



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1DZ6 / pdb_00001dz6
Title : ferrous 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

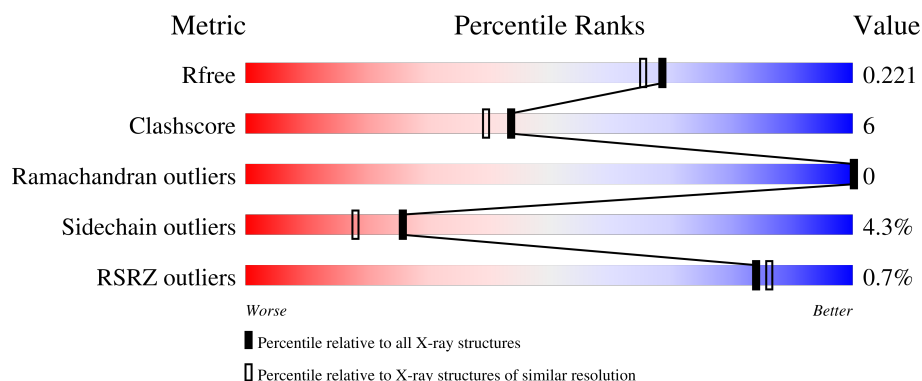
1 Overall quality at a glance

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	
1	B	414	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TRS	A	503	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7197 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.

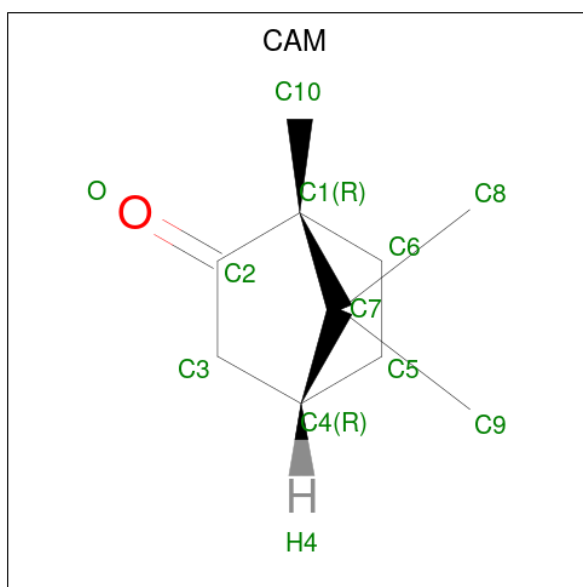
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3200	2029	559	594	18			
1	B	405	Total	C	N	O	S	0	1	0
			3211	2035	561	597	18			

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



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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



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

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

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

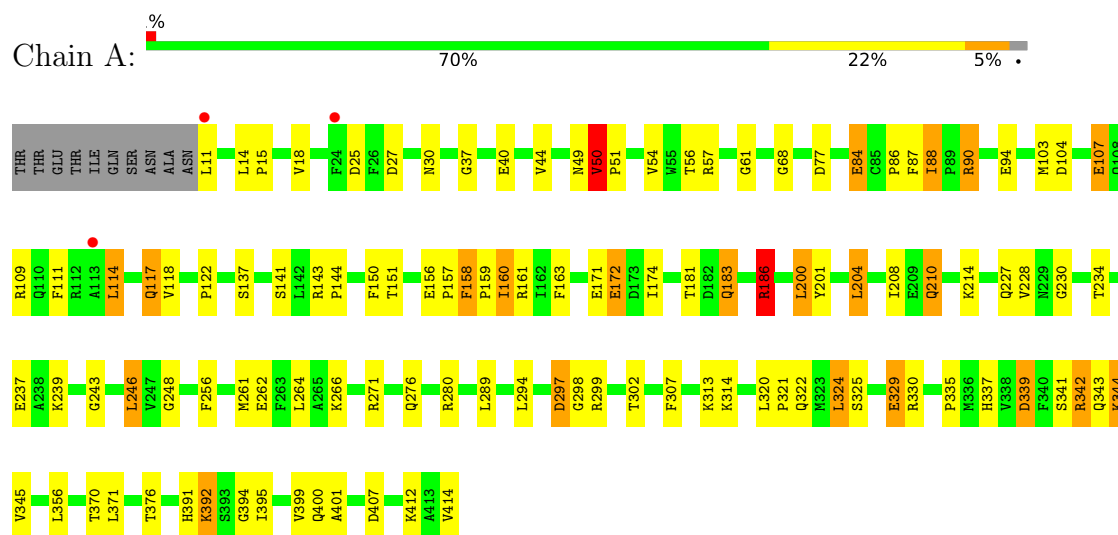
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	289	Total 289	O 289	0	0
6	B	378	Total 378	O 378	0	0

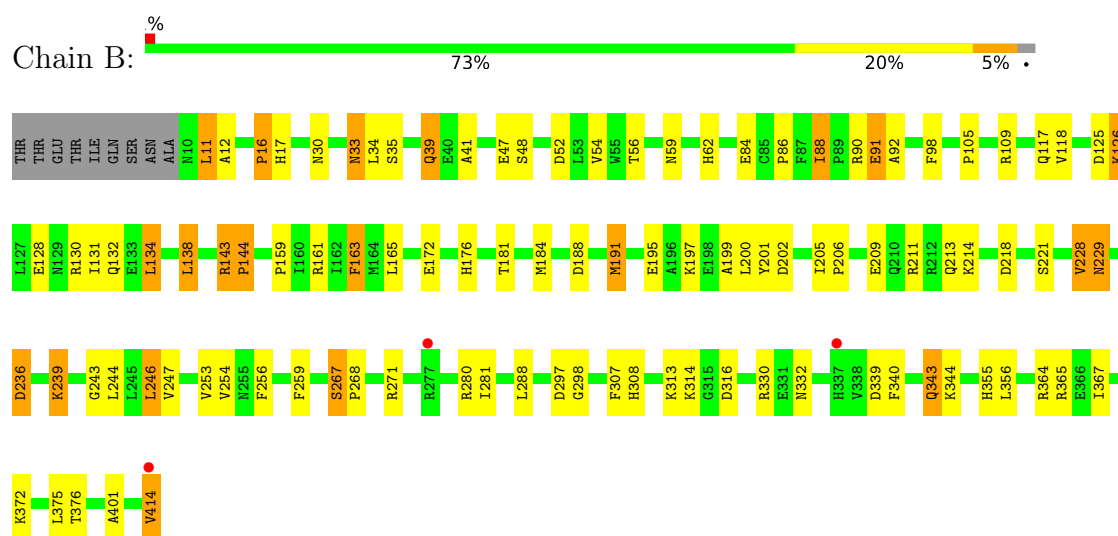
3 Residue-property plots [i](#)

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	67.80Å 62.80Å 95.50Å 90.00° 90.60° 90.00°	Depositor
Resolution (Å)	19.00 – 1.90 19.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.00-1.90) 97.5 (19.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.188 , 0.268 (Not available) , 0.221	Depositor DCC
R_{free} test set	4155 reflections (6.70%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 64.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7197	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 4.60% 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, CAM, HEM, TRS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.84	0/3279	1.95	86/4454 (1.9%)
1	B	0.94	1/3294 (0.0%)	1.95	89/4475 (2.0%)
All	All	0.89	1/6573 (0.0%)	1.95	175/8929 (2.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	86	PRO	N-CA	-5.02	1.41	1.47

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	VAL	CA-C-O	10.98	126.33	119.19
1	B	48	SER	N-CA-C	10.74	122.99	111.28
1	A	297	ASP	CA-CB-CG	10.43	123.03	112.60
1	B	105	PRO	O-C-N	10.40	126.09	121.31
1	B	343	GLN	N-CA-C	9.46	121.19	111.07
1	A	172	GLU	CB-CA-C	9.34	127.00	110.37
1	A	307	PHE	CA-CB-CG	9.13	122.94	113.80
1	A	114	LEU	N-CA-C	-8.83	100.83	111.69
1	A	172	GLU	CB-CG-CD	8.79	127.54	112.60
1	B	229	ASN	CA-CB-CG	-8.73	103.87	112.60
1	B	105	PRO	CA-C-O	-8.56	114.73	120.90
1	A	163	PHE	CA-CB-CG	-8.23	105.57	113.80
1	B	259	PHE	CA-C-N	8.12	131.00	120.44
1	B	259	PHE	C-N-CA	8.12	131.00	120.44
1	A	104	ASP	CA-CB-CG	8.12	120.72	112.60
1	A	407	ASP	CA-C-O	7.93	124.45	119.29
1	A	27	ASP	CA-CB-CG	7.70	120.30	112.60
1	A	84	GLU	CA-C-O	-7.61	112.41	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	GLY	CA-C-O	-7.42	115.18	121.04
1	B	246	LEU	CA-C-O	-7.38	112.73	120.55
1	B	308	HIS	CA-CB-CG	-7.33	106.47	113.80
1	B	90	ARG	CD-NE-CZ	7.32	134.65	124.40
1	A	171	GLU	CA-C-N	-7.29	110.03	122.56
1	A	171	GLU	C-N-CA	-7.29	110.03	122.56
1	B	92	ALA	CA-C-N	7.26	128.16	120.03
1	B	92	ALA	C-N-CA	7.26	128.16	120.03
1	A	325	SER	CA-C-O	-7.25	112.87	120.55
1	B	109	ARG	N-CA-C	7.25	119.18	111.28
1	B	176	HIS	CA-CB-CG	7.14	120.94	113.80
1	A	210	GLN	CB-CG-CD	7.06	124.61	112.60
1	A	280	ARG	CA-C-N	-7.04	115.80	120.24
1	A	280	ARG	C-N-CA	-7.04	115.80	120.24
1	A	18	VAL	N-CA-C	7.04	114.86	107.76
1	B	35	SER	O-C-N	-7.00	113.23	122.33
1	B	16	PRO	O-C-N	-6.94	114.26	122.24
1	A	77	ASP	CA-CB-CG	6.93	119.53	112.60
1	B	200	LEU	CA-C-N	6.91	129.54	120.28
1	B	200	LEU	C-N-CA	6.91	129.54	120.28
1	B	236	ASP	CA-CB-CG	6.89	119.50	112.60
1	B	271	ARG	CD-NE-CZ	6.85	133.99	124.40
1	B	34	LEU	N-CA-C	6.74	119.49	111.33
1	B	307	PHE	CA-CB-CG	6.62	120.42	113.80
1	B	267	SER	CA-C-N	6.58	125.81	118.97
1	B	267	SER	C-N-CA	6.58	125.81	118.97
1	A	248	GLY	N-CA-C	-6.57	104.87	112.50
1	A	395	ILE	CA-C-N	-6.57	114.53	123.14
1	A	395	ILE	C-N-CA	-6.57	114.53	123.14
1	A	186	ARG	NE-CZ-NH1	-6.57	114.93	121.50
1	B	117	GLN	CB-CG-CD	6.56	123.75	112.60
1	B	163	PHE	CA-CB-CG	-6.55	107.25	113.80
1	A	401	ALA	CA-C-N	-6.51	114.41	122.42
1	A	401	ALA	C-N-CA	-6.51	114.41	122.42
1	A	345	VAL	CA-C-N	-6.50	113.75	122.72
1	A	345	VAL	C-N-CA	-6.50	113.75	122.72
1	B	340	PHE	CA-CB-CG	6.47	120.27	113.80
1	B	90	ARG	NE-CZ-NH2	-6.39	113.44	119.20
1	B	228	VAL	N-CA-CB	6.37	119.92	111.90
1	A	183	GLN	CA-CB-CG	6.34	126.77	114.10
1	B	17	HIS	N-CA-C	6.33	120.74	112.89
1	B	105	PRO	N-CA-C	-6.31	104.41	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	PHE	CA-C-N	6.30	128.81	123.33
1	A	87	PHE	C-N-CA	6.30	128.81	123.33
1	A	344	LYS	N-CA-CB	6.27	121.03	110.69
1	A	90	ARG	CD-NE-CZ	6.26	133.17	124.40
1	A	161	ARG	CA-C-O	-6.21	112.82	119.97
1	B	256	PHE	CA-CB-CG	-6.17	107.63	113.80
1	A	14	LEU	CA-C-N	6.16	124.16	119.66
1	A	14	LEU	C-N-CA	6.16	124.16	119.66
1	B	218	ASP	CA-CB-CG	-6.12	106.48	112.60
1	B	59	ASN	CA-CB-CG	-6.12	106.48	112.60
1	A	88	ILE	N-CA-C	-6.11	100.34	107.61
1	A	204	LEU	N-CA-C	6.09	118.89	111.82
1	A	394	GLY	O-C-N	6.05	128.82	123.80
1	A	158	PHE	CA-C-N	6.04	125.43	118.85
1	A	158	PHE	C-N-CA	6.04	125.43	118.85
1	B	52	ASP	CA-CB-CG	6.02	118.62	112.60
1	B	339	ASP	CA-C-O	6.01	127.82	120.25
1	A	256	PHE	CA-CB-CG	-5.99	107.81	113.80
1	A	322	GLN	CA-C-N	5.97	128.28	120.28
1	A	322	GLN	C-N-CA	5.97	128.28	120.28
1	B	256	PHE	CA-C-O	5.96	127.28	120.90
1	B	401	ALA	CA-C-O	-5.95	113.41	120.43
1	A	122	PRO	CA-C-N	5.94	128.86	120.42
1	A	122	PRO	C-N-CA	5.94	128.86	120.42
1	A	109	ARG	NE-CZ-NH2	5.93	124.54	119.20
1	B	243	GLY	N-CA-C	-5.92	105.63	112.50
1	B	211	ARG	CA-CB-CG	-5.91	102.27	114.10
1	B	131	ILE	CA-C-O	5.91	127.61	121.05
1	B	62	HIS	CA-C-N	5.90	130.21	120.94
1	B	62	HIS	C-N-CA	5.90	130.21	120.94
1	A	88	ILE	CA-C-O	-5.89	115.86	119.51
1	A	174	ILE	N-CA-CB	5.89	115.04	110.45
1	A	109	ARG	CA-C-O	-5.82	114.34	120.63
1	B	298	GLY	CA-C-O	5.81	127.59	121.08
1	A	370	THR	O-C-N	-5.80	116.10	122.07
1	A	54	VAL	CB-CA-C	-5.79	103.83	111.70
1	A	392	LYS	CA-C-O	-5.79	114.34	121.11
1	B	35	SER	CA-C-O	5.78	126.43	119.61
1	A	160	ILE	N-CA-C	5.76	115.95	110.53
1	A	109	ARG	CD-NE-CZ	-5.75	116.35	124.40
1	B	297	ASP	N-CA-CB	5.75	120.20	110.49
1	B	143	ARG	CA-C-N	5.69	125.37	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	ARG	C-N-CA	5.69	125.37	119.56
1	A	181	THR	N-CA-CB	5.67	118.45	110.12
1	B	288	LEU	CA-C-O	5.65	126.46	119.97
1	B	297	ASP	CA-CB-CG	5.60	118.20	112.60
1	A	320	LEU	N-CA-CB	-5.59	102.03	111.30
1	A	107	GLU	CA-C-N	5.57	128.01	120.38
1	A	107	GLU	C-N-CA	5.57	128.01	120.38
1	A	343	GLN	CA-C-O	-5.57	114.52	120.42
1	B	11	LEU	O-C-N	-5.54	117.00	123.27
1	A	401	ALA	CA-C-O	-5.54	114.80	120.89
1	A	68	GLY	CA-C-O	5.52	126.36	120.40
1	B	364	ARG	CA-C-O	-5.51	114.57	120.42
1	A	271	ARG	N-CA-C	-5.51	105.19	111.14
1	B	84	GLU	CA-C-O	-5.49	114.73	120.55
1	A	407	ASP	CA-C-N	5.48	125.83	119.47
1	A	407	ASP	C-N-CA	5.48	125.83	119.47
1	A	44	VAL	CB-CA-C	-5.46	103.70	112.16
1	B	144	PRO	N-CA-C	5.45	120.93	113.84
1	B	280	ARG	NE-CZ-NH1	5.45	126.95	121.50
1	B	91	GLU	CB-CG-CD	5.45	121.86	112.60
1	A	299	ARG	CG-CD-NE	5.45	123.98	112.00
1	B	88	ILE	CA-CB-CG1	5.44	119.65	110.40
1	A	163	PHE	O-C-N	-5.43	116.48	122.07
1	B	202	ASP	O-C-N	-5.42	116.37	122.12
1	B	125	ASP	CA-C-N	5.42	127.54	120.28
1	B	125	ASP	C-N-CA	5.42	127.54	120.28
1	A	117	GLN	CA-CB-CG	5.41	124.91	114.10
1	B	132	GLN	CA-C-O	5.38	126.65	120.90
1	A	88	ILE	CB-CA-C	5.37	115.34	110.13
1	A	243	GLY	CA-C-O	5.35	126.26	120.75
1	B	161	ARG	CD-NE-CZ	-5.35	116.91	124.40
1	B	188	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	30	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	B	239	LYS	CA-C-O	5.31	126.17	120.70
1	B	316	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	107	GLU	N-CA-C	5.30	117.47	111.11
1	A	399	VAL	O-C-N	-5.29	117.55	123.26
1	B	144	PRO	CB-CA-C	-5.29	104.34	111.85
1	B	253	VAL	CA-C-O	5.28	126.44	120.95
1	B	191	MET	CA-C-O	-5.28	114.94	121.06
1	A	298	GLY	O-C-N	-5.28	117.62	123.58
1	B	267	SER	CA-C-O	5.25	127.36	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	VAL	CA-C-O	-5.25	116.16	121.67
1	A	50	VAL	N-CA-C	5.23	114.22	108.05
1	B	30	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	B	330	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	B	48	SER	CA-C-N	-5.19	114.37	122.73
1	B	48	SER	C-N-CA	-5.19	114.37	122.73
1	B	367	ILE	O-C-N	5.19	127.30	121.90
1	A	25	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	197	LYS	CA-C-N	5.14	127.16	120.28
1	B	197	LYS	C-N-CA	5.14	127.16	120.28
1	B	88	ILE	CB-CG1-CD1	5.13	124.57	113.80
1	B	221	SER	CA-C-O	5.13	125.98	120.55
1	B	105	PRO	N-CA-CB	5.12	106.06	103.19
1	A	114	LEU	N-CA-CB	5.10	117.80	110.20
1	B	12	ALA	N-CA-C	-5.09	102.81	110.24
1	A	15	PRO	N-CA-C	5.09	115.36	110.47
1	B	199	ALA	CA-C-O	-5.08	115.48	120.82
1	A	330	ARG	CD-NE-CZ	5.08	131.51	124.40
1	A	342	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	B	109	ARG	CA-C-O	-5.07	115.17	120.55
1	A	391	HIS	CA-CB-CG	5.07	118.87	113.80
1	B	375	LEU	CA-C-N	5.07	127.49	120.29
1	B	375	LEU	C-N-CA	5.07	127.49	120.29
1	B	56	THR	N-CA-CB	5.07	118.85	110.69
1	B	17	HIS	CA-CB-CG	5.06	118.86	113.80
1	A	339	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	230	GLY	CA-C-O	-5.05	113.69	119.04
1	B	47	GLU	O-C-N	-5.04	117.04	122.79
1	A	90	ARG	NE-CZ-NH2	-5.04	114.67	119.20
1	A	289	LEU	O-C-N	-5.03	116.34	122.22
1	B	332	ASN	N-CA-C	5.02	116.60	108.26

There are no chirality outliers.

There are no planarity outliers.

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	3200	0	3152	44	0
1	B	3211	0	3161	33	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
3	A	11	0	16	0	0
3	B	11	0	16	0	0
4	A	8	0	12	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
6	A	289	0	0	4	0
6	B	378	0	0	2	0
All	All	7197	0	6417	79	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 6.

All (79) 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:B:236:ASP:HB3	6:B:899:HOH:O	1.74	0.87
1:A:376:THR:HG22	1:A:414:VAL:HG21	1.57	0.87
1:B:130:ARG:HD2	1:B:165:LEU:HD21	1.61	0.83
1:A:392:LYS:HD3	1:A:400:GLN:HG2	1.62	0.81
1:B:134:LEU:HD22	1:B:138:LEU:HD22	1.66	0.77
1:A:210:GLN:HE22	1:A:214:LYS:HE3	1.50	0.76
1:A:90:ARG:O	1:A:94:GLU:HG3	1.87	0.74
1:B:128:GLU:HG3	1:B:365:ARG:HH12	1.54	0.72
2:B:501:HEM:HMB2	2:B:501:HEM:HBB2	1.73	0.69
1:A:276:GLN:HE21	1:B:172:GLU:N	1.94	0.65
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.80	0.63
1:A:11:LEU:HD21	1:A:57:ARG:HH21	1.64	0.63
1:A:56:THR:O	1:A:61:GLY:HA2	1.99	0.63
1:B:159:PRO:HG2	1:B:254:VAL:HG22	1.79	0.62
1:A:276:GLN:HE21	1:B:172:GLU:H	1.49	0.61
1:B:376:THR:HG21	1:B:414:VAL:HG11	1.84	0.59
1:A:200:LEU:HD21	1:A:246:LEU:HD13	1.85	0.59
1:A:151:THR:HG22	6:A:732:HOH:O	2.04	0.58
1:B:372:LYS:NZ	1:B:372:LYS:HB3	2.22	0.55
1:A:114:LEU:HD13	1:A:227:GLN:O	2.06	0.55
1:B:163:PHE:HE2	1:B:246:LEU:HD23	1.72	0.54
1:B:281:ILE:HD12	1:B:372:LYS:HG2	1.88	0.54
1:A:329:GLU:HG3	1:A:335:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.37	0.53
1:A:302:THR:O	1:A:314:LYS:HD2	2.11	0.51
1:B:33:ASN:HB3	1:B:41:ALA:HA	1.93	0.51
1:B:128:GLU:CG	1:B:365:ARG:HH12	2.22	0.50
1:A:376:THR:CG2	1:A:414:VAL:HG21	2.34	0.50
1:B:91:GLU:HB3	6:B:642:HOH:O	2.10	0.50
1:B:201:TYR:CD2	1:B:239:LYS:HE3	2.47	0.49
1:A:412:LYS:HE2	1:A:414:VAL:HG22	1.94	0.49
1:B:134:LEU:HD22	1:B:138:LEU:CD2	2.37	0.49
1:A:356:LEU:HB2	6:A:792:HOH:O	2.13	0.48
2:A:501:HEM:HBB2	2:A:501:HEM:CMB	2.43	0.48
1:B:228:VAL:O	1:B:229:ASN:C	2.56	0.48
1:A:412:LYS:HE2	1:A:414:VAL:CG2	2.44	0.47
1:A:294:LEU:HD23	1:A:294:LEU:H	1.80	0.47
1:B:191:MET:HE2	1:B:195:GLU:HB3	1.95	0.47
1:A:262:GLU:O	1:A:266:LYS:HG3	2.15	0.46
1:A:151:THR:HG23	6:A:725:HOH:O	2.14	0.46
1:A:204:LEU:HD11	1:A:246:LEU:CD1	2.46	0.46
1:B:98:PHE:HB3	1:B:244:LEU:HB2	1.98	0.46
1:A:297:ASP:OD2	2:A:501:HEM:O2A	2.34	0.45
1:A:321:PRO:HB2	1:A:324:LEU:HD22	1.97	0.45
1:A:103:MET:HE1	1:A:111:PHE:CE2	2.50	0.45
1:B:143:ARG:HB3	1:B:144:PRO:CD	2.47	0.45
1:B:355:HIS:O	1:B:356:LEU:C	2.59	0.45
1:A:210:GLN:NE2	1:A:214:LYS:HE3	2.26	0.44
1:B:209:GLU:OE2	1:B:213:GLN:NE2	2.50	0.44
1:A:50:VAL:HA	1:A:51:PRO:HD3	1.94	0.44
1:A:158:PHE:HB3	1:A:159:PRO:HD3	2.00	0.44
1:A:264:LEU:HD11	1:A:371:LEU:HD22	2.00	0.44
1:A:186:ARG:HD2	1:A:392:LYS:HG3	1.99	0.44
1:A:294:LEU:HD23	1:A:294:LEU:N	2.33	0.43
1:B:126:LYS:HD3	1:B:130:ARG:HH22	1.83	0.43
1:B:344:LYS:HD3	1:B:344:LYS:HA	1.79	0.43
1:A:107:GLU:HB2	6:A:738:HOH:O	2.17	0.43
1:B:39:GLN:NE2	1:B:39:GLN:H	2.15	0.43
1:B:143:ARG:N	1:B:144:PRO:HD2	2.34	0.43
1:A:37:GLY:HA3	1:A:40:GLU:OE1	2.18	0.43
1:A:201:TYR:HB3	1:A:239:LYS:HD2	2.00	0.43
1:A:329:GLU:HG3	1:A:335:PRO:CD	2.49	0.42
1:A:341:SER:O	1:A:342:ARG:C	2.60	0.42
1:B:267:SER:HA	1:B:268:PRO:HD2	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLU:O	1:A:160:ILE:HG13	2.18	0.42
1:A:321:PRO:HG2	1:A:324:LEU:HD22	2.01	0.42
1:B:205:ILE:N	1:B:206:PRO:HD2	2.35	0.42
1:A:313:LYS:O	1:A:314:LYS:C	2.63	0.41
1:A:234:THR:OG1	1:A:237:GLU:HG3	2.20	0.41
1:A:337:HIS:CE1	1:A:339:ASP:HB2	2.55	0.41
1:A:204:LEU:O	1:A:208:ILE:HG13	2.21	0.41
1:B:163:PHE:CE2	1:B:246:LEU:HD23	2.53	0.41
1:B:181[B]:THR:HG23	1:B:247:VAL:HG13	2.02	0.41
1:A:156:GLU:HB2	1:A:157:PRO:HD3	2.03	0.41
1:A:150:PHE:CZ	1:A:261:MET:HG3	2.56	0.41
1:B:372:LYS:HB3	1:B:372:LYS:HZ3	1.85	0.40
1:A:143:ARG:HB3	1:A:144:PRO:HD3	2.03	0.40
1:B:313:LYS:O	1:B:314:LYS:C	2.63	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	402/414 (97%)	386 (96%)	16 (4%)	0	100	100
1	B	404/414 (98%)	393 (97%)	11 (3%)	0	100	100
All	All	806/828 (97%)	779 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	349/358 (98%)	331 (95%)	18 (5%)	21	13
1	B	351/358 (98%)	339 (97%)	12 (3%)	32	25
All	All	700/716 (98%)	670 (96%)	30 (4%)	26	18

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	50	VAL
1	A	84	GLU
1	A	86	PRO
1	A	88	ILE
1	A	117	GLN
1	A	118	VAL
1	A	137	SER
1	A	141	SER
1	A	172	GLU
1	A	183	GLN
1	A	186	ARG
1	A	200	LEU
1	A	228	VAL
1	A	246	LEU
1	A	324	LEU
1	A	329	GLU
1	A	344	LYS
1	B	11	LEU
1	B	16	PRO
1	B	33	ASN
1	B	39	GLN
1	B	88	ILE
1	B	118	VAL
1	B	126	LYS
1	B	134	LEU
1	B	138	LEU
1	B	214	LYS
1	B	343	GLN
1	B	414	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	46	GLN
1	A	49	ASN
1	A	210	GLN
1	A	225	ASN
1	A	272	GLN
1	A	276	GLN
1	A	311	GLN
1	A	337	HIS
1	A	388	GLN
1	B	30	ASN
1	B	33	ASN
1	B	39	GLN
1	B	46	GLN
1	B	69	GLN
1	B	117	GLN
1	B	132	GLN
1	B	145	GLN
1	B	147	GLN
1	B	210	GLN
1	B	225	ASN
1	B	272	GLN
1	B	276	GLN
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 8 ligands modelled in this entry, 3 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	$\# Z > 2$
2	HEM	B	501	1	50,50,50	1.42	12 (24%)	67,82,82	1.19	4 (5%)
3	CAM	B	502	-	12,12,12	0.97	1 (8%)	20,21,21	2.37	7 (35%)
2	HEM	A	501	1	50,50,50	1.42	9 (18%)	67,82,82	1.29	10 (14%)
3	CAM	A	502	-	12,12,12	0.95	1 (8%)	20,21,21	2.85	10 (50%)
4	TRS	A	503	-	7,7,7	2.02	3 (42%)	9,9,9	2.66	4 (44%)

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

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	TRS	O3-C3	3.32	1.52	1.42
2	A	501	HEM	FE-NC	3.29	2.06	1.95
2	A	501	HEM	CAB-C3B	3.06	1.55	1.47
2	B	501	HEM	CAC-C3C	2.97	1.55	1.47
4	A	503	TRS	O1-C1	2.97	1.51	1.42
2	A	501	HEM	FE-NB	2.94	2.04	1.94
2	B	501	HEM	FE-NC	2.85	2.04	1.95
2	B	501	HEM	FE-NA	2.65	2.03	1.95
3	A	502	CAM	C1-C2	2.65	1.56	1.52
2	B	501	HEM	CAA-C2A	2.64	1.58	1.51
4	A	503	TRS	O2-C2	2.56	1.50	1.42
2	B	501	HEM	CAB-C3B	2.48	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	CMA-C3A	2.40	1.55	1.50
3	B	502	CAM	C1-C2	2.39	1.56	1.52
2	A	501	HEM	FE-ND	2.35	2.02	1.94
2	B	501	HEM	CMD-C2D	2.31	1.55	1.50
2	A	501	HEM	CAC-C3C	2.26	1.53	1.47
2	A	501	HEM	C3C-C2C	-2.24	1.32	1.37
2	A	501	HEM	CMC-C2C	2.24	1.55	1.50
2	B	501	HEM	FE-NB	2.21	2.01	1.94
2	A	501	HEM	CMD-C2D	2.17	1.55	1.50
2	A	501	HEM	FE-NA	2.17	2.02	1.95
2	B	501	HEM	C1A-C2A	2.14	1.48	1.44
2	B	501	HEM	FE-ND	2.12	2.01	1.94
2	B	501	HEM	C2A-C3A	-2.11	1.33	1.38
2	B	501	HEM	CMB-C2B	2.02	1.54	1.50

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	CAM	O-C2-C3	6.31	139.39	126.39
3	B	502	CAM	C5-C4-C3	-5.29	92.06	106.39
3	A	502	CAM	C5-C4-C3	-4.91	93.09	106.39
3	B	502	CAM	C3-C2-C1	-4.81	95.96	107.43
3	A	502	CAM	C7-C1-C2	4.75	108.44	100.33
3	A	502	CAM	C3-C2-C1	-4.62	96.42	107.43
4	A	503	TRS	C3-C-N	4.46	119.54	108.17
4	A	503	TRS	C3-C-C2	-4.45	98.81	110.66
2	A	501	HEM	CBD-CAD-C3D	4.41	124.74	112.53
2	B	501	HEM	CBD-CAD-C3D	4.00	123.59	112.53
3	A	502	CAM	C4-C3-C2	3.92	108.94	102.05
2	B	501	HEM	CMA-C3A-C4A	-3.70	119.78	125.42
3	B	502	CAM	O-C2-C3	3.62	133.85	126.39
3	B	502	CAM	C4-C3-C2	3.43	108.07	102.05
3	A	502	CAM	C9-C7-C4	-3.37	105.29	113.44
4	A	503	TRS	C2-C-C1	-3.12	102.34	110.66
4	A	503	TRS	C3-C-C1	2.81	118.14	110.66
2	B	501	HEM	CMA-C3A-C2A	2.74	131.44	125.62
3	B	502	CAM	C6-C1-C7	2.72	107.27	101.52
2	A	501	HEM	CAA-CBA-CGA	2.72	120.88	113.67
3	B	502	CAM	C7-C1-C2	2.70	104.93	100.33
2	A	501	HEM	O1D-CGD-CBD	-2.61	114.81	123.09
3	B	502	CAM	C9-C7-C8	2.61	114.28	107.67
2	A	501	HEM	CMA-C3A-C4A	-2.50	121.61	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CBA-CAA-C2A	2.44	119.27	112.53
2	A	501	HEM	CHC-C1C-NC	2.31	126.97	124.45
3	A	502	CAM	C6-C1-C7	2.27	106.32	101.52
3	A	502	CAM	C5-C6-C1	-2.25	100.19	104.73
2	A	501	HEM	O1A-CGA-CBA	-2.18	116.17	123.09
2	A	501	HEM	CHD-C4C-NC	2.10	126.75	124.45
2	A	501	HEM	CHB-C4A-NA	2.06	127.60	123.86
3	A	502	CAM	O-C2-C1	-2.05	122.87	125.33
2	A	501	HEM	CMA-C3A-C2A	2.04	129.96	125.62
3	A	502	CAM	C8-C7-C1	2.04	117.59	113.05
2	B	501	HEM	CMD-C2D-C1D	-2.01	121.90	125.03

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	TRS	C1-C-C3-O3
4	A	503	TRS	N-C-C3-O3
4	A	503	TRS	C2-C-C3-O3
2	B	501	HEM	C2C-C3C-CAC-CBC
2	B	501	HEM	C4C-C3C-CAC-CBC
4	A	503	TRS	C1-C-C2-O2
2	A	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAD-CBD-CGD-O2D

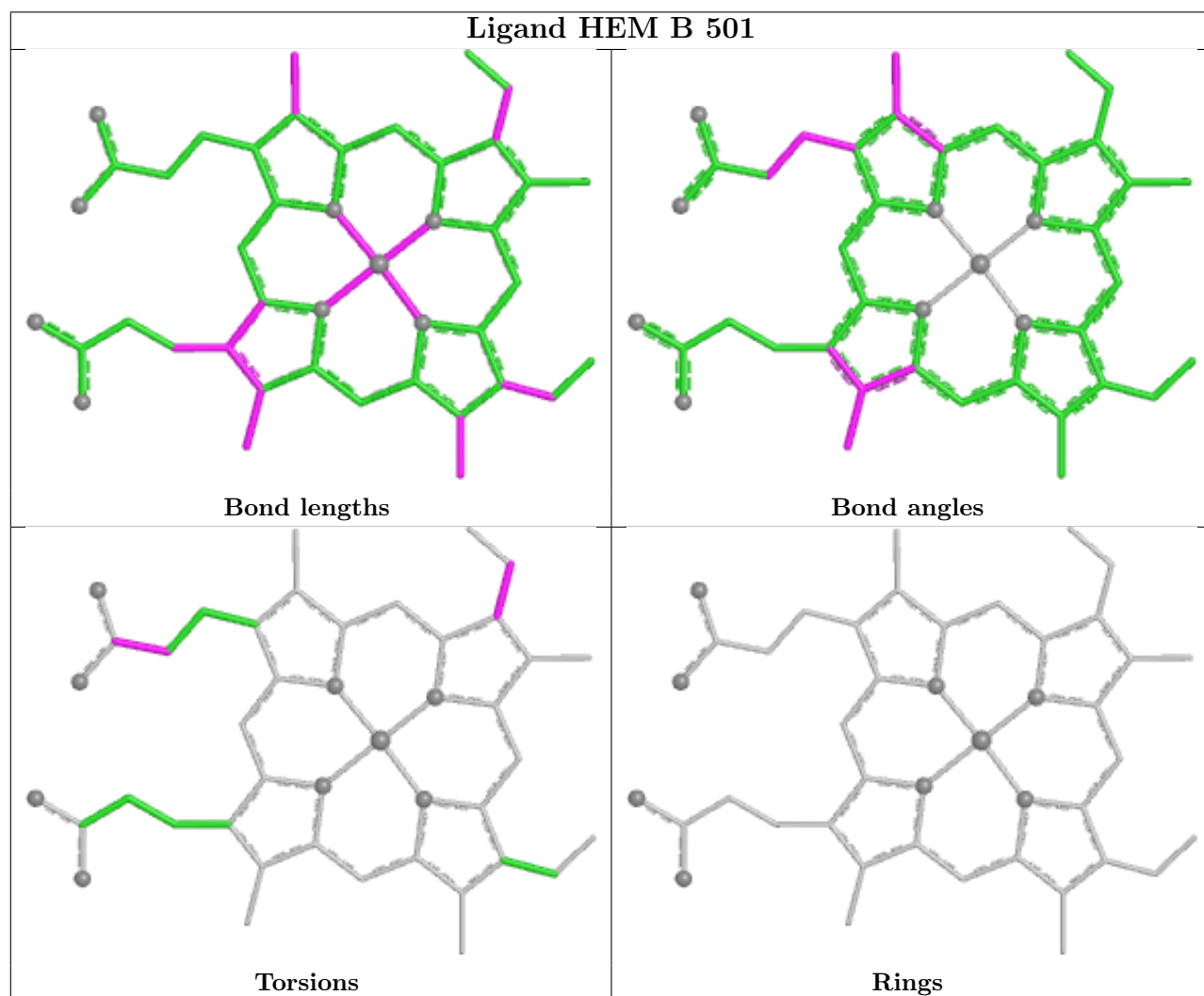
There are no ring outliers.

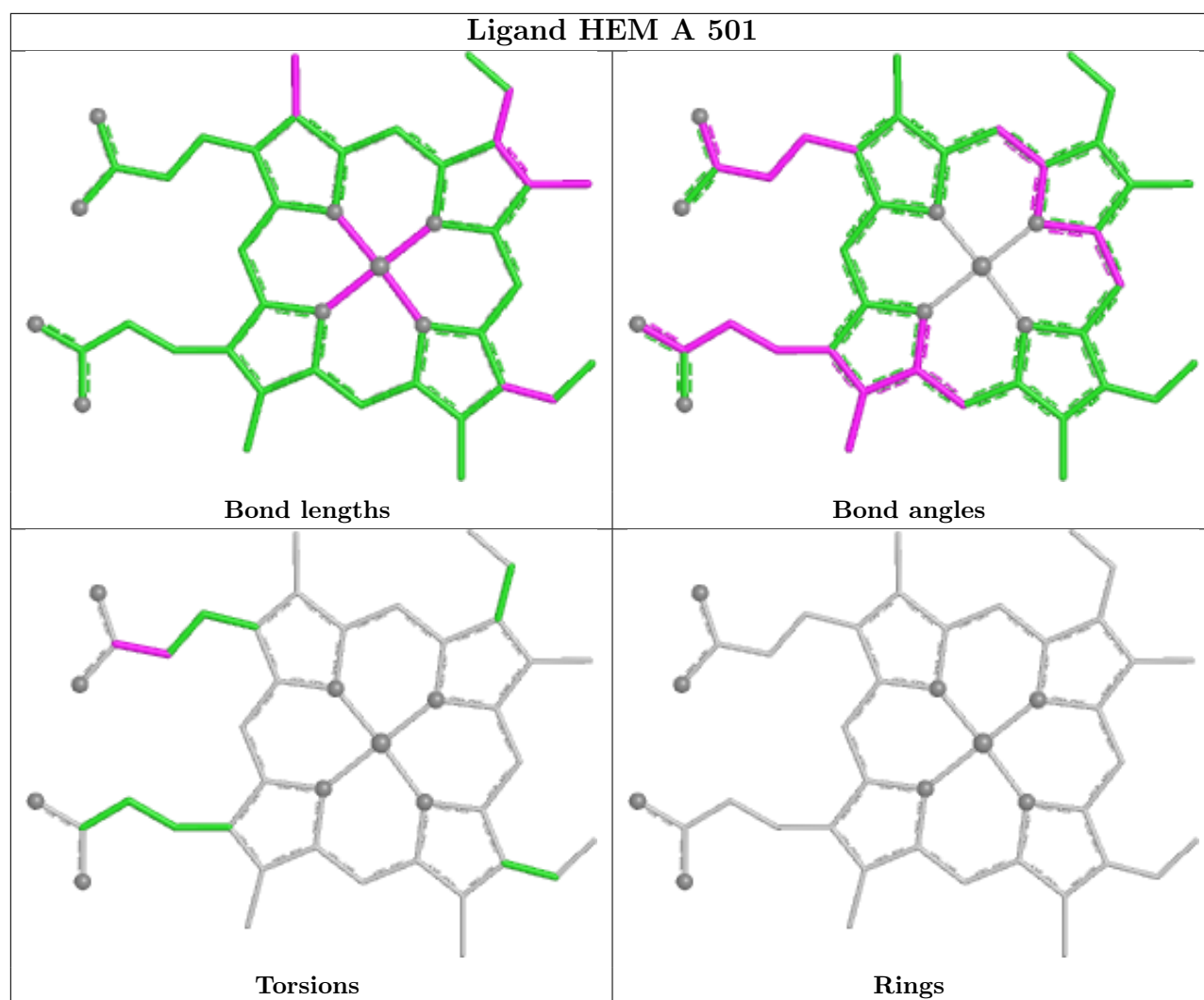
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	2	0
2	A	501	HEM	3	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%)	-0.15	3 (0%) 84 86	11, 23, 46, 64	0
1	B	405/414 (97%)	-0.43	3 (0%) 84 86	9, 18, 37, 69	1 (0%)
All	All	809/828 (97%)	-0.29	6 (0%) 84 86	9, 20, 43, 69	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	HIS	2.6
1	A	11	LEU	2.3
1	B	277	ARG	2.3
1	A	24	PHE	2.2
1	B	414	VAL	2.1
1	A	113	ALA	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](#)

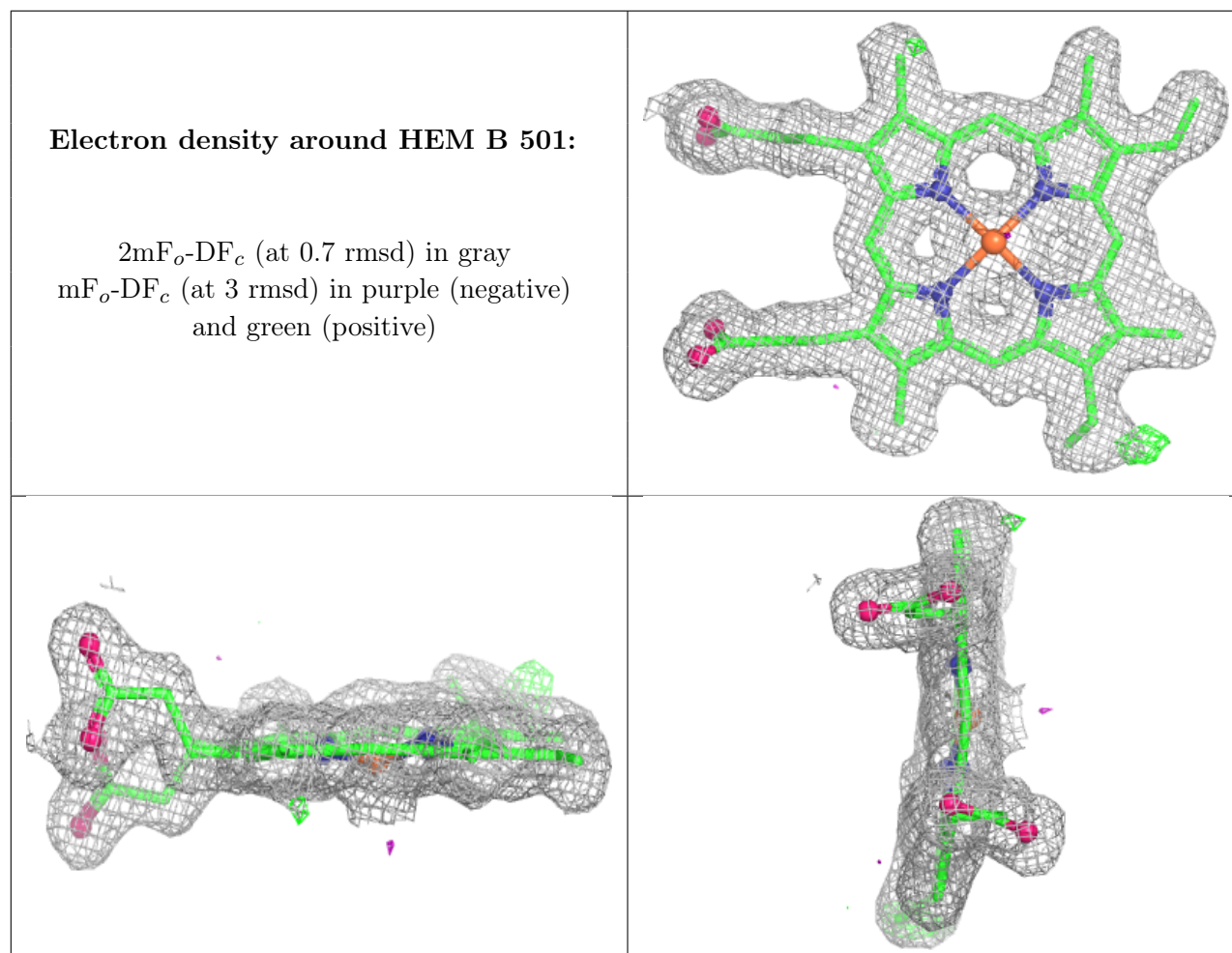
There are no oligosaccharides in this entry.

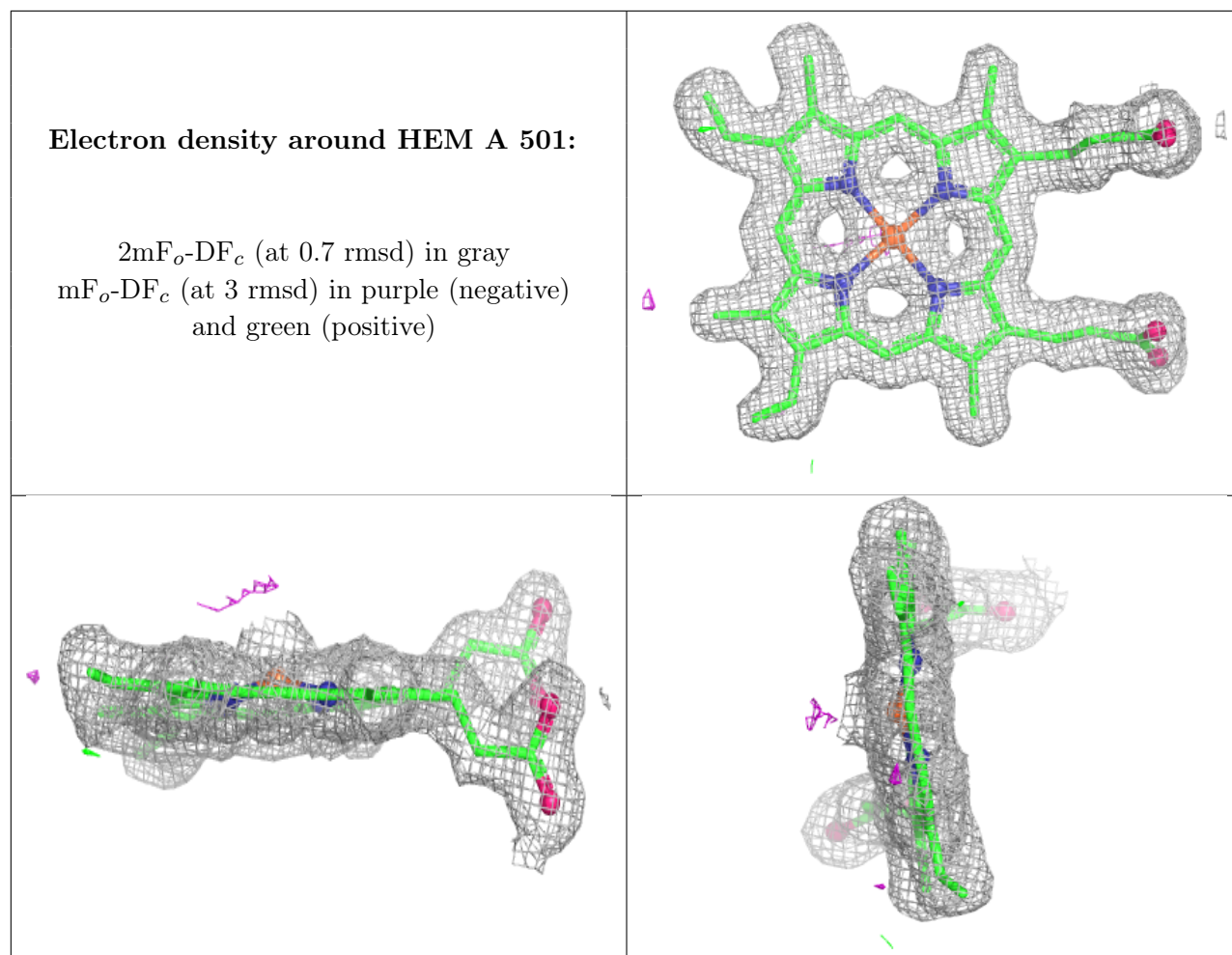
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
3	CAM	A	502	11/11	0.93	0.07	9,14,21,21	0
3	CAM	B	502	11/11	0.96	0.05	6,11,21,23	0
4	TRS	A	503	8/8	0.96	0.05	10,17,23,27	0
2	HEM	B	501	43/43	0.98	0.05	7,13,25,33	0
2	HEM	A	501	43/43	0.98	0.05	6,17,25,31	0
5	K	A	504	1/1	0.98	0.03	21,21,21,21	0
5	K	B	504	1/1	0.99	0.02	18,18,18,18	0
5	K	B	503	1/1	1.00	0.03	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.