Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:18 PM GMT

PDB ID	:	4C27
Title	:	Crystal structure of Trypanosoma cruzi CYP51 bound to the inhibitor (R)-N-(3-(1H-indol-3-yl)-1-oxo-1-(pyridin-4-ylamino)propan-2-yl)-2-fluoro-4-(4-(4-(trifluoromethyl)phenyl)piperazin-1-yl)benzamide
Authors	:	Vieira, D.F.; Calvet, C.M.; Choi, J.Y.; Cameron, M.D.; Gut, J.; Kellar, D.; Siqueira-Neto, J.L.; McKerrow, J.H.; Roush, W.R.; Podust, L.M.
Deposited on	:	2013-08-16
Resolution	:	1.95 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:

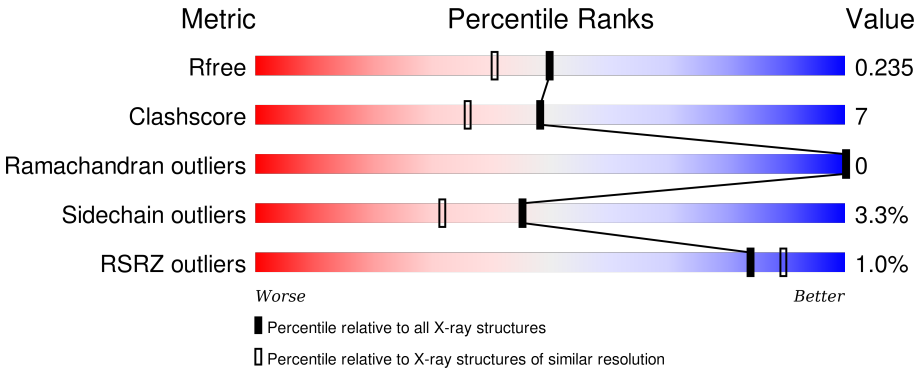
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	467	% 82% 12% • 5%
1	B	467	% 80% 14% • 5%

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
4	EDO	A	1480	-	-	-	X
4	EDO	B	1479	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7823 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 STEROL 14-ALPHA DEMETHYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	8	0
			3613	2306	639	640	28			
1	B	443	Total	C	N	O	S	0	4	0
			3546	2265	619	634	28			

There are 28 discrepancies between the modelled and reference sequences:

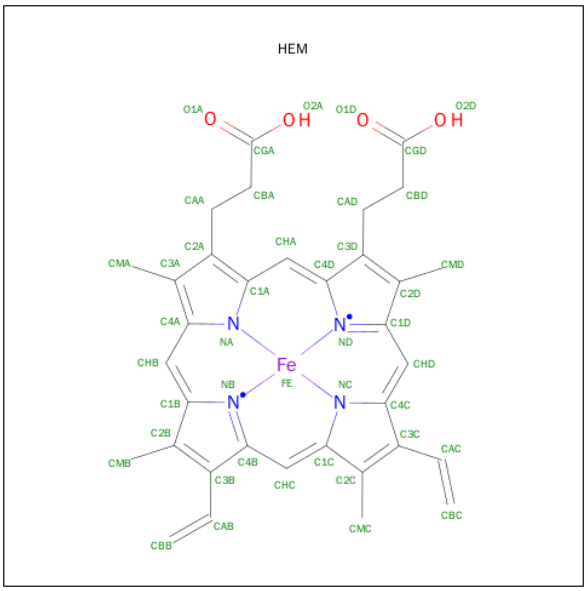
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	EXPRESSION TAG	UNP Q5I4E1
A	22	ALA	-	EXPRESSION TAG	UNP Q5I4E1
A	23	LYS	-	EXPRESSION TAG	UNP Q5I4E1
A	24	LYS	-	EXPRESSION TAG	UNP Q5I4E1
A	25	THR	-	EXPRESSION TAG	UNP Q5I4E1
A	26	SER	-	EXPRESSION TAG	UNP Q5I4E1
A	27	SER	-	EXPRESSION TAG	UNP Q5I4E1
A	28	LYS	-	EXPRESSION TAG	UNP Q5I4E1
A	482	HIS	-	EXPRESSION TAG	UNP Q5I4E1
A	483	HIS	-	EXPRESSION TAG	UNP Q5I4E1
A	484	HIS	-	EXPRESSION TAG	UNP Q5I4E1
A	485	HIS	-	EXPRESSION TAG	UNP Q5I4E1
A	486	HIS	-	EXPRESSION TAG	UNP Q5I4E1
A	487	HIS	-	EXPRESSION TAG	UNP Q5I4E1
B	21	MET	-	EXPRESSION TAG	UNP Q5I4E1
B	22	ALA	-	EXPRESSION TAG	UNP Q5I4E1
B	23	LYS	-	EXPRESSION TAG	UNP Q5I4E1
B	24	LYS	-	EXPRESSION TAG	UNP Q5I4E1
B	25	THR	-	EXPRESSION TAG	UNP Q5I4E1
B	26	SER	-	EXPRESSION TAG	UNP Q5I4E1
B	27	SER	-	EXPRESSION TAG	UNP Q5I4E1
B	28	LYS	-	EXPRESSION TAG	UNP Q5I4E1
B	482	HIS	-	EXPRESSION TAG	UNP Q5I4E1
B	483	HIS	-	EXPRESSION TAG	UNP Q5I4E1
B	484	HIS	-	EXPRESSION TAG	UNP Q5I4E1

Continued on next page...

Continued from previous page...

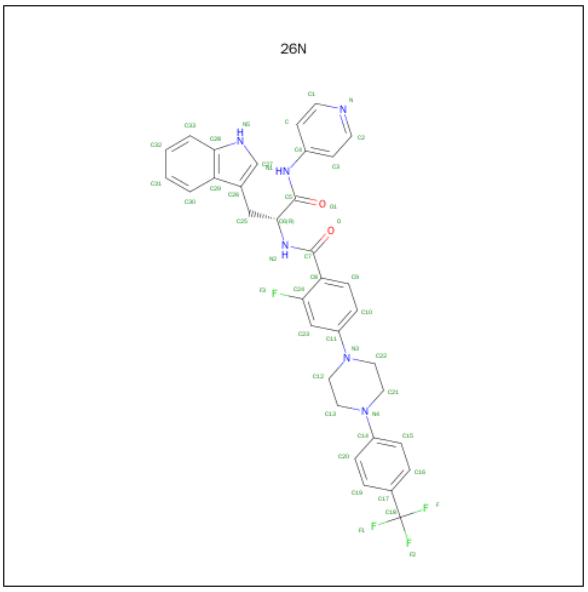
Chain	Residue	Modelled	Actual	Comment	Reference
B	485	HIS	-	EXPRESSION TAG	UNP Q5I4E1
B	486	HIS	-	EXPRESSION TAG	UNP Q5I4E1
B	487	HIS	-	EXPRESSION TAG	UNP Q5I4E1

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



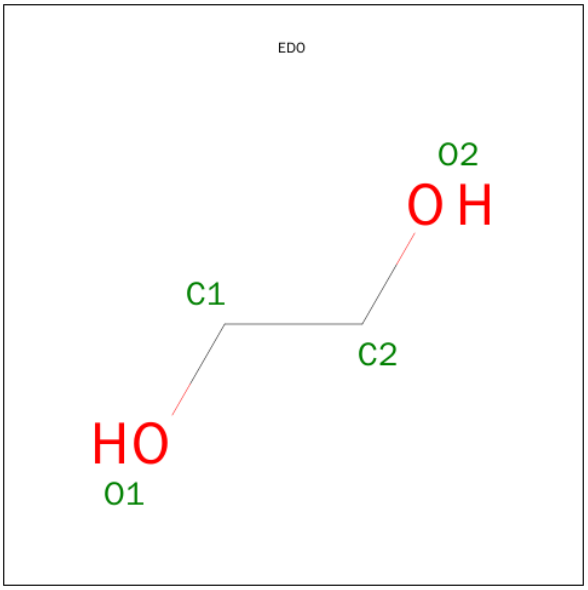
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is NALPHA-(2-FLUORO-4-{4-[4-(TRIFLUOROMETHYL)PHENYL]PIPERAZIN-1-YL}BENZOYL)-N-PYRIDIN-4-YL-D-TRYPTOPHANAMIDE (three-letter code: 26N) (formula: $C_{34}H_{30}F_4N_6O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			46	34	4	6	2		
3	B	1	Total	C	F	N	O	0	1
			92	68	8	12	4		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is water.

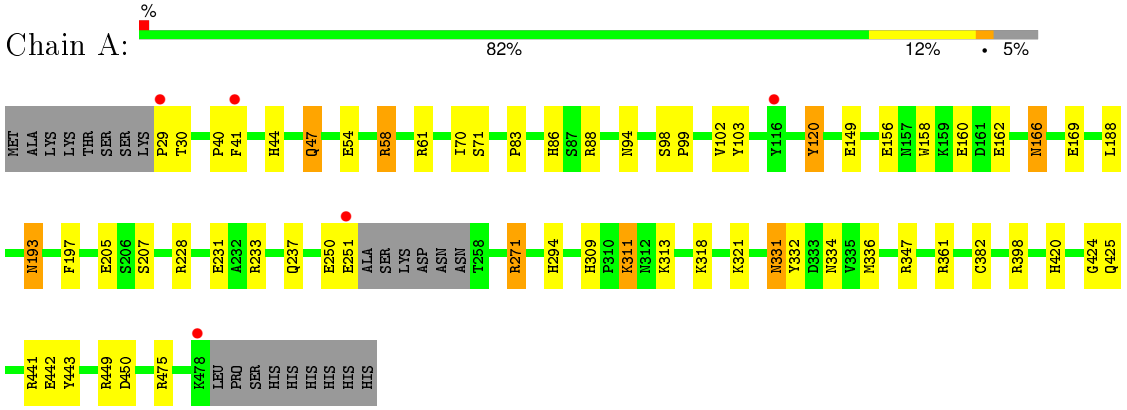
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	246	Total O 246 246	0	0
6	B	181	Total O 181 181	0	0

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.

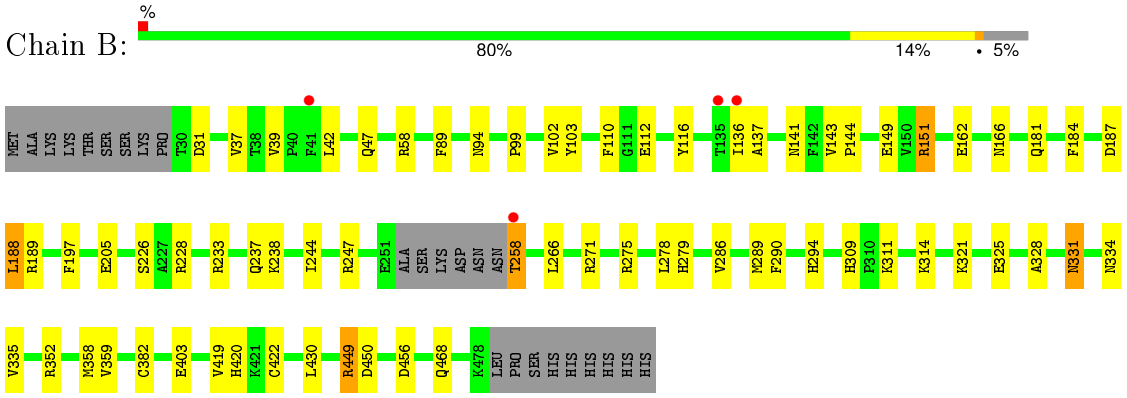
- Molecule 1: STEROL 14-ALPHA DEMETHYLASE

Chain A:



- Molecule 1: STEROL 14-ALPHA DEMETHYLASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.10Å 79.16Å 176.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.36 – 1.95 72.26 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.9 (72.36-1.95) 98.9 (72.26-1.95)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.183 , 0.233 0.190 , 0.235	Depositor DCC
R_{free} test set	3773 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 37.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 74813 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7823	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: HEM, CL, 26N, EDO

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	0.93	2/3698 (0.1%)	1.02	15/4998 (0.3%)
1	B	0.93	0/3630	0.97	10/4915 (0.2%)
All	All	0.93	2/7328 (0.0%)	1.00	25/9913 (0.3%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	ARG	CD-NE	-5.35	1.37	1.46
1	A	207	SER	CB-OG	5.06	1.48	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	58	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	A	61	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	A	58	ARG	NE-CZ-NH1	9.97	125.29	120.30
1	A	61	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	271	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	A	271	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	361	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	A	361	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	A	441	ARG	NE-CZ-NH2	-6.67	116.97	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	189	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	441	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	398	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	B	187	ASP	CB-CG-OD1	5.96	123.67	118.30
1	B	271	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	449	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	456	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	425	GLN	N-CA-CB	-5.65	100.43	110.60
1	B	352	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	88	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	31	ASP	CB-CG-OD1	5.47	123.22	118.30
1	B	456	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	B	151	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	B	228	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	358	MET	CG-SD-CE	-5.28	91.75	100.20
1	A	120	TYR	CB-CG-CD1	-5.24	117.85	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29	PRO	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	3613	0	3616	45	0
1	B	3546	0	3523	51	0
2	A	43	0	30	8	0
2	B	43	0	30	8	0
3	A	46	0	30	3	0
3	B	92	0	60	7	0
4	A	8	0	12	0	0
4	B	4	0	6	0	0
5	A	1	0	0	0	0
6	A	246	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	181	0	0	5	0
All	All	7823	0	7307	108	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (108) 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:B:141[B]:ASN:HD22	1:B:141[B]:ASN:H	1.03	0.98
1:B:149:GLU:HG2	1:B:181:GLN:HG3	1.62	0.81
1:A:44:HIS:HD2	1:A:71:SER:H	1.33	0.75
1:B:449[A]:ARG:CG	1:B:449[A]:ARG:HH11	1.98	0.75
1:A:149:GLU:OE2	6:A:2091:HOH:O	2.06	0.74
1:A:47:GLN:H	1:A:47:GLN:HE21	1.38	0.70
1:B:141[B]:ASN:ND2	1:B:141[B]:ASN:H	1.83	0.70
1:B:149:GLU:CG	1:B:181:GLN:HG3	2.22	0.69
1:B:141[B]:ASN:N	1:B:141[B]:ASN:HD22	1.83	0.65
1:B:99:PRO:O	1:B:102:VAL:HG22	1.96	0.65
1:B:47:GLN:HG3	6:B:2011:HOH:O	1.95	0.65
1:B:275:ARG:HD2	6:B:2102:HOH:O	1.96	0.64
1:A:160[B]:GLU:HG3	1:A:162:GLU:O	1.98	0.63
1:B:449[A]:ARG:CG	1:B:449[A]:ARG:NH1	2.59	0.63
2:B:1450:HEM:HHC	2:B:1450:HEM:HBB2	1.82	0.62
1:A:102:VAL:HG23	1:A:103:TYR:CD2	2.36	0.60
1:B:449[A]:ARG:HG2	1:B:449[A]:ARG:NH1	2.15	0.60
1:A:228:ARG:NH2	6:A:2134:HOH:O	2.33	0.60
1:A:44:HIS:CD2	1:A:71:SER:H	2.18	0.58
1:A:420:HIS:HD2	2:A:1450:HEM:O2D	1.88	0.57
1:B:325:GLU:HB2	6:B:2125:HOH:O	2.05	0.56
1:A:271:ARG:NH2	6:A:2156:HOH:O	2.38	0.56
1:A:331:ASN:H	1:A:334:ASN:HD22	1.53	0.56
1:A:309:HIS:CD2	1:A:311:LYS:HG2	2.41	0.56
1:B:422:CYS:HA	2:B:1450:HEM:C4D	2.40	0.55
2:A:1450:HEM:HBC2	2:A:1450:HEM:HHD	1.87	0.55
1:A:420:HIS:O	2:A:1450:HEM:HBD1	2.07	0.55
1:B:309:HIS:HD2	1:B:311:LYS:H	1.54	0.54
1:A:347[A]:ARG:NH1	1:A:347[A]:ARG:HB3	2.23	0.53
1:A:98:SER:OG	1:A:120:TYR:OH	2.21	0.53
1:A:205:GLU:OE1	1:A:294:HIS:HE1	1.92	0.53
1:B:39:VAL:HG23	1:B:42:LEU:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:HIS:HD2	1:A:311:LYS:H	1.58	0.52
1:A:233:ARG:HH12	1:A:237:GLN:NE2	2.09	0.51
1:B:110:PHE:HZ	3:B:1460[B]:26N:C27	2.23	0.51
1:B:112[A]:GLU:CD	1:B:112[A]:GLU:H	2.13	0.50
1:B:233:ARG:HH12	1:B:237:GLN:NE2	2.09	0.50
1:A:54:GLU:OE2	1:A:58:ARG:HD3	2.12	0.50
1:B:39:VAL:HG23	1:B:39:VAL:O	2.10	0.50
1:B:197:PHE:CE2	1:B:289:MET:HG3	2.46	0.49
1:A:309:HIS:CD2	1:A:311:LYS:H	2.30	0.49
1:A:166:ASN:HD22	1:A:169:GLU:H	1.61	0.49
1:B:103:TYR:CD2	1:B:116:TYR:CE2	3.00	0.49
1:A:347[A]:ARG:HH11	1:A:347[A]:ARG:CB	2.25	0.49
1:A:332:TYR:CZ	1:A:336:MET:HG3	2.48	0.49
1:B:143:VAL:HB	1:B:144:PRO:HD3	1.93	0.49
1:B:325:GLU:N	6:B:2125:HOH:O	2.44	0.48
1:B:247:ARG:HD3	1:B:258:THR:HG23	1.96	0.48
1:B:244:ILE:HG12	1:B:266:LEU:HD11	1.96	0.48
1:B:151:ARG:NH2	1:B:328:ALA:O	2.46	0.47
1:A:331:ASN:HD22	1:A:331:ASN:C	2.18	0.47
1:A:318:LYS:HA	1:A:321[B]:LYS:HE2	1.96	0.47
1:B:286:VAL:O	1:B:290:PHE:HB2	2.15	0.47
2:A:1450:HEM:C4D	3:A:1460:26N:H2	2.49	0.47
3:B:1460[A]:26N:H22	3:B:1460[A]:26N:H10	1.58	0.47
1:B:184:PHE:CG	1:B:188:LEU:HD13	2.50	0.46
1:B:112[B]:GLU:O	1:B:279:HIS:HE1	1.98	0.46
1:A:228:ARG:HD3	1:A:231[B]:GLU:OE1	2.15	0.46
1:B:89:PHE:CZ	1:B:359:VAL:HG12	2.51	0.46
2:B:1450:HEM:C4D	3:B:1460[B]:26N:H2	2.51	0.46
1:A:228:ARG:CZ	6:A:2134:HOH:O	2.64	0.46
1:A:250:GLU:O	1:A:251:GLU:CB	2.64	0.46
3:B:1460[B]:26N:H20	3:B:1460[B]:26N:H13A	1.69	0.45
1:B:331:ASN:HD22	1:B:331:ASN:C	2.19	0.45
2:B:1450:HEM:HHD	2:B:1450:HEM:HBC2	1.98	0.45
1:A:347[A]:ARG:HH11	1:A:347[A]:ARG:HB3	1.81	0.45
1:A:442:GLU:HB2	1:A:443:TYR:CD1	2.52	0.45
2:A:1450:HEM:C1A	3:A:1460:26N:H2	2.52	0.44
1:B:331:ASN:ND2	1:B:334:ASN:H	2.15	0.44
1:B:136:ILE:HD12	1:B:137:ALA:N	2.33	0.44
2:B:1450:HEM:C1A	3:B:1460[A]:26N:H2	2.51	0.44
1:B:420:HIS:HD2	2:B:1450:HEM:O2D	2.01	0.44
1:A:94:ASN:OD1	1:A:420:HIS:CE1	2.70	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:HIS:HE1	1:A:450:ASP:O	2.01	0.44
1:B:449[B]:ARG:CD	1:B:468:GLN:HB3	2.48	0.44
2:B:1450:HEM:HBC2	2:B:1450:HEM:CHD	2.48	0.43
1:B:141[B]:ASN:N	1:B:141[B]:ASN:ND2	2.53	0.43
1:B:309:HIS:CD2	1:B:311:LYS:H	2.34	0.43
1:B:309:HIS:HE1	1:B:450:ASP:O	2.01	0.43
1:B:47:GLN:HE22	1:B:58:ARG:HH12	1.66	0.43
1:B:205:GLU:OE2	1:B:294:HIS:CE1	2.71	0.43
1:B:47:GLN:NE2	1:B:58:ARG:HH12	2.17	0.43
1:A:94:ASN:OD1	1:A:420:HIS:HE1	2.01	0.43
1:B:110:PHE:HZ	3:B:1460[B]:26N:N5	2.17	0.43
1:A:309:HIS:CD2	1:A:311:LYS:CG	3.02	0.43
1:A:99:PRO:O	1:A:102:VAL:HG22	2.19	0.42
1:B:149:GLU:CG	1:B:181:GLN:CG	2.95	0.42
1:B:422:CYS:HA	2:B:1450:HEM:CHA	2.50	0.42
1:A:331:ASN:H	1:A:334:ASN:ND2	2.16	0.42
1:B:205:GLU:OE2	1:B:294:HIS:HE1	2.03	0.42
1:B:335:VAL:HG11	1:B:430:LEU:HD12	2.02	0.42
3:A:1460:26N:H23	3:A:1460:26N:H12A	1.89	0.41
1:B:112[A]:GLU:O	1:B:279:HIS:HE1	2.02	0.41
1:B:197:PHE:CZ	1:B:289:MET:HG3	2.56	0.41
3:B:1460[A]:26N:H20	3:B:1460[A]:26N:H13	1.92	0.41
1:A:424:GLY:HA3	2:A:1450:HEM:C3C	2.56	0.41
1:A:475[B]:ARG:HB2	1:A:475[B]:ARG:HE	1.31	0.41
1:B:294:HIS:HD2	6:B:2026:HOH:O	2.04	0.41
1:A:158:TRP:O	1:A:475[B]:ARG:NH2	2.53	0.41
1:B:244:ILE:HD12	1:B:278:LEU:HD13	2.02	0.41
1:A:83:PRO:HA	1:A:86:HIS:CD2	2.56	0.41
1:B:94:ASN:OD1	1:B:420:HIS:HE1	2.04	0.40
1:A:44:HIS:CD2	1:A:70:ILE:HB	2.56	0.40
1:A:424:GLY:HA3	2:A:1450:HEM:C2C	2.56	0.40
1:A:420:HIS:CD2	2:A:1450:HEM:O2D	2.73	0.40
1:A:40:PRO:O	1:A:41:PHE:C	2.58	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	448/467 (96%)	440 (98%)	8 (2%)	0	100	100
1	B	443/467 (95%)	435 (98%)	8 (2%)	0	100	100
All	All	891/934 (95%)	875 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	390/409 (95%)	379 (97%)	11 (3%)	51	39
1	B	382/409 (93%)	367 (96%)	15 (4%)	39	24
All	All	772/818 (94%)	746 (97%)	26 (3%)	45	30

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	47	GLN
1	A	156	GLU
1	A	166	ASN
1	A	188	LEU
1	A	193	ASN
1	A	197	PHE
1	A	311	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	313	LYS
1	A	331	ASN
1	A	382	CYS
1	B	37	VAL
1	B	162	GLU
1	B	166	ASN
1	B	188	LEU
1	B	226	SER
1	B	238	LYS
1	B	258	THR
1	B	314	LYS
1	B	321	LYS
1	B	331	ASN
1	B	382	CYS
1	B	403	GLU
1	B	419	VAL
1	B	449[A]	ARG
1	B	449[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	47	GLN
1	A	57	GLN
1	A	128	ASN
1	A	166	ASN
1	A	193	ASN
1	A	237	GLN
1	A	279	HIS
1	A	294	HIS
1	A	309	HIS
1	A	331	ASN
1	A	334	ASN
1	A	420	HIS
1	B	47	GLN
1	B	166	ASN
1	B	237	GLN
1	B	279	HIS
1	B	294	HIS
1	B	309	HIS
1	B	331	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	334	ASN
1	B	420	HIS

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)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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	2.28	6 (20%)	24,82,82	2.32	9 (37%)
3	26N	A	1460	2	50,51,51	1.22	3 (6%)	64,73,73	1.81	13 (20%)
4	EDO	A	1479	-	3,3,3	0.42	0	2,2,2	0.00	0
4	EDO	A	1480	-	3,3,3	0.32	0	2,2,2	1.58	1 (50%)
2	HEM	B	1450	1,3	30,50,50	2.30	8 (26%)	24,82,82	2.39	11 (45%)
3	26N	B	1460[A]	2	50,51,51	1.29	4 (8%)	64,73,73	1.70	12 (18%)
3	26N	B	1460[B]	2	50,51,51	1.41	5 (10%)	64,73,73	1.61	9 (14%)
4	EDO	B	1479	-	3,3,3	0.30	0	2,2,2	0.65	0

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	26N	A	1460	2	-	0/33/44/44	0/6/6/6
4	EDO	A	1479	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1480	-	-	0/1/1/1	0/0/0/0
2	HEM	B	1450	1,3	-	0/10/54/54	0/0/8/8
3	26N	B	1460[A]	2	-	0/33/44/44	0/6/6/6
3	26N	B	1460[B]	2	-	0/33/44/44	0/6/6/6
4	EDO	B	1479	-	-	0/1/1/1	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1450	HEM	C2D-C3D	-7.47	1.32	1.54
2	B	1450	HEM	C2D-C3D	-6.40	1.35	1.54
2	A	1450	HEM	C2C-C1C	-5.83	1.41	1.52
2	B	1450	HEM	C2C-C1C	-5.14	1.42	1.52
2	B	1450	HEM	C3B-C4B	-4.61	1.47	1.51
2	A	1450	HEM	C3B-C4B	-3.90	1.48	1.51
2	B	1450	HEM	C3D-C4D	-3.51	1.47	1.51
2	B	1450	HEM	C2B-C1B	-3.21	1.41	1.51
3	A	1460	26N	C12-N3	-2.86	1.42	1.46
2	B	1450	HEM	C3B-CAB	-2.84	1.46	1.51
3	B	1460[A]	26N	C4-N1	-2.59	1.36	1.41
2	A	1450	HEM	C3D-C4D	-2.54	1.48	1.51
3	B	1460[B]	26N	C19-C17	-2.29	1.35	1.39
3	B	1460[B]	26N	C33-C28	-2.12	1.38	1.41
3	B	1460[A]	26N	C19-C17	-2.07	1.35	1.39
3	B	1460[B]	26N	C4-N1	-2.05	1.37	1.41
3	B	1460[A]	26N	C31-C30	2.00	1.41	1.36
3	B	1460[B]	26N	C29-C28	2.12	1.48	1.42
3	A	1460	26N	O-C7	2.22	1.27	1.23
2	A	1450	HEM	CHC-C1C	2.46	1.42	1.36
2	B	1450	HEM	FE-NC	2.79	2.06	1.95
2	B	1450	HEM	C4C-NC	3.14	1.39	1.36
2	A	1450	HEM	FE-NC	3.22	2.08	1.95
3	A	1460	26N	C8-C24	4.75	1.45	1.38
3	B	1460[A]	26N	C8-C24	6.07	1.47	1.38
3	B	1460[B]	26N	C8-C24	7.13	1.49	1.38

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1460	26N	C25-C26-C27	-4.31	122.65	127.97
3	A	1460	26N	C31-C30-C29	-3.99	115.23	120.88
3	B	1460[B]	26N	C23-C24-C8	-3.99	119.29	123.70
2	B	1450	HEM	C3B-C4B-NB	-3.92	104.12	111.63
2	B	1450	HEM	C3C-CAC-CBC	-3.83	118.59	124.46
3	B	1460[A]	26N	C10-C11-N3	-3.80	116.27	121.38
3	B	1460[B]	26N	C25-C6-N2	-3.62	103.22	110.80
3	B	1460[A]	26N	F2-C18-C17	-3.44	105.59	112.95
3	B	1460[B]	26N	C31-C30-C29	-3.19	116.37	120.88
3	B	1460[A]	26N	O-C7-N2	-2.82	117.35	122.44
3	B	1460[A]	26N	C3-C4-C	-2.75	115.25	119.06
3	B	1460[B]	26N	C3-C4-C	-2.70	115.31	119.06
2	B	1450	HEM	CBA-CAA-C2A	-2.57	107.92	112.53
3	A	1460	26N	C3-C4-C	-2.39	115.74	119.06
3	B	1460[A]	26N	C33-C28-C29	-2.34	117.10	121.11
3	B	1460[A]	26N	C23-C24-C8	-2.33	121.12	123.70
2	A	1450	HEM	CAD-CBD-CGD	-2.24	103.89	113.02
4	A	1480	EDO	O2-C2-C1	-2.08	97.63	112.54
3	A	1460	26N	O-C7-C8	-2.03	117.06	120.95
2	B	1450	HEM	C2C-C1C-CHC	2.04	126.78	123.68
3	B	1460[B]	26N	C22-C21-N4	2.09	114.77	110.63
3	A	1460	26N	C2-C3-C4	2.09	122.12	118.94
3	A	1460	26N	C8-C7-N2	2.10	120.81	116.88
3	B	1460[A]	26N	C-C4-N1	2.14	127.55	120.41
3	B	1460[B]	26N	C31-C32-C33	2.16	123.59	120.45
2	B	1450	HEM	CMD-C2D-C3D	2.17	123.94	114.35
3	B	1460[A]	26N	C9-C10-C11	2.27	123.30	120.36
3	A	1460	26N	C32-C31-C30	2.32	123.83	120.45
3	A	1460	26N	C16-C15-C14	2.33	123.38	120.36
2	A	1450	HEM	C2C-C1C-CHC	2.51	127.50	123.68
2	A	1450	HEM	CBD-CAD-C3D	2.52	120.88	113.55
3	B	1460[A]	26N	C23-C11-N3	2.55	124.11	121.36
3	A	1460	26N	C5-C6-N2	2.57	118.50	111.26
2	B	1450	HEM	CMB-C2B-C3B	2.71	123.29	116.53
2	A	1450	HEM	CAD-C3D-C2D	2.78	121.22	113.22
3	B	1460[B]	26N	C-C4-N1	2.83	129.87	120.41
2	B	1450	HEM	C3B-C4B-CHC	2.84	127.16	123.16
2	B	1450	HEM	CMC-C2C-C3C	2.85	123.64	116.53
2	A	1450	HEM	CMD-C2D-C3D	2.94	127.35	114.35
3	A	1460	26N	C12-C13-N4	3.17	116.91	110.63
2	B	1450	HEM	C2D-C3D-C4D	3.22	106.97	101.50
2	A	1450	HEM	CMC-C2C-C3C	3.41	125.04	116.53
3	B	1460[B]	26N	C22-N3-C12	4.04	120.08	111.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1450	HEM	CAD-C3D-C4D	4.08	126.85	112.47
3	B	1460[A]	26N	C22-N3-C12	4.09	120.18	111.59
2	A	1450	HEM	CMB-C2B-C3B	4.12	126.81	116.53
2	A	1450	HEM	C2D-C3D-C4D	4.14	108.52	101.50
3	A	1460	26N	C21-C22-N3	4.33	119.21	110.63
2	B	1450	HEM	CAD-C3D-C2D	4.39	125.84	113.22
3	B	1460[A]	26N	C21-N4-C13	4.58	121.20	111.59
3	B	1460[A]	26N	C8-C7-N2	4.60	125.49	116.88
2	A	1450	HEM	CAD-C3D-C4D	4.94	129.91	112.47
3	A	1460	26N	C22-N3-C12	5.61	123.36	111.59
3	A	1460	26N	C21-N4-C13	5.72	123.61	111.59
3	B	1460[B]	26N	C21-N4-C13	5.79	123.75	111.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1450	HEM	8	0
3	A	1460	26N	3	0
2	B	1450	HEM	8	0
3	B	1460[A]	26N	3	0
3	B	1460[B]	26N	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	444/467 (95%)	0.07	5 (1%)	82	88	15, 25, 43, 73	0
1	B	443/467 (94%)	0.10	4 (0%)	85	90	16, 26, 46, 70	0
All	All	887/934 (94%)	0.08	9 (1%)	84	89	15, 26, 45, 73	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	258	THR	5.0
1	A	41	PHE	4.3
1	A	29	PRO	3.1
1	A	251	GLU	2.8
1	A	478	LYS	2.6
1	B	41	PHE	2.5
1	B	136	ILE	2.4
1	A	116	TYR	2.1
1	B	135	THR	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
4	EDO	A	1480	4/4	0.87	0.30	6.51	43,49,52,53	0
4	EDO	B	1479	4/4	0.91	0.19	3.62	48,53,53,65	0
4	EDO	A	1479	4/4	0.96	0.15	1.89	31,35,41,43	0
3	26N	B	1460[A]	46/46	0.96	0.13	1.10	15,19,23,25	46
3	26N	B	1460[B]	46/46	0.96	0.13	1.09	15,20,26,27	46
2	HEM	B	1450	43/43	0.97	0.13	0.57	17,21,31,34	0
2	HEM	A	1450	43/43	0.97	0.12	0.18	16,18,26,35	0
3	26N	A	1460	46/46	0.96	0.10	-0.48	18,23,28,33	0
5	CL	A	1481	1/1	0.92	0.07	-1.55	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.