



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:52 am GMT

PDB ID : 1W0F  
Title : CRYSTAL STRUCTURE OF HUMAN CYTOCHROME P450 3A4  
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Deposited on : 2004-06-03  
Resolution : 2.65 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

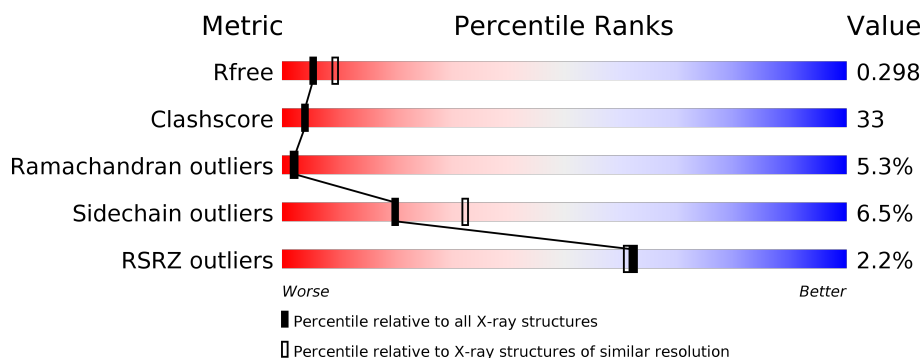
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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	<div> <div>2%</div> <div> <div></div> <div>46%</div> <div>40%</div> <div>8%</div> <div>5%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3794 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.

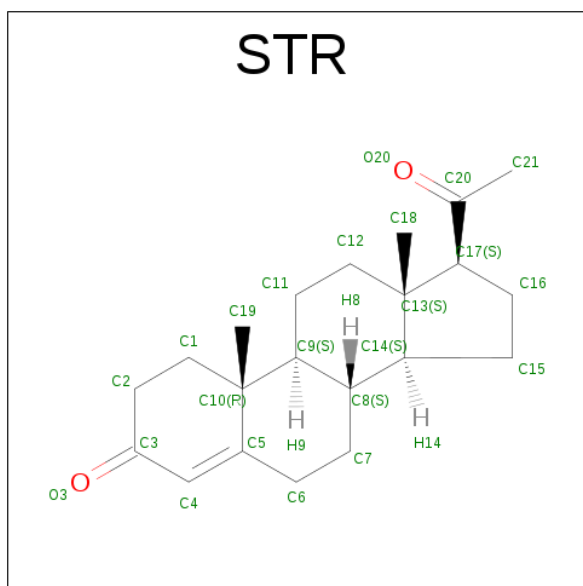
- Molecule 1 is a protein called CYTOCHROME P450 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	459	3681	2398	603	656	24	0	0	0

There is a discrepancy between the modelled and reference sequences:

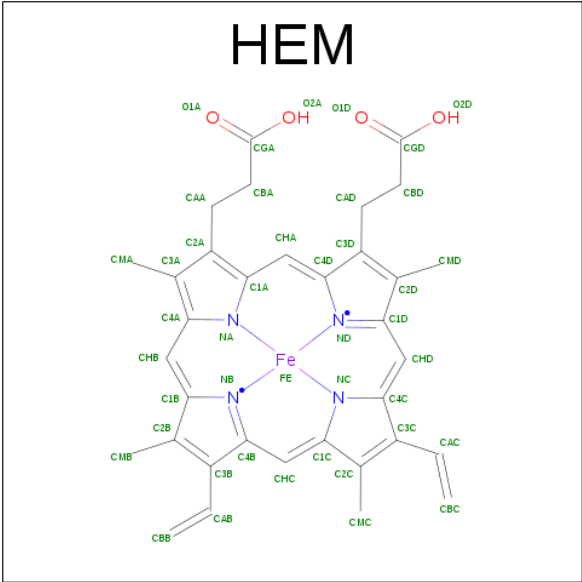
Chain	Residue	Modelled	Actual	Comment	Reference
A	392	VAL	TRP	CONFLICT SEE REMARK 9	UNP P08684

- Molecule 2 is PROGESTERONE (three-letter code: STR) (formula:  $C_{21}H_{30}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	23	21	2	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		

### 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.41Å 101.51Å 128.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.00 – 2.65 64.33 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.1 (65.00-2.65) 97.1 (64.33-2.65)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.19 (at 2.65Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.239 , 0.303 0.236 , 0.298	Depositor DCC
$R_{free}$ test set	739 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3794	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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, STR

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	0.31	0/3771	0.52	0/5103

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	322	ALA	Peptide
1	A	425	ASP	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	3681	0	3754	249	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	23	0	30	0	0
3	A	43	0	30	1	0
4	A	47	0	0	3	0
All	All	3794	0	3814	249	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 33.

All (249) 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:260:ARG:HH21	1:A:273:GLN:HG2	1.27	1.00
1:A:102:PHE:HB3	1:A:375:ARG:HG2	1.47	0.95
1:A:178:ALA:HB1	1:A:196:LEU:HA	1.48	0.92
1:A:346:THR:HB	1:A:349:THR:OG1	1.73	0.88
1:A:101:VAL:HG11	1:A:381:VAL:HG21	1.57	0.85
1:A:140:GLY:HA2	1:A:143:LYS:HG3	1.60	0.84
1:A:355:TYR:HA	1:A:358:MET:HE2	1.61	0.80
1:A:339:LEU:HB2	1:A:343:ALA:HB3	1.64	0.79
1:A:335:ILE:HG12	1:A:353:MET:HE1	1.64	0.78
1:A:475:LEU:H	1:A:475:LEU:HD23	1.50	0.76
1:A:178:ALA:CB	1:A:196:LEU:HA	2.16	0.75
1:A:163:GLU:HB3	1:A:170:VAL:HG22	1.68	0.74
1:A:162:ARG:NE	1:A:163:GLU:HG2	2.03	0.74
1:A:99:TYR:HE2	1:A:127:LYS:HD2	1.51	0.73
1:A:291:SER:HB3	1:A:294:GLU:HB3	1.68	0.73
1:A:323:THR:HG23	1:A:324:HIS:ND1	2.03	0.73
1:A:308:GLU:O	1:A:312:SER:HB2	1.89	0.73
1:A:468:CYS:HB3	1:A:492:LYS:HG3	1.71	0.72
1:A:155:VAL:HG12	1:A:196:LEU:HD23	1.72	0.71
1:A:328:GLN:O	1:A:332:GLN:HB2	1.90	0.71
1:A:131:SER:O	1:A:132:LEU:HB2	1.92	0.70
1:A:252:SER:O	1:A:256:MET:HG3	1.91	0.70
1:A:178:ALA:HB3	1:A:196:LEU:HD13	1.74	0.70
1:A:169:PRO:HB3	1:A:468:CYS:SG	2.33	0.69
1:A:195:SER:O	1:A:197:ASN:N	2.25	0.69
1:A:211:LEU:HD22	1:A:308:GLU:OE2	1.92	0.69
1:A:335:ILE:O	1:A:339:LEU:HD12	1.93	0.69
1:A:201:ASP:H	1:A:202:PRO:HD2	1.57	0.68
1:A:201:ASP:H	1:A:202:PRO:CD	2.07	0.68
1:A:178:ALA:HB1	1:A:196:LEU:CA	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:VAL:HG11	1:A:386:MET:HE1	1.75	0.67
1:A:38:ILE:HD12	1:A:38:ILE:N	2.10	0.66
1:A:193:ILE:H	1:A:193:ILE:HD13	1.61	0.65
1:A:162:ARG:HE	1:A:163:GLU:HG2	1.60	0.65
1:A:141:LYS:O	1:A:145:MET:HG3	1.96	0.65
1:A:189:PHE:HE1	1:A:303:ILE:HD11	1.61	0.64
1:A:419:PHE:O	1:A:424:LYS:HD3	1.98	0.64
1:A:485:PRO:O	1:A:486:GLU:HB3	1.97	0.64
1:A:158:ARG:HB3	1:A:158:ARG:HH11	1.63	0.64
1:A:202:PRO:HG2	1:A:203:PHE:H	1.63	0.64
1:A:270:ASP:HB3	1:A:273:GLN:HB2	1.80	0.64
1:A:403:ARG:O	1:A:405:PRO:HD3	1.98	0.64
1:A:200:GLN:HG3	1:A:201:ASP:OD1	1.98	0.63
1:A:354:GLU:OE1	1:A:421:LYS:HE3	1.98	0.63
1:A:291:SER:HB3	1:A:294:GLU:CB	2.29	0.63
1:A:270:ASP:O	1:A:273:GLN:HB2	1.98	0.63
1:A:368:PRO:HG3	1:A:399:TYR:HA	1.80	0.63
1:A:369:ILE:HD13	1:A:483:LEU:HD12	1.82	0.62
1:A:76:ASP:OD2	1:A:106:ARG:NH1	2.24	0.62
1:A:355:TYR:HD2	1:A:358:MET:HE3	1.64	0.62
1:A:127:LYS:HE3	1:A:127:LYS:HA	1.82	0.61
1:A:158:ARG:NH1	1:A:158:ARG:HB3	2.15	0.61
1:A:327:VAL:HG13	1:A:355:TYR:OH	2.01	0.61
1:A:335:ILE:HG12	1:A:353:MET:CE	2.28	0.61
1:A:106:ARG:HD2	1:A:374:GLU:OE2	2.01	0.60
1:A:164:ALA:HB2	1:A:493:VAL:HG12	1.82	0.60
1:A:466:LYS:O	1:A:492:LYS:HB2	2.02	0.60
1:A:251:LYS:HD2	4:A:2025:HOH:O	2.02	0.60
1:A:373:LEU:HD22	1:A:398:SER:OG	2.02	0.60
1:A:410:GLU:HB3	1:A:413:LYS:HG3	1.84	0.59
1:A:260:ARG:NH2	1:A:273:GLN:HG2	2.09	0.59
1:A:408:TRP:O	1:A:411:PRO:HG3	2.02	0.59
1:A:99:TYR:CE2	1:A:127:LYS:HD2	2.36	0.59
1:A:421:LYS:HA	1:A:424:LYS:HE2	1.85	0.59
1:A:476:LYS:O	1:A:485:PRO:O	2.21	0.59
1:A:331:LEU:O	1:A:335:ILE:HG13	2.02	0.58
1:A:322:ALA:O	1:A:323:THR:HG22	2.03	0.58
1:A:206:ASN:HB3	1:A:245:VAL:HG13	1.86	0.58
1:A:161:ARG:HH11	1:A:161:ARG:HG3	1.69	0.58
1:A:163:GLU:HB3	1:A:170:VAL:CG2	2.33	0.58
1:A:152:TYR:OH	1:A:192:ASN:ND2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LYS:NZ	1:A:462:ASN:HA	2.19	0.57
1:A:248:PHE:HD1	1:A:249:LEU:HD22	1.69	0.57
1:A:47:LEU:HD22	1:A:50:ILE:HD11	1.85	0.57
1:A:178:ALA:CB	1:A:196:LEU:HD13	2.33	0.57
1:A:339:LEU:HD22	1:A:343:ALA:O	2.04	0.57
1:A:415:LEU:HD11	1:A:418:ARG:CZ	2.34	0.57
1:A:339:LEU:HD23	1:A:349:THR:HG21	1.85	0.56
1:A:323:THR:HG23	1:A:324:HIS:CE1	2.39	0.56
1:A:194:ASP:O	1:A:199:PRO:HD2	2.05	0.56
1:A:189:PHE:CE1	1:A:303:ILE:HD11	2.40	0.56
1:A:453:LYS:O	1:A:457:ILE:HG12	2.05	0.56
1:A:71:VAL:HG13	1:A:82:LEU:HD21	1.87	0.56
1:A:328:GLN:OE1	1:A:464:SER:HA	2.07	0.55
1:A:201:ASP:N	1:A:202:PRO:HD2	2.21	0.55
1:A:250:ARG:HD2	1:A:296:VAL:HG11	1.89	0.55
1:A:198:ASN:CB	1:A:199:PRO:HD3	2.37	0.55
1:A:317:ILE:HG13	1:A:363:THR:HG21	1.89	0.55
1:A:64:CYS:O	1:A:68:TYR:HB2	2.07	0.55
1:A:415:LEU:HD11	1:A:418:ARG:NH1	2.21	0.55
1:A:475:LEU:N	1:A:475:LEU:HD23	2.20	0.55
1:A:269:VAL:O	1:A:270:ASP:HB2	2.06	0.54
1:A:410:GLU:HB3	1:A:413:LYS:CG	2.37	0.54
1:A:249:LEU:O	1:A:253:VAL:HG23	2.08	0.54
1:A:83:ALA:HA	1:A:395:MET:O	2.08	0.54
1:A:111:VAL:O	1:A:114:MET:HB2	2.08	0.54
1:A:381:VAL:HG12	1:A:382:GLU:N	2.23	0.54
1:A:38:ILE:H	1:A:38:ILE:HD12	1.72	0.54
1:A:98:CYS:SG	1:A:439:PRO:HB2	2.47	0.54
1:A:406:LYS:HG3	1:A:407:TYR:N	2.22	0.54
1:A:137:PHE:O	1:A:446:ARG:NH2	2.41	0.53
1:A:375:ARG:HH22	1:A:440:ARG:HB3	1.72	0.53
1:A:396:ILE:N	1:A:396:ILE:HD12	2.23	0.53
1:A:420:SER:O	1:A:424:LYS:HG2	2.08	0.53
1:A:195:SER:OG	1:A:196:LEU:N	2.41	0.53
1:A:278:SER:O	1:A:279:GLN:HG2	2.08	0.53
1:A:293:LEU:N	1:A:293:LEU:HD22	2.24	0.53
1:A:91:LYS:HE2	1:A:96:LYS:HE3	1.90	0.53
1:A:330:LYS:HE3	1:A:355:TYR:CE2	2.44	0.53
1:A:296:VAL:O	1:A:300:ILE:HG13	2.09	0.52
1:A:475:LEU:HG	1:A:476:LYS:H	1.74	0.52
1:A:483:LEU:O	1:A:483:LEU:HD13	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASP:N	1:A:202:PRO:CD	2.72	0.52
1:A:419:PHE:HA	1:A:424:LYS:HB3	1.90	0.52
1:A:213:PHE:CZ	1:A:240:VAL:HG13	2.43	0.52
1:A:144:GLU:HB3	1:A:269:VAL:HG21	1.91	0.52
1:A:389:PRO:HG2	1:A:392:VAL:CG2	2.39	0.52
1:A:485:PRO:O	1:A:486:GLU:CB	2.58	0.52
1:A:140:GLY:HA2	1:A:143:LYS:CG	2.37	0.52
1:A:146:VAL:HB	1:A:147:PRO:HD3	1.92	0.51
1:A:133:LEU:O	1:A:136:THR:HB	2.11	0.51
1:A:184:ILE:CG2	1:A:303:ILE:HG12	2.41	0.51
1:A:164:ALA:HB2	1:A:493:VAL:CG1	2.40	0.51
1:A:355:TYR:HA	1:A:358:MET:CE	2.35	0.51
1:A:101:VAL:HG11	1:A:381:VAL:CG2	2.37	0.51
1:A:277:ASP:O	1:A:279:GLN:N	2.43	0.51
1:A:162:ARG:HH11	1:A:162:ARG:HG2	1.76	0.51
1:A:279:GLN:O	1:A:280:ASN:C	2.49	0.51
1:A:397:PRO:O	1:A:398:SER:C	2.48	0.51
1:A:382:GLU:O	1:A:386:MET:O	2.29	0.50
1:A:38:ILE:HG23	1:A:71:VAL:HG12	1.92	0.50
1:A:452:MET:O	1:A:456:LEU:HD22	2.12	0.50
1:A:257:LYS:HE2	1:A:292:ASP:OD1	2.11	0.50
1:A:27:THR:CG2	1:A:45:PRO:HA	2.42	0.50
1:A:317:ILE:CG1	1:A:363:THR:HG21	2.42	0.50
1:A:132:LEU:HD21	1:A:290:LEU:HG	1.94	0.49
1:A:339:LEU:CD2	1:A:349:THR:HG21	2.43	0.49
1:A:245:VAL:O	1:A:249:LEU:HD23	2.13	0.49
1:A:44:LEU:CD2	1:A:51:LEU:HD12	2.42	0.49
1:A:479:LEU:HD23	1:A:479:LEU:N	2.27	0.49
1:A:159:ASN:ND2	1:A:196:LEU:HG	2.27	0.49
1:A:346:THR:HG22	1:A:348:ASP:H	1.76	0.49
1:A:365:ARG:O	1:A:368:PRO:HD3	2.12	0.48
1:A:226:PHE:O	1:A:229:LEU:HB2	2.12	0.48
1:A:101:VAL:HG23	1:A:102:PHE:CD1	2.48	0.48
1:A:193:ILE:CD1	1:A:193:ILE:H	2.25	0.48
1:A:191:VAL:HG12	1:A:193:ILE:HG23	1.96	0.48
1:A:134:SER:N	1:A:135:PRO:CD	2.77	0.48
1:A:339:LEU:CB	1:A:343:ALA:HB3	2.41	0.48
1:A:465:PHE:CE1	1:A:493:VAL:HG22	2.48	0.48
1:A:223:ILE:HD11	1:A:233:LEU:CD1	2.44	0.48
1:A:144:GLU:O	1:A:147:PRO:HD2	2.14	0.48
1:A:460:LEU:C	1:A:462:ASN:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ILE:HG13	1:A:90:ILE:HG12	1.96	0.47
1:A:317:ILE:O	1:A:321:LEU:HG	2.14	0.47
1:A:461:GLN:HG3	1:A:461:GLN:O	2.13	0.47
1:A:198:ASN:CB	1:A:199:PRO:CD	2.93	0.47
1:A:256:MET:O	1:A:260:ARG:HG3	2.15	0.47
1:A:484:GLN:HB2	1:A:485:PRO:HD2	1.97	0.47
1:A:90:ILE:O	1:A:94:LEU:HB2	2.14	0.47
1:A:136:THR:O	1:A:136:THR:HG22	2.14	0.47
1:A:254:LYS:HD2	1:A:254:LYS:HA	1.79	0.47
1:A:375:ARG:NH2	1:A:440:ARG:HB3	2.30	0.47
1:A:228:PHE:CE1	1:A:229:LEU:HD13	2.49	0.46
1:A:386:MET:HB2	4:A:2003:HOH:O	2.15	0.46
1:A:389:PRO:HG2	1:A:392:VAL:HG23	1.95	0.46
1:A:410:GLU:O	1:A:418:ARG:NH1	2.47	0.46
1:A:469:LYS:HD3	1:A:469:LYS:C	2.36	0.46
1:A:298:GLN:O	1:A:301:ILE:HG22	2.15	0.46
1:A:293:LEU:HB3	4:A:2026:HOH:O	2.16	0.46
1:A:326:ASP:OD1	1:A:327:VAL:HG23	2.15	0.46
1:A:354:GLU:O	1:A:358:MET:HG3	2.15	0.46
1:A:25:TYR:HE1	1:A:28:HIS:ND1	2.14	0.46
1:A:295:LEU:O	1:A:295:LEU:HD23	2.16	0.46
1:A:44:LEU:HD22	1:A:51:LEU:HD12	1.97	0.46
1:A:178:ALA:O	1:A:182:ASP:OD1	2.34	0.46
1:A:134:SER:OG	1:A:135:PRO:HD3	2.15	0.46
1:A:269:VAL:HG12	1:A:270:ASP:N	2.30	0.46
1:A:429:PRO:O	1:A:430:TYR:HB2	2.15	0.46
1:A:76:ASP:HB2	1:A:106:ARG:NH1	2.31	0.46
1:A:140:GLY:O	1:A:143:LYS:HB2	2.16	0.46
1:A:406:LYS:CG	1:A:407:TYR:N	2.79	0.45
1:A:457:ILE:O	1:A:461:GLN:HG2	2.15	0.45
1:A:194:ASP:OD1	1:A:196:LEU:HB3	2.16	0.45
1:A:474:PRO:HB3	1:A:475:LEU:HD23	1.98	0.45
1:A:193:ILE:HG12	1:A:195:SER:H	1.82	0.45
1:A:178:ALA:O	1:A:181:MET:HB3	2.16	0.45
1:A:230:ILE:HB	1:A:231:PRO:HD3	1.99	0.45
1:A:235:VAL:C	1:A:237:ASN:H	2.20	0.45
1:A:356:LEU:HD22	1:A:457:ILE:HD11	1.97	0.45
1:A:162:ARG:HE	1:A:163:GLU:CG	2.29	0.45
1:A:232:ILE:O	1:A:235:VAL:HB	2.17	0.45
1:A:331:LEU:HD22	1:A:460:LEU:HG	1.99	0.45
1:A:278:SER:O	1:A:280:ASN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:VAL:HG12	1:A:270:ASP:H	1.82	0.44
1:A:429:PRO:O	1:A:430:TYR:CB	2.65	0.44
1:A:322:ALA:HB1	1:A:467:PRO:HD3	1.98	0.44
1:A:223:ILE:CG2	1:A:223:ILE:O	2.65	0.44
1:A:458:ARG:HD3	1:A:458:ARG:HA	1.79	0.44
1:A:181:MET:SD	1:A:207:THR:CG2	3.06	0.44
1:A:227:PRO:C	1:A:229:LEU:H	2.20	0.44
1:A:246:THR:O	1:A:250:ARG:HB2	2.17	0.44
1:A:360:VAL:HG21	1:A:453:LYS:HZ3	1.81	0.43
1:A:108:PHE:HE2	1:A:120:ILE:HD12	1.83	0.43
1:A:158:ARG:CB	1:A:158:ARG:NH1	2.80	0.43
1:A:229:LEU:HA	1:A:229:LEU:HD12	1.85	0.43
1:A:474:PRO:CB	1:A:475:LEU:HD23	2.48	0.43
1:A:226:PHE:CD2	1:A:226:PHE:N	2.83	0.43
1:A:375:ARG:NH1	3:A:1501:HEM:O1A	2.51	0.43
1:A:250:ARG:CD	1:A:296:VAL:HG11	2.49	0.43
1:A:275:MET:O	1:A:278:SER:HB3	2.18	0.43
1:A:479:LEU:HD23	1:A:479:LEU:H	1.83	0.43
1:A:38:ILE:CD1	1:A:38:ILE:N	2.80	0.43
1:A:198:ASN:HB3	1:A:199:PRO:HD3	2.01	0.43
1:A:229:LEU:HD12	1:A:232:ILE:HD12	2.00	0.42
1:A:198:ASN:HB2	1:A:199:PRO:CD	2.49	0.42
1:A:334:GLU:OE1	1:A:355:TYR:HB3	2.20	0.42
1:A:85:THR:HG23	1:A:401:LEU:HD21	2.00	0.42
1:A:460:LEU:O	1:A:462:ASN:N	2.48	0.42
1:A:278:SER:C	1:A:280:ASN:H	2.22	0.42
1:A:184:ILE:HG21	1:A:303:ILE:HG12	2.02	0.42
1:A:381:VAL:CG1	1:A:382:GLU:N	2.83	0.42
1:A:44:LEU:HA	1:A:45:PRO:HD3	1.94	0.42
1:A:169:PRO:CB	1:A:468:CYS:SG	3.05	0.42
1:A:344:PRO:HA	1:A:458:ARG:NH1	2.34	0.41
1:A:202:PRO:HG2	1:A:203:PHE:N	2.33	0.41
1:A:322:ALA:O	1:A:323:THR:CB	2.69	0.41
1:A:347:TYR:O	1:A:351:LEU:HG	2.20	0.41
1:A:270:ASP:HB3	1:A:273:GLN:CB	2.49	0.41
1:A:171:THR:HA	1:A:490:VAL:HG12	2.03	0.41
1:A:154:ASP:O	1:A:157:VAL:HG22	2.21	0.41
1:A:162:ARG:O	1:A:165:GLU:HB2	2.20	0.41
1:A:260:ARG:NH2	1:A:270:ASP:OD1	2.45	0.41
1:A:161:ARG:HG3	1:A:161:ARG:NH1	2.33	0.41
1:A:25:TYR:CZ	1:A:28:HIS:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:THR:O	1:A:136:THR:CG2	2.69	0.41
1:A:181:MET:CE	1:A:208:LYS:HG3	2.51	0.41
1:A:185:THR:HG21	1:A:193:ILE:HD11	2.03	0.41
1:A:142:LEU:O	1:A:146:VAL:HG23	2.20	0.40
1:A:322:ALA:O	1:A:323:THR:CG2	2.69	0.40
1:A:140:GLY:O	1:A:144:GLU:HG3	2.22	0.40
1:A:198:ASN:HB2	1:A:199:PRO:HD3	2.03	0.40
1:A:216:LEU:HD22	1:A:481:GLY:HA2	2.03	0.40
1:A:377:CYS:SG	1:A:388:ILE:HG22	2.62	0.40
1:A:415:LEU:CD1	1:A:418:ARG:NE	2.84	0.40
1:A:145:MET:HG2	1:A:269:VAL:HG11	2.04	0.40
1:A:330:LYS:HG2	1:A:355:TYR:CE1	2.56	0.40
1:A:92:THR:HA	1:A:96:LYS:HB2	2.03	0.40
1:A:104:ASN:HA	1:A:440:ARG:NH2	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	453/485 (93%)	371 (82%)	58 (13%)	24 (5%)	<b>2</b> <b>2</b>

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	196	LEU
1	A	198	ASN
1	A	270	ASP
1	A	341	ASN
1	A	369	ILE
1	A	406	LYS

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Mol	Chain	Res	Type
1	A	36	LEU
1	A	132	LEU
1	A	139	SER
1	A	201	ASP
1	A	279	GLN
1	A	457	ILE
1	A	462	ASN
1	A	202	PRO
1	A	278	SER
1	A	461	GLN
1	A	476	LYS
1	A	100	SER
1	A	195	SER
1	A	273	GLN
1	A	487	LYS
1	A	383	ILE
1	A	474	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	416/441 (94%)	389 (94%)	27 (6%)	20	32

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	PRO
1	A	82	LEU
1	A	93	VAL
1	A	111	VAL
1	A	127	LYS
1	A	162	ARG
1	A	193	ILE
1	A	196	LEU
1	A	216	LEU

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Mol	Chain	Res	Type
1	A	221	LEU
1	A	226	PHE
1	A	240	VAL
1	A	250	ARG
1	A	272	LEU
1	A	273	GLN
1	A	280	ASN
1	A	332	GLN
1	A	339	LEU
1	A	349	THR
1	A	373	LEU
1	A	375	ARG
1	A	415	LEU
1	A	456	LEU
1	A	475	LEU
1	A	479	LEU
1	A	485	PRO
1	A	486	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	159	ASN
1	A	192	ASN
1	A	200	GLN
1	A	206	ASN
1	A	273	GLN
1	A	280	ASN
1	A	332	GLN
1	A	451	ASN
1	A	472	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	STR	A	1499	-	26,26,26	3.12	17 (65%)	42,42,42	1.23	4 (9%)
3	HEM	A	1501	1	28,50,50	0.80	2 (7%)	17,82,82	1.46	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	STR	A	1499	-	-	0/4/62/62	0/4/4/4
3	HEM	A	1501	1	-	0/6/54/54	0/0/8/8

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1501	HEM	C3B-C2B	-2.21	1.37	1.40
3	A	1501	HEM	C3C-C2C	-2.05	1.37	1.40
2	A	1499	STR	C13-C17	2.10	1.59	1.56
2	A	1499	STR	C4-C5	2.39	1.37	1.34
2	A	1499	STR	C12-C11	2.56	1.58	1.53
2	A	1499	STR	C7-C8	2.99	1.59	1.53
2	A	1499	STR	C10-C5	3.01	1.58	1.52
2	A	1499	STR	C1-C2	3.22	1.60	1.53
2	A	1499	STR	C12-C13	3.23	1.60	1.54
2	A	1499	STR	C17-C20	3.82	1.57	1.51
2	A	1499	STR	C1-C10	3.86	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1499	STR	C4-C3	4.03	1.54	1.45
2	A	1499	STR	C2-C3	4.20	1.59	1.49
2	A	1499	STR	C18-C13	4.27	1.62	1.54
2	A	1499	STR	C13-C14	4.27	1.63	1.55
2	A	1499	STR	C6-C5	4.29	1.57	1.50
2	A	1499	STR	C11-C9	4.51	1.61	1.53
2	A	1499	STR	C10-C9	4.54	1.63	1.56
2	A	1499	STR	C8-C9	4.86	1.63	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1499	STR	C6-C5-C4	-2.52	116.70	120.87
2	A	1499	STR	C17-C13-C14	-2.35	97.21	99.71
3	A	1501	HEM	CAD-CBD-CGD	-2.22	108.87	112.66
2	A	1499	STR	C16-C15-C14	-2.08	100.97	105.12
3	A	1501	HEM	CMA-C3A-C4A	-2.06	125.30	128.46
2	A	1499	STR	C18-C13-C17	2.10	113.59	110.14
3	A	1501	HEM	CMC-C2C-C3C	2.13	128.84	124.89
3	A	1501	HEM	CAA-CBA-CGA	2.17	116.37	112.66
3	A	1501	HEM	CMB-C2B-C3B	2.24	129.04	124.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1501	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 [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	459/485 (94%)	0.14	10 (2%) 62 61	31, 60, 89, 109	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	25	TYR	4.7
1	A	196	LEU	3.7
1	A	341	ASN	3.0
1	A	493	VAL	2.8
1	A	352	GLN	2.4
1	A	498	GLY	2.1
1	A	490	VAL	2.1
1	A	494	GLU	2.1
1	A	427	ILE	2.1
1	A	197	ASN	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
2	STR	A	1499	23/23	0.94	0.19	1.49	43,44,46,48	0
3	HEM	A	1501	43/43	0.98	0.20	0.72	31,35,40,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.