



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:53 AM GMT

PDB ID : 3MDR  
Title : Tranlylcypromine complex of Cytochrome P450 46A1  
Authors : Mast, N.; Charvet, C.; Pikuleva, I.; Stout, C.D.  
Deposited on : 2010-03-30  
Resolution : 2.00 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

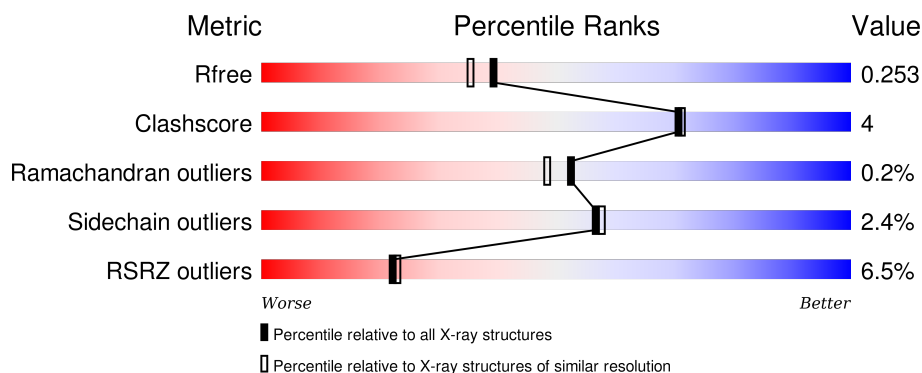
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	456	<div> <div>7%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>• 6%</div> </div> </div>
1	B	456	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7322 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 Cholesterol 24-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3447	2200	605	625	17			
1	B	425	Total	C	N	O	S	0	0	0
			3429	2187	602	623	17			

There are 12 discrepancies between the modelled and reference sequences:

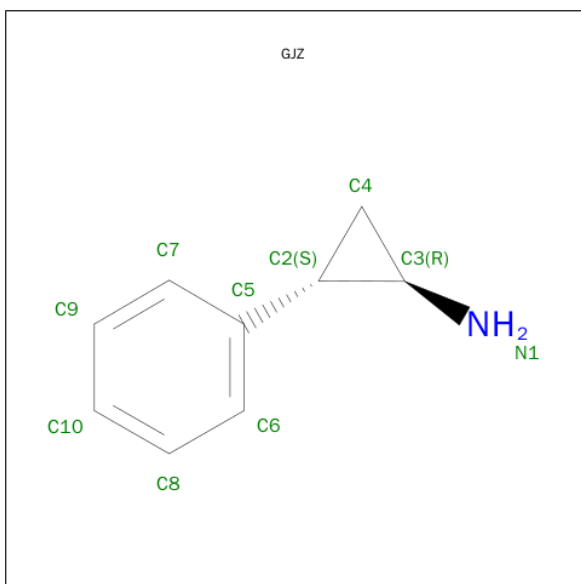
Chain	Residue	Modelled	Actual	Comment	Reference
A	49	MET	-	EXPRESSION TAG	UNP Q9Y6A2
A	50	ALA	-	EXPRESSION TAG	UNP Q9Y6A2
A	501	HIS	-	EXPRESSION TAG	UNP Q9Y6A2
A	502	HIS	-	EXPRESSION TAG	UNP Q9Y6A2
A	503	HIS	-	EXPRESSION TAG	UNP Q9Y6A2
A	504	HIS	-	EXPRESSION TAG	UNP Q9Y6A2
B	49	MET	-	EXPRESSION TAG	UNP Q9Y6A2
B	50	ALA	-	EXPRESSION TAG	UNP Q9Y6A2
B	501	HIS	-	EXPRESSION TAG	UNP Q9Y6A2
B	502	HIS	-	EXPRESSION TAG	UNP Q9Y6A2
B	503	HIS	-	EXPRESSION TAG	UNP Q9Y6A2
B	504	HIS	-	EXPRESSION TAG	UNP Q9Y6A2

- 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		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is (1R,2S)-2-PHENYLCYCLOPROPANAMINE (three-letter code: GJZ) (formula: C<sub>9</sub>H<sub>11</sub>N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			10	9	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			10	9	1		

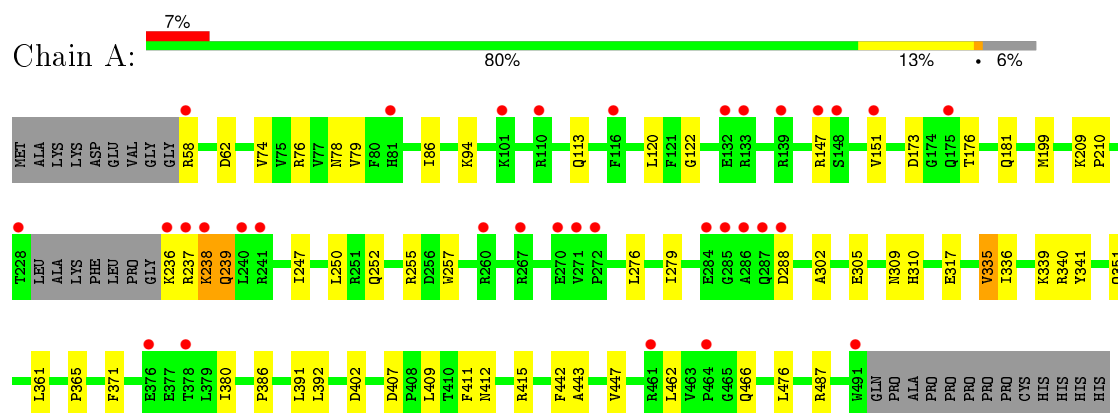
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	172	Total	O	0	0
			172	172		
4	B	168	Total	O	0	0
			168	168		

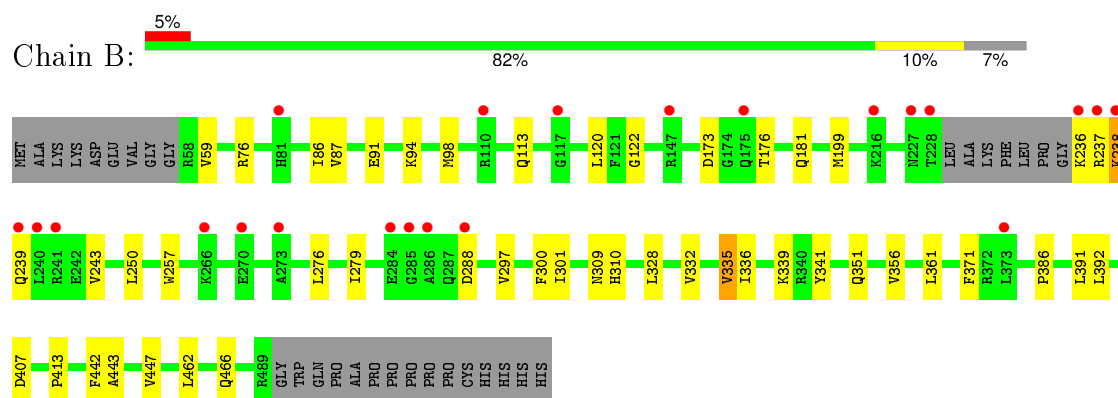
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: Cholesterol 24-hydroxylase



#### • Molecule 1: Cholesterol 24-hydroxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.19Å 121.19Å 143.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 38.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.2 (30.00-2.00) 94.1 (38.89-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.225 , 0.244 0.232 , 0.253	Depositor DCC
$R_{free}$ test set	3387 reflections (5.44%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 35.6	EDS
Estimated twinning fraction	0.532 for H, K, L 0.468 for -H, K, -L 0.289 for -h,k,-l	Xtriage
Reported twinning fraction	0.532 for H, K, L 0.468 for -H, K, -L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	1 of 65726 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7322	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, GJZ

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	0.65	0/3516	0.66	0/4742
1	B	0.65	0/3496	0.65	0/4714
All	All	0.65	0/7012	0.66	0/9456

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 ⓘ

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	3447	0	3492	35	0
1	B	3429	0	3479	25	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
3	A	10	0	10	1	0
3	B	10	0	10	0	0
4	A	172	0	0	4	0
4	B	168	0	0	6	0
All	All	7322	0	7051	61	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 4.



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:58:ARG:NH1	1:A:62:ASP:HB3	1.86	0.91
1:A:58:ARG:HH11	1:A:62:ASP:HB3	1.38	0.87
1:A:86:ILE:HD12	1:A:392:LEU:HD22	1.64	0.80
1:A:305:GLU:OE2	4:A:629:HOH:O	2.03	0.76
1:B:87:VAL:HG13	4:B:603:HOH:O	1.91	0.68
1:B:309:ASN:ND2	4:B:623:HOH:O	1.85	0.67
1:B:91:GLU:HB2	4:B:540:HOH:O	1.95	0.65
1:B:236:LYS:O	1:B:238:LYS:N	2.34	0.60
1:A:113:GLN:HG2	1:A:122:GLY:O	2.01	0.60
1:B:113:GLN:HG2	1:B:122:GLY:O	2.04	0.57
1:A:236:LYS:O	1:A:238:LYS:N	2.38	0.57
1:B:86:ILE:HD12	1:B:392:LEU:HD22	1.87	0.57
1:A:309:ASN:ND2	4:A:620:HOH:O	2.03	0.57
1:B:173:ASP:OD2	1:B:176:THR:OG1	2.23	0.56
2:A:505:HEM:HBC2	2:A:505:HEM:CMC	2.38	0.54
1:B:328:LEU:HD21	1:B:356:VAL:HG21	1.91	0.53
1:A:276:LEU:HA	1:A:279:ILE:HG12	1.89	0.53
1:B:443:ALA:O	1:B:447:VAL:HG13	2.09	0.52
1:A:120:LEU:HD13	1:A:247:ILE:HG12	1.92	0.52
1:A:147:ARG:O	1:A:151:VAL:HG23	2.10	0.51
1:B:300:PHE:HD2	1:B:301:ILE:HD13	1.75	0.51
1:A:173:ASP:OD2	1:A:176:THR:OG1	2.27	0.50
1:A:402:ASP:HB2	4:B:643:HOH:O	2.10	0.50
1:A:173:ASP:O	1:A:487:ARG:NH2	2.45	0.49
1:A:199:MET:HG3	1:A:257:TRP:CD2	2.47	0.49
1:B:335:VAL:HG23	1:B:336:ILE:HG23	1.92	0.49
1:B:76:ARG:HH22	1:B:386:PRO:HG2	1.77	0.49
1:A:412:ASN:O	1:A:415:ARG:HG3	2.12	0.49
1:A:335:VAL:HG23	1:A:336:ILE:HG23	1.95	0.49
1:A:252:GLN:OE1	1:A:255:ARG:NH1	2.42	0.49
1:B:310:HIS:CE1	1:B:361:LEU:HG	2.48	0.48
1:B:94:LYS:O	1:B:98:MET:HB2	2.15	0.47
1:A:76:ARG:HH22	1:A:386:PRO:HG2	1.79	0.47
1:A:443:ALA:O	1:A:447:VAL:HG13	2.15	0.47
1:A:462:LEU:HG	1:A:466:GLN:HB2	1.95	0.47
1:A:365:PRO:O	1:A:476:LEU:HD12	2.14	0.47
1:A:310:HIS:CE1	1:A:361:LEU:HG	2.50	0.47
1:B:339:LYS:HE2	1:B:341:TYR:O	2.15	0.47
1:B:413:PRO:HD2	4:B:585:HOH:O	2.14	0.47
1:A:78:ASN:HB3	4:A:573:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:LEU:HG	1:B:466:GLN:HB2	1.97	0.45
1:A:236:LYS:HD3	1:A:238:LYS:HE2	1.99	0.45
1:A:317:GLU:HG2	1:A:411:PHE:CD1	2.51	0.45
1:A:339:LYS:HE2	1:A:341:TYR:O	2.17	0.45
1:B:371:PHE:HA	1:B:391:LEU:O	2.17	0.45
1:A:302:ALA:HB1	3:A:506:GJZ:HN1	1.82	0.45
1:A:94:LYS:HD2	1:B:91:GLU:HG2	2.00	0.45
1:A:371:PHE:HA	1:A:391:LEU:O	2.17	0.44
2:B:505:HEM:HBC2	2:B:505:HEM:CMC	2.48	0.43
1:A:340:ARG:NH2	4:A:646:HOH:O	2.50	0.43
1:B:276:LEU:HA	1:B:279:ILE:HG12	2.01	0.43
1:B:199:MET:HG3	1:B:257:TRP:CD2	2.55	0.42
1:A:79:VAL:HG11	1:A:392:LEU:HD12	2.02	0.41
1:A:409:LEU:HA	1:A:409:LEU:HD23	1.83	0.41
1:A:238:LYS:HG2	1:A:239:GLN:N	2.34	0.41
1:B:239:GLN:O	1:B:243:VAL:HG23	2.20	0.41
1:B:120:LEU:HD12	1:B:297:VAL:HG11	2.03	0.41
1:B:236:LYS:HD3	1:B:238:LYS:HE2	2.03	0.41
1:A:209:LYS:HB2	1:A:210:PRO:HD3	2.02	0.41
1:A:74:VAL:HG21	1:A:380:ILE:O	2.21	0.41
1:B:59:VAL:HB	4:B:622:HOH:O	2.21	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	423/456 (93%)	407 (96%)	15 (4%)	1 (0%)	52	48
1	B	421/456 (92%)	408 (97%)	12 (3%)	1 (0%)	52	48
All	All	844/912 (92%)	815 (97%)	27 (3%)	2 (0%)	52	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	ARG
1	B	237	ARG

### 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	374/397 (94%)	365 (98%)	9 (2%)	57	58
1	B	373/397 (94%)	364 (98%)	9 (2%)	57	58
All	All	747/794 (94%)	729 (98%)	18 (2%)	57	58

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	A	238	LYS
1	A	239	GLN
1	A	250	LEU
1	A	288	ASP
1	A	335	VAL
1	A	351	GLN
1	A	407	ASP
1	A	442	PHE
1	B	181	GLN
1	B	238	LYS
1	B	250	LEU
1	B	288	ASP
1	B	332	VAL
1	B	335	VAL
1	B	351	GLN
1	B	407	ASP
1	B	442	PHE

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	213	GLN
1	A	351	GLN
1	A	355	GLN
1	A	473	GLN
1	B	213	GLN
1	B	351	GLN
1	B	355	GLN
1	B	473	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 ⓘ

4 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	505	1,3	30,50,50	3.58	12 (40%)	24,82,82	2.37	12 (50%)
3	GJZ	A	506	2	10,11,11	0.88	0	11,15,15	1.18	1 (9%)
2	HEM	B	505	1,3	30,50,50	3.63	13 (43%)	24,82,82	2.31	12 (50%)
3	GJZ	B	506	2	10,11,11	0.90	0	11,15,15	1.65	3 (27%)

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	505	1,3	-	0/10/54/54	0/0/8/8
3	GJZ	A	506	2	-	0/4/9/9	0/1/2/2
2	HEM	B	505	1,3	-	0/10/54/54	0/0/8/8
3	GJZ	B	506	2	-	0/4/9/9	0/1/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	505	HEM	C2C-C1C	-9.47	1.34	1.52
2	B	505	HEM	C3B-CAB	-9.38	1.33	1.51
2	B	505	HEM	C2C-C1C	-9.28	1.34	1.52
2	A	505	HEM	C3B-CAB	-9.11	1.34	1.51
2	A	505	HEM	C2D-C3D	-6.65	1.34	1.54
2	B	505	HEM	C2D-C3D	-6.56	1.34	1.54
2	A	505	HEM	C3B-C4B	-5.63	1.46	1.51
2	B	505	HEM	C2B-C1B	-5.51	1.33	1.51
2	A	505	HEM	C2B-C1B	-5.23	1.34	1.51
2	B	505	HEM	C3B-C4B	-4.51	1.47	1.51
2	A	505	HEM	C3D-C4D	-2.74	1.48	1.51
2	A	505	HEM	CHC-C4B	-2.32	1.32	1.38
2	B	505	HEM	C4A-CHB	-2.27	1.33	1.39
2	B	505	HEM	CHD-C1D	-2.22	1.32	1.38
2	A	505	HEM	FE-NC	2.50	2.05	1.95
2	B	505	HEM	FE-NC	2.71	2.06	1.95
2	B	505	HEM	FE-NB	3.25	2.14	1.97
2	A	505	HEM	CBB-CAB	3.45	1.49	1.29
2	A	505	HEM	C1A-CHA	3.61	1.49	1.39
2	B	505	HEM	C1A-CHA	3.94	1.50	1.39
2	B	505	HEM	CBB-CAB	3.99	1.52	1.29
2	A	505	HEM	CHC-C1C	4.15	1.46	1.36
2	B	505	HEM	CHC-C1C	5.09	1.48	1.36
2	A	505	HEM	CHD-C4C	5.18	1.48	1.36
2	B	505	HEM	CHD-C4C	5.18	1.48	1.36

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	505	HEM	CAA-C2A-C1A	-4.29	122.35	127.01
2	B	505	HEM	CAA-C2A-C1A	-3.72	122.97	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	505	HEM	C3C-CAC-CBC	-3.08	119.73	124.46
2	B	505	HEM	C3C-CAC-CBC	-2.98	119.88	124.46
2	A	505	HEM	CBA-CAA-C2A	-2.97	107.20	112.53
3	B	506	GJZ	C7-C5-C2	-2.78	115.52	121.08
2	A	505	HEM	C3B-C4B-CHC	-2.40	119.79	123.16
3	A	506	GJZ	C7-C5-C2	-2.27	116.54	121.08
2	B	505	HEM	CAA-CBA-CGA	-2.23	108.65	112.75
2	B	505	HEM	CBA-CAA-C2A	-2.18	108.62	112.53
2	B	505	HEM	C3B-C4B-NB	-2.14	107.53	111.63
2	A	505	HEM	CMA-C3A-C4A	-2.02	125.03	128.36
2	A	505	HEM	CHC-C4B-NB	2.06	129.48	124.52
2	B	505	HEM	CHC-C4B-NB	2.12	129.63	124.52
3	B	506	GJZ	C4-C2-C5	2.30	126.43	122.30
2	A	505	HEM	CMB-C2B-C3B	2.39	122.51	116.53
2	A	505	HEM	C2D-C3D-C4D	2.71	106.09	101.50
2	A	505	HEM	CMD-C2D-C3D	2.79	126.70	114.35
2	B	505	HEM	C2D-C3D-C4D	2.83	106.29	101.50
2	B	505	HEM	CMD-C2D-C3D	3.15	128.30	114.35
3	B	506	GJZ	C4-C2-C3	3.25	61.10	59.21
2	B	505	HEM	CMB-C2B-C3B	3.28	124.72	116.53
2	B	505	HEM	CMC-C2C-C3C	3.57	125.45	116.53
2	B	505	HEM	CAD-C3D-C4D	3.66	125.38	112.47
2	A	505	HEM	CAD-C3D-C4D	3.81	125.91	112.47
2	A	505	HEM	CMC-C2C-C3C	3.85	126.14	116.53
2	B	505	HEM	CAD-C3D-C2D	4.71	126.77	113.22
2	A	505	HEM	CAD-C3D-C2D	4.80	127.00	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	505	HEM	1	0
3	A	506	GJZ	1	0
2	B	505	HEM	1	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

### 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	427/456 (93%)	0.49	33 (7%) 16 17	19, 37, 56, 77	0
1	B	425/456 (93%)	0.48	22 (5%) 31 33	18, 37, 55, 77	0
All	All	852/912 (93%)	0.49	55 (6%) 22 23	18, 37, 56, 77	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	ARG	8.2
1	B	228	THR	7.4
1	A	228	THR	6.9
1	B	238	LYS	6.8
1	A	236	LYS	6.7
1	B	237	ARG	6.7
1	B	236	LYS	5.7
1	A	285	GLY	5.2
1	A	238	LYS	5.1
1	B	284	GLU	5.1
1	B	285	GLY	4.0
1	A	270	GLU	3.6
1	B	227	ASN	3.5
1	B	117	GLY	3.4
1	B	175	GLN	3.3
1	A	287	GLN	3.3
1	B	266	LYS	3.2
1	B	270	GLU	3.2
1	A	241	ARG	3.2
1	A	491	TRP	3.1
1	A	139	ARG	3.0
1	B	240	LEU	3.0
1	B	241	ARG	3.0
1	A	81	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	267	ARG	2.8
1	A	271	VAL	2.8
1	B	239	GLN	2.7
1	A	378	THR	2.7
1	A	147	ARG	2.7
1	A	101	LYS	2.7
1	A	284	GLU	2.7
1	B	110	ARG	2.6
1	A	286	ALA	2.5
1	B	81	HIS	2.5
1	A	58	ARG	2.5
1	A	464	PRO	2.5
1	B	286	ALA	2.5
1	A	288	ASP	2.4
1	A	116	PHE	2.4
1	A	260	ARG	2.3
1	A	133	ARG	2.3
1	B	216	LYS	2.3
1	A	240	LEU	2.3
1	A	110	ARG	2.2
1	A	461	ARG	2.2
1	A	148	SER	2.2
1	A	132	GLU	2.2
1	A	175	GLN	2.1
1	A	376	GLU	2.1
1	A	272	PRO	2.1
1	B	273	ALA	2.0
1	B	147	ARG	2.0
1	B	373	LEU	2.0
1	A	151	VAL	2.0
1	B	288	ASP	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( $\text{\AA}^2$ )	Q<0.9
3	GJZ	A	506	10/10	0.94	0.16	1.36	34,37,41,41	0
3	GJZ	B	506	10/10	0.89	0.15	1.00	30,37,40,41	0
2	HEM	A	505	43/43	0.96	0.13	0.62	16,23,29,32	0
2	HEM	B	505	43/43	0.98	0.11	-0.70	17,23,29,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.