Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:22 AM GMT

PDB ID	:	2WUZ
Title	:	X-ray structure of CYP51 from Trypanosoma cruzi in complex with fluconazole in alternative conformation
Authors	:	Chen, C.-K.; Leung, S.S.F.; Guilbert, C.; Jacobson, M.; Mckerrow, J.H.; Podust, L.M.
Deposited on	:	2009-10-11
Resolution	:	2.35 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:

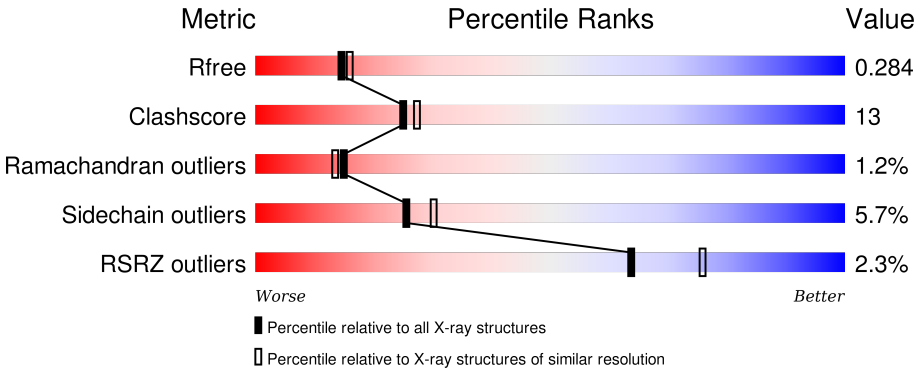
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	473	2% 71% 20% 6%
1	B	473	2% 67% 24% 6%

2 Entry composition

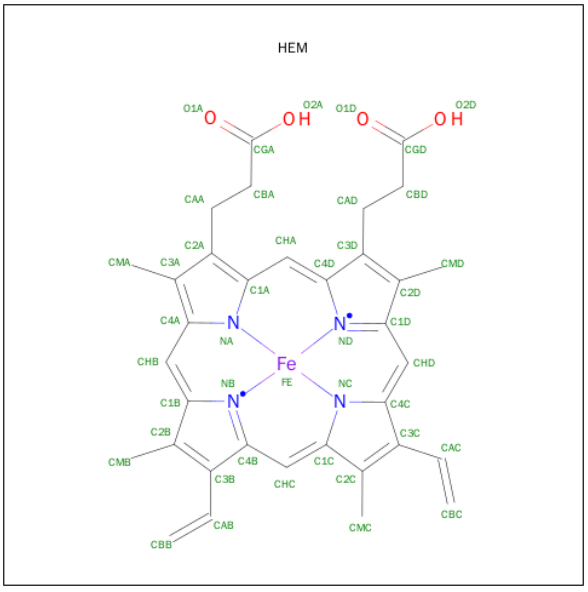
There are 4 unique types of molecules in this entry. The entry contains 7300 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, PUTATIVE.

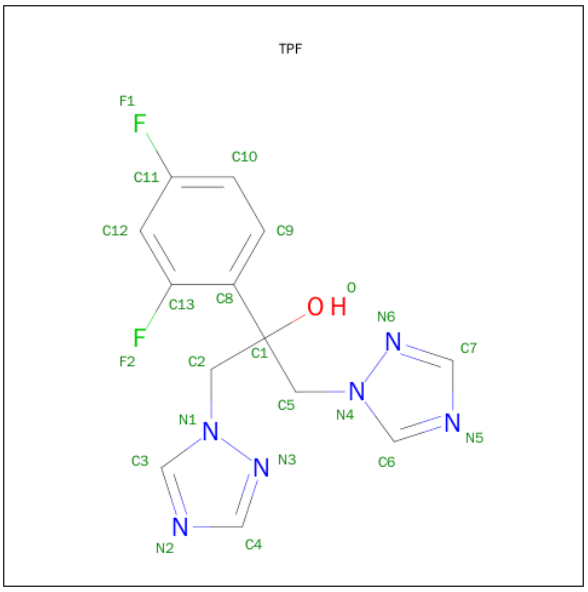
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	2	0
			3490	2233	615	614	28			
1	B	444	Total	C	N	O	S	0	2	0
			3504	2249	607	620	28			

- 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 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
3	A	1	Total	C	F	N	O	0	0
			22	13	2	6	1		
3	B	1	Total	C	F	N	O	0	0
			22	13	2	6	1		

- Molecule 4 is water.

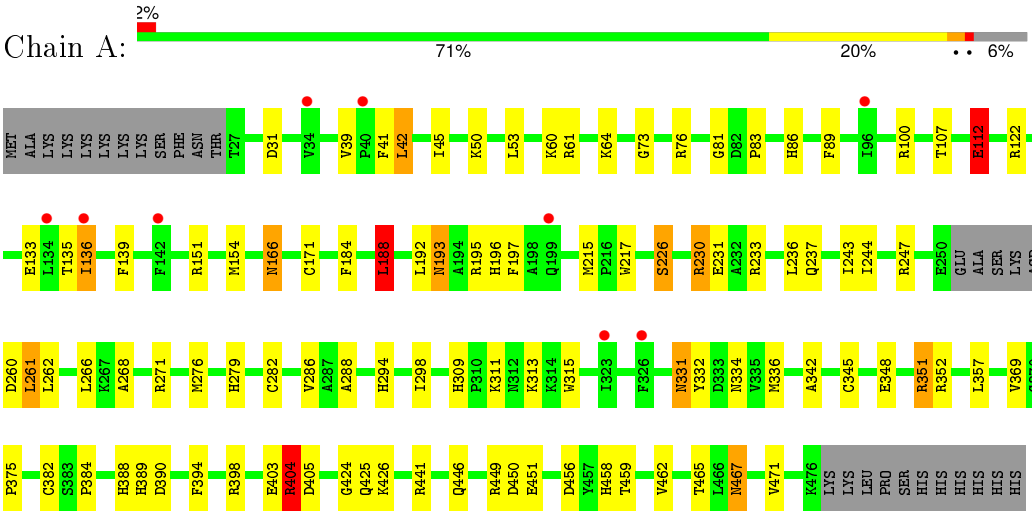
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	83	Total	O	0	0
			83	83		
4	B	93	Total	O	0	0
			93	93		

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.

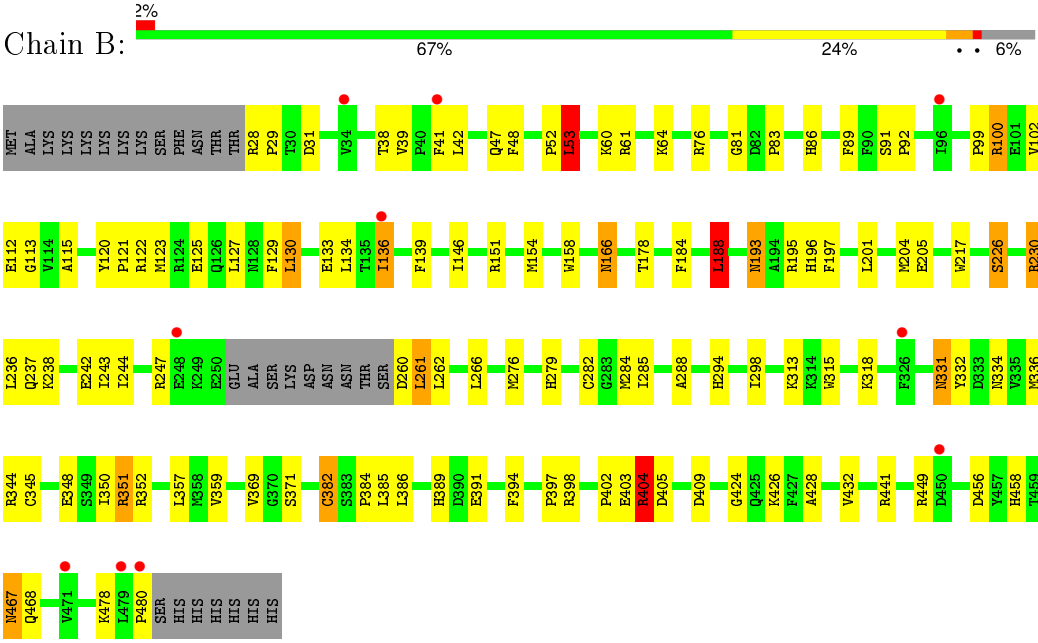
- Molecule 1: LANOSTEROL 14-ALPHA-DEMETHYLASE, PUTATIVE

Chain A:



- Molecule 1: LANOSTEROL 14-ALPHA-DEMETHYLASE, PUTATIVE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.86Å 92.57Å 78.28Å 90.00° 102.14° 90.00°	Depositor
Resolution (Å)	76.53 – 2.35 76.53 – 2.35	Depositor EDS
% Data completeness (in resolution range)	93.6 (76.53-2.35) 93.6 (76.53-2.35)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.217 , 0.275 0.237 , 0.284	Depositor DCC
R_{free} test set	2046 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	42.6	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.6	EDS
Estimated twinning fraction	0.020 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 40834 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7300	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.20% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.88	5/3574 (0.1%)	0.92	10/4844 (0.2%)
1	B	0.88	3/3588 (0.1%)	0.91	11/4860 (0.2%)
All	All	0.88	8/7162 (0.1%)	0.92	21/9704 (0.2%)

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
1	B	0	2
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382	CYS	CB-SG	-6.08	1.72	1.82
1	A	171	CYS	CB-SG	-5.99	1.72	1.82
1	A	231	GLU	CG-CD	5.83	1.60	1.51
1	B	231	GLU	CG-CD	5.75	1.60	1.51
1	A	348	GLU	CD-OE1	-5.73	1.19	1.25
1	A	53	LEU	CG-CD1	-5.58	1.31	1.51
1	A	348	GLU	CD-OE2	-5.47	1.19	1.25
1	B	348	GLU	CD-OE2	-5.40	1.19	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	404	ARG	NE-CZ-NH1	8.36	124.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	404	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	A	351	ARG	NE-CZ-NH2	7.81	124.21	120.30
1	A	230	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	A	31	ASP	CB-CG-OD2	7.05	124.64	118.30
1	A	348	GLU	OE1-CD-OE2	-7.03	114.87	123.30
1	B	53	LEU	CB-CG-CD1	6.94	122.81	111.00
1	B	348	GLU	OE1-CD-OE2	-6.60	115.38	123.30
1	B	351	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	230	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	A	112	GLU	CA-C-N	6.23	128.66	116.20
1	B	404	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	404	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	352	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	480	PRO	N-CA-CB	5.59	110.01	103.30
1	B	31	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	188	LEU	CA-CB-CG	5.43	127.79	115.30
1	B	352	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	390	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	409	ASP	CB-CG-OD1	5.33	123.10	118.30
1	B	188	LEU	CA-CB-CG	5.25	127.38	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	42	LEU	Peptide
1	B	42	LEU	Peptide
1	B	478	LYS	Peptide

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	3490	0	3453	85	0
1	B	3504	0	3480	99	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	22	0	12	0	0
3	B	22	0	12	4	0
4	A	83	0	0	3	0
4	B	93	0	0	7	0
All	All	7300	0	7017	180	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 13.

All (180) 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:136:ILE:CD1	1:A:426:LYS:NZ	2.35	0.89
1:B:331:ASN:ND2	1:B:334:ASN:H	1.71	0.89
1:A:331:ASN:ND2	1:A:334:ASN:H	1.74	0.86
1:A:193:ASN:ND2	1:A:196:HIS:H	1.75	0.85
1:A:217:TRP:CH2	1:B:217:TRP:HH2	1.95	0.84
1:A:449:ARG:O	1:A:449:ARG:HG2	1.77	0.84
1:B:136:ILE:HD12	1:B:426:LYS:NZ	1.95	0.82
1:A:217:TRP:HH2	1:B:217:TRP:CH2	1.97	0.82
1:B:136:ILE:CD1	1:B:426:LYS:NZ	2.44	0.81
1:B:369:VAL:O	1:B:371:SER:O	1.99	0.81
1:B:130[B]:LEU:HD11	1:B:288:ALA:HB2	1.64	0.80
1:B:404:ARG:HG3	4:B:2061:HOH:O	1.81	0.79
1:A:369:VAL:O	1:A:371:SER:O	2.01	0.78
1:A:136:ILE:HD12	1:A:426:LYS:NZ	2.01	0.76
1:A:136:ILE:HD11	1:A:426:LYS:HE2	1.69	0.75
1:A:217:TRP:CH2	1:B:217:TRP:CH2	2.74	0.75
1:B:460:MET:HG2	3:B:1460:TPF:HC7	1.70	0.73
1:B:136:ILE:CD1	1:B:426:LYS:HZ1	2.00	0.73
1:A:193:ASN:HD21	1:A:196:HIS:H	1.32	0.73
1:A:136:ILE:HD12	1:A:426:LYS:HZ3	1.53	0.72
1:A:217:TRP:HH2	1:B:217:TRP:HH2	1.34	0.72
1:B:130[A]:LEU:HD23	1:B:284:MET:HB3	1.73	0.70
1:A:136:ILE:HD11	1:A:426:LYS:CE	2.21	0.70
1:A:315:TRP:HZ3	1:A:403:GLU:OE2	1.72	0.70
1:A:136:ILE:CD1	1:A:426:LYS:HE2	2.23	0.69
1:B:136:ILE:HD12	1:B:426:LYS:HZ3	1.56	0.69
1:A:136:ILE:CD1	1:A:426:LYS:CE	2.71	0.69
1:B:193:ASN:ND2	1:B:196:HIS:H	1.91	0.67
1:B:331:ASN:HD21	1:B:334:ASN:H	1.39	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:HIS:CD2	1:B:298:ILE:HD11	2.30	0.67
1:A:136:ILE:CD1	1:A:426:LYS:HZ1	2.06	0.67
1:B:151:ARG:HA	1:B:154:MET:HE2	1.79	0.65
1:B:61:ARG:O	1:B:64:LYS:HD3	1.97	0.65
1:A:151:ARG:HA	1:A:154:MET:HE2	1.76	0.65
1:B:404:ARG:HG2	1:B:405:ASP:N	2.12	0.64
1:B:331:ASN:HD22	1:B:331:ASN:C	2.00	0.64
1:A:424:GLY:HA3	2:A:1450:HEM:C3C	2.32	0.64
1:B:233:ARG:HB3	4:B:2032:HOH:O	1.97	0.64
3:B:1460:TPF:O	3:B:1460:TPF:C6	2.46	0.64
1:A:404:ARG:HG2	1:A:405:ASP:N	2.13	0.63
1:B:242:GLU:OE2	4:B:2036:HOH:O	2.15	0.63
1:A:331:ASN:H	1:A:334:ASN:HD22	1.44	0.63
1:B:318:LYS:HD2	4:B:2059:HOH:O	1.98	0.62
1:A:76:ARG:HD2	4:A:2007:HOH:O	1.99	0.62
1:A:331:ASN:HD21	1:A:334:ASN:H	1.47	0.62
1:B:351:ARG:HD3	1:B:394:PHE:CD1	2.34	0.61
1:A:456:ASP:OD1	1:A:458:HIS:HD2	1.84	0.60
1:A:351:ARG:HD3	1:A:394:PHE:CD1	2.37	0.59
1:A:61:ARG:O	1:A:64:LYS:HD3	2.03	0.59
1:A:449:ARG:O	1:A:451:GLU:N	2.36	0.59
1:A:357:LEU:O	1:A:384:PRO:HD2	2.02	0.58
1:B:136:ILE:O	1:B:136:ILE:HG12	2.03	0.58
3:B:1460:TPF:O	3:B:1460:TPF:HC6	2.03	0.58
1:B:244:ILE:HG12	1:B:266:LEU:HD11	1.86	0.58
1:B:315:TRP:HZ3	1:B:403:GLU:OE2	1.84	0.58
1:A:244:ILE:HD11	1:A:262:LEU:HD11	1.84	0.58
1:A:449:ARG:O	1:A:449:ARG:CG	2.44	0.57
1:B:129:PHE:HD2	1:B:276:MET:HE2	1.70	0.57
1:B:386:LEU:HD12	4:B:2055:HOH:O	2.04	0.57
1:A:217:TRP:CZ2	1:B:217:TRP:HH2	2.22	0.57
1:A:237:GLN:NE2	1:A:279:HIS:HA	2.19	0.57
1:B:237:GLN:NE2	1:B:279:HIS:HA	2.19	0.57
1:A:129:PHE:HD2	1:A:276:MET:HE2	1.69	0.57
1:B:424:GLY:HA3	2:B:1450:HEM:C3C	2.40	0.56
1:A:130:LEU:HD11	1:A:288:ALA:HB2	1.87	0.56
1:A:60:LYS:NZ	1:A:81:GLY:O	2.35	0.56
1:A:226:SER:O	1:A:230:ARG:HG3	2.04	0.56
1:B:357:LEU:O	1:B:384:PRO:HD2	2.06	0.55
1:A:331:ASN:C	1:A:331:ASN:HD22	2.08	0.55
1:B:60:LYS:NZ	1:B:81:GLY:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ASN:C	1:A:193:ASN:HD22	2.10	0.55
1:A:309:HIS:ND1	1:A:311[B]:LYS:HG2	2.22	0.55
1:A:184:PHE:HB3	1:A:188:LEU:HG	1.91	0.53
1:B:129:PHE:HD2	1:B:276:MET:CE	2.22	0.53
1:B:332:TYR:CE1	1:B:336:MET:HG3	2.44	0.53
1:B:389:HIS:NE2	1:B:398:ARG:HD2	2.25	0.52
1:B:331:ASN:H	1:B:334:ASN:HD22	1.57	0.52
1:B:237:GLN:HE21	1:B:282:CYS:CB	2.22	0.51
1:B:107:THR:HG23	1:B:112:GLU:HA	1.91	0.51
1:A:127:LEU:HD13	2:A:1450:HEM:CGD	2.41	0.51
1:B:136:ILE:CD1	1:B:426:LYS:CE	2.89	0.51
1:B:237:GLN:HE21	1:B:282:CYS:HB3	1.74	0.51
1:A:129:PHE:HD2	1:A:276:MET:CE	2.23	0.51
1:A:136:ILE:HD12	1:A:426:LYS:CE	2.40	0.51
1:A:351:ARG:HD2	1:A:388:HIS:HB3	1.92	0.51
1:A:331:ASN:H	1:A:334:ASN:ND2	2.10	0.50
1:B:261:LEU:HD13	1:B:285:ILE:HG12	1.92	0.50
1:B:244:ILE:HD11	1:B:262:LEU:HD11	1.92	0.50
1:B:28:ARG:CB	1:B:29:PRO:HD3	2.42	0.50
1:B:357:LEU:HD22	1:B:385:LEU:HD22	1.93	0.49
1:B:184:PHE:HB3	1:B:188:LEU:HG	1.92	0.49
1:A:332:TYR:CE1	1:A:336:MET:HG3	2.46	0.49
1:A:83:PRO:HA	1:A:86:HIS:CD2	2.47	0.49
1:B:456:ASP:OD1	1:B:458:HIS:HD2	1.96	0.49
1:A:107:THR:CG2	1:A:112:GLU:HA	2.43	0.48
1:A:282:CYS:O	1:A:286:VAL:HG23	2.12	0.48
1:A:342:ALA:O	1:A:345:CYS:HB2	2.13	0.48
1:B:318:LYS:HD3	1:B:341:PHE:CE1	2.47	0.48
1:A:217:TRP:HH2	1:B:217:TRP:CZ2	2.32	0.48
1:B:332:TYR:CZ	1:B:336:MET:HG3	2.49	0.48
1:A:136:ILE:HD11	1:A:426:LYS:NZ	2.26	0.47
1:A:129:PHE:CD2	1:A:268:ALA:HB1	2.49	0.47
1:A:331:ASN:HD22	1:A:334:ASN:H	1.55	0.47
1:A:136:ILE:HG13	1:A:139:PHE:CD2	2.49	0.47
1:A:233:ARG:HB3	4:A:2038:HOH:O	2.14	0.47
1:A:389:HIS:NE2	1:A:398:ARG:HD2	2.30	0.47
1:B:133:GLU:HG2	1:B:261:LEU:HA	1.97	0.47
1:A:446:GLN:O	1:A:471:VAL:HG23	2.15	0.47
1:A:424:GLY:HA3	2:A:1450:HEM:C2C	2.50	0.46
1:A:244:ILE:HG12	1:A:266:LEU:HD11	1.97	0.46
1:B:342:ALA:O	1:B:345:CYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ILE:HD13	1:A:462:VAL:O	2.16	0.46
1:B:48:PHE:O	1:B:52:PRO:HD3	2.15	0.46
1:A:107:THR:HG23	1:A:112:GLU:HA	1.98	0.46
1:A:315:TRP:CZ3	1:A:403:GLU:OE2	2.61	0.46
1:B:226:SER:O	1:B:230:ARG:HG3	2.15	0.46
1:A:133:GLU:HG2	1:A:261:LEU:HD23	1.97	0.46
1:B:136:ILE:HD12	1:B:426:LYS:CE	2.45	0.46
1:B:107:THR:CG2	1:B:112:GLU:HA	2.46	0.46
1:B:91:SER:HB2	1:B:92:PRO:HD3	1.98	0.46
2:B:1450:HEM:HBC2	2:B:1450:HEM:HHD	1.98	0.45
1:B:201:LEU:O	1:B:205[B]:GLU:HB2	2.15	0.45
1:A:217:TRP:CE3	1:B:41:PHE:HE2	2.35	0.45
1:B:193:ASN:HD21	1:B:196:HIS:H	1.61	0.45
1:A:237:GLN:HE21	1:A:282:CYS:HB3	1.81	0.45
1:B:243:ILE:O	1:B:247:ARG:HB2	2.16	0.45
1:B:136:ILE:HG13	1:B:139:PHE:CD2	2.52	0.44
1:B:76:ARG:HD2	4:B:2010:HOH:O	2.17	0.44
1:B:146:ILE:HG23	1:B:178:THR:HG21	2.00	0.44
1:A:294:HIS:CD2	1:A:298:ILE:HD11	2.52	0.44
1:B:136:ILE:HD11	1:B:426:LYS:CE	2.48	0.44
1:B:188:LEU:HD12	1:B:188:LEU:C	2.38	0.44
1:A:89:PHE:CD2	1:A:382:CYS:HB2	2.53	0.44
1:B:28:ARG:CB	1:B:29:PRO:CD	2.95	0.43
1:A:45:ILE:HD12	1:A:215:MET:CE	2.49	0.43
1:B:389:HIS:CD2	1:B:397:PRO:HB2	2.53	0.43
1:B:133:GLU:HG2	1:B:261:LEU:HD23	2.00	0.43
1:B:465:THR:HG22	1:B:467:ASN:HB2	2.01	0.43
1:A:332:TYR:CZ	1:A:336:MET:HG3	2.54	0.43
1:A:247:ARG:NH1	1:A:257:ASN:HA	2.34	0.43
1:B:136:ILE:HD11	1:B:426:LYS:HZ1	1.82	0.43
1:B:294:HIS:CD2	1:B:298:ILE:CD1	3.01	0.43
1:A:133:GLU:HG2	1:A:261:LEU:HA	2.01	0.43
1:A:166:ASN:HD22	1:A:166:ASN:C	2.23	0.42
1:B:331:ASN:HD22	1:B:334:ASN:H	1.60	0.42
1:B:99:PRO:O	1:B:102:VAL:HG22	2.19	0.42
1:B:89:PHE:CD2	1:B:382:CYS:HB2	2.55	0.42
1:B:115:ALA:C	1:B:123:MET:HG3	2.39	0.42
1:B:100:ARG:HE	1:B:100:ARG:HB2	1.35	0.42
1:B:350:ILE:HG21	1:B:350:ILE:HD13	1.84	0.42
1:B:238:LYS:O	1:B:242:GLU:HG3	2.20	0.42
1:B:201:LEU:HD23	1:B:204:MET:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HB3	1:A:45:ILE:HG22	2.01	0.42
1:B:53:LEU:HG	1:B:385:LEU:HD11	2.02	0.42
1:A:217:TRP:CZ3	1:B:41:PHE:HE2	2.38	0.42
1:B:130[A]:LEU:HD11	1:B:288:ALA:HB2	2.01	0.42
3:B:1460:TPF:O	3:B:1460:TPF:F2	2.27	0.42
1:B:121:PRO:O	1:B:125:GLU:HG3	2.19	0.42
1:B:127:LEU:HD13	2:B:1450:HEM:CGD	2.50	0.41
1:B:83:PRO:HA	1:B:86:HIS:CD2	2.55	0.41
1:A:465:THR:HG22	1:A:467:ASN:HB2	2.02	0.41
1:A:41:PHE:O	1:A:73:GLY:HA2	2.20	0.41
1:B:136:ILE:CD1	1:B:426:LYS:HE2	2.50	0.41
1:B:107:THR:N	1:B:108:PRO:HD2	2.36	0.41
1:A:243:ILE:O	1:A:247:ARG:HB2	2.20	0.41
1:B:89:PHE:CZ	1:B:359:VAL:HG12	2.56	0.41
1:B:120:TYR:O	1:B:123:MET:HB3	2.20	0.41
1:B:166:ASN:C	1:B:166:ASN:HD22	2.23	0.41
1:B:154:MET:HG2	1:B:158:TRP:CE3	2.55	0.41
1:A:459:THR:HG22	4:B:2030:HOH:O	2.20	0.41
1:A:188:LEU:HD12	1:A:188:LEU:C	2.41	0.41
1:A:425:GLN:NE2	4:A:2068:HOH:O	2.54	0.41
1:A:331:ASN:N	1:A:334:ASN:HD22	2.15	0.41
1:B:344:ARG:HB3	1:B:402:PRO:O	2.21	0.41
1:B:115:ALA:O	1:B:123:MET:HG3	2.20	0.40
1:B:428:ALA:O	1:B:432:VAL:HG23	2.21	0.40
1:B:266:LEU:HA	1:B:266:LEU:HD23	1.90	0.40
1:A:374:VAL:HA	1:A:375:PRO:HD3	1.85	0.40
1:A:107:THR:HG22	1:A:112:GLU:OE2	2.22	0.40
1:B:449:ARG:CD	1:B:468:GLN:HB3	2.51	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	442/473 (93%)	412 (93%)	23 (5%)	7 (2%)	12	10
1	B	442/473 (93%)	413 (93%)	25 (6%)	4 (1%)	21	22
All	All	884/946 (93%)	825 (93%)	48 (5%)	11 (1%)	15	15

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	GLU
1	A	258	THR
1	A	135	THR
1	A	450	ASP
1	A	467	ASN
1	B	53	LEU
1	B	467	ASN
1	A	372	TYR
1	A	136	ILE
1	B	136	ILE
1	B	113	GLY

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	368/415 (89%)	348 (95%)	20 (5%)	27	33
1	B	372/415 (90%)	349 (94%)	23 (6%)	23	26
All	All	740/830 (89%)	697 (94%)	43 (6%)	25	29

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	VAL
1	A	50	LYS
1	A	100	ARG
1	A	122	ARG
1	A	166	ASN

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Mol	Chain	Res	Type
1	A	188	LEU
1	A	192	LEU
1	A	193	ASN
1	A	195	ARG
1	A	197	PHE
1	A	226	SER
1	A	236	LEU
1	A	260	ASP
1	A	261	LEU
1	A	271	ARG
1	A	313	LYS
1	A	331	ASN
1	A	371	SER
1	A	404	ARG
1	A	441	ARG
1	B	38	THR
1	B	39	VAL
1	B	47	GLN
1	B	53	LEU
1	B	100	ARG
1	B	122	ARG
1	B	130[A]	LEU
1	B	130[B]	LEU
1	B	134	LEU
1	B	166	ASN
1	B	188	LEU
1	B	193	ASN
1	B	195	ARG
1	B	197	PHE
1	B	226	SER
1	B	236	LEU
1	B	260	ASP
1	B	261	LEU
1	B	313	LYS
1	B	331	ASN
1	B	391	GLU
1	B	404	ARG
1	B	441	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	193	ASN
1	A	237	GLN
1	A	293	GLN
1	A	320	HIS
1	A	331	ASN
1	A	334	ASN
1	A	458	HIS
1	B	166	ASN
1	B	193	ASN
1	B	237	GLN
1	B	294	HIS
1	B	320	HIS
1	B	331	ASN
1	B	334	ASN
1	B	425	GLN
1	B	458	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

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	1450	1,3	30,50,50	2.48	7 (23%)	24,82,82	2.81	11 (45%)
3	TPF	A	1460	2	16,24,24	2.64	5 (31%)	22,34,34	4.88	12 (54%)
2	HEM	B	1450	1,3	30,50,50	2.80	6 (20%)	24,82,82	2.34	7 (29%)
3	TPF	B	1460	2	16,24,24	2.67	7 (43%)	22,34,34	5.02	14 (63%)

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	1450	1,3	-	0/10/54/54	0/0/8/8
3	TPF	A	1460	2	-	2/16/16/16	0/3/3/3
2	HEM	B	1450	1,3	-	0/10/54/54	0/0/8/8
3	TPF	B	1460	2	-	1/16/16/16	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1450	HEM	C3B-C4B	-10.91	1.42	1.51
2	A	1450	HEM	C3B-C4B	-9.70	1.43	1.51
2	B	1450	HEM	C3D-C4D	-5.46	1.44	1.51
2	A	1450	HEM	C3D-C4D	-5.21	1.44	1.51
2	B	1450	HEM	C2C-C1C	-4.65	1.43	1.52
3	A	1460	TPF	C1-C8	-4.65	1.48	1.53
2	A	1450	HEM	C2C-C1C	-3.87	1.45	1.52
3	B	1460	TPF	C1-C8	-3.50	1.49	1.53
3	A	1460	TPF	C6-N4	-2.56	1.31	1.33
2	A	1450	HEM	C1C-NC	2.09	1.38	1.36
3	A	1460	TPF	N6-N4	2.13	1.38	1.35
3	B	1460	TPF	C12-C11	2.20	1.41	1.37
3	B	1460	TPF	C10-C11	2.23	1.41	1.37
2	A	1450	HEM	CMA-C3A	2.31	1.56	1.51
2	A	1450	HEM	FE-ND	2.32	2.09	1.97
2	B	1450	HEM	CAA-C2A	2.34	1.56	1.52
2	A	1450	HEM	C4C-NC	2.35	1.38	1.36
3	B	1460	TPF	F2-C13	2.62	1.41	1.35
3	B	1460	TPF	N3-N1	3.03	1.39	1.35
3	B	1460	TPF	N6-N4	3.37	1.40	1.35
2	B	1450	HEM	FE-ND	3.45	2.15	1.97
3	A	1460	TPF	N3-N1	3.57	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1450	HEM	FE-NC	4.58	2.13	1.95
3	B	1460	TPF	C8-C13	7.37	1.50	1.38
3	A	1460	TPF	C8-C13	7.38	1.50	1.38

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1460	TPF	C1-C8-C13	-11.23	114.16	122.92
3	B	1460	TPF	C12-C13-C8	-10.93	115.76	124.21
3	A	1460	TPF	C12-C13-C8	-8.35	117.76	124.21
3	B	1460	TPF	C1-C8-C13	-7.78	116.85	122.92
3	B	1460	TPF	O-C1-C2	-6.29	94.19	108.30
2	A	1450	HEM	C3B-CAB-CBB	-5.21	116.46	124.46
3	A	1460	TPF	C10-C9-C8	-3.54	115.66	121.70
2	A	1450	HEM	CAA-CBA-CGA	-3.41	106.49	112.75
3	A	1460	TPF	O-C1-C5	-3.12	101.31	108.30
2	A	1450	HEM	CAA-C2A-C1A	-2.98	123.77	127.01
2	A	1450	HEM	CMA-C3A-C4A	-2.64	123.99	128.36
2	A	1450	HEM	CBD-CAD-C3D	-2.41	106.54	113.55
3	A	1460	TPF	C2-C1-C8	-2.33	104.77	110.78
3	B	1460	TPF	F2-C13-C8	2.01	120.84	118.88
3	B	1460	TPF	O-C1-C5	2.07	112.93	108.30
2	B	1450	HEM	C2C-C1C-CHC	2.09	126.86	123.68
3	B	1460	TPF	C9-C10-C11	2.10	120.62	118.35
2	A	1450	HEM	C2C-C1C-CHC	2.21	127.05	123.68
2	A	1450	HEM	CMA-C3A-C2A	2.25	129.93	125.24
3	A	1460	TPF	F2-C13-C12	2.34	122.99	118.59
3	B	1460	TPF	C5-C1-C2	2.44	114.11	109.15
3	B	1460	TPF	F2-C13-C12	2.54	123.37	118.59
2	B	1450	HEM	C4B-CHC-C1C	2.55	130.09	125.82
3	B	1460	TPF	C2-C1-C8	2.67	117.69	110.78
2	B	1450	HEM	CMD-C2D-C3D	2.74	126.45	114.35
2	A	1450	HEM	CMC-C2C-C3C	3.31	124.79	116.53
2	B	1450	HEM	CMC-C2C-C3C	3.42	125.08	116.53
3	A	1460	TPF	C3-N1-N3	3.54	113.63	108.84
3	B	1460	TPF	C13-C12-C11	3.71	120.51	116.63
3	B	1460	TPF	C6-N4-N6	3.73	113.89	108.84
3	A	1460	TPF	C9-C10-C11	3.93	122.60	118.35
2	B	1450	HEM	CAD-C3D-C4D	4.29	127.62	112.47
2	A	1450	HEM	CAD-C3D-C4D	4.30	127.62	112.47
2	A	1450	HEM	CAD-C3D-C2D	4.97	127.49	113.22
2	B	1450	HEM	CAD-C3D-C2D	5.02	127.64	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1450	HEM	CMB-C2B-C3B	5.74	130.87	116.53
3	A	1460	TPF	C5-C1-C2	5.99	121.31	109.15
3	B	1460	TPF	C9-C8-C13	6.46	122.65	116.01
3	A	1460	TPF	C9-C8-C13	6.79	122.99	116.01
2	A	1450	HEM	CMB-C2B-C3B	6.82	133.55	116.53
3	A	1460	TPF	C6-N5-C7	8.77	108.09	102.25
3	B	1460	TPF	C3-N2-C4	9.15	108.34	102.25
3	A	1460	TPF	C3-N2-C4	9.91	108.84	102.25
3	B	1460	TPF	C6-N5-C7	11.82	110.12	102.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1460	TPF	C1-C5-N4-C6
3	A	1460	TPF	O-C1-C8-C13
3	B	1460	TPF	O-C1-C8-C13

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1450	HEM	3	0
2	B	1450	HEM	3	0
3	B	1460	TPF	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	444/473 (93%)	0.52	10 (2%)	64	76	31, 44, 56, 62	0
1	B	444/473 (93%)	0.51	10 (2%)	64	76	32, 44, 56, 62	0
All	All	888/946 (93%)	0.52	20 (2%)	64	76	31, 44, 56, 62	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	PRO	2.9
1	B	326	PHE	2.9
1	B	480	PRO	2.8
1	A	96	ILE	2.6
1	A	259	SER	2.6
1	B	479	LEU	2.5
1	B	136	ILE	2.4
1	B	34	VAL	2.3
1	B	41	PHE	2.3
1	A	134	LEU	2.3
1	A	34	VAL	2.3
1	A	326	PHE	2.3
1	B	248	GLU	2.3
1	B	471	VAL	2.2
1	B	450	ASP	2.2
1	A	136	ILE	2.2
1	A	142	PHE	2.2
1	A	199	GLN	2.2
1	A	323	ILE	2.1
1	B	96	ILE	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	TPF	B	1460	22/22	0.95	0.15	-0.25	42,48,55,57	0
2	HEM	A	1450	43/43	0.96	0.15	-0.33	27,41,51,52	0
2	HEM	B	1450	43/43	0.96	0.16	-0.34	32,39,52,55	0
3	TPF	A	1460	22/22	0.94	0.15	-0.58	38,45,46,47	0

6.5 Other polymers (i)

There are no such residues in this entry.