



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:40 am BST

PDB ID : 2JJN  
Title : Structure of closed cytochrome P450 EryK  
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Deposited on : 2008-04-15  
Resolution : 1.59 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 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) : 2.11

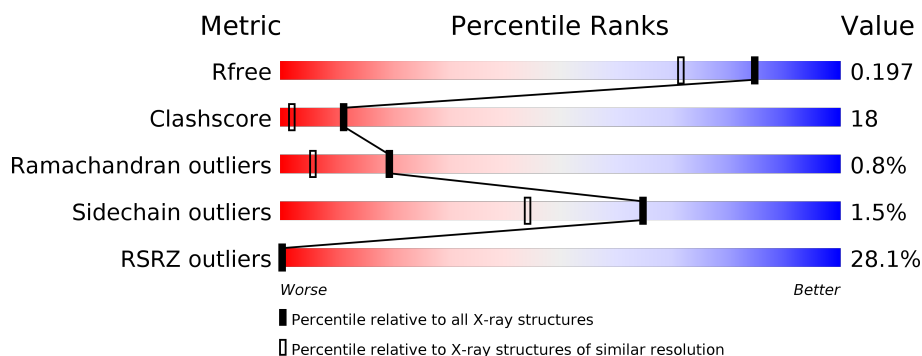
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.59 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))
$R_{free}$	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	411	<div> <div>27%</div> <div>75%</div> <div>19%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3842 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 113A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	395	3223	2015	569	626	13	0	50	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	LEU	MET	engineered mutation	UNP P48635
A	344	LEU	PHE	engineered mutation	UNP P48635

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



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

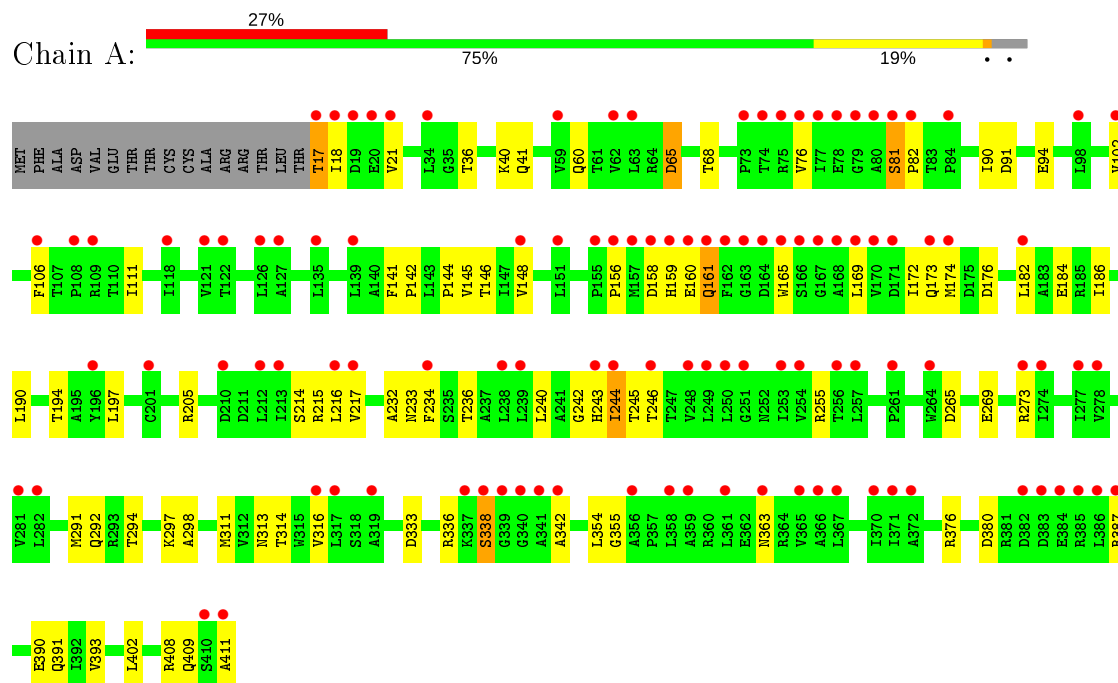
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	551	Total	O	0	0
			551	551		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 113A1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.46Å 68.00Å 57.41Å 90.00° 101.05° 90.00°	Depositor
Resolution (Å)	56.34 – 1.59 26.23 – 1.59	Depositor EDS
% Data completeness (in resolution range)	98.8 (56.34-1.59) 98.8 (26.23-1.59)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.86 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.160 , 0.195 0.163 , 0.197	Depositor DCC
$R_{free}$ test set	2725 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.2	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 64.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3842	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.84% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: HEM, SO4

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	0.76	0/3561	0.87	13/4859 (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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273[A]	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	273[B]	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	376	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	408[A]	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	408[B]	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	408[A]	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	408[B]	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	273[A]	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	273[B]	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	255	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	A	376	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	205	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	65	ASP	CB-CG-OD2	-5.05	113.76	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	THR	Peptide

## 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	3223	0	3200	116	1
2	A	43	0	30	4	0
3	A	25	0	0	3	0
4	A	551	0	0	23	1
All	All	3842	0	3230	118	2

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 18.

All (118) 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:102[B]:VAL:HG11	1:A:234:PHE:CZ	1.78	1.18
1:A:165[B]:TRP:CD1	1:A:243[B]:HIS:NE2	2.25	1.04
1:A:174[B]:MET:HG2	1:A:182[B]:LEU:HD11	1.38	1.03
1:A:18:ILE:HG12	4:A:2005:HOH:O	1.55	1.03
1:A:165[B]:TRP:HE1	1:A:243[B]:HIS:CE1	1.76	1.02
1:A:194[B]:THR:HG22	1:A:236[B]:THR:HG21	1.07	1.01
1:A:165[B]:TRP:HE3	1:A:169[B]:LEU:HD13	1.20	1.01
1:A:102[B]:VAL:HG11	1:A:234:PHE:CE2	1.97	1.00
1:A:145:VAL:CG1	1:A:243[A]:HIS:CE1	2.51	0.93
1:A:194[B]:THR:HG22	1:A:236[B]:THR:CG2	1.99	0.90
1:A:194[B]:THR:CG2	1:A:236[B]:THR:HG21	2.00	0.90
1:A:17:THR:HG22	1:A:18:ILE:H	1.38	0.89
1:A:145:VAL:HG12	1:A:243[A]:HIS:CE1	2.07	0.88
1:A:165[B]:TRP:CE3	1:A:169[B]:LEU:HD13	2.09	0.87
1:A:165[B]:TRP:CD1	1:A:243[B]:HIS:CD2	2.62	0.86
1:A:165[B]:TRP:NE1	1:A:243[B]:HIS:NE2	2.24	0.85
1:A:342:ALA:O	3:A:417:SO4:O4	1.96	0.83
1:A:76:VAL:HG21	1:A:311[B]:MET:CG	2.10	0.81
1:A:165[A]:TRP:CZ3	1:A:244[A]:ILE:HD13	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165[B]:TRP:NE1	1:A:243[B]:HIS:CE1	2.50	0.79
1:A:338:SER:HB3	4:A:2543:HOH:O	1.82	0.79
1:A:194[B]:THR:HG21	4:A:2324:HOH:O	1.83	0.78
1:A:36[A]:THR:HG21	4:A:2035:HOH:O	1.83	0.78
1:A:165[B]:TRP:CD2	1:A:244[B]:ILE:HG12	2.20	0.76
1:A:102[B]:VAL:CG1	1:A:234:PHE:CE2	2.69	0.76
1:A:291[B]:MET:CE	1:A:316[B]:VAL:HG11	2.17	0.75
1:A:18:ILE:CG1	4:A:2005:HOH:O	2.22	0.74
3:A:414:SO4:O2	4:A:2543:HOH:O	2.04	0.74
1:A:165[A]:TRP:CE3	1:A:244[A]:ILE:HD13	2.21	0.74
1:A:144:PRO:HG3	1:A:246[B]:THR:HG22	1.69	0.73
1:A:21:VAL:HG21	4:A:2404:HOH:O	1.87	0.72
1:A:165[B]:TRP:HD1	1:A:243[B]:HIS:NE2	1.85	0.72
1:A:90:ILE:HG23	1:A:94[B]:GLU:HG3	1.70	0.71
1:A:165[A]:TRP:HE1	1:A:243[A]:HIS:CE1	2.09	0.71
1:A:76:VAL:HG13	1:A:294[B]:THR:HG21	1.70	0.71
1:A:148[A]:VAL:HG23	4:A:2475:HOH:O	1.90	0.70
1:A:91:ASP:O	1:A:94[B]:GLU:HG2	1.91	0.70
1:A:76:VAL:HG21	1:A:311[B]:MET:HG3	1.74	0.69
1:A:232:ALA:O	1:A:236[B]:THR:HG23	1.93	0.69
1:A:142:PRO:O	1:A:145:VAL:HG22	1.92	0.69
1:A:17:THR:HG22	1:A:18:ILE:N	2.08	0.69
1:A:102[B]:VAL:HG13	1:A:216:LEU:HD21	1.77	0.66
1:A:165[B]:TRP:HD1	1:A:243[B]:HIS:CD2	2.12	0.66
1:A:90:ILE:CG2	1:A:94[B]:GLU:HG3	2.26	0.65
1:A:165[B]:TRP:CZ3	1:A:244[B]:ILE:HG23	2.32	0.65
1:A:380:ASP:HB2	1:A:402[A]:LEU:HG	1.79	0.64
1:A:76:VAL:HG21	1:A:311[B]:MET:HG2	1.79	0.64
1:A:165[A]:TRP:CZ3	1:A:244[A]:ILE:CD1	2.82	0.63
1:A:246[A]:THR:HG23	1:A:363:ASN:HD21	1.64	0.63
1:A:165[B]:TRP:HE3	1:A:169[B]:LEU:CD1	2.04	0.62
1:A:174[B]:MET:HG2	1:A:182[B]:LEU:CD1	2.24	0.61
1:A:18:ILE:CD1	4:A:2005:HOH:O	2.46	0.60
1:A:233:ASN:O	1:A:236[B]:THR:OG1	2.18	0.60
1:A:390[B]:GLU:CG	4:A:2511:HOH:O	2.51	0.58
1:A:291[B]:MET:HE1	1:A:316[B]:VAL:HG11	1.85	0.58
1:A:297[A]:LYS:HE2	4:A:2128:HOH:O	2.04	0.58
1:A:102[B]:VAL:CG1	1:A:234:PHE:CZ	2.71	0.57
1:A:76:VAL:HG13	1:A:294[B]:THR:CG2	2.34	0.57
1:A:246[A]:THR:HG23	1:A:363:ASN:ND2	2.21	0.56
1:A:165[B]:TRP:HZ3	1:A:169[B]:LEU:HD22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244[A]:ILE:HG23	1:A:245:THR:N	2.20	0.56
1:A:145:VAL:HG13	1:A:243[A]:HIS:NE2	2.22	0.55
1:A:240:LEU:O	1:A:244[A]:ILE:HG22	2.07	0.55
1:A:68[B]:THR:HG21	4:A:2414:HOH:O	2.07	0.55
1:A:354:LEU:HD11	4:A:2202:HOH:O	2.05	0.54
1:A:242:GLY:HA2	2:A:412:HEM:C2C	2.43	0.54
1:A:60:GLN:NE2	4:A:2106:HOH:O	2.39	0.54
1:A:65:ASP:CG	1:A:68[B]:THR:OG1	2.46	0.54
1:A:18:ILE:HG13	1:A:18:ILE:O	2.07	0.54
1:A:390[B]:GLU:CD	4:A:2511:HOH:O	2.46	0.53
1:A:244[A]:ILE:HG23	1:A:245:THR:HG23	1.91	0.52
1:A:106[B]:PHE:CE2	1:A:111:ILE:HD11	2.44	0.52
1:A:161:GLN:NE2	4:A:2290:HOH:O	2.40	0.51
1:A:165[B]:TRP:CE3	1:A:244[B]:ILE:HG12	2.45	0.51
1:A:291[B]:MET:HG3	1:A:314:THR:OG1	2.12	0.50
1:A:215[B]:ARG:HD2	4:A:2342:HOH:O	2.12	0.50
1:A:145:VAL:CG1	1:A:243[A]:HIS:NE2	2.76	0.49
1:A:18:ILE:HD11	4:A:2005:HOH:O	2.12	0.48
1:A:81[A]:SER:OG	1:A:82:PRO:HD2	2.14	0.48
3:A:416:SO4:O3	4:A:2547:HOH:O	2.19	0.47
1:A:292[A]:GLN:HG3	1:A:313[A]:ASN:ND2	2.29	0.47
1:A:294[A]:THR:HG23	4:A:2410:HOH:O	2.15	0.47
1:A:355:GLY:HA3	2:A:412:HEM:C3C	2.50	0.46
1:A:333:ASP:O	1:A:336:ARG:HG2	2.16	0.46
1:A:402[B]:LEU:HD21	4:A:2282:HOH:O	2.15	0.46
1:A:245:THR:HB	2:A:412:HEM:CAB	2.45	0.46
1:A:65:ASP:OD2	1:A:68[B]:THR:OG1	2.34	0.46
1:A:145:VAL:HG13	1:A:243[A]:HIS:CE1	2.45	0.46
1:A:145:VAL:HG23	1:A:146:THR:N	2.30	0.46
1:A:269[B]:GLU:HG3	4:A:2390:HOH:O	2.16	0.46
1:A:158:ASP:O	1:A:160:GLU:N	2.49	0.45
1:A:182[B]:LEU:HD23	1:A:186:ILE:HD12	1.99	0.45
1:A:172:ILE:O	1:A:174[A]:MET:HG3	2.18	0.44
1:A:265:ASP:O	1:A:269[B]:GLU:HG3	2.17	0.44
1:A:76:VAL:CG1	1:A:294[B]:THR:CG2	2.96	0.44
1:A:242:GLY:HA2	2:A:412:HEM:CMC	2.47	0.44
1:A:197:LEU:HD12	1:A:236[B]:THR:HG22	1.99	0.44
1:A:214:SER:HA	1:A:217[B]:VAL:HG22	2.00	0.43
1:A:36[B]:THR:CG2	1:A:40[B]:LYS:HD2	2.49	0.43
1:A:18:ILE:CG1	1:A:18:ILE:O	2.67	0.43
1:A:165[B]:TRP:CG	1:A:244[B]:ILE:HG12	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102[B]:VAL:HG13	1:A:216:LEU:CD2	2.48	0.42
1:A:145:VAL:HG12	1:A:243[A]:HIS:ND1	2.32	0.42
1:A:297[B]:LYS:NZ	1:A:298:ALA:O	2.48	0.42
1:A:41:GLN:HE21	1:A:41:GLN:HA	1.84	0.42
1:A:190:LEU:HD22	1:A:240:LEU:HD11	2.03	0.41
1:A:184:GLU:HB3	4:A:2314:HOH:O	2.20	0.41
1:A:244[A]:ILE:HD11	1:A:393:VAL:HG11	2.03	0.41
1:A:141:PHE:HB3	1:A:142:PRO:HD3	2.02	0.40
1:A:145:VAL:CG2	1:A:146:THR:N	2.83	0.40
1:A:165[B]:TRP:CZ3	1:A:169[B]:LEU:HD22	2.52	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ILE:CD1	1:A:411:ALA:O[1_554]	1.72	0.48
4:A:2162:HOH:O	4:A:2282:HOH:O[1_655]	1.99	0.21

## 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	446/411 (108%)	432 (97%)	11 (2%)	3 (1%)	22   7

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	SER
1	A	156	PRO
1	A	159	HIS

### 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	378/343 (110%)	369 (98%)	9 (2%)	49 24

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81[A]	SER
1	A	81[B]	SER
1	A	81[C]	SER
1	A	161	GLN
1	A	244[A]	ILE
1	A	244[B]	ILE
1	A	387[A]	ARG
1	A	387[B]	ARG
1	A	391	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	45	GLN
1	A	60	GLN
1	A	363	ASN
1	A	409	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 carbohydrates in this entry.

## 5.6 Ligand geometry

6 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	SO4	A	415	-	4,4,4	0.15	0	6,6,6	0.33	0
2	HEM	A	412	1,4	27,50,50	2.00	9 (33%)	17,82,82	1.64	3 (17%)
3	SO4	A	414	-	4,4,4	0.25	0	6,6,6	0.61	0
3	SO4	A	413	-	4,4,4	0.14	0	6,6,6	0.34	0
3	SO4	A	417	-	4,4,4	0.37	0	6,6,6	0.74	0
3	SO4	A	416	-	4,4,4	0.19	0	6,6,6	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	412	1,4	-	0/6/54/54	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	412	HEM	C3D-C2D	4.12	1.49	1.37
2	A	412	HEM	C3C-C2C	-3.54	1.35	1.40
2	A	412	HEM	C3B-C2B	-3.31	1.35	1.40
2	A	412	HEM	C3C-CAC	3.28	1.54	1.47
2	A	412	HEM	C3B-CAB	3.25	1.54	1.47
2	A	412	HEM	C1D-ND	2.55	1.41	1.36
2	A	412	HEM	C1A-NA	2.33	1.41	1.36
2	A	412	HEM	CMD-C2D	2.22	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	412	HEM	C4A-NA	2.15	1.40	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	412	HEM	CMB-C2B-C3B	3.86	131.90	124.68
2	A	412	HEM	CMC-C2C-C3C	2.72	129.78	124.68
2	A	412	HEM	CMA-C3A-C4A	-2.29	124.94	128.46

There are no chirality outliers.

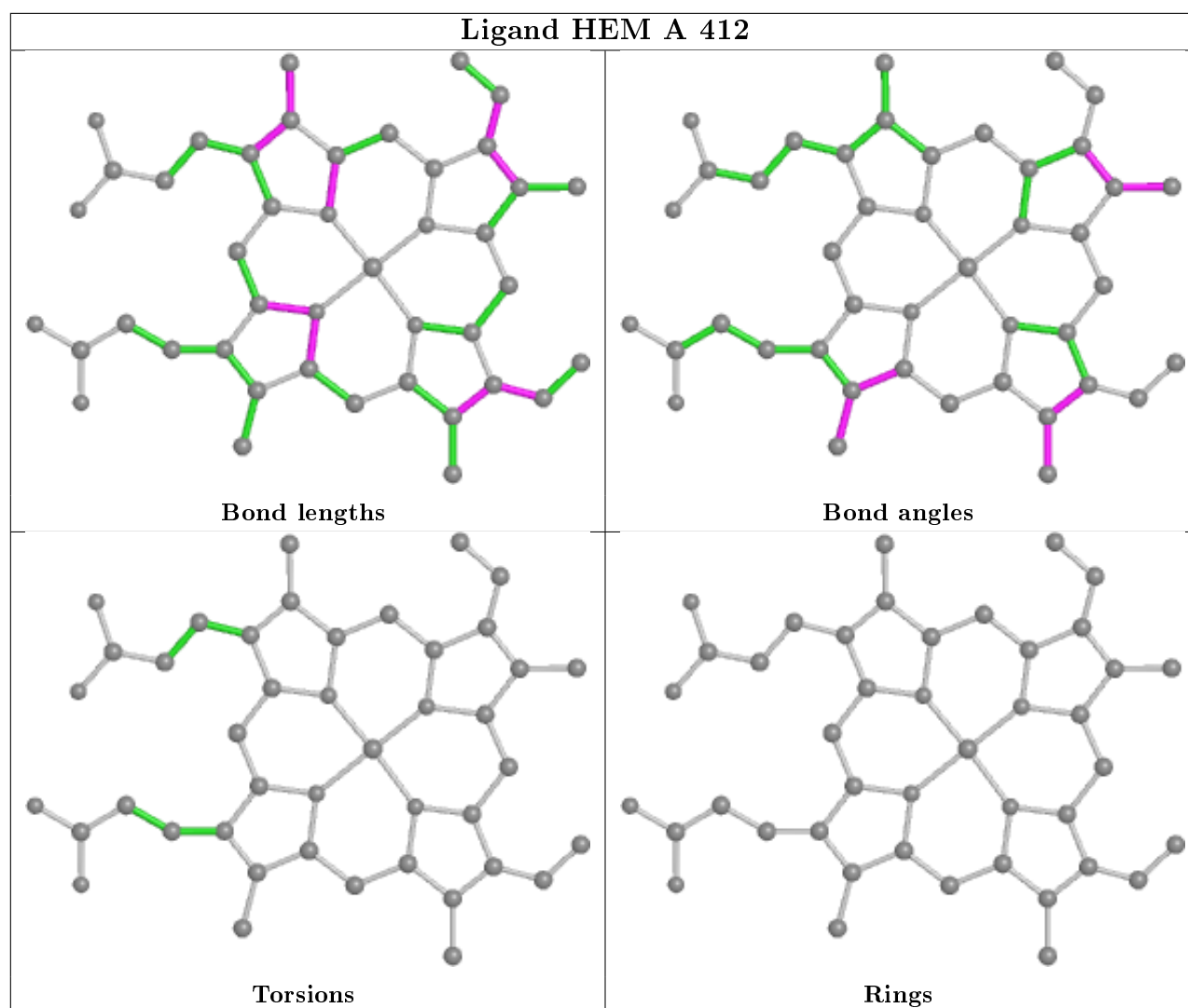
There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	412	HEM	4	0
3	A	414	SO4	1	0
3	A	417	SO4	1	0
3	A	416	SO4	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	395/411 (96%)	1.49	111 (28%) 0 0	10, 20, 38, 65	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	ILE	17.2
1	A	17	THR	13.7
1	A	156	PRO	12.3
1	A	339	GLY	11.3
1	A	158	ASP	9.9
1	A	159	HIS	8.6
1	A	162	PHE	7.9
1	A	341	ALA	7.8
1	A	161	GLN	7.8
1	A	157	MET	7.6
1	A	383	ASP	7.3
1	A	338	SER	7.0
1	A	340	GLY	6.9
1	A	165[A]	TRP	6.8
1	A	160	GLU	6.6
1	A	337	LYS	6.2
1	A	21	VAL	6.0
1	A	80	ALA	5.9
1	A	79	GLY	5.4
1	A	370	ILE	5.3
1	A	411	ALA	5.1
1	A	81[A]	SER	5.0
1	A	249	LEU	4.9
1	A	74	THR	4.7
1	A	77	ILE	4.6
1	A	382	ASP	4.6
1	A	155	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	384	GLU	4.5
1	A	126	LEU	4.4
1	A	316[A]	VAL	4.4
1	A	78[A]	GLU	4.4
1	A	254	VAL	4.3
1	A	163	GLY	4.2
1	A	82	PRO	4.2
1	A	250	LEU	4.0
1	A	253	ILE	3.9
1	A	164	ASP	3.7
1	A	106[A]	PHE	3.7
1	A	257	LEU	3.6
1	A	108	PRO	3.6
1	A	282	LEU	3.5
1	A	173[A]	GLN	3.5
1	A	76	VAL	3.5
1	A	217[A]	VAL	3.5
1	A	239[A]	LEU	3.4
1	A	73	PRO	3.4
1	A	212	LEU	3.4
1	A	59	VAL	3.4
1	A	365	VAL	3.4
1	A	281	VAL	3.2
1	A	139	LEU	3.1
1	A	367	LEU	3.1
1	A	62	VAL	3.1
1	A	371	ILE	3.1
1	A	210[A]	ASP	3.1
1	A	358	LEU	3.1
1	A	135	LEU	3.0
1	A	385	ARG	3.0
1	A	342	ALA	3.0
1	A	216	LEU	3.0
1	A	118	ILE	2.9
1	A	244[A]	ILE	2.9
1	A	63	LEU	2.9
1	A	264	TRP	2.9
1	A	151	LEU	2.8
1	A	102[A]	VAL	2.8
1	A	387[A]	ARG	2.8
1	A	234	PHE	2.8
1	A	170	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	278	VAL	2.7
1	A	238	LEU	2.7
1	A	366	ALA	2.7
1	A	248	VAL	2.7
1	A	168	ALA	2.7
1	A	277	ILE	2.6
1	A	19	ASP	2.6
1	A	201	CYS	2.6
1	A	109	ARG	2.6
1	A	98[A]	LEU	2.6
1	A	213	ILE	2.6
1	A	34	LEU	2.4
1	A	356	ALA	2.4
1	A	273[A]	ARG	2.4
1	A	20	GLU	2.4
1	A	75	ARG	2.4
1	A	243[A]	HIS	2.4
1	A	363	ASN	2.4
1	A	410	SER	2.3
1	A	319	ALA	2.3
1	A	256	THR	2.3
1	A	174[A]	MET	2.3
1	A	246[A]	THR	2.3
1	A	361	LEU	2.3
1	A	171	ASP	2.2
1	A	386	LEU	2.2
1	A	166	SER	2.2
1	A	84	PRO	2.2
1	A	317	LEU	2.2
1	A	122	THR	2.2
1	A	372	ALA	2.2
1	A	121	VAL	2.2
1	A	274	ILE	2.2
1	A	182[A]	LEU	2.1
1	A	148[A]	VAL	2.1
1	A	127	ALA	2.1
1	A	261	PRO	2.1
1	A	359	ALA	2.0
1	A	169[A]	LEU	2.0
1	A	167	GLY	2.0
1	A	251	GLY	2.0
1	A	196	TYR	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

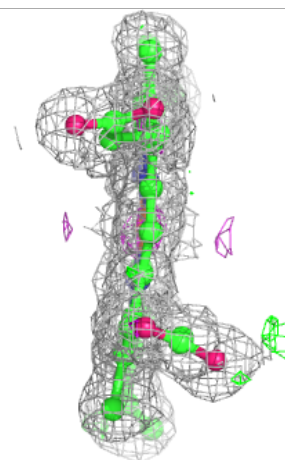
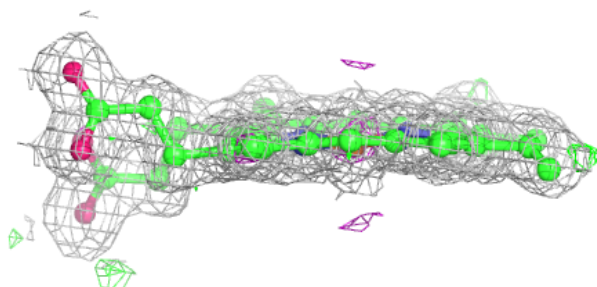
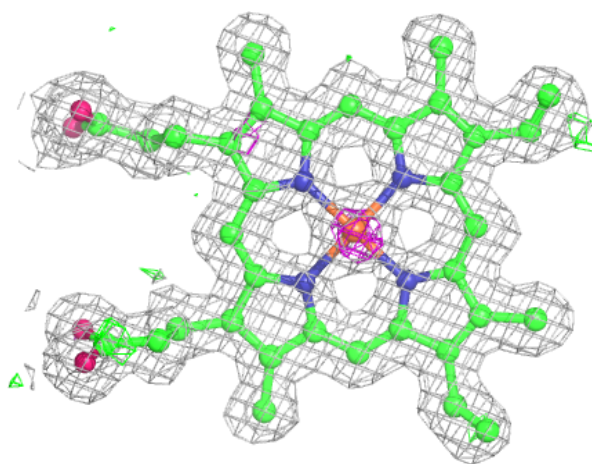
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	417	5/5	0.71	0.26	20,22,28,29	5
3	SO4	A	415	5/5	0.85	0.22	28,29,30,30	5
3	SO4	A	416	5/5	0.88	0.23	40,41,43,43	5
3	SO4	A	414	5/5	0.92	0.14	32,33,35,38	5
3	SO4	A	413	5/5	0.97	0.14	28,29,32,33	5
2	HEM	A	412	43/43	0.98	0.07	10,12,15,22	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 412:**

$2mF_o-DF_c$  (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.