



Full wwPDB X-ray Structure Validation Report

Sep 2, 2014 – 05:29 PM EDT

PDB ID : 3MDT
Title : Voriconazole complex of Cytochrome P450 46A1
Authors : Mast, N.; Charvet, C.; Pikuleva, I.; Stout, C.D.
Deposited on : 2010-03-30
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

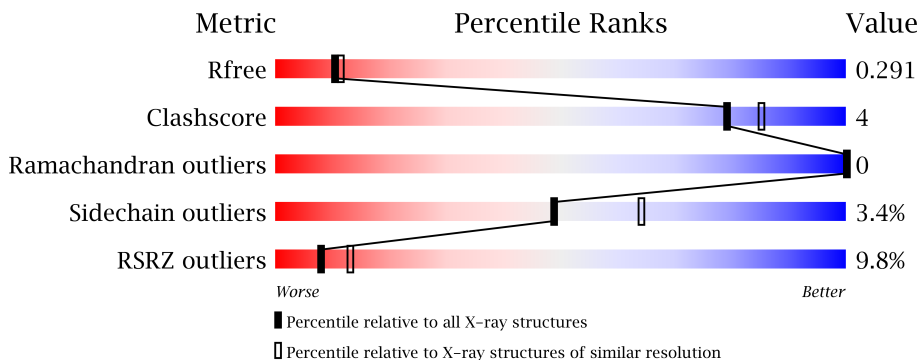
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance



The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	456	
1	B	456	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	VOR	A	506	X	X
3	VOR	B	506	X	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7350 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

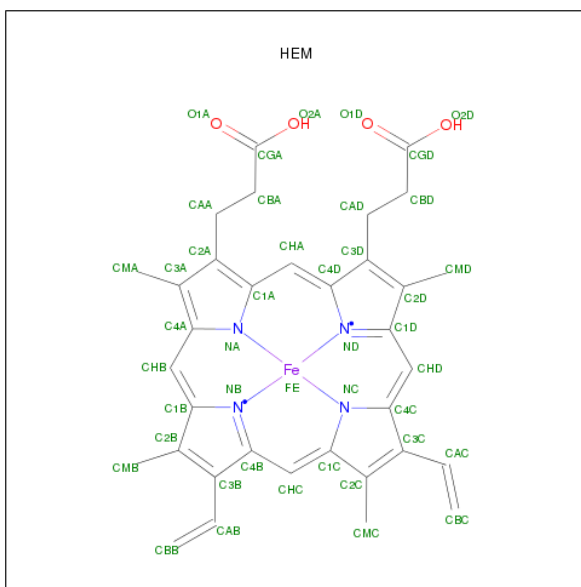
- Molecule 1 is a protein called Cholesterol 24-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3418	2181	598	622	17			
1	B	424	Total	C	N	O	S	0	0	0
			3418	2181	598	622	17			

There are 12 discrepancies between the modelled and reference sequences:

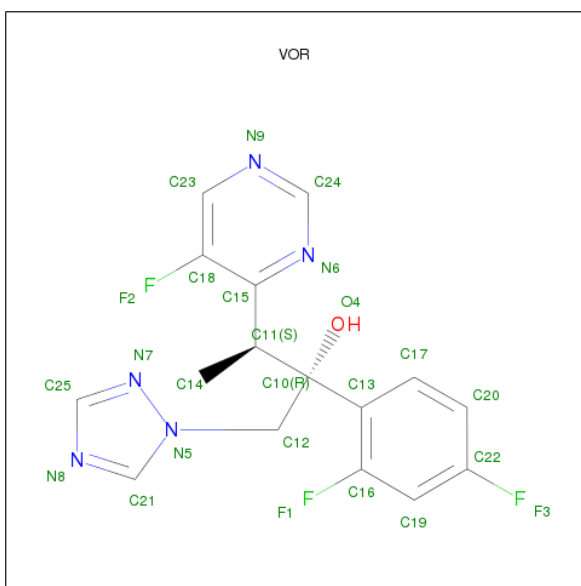
Chain	Residue	Modelled	Actual	Comment	Reference
A	49	MET	-	EXPRESSION TAG	UNP Q9Y6A2
A	50	ALA	-	EXPRESSION TAG	UNP Q9Y6A2
A	501	HIS	-	EXPRESSION TAG	UNP Q9Y6A2
A	502	HIS	-	EXPRESSION TAG	UNP Q9Y6A2
A	503	HIS	-	EXPRESSION TAG	UNP Q9Y6A2
A	504	HIS	-	EXPRESSION TAG	UNP Q9Y6A2
B	49	MET	-	EXPRESSION TAG	UNP Q9Y6A2
B	50	ALA	-	EXPRESSION TAG	UNP Q9Y6A2
B	501	HIS	-	EXPRESSION TAG	UNP Q9Y6A2
B	502	HIS	-	EXPRESSION TAG	UNP Q9Y6A2
B	503	HIS	-	EXPRESSION TAG	UNP Q9Y6A2
B	504	HIS	-	EXPRESSION TAG	UNP Q9Y6A2

- 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 VORICONAZOLE (three-letter code: VOR) (formula: $C_{16}H_{14}F_3N_5O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			25	16	3	5	1		
3	B	1	Total	C	F	N	O	0	0
			25	16	3	5	1		

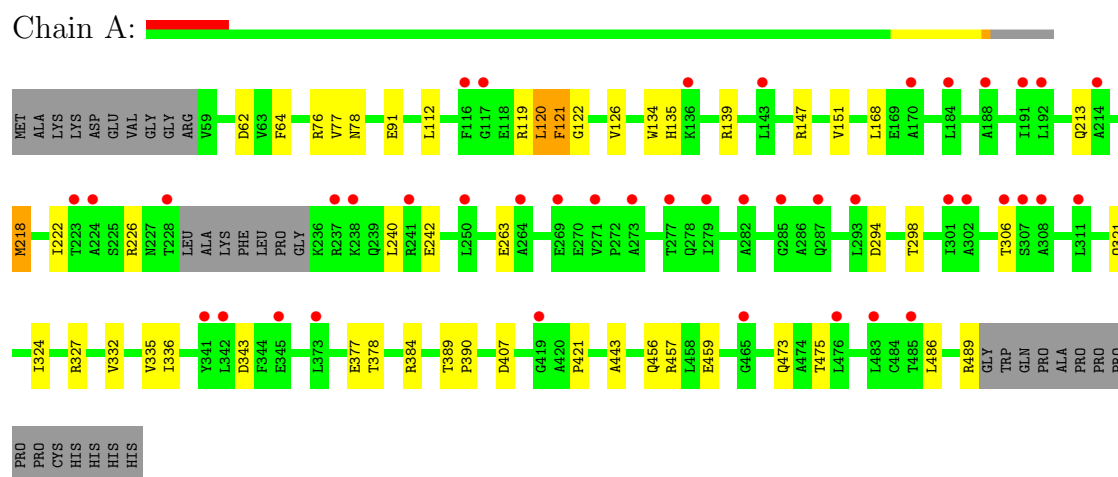
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	182	Total 182	O 182	0	0
4	B	196	Total 196	O 196	0	0

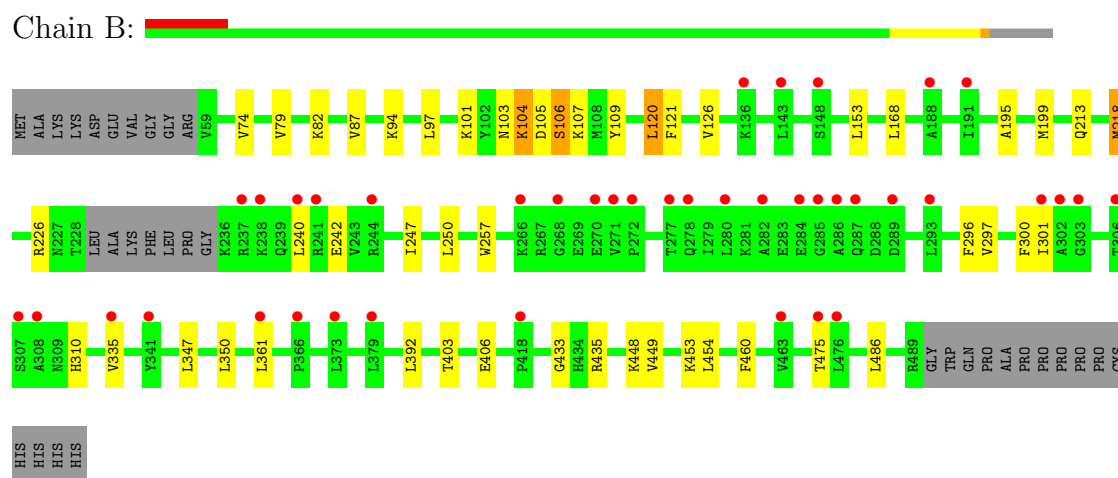
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cholesterol 24-hydroxylase



- Molecule 1: Cholesterol 24-hydroxylase



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	121.60Å 121.60Å 143.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.86 – 2.30 42.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (92.86-2.30) 99.4 (42.99-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.229 , 0.287 0.235 , 0.291	Depositor DCC
R_{free} test set	2340 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 14.8	EDS
Estimated twinning fraction	0.500 for H, K, L 0.500 for -H, K, -L 0.208 for -h,k,-l	Xtriage
Reported twinning fraction	0.500 for H, K, L 0.500 for -H, K, -L	Depositor
L-test for twinning	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	1 of 46043 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7350	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.41	2/3485 (0.1%)	0.65	6/4700 (0.1%)
1	B	0.43	2/3485 (0.1%)	0.62	8/4700 (0.2%)
All	All	0.42	4/6970 (0.1%)	0.63	14/9400 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	120	LEU	C-N	-5.97	1.20	1.34
1	A	120	LEU	C-N	-5.84	1.20	1.34
1	A	119	ARG	NE-CZ	-5.50	1.25	1.33
1	B	101	LYS	C-N	-5.13	1.22	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ARG	CD-NE-CZ	20.15	151.81	123.60
1	A	119	ARG	NE-CZ-NH1	10.49	125.54	120.30
1	A	120	LEU	O-C-N	-9.48	107.53	122.70
1	A	119	ARG	O-C-N	-8.31	109.41	122.70
1	A	121	PHE	O-C-N	-7.78	109.98	123.20
1	B	105	ASP	CB-CG-OD1	7.75	125.28	118.30
1	B	120	LEU	C-N-CA	6.25	137.31	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	ASN	O-C-N	6.17	132.58	122.70
1	B	103	ASN	C-N-CA	5.68	135.89	121.70
1	B	121	PHE	O-C-N	-5.67	113.55	123.20
1	A	119	ARG	C-N-CA	5.52	135.50	121.70
1	B	106	SER	O-C-N	-5.51	113.88	122.70
1	B	120	LEU	O-C-N	-5.36	114.12	122.70
1	B	105	ASP	N-CA-CB	5.29	120.11	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	PHE	Mainchain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3418	0	3463	24	0
1	B	3418	0	3463	23	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
3	A	25	0	13	4	0
3	B	25	0	14	2	0
4	A	182	0	0	0	0
4	B	196	0	0	1	0
All	All	7350	0	7013	49	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (49) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:120:LEU:HD11	1:B:218:MET:HE2	1.34	1.06
1:A:421:PRO:HD3	1:B:406:GLU:HB2	1.70	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:475:THR:HG22	3:B:506:VOR:H14	1.77	0.67
1:A:120:LEU:HD21	1:A:218:MET:CE	2.28	0.63
1:A:64:PHE:CE1	1:A:77:VAL:HG11	2.33	0.63
1:B:168:LEU:HB3	1:B:486:LEU:HD22	1.82	0.62
1:A:120:LEU:HD21	1:A:218:MET:HE1	1.85	0.59
1:B:310:HIS:CE1	1:B:361:LEU:HG	2.38	0.58
1:A:77:VAL:HG12	1:A:78:ASN:N	2.21	0.55
1:B:104:LYS:HD2	1:B:435:ARG:CZ	2.41	0.50
1:A:456:GLN:HB3	1:A:457:ARG:HG2	1.93	0.50
1:B:347:LEU:HD22	1:B:448:LYS:HB3	1.93	0.50
1:A:443:ALA:HB2	2:A:505:HEM:HHC	1.94	0.50
1:A:321:GLN:HB3	1:A:324:ILE:HD12	1.93	0.50
1:B:350:LEU:HB2	1:B:448:LYS:HE2	1.94	0.50
1:A:126:VAL:HG23	1:A:298:THR:HG23	1.94	0.49
2:B:505:HEM:HBC2	2:B:505:HEM:HMC2	1.93	0.49
1:A:91:GLU:HG2	1:B:94:LYS:HD2	1.94	0.49
1:B:120:LEU:HD13	1:B:247:ILE:HG12	1.95	0.48
1:A:475:THR:HG22	3:A:506:VOR:H14	1.96	0.48
1:B:199:MET:HG3	1:B:257:TRP:CG	2.48	0.47
1:A:306:THR:OG1	3:A:506:VOR:H25	2.15	0.47
2:B:505:HEM:C1A	3:B:506:VOR:H21	2.50	0.46
1:A:147:ARG:O	1:A:151:VAL:HG23	2.16	0.46
2:A:505:HEM:HBB2	2:A:505:HEM:HMB1	1.98	0.46
1:A:112:LEU:HD23	1:A:222:ILE:HD12	1.97	0.45
2:A:505:HEM:C4B	3:A:506:VOR:H25	2.51	0.45
1:B:296:PHE:O	1:B:300:PHE:HB2	2.16	0.45
1:A:120:LEU:HD21	1:A:218:MET:HE2	2.00	0.43
1:B:250:LEU:HD23	1:B:297:VAL:HG13	2.00	0.43
1:A:459:GLU:HG3	1:A:489:ARG:HG3	2.00	0.43
1:B:104:LYS:HG2	1:B:109:TYR:CE1	2.54	0.43
1:B:153:LEU:HD22	1:B:195:ALA:HB1	2.01	0.42
1:B:82:LYS:HE3	1:B:107:LYS:O	2.19	0.42
1:B:104:LYS:HE3	4:B:616:HOH:O	2.19	0.42
1:A:112:LEU:HD22	3:A:506:VOR:H23	2.01	0.42
1:B:79:VAL:HG11	1:B:392:LEU:HD12	2.01	0.42
1:A:168:LEU:HB3	1:A:486:LEU:CD2	2.50	0.42
1:A:389:THR:HA	1:A:390:PRO:HD3	1.90	0.41
1:A:77:VAL:CG1	1:A:78:ASN:N	2.82	0.41
1:B:454:LEU:HD22	1:B:460:PHE:HZ	1.84	0.41
1:A:377:GLU:OE1	1:A:384:ARG:HD3	2.21	0.41
1:A:122:GLY:HA3	1:A:294:ASP:CG	2.41	0.41
1:B:218:MET:CE	1:B:301:ILE:HG13	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:74:VAL:HG22	1:B:87:VAL:HG13	2.03	0.40
1:B:97:LEU:O	1:B:433:GLY:HA3	2.21	0.40
1:B:449:VAL:O	1:B:453:LYS:HG3	2.21	0.40
1:A:134:TRP:CZ3	1:A:135:HIS:HD2	2.39	0.40
1:A:332:VAL:HG13	1:A:336:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	420/456 (92%)	407 (97%)	13 (3%)	0	100	100
1	B	420/456 (92%)	408 (97%)	12 (3%)	0	100	100
All	All	840/912 (92%)	815 (97%)	25 (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	372/397 (94%)	357 (96%)	15 (4%)	42	56
1	B	372/397 (94%)	362 (97%)	10 (3%)	57	74
All	All	744/794 (94%)	719 (97%)	25 (3%)	49	64

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ASP
1	A	76	ARG
1	A	139	ARG
1	A	213	GLN
1	A	218	MET
1	A	226	ARG
1	A	240	LEU
1	A	242	GLU
1	A	263	GLU
1	A	327	ARG
1	A	335	VAL
1	A	343	ASP
1	A	378	THR
1	A	407	ASP
1	A	473	GLN
1	B	104	LYS
1	B	106	SER
1	B	126	VAL
1	B	213	GLN
1	B	218	MET
1	B	226	ARG
1	B	240	LEU
1	B	242	GLU
1	B	335	VAL
1	B	403	THR

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	135	HIS
1	A	434	HIS
1	B	81	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	505	1,3	42,50,50	4.43	20 (47%)	27,82,82	1.32	4 (14%)
3	VOR	A	506	2	27,27,27	3.91	17 (62%)	39,39,39	3.81	27 (69%)
2	HEM	B	505	1,3	42,50,50	4.49	20 (47%)	27,82,82	1.44	6 (22%)
3	VOR	B	506	2	27,27,27	3.65	18 (66%)	39,39,39	3.39	22 (56%)

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	505	1,3	-	0/14/114/114	0/0/8/8
3	VOR	A	506	2	-	0/21/21/21	0/3/3/3
2	HEM	B	505	1,3	-	0/14/114/114	0/0/8/8
3	VOR	B	506	2	-	0/21/21/21	0/3/3/3

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	505	HEM	C3C-C4C	-16.34	1.32	1.45
2	A	505	HEM	C3C-C4C	-15.68	1.33	1.45
2	B	505	HEM	C1B-C2B	-15.04	1.33	1.45
2	A	505	HEM	C1B-C2B	-14.83	1.33	1.45
2	A	505	HEM	FE-NB	8.42	2.26	1.95
2	B	505	HEM	FE-NB	8.26	2.25	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	506	VOR	C23-C18	7.80	1.44	1.37
3	B	506	VOR	C25-N8	7.34	1.40	1.34
3	B	506	VOR	C12-C10	-7.18	1.47	1.55
3	A	506	VOR	C25-N8	6.80	1.40	1.34
2	A	505	HEM	CHC-C4B	-6.30	1.32	1.39
3	B	506	VOR	C21-N5	6.29	1.40	1.33
3	B	506	VOR	C23-C18	6.16	1.43	1.37
2	B	505	HEM	CHC-C4B	-6.02	1.32	1.39
3	A	506	VOR	C21-N5	5.79	1.39	1.33
3	A	506	VOR	C12-C10	-5.72	1.49	1.55
2	B	505	HEM	C1A-NA	5.57	1.45	1.36
3	A	506	VOR	C19-C16	5.52	1.47	1.37
2	A	505	HEM	C1A-NA	5.23	1.45	1.36
3	A	506	VOR	C18-C15	5.03	1.44	1.38
3	A	506	VOR	C25-N7	5.02	1.40	1.32
2	A	505	HEM	C3B-C2B	4.83	1.50	1.45
3	A	506	VOR	C24-N9	4.71	1.39	1.33
3	B	506	VOR	C18-C15	4.59	1.44	1.38
3	B	506	VOR	C25-N7	4.53	1.40	1.32
2	B	505	HEM	C1A-C2A	4.53	1.50	1.43
3	A	506	VOR	C17-C13	4.51	1.45	1.39
2	B	505	HEM	C4A-C3A	4.50	1.50	1.43
2	B	505	HEM	C3C-C2C	4.50	1.48	1.45
2	A	505	HEM	C3C-C2C	4.49	1.48	1.45
2	A	505	HEM	C4A-C3A	4.41	1.50	1.43
3	A	506	VOR	C15-N6	4.40	1.39	1.34
3	A	506	VOR	C24-N6	4.39	1.42	1.33
2	A	505	HEM	C1C-C2C	-4.36	1.32	1.43
2	A	505	HEM	C1A-C2A	4.34	1.50	1.43
2	B	505	HEM	C3B-C2B	4.32	1.49	1.45
2	A	505	HEM	CMC-C2C	4.05	1.52	1.45
2	B	505	HEM	C1C-C2C	-4.03	1.33	1.43
2	A	505	HEM	CBB-CAB	4.00	1.51	1.29
3	B	506	VOR	C13-C16	3.97	1.44	1.38
2	B	505	HEM	CBB-CAB	3.94	1.51	1.29
2	B	505	HEM	CMC-C2C	3.93	1.52	1.45
2	A	505	HEM	CMB-C2B	3.92	1.52	1.45
3	B	506	VOR	C24-N9	3.91	1.38	1.33
2	B	505	HEM	C3D-C2D	-3.87	1.33	1.43
2	B	505	HEM	CMD-C2D	3.86	1.51	1.45
2	A	505	HEM	C3D-C2D	-3.85	1.33	1.43
2	A	505	HEM	CMD-C2D	3.79	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	505	HEM	CMB-C2B	3.76	1.51	1.45
3	B	506	VOR	C19-C22	3.45	1.43	1.37
3	A	506	VOR	C14-C11	-3.42	1.47	1.53
3	A	506	VOR	C19-C22	3.35	1.43	1.37
3	A	506	VOR	C20-C17	3.29	1.44	1.38
3	A	506	VOR	C23-N9	3.29	1.41	1.34
3	B	506	VOR	C24-N6	3.22	1.40	1.33
3	B	506	VOR	C19-C16	3.11	1.43	1.37
3	A	506	VOR	C21-N8	3.11	1.40	1.34
2	B	505	HEM	C3C-CAC	3.10	1.50	1.40
3	B	506	VOR	C15-N6	3.07	1.37	1.34
3	B	506	VOR	C20-C22	2.98	1.42	1.37
3	B	506	VOR	C17-C13	2.93	1.43	1.39
2	A	505	HEM	C3C-CAC	2.91	1.49	1.40
3	B	506	VOR	C21-N8	2.89	1.40	1.34
3	A	506	VOR	C20-C22	2.82	1.42	1.37
3	B	506	VOR	C20-C17	2.75	1.43	1.38
2	B	505	HEM	C4D-C3D	2.50	1.50	1.43
3	B	506	VOR	C23-N9	2.44	1.39	1.34
2	B	505	HEM	FE-NC	2.34	2.05	1.95
2	A	505	HEM	C4D-C3D	2.29	1.49	1.43
2	B	505	HEM	C3B-CAB	-2.28	1.32	1.40
3	B	506	VOR	C12-N5	-2.27	1.39	1.48
2	A	505	HEM	C1D-C2D	2.27	1.49	1.43
2	A	505	HEM	FE-NC	2.14	2.04	1.95
2	B	505	HEM	C1D-C2D	2.09	1.49	1.43
2	A	505	HEM	C3B-CAB	-2.06	1.33	1.40

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	506	VOR	F1-C16-C13	9.84	129.45	118.86
3	B	506	VOR	N9-C24-N6	-7.81	119.76	127.90
3	A	506	VOR	N9-C24-N6	-7.42	120.17	127.90
3	B	506	VOR	C25-N7-N5	7.31	109.25	102.81
3	A	506	VOR	C25-N7-N5	7.14	109.09	102.81
3	B	506	VOR	C21-N8-C25	6.58	107.14	102.31
3	A	506	VOR	C21-N8-C25	6.45	107.04	102.31
3	B	506	VOR	C10-C12-N5	6.36	129.65	113.53
3	A	506	VOR	C14-C11-C10	5.41	118.65	111.95
3	B	506	VOR	C11-C15-N6	5.34	123.79	116.13
3	A	506	VOR	C17-C13-C10	-4.95	114.15	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	506	VOR	C14-C11-C10	4.95	118.07	111.95
3	A	506	VOR	C11-C15-N6	4.91	123.18	116.13
3	A	506	VOR	C10-C13-C16	4.82	127.28	122.98
3	B	506	VOR	F1-C16-C13	4.61	123.82	118.86
3	A	506	VOR	F1-C16-C19	-4.56	109.94	118.58
3	A	506	VOR	C14-C11-C15	4.38	119.17	111.21
3	B	506	VOR	C16-C19-C22	4.36	121.35	116.65
3	A	506	VOR	C23-N9-C24	4.31	120.42	115.88
3	A	506	VOR	F2-C18-C15	4.14	122.56	118.06
3	A	506	VOR	C12-C10-C11	4.02	114.16	109.98
3	B	506	VOR	C23-N9-C24	3.93	120.03	115.88
3	A	506	VOR	C19-C16-C13	-3.83	120.61	124.20
3	A	506	VOR	C18-C15-C11	-3.74	116.78	122.94
3	A	506	VOR	C10-C11-C15	-3.71	107.06	113.04
3	B	506	VOR	C18-C15-C11	-3.71	116.84	122.94
3	B	506	VOR	F2-C18-C15	3.69	122.07	118.06
3	B	506	VOR	C20-C22-C19	-3.57	118.56	123.32
3	B	506	VOR	O4-C10-C13	-3.35	102.17	108.33
3	B	506	VOR	C19-C16-C13	-3.34	121.06	124.20
3	A	506	VOR	C10-C12-N5	3.18	121.59	113.53
2	A	505	HEM	C4A-C3A-C2A	3.01	109.09	107.00
3	A	506	VOR	C16-C19-C22	2.89	119.76	116.65
3	B	506	VOR	C12-C10-C11	2.83	112.92	109.98
3	B	506	VOR	C13-C10-C11	2.77	116.19	110.40
3	A	506	VOR	C17-C13-C16	2.75	118.56	115.92
2	B	505	HEM	C4A-C3A-C2A	2.71	108.88	107.00
3	A	506	VOR	N8-C21-N5	-2.66	108.22	111.79
3	B	506	VOR	N8-C21-N5	-2.66	108.22	111.79
2	A	505	HEM	CBD-CAD-C3D	-2.57	108.94	114.51
2	B	505	HEM	C2A-C1A-NA	-2.53	106.23	109.73
3	B	506	VOR	C21-N5-N7	-2.48	107.93	110.33
3	A	506	VOR	N7-C25-N8	-2.47	107.35	114.89
3	A	506	VOR	C18-C23-N9	-2.45	120.19	122.71
2	B	505	HEM	C3A-C4A-NA	-2.44	107.87	109.50
3	B	506	VOR	N7-C25-N8	-2.44	107.42	114.89
3	A	506	VOR	O4-C10-C13	-2.40	103.92	108.33
3	A	506	VOR	F3-C22-C19	2.38	121.70	118.21
2	B	505	HEM	CMA-C3A-C4A	-2.34	124.87	128.46
3	A	506	VOR	C20-C22-C19	-2.34	120.20	123.32
2	B	505	HEM	O2A-CGA-CBA	2.28	122.08	114.19
3	B	506	VOR	C14-C11-C15	2.27	115.33	111.21
3	B	506	VOR	C24-N6-C15	2.20	122.18	118.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	506	VOR	C21-N5-N7	-2.15	108.25	110.33
2	A	505	HEM	CMA-C3A-C4A	-2.14	125.17	128.46
3	A	506	VOR	O4-C10-C12	2.13	112.65	108.42
2	A	505	HEM	C2A-C1A-NA	-2.09	106.83	109.73
2	B	505	HEM	CAD-CBD-CGD	-2.08	109.61	113.53
3	B	506	VOR	C23-C18-C15	-2.07	117.61	122.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	424/456 (92%)	0.77	42 (9%)	8 13	9, 20, 29, 35	0
1	B	424/456 (92%)	0.80	41 (9%)	8 13	8, 21, 33, 37	0
All	All	848/912 (92%)	0.78	83 (9%)	8 13	8, 20, 32, 37	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	271	VAL	3.9
1	B	268	GLY	3.8
1	B	335	VAL	3.5
1	B	286	ALA	3.5
1	A	224	ALA	3.4
1	B	463	VAL	3.4
1	B	285	GLY	3.4
1	B	266	LYS	3.2
1	B	277	THR	3.2
1	A	237	ARG	3.1
1	B	306	THR	3.1
1	B	341	TYR	3.1
1	A	228	THR	3.0
1	A	306	THR	3.0
1	A	293	LEU	2.9
1	A	485	THR	2.9
1	B	241	ARG	2.9
1	B	284	GLU	2.9
1	B	418	PRO	2.9
1	B	303	GLY	2.8
1	B	373	LEU	2.7
1	B	289	ASP	2.7
1	B	237	ARG	2.7
1	B	280	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	188	ALA	2.6
1	B	302	ALA	2.6
1	B	475	THR	2.6
1	A	465	GLY	2.6
1	A	301	ILE	2.6
1	B	238	LYS	2.6
1	B	476	LEU	2.6
1	A	184	LEU	2.5
1	A	117	GLY	2.5
1	B	366	PRO	2.5
1	A	373	LEU	2.5
1	B	301	ILE	2.5
1	A	419	GLY	2.4
1	B	293	LEU	2.4
1	B	282	ALA	2.4
1	A	311	LEU	2.3
1	A	285	GLY	2.3
1	A	188	ALA	2.3
1	A	282	ALA	2.3
1	A	238	LYS	2.3
1	A	287	GLN	2.3
1	B	244	ARG	2.3
1	A	273	ALA	2.3
1	A	192	LEU	2.3
1	A	250	LEU	2.3
1	B	240	LEU	2.2
1	A	302	ALA	2.2
1	A	277	THR	2.2
1	B	287	GLN	2.2
1	B	307	SER	2.2
1	A	223	THR	2.2
1	A	264	ALA	2.2
1	A	483	LEU	2.2
1	A	341	TYR	2.2
1	B	136	LYS	2.1
1	A	116	PHE	2.1
1	A	308	ALA	2.1
1	A	143	LEU	2.1
1	A	307	SER	2.1
1	B	278	GLN	2.1
1	A	191	ILE	2.1
1	A	279	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	191	ILE	2.1
1	A	214	ALA	2.1
1	A	476	LEU	2.1
1	A	136	LYS	2.1
1	B	272	PRO	2.1
1	B	270	GLU	2.1
1	B	361	LEU	2.1
1	B	379	LEU	2.1
1	A	241	ARG	2.0
1	B	143	LEU	2.0
1	A	271	VAL	2.0
1	B	148	SER	2.0
1	A	342	LEU	2.0
1	A	345	GLU	2.0
1	A	170	ALA	2.0
1	B	308	ALA	2.0
1	A	269	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	VOR	B	506	25/25	0.37	3.80	40,44,45,46	0
3	VOR	A	506	25/25	0.36	3.69	40,44,45,46	0
2	HEM	B	505	43/43	0.29	1.94	18,20,24,27	0
2	HEM	A	505	43/43	0.27	1.82	12,17,23,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.