



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 26, 2016 – 12:00 AM EDT

PDB ID : 5CWE  
Title : Structure of CYP107L2 from *Streptomyces avermitilis* with lauric acid  
Authors : Pham, T.-V.; Han, S.-H.; Kim, J.-H.; Kim, D.-H.; Kang, L.-W.  
Deposited on : 2015-07-28  
Resolution : 2.39 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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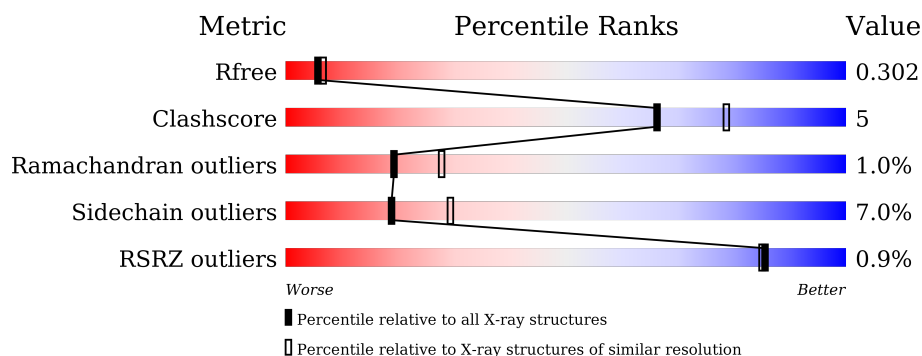
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : rb-20027939

**i**

## X-RAY DIFFRACTION

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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	393	<div> <div></div> <div>83%</div> <div>15%</div> <div></div> </div>
1	B	393	<div> <div></div> <div>83%</div> <div>16%</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	DAO	A	402	-	-	-	X
3	DAO	B	402	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6370 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 hydroxylase.

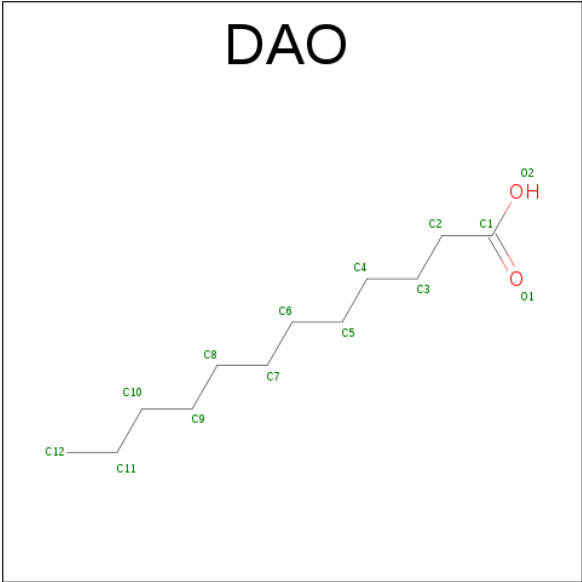
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3036	1912	545	567	12			
1	B	393	Total	C	N	O	S	0	0	0
			3036	1912	545	567	12			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



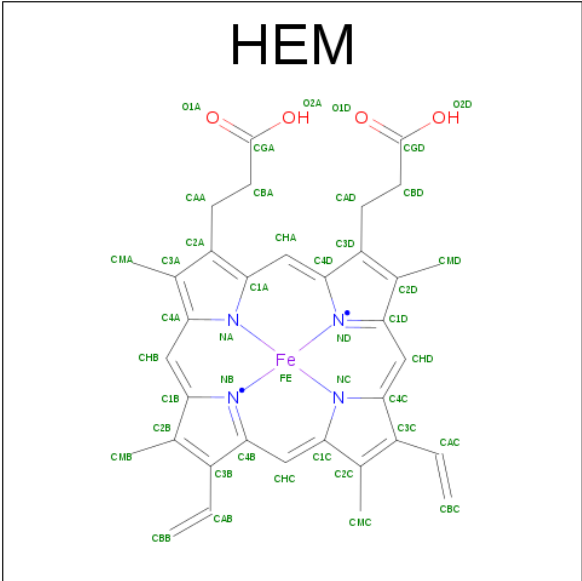
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is LAURIC ACID (three-letter code: DAO) (formula: C<sub>12</sub>H<sub>24</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	12	2		
3	B	1	Total	C	O	0	0
			14	12	2		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



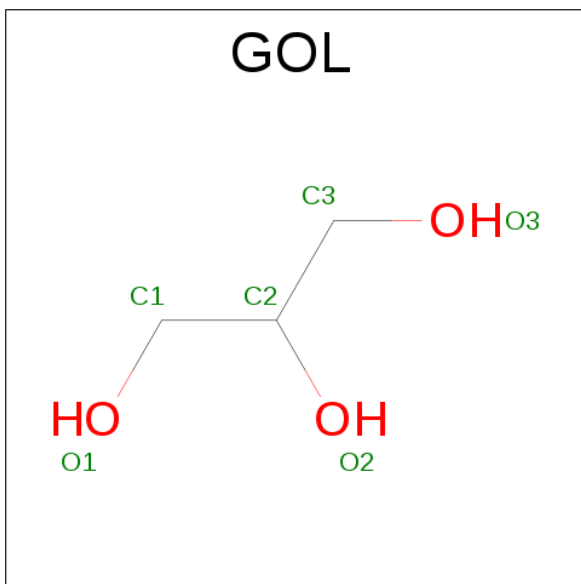
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

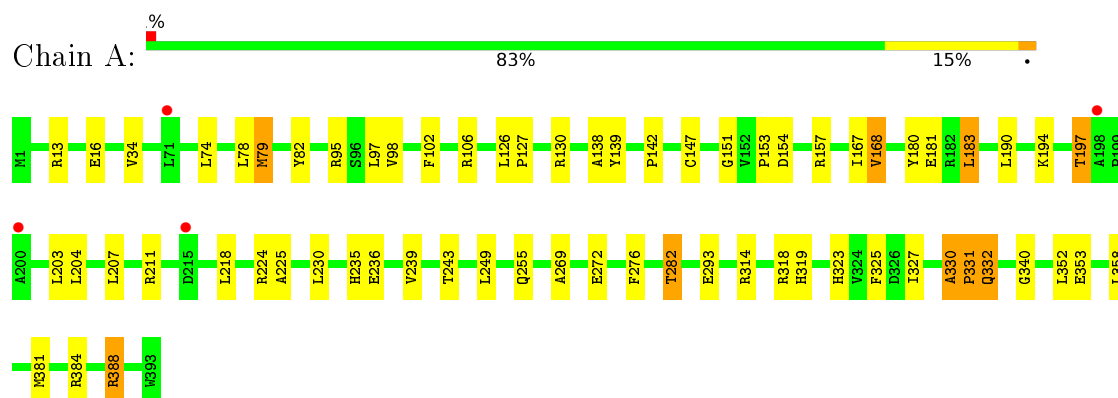
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	80	Total	O	0	0
			80	80		
6	B	88	Total	O	0	0
			88	88		

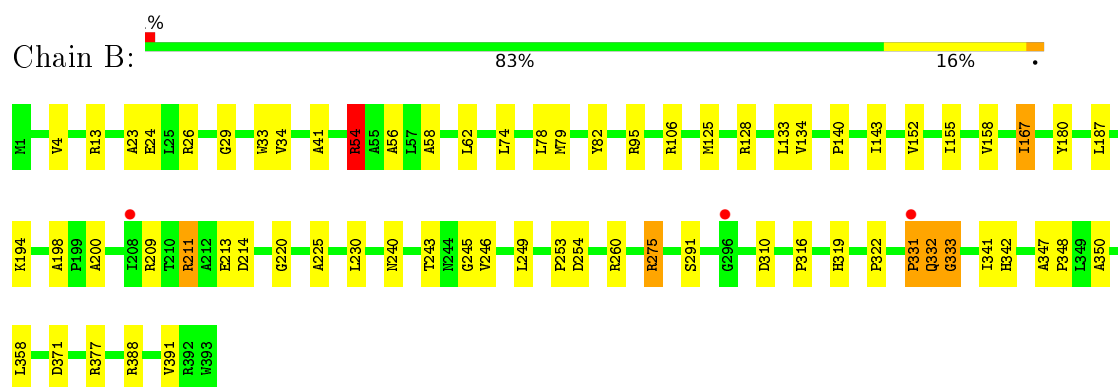
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 hydroxylase



- Molecule 1: Cytochrome P450 hydroxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.08Å 118.37Å 66.04Å 90.00° 105.51° 90.00°	Depositor
Resolution (Å)	47.43 – 2.39 43.34 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.43-2.39) 98.8 (43.34-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.63 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.226 , 0.301 0.229 , 0.302	Depositor DCC
$R_{free}$ test set	1862 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 19.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.075 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6370	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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: GOL, DAO, SO4, 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	0.63	0/3103	0.89	3/4227 (0.1%)
1	B	0.66	0/3103	0.92	10/4227 (0.2%)
All	All	0.64	0/6206	0.90	13/8454 (0.2%)

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	ARG	NE-CZ-NH1	-8.97	115.81	120.30
1	B	95	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	B	54	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	B	275	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	B	275	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	A	388	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	B	388	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	95	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	310	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	384	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	260	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	377	ARG	NE-CZ-NH1	5.05	122.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	331	PRO	Peptide
1	B	331	PRO	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	3036	0	3025	28	0
1	B	3036	0	3025	28	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
3	A	14	0	23	0	0
3	B	14	0	23	0	0
4	A	43	0	30	0	0
4	B	43	0	30	4	0
5	B	6	0	8	3	0
6	A	80	0	0	0	0
6	B	88	0	0	3	0
All	All	6370	0	6164	60	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 (60) 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:275:ARG:NH2	1:B:322:PRO:O	2.18	0.75
1:A:82:TYR:HB3	1:A:225:ALA:HB1	1.80	0.64
1:B:82:TYR:HB3	1:B:225:ALA:HB1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LEU:CD2	1:B:246:VAL:HG11	2.30	0.60
1:B:79:MET:CE	1:B:187:LEU:HD12	2.31	0.60
1:A:340:GLY:O	1:B:54:ARG:NH1	2.37	0.58
1:A:282:THR:HG23	1:A:381:MET:O	2.05	0.57
2:B:401:SO4:O3	5:B:404:GOL:H2	2.05	0.56
1:A:330:ALA:HB3	1:A:331:PRO:HD3	1.87	0.56
1:B:347:ALA:HB3	1:B:348:PRO:HD3	1.88	0.55
1:A:147:CYS:O	1:A:151:GLY:HA2	2.06	0.55
1:A:168:VAL:HG11	1:A:236:GLU:HG2	1.90	0.54
1:A:78:LEU:HD23	1:A:180:TYR:HB3	1.90	0.53
1:B:79:MET:HE1	1:B:187:LEU:HD12	1.92	0.52
1:B:341:ILE:HG13	1:B:342:HIS:CD2	2.45	0.52
4:B:403:HEM:HMC2	4:B:403:HEM:HBC2	1.93	0.51
1:B:134:VAL:HG22	1:B:243:THR:HG21	1.93	0.50
1:B:200:ALA:O	1:B:209:ARG:NH2	2.41	0.50
1:A:139:TYR:HA	1:A:239:VAL:HG22	1.94	0.49
1:A:318:ARG:HG3	1:A:319:HIS:CE1	2.48	0.48
1:B:56:ALA:O	1:B:62:LEU:HD12	2.14	0.48
1:B:152:VAL:HG13	1:B:152:VAL:O	2.14	0.48
1:B:78:LEU:HD12	1:B:180:TYR:HB3	1.95	0.48
1:B:316:PRO:HA	1:B:319:HIS:O	2.15	0.47
1:A:272:GLU:HG3	1:A:325:PHE:CD1	2.50	0.46
1:B:4:VAL:HG22	1:B:33:TRP:CD1	2.51	0.46
1:B:333:GLY:HA2	5:B:404:GOL:C3	2.46	0.46
1:B:371:ASP:O	1:B:371:ASP:CG	2.53	0.46
1:A:194:LYS:O	1:A:197:THR:HG22	2.15	0.45
1:A:126:LEU:N	1:A:127:PRO:HD2	2.30	0.45
1:B:167:ILE:C	1:B:167:ILE:HD12	2.36	0.45
1:B:133:LEU:HD21	1:B:246:VAL:HG11	1.98	0.45
1:B:332:GLN:HA	6:B:548:HOH:O	2.17	0.45
1:A:98:VAL:HG12	1:A:203:LEU:HD11	1.99	0.44
1:B:26:ARG:HA	1:B:29:GLY:O	2.17	0.44
1:B:23:ALA:O	1:B:24:GLU:C	2.56	0.44
4:B:403:HEM:CMC	4:B:403:HEM:HBC2	2.48	0.44
1:A:138:ALA:O	1:A:142:PRO:HD2	2.18	0.44
1:A:239:VAL:O	1:A:243:THR:HG23	2.18	0.44
1:A:332:GLN:O	1:A:332:GLN:NE2	2.51	0.44
4:B:403:HEM:HHC	4:B:403:HEM:HBB2	1.99	0.44
1:A:255:GLN:HE21	1:A:327:ILE:HG12	1.83	0.43
1:B:58:ALA:HA	6:B:545:HOH:O	2.17	0.43
1:A:79:MET:HE3	1:A:183:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HD23	1:A:180:TYR:CB	2.49	0.42
1:B:350:ALA:HB1	4:B:403:HEM:CBB	2.48	0.42
1:B:140:PRO:HA	1:B:143:ILE:HG22	2.02	0.42
1:A:269:ALA:HB2	1:A:327:ILE:HG23	2.02	0.42
1:A:276:PHE:O	1:A:314:ARG:NH2	2.49	0.42
1:B:240:ASN:HA	1:B:243:THR:OG1	2.20	0.42
1:A:97:LEU:CD1	1:A:218:LEU:HD13	2.50	0.42
1:B:125:MET:O	1:B:128:ARG:HG2	2.20	0.42
1:A:102:PHE:CZ	1:A:230:LEU:HD22	2.55	0.41
5:B:404:GOL:H12	6:B:518:HOH:O	2.19	0.41
1:A:255:GLN:HB3	1:A:327:ILE:HG12	2.03	0.41
1:A:314:ARG:HH11	1:A:323:HIS:HD2	1.67	0.41
1:A:272:GLU:HG3	1:A:325:PHE:CE1	2.55	0.41
1:B:211:ARG:CD	1:B:220:GLY:HA2	2.52	0.40
1:A:352:LEU:O	1:A:353:GLU:C	2.59	0.40
1:A:79:MET:CE	1:A:183:LEU:HD13	2.51	0.40

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	391/393 (100%)	370 (95%)	19 (5%)	2 (0%)	34	48
1	B	391/393 (100%)	356 (91%)	29 (7%)	6 (2%)	13	17
All	All	782/786 (100%)	726 (93%)	48 (6%)	8 (1%)	19	28

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	ALA
1	B	333	GLY

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Mol	Chain	Res	Type
1	A	330	ALA
1	B	198	ALA
1	B	155	ILE
1	B	245	GLY
1	A	153	PRO
1	B	331	PRO

### 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	315/315 (100%)	289 (92%)	26 (8%)	14	21
1	B	315/315 (100%)	297 (94%)	18 (6%)	25	40
All	All	630/630 (100%)	586 (93%)	44 (7%)	19	29

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	16	GLU
1	A	34	VAL
1	A	74	LEU
1	A	79	MET
1	A	106	ARG
1	A	130	ARG
1	A	154	ASP
1	A	157	ARG
1	A	167	ILE
1	A	168	VAL
1	A	181	GLU
1	A	183	LEU
1	A	190	LEU
1	A	197	THR
1	A	204	LEU
1	A	207	LEU

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Mol	Chain	Res	Type
1	A	211	ARG
1	A	224	ARG
1	A	235	HIS
1	A	249	LEU
1	A	282	THR
1	A	293	GLU
1	A	332	GLN
1	A	358	LEU
1	A	388	ARG
1	B	34	VAL
1	B	54	ARG
1	B	74	LEU
1	B	106	ARG
1	B	158	VAL
1	B	167	ILE
1	B	194	LYS
1	B	211	ARG
1	B	213	GLU
1	B	214	ASP
1	B	230	LEU
1	B	249	LEU
1	B	253	PRO
1	B	254	ASP
1	B	291	SER
1	B	332	GLN
1	B	358	LEU
1	B	391	VAL

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

Mol	Chain	Res	Type
1	A	32	HIS
1	A	165	ASN
1	A	240	ASN
1	A	255	GLN
1	A	319	HIS
1	A	323	HIS
1	A	334	HIS
1	B	165	ASN
1	B	247	HIS
1	B	255	GLN
1	B	332	GLN

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Mol	Chain	Res	Type
1	B	334	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 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	SO4	A	401	-	4,4,4	0.29	0	6,6,6	0.56	0
3	DAO	A	402	-	10,13,13	0.43	0	10,13,13	0.36	0
4	HEM	A	403	1	24,50,50	1.04	2 (8%)	16,82,82	1.54	5 (31%)
2	SO4	B	401	-	4,4,4	0.21	0	6,6,6	0.62	0
3	DAO	B	402	-	10,13,13	0.47	0	10,13,13	0.21	0
4	HEM	B	403	1	24,50,50	1.45	4 (16%)	16,82,82	1.17	1 (6%)
5	GOL	B	404	-	5,5,5	0.56	0	5,5,5	0.71	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	SO4	A	401	-	-	0/0/0/0	0/0/0/0
3	DAO	A	402	-	-	0/9/11/11	0/0/0/0
4	HEM	A	403	1	-	0/6/54/54	0/0/8/8
2	SO4	B	401	-	-	0/0/0/0	0/0/0/0
3	DAO	B	402	-	-	0/9/11/11	0/0/0/0
4	HEM	B	403	1	-	0/6/54/54	0/0/8/8
5	GOL	B	404	-	-	0/4/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	HEM	C4D-ND	-3.69	1.31	1.36
4	B	403	HEM	C4C-NC	-3.09	1.32	1.36
4	B	403	HEM	C1B-NB	-2.91	1.32	1.36
4	A	403	HEM	C4C-NC	-2.56	1.33	1.36
4	A	403	HEM	C3B-C2B	-2.48	1.37	1.40
4	B	403	HEM	C4A-CHB	-2.15	1.34	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	403	HEM	C3B-C4B-NB	-2.89	105.47	109.21
4	A	403	HEM	C3B-C4B-NB	-2.38	106.13	109.21
4	A	403	HEM	CMA-C3A-C4A	-2.36	124.30	128.31
4	A	403	HEM	CMD-C2D-C1D	-2.17	124.62	128.31
4	A	403	HEM	CMD-C2D-C3D	2.21	129.86	125.24
4	A	403	HEM	CMC-C2C-C3C	2.59	130.15	125.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	SO4	1	0
4	B	403	HEM	4	0
5	B	404	GOL	3	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

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	393/393 (100%)	0.03	4 (1%) 84 83	24, 43, 71, 103	0
1	B	393/393 (100%)	0.08	3 (0%) 87 87	22, 42, 67, 99	0
All	All	786/786 (100%)	0.05	7 (0%) 85 85	22, 43, 69, 103	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	ILE	3.7
1	A	215	ASP	3.3
1	A	198	ALA	3.2
1	B	331	PRO	2.7
1	A	200	ALA	2.4
1	A	71	LEU	2.3
1	B	296	GLY	2.1

### 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( $\text{\AA}^2$ )	Q<0.9
3	DAO	B	402	14/14	0.88	0.33	7.08	53,69,84,86	0
3	DAO	A	402	14/14	0.86	0.28	6.10	55,74,84,85	0
4	HEM	A	403	43/43	0.97	0.14	0.44	21,24,31,35	0
2	SO4	A	401	5/5	0.99	0.13	0.38	33,33,38,38	0
5	GOL	B	404	6/6	0.93	0.18	0.31	34,41,42,46	0
2	SO4	B	401	5/5	0.99	0.12	0.27	31,32,34,40	0
4	HEM	B	403	43/43	0.98	0.15	0.23	18,22,29,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.