

Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 08:22 AM EST

PDB ID : 3P6N

Title: Crystal Structure of Cytochrome P450cam crystallized in the presence of a

tethered substrate analog AdaC1-C8-Dans

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Deposited on : 2010-10-11

Resolution : 1.70 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.orgA user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

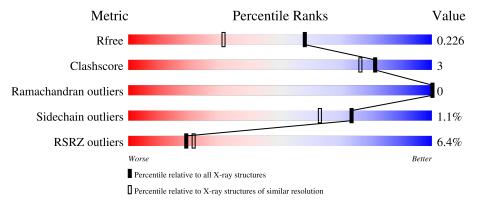
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 1.70 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	
			6%	
1	A	414	91%	6% •



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3617 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.

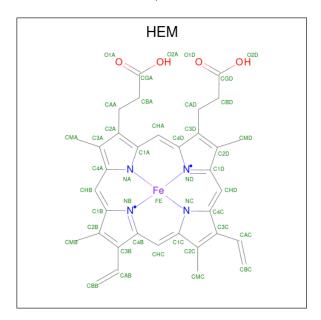
• Molecule 1 is a protein called Camphor 5-monoxygenase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	404	Total	С	N	О	S	0	0	0
1	A	404	3239	2061	560	597	21	0	0	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	ALA	CYS	engineered mutation	UNP P00183

Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



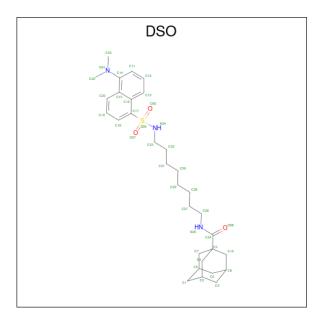
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
2	A	1	Total		Fe	N	O	0	0
			43	34	1	4	4		

• Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0

 \bullet Molecule 4 is ADAMANTANE-1-CARBOXYLIC ACID-5-DIMETHYLAMINO-NAPH THALENE-1-SULFONYLAMINO-OCTYL-AMIDE (three-letter code: DSO) (formula: $C_{31}H_{45}N_3O_3S).$



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
4	A	1	Total 38	C 31	N 3	O 3	S 1	0	0

• Molecule 5 is water.

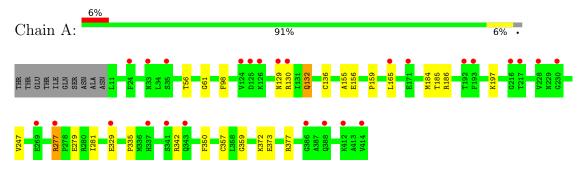
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	296	Total O 296 296	0	0



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: Camphor 5-monooxygenase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	65.24Å 74.76Å 92.86Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 - 1.70	Depositor
Resolution (A)	9.98 - 1.70	EDS
% Data completeness	98.4 (10.00-1.70)	Depositor
(in resolution range)	98.4 (9.98-1.70)	EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	4.09 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
D D.	0.204 , 0.227	Depositor
R, R_{free}	0.204 , 0.226	DCC
R_{free} test set	2520 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.51, 59.6	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3617	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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, K, DSO

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).

Mal	Mol Chain		$\mathbf{lengths}$	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.50	0/3340	0.60	0/4537	

There are no bond length outliers.

There are no bond angle outliers.

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	3239	0	3210	17	0
2	A	43	0	30	1	0
3	A	1	0	0	0	0
4	A	38	0	45	1	0
5	A	296	0	0	2	0
All	All	3617	0	3285	17	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 3.

All (17) 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:377:ARG:HD3	5:A:577:HOH:O	1.79	0.81
1:A:329:GLU:HG3	1:A:335:PRO:HD3	1.73	0.71
1:A:155:ALA:O	1:A:159:PRO:HD2	2.03	0.58
1:A:373:GLU:OE1	1:A:377:ARG:NH1	2.28	0.56
1:A:277:ARG:HG3	1:A:279:GLU:OE2	2.04	0.56
1:A:98:PHE:HE2	1:A:247:VAL:HG21	1.75	0.51
1:A:184:MET:CE	1:A:197:LYS:HA	2.43	0.49
1:A:350:PHE:HB3	1:A:357:CYS:HB3	1.96	0.48
1:A:130:ARG:HG2	1:A:165:LEU:CD2	2.45	0.47
1:A:359:GLY:HA3	2:A:420:HEM:C3C	2.52	0.44
1:A:130:ARG:HG2	1:A:165:LEU:HD21	1.99	0.44
1:A:156:GLU:CD	1:A:186:ARG:HH12	2.21	0.44
1:A:281:ILE:HD13	1:A:372:LYS:HG3	1.99	0.44
1:A:136[B]:CYS:SG	1:A:377:ARG:NH2	2.90	0.44
1:A:185:THR:HG22	4:A:440:DSO:H262	2.00	0.44
1:A:132:GLN:NE2	5:A:706:HOH:O	2.51	0.43
1:A:56:THR:O	1:A:61:GLY:HA2	2.17	0.43

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			
1	A	410/414 (99%)	403 (98%)	7 (2%)	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	Analysed Rotameric Outliers		Percentiles	
1	A	356/357 (100%)	352 (99%)	4 (1%)	73 63	

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	132	GLN
1	A	277	ARG
1	A	342	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	GLN
1	A	213	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	Tuno	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	gles
WIOI	Туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	DSO	A	440	-	42,42,42	2.46	1 (2%)	61,61,61	1.61	7 (11%)
2	HEM	A	420	1	41,50,50	1.88	6 (14%)	45,82,82	1.63	11 (24%)

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
4	DSO	A	440	-	-	6/30/57/57	0/6/5/5
2	HEM	A	420	1	-	2/12/54/54	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
4	A	440	DSO	C17-S36	-15.24	1.62	1.77
2	A	420	HEM	C3D-C2D	7.35	1.52	1.36
2	A	420	HEM	C3C-C2C	-4.30	1.34	1.40
2	A	420	HEM	C3C-CAC	3.38	1.54	1.47
2	A	420	HEM	CAA-C2A	3.02	1.56	1.52
2	A	420	HEM	CAB-C3B	2.70	1.54	1.47
2	A	420	HEM	CMD-C2D	2.14	1.55	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
4	A	440	DSO	O37-S36-O35	-8.45	109.17	119.55
2	A	420	HEM	C4D-ND-C1D	5.36	110.61	105.07
4	A	440	DSO	C26-N25-C24	3.66	128.79	122.12
2	A	420	HEM	CAD-CBD-CGD	-3.22	106.68	113.60
4	A	440	DSO	C15-C14-N21	3.08	122.66	118.23
4	A	440	DSO	O35-S36-N34	2.59	111.09	107.04
2	A	420	HEM	C4C-CHD-C1D	2.55	125.92	122.56
4	A	440	DSO	C11-C14-N21	-2.50	117.91	121.68
2	A	420	HEM	C1B-NB-C4B	2.37	107.52	105.07
2	A	420	HEM	CMA-C3A-C4A	-2.34	124.88	128.46
4	A	440	DSO	C23-N21-C14	2.33	121.05	114.12
2	A	420	HEM	C1D-C2D-C3D	-2.21	104.63	106.96

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Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	420	HEM	O1A-CGA-CBA	-2.19	116.04	123.08
2	A	420	HEM	C4B-CHC-C1C	2.14	125.39	122.56
2	A	420	HEM	C4A-C3A-C2A	2.14	108.48	107.00
2	A	420	HEM	CHA-C4D-ND	2.13	127.02	124.38
4	A	440	DSO	C13-C16-C17	-2.11	120.83	123.60
2	A	420	HEM	O2A-CGA-CBA	2.02	120.50	114.03

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	440	DSO	C31-C32-C33-N34
4	A	440	DSO	C27-C28-C29-C30
4	A	440	DSO	C28-C29-C30-C31
4	A	440	DSO	C26-C27-C28-C29
4	A	440	DSO	C29-C30-C31-C32
2	A	420	HEM	CAD-CBD-CGD-O2D
4	A	440	DSO	C30-C31-C32-C33
2	A	420	HEM	CAD-CBD-CGD-O1D

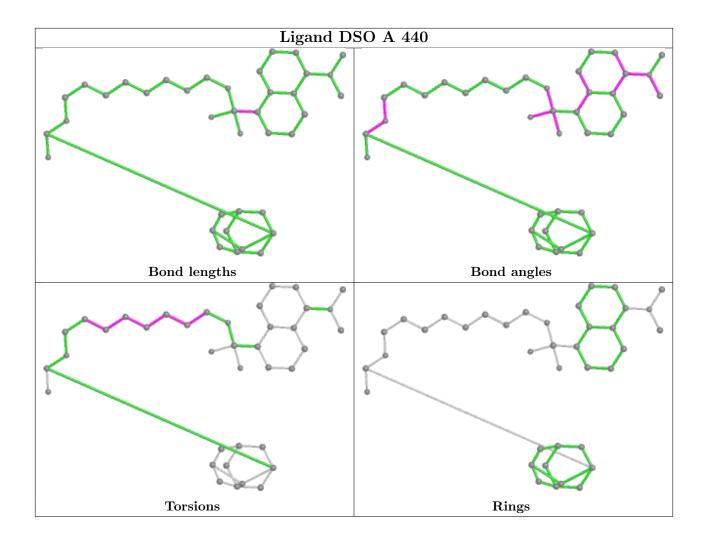
There are no ring outliers.

2 monomers are involved in 2 short contacts:

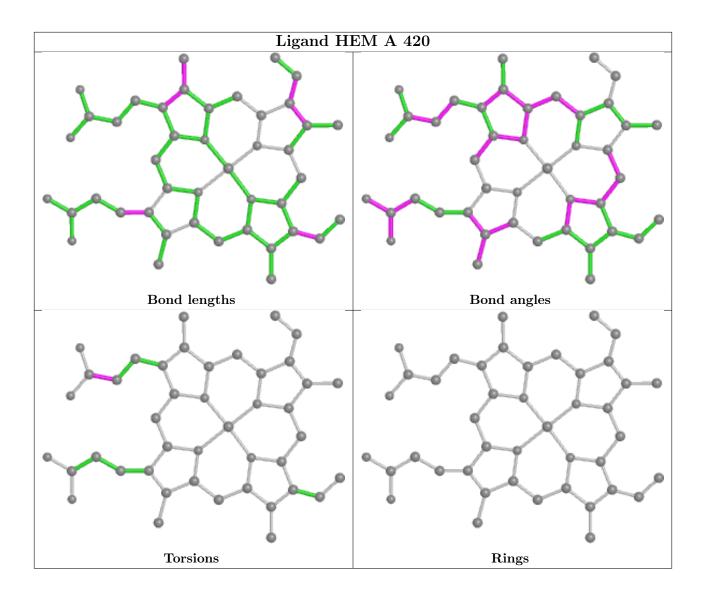
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	440	DSO	1	0
2	A	420	HEM	1	0

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 then 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, 95^{th} 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	$\langle { m RSRZ} \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q < 0.9
1	A	404/414 (97%)	0.26	26 (6%) 19 21	9, 18, 30, 37	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	414	VAL	5.0
1	A	33	ASN	4.0
1	A	386	GLY	3.5
1	A	126	LYS	3.4
1	A	165	LEU	3.3
1	A	125	ASP	3.1
1	A	217	THR	3.1
1	A	343	GLN	3.0
1	A	35	SER	2.9
1	A	269	GLU	2.8
1	A	193	PHE	2.8
1	A	412	LYS	2.6
1	A	129	ASN	2.6
1	A	171	GLU	2.6
1	A	130	ARG	2.5
1	A	192	THR	2.4
1	A	388	GLN	2.3
1	A	341	SER	2.3
1	A	216	GLY	2.3
1	A	228	VAL	2.2
1	A	329	GLU	2.2
1	A	124	VAL	2.1
1	A	337	HIS	2.1
1	A	24[A]	PHE	2.1
1	A	277	ARG	2.0
1	A	230	GLY	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 monosaccharides in this entry.

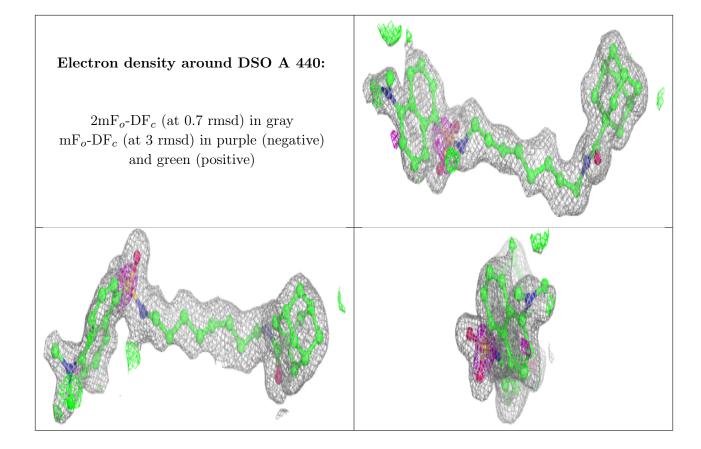
6.4 Ligands (i)

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, 95^{th} 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.

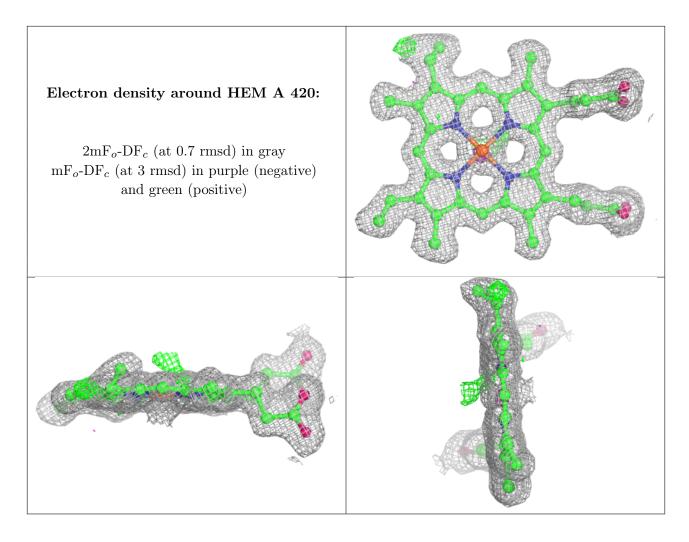
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	DSO	A	440	38/38	0.89	0.12	14,31,36,37	0
2	HEM	A	420	43/43	0.98	0.07	8,10,12,15	0
3	K	A	430	1/1	0.99	0.12	20,20,20,20	0

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 (i)

There are no such residues in this entry.

