



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:49 am GMT

PDB ID : 2J0D  
Title : CRYSTAL STRUCTURE OF HUMAN P450 3A4 IN COMPLEX WITH ERY-  
THROMYCIN  
Authors : Sjogren, T.; Ekroos, M.  
Deposited on : 2006-08-02  
Resolution : 2.75 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.

---

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

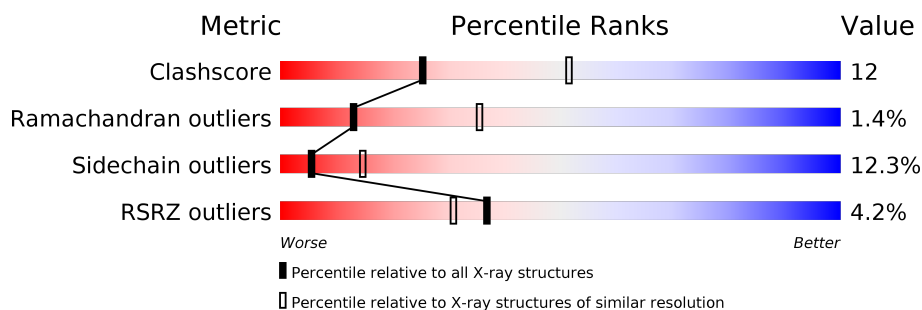
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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	485	
1	B	485	

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	ERY	A	1498	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7326 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 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3578	2331	588	635	24			
1	B	445	Total	C	N	O	S	0	0	0
			3562	2320	585	633	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	VAL	TRP	CONFLICT	UNP P08684
B	392	VAL	TRP	CONFLICT	UNP P08684

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



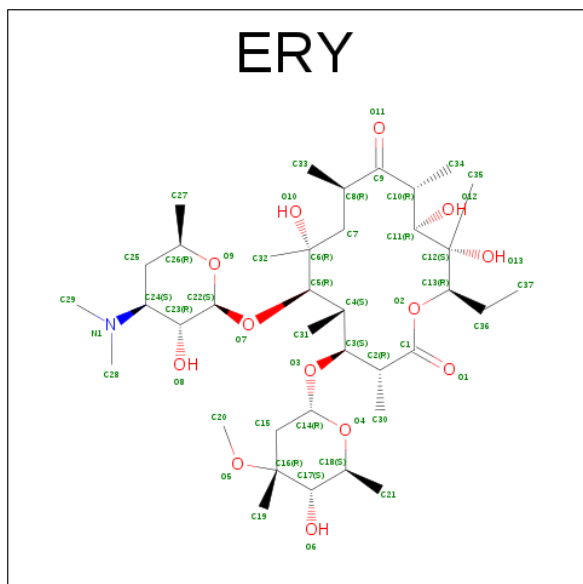
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

*Continued on next page...*

Continued from previous page...

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

- Molecule 3 is ERYTHROMYCIN A (three-letter code: ERY) (formula:  $C_{37}H_{67}NO_{13}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			51	37	1	13		

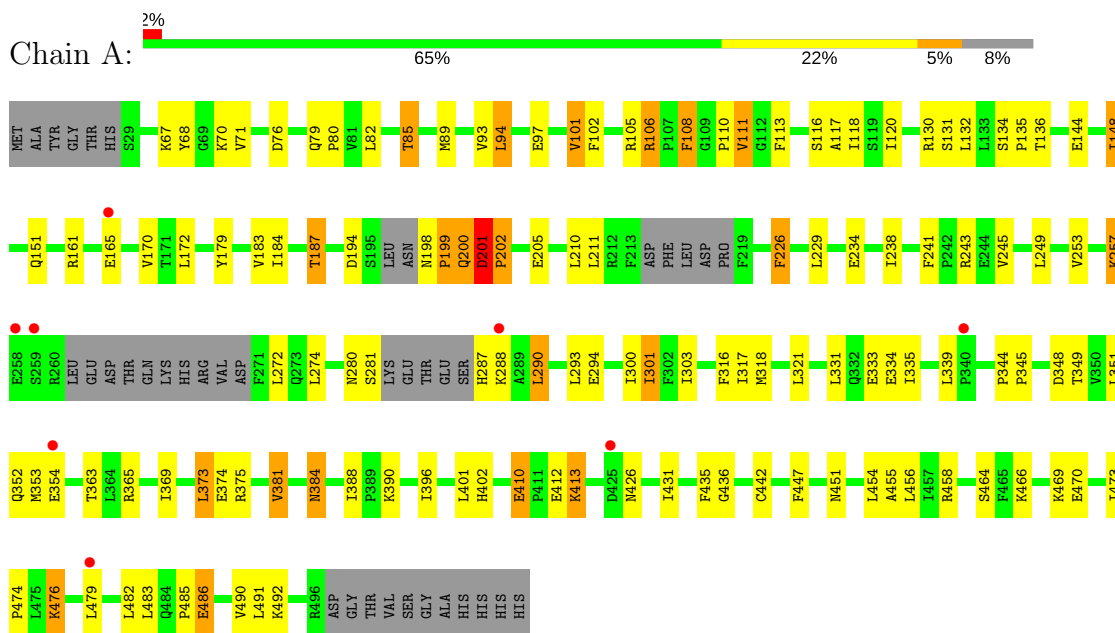
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	27	Total O	0	0
			27 27		
4	B	22	Total O	0	0
			22 22		

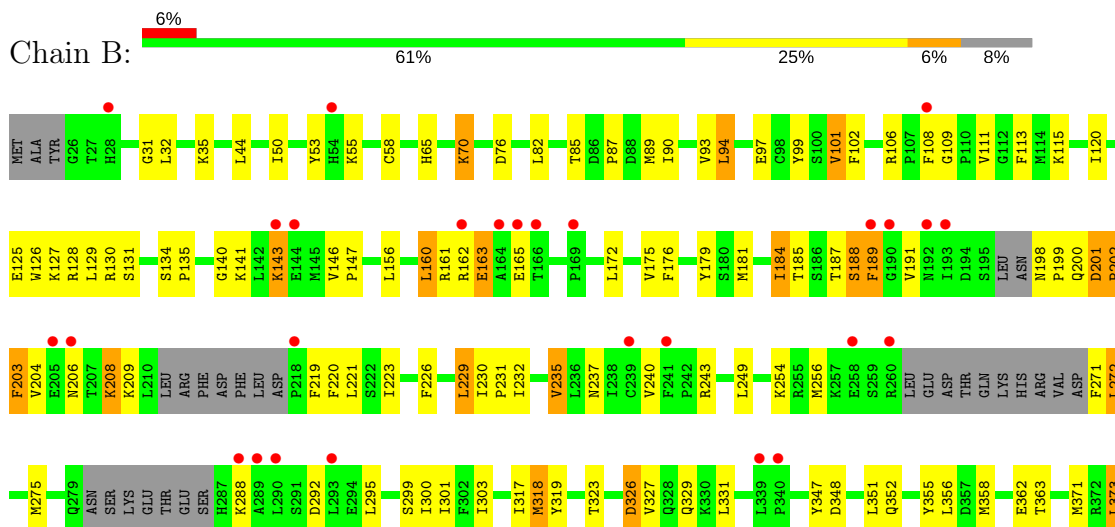
### 3 Residue-property plots

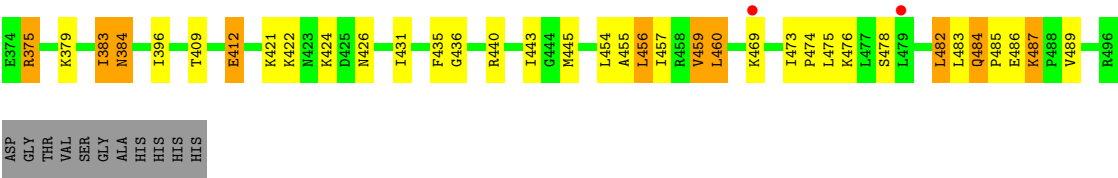
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 3A4



#### • Molecule 1: CYTOCHROME P450 3A4





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.25Å 210.71Å 161.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75 29.77 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.3 (30.00-2.75) 97.3 (29.77-2.75)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.87 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.238 , 0.315 0.233 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	54.6	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7326	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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, ERY

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	0.49	0/3662	0.61	0/4948
1	B	0.48	0/3647	0.61	0/4929
All	All	0.48	0/7309	0.61	0/9877

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	3578	0	3665	83	0
1	B	3562	0	3646	87	0
2	A	43	0	30	9	0
2	B	43	0	30	1	0
3	A	51	0	67	3	0
4	A	27	0	0	0	0
4	B	22	0	0	0	0
All	All	7326	0	7438	177	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 12.



All (177) 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)
2:A:1497:HEM:HMB1	2:A:1497:HEM:HBB2	1.24	1.11
2:A:1497:HEM:CMB	2:A:1497:HEM:HBB2	1.86	1.02
1:A:117:ALA:HB1	1:A:301:ILE:HG13	1.54	0.90
1:A:108:PHE:HE1	1:A:120:ILE:HD12	1.40	0.86
1:A:201:ASP:H	1:A:202:PRO:HD3	1.40	0.84
1:A:102:PHE:HB3	1:A:375:ARG:HG2	1.59	0.83
1:A:344:PRO:HA	1:A:458:ARG:HH21	1.44	0.82
1:A:198:ASN:HB3	1:A:199:PRO:HD2	1.61	0.81
1:A:97:GLU:HB3	1:A:101:VAL:CG1	2.12	0.80
1:B:113:PHE:HA	1:B:115:LYS:HE2	1.62	0.79
1:A:108:PHE:CE1	1:A:120:ILE:HD12	2.23	0.74
1:A:194:ASP:O	1:A:198:ASN:HB2	1.90	0.71
1:B:226:PHE:HB2	1:B:229:LEU:HD22	1.71	0.71
1:A:179:TYR:CZ	1:A:455:ALA:HB2	2.27	0.70
1:B:97:GLU:HB3	1:B:101:VAL:HG13	1.72	0.70
1:B:356:LEU:HD22	1:B:457:ILE:HD11	1.73	0.69
1:A:201:ASP:N	1:A:202:PRO:HD3	2.09	0.68
1:B:176:PHE:HE2	1:B:318:MET:HG2	1.59	0.68
1:B:201:ASP:H	1:B:202:PRO:HD3	1.59	0.68
1:A:470:GLU:O	1:A:470:GLU:HG2	1.94	0.68
1:A:106:ARG:HH12	3:A:1498:ERY:H193	1.60	0.66
1:A:476:LYS:HB3	1:A:486:GLU:HG2	1.78	0.66
1:A:198:ASN:HB3	1:A:199:PRO:CD	2.26	0.65
1:A:136:THR:HG23	1:A:274:LEU:HB2	1.78	0.65
1:B:146:VAL:HG21	1:B:347:TYR:HB2	1.79	0.65
1:B:94:LEU:HD12	1:B:375:ARG:HH11	1.62	0.65
1:A:110:PRO:HB3	1:A:234:GLU:HG2	1.80	0.64
1:A:198:ASN:CB	1:A:199:PRO:HD2	2.28	0.64
1:B:201:ASP:H	1:B:202:PRO:CD	2.12	0.64
1:A:97:GLU:HB3	1:A:101:VAL:HG13	1.79	0.63
1:A:117:ALA:HB1	1:A:301:ILE:CG1	2.26	0.62
1:B:317:ILE:HD13	1:B:456:LEU:HD21	1.81	0.61
1:A:172:LEU:HD11	1:A:491:LEU:HD12	1.82	0.61
1:B:319:TYR:O	1:B:323:THR:HG22	2.01	0.61
1:A:375:ARG:NH2	2:A:1497:HEM:O1A	2.34	0.61
1:B:140:GLY:HA2	1:B:143:LYS:HG2	1.83	0.61
3:A:1498:ERY:H373	3:A:1498:ERY:H351	1.81	0.61
1:B:113:PHE:HA	1:B:115:LYS:CE	2.31	0.60
2:A:1497:HEM:CBB	2:A:1497:HEM:CMB	2.72	0.59
1:B:189:PHE:HZ	1:B:303:ILE:HD11	1.67	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:CYS:SG	1:B:371:MET:CE	2.91	0.59
1:B:219:PHE:CE2	1:B:223:ILE:HD11	2.38	0.59
1:A:108:PHE:HE1	1:A:120:ILE:CD1	2.14	0.58
1:B:58:CYS:SG	1:B:371:MET:HE2	2.44	0.58
1:A:161:ARG:O	1:A:165:GLU:HG2	2.04	0.57
1:B:355:TYR:HD1	1:B:358:MET:HE3	1.70	0.57
1:B:230:ILE:HB	1:B:231:PRO:HD3	1.86	0.57
1:A:287:HIS:O	1:A:288:LYS:HG3	2.05	0.56
3:A:1498:ERY:H202	3:A:1498:ERY:H303	1.87	0.56
1:B:102:PHE:CE2	1:B:383:ILE:HD11	2.41	0.55
1:A:105:ARG:HH21	2:A:1497:HEM:HAA1	1.72	0.55
1:B:189:PHE:CZ	1:B:303:ILE:HD11	2.41	0.55
2:A:1497:HEM:HMB1	2:A:1497:HEM:CBB	2.17	0.55
1:A:375:ARG:HH22	2:A:1497:HEM:CGA	2.20	0.55
1:B:94:LEU:CD1	1:B:375:ARG:HH11	2.19	0.55
1:B:373:LEU:HD21	1:B:436:GLY:HA2	1.89	0.55
1:B:163:GLU:HA	1:B:163:GLU:OE1	2.06	0.54
1:A:249:LEU:HD23	1:A:300:ILE:HG12	1.89	0.54
1:B:70:LYS:O	1:B:85:THR:HB	2.07	0.54
1:B:220:PHE:CZ	1:B:240:VAL:HG21	2.42	0.54
1:B:102:PHE:HE2	1:B:383:ILE:HD11	1.73	0.54
1:A:384:ASN:HD22	1:A:384:ASN:N	2.06	0.54
1:B:318:MET:HE3	1:B:318:MET:HA	1.88	0.53
1:A:335:ILE:HA	1:A:353:MET:HE1	1.90	0.53
1:B:130:ARG:HD2	1:B:443:ILE:HD12	1.91	0.53
1:A:280:ASN:O	1:A:281:SER:HB3	2.09	0.53
1:B:326:ASP:N	1:B:326:ASP:OD1	2.42	0.53
1:B:87:PRO:HG3	1:B:431:ILE:HD11	1.90	0.52
1:A:67:LYS:HD3	1:A:68:TYR:CZ	2.44	0.52
1:B:102:PHE:HB3	1:B:375:ARG:HG2	1.91	0.52
1:A:198:ASN:CB	1:A:199:PRO:CD	2.87	0.52
1:A:210:LEU:HD21	1:A:300:ILE:HG23	1.92	0.52
1:B:317:ILE:HG13	1:B:363:THR:HG21	1.91	0.52
1:A:183:VAL:O	1:A:187:THR:OG1	2.26	0.51
1:B:204:VAL:O	1:B:208:LYS:HB2	2.11	0.51
1:A:226:PHE:HB2	1:A:229:LEU:HB2	1.93	0.51
1:B:232:ILE:O	1:B:235:VAL:HG12	2.12	0.50
1:A:132:LEU:HD13	1:A:290:LEU:HB2	1.93	0.50
1:A:317:ILE:HG13	1:A:363:THR:HG21	1.92	0.50
1:B:31:GLY:O	1:B:35:LYS:HG3	2.10	0.50
1:A:201:ASP:N	1:A:202:PRO:CD	2.72	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:GLU:O	1:B:129:LEU:HD12	2.11	0.50
1:A:344:PRO:HA	1:A:458:ARG:NH2	2.20	0.50
1:B:203:PHE:HA	1:B:206:ASN:HD22	1.76	0.50
1:A:70:LYS:O	1:A:85:THR:HB	2.12	0.49
1:B:355:TYR:HA	1:B:358:MET:HE3	1.94	0.49
2:B:1497:HEM:HMB2	2:B:1497:HEM:HBB2	1.92	0.49
1:B:58:CYS:SG	1:B:371:MET:HE3	2.53	0.49
1:A:111:VAL:HG12	1:A:241:PHE:HE2	1.77	0.49
1:B:161:ARG:O	1:B:165:GLU:HG2	2.13	0.49
1:B:319:TYR:CZ	1:B:475:LEU:HB2	2.48	0.48
1:A:179:TYR:OH	1:A:451:ASN:ND2	2.46	0.48
1:B:187:THR:O	1:B:271:PHE:N	2.46	0.48
1:B:482:LEU:HG	1:B:484:GLN:NE2	2.28	0.48
1:A:211:LEU:HD21	1:A:303:ILE:HG22	1.94	0.48
1:B:362:GLU:HA	1:B:362:GLU:OE1	2.13	0.48
1:B:355:TYR:HA	1:B:358:MET:CE	2.43	0.48
1:A:447:PHE:HD2	2:A:1497:HEM:HMC3	1.79	0.48
1:A:134:SER:HB2	1:A:135:PRO:HD3	1.96	0.47
1:A:369:ILE:HG22	1:A:482:LEU:HG	1.95	0.47
1:B:146:VAL:N	1:B:147:PRO:HD2	2.30	0.47
1:B:275:MET:HB3	1:B:295:LEU:HD11	1.96	0.47
1:B:99:TYR:CE1	1:B:127:LYS:HD3	2.50	0.47
1:A:401:LEU:HD22	1:A:431:ILE:HD12	1.97	0.46
1:A:89:MET:O	1:A:93:VAL:HG13	2.14	0.46
1:B:179:TYR:CZ	1:B:455:ALA:HB2	2.50	0.46
1:B:383:ILE:HG23	1:B:384:ASN:HD22	1.81	0.46
1:B:478:SER:HA	1:B:486:GLU:HB2	1.98	0.46
1:B:486:GLU:O	1:B:487:LYS:HB3	2.14	0.46
1:A:198:ASN:O	1:A:200:GLN:N	2.49	0.46
1:A:339:LEU:HD21	1:A:349:THR:HG21	1.98	0.45
1:B:184:ILE:O	1:B:188:SER:HB2	2.16	0.45
1:B:32:LEU:HA	1:B:35:LYS:HE2	1.99	0.45
1:A:381:VAL:HG23	1:A:388:ILE:HB	1.99	0.45
1:B:482:LEU:HG	1:B:484:GLN:HE21	1.82	0.45
1:A:373:LEU:HD21	1:A:436:GLY:HA2	1.98	0.45
1:B:181:MET:O	1:B:185:THR:HG23	2.17	0.45
1:B:126:TRP:CZ2	1:B:440:ARG:HD2	2.52	0.45
1:A:334:GLU:OE2	1:A:353:MET:HB3	2.16	0.44
1:A:179:TYR:CE2	1:A:455:ALA:HB2	2.52	0.44
1:B:189:PHE:O	1:B:191:VAL:HG23	2.16	0.44
1:A:210:LEU:HB2	1:A:245:VAL:HG11	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ILE:HA	1:B:303:ILE:HD12	2.00	0.44
1:B:134:SER:HB2	1:B:135:PRO:HD3	2.00	0.44
1:A:318:MET:HE3	1:A:321:LEU:HD12	2.00	0.44
1:B:128:ARG:HA	1:B:288:LYS:HD3	2.00	0.44
1:B:435:PHE:CG	1:B:445:MET:HG3	2.53	0.44
1:B:473:ILE:HA	1:B:474:PRO:HA	1.85	0.44
1:B:65:HIS:HE1	1:B:85:THR:HG21	1.83	0.44
1:A:113:PHE:CD2	1:A:293:LEU:HD11	2.53	0.43
1:B:412:GLU:CD	1:B:412:GLU:H	2.22	0.43
1:B:127:LYS:HD2	1:B:127:LYS:HA	1.80	0.43
1:B:65:HIS:CE1	1:B:85:THR:HG21	2.53	0.43
1:B:160:LEU:HD23	1:B:175:VAL:HG21	2.01	0.43
1:B:108:PHE:HE1	1:B:120:ILE:HD12	1.83	0.43
1:B:272:LEU:HA	1:B:275:MET:HB2	2.01	0.43
1:A:110:PRO:HB2	1:A:238:ILE:O	2.18	0.43
1:A:253:VAL:O	1:A:257:LYS:HB2	2.19	0.43
1:A:410:GLU:OE1	1:A:413:LYS:HG3	2.18	0.43
1:A:170:VAL:O	1:A:490:VAL:HA	2.19	0.43
1:A:280:ASN:O	1:A:281:SER:CB	2.66	0.43
1:B:327:VAL:HG13	1:B:355:TYR:OH	2.19	0.43
1:A:316:PHE:CZ	1:A:485:PRO:HD3	2.54	0.42
1:B:156:LEU:HD13	1:B:179:TYR:HB2	2.01	0.42
1:A:301:ILE:HA	1:A:301:ILE:HD13	1.87	0.42
1:B:113:PHE:C	1:B:115:LYS:H	2.22	0.42
1:B:475:LEU:HD11	1:B:485:PRO:HB3	2.01	0.42
1:A:116:SER:HB3	1:A:294:GLU:HG2	2.01	0.42
1:A:148:ILE:HG12	1:A:148:ILE:H	1.72	0.42
1:A:111:VAL:HG12	1:A:241:PHE:CE2	2.55	0.41
1:A:105:ARG:NH2	2:A:1497:HEM:HAA1	2.33	0.41
1:A:365:ARG:O	1:A:402:HIS:HB3	2.20	0.41
1:A:201:ASP:HA	1:A:205:GLU:HG3	2.02	0.41
1:A:373:LEU:HB2	1:A:396:ILE:HB	2.01	0.41
1:B:109:GLY:HA2	1:B:111:VAL:HG23	2.01	0.41
1:B:202:PRO:HB2	1:B:203:PHE:H	1.57	0.41
1:A:384:ASN:N	1:A:384:ASN:ND2	2.69	0.41
1:A:94:LEU:HD21	1:A:373:LEU:HD23	2.02	0.41
1:B:373:LEU:HB2	1:B:396:ILE:HB	2.02	0.41
1:A:76:ASP:OD2	1:A:106:ARG:NH2	2.53	0.41
1:A:344:PRO:HA	1:A:345:PRO:HD3	1.92	0.41
1:B:318:MET:CE	1:B:318:MET:HA	2.49	0.41
1:B:50:ILE:O	1:B:53:TYR:HB2	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:MET:HE2	1:B:89:MET:HB3	1.69	0.41
1:B:90:ILE:HG23	1:B:94:LEU:HD22	2.02	0.41
1:A:106:ARG:NH1	1:A:374:GLU:OE1	2.53	0.41
1:A:435:PHE:HB3	1:A:442:CYS:HB3	2.01	0.41
1:B:220:PHE:HZ	1:B:240:VAL:HG21	1.83	0.41
1:B:459:VAL:HG12	1:B:460:LEU:HD13	2.03	0.41
1:A:118:ILE:HD11	1:A:130:ARG:HD2	2.01	0.41
1:B:237:ASN:HB3	1:B:243:ARG:NH2	2.36	0.41
1:A:287:HIS:C	1:A:288:LYS:HG3	2.40	0.41
1:A:94:LEU:HA	1:A:94:LEU:HD12	1.93	0.41
1:A:473:ILE:HA	1:A:474:PRO:HA	1.75	0.40
1:B:198:ASN:O	1:B:200:GLN:N	2.53	0.40
1:B:172:LEU:HD12	1:B:489:VAL:HB	2.04	0.40
1:A:79:GLN:NE2	1:A:80:PRO:HD2	2.36	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	436/485 (90%)	398 (91%)	32 (7%)	6 (1%)	13	35
1	B	435/485 (90%)	395 (91%)	34 (8%)	6 (1%)	13	35
All	All	871/970 (90%)	793 (91%)	66 (8%)	12 (1%)	13	35

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	PRO
1	A	354	GLU
1	B	201	ASP
1	A	199	PRO

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	290	LEU
1	B	202	PRO
1	A	201	ASP
1	B	199	PRO
1	B	384	ASN
1	B	487	LYS
1	B	426	ASN
1	A	351	LEU

### 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	405/441 (92%)	362 (89%)	43 (11%)	8	20
1	B	403/441 (91%)	347 (86%)	56 (14%)	4	10
All	All	808/882 (92%)	709 (88%)	99 (12%)	5	15

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	VAL
1	A	82	LEU
1	A	85	THR
1	A	94	LEU
1	A	101	VAL
1	A	106	ARG
1	A	108	PHE
1	A	111	VAL
1	A	131	SER
1	A	144	GLU
1	A	148	ILE
1	A	151	GLN
1	A	184	ILE
1	A	187	THR
1	A	200	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	201	ASP
1	A	226	PHE
1	A	243	ARG
1	A	257	LYS
1	A	272	LEU
1	A	301	ILE
1	A	331	LEU
1	A	333	GLU
1	A	348	ASP
1	A	352	GLN
1	A	373	LEU
1	A	381	VAL
1	A	384	ASN
1	A	390	LYS
1	A	410	GLU
1	A	412	GLU
1	A	413	LYS
1	A	426	ASN
1	A	454	LEU
1	A	456	LEU
1	A	464	SER
1	A	466	LYS
1	A	469	LYS
1	A	476	LYS
1	A	479	LEU
1	A	483	LEU
1	A	486	GLU
1	A	492	LYS
1	B	44	LEU
1	B	55	LYS
1	B	70	LYS
1	B	76	ASP
1	B	82	LEU
1	B	93	VAL
1	B	94	LEU
1	B	101	VAL
1	B	106	ARG
1	B	131	SER
1	B	141	LYS
1	B	143	LYS
1	B	160	LEU
1	B	162	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	163	GLU
1	B	184	ILE
1	B	188	SER
1	B	189	PHE
1	B	203	PHE
1	B	208	LYS
1	B	209	LYS
1	B	221	LEU
1	B	229	LEU
1	B	235	VAL
1	B	249	LEU
1	B	254	LYS
1	B	256	MET
1	B	272	LEU
1	B	292	ASP
1	B	299	SER
1	B	301	ILE
1	B	318	MET
1	B	326	ASP
1	B	329	GLN
1	B	331	LEU
1	B	348	ASP
1	B	351	LEU
1	B	352	GLN
1	B	373	LEU
1	B	375	ARG
1	B	379	LYS
1	B	383	ILE
1	B	409	THR
1	B	412	GLU
1	B	421	LYS
1	B	422	LYS
1	B	424	LYS
1	B	454	LEU
1	B	456	LEU
1	B	459	VAL
1	B	460	LEU
1	B	469	LYS
1	B	476	LYS
1	B	482	LEU
1	B	483	LEU
1	B	484	GLN



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	78	GLN
1	A	79	GLN
1	A	247	ASN
1	A	384	ASN
1	A	423	ASN
1	A	426	ASN
1	A	451	ASN
1	B	151	GLN
1	B	206	ASN
1	B	423	ASN
1	B	451	ASN
1	B	484	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	1497	1	28,50,50	2.85	12 (42%)	17,82,82	2.25	7 (41%)
3	ERY	A	1498	-	53,53,53	0.71	0	82,82,82	2.20	19 (23%)
2	HEM	B	1497	1	28,50,50	2.12	6 (21%)	17,82,82	1.57	5 (29%)

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	1497	1	-	0/6/54/54	0/0/8/8
3	ERY	A	1498	-	-	0/72/107/107	0/3/3/3
2	HEM	B	1497	1	-	0/6/54/54	0/0/8/8

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1497	HEM	C3C-C2C	-4.73	1.34	1.40
2	B	1497	HEM	C3C-C2C	-4.39	1.34	1.40
2	A	1497	HEM	C3B-C2B	-4.27	1.34	1.40
2	B	1497	HEM	C3B-C2B	-3.66	1.35	1.40
2	A	1497	HEM	C3B-CAB	-2.18	1.43	1.47
2	A	1497	HEM	CMC-C2C	2.21	1.56	1.51
2	A	1497	HEM	C4B-NB	2.29	1.41	1.36
2	B	1497	HEM	C4D-ND	2.30	1.39	1.36
2	A	1497	HEM	C1A-NA	2.40	1.41	1.36
2	A	1497	HEM	C4C-NC	2.94	1.40	1.36
2	A	1497	HEM	CMB-C2B	3.31	1.58	1.51
2	B	1497	HEM	C3C-CAC	3.60	1.54	1.47
2	B	1497	HEM	C3B-CAB	3.78	1.55	1.47
2	A	1497	HEM	C3D-C2D	4.75	1.51	1.37
2	A	1497	HEM	C3C-CAC	5.06	1.57	1.47
2	A	1497	HEM	CAA-C2A	5.09	1.60	1.52
2	B	1497	HEM	C3D-C2D	5.15	1.52	1.37
2	A	1497	HEM	CAD-C3D	7.31	1.66	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1497	HEM	CBD-CAD-C3D	-2.94	106.86	112.47
2	A	1497	HEM	C3B-C4B-NB	-2.83	105.55	109.21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1497	HEM	CAA-C2A-C3A	-2.66	121.40	129.00
3	A	1498	ERY	O11-C9-C8	-2.59	116.10	121.15
2	B	1497	HEM	CMA-C3A-C4A	-2.53	124.57	128.46
3	A	1498	ERY	O1-C1-C2	-2.31	117.71	124.02
3	A	1498	ERY	O10-C6-C32	-2.22	103.34	108.48
2	B	1497	HEM	C1D-C2D-C3D	-2.15	105.50	107.00
2	B	1497	HEM	C3C-C4C-NC	-2.12	106.94	110.94
3	A	1498	ERY	O5-C16-C19	-2.02	107.42	110.96
2	A	1497	HEM	C1D-C2D-C3D	2.05	108.42	107.00
2	B	1497	HEM	C4A-C3A-C2A	2.05	108.42	107.00
3	A	1498	ERY	O7-C5-C4	2.17	114.84	111.48
3	A	1498	ERY	C31-C4-C5	2.25	117.40	112.89
3	A	1498	ERY	C14-O4-C18	2.38	120.02	114.19
2	B	1497	HEM	C4C-C3C-C2C	2.52	108.66	106.90
3	A	1498	ERY	C7-C6-C5	2.57	115.62	110.46
3	A	1498	ERY	C12-C11-C10	2.76	120.12	116.44
3	A	1498	ERY	C22-C23-C24	2.90	114.18	109.27
3	A	1498	ERY	O3-C3-C4	3.02	111.79	108.16
2	A	1497	HEM	C4C-C3C-C2C	3.03	109.01	106.90
3	A	1498	ERY	O2-C13-C12	3.12	112.62	107.32
3	A	1498	ERY	C8-C9-C10	3.23	124.98	119.12
2	A	1497	HEM	CMB-C2B-C3B	3.38	131.17	124.89
3	A	1498	ERY	O2-C1-C2	3.52	119.53	111.58
3	A	1498	ERY	O5-C16-C17	3.71	109.56	103.84
3	A	1498	ERY	O2-C13-C36	3.97	115.24	107.44
2	A	1497	HEM	CMC-C2C-C3C	5.06	134.28	124.89
3	A	1498	ERY	C13-O2-C1	6.15	129.15	118.14
3	A	1498	ERY	C22-O7-C5	6.36	127.59	116.29
3	A	1498	ERY	O7-C5-C6	10.59	120.03	106.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1497	HEM	9	0
3	A	1498	ERY	3	0
2	B	1497	HEM	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

### 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	446/485 (91%)	0.20	8 (1%) 69 65	22, 47, 71, 79	0
1	B	445/485 (91%)	0.40	29 (6%) 20 15	22, 56, 93, 105	0
All	All	891/970 (91%)	0.30	37 (4%) 37 31	22, 51, 83, 105	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	GLU	5.0
1	B	479	LEU	4.9
1	A	165	GLU	3.4
1	A	479	LEU	3.2
1	B	340	PRO	2.9
1	B	54	HIS	2.9
1	B	290	LEU	2.8
1	B	293	LEU	2.8
1	B	192	ASN	2.8
1	B	193	ILE	2.8
1	B	205	GLU	2.7
1	B	164	ALA	2.7
1	B	169	PRO	2.7
1	A	425	ASP	2.7
1	B	189	PHE	2.7
1	B	239	CYS	2.7
1	B	289	ALA	2.6
1	B	162	ARG	2.5
1	B	241	PHE	2.5
1	A	259	SER	2.5
1	B	28	HIS	2.4
1	B	258	GLU	2.4
1	A	258	GLU	2.4
1	B	166	THR	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	190	GLY	2.3
1	B	469	LYS	2.3
1	B	108	PHE	2.2
1	B	218	PRO	2.1
1	B	260	ARG	2.1
1	B	143	LYS	2.1
1	A	288	LYS	2.1
1	B	339	LEU	2.1
1	A	340	PRO	2.1
1	B	206	ASN	2.1
1	B	144	GLU	2.1
1	B	288	LYS	2.0
1	A	354	GLU	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	ERY	A	1498	51/51	0.76	0.33	3.50	88,93,100,100	0
2	HEM	A	1497	43/43	0.96	0.22	0.52	22,24,31,36	0
2	HEM	B	1497	43/43	0.97	0.20	-0.11	27,29,33,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.