



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1DZ8 / pdb_00001dz8
Title : oxygen complex of p450cam from pseudomonas putida
Authors : Schlichting, I.; Berendzen, J.; Chu, K.; Stock, A.M.; Maves, S.A.; Benson, D.E.; Sweet, R.M.; Ringe, D.; Petsko, G.A.; Sligar, S.G.
Deposited on : 2000-02-18
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

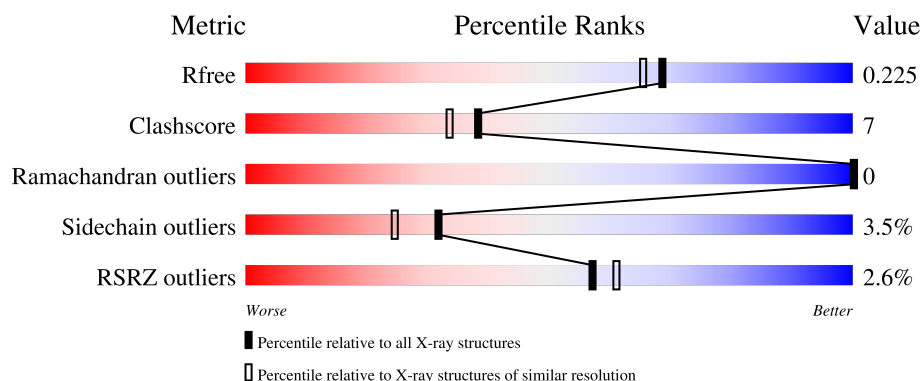
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	414	4% 71% 24% ..
1	B	414	% 71% 24% ...

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
5	TRS	A	504	-	X	-	-

2 Entry composition [i](#)

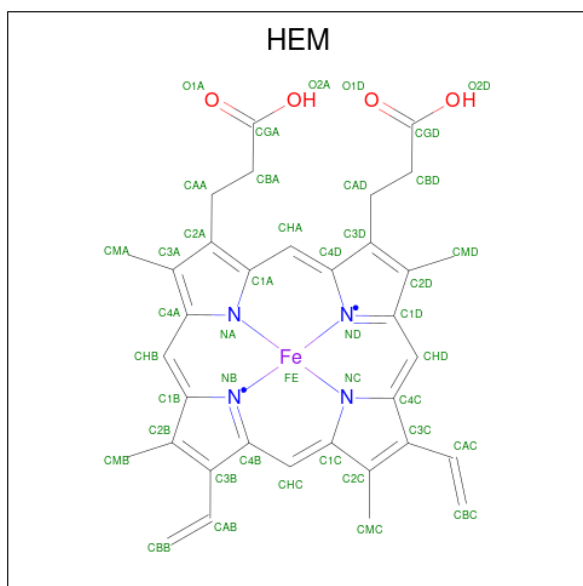
There are 7 unique types of molecules in this entry. The entry contains 7207 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

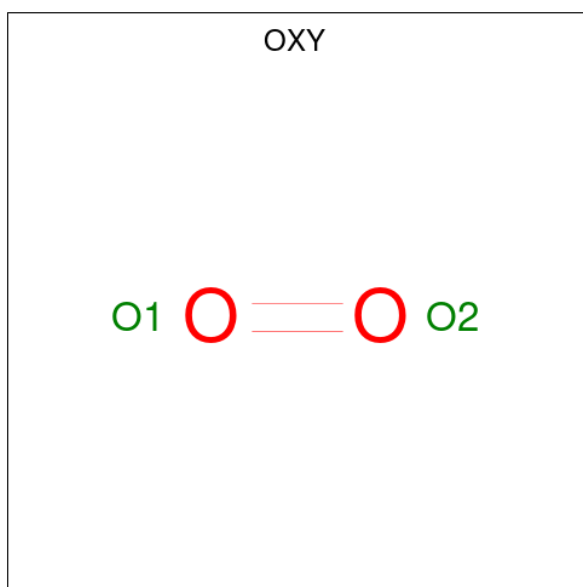
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	2	0
			3210	2038	559	595	18			
1	B	405	Total	C	N	O	S	0	3	0
			3226	2043	563	602	18			

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



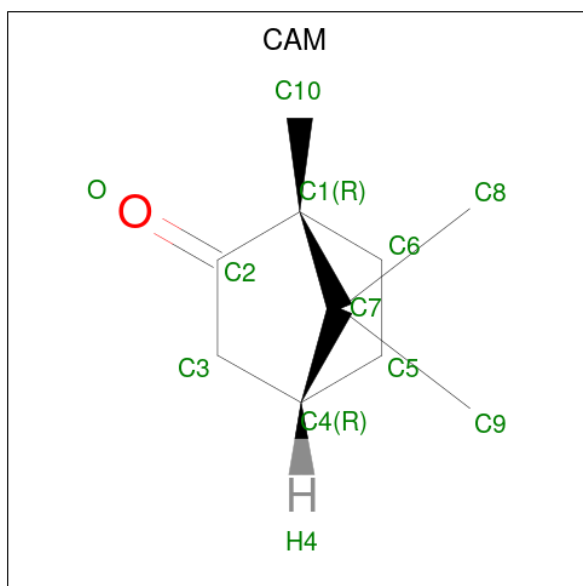
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			2	2		

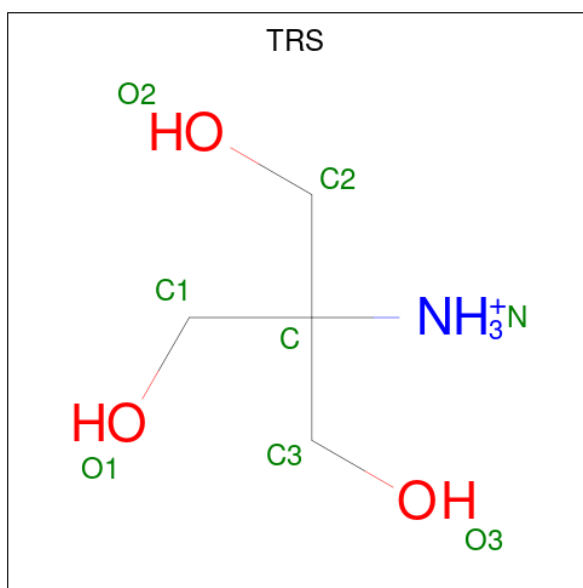
- Molecule 4 is CAMPHOR (CCD ID: CAM) (formula: $C_{10}H_{16}O$).



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

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS)

(formula: C₄H₁₂NO₃).



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

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

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

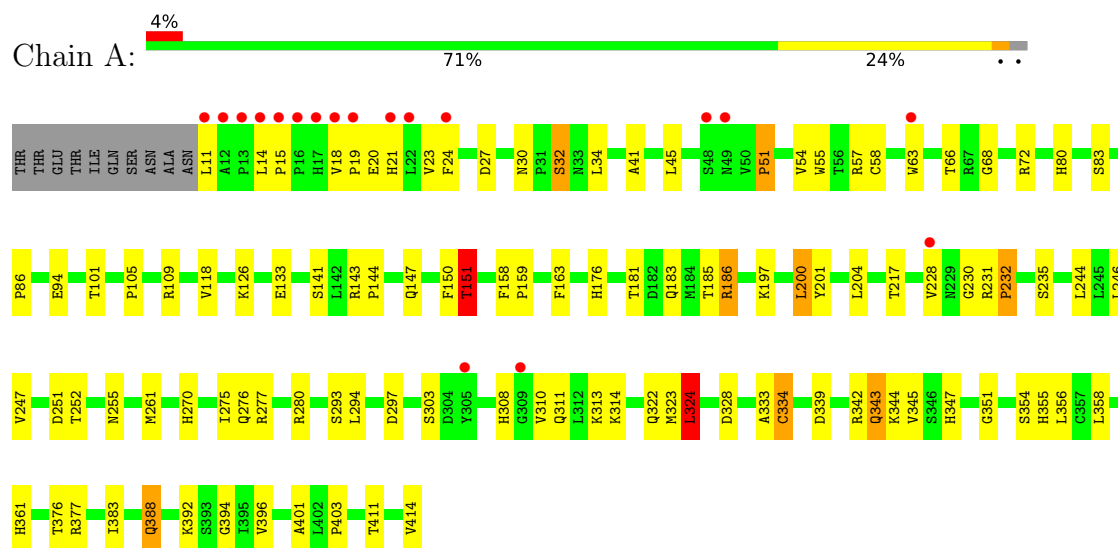
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	276	Total	O	0	0
			276	276		
7	B	374	Total	O	0	0
			374	374		

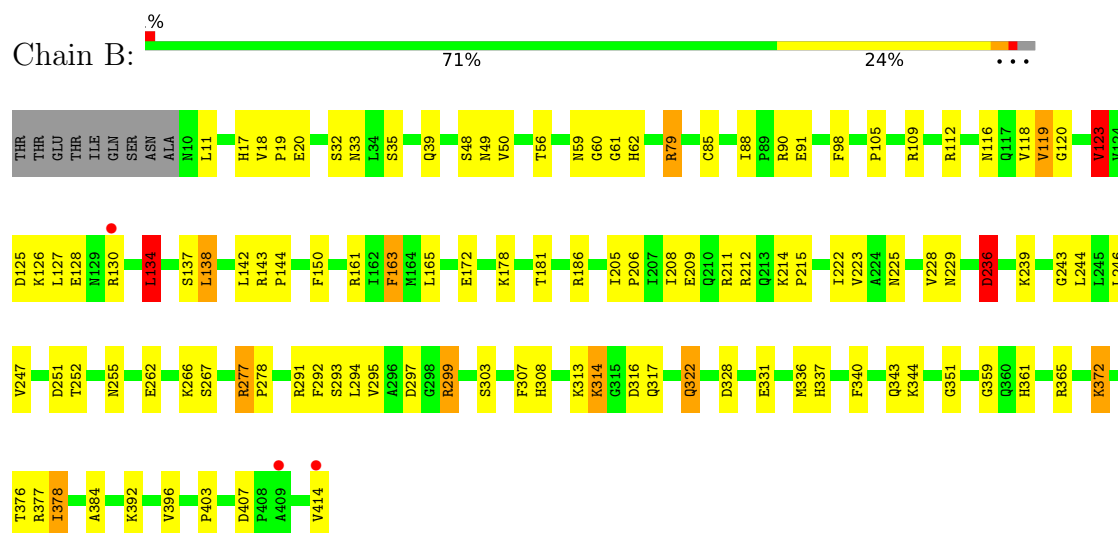
3 Residue-property plots [i](#)

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	67.00Å 61.80Å 94.70Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	19.00 – 1.90 19.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.6 (19.00-1.90) 98.4 (19.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.248 (Not available) , 0.225	Depositor DCC
R_{free} test set	4868 reflections (7.02%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7207	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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: TRS, OXY, CAM, HEM, K

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	0.92	1/3298 (0.0%)	1.85	67/4480 (1.5%)
1	B	0.98	1/3309 (0.0%)	1.86	86/4496 (1.9%)
All	All	0.95	2/6607 (0.0%)	1.85	153/8976 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	PRO	CA-C	6.67	1.55	1.51
1	B	49	ASN	N-CA	5.11	1.52	1.46

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	ARG	NE-CZ-NH2	-14.01	106.59	119.20
1	A	105	PRO	O-C-N	11.05	126.39	121.31
1	A	255	ASN	CA-CB-CG	-10.61	101.99	112.60
1	B	90	ARG	CD-NE-CZ	10.16	138.62	124.40
1	A	151	THR	N-CA-CB	-9.92	95.54	110.12
1	B	163	PHE	CA-CB-CG	-9.59	104.21	113.80
1	B	236	ASP	CA-CB-CG	-9.40	103.20	112.60
1	B	39	GLN	OE1-CD-NE2	-9.34	113.26	122.60
1	B	255	ASN	CA-CB-CG	-9.25	103.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	SER	N-CA-C	8.63	122.91	112.38
1	B	308	HIS	CA-CB-CG	-8.38	105.42	113.80
1	A	361	HIS	CA-CB-CG	-8.33	105.47	113.80
1	A	32	SER	N-CA-C	7.72	119.33	111.07
1	B	343	GLN	N-CA-C	7.68	119.43	111.14
1	A	324	LEU	N-CA-C	7.56	120.59	111.82
1	A	105	PRO	CA-C-O	-7.48	115.51	120.90
1	A	18	VAL	CA-C-O	7.36	124.58	119.20
1	B	328	ASP	CA-CB-CG	7.36	119.96	112.60
1	B	186	ARG	NH1-CZ-NH2	7.32	128.81	119.30
1	A	109	ARG	CA-C-O	-7.30	112.75	120.63
1	A	105	PRO	N-CA-C	-7.15	103.61	110.47
1	A	308	HIS	CA-CB-CG	-7.05	106.75	113.80
1	B	90	ARG	NH1-CZ-NH2	-7.05	110.14	119.30
1	A	270	HIS	CA-CB-CG	-7.04	106.76	113.80
1	A	230	GLY	N-CA-C	7.00	124.64	115.40
1	B	90	ARG	NE-CZ-NH1	7.00	128.50	121.50
1	B	228	VAL	N-CA-CB	6.97	120.68	111.90
1	B	33	ASN	CA-CB-CG	6.96	119.56	112.60
1	B	112	ARG	NE-CZ-NH2	-6.92	112.97	119.20
1	B	59	ASN	CA-CB-CG	-6.87	105.73	112.60
1	A	217	THR	CA-CB-OG1	-6.83	99.35	109.60
1	A	280	ARG	CA-C-N	-6.83	115.94	120.24
1	A	280	ARG	C-N-CA	-6.83	115.94	120.24
1	B	178	LYS	CA-C-O	-6.83	113.18	120.42
1	A	68	GLY	CA-C-O	6.80	127.75	120.75
1	B	336	MET	CA-C-N	6.74	131.13	121.50
1	B	336	MET	C-N-CA	6.74	131.13	121.50
1	A	396	VAL	CA-C-O	-6.73	113.39	120.39
1	B	291	ARG	CD-NE-CZ	6.69	133.77	124.40
1	B	337	HIS	CA-CB-CG	6.65	120.45	113.80
1	B	314	LYS	O-C-N	-6.52	115.29	123.12
1	A	151	THR	CB-CA-C	6.49	121.57	110.79
1	A	342	ARG	CG-CD-NE	6.48	126.25	112.00
1	A	72	ARG	NE-CZ-NH2	6.46	125.02	119.20
1	B	60	GLY	CA-C-N	6.45	134.06	121.41
1	B	60	GLY	C-N-CA	6.45	134.06	121.41
1	B	361	HIS	CA-CB-CG	-6.44	107.36	113.80
1	A	18	VAL	N-CA-C	6.39	114.93	107.77
1	B	292	PHE	CA-CB-CG	-6.38	107.42	113.80
1	A	251	ASP	CA-C-N	6.37	129.06	120.65
1	A	251	ASP	C-N-CA	6.37	129.06	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	SER	CA-C-N	-6.36	112.56	122.67
1	B	48	SER	C-N-CA	-6.36	112.56	122.67
1	A	133	GLU	CB-CG-CD	6.35	123.40	112.60
1	B	212	ARG	CD-NE-CZ	6.31	133.23	124.40
1	A	297	ASP	N-CA-CB	6.29	121.13	110.49
1	B	161	ARG	NE-CZ-NH2	6.26	124.84	119.20
1	A	280	ARG	CD-NE-CZ	6.21	133.09	124.40
1	B	243	GLY	N-CA-C	-6.19	104.84	112.77
1	B	119	VAL	CA-C-N	6.17	130.35	121.54
1	B	119	VAL	C-N-CA	6.17	130.35	121.54
1	A	342	ARG	NE-CZ-NH2	6.11	124.70	119.20
1	B	32	SER	CA-C-N	-6.11	112.70	122.66
1	B	32	SER	C-N-CA	-6.11	112.70	122.66
1	A	401	ALA	CA-C-O	-6.03	114.26	120.89
1	B	209	GLU	CA-C-O	-6.02	114.50	120.82
1	B	208	ILE	O-C-N	5.98	127.99	121.83
1	A	339	ASP	CA-CB-CG	5.91	118.51	112.60
1	B	109	ARG	N-CA-C	5.91	117.40	111.07
1	A	126	LYS	CA-CB-CG	5.91	125.91	114.10
1	A	230	GLY	CA-C-O	-5.90	112.78	119.04
1	B	35	SER	O-C-N	-5.88	114.34	122.46
1	B	123	VAL	CG1-CB-CG2	-5.86	97.90	110.80
1	B	79	ARG	NE-CZ-NH1	-5.84	115.66	121.50
1	B	85	CYS	N-CA-CB	-5.84	102.63	111.21
1	A	186	ARG	O-C-N	-5.77	116.20	121.34
1	B	322	GLN	CA-C-N	5.76	128.58	120.28
1	B	322	GLN	C-N-CA	5.76	128.58	120.28
1	A	347	HIS	CA-C-O	5.75	127.48	121.38
1	B	407	ASP	CA-C-N	5.74	125.60	119.28
1	B	407	ASP	C-N-CA	5.74	125.60	119.28
1	B	307	PHE	CA-CB-CG	5.72	119.53	113.80
1	B	229	ASN	CA-CB-CG	-5.71	106.89	112.60
1	B	316	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	116	ASN	OD1-CG-ND2	5.69	128.29	122.60
1	B	125	ASP	CA-C-N	5.68	127.89	120.28
1	B	125	ASP	C-N-CA	5.68	127.89	120.28
1	A	275	ILE	N-CA-C	-5.68	104.99	110.72
1	A	345	VAL	CA-C-N	-5.67	114.19	122.65
1	A	345	VAL	C-N-CA	-5.67	114.19	122.65
1	B	35	SER	CA-C-O	5.67	126.42	119.05
1	B	50	VAL	CA-C-O	5.67	123.34	119.20
1	B	377	ARG	CD-NE-CZ	5.65	132.31	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	403	PRO	CB-CA-C	5.64	116.53	111.40
1	B	112	ARG	NH1-CZ-NH2	5.63	126.61	119.30
1	A	328	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	147	GLN	CA-C-O	-5.61	114.93	121.10
1	B	267	SER	CA-C-O	5.60	127.79	120.74
1	B	62	HIS	CA-CB-CG	5.60	119.40	113.80
1	B	211	ARG	CB-CG-CD	5.59	124.16	111.30
1	B	299	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	A	126	LYS	CB-CA-C	-5.55	101.57	110.79
1	B	32	SER	N-CA-C	5.53	118.02	111.33
1	B	105	PRO	N-CA-C	-5.52	105.17	110.47
1	A	204	LEU	N-CA-C	5.50	118.20	111.82
1	A	297	ASP	CA-C-N	-5.47	112.84	121.37
1	A	297	ASP	C-N-CA	-5.47	112.84	121.37
1	A	235	SER	CA-C-N	5.46	127.54	120.44
1	A	235	SER	C-N-CA	5.46	127.54	120.44
1	B	378	ILE	CA-C-N	5.46	125.28	119.28
1	B	378	ILE	C-N-CA	5.46	125.28	119.28
1	A	232	PRO	CA-C-O	5.42	127.21	121.03
1	B	134	LEU	CB-CA-C	-5.40	102.36	110.90
1	A	403	PRO	N-CA-CB	5.40	106.84	103.23
1	A	383	ILE	CA-C-N	5.39	128.33	120.51
1	A	383	ILE	C-N-CA	5.39	128.33	120.51
1	B	186	ARG	CD-NE-CZ	5.39	131.95	124.40
1	B	295	VAL	O-C-N	5.39	128.59	122.98
1	A	394	GLY	CA-C-O	-5.37	116.80	121.04
1	B	297	ASP	N-CA-CB	5.37	119.56	110.49
1	B	32	SER	CB-CA-C	-5.35	101.58	110.68
1	A	388	GLN	CA-C-O	-5.33	114.80	120.40
1	B	340	PHE	CA-CB-CG	5.33	119.14	113.80
1	B	223	VAL	CB-CA-C	-5.31	105.06	112.02
1	A	51	PRO	CA-C-N	5.29	127.90	120.28
1	A	51	PRO	C-N-CA	5.29	127.90	120.28
1	A	176	HIS	CA-C-O	5.29	126.15	120.70
1	A	80	HIS	CA-CB-CG	-5.28	108.52	113.80
1	B	331	GLU	N-CA-C	-5.26	106.92	113.55
1	A	183	GLN	CA-CB-CG	5.25	124.60	114.10
1	B	142	LEU	O-C-N	5.24	129.05	122.23
1	A	94	GLU	CA-C-O	-5.22	115.01	120.55
1	A	277	ARG	CA-C-N	5.22	124.88	119.56
1	A	277	ARG	C-N-CA	5.22	124.88	119.56
1	B	277	ARG	CA-C-N	5.20	124.86	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	ARG	C-N-CA	5.20	124.86	119.56
1	B	299	ARG	NH1-CZ-NH2	5.20	126.06	119.30
1	A	185	THR	CA-C-O	-5.18	113.71	119.67
1	B	384	ALA	CA-C-O	5.16	125.54	120.17
1	A	310	VAL	CA-C-O	-5.16	114.84	120.72
1	B	62	HIS	CA-C-O	-5.13	115.45	121.10
1	A	354	SER	CA-C-N	-5.13	114.47	122.73
1	A	354	SER	C-N-CA	-5.13	114.47	122.73
1	B	294	LEU	N-CA-C	5.09	121.24	113.19
1	B	150	PHE	O-C-N	5.07	127.49	122.12
1	A	252	THR	CA-C-O	-5.06	115.68	121.00
1	B	20	GLU	CG-CD-OE2	-5.06	106.75	118.40
1	A	151	THR	OG1-CB-CG2	5.03	119.35	109.30
1	B	293	SER	O-C-N	-5.01	116.64	122.81
1	A	334	CYS	CA-C-N	5.01	124.50	119.19
1	A	334	CYS	C-N-CA	5.01	124.50	119.19
1	B	17	HIS	N-CA-C	5.00	119.23	113.18
1	B	150	PHE	CA-C-O	-5.00	115.22	120.63

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	252[B]	THR	Mainchain
1	B	91	GLU	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	3210	0	3160	45	0
1	B	3226	0	3171	43	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
3	A	2	0	0	1	0
4	A	11	0	16	1	0
4	B	11	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	8	0	12	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
7	A	276	0	0	2	0
7	B	374	0	0	2	0
All	All	7207	0	6435	90	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 7.

All (90) 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:130:ARG:HD2	1:B:165:LEU:HD21	1.52	0.89
1:B:128:GLU:HB2	1:B:365:ARG:HH12	1.51	0.76
1:A:51:PRO:HG2	1:A:54:VAL:HG12	1.71	0.72
1:B:120:GLY:O	1:B:123:VAL:HG12	1.91	0.70
1:A:294:LEU:HA	1:A:323:MET:HE2	1.75	0.69
1:A:163[A]:PHE:CE2	1:A:246:LEU:HD22	2.27	0.69
1:A:11:LEU:HD12	1:A:57:ARG:HB2	1.73	0.68
1:A:358:LEU:HD12	2:A:501:HEM:HBD2	1.75	0.68
1:B:236:ASP:HB3	7:B:612:HOH:O	1.94	0.68
1:B:127:LEU:HD23	1:B:130:ARG:NH2	2.10	0.67
1:A:200:LEU:HD21	1:A:246:LEU:HD12	1.77	0.65
1:B:181[B]:THR:HG21	1:B:251[B]:ASP:HB2	1.82	0.62
1:A:143:ARG:HB3	1:A:144:PRO:HD3	1.81	0.61
1:B:130:ARG:HD2	1:B:165:LEU:CD2	2.29	0.61
1:B:181[A]:THR:HG22	1:B:247:VAL:HG22	1.82	0.61
1:B:143:ARG:HB3	1:B:144:PRO:HD3	1.83	0.60
1:B:134:LEU:HD22	1:B:138:LEU:HD22	1.85	0.59
1:A:151:THR:HG23	7:A:634:HOH:O	2.03	0.58
1:B:163:PHE:HE2	1:B:246:LEU:HD23	1.68	0.57
1:A:19:PRO:HB2	1:A:21:HIS:CE1	2.40	0.57
1:A:343:GLN:HB3	1:A:344:LYS:HD3	1.87	0.57
1:A:276:GLN:HE21	1:B:172:GLU:H	1.53	0.56
1:B:127:LEU:HA	1:B:130:ARG:HH21	1.69	0.56
1:A:163[A]:PHE:HE2	1:A:246:LEU:HD22	1.69	0.56
1:B:163:PHE:CE2	1:B:246:LEU:HD23	2.40	0.56
1:B:372:LYS:HZ2	1:B:372:LYS:HB3	1.71	0.56
1:B:372:LYS:HB3	1:B:372:LYS:NZ	2.20	0.56
1:B:181[B]:THR:CG2	1:B:251[B]:ASP:HB2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LYS:HE3	1:A:201:TYR:CE2	2.41	0.54
1:A:163[A]:PHE:CZ	1:A:246:LEU:HD22	2.41	0.54
1:B:251[B]:ASP:O	1:B:396:VAL:HG11	2.09	0.53
1:B:98:PHE:HB3	1:B:244:LEU:HB2	1.91	0.53
1:A:231:ARG:HB2	1:A:232:PRO:CD	2.39	0.53
1:B:56:THR:O	1:B:61:GLY:HA2	2.10	0.52
1:B:123:VAL:O	1:B:126:LYS:HB3	2.10	0.52
1:B:126:LYS:HG2	1:B:130:ARG:NH2	2.25	0.52
1:B:19:PRO:HD3	7:B:653:HOH:O	2.10	0.51
1:A:23:VAL:HG11	1:A:57:ARG:NH1	2.26	0.51
1:B:127:LEU:HD23	1:B:130:ARG:CZ	2.41	0.50
1:A:66:THR:HA	1:A:324:LEU:HD23	1.94	0.49
1:A:376:THR:HG22	1:A:414:VAL:HG21	1.93	0.49
1:B:303:SER:HA	1:B:314:LYS:HB2	1.94	0.49
1:A:186:ARG:HD2	1:A:392:LYS:HG3	1.94	0.49
2:A:501:HEM:CMB	2:A:501:HEM:HBB2	2.42	0.49
1:A:181[A]:THR:HG22	1:A:247:VAL:HG22	1.94	0.49
1:A:231:ARG:HB2	1:A:232:PRO:HD2	1.96	0.48
1:B:215:PRO:HB3	1:B:225:ASN:ND2	2.29	0.48
1:A:197:LYS:HE3	1:A:201:TYR:HE2	1.76	0.47
2:B:501:HEM:HMB2	2:B:501:HEM:HBB2	1.94	0.47
1:A:303:SER:HA	1:A:314:LYS:HB2	1.96	0.47
1:A:163[A]:PHE:CZ	1:A:246:LEU:CD2	2.97	0.47
1:A:27:ASP:HB2	1:A:58:CYS:SG	2.55	0.47
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.96	0.46
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.97	0.46
1:A:150:PHE:CZ	1:A:261:MET:HG3	2.50	0.46
1:B:376:THR:HG22	1:B:414:VAL:HG21	1.98	0.45
1:A:333:ALA:O	1:A:334:CYS:C	2.59	0.45
1:A:34:LEU:HA	1:A:41:ALA:HB2	1.98	0.44
1:A:163[A]:PHE:HZ	1:A:246:LEU:CD2	2.30	0.44
1:A:293:SER:HB3	1:A:323:MET:HA	1.99	0.44
1:B:262:GLU:CG	1:B:266:LYS:HE3	2.48	0.44
1:A:14:LEU:HA	1:A:15:PRO:HD3	1.87	0.44
1:B:126:LYS:HG2	1:B:130:ARG:HH22	1.83	0.44
1:B:313:LYS:O	1:B:314:LYS:C	2.59	0.44
1:A:163[A]:PHE:CZ	1:A:246:LEU:HA	2.53	0.43
1:A:276:GLN:HE21	1:B:172:GLU:N	2.15	0.43
1:A:11:LEU:CD1	1:A:57:ARG:HB2	2.46	0.43
1:A:55:TRP:HE3	1:A:63:TRP:CD2	2.36	0.43
3:A:502:OXY:O1	4:A:503:CAM:H52	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ARG:HH11	1:B:299:ARG:HD3	1.61	0.43
1:B:118:VAL:HG12	1:B:222:ILE:HG21	2.00	0.43
1:B:18:VAL:HA	1:B:19:PRO:HD3	1.91	0.43
1:A:356:LEU:HB2	7:A:741:HOH:O	2.19	0.43
1:B:205:ILE:N	1:B:206:PRO:HD2	2.34	0.43
1:B:359:GLY:HA3	2:B:501:HEM:C3C	2.54	0.42
1:A:377:ARG:O	1:A:411:THR:HB	2.20	0.42
1:A:19:PRO:HB2	1:A:21:HIS:ND1	2.33	0.42
1:A:163[A]:PHE:HZ	1:A:246:LEU:HD23	1.85	0.42
1:B:88:ILE:HD11	1:B:317:GLN:HB3	2.01	0.42
1:B:239:LYS:HE2	1:B:239:LYS:HB3	1.95	0.42
1:A:313:LYS:O	1:A:314:LYS:C	2.63	0.42
1:B:119:VAL:HA	1:B:123:VAL:HG11	2.01	0.42
1:A:322:GLN:HG2	1:A:351:GLY:HA2	2.03	0.41
1:A:24:PHE:CE2	1:A:45:LEU:HD23	2.55	0.41
1:A:83:SER:HB3	1:A:101:THR:O	2.21	0.41
1:B:79:ARG:HH11	1:B:79:ARG:HD2	1.58	0.41
1:B:277:ARG:HA	1:B:278:PRO:HD2	1.88	0.41
1:A:355:HIS:O	1:A:356:LEU:C	2.64	0.41
1:B:378:ILE:HD13	1:B:378:ILE:HG21	1.86	0.40
1:B:322:GLN:HG2	1:B:351:GLY:HA2	2.03	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	404/414 (98%)	389 (96%)	15 (4%)	0	100	100
1	B	406/414 (98%)	392 (97%)	14 (3%)	0	100	100
All	All	810/828 (98%)	781 (96%)	29 (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	346/358 (97%)	332 (96%)	14 (4%)	28	20
1	B	353/358 (99%)	343 (97%)	10 (3%)	38	32
All	All	699/716 (98%)	675 (97%)	24 (3%)	32	25

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	30	ASN
1	A	32	SER
1	A	86	PRO
1	A	118	VAL
1	A	141	SER
1	A	151	THR
1	A	200	LEU
1	A	228	VAL
1	A	244	LEU
1	A	311	GLN
1	A	324	LEU
1	A	343	GLN
1	A	388	GLN
1	B	11	LEU
1	B	123	VAL
1	B	134	LEU
1	B	137	SER
1	B	138	LEU
1	B	214	LYS
1	B	236	ASP
1	B	344	LYS
1	B	372	LYS
1	B	392	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	183	GLN
1	A	227	GLN
1	A	272	GLN
1	A	276	GLN
1	A	311	GLN
1	A	388	GLN
1	B	30	ASN
1	B	49	ASN
1	B	388	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	$\# Z > 2$
3	OXY	A	502	2	1,1,1	0.06	0	-		
5	TRS	A	504	-	7,7,7	2.07	4 (57%)	9,9,9	2.39	4 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CAM	A	503	-	12,12,12	0.87	1 (8%)	20,21,21	2.73	6 (30%)
4	CAM	B	502	-	12,12,12	1.00	1 (8%)	20,21,21	2.65	9 (45%)
2	HEM	B	501	1	50,50,50	1.42	8 (16%)	67,82,82	1.27	7 (10%)
2	HEM	A	501	1,3	50,50,50	1.45	11 (22%)	67,82,82	1.24	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TRS	A	504	-	-	2/9/9/9	-
4	CAM	A	503	-	-	-	0/3/2/2
4	CAM	B	502	-	-	-	0/3/2/2
2	HEM	B	501	1	-	4/14/54/54	-
2	HEM	A	501	1,3	-	3/14/54/54	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	CBD-CGD	3.23	1.58	1.50
2	B	501	HEM	FE-NC	3.14	2.05	1.95
5	A	504	TRS	O2-C2	3.01	1.51	1.42
2	B	501	HEM	CAC-C3C	3.00	1.55	1.47
5	A	504	TRS	O3-C3	2.93	1.51	1.42
2	A	501	HEM	FE-NC	2.82	2.04	1.95
2	B	501	HEM	CAB-C3B	2.78	1.54	1.47
4	B	502	CAM	C1-C2	2.69	1.56	1.52
2	A	501	HEM	CAC-C3C	2.64	1.54	1.47
2	B	501	HEM	FE-NA	2.57	2.03	1.95
2	B	501	HEM	CMD-C2D	2.44	1.55	1.50
2	B	501	HEM	C3C-C2C	-2.40	1.32	1.37
2	A	501	HEM	CAB-C3B	2.37	1.53	1.47
5	A	504	TRS	O1-C1	2.37	1.49	1.42
2	A	501	HEM	FE-NB	2.35	2.02	1.94
2	A	501	HEM	CBA-CGA	2.32	1.55	1.50
2	A	501	HEM	FE-ND	2.30	2.02	1.94
2	A	501	HEM	CMD-C2D	2.23	1.55	1.50
2	A	501	HEM	O2D-CGD	-2.23	1.23	1.30
4	A	503	CAM	C1-C2	2.21	1.55	1.52
2	A	501	HEM	CMC-C2C	2.17	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	CAA-C2A	2.17	1.56	1.51
2	A	501	HEM	C2A-C3A	-2.13	1.33	1.38
2	B	501	HEM	C4C-NC	-2.08	1.35	1.39
5	A	504	TRS	C1-C	2.04	1.58	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	CAM	O-C2-C3	5.33	137.37	126.39
4	A	503	CAM	C7-C1-C2	5.26	109.29	100.33
4	A	503	CAM	C5-C4-C3	-5.23	92.21	106.39
4	B	502	CAM	C3-C2-C1	-5.14	95.17	107.43
4	B	502	CAM	C5-C4-C3	-4.85	93.25	106.39
4	A	503	CAM	C4-C3-C2	4.71	110.33	102.05
4	A	503	CAM	C3-C2-C1	-4.69	96.26	107.43
4	B	502	CAM	C9-C7-C8	4.48	119.02	107.67
4	B	502	CAM	O-C2-C3	4.32	135.29	126.39
2	A	501	HEM	O1D-CGD-CBD	-3.83	110.95	123.09
5	A	504	TRS	C3-C-C2	-3.79	100.55	110.66
5	A	504	TRS	C2-C-C1	-3.78	100.60	110.66
2	A	501	HEM	O2D-CGD-O1D	3.74	132.96	123.33
2	B	501	HEM	CBC-CAC-C3C	-3.66	109.24	127.53
4	B	502	CAM	C4-C3-C2	3.55	108.30	102.05
2	B	501	HEM	CBD-CAD-C3D	3.35	121.79	112.53
2	B	501	HEM	CMD-C2D-C1D	-3.18	120.07	125.03
4	B	502	CAM	C6-C1-C7	3.16	108.19	101.52
5	A	504	TRS	C2-C-N	2.90	115.56	108.17
4	A	503	CAM	C9-C7-C8	2.75	114.63	107.67
4	B	502	CAM	C9-C7-C4	-2.59	107.17	113.44
4	B	502	CAM	C7-C1-C2	2.52	104.62	100.33
2	B	501	HEM	CMA-C3A-C4A	-2.41	121.74	125.42
5	A	504	TRS	C3-C-C1	2.41	117.08	110.66
2	B	501	HEM	CMA-C3A-C2A	2.38	130.68	125.62
4	B	502	CAM	C5-C6-C1	-2.37	99.95	104.73
2	B	501	HEM	O1A-CGA-CBA	-2.31	115.75	123.09
2	A	501	HEM	CBD-CAD-C3D	2.27	118.82	112.53
2	B	501	HEM	O1D-CGD-CBD	-2.27	115.89	123.09
2	A	501	HEM	CMA-C3A-C4A	-2.13	122.18	125.42
2	A	501	HEM	CHB-C4A-NA	2.05	127.57	123.86

There are no chirality outliers.

All (9) torsion outliers are listed below:

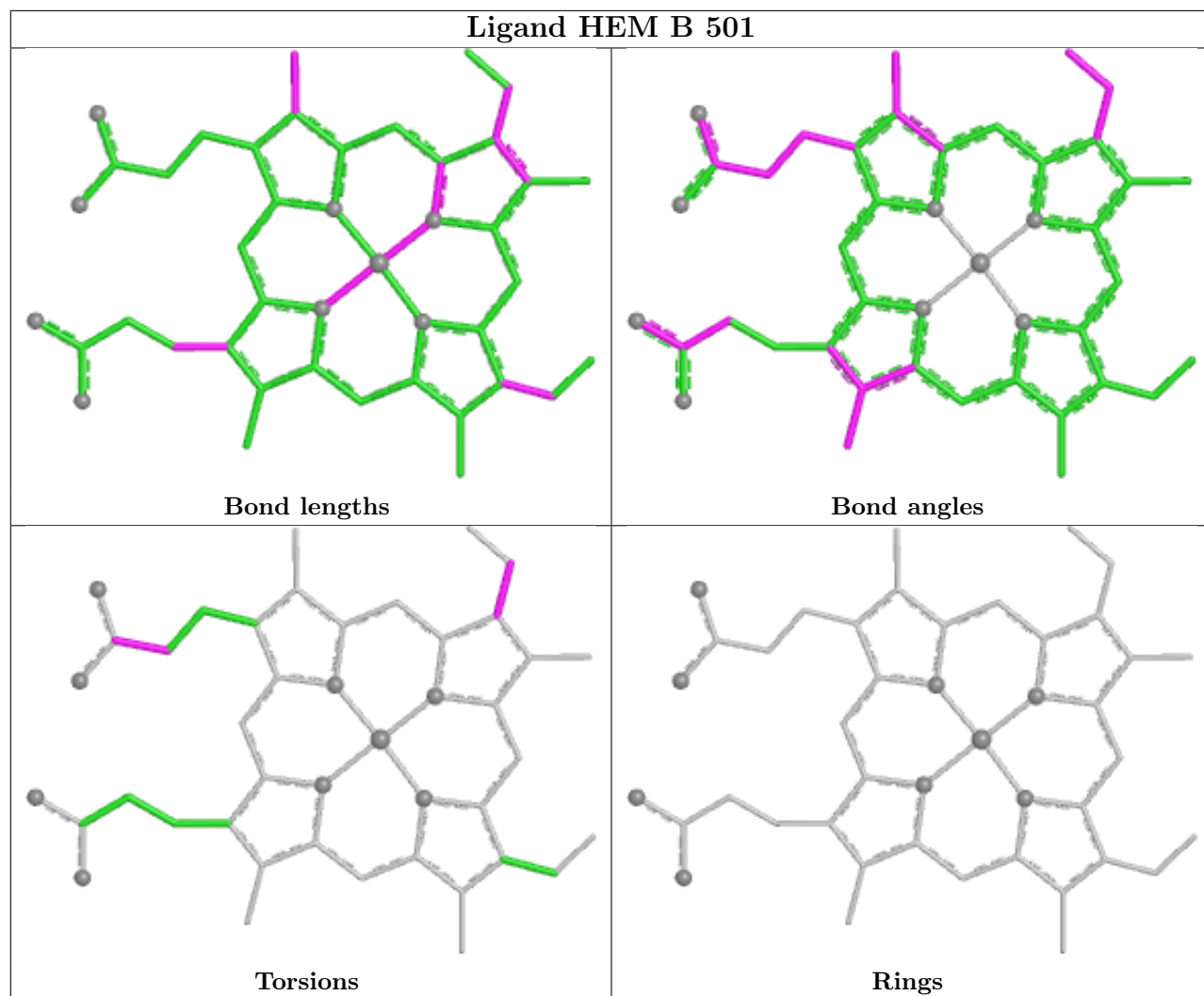
Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C2C-C3C-CAC-CBC
5	A	504	TRS	C1-C-C3-O3
2	B	501	HEM	C2C-C3C-CAC-CBC
5	A	504	TRS	N-C-C3-O3
2	A	501	HEM	C4C-C3C-CAC-CBC
2	B	501	HEM	C4C-C3C-CAC-CBC
2	B	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O1D

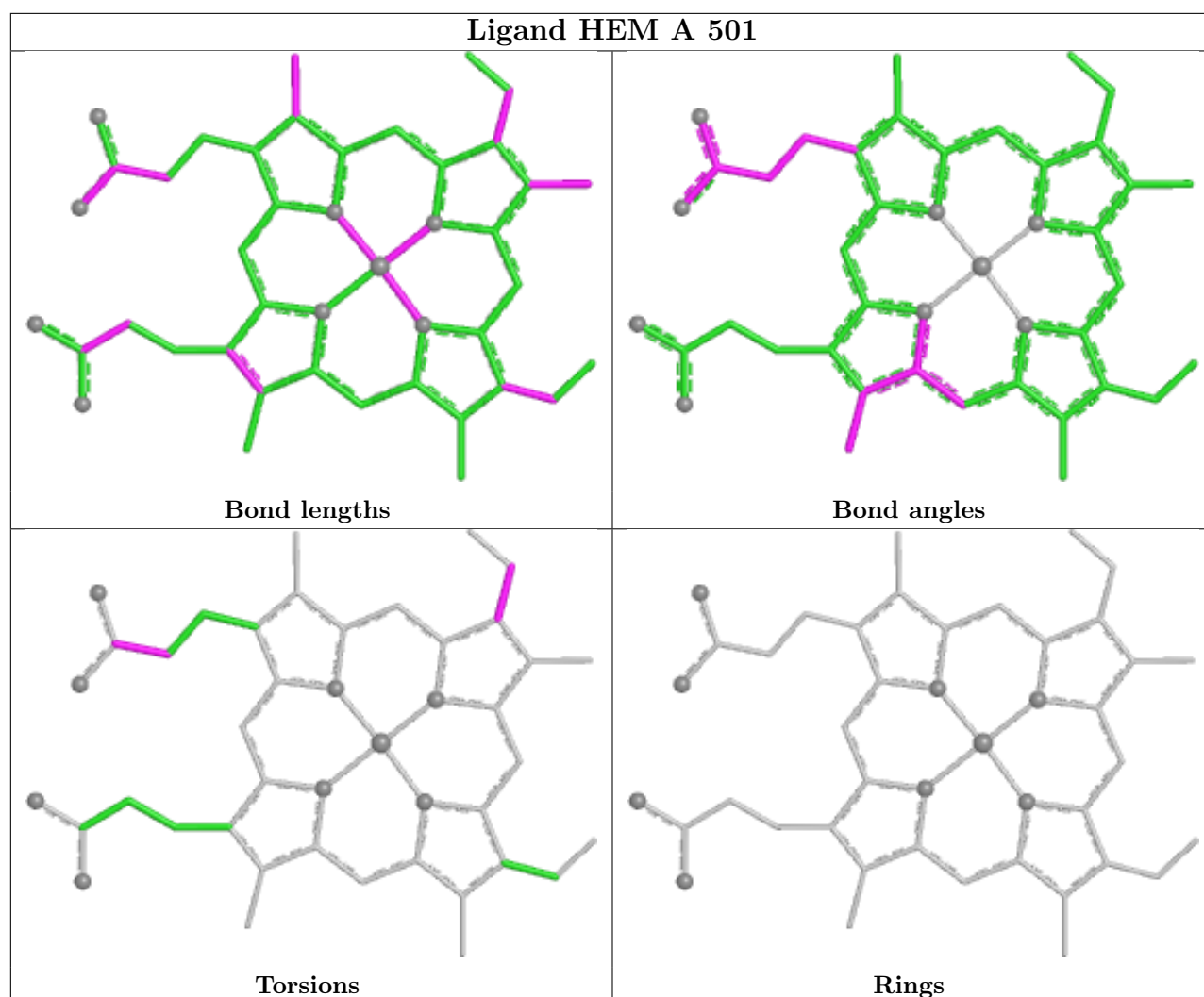
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	OXY	1	0
4	A	503	CAM	1	0
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

6.1 Protein, DNA and RNA chains

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%)	0.27	18 (4%) 38 40	8, 21, 47, 69	3 (0%)
1	B	405/414 (97%)	-0.40	3 (0%) 84 86	7, 15, 35, 55	3 (0%)
All	All	809/828 (97%)	-0.06	21 (2%) 57 61	7, 18, 42, 69	6 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	PRO	4.0
1	A	11	LEU	3.8
1	A	21	HIS	3.6
1	A	13	PRO	3.2
1	A	14	LEU	3.2
1	A	18	VAL	2.9
1	A	228	VAL	2.9
1	A	12	ALA	2.9
1	A	22	LEU	2.8
1	A	15	PRO	2.7
1	A	63	TRP	2.5
1	A	309	GLY	2.4
1	B	409	ALA	2.4
1	A	24	PHE	2.3
1	A	17	HIS	2.3
1	B	414	VAL	2.2
1	A	305	TYR	2.1
1	B	130	ARG	2.1
1	A	19	PRO	2.1
1	A	49	ASN	2.0
1	A	48	SER	2.0

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](#)

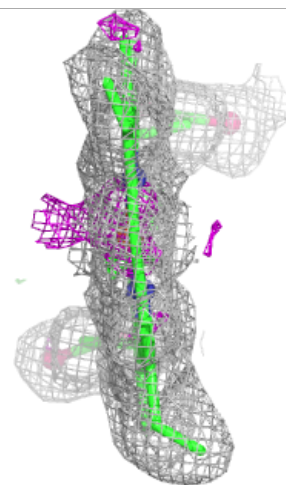
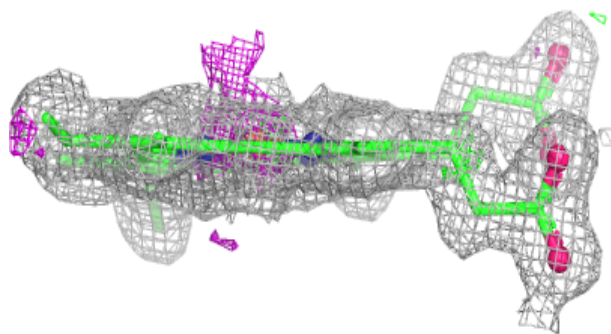
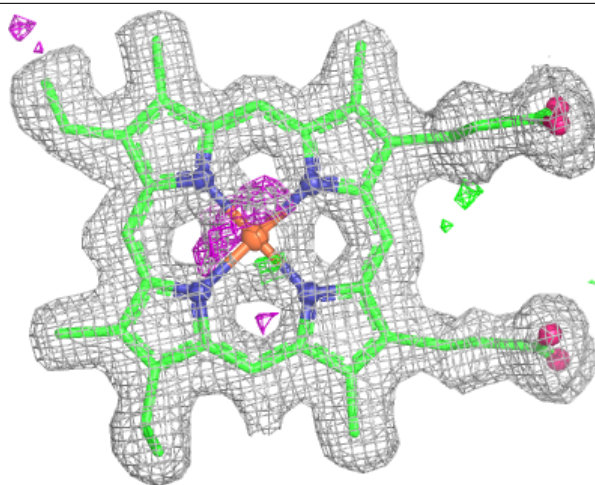
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	CAM	A	503	11/11	0.92	0.08	15,20,26,26	0
6	K	A	505	1/1	0.93	0.07	18,18,18,18	0
4	CAM	B	502	11/11	0.94	0.06	8,11,17,18	0
3	OXY	A	502	2/2	0.94	0.14	22,22,22,46	0
5	TRS	A	504	8/8	0.97	0.05	8,14,21,22	0
2	HEM	A	501	43/43	0.97	0.07	7,14,20,25	0
6	K	B	504	1/1	0.98	0.03	17,17,17,17	0
2	HEM	B	501	43/43	0.99	0.05	5,11,16,18	0
6	K	B	503	1/1	1.00	0.02	10,10,10,10	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

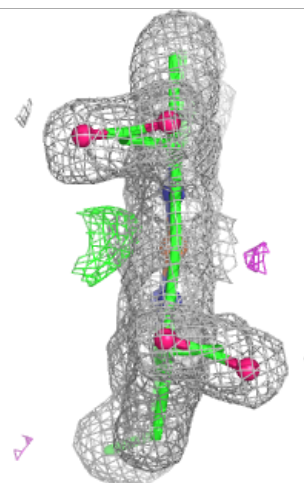
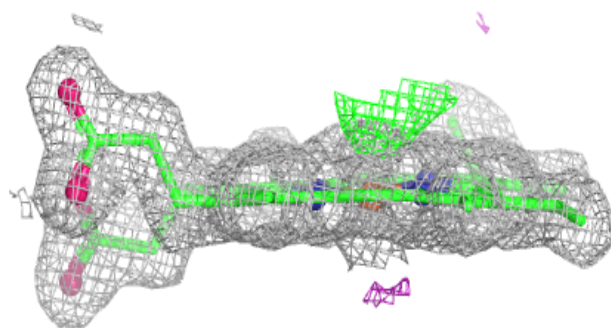
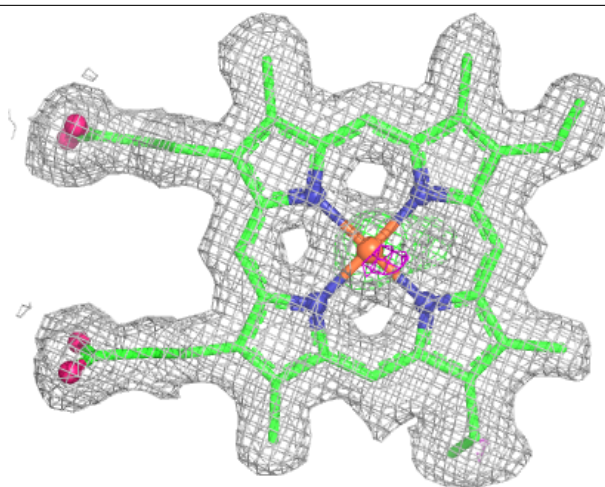
Electron density around HEM A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.