5.26	1.52	1.46
1	A	293	SER	CA-C	5.21	1.61	1.52
1	A	352	HIS	CG-ND1	5.21	1.44	1.38
1	A	72	ARG	CA-CB	5.18	1.62	1.53
1	A	51	PRO	CA-C	5.16	1.58	1.52
1	A	410	THR	C-N	5.14	1.40	1.33
1	A	315	GLY	CA-C	5.13	1.58	1.51
1	A	52	ASP	CA-C	5.09	1.59	1.52
1	A	355	HIS	N-CA	-5.08	1.38	1.46
1	A	175	PRO	C-N	-5.08	1.27	1.33
1	A	165	LEU	N-CA	5.06	1.52	1.46
1	A	308	HIS	CD2-NE2	5.06	1.43	1.37
1	A	238	ALA	CA-C	5.03	1.59	1.52
1	A	377	ARG	C-N	-5.02	1.27	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ASP	CA-CB-CG	11.37	123.97	112.60
1	A	186	ARG	CA-C-N	10.74	132.47	120.98
1	A	186	ARG	C-N-CA	10.74	132.47	120.98
1	A	80	HIS	CA-CB-CG	10.15	123.95	113.80
1	A	322	GLN	OE1-CD-NE2	-9.24	113.36	122.60
1	A	130	ARG	NE-CZ-NH1	9.17	130.67	121.50
1	A	188	ASP	CA-C-N	9.08	130.51	122.43
1	A	188	ASP	C-N-CA	9.08	130.51	122.43
1	A	39	GLN	OE1-CD-NE2	-9.02	113.58	122.60
1	A	174	ILE	N-CA-CB	-9.01	104.83	110.50
1	A	183	GLN	OE1-CD-NE2	-8.92	113.68	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	ASP	CA-CB-CG	8.76	121.36	112.60
1	A	108	GLN	OE1-CD-NE2	-8.49	114.11	122.60
1	A	30	ASN	OD1-CG-ND2	-8.41	114.19	122.60
1	A	62	HIS	N-CA-C	8.31	121.16	108.52
1	A	176	HIS	ND1-CE1-NE2	8.22	116.62	108.40
1	A	147	GLN	OE1-CD-NE2	-8.11	114.49	122.60
1	A	31	PRO	O-C-N	-8.10	111.71	122.64
1	A	332	ASN	O-C-N	-8.09	113.72	123.27
1	A	105	PRO	N-CA-CB	7.71	110.55	103.08
1	A	324	LEU	CA-C-O	7.63	127.14	118.97
1	A	176	HIS	CB-CG-CD2	-7.62	121.30	131.20
1	A	244	LEU	O-C-N	-7.43	114.42	122.07
1	A	256	PHE	O-C-N	7.42	129.99	122.12
1	A	237	GLU	CA-C-N	7.41	130.54	120.54
1	A	237	GLU	C-N-CA	7.41	130.54	120.54
1	A	238	ALA	O-C-N	7.35	129.73	122.09
1	A	132	GLN	CA-C-N	7.29	129.91	120.44
1	A	132	GLN	C-N-CA	7.29	129.91	120.44
1	A	108	GLN	CG-CD-NE2	7.28	127.32	116.40
1	A	62	HIS	ND1-CE1-NE2	7.08	115.48	108.40
1	A	256	PHE	CA-C-O	-7.05	113.08	120.55
1	A	179	TYR	CA-C-N	7.01	129.56	120.44
1	A	179	TYR	C-N-CA	7.01	129.56	120.44
1	A	111	PHE	CA-C-N	6.98	129.64	120.28
1	A	111	PHE	C-N-CA	6.98	129.64	120.28
1	A	380	ASP	CA-C-O	-6.97	112.79	120.38
1	A	77	ASP	CA-CB-CG	-6.89	105.71	112.60
1	A	257	LEU	CA-C-N	6.86	130.04	120.29
1	A	257	LEU	C-N-CA	6.86	130.04	120.29
1	A	43	ALA	CA-C-O	-6.80	112.58	120.20
1	A	397	SER	N-CA-CB	-6.76	100.01	110.56
1	A	225	ASN	CA-C-N	6.73	126.49	120.10
1	A	225	ASN	C-N-CA	6.73	126.49	120.10
1	A	389	ILE	CA-C-N	6.68	132.49	122.47
1	A	389	ILE	C-N-CA	6.68	132.49	122.47
1	A	290	ARG	N-CA-C	-6.68	103.62	111.03
1	A	167	ALA	N-CA-CB	-6.67	100.54	110.61
1	A	260	SER	O-C-N	6.65	130.45	122.27
1	A	402	LEU	CA-C-N	6.62	128.11	119.84
1	A	402	LEU	C-N-CA	6.62	128.11	119.84
1	A	33	ASN	OD1-CG-ND2	-6.61	115.99	122.60
1	A	205	ILE	CA-C-N	6.61	125.85	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ILE	C-N-CA	6.61	125.85	118.97
1	A	62	HIS	CA-CB-CG	6.60	120.40	113.80
1	A	347	HIS	CB-CG-CD2	-6.58	122.64	131.20
1	A	400	GLN	OE1-CD-NE2	-6.54	116.06	122.60
1	A	329	GLU	CA-C-N	6.50	130.19	120.31
1	A	329	GLU	C-N-CA	6.50	130.19	120.31
1	A	254	VAL	CA-CB-CG1	6.47	121.41	110.40
1	A	210	GLN	OE1-CD-NE2	-6.46	116.14	122.60
1	A	98	PHE	CA-CB-CG	6.45	120.25	113.80
1	A	23	VAL	CA-C-O	-6.43	114.29	121.36
1	A	332	ASN	CA-C-O	6.42	127.38	120.32
1	A	140	GLU	O-C-N	-6.42	113.83	122.43
1	A	364	ARG	CA-C-O	-6.37	112.90	120.10
1	A	257	LEU	O-C-N	-6.36	115.47	122.09
1	A	118	VAL	N-CA-C	-6.32	103.73	110.36
1	A	300	ILE	O-C-N	-6.32	115.80	122.81
1	A	55	TRP	CA-C-N	6.28	131.39	122.72
1	A	55	TRP	C-N-CA	6.28	131.39	122.72
1	A	155	ALA	CA-C-O	-6.28	114.23	120.82
1	A	332	ASN	CA-C-N	6.24	128.92	120.44
1	A	332	ASN	C-N-CA	6.24	128.92	120.44
1	A	334	CYS	CA-C-N	6.21	127.61	119.84
1	A	334	CYS	C-N-CA	6.21	127.61	119.84
1	A	411	THR	O-C-N	-6.21	115.01	122.65
1	A	352	HIS	CB-CG-CD2	-6.21	123.13	131.20
1	A	71	ILE	CA-CB-CG2	6.21	121.05	110.50
1	A	156	GLU	CB-CG-CD	-6.14	102.16	112.60
1	A	92	ALA	N-CA-CB	-6.13	101.07	110.20
1	A	106	PRO	N-CD-CG	6.09	111.11	103.80
1	A	238	ALA	CA-C-O	-6.06	114.42	120.90
1	A	396	VAL	O-C-N	-6.06	116.64	123.18
1	A	361	HIS	CB-CG-CD2	-6.06	123.33	131.20
1	A	115	ALA	CA-C-N	6.03	128.65	120.38
1	A	115	ALA	C-N-CA	6.03	128.65	120.38
1	A	222	ILE	N-CA-C	6.01	116.18	110.53
1	A	174	ILE	O-C-N	5.99	124.32	120.07
1	A	176	HIS	CG-ND1-CE1	-5.99	99.12	109.30
1	A	170	PRO	N-CD-CG	5.98	112.17	103.20
1	A	255	ASN	OD1-CG-ND2	5.95	128.55	122.60
1	A	28	MET	N-CA-C	5.94	118.54	111.71
1	A	49	ASN	CA-CB-CG	5.93	118.53	112.60
1	A	208	ILE	CA-CB-CG1	5.92	120.47	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	LEU	CA-C-N	5.92	123.97	120.24
1	A	204	LEU	C-N-CA	5.92	123.97	120.24
1	A	132	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	A	234	THR	N-CA-C	5.91	119.30	110.14
1	A	145	GLN	OE1-CD-NE2	-5.89	116.71	122.60
1	A	117	GLN	CA-C-N	5.88	128.19	120.60
1	A	117	GLN	C-N-CA	5.88	128.19	120.60
1	A	30	ASN	N-CA-C	5.84	119.89	108.21
1	A	365	ARG	CD-NE-CZ	5.82	132.55	124.40
1	A	270	HIS	CA-CB-CG	5.82	119.62	113.80
1	A	338	VAL	N-CA-C	5.82	117.01	107.24
1	A	92	ALA	CB-CA-C	5.81	121.33	110.70
1	A	364	ARG	NH1-CZ-NH2	-5.78	111.78	119.30
1	A	283	ALA	N-CA-C	5.78	117.44	111.03
1	A	374	TRP	CA-C-N	5.78	128.29	120.44
1	A	374	TRP	C-N-CA	5.78	128.29	120.44
1	A	79	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	A	337	HIS	ND1-CG-CD2	5.68	111.78	106.10
1	A	333	ALA	CA-C-O	-5.66	114.87	120.70
1	A	329	GLU	N-CA-C	-5.65	106.36	113.20
1	A	67	ARG	NE-CZ-NH2	-5.64	114.13	119.20
1	A	192	THR	CA-C-N	5.63	127.76	120.44
1	A	192	THR	C-N-CA	5.63	127.76	120.44
1	A	375	LEU	CA-C-N	5.63	128.09	120.38
1	A	375	LEU	C-N-CA	5.63	128.09	120.38
1	A	287	GLU	O-C-N	-5.63	116.15	122.12
1	A	278	PRO	CA-C-N	5.61	127.73	120.44
1	A	278	PRO	C-N-CA	5.61	127.73	120.44
1	A	365	ARG	CA-C-O	-5.59	114.94	120.70
1	A	360	GLN	CA-CB-CG	5.56	125.22	114.10
1	A	134	LEU	CA-C-O	-5.55	114.96	120.90
1	A	374	TRP	CB-CA-C	5.55	120.28	110.85
1	A	17	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	A	245	LEU	N-CA-C	5.53	118.02	111.33
1	A	220	ILE	CA-CB-CG1	5.51	119.77	110.40
1	A	322	GLN	CA-C-O	-5.50	113.89	120.10
1	A	349	THR	CA-C-N	5.50	132.04	121.54
1	A	349	THR	C-N-CA	5.50	132.04	121.54
1	A	322	GLN	CG-CD-NE2	5.48	124.62	116.40
1	A	294	LEU	N-CA-C	5.48	122.47	110.80
1	A	347	HIS	ND1-CG-CD2	5.48	111.58	106.10
1	A	308	HIS	CA-C-N	5.47	131.34	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	HIS	C-N-CA	5.47	131.34	122.09
1	A	191	MET	CA-CB-CG	-5.47	103.16	114.10
1	A	218	ASP	CA-C-N	5.43	128.31	120.38
1	A	218	ASP	C-N-CA	5.43	128.31	120.38
1	A	101	THR	CA-CB-OG1	-5.42	101.47	109.60
1	A	34	LEU	CA-C-O	5.38	126.05	119.05
1	A	297	ASP	CA-C-N	5.38	131.95	121.41
1	A	297	ASP	C-N-CA	5.38	131.95	121.41
1	A	202	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	59	ASN	CA-CB-CG	-5.37	107.23	112.60
1	A	336	MET	N-CA-C	5.35	118.27	111.69
1	A	139	ILE	O-C-N	-5.32	116.35	121.83
1	A	407	ASP	O-C-N	-5.31	116.69	121.31
1	A	260	SER	CA-C-O	-5.28	113.90	119.97
1	A	65	ALA	O-C-N	-5.27	117.05	123.16
1	A	365	ARG	NE-CZ-NH1	5.27	126.77	121.50
1	A	137	SER	N-CA-C	5.26	117.70	111.33
1	A	187	PRO	CA-N-CD	-5.23	104.67	112.00
1	A	313	LYS	O-C-N	-5.23	116.10	123.11
1	A	272	GLN	OE1-CD-NE2	-5.23	117.37	122.60
1	A	67	ARG	CA-C-N	5.21	125.86	120.03
1	A	67	ARG	C-N-CA	5.21	125.86	120.03
1	A	133	GLU	CA-C-N	5.20	127.56	120.54
1	A	133	GLU	C-N-CA	5.20	127.56	120.54
1	A	30	ASN	N-CA-CB	-5.20	102.67	111.30
1	A	343	GLN	O-C-N	-5.19	116.93	122.85
1	A	81	PHE	CA-CB-CG	5.19	118.99	113.80
1	A	272	GLN	CA-C-N	5.19	127.48	120.38
1	A	272	GLN	C-N-CA	5.19	127.48	120.38
1	A	183	GLN	N-CA-CB	5.18	117.73	110.12
1	A	211	ARG	N-CA-C	-5.17	105.07	111.33
1	A	312	LEU	O-C-N	-5.17	117.19	123.03
1	A	210	GLN	CG-CD-NE2	5.16	124.14	116.40
1	A	232	PRO	CA-C-N	5.16	127.52	120.35
1	A	232	PRO	C-N-CA	5.16	127.52	120.35
1	A	57	ARG	CD-NE-CZ	5.15	131.61	124.40
1	A	288	LEU	N-CA-C	-5.14	105.76	111.36
1	A	124	VAL	CA-C-N	5.11	129.36	120.68
1	A	124	VAL	C-N-CA	5.11	129.36	120.68
1	A	361	HIS	N-CA-C	5.10	117.50	111.33
1	A	354	SER	CA-C-O	-5.10	114.58	120.24
1	A	156	GLU	O-C-N	-5.08	115.47	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	LEU	CA-C-N	5.08	127.09	120.28
1	A	177	LEU	C-N-CA	5.08	127.09	120.28
1	A	377	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	A	149	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	A	141	SER	N-CA-C	5.05	119.07	113.01
1	A	311	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	A	210	GLN	CA-C-O	-5.04	115.71	120.90
1	A	143	ARG	CD-NE-CZ	5.04	131.45	124.40
1	A	164	MET	CA-C-O	-5.04	115.08	120.42
1	A	88	ILE	N-CA-C	5.03	119.75	108.88
1	A	313	LYS	CA-C-O	5.03	127.34	121.46
1	A	203	TYR	CD1-CG-CD2	5.02	125.63	118.10
1	A	300	ILE	CA-C-O	5.02	126.57	120.85
1	A	281	ILE	CA-CB-CG1	-5.01	101.88	110.40
1	A	318	ILE	N-CA-C	5.01	115.48	108.17
1	A	129	ASN	OD1-CG-ND2	-5.01	117.59	122.60

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	17	HIS	Mainchain
1	A	72	ARG	Sidechain
1	A	79	ARG	Sidechain
1	A	90	ARG	Sidechain
1	A	96	TYR	Sidechain
1	A	98	PHE	Sidechain
1	A	134	LEU	Mainchain
1	A	186	ARG	Sidechain
1	A	280	ARG	Sidechain
1	A	305	TYR	Sidechain
1	A	377	ARG	Sidechain
1	A	387	ALA	Mainchain

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	1
All	All	3281	3241	3186	1

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:158:PHE:CE1	1:A:162:ILE:HD11	0.45	2.47

6.3 Torsion angles [i](#)

6.3.1 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 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	403/413 (98%)	355 (88%)	39 (10%)	9 (2%)	7	47
All	All	403/413 (98%)	355 (88%)	39 (10%)	9 (2%)	7	47

All 9 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	119	VAL
1	A	188	ASP
1	A	294	LEU
1	A	308	HIS
1	A	335	PRO
1	A	347	HIS
1	A	349	THR
1	A	350	PHE
1	A	352	HIS

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	350/357 (98%)	339 (97%)	11 (3%)	36	85
All	All	350/357 (98%)	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	39	GLN
1	A	44	VAL
1	A	53	LEU
1	A	164	MET
1	A	178	LYS
1	A	207	ILE
1	A	223	VAL
1	A	253	VAL
1	A	293	SER
1	A	297	ASP
1	A	366	GLU

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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
3	CMO	A	502	2	0,1,1	0.00	-
2	HEM	A	501	3,1	50,50,50	1.86	15 (30%)

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
3	CMO	A	502	2	-	-	-
2	HEM	A	501	3,1	67,82,82	1.74	15 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	501	3,1	-	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)
2	A	501	HEM	FE-NA	4.07	2.08	1.95
2	A	501	HEM	FE-NB	4.06	2.07	1.94
2	A	501	HEM	C4D-C3D	3.81	1.51	1.45
2	A	501	HEM	C4A-C3A	3.34	1.51	1.43
2	A	501	HEM	C3C-C4C	3.19	1.40	1.46
2	A	501	HEM	C1D-ND	3.12	1.45	1.38
2	A	501	HEM	C3D-C2D	2.84	1.42	1.36
2	A	501	HEM	FE-NC	2.82	2.04	1.95
2	A	501	HEM	C1A-C2A	2.81	1.50	1.44
2	A	501	HEM	C4A-NA	2.62	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-ND	2.55	2.02	1.94
2	A	501	HEM	CHA-C1A	2.47	1.45	1.39
2	A	501	HEM	CAC-C3C	2.06	1.52	1.47
2	A	501	HEM	CBD-CGD	2.06	1.45	1.50
2	A	501	HEM	C1D-C2D	2.06	1.48	1.44

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

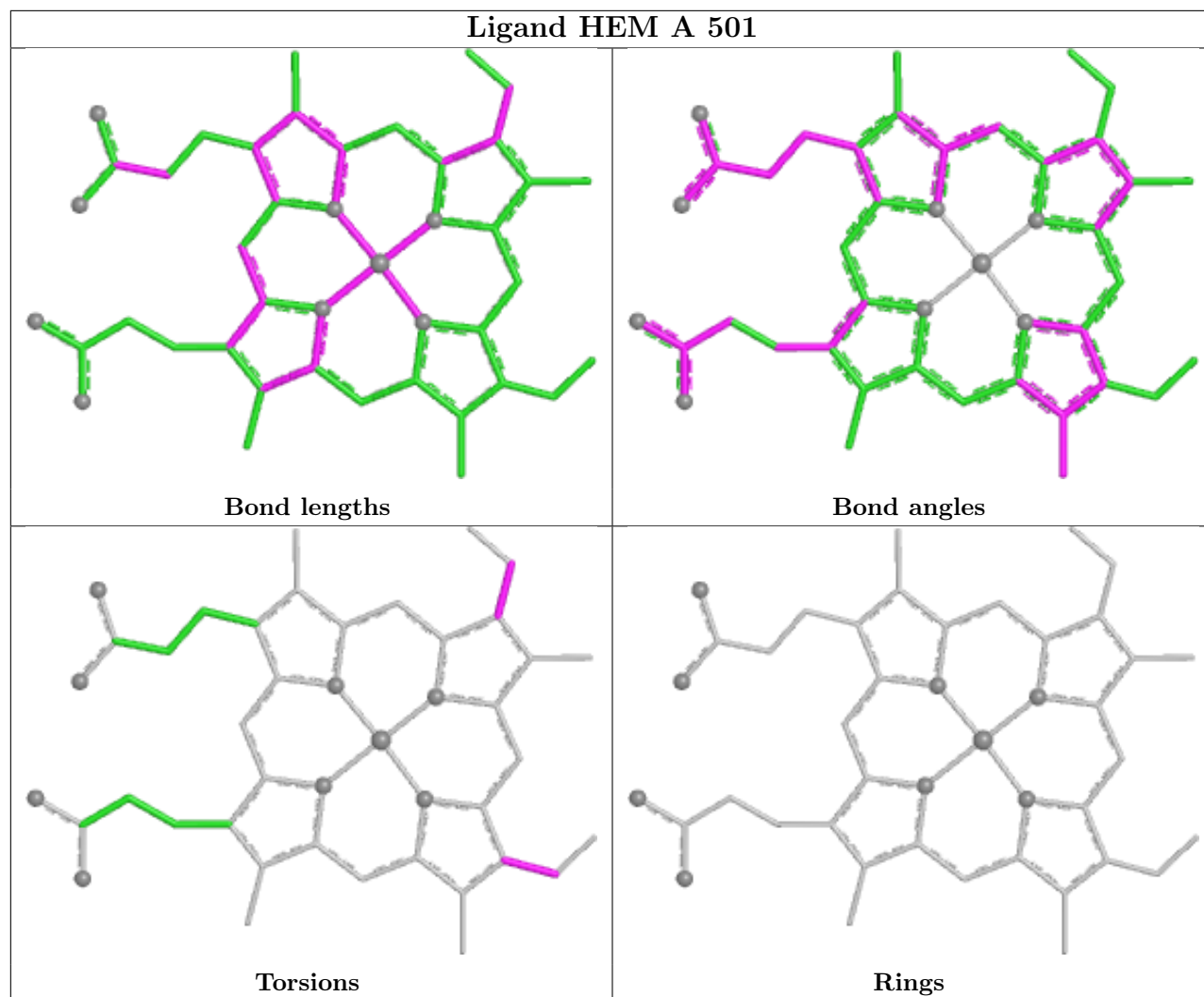
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C3B-C2B-C1B	5.11	110.25	106.41
2	A	501	HEM	C3B-C4B-NB	4.83	112.94	109.47
2	A	501	HEM	C3C-C2C-C1C	4.17	110.99	107.05
2	A	501	HEM	C4B-C3B-C2B	3.89	103.70	107.28
2	A	501	HEM	CAD-CBD-CGD	3.47	122.86	113.67
2	A	501	HEM	O2D-CGD-CBD	2.61	122.24	114.00
2	A	501	HEM	CMB-C2B-C1B	2.57	121.01	125.03
2	A	501	HEM	CAA-C2A-C1A	2.50	129.82	124.94
2	A	501	HEM	O2A-CGA-CBA	2.50	121.89	114.00
2	A	501	HEM	CAD-C3D-C4D	2.40	128.89	124.70
2	A	501	HEM	O1A-CGA-CBA	2.34	115.68	123.09
2	A	501	HEM	CHD-C1D-C2D	2.20	128.50	125.03
2	A	501	HEM	C4C-C3C-C2C	2.07	105.02	106.81
2	A	501	HEM	O2D-CGD-O1D	2.05	118.07	123.33
2	A	501	HEM	C2D-C1D-ND	2.03	107.55	109.90

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: *assigned_chem_shift_list_1*

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 ⓘ

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 ⓘ

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:

