WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:21 AM GMT

PDB ID : 2WV2

Title : X-ray structure of CYP51 from the human pathogen Trypanosoma brucei in complex with fluconazole

Authors : Chen, C.-K.; Leung, S.S.F.; Guilbert, C.; Jacobson, M.; Mckerrow, J.H.; Podust, L.M.

Deposited on : 2009-10-12

Resolution : 2.70 Å(reported)

The following versions of software and data (see references (i)) 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 (i)

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

The reported resolution of this entry is 2.70 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	Percentile Ranks	Value
Rfree		0.261
Clashscore		15
Ramachandran outliers		2.1%
Sidechain outliers		10.7%
RSRZ outliers		2.9%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
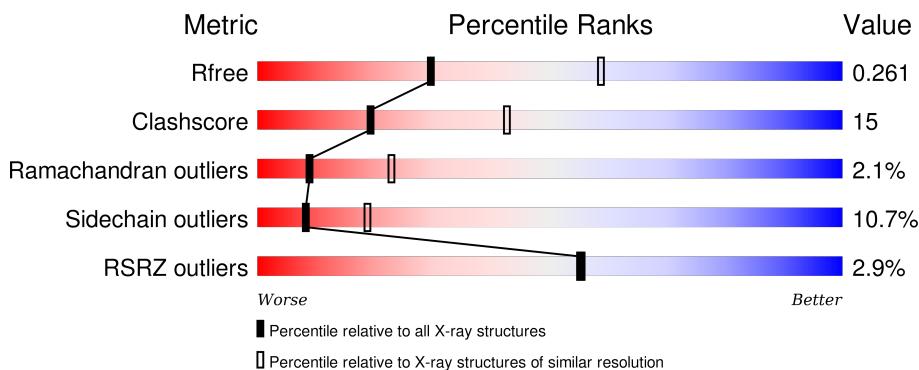
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	475	3% red; 63% green; 25% yellow; 5% orange; 7% grey
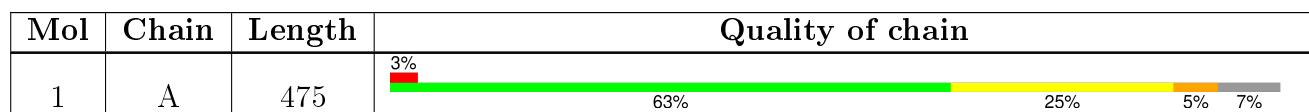
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3508 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 LANOSTEROL 14-ALPHA-DEMETHYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total 3428	C 2192	N 594	O 615	S 27	0	0	0

- Molecule 2 is 2-(2,4-DIFLUOROPHENYL)-1,3-DI(1H-1,2,4-TRIAZOL-1-YL)PROPAN-2-OL (three-letter code: TPF) (formula: $C_{13}H_{12}F_2N_6O$).
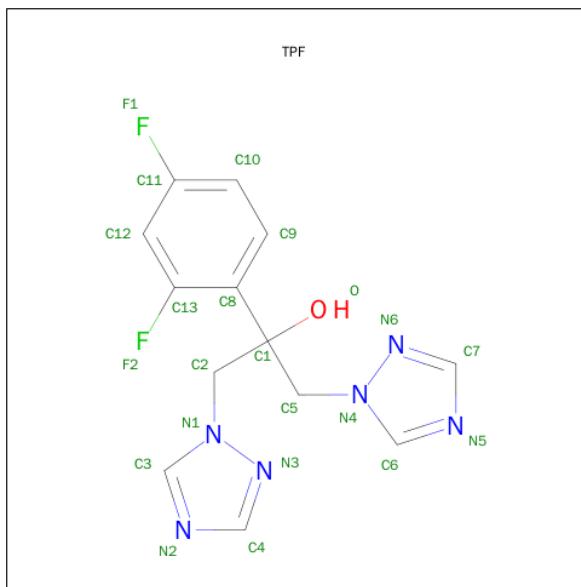
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 22	C 13	F 2	N 6	O 1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

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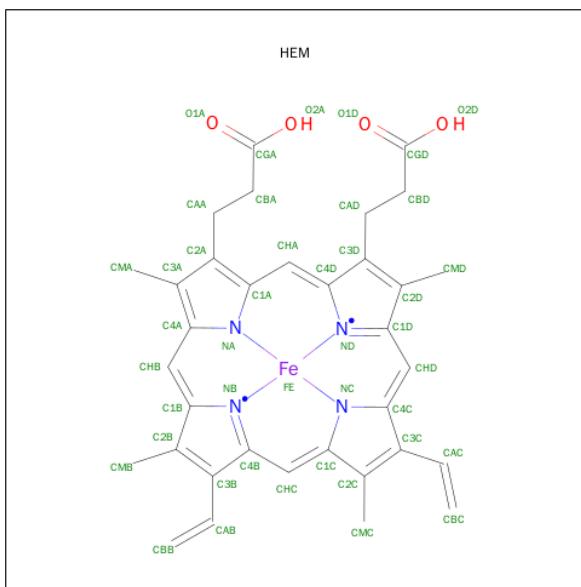
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		

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: LANOSTEROL 14-ALPHA-DEMETHYLASE
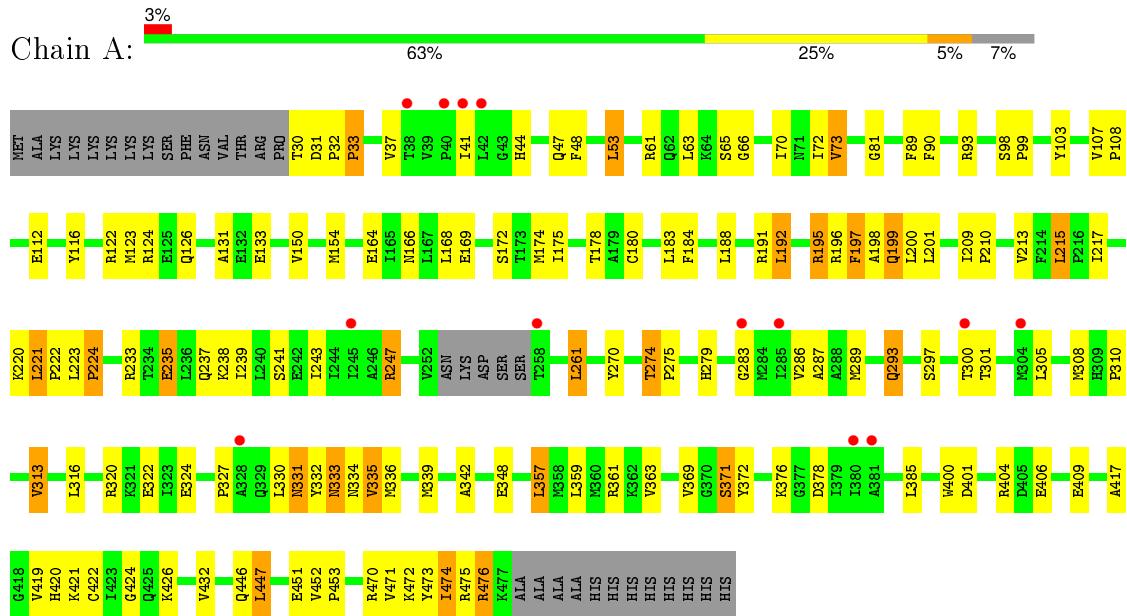
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	106.18Å 106.18Å 99.73Å	Depositor
a, b, c, α, β, γ	90.00° 90.00° 120.00°	
Resolution (Å)	92.06 – 2.70	Depositor
	21.10 – 2.70	EDS
% Data completeness	98.4 (92.06-2.70)	Depositor
(in resolution range)	96.4 (21.10-2.70)	EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.210 , 0.274	Depositor
	0.205 , 0.261	DCC
R_{free} test set	898 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	100.8	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 65.3	EDS
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
L-test for twinning[2]	$< |L| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 17553 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3508	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: TPF, 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	0.80	2/3509 (0.1%)	0.84	2/4761 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	CYS	CB-SG	-6.20	1.71	1.82
1	A	451	GLU	CG-CD	5.10	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	LEU	CB-CG-CD1	-6.78	99.47	111.00
1	A	359	LEU	CA-CB-CG	-5.13	103.49	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3428	0	3342	96	0
2	A	22	0	12	3	0
3	A	43	0	30	10	0
4	A	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3508	0	3384	104	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 15.

All (104) 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:A:1450:HEM:HMB2	3:A:1450:HEM:HBB2	1.58	0.85
1:A:237:GLN:NE2	1:A:279:HIS:HA	1.93	0.83
1:A:30:THR:O	1:A:372:TYR:HA	1.79	0.82
1:A:335:VAL:HB	1:A:339:MET:HE1	1.68	0.74
3:A:1450:HEM:CMB	3:A:1450:HEM:HBB2	2.19	0.72
1:A:320:ARG:O	1:A:324:GLU:HG2	1.89	0.72
1:A:327:PRO:HD2	1:A:334:ASN:HD21	1.54	0.72
1:A:270:TYR:HD1	1:A:274:THR:HG23	1.54	0.71
1:A:33:PRO:HB2	1:A:63:LEU:HD13	1.73	0.70
1:A:293:GLN:HA	1:A:293:GLN:NE2	2.07	0.69
1:A:192:LEU:HD21	1:A:197:PHE:CD1	2.27	0.69
1:A:327:PRO:HD2	1:A:334:ASN:ND2	2.08	0.69
1:A:221:LEU:CB	1:A:222:PRO:HD3	2.24	0.68
1:A:150:VAL:O	1:A:154:MET:HG3	1.93	0.68
1:A:331:ASN:ND2	1:A:334:ASN:OD1	2.27	0.66
1:A:172:SER:HA	1:A:297:SER:OG	1.94	0.66
1:A:166:ASN:HD22	1:A:169:GLU:H	1.40	0.66
1:A:348:GLU:HA	1:A:348:GLU:OE1	1.96	0.66
1:A:316:LEU:HD11	1:A:320:ARG:NH1	2.15	0.62
1:A:330:LEU:HD23	1:A:334:ASN:HD22	1.65	0.62
1:A:192:LEU:HD21	1:A:197:PHE:HD1	1.65	0.60
1:A:166:ASN:ND2	1:A:169:GLU:H	1.99	0.60
1:A:357:LEU:HD22	1:A:385:LEU:HD22	1.84	0.60
1:A:335:VAL:HA	1:A:339:MET:HE3	1.84	0.59
1:A:237:GLN:HE22	1:A:279:HIS:HA	1.68	0.59
1:A:422:CYS:HA	3:A:1450:HEM:CHA	2.33	0.59
1:A:310:PRO:O	1:A:313:VAL:HG22	2.03	0.59
1:A:401:ASP:O	1:A:404:ARG:HG2	2.03	0.58
1:A:363:VAL:HG12	1:A:376:LYS:HA	1.87	0.57
1:A:239:ILE:O	1:A:243:ILE:HG12	2.04	0.57
1:A:327:PRO:CD	1:A:334:ASN:HD21	2.17	0.56
1:A:72:ILE:HG22	1:A:73:VAL:HG23	1.86	0.56
1:A:184:PHE:HB3	1:A:188:LEU:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:CB	1:A:222:PRO:CD	2.83	0.56
1:A:369:VAL:O	1:A:371:SER:O	2.25	0.55
1:A:316:LEU:HD11	1:A:320:ARG:HH11	1.72	0.55
1:A:335:VAL:HA	1:A:339:MET:CE	2.37	0.54
1:A:452:VAL:HG13	1:A:453:PRO:HD2	1.90	0.54
1:A:348:GLU:HG3	1:A:400:TRP:CD1	2.43	0.54
1:A:332:TYR:CE1	1:A:336:MET:HG3	2.43	0.53
2:A:1:TPF:C3	2:A:1:TPF:O	2.58	0.52
1:A:422:CYS:HA	3:A:1450:HEM:C4D	2.45	0.51
1:A:420:HIS:ND1	3:A:1450:HEM:O1D	2.41	0.51
1:A:122:ARG:O	1:A:126:GLN:HG3	2.10	0.51
1:A:61:ARG:HD3	4:A:2001:HOH:O	2.10	0.51
3:A:1450:HEM:HBC2	3:A:1450:HEM:CHD	2.41	0.50
1:A:90:PHE:CG	1:A:417:ALA:HB3	2.47	0.50
1:A:166:ASN:ND2	1:A:168:LEU:H	2.09	0.50
2:A:1:TPF:F2	2:A:1:TPF:O	2.08	0.50
2:A:1:TPF:HC3	2:A:1:TPF:O	2.12	0.49
1:A:168:LEU:O	1:A:172:SER:HB2	2.13	0.49
1:A:237:GLN:HE21	1:A:279:HIS:HA	1.77	0.49
1:A:331:ASN:C	1:A:331:ASN:HD22	2.17	0.48
1:A:200:LEU:HD11	1:A:235:GLU:HG2	1.95	0.48
1:A:243:ILE:O	1:A:247:ARG:HB2	2.13	0.48
1:A:417:ALA:HA	1:A:421:LYS:HD2	1.95	0.47
1:A:330:LEU:CD2	1:A:334:ASN:HD22	2.27	0.47
3:A:1450:HEM:HBC2	3:A:1450:HEM:HHD	1.97	0.46
1:A:371:SER:O	1:A:372:TYR:HB2	2.15	0.46
1:A:131:ALA:C	1:A:133:GLU:H	2.18	0.46
1:A:210:PRO:O	1:A:213:VAL:HG23	2.15	0.46
1:A:474:ILE:O	1:A:474:ILE:HG13	2.16	0.46
1:A:32:PRO:HA	1:A:372:TYR:CD1	2.51	0.46
1:A:32:PRO:HA	1:A:372:TYR:CE1	2.50	0.46
1:A:223:LEU:N	1:A:224:PRO:HD3	2.31	0.46
1:A:322:GLU:CD	1:A:339:MET:HA	2.37	0.45
1:A:73:VAL:HG11	1:A:215:LEU:HD11	1.97	0.45
1:A:308:MET:SD	1:A:447:LEU:HD13	2.56	0.45
1:A:327:PRO:CG	1:A:334:ASN:HD21	2.30	0.45
1:A:195:ARG:O	1:A:196:ARG:C	2.55	0.45
1:A:476:ARG:H	1:A:476:ARG:HG2	1.68	0.44
3:A:1450:HEM:HMB2	3:A:1450:HEM:CBB	2.39	0.43
1:A:70:ILE:HD11	1:A:72:ILE:HD11	1.99	0.43
1:A:191:ARG:O	1:A:196:ARG:HD2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:GLY:HA3	3:A:1450:HEM:C3C	2.54	0.43
1:A:37:VAL:HG22	1:A:44:HIS:HE1	1.82	0.43
1:A:103:TYR:HD2	1:A:116:TYR:CD2	2.36	0.43
1:A:300:THR:OG1	1:A:432:VAL:HG22	2.19	0.43
1:A:107:VAL:N	1:A:108:PRO:CD	2.82	0.43
1:A:89:PHE:CZ	1:A:361:ARG:HG2	2.53	0.43
1:A:233:ARG:HH21	1:A:279:HIS:CE1	2.36	0.43
1:A:270:TYR:HD1	1:A:274:THR:CG2	2.28	0.43
1:A:286:VAL:O	1:A:287:ALA:C	2.55	0.43
1:A:198:ALA:O	1:A:199:GLN:C	2.54	0.43
1:A:73:VAL:O	1:A:73:VAL:HG12	2.19	0.43
1:A:322:GLU:OE1	1:A:339:MET:HA	2.19	0.42
1:A:166:ASN:ND2	1:A:168:LEU:N	2.67	0.42
1:A:183:LEU:HD13	1:A:261:LEU:HD12	2.02	0.42
1:A:174:MET:O	1:A:178:THR:HG23	2.20	0.41
1:A:72:ILE:CG2	1:A:73:VAL:HG23	2.50	0.41
1:A:293:GLN:CA	1:A:293:GLN:NE2	2.80	0.41
1:A:98:SER:HA	1:A:99:PRO:HD3	1.86	0.41
1:A:48:PHE:CD2	1:A:48:PHE:C	2.93	0.41
1:A:301:THR:O	1:A:305:LEU:HG	2.20	0.41
1:A:333:ASN:HD22	1:A:333:ASN:N	2.18	0.41
1:A:175:ILE:HA	1:A:175:ILE:HD13	1.90	0.41
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.83	0.41
1:A:164:GLU:HB3	1:A:470:ARG:HE	1.85	0.41
1:A:339:MET:HB3	1:A:342:ALA:HB3	2.03	0.41
1:A:66:GLY:O	1:A:81:GLY:N	2.54	0.41
1:A:283:GLY:HA2	1:A:286:VAL:HG22	2.03	0.40
1:A:289:MET:HE3	1:A:289:MET:HA	2.03	0.40
1:A:473:TYR:CD1	1:A:473:TYR:C	2.95	0.40
1:A:422:CYS:HB2	3:A:1450:HEM:C1A	2.56	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	439/475 (92%)	392 (89%)	38 (9%)	9 (2%)	9	23

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ILE
1	A	220	LYS
1	A	65	SER
1	A	476	ARG
1	A	73	VAL
1	A	195	ARG
1	A	221	LEU
1	A	224	PRO
1	A	275	PRO

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	356/413 (86%)	318 (89%)	38 (11%)	8	19

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASP
1	A	33	PRO
1	A	47	GLN
1	A	53	LEU
1	A	93	ARG
1	A	112	GLU
1	A	123	MET
1	A	124	ARG
1	A	192	LEU
1	A	197	PHE

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Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type
1	A	199	GLN
1	A	201	LEU
1	A	209	ILE
1	A	215	LEU
1	A	217	ILE
1	A	235	GLU
1	A	238	LYS
1	A	241	SER
1	A	247	ARG
1	A	261	LEU
1	A	274	THR
1	A	293	GLN
1	A	313	VAL
1	A	331	ASN
1	A	333	ASN
1	A	335	VAL
1	A	371	SER
1	A	378	ASP
1	A	406	GLU
1	A	409	GLU
1	A	419	VAL
1	A	426	LYS
1	A	446	GLN
1	A	447	LEU
1	A	471	VAL
1	A	472	LYS
1	A	474	ILE
1	A	475	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	157	ASN
1	A	166	ASN
1	A	237	GLN
1	A	293	GLN
1	A	331	ASN
1	A	333	ASN
1	A	334	ASN
1	A	425	GLN

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)

2 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	TPF	A	1	3	16,24,24	3.34	8 (50%)	22,34,34	6.44	17 (77%)
3	HEM	A	1450	1,2	30,50,50	2.12	4 (13%)	24,82,82	3.57	14 (58%)

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	TPF	A	1	3	-	3/16/16/16	0/3/3/3
3	HEM	A	1450	1,2	-	0/10/54/54	0/0/8/8

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1450	HEM	C3B-C4B	-8.47	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1450	HEM	C2C-C1C	-4.03	1.44	1.52
3	A	1450	HEM	C3D-C4D	-3.93	1.46	1.51
2	A	1	TPF	C1-C8	-3.45	1.49	1.53
3	A	1450	HEM	CHC-C4B	-2.35	1.32	1.38
2	A	1	TPF	C6-N5	2.25	1.38	1.34
2	A	1	TPF	C10-C11	2.53	1.42	1.37
2	A	1	TPF	C10-C9	2.84	1.43	1.38
2	A	1	TPF	C6-N4	5.21	1.39	1.33
2	A	1	TPF	N3-N1	5.75	1.43	1.35
2	A	1	TPF	C8-C13	5.96	1.48	1.38
2	A	1	TPF	N6-N4	6.33	1.44	1.35

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	TPF	C1-C8-C13	-15.59	110.76	122.92
3	A	1450	HEM	C3C-CAC-CBC	-10.15	108.89	124.46
2	A	1	TPF	F2-C13-C8	-6.28	112.75	118.88
2	A	1	TPF	C10-C9-C8	-5.83	111.73	121.70
3	A	1450	HEM	C3B-CAB-CBB	-5.38	116.21	124.46
2	A	1	TPF	C5-C1-C8	-4.97	97.95	110.78
3	A	1450	HEM	C1D-CHD-C4C	-4.91	117.61	125.82
3	A	1450	HEM	CBA-CAA-C2A	-3.97	105.42	112.53
3	A	1450	HEM	CMA-C3A-C4A	-3.66	122.30	128.36
2	A	1	TPF	O-C1-C2	-3.44	100.58	108.30
2	A	1	TPF	C13-C12-C11	-3.08	113.41	116.63
3	A	1450	HEM	C3B-C4B-CHC	-2.09	120.23	123.16
3	A	1450	HEM	CHC-C4B-NB	2.03	129.40	124.52
3	A	1450	HEM	CMA-C3A-C2A	2.21	129.86	125.24
2	A	1	TPF	C5-C1-C2	2.38	113.97	109.15
2	A	1	TPF	F2-C13-C12	2.49	123.28	118.59
3	A	1450	HEM	CMD-C2D-C3D	2.55	125.62	114.35
2	A	1	TPF	C2-C1-C8	2.74	117.87	110.78
3	A	1450	HEM	CMC-C2C-C3C	3.24	124.61	116.53
3	A	1450	HEM	C4B-CHC-C1C	3.27	131.29	125.82
2	A	1	TPF	O-C1-C5	3.32	115.74	108.30
2	A	1	TPF	C6-N4-N6	3.80	113.99	108.84
3	A	1450	HEM	CAD-C3D-C4D	4.62	128.76	112.47
2	A	1	TPF	C9-C8-C1	4.68	126.08	121.02
3	A	1450	HEM	CAD-C3D-C2D	4.83	127.09	113.22
3	A	1450	HEM	CMB-C2B-C3B	4.86	128.66	116.53
2	A	1	TPF	C3-N1-N3	5.85	116.76	108.84

Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	TPF	C9-C8-C13	6.16	122.34	116.01
2	A	1	TPF	C9-C10-C11	6.46	125.33	118.35
2	A	1	TPF	C6-N5-C7	11.11	109.64	102.25
2	A	1	TPF	C3-N2-C4	15.46	112.54	102.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	TPF	C1-C2-N1-C3
2	A	1	TPF	C2-C1-C8-C13
2	A	1	TPF	O-C1-C8-C13

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	TPF	3	0
3	A	1450	HEM	10	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, 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	443/475 (93%)	-0.15	13 (2%)	55	55	33, 45, 57, 81	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	PRO	5.2
1	A	258	THR	2.7
1	A	381	ALA	2.6
1	A	285	ILE	2.4
1	A	380	ILE	2.3
1	A	304	MET	2.3
1	A	328	ALA	2.3
1	A	38	THR	2.3
1	A	283	GLY	2.3
1	A	245	ILE	2.2
1	A	42	LEU	2.2
1	A	41	ILE	2.1
1	A	300	THR	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, 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	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	TPF	A	1	22/22	0.92	0.14	-0.51	62,67,82,85	0
3	HEM	A	1450	43/43	0.98	0.12	-1.06	49,55,65,72	0

6.5 Other polymers (i)

There are no such residues in this entry.