



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:54 PM UTC

PDB ID : 5FYF / pdb_00005fyf
Title : Structure of CYP153A from *Marinobacter aquaeolei*
Authors : Danesh Azari, H.R.; Spandolf, C.; Hoffman, S.M.; Weissenborn, M.; Hauer, B.; Grogan, G.
Deposited on : 2016-03-07
Resolution : 2.04 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

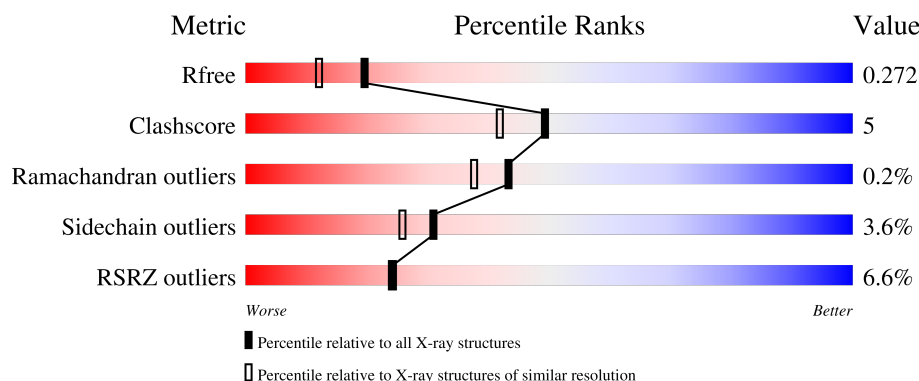
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	470	 4% 78% 9% 11%
1	B	470	 7% 76% 11% 13%

2 Entry composition [i](#)

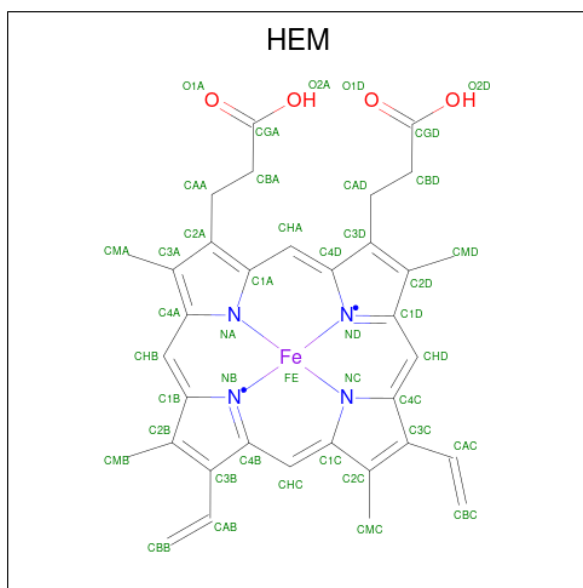
There are 4 unique types of molecules in this entry. The entry contains 6869 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

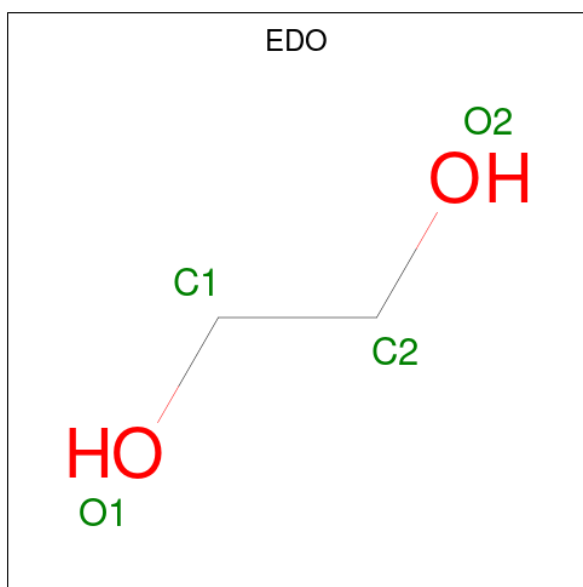
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3281	2080	576	608	17			
1	B	411	Total	C	N	O	S	0	0	0
			3204	2037	559	592	16			

- 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 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

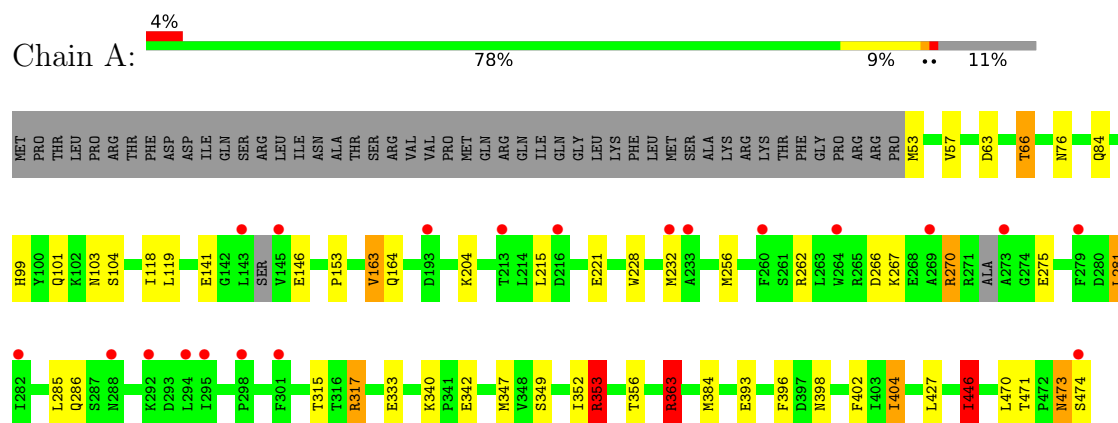
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	184	Total	O	0	0
			184	184		
4	B	102	Total	O	0	0
			102	102		

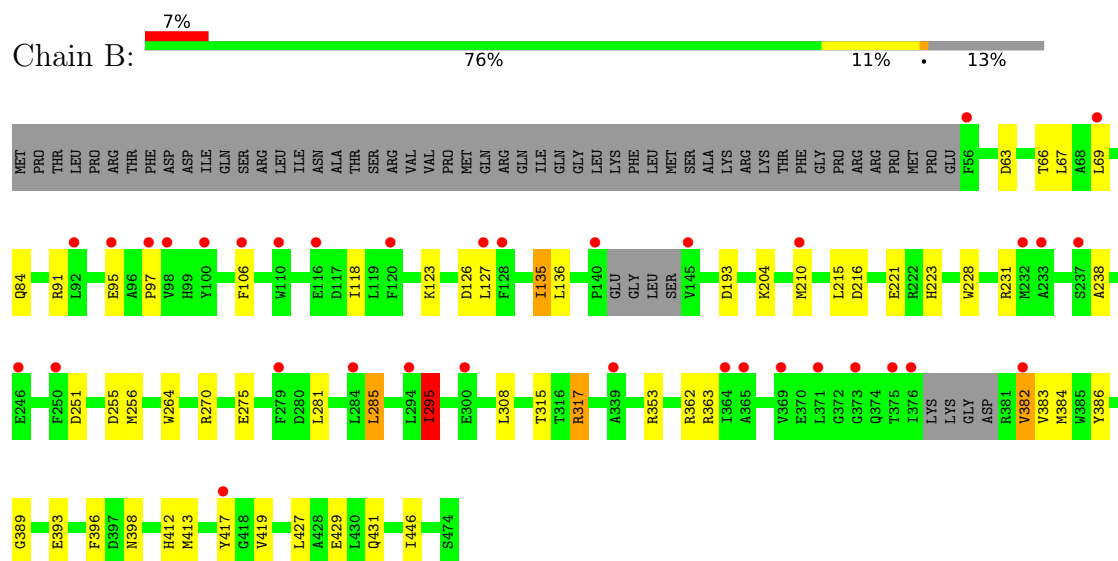
3 Residue-property plots [i](#)

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



• Molecule 1: CYTOCHROME P450



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.59Å 71.11Å 215.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.59 – 2.04 107.59 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.9 (107.59-2.04) 99.9 (107.59-2.04)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.198 , 0.237 0.261 , 0.272	Depositor DCC
R_{free} test set	2918 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6869	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: EDO, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the 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	1.28	11/3356 (0.3%)	1.19	19/4550 (0.4%)
1	B	1.10	3/3279 (0.1%)	1.10	11/4451 (0.2%)
All	All	1.19	14/6635 (0.2%)	1.14	30/9001 (0.3%)

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	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	ARG	C-N	18.96	1.57	1.33
1	A	363	ARG	CD-NE	-7.14	1.36	1.46
1	B	398	ASN	C-O	-7.02	1.20	1.23
1	B	215	LEU	C-N	-6.35	1.26	1.33
1	A	153	PRO	CA-C	6.07	1.55	1.51
1	A	76	ASN	CA-C	5.91	1.59	1.52
1	A	317	ARG	CD-NE	-5.88	1.38	1.46
1	A	349	SER	N-CA	-5.66	1.39	1.46
1	A	99	HIS	N-CA	5.64	1.52	1.46
1	A	398	ASN	C-O	-5.30	1.21	1.23
1	A	104	SER	CA-C	-5.30	1.46	1.52
1	B	429	GLU	CA-C	-5.30	1.45	1.52
1	A	57	VAL	CA-CB	5.26	1.60	1.54
1	A	119	LEU	C-O	-5.25	1.18	1.24

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	LEU	CA-C-N	-14.27	103.67	122.79
1	B	215	LEU	C-N-CA	-14.27	103.67	122.79
1	A	353	ARG	O-C-N	14.08	136.67	122.03
1	A	215	LEU	CA-C-N	-13.58	104.59	122.79
1	A	215	LEU	C-N-CA	-13.58	104.59	122.79
1	A	363	ARG	NE-CZ-NH2	-12.19	108.23	119.20
1	A	363	ARG	NE-CZ-NH1	9.90	131.40	121.50
1	A	363	ARG	CD-NE-CZ	7.49	134.88	124.40
1	B	295	ILE	CB-CA-C	-7.33	101.35	112.05
1	A	317	ARG	NE-CZ-NH2	-6.67	113.20	119.20
1	A	473	ASN	N-CA-C	6.10	120.46	112.89
1	B	295	ILE	N-CA-CB	6.03	120.01	110.54
1	B	215	LEU	N-CA-C	-6.03	100.47	109.94
1	A	317	ARG	NE-CZ-NH1	6.03	127.53	121.50
1	B	215	LEU	O-C-N	-5.89	114.60	122.14
1	B	317	ARG	NE-CZ-NH2	-5.81	113.97	119.20
1	A	317	ARG	CB-CG-CD	-5.76	98.06	111.30
1	A	352	ILE	CA-C-N	-5.66	113.18	120.65
1	A	352	ILE	C-N-CA	-5.66	113.18	120.65
1	A	215	LEU	O-C-N	-5.59	114.98	122.14
1	B	216	ASP	N-CA-C	-5.54	101.25	109.11
1	A	215	LEU	N-CA-C	-5.45	101.39	109.94
1	B	317	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	A	363	ARG	CG-CD-NE	-5.38	100.16	112.00
1	A	446	ILE	CB-CA-C	5.32	120.01	111.29
1	B	216	ASP	CB-CA-C	5.30	119.83	111.72
1	A	163	VAL	N-CA-CB	-5.28	106.40	112.21
1	A	286	GLN	CB-CA-C	5.24	119.45	110.01
1	B	317	ARG	CB-CG-CD	-5.14	99.47	111.30
1	A	363	ARG	CB-CG-CD	5.11	123.06	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	ARG	Mainchain

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	3281	0	3129	33	0
1	B	3204	0	3035	35	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
3	A	8	0	12	1	0
3	B	4	0	6	0	0
4	A	184	0	0	2	0
4	B	102	0	0	3	0
All	All	6869	0	6242	69	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 5.

All (69) 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:386:TYR:HA	1:B:413:MET:HE3	1.41	0.99
1:B:118:ILE:HD13	1:B:413:MET:HE1	1.50	0.92
1:B:210:MET:HE2	1:B:427:LEU:HD11	1.53	0.91
1:A:232:MET:CE	1:A:256:MET:HE1	2.02	0.89
1:B:386:TYR:HA	1:B:413:MET:CE	2.09	0.81
1:B:118:ILE:CD1	1:B:413:MET:HE1	2.11	0.79
1:A:163:VAL:HG23	1:A:281:LEU:HD21	1.64	0.78
1:A:101:GLN:HE21	1:A:103:ASN:H	1.35	0.72
1:B:193:ASP:OD1	4:B:2034:HOH:O	2.07	0.71
1:B:270:ARG:HD2	1:B:275:GLU:OE1	1.90	0.71
1:B:389:GLY:HA3	1:B:413:MET:HE2	1.72	0.70
1:B:136:LEU:HD12	1:B:383:VAL:HG21	1.74	0.70
1:A:363:ARG:HD2	3:A:1476:EDO:O1	1.93	0.69
1:B:204:LYS:HG2	1:B:317:ARG:HD2	1.76	0.68
1:A:204:LYS:HG2	1:A:317:ARG:HD2	1.75	0.68
1:A:402:PHE:CE2	1:A:404:ILE:HD11	2.29	0.67
1:A:232:MET:HE2	1:A:256:MET:HE1	1.77	0.66
1:B:353:ARG:HB2	1:B:412:HIS:HB3	1.79	0.65
1:B:91:ARG:NH1	1:B:95:GLU:OE1	2.29	0.64
1:A:317:ARG:HD3	4:A:2114:HOH:O	1.98	0.64
1:B:264:TRP:NE1	1:B:295:ILE:HG12	2.13	0.63
1:A:471:THR:HG23	4:A:2184:HOH:O	1.98	0.63
1:B:97:PRO:HB3	4:B:2010:HOH:O	2.00	0.61
1:B:210:MET:HG2	1:B:431:GLN:NE2	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ARG:O	1:A:356:THR:OG1	2.21	0.58
1:A:347:MET:HG3	1:A:404:ILE:HD12	1.86	0.56
1:A:232:MET:HE3	1:A:256:MET:HE1	1.86	0.56
1:B:281:LEU:HD22	1:B:308:LEU:HD22	1.87	0.55
1:B:353:ARG:HB2	1:B:412:HIS:CB	2.37	0.55
1:A:204:LYS:CG	1:A:317:ARG:HD2	2.36	0.55
1:B:123:LYS:NZ	1:B:417:TYR:HB3	2.21	0.54
1:B:118:ILE:HD13	1:B:413:MET:CE	2.32	0.54
1:B:204:LYS:CG	1:B:317:ARG:HD2	2.37	0.54
1:B:389:GLY:HA3	1:B:413:MET:CE	2.39	0.53
1:B:135:ILE:O	1:B:362:ARG:HD3	2.10	0.52
1:A:333:GLU:HB3	1:A:404:ILE:HG12	1.91	0.51
1:A:315:THR:HB	2:A:1475:HEM:C3B	2.44	0.51
1:A:266:ASP:O	1:A:270:ARG:CG	2.59	0.50
1:A:340:LYS:CG	1:A:342:GLU:OE2	2.60	0.50
1:A:118:ILE:HG23	1:A:384:MET:HB3	1.94	0.49
1:A:63:ASP:O	1:A:66:THR:HG22	2.13	0.49
1:B:251:ASP:O	1:B:255:ASP:HB2	2.13	0.49
1:B:118:ILE:HG23	1:B:384:MET:HB3	1.95	0.48
1:A:473:ASN:O	1:A:474:SER:OG	2.19	0.48
1:B:363:ARG:HB2	1:B:382:VAL:HG13	1.95	0.48
1:A:228:TRP:CE3	1:A:256:MET:HG3	2.48	0.48
1:A:270:ARG:NE	1:A:275:GLU:OE2	2.46	0.48
1:A:267:LYS:HA	1:A:270:ARG:HG3	1.95	0.48
1:A:266:ASP:O	1:A:270:ARG:HG3	2.14	0.48
1:B:210:MET:CE	1:B:427:LEU:HD11	2.36	0.47
1:B:228:TRP:CE3	1:B:256:MET:HG3	2.50	0.47
1:B:123:LYS:HZ2	1:B:417:TYR:HB3	1.78	0.47
1:A:281:LEU:HD22	1:A:281:LEU:O	2.14	0.46
1:B:315:THR:HB	2:B:1475:HEM:C3B	2.51	0.46
1:A:446:ILE:HG13	1:A:470:LEU:CD2	2.46	0.45
1:A:446:ILE:HG13	1:A:470:LEU:HD23	1.98	0.45
1:B:393:GLU:HA	1:B:396:PHE:O	2.16	0.45
1:A:393:GLU:HA	1:A:396:PHE:O	2.16	0.45
1:A:266:ASP:O	1:A:270:ARG:HG2	2.17	0.45
1:A:163:VAL:HG23	1:A:281:LEU:CD2	2.41	0.44
1:B:223:HIS:HB3	4:B:2014:HOH:O	2.17	0.44
1:B:63:ASP:HB3	1:B:66:THR:HG23	2.00	0.43
1:B:135:ILE:HD12	1:B:238:ALA:HB1	2.01	0.43
1:A:281:LEU:HD22	1:A:285:LEU:HG	2.02	0.42
1:B:281:LEU:HG	1:B:285:LEU:HD22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LEU:HD23	2:A:1475:HEM:HBC2	2.02	0.41
1:A:402:PHE:CE2	1:A:404:ILE:CD1	3.03	0.41
1:B:106:PHE:CB	1:B:136:LEU:HD23	2.50	0.41
2:B:1475:HEM:HMC1	2:B:1475:HEM:HBC2	2.02	0.41

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	414/470 (88%)	401 (97%)	11 (3%)	2 (0%)	24	16
1	B	405/470 (86%)	395 (98%)	10 (2%)	0	100	100
All	All	819/940 (87%)	796 (97%)	21 (3%)	2 (0%)	43	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	GLU
1	A	146	GLU

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	337/413 (82%)	326 (97%)	11 (3%)	33	28
1	B	326/413 (79%)	313 (96%)	13 (4%)	28	22
All	All	663/826 (80%)	639 (96%)	24 (4%)	31	26

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

Mol	Chain	Res	Type
1	A	53	MET
1	A	66	THR
1	A	84	GLN
1	A	164	GLN
1	A	221	GLU
1	A	262	ARG
1	A	270	ARG
1	A	281	LEU
1	A	363	ARG
1	A	404	ILE
1	A	446	ILE
1	B	67	LEU
1	B	69	LEU
1	B	84	GLN
1	B	126	ASP
1	B	127	LEU
1	B	135	ILE
1	B	221	GLU
1	B	231	ARG
1	B	285	LEU
1	B	295	ILE
1	B	382	VAL
1	B	419	VAL
1	B	446	ILE

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

Mol	Chain	Res	Type
1	A	84	GLN
1	A	101	GLN
1	A	133	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	164	GLN
1	A	313	ASN
1	A	411	ASN
1	A	425	ASN
1	B	84	GLN
1	B	133	GLN
1	B	313	ASN
1	B	398	ASN
1	B	431	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](#)

5 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	EDO	B	1476	-	3,3,3	0.34	0	2,2,2	0.34	0
3	EDO	A	1476	-	3,3,3	0.72	0	2,2,2	0.29	0
3	EDO	A	1477	-	3,3,3	0.49	0	2,2,2	0.35	0
2	HEM	B	1475	1	50,50,50	1.86	9 (18%)	67,82,82	1.58	16 (23%)
2	HEM	A	1475	1	50,50,50	1.66	9 (18%)	67,82,82	1.91	17 (25%)

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	EDO	B	1476	-	-	0/1/1/1	-
3	EDO	A	1476	-	-	0/1/1/1	-
3	EDO	A	1477	-	-	1/1/1/1	-
2	HEM	B	1475	1	-	0/14/54/54	-
2	HEM	A	1475	1	-	1/14/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1475	HEM	FE-NB	5.22	2.11	1.94
2	B	1475	HEM	C3B-C4B	4.59	1.53	1.44
2	A	1475	HEM	C1B-NB	-4.52	1.32	1.40
2	B	1475	HEM	C4D-ND	-4.36	1.32	1.40
2	A	1475	HEM	C4A-NA	-4.31	1.31	1.39
2	A	1475	HEM	C4D-ND	-4.24	1.32	1.40
2	B	1475	HEM	FE-NC	4.09	2.08	1.95
2	B	1475	HEM	C4B-NB	-3.86	1.31	1.38
2	A	1475	HEM	C3C-C2C	3.29	1.43	1.37
2	B	1475	HEM	C1B-NB	-3.24	1.34	1.40
2	A	1475	HEM	FE-NC	3.19	2.05	1.95
2	B	1475	HEM	C1D-ND	-2.92	1.33	1.38
2	A	1475	HEM	C3D-C2D	-2.63	1.31	1.36
2	B	1475	HEM	C3C-C2C	2.61	1.42	1.37
2	A	1475	HEM	FE-NA	2.48	2.03	1.95
2	A	1475	HEM	O1A-CGA	2.46	1.30	1.22
2	B	1475	HEM	O2A-CGA	-2.12	1.23	1.30
2	A	1475	HEM	FE-NB	2.03	2.01	1.94

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1475	HEM	CHC-C4B-NB	4.80	129.59	124.42
2	A	1475	HEM	CHD-C4C-NC	4.65	129.51	124.45
2	B	1475	HEM	C1B-NB-C4B	3.76	109.66	105.21
2	A	1475	HEM	C2D-C1D-ND	3.66	114.14	109.90
2	A	1475	HEM	C3D-C4D-ND	3.59	114.11	110.17
2	A	1475	HEM	CHD-C1D-C2D	-3.52	119.47	125.03
2	B	1475	HEM	C4B-C3B-C2B	-3.52	104.05	107.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1475	HEM	C4D-ND-C1D	-3.45	101.12	105.21
2	A	1475	HEM	CHA-C4D-C3D	-3.36	119.03	125.23
2	B	1475	HEM	CHD-C1D-C2D	-3.28	119.86	125.03
2	A	1475	HEM	O2D-CGD-CBD	3.27	124.33	114.00
2	B	1475	HEM	CHC-C4B-NB	3.24	127.91	124.42
2	B	1475	HEM	O2D-CGD-CBD	2.97	123.38	114.00
2	A	1475	HEM	C1B-NB-C4B	2.85	108.58	105.21
2	A	1475	HEM	C4C-NC-C1C	2.81	110.40	105.82
2	A	1475	HEM	C3B-C2B-C1B	2.76	108.48	106.41
2	B	1475	HEM	CHD-C1D-ND	2.70	127.33	124.42
2	A	1475	HEM	CMD-C2D-C1D	2.63	129.15	125.03
2	B	1475	HEM	CHA-C4D-C3D	-2.62	120.39	125.23
2	A	1475	HEM	C4B-C3B-C2B	-2.58	104.91	107.28
2	B	1475	HEM	C2D-C1D-ND	2.51	112.80	109.90
2	B	1475	HEM	C3C-C2C-C1C	-2.50	104.68	107.05
2	A	1475	HEM	O2D-CGD-O1D	-2.49	116.94	123.33
2	B	1475	HEM	CMD-C2D-C1D	2.45	128.86	125.03
2	B	1475	HEM	CHA-C4D-ND	2.33	127.25	124.37
2	B	1475	HEM	CMB-C2B-C1B	2.28	128.59	125.03
2	B	1475	HEM	C1D-C2D-C3D	-2.23	104.64	106.98
2	B	1475	HEM	O1D-CGD-CBD	-2.14	116.32	123.09
2	A	1475	HEM	C1A-CHA-C4D	-2.11	121.28	126.25
2	B	1475	HEM	CAC-C3C-C4C	-2.08	119.85	124.82
2	B	1475	HEM	CAA-C2A-C1A	2.06	128.97	124.94
2	A	1475	HEM	C4C-CHD-C1D	-2.03	121.70	126.02
2	A	1475	HEM	CAD-C3D-C4D	2.03	128.24	124.70

There are no chirality outliers.

All (2) torsion outliers are listed below:

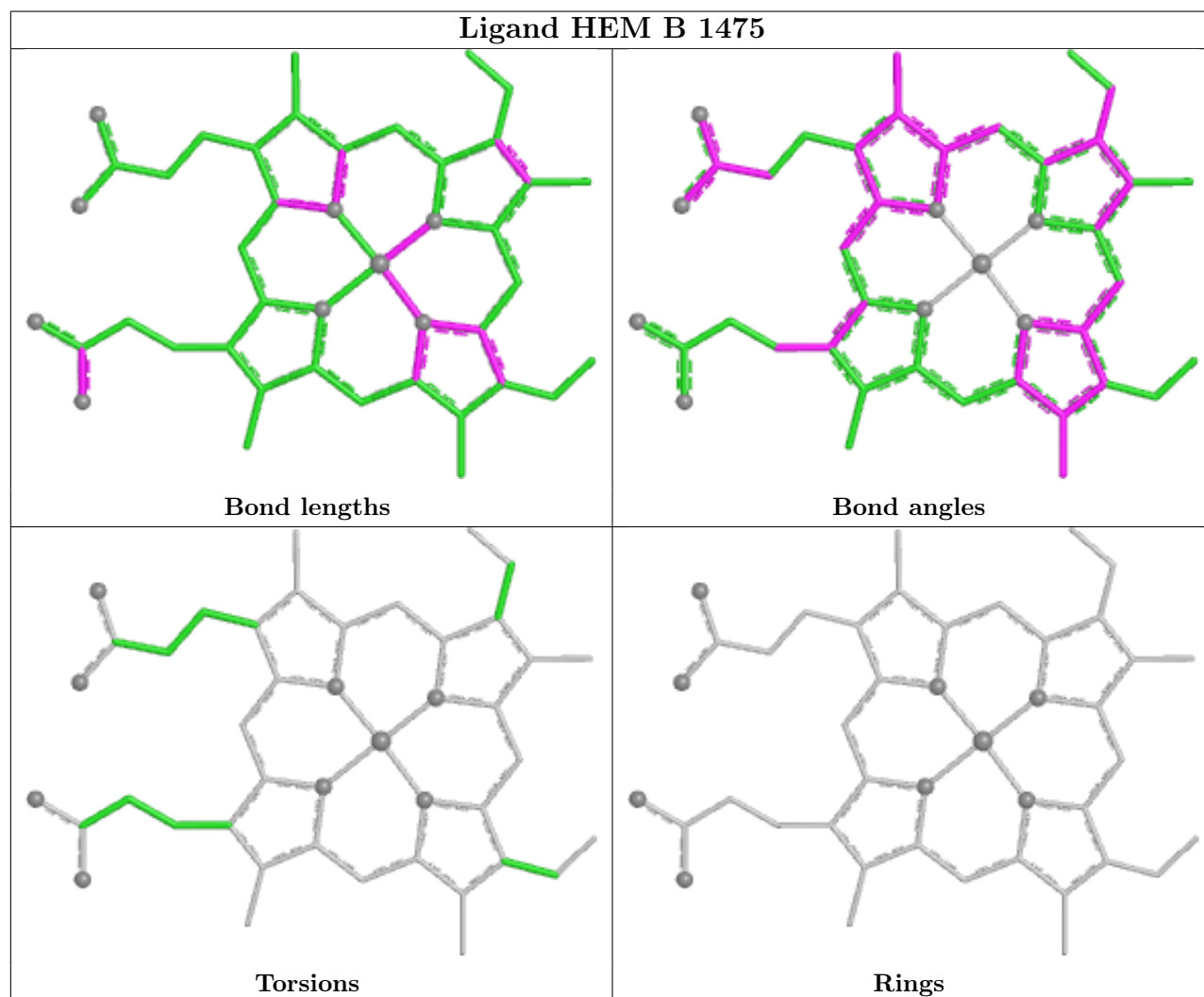
Mol	Chain	Res	Type	Atoms
3	A	1477	EDO	O1-C1-C2-O2
2	A	1475	HEM	C3A-C2A-CAA-CBA

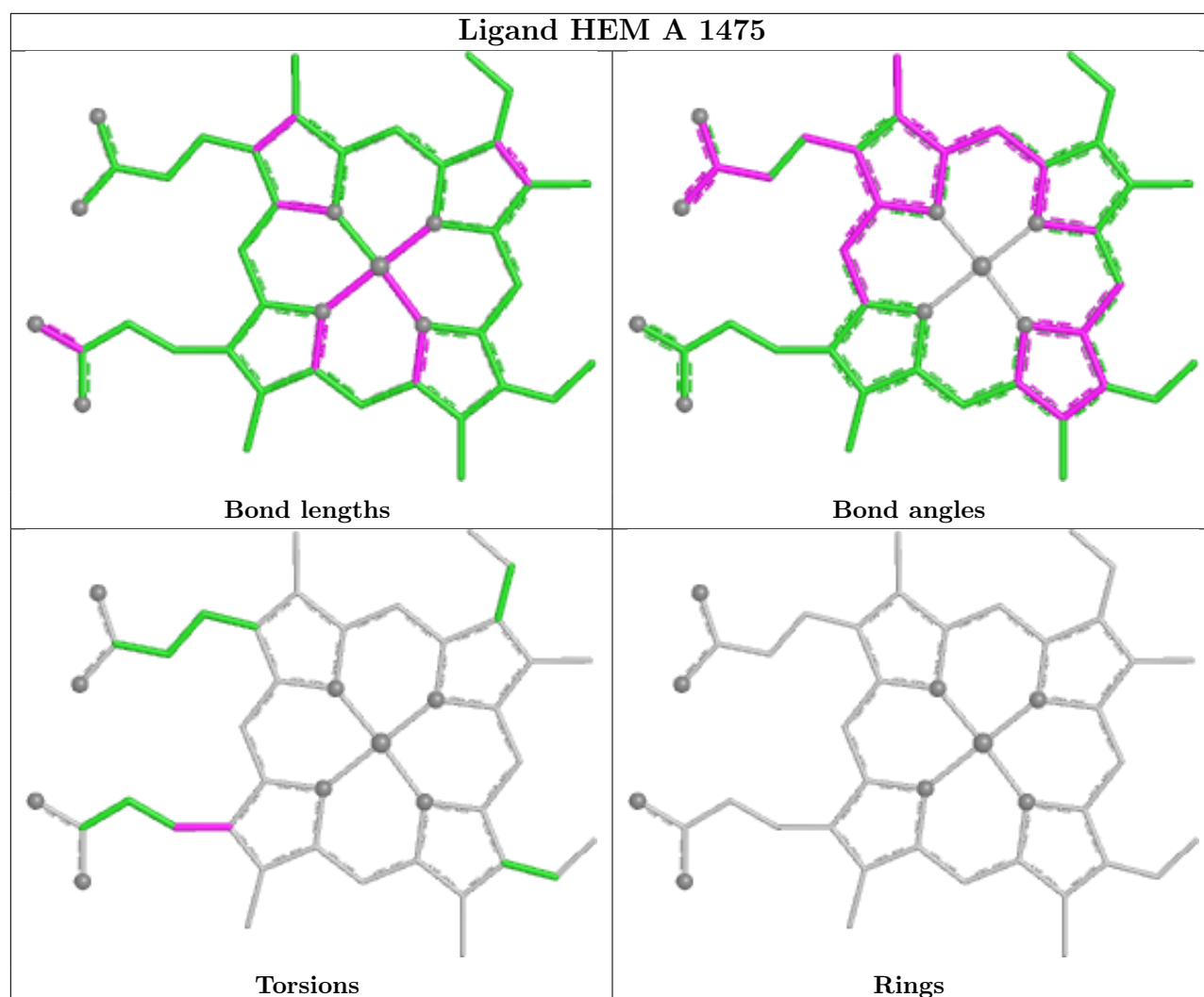
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1476	EDO	1	0
2	B	1475	HEM	2	0
2	A	1475	HEM	2	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	420/470 (89%)	0.18	20 (4%) 35 36	25, 40, 68, 84	0
1	B	411/470 (87%)	0.71	35 (8%) 16 17	30, 51, 78, 97	0
All	All	831/940 (88%)	0.44	55 (6%) 24 24	25, 45, 75, 97	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	145	VAL	5.0
1	B	376	ILE	4.8
1	B	128	PHE	3.9
1	A	264	TRP	3.7
1	A	288	ASN	3.5
1	B	382	VAL	3.5
1	B	284	LEU	3.2
1	B	92	LEU	3.2
1	A	294	LEU	3.2
1	B	369	VAL	3.1
1	B	100	TYR	3.1
1	B	110	TRP	3.1
1	A	269	ALA	3.0
1	B	145	VAL	3.0
1	B	69	LEU	3.0
1	B	365	ALA	2.9
1	B	127	LEU	2.9
1	B	120	PHE	2.9
1	A	295	ILE	2.8
1	A	143	LEU	2.8
1	B	375	THR	2.8
1	B	140	PRO	2.7
1	A	232	MET	2.6
1	B	98	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	371	LEU	2.6
1	A	474	SER	2.6
1	B	116	GLU	2.6
1	A	213	THR	2.6
1	B	97	PRO	2.6
1	A	273	ALA	2.5
1	B	339	ALA	2.5
1	A	301	PHE	2.5
1	A	260	PHE	2.4
1	B	232	MET	2.4
1	B	233	ALA	2.4
1	B	417	TYR	2.3
1	B	373	GLY	2.3
1	B	210	MET	2.3
1	B	56	PHE	2.3
1	B	364	ILE	2.3
1	B	294	LEU	2.2
1	A	193	ASP	2.2
1	A	233	ALA	2.2
1	B	106	PHE	2.2
1	B	250	PHE	2.2
1	B	246	GLU	2.2
1	A	279	PHE	2.1
1	B	95	GLU	2.1
1	A	216	ASP	2.1
1	A	298	PRO	2.1
1	A	282	ILE	2.1
1	B	279	PHE	2.1
1	B	237	SER	2.1
1	B	300	GLU	2.0
1	A	292	LYS	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 ⓘ

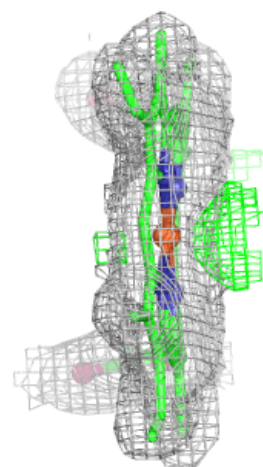
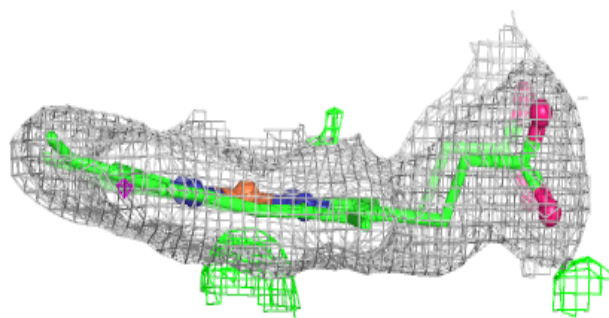
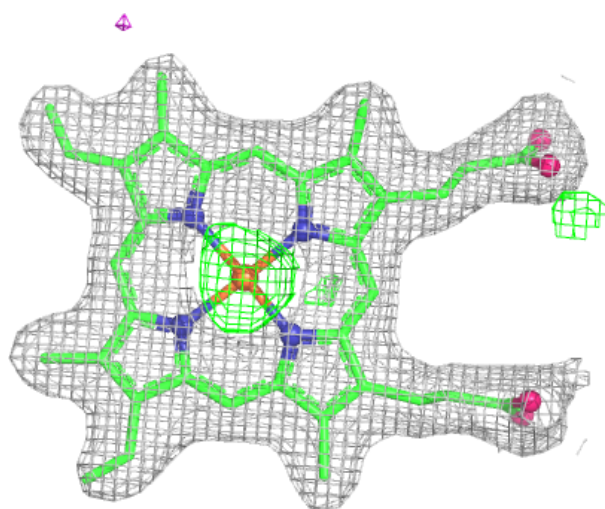
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EDO	A	1477	4/4	0.92	0.10	29,36,37,37	0
3	EDO	A	1476	4/4	0.95	0.09	34,39,40,41	0
3	EDO	B	1476	4/4	0.95	0.08	38,46,46,47	0
2	HEM	B	1475	43/43	0.97	0.08	32,40,46,49	0
2	HEM	A	1475	43/43	0.99	0.05	21,26,30,37	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.

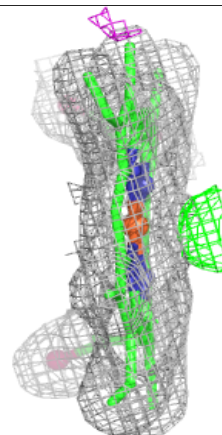
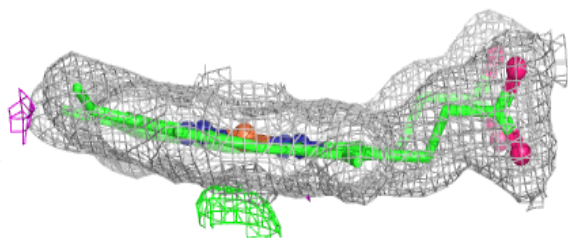
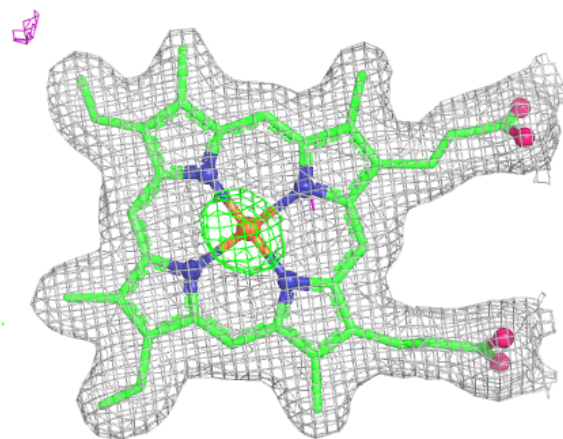
Electron density around HEM B 1475:

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 A 1475:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.