wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 10:24 PM GMT

PDB ID	:	1TH4
Title	:	crystal structure of NADPH depleted bovine liver catalase complexed with 3-amino-1,2,4-triazole
Authors	:	Sugadev, R.; Ponnuswamy, M.N.; Kumaran, D.; Swaminathan, S.; Sekar, K.
Deposited on	:	2004-06-01
Resolution	:	2.98 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

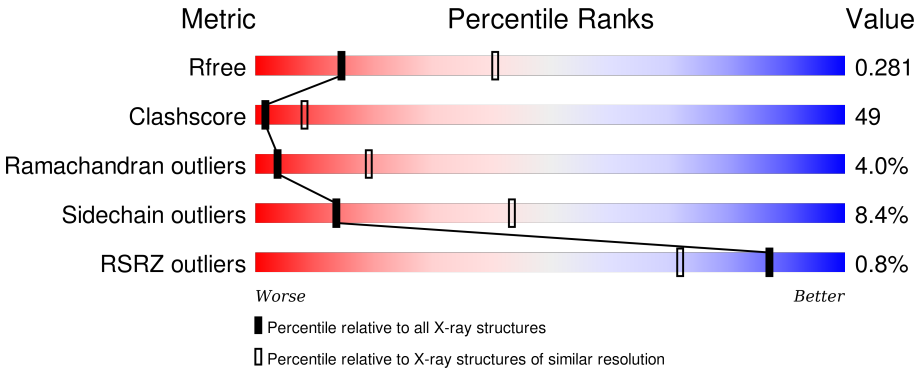
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.98 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	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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	506	32% 58% 8%
1	B	506	% 35% 53% 9%
1	C	506	% 38% 51% 9%
1	D	506	% 39% 52% 7%

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
2	3TR	D	3074	-	-	X	-
3	HEM	A	2000	-	-	X	X
3	HEM	B	2001	-	-	X	X
3	HEM	C	2002	-	-	X	X
3	HEM	D	2003	-	-	X	-

2 Entry composition

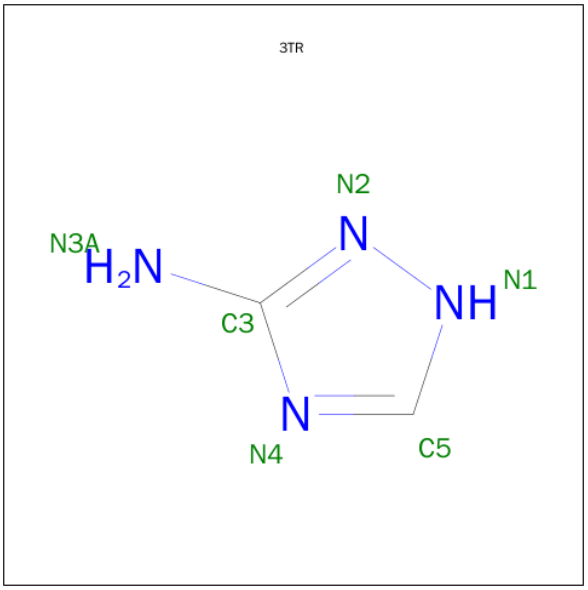
There are 4 unique types of molecules in this entry. The entry contains 16915 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Catalase.

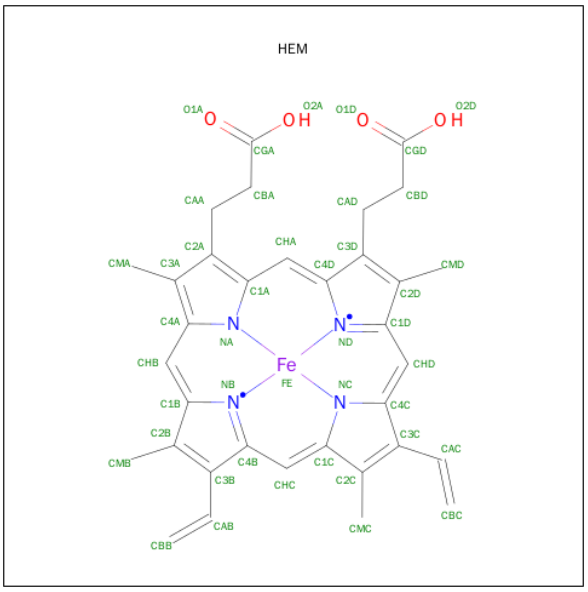
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			
1	B	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			
1	C	499	Total	C	N	O	S	1	0	0
			4017	2548	715	740	14			
1	D	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			

- Molecule 2 is 3-AMINO-1,2,4-TRIAZOLE (three-letter code: 3TR) (formula: $C_2H_4N_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	N	0	0
			6	2	4		

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



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

- Molecule 4 is water.

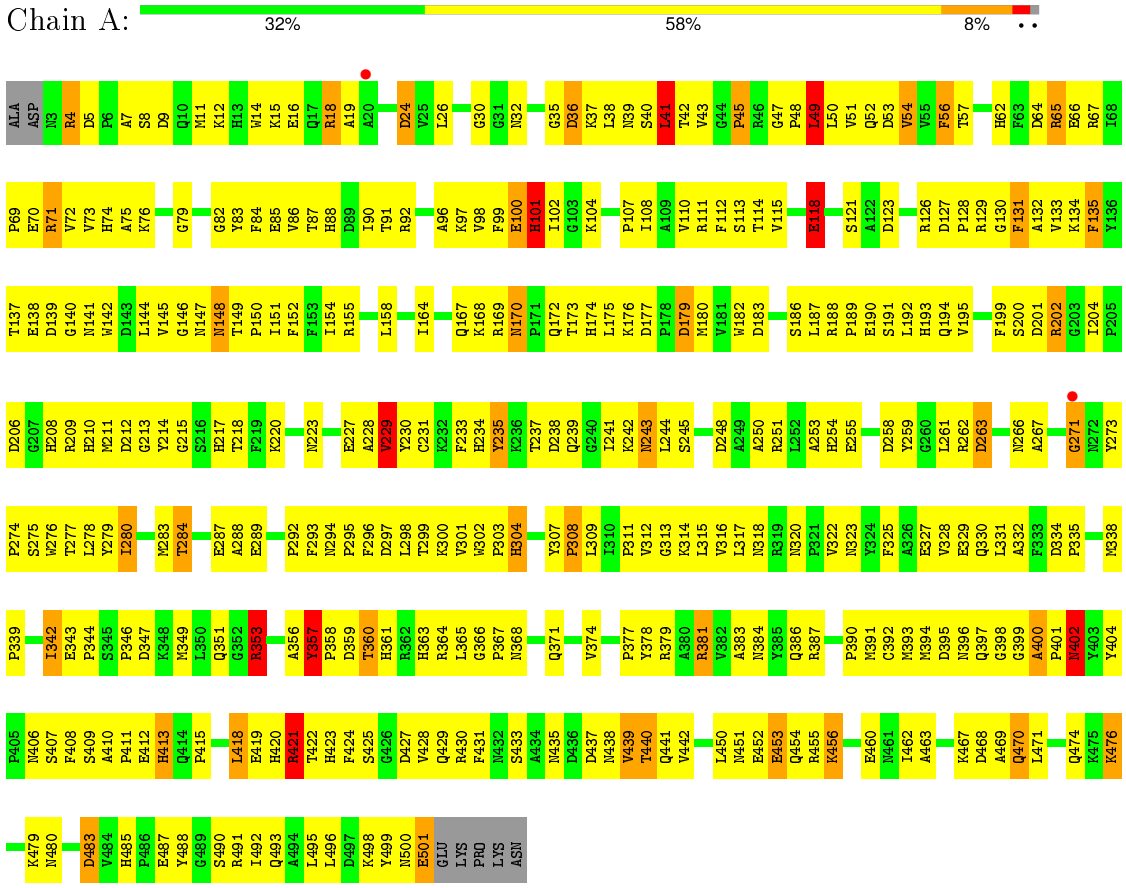
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	154	Total	O	0	0
			154	154		
4	B	145	Total	O	0	0
			145	145		
4	C	188	Total	O	0	0
			188	188		
4	D	182	Total	O	0	0
			182	182		

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.

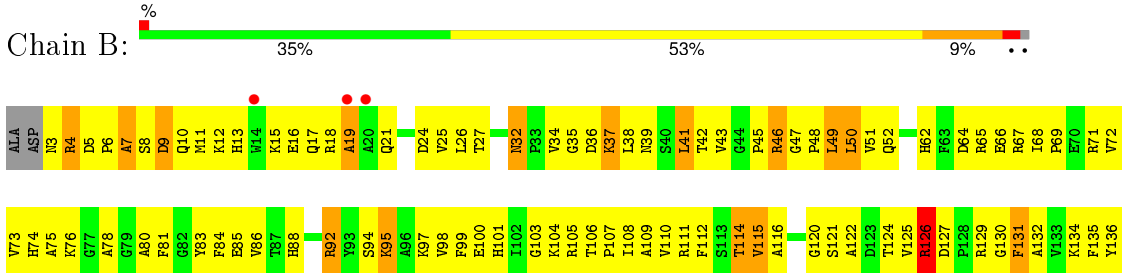
- Molecule 1: Catalase

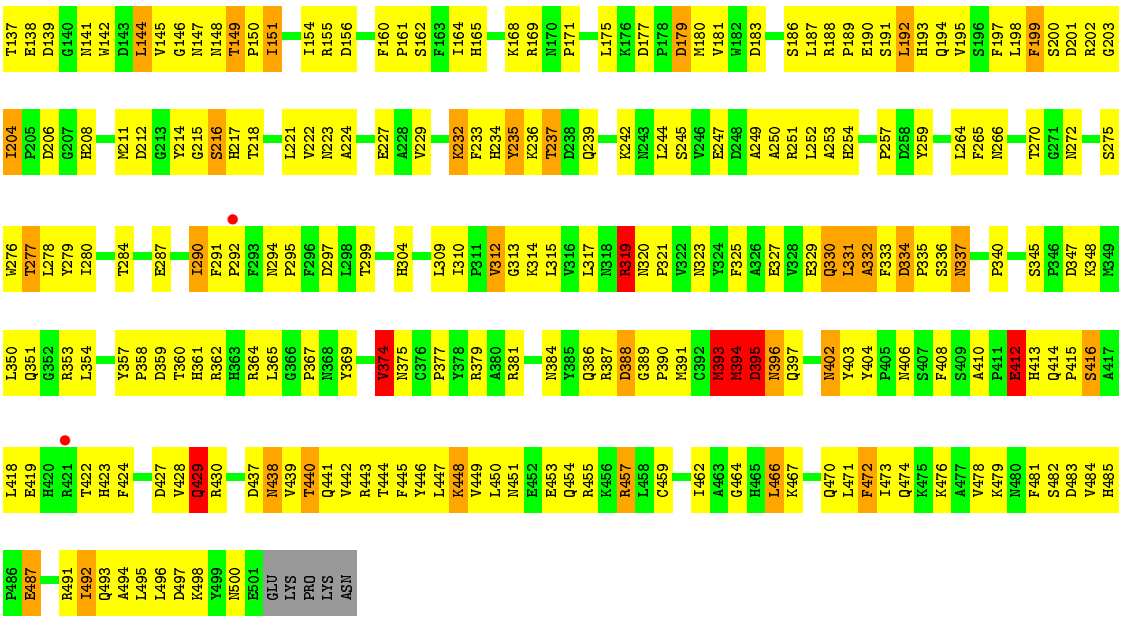
Chain A:



- Molecule 1: Catalase

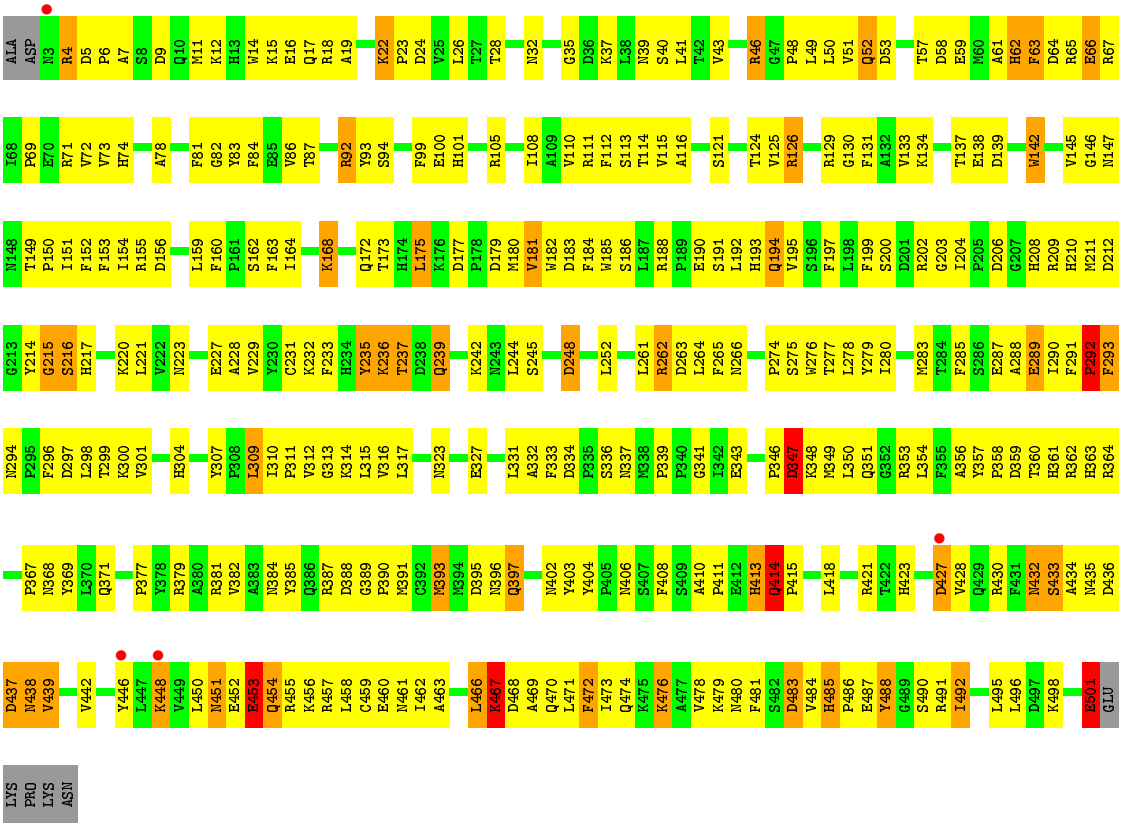
Chain B:





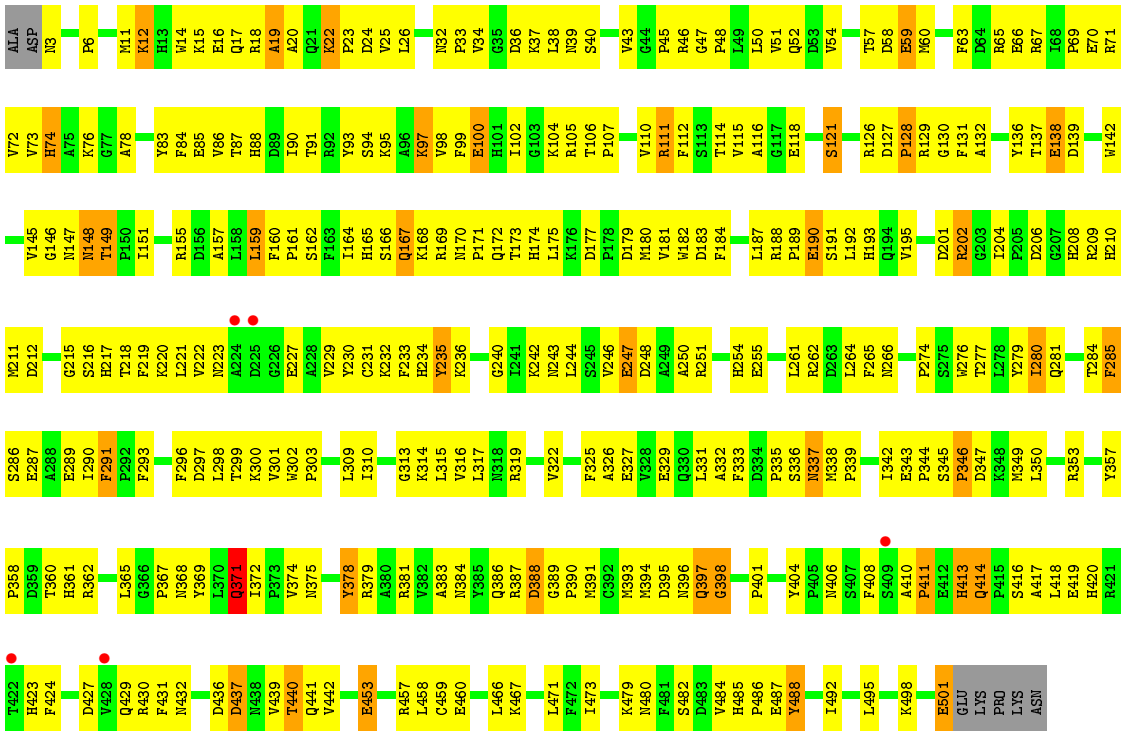
• Molecule 1: Catalase

Chain C:



• Molecule 1: Catalase

Chain D:


ALA ASP N3 P6 M11 K12 H13 W14 K15 E16 Q17 R18 A19 A20 Q21 K22 P23 D24 V25 L26 N32 P33 V34 G35 D36 K37 L38 N39 S40 V43 G44 P45 R46 G47 P48 L49 L50 V51 Q52 D53 V54 T57 D58 E59 M60 F63 D64 R65 E66 R67 I68 P69 E70 R71
V72 V73 H74 A75 K76 G77 A78 Y83 F84 E85 V86 T87 H88 D89 I90 T91 R92 Y93 S94 K95 A96 K97 V98 F99 E100 H101 I102 G103 K104 R105 T106 P107 V110 R111 F112 S113 T114 V115 A116 G117 E118 S121 R126 D127 P128 R129 G130 F131 A132 Y136 T137 E138 D139 W142
V145 G146 N147 N148 T149 P150 I151 R155 D156 A157 L158 L159 F160 P161 S162 F163 I164 H165 S166 Q167 K168 R169 N170 P171 Q172 T173 H174 L175 K176 D177 P178 D179 M180 V181 W182 D183 F184 L187 R188 P189 E190 S191 L192 H193 Q194 V195 D201 R202 G203 I204 P205 D206 G207 H208 R209 H210
W211 D212 G215 S216 H217 T218 F219 K220 I221 V222 N223 A224 D225 G226 E227 A228 V229 Y230 C231 K232 F233 H234 Y235 K236 G240 I241 K242 N243 L244 S245 V246 E247 D248 A249 A250 R251 H254 E255 L261 R262 D263 L264 F265 N266 P274 S275 W276 T277 L278 Y279 I280 Q281 T284 F285
S286 E287 A288 E289 I290 F291 P292 F293 F296 D297 L298 T299 K300 V301 W302 P303 L309 I310 G313 K314 L315 V316 L317 N318 R319 V322 F325 A326 E327 V328 E329 Q330 L331 A332 F333 D334 P335 S336 N337 M338 P339 I342 E343 P344 S345 P346 D347 K348 M349 L350 R353 Y357
P358 D359 T360 H361 R362 L365 G366 P367 N368 Y369 L370 Q371 I372 P373 V374 N375 Y378 R379 A380 R381 V382 A383 N384 Y385 Q386 R387 D388 G389 P390 M391 C392 M393 M394 D395 N396 Q397 G398 P401 Y404 P405 N406 S407 F408 S409 A410 P411 E412 H413 Q414 P415 S416 A417 L418 E419 H420 R421
T422 H423 F424 D427 Y428 Q429 R430 F431 N432 D436 D437 N438 Y439 T440 Q441 V442 E453 R457 L458 C459 E460 L466 K467 L471 F472 I473 K479 N480 F481 S482 D483 Y484 H485 P486 E487 Y488 I492 L495 K498 E501 GLU LYS PRO LYS ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.03Å 141.09Å 231.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 2.98 44.37 – 2.98	Depositor EDS
% Data completeness (in resolution range)	57.6 (39.90-2.98) 57.6 (44.37-2.98)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	0.30	Depositor
$< I/\sigma(I) >$ [1]	0.73 (at 2.96Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.235 , 0.292 0.227 , 0.281	Depositor DCC
R_{free} test set	1000 reflections (3.10%)	DCC
Wilson B-factor (Å^2)	53.3	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 57.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 33297 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	16915	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 2.54% 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, 3TR

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	0.60	5/4137 (0.1%)	1.78	61/5619 (1.1%)
1	B	0.99	6/4137 (0.1%)	1.45	31/5619 (0.6%)
1	C	0.66	8/4137 (0.2%)	1.49	33/5619 (0.6%)
1	D	0.61	1/4137 (0.0%)	0.92	9/5619 (0.2%)
All	All	0.73	20/16548 (0.1%)	1.44	134/22476 (0.6%)

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	1	2
1	B	1	3
1	C	2	2
1	D	1	0
All	All	5	7

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	319	ARG	CD-NE	49.16	2.30	1.46
1	D	413	HIS	CA-CB	-20.41	1.09	1.53
1	C	202	ARG	NE-CZ	16.91	1.55	1.33
1	B	319	ARG	NE-CZ	16.04	1.53	1.33
1	A	304	HIS	CA-CB	12.45	1.81	1.53

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	357	TYR	CB-CG-CD2	-68.04	80.18	121.00
1	C	202	ARG	NE-CZ-NH2	-52.67	93.97	120.30
1	B	319	ARG	NE-CZ-NH1	-46.60	97.00	120.30
1	C	202	ARG	NE-CZ-NH1	44.10	142.35	120.30
1	B	319	ARG	CG-CD-NE	-41.12	25.46	111.80

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	395	ASP	CA
1	B	395	ASP	CA
1	C	453	GLU	CA
1	C	501	GLU	CA
1	D	371	GLN	CA

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	357	TYR	Sidechain
1	A	421	ARG	Sidechain
1	B	126	ARG	Sidechain
1	B	319	ARG	Sidechain
1	B	394	MET	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	4017	0	3838	473	1
1	B	4017	0	3839	431	0
1	C	4017	0	3840	429	0
1	D	4017	0	3839	389	0
2	D	6	0	3	12	0
3	A	43	0	30	79	0
3	B	43	0	30	39	0
3	C	43	0	30	49	0
3	D	43	0	30	25	0
4	A	154	0	0	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	145	0	0	28	0
4	C	188	0	0	17	1
4	D	182	0	0	14	0
All	All	16915	0	15479	1562	1

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 49.

The worst 5 of 1562 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:304:HIS:CB	1:A:304:HIS:CA	1.81	1.58
1:A:100:GLU:HG2	1:A:101:HIS:CE1	1.43	1.52
3:A:2000:HEM:CBC	3:A:2000:HEM:CAC	1.87	1.47
1:A:353:ARG:HD2	3:A:2000:HEM:CHC	1.53	1.37
1:C:111:ARG:NE	3:C:2002:HEM:O1D	1.57	1.36

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:GLU:OE1	4:C:2061:HOH:O[3_655]	2.18	0.02

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	497/506 (98%)	400 (80%)	80 (16%)	17 (3%)	5 23
1	B	497/506 (98%)	408 (82%)	65 (13%)	24 (5%)	3 15
1	C	497/506 (98%)	398 (80%)	82 (16%)	17 (3%)	5 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	497/506 (98%)	402 (81%)	74 (15%)	21 (4%)	3 18
All	All	1988/2024 (98%)	1608 (81%)	301 (15%)	79 (4%)	4 19

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	GLU
1	B	19	ALA
1	B	100	GLU
1	B	331	LEU
1	B	394	MET

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	431/437 (99%)	396 (92%)	35 (8%)	15 45
1	B	431/437 (99%)	387 (90%)	44 (10%)	9 32
1	C	431/437 (99%)	394 (91%)	37 (9%)	13 42
1	D	431/437 (99%)	403 (94%)	28 (6%)	21 57
All	All	1724/1748 (99%)	1580 (92%)	144 (8%)	14 43

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	374	VAL
1	C	22	LYS
1	D	378	TYR
1	B	395	ASP
1	B	438	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	429	GLN
1	C	32	ASN
1	D	371	GLN
1	B	435	ASN
1	C	3	ASN

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

5 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	$\#\|Z\| > 2$
3	HEM	A	2000	1	30,50,50	3.58	12 (40%)	24,82,82	3.55	9 (37%)
3	HEM	B	2001	1	30,50,50	3.57	15 (50%)	24,82,82	3.37	12 (50%)
3	HEM	C	2002	1	30,50,50	2.73	10 (33%)	24,82,82	2.35	9 (37%)
3	HEM	D	2003	1,2	30,50,50	4.44	16 (53%)	24,82,82	6.41	13 (54%)
2	3TR	D	3074	1,3	4,6,6	2.33	2 (50%)	1,7,7	4.31	1 (100%)

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
3	HEM	A	2000	1	-	0/10/54/54	0/0/8/8
3	HEM	B	2001	1	-	0/10/54/54	0/0/8/8
3	HEM	C	2002	1	-	0/10/54/54	0/0/8/8
3	HEM	D	2003	1,2	-	0/10/54/54	0/0/8/8
2	3TR	D	3074	1,3	-	0/0/0/0	0/1/1/1

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2003	HEM	CHC-C4B	-10.25	1.10	1.38
3	D	2003	HEM	CHD-C1D	-7.60	1.17	1.38
3	C	2002	HEM	C3B-C4B	-6.97	1.45	1.51
3	A	2000	HEM	C3B-C4B	-6.83	1.45	1.51
3	D	2003	HEM	C3B-C4B	-6.82	1.45	1.51

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2000	HEM	C3C-CAC-CBC	-12.74	104.92	124.46
3	B	2001	HEM	C1D-CHD-C4C	-10.37	108.49	125.82
3	D	2003	HEM	C1D-CHD-C4C	-6.36	115.20	125.82
3	B	2001	HEM	C4B-CHC-C1C	-5.57	116.52	125.82
2	D	3074	3TR	N3A-C3-N4	-4.31	117.62	123.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 192 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2000	HEM	79	0
3	B	2001	HEM	39	0
3	C	2002	HEM	49	0
3	D	2003	HEM	25	0
2	D	3074	3TR	12	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	499/506 (98%)	-0.37	2 (0%)	93	83	10, 40, 76, 97	0
1	B	499/506 (98%)	-0.29	5 (1%)	84	66	16, 44, 78, 102	0
1	C	499/506 (98%)	-0.16	4 (0%)	87	72	16, 41, 81, 100	1 (0%)
1	D	499/506 (98%)	-0.28	5 (1%)	84	66	15, 45, 84, 101	0
All	All	1996/2024 (98%)	-0.27	16 (0%)	87	72	10, 43, 80, 102	1 (0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	421	ARG	3.3
1	D	422	THR	3.2
1	B	19	ALA	3.1
1	B	20	ALA	3.0
1	C	448	LYS	2.9

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	HEM	A	2000	43/43	0.80	0.42	6.46	80,94,101,101	0
3	HEM	C	2002	43/43	0.83	0.38	4.51	41,58,72,92	0
3	HEM	B	2001	43/43	0.89	0.29	4.13	21,56,83,101	0
2	3TR	D	3074	6/6	0.94	0.20	0.59	89,96,99,101	0
3	HEM	D	2003	43/43	0.96	0.17	0.25	20,38,56,59	0

6.5 Other polymers (i)

There are no such residues in this entry.