Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2016 – 04:56 PM EDT

PDB ID	:	5IUZ
Title	:	STRUCTURE OF P450 2B4 F202W MUTANT (CYMAL-5)
Authors	:	Jang, H.-H.; Halpert, J.R.; Shah, M.B.
Deposited on	:	2016-03-18
Resolution	:	2.73 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

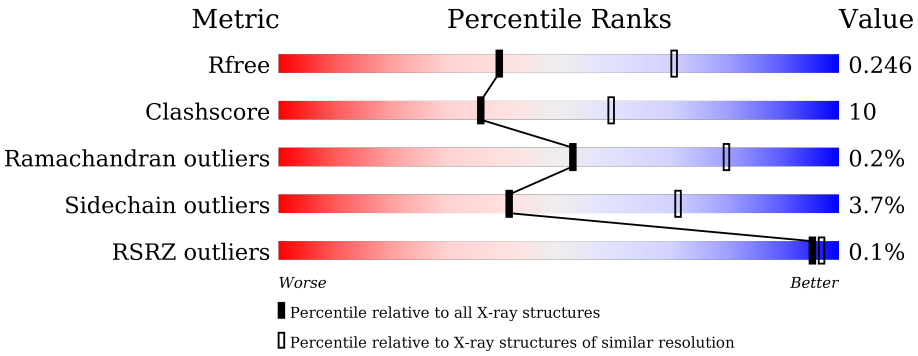
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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 >=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 <=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	478	79% 16%
1	B	478	78% 18%

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	502	-	-	-	X
3	CM5	A	503	-	-	-	X
3	CM5	B	502	-	-	-	X
3	CM5	B	503	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7914 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
1	A	459	Total	C	N	O	S	0	1	0
			3692	2382	637	663	10			
1	B	464	Total	C	N	O	S	0	1	0
			3720	2395	647	667	11			

There are 72 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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	27	LYS	HIS	engineered mutation	UNP P00178
A	29	LYS	ARG	engineered mutation	UNP P00178
A	202	TRP	PHE	engineered mutation	UNP P00178
A	221	SER	PRO	SEE REMARK 999	UNP P00178
A	226	TYR	HIS	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
B	21	ALA	GLU	engineered mutation	UNP P00178
B	?	-	PHE	DELETION	UNP P00178
B	?	-	SER	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	ALA	DELETION	UNP P00178
B	?	-	PHE	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	ALA	DELETION	UNP P00178
B	?	-	GLY	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	PHE	DELETION	UNP P00178
B	?	-	ARG	DELETION	UNP P00178
B	22	LYS	GLY	engineered mutation	UNP P00178
B	23	LYS	HIS	engineered mutation	UNP P00178
B	24	THR	PRO	engineered mutation	UNP P00178
B	25	SER	LYS	engineered mutation	UNP P00178
B	26	SER	ALA	engineered mutation	UNP P00178
B	27	LYS	HIS	engineered mutation	UNP P00178
B	29	LYS	ARG	engineered mutation	UNP P00178
B	202	TRP	PHE	engineered mutation	UNP P00178
B	221	SER	PRO	variant	UNP P00178
B	226	TYR	HIS	engineered mutation	UNP P00178
B	492	HIS	-	expression tag	UNP P00178

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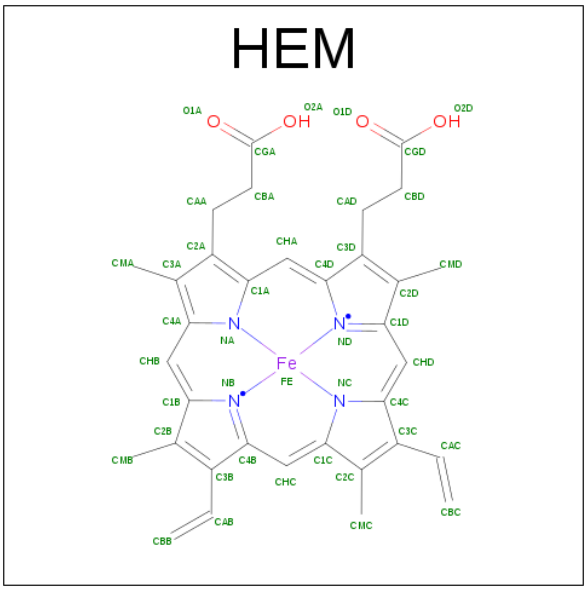
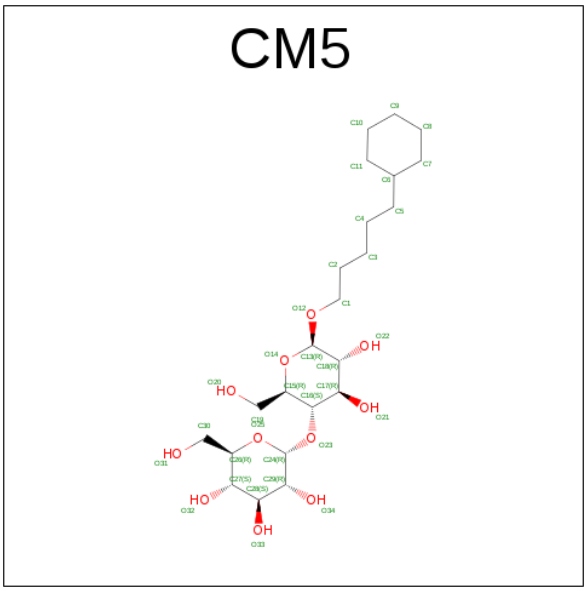
Chain	Residue	Modelled	Actual	Comment	Reference
B	493	HIS	-	expression tag	UNP P00178
B	494	HIS	-	expression tag	UNP P00178
B	495	HIS	-	expression tag	UNP P00178
B	496	HIS	-	expression tag	UNP P00178
B	497	HIS	-	expression tag	UNP P00178

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



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

- Molecule 3 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSIDE (three-letter code: CM5) (formula: $C_{23}H_{42}O_{11}$).



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

- Molecule 4 is water.

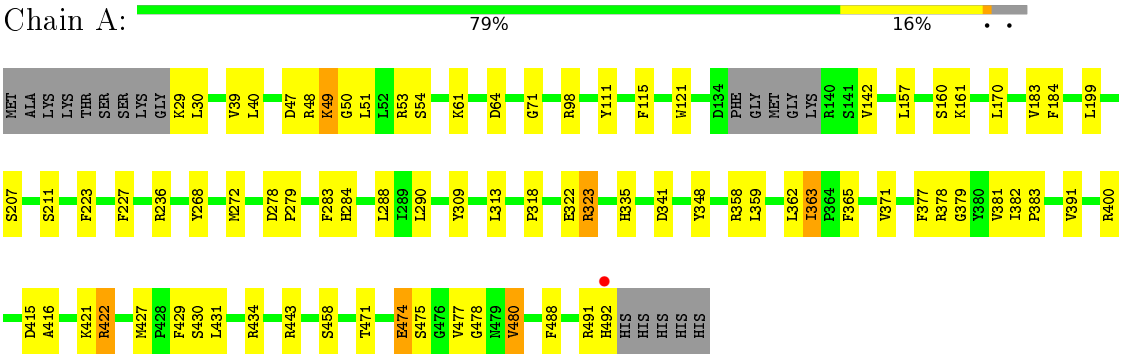
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	136	Total O 136 136	0	0
4	B	144	Total O 144 144	0	0

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 (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.

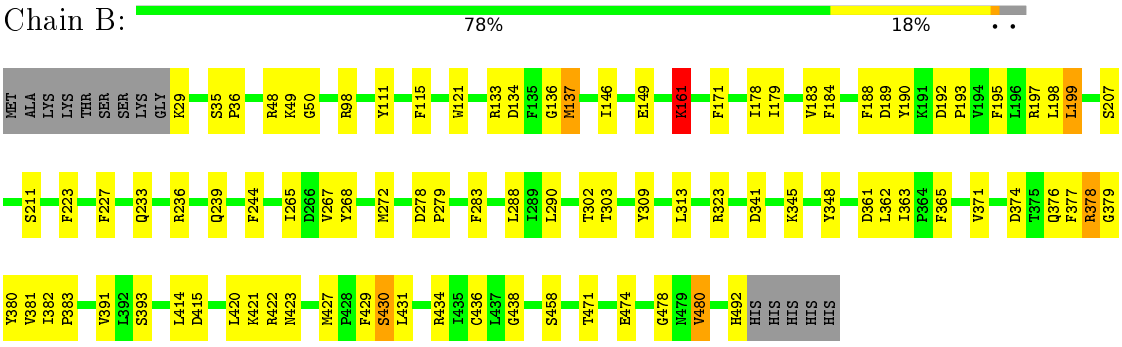
- Molecule 1: Cytochrome P450 2B4

Chain A:



- Molecule 1: Cytochrome P450 2B4

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	91.61Å 91.61Å 150.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.73 19.89 – 2.73	Depositor EDS
% Data completeness (in resolution range)	90.5 (20.00-2.73) 90.5 (19.89-2.73)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.75Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.180 , 0.248 0.191 , 0.246	Depositor DCC
R_{free} test set	1705 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	45.1	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 10.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l 0.459 for h,-h-k,-l 0.028 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7914	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CM5

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	0.87	0/3789	0.80	2/5133 (0.0%)
1	B	0.85	3/3815 (0.1%)	0.80	2/5170 (0.0%)
All	All	0.86	3/7604 (0.0%)	0.80	4/10303 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	171	PHE	CE2-CZ	-5.26	1.27	1.37
1	B	171	PHE	CE1-CZ	-5.10	1.27	1.37
1	B	171	PHE	CG-CD2	-5.09	1.31	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	199	LEU	CA-CB-CG	5.94	128.96	115.30
1	A	443	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	161	LYS	CB-CA-C	-5.13	100.14	110.40
1	A	64	ASP	CB-CG-OD1	5.07	122.86	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	3692	0	3690	66	0
1	B	3720	0	3706	76	0
2	A	43	0	30	5	0
2	B	43	0	30	2	0
3	A	68	0	84	2	0
3	B	68	0	83	20	0
4	A	136	0	0	10	0
4	B	144	0	0	8	0
All	All	7914	0	7623	147	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 10.

All (147) 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)
3:B:503:CM5:C29	3:B:503:CM5:H192	1.44	1.45
1:B:423:ASN:HB2	4:B:712:HOH:O	1.50	1.10
3:B:503:CM5:H29	3:B:503:CM5:C19	1.85	1.07
1:A:422:ARG:HB2	1:A:422:ARG:HH21	1.12	1.05
3:B:503:CM5:H29	3:B:503:CM5:H192	0.99	0.99
1:A:422:ARG:HH21	1:A:422:ARG:CB	1.75	0.97
3:B:503:CM5:C24	3:B:503:CM5:H192	1.96	0.96
3:B:503:CM5:C19	3:B:503:CM5:C29	2.41	0.94
1:B:422:ARG:HD2	4:B:645:HOH:O	1.67	0.93
1:B:50:GLY:HA2	3:B:503:CM5:H82	1.58	0.85
1:A:422:ARG:HB2	1:A:422:ARG:NH2	1.92	0.84
1:B:474:GLU:O	1:B:480:VAL:HG23	1.82	0.80
1:B:244:PHE:CZ	3:B:502:CM5:H31A	2.18	0.79
1:B:244:PHE:CE1	3:B:502:CM5:O12	2.37	0.78
1:A:474:GLU:O	1:A:480:VAL:HG23	1.85	0.76
1:A:427:MET:O	1:A:427:MET:HG3	1.87	0.75
1:B:377:PHE:O	1:B:378:ARG:C	2.25	0.75
1:A:115:PHE:HB3	4:A:667:HOH:O	1.89	0.71
1:A:474:GLU:HG2	4:A:606:HOH:O	1.93	0.68
3:B:503:CM5:C19	3:B:503:CM5:C24	2.70	0.68
1:B:345:LYS:HD2	4:B:637:HOH:O	1.92	0.68
1:A:49:LYS:HD3	1:A:53:ARG:HG2	1.76	0.67
1:A:71:GLY:HA3	4:A:613:HOH:O	1.95	0.66
1:A:268:TYR:CE1	1:A:288:LEU:HB2	2.30	0.66
1:B:430:SER:O	1:B:431:LEU:HD23	1.96	0.65
1:B:377:PHE:O	1:B:379:GLY:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LYS:HA	4:A:681:HOH:O	1.97	0.64
1:A:491:ARG:O	1:A:492:HIS:C	2.35	0.64
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.78	0.64
1:A:416:ALA:H	1:B:233:GLN:HE22	1.45	0.62
3:B:503:CM5:O34	3:B:503:CM5:H192	1.99	0.62
1:A:379:GLY:HA2	1:B:161:LYS:HD3	1.82	0.61
1:B:268:TYR:CE1	1:B:288:LEU:HB2	2.35	0.61
1:B:420:LEU:HD21	1:B:422:ARG:HE	1.66	0.61
1:A:160:SER:O	1:A:161:LYS:HB2	2.02	0.60
1:B:198:LEU:HD22	3:B:502:CM5:H22A	1.83	0.59
1:A:415:ASP:HB2	1:B:233:GLN:NE2	2.17	0.59
1:A:236:ARG:HD3	4:A:695:HOH:O	2.02	0.59
1:B:189:ASP:HB2	4:B:686:HOH:O	2.02	0.59
1:B:381:VAL:O	1:B:383:PRO:HD3	2.03	0.58
1:A:272:MET:HG2	1:A:283:PHE:O	2.04	0.58
2:A:501:HEM:HMB2	2:A:501:HEM:HBB2	1.85	0.57
1:B:183:VAL:HG12	1:B:184:PHE:CD1	2.39	0.57
1:A:379:GLY:HA2	1:B:161:LYS:CD	2.35	0.57
1:A:416:ALA:H	1:B:233:GLN:NE2	2.02	0.56
1:B:420:LEU:CD2	1:B:422:ARG:HE	2.18	0.56
1:A:415:ASP:C	1:A:415:ASP:OD1	2.45	0.56
1:A:371:VAL:HG21	1:A:382:ILE:HG22	1.88	0.56
1:A:400:ARG:O	1:B:197:ARG:HG3	2.06	0.55
1:A:323:ARG:HB3	1:A:348:TYR:CE2	2.40	0.55
1:B:323:ARG:HB3	1:B:348:TYR:CE2	2.40	0.55
1:A:458:SER:HB2	4:A:716:HOH:O	2.06	0.55
1:B:98:ARG:HG2	1:B:115:PHE:HA	1.89	0.55
1:A:30:LEU:HD21	1:A:383:PRO:HD2	1.89	0.55
1:A:30:LEU:HD21	1:A:382:ILE:HA	1.89	0.54
1:B:421:LYS:HG3	1:B:421:LYS:O	2.06	0.54
1:B:458:SER:HB2	4:B:727:HOH:O	2.06	0.54
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.38	0.54
1:A:98:ARG:HG2	1:A:115:PHE:HA	1.89	0.54
1:A:379:GLY:CA	1:B:161:LYS:HD3	2.37	0.54
1:A:47:ASP:OD1	1:A:49:LYS:CD	2.56	0.53
1:B:362:LEU:O	1:B:478:GLY:HA2	2.07	0.53
1:A:377:PHE:O	1:A:378:ARG:C	2.47	0.53
1:A:422:ARG:CG	1:A:422:ARG:HH21	2.21	0.53
1:B:415:ASP:C	1:B:415:ASP:OD1	2.47	0.52
1:B:371:VAL:HG21	1:B:382:ILE:HG22	1.92	0.52
1:B:272:MET:HG2	1:B:283:PHE:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:TYR:CD1	1:B:288:LEU:HD13	2.44	0.52
1:B:244:PHE:CZ	3:B:502:CM5:C3	2.93	0.51
1:A:421:LYS:HG3	1:A:421:LYS:O	2.11	0.51
1:A:415:ASP:HB2	1:B:233:GLN:HE22	1.74	0.51
1:A:362:LEU:O	1:A:478:GLY:HA2	2.11	0.51
1:B:111:TYR:HB2	1:B:290:LEU:HD12	1.92	0.51
1:B:236:ARG:HD3	4:B:667:HOH:O	2.10	0.51
1:B:188:PHE:CE2	3:B:502:CM5:H11	2.46	0.50
1:A:268:TYR:CG	1:A:288:LEU:HD13	2.47	0.50
1:B:244:PHE:CE2	3:B:502:CM5:H31A	2.47	0.50
1:A:381:VAL:O	1:A:383:PRO:HD3	2.11	0.50
1:B:302:THR:HG21	1:B:363:ILE:HD11	1.93	0.50
1:B:134:ASP:C	1:B:136:GLY:H	2.14	0.50
1:A:268:TYR:CD1	1:A:288:LEU:HD13	2.46	0.50
1:A:379:GLY:HA2	1:B:161:LYS:HB2	1.94	0.50
1:A:430:SER:OG	1:A:431:LEU:N	2.45	0.49
1:A:475:SER:N	4:A:606:HOH:O	2.45	0.49
1:A:111:TYR:HB2	1:A:290:LEU:HD12	1.95	0.49
3:A:503:CM5:H24	3:A:503:CM5:O20	2.13	0.49
1:B:195:PHE:HA	3:B:502:CM5:H21A	1.94	0.49
1:A:39:VAL:HG12	1:A:40:LEU:HD12	1.96	0.48
1:A:47:ASP:OD1	1:A:49:LYS:HD3	2.13	0.48
1:B:137:MET:HG2	1:B:267:VAL:HG21	1.95	0.48
1:A:183:VAL:HG12	1:A:184:PHE:CD1	2.49	0.48
1:B:309:TYR:HE2	1:B:313:LEU:HD11	1.79	0.47
1:A:429:PHE:O	1:A:430:SER:HB3	2.15	0.47
1:B:244:PHE:HE1	3:B:502:CM5:O12	1.92	0.47
1:A:358:ARG:NH2	1:A:359:LEU:HD13	2.30	0.47
1:B:268:TYR:CG	1:B:288:LEU:HD13	2.49	0.47
1:B:278:ASP:HA	1:B:279:PRO:HD3	1.79	0.46
1:B:98:ARG:NH2	2:B:501:HEM:O2D	2.40	0.46
1:B:429:PHE:HB3	1:B:436:CYS:CB	2.45	0.46
1:A:284:HIS:HB2	4:A:701:HOH:O	2.15	0.46
1:B:438:GLY:HA3	2:B:501:HEM:C3C	2.51	0.46
3:B:503:CM5:C16	3:B:503:CM5:O34	2.64	0.46
1:B:50:GLY:CA	3:B:503:CM5:H82	2.38	0.46
2:A:501:HEM:CMB	2:A:501:HEM:HBB2	2.46	0.45
1:B:430:SER:OG	1:B:431:LEU:N	2.50	0.45
1:A:365:PHE:HA	1:A:391:VAL:HA	1.98	0.45
1:A:309:TYR:CE2	1:A:313:LEU:HD11	2.52	0.45
1:B:146:ILE:HG12	1:B:178:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:VAL:HG23	4:A:614:HOH:O	2.16	0.45
1:B:29:LYS:O	1:B:380:TYR:HB3	2.17	0.44
1:B:121:TRP:CZ2	1:B:434:ARG:HD3	2.52	0.44
1:A:121:TRP:CZ2	1:A:434:ARG:HD3	2.52	0.44
1:B:309:TYR:CE2	1:B:313:LEU:HD11	2.52	0.44
1:A:309:TYR:HE2	1:A:313:LEU:HD11	1.82	0.44
1:A:318:PRO:O	1:A:322:GLU:HG3	2.18	0.44
1:B:377:PHE:C	1:B:379:GLY:N	2.72	0.43
1:A:157:LEU:HD22	1:A:488:PHE:CD2	2.54	0.43
1:B:427:MET:HA	4:B:648:HOH:O	2.17	0.43
1:A:50:GLY:HA2	3:A:503:CM5:C10	2.49	0.43
1:B:348:TYR:HD1	1:B:414:LEU:HD11	1.84	0.43
1:B:429:PHE:HB3	1:B:436:CYS:HB3	2.00	0.43
1:B:183:VAL:O	1:B:265:ILE:HG13	2.19	0.43
1:B:188:PHE:CZ	3:B:502:CM5:H32A	2.54	0.43
1:B:278:ASP:OD1	1:B:278:ASP:C	2.57	0.42
1:B:421:LYS:HA	4:B:734:HOH:O	2.19	0.42
1:B:361:ASP:OD2	1:B:393:SER:OG	2.27	0.42
1:B:365:PHE:HA	1:B:391:VAL:HA	2.01	0.42
1:B:149:GLU:OE2	1:B:190:TYR:OH	2.30	0.42
1:B:429:PHE:O	1:B:430:SER:HB3	2.20	0.42
3:B:503:CM5:O34	3:B:503:CM5:O14	2.35	0.42
1:B:192:ASP:HA	1:B:193:PRO:HD3	1.92	0.42
1:A:98:ARG:NH2	2:A:501:HEM:O2D	2.49	0.41
1:B:111:TYR:HB2	1:B:290:LEU:CD1	2.49	0.41
1:A:278:ASP:OD1	1:A:278:ASP:C	2.57	0.41
1:A:335:HIS:CE1	4:A:638:HOH:O	2.73	0.41
1:B:374:ASP:OD2	1:B:383:PRO:HA	2.20	0.41
1:B:133:ARG:O	1:B:133:ARG:HG2	2.21	0.41
1:A:30:LEU:CD2	1:A:382:ILE:HA	2.50	0.41
1:A:422:ARG:CG	1:A:422:ARG:NH2	2.84	0.41
1:A:227:PHE:CD1	1:A:227:PHE:N	2.88	0.41
1:B:227:PHE:N	1:B:227:PHE:CD1	2.88	0.41
1:A:51:LEU:O	1:A:54:SER:HB2	2.22	0.40
1:A:363:ILE:HA	1:A:477:VAL:O	2.20	0.40
1:A:47:ASP:OD1	1:A:49:LYS:HD2	2.21	0.40
1:B:179:ILE:O	1:B:183:VAL:HB	2.21	0.40
1:B:35:SER:HA	1:B:36:PRO:HD2	1.89	0.40
1:A:170:LEU:HA	1:A:170:LEU:HD23	1.93	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	456/478 (95%)	435 (95%)	21 (5%)	0	100 100
1	B	463/478 (97%)	437 (94%)	24 (5%)	2 (0%)	39 68
All	All	919/956 (96%)	872 (95%)	45 (5%)	2 (0%)	52 80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	378	ARG
1	B	430	SER

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	406/423 (96%)	391 (96%)	15 (4%)	41 71
1	B	407/423 (96%)	392 (96%)	15 (4%)	41 71
All	All	813/846 (96%)	783 (96%)	30 (4%)	41 71

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	49	LYS
1	A	61	LYS
1	A	199	LEU

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Mol	Chain	Res	Type
1	A	207	SER
1	A	211	SER
1	A	223	PHE
1	A	279	PRO
1	A	323	ARG
1	A	341	ASP
1	A	363	ILE
1	A	422	ARG
1	A	471	THR
1	A	474	GLU
1	A	480	VAL
1	B	48	ARG
1	B	49	LYS
1	B	137	MET
1	B	161	LYS
1	B	199	LEU
1	B	207	SER
1	B	211	SER
1	B	223	PHE
1	B	239	GLN
1	B	303	THR
1	B	341	ASP
1	B	376	GLN
1	B	471	THR
1	B	480	VAL
1	B	492	HIS

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	24,50,50	2.41	6 (25%)	16,82,82	1.84	4 (25%)
3	CM5	A	502	-	36,36,36	1.48	2 (5%)	49,49,49	2.30	7 (14%)
3	CM5	A	503	-	36,36,36	0.89	2 (5%)	49,49,49	2.93	5 (10%)
2	HEM	B	501	1	24,50,50	2.63	6 (25%)	16,82,82	1.67	4 (25%)
3	CM5	B	502	-	36,36,36	2.01	3 (8%)	49,49,49	3.24	6 (12%)
3	CM5	B	503	-	36,36,36	2.80	8 (22%)	49,49,49	3.86	16 (32%)

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	-	0/6/54/54	0/0/8/8
3	CM5	A	502	-	-	0/17/65/65	0/3/3/3
3	CM5	A	503	-	-	0/17/65/65	0/3/3/3
2	HEM	B	501	1	-	0/6/54/54	0/0/8/8
3	CM5	B	502	-	-	0/17/65/65	0/3/3/3
3	CM5	B	503	-	-	0/17/65/65	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	CM5	O12-C13	-7.19	1.27	1.40
2	B	501	HEM	C3C-C2C	-7.12	1.31	1.40
2	A	501	HEM	C3C-C2C	-5.83	1.32	1.40
2	B	501	HEM	C3B-C2B	-5.60	1.33	1.40
2	A	501	HEM	C3B-C2B	-4.85	1.34	1.40
3	A	503	CM5	O23-C16	-2.98	1.36	1.43
2	B	501	HEM	C1A-CHA	-2.14	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	CAD-C3D	2.01	1.54	1.52
2	A	501	HEM	C3B-CAB	3.00	1.54	1.47
3	A	502	CM5	C13-C18	3.34	1.62	1.52
3	B	502	CM5	C13-C18	3.35	1.62	1.52
2	B	501	HEM	C3C-CAC	3.53	1.55	1.47
2	B	501	HEM	C3B-CAB	3.56	1.55	1.47
3	A	503	CM5	O12-C13	3.56	1.46	1.40
2	A	501	HEM	C3C-CAC	3.62	1.55	1.47
3	B	503	CM5	C13-C18	3.78	1.63	1.52
3	B	503	CM5	C16-C15	4.07	1.64	1.52
3	B	503	CM5	C17-C16	4.11	1.63	1.52
3	B	503	CM5	C17-C18	4.20	1.63	1.52
2	B	501	HEM	C3D-C2D	5.13	1.52	1.37
2	A	501	HEM	C3D-C2D	5.15	1.52	1.37
3	B	503	CM5	O23-C16	6.62	1.60	1.43
3	B	503	CM5	O12-C1	7.16	1.62	1.42
3	A	502	CM5	O14-C13	7.59	1.61	1.41
3	B	502	CM5	O14-C13	7.59	1.61	1.41
3	B	503	CM5	O23-C24	7.88	1.63	1.41
3	B	502	CM5	O12-C13	8.15	1.55	1.40

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	503	CM5	O23-C16-C17	-13.93	70.85	107.18
3	A	503	CM5	O12-C13-C18	-13.17	91.80	108.00
3	B	503	CM5	C1-O12-C13	-11.70	93.55	114.00
3	B	502	CM5	C1-O12-C13	-10.93	94.89	114.00
3	B	503	CM5	C18-C17-C16	-9.69	88.25	109.63
3	B	502	CM5	O14-C13-C18	-7.07	95.59	110.28
3	A	502	CM5	O14-C13-C18	-7.06	95.60	110.28
3	B	503	CM5	C13-C18-C17	-5.44	99.20	109.98
3	B	503	CM5	C13-O14-C15	-5.34	103.26	113.74
3	B	503	CM5	O14-C15-C16	-5.13	98.84	109.78
3	B	503	CM5	O23-C16-C15	-4.62	97.03	109.33
3	B	503	CM5	C17-C16-C15	-4.43	100.73	110.85
2	A	501	HEM	CAA-CBA-CGA	-4.03	104.94	112.78
2	A	501	HEM	CBD-CAD-C3D	-3.91	105.60	112.47
3	B	503	CM5	O14-C13-C18	-3.77	102.44	110.28
2	B	501	HEM	CAA-CBA-CGA	-3.41	106.14	112.78
2	B	501	HEM	CBD-CAD-C3D	-3.33	106.62	112.47
3	B	503	CM5	C19-C15-C16	-3.31	103.53	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	503	CM5	C24-O23-C16	-2.96	110.13	118.00
3	B	503	CM5	O21-C17-C16	-2.78	103.31	109.89
3	B	502	CM5	O22-C18-C13	-2.55	104.35	110.01
3	A	502	CM5	O22-C18-C13	-2.55	104.35	110.01
3	B	503	CM5	O21-C17-C18	-2.20	105.39	110.36
3	B	502	CM5	C13-C18-C17	-2.20	105.62	109.98
3	A	502	CM5	C13-C18-C17	-2.19	105.65	109.98
2	B	501	HEM	CMB-C2B-C3B	2.01	129.02	125.09
3	B	503	CM5	O23-C24-C29	2.01	113.13	108.12
3	A	503	CM5	O14-C15-C16	2.07	114.19	109.78
3	B	502	CM5	O14-C15-C16	2.07	114.20	109.78
3	A	502	CM5	O14-C15-C16	2.08	114.22	109.78
2	A	501	HEM	CBA-CAA-C2A	2.21	116.38	112.49
3	A	502	CM5	C9-C8-C7	2.25	116.08	111.44
3	B	503	CM5	O12-C1-C2	2.37	116.45	109.63
2	A	501	HEM	CMB-C2B-C3B	2.50	129.98	125.09
2	B	501	HEM	CBA-CAA-C2A	2.60	117.06	112.49
3	A	503	CM5	O23-C16-C15	4.24	120.62	109.33
3	A	502	CM5	O14-C13-O12	4.79	121.48	109.99
3	B	503	CM5	O12-C13-C18	5.53	114.80	108.00
3	B	503	CM5	O14-C13-O12	10.41	134.94	109.99
3	A	502	CM5	O12-C13-C18	11.85	122.58	108.00
3	B	503	CM5	O23-C16-C17	13.21	141.64	107.18
3	B	502	CM5	O12-C13-C18	17.47	129.50	108.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	5	0
3	A	503	CM5	2	0
2	B	501	HEM	2	0
3	B	502	CM5	9	0
3	B	503	CM5	11	0

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^{th} 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^2)	Q<0.9
1	A	459/478 (96%)	-0.40	1 (0%) 95 96	17, 36, 58, 73	0
1	B	464/478 (97%)	-0.38	0 100 100	17, 36, 59, 73	0
All	All	923/956 (96%)	-0.39	1 (0%) 95 97	17, 36, 58, 73	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	492	HIS	2.1

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^{th} 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^2)	Q<0.9
3	CM5	B	502	34/34	0.78	0.29	6.71	48,88,101,102	0
3	CM5	A	502	34/34	0.82	0.32	5.43	52,97,107,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CM5	A	503	34/34	0.87	0.30	2.59	63,106,117,117	0
3	CM5	B	503	34/34	0.83	0.27	2.19	66,142,167,172	0
2	HEM	B	501	43/43	0.98	0.15	0.06	16,20,32,39	0
2	HEM	A	501	43/43	0.98	0.14	-0.04	14,21,28,31	0

6.5 Other polymers (i)

There are no such residues in this entry.