



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:10 PM GMT

PDB ID : 4HGF  
Title : Crystal structure of P450 BM3 5F5K heme domain variant complexed with styrene  
Authors : Shehzad, A.; Panneerselvam, S.; Bocola, M.; Mueller-Dieckmann, J.; Wilmanns, M.; Schwaneberg, U.  
Deposited on : 2012-10-08  
Resolution : 1.70 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.

---

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

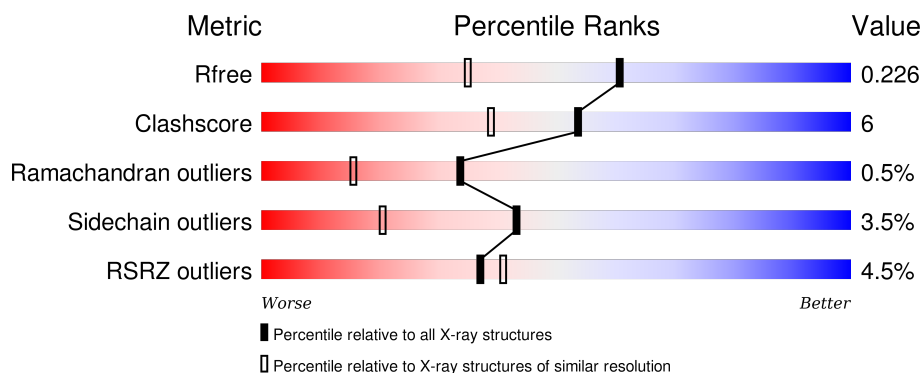
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	455	 4% 82% 13% . .
1	B	455	 4% 84% 11% . .

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	SYN	A	502	-	-	-	X
3	SYN	B	502	-	-	X	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8178 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.

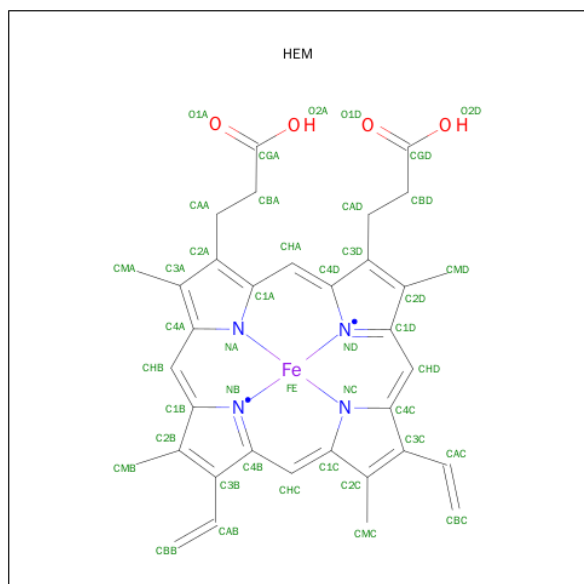
- Molecule 1 is a protein called Bifunctional P-450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	9	0
			3607	2314	608	668	17			
1	B	441	Total	C	N	O	S	0	8	0
			3599	2303	609	669	18			

There are 6 discrepancies between the modelled and reference sequences:

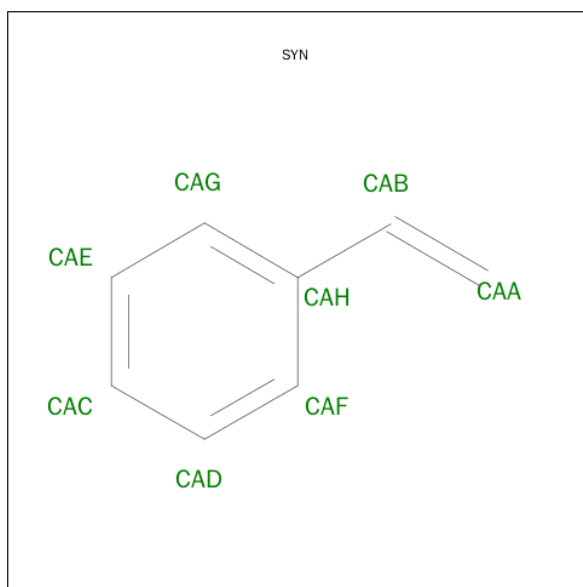
Chain	Residue	Modelled	Actual	Comment	Reference
A	87	ALA	PHE	ENGINEERED MUTATION	UNP P14779
A	184	LYS	ALA	ENGINEERED MUTATION	UNP P14779
A	235	ALA	THR	ENGINEERED MUTATION	UNP P14779
B	87	ALA	PHE	ENGINEERED MUTATION	UNP P14779
B	184	LYS	ALA	ENGINEERED MUTATION	UNP P14779
B	235	ALA	THR	ENGINEERED MUTATION	UNP P14779

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

- Molecule 3 is ETHENYLBENZENE (three-letter code: SYN) (formula: C<sub>8</sub>H<sub>8</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C		
			8	8	0	0
3	B	1	Total	C		
			8	8	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl		
			1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	423	Total	O		
			423	423	0	0
5	B	446	Total	O		
			446	446	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.14Å 148.12Å 64.07Å 90.00° 98.16° 90.00°	Depositor
Resolution (Å)	19.51 – 1.70 19.51 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.51-1.70) 98.4 (19.51-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.189 , 0.228 0.189 , 0.226	Depositor DCC
$R_{free}$ test set	824 reflections (0.71%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 55.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 117395 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8178	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% 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, SYN, CL

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	1.19	2/3714 (0.1%)	1.05	10/5012 (0.2%)
1	B	1.20	2/3700 (0.1%)	1.05	10/4993 (0.2%)
All	All	1.20	4/7414 (0.1%)	1.05	20/10005 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	TRP	CD2-CE2	5.84	1.48	1.41
1	A	130	TRP	CD2-CE2	5.64	1.48	1.41
1	B	244	GLU	CG-CD	5.45	1.60	1.51
1	B	256	TYR	CG-CD2	5.11	1.45	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	MET	CG-SD-CE	5.87	109.60	100.20
1	A	161	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	398	ARG	NE-CZ-NH1	-5.71	117.45	120.30
1	B	237	MET	CG-SD-CE	5.64	109.23	100.20
1	A	232	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	296	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	356	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	B	280	LEU	CB-CG-CD2	5.48	120.32	111.00
1	A	233	LEU	CB-CG-CD2	5.47	120.30	111.00
1	B	353	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	B	66	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	B	398	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	B	250	ASP	CB-CG-OD1	5.19	122.97	118.30
1	B	249	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	A	71	LEU	CB-CG-CD2	-5.11	102.31	111.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	444	PHE	CB-CG-CD2	-5.08	117.25	120.80
1	B	151	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	B	244	GLU	OE1-CD-OE2	-5.02	117.28	123.30
1	A	250	ASP	CB-CG-OD1	5.01	122.81	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	3607	0	3636	47	0
1	B	3599	0	3603	45	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	8	0	8	3	0
3	B	8	0	7	4	0
4	A	1	0	0	0	0
5	A	423	0	0	10	0
5	B	446	0	0	13	0
All	All	8178	0	7314	95	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 6.

All (95) 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:370:ASP:OD2	1:A:375:ARG:NH1	1.91	1.03
1:A:128:GLN:HG3	5:B:604:HOH:O	1.59	1.01
1:B:128:GLN:NE2	5:B:1003:HOH:O	1.92	0.98
1:B:183:GLU:OE1	1:B:201:ASN:HB3	1.71	0.90
1:A:267[B]:GLU:HG2	1:A:438:THR:HG21	1.54	0.89
1:A:199:ASP:O	1:A:202:LYS:HD3	1.74	0.87

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:MET:HG2	5:A:941:HOH:O	1.73	0.87
1:B:128:GLN:HG2	5:B:1004:HOH:O	1.77	0.85
1:A:310:GLN:HG3	5:A:899:HOH:O	1.78	0.82
1:A:43:GLU:HG2	1:A:48[B]:VAL:HG12	1.61	0.82
1:A:267[B]:GLU:CG	1:A:438:THR:HG21	2.13	0.78
1:B:204:GLN:HA	1:B:204:GLN:NE2	2.00	0.75
1:A:267[B]:GLU:HG2	1:A:438:THR:CG2	2.16	0.75
1:B:222:ASP:OD2	5:B:885:HOH:O	2.05	0.75
1:B:183:GLU:HG3	1:B:183:GLU:O	1.86	0.75
1:A:179:ARG:CD	1:A:204:GLN:OE1	2.35	0.74
1:B:226:SER:C	1:B:228:GLU:H	1.95	0.70
1:B:182:ASP:C	1:B:184:LYS:H	1.95	0.69
1:A:229:GLN:HA	1:A:229:GLN:OE1	1.93	0.67
1:A:309:LYS:O	1:A:312[B]:LYS:HE3	1.95	0.67
1:B:31[A]:LYS:HD2	5:B:811:HOH:O	1.95	0.66
1:A:179:ARG:HD2	1:A:204:GLN:OE1	1.95	0.66
1:A:212:MET:SD	5:A:1005:HOH:O	2.54	0.66
1:B:204:GLN:HA	1:B:204:GLN:HE21	1.59	0.64
3:B:502:SYN:H8	5:B:1046:HOH:O	1.97	0.64
1:A:183:GLU:HG2	1:A:205:PHE:HB2	1.79	0.64
1:B:224:LYS:HZ3	1:B:225:ALA:HB2	1.63	0.64
1:A:183:GLU:HG3	1:A:183:GLU:O	1.98	0.64
1:A:147:ARG:HG2	1:A:164[B]:SER:OG	1.98	0.63
1:A:199:ASP:N	1:A:199:ASP:OD2	2.30	0.63
1:A:177:MET:HG2	1:A:212:MET:HE1	1.81	0.62
1:B:183:GLU:OE1	1:B:201:ASN:CB	2.47	0.61
3:A:502:SYN:H8	5:A:874:HOH:O	2.01	0.60
1:B:303:PRO:HG3	5:B:883:HOH:O	2.01	0.60
1:B:404:GLN:HG3	5:B:1024:HOH:O	2.02	0.60
1:A:7:GLN:HB2	1:A:41[A]:LYS:HG3	1.83	0.59
1:A:264:ALA:O	3:A:502:SYN:H9	2.02	0.59
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.86	0.58
1:B:224:LYS:NZ	1:B:225:ALA:HB2	2.19	0.57
1:B:74:ALA:O	1:B:78:VAL:HG23	2.05	0.57
1:B:80:ASP:HB2	1:B:184:LYS:NZ	2.20	0.55
1:B:182:ASP:C	1:B:184:LYS:N	2.59	0.55
1:A:316:MET:CE	1:A:380:GLU:HG3	2.36	0.55
1:A:272:LEU:HD13	1:A:322:LEU:HG	1.87	0.55
1:B:306:LYS:HG2	5:B:844:HOH:O	2.06	0.55
1:B:109:GLN:OE1	1:B:305:TYR:OH	2.18	0.55
1:A:316:MET:HE1	1:A:380:GLU:HG3	1.87	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ALA:HB1	3:B:502:SYN:H4	1.90	0.54
1:A:182:ASP:C	1:A:184:LYS:H	2.11	0.54
1:A:201:ASN:OD1	1:A:201:ASN:N	2.40	0.53
1:B:226:SER:C	1:B:228:GLU:N	2.62	0.53
1:B:35:GLU:HG3	5:B:979:HOH:O	2.08	0.53
1:A:296:ARG:NH2	5:A:849:HOH:O	2.38	0.53
1:A:267[B]:GLU:CG	1:A:438:THR:CG2	2.84	0.51
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.91	0.51
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.93	0.51
1:B:136[A]:ASP:O	1:B:136[A]:ASP:OD2	2.29	0.50
1:B:182:ASP:O	1:B:184:LYS:N	2.39	0.50
1:B:226:SER:O	1:B:228:GLU:N	2.45	0.50
1:B:101:ASN:HD21	1:B:244:GLU:CD	2.15	0.49
1:B:370:ASP:OD2	1:B:375[B]:ARG:NH1	2.41	0.49
1:B:53:SER:HB3	1:B:359:GLN:HB3	1.94	0.49
1:A:94[B]:LYS:HE3	5:A:784:HOH:O	2.12	0.49
1:A:7:GLN:HB2	1:A:41[A]:LYS:HE2	1.95	0.49
1:A:204:GLN:HG3	1:A:205:PHE:N	2.27	0.49
3:B:502:SYN:H8	5:B:821:HOH:O	2.14	0.48
1:B:287:LEU:HD23	1:B:287:LEU:C	2.34	0.47
1:B:209:ILE:HA	1:B:209:ILE:HD13	1.70	0.47
1:A:81:PHE:HE2	1:A:209:ILE:HD11	1.80	0.47
1:A:47:ARG:NH2	5:A:767:HOH:O	2.48	0.46
5:A:855:HOH:O	1:B:218:LYS:HE2	2.15	0.46
1:A:264:ALA:O	3:A:502:SYN:CAA	2.63	0.46
1:A:222:ASP:OD2	5:A:824:HOH:O	2.21	0.46
1:A:205:PHE:HD2	1:A:206:GLN:HG2	1.79	0.45
1:A:177:MET:HG2	1:A:212:MET:CE	2.44	0.45
1:A:200:GLU:O	1:A:202:LYS:N	2.47	0.45
1:A:170:PRO:HA	5:A:873:HOH:O	2.18	0.44
1:B:31[A]:LYS:HE2	1:B:31[A]:LYS:HB3	1.40	0.44
1:A:41[B]:LYS:CB	1:A:41[B]:LYS:NZ	2.81	0.44
1:B:81:PHE:HE1	1:B:209:ILE:HD11	1.83	0.43
1:A:182:ASP:O	1:A:184:LYS:N	2.52	0.43
1:A:74:ALA:O	1:A:78:VAL:HG23	2.18	0.43
1:A:124:VAL:HG13	1:A:455:LEU:HD13	2.01	0.42
1:B:51:TYR:HD2	1:B:356:LEU:HD13	1.85	0.42
1:B:62:CYS:SG	1:B:391:LYS:HE2	2.59	0.42
1:A:2:ILE:HG13	1:A:346:PRO:HG3	2.02	0.42
1:B:31[A]:LYS:NZ	5:B:716:HOH:O	2.52	0.42
1:B:183:GLU:CG	1:B:183:GLU:O	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ALA:O	3:B:502:SYN:CAA	2.68	0.42
1:B:370:ASP:OD2	1:B:375[B]:ARG:NH2	2.49	0.41
1:A:439:LEU:O	1:A:440[A]:LYS:HG2	2.20	0.41
1:B:52:LEU:HD11	1:B:353:LEU:HD13	2.02	0.41
1:B:380:GLU:HB3	5:B:769:HOH:O	2.20	0.41
1:B:179:ARG:HG3	1:B:179:ARG:HH11	1.86	0.41
1:B:120:VAL:HG11	1:B:302:VAL:CG1	2.52	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	447/455 (98%)	436 (98%)	9 (2%)	2 (0%)	39	20
1	B	445/455 (98%)	429 (96%)	14 (3%)	2 (0%)	39	20
All	All	892/910 (98%)	865 (97%)	23 (3%)	4 (0%)	34	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	GLU
1	B	183	GLU
1	B	227	GLY
1	A	370	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	396/398 (100%)	380 (96%)	16 (4%)	38	16
1	B	394/398 (99%)	382 (97%)	12 (3%)	48	26
All	All	790/796 (99%)	762 (96%)	28 (4%)	43	20

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	59	LYS
1	A	148	LEU
1	A	179	ARG
1	A	182	ASP
1	A	184	LYS
1	A	199	ASP
1	A	201	ASN
1	A	203	ARG
1	A	204	GLN
1	A	207	GLU
1	A	210	LYS
1	A	226	SER
1	A	233	LEU
1	A	302	VAL
1	A	369	ASP
1	B	2	ILE
1	B	31[A]	LYS
1	B	31[B]	LYS
1	B	41	LYS
1	B	110	GLN
1	B	148	LEU
1	B	184	LYS
1	B	200	GLU
1	B	224	LYS
1	B	226	SER
1	B	228	GLU
1	B	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	403	GLN
1	B	101	ASN
1	B	110	GLN
1	B	236	HIS

### 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 ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	2.24	8 (26%)	24,82,82	2.51	10 (41%)
3	SYN	A	502	-	8,8,8	1.95	3 (37%)	9,9,9	0.85	0
2	HEM	B	501	1	30,50,50	2.15	7 (23%)	24,82,82	2.71	12 (50%)
3	SYN	B	502	-	8,8,8	1.70	2 (25%)	9,9,9	0.94	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	SYN	A	502	-	-	0/2/2/2	0/1/1/1
2	HEM	B	501	1	-	0/10/54/54	0/0/8/8
3	SYN	B	502	-	-	0/2/2/2	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3B-C4B	-7.67	1.45	1.51
2	B	501	HEM	C3B-C4B	-7.57	1.45	1.51
2	A	501	HEM	C3D-C4D	-5.21	1.44	1.51
2	B	501	HEM	C3D-C4D	-4.47	1.45	1.51
2	A	501	HEM	C2C-C1C	-3.79	1.45	1.52
2	A	501	HEM	C2D-C1D	-2.83	1.42	1.51
2	A	501	HEM	C2B-C1B	-2.37	1.44	1.51
2	B	501	HEM	C2C-C1C	-2.32	1.48	1.52
2	A	501	HEM	C2D-C3D	-2.26	1.47	1.54
2	B	501	HEM	C2D-C1D	-2.22	1.44	1.51
3	A	502	SYN	CAH-CAB	-2.06	1.41	1.49
3	B	502	SYN	CAH-CAB	-2.04	1.41	1.49
3	A	502	SYN	CAE-CAG	2.27	1.43	1.38
2	B	501	HEM	FE-ND	2.31	2.09	1.97
2	A	501	HEM	FE-NB	2.62	2.11	1.97
2	B	501	HEM	FE-NB	2.99	2.13	1.97
2	A	501	HEM	FE-ND	3.00	2.13	1.97
3	B	502	SYN	CAA-CAB	3.68	1.55	1.28
2	B	501	HEM	FE-NC	3.82	2.10	1.95
3	A	502	SYN	CAA-CAB	3.88	1.57	1.28

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C2C-C1C-NC	-3.52	104.28	110.21
2	B	501	HEM	C3B-C4B-NB	-3.50	104.93	111.63
2	A	501	HEM	C3C-CAC-CBC	-3.09	119.72	124.46
2	A	501	HEM	CBD-CAD-C3D	-2.77	105.51	113.55
2	B	501	HEM	CMA-C3A-C4A	-2.74	123.83	128.36
2	A	501	HEM	C3B-C4B-NB	-2.16	107.50	111.63
2	B	501	HEM	CHD-C1D-ND	2.11	129.61	124.52
2	B	501	HEM	C2D-C3D-C4D	2.28	105.36	101.50
2	B	501	HEM	C2C-C1C-CHC	2.66	127.73	123.68
2	B	501	HEM	C3B-C4B-CHC	2.80	127.10	123.16
2	A	501	HEM	CMD-C2D-C3D	3.13	128.21	114.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CMD-C2D-C3D	3.34	129.14	114.35
2	A	501	HEM	C2D-C3D-C4D	3.42	107.30	101.50
2	A	501	HEM	C3B-C4B-CHC	3.52	128.12	123.16
2	A	501	HEM	CAD-C3D-C2D	4.07	124.92	113.22
2	B	501	HEM	CAD-C3D-C4D	4.16	127.15	112.47
2	A	501	HEM	CAD-C3D-C4D	4.34	127.78	112.47
2	A	501	HEM	CMB-C2B-C3B	4.56	127.91	116.53
2	B	501	HEM	CMC-C2C-C3C	4.74	128.37	116.53
2	A	501	HEM	CMC-C2C-C3C	4.84	128.62	116.53
2	B	501	HEM	CAD-C3D-C2D	4.96	127.48	113.22
2	B	501	HEM	CMB-C2B-C3B	5.23	129.59	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	SYN	3	0
3	B	502	SYN	4	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	442/455 (97%)	-0.08	20 (4%) 37 41	9, 15, 50, 125	1 (0%)
1	B	441/455 (96%)	-0.03	20 (4%) 37 41	9, 16, 44, 104	0
All	All	883/910 (97%)	-0.05	40 (4%) 37 41	9, 16, 49, 125	1 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ILE	7.3
1	B	185	MET	6.3
1	B	227	GLY	5.8
1	A	199	ASP	5.3
1	A	2	ILE	5.1
1	B	229	GLN	5.0
1	B	228	GLU	4.4
1	A	229	GLN	4.1
1	A	77	PHE	4.0
1	A	1	THR	4.0
1	A	200	GLU	4.0
1	A	182	ASP	3.7
1	A	185	MET	3.6
1	B	46	GLY	3.6
1	A	202	LYS	3.5
1	A	180	ALA	3.5
1	A	227	GLY	3.5
1	A	228	GLU	3.4
1	B	199	ASP	3.4
1	B	77	PHE	3.3
1	A	170	PRO	3.3
1	B	200	GLU	3.1
1	B	225	ALA	2.8
1	B	202	LYS	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	201	ASN	2.8
1	B	184	LYS	2.7
1	A	169	GLN	2.6
1	A	203	ARG	2.5
1	A	206	GLN	2.5
1	B	203	ARG	2.4
1	B	226	SER	2.4
1	B	182	ASP	2.3
1	A	201	ASN	2.2
1	B	231	ASP	2.2
1	B	383	SER	2.2
1	A	369	ASP	2.2
1	A	183	GLU	2.1
1	B	183	GLU	2.1
1	A	181	LEU	2.1
1	B	4	GLU	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
3	SYN	B	502	8/8	0.87	0.13	4.59	21,32,37,38	0
3	SYN	A	502	8/8	0.89	0.13	3.01	19,30,38,41	0
2	HEM	A	501	43/43	0.98	0.07	0.10	8,10,13,15	0
2	HEM	B	501	43/43	0.98	0.08	-0.12	8,9,12,15	0
4	CL	A	503	1/1	0.93	0.07	-	53,53,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.