



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:29 PM UTC

PDB ID : 3KOH / pdb_00003koh
Title : Cytochrome P450 2E1 with omega-imidazolyl octanoic acid
Authors : Scott, E.E.; Porubsky, P.R.
Deposited on : 2009-11-13
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

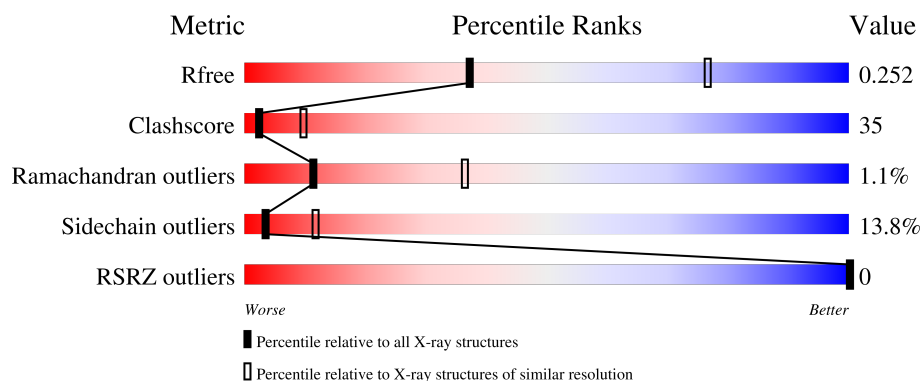
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

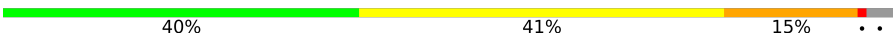
The reported resolution of this entry is 2.90 Å.

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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	476	
1	B	476	

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
3	OIO	A	1	-	-	X	-
3	OIO	B	1	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7681 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 2E1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3777	2444	648	667	18			
1	B	463	Total	C	N	O	S	0	0	0
			3777	2444	648	667	18			

There are 28 discrepancies between the modelled and reference sequences:

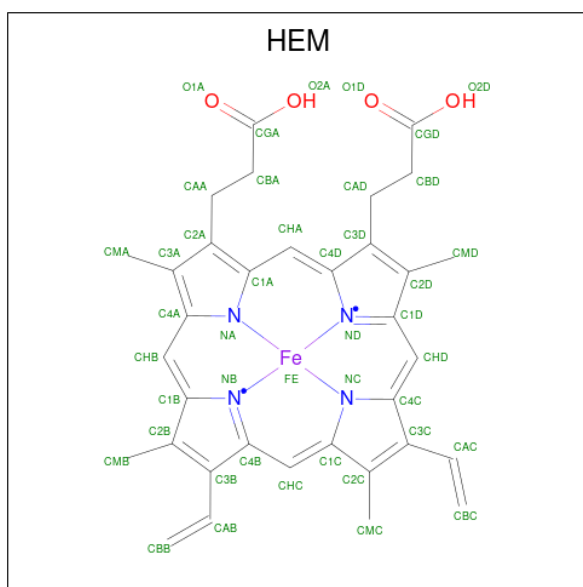
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	expression tag	UNP P05181
A	23	ALA	-	expression tag	UNP P05181
A	24	LYS	-	expression tag	UNP P05181
A	25	LYS	-	expression tag	UNP P05181
A	26	THR	-	expression tag	UNP P05181
A	27	SER	-	expression tag	UNP P05181
A	28	SER	-	expression tag	UNP P05181
A	29	LYS	-	expression tag	UNP P05181
A	30	GLY	-	expression tag	UNP P05181
A	31	LYS	-	expression tag	UNP P05181
A	494	HIS	-	expression tag	UNP P05181
A	495	HIS	-	expression tag	UNP P05181
A	496	HIS	-	expression tag	UNP P05181
A	497	HIS	-	expression tag	UNP P05181
B	22	MET	-	expression tag	UNP P05181
B	23	ALA	-	expression tag	UNP P05181
B	24	LYS	-	expression tag	UNP P05181
B	25	LYS	-	expression tag	UNP P05181
B	26	THR	-	expression tag	UNP P05181
B	27	SER	-	expression tag	UNP P05181
B	28	SER	-	expression tag	UNP P05181
B	29	LYS	-	expression tag	UNP P05181
B	30	GLY	-	expression tag	UNP P05181
B	31	LYS	-	expression tag	UNP P05181
B	494	HIS	-	expression tag	UNP P05181

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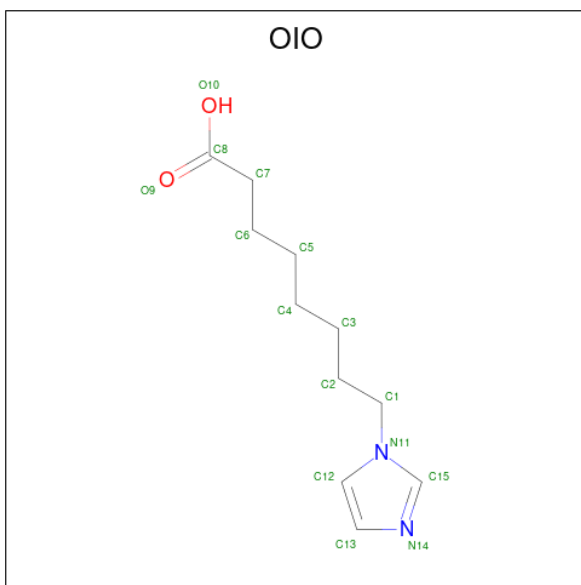
Chain	Residue	Modelled	Actual	Comment	Reference
B	495	HIS	-	expression tag	UNP P05181
B	496	HIS	-	expression tag	UNP P05181
B	497	HIS	-	expression tag	UNP P05181

- 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 8-(1H-imidazol-1-yl)octanoic acid (CCD ID: OIO) (formula: $C_{11}H_{18}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	2	2		
3	B	1	Total	C	N	O	0	0
			15	11	2	2		

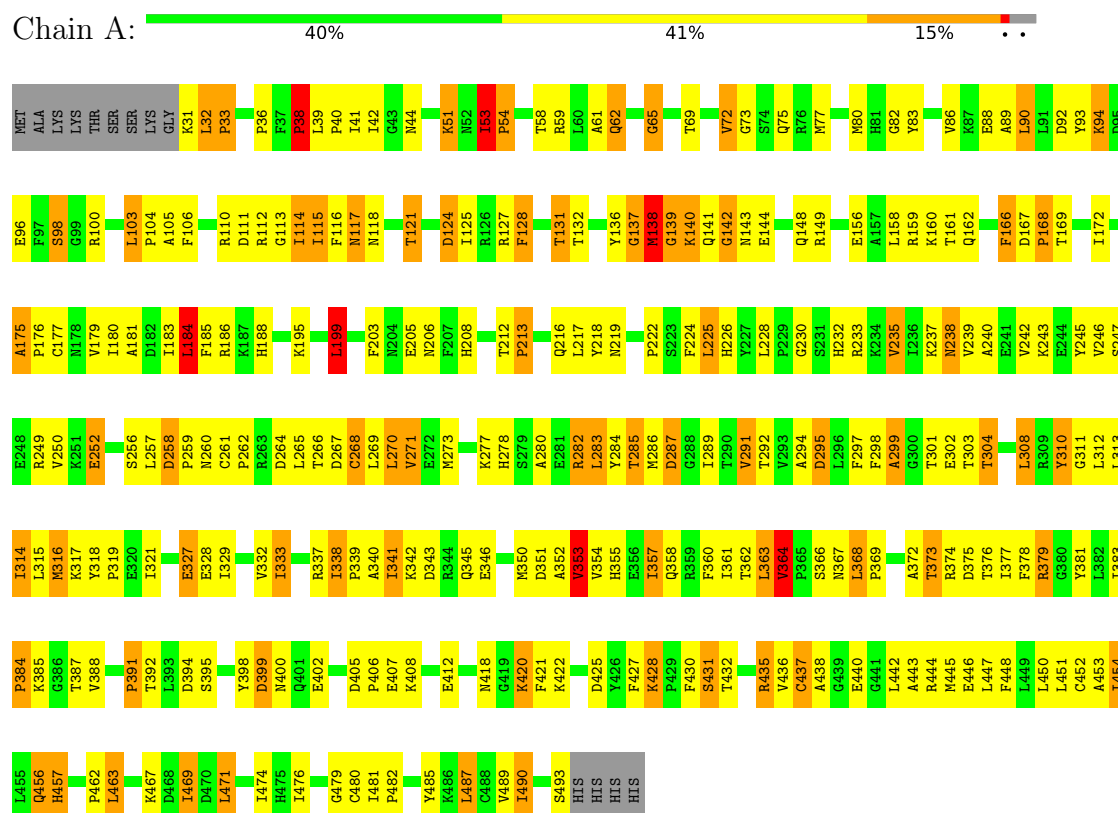
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	5	Total	O	0	0
			5	5		

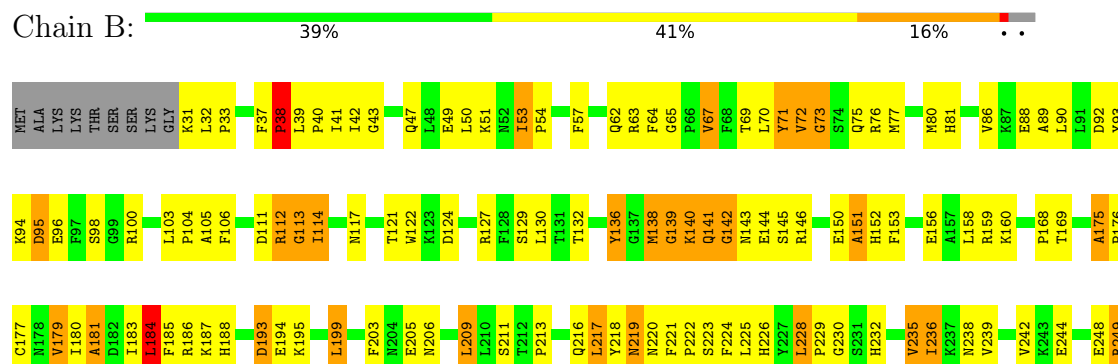
3 Residue-property plots [i](#)

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 2E1



• Molecule 1: Cytochrome P450 2E1



P466	I469	D470	L471	I474	H475	I476	G477	F478	G479	C480	I481	P482	P483	R484	Y485	K486	L487	C488	V489	I490	S493	HIS	HIS	HIS	HIS	K250	V251	E252	H253	H254	L257	D258	C261	P262	R263	D264	L265	T266	D267	C268	L269	L270	V271	E272	M273	H278	E281	R282	L283	Y284	T285	M286	D287	G288	I289	T290	V291	T292	V293	F298	A299	G300	T301	E302	T303	R309	Y310	G311	L312	L313	I314	L315	M316	K317	Y318	P319	E320	I321	E322
L393	D394	S395	V396	Y398	D399	M400	Q401	E402	F403	P404	D405	P406	K410	P411	E412	M416	E417	N418	G419	K420	F421	K422	Y423	S424	D425	K428	F429	F430	S431	T432	G433	K434	R435	V436	C437	A443	R444	M445	E446	L447	L450	L451	C452	A453	I454	L455	Q456	H457	P462	L463	V464	D465																											
L325	H326	E327	E328	Y329	V332	I333	I338	P339	A340	I341	K342	D343	E346	M347	P348	Y349	M350	D351	A352	V353	V354	H355	E356	I357	Q358	I361	T362	L363	V364	P365	S366	N367	L368	P369	H370	E371	A372	T373	R374	D375	I376	I377	F378	R379	L382	I383	P384	K385	G386	T387	V388	P391	T392																										

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	71.19Å 71.19Å 224.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.59 – 2.90 35.59 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (35.59-2.90) 98.1 (35.59-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.206 , 0.292 (Not available) , 0.252	Depositor DCC
R_{free} test set	1217 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	56.8	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.459 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7681	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	2.12	39/3882 (1.0%)	1.39	61/5257 (1.2%)
1	B	2.10	34/3882 (0.9%)	1.36	57/5257 (1.1%)
All	All	2.11	73/7764 (0.9%)	1.38	118/10514 (1.1%)

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	482	PRO	CA-C	-11.06	1.44	1.52
1	B	405	ASP	C-O	-10.36	1.19	1.23
1	A	405	ASP	C-O	-10.14	1.18	1.23
1	B	464	VAL	CA-CB	-9.58	1.45	1.55
1	A	53	ILE	CA-CB	-9.31	1.47	1.53

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ASN	N-CA-C	-11.60	98.44	112.59
1	B	139	GLY	N-CA-C	-10.59	98.20	115.46
1	B	220	ASN	N-CA-C	9.87	123.27	111.82
1	A	435	ARG	O-C-N	9.87	135.41	122.19
1	B	271	VAL	O-C-N	-9.73	112.37	121.91

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3777	0	3780	282	0
1	B	3777	0	3781	257	0
2	A	43	0	30	11	0
2	B	43	0	30	4	0
3	A	15	0	17	7	0
3	B	15	0	17	10	0
4	A	6	0	0	0	0
4	B	5	0	0	0	0
All	All	7681	0	7655	539	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 35.

The worst 5 of 539 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:303:THR:CG2	3:A:1:OIO:H15	1.48	1.42
1:B:257:LEU:HD12	1:B:258:ASP:N	1.36	1.34
1:B:265:LEU:HD23	1:B:265:LEU:C	1.50	1.29
1:B:265:LEU:HD23	1:B:265:LEU:O	1.37	1.24
1:A:265:LEU:O	1:A:265:LEU:HD23	1.35	1.23

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	461/476 (97%)	444 (96%)	12 (3%)	5 (1%)	11	36
1	B	461/476 (97%)	445 (96%)	11 (2%)	5 (1%)	11	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	922/952 (97%)	889 (96%)	23 (2%)	10 (1%)	11	36

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	342	LYS
1	B	419	GLY
1	B	437	CYS
1	A	38	PRO
1	A	437	CYS

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	417/428 (97%)	363 (87%)	54 (13%)	4	13
1	B	417/428 (97%)	356 (85%)	61 (15%)	3	10
All	All	834/856 (97%)	719 (86%)	115 (14%)	3	12

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	62	GLN
1	B	445	MET
1	B	145	SER
1	B	425	ASP
1	B	368	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	164	GLN
1	B	117	ASN
1	A	358	GLN

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Mol	Chain	Res	Type
1	A	326	HIS
1	A	459	ASN

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 ⓘ

4 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$
3	OIO	B	1	2	15,15,15	0.97	2 (13%)	17,17,17	1.10	1 (5%)
2	HEM	B	500	1,3	50,50,50	1.85	11 (22%)	67,82,82	1.36	7 (10%)
2	HEM	A	500	1,3	50,50,50	1.90	8 (16%)	67,82,82	1.52	12 (17%)
3	OIO	A	1	2	15,15,15	0.97	2 (13%)	17,17,17	1.11	2 (11%)

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
3	OIO	B	1	2	-	5/10/10/10	0/1/1/1
2	HEM	B	500	1,3	-	5/14/54/54	-
2	HEM	A	500	1,3	-	9/14/54/54	-
3	OIO	A	1	2	-	5/10/10/10	0/1/1/1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3D-C2D	7.11	1.52	1.36
2	A	500	HEM	C3D-C2D	6.89	1.51	1.36
2	A	500	HEM	FE-NB	5.06	2.10	1.94
2	A	500	HEM	FE-NC	4.77	2.10	1.95
2	B	500	HEM	FE-NB	4.27	2.08	1.94

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	HEM	C4D-ND-C1D	5.66	111.91	105.21
2	B	500	HEM	C4D-ND-C1D	5.01	111.14	105.21
2	B	500	HEM	CAD-CBD-CGD	-2.86	106.09	113.67
2	A	500	HEM	CHC-C4B-NB	2.67	127.30	124.42
2	A	500	HEM	CHD-C4C-C3C	2.67	129.70	125.21

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

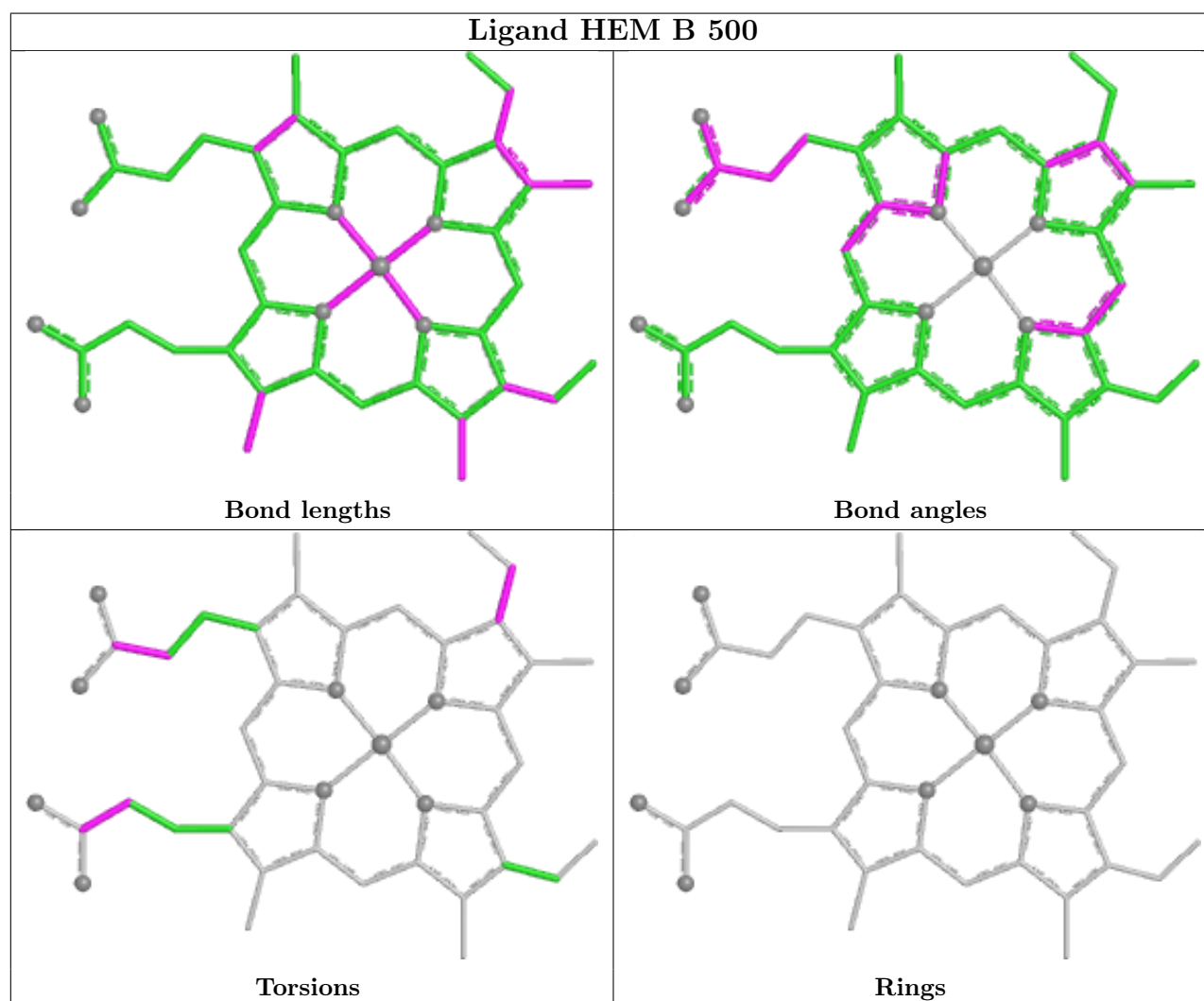
Mol	Chain	Res	Type	Atoms
2	A	500	HEM	C2B-C3B-CAB-CBB
3	A	1	OIO	C2-C3-C4-C5
3	B	1	OIO	C2-C3-C4-C5
2	A	500	HEM	C4B-C3B-CAB-CBB
3	A	1	OIO	C1-C2-C3-C4

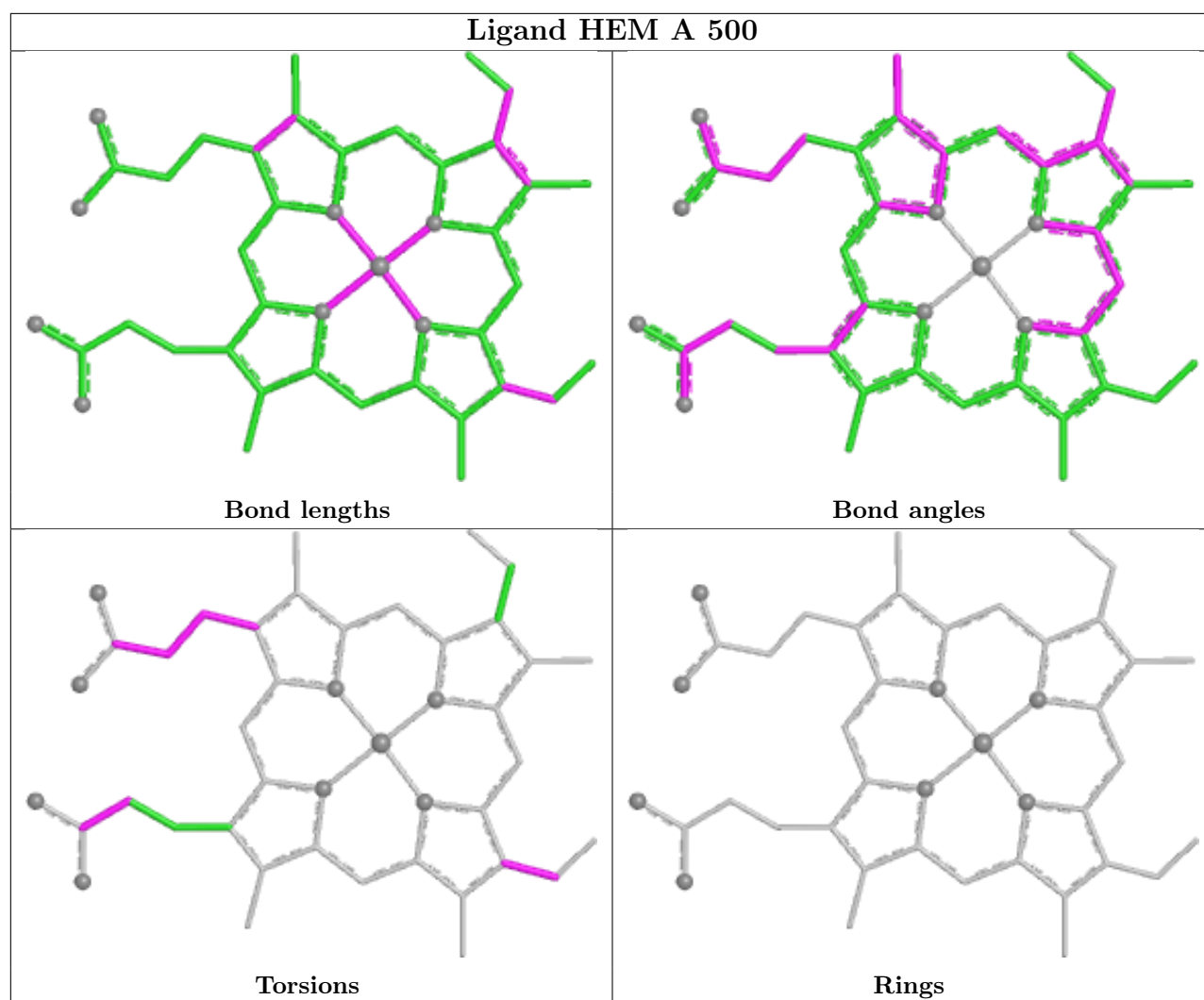
There are no ring outliers.

4 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	OIO	10	0
2	B	500	HEM	4	0
2	A	500	HEM	11	0
3	A	1	OIO	7	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	463/476 (97%)	-1.66	0 100 100	24, 48, 76, 92	0
1	B	463/476 (97%)	-1.65	0 100 100	27, 48, 74, 91	0
All	All	926/952 (97%)	-1.65	0 100 100	24, 48, 75, 92	0

There are no RSRZ outliers to report.

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.

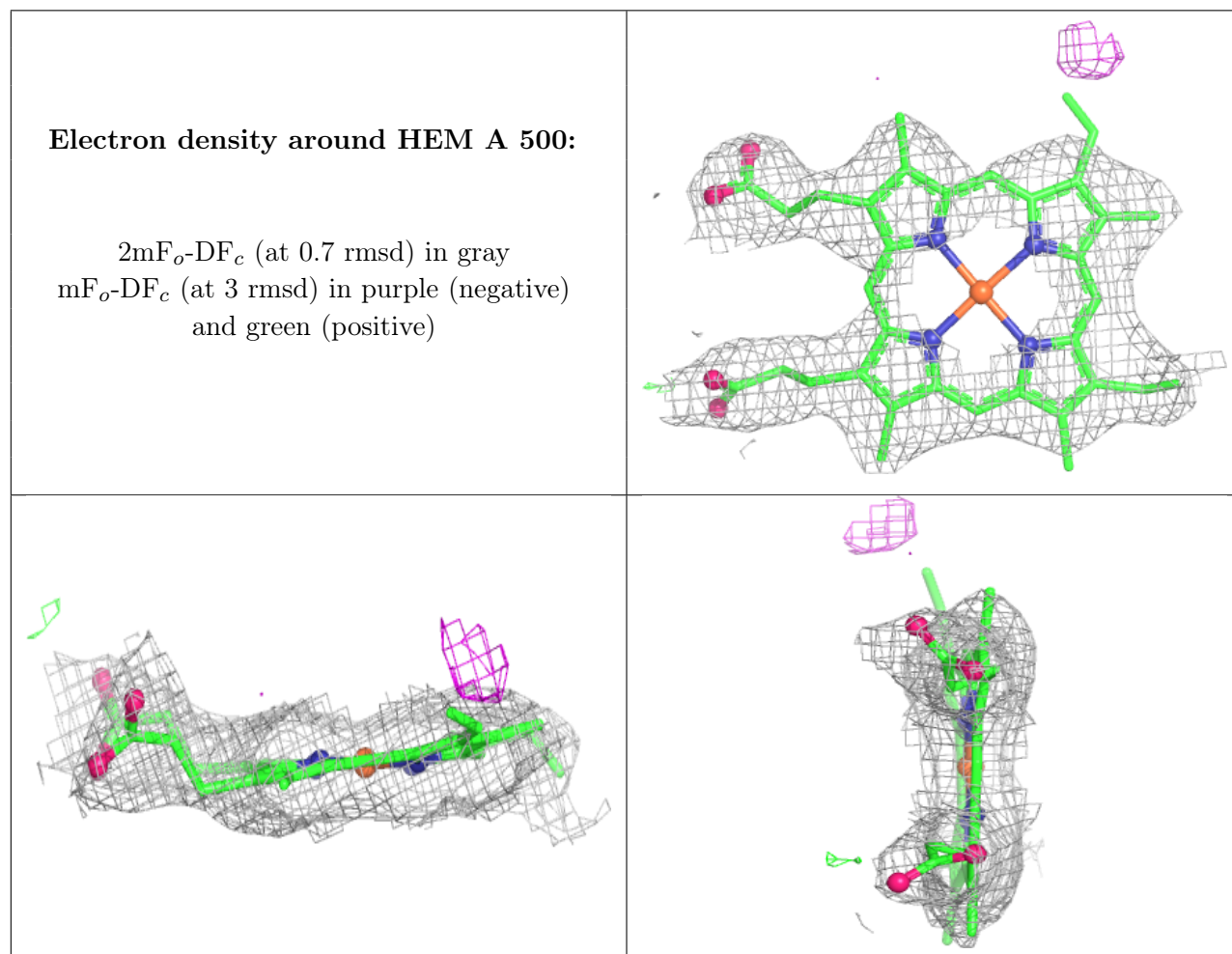
6.4 Ligands [i](#)

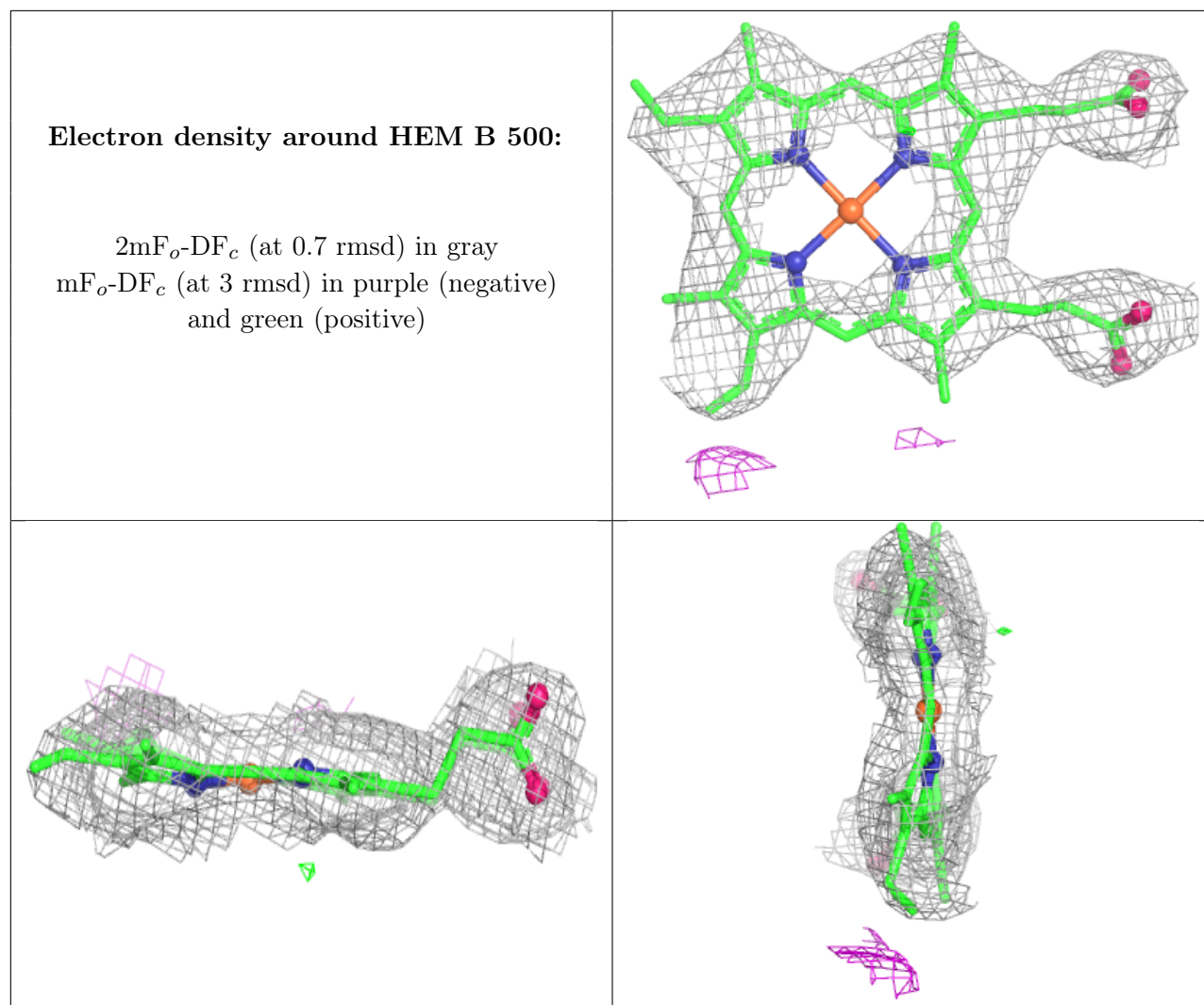
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OIO	A	1	15/15	0.99	0.04	56,61,62,63	0
3	OIO	B	1	15/15	0.99	0.04	56,61,62,63	0
2	HEM	A	500	43/43	1.00	0.03	25,30,37,41	0
2	HEM	B	500	43/43	1.00	0.03	37,41,44,44	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.