



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2017 – 11:39 PM EST

PDB ID : 5CPP
Title : THE STRUCTURAL BASIS FOR SUBSTRATE-INDUCED CHANGES IN REDOX POTENTIAL AND SPIN EQUILIBRIUM IN CYTOCHROME P-450(CAM)
Authors : Raag, R.; Poulos, T.L.
Deposited on : unknown
Resolution : 2.08 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

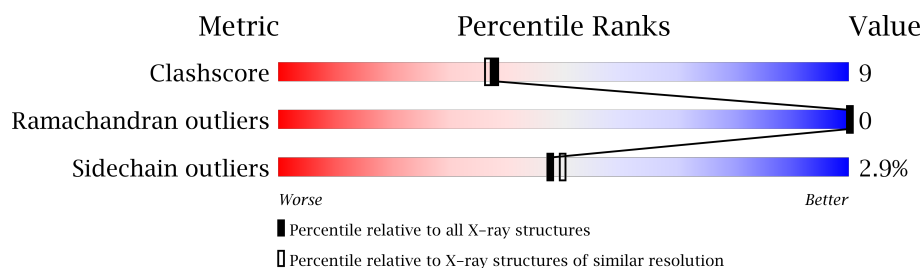
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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))
Clashscore	112137	5537 (2.10-2.06)
Ramachandran outliers	110173	5483 (2.10-2.06)
Sidechain outliers	110143	5484 (2.10-2.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	414	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3462 atoms, of which 0 are hydrogens and 0 are deuteriums.

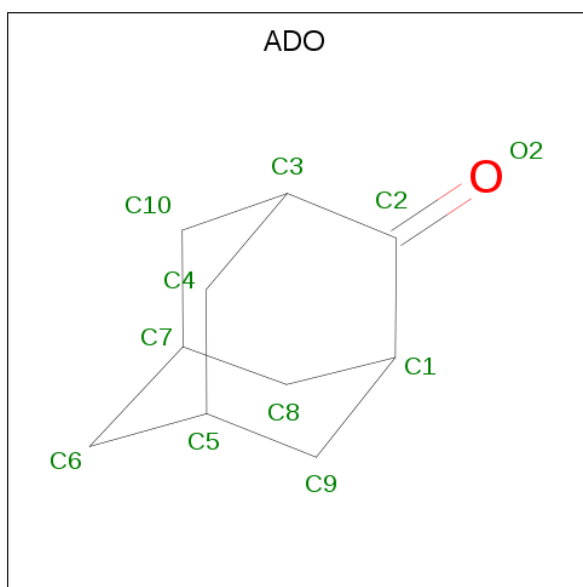
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CYTOCHROME P450-CAM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3204	2030	559	597	18			

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





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

- Molecule 4 is water.

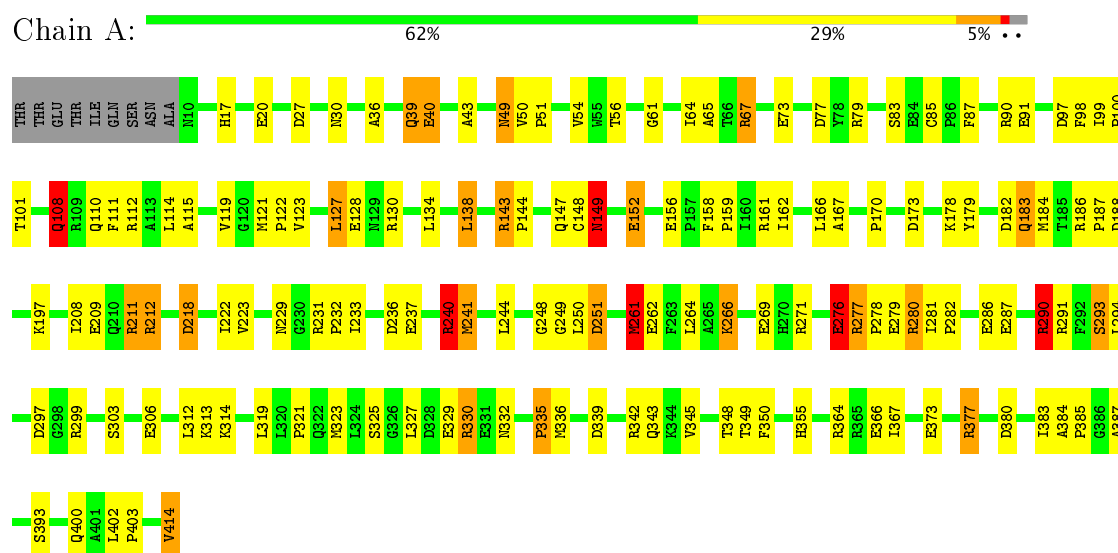
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	204	Total	O	0	0
			204	204		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: CYTOCHROME P450-CAM



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.67Å 103.90Å 36.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.08	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.08)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3462	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ADO

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	1.49	20/3283 (0.6%)	2.01	91/4461 (2.0%)

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 outliers	#Planarity outliers
1	A	0	18

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	GLU	CD-OE2	9.23	1.35	1.25
1	A	276	GLU	CD-OE2	8.06	1.34	1.25
1	A	251	ASP	C-O	7.89	1.38	1.23
1	A	287	GLU	CD-OE1	-7.34	1.17	1.25
1	A	393	SER	CA-CB	7.32	1.64	1.52
1	A	287	GLU	CG-CD	7.25	1.62	1.51
1	A	286	GLU	CD-OE1	-6.97	1.18	1.25
1	A	64	ILE	C-O	6.65	1.35	1.23
1	A	262	GLU	CD-OE1	-6.53	1.18	1.25
1	A	211	ARG	CD-NE	-6.24	1.35	1.46
1	A	350	PHE	C-N	6.16	1.44	1.33
1	A	335	PRO	N-CD	5.91	1.56	1.47
1	A	286	GLU	CD-OE2	5.60	1.31	1.25
1	A	342	ARG	NE-CZ	5.54	1.40	1.33
1	A	248	GLY	C-N	5.37	1.42	1.33
1	A	364	ARG	CB-CG	5.34	1.67	1.52
1	A	325	SER	CB-OG	-5.21	1.35	1.42
1	A	367	ILE	CA-CB	5.06	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	GLU	CD-OE1	-5.01	1.20	1.25
1	A	299	ARG	NE-CZ	5.00	1.39	1.33

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	CD-NE-CZ	33.99	171.19	123.60
1	A	212	ARG	CD-NE-CZ	21.71	153.99	123.60
1	A	299	ARG	NE-CZ-NH2	-17.98	111.31	120.30
1	A	212	ARG	NE-CZ-NH1	15.06	127.83	120.30
1	A	67	ARG	NE-CZ-NH2	-13.97	113.32	120.30
1	A	330	ARG	NE-CZ-NH1	13.56	127.08	120.30
1	A	161	ARG	NE-CZ-NH2	-13.55	113.52	120.30
1	A	143	ARG	NE-CZ-NH2	-12.39	114.10	120.30
1	A	112	ARG	NE-CZ-NH1	12.10	126.35	120.30
1	A	211	ARG	NE-CZ-NH2	11.62	126.11	120.30
1	A	240	ARG	NE-CZ-NH2	-11.37	114.61	120.30
1	A	280	ARG	NE-CZ-NH2	-10.54	115.03	120.30
1	A	240	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	A	182	ASP	CB-CG-OD1	-10.29	109.04	118.30
1	A	161	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	A	143	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	A	130	ARG	NE-CZ-NH1	-9.12	115.74	120.30
1	A	277	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	A	130	ARG	NE-CZ-NH2	8.84	124.72	120.30
1	A	280	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	A	67	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	A	65	ALA	CB-CA-C	7.94	122.01	110.10
1	A	130	ARG	CD-NE-CZ	7.92	134.69	123.60
1	A	299	ARG	NH1-CZ-NH2	7.89	128.08	119.40
1	A	90	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	A	364	ARG	NE-CZ-NH2	7.65	124.13	120.30
1	A	291	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	364	ARG	CD-NE-CZ	7.44	134.01	123.60
1	A	261	MET	CG-SD-CE	7.32	111.91	100.20
1	A	67	ARG	CD-NE-CZ	7.29	133.81	123.60
1	A	348	THR	CA-CB-CG2	7.23	122.53	112.40
1	A	241	MET	N-CA-CB	7.05	123.29	110.60
1	A	87	PHE	CB-CG-CD1	-7.04	115.88	120.80
1	A	350	PHE	CB-CG-CD1	-7.00	115.90	120.80
1	A	149	ASN	N-CA-CB	6.96	123.13	110.60
1	A	290	ARG	CD-NE-CZ	6.90	133.26	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	A	297	ASP	CB-CG-OD1	6.85	124.47	118.30
1	A	79	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	A	287	GLU	CG-CD-OE2	-6.73	104.84	118.30
1	A	123	VAL	CA-CB-CG1	6.66	120.89	110.90
1	A	39	GLN	N-CA-CB	6.46	122.24	110.60
1	A	127	LEU	CA-CB-CG	6.38	129.97	115.30
1	A	269	GLU	CG-CD-OE2	-6.30	105.70	118.30
1	A	108	GLN	CA-CB-CG	6.25	127.14	113.40
1	A	90	ARG	CD-NE-CZ	6.22	132.31	123.60
1	A	251	ASP	O-C-N	-6.17	112.82	122.70
1	A	54	VAL	CA-CB-CG2	6.02	119.93	110.90
1	A	349	THR	CA-CB-OG1	-5.93	96.55	109.00
1	A	327	LEU	C-N-CA	5.92	136.51	121.70
1	A	339	ASP	CB-CG-OD1	-5.92	112.98	118.30
1	A	414	VAL	CB-CA-C	5.90	122.61	111.40
1	A	279	GLU	CA-CB-CG	5.88	126.32	113.40
1	A	183	GLN	N-CA-CB	5.87	121.17	110.60
1	A	287	GLU	OE1-CD-OE2	5.87	130.34	123.30
1	A	330	ARG	NH1-CZ-NH2	-5.80	113.02	119.40
1	A	312	LEU	CB-CA-C	5.78	121.19	110.20
1	A	366	GLU	OE1-CD-OE2	-5.77	116.38	123.30
1	A	115	ALA	CB-CA-C	5.75	118.72	110.10
1	A	209	GLU	C-N-CA	5.72	136.00	121.70
1	A	211	ARG	NH1-CZ-NH2	-5.70	113.14	119.40
1	A	179	TYR	CB-CG-CD2	-5.69	117.59	121.00
1	A	87	PHE	CB-CG-CD2	5.65	124.75	120.80
1	A	152	GLU	OE1-CD-OE2	5.60	130.02	123.30
1	A	266	LYS	CB-CG-CD	5.58	126.10	111.60
1	A	400	GLN	CA-CB-CG	5.57	125.65	113.40
1	A	67	ARG	O-C-N	5.52	132.58	123.20
1	A	241	MET	CG-SD-CE	-5.50	91.39	100.20
1	A	85	CYS	CB-CA-C	5.49	121.38	110.40
1	A	329	GLU	CA-CB-CG	5.48	125.46	113.40
1	A	269	GLU	CG-CD-OE1	5.40	129.10	118.30
1	A	27	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	149	ASN	CA-C-O	-5.28	109.00	120.10
1	A	373	GLU	OE1-CD-OE2	-5.26	116.99	123.30
1	A	251	ASP	CA-C-O	-5.24	109.10	120.10
1	A	218	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	312	LEU	CA-CB-CG	5.23	127.32	115.30
1	A	43	ALA	N-CA-CB	5.21	117.40	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	LYS	CA-CB-CG	5.21	124.87	113.40
1	A	20	GLU	CA-CB-CG	5.21	124.86	113.40
1	A	209	GLU	CA-CB-CG	5.20	124.84	113.40
1	A	294	LEU	CB-CG-CD1	-5.20	102.17	111.00
1	A	36	ALA	CB-CA-C	-5.18	102.34	110.10
1	A	156	GLU	CA-CB-CG	5.17	124.77	113.40
1	A	43	ALA	CB-CA-C	5.15	117.82	110.10
1	A	343	GLN	N-CA-CB	5.09	119.77	110.60
1	A	306	GLU	O-C-N	5.09	130.85	122.70
1	A	90	ARG	NH1-CZ-NH2	-5.07	113.82	119.40
1	A	236	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	A	108	GLN	CB-CG-CD	5.04	124.70	111.60
1	A	138	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	VAL	Mainchain
1	A	147	GLN	Mainchain
1	A	148	CYS	Mainchain
1	A	149	ASN	Mainchain
1	A	167	ALA	Mainchain
1	A	186	ARG	Sidechain
1	A	240	ARG	Sidechain
1	A	249	GLY	Mainchain
1	A	250	LEU	Mainchain
1	A	251	ASP	Mainchain
1	A	271	ARG	Sidechain
1	A	280	ARG	Sidechain
1	A	290	ARG	Sidechain
1	A	330	ARG	Sidechain
1	A	377	ARG	Sidechain
1	A	40	GLU	Mainchain
1	A	67	ARG	Sidechain
1	A	77	ASP	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3204	0	3144	56	0
2	A	43	0	30	0	0
3	A	11	0	14	0	0
4	A	204	0	0	4	0
All	All	3462	0	3188	56	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 9.

All (56) 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:183:GLN:HE22	1:A:188:ASP:HB2	1.30	0.97
1:A:40:GLU:HG3	1:A:336:MET:HE2	1.65	0.79
1:A:208:ILE:O	1:A:212:ARG:HG3	1.91	0.69
1:A:127:LEU:HD11	1:A:166:LEU:HD13	1.75	0.69
1:A:231:ARG:HB2	1:A:232:PRO:HD2	1.76	0.66
1:A:121:MET:HB2	1:A:122:PRO:HD3	1.79	0.64
1:A:183:GLN:NE2	1:A:188:ASP:HB2	2.08	0.63
1:A:40:GLU:HG3	1:A:336:MET:CE	2.33	0.58
1:A:149:ASN:ND2	1:A:402:LEU:H	2.02	0.56
1:A:184:MET:CE	1:A:197:LYS:HA	2.35	0.56
1:A:49:ASN:H	1:A:49:ASN:HD22	1.57	0.53
1:A:152:GLU:HB3	4:A:563:HOH:O	2.10	0.51
1:A:184:MET:HE2	1:A:197:LYS:HA	1.92	0.51
1:A:98:PHE:HB3	1:A:244:LEU:HB2	1.92	0.51
1:A:387:ALA:HB1	1:A:403:PRO:HG2	1.92	0.50
1:A:122:PRO:HD2	4:A:701:HOH:O	2.10	0.50
1:A:290:ARG:HD3	1:A:345:VAL:HG13	1.93	0.50
1:A:121:MET:CB	1:A:122:PRO:HD3	2.42	0.50
1:A:30:ASN:ND2	4:A:555:HOH:O	2.44	0.49
1:A:56:THR:O	1:A:61:GLY:HA2	2.13	0.49
1:A:277:ARG:N	1:A:278:PRO:HD3	2.29	0.48
1:A:138:LEU:HD23	1:A:158:PHE:HB2	1.95	0.48
1:A:261:MET:HA	1:A:261:MET:HE2	1.96	0.48
1:A:303:SER:HA	1:A:314:LYS:HG3	1.96	0.47
1:A:223:VAL:O	1:A:233:ILE:HG21	2.14	0.47
1:A:387:ALA:CB	1:A:403:PRO:HG2	2.45	0.47
1:A:110:GLN:NE2	1:A:229:ASN:HA	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLN:HG3	1:A:355:HIS:CE1	2.51	0.46
1:A:111:PHE:HD2	1:A:241:MET:HE2	1.81	0.46
1:A:30:ASN:ND2	4:A:556:HOH:O	2.49	0.46
1:A:158:PHE:CE1	1:A:162:ILE:HD11	2.50	0.46
1:A:114:LEU:HD23	1:A:241:MET:HE3	1.96	0.46
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.98	0.45
1:A:97:ASP:O	1:A:240:ARG:HD2	2.16	0.44
1:A:281:ILE:N	1:A:282:PRO:CD	2.80	0.44
1:A:266:LYS:HD3	1:A:383:ILE:CD1	2.48	0.44
1:A:170:PRO:HG2	1:A:173:ASP:OD1	2.18	0.44
1:A:266:LYS:HD3	1:A:383:ILE:HD11	2.00	0.44
1:A:17:HIS:CD2	1:A:313:LYS:HG3	2.53	0.43
1:A:384:ALA:HA	1:A:385:PRO:HD3	1.86	0.43
1:A:134:LEU:O	1:A:138:LEU:HB2	2.18	0.43
1:A:261:MET:HE2	1:A:264:LEU:HD12	1.99	0.43
1:A:293:SER:HB3	1:A:323:MET:HA	2.01	0.43
1:A:183:GLN:HE22	1:A:188:ASP:CB	2.14	0.43
1:A:332:ASN:O	1:A:335:PRO:HD3	2.19	0.43
1:A:99:ILE:HG23	1:A:100:PRO:HA	2.01	0.42
1:A:83:SER:HB3	1:A:101:THR:O	2.19	0.42
1:A:143:ARG:HB3	1:A:144:PRO:HD3	2.01	0.42
1:A:319:LEU:C	1:A:321:PRO:HD3	2.40	0.42
1:A:377:ARG:HH21	1:A:414:VAL:HG12	1.85	0.41
1:A:319:LEU:O	1:A:321:PRO:HD3	2.21	0.41
1:A:110:GLN:CD	1:A:229:ASN:H	2.24	0.41
1:A:218:ASP:O	1:A:222:ILE:HG12	2.21	0.41
1:A:276:GLU:C	1:A:278:PRO:HD3	2.41	0.41
1:A:91:GLU:H	1:A:91:GLU:CD	2.24	0.41
1:A:50:VAL:HA	1:A:51:PRO:HD3	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/414 (97%)	387 (96%)	16 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/358 (98%)	339 (97%)	10 (3%)	48	50

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	49	ASN
1	A	108	GLN
1	A	128	GLU
1	A	187	PRO
1	A	211	ARG
1	A	261	MET
1	A	276	GLU
1	A	293	SER
1	A	380	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	39	GLN
1	A	46	GLN
1	A	49	ASN
1	A	59	ASN
1	A	69	GLN
1	A	108	GLN
1	A	110	GLN

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Mol	Chain	Res	Type
1	A	149	ASN
1	A	225	ASN
1	A	227	GLN
1	A	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	HEM	A	417	1	28,50,50	2.91	13 (46%)	17,82,82	3.06	8 (47%)
3	ADO	A	422	-	13,13,13	2.52	8 (61%)	20,20,20	1.08	1 (5%)

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	417	1	-	0/6/54/54	0/0/8/8
3	ADO	A	422	-	-	0/0/28/28	0/0/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	417	HEM	C3B-C2B	-7.14	1.30	1.40
2	A	417	HEM	C4C-NC	-5.24	1.30	1.36
2	A	417	HEM	C3C-C2C	-3.67	1.35	1.40
2	A	417	HEM	C4A-NA	-2.39	1.31	1.36
2	A	417	HEM	C1D-CHD	-2.32	1.34	1.40
2	A	417	HEM	C3D-C2D	-2.01	1.31	1.37
3	A	422	ADO	C1-C2	2.10	1.56	1.51
3	A	422	ADO	C6-C7	2.23	1.58	1.52
3	A	422	ADO	C9-C5	2.34	1.58	1.52
3	A	422	ADO	C3-C2	2.63	1.58	1.51
2	A	417	HEM	C4D-ND	2.86	1.40	1.36
2	A	417	HEM	C3B-CAB	2.87	1.53	1.47
3	A	422	ADO	C10-C7	3.03	1.60	1.52
3	A	422	ADO	C6-C5	3.38	1.61	1.52
2	A	417	HEM	C3C-CAC	3.48	1.54	1.47
3	A	422	ADO	C4-C3	3.56	1.61	1.53
2	A	417	HEM	CMB-C2B	4.04	1.60	1.51
2	A	417	HEM	CMD-C2D	4.36	1.60	1.51
2	A	417	HEM	C1D-ND	4.46	1.45	1.36
3	A	422	ADO	C8-C1	4.70	1.64	1.53
2	A	417	HEM	C1B-NB	5.76	1.43	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	417	HEM	CMA-C3A-C4A	-6.39	118.64	128.46
2	A	417	HEM	CMD-C2D-C1D	-3.53	123.03	128.46
2	A	417	HEM	C4A-C3A-C2A	-2.69	105.13	107.00
2	A	417	HEM	C3B-C4B-NB	2.10	111.93	109.21
2	A	417	HEM	CMC-C2C-C3C	2.16	128.89	124.89
3	A	422	ADO	O2-C2-C1	2.16	127.01	123.50
2	A	417	HEM	CBD-CAD-C3D	4.70	121.42	112.47
2	A	417	HEM	C1D-C2D-C3D	4.87	110.39	107.00
2	A	417	HEM	CMA-C3A-C2A	5.98	136.21	124.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.