



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 02:51 am 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

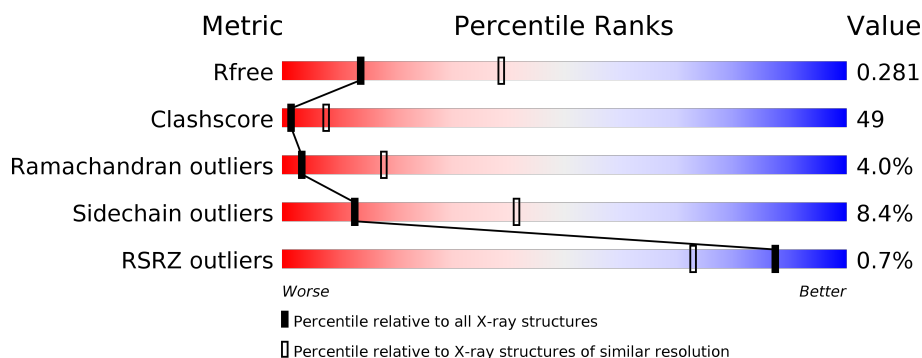
1 Overall quality at a glance ⓘ

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}	100719	2168 (3.00-2.96)
Clashscore	112137	2535 (3.00-2.96)
Ramachandran outliers	110173	2451 (3.00-2.96)
Sidechain outliers	110143	2454 (3.00-2.96)
RSRZ outliers	101464	2192 (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 $\leq 5\%$. 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	<div> <div>32%</div> <div>58%</div> <div>8%</div> <div>..</div> </div>
1	B	506	<div> <div>%</div> <div>35%</div> <div>53%</div> <div>9%</div> <div>..</div> </div>
1	C	506	<div> <div>%</div> <div>38%</div> <div>51%</div> <div>9%</div> <div>..</div> </div>
1	D	506	<div> <div>%</div> <div>39%</div> <div>52%</div> <div>7%</div> <div>.</div> </div>

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 crite-

ria:

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 [i](#)

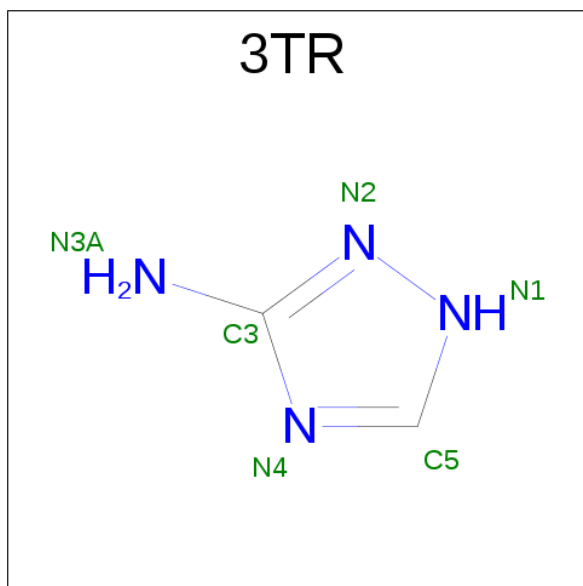
There are 4 unique types of molecules in this entry. The entry contains 16915 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

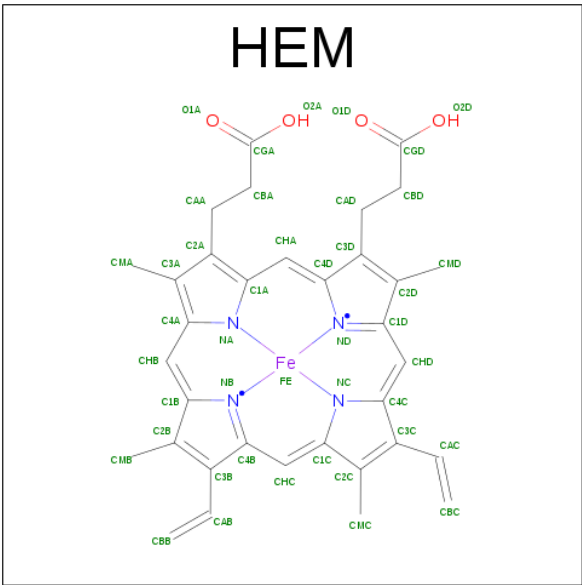
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			
1	B	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			
1	C	499	Total	C	N	O	S	1	0	0
			4017	2548	715	740	14			
1	D	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			

- Molecule 2 is 3-AMINO-1,2,4-TRIAZOLE (three-letter code: 3TR) (formula: C₂H₄N₄).



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: C₃₄H₃₂FeN₄O₄).



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

- Molecule 4 is water.

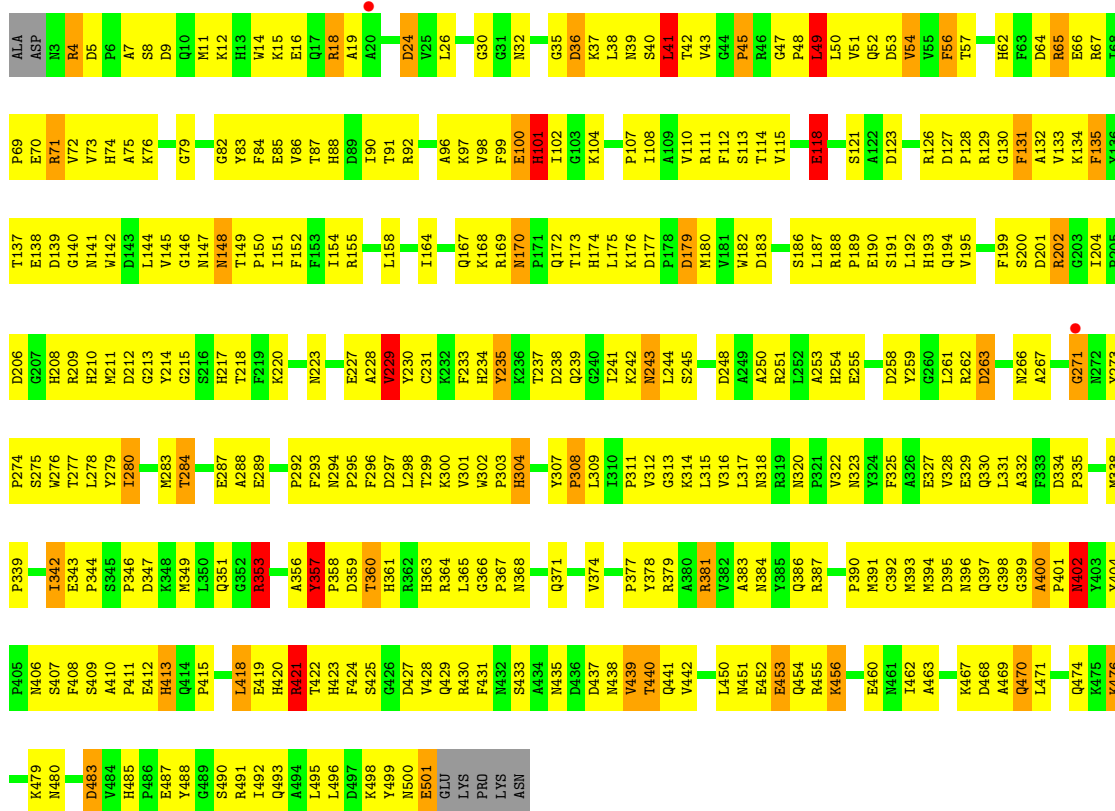
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	154	Total	O	0	0
			154	154		
4	B	145	Total	O	0	0
			145	145		
4	C	188	Total	O	0	0
			188	188		
4	D	182	Total	O	0	0
			182	182		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

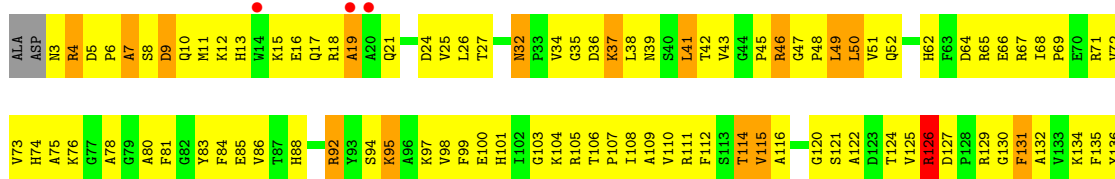
• Molecule 1: Catalase

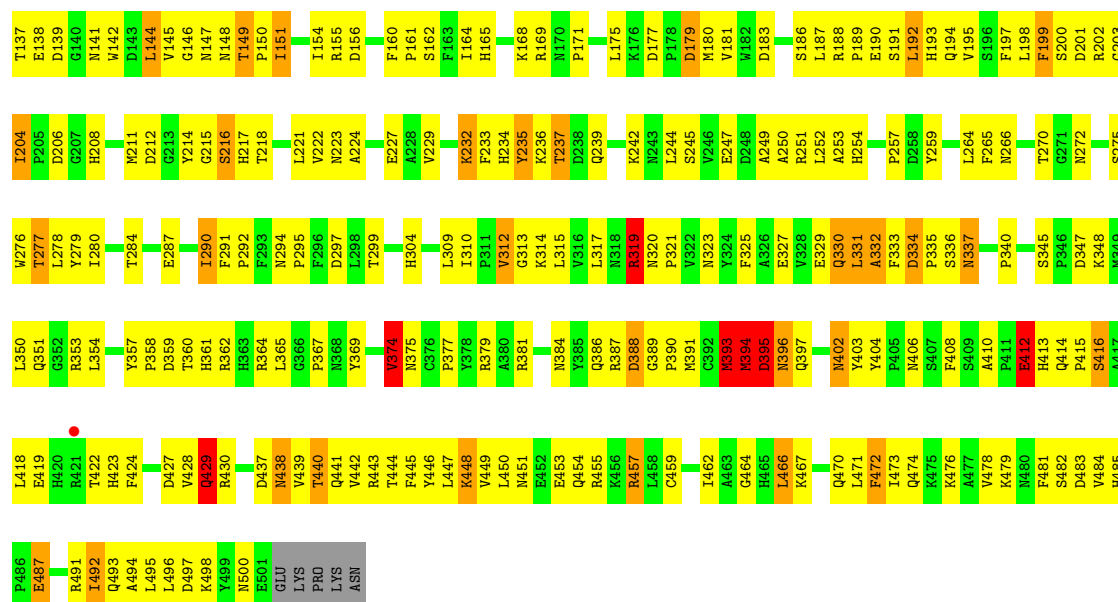
Chain A: 



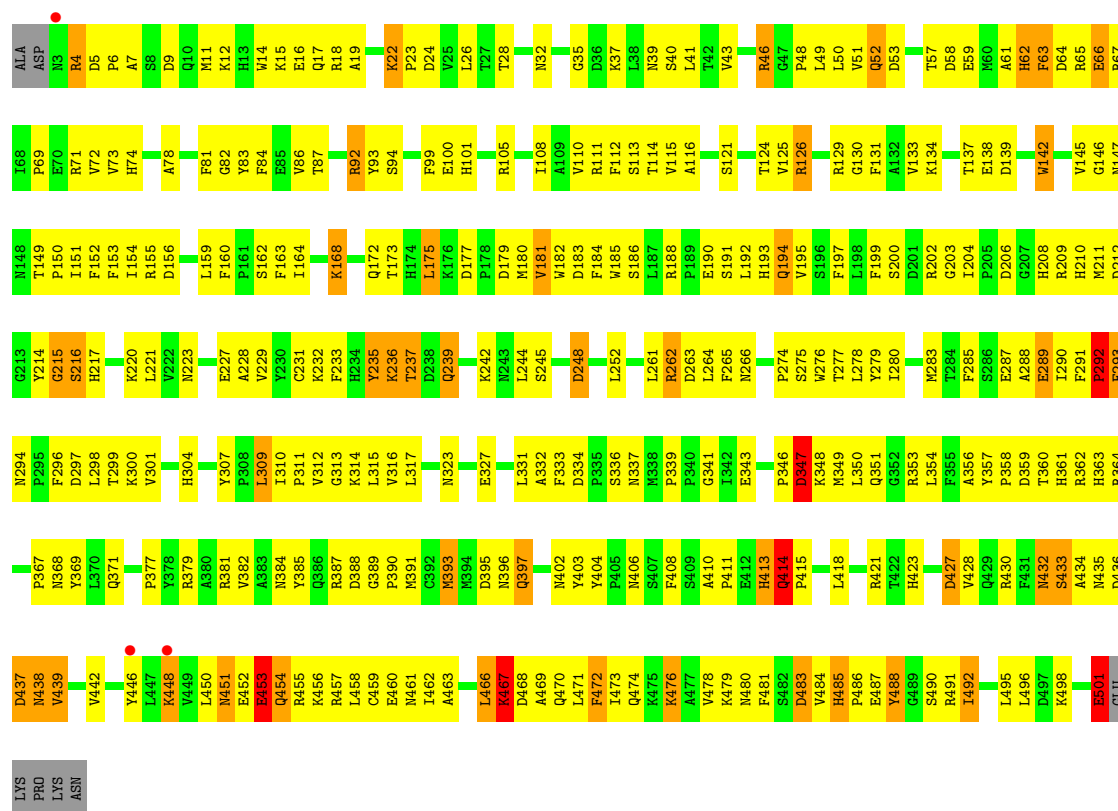
• Molecule 1: Catalase

Chain B: 





● Molecule 1: Catalase



● Molecule 1: Catalase



H423	F424	D427	V428	Q429	R430	F431	N432	D436	D437	N438	V439	T440	Q441	V442	E453	R457	L458	C459	E460	L466	K467	L471	F472	I473	K479	N480	F481	S482	P483	V484	H485	P486	E487	Y488	I492	L495	K498	E501	GLU	LYS	PRO	LYS	ASN												
D359	T360	H361	R362	L365	G366	P367	N368	Y369	L370	Q371	L372	F373	V374	N375	Y378	R379	A380	R381	V382	A383	N384	Y385	Q386	R387	D388	P389	P390	M391	G392	M393	M394	D395	N396	Q397	G398	P401	Y404	P405	N406	S407	F408	A409	A410	P411	E412	H413	Q414	P415	S416	A417	L418	E419	H420	R421	T422
E287	A288	E289	I290	F291	P292	F293	F296	D297	L298	T299	K300	V301	W302	P303	L309	I310	G313	K314	L315	Y316	L317	K318	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				
M211	D212	G215	S216	H217	T218	F219	K220	L221	V222	N223	A224	E227	A228	V229	Y230	C231	K232	F233	H234	Y235	K236	G240	T241	K242	N243	L244	F245	S246	A247	V248	E249	Q250	L251	K252	D253	P254	S255	L261	R262	M263	S264	F265	N266	P274	S275	H276	T277	L278	Y279	I280	Q281	T284	P285	S286	
V145	G146	M147	N148	T149	P150	I151	R155	D156	A157	L158	L159	F160	P161	S162	F163	I164	H165	S166	G167	L168	M169	N170	P171	Q172	T173	H174	L175	K176	D177	P178	D179	M180	R181	W182	K183	F184	L187	R188	P189	E190	S191	L192	H193	Q194	V195	D201	R202	G203	T204	P205	D206	G207	H208	R209	H210
V72	V73	H74	A75	K76	G77	A78	Y83	F84	E85	V86	T87	H88	D89	F90	A92	R92	Y93	S94	K95	A96	K97	F98	P99	E100	H101	D102	K103	L104	R105	T106	P107	V110	R111	F112	S113	T114	V115	A116	G117	E118	S121	R126	D127	P128	R129	G130	F131	A132	R65	E66	Y136	T137	E138	D139	W142
ALA	ASP	N3	P6	M11	K12	H13	K15	E16	Q17	R18	A19	A20	Q21	K22	P23	D24	V25	L26	N32	P33	V34	G35	K37	L38	N39	S40	V43	G44	P45	R46	G47	P48	L49	L50	V51	Q52	D53	V54	T57	D58	E59	M60	F63	D64	R65	E66	T68	P69	E70	R71					

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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(°)	Ideal(°)
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

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%)	4	22
1	B	497/506 (98%)	408 (82%)	65 (13%)	24 (5%)	2	14
1	C	497/506 (98%)	398 (80%)	82 (16%)	17 (3%)	4	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	497/506 (98%)	402 (81%)	74 (15%)	21 (4%)	3	17
All	All	1988/2024 (98%)	1608 (81%)	301 (15%)	79 (4%)	3	18

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 ⓘ

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%)	14	43
1	B	431/437 (99%)	387 (90%)	44 (10%)	8	30
1	C	431/437 (99%)	394 (91%)	37 (9%)	12	40
1	D	431/437 (99%)	403 (94%)	28 (6%)	20	54
All	All	1724/1748 (99%)	1580 (92%)	144 (8%)	13	41

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 [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](#)

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	28,50,50	2.53	8 (28%)	17,82,82	1.51	2 (11%)
3	HEM	B	2001	1	28,50,50	2.51	10 (35%)	17,82,82	0.86	1 (5%)
3	HEM	C	2002	1	28,50,50	1.91	7 (25%)	17,82,82	0.88	1 (5%)
3	HEM	D	2003	1,2	28,50,50	3.35	11 (39%)	17,82,82	6.42	1 (5%)
2	3TR	D	3074	1,3	4,6,6	2.23	2 (50%)	0,7,7	0.00	-

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	-	0/6/54/54	0/0/8/8
3	HEM	B	2001	1	-	0/6/54/54	0/0/8/8
3	HEM	C	2002	1	-	0/6/54/54	0/0/8/8
3	HEM	D	2003	1,2	-	0/6/54/54	0/0/8/8
2	3TR	D	3074	1,3	-	0/0/0/0	0/1/1/1

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2003	HEM	C4B-CHC	-11.21	1.10	1.40
3	D	2003	HEM	C1D-CHD	-8.43	1.17	1.40
3	B	2001	HEM	C3B-CAB	-4.62	1.38	1.47
3	D	2003	HEM	C3B-CAB	-4.60	1.38	1.47
3	C	2002	HEM	C3B-CAB	-4.55	1.38	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	HEM	CBA-CAA-C2A	-2.32	108.05	112.48
3	C	2002	HEM	CBA-CAA-C2A	-2.26	108.17	112.48
3	A	2000	HEM	CBA-CAA-C2A	-2.24	108.19	112.48
3	A	2000	HEM	CMC-C2C-C3C	5.34	134.79	124.89
3	D	2003	HEM	CBA-CAA-C2A	26.29	162.74	112.48

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 [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	499/506 (98%)	-0.37	2 (0%) 92 81	10, 40, 76, 97	0
1	B	499/506 (98%)	-0.29	4 (0%) 86 69	16, 44, 78, 102	0
1	C	499/506 (98%)	-0.17	3 (0%) 89 75	16, 41, 81, 100	1 (0%)
1	D	499/506 (98%)	-0.29	4 (0%) 86 69	15, 45, 84, 101	0
All	All	1996/2024 (98%)	-0.28	13 (0%) 87 73	10, 43, 80, 102	1 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	421	ARG	3.4
1	B	19	ALA	3.1
1	D	422	THR	3.1
1	B	20	ALA	3.1
1	C	448	LYS	2.9

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(\AA^2)	Q<0.9
3	HEM	A	2000	43/43	0.80	0.42	6.45	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	4.15	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.