



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:36 am GMT

PDB ID : 2WI9  
Title : SELECTIVE OXIDATION OF CARBOLIDE C-H BONDS BY ENGINEERED MACROLIDE P450 MONOOXYGENASE  
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Deposited on : 2009-05-08  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (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

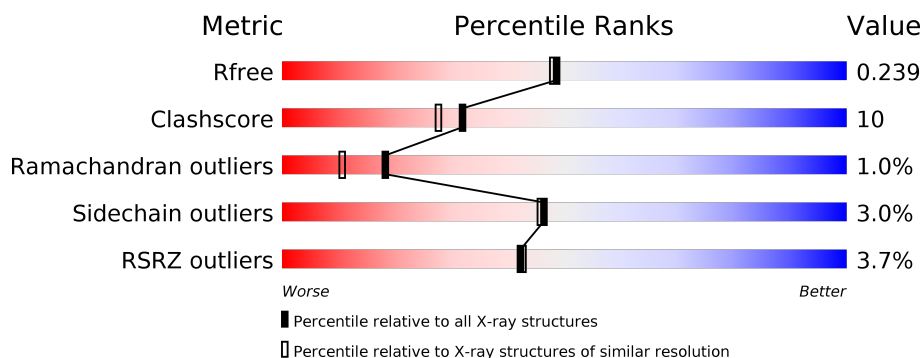
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	436	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	436	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>•</div> <div>10%</div> </div> </div>

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	1D2	B	1409[A]	-	-	-	X
3	1D2	B	1409[B]	-	-	-	X
4	SO4	B	1410	-	-	-	X
4	SO4	B	1412	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6978 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 HYDROXYLASE PIKC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	10	0
			3137	1986	561	575	15			
1	B	394	Total	C	N	O	S	0	5	0
			3092	1952	559	567	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605
B	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605

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



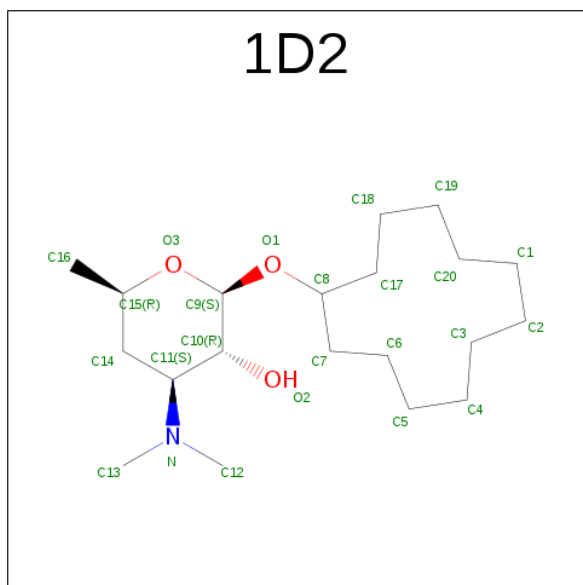
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 3 is CYCLODODECYL 3,4,6-TRIDEOXY-3-(DIMETHYLAMINO)-BETA-D-XYLO-HEXOPYRANOSIDE (three-letter code: 1D2) (formula:  $C_{20}H_{39}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	24	20	1	3	0	0
3	B	1	48	40	2	6	0	1

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

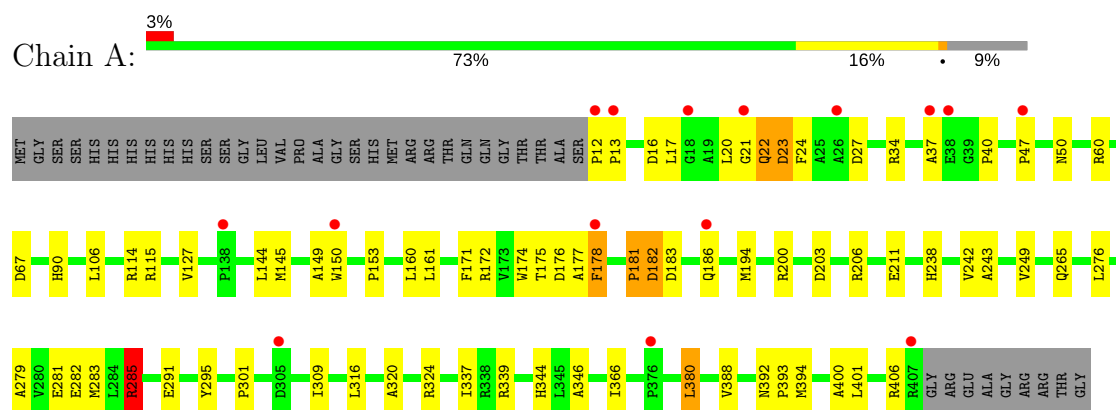
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	296	Total	O	0	0
			296	296		
5	B	280	Total	O	0	0
			280	280		

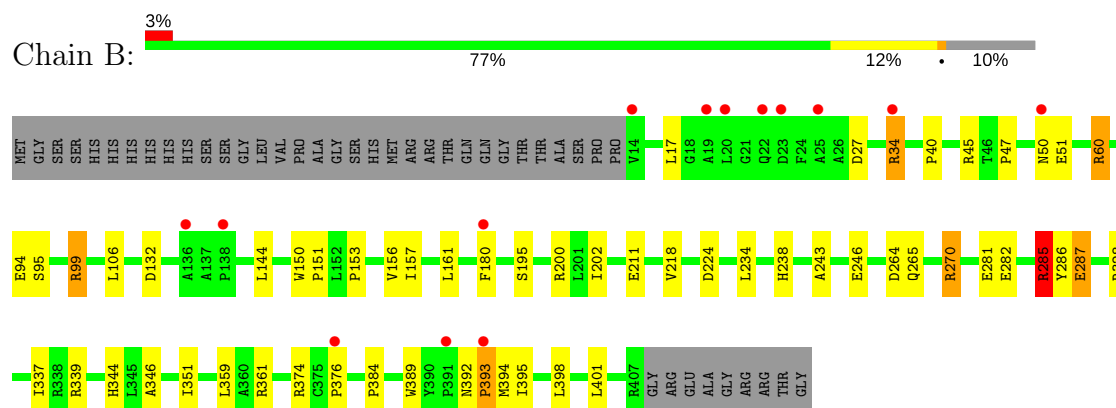
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 HYDROXYLASE PIKC



#### • Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.25Å 109.09Å 153.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.74 – 2.00 46.26 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (88.74-2.00) 97.8 (46.26-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.13 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.184 , 0.239 0.185 , 0.239	Depositor DCC
$R_{free}$ test set	6789 reflections (11.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.2	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	0.95	EDS
Total number of atoms	6978	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.71% 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, 1D2, SO4

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	1.03	2/3215 (0.1%)	1.00	7/4389 (0.2%)
1	B	1.02	1/3166 (0.0%)	0.98	12/4317 (0.3%)
All	All	1.02	3/6381 (0.0%)	0.99	19/8706 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	GLU	CG-CD	6.46	1.61	1.51
1	A	285	ARG	CD-NE	-5.73	1.36	1.46
1	B	285	ARG	CD-NE	-5.42	1.37	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ARG	NE-CZ-NH2	-19.83	110.38	120.30
1	B	285	ARG	NE-CZ-NH2	-15.11	112.74	120.30
1	A	285	ARG	NE-CZ-NH1	12.95	126.78	120.30
1	B	285	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	B	99	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	B	99	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	A	67	ASP	CB-CG-OD1	6.45	124.10	118.30
1	B	270[A]	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	270[B]	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	270[A]	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	270[B]	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	224	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	B	60	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	12	PRO	N-CA-CB	5.55	109.96	103.30
1	A	206	ARG	CG-CD-NE	-5.49	100.26	111.80
1	A	380	LEU	CA-CB-CG	5.44	127.81	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ARG	CG-CD-NE	-5.41	100.43	111.80
1	B	361	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	B	264	ASP	CB-CG-OD1	5.13	122.92	118.30

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	3137	0	3087	64	0
1	B	3092	0	3065	45	0
2	A	43	0	30	0	0
2	B	43	0	30	1	0
3	A	24	0	39	5	0
3	B	48	0	78	22	0
4	B	15	0	0	0	0
5	A	296	0	0	17	2
5	B	280	0	0	11	0
All	All	6978	0	6329	129	2

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 10.

All (129) 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:174:TRP:HB3	1:A:178[A]:PHE:CZ	1.77	1.20
1:A:22:GLN:CB	1:A:23:ASP:HB2	1.83	1.08
1:B:34[A]:ARG:HH11	1:B:34[A]:ARG:HG3	1.16	1.04
1:A:34:ARG:O	5:A:2011:HOH:O	1.77	1.03
3:B:1409[A]:1D2:H202	3:B:1409[A]:1D2:H52C	1.41	1.01
3:B:1409[A]:1D2:H181	3:B:1409[A]:1D2:C6	1.99	0.93
1:B:200:ARG:NE	5:B:2150:HOH:O	1.96	0.93
1:B:200:ARG:NH2	5:B:2150:HOH:O	1.91	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291[A]:GLU:HG3	1:A:320:ALA:HB2	1.56	0.88
3:B:1409[A]:1D2:H181	3:B:1409[A]:1D2:H61C	1.58	0.84
1:B:34[A]:ARG:HH11	1:B:34[A]:ARG:CG	1.91	0.84
1:A:282:GLU:OE1	1:A:285:ARG:HD3	1.77	0.83
3:B:1409[A]:1D2:H181	3:B:1409[A]:1D2:H52C	1.63	0.80
1:A:22:GLN:CB	1:A:23:ASP:CB	2.62	0.78
1:A:394[C]:MET:HG2	5:A:2237:HOH:O	1.85	0.77
1:A:175:THR:C	1:A:177:ALA:H	1.87	0.76
3:B:1409[A]:1D2:H181	3:B:1409[A]:1D2:C5	2.15	0.76
1:B:282:GLU:OE1	1:B:285:ARG:HD3	1.87	0.73
1:B:394[A]:MET:SD	3:B:1409[A]:1D2:H171	2.29	0.73
1:A:174:TRP:HB3	1:A:178[A]:PHE:CE1	2.24	0.72
1:A:21:GLY:N	1:A:22:GLN:CB	2.52	0.72
1:B:34[A]:ARG:HG3	1:B:34[A]:ARG:NH1	1.98	0.71
1:A:282:GLU:OE1	1:A:285:ARG:CD	2.41	0.69
1:A:203:ASP:OD1	5:A:2171:HOH:O	2.09	0.69
3:B:1409[B]:1D2:O2	5:B:2277:HOH:O	1.95	0.69
3:B:1409[A]:1D2:C20	3:B:1409[A]:1D2:H52C	2.19	0.69
3:B:1409[B]:1D2:H181	3:B:1409[B]:1D2:H62C	1.75	0.67
1:A:21:GLY:H	1:A:22:GLN:CB	2.08	0.67
1:B:344:HIS:HD2	1:B:346:ALA:H	1.43	0.67
1:B:238:HIS:CE1	3:B:1409[B]:1D2:H15	2.30	0.67
1:B:392:ASN:OD1	1:B:393:PRO:HD2	1.96	0.66
1:A:344:HIS:HD2	1:A:346:ALA:H	1.43	0.66
1:A:200:ARG:NH1	5:A:2170:HOH:O	2.25	0.66
3:B:1409[A]:1D2:H162	5:B:2072:HOH:O	1.96	0.64
1:B:144:LEU:HD23	1:B:401:LEU:HD23	1.80	0.64
1:A:171:PHE:O	1:A:175:THR:HG23	1.98	0.64
1:B:392:ASN:CG	1:B:393:PRO:HD2	2.18	0.63
1:A:291[A]:GLU:HG3	1:A:320:ALA:CB	2.28	0.63
1:B:34[A]:ARG:CG	1:B:34[A]:ARG:NH1	2.56	0.61
1:B:395:ILE:HD11	3:B:1409[A]:1D2:H191	1.81	0.61
1:A:174:TRP:CB	1:A:178[A]:PHE:CZ	2.70	0.60
1:A:178[A]:PHE:CE1	1:A:194:MET:SD	2.95	0.60
1:A:178[A]:PHE:CZ	1:A:194:MET:HE2	2.37	0.59
1:A:175:THR:C	1:A:177:ALA:N	2.55	0.59
1:B:282:GLU:OE1	1:B:285:ARG:CD	2.51	0.58
1:A:281:GLU:OE1	1:A:344:HIS:HE1	1.87	0.58
1:A:27:ASP:O	5:A:2005:HOH:O	2.17	0.57
1:B:265:GLN:NE2	1:B:337:ILE:H	2.02	0.57
1:A:178[A]:PHE:CZ	1:A:194:MET:SD	2.98	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ARG:CZ	5:B:2150:HOH:O	2.23	0.56
1:A:285:ARG:HD2	1:A:339:ARG:HD2	1.88	0.55
1:A:175:THR:O	1:A:177:ALA:N	2.40	0.55
3:B:1409[B]:1D2:H62C	3:B:1409[B]:1D2:C18	2.34	0.55
1:A:17:LEU:HB2	1:A:47:PRO:HD3	1.88	0.55
1:B:157:ILE:HG13	1:B:161[A]:LEU:HD12	1.89	0.55
1:B:180:PHE:HD1	1:B:180:PHE:O	1.91	0.54
1:A:265:GLN:NE2	1:A:337:ILE:H	2.05	0.54
3:B:1409[A]:1D2:H15	5:B:2278:HOH:O	2.08	0.53
1:B:180:PHE:CD1	1:B:180:PHE:O	2.62	0.53
1:B:286:TYR:CD2	1:B:287:GLU:HG2	2.42	0.53
1:B:94:GLU:OE1	3:B:1409[B]:1D2:C12	2.56	0.52
1:A:295:TYR:CE1	1:A:316:LEU:HD21	2.45	0.52
1:A:265:GLN:NE2	1:A:337:ILE:HG12	2.25	0.52
1:A:178[A]:PHE:CZ	1:A:194:MET:CE	2.92	0.51
1:A:285:ARG:HD2	1:A:339:ARG:CD	2.41	0.51
1:A:392:ASN:OD1	1:A:393:PRO:HD2	2.09	0.51
1:A:90:HIS:HE1	5:A:2072:HOH:O	1.94	0.51
1:B:246:GLU:OE1	3:B:1409[A]:1D2:H182	2.10	0.51
3:B:1409[A]:1D2:C18	3:B:1409[A]:1D2:H52C	2.36	0.51
1:A:16:ASP:HB2	5:A:2001:HOH:O	2.10	0.51
1:A:20:LEU:HD23	1:A:24:PHE:CD1	2.47	0.50
3:A:1409:1D2:H163	5:A:2086:HOH:O	2.12	0.49
1:B:328:ARG:HG3	1:B:328:ARG:HH11	1.77	0.49
1:A:324:ARG:NH1	5:A:2251:HOH:O	1.93	0.49
1:A:150[A]:TRP:O	1:A:153:PRO:HD2	2.12	0.49
3:A:1409:1D2:H51C	3:A:1409:1D2:O1	2.13	0.49
1:A:145[B]:MET:HB3	1:A:150[B]:TRP:HD1	1.78	0.48
1:B:285:ARG:HD2	1:B:339:ARG:HD2	1.95	0.48
1:B:17:LEU:HB2	1:B:47:PRO:HD3	1.97	0.47
3:A:1409:1D2:H11C	5:A:2294:HOH:O	2.13	0.47
1:A:90:HIS:HD2	5:A:2215:HOH:O	1.98	0.46
1:B:281:GLU:OE1	1:B:344:HIS:HE1	1.99	0.46
1:A:316:LEU:HD22	1:A:394[A]:MET:HE3	1.96	0.46
1:A:406:ARG:CB	5:A:2277:HOH:O	2.64	0.46
1:A:37:ALA:HB3	5:A:2011:HOH:O	2.15	0.46
1:A:145[B]:MET:HA	1:A:149:ALA:HB3	1.98	0.46
1:A:279:ALA:O	1:A:283:MET:HG3	2.16	0.46
1:A:90:HIS:CE1	5:A:2072:HOH:O	2.69	0.46
1:A:150[B]:TRP:CE3	1:A:172:ARG:HG3	2.51	0.45
1:A:127:VAL:HG21	1:A:366:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:TRP:CB	1:A:178[A]:PHE:CE1	2.99	0.45
1:A:243:ALA:HB1	5:A:2294:HOH:O	2.16	0.45
2:B:1408:HEM:C4D	3:B:1409[B]:1D2:H201	2.52	0.45
1:B:238:HIS:ND1	5:B:2197:HOH:O	2.14	0.45
1:B:211:GLU:OE2	5:B:2167:HOH:O	2.21	0.44
1:B:389:TRP:CE2	1:B:398:LEU:HD21	2.51	0.44
1:B:45:ARG:HA	1:B:50:ASN:O	2.16	0.44
1:A:178[A]:PHE:CE2	1:A:194:MET:HE2	2.52	0.44
3:A:1409:1D2:H42C	3:A:1409:1D2:H72C	1.81	0.44
1:A:316:LEU:HD22	1:A:394[A]:MET:CE	2.47	0.44
1:B:202:ILE:HG23	1:B:218:VAL:HG22	1.99	0.44
1:A:394[C]:MET:CG	5:A:2237:HOH:O	2.56	0.44
1:A:150[B]:TRP:CZ3	1:A:172:ARG:HG3	2.53	0.43
1:A:145[B]:MET:HB3	1:A:150[B]:TRP:CD1	2.53	0.43
1:A:40:PRO:HB2	1:A:60:ARG:HG2	2.01	0.43
1:B:243:ALA:HA	3:B:1409[A]:1D2:H41C	2.00	0.43
1:A:238:HIS:O	1:A:242[A]:VAL:HG23	2.19	0.43
1:B:60:ARG:HA	1:B:60:ARG:HD3	1.84	0.43
1:B:376:PRO:HA	5:B:2269:HOH:O	2.19	0.42
1:A:144:LEU:HD23	1:A:401:LEU:HD23	2.00	0.42
1:A:145[B]:MET:HG3	1:A:400:ALA:HA	2.00	0.42
3:B:1409[A]:1D2:C18	3:B:1409[A]:1D2:H61C	2.41	0.42
1:A:301:PRO:HA	1:A:309:ILE:O	2.19	0.42
1:A:115:ARG:HD2	5:A:2117:HOH:O	2.19	0.42
1:B:392:ASN:OD1	1:B:393:PRO:CD	2.65	0.42
1:B:150:TRP:N	1:B:151:PRO:HD2	2.35	0.42
1:A:145[A]:MET:SD	1:A:249:VAL:CG1	3.07	0.41
3:A:1409:1D2:H42C	3:A:1409:1D2:H12C	1.34	0.41
3:B:1409[B]:1D2:H181	3:B:1409[B]:1D2:H11C	1.49	0.41
1:B:95:SER:HB3	1:B:99:ARG:HD2	2.01	0.41
1:B:238:HIS:HE1	3:B:1409[B]:1D2:H15	1.82	0.41
1:B:40:PRO:HB2	1:B:60:ARG:HG2	2.01	0.41
1:A:160[B]:LEU:HD12	1:A:160[B]:LEU:HA	1.88	0.41
1:B:27:ASP:O	5:B:2003:HOH:O	2.22	0.41
1:B:132:ASP:OD1	1:B:374:ARG:NH2	2.41	0.41
1:A:181:PRO:HB2	1:A:182:ASP:H	1.63	0.40
1:B:150:TRP:O	1:B:153:PRO:HD2	2.21	0.40
1:B:351:ILE:HG12	5:B:2256:HOH:O	2.21	0.40
1:B:156:VAL:HG11	1:B:359:LEU:HD11	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2035:HOH:O	5:A:2209:HOH:O[4_456]	2.09	0.11
5:A:2202:HOH:O	5:A:2266:HOH:O[4_556]	2.11	0.09

### 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	404/436 (93%)	380 (94%)	16 (4%)	8 (2%)	9	3
1	B	397/436 (91%)	382 (96%)	14 (4%)	1 (0%)	44	40
All	All	801/872 (92%)	762 (95%)	30 (4%)	9 (1%)	18	9

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	ASP
1	A	182	ASP
1	A	178[A]	PHE
1	A	178[B]	PHE
1	A	181	PRO
1	A	13	PRO
1	B	393	PRO
1	A	22	GLN
1	A	183	ASP

#### 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	325/354 (92%)	315 (97%)	10 (3%)	45	44
1	B	321/354 (91%)	310 (97%)	11 (3%)	42	40
All	All	646/708 (91%)	625 (97%)	21 (3%)	46	41

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	50	ASN
1	A	106	LEU
1	A	114	ARG
1	A	161	LEU
1	A	186	GLN
1	A	276	LEU
1	A	285	ARG
1	A	380	LEU
1	A	388	VAL
1	B	34[A]	ARG
1	B	34[B]	ARG
1	B	51	GLU
1	B	106	LEU
1	B	195	SER
1	B	234	LEU
1	B	270[A]	ARG
1	B	270[B]	ARG
1	B	285	ARG
1	B	287	GLU
1	B	384	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	186	GLN
1	A	188	GLN
1	A	208	GLN
1	A	238	HIS
1	A	265	GLN
1	A	344	HIS
1	B	188	GLN
1	B	208	GLN

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Mol	Chain	Res	Type
1	B	238	HIS
1	B	265	GLN
1	B	333	HIS
1	B	344	HIS

### 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](#)

8 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	1408	1	28,50,50	2.06	10 (35%)	17,82,82	2.12	6 (35%)
3	1D2	A	1409	-	25,25,25	0.78	0	32,32,32	2.40	9 (28%)
2	HEM	B	1408	1	28,50,50	2.07	9 (32%)	17,82,82	2.72	6 (35%)
3	1D2	B	1409[A]	-	25,25,25	0.68	0	32,32,32	2.62	12 (37%)
3	1D2	B	1409[B]	-	25,25,25	0.53	0	32,32,32	2.41	10 (31%)
4	SO4	B	1410	-	4,4,4	0.39	0	6,6,6	0.48	0
4	SO4	B	1411	-	4,4,4	0.21	0	6,6,6	0.13	0
4	SO4	B	1412	-	4,4,4	0.18	0	6,6,6	0.72	0



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	1408	1	-	0/6/54/54	0/0/8/8
3	1D2	A	1409	-	-	0/22/38/38	1/2/2/2
2	HEM	B	1408	1	-	0/6/54/54	0/0/8/8
3	1D2	B	1409[A]	-	-	0/22/38/38	1/2/2/2
3	1D2	B	1409[B]	-	-	0/22/38/38	1/2/2/2
4	SO4	B	1410	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1411	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1412	-	-	0/0/0/0	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1408	HEM	C3B-C2B	-4.78	1.34	1.40
2	B	1408	HEM	C3C-C2C	-4.16	1.34	1.40
2	A	1408	HEM	C1B-NB	-2.60	1.33	1.36
2	A	1408	HEM	C4B-NB	-2.17	1.31	1.36
2	A	1408	HEM	C3C-C2C	-2.11	1.37	1.40
2	B	1408	HEM	C1D-ND	2.06	1.40	1.36
2	B	1408	HEM	C3B-CAB	2.26	1.52	1.47
2	B	1408	HEM	C1C-NC	2.28	1.39	1.36
2	A	1408	HEM	C1A-NA	2.34	1.41	1.36
2	B	1408	HEM	CMC-C2C	2.49	1.56	1.51
2	A	1408	HEM	C1C-NC	2.57	1.39	1.36
2	B	1408	HEM	C1A-NA	2.58	1.41	1.36
2	A	1408	HEM	CMD-C2D	2.61	1.56	1.51
2	A	1408	HEM	C3B-CAB	2.72	1.53	1.47
2	B	1408	HEM	CMD-C2D	3.23	1.58	1.51
2	A	1408	HEM	C3C-CAC	3.50	1.54	1.47
2	A	1408	HEM	C3D-C2D	4.50	1.51	1.37
2	B	1408	HEM	C3C-CAC	4.81	1.57	1.47
2	B	1408	HEM	C3D-C2D	4.88	1.52	1.37

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1409[B]	1D2	C9-C10-C11	-7.32	96.88	109.27
2	B	1408	HEM	C1D-C2D-C3D	-6.15	102.71	107.00
3	B	1409[B]	1D2	C12-N-C11	-6.10	95.27	113.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1408	HEM	CBD-CAD-C3D	-5.67	101.66	112.47
2	A	1408	HEM	CBD-CAD-C3D	-4.95	103.03	112.47
3	A	1409	1D2	C9-O3-C15	-4.75	105.05	112.91
3	B	1409[A]	1D2	C14-C11-C10	-4.65	103.50	110.07
3	B	1409[A]	1D2	C12-N-C11	-4.52	99.87	113.08
3	B	1409[B]	1D2	C15-C14-C11	-4.00	103.26	110.42
2	A	1408	HEM	CAD-CBD-CGD	-3.78	106.20	112.66
3	B	1409[A]	1D2	C16-C15-C14	-3.67	107.50	113.39
3	B	1409[A]	1D2	C9-C10-C11	-3.56	103.24	109.27
3	A	1409	1D2	C14-C11-N	-3.40	106.14	115.83
3	B	1409[A]	1D2	C15-C14-C11	-3.25	104.59	110.42
2	B	1408	HEM	CMA-C3A-C4A	-3.23	123.50	128.46
3	B	1409[B]	1D2	C14-C11-C10	-2.97	105.87	110.07
3	B	1409[A]	1D2	C14-C11-N	-2.87	107.67	115.83
3	B	1409[B]	1D2	O3-C9-C10	-2.80	104.89	110.30
2	A	1408	HEM	C1D-C2D-C3D	-2.76	105.08	107.00
2	A	1408	HEM	C3B-C4B-NB	-2.41	106.09	109.21
2	B	1408	HEM	CAD-CBD-CGD	-2.32	108.69	112.66
3	B	1409[B]	1D2	C13-N-C12	-2.13	103.91	110.41
2	A	1408	HEM	CMA-C3A-C4A	-2.11	125.22	128.46
3	A	1409	1D2	O1-C8-C7	-2.01	104.82	108.34
3	B	1409[A]	1D2	O3-C15-C16	2.25	111.60	106.88
3	A	1409	1D2	O2-C10-C11	2.30	113.90	109.78
3	B	1409[A]	1D2	C9-O1-C8	2.30	119.66	114.93
2	A	1408	HEM	CMC-C2C-C3C	2.35	129.25	124.89
3	A	1409	1D2	C13-N-C11	2.39	120.06	113.08
3	B	1409[A]	1D2	O2-C10-C11	2.45	114.17	109.78
3	B	1409[B]	1D2	O1-C9-O3	2.47	116.70	110.70
3	B	1409[B]	1D2	O3-C15-C16	2.48	112.06	106.88
2	B	1408	HEM	CMB-C2B-C3B	2.95	130.37	124.89
3	B	1409[B]	1D2	O1-C8-C17	2.98	113.56	108.34
3	B	1409[B]	1D2	O2-C10-C11	3.46	115.99	109.78
2	B	1408	HEM	C4A-C3A-C2A	3.67	109.55	107.00
3	A	1409	1D2	C15-C14-C11	3.69	117.04	110.42
3	A	1409	1D2	O1-C9-C10	4.29	117.77	108.11
3	B	1409[A]	1D2	O1-C8-C17	4.34	115.96	108.34
3	A	1409	1D2	C9-O1-C8	4.71	124.62	114.93
3	B	1409[A]	1D2	O3-C15-C14	5.51	117.68	109.10
3	B	1409[A]	1D2	C9-O3-C15	6.97	124.44	112.91
3	A	1409	1D2	O1-C8-C17	7.34	121.22	108.34

There are no chirality outliers.

There are no torsion outliers.

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1409	1D2	C1-C17-C18-C19-C2-C20-C3-C4-C5-C6-C7-C8
3	B	1409[A]	1D2	C1-C17-C18-C19-C2-C20-C3-C4-C5-C6-C7-C8
3	B	1409[B]	1D2	C1-C17-C18-C19-C2-C20-C3-C4-C5-C6-C7-C8

4 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1409	1D2	5	0
2	B	1408	HEM	1	0
3	B	1409[A]	1D2	14	0
3	B	1409[B]	1D2	8	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	396/436 (90%)	-0.12	15 (3%) 41 41	14, 27, 61, 73	0
1	B	394/436 (90%)	-0.24	14 (3%) 43 44	13, 26, 61, 78	0
All	All	790/872 (90%)	-0.18	29 (3%) 42 43	13, 27, 61, 78	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178[A]	PHE	5.3
1	A	47	PRO	3.8
1	A	18	GLY	3.5
1	A	13	PRO	3.3
1	A	407	ARG	3.1
1	B	25	ALA	3.1
1	B	138	PRO	3.1
1	B	22	GLN	2.9
1	B	180	PHE	2.9
1	B	23	ASP	2.7
1	A	305[A]	ASP	2.7
1	A	26	ALA	2.5
1	A	21	GLY	2.5
1	A	37	ALA	2.5
1	B	136	ALA	2.4
1	A	138	PRO	2.4
1	A	376	PRO	2.4
1	B	50	ASN	2.3
1	A	186	GLN	2.3
1	A	12	PRO	2.3
1	B	391	PRO	2.2
1	A	38	GLU	2.2
1	B	19	ALA	2.2
1	B	20	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	150[A]	TRP	2.2
1	B	34[A]	ARG	2.2
1	B	14	VAL	2.1
1	B	376	PRO	2.1
1	B	393	PRO	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, 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
4	SO4	B	1412	5/5	0.86	0.17	6.55	78,79,80,81	0
3	1D2	B	1409[B]	24/24	0.85	0.26	4.20	12,28,32,34	24
3	1D2	B	1409[A]	24/24	0.85	0.26	3.28	35,42,50,51	24
4	SO4	B	1410	5/5	0.86	0.16	2.87	67,67,70,71	0
3	1D2	A	1409	24/24	0.74	0.23	1.06	46,62,72,72	0
2	HEM	B	1408	43/43	0.99	0.13	1.04	9,15,19,28	0
2	HEM	A	1408	43/43	0.99	0.14	0.29	12,16,19,25	0
4	SO4	B	1411	5/5	0.72	0.20	-	106,106,106,106	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.