Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:54 PM GMT

PDB ID	:	4GL7
Title	:	Structure of human placental aromatase complexed with designed inhibitor HDDG046 (compound 5)
Authors	:	Ghosh, D.
Deposited on	:	2012-08-13
Resolution	:	3.90 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

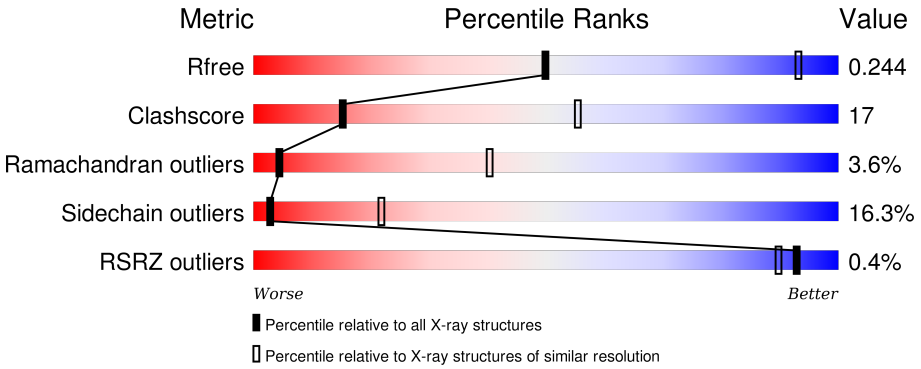
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.90 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	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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	503	50% 32% 6% • 10%

2 Entry composition

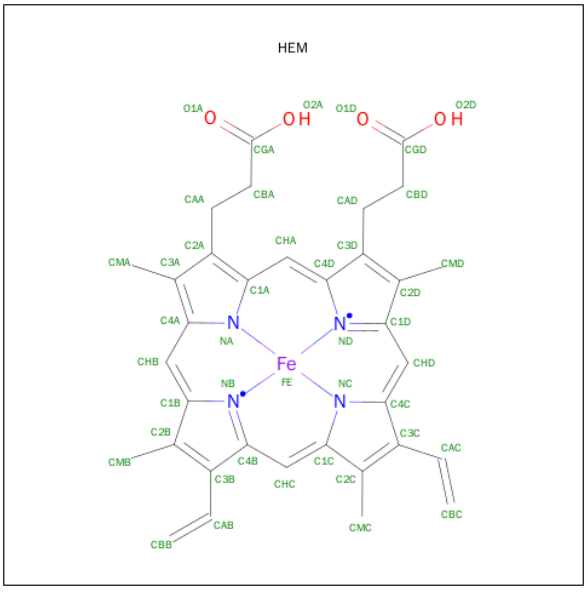
There are 3 unique types of molecules in this entry. The entry contains 3728 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 19A1.

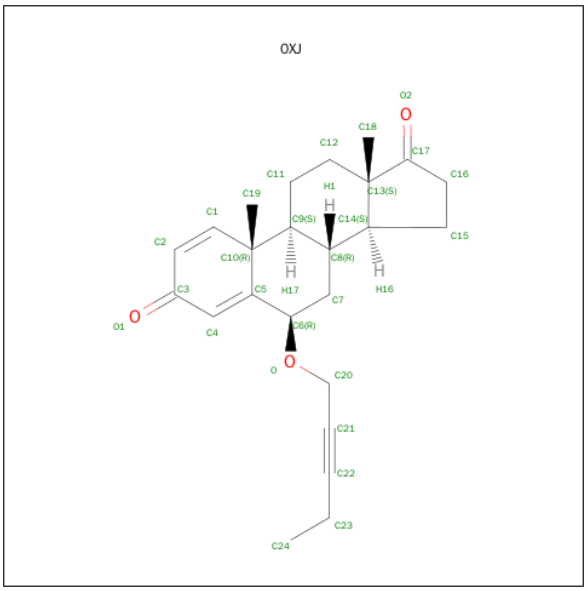
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	452	3658	2361	617	650	30	0	0	0

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

- Molecule 3 is (6ALPHA,8ALPHA)-6-(PENT-2-YN-1-YLOXY)ANDROSTA-1,4-DIENE-3,17-DIONE (three-letter code: 0XJ) (formula: $C_{24}H_{30}O_3$).



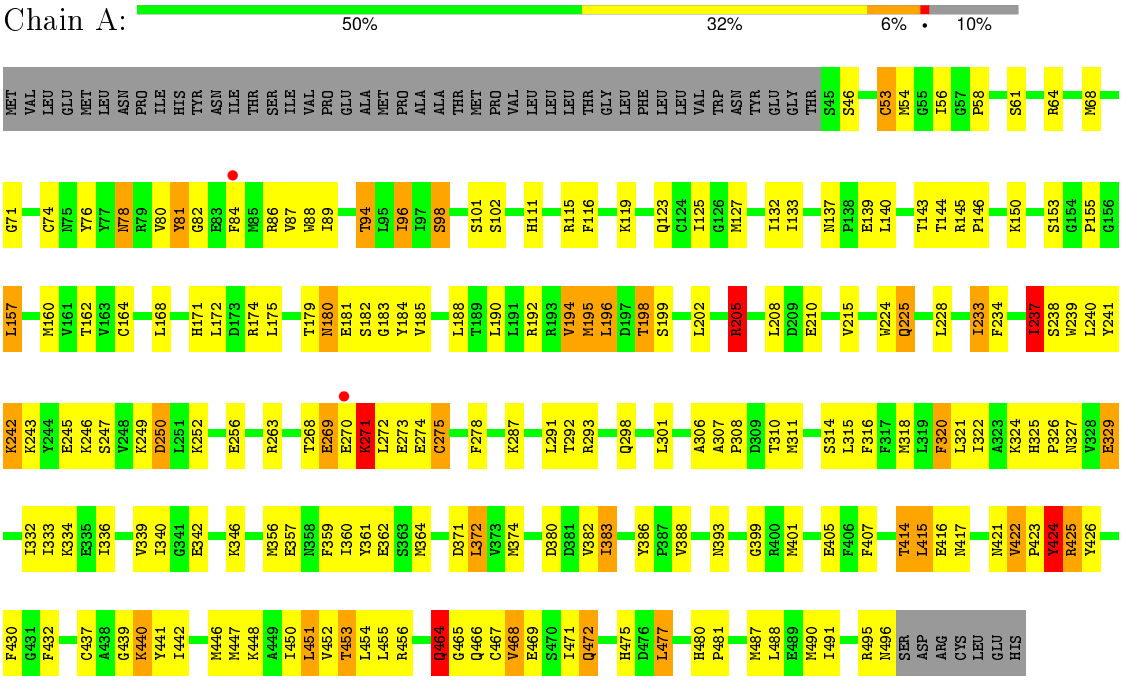
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			27	24	3		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cytochrome P450 19A1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.44Å 141.44Å 118.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.90 46.30 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-3.90) 99.1 (46.30-3.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.214 , 0.254 0.207 , 0.244	Depositor DCC
R_{free} test set	628 reflections (5.18%)	DCC
Wilson B-factor (Å^2)	137.5	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 81.2	EDS
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 12747 reflections (0.008%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3728	wwPDB-VP
Average B, all atoms (Å^2)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0XJ, 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	0.56	0/3737	0.69	1/5035 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	301	LEU	CA-CB-CG	5.17	127.19	115.30

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	3658	0	3735	130	0
2	A	43	0	30	5	0
3	A	27	0	30	3	0
All	All	3728	0	3795	131	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 17.

All (131) 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:310:THR:HG22	3:A:601:0XJ:H24	1.51	0.90
1:A:115:ARG:HH22	2:A:600:HEM:HBA2	1.46	0.80
1:A:171:HIS:HD2	1:A:194:VAL:HG12	1.44	0.80
1:A:195:MET:HA	1:A:195:MET:CE	2.11	0.80
1:A:225:GLN:HG3	1:A:477:LEU:HB2	1.62	0.78
1:A:424:TYR:HD1	1:A:424:TYR:O	1.66	0.77
1:A:320:PHE:HB3	1:A:468:VAL:HG12	1.66	0.77
1:A:315:LEU:HD22	1:A:450:ILE:HD11	1.67	0.76
1:A:188:LEU:HD23	1:A:192:ARG:HH12	1.52	0.73
1:A:407:PHE:HD1	1:A:417:ASN:HB3	1.51	0.73
1:A:58:PRO:HA	1:A:88:TRP:HB2	1.71	0.72
1:A:356:MET:CE	1:A:448:LYS:HG2	2.21	0.71
1:A:87:VAL:HG12	1:A:88:TRP:N	2.06	0.71
1:A:171:HIS:CD2	1:A:194:VAL:HG12	2.27	0.70
1:A:101:SER:HA	1:A:425:ARG:HH22	1.55	0.70
1:A:234:PHE:HE2	1:A:241:TYR:HB3	1.57	0.70
1:A:71:GLY:HA2	1:A:372:LEU:HD21	1.76	0.68
1:A:87:VAL:CG1	1:A:88:TRP:N	2.56	0.68
1:A:424:TYR:CD1	1:A:424:TYR:O	2.48	0.67
1:A:271:LYS:O	1:A:274:GLU:HG3	1.97	0.65
1:A:407:PHE:CD1	1:A:417:ASN:HB3	2.34	0.63
1:A:270:GLU:HG3	1:A:270:GLU:O	1.99	0.62
1:A:87:VAL:CG1	1:A:88:TRP:H	2.13	0.62
1:A:195:MET:HE3	1:A:195:MET:HA	1.82	0.61
1:A:424:TYR:C	1:A:424:TYR:CD1	2.73	0.61
1:A:61:SER:HB2	1:A:87:VAL:HG13	1.83	0.60
1:A:168:LEU:O	1:A:172:LEU:HG	2.01	0.60
1:A:321:LEU:HG	1:A:468:VAL:HG11	1.82	0.59
1:A:81:TYR:CD2	1:A:81:TYR:N	2.70	0.59
1:A:238:SER:HB2	1:A:242:LYS:HE3	1.84	0.59
1:A:383:ILE:CG2	1:A:388:VAL:HG21	2.32	0.59
1:A:356:MET:HE3	1:A:448:LYS:HG2	1.83	0.59
1:A:64:ARG:O	1:A:68:MET:HB2	2.04	0.58
1:A:332:ILE:O	1:A:336:ILE:HG13	2.03	0.58
1:A:315:LEU:HD21	1:A:447:MET:HG2	1.84	0.57
1:A:359:PHE:HA	1:A:415:LEU:HD21	1.87	0.56
1:A:439:GLY:O	1:A:441:TYR:N	2.39	0.56
1:A:247:SER:HA	1:A:250:ASP:HB2	1.87	0.55
1:A:171:HIS:NE2	1:A:210:GLU:OE1	2.39	0.55
1:A:315:LEU:HD13	1:A:450:ILE:HD11	1.88	0.54
1:A:362:GLU:OE2	1:A:362:GLU:HA	2.06	0.54
1:A:234:PHE:CE2	1:A:241:TYR:HB3	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ASN:HB2	1:A:184:TYR:HB2	1.90	0.53
1:A:175:LEU:HD12	1:A:185:VAL:HG11	1.90	0.53
1:A:132:ILE:HD11	2:A:600:HEM:CMD	2.39	0.53
1:A:423:PRO:HG2	1:A:426:TYR:HD2	1.74	0.53
1:A:196:LEU:O	1:A:196:LEU:HG	2.07	0.52
1:A:242:LYS:HA	1:A:245:GLU:HB3	1.91	0.51
1:A:471:ILE:HG22	1:A:472:GLN:N	2.25	0.51
1:A:132:ILE:HD11	2:A:600:HEM:HMD3	1.93	0.51
1:A:271:LYS:O	1:A:274:GLU:CG	2.58	0.51
1:A:322:ILE:HD13	1:A:455:LEU:HD11	1.92	0.51
1:A:310:THR:HG22	3:A:601:0XJ:C20	2.30	0.51
1:A:133:ILE:HA	2:A:600:HEM:HAD1	1.92	0.51
1:A:198:THR:HG22	1:A:199:SER:N	2.25	0.51
1:A:61:SER:CB	1:A:87:VAL:HG13	2.40	0.50
1:A:168:LEU:HD21	1:A:454:LEU:HB2	1.92	0.50
1:A:430:PHE:HB3	1:A:437:CYS:HB3	1.94	0.50
1:A:455:LEU:O	1:A:495:ARG:NH1	2.45	0.49
1:A:101:SER:HA	1:A:425:ARG:NH2	2.24	0.49
1:A:339:VAL:C	1:A:340:ILE:HG13	2.33	0.49
1:A:188:LEU:CD1	1:A:316:PHE:CD1	2.96	0.49
1:A:238:SER:C	1:A:240:LEU:H	2.15	0.48
1:A:190:LEU:O	1:A:194:VAL:HG13	2.14	0.48
1:A:307:ALA:HB3	1:A:308:PRO:HD3	1.95	0.48
1:A:306:ALA:HA	3:A:601:0XJ:O1	2.13	0.48
2:A:600:HEM:HBC2	2:A:600:HEM:HMC2	1.96	0.48
1:A:225:GLN:CG	1:A:477:LEU:HB2	2.37	0.48
1:A:205:ARG:HH22	1:A:275:CYS:HB2	1.79	0.48
1:A:329:GLU:O	1:A:333:ILE:HG12	2.14	0.48
1:A:132:ILE:HG13	1:A:133:ILE:N	2.28	0.48
1:A:119:LYS:O	1:A:123:GLN:HB2	2.14	0.47
1:A:195:MET:HE2	1:A:195:MET:HA	1.92	0.47
1:A:315:LEU:CD2	1:A:450:ILE:HD11	2.42	0.47
1:A:137:ASN:HB3	1:A:140:LEU:HB3	1.95	0.47
1:A:452:VAL:HG12	1:A:453:THR:N	2.29	0.47
1:A:87:VAL:HG13	1:A:88:TRP:H	1.80	0.47
1:A:74:CYS:O	1:A:78:ASN:HB2	2.14	0.47
1:A:153:SER:O	1:A:155:PRO:HD2	2.14	0.47
1:A:383:ILE:CG2	1:A:388:VAL:CG2	2.93	0.47
1:A:53:CYS:HB3	1:A:56:ILE:HB	1.96	0.47
1:A:139:GLU:O	1:A:143:THR:HG23	2.15	0.46
1:A:233:ILE:HG13	1:A:233:ILE:H	1.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ARG:O	1:A:146:PRO:C	2.54	0.46
1:A:432:PHE:CD1	1:A:432:PHE:C	2.89	0.46
1:A:102:SER:HB3	1:A:383:ILE:HD11	1.99	0.45
1:A:357:GLU:HG2	1:A:361:TYR:CE1	2.50	0.45
1:A:98:SER:O	1:A:401:MET:HG3	2.17	0.45
1:A:469:GLU:OE1	1:A:469:GLU:N	2.48	0.45
1:A:371:ASP:HB2	1:A:399:GLY:HA3	1.99	0.45
1:A:480:HIS:HB2	1:A:481:PRO:HD2	1.99	0.44
1:A:237:ILE:HD12	1:A:240:LEU:HD22	2.00	0.44
1:A:324:LYS:HE2	1:A:466:GLN:O	2.17	0.44
1:A:271:LYS:HE2	1:A:271:LYS:N	2.33	0.44
1:A:127:MET:HG2	1:A:298:GLN:NE2	2.33	0.44
1:A:157:LEU:O	1:A:157:LEU:HD23	2.18	0.44
1:A:311:MET:HE3	1:A:315:LEU:HD11	1.99	0.43
1:A:271:LYS:H	1:A:271:LYS:HE2	1.82	0.43
1:A:464:GLN:HB3	1:A:465:GLY:H	1.45	0.43
1:A:269:GLU:HG2	1:A:272:LEU:HD23	1.99	0.43
1:A:315:LEU:HD22	1:A:450:ILE:CD1	2.44	0.43
1:A:116:PHE:CE1	1:A:374:MET:HB3	2.54	0.42
1:A:477:LEU:HD23	1:A:477:LEU:HA	1.75	0.42
1:A:71:GLY:HA3	1:A:475:HIS:CD2	2.54	0.42
1:A:74:CYS:HB3	1:A:96:ILE:HD13	2.00	0.42
1:A:125:ILE:HD13	1:A:224:TRP:HA	2.01	0.42
1:A:82:GLY:C	1:A:84:PHE:H	2.22	0.42
1:A:447:MET:O	1:A:451:LEU:HB2	2.19	0.42
1:A:414:THR:C	1:A:416:GLU:H	2.22	0.42
1:A:94:THR:HB	1:A:393:ASN:HB2	2.01	0.42
1:A:360:ILE:O	1:A:364:MET:HG3	2.18	0.42
1:A:356:MET:HE1	1:A:448:LYS:HA	2.01	0.42
1:A:422:VAL:HA	1:A:423:PRO:HD3	1.73	0.42
1:A:160:MET:HE2	1:A:442:ILE:HD11	2.00	0.42
1:A:132:ILE:O	1:A:133:ILE:C	2.58	0.42
1:A:225:GLN:HE21	1:A:225:GLN:HB3	1.67	0.42
1:A:423:PRO:C	1:A:425:ARG:H	2.23	0.42
1:A:185:VAL:HG22	1:A:490:MET:O	2.20	0.41
1:A:311:MET:HE1	1:A:446:MET:HB2	2.02	0.41
1:A:263:ARG:NH2	1:A:293:ARG:HG3	2.34	0.41
1:A:89:ILE:H	1:A:94:THR:CG2	2.33	0.41
1:A:325:HIS:HA	1:A:326:PRO:HD3	1.92	0.41
1:A:181:GLU:C	1:A:183:GLY:H	2.23	0.41
1:A:382:VAL:HA	1:A:386:TYR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:TYR:CD2	1:A:241:TYR:C	2.94	0.41
1:A:437:CYS:HB3	1:A:440:LYS:HB3	2.03	0.41
1:A:184:TYR:CE2	1:A:491:ILE:HD11	2.56	0.40
1:A:76:TYR:CZ	1:A:80:VAL:HG21	2.56	0.40
1:A:180:ASN:HB3	1:A:184:TYR:H	1.86	0.40
1:A:357:GLU:HG2	1:A:361:TYR:HE1	1.86	0.40
1:A:467:CYS:O	1:A:471:ILE:HG13	2.20	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	450/503 (90%)	374 (83%)	60 (13%)	16 (4%)	4 40

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	ARG
1	A	271	LYS
1	A	239	TRP
1	A	111	HIS
1	A	180	ASN
1	A	243	LYS
1	A	440	LYS
1	A	464	GLN
1	A	487	MET
1	A	182	SER
1	A	205	ARG
1	A	278	PHE
1	A	421	ASN
1	A	424	TYR

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Mol	Chain	Res	Type
1	A	46	SER
1	A	237	ILE

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	406/452 (90%)	340 (84%)	66 (16%)	3 22

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	CYS
1	A	54	MET
1	A	78	ASN
1	A	81	TYR
1	A	86	ARG
1	A	94	THR
1	A	96	ILE
1	A	98	SER
1	A	144	THR
1	A	150	LYS
1	A	157	LEU
1	A	162	THR
1	A	164	CYS
1	A	179	THR
1	A	194	VAL
1	A	195	MET
1	A	196	LEU
1	A	198	THR
1	A	202	LEU
1	A	205	ARG
1	A	208	LEU
1	A	215	VAL
1	A	225	GLN
1	A	228	LEU

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Mol	Chain	Res	Type
1	A	233	ILE
1	A	237	ILE
1	A	242	LYS
1	A	246	LYS
1	A	249	LYS
1	A	250	ASP
1	A	252	LYS
1	A	256	GLU
1	A	268	THR
1	A	269	GLU
1	A	271	LYS
1	A	273	GLU
1	A	275	CYS
1	A	287	LYS
1	A	291	LEU
1	A	292	THR
1	A	314	SER
1	A	318	MET
1	A	320	PHE
1	A	327	ASN
1	A	329	GLU
1	A	334	LYS
1	A	342	GLU
1	A	346	LYS
1	A	372	LEU
1	A	380	ASP
1	A	383	ILE
1	A	405	GLU
1	A	414	THR
1	A	415	LEU
1	A	422	VAL
1	A	424	TYR
1	A	425	ARG
1	A	451	LEU
1	A	453	THR
1	A	456	ARG
1	A	464	GLN
1	A	468	VAL
1	A	472	GLN
1	A	477	LEU
1	A	488	LEU
1	A	496	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	128	HIS
1	A	464	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

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	HEM	A	600	1	30,50,50	2.54	8 (26%)	24,82,82	2.41	9 (37%)
3	0XJ	A	601	-	30,30,30	1.68	6 (20%)	43,46,46	1.62	9 (20%)

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	600	1	-	0/10/54/54	0/0/8/8
3	0XJ	A	601	-	-	0/4/67/67	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	HEM	C3B-C4B	-9.03	1.43	1.51
2	A	600	HEM	C3D-C4D	-6.24	1.43	1.51
2	A	600	HEM	C2C-C1C	-4.45	1.44	1.52
3	A	601	0XJ	C10-C9	-3.75	1.52	1.57
3	A	601	0XJ	C10-C1	-3.61	1.45	1.50
3	A	601	0XJ	C2-C3	-3.21	1.38	1.45
2	A	600	HEM	C2D-C1D	-2.39	1.44	1.51
3	A	601	0XJ	C4-C3	-2.26	1.39	1.45
2	A	600	HEM	CAA-C2A	2.09	1.55	1.52
2	A	600	HEM	FE-ND	2.35	2.09	1.97
2	A	600	HEM	FE-NC	2.38	2.05	1.95
2	A	600	HEM	C3C-CAC	2.83	1.56	1.51
3	A	601	0XJ	C2-C1	3.26	1.39	1.33
3	A	601	0XJ	C4-C5	4.16	1.40	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	0XJ	C10-C9-C8	-4.91	107.44	111.97
2	A	600	HEM	CBD-CAD-C3D	-3.49	103.40	113.55
3	A	601	0XJ	C15-C16-C17	-3.06	102.47	105.65
2	A	600	HEM	C3B-CAB-CBB	-3.04	119.79	124.46
3	A	601	0XJ	O2-C17-C16	-2.90	122.00	125.71
2	A	600	HEM	CAA-C2A-C1A	-2.72	124.06	127.01
3	A	601	0XJ	O1-C3-C2	-2.64	117.34	121.51
3	A	601	0XJ	C14-C13-C17	-2.63	97.27	100.56
3	A	601	0XJ	C10-C5-C6	2.30	120.11	111.50
3	A	601	0XJ	C16-C17-C13	2.39	111.01	108.64
3	A	601	0XJ	O-C20-C21	2.43	118.55	112.18
2	A	600	HEM	C2D-C3D-C4D	2.49	105.72	101.50
3	A	601	0XJ	C2-C3-C4	3.00	120.38	117.12
2	A	600	HEM	CMB-C2B-C3B	3.06	124.17	116.53
2	A	600	HEM	CMD-C2D-C3D	3.52	129.93	114.35
2	A	600	HEM	CAD-C3D-C4D	3.92	126.29	112.47
2	A	600	HEM	CMC-C2C-C3C	5.09	129.23	116.53
2	A	600	HEM	CAD-C3D-C2D	5.13	127.97	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	HEM	5	0
3	A	601	0XJ	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} 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	452/503 (89%)	-0.12	2 (0%)	93	90	116, 147, 176, 192	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	GLU	2.9
1	A	84	PHE	2.7

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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^{th} 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^2)	Q<0.9
3	0XJ	A	601	27/27	0.96	0.34	1.34	113,116,120,120	0
2	HEM	A	600	43/43	0.99	0.25	0.06	95,97,111,115	0

6.5 Other polymers (i)

There are no such residues in this entry.