



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:03 PM GMT

PDB ID : 4H1N  
Title : Crystal Structure of P450 2B4 F297A Mutant in Complex with Anti-platelet Drug Clopidogrel  
Authors : Shah, M.B.; Jang, H.H.; Stout, C.D.; Halpert, J.R.  
Deposited on : 2012-09-10  
Resolution : 2.99 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 (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

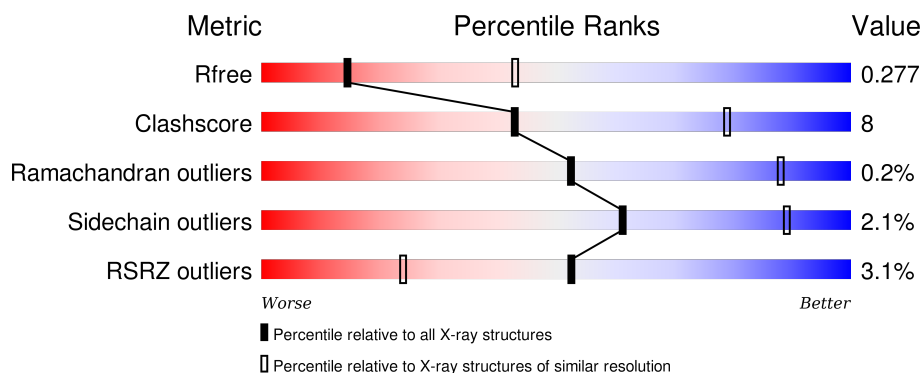
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	479	<div> <div>3%</div> <div>81%</div> <div>14%</div> <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	CM5	A	504	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3766 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 2B4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	459	3621	2332	620	659	10	0	1	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
A	?	-	PHE	DELETION	UNP P00178
A	?	-	SER	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	ALA	DELETION	UNP P00178
A	?	-	PHE	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	ALA	DELETION	UNP P00178
A	?	-	GLY	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	PHE	DELETION	UNP P00178
A	?	-	ARG	DELETION	UNP P00178
A	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178
A	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
A	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
A	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
A	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
A	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
A	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178

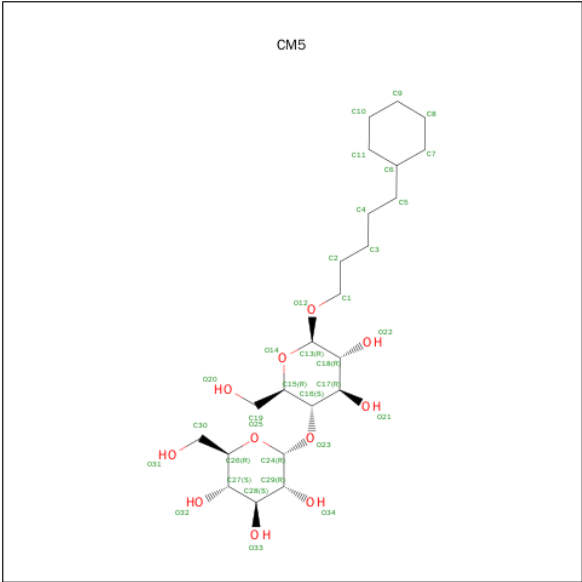
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Chain	Residue	Modelled	Actual	Comment	Reference
A	221	SER	PRO	SEE REMARK 999	UNP P00178
A	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
A	297	ALA	PHE	ENGINEERED MUTATION	UNP P00178
A	492	HIS	-	EXPRESSION TAG	UNP P00178
A	493	HIS	-	EXPRESSION TAG	UNP P00178
A	494	HIS	-	EXPRESSION TAG	UNP P00178
A	495	HIS	-	EXPRESSION TAG	UNP P00178
A	496	HIS	-	EXPRESSION TAG	UNP P00178
A	497	HIS	-	EXPRESSION TAG	UNP P00178
A	498	HIS	-	EXPRESSION TAG	UNP P00178

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- Chemical structure of HEM (Heme) showing a central iron atom coordinated by four nitrogen atoms in a porphyrin-like ring, with various side chains and a central heme group.

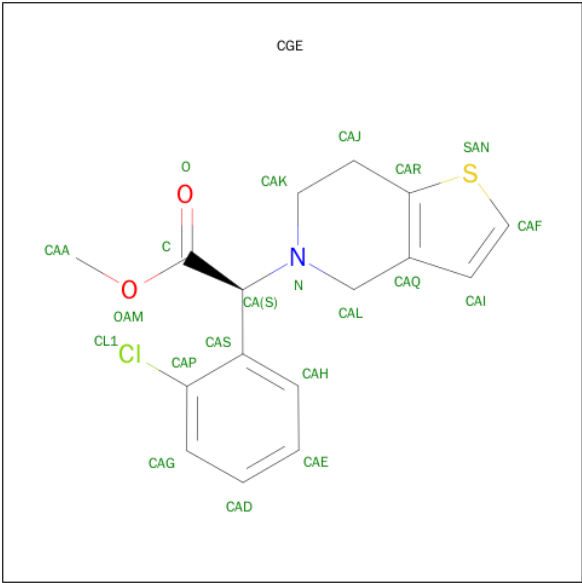
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			12	11	1		
3	A	1	Total	C	O	0	0
			34	23	11		

- Molecule 4 is CLOPIDOGREL (three-letter code: CGE) (formula: C<sub>16</sub>H<sub>16</sub>ClNO<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	Cl	N	O	S	0	0
			21	16	1	1	2	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

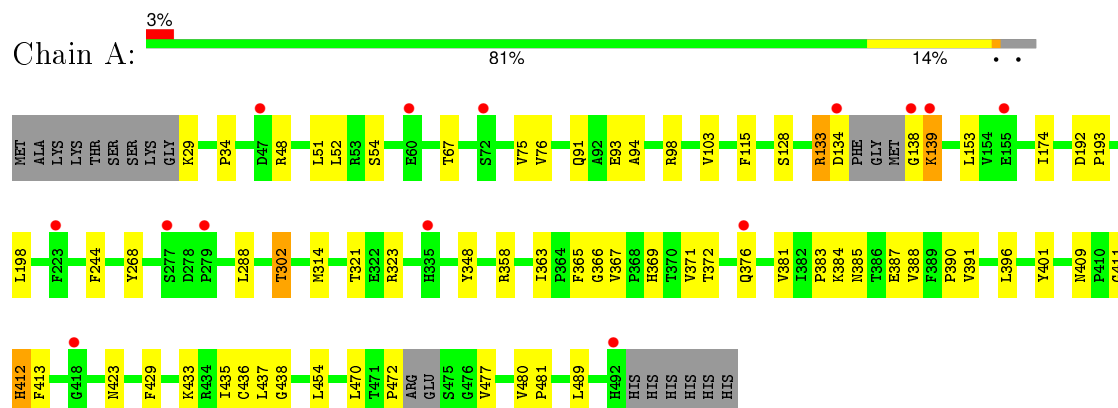
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total	O	0	0
			19	19		

### 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 ( $\text{RSRZ} > 2$ ). 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 2B4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.39Å 91.39Å 152.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.99 19.94 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.99) 99.7 (19.94-2.99)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.233 , 0.286 0.247 , 0.277	Depositor DCC
$R_{free}$ test set	777 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	83.5	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.8	EDS
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 15327 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3766	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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, 0.375 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: HEM, CM5, CGE, 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	0.42	0/3711	0.53	0/5038

There are no bond length outliers.

There are no bond angle outliers.

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	3621	0	3546	55	0
2	A	43	0	30	3	0
3	A	57	0	68	6	0
4	A	21	0	16	5	0
5	A	5	0	0	0	0
6	A	19	0	0	0	0
All	All	3766	0	3660	61	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 8.

All (61) 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:75:VAL:HG12	1:A:387:GLU:HB2	1.41	0.98
3:A:504:CM5:C24	3:A:504:CM5:H192	2.05	0.86
1:A:139:LYS:O	1:A:139:LYS:HD2	1.76	0.85
1:A:381:VAL:O	1:A:383:PRO:HD3	1.76	0.84
1:A:244:PHE:CE2	3:A:504:CM5:O12	2.32	0.82
1:A:139:LYS:CD	1:A:139:LYS:O	2.32	0.78
1:A:198:LEU:HD12	3:A:504:CM5:H22A	1.66	0.76
3:A:504:CM5:H24	3:A:504:CM5:H192	1.68	0.73
1:A:391:VAL:O	1:A:391:VAL:HG12	1.92	0.69
1:A:93:GLU:OE1	1:A:433:LYS:HE3	1.99	0.62
1:A:133:ARG:O	1:A:134:ASP:CG	2.37	0.62
1:A:477:VAL:HB	4:A:505:CGE:HAD	1.80	0.62
1:A:98:ARG:HG2	1:A:115:PHE:HA	1.82	0.62
1:A:75:VAL:CG1	1:A:387:GLU:HB2	2.26	0.58
1:A:76:VAL:HB	1:A:388:VAL:HG22	1.86	0.58
1:A:98:ARG:NH2	2:A:501:HEM:O2D	2.33	0.57
1:A:401:TYR:HB3	1:A:423:ASN:OD1	2.05	0.55
1:A:358:ARG:HD3	1:A:396:LEU:O	2.07	0.54
1:A:51:LEU:O	1:A:54:SER:N	2.39	0.54
1:A:268:TYR:CE1	1:A:288:LEU:HB2	2.44	0.53
1:A:51:LEU:O	1:A:54:SER:HB2	2.08	0.53
1:A:363:ILE:HG22	1:A:366:GLY:HA2	1.91	0.53
1:A:384:LYS:O	1:A:385:ASN:HB2	2.09	0.52
1:A:91:GLN:NE2	1:A:376:GLN:O	2.42	0.52
1:A:133:ARG:O	1:A:134:ASP:OD1	2.28	0.51
1:A:388:VAL:O	1:A:390:PRO:HD3	2.10	0.51
1:A:138:GLY:O	1:A:139:LYS:HB3	2.11	0.51
1:A:429:PHE:HB3	1:A:436:CYS:HB3	1.93	0.50
1:A:323:ARG:HB3	1:A:348:TYR:CE2	2.47	0.49
3:A:504:CM5:H192	3:A:504:CM5:O25	2.11	0.49
1:A:371:VAL:HG23	1:A:384:LYS:HA	1.95	0.48
1:A:369:HIS:HE1	2:A:501:HEM:O2A	1.97	0.47
4:A:505:CGE:HAK	4:A:505:CGE:CAH	2.44	0.47
1:A:314:MET:HB3	1:A:321:THR:HG21	1.95	0.47
1:A:383:PRO:O	1:A:384:LYS:C	2.53	0.47
1:A:302:THR:HG21	1:A:363:ILE:HD11	1.95	0.47
1:A:29:LYS:HG3	1:A:381:VAL:HB	1.97	0.47
4:A:505:CGE:CAK	4:A:505:CGE:CAH	2.93	0.47
1:A:314:MET:HB3	1:A:321:THR:CG2	2.45	0.46
1:A:314:MET:SD	1:A:454:LEU:HD11	2.55	0.46
1:A:409:ASN:HB3	1:A:412:HIS:CE1	2.52	0.45
1:A:93:GLU:O	1:A:94:ALA:C	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:505:CGE:HAH	4:A:505:CGE:CAK	2.46	0.45
1:A:153:LEU:HD22	1:A:174:ILE:HG21	1.98	0.44
1:A:365:PHE:HA	1:A:391:VAL:HA	2.00	0.44
1:A:34:PRO:HD2	1:A:67:THR:O	2.17	0.44
1:A:438:GLY:HA3	2:A:501:HEM:C3C	2.53	0.43
1:A:138:GLY:O	1:A:139:LYS:CB	2.66	0.43
1:A:128:SER:HB2	1:A:437:LEU:HD21	2.01	0.43
1:A:139:LYS:CG	1:A:139:LYS:O	2.67	0.43
1:A:51:LEU:O	1:A:52:LEU:C	2.57	0.43
1:A:139:LYS:HD3	1:A:139:LYS:HA	1.46	0.42
1:A:94:ALA:O	1:A:371:VAL:HA	2.18	0.42
1:A:192:ASP:HA	1:A:193:PRO:HD3	1.85	0.42
1:A:372:THR:O	1:A:384:LYS:HG3	2.18	0.42
1:A:472:PRO:HB3	1:A:481:PRO:HA	2.02	0.41
1:A:48:ARG:HA	3:A:503:CM5:H72	2.01	0.41
1:A:93:GLU:OE1	1:A:433:LYS:CE	2.66	0.41
1:A:367:VAL:HG21	4:A:505:CGE:CAA	2.51	0.41
1:A:411:GLY:O	1:A:413:PHE:N	2.55	0.40
1:A:358:ARG:CD	1:A:396:LEU:O	2.68	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	454/479 (95%)	427 (94%)	26 (6%)	1 (0%)	52 88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	HIS

### 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	390/423 (92%)	382 (98%)	8 (2%)	61 89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	VAL
1	A	133	ARG
1	A	139	LYS
1	A	302	THR
1	A	435	ILE
1	A	470	LEU
1	A	480	VAL
1	A	489	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

6 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	501	1	30,50,50	2.05	5 (16%)	24,82,82	2.40	10 (41%)
3	CM5	A	502	-	11,11,36	2.11	2 (18%)	14,15,49	4.03	7 (50%)
3	CM5	A	503	-	12,12,36	0.57	0	13,13,49	0.61	0
3	CM5	A	504	-	36,36,36	1.78	8 (22%)	49,49,49	3.41	18 (36%)
4	CGE	A	505	-	19,23,23	1.85	3 (15%)	19,32,32	2.59	4 (21%)
5	SO4	A	506	-	4,4,4	1.02	0	6,6,6	0.26	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	501	1	-	0/10/54/54	0/0/8/8
3	CM5	A	502	-	-	0/2/19/65	0/1/1/3
3	CM5	A	503	-	-	0/6/14/65	0/1/1/3
3	CM5	A	504	-	-	0/17/65/65	0/3/3/3
4	CGE	A	505	-	-	0/14/23/23	0/3/3/3
5	SO4	A	506	-	-	0/0/0/0	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3B-C4B	-6.81	1.45	1.51
4	A	505	CGE	CAJ-CAR	-6.61	1.45	1.50
3	A	504	CM5	C30-C26	-5.09	1.33	1.51
2	A	501	HEM	C3D-C4D	-4.70	1.45	1.51
3	A	504	CM5	O12-C13	-4.02	1.32	1.40
3	A	502	CM5	O21-C17	-3.84	1.33	1.43
2	A	501	HEM	C2C-C1C	-3.66	1.45	1.52
3	A	504	CM5	O21-C17	-2.36	1.37	1.43
2	A	501	HEM	C3C-CAC	2.02	1.55	1.51
3	A	504	CM5	O25-C24	2.04	1.47	1.41
3	A	504	CM5	O23-C24	2.18	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	505	CGE	CAF-SAN	2.22	1.81	1.70
2	A	501	HEM	FE-ND	2.66	2.11	1.97
3	A	504	CM5	C17-C18	2.84	1.59	1.52
4	A	505	CGE	CAI-CAF	3.07	1.49	1.37
3	A	504	CM5	O34-C29	3.19	1.50	1.43
3	A	504	CM5	O23-C16	3.38	1.52	1.43
3	A	502	CM5	C18-C17	5.22	1.59	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	CM5	C19-C15-C16	-11.31	85.11	113.02
3	A	504	CM5	O22-C18-C17	-8.51	91.19	110.34
4	A	505	CGE	CAL-CAQ-CAI	-7.33	119.80	127.31
3	A	504	CM5	C24-O23-C16	-4.38	106.55	118.01
3	A	504	CM5	C1-O12-C13	-4.24	106.54	113.94
4	A	505	CGE	O-C-CA	-4.11	119.80	125.30
3	A	504	CM5	C19-C15-C16	-3.95	101.74	113.25
3	A	502	CM5	C13-C18-C17	-3.70	105.16	109.54
2	A	501	HEM	CAA-CBA-CGA	-3.53	106.28	112.75
3	A	504	CM5	O12-C13-C18	-3.45	103.68	108.04
3	A	502	CM5	O22-C18-C17	-3.43	103.23	110.12
2	A	501	HEM	C3B-CAB-CBB	-3.25	119.48	124.46
3	A	504	CM5	C13-C18-C17	-2.36	105.32	109.97
2	A	501	HEM	CBD-CAD-C3D	-2.31	106.84	113.55
3	A	504	CM5	O23-C16-C17	2.07	112.51	107.17
2	A	501	HEM	C2D-C3D-C4D	2.20	105.23	101.50
3	A	502	CM5	O23-C16-C15	2.22	115.12	109.24
2	A	501	HEM	C3B-C4B-CHC	2.52	126.71	123.16
3	A	504	CM5	O21-C17-C16	2.72	116.30	109.87
2	A	501	HEM	CMD-C2D-C3D	2.75	126.52	114.35
3	A	504	CM5	O23-C16-C15	2.79	116.66	109.32
4	A	505	CGE	CAA-OAM-C	2.81	122.59	115.99
3	A	502	CM5	C18-C17-C16	2.93	116.02	111.04
3	A	504	CM5	C30-C26-C27	3.15	120.78	113.02
3	A	504	CM5	C3-C2-C1	3.49	129.06	113.47
2	A	501	HEM	CMB-C2B-C3B	4.00	126.51	116.53
2	A	501	HEM	CAD-C3D-C4D	4.39	127.96	112.47
3	A	504	CM5	C17-C16-C15	4.54	121.11	110.84
2	A	501	HEM	CMC-C2C-C3C	4.54	127.87	116.53
3	A	502	CM5	O21-C17-C18	4.61	118.32	110.00
3	A	504	CM5	O32-C27-C26	4.62	121.48	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CAD-C3D-C2D	4.73	126.80	113.22
3	A	502	CM5	O21-C17-C16	5.57	122.88	110.34
3	A	504	CM5	O25-C26-C30	5.73	120.84	106.36
4	A	505	CGE	OAM-C-CA	5.97	120.42	110.83
3	A	504	CM5	O32-C27-C28	6.14	124.16	110.34
3	A	504	CM5	O34-C29-C24	7.68	126.85	110.02
3	A	504	CM5	O12-C1-C2	8.76	144.72	109.88
3	A	504	CM5	O14-C13-O12	11.04	136.63	110.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	3	0
3	A	503	CM5	1	0
3	A	504	CM5	5	0
4	A	505	CGE	5	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	459/479 (95%)	0.06	14 (3%)	52 24	25, 78, 100, 106	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	138	GLY	5.0
1	A	277	SER	3.1
1	A	279	PRO	3.0
1	A	376	GLN	3.0
1	A	72	SER	2.9
1	A	60	GLU	2.8
1	A	134	ASP	2.8
1	A	335	HIS	2.6
1	A	492	HIS	2.6
1	A	139	LYS	2.3
1	A	155	GLU	2.3
1	A	47	ASP	2.2
1	A	418	GLY	2.2
1	A	223	PHE	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.



## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CM5	A	504	34/34	0.70	0.43	3.72	125,132,134,135	0
4	CGE	A	505	21/21	0.84	0.26	2.00	109,110,111,111	0
3	CM5	A	503	12/34	0.83	0.27	0.52	84,85,85,85	0
2	HEM	A	501	43/43	0.97	0.15	-0.73	51,56,60,61	0
3	CM5	A	502	11/34	0.82	0.44	-	110,111,111,111	0
5	SO4	A	506	5/5	0.94	0.25	-	114,114,114,115	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.