



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:38 PM GMT

PDB ID : 2PG7  
Title : Crystal Structure of Human Microsomal P450 2A6 N297Q/I300V  
Authors : Sansen, S.; Hsu, M.H.; Stout, C.D.; Johnson, E.F.  
Deposited on : 2007-04-06  
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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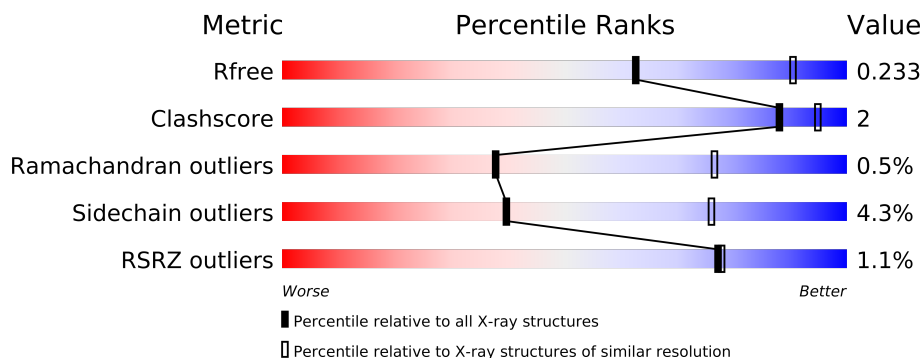
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	476	
1	B	476	
1	C	476	
1	D	476	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15273 atoms, of which 0 are hydrogen and 0 are deuterium.

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 2A6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			
1	B	464	Total	C	N	O	S	0	0	0
			3757	2412	650	677	18			
1	C	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			
1	D	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			

There are 52 discrepancies between the modelled and reference sequences:

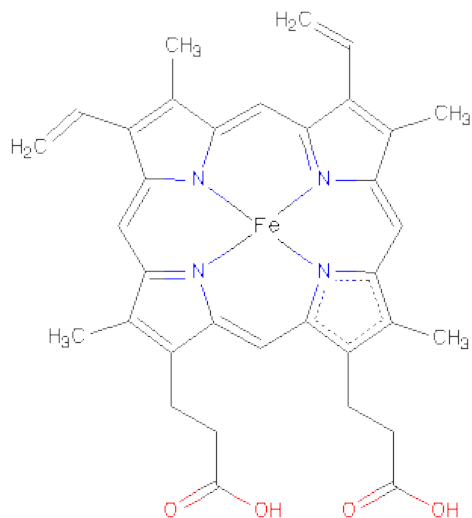
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	CLONING ARTIFACT	UNP P11509
A	24	ALA	-	CLONING ARTIFACT	UNP P11509
A	25	LYS	-	CLONING ARTIFACT	UNP P11509
A	26	LYS	-	CLONING ARTIFACT	UNP P11509
A	27	THR	-	CLONING ARTIFACT	UNP P11509
A	28	SER	-	CLONING ARTIFACT	UNP P11509
A	160	LEU	HIS	VARIANT	UNP P11509
A	297	GLN	ASN	ENGINEERED	UNP P11509
A	300	VAL	ILE	ENGINEERED	UNP P11509
A	495	HIS	-	EXPRESSION TAG	UNP P11509
A	496	HIS	-	EXPRESSION TAG	UNP P11509
A	497	HIS	-	EXPRESSION TAG	UNP P11509
A	498	HIS	-	EXPRESSION TAG	UNP P11509
B	23	MET	-	CLONING ARTIFACT	UNP P11509
B	24	ALA	-	CLONING ARTIFACT	UNP P11509
B	25	LYS	-	CLONING ARTIFACT	UNP P11509
B	26	LYS	-	CLONING ARTIFACT	UNP P11509
B	27	THR	-	CLONING ARTIFACT	UNP P11509
B	28	SER	-	CLONING ARTIFACT	UNP P11509
B	160	LEU	HIS	VARIANT	UNP P11509
B	297	GLN	ASN	ENGINEERED	UNP P11509

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Chain	Residue	Modelled	Actual	Comment	Reference
B	300	VAL	ILE	ENGINEERED	UNP P11509
B	495	HIS	-	EXPRESSION TAG	UNP P11509
B	496	HIS	-	EXPRESSION TAG	UNP P11509
B	497	HIS	-	EXPRESSION TAG	UNP P11509
B	498	HIS	-	EXPRESSION TAG	UNP P11509
C	23	MET	-	CLONING ARTIFACT	UNP P11509
C	24	ALA	-	CLONING ARTIFACT	UNP P11509
C	25	LYS	-	CLONING ARTIFACT	UNP P11509
C	26	LYS	-	CLONING ARTIFACT	UNP P11509
C	27	THR	-	CLONING ARTIFACT	UNP P11509
C	28	SER	-	CLONING ARTIFACT	UNP P11509
C	160	LEU	HIS	VARIANT	UNP P11509
C	297	GLN	ASN	ENGINEERED	UNP P11509
C	300	VAL	ILE	ENGINEERED	UNP P11509
C	495	HIS	-	EXPRESSION TAG	UNP P11509
C	496	HIS	-	EXPRESSION TAG	UNP P11509
C	497	HIS	-	EXPRESSION TAG	UNP P11509
C	498	HIS	-	EXPRESSION TAG	UNP P11509
D	23	MET	-	CLONING ARTIFACT	UNP P11509
D	24	ALA	-	CLONING ARTIFACT	UNP P11509
D	25	LYS	-	CLONING ARTIFACT	UNP P11509
D	26	LYS	-	CLONING ARTIFACT	UNP P11509
D	27	THR	-	CLONING ARTIFACT	UNP P11509
D	28	SER	-	CLONING ARTIFACT	UNP P11509
D	160	LEU	HIS	VARIANT	UNP P11509
D	297	GLN	ASN	ENGINEERED	UNP P11509
D	300	VAL	ILE	ENGINEERED	UNP P11509
D	495	HIS	-	EXPRESSION TAG	UNP P11509
D	496	HIS	-	EXPRESSION TAG	UNP P11509
D	497	HIS	-	EXPRESSION TAG	UNP P11509
D	498	HIS	-	EXPRESSION TAG	UNP P11509

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

- Molecule 3 is water.

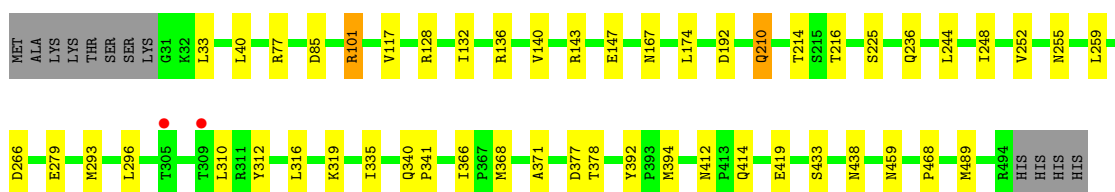
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	23	Total	O	0	0
			23	23		
3	C	25	Total	O	0	0
			25	25		
3	D	23	Total	O	0	0
			23	23		

### 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.

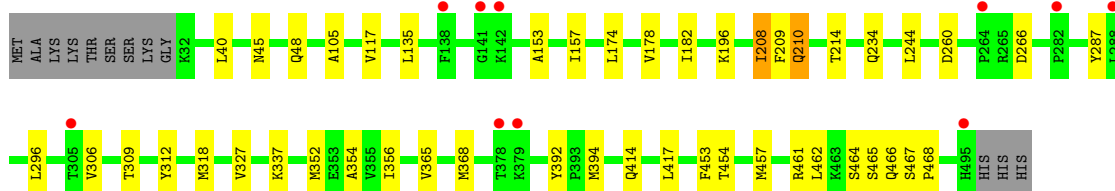
#### • Molecule 1: Cytochrome P450 2A6

Chain A:



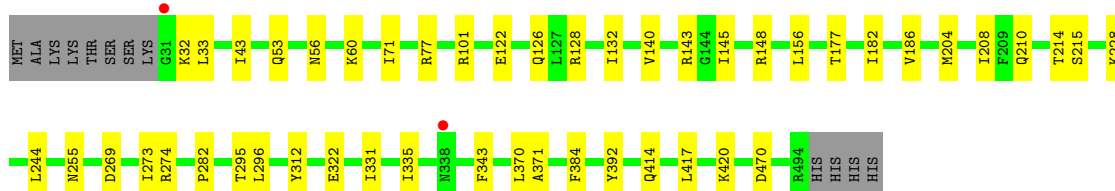
#### • Molecule 1: Cytochrome P450 2A6

Chain B:



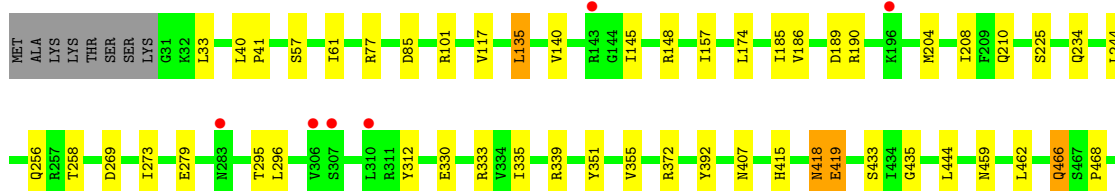
#### • Molecule 1: Cytochrome P450 2A6

Chain C:



#### • Molecule 1: Cytochrome P450 2A6

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.89Å 159.39Å 104.10Å 90.00° 91.92° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80 36.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-2.80) 99.6 (36.65-2.80)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.235 , 0.289 0.230 , 0.233	Depositor DCC
$R_{free}$ test set	2865 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.3	Xtriage
Anisotropy	0.849	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 10.1	EDS
Estimated twinning fraction	0.041 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 56548 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15273	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

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	0.68	0/3842	0.74	2/5175 (0.0%)
1	B	0.70	0/3849	0.75	0/5185
1	C	0.69	0/3842	0.75	1/5175 (0.0%)
1	D	0.68	0/3842	0.74	1/5175 (0.0%)
All	All	0.69	0/15375	0.75	4/20710 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	LEU	CA-CB-CG	6.04	129.20	115.30
1	D	135	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	366	ILE	CG1-CB-CG2	-5.14	100.08	111.40
1	A	33	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3751	0	3734	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3757	0	3738	16	0
1	C	3751	0	3734	15	0
1	D	3751	0	3734	25	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	0	0
2	D	43	0	30	2	0
3	A	20	0	0	0	0
3	B	23	0	0	0	0
3	C	25	0	0	0	0
3	D	23	0	0	0	0
All	All	15273	0	15060	73	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (73) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:145:ILE:HD13	1:D:185:ILE:HD11	1.75	0.69
1:C:32:LYS:HB3	1:C:384:PHE:HB3	1.75	0.67
1:D:244:LEU:HB3	1:D:296:LEU:HD11	1.79	0.64
1:B:368:MET:HG2	1:B:394:MET:SD	2.40	0.62
1:A:244:LEU:HB3	1:A:296:LEU:HD11	1.83	0.60
1:D:117:VAL:HG22	2:D:500:HEM:HAD1	1.84	0.60
1:D:101:ARG:HD3	1:D:117:VAL:O	2.01	0.60
1:C:128:ARG:HE	1:C:132:ILE:HD11	1.67	0.59
1:D:335:ILE:HA	1:D:339:ARG:HH21	1.70	0.56
1:A:132:ILE:HG22	1:A:136:ARG:NH1	2.21	0.55
1:C:53:GLN:HB3	1:C:56:ASN:HB2	1.89	0.55
1:A:225:SER:HB2	1:D:225:SER:HB2	1.88	0.55
1:A:40:LEU:HD21	1:C:43:ILE:HD13	1.89	0.55
1:A:433:SER:HB3	2:A:500:HEM:HBA1	1.89	0.54
1:C:156:LEU:HB2	1:C:177:THR:HG21	1.90	0.54
1:B:352:MET:HE3	1:B:454:THR:HG22	1.90	0.54
1:D:407:ASN:H	1:D:415:HIS:HE1	1.55	0.53
1:A:128:ARG:O	1:A:132:ILE:HG13	2.08	0.52
1:D:140:VAL:HG22	1:D:444:LEU:HD13	1.92	0.52
1:D:433:SER:HB3	2:D:500:HEM:HBA1	1.92	0.52
1:D:204:MET:O	1:D:208:ILE:HG12	2.11	0.51
1:D:330:GLU:HG3	1:D:333:ARG:NH2	2.27	0.50
1:B:244:LEU:HB3	1:B:296:LEU:HD11	1.94	0.50
1:C:269:ASP:O	1:C:273:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:269:ASP:O	1:D:273:ILE:HG12	2.11	0.49
1:A:412:ASN:HD21	1:A:414:GLN:HB2	1.78	0.49
1:C:214:THR:HG22	1:C:215:SER:H	1.77	0.49
1:A:248:ILE:O	1:A:252:VAL:HG23	2.13	0.49
1:D:462:LEU:HD22	1:D:489:MET:HE1	1.93	0.49
1:B:153:ALA:O	1:B:157:ILE:HG12	2.13	0.49
1:B:45:ASN:HD22	1:B:48:GLN:NE2	2.10	0.49
1:A:132:ILE:HG22	1:A:136:ARG:HH12	1.78	0.48
1:B:414:GLN:NE2	1:B:417:LEU:HD23	2.29	0.48
1:C:77:ARG:HG2	1:C:77:ARG:HH11	1.78	0.48
1:B:327:VAL:HG13	1:B:352:MET:HE1	1.96	0.47
1:D:419:GLU:H	1:D:419:GLU:CD	2.17	0.47
1:C:122:GLU:O	1:C:126:GLN:HB2	2.15	0.47
1:D:466:GLN:HG3	1:D:471:ILE:HG12	1.96	0.47
1:D:351:TYR:O	1:D:355:VAL:HG23	2.15	0.47
1:D:157:ILE:HG21	1:D:459:ASN:HD22	1.80	0.47
1:C:186:VAL:HG13	1:C:295:THR:HG23	1.96	0.46
1:C:331:ILE:HG23	1:C:335:ILE:HD12	1.97	0.46
1:B:352:MET:O	1:B:356:ILE:HG12	2.17	0.45
1:B:117:VAL:HG22	2:B:500:HEM:HAD1	1.98	0.45
1:A:210:GLN:O	1:A:214:THR:HG23	2.16	0.45
1:B:210:GLN:O	1:B:214:THR:HG23	2.17	0.44
1:A:117:VAL:HG22	2:A:500:HEM:HAD1	2.00	0.44
1:C:244:LEU:HB3	1:C:296:LEU:HD11	1.98	0.44
1:B:178:VAL:HG11	1:B:306:VAL:HB	2.00	0.44
1:D:33:LEU:HD11	1:D:77:ARG:NH1	2.33	0.44
1:D:57:SER:O	1:D:61:ILE:HG12	2.18	0.44
1:C:204:MET:O	1:C:208:ILE:HG12	2.17	0.43
1:D:148:ARG:HH21	1:D:190:ARG:HB3	1.83	0.43
1:A:319:LYS:HD2	1:A:468:PRO:O	2.18	0.43
1:B:318:MET:HE3	1:B:462:LEU:HB3	1.99	0.43
1:A:335:ILE:HG21	1:A:341:PRO:HG3	2.00	0.43
1:D:462:LEU:HD22	1:D:489:MET:CE	2.49	0.42
1:D:189:ASP:CG	1:D:190:ARG:H	2.23	0.42
1:A:143:ARG:O	1:A:147:GLU:HG2	2.19	0.42
1:B:208:ILE:HD13	1:B:208:ILE:HA	1.93	0.42
1:D:186:VAL:HG13	1:D:295:THR:HG23	2.02	0.42
1:C:214:THR:HG22	1:C:215:SER:N	2.34	0.42
1:D:372:ARG:HH22	1:D:435:GLY:HA3	1.84	0.41
1:B:453:PHE:O	1:B:457:MET:HG2	2.20	0.41
1:C:101:ARG:NH2	1:C:370:LEU:O	2.53	0.41
1:B:309:THR:OG1	1:B:365:VAL:HG21	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:368:MET:HG2	1:A:394:MET:SD	2.60	0.41
1:A:489:MET:HE2	1:A:489:MET:HB2	1.90	0.41
1:D:135:LEU:HG	1:D:140:VAL:HG21	2.03	0.41
1:A:174:LEU:HD22	1:A:310:LEU:HD13	2.03	0.41
1:A:101:ARG:HD2	1:A:117:VAL:O	2.22	0.40
1:B:354:ALA:HB2	1:B:417:LEU:HD13	2.03	0.40
1:A:255:ASN:O	1:A:259:LEU:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	462/476 (97%)	436 (94%)	23 (5%)	3 (1%)	33	72
1	B	462/476 (97%)	429 (93%)	31 (7%)	2 (0%)	43	80
1	C	462/476 (97%)	440 (95%)	19 (4%)	3 (1%)	33	72
1	D	462/476 (97%)	430 (93%)	30 (6%)	2 (0%)	43	80
All	All	1848/1904 (97%)	1735 (94%)	103 (6%)	10 (0%)	38	76

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	VAL
1	C	371	ALA
1	A	371	ALA
1	B	468	PRO
1	A	438	ASN
1	B	105	ALA
1	C	282	PRO
1	D	418	ASN
1	D	468	PRO
1	C	140	VAL

### 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	411/422 (97%)	392 (95%)	19 (5%)	37	73
1	B	412/422 (98%)	392 (95%)	20 (5%)	35	71
1	C	411/422 (97%)	393 (96%)	18 (4%)	39	75
1	D	411/422 (97%)	397 (97%)	14 (3%)	49	84
All	All	1645/1688 (98%)	1574 (96%)	71 (4%)	40	76

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ARG
1	A	85	ASP
1	A	101	ARG
1	A	167	ASN
1	A	192	ASP
1	A	210	GLN
1	A	216	THR
1	A	236	GLN
1	A	266	ASP
1	A	279	GLU
1	A	293	MET
1	A	312	TYR
1	A	316	LEU
1	A	340	GLN
1	A	377	ASP
1	A	378	THR
1	A	392	TYR
1	A	419	GLU
1	A	459	ASN
1	B	40	LEU
1	B	135	LEU
1	B	174	LEU
1	B	182	ILE
1	B	196	LYS
1	B	208	ILE
1	B	209	PHE

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Mol	Chain	Res	Type
1	B	210	GLN
1	B	234	GLN
1	B	260	ASP
1	B	266	ASP
1	B	287	TYR
1	B	312	TYR
1	B	337	LYS
1	B	392	TYR
1	B	461	ARG
1	B	464	SER
1	B	465	SER
1	B	466	GLN
1	B	467	SER
1	C	60	LYS
1	C	71	ILE
1	C	143	ARG
1	C	145	ILE
1	C	148	ARG
1	C	182	ILE
1	C	210	GLN
1	C	228	LYS
1	C	255	ASN
1	C	274	ARG
1	C	312	TYR
1	C	322	GLU
1	C	343	PHE
1	C	392	TYR
1	C	414	GLN
1	C	417	LEU
1	C	420	LYS
1	C	470	ASP
1	D	40	LEU
1	D	41	PRO
1	D	85	ASP
1	D	174	LEU
1	D	210	GLN
1	D	234	GLN
1	D	256	GLN
1	D	258	THR
1	D	279	GLU
1	D	312	TYR
1	D	392	TYR

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Mol	Chain	Res	Type
1	D	418	ASN
1	D	419	GLU
1	D	466	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	210	GLN
1	A	412	ASN
1	A	414	GLN
1	A	458	GLN
1	B	48	GLN
1	B	255	ASN
1	B	414	GLN
1	B	418	ASN
1	C	150	GLN
1	C	167	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	500	1	49,50,50	4.31	21 (42%)	46,82,82	1.90	17 (36%)
2	HEM	B	500	1	49,50,50	4.15	20 (40%)	46,82,82	1.88	12 (26%)
2	HEM	C	500	1	49,50,50	4.20	22 (44%)	46,82,82	1.76	11 (23%)
2	HEM	D	500	1	49,50,50	4.16	19 (38%)	46,82,82	1.85	13 (28%)

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	500	1	-	0/14/114/114	0/0/8/8
2	HEM	B	500	1	-	0/14/114/114	0/0/8/8
2	HEM	C	500	1	-	0/14/114/114	0/0/8/8
2	HEM	D	500	1	-	0/14/114/114	0/0/8/8

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	HEM	C2D-C1D	-21.10	1.39	1.44
2	B	500	HEM	C2D-C1D	-18.96	1.39	1.44
2	A	500	HEM	C2D-C1D	-18.83	1.39	1.44
2	D	500	HEM	C2D-C1D	-18.63	1.39	1.44
2	A	500	HEM	C3D-C4D	-16.08	1.40	1.44
2	D	500	HEM	C3D-C4D	-15.15	1.40	1.44
2	B	500	HEM	C3D-C4D	-13.52	1.41	1.44
2	C	500	HEM	C3D-C4D	-12.66	1.41	1.44
2	B	500	HEM	C2B-C1B	-9.72	1.42	1.44
2	A	500	HEM	C2B-C1B	-9.04	1.42	1.44
2	D	500	HEM	C2B-C1B	-8.37	1.42	1.44
2	C	500	HEM	C2B-C1B	-6.98	1.42	1.44
2	C	500	HEM	C1C-NC	-4.68	1.31	1.38
2	B	500	HEM	C1C-NC	-4.66	1.31	1.38
2	A	500	HEM	C1C-NC	-4.47	1.31	1.38
2	C	500	HEM	C3D-C2D	-4.29	1.36	1.43
2	D	500	HEM	C1C-NC	-4.19	1.32	1.38
2	B	500	HEM	C3D-C2D	-4.19	1.36	1.43
2	A	500	HEM	C3D-C2D	-4.07	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C1D-ND	-4.02	1.28	1.37
2	A	500	HEM	C1B-NB	-3.93	1.31	1.39
2	D	500	HEM	C1D-ND	-3.88	1.28	1.37
2	B	500	HEM	C1D-ND	-3.85	1.28	1.37
2	C	500	HEM	C1D-ND	-3.82	1.28	1.37
2	D	500	HEM	C1B-NB	-3.69	1.31	1.39
2	D	500	HEM	C3D-C2D	-3.65	1.37	1.43
2	B	500	HEM	C4A-NA	-3.60	1.29	1.36
2	B	500	HEM	C1B-NB	-3.57	1.32	1.39
2	A	500	HEM	C4A-NA	-3.55	1.29	1.36
2	A	500	HEM	CBB-CAB	3.49	1.49	1.28
2	D	500	HEM	CBB-CAB	3.48	1.49	1.28
2	B	500	HEM	CBB-CAB	3.46	1.49	1.28
2	C	500	HEM	CBB-CAB	3.44	1.48	1.28
2	C	500	HEM	C1B-NB	-3.32	1.32	1.39
2	D	500	HEM	CMA-C3A	3.21	1.58	1.51
2	D	500	HEM	C4A-NA	-3.18	1.30	1.36
2	C	500	HEM	FE-NA	3.15	2.06	1.92
2	D	500	HEM	FE-NA	3.15	2.06	1.92
2	D	500	HEM	C4C-NC	-3.12	1.33	1.38
2	C	500	HEM	C4A-NA	-3.05	1.30	1.36
2	B	500	HEM	C4D-ND	-3.02	1.33	1.39
2	C	500	HEM	C4D-ND	-3.01	1.33	1.39
2	A	500	HEM	C4B-NB	-2.98	1.30	1.37
2	B	500	HEM	C4B-NB	-2.93	1.30	1.37
2	A	500	HEM	CMA-C3A	2.89	1.57	1.51
2	C	500	HEM	C4C-NC	-2.87	1.34	1.38
2	A	500	HEM	O2A-CGA	-2.87	1.20	1.30
2	A	500	HEM	C4C-NC	-2.87	1.34	1.38
2	D	500	HEM	CMC-C2C	2.85	1.56	1.47
2	B	500	HEM	CMC-C2C	2.85	1.56	1.47
2	B	500	HEM	FE-NA	2.84	2.04	1.92
2	C	500	HEM	CMC-C2C	2.82	1.56	1.47
2	A	500	HEM	CMC-C2C	2.80	1.56	1.47
2	A	500	HEM	FE-NA	2.77	2.04	1.92
2	C	500	HEM	CMA-C3A	2.77	1.57	1.51
2	C	500	HEM	C4B-NB	-2.76	1.31	1.37
2	D	500	HEM	C4D-ND	-2.68	1.34	1.39
2	D	500	HEM	C4B-NB	-2.67	1.31	1.37
2	C	500	HEM	O2A-CGA	-2.63	1.20	1.30
2	A	500	HEM	C4D-ND	-2.61	1.34	1.39
2	B	500	HEM	O2A-CGA	-2.60	1.21	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HEM	O2A-CGA	-2.56	1.21	1.30
2	B	500	HEM	CMA-C3A	2.55	1.57	1.51
2	A	500	HEM	FE-NB	2.50	2.06	1.97
2	B	500	HEM	FE-ND	2.48	2.06	1.97
2	D	500	HEM	FE-ND	2.46	2.06	1.97
2	C	500	HEM	FE-ND	2.35	2.06	1.97
2	C	500	HEM	CHB-C1B	2.35	1.39	1.35
2	C	500	HEM	CBC-CAC	2.33	1.42	1.28
2	A	500	HEM	CBC-CAC	2.27	1.42	1.28
2	B	500	HEM	CBC-CAC	2.27	1.42	1.28
2	A	500	HEM	FE-ND	2.24	2.06	1.97
2	D	500	HEM	CBC-CAC	2.21	1.41	1.28
2	C	500	HEM	FE-NB	2.20	2.05	1.97
2	C	500	HEM	C3C-C2C	-2.16	1.40	1.43
2	B	500	HEM	C4C-NC	-2.12	1.35	1.38
2	C	500	HEM	C1A-C2A	-2.10	1.39	1.43
2	B	500	HEM	CMD-C2D	2.08	1.53	1.47
2	A	500	HEM	CBD-CGD	2.06	1.55	1.50
2	B	500	HEM	CBD-CGD	2.03	1.55	1.50
2	A	500	HEM	C3C-C2C	-2.03	1.40	1.43
2	D	500	HEM	CMD-C2D	2.02	1.53	1.47

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	HEM	CHD-C4C-NC	-5.57	119.89	124.73
2	B	500	HEM	CHD-C4C-NC	-5.28	120.15	124.73
2	D	500	HEM	CHD-C4C-NC	-4.18	121.10	124.73
2	C	500	HEM	CHD-C4C-NC	-4.16	121.12	124.73
2	B	500	HEM	C3B-C4B-NB	-4.10	111.07	114.00
2	D	500	HEM	C3B-C4B-NB	-3.98	111.15	114.00
2	B	500	HEM	CHC-C1C-NC	-3.70	121.52	124.73
2	D	500	HEM	CHB-C1B-NB	-3.63	119.31	124.31
2	D	500	HEM	C1B-NB-C4B	3.46	108.70	105.16
2	C	500	HEM	C3B-C4B-NB	-3.41	111.56	114.00
2	D	500	HEM	C3A-C4A-NA	3.38	111.96	109.41
2	A	500	HEM	C3A-C4A-NA	3.37	111.96	109.41
2	C	500	HEM	C4A-CHB-C1B	3.25	131.75	127.47
2	A	500	HEM	C3B-C4B-NB	-3.19	111.72	114.00
2	A	500	HEM	C4D-ND-C1D	3.13	108.36	105.16
2	B	500	HEM	C1B-NB-C4B	3.12	108.35	105.16
2	B	500	HEM	C3A-C4A-NA	3.08	111.74	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	HEM	C4A-CHB-C1B	3.08	131.53	127.47
2	D	500	HEM	C4D-ND-C1D	3.07	108.30	105.16
2	C	500	HEM	CHC-C1C-NC	-3.04	122.09	124.73
2	B	500	HEM	C4D-ND-C1D	3.04	108.27	105.16
2	C	500	HEM	C1B-NB-C4B	2.99	108.22	105.16
2	C	500	HEM	C4D-ND-C1D	2.97	108.20	105.16
2	C	500	HEM	C3A-C4A-NA	2.94	111.63	109.41
2	B	500	HEM	CHB-C1B-NB	-2.89	120.34	124.31
2	A	500	HEM	C1B-NB-C4B	2.75	107.97	105.16
2	A	500	HEM	CHB-C1B-NB	-2.70	120.59	124.31
2	D	500	HEM	C4A-CHB-C1B	2.69	131.01	127.47
2	B	500	HEM	C4A-CHB-C1B	2.69	131.01	127.47
2	C	500	HEM	CHC-C4B-NB	-2.68	122.36	124.58
2	A	500	HEM	C2D-C1D-ND	-2.62	109.84	112.93
2	A	500	HEM	CHC-C4B-NB	-2.58	122.44	124.58
2	A	500	HEM	CMA-C3A-C4A	-2.54	124.72	128.62
2	D	500	HEM	CHC-C1C-NC	-2.52	122.54	124.73
2	B	500	HEM	C2D-C1D-ND	-2.45	110.04	112.93
2	D	500	HEM	CHC-C4B-NB	-2.43	122.57	124.58
2	B	500	HEM	CHC-C4B-NB	-2.42	122.57	124.58
2	A	500	HEM	C4C-NC-C1C	2.40	108.03	105.53
2	D	500	HEM	C2D-C1D-ND	-2.34	110.16	112.93
2	D	500	HEM	C4C-NC-C1C	2.24	107.86	105.53
2	A	500	HEM	CHC-C1C-NC	-2.23	122.79	124.73
2	C	500	HEM	C2D-C1D-ND	-2.23	110.30	112.93
2	D	500	HEM	CMA-C3A-C4A	-2.15	125.32	128.62
2	D	500	HEM	O2A-CGA-CBA	2.14	121.77	114.22
2	B	500	HEM	CMA-C3A-C4A	-2.11	125.38	128.62
2	B	500	HEM	C4C-NC-C1C	2.08	107.69	105.53
2	C	500	HEM	CBA-CAA-C2A	2.05	116.31	112.69
2	A	500	HEM	CMA-C3A-C2A	2.05	128.81	124.94
2	A	500	HEM	CAD-C3D-C4D	2.05	128.21	124.53
2	A	500	HEM	C1A-C2A-C3A	-2.04	104.81	106.92
2	A	500	HEM	O2A-CGA-CBA	2.03	121.41	114.22
2	A	500	HEM	C4B-CHC-C1C	2.03	131.91	126.57
2	C	500	HEM	CAD-C3D-C4D	2.01	128.14	124.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<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	464/476 (97%)	-0.20	2 (0%) 90 91	21, 48, 81, 107	1 (0%)
1	B	464/476 (97%)	-0.08	10 (2%) 59 60	24, 53, 86, 136	0
1	C	464/476 (97%)	-0.17	2 (0%) 90 91	22, 49, 81, 120	0
1	D	464/476 (97%)	-0.14	6 (1%) 74 75	23, 50, 79, 134	0
All	All	1856/1904 (97%)	-0.15	20 (1%) 77 78	21, 50, 82, 136	1 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	338	ASN	4.5
1	C	31	GLY	4.2
1	D	143	ARG	3.4
1	A	305	THR	2.8
1	D	307	SER	2.7
1	B	264	PRO	2.5
1	B	305	THR	2.5
1	B	138	PHE	2.4
1	B	495	HIS	2.4
1	D	310	LEU	2.4
1	D	196	LYS	2.2
1	D	306	VAL	2.2
1	D	283	ASN	2.2
1	B	141	GLY	2.2
1	B	142	LYS	2.2
1	B	378	THR	2.1
1	B	379	LYS	2.1
1	B	282	PRO	2.0
1	A	309	THR	2.0
1	B	288	LEU	2.0

## 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<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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	HEM	B	500	43/43	0.28	1.14	48,48,48,48	0
2	HEM	C	500	43/43	0.24	1.02	48,48,48,48	0
2	HEM	A	500	43/43	0.26	0.83	48,48,48,48	0
2	HEM	D	500	43/43	0.23	0.33	48,48,48,48	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.