



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:23 PM GMT

PDB ID : 4RRT  
Title : Crystal structure of a human cytochrome P450 2B6 (Y226H/K262R) in complex with (+)-3-carene  
Authors : Shah, M.B.  
Deposited on : 2014-11-06  
Resolution : 2.20 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

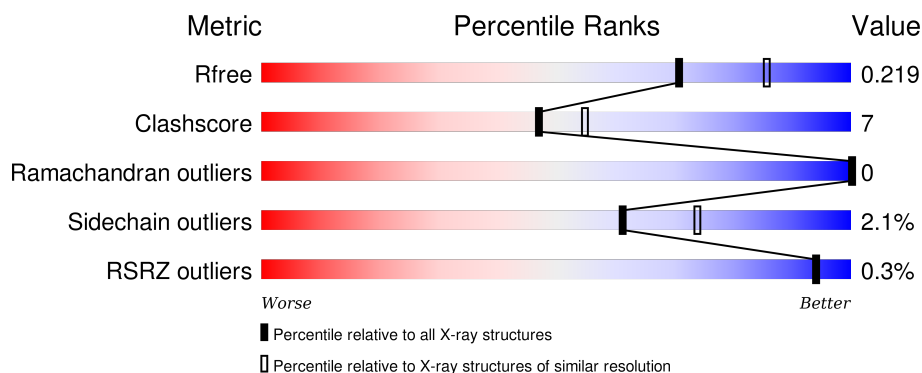
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	476	 81% 15% . .
1	B	476	 83% 13% . .

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	3V4	A	502	-	-	-	X
3	3V4	B	502	-	-	-	X
4	CM5	A	503	-	-	-	X
4	CM5	A	504	-	-	-	X
4	CM5	A	505	-	-	-	X
4	CM5	B	504	-	-	-	X
4	CM5	B	505	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8095 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 2B6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3700	2400	629	655	16			
1	B	461	Total	C	N	O	S	0	0	0
			3702	2403	629	654	16			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ALA	GLU	ENGINEERED MUTATION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	SER	DELETION	UNP P20813
A	?	-	VAL	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	PHE	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	ALA	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	THR	DELETION	UNP P20813
A	?	-	GLY	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	LEU	DELETION	UNP P20813
A	?	-	VAL	DELETION	UNP P20813
A	?	-	GLN	DELETION	UNP P20813
A	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
A	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
A	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
A	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
A	26	SER	THR	ENGINEERED MUTATION	UNP P20813

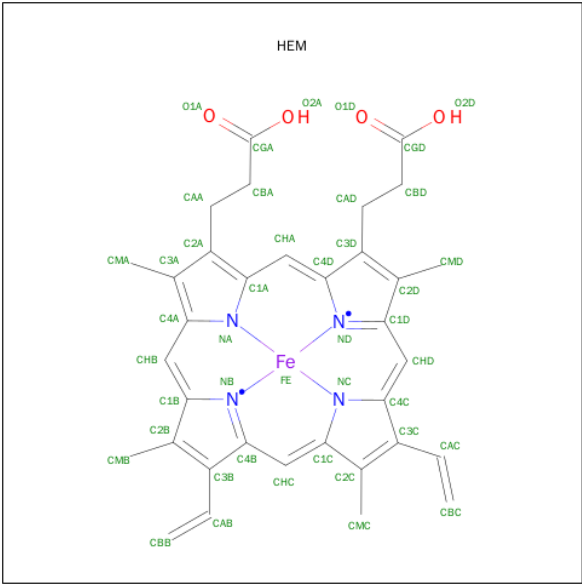
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Chain	Residue	Modelled	Actual	Comment	Reference
A	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
A	29	LYS	ASP	ENGINEERED MUTATION	UNP P20813
A	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
A	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
A	492	HIS	-	EXPRESSION TAG	UNP P20813
A	493	HIS	-	EXPRESSION TAG	UNP P20813
A	494	HIS	-	EXPRESSION TAG	UNP P20813
A	495	HIS	-	EXPRESSION TAG	UNP P20813
B	21	ALA	GLU	ENGINEERED MUTATION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	SER	DELETION	UNP P20813
B	?	-	VAL	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	PHE	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	ALA	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	THR	DELETION	UNP P20813
B	?	-	GLY	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	LEU	DELETION	UNP P20813
B	?	-	VAL	DELETION	UNP P20813
B	?	-	GLN	DELETION	UNP P20813
B	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
B	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
B	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
B	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
B	26	SER	THR	ENGINEERED MUTATION	UNP P20813
B	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
B	29	LYS	ASP	ENGINEERED MUTATION	UNP P20813
B	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
B	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
B	492	HIS	-	EXPRESSION TAG	UNP P20813
B	493	HIS	-	EXPRESSION TAG	UNP P20813
B	494	HIS	-	EXPRESSION TAG	UNP P20813
B	495	HIS	-	EXPRESSION TAG	UNP P20813

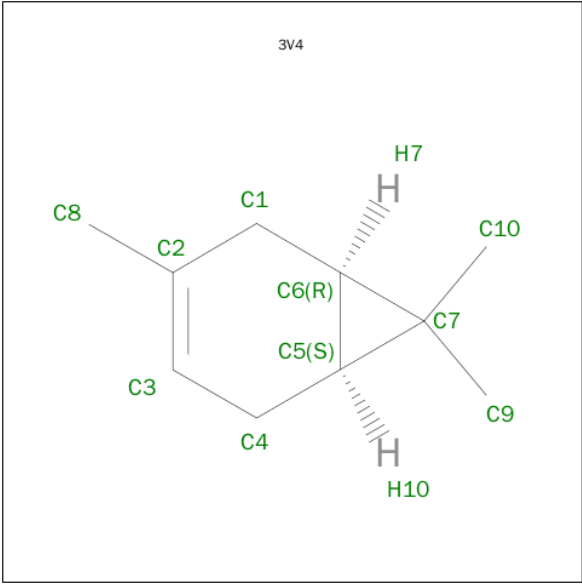
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 3 is (+)-3-CARENE (three-letter code: 3V4) (formula: C<sub>10</sub>H<sub>16</sub>).



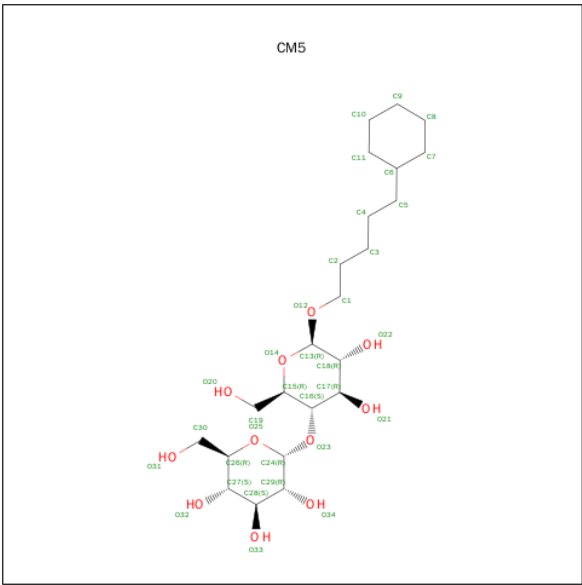
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			10	10		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C 10 10	0	0

- Molecule 4 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSIDE (three-letter code: CM5) (formula: C<sub>23</sub>H<sub>42</sub>O<sub>11</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	228	Total	O	0	0
			228	228		
6	B	231	Total	O	0	0
			231	231		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.07 Å 78.07 Å 203.08 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	67.69 – 2.20 40.60 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.9 (67.69-2.20) 95.9 (40.60-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.40 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.170 , 0.222 0.176 , 0.219	Depositor DCC
$R_{free}$ test set	3377 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 28.5	EDS
Estimated twinning fraction	0.039 for -h,-k,l 0.478 for h,-h-k,-l 0.044 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 67074 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8095	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 3V4, CM5, 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	1.07	2/3800 (0.1%)	0.90	4/5146 (0.1%)
1	B	1.09	3/3802 (0.1%)	0.89	7/5147 (0.1%)
All	All	1.08	5/7602 (0.1%)	0.90	11/10293 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	155	GLU	CG-CD	5.84	1.60	1.51
1	A	402	PHE	CE1-CZ	5.41	1.47	1.37
1	B	474	GLU	CB-CG	5.26	1.62	1.52
1	B	296	PHE	CB-CG	-5.25	1.42	1.51
1	A	155	GLU	CG-CD	5.25	1.59	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	336	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	B	487	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	487	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	293	LEU	CA-CB-CG	5.70	128.42	115.30
1	B	64	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	B	109	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	434	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	326	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	308	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	326	ARG	NE-CZ-NH1	5.09	122.84	120.30

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	3700	0	3654	56	0
1	B	3702	0	3663	52	0
2	A	43	0	30	5	0
2	B	43	0	30	3	0
3	A	10	0	16	0	0
3	B	10	0	16	0	0
4	A	58	0	84	7	0
4	B	58	0	84	8	0
5	A	12	0	16	0	0
6	A	228	0	0	10	0
6	B	231	0	0	7	0
All	All	8095	0	7593	114	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 7.

All (114) 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:384:LYS:O	1:A:385:ASP:HB2	1.68	0.91
1:A:49:ARG:HH21	1:A:53:LYS:HD2	1.42	0.84
1:A:168:THR:OG1	1:A:308:ARG:HD3	1.83	0.78
1:A:141:SER:HB2	6:A:777:HOH:O	1.85	0.75
1:B:131:THR:CG2	1:B:264:LEU:HD12	2.15	0.75
1:B:128:SER:O	1:B:132:MET:HG3	1.87	0.75
1:B:223:PHE:HB2	4:B:503:CM5:H22A	1.68	0.75
1:B:127:PHE:O	1:B:131:THR:HB	1.85	0.75
1:B:184:PHE:CE2	1:B:296:PHE:CZ	2.74	0.74
1:B:131:THR:HG22	1:B:264:LEU:HD12	1.69	0.73
1:A:128:SER:O	1:A:132:MET:HG3	1.90	0.72
1:A:184:PHE:CE2	1:A:296:PHE:CZ	2.77	0.72
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.72	0.72
1:B:184:PHE:CE2	1:B:296:PHE:CE2	2.79	0.71
1:B:345:LYS:HG3	6:B:805:HOH:O	1.91	0.69
1:B:37:LEU:HB3	1:B:38:PRO:HD2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ARG:HA	4:B:505:CM5:H52	1.78	0.66
1:B:140:ARG:HH21	1:B:145:ARG:HG2	1.60	0.65
1:B:296:PHE:CE1	4:B:504:CM5:H82	2.33	0.64
2:A:501:HEM:HMB2	2:A:501:HEM:HBB2	1.81	0.63
1:A:274:LYS:NZ	6:A:821:HOH:O	2.32	0.62
1:A:296:PHE:CE1	4:A:504:CM5:H82	2.34	0.61
1:B:131:THR:CG2	1:B:264:LEU:CD1	2.78	0.61
1:B:140:ARG:HD2	1:B:148:GLU:OE2	2.01	0.60
1:A:30:LEU:HD21	1:A:383:PRO:HD2	1.85	0.59
1:A:345:LYS:HG3	6:A:785:HOH:O	2.03	0.58
1:B:330:GLN:HB2	6:B:665:HOH:O	2.05	0.57
1:A:111:TYR:HB2	1:A:290:LEU:HD12	1.86	0.57
1:A:88:LEU:HD21	1:A:390:LEU:HD21	1.87	0.56
6:A:810:HOH:O	1:B:194:GLU:HG3	2.04	0.56
1:B:335:HIS:ND1	6:B:667:HOH:O	2.32	0.56
1:A:360:SER:O	1:A:479:LYS:HD3	2.06	0.56
1:A:443:ARG:HD2	6:A:823:HOH:O	2.05	0.56
1:B:70:LEU:HD12	1:B:75:VAL:HG21	1.88	0.55
1:B:244:TYR:CD2	4:B:504:CM5:H112	2.42	0.55
1:A:126:ARG:O	1:A:130:THR:HB	2.05	0.55
1:B:37:LEU:HB3	1:B:38:PRO:CD	2.38	0.54
1:A:244:TYR:HA	4:A:504:CM5:H192	1.88	0.54
1:B:111:TYR:HB2	1:B:290:LEU:HD12	1.88	0.54
1:A:456:ASN:O	1:A:491:ARG:HG3	2.08	0.54
1:A:140:ARG:HD2	1:A:148:GLU:OE2	2.09	0.53
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.36	0.53
1:B:326:ARG:NH2	6:B:824:HOH:O	2.42	0.52
1:B:296:PHE:CD1	4:B:504:CM5:H82	2.45	0.52
1:A:384:LYS:O	1:A:385:ASP:CB	2.48	0.52
1:B:429:PHE:O	1:B:430:SER:HB3	2.09	0.52
1:B:194:GLU:HB3	4:B:504:CM5:H11	1.91	0.52
1:B:200:ASN:O	1:B:204:GLN:HG2	2.09	0.52
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.40	0.52
1:A:140:ARG:NH2	1:A:145:ARG:HG2	2.24	0.51
1:B:184:PHE:HE2	1:B:296:PHE:CZ	2.27	0.51
1:A:198:MET:HG3	4:A:504:CM5:H41	1.92	0.51
1:A:127:PHE:O	1:A:130:THR:HG22	2.10	0.50
1:A:436:CYS:HB2	2:A:501:HEM:NA	2.27	0.49
1:A:184:PHE:CE2	1:A:296:PHE:CE2	3.01	0.49
1:A:454:LEU:HD21	1:A:459:MET:CE	2.43	0.49
1:B:179:ILE:HG13	1:B:299:GLY:HA3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ALA:HB3	6:B:676:HOH:O	2.13	0.48
1:B:131:THR:HG21	1:B:264:LEU:HG	1.95	0.48
1:A:82:GLU:HG2	6:A:608:HOH:O	2.13	0.48
1:A:430:SER:OG	1:A:431:LEU:N	2.47	0.48
1:B:459:MET:HG2	1:B:486:ILE:HD11	1.95	0.48
1:A:319:HIS:CE1	6:A:780:HOH:O	2.66	0.47
1:B:219:LEU:HD13	6:B:628:HOH:O	2.14	0.47
1:A:49:ARG:NH2	1:A:53:LYS:HD2	2.19	0.47
1:A:36:PRO:HG3	1:A:69:HIS:CD2	2.49	0.47
1:B:105:ASP:N	1:B:106:PRO:CD	2.77	0.47
2:A:501:HEM:HBC2	2:A:501:HEM:HMC2	1.97	0.47
1:A:296:PHE:CG	4:A:504:CM5:H92	2.49	0.47
1:A:179:ILE:HG13	1:A:299:GLY:HA3	1.97	0.47
1:A:429:PHE:O	1:A:430:SER:HB3	2.14	0.47
1:A:296:PHE:CD1	4:A:504:CM5:H82	2.50	0.47
1:B:430:SER:OG	1:B:431:LEU:N	2.48	0.47
1:B:374:HIS:HB3	6:B:673:HOH:O	2.16	0.46
1:B:466:GLU:CD	1:B:466:GLU:H	2.19	0.46
1:B:430:SER:HB3	2:B:501:HEM:HBA1	1.98	0.45
1:B:179:ILE:HG23	1:B:179:ILE:HD12	1.69	0.45
1:A:371:VAL:HG21	1:A:382:ILE:HG22	1.99	0.45
1:B:85:ARG:O	1:B:86:GLU:C	2.54	0.45
1:A:142:VAL:HA	1:A:145:ARG:HD2	1.99	0.45
1:B:131:THR:HG22	1:B:264:LEU:CD1	2.42	0.44
1:A:184:PHE:CE2	1:A:296:PHE:HZ	2.34	0.44
1:B:88:LEU:HD11	1:B:390:LEU:HG	1.99	0.44
1:A:49:ARG:HE	1:A:53:LYS:HG3	1.80	0.44
1:A:491:ARG:NH2	6:A:655:HOH:O	2.51	0.44
1:A:374:HIS:HB3	6:A:765:HOH:O	2.17	0.43
1:A:184:PHE:CZ	1:A:296:PHE:CE2	3.07	0.43
1:A:81:VAL:HG12	6:A:824:HOH:O	2.19	0.43
1:B:382:ILE:HA	1:B:383:PRO:HD3	1.81	0.43
1:A:168:THR:OG1	1:A:308:ARG:CD	2.61	0.43
1:A:202:PHE:HE2	4:A:504:CM5:H91	1.83	0.43
1:B:180:CYS:HG	1:B:296:PHE:HE1	1.64	0.43
1:A:105:ASP:N	1:A:106:PRO:CD	2.82	0.43
1:B:49:ARG:HG3	1:B:53:LYS:HG2	2.01	0.42
1:A:200:ASN:O	1:A:204:GLN:HG2	2.19	0.42
1:A:156:GLU:HG2	1:A:170:LEU:HD21	2.01	0.42
1:A:371:VAL:HG23	1:A:384:LYS:HA	2.00	0.42
1:B:245:ILE:O	1:B:249:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ASN:OD1	1:B:289:ASN:HB3	2.20	0.41
1:B:434:ARG:HD3	1:B:434:ARG:HA	1.87	0.41
2:A:501:HEM:CMB	2:A:501:HEM:HBB2	2.48	0.41
1:B:296:PHE:CG	4:B:504:CM5:H92	2.55	0.41
1:A:456:ASN:C	1:A:491:ARG:HG3	2.41	0.41
1:A:434:ARG:HD3	1:A:434:ARG:HA	1.87	0.41
1:A:220:PHE:CD2	4:A:503:CM5:H111	2.56	0.41
1:B:213:PHE:C	1:B:213:PHE:CD1	2.94	0.41
1:B:70:LEU:HD22	1:B:219:LEU:HD22	2.02	0.41
1:A:82:GLU:O	1:A:86:GLU:HB2	2.21	0.41
1:B:131:THR:HG21	1:B:264:LEU:CD1	2.51	0.40
1:B:244:TYR:HA	4:B:504:CM5:H192	2.03	0.40
1:A:349:THR:HG21	1:A:451:THR:HG22	2.02	0.40
1:A:360:SER:O	1:A:361:ASP:HB3	2.22	0.40
1:A:268:TYR:CG	1:A:288:LEU:HD13	2.57	0.40
1:A:466:GLU:CD	1:A:466:GLU:H	2.25	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	457/476 (96%)	444 (97%)	13 (3%)	0	100	100
1	B	457/476 (96%)	443 (97%)	14 (3%)	0	100	100
All	All	914/952 (96%)	887 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	396/418 (95%)	387 (98%)	9 (2%)	58	71
1	B	396/418 (95%)	388 (98%)	8 (2%)	63	76
All	All	792/836 (95%)	775 (98%)	17 (2%)	61	74

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	53	LYS
1	A	57	ARG
1	A	73	ARG
1	A	130	THR
1	A	135	PHE
1	A	293	LEU
1	A	309	TYR
1	A	384	LYS
1	B	39	LEU
1	B	49	ARG
1	B	73	ARG
1	B	131	THR
1	B	133	ARG
1	B	293	LEU
1	B	309	TYR
1	B	335	HIS

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

Mol	Chain	Res	Type
1	A	69	HIS
1	A	247	HIS
1	B	69	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 ⓘ

12 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	2.72	11 (36%)	24,82,82	2.72	8 (33%)
3	3V4	A	502	-	11,11,11	1.82	2 (18%)	18,18,18	3.85	7 (38%)
4	CM5	A	503	-	12,12,36	0.28	0	13,13,49	0.81	0
4	CM5	A	504	-	36,36,36	0.77	1 (2%)	49,49,49	1.33	6 (12%)
4	CM5	A	505	-	12,12,36	0.43	0	13,13,49	0.69	0
5	GOL	A	506	-	5,5,5	0.39	0	5,5,5	0.53	0
5	GOL	A	507	-	5,5,5	0.42	0	5,5,5	0.57	0
2	HEM	B	501	1	30,50,50	2.28	9 (30%)	24,82,82	2.74	9 (37%)
3	3V4	B	502	-	11,11,11	1.83	2 (18%)	18,18,18	3.85	7 (38%)
4	CM5	B	503	-	12,12,36	0.33	0	13,13,49	0.75	0
4	CM5	B	504	-	36,36,36	0.77	1 (2%)	49,49,49	1.22	6 (12%)
4	CM5	B	505	-	12,12,36	0.47	0	13,13,49	1.16	1 (7%)

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	3V4	A	502	-	-	0/0/22/22	0/1/2/2
4	CM5	A	503	-	-	0/6/14/65	0/1/1/3
4	CM5	A	504	-	-	0/17/65/65	0/3/3/3
4	CM5	A	505	-	-	0/6/14/65	0/1/1/3
5	GOL	A	506	-	-	0/4/4/4	0/0/0/0
5	GOL	A	507	-	-	0/4/4/4	0/0/0/0
2	HEM	B	501	1	-	0/10/54/54	0/0/8/8
3	3V4	B	502	-	-	0/0/22/22	0/1/2/2
4	CM5	B	503	-	-	0/6/14/65	0/1/1/3
4	CM5	B	504	-	-	0/17/65/65	0/3/3/3
4	CM5	B	505	-	-	0/6/14/65	0/1/1/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3B-C4B	-10.32	1.42	1.51
2	B	501	HEM	C3B-C4B	-7.75	1.44	1.51
2	A	501	HEM	C2C-C1C	-4.33	1.44	1.52
2	A	501	HEM	C3D-C4D	-3.74	1.46	1.51
2	B	501	HEM	C2C-C1C	-3.63	1.45	1.52
2	B	501	HEM	C3D-C4D	-3.47	1.47	1.51
2	B	501	HEM	C2D-C1D	-2.27	1.44	1.51
2	A	501	HEM	C2D-C1D	-2.14	1.44	1.51
2	A	501	HEM	C2B-C1B	-2.03	1.45	1.51
4	B	504	CM5	O12-C13	2.03	1.43	1.40
2	A	501	HEM	C3C-CAC	2.03	1.55	1.51
2	B	501	HEM	C3C-CAC	2.09	1.55	1.51
2	B	501	HEM	CMA-C3A	2.21	1.56	1.51
4	A	504	CM5	O12-C13	2.23	1.44	1.40
2	B	501	HEM	CAA-C2A	2.27	1.55	1.52
3	B	502	3V4	C7-C6	2.45	1.56	1.51
3	A	502	3V4	C7-C6	2.45	1.56	1.51
2	A	501	HEM	FE-NB	2.81	2.12	1.97
2	A	501	HEM	CMA-C3A	2.92	1.57	1.51
2	A	501	HEM	FE-ND	3.43	2.15	1.97
2	A	501	HEM	CAA-C2A	3.69	1.58	1.52
2	B	501	HEM	FE-ND	3.71	2.17	1.97
2	A	501	HEM	C4C-NC	4.09	1.41	1.36
2	B	501	HEM	C4C-NC	4.13	1.41	1.36
3	B	502	3V4	C3-C2	4.49	1.50	1.33
3	A	502	3V4	C3-C2	4.49	1.50	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	3V4	C1-C2-C3	-10.65	109.08	121.50
3	B	502	3V4	C1-C2-C3	-10.65	109.10	121.50
3	B	502	3V4	C8-C2-C3	-6.79	107.85	122.63
3	B	502	3V4	C4-C5-C7	-6.78	113.81	123.50
3	A	502	3V4	C4-C5-C7	-6.78	113.81	123.50
3	A	502	3V4	C8-C2-C3	-6.77	107.89	122.63
2	A	501	HEM	C3C-CAC-CBC	-5.49	116.03	124.46
2	B	501	HEM	C3C-CAC-CBC	-4.27	117.91	124.46
3	B	502	3V4	C1-C6-C7	-4.14	117.67	123.55
3	A	502	3V4	C1-C6-C7	-4.13	117.67	123.55
2	B	501	HEM	C3B-CAB-CBB	-3.99	118.33	124.46
3	B	502	3V4	C4-C3-C2	-3.47	111.52	123.85
3	A	502	3V4	C4-C3-C2	-3.47	111.52	123.85
3	B	502	3V4	C9-C7-C5	-3.19	109.18	118.43
3	A	502	3V4	C9-C7-C5	-3.18	109.20	118.43
2	B	501	HEM	CAA-CBA-CGA	-2.86	107.50	112.75
2	A	501	HEM	CBD-CAD-C3D	-2.14	107.33	113.55
2	A	501	HEM	C3B-C4B-CHC	2.03	126.02	123.16
4	A	504	CM5	C13-O14-C15	2.09	117.81	113.75
4	A	504	CM5	O25-C26-C30	2.09	111.64	106.36
4	B	504	CM5	C5-C6-C11	2.10	116.55	112.10
4	A	504	CM5	C18-C17-C16	2.18	114.39	109.60
4	B	504	CM5	O25-C26-C30	2.27	112.10	106.36
4	B	505	CM5	C5-C6-C7	2.33	117.04	112.10
2	B	501	HEM	C2D-C3D-C4D	2.44	105.63	101.50
4	B	504	CM5	O14-C15-C16	2.46	114.95	109.75
4	B	504	CM5	C13-O14-C15	2.60	118.80	113.75
4	B	504	CM5	C24-O25-C26	2.66	118.92	113.75
4	A	504	CM5	C9-C10-C11	3.10	117.95	111.44
4	A	504	CM5	C8-C7-C6	3.25	117.47	112.22
2	B	501	HEM	CAD-C3D-C4D	3.25	123.95	112.47
2	A	501	HEM	CAD-C3D-C4D	3.43	124.56	112.47
4	B	504	CM5	C9-C10-C11	3.44	118.65	111.44
2	A	501	HEM	CMD-C2D-C3D	3.66	130.53	114.35
3	B	502	3V4	C5-C4-C3	3.68	118.83	112.30
3	A	502	3V4	C5-C4-C3	3.68	118.83	112.30
2	B	501	HEM	CMD-C2D-C3D	3.78	131.08	114.35
4	A	504	CM5	C24-O25-C26	3.98	121.47	113.75
2	A	501	HEM	CMC-C2C-C3C	4.94	128.87	116.53
2	B	501	HEM	CMC-C2C-C3C	4.97	128.93	116.53
2	A	501	HEM	CMB-C2B-C3B	5.10	129.27	116.53
2	B	501	HEM	CMB-C2B-C3B	5.36	129.91	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CAD-C3D-C2D	5.94	130.30	113.22
2	A	501	HEM	CAD-C3D-C2D	6.05	130.61	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	5	0
4	A	503	CM5	1	0
4	A	504	CM5	6	0
2	B	501	HEM	3	0
4	B	503	CM5	1	0
4	B	504	CM5	6	0
4	B	505	CM5	1	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	461/476 (96%)	-0.57	2 (0%) 93 93	18, 31, 51, 82	9 (1%)
1	B	461/476 (96%)	-0.60	1 (0%) 95 95	18, 31, 49, 74	9 (1%)
All	All	922/952 (96%)	-0.59	3 (0%) 94 94	18, 31, 49, 82	18 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	ARG	2.8
1	A	135	PHE	2.5
1	B	296	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( $\text{\AA}^2$ )	Q<0.9
4	CM5	A	505	12/34	0.89	0.21	6.81	55,60,66,66	0
3	3V4	A	502	10/10	0.84	0.28	6.02	45,49,53,54	0
3	3V4	B	502	10/10	0.84	0.29	5.95	55,58,60,61	0
4	CM5	A	504	34/34	0.81	0.26	5.14	55,82,89,89	0
4	CM5	B	505	12/34	0.82	0.18	4.52	57,60,66,67	0
4	CM5	B	504	34/34	0.81	0.24	2.97	49,87,91,92	0
4	CM5	A	503	12/34	0.91	0.18	2.24	64,68,70,70	0
4	CM5	B	503	12/34	0.83	0.17	1.55	67,69,71,71	0
2	HEM	A	501	43/43	0.99	0.09	-0.43	17,22,27,31	0
2	HEM	B	501	43/43	0.99	0.09	-0.56	15,23,29,31	0
5	GOL	A	507	6/6	0.58	0.17	-	75,77,78,78	0
5	GOL	A	506	6/6	0.58	0.26	-	82,86,87,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.