Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:22 PM GMT

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PDB ID	:	4I3Q
Title	:	Crystal structure of human CYP3A4 coordinated to a water molecule
Authors	:	Sevrioukova, I.F.; Poulos, T.L.
Deposited on	:	2012-11-26
Resolution	:	2.60 Å(reported)

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1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	Percentile Ranks	Value
Rfree		0.294
Clashscore		15
Ramachandran outliers		1.3%
Sidechain outliers		10.6%
RSRZ outliers		1.7%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 >=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 <=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	487	2% ... 62% ... 28% ... 6% ... 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3798 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.
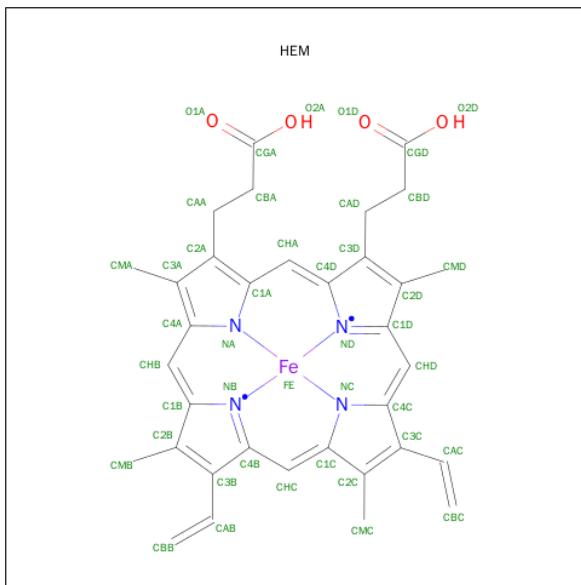
- Molecule 1 is a protein called Cytochrome P450 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	465	3749	2436	620	669	24	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	DELETION	UNP P08684
A	?	-	ILE	DELETION	UNP P08684
A	?	-	PRO	DELETION	UNP P08684
A	?	-	ASP	DELETION	UNP P08684
A	?	-	LEU	DELETION	UNP P08684
A	?	-	ALA	DELETION	UNP P08684
A	?	-	MET	DELETION	UNP P08684
A	?	-	GLU	DELETION	UNP P08684
A	?	-	THR	DELETION	UNP P08684
A	?	-	TRP	DELETION	UNP P08684
A	?	-	LEU	DELETION	UNP P08684
A	?	-	LEU	DELETION	UNP P08684
A	?	-	LEU	DELETION	UNP P08684
A	?	-	ALA	DELETION	UNP P08684
A	?	-	VAL	DELETION	UNP P08684
A	?	-	SER	DELETION	UNP P08684
A	?	-	LEU	DELETION	UNP P08684
A	?	-	VAL	DELETION	UNP P08684
A	?	-	LEU	DELETION	UNP P08684
A	?	-	LEU	DELETION	UNP P08684
A	504	HIS	-	EXPRESSION TAG	UNP P08684
A	505	HIS	-	EXPRESSION TAG	UNP P08684
A	506	HIS	-	EXPRESSION TAG	UNP P08684
A	507	HIS	-	EXPRESSION TAG	UNP P08684

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

HEM

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
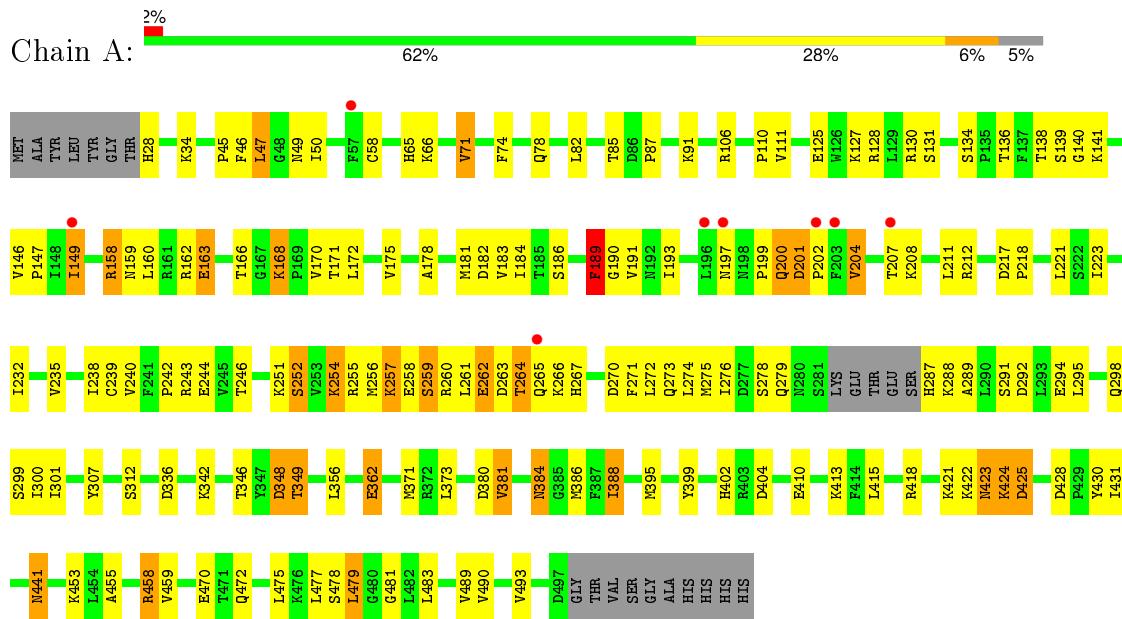
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		

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 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 3A4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	79.11Å 101.47Å 130.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.27 – 2.60 65.27 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (65.27-2.60) 98.4 (65.27-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.220 , 0.298 0.218 , 0.294	Depositor DCC
R_{free} test set	834 reflections (5.41%)	DCC
Wilson B-factor (Å^2)	85.2	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \vert L \vert > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 16252 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3798	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< \vert L \vert >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM

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	0.60	1/3841 (0.0%)	0.79	6/5195 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	418	ARG	CZ-NH1	5.81	1.40	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	GLN	N-CA-C	9.15	135.72	111.00
1	A	201	ASP	N-CA-CB	-8.64	95.04	110.60
1	A	200	GLN	CB-CA-C	-8.38	93.65	110.40
1	A	418	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	257	LYS	CB-CA-C	-6.33	97.75	110.40
1	A	336	ASP	CB-CG-OD1	5.17	122.96	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3749	0	3829	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	43	0	30	0	0
3	A	6	0	0	3	0
All	All	3798	0	3859	117	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 15.

All (117) 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:189:PHE:HE1	1:A:273:GLN:HG2	1.22	0.99
1:A:410:GLU:HB3	1:A:413:LYS:HG3	1.43	0.98
1:A:163:GLU:HG2	1:A:170:VAL:HG22	1.57	0.84
1:A:189:PHE:CE1	1:A:273:GLN:HG2	2.13	0.80
1:A:189:PHE:HA	1:A:270:ASP:OD1	1.82	0.79
1:A:191:VAL:HG12	1:A:193:ILE:HD11	1.67	0.77
1:A:256:MET:HA	1:A:260:ARG:CB	2.16	0.75
1:A:138:THR:HG22	1:A:140:GLY:H	1.51	0.74
1:A:265:GLN:HG3	1:A:266:LYS:HG2	1.73	0.71
1:A:189:PHE:HD1	1:A:270:ASP:OD1	1.73	0.70
1:A:256:MET:HA	1:A:260:ARG:HB2	1.73	0.70
1:A:257:LYS:NZ	1:A:292:ASP:OD2	2.26	0.69
1:A:130:ARG:HH22	1:A:441:ASN:ND2	1.90	0.68
1:A:258:GLU:C	1:A:262:GLU:HG2	2.15	0.67
1:A:479:LEU:HD22	1:A:479:LEU:H	1.58	0.67
1:A:138:THR:HG22	1:A:140:GLY:N	2.10	0.66
1:A:189:PHE:CZ	1:A:261:LEU:HD12	2.32	0.65
1:A:189:PHE:CG	1:A:272:LEU:HD23	2.31	0.65
1:A:136:THR:HG22	1:A:271:PHE:HD1	1.62	0.64
1:A:212:ARG:NH1	3:A:705:HOH:O	2.32	0.63
1:A:136:THR:CG2	1:A:271:PHE:HD1	2.13	0.62
1:A:172:LEU:HD12	1:A:489:VAL:HB	1.83	0.61
1:A:271:PHE:O	1:A:275:MET:HG3	2.02	0.60
1:A:256:MET:HA	1:A:260:ARG:HB3	1.84	0.60
1:A:264:THR:O	1:A:265:GLN:HB3	2.02	0.59
1:A:348:ASP:N	1:A:348:ASP:OD2	2.22	0.59
1:A:189:PHE:CD1	1:A:270:ASP:OD1	2.55	0.58
1:A:428:ASP:HB3	1:A:431:ILE:HG12	1.86	0.57
1:A:138:THR:HG22	1:A:139:SER:N	2.20	0.57
1:A:232:ILE:O	1:A:235:VAL:HG12	2.04	0.56
1:A:265:GLN:HE21	1:A:266:LYS:HG2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ARG:CZ	1:A:158:ARG:HB2	2.35	0.56
1:A:47:LEU:HG	1:A:50:ILE:HD11	1.88	0.55
1:A:149:ILE:HG22	1:A:183:VAL:HG13	1.89	0.55
1:A:191:VAL:O	1:A:193:ILE:HG13	2.08	0.53
1:A:240:VAL:O	1:A:242:PRO:HD3	2.08	0.53
1:A:276:ILE:O	1:A:279:GLN:HB2	2.08	0.52
1:A:294:GLU:O	1:A:298:GLN:HG2	2.10	0.52
1:A:256:MET:O	1:A:260:ARG:HB3	2.10	0.52
1:A:170:VAL:O	1:A:490:VAL:HA	2.09	0.51
1:A:130:ARG:HH22	1:A:441:ASN:HD21	1.57	0.51
1:A:189:PHE:H	1:A:270:ASP:HB2	1.74	0.51
1:A:288:LYS:O	1:A:289:ALA:HB3	2.10	0.51
1:A:472:GLN:OE1	1:A:475:LEU:HD12	2.10	0.51
1:A:217:ASP:HB2	1:A:218:PRO:HD2	1.93	0.51
1:A:402:HIS:CD2	1:A:431:ILE:O	2.63	0.51
1:A:264:THR:HG22	1:A:265:GLN:H	1.76	0.50
1:A:270:ASP:O	1:A:274:LEU:HG	2.12	0.50
1:A:191:VAL:HG12	1:A:193:ILE:CD1	2.40	0.50
1:A:423:ASN:O	1:A:425:ASP:N	2.45	0.49
1:A:252:SER:O	1:A:255:ARG:HG3	2.12	0.49
1:A:184:ILE:CD1	1:A:307:TYR:HA	2.43	0.49
1:A:58:CYS:HB3	1:A:399:TYR:CD2	2.48	0.49
1:A:270:ASP:OD2	1:A:273:GLN:HB2	2.13	0.48
1:A:191:VAL:CG1	1:A:193:ILE:HD11	2.40	0.48
1:A:295:LEU:O	1:A:299:SER:OG	2.29	0.48
1:A:402:HIS:HD2	1:A:431:ILE:O	1.97	0.48
1:A:138:THR:HB	1:A:141:LYS:HG2	1.96	0.47
1:A:65:HIS:HE1	1:A:404:ASP:OD2	1.97	0.47
1:A:181:MET:SD	1:A:207:THR:HB	2.55	0.47
1:A:138:THR:CG2	1:A:139:SER:N	2.77	0.47
1:A:159:ASN:OD1	1:A:162:ARG:NH1	2.48	0.47
1:A:49:ASN:OD1	1:A:74:PHE:HB2	2.16	0.46
1:A:477:LEU:HD22	1:A:483:LEU:HD12	1.98	0.46
1:A:149:ILE:CG2	1:A:183:VAL:HG13	2.45	0.46
1:A:91:LYS:HG3	1:A:430:TYR:CZ	2.51	0.45
1:A:178:ALA:O	1:A:182:ASP:OD2	2.34	0.45
1:A:34:LYS:HB3	1:A:34:LYS:HE2	1.66	0.45
1:A:254:LYS:NZ	1:A:254:LYS:HA	2.31	0.45
1:A:455:ALA:O	1:A:459:VAL:HG23	2.15	0.45
1:A:258:GLU:O	1:A:260:ARG:N	2.49	0.45
1:A:171:THR:O	1:A:175:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:PRO:HA	3:A:702:HOH:O	2.17	0.44
1:A:172:LEU:HA	1:A:175:VAL:CG2	2.47	0.44
1:A:201:ASP:O	1:A:202:PRO:C	2.53	0.44
1:A:246:THR:HG22	1:A:300:ILE:HD13	2.00	0.44
1:A:258:GLU:O	1:A:262:GLU:HG2	2.17	0.44
1:A:470:GLU:N	1:A:470:GLU:CD	2.71	0.44
1:A:458:ARG:HH21	1:A:458:ARG:HG2	1.83	0.44
1:A:87:PRO:HG3	1:A:431:ILE:HD11	2.00	0.43
1:A:172:LEU:HA	1:A:175:VAL:HG22	2.00	0.43
1:A:110:PRO:O	1:A:240:VAL:HG22	2.19	0.43
1:A:189:PHE:CA	1:A:270:ASP:OD1	2.60	0.43
1:A:71:VAL:HG13	1:A:82:LEU:HD11	1.99	0.42
1:A:186:SER:HA	1:A:190:GLY:HA2	2.01	0.42
1:A:197:ASN:O	1:A:199:PRO:HD3	2.19	0.42
1:A:127:LYS:HB2	1:A:127:LYS:HE3	1.66	0.42
1:A:362:GLU:HG3	1:A:415:LEU:C	2.40	0.42
1:A:136:THR:HG22	1:A:271:PHE:CD1	2.48	0.42
1:A:410:GLU:HB3	1:A:413:LYS:CG	2.31	0.42
1:A:381:VAL:O	1:A:388:ILE:N	2.46	0.42
1:A:128:ARG:HA	1:A:287:HIS:CE1	2.55	0.42
1:A:204:VAL:O	1:A:208:LYS:HB2	2.20	0.42
1:A:221:LEU:HA	1:A:221:LEU:HD23	1.79	0.42
1:A:264:THR:O	1:A:265:GLN:CB	2.66	0.42
1:A:184:ILE:HD11	1:A:307:TYR:HA	2.01	0.42
1:A:422:LYS:H	1:A:422:LYS:HG2	1.54	0.42
1:A:166:THR:HG22	1:A:168:LYS:H	1.85	0.42
1:A:371:MET:HE1	1:A:481:GLY:O	2.20	0.42
1:A:189:PHE:H	1:A:270:ASP:CB	2.33	0.42
1:A:45:PRO:O	1:A:46:PHE:HB2	2.19	0.42
1:A:158:ARG:HG2	3:A:701:HOH:O	2.20	0.42
1:A:346:THR:OG1	1:A:349:THR:HB	2.20	0.42
1:A:65:HIS:CD2	1:A:85:THR:HG21	2.55	0.41
1:A:267:HIS:HE1	1:A:273:GLN:HB3	1.85	0.41
1:A:271:PHE:HA	1:A:274:LEU:HD12	2.01	0.41
1:A:291:SER:HB3	1:A:294:GLU:OE1	2.21	0.41
1:A:270:ASP:O	1:A:270:ASP:OD2	2.38	0.41
1:A:146:VAL:HB	1:A:147:PRO:HD3	2.03	0.41
1:A:362:GLU:OE2	1:A:362:GLU:HA	2.20	0.41
1:A:395:MET:C	1:A:395:MET:SD	2.98	0.41
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.96	0.41
1:A:421:LYS:HG3	1:A:424:LYS:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:HG22	1:A:239:CYS:N	2.36	0.40
1:A:301:ILE:HA	1:A:301:ILE:HD12	1.98	0.40
1:A:356:LEU:HD21	1:A:453:LYS:HB3	2.02	0.40
1:A:170:VAL:HG21	1:A:493:VAL:HG21	2.03	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	461/487 (95%)	410 (89%)	45 (10%)	6 (1%)	15	30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ASP
1	A	384	ASN
1	A	259	SER
1	A	342	LYS
1	A	424	LYS
1	A	189	PHE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/443 (96%)	381 (89%)	45 (11%)	8	15

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	47	LEU
1	A	66	LYS
1	A	71	VAL
1	A	78	GLN
1	A	106	ARG
1	A	111	VAL
1	A	125	GLU
1	A	131	SER
1	A	134	SER
1	A	149	ILE
1	A	158	ARG
1	A	160	LEU
1	A	163	GLU
1	A	168	LYS
1	A	189	PHE
1	A	200	GLN
1	A	204	VAL
1	A	211	LEU
1	A	223	ILE
1	A	243	ARG
1	A	244	GLU
1	A	251	LYS
1	A	252	SER
1	A	254	LYS
1	A	259	SER
1	A	262	GLU
1	A	264	THR
1	A	278	SER
1	A	312	SER
1	A	348	ASP
1	A	349	THR
1	A	362	GLU
1	A	373	LEU
1	A	380	ASP
1	A	381	VAL
1	A	384	ASN
1	A	386	MET

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Mol	Chain	Res	Type
1	A	388	ILE
1	A	423	ASN
1	A	425	ASP
1	A	441	ASN
1	A	458	ARG
1	A	478	SER
1	A	479	LEU

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	65	HIS
1	A	78	GLN
1	A	79	GLN
1	A	247	ASN
1	A	265	GLN
1	A	267	HIS
1	A	279	GLN
1	A	441	ASN
1	A	451	ASN
1	A	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)

1 ligand is 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	601	1,3	30,50,50	3.01	12 (40%)	24,82,82	2.89	11 (45%)

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	601	1,3	-	0/10/54/54	0/0/8/8

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C3B-C4B	-3.12	1.49	1.51
2	A	601	HEM	C2D-C3D	-2.81	1.46	1.54
2	A	601	HEM	C1A-CHA	2.21	1.45	1.39
2	A	601	HEM	CHD-C1D	2.45	1.45	1.38
2	A	601	HEM	FE-NB	2.58	2.11	1.97
2	A	601	HEM	FE-ND	2.94	2.13	1.97
2	A	601	HEM	CHC-C4B	3.07	1.47	1.38
2	A	601	HEM	C2A-C3A	3.08	1.46	1.37
2	A	601	HEM	CHD-C4C	4.31	1.46	1.36
2	A	601	HEM	CHC-C1C	4.41	1.46	1.36
2	A	601	HEM	C4C-NC	8.55	1.46	1.36
2	A	601	HEM	C1C-NC	8.94	1.47	1.36

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	CBD-CAD-C3D	-3.88	102.28	113.55
2	A	601	HEM	CAA-CBA-CGA	-3.29	106.71	112.75
2	A	601	HEM	C3B-CAB-CBB	-2.48	120.66	124.46
2	A	601	HEM	C1D-CHD-C4C	-2.36	121.87	125.82
2	A	601	HEM	C3C-CAC-CBC	-2.11	121.22	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	CMD-C2D-C3D	3.59	130.21	114.35
2	A	601	HEM	C2C-C1C-NC	3.73	116.50	110.21
2	A	601	HEM	CAD-C3D-C4D	4.65	128.88	112.47
2	A	601	HEM	CMC-C2C-C3C	4.94	128.87	116.53
2	A	601	HEM	CAD-C3D-C2D	5.41	128.78	113.22
2	A	601	HEM	CMB-C2B-C3B	6.43	132.58	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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^2)	Q<0.9
1	A	465/487 (95%)	0.06	8 (1%)	73	68	59, 91, 137, 180	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	LEU	3.9
1	A	203	PHE	2.8
1	A	149	ILE	2.8
1	A	265	GLN	2.5
1	A	207	THR	2.4
1	A	57	PHE	2.3
1	A	202	PRO	2.1
1	A	197	ASN	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, 95th 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(Å²)	Q<0.9
2	HEM	A	601	43/43	0.99	0.21	0.52	57,62,70,71	0

6.5 Other polymers (i)

There are no such residues in this entry.