



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:15 am GMT

PDB ID : 4G46  
Title : Structure of cytochrome P450 CYP121 in complex with 4-oxo-4,5,6,7-tetrahydrobenzofuran-3-carboxylate  
Authors : Hudson, S.A.; McLean, K.J.; Surade, S.; Yang, Y.-Q.; Leys, D.; Ciulli, A.; Munro, A.W.; Abell, C.  
Deposited on : 2012-07-16  
Resolution : 1.52 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

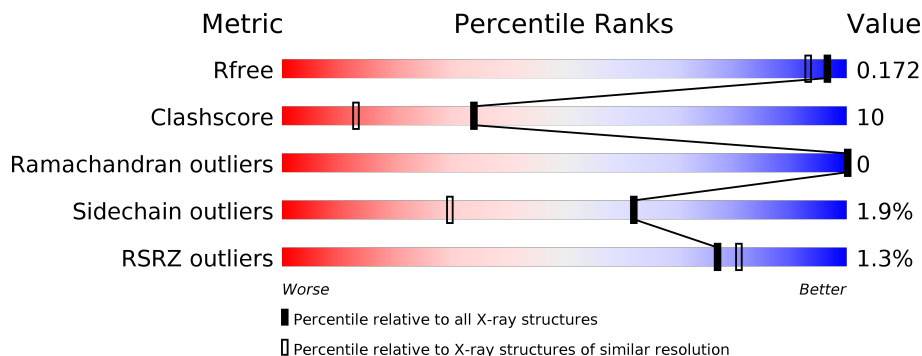
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.52 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))
$R_{free}$	100719	2964 (1.54-1.50)
Clashscore	112137	3216 (1.54-1.50)
Ramachandran outliers	110173	3145 (1.54-1.50)
Sidechain outliers	110143	3143 (1.54-1.50)
RSRZ outliers	101464	2990 (1.54-1.50)

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. 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	396	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; right: 0;">%</div> <div style="position: absolute; top: 5px; left: 0; right: 0;"> <div style="width: 1%; height: 10px; background-color: red;"></div> <div style="width: 77%, height: 10px; background-color: orange;"></div> <div style="width: 19%, height: 10px; background-color: yellow;"></div> <div style="width: 3%, height: 10px; background-color: green;"></div> </div> <div style="position: absolute; bottom: 5px; left: 0; right: 0;"> <div style="width: 1%;"></div> <div style="width: 78%; text-align: center;">78%</div> <div style="width: 19%; text-align: center;">19%</div> <div style="width: 3%; text-align: center;">•</div> </div> </div> </div>

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	SO4	A	402	-	X	X	X
3	SO4	A	403	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	405	-	-	-	X
4	TTY	A	406	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3886 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 121.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	31	1
			3078	1972	531	563	12			

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



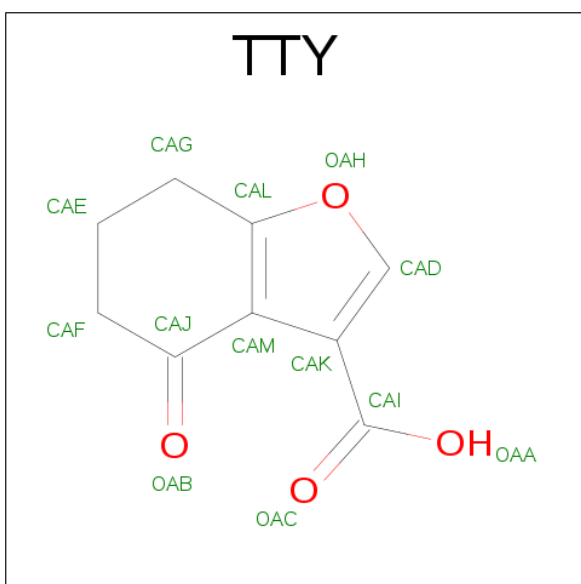
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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		

- Molecule 4 is 4-OXO-4,5,6,7-TETRAHYDRO-1-BENZOFURAN-3-CARBOXYLIC ACID (three-letter code: TTY) (formula: C<sub>9</sub>H<sub>8</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	9	4		

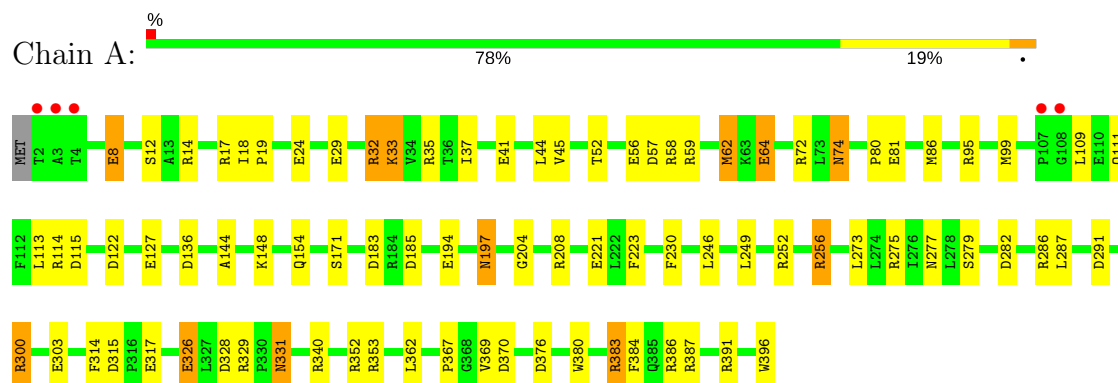
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	732	Total	O	0	0
			732	732		

### 3 Residue-property plots

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 121



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.57Å 77.57Å 262.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.99 – 1.52 46.99 – 1.52	Depositor EDS
% Data completeness (in resolution range)	96.8 (46.99-1.52) 96.8 (46.99-1.52)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.41 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.149 , 0.172 0.147 , 0.172	Depositor DCC
$R_{free}$ test set	3565 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.0	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3886	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, TTY, 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	3.64	31/3298 (0.9%)	1.84	68/4486 (1.5%)

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 (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64[A]	GLU	CG-CD	103.06	3.06	1.51
1	A	64[B]	GLU	CG-CD	103.06	3.06	1.51
1	A	194[A]	GLU	CG-CD	63.64	2.47	1.51
1	A	194[B]	GLU	CG-CD	63.64	2.47	1.51
1	A	300[A]	ARG	CG-CD	58.66	2.98	1.51
1	A	300[B]	ARG	CG-CD	58.66	2.98	1.51
1	A	33[A]	LYS	CD-CE	14.71	1.88	1.51
1	A	33[B]	LYS	CD-CE	14.71	1.88	1.51
1	A	221	GLU	CG-CD	10.38	1.67	1.51
1	A	81	GLU	CD-OE1	9.86	1.36	1.25
1	A	221	GLU	CD-OE2	9.85	1.36	1.25
1	A	326	GLU	CD-OE2	-9.65	1.15	1.25
1	A	221	GLU	CD-OE1	7.40	1.33	1.25
1	A	62	MET	CB-CG	7.35	1.74	1.51
1	A	221	GLU	CB-CG	7.32	1.66	1.52
1	A	59	ARG	CZ-NH1	6.52	1.41	1.33
1	A	396	TRP	CG-CD1	6.48	1.45	1.36
1	A	256	ARG	CZ-NH2	6.16	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	GLY	N-CA	5.78	1.54	1.46
1	A	396	TRP	CD2-CE2	5.59	1.48	1.41
1	A	380	TRP	CD2-CE2	5.54	1.48	1.41
1	A	12[A]	SER	CB-OG	5.49	1.49	1.42
1	A	12[B]	SER	CB-OG	5.49	1.49	1.42
1	A	352	ARG	CZ-NH1	5.43	1.40	1.33
1	A	32	ARG	CZ-NH2	-5.40	1.26	1.33
1	A	171	SER	CB-OG	5.37	1.49	1.42
1	A	8	GLU	CD-OE2	-5.23	1.19	1.25
1	A	24	GLU	C-O	5.21	1.33	1.23
1	A	32	ARG	CZ-NH1	5.18	1.39	1.33
1	A	367	PRO	N-CA	-5.10	1.38	1.47
1	A	384	PHE	CG-CD2	5.01	1.46	1.38

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64[A]	GLU	CG-CD-OE2	-24.53	69.23	118.30
1	A	64[B]	GLU	CG-CD-OE2	-24.53	69.23	118.30
1	A	64[A]	GLU	CG-CD-OE1	24.08	166.46	118.30
1	A	64[B]	GLU	CG-CD-OE1	24.08	166.46	118.30
1	A	32	ARG	NE-CZ-NH1	20.38	130.49	120.30
1	A	300[A]	ARG	CB-CG-CD	-20.09	59.37	111.60
1	A	300[B]	ARG	CB-CG-CD	-20.09	59.37	111.60
1	A	64[A]	GLU	CB-CG-CD	-19.96	60.32	114.20
1	A	64[B]	GLU	CB-CG-CD	-19.96	60.32	114.20
1	A	32	ARG	NE-CZ-NH2	-19.11	110.75	120.30
1	A	33[A]	LYS	CD-CE-NZ	17.60	152.18	111.70
1	A	33[B]	LYS	CD-CE-NZ	17.60	152.18	111.70
1	A	35	ARG	NE-CZ-NH1	12.65	126.63	120.30
1	A	300[A]	ARG	CG-CD-NE	9.71	132.18	111.80
1	A	300[B]	ARG	CG-CD-NE	9.71	132.18	111.80
1	A	33[A]	LYS	CG-CD-CE	-9.54	83.29	111.90
1	A	33[B]	LYS	CG-CD-CE	-9.54	83.29	111.90
1	A	352	ARG	NE-CZ-NH1	-9.36	115.62	120.30
1	A	194[A]	GLU	CG-CD-OE2	9.27	136.85	118.30
1	A	194[B]	GLU	CG-CD-OE2	9.27	136.85	118.30
1	A	387	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	286	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	57	ASP	CB-CG-OD2	-8.06	111.05	118.30
1	A	58	ARG	NE-CZ-NH1	-7.60	116.50	120.30
1	A	286	ARG	NE-CZ-NH2	-7.42	116.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194[A]	GLU	CG-CD-OE1	-7.36	103.58	118.30
1	A	194[B]	GLU	CG-CD-OE1	-7.36	103.58	118.30
1	A	194[A]	GLU	CB-CG-CD	-7.17	94.85	114.20
1	A	194[B]	GLU	CB-CG-CD	-7.17	94.85	114.20
1	A	291	ASP	CB-CG-OD1	7.13	124.72	118.30
1	A	256	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	A	391	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	59	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	A	115	ASP	CB-CG-OD2	-6.77	112.20	118.30
1	A	208[A]	ARG	CD-NE-CZ	6.70	132.98	123.60
1	A	208[B]	ARG	CD-NE-CZ	6.70	132.98	123.60
1	A	328	ASP	CB-CG-OD2	6.64	124.27	118.30
1	A	303	GLU	OE1-CD-OE2	-6.62	115.36	123.30
1	A	113	LEU	CA-CB-CG	6.60	130.49	115.30
1	A	252	ARG	NE-CZ-NH1	-6.35	117.12	120.30
1	A	376	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	208[A]	ARG	CA-CB-CG	6.23	127.10	113.40
1	A	208[B]	ARG	CA-CB-CG	6.23	127.10	113.40
1	A	35	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	383	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	A	315	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	99[A]	MET	CB-CA-C	-5.97	98.45	110.40
1	A	99[B]	MET	CB-CA-C	-5.97	98.45	110.40
1	A	370	ASP	CB-CG-OD1	5.92	123.62	118.30
1	A	183	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	279[A]	SER	N-CA-CB	-5.82	101.77	110.50
1	A	279[B]	SER	N-CA-CB	-5.82	101.77	110.50
1	A	221	GLU	CB-CG-CD	5.80	129.85	114.20
1	A	329	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	A	183	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	A	208[A]	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	208[B]	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	282	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	14	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	136	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	275	ARG	NE-CZ-NH2	5.25	122.93	120.30
1	A	314	PHE	CB-CG-CD1	5.24	124.47	120.80
1	A	223	PHE	CB-CG-CD2	5.17	124.42	120.80
1	A	197	ASN	CB-CA-C	-5.16	100.08	110.40
1	A	185	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	62	MET	CB-CG-SD	-5.08	97.15	112.40
1	A	185	ASP	CB-CG-OD2	-5.07	113.74	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	ARG	Sidechain

## 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	3078	0	3090	57	0
2	A	43	0	30	3	0
3	A	20	0	0	2	0
4	A	13	0	7	1	0
5	A	732	0	0	31	1
All	All	3886	0	3127	61	1

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 10.

All (61) 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:62:MET:CB	1:A:62:MET:CG	1.74	1.58
1:A:37[A]:ILE:HD11	5:A:1073:HOH:O	1.41	1.20
1:A:326:GLU:OE2	5:A:844:HOH:O	1.57	1.20
1:A:383:ARG:NE	5:A:1073:HOH:O	1.95	0.97
1:A:8:GLU:CD	5:A:1151:HOH:O	2.05	0.92
1:A:148:LYS:CD	5:A:1199:HOH:O	2.20	0.87
1:A:62:MET:SD	1:A:62:MET:CB	2.70	0.80
1:A:8:GLU:CG	5:A:1151:HOH:O	2.31	0.78
1:A:111:GLN:NE2	1:A:114[B]:ARG:HH21	1.81	0.77
1:A:197:ASN:OD1	5:A:1101:HOH:O	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LYS:CD	5:A:1164:HOH:O	2.32	0.76
3:A:402:SO4:O3	5:A:749:HOH:O	2.03	0.76
4:A:406:TTY:H3	5:A:1231:HOH:O	1.86	0.76
1:A:383:ARG:CD	5:A:1073:HOH:O	2.32	0.74
1:A:37[A]:ILE:CD1	5:A:1073:HOH:O	2.13	0.73
1:A:64[A]:GLU:CG	1:A:287:LEU:HD23	2.19	0.72
1:A:326:GLU:CG	5:A:844:HOH:O	2.37	0.71
1:A:80[A]:PRO:HG3	5:A:1172:HOH:O	1.89	0.70
3:A:402:SO4:S	5:A:749:HOH:O	2.50	0.68
1:A:340[A]:ARG:NH2	5:A:1075:HOH:O	2.26	0.67
1:A:64[A]:GLU:HG3	1:A:287:LEU:HD23	1.77	0.66
1:A:317:GLU:CG	5:A:1160:HOH:O	2.46	0.63
1:A:17:ARG:NE	5:A:1128:HOH:O	2.31	0.63
1:A:41[B]:GLU:OE2	5:A:798:HOH:O	2.16	0.61
1:A:114[A]:ARG:HG3	1:A:114[A]:ARG:HH11	1.67	0.60
1:A:8:GLU:OE2	5:A:1151:HOH:O	2.16	0.59
1:A:29:GLU:OE1	5:A:1084:HOH:O	2.17	0.57
1:A:64[A]:GLU:HG2	1:A:287:LEU:HD23	1.86	0.56
1:A:64[A]:GLU:HG3	1:A:287:LEU:CD2	2.37	0.55
1:A:353:ARG:CG	5:A:1069:HOH:O	2.53	0.55
1:A:52[B]:THR:CG2	1:A:56:GLU:OE2	2.56	0.54
1:A:74:ASN:HD22	1:A:74:ASN:C	2.10	0.54
1:A:383:ARG:HG2	5:A:1073:HOH:O	2.08	0.53
1:A:114[A]:ARG:HG3	1:A:114[A]:ARG:NH1	2.23	0.53
1:A:331:ASN:H	1:A:331:ASN:HD22	1.55	0.53
1:A:86[A]:MET:HE3	5:A:819:HOH:O	2.09	0.53
1:A:52[B]:THR:HG23	1:A:56:GLU:OE2	2.10	0.51
1:A:62:MET:CA	1:A:62:MET:CG	2.82	0.51
1:A:111:GLN:HE22	1:A:114[B]:ARG:HH21	1.58	0.50
1:A:114[B]:ARG:HD2	5:A:1218:HOH:O	2.14	0.48
1:A:246:LEU:HD22	1:A:362[B]:LEU:CD2	2.44	0.48
1:A:86[A]:MET:CE	5:A:819:HOH:O	2.63	0.47
1:A:17:ARG:NE	5:A:1118:HOH:O	2.48	0.46
2:A:401:HEM:HBC2	2:A:401:HEM:HMC1	1.98	0.45
1:A:256:ARG:NH1	5:A:858:HOH:O	2.48	0.45
1:A:86[A]:MET:HG3	2:A:401:HEM:HBD2	1.99	0.45
1:A:86[B]:MET:HE1	1:A:230:PHE:HZ	1.82	0.45
1:A:95:ARG:NE	5:A:819:HOH:O	2.34	0.44
1:A:86[A]:MET:HG3	2:A:401:HEM:CGD	2.49	0.42
1:A:18:ILE:HA	1:A:19:PRO:HD3	1.95	0.42
1:A:144:ALA:HA	1:A:154:GLN:HE22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249[A]:LEU:HD21	1:A:273:LEU:HD11	2.01	0.42
1:A:331:ASN:N	1:A:331:ASN:HD22	2.16	0.41
1:A:362[A]:LEU:HD21	1:A:369:VAL:HG11	2.03	0.41
1:A:246:LEU:HD22	1:A:362[B]:LEU:HD22	2.02	0.41
1:A:44[B]:LEU:HD13	1:A:45:VAL:N	2.36	0.40
1:A:326:GLU:CD	5:A:844:HOH:O	2.19	0.40
1:A:127[B]:GLU:CG	5:A:871:HOH:O	2.69	0.40

All (1) 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)
5:A:1036:HOH:O	5:A:1036:HOH:O[10_665]	1.81	0.39

## 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	424/396 (107%)	419 (99%)	5 (1%)	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	Rotameric	Outliers	Percentiles
1	A	338/326 (104%)	330 (98%)	8 (2%)	54 21

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	33[A]	LYS
1	A	33[B]	LYS
1	A	74	ASN
1	A	277	ASN
1	A	300[A]	ARG
1	A	300[B]	ARG
1	A	331	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	111	GLN
1	A	154	GLN
1	A	197	ASN
1	A	251	GLN
1	A	331	ASN
1	A	342	GLN
1	A	356	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
2	HEM	A	401	1,5	28,50,50	1.90	6 (21%)	17,82,82	2.62	6 (35%)
3	SO4	A	402	-	4,4,4	2.15	2 (50%)	6,6,6	1.08	0
3	SO4	A	403	-	4,4,4	0.44	0	6,6,6	0.48	0
3	SO4	A	404	-	4,4,4	1.33	1 (25%)	6,6,6	1.02	0
3	SO4	A	405	-	4,4,4	1.78	2 (50%)	6,6,6	0.96	0
4	TTY	A	406	-	8,14,14	3.50	5 (62%)	7,20,20	1.44	2 (28%)

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	401	1,5	-	0/6/54/54	0/0/8/8
3	SO4	A	402	-	-	0/0/0/0	0/0/0/0
3	SO4	A	403	-	-	0/0/0/0	0/0/0/0
3	SO4	A	404	-	-	0/0/0/0	0/0/0/0
3	SO4	A	405	-	-	0/0/0/0	0/0/0/0
4	TTY	A	406	-	-	0/0/14/14	0/1/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	406	TTY	CAG-CAL	-8.21	1.44	1.50
3	A	402	SO4	O2-S	-3.19	1.28	1.45
4	A	406	TTY	CAF-CAJ	-2.61	1.44	1.50
4	A	406	TTY	CAK-CAM	-2.47	1.38	1.41
4	A	406	TTY	CAM-CAJ	-2.44	1.41	1.46
3	A	404	SO4	O4-S	-2.07	1.29	1.47
2	A	401	HEM	C3D-C2D	2.00	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	C3C-C2C	2.12	1.43	1.40
3	A	402	SO4	O1-S	2.16	1.57	1.45
2	A	401	HEM	C3C-CAC	2.26	1.52	1.47
3	A	405	SO4	O2-S	2.29	1.58	1.45
3	A	405	SO4	O1-S	2.72	1.60	1.45
4	A	406	TTY	OAB-CAJ	2.89	1.27	1.22
2	A	401	HEM	C1C-NC	4.06	1.41	1.36
2	A	401	HEM	C4A-NA	4.11	1.44	1.36
2	A	401	HEM	C4C-NC	5.75	1.43	1.36

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HEM	CMD-C2D-C1D	-3.14	123.64	128.46
2	A	401	HEM	CAA-CBA-CGA	-2.35	108.64	112.66
4	A	406	TTY	OAB-CAJ-CAF	-2.08	117.61	120.77
4	A	406	TTY	CAF-CAJ-CAM	2.08	120.52	118.17
2	A	401	HEM	CAD-CBD-CGD	2.63	117.15	112.66
2	A	401	HEM	CMB-C2B-C3B	2.79	130.07	124.89
2	A	401	HEM	CMC-C2C-C3C	4.84	133.87	124.89
2	A	401	HEM	C4C-C3C-C2C	7.11	111.86	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HEM	3	0
3	A	402	SO4	2	0
4	A	406	TTY	1	0

## 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<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	395/396 (99%)	-0.12	5 (1%) 77 81	4, 9, 20, 43	3 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	THR	4.7
1	A	4	THR	3.0
1	A	107	PRO	2.8
1	A	3	ALA	2.3
1	A	108	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	A	402	5/5	0.93	0.35	30.20	15,23,32,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	TTY	A	406	13/13	0.89	0.19	8.90	18,22,28,32	0
3	SO4	A	405	5/5	0.96	0.15	8.05	20,25,31,45	0
3	SO4	A	403	5/5	0.95	0.17	7.43	18,21,21,22	5
3	SO4	A	404	5/5	0.98	0.10	0.54	12,14,17,21	0
2	HEM	A	401	43/43	0.99	0.07	-0.06	4,5,9,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.