



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:38 PM GMT

PDB ID : 4CWX  
Title : ALPHA-KETOGLUTARATE-DEPENDENT DIOXYGENASE COMPLEX1  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2014-04-03  
Resolution : 2.15 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](mailto: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.

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

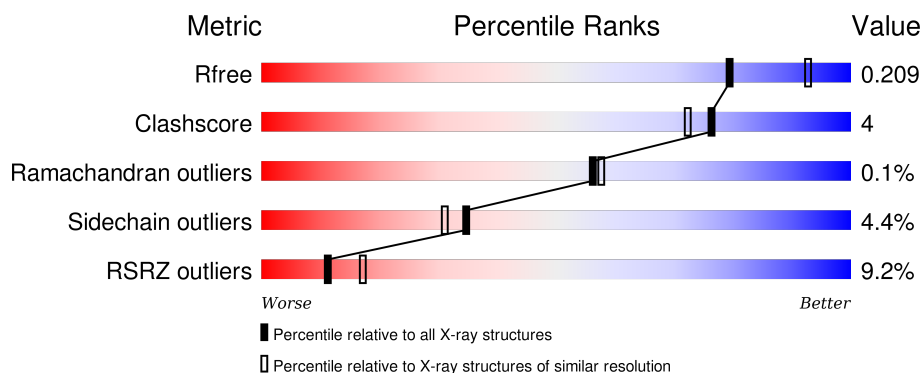
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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  $\geq 3$ , 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	443	<div> <div>10%</div> <div>81%</div> <div>8%</div> <div>9%</div> </div>
1	B	443	<div> <div>7%</div> <div>80%</div> <div>9%</div> <div>9%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ACT	A	860	-	-	-	X
6	ACT	B	860	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6914 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.

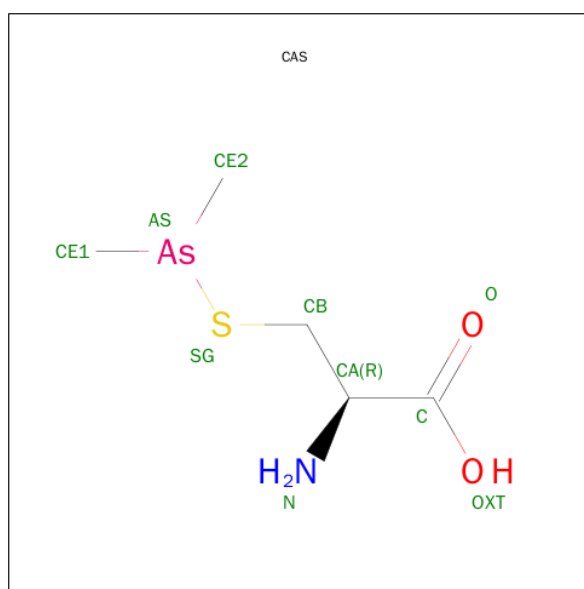
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, ENDOTHELIAL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	404	Total	As	C	N	O	S	0	1	0
			3220	1	2048	567	588	16			
1	B	402	Total	C	N	O	S		0	1	0
			3201	2036	562	586	17				

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29473
B	100	ARG	CYS	SEE REMARK 999	UNP P29473

- Molecule 2 is S-(DIMETHYLARSENIC)CYSTEINE (three-letter code: CAS) (formula:  $C_5H_{12}AsNO_2S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	As	C	0	0
			3	1	2		

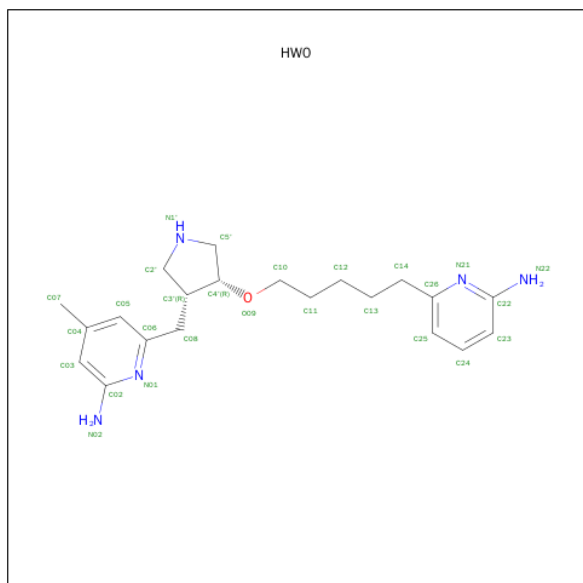
- 
- Chemical structure of HEM (Heme) showing a central iron atom coordinated by four nitrogen atoms in a porphyrin-like ring, with various side chains and a central heme group.

H4B

Chemical structure of H4B (Hydroquinone) showing a benzene ring with two hydroxyl groups at the para position. The structure is labeled with atom names: C1, C2, C3, C4, C5, C6 for the ring carbons; O1, O2 for the hydroxyl oxygens; H1, H2 for the hydroxyl hydrogens. The stereochemistry is indicated with wedges and dashes.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	5	3		
4	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 5 is 6-{[(3R,4R)-4-{[5-(6-AMINOPYRIDIN-2-YL)PENTYL]OXY}PYRROLIDIN-3-YL]METHYL}-4-METHYLPYRIDIN-2-AMINE (three-letter code: HW0) (formula: C<sub>21</sub>H<sub>31</sub>N<sub>5</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			27	21	5	1		
5	B	1	Total	C	N	O	0	0
			27	21	5	1		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Zn	0	0
			1	1		

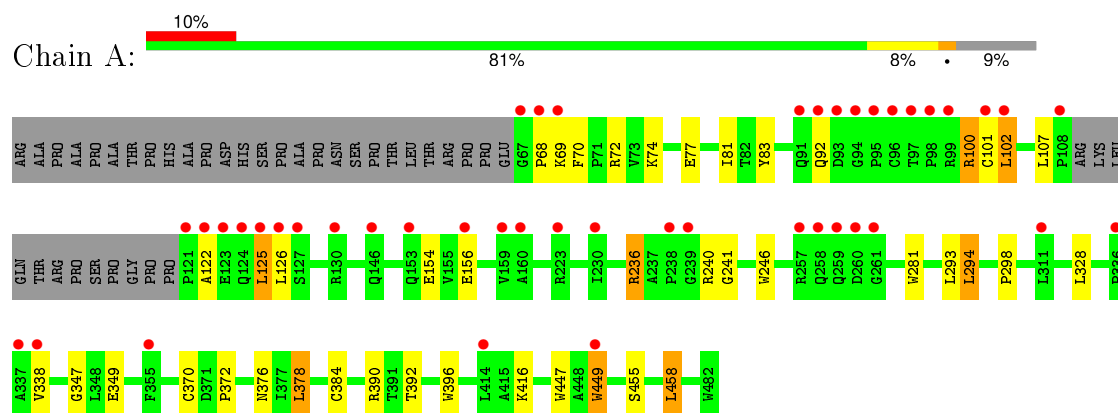
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	152	Total	O	0	0
			152	152		
8	B	147	Total	O	0	0
			147	147		

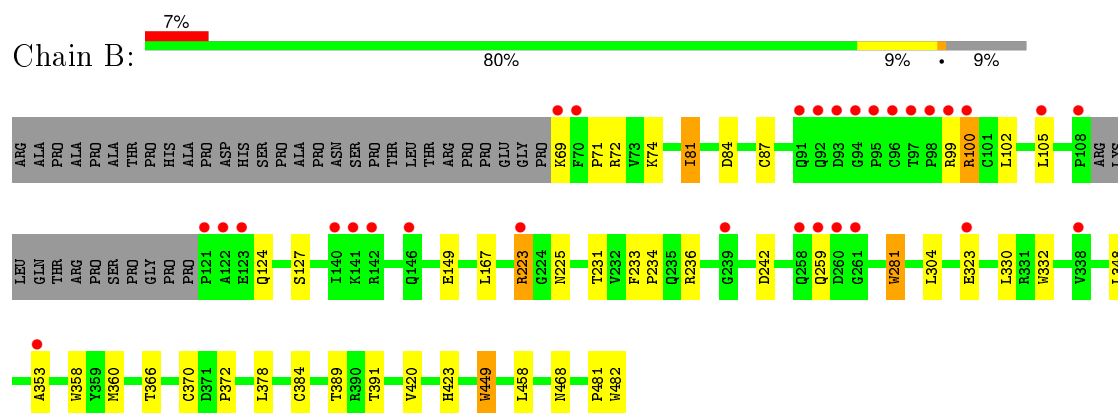
### 3 Residue-property plots [i](#)

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: NITRIC OXIDE SYNTHASE, ENDOTHELIAL



#### • Molecule 1: NITRIC OXIDE SYNTHASE, ENDOTHELIAL





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.94Å 106.49Å 156.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.70 – 2.15 39.21 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.70-2.15) 99.7 (39.21-2.15)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.171 , 0.210 0.169 , 0.209	Depositor DCC
$R_{free}$ test set	2690 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.3	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 53730 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6914	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, H4B, CAS, ACT, HEM, HW0

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	0.65	4/3303 (0.1%)	0.65	0/4497
1	B	0.63	3/3286 (0.1%)	0.63	0/4474
All	All	0.64	7/6589 (0.1%)	0.64	0/8971

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	447	TRP	CD2-CE2	5.97	1.48	1.41
1	A	281	TRP	CD2-CE2	5.85	1.48	1.41
1	A	396	TRP	CD2-CE2	5.62	1.48	1.41
1	B	332	TRP	CD2-CE2	5.42	1.47	1.41
1	B	449	TRP	CD2-CE2	5.28	1.47	1.41
1	A	449	TRP	CD2-CE2	5.21	1.47	1.41
1	B	281	TRP	CD2-CE2	5.17	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3220	0	3127	26	0
1	B	3201	0	3109	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3	0	0	1	0
3	A	43	0	30	2	0
3	B	43	0	30	5	0
4	A	17	0	15	2	0
4	B	17	0	15	1	0
5	A	27	0	31	2	0
5	B	27	0	31	2	0
6	A	8	0	6	0	0
6	B	8	0	6	0	0
7	B	1	0	0	0	0
8	A	152	0	0	1	0
8	B	147	0	0	0	0
All	All	6914	0	6400	50	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 4.

All (50) 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:384:CAS:AS	1:A:384:CAS:SG	2.53	1.27
1:B:384:CAS:SG	2:B:950:CAS:AS	2.56	1.23
3:B:500:HEM:HBC2	3:B:500:HEM:HMC2	1.57	0.84
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.73	0.70
1:A:384:CAS:CB	1:A:384:CAS:AS	3.00	0.70
1:A:100:ARG:HB3	1:B:87[B]:CYS:SG	2.33	0.68
1:B:236:ARG:HD2	1:B:242:ASP:OD1	1.94	0.68
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.81	0.61
1:B:358:TRP:H	3:B:500:HEM:HAB	1.68	0.59
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.83	0.59
3:B:500:HEM:HBC2	3:B:500:HEM:CMC	2.31	0.57
1:A:384:CAS:HB2	1:A:384:CAS:AS	2.65	0.57
1:A:102:LEU:HD11	1:B:71:PRO:HB3	1.88	0.56
1:B:99:ARG:HG2	1:B:100:ARG:HD2	1.88	0.55
1:B:71:PRO:HG2	1:B:84:ASP:HB3	1.87	0.55
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.38	0.54
1:A:449:TRP:HA	4:A:600:H4B:N1	2.24	0.53
1:A:236:ARG:HG3	1:A:349:GLU:HB2	1.92	0.51
3:A:500:HEM:HBA2	5:A:800:HW0:H9	1.93	0.51
1:B:449:TRP:HA	4:B:600:H4B:N1	2.25	0.51
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PRO:HB2	1:A:70:PHE:HD2	1.78	0.48
1:A:338:VAL:HG23	5:A:800:HW0:H5	1.96	0.47
1:A:107:LEU:HD12	1:B:72:ARG:HH22	1.80	0.46
1:A:240:ARG:HD2	1:A:241:GLY:O	2.15	0.46
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.42	0.46
1:B:99:ARG:HG2	1:B:100:ARG:CD	2.46	0.45
1:A:126:LEU:HD11	1:A:156:GLU:HA	1.98	0.45
1:B:74:LYS:HD2	1:B:81:ILE:HD11	1.97	0.45
3:B:500:HEM:HBA2	5:B:800:HW0:H9	1.98	0.45
1:A:378:LEU:HB2	8:A:2113:HOH:O	2.17	0.45
1:A:72:ARG:HB2	1:A:83:TYR:CE1	2.52	0.44
3:B:500:HEM:C4B	5:B:800:HW0:H3	2.53	0.44
1:B:481:PRO:HD2	1:B:482:TRP:CE3	2.53	0.44
1:B:366:THR:O	1:B:370:CYS:HB2	2.18	0.43
1:A:101:CYS:HB3	1:B:468:ASN:HB3	1.99	0.43
1:A:74:LYS:HD2	1:A:81:ILE:HD11	2.01	0.42
1:A:392:THR:HB	1:B:423:HIS:HB2	2.02	0.42
1:A:125:LEU:HD23	1:A:347:GLY:HA3	2.02	0.41
1:B:231:THR:O	1:B:353:ALA:HA	2.20	0.41
1:A:77:GLU:HG3	1:B:372:PRO:HG2	2.03	0.41
1:B:223:ARG:NH1	1:B:223:ARG:HB2	2.35	0.41
1:B:360:MET:HA	1:B:420:VAL:O	2.21	0.41
1:B:223:ARG:CZ	1:B:223:ARG:HB2	2.50	0.41
1:B:167:LEU:HG	1:B:348:LEU:HD12	2.03	0.41
1:A:455:SER:O	1:A:458:LEU:HB2	2.20	0.41
1:B:481:PRO:HD2	1:B:482:TRP:CZ3	2.56	0.41
3:A:500:HEM:O1A	4:A:600:H4B:N3	2.48	0.41
1:A:390:ARG:HB2	1:A:390:ARG:HE	1.65	0.41
1:A:372:PRO:HA	1:A:376:ASN:ND2	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	400/443 (90%)	392 (98%)	7 (2%)	1 (0%)	46	42
1	B	398/443 (90%)	390 (98%)	8 (2%)	0	100	100
All	All	798/886 (90%)	782 (98%)	15 (2%)	1 (0%)	56	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ALA

### 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	343/375 (92%)	330 (96%)	13 (4%)	40	37
1	B	342/375 (91%)	325 (95%)	17 (5%)	30	25
All	All	685/750 (91%)	655 (96%)	30 (4%)	35	31

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	92	GLN
1	A	100	ARG
1	A	102	LEU
1	A	125	LEU
1	A	154	GLU
1	A	236	ARG
1	A	293	LEU
1	A	294	LEU
1	A	328	LEU
1	A	378	LEU
1	A	416	LYS
1	A	458	LEU
1	B	69	LYS
1	B	81	ILE

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Mol	Chain	Res	Type
1	B	100	ARG
1	B	102	LEU
1	B	105	LEU
1	B	124	GLN
1	B	127	SER
1	B	149	GLU
1	B	223	ARG
1	B	225	ASN
1	B	259	GLN
1	B	323	GLU
1	B	330	LEU
1	B	378	LEU
1	B	389	THR
1	B	391	THR
1	B	458	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	166	HIS
1	A	191	GLN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	178	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	376	ASN
1	B	405	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CAS	A	384	1	5,8,9	1.11	0	2,9,11	1.31	0
1	CAS	B	384	1	4,5,9	0.44	0	3,5,11	1.25	1 (33%)

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
1	CAS	A	384	1	-	0/0/7/9	0/0/0/0
1	CAS	B	384	1	-	0/1/4/9	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	384	CAS	O-C-CA	-2.16	119.86	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	384	CAS	3	0
1	B	384	CAS	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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$
3	HEM	A	500	1	30,50,50	2.67	13 (43%)	24,82,82	2.77	9 (37%)
4	H4B	A	600	-	13,18,18	0.56	0	11,26,26	2.58	6 (54%)
5	HW0	A	800	-	26,29,29	0.73	0	29,38,38	2.02	5 (17%)
6	ACT	A	860	-	1,3,3	1.16	0	0,3,3	0.00	-
6	ACT	A	861	-	1,3,3	2.68	1 (100%)	0,3,3	0.00	-
3	HEM	B	500	1	30,50,50	2.70	13 (43%)	24,82,82	2.92	11 (45%)
4	H4B	B	600	-	13,18,18	0.72	0	11,26,26	2.23	5 (45%)
5	HW0	B	800	-	26,29,29	0.72	0	29,38,38	1.80	6 (20%)
6	ACT	B	860	-	1,3,3	1.44	0	0,3,3	0.00	-
6	ACT	B	861	-	1,3,3	1.58	0	0,3,3	0.00	-
2	CAS	B	950	-	0,2,9	0.00	-	0,1,11	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	500	1	-	0/10/54/54	0/0/8/8
4	H4B	A	600	-	-	0/8/17/17	0/2/2/2
5	HW0	A	800	-	-	0/13/23/23	0/3/3/3
6	ACT	A	860	-	-	0/0/0/0	0/0/0/0
6	ACT	A	861	-	-	0/0/0/0	0/0/0/0
3	HEM	B	500	1	-	0/10/54/54	0/0/8/8
4	H4B	B	600	-	-	0/8/17/17	0/2/2/2
5	HW0	B	800	-	-	0/13/23/23	0/3/3/3
6	ACT	B	860	-	-	0/0/0/0	0/0/0/0
6	ACT	B	861	-	-	0/0/0/0	0/0/0/0
2	CAS	B	950	-	-	0/0/0/9	0/0/0/0



All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	HEM	C3B-C4B	-4.46	1.47	1.51
3	A	500	HEM	C3B-C4B	-3.41	1.48	1.51
3	B	500	HEM	C2D-C3D	-2.78	1.46	1.54
3	B	500	HEM	C3D-C4D	-2.57	1.48	1.51
3	A	500	HEM	C2D-C3D	-2.51	1.47	1.54
3	A	500	HEM	C3D-C4D	-2.27	1.48	1.51
3	A	500	HEM	CAD-C3D	-2.06	1.50	1.54
3	A	500	HEM	FE-ND	2.01	2.08	1.97
3	B	500	HEM	CHD-C1D	2.15	1.44	1.38
3	A	500	HEM	C1A-CHA	2.23	1.46	1.39
3	B	500	HEM	C4A-CHB	2.35	1.46	1.39
3	B	500	HEM	FE-ND	2.37	2.10	1.97
3	B	500	HEM	FE-NB	2.43	2.10	1.97
3	A	500	HEM	FE-NB	2.47	2.10	1.97
3	A	500	HEM	CHC-C4B	2.54	1.45	1.38
6	A	861	ACT	CH3-C	2.68	1.52	1.48
3	B	500	HEM	CHC-C4B	2.79	1.46	1.38
3	B	500	HEM	C2A-C3A	3.33	1.47	1.37
3	A	500	HEM	C2A-C3A	3.56	1.48	1.37
3	A	500	HEM	CHD-C4C	3.72	1.45	1.36
3	B	500	HEM	CHD-C4C	4.00	1.45	1.36
3	B	500	HEM	CHC-C1C	4.02	1.45	1.36
3	A	500	HEM	CHC-C1C	4.37	1.46	1.36
3	B	500	HEM	C1C-NC	6.62	1.44	1.36
3	A	500	HEM	C1C-NC	6.89	1.44	1.36
3	B	500	HEM	C4C-NC	7.24	1.45	1.36
3	A	500	HEM	C4C-NC	7.33	1.45	1.36

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	HEM	CBA-CAA-C2A	-6.39	101.08	112.53
3	A	500	HEM	CBA-CAA-C2A	-5.66	102.38	112.53
4	B	600	H4B	N3-C2-N1	-3.43	119.91	125.53
3	B	500	HEM	C3B-CAB-CBB	-3.41	119.22	124.46
3	B	500	HEM	C3C-CAC-CBC	-3.17	119.60	124.46
4	A	600	H4B	N3-C2-N1	-3.14	120.39	125.53
5	A	800	HW0	C04-C05-C06	-2.77	118.54	120.28
5	A	800	HW0	C05-C06-N01	-2.61	120.02	122.96
5	B	800	HW0	C05-C06-N01	-2.59	120.03	122.96
3	A	500	HEM	C3B-C4B-CHC	-2.58	119.53	123.16
3	B	500	HEM	CBD-CAD-C3D	-2.49	106.32	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	HEM	CBD-CAD-C3D	-2.47	106.37	113.55
5	B	800	HW0	C04-C05-C06	-2.23	118.88	120.28
3	B	500	HEM	C1D-CHD-C4C	-2.21	122.14	125.82
5	A	800	HW0	C25-C26-N21	-2.17	119.75	122.41
5	B	800	HW0	C25-C24-C23	-2.11	117.22	120.24
3	B	500	HEM	C2C-C1C-NC	2.02	113.61	110.21
4	A	600	H4B	C4A-C8A-N8	2.02	120.81	118.43
3	A	500	HEM	C3B-C4B-NB	2.19	115.82	111.63
4	B	600	H4B	N2-C2-N3	2.20	120.85	117.20
4	A	600	H4B	N2-C2-N1	2.26	120.95	117.20
5	B	800	HW0	C14-C26-N21	2.32	119.12	115.69
4	A	600	H4B	C2-N1-C8A	2.57	120.31	114.54
4	B	600	H4B	C2-N1-C8A	2.88	121.01	114.54
5	B	800	HW0	C22-N21-C26	3.34	120.60	118.23
3	B	500	HEM	CMD-C2D-C3D	3.41	129.43	114.35
4	B	600	H4B	C4-N3-C2	3.42	120.69	115.94
3	A	500	HEM	CMD-C2D-C3D	3.51	129.89	114.35
4	B	600	H4B	C4-C4A-C8A	3.66	117.88	114.56
4	A	600	H4B	C4-N3-C2	4.24	121.83	115.94
3	A	500	HEM	CMC-C2C-C3C	4.45	127.64	116.53
3	A	500	HEM	CAD-C3D-C4D	4.53	128.46	112.47
3	B	500	HEM	CMC-C2C-C3C	4.63	128.08	116.53
3	B	500	HEM	CAD-C3D-C4D	4.67	128.95	112.47
3	B	500	HEM	CAD-C3D-C2D	5.26	128.34	113.22
4	A	600	H4B	C4-C4A-C8A	5.29	119.35	114.56
3	A	500	HEM	CAD-C3D-C2D	5.44	128.86	113.22
3	A	500	HEM	CMB-C2B-C3B	5.74	130.85	116.53
3	B	500	HEM	CMB-C2B-C3B	5.98	131.46	116.53
5	A	800	HW0	C22-N21-C26	6.02	122.50	118.23
5	B	800	HW0	C02-N01-C06	6.26	122.67	118.23
5	A	800	HW0	C02-N01-C06	6.34	122.73	118.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	HEM	2	0
4	A	600	H4B	2	0
5	A	800	HW0	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	500	HEM	5	0
4	B	600	H4B	1	0
5	B	800	HW0	2	0
2	B	950	CAS	1	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	403/443 (90%)	0.60	44 (10%) 7 12	32, 45, 77, 97	0
1	B	401/443 (90%)	0.50	30 (7%) 17 23	33, 48, 80, 112	0
All	All	804/886 (90%)	0.55	74 (9%) 11 17	32, 46, 78, 112	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	GLY	5.8
1	A	123	GLU	5.8
1	A	98	PRO	5.7
1	A	121	PRO	5.6
1	B	259	GLN	5.6
1	A	69	LYS	5.5
1	A	259	GLN	5.5
1	A	99	ARG	5.4
1	A	160	ALA	5.2
1	B	99	ARG	5.2
1	A	122	ALA	4.8
1	A	91	GLN	4.8
1	B	121	PRO	4.7
1	B	239	GLY	4.7
1	A	238	PRO	4.5
1	A	239	GLY	4.2
1	A	94	GLY	4.2
1	A	92	GLN	4.2
1	B	122	ALA	4.1
1	B	92	GLN	4.0
1	A	126	LEU	3.9
1	A	124	GLN	3.9
1	B	93	ASP	3.9
1	A	95	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	97	THR	3.7
1	A	338	VAL	3.7
1	B	146	GLN	3.7
1	A	261	GLY	3.6
1	B	98	PRO	3.6
1	B	108	PRO	3.6
1	A	97	THR	3.6
1	B	94	GLY	3.5
1	A	153	GLN	3.4
1	A	156	GLU	3.4
1	A	93	ASP	3.4
1	B	91	GLN	3.3
1	B	260	ASP	3.3
1	A	230	ILE	3.3
1	B	123	GLU	3.3
1	A	260	ASP	3.2
1	B	70	PHE	3.2
1	A	102	LEU	3.2
1	B	100	ARG	3.1
1	A	414	LEU	3.0
1	A	337	ALA	3.0
1	A	68	PRO	2.9
1	A	96	CYS	2.9
1	B	223	ARG	2.9
1	A	257	ARG	2.9
1	A	130	ARG	2.8
1	A	108	PRO	2.7
1	B	261	GLY	2.7
1	A	355	PHE	2.7
1	B	258	GLN	2.6
1	B	141	LYS	2.6
1	A	159	VAL	2.5
1	B	140	ILE	2.5
1	A	449	TRP	2.5
1	B	69	LYS	2.5
1	B	96	CYS	2.4
1	A	127	SER	2.4
1	B	323	GLU	2.3
1	A	125	LEU	2.3
1	B	105	LEU	2.3
1	A	258	GLN	2.3
1	B	338	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	146	GLN	2.2
1	A	223	ARG	2.2
1	A	311	LEU	2.2
1	A	101	CYS	2.1
1	B	95	PRO	2.1
1	B	142	ARG	2.1
1	A	336	PRO	2.1
1	B	353	ALA	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CAS	B	384	6/10	0.97	0.07	-	53,54,57,62	0
1	CAS	A	384	9/10	0.97	0.09	-	44,45,61,61	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	ACT	B	860	4/4	0.97	0.26	9.95	54,56,60,61	0
6	ACT	A	860	4/4	0.96	0.18	3.54	53,57,58,59	0
5	HW0	B	800	27/27	0.93	0.20	1.05	38,43,53,55	0
3	HEM	A	500	43/43	0.98	0.20	0.97	28,32,40,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	HW0	A	800	27/27	0.94	0.22	0.63	36,46,58,59	0
3	HEM	B	500	43/43	0.99	0.16	0.46	32,35,43,50	0
6	ACT	A	861	4/4	0.95	0.16	0.33	37,37,41,43	0
4	H4B	B	600	17/17	0.98	0.16	0.25	35,40,43,43	0
4	H4B	A	600	17/17	0.98	0.15	-0.14	36,40,45,48	0
6	ACT	B	861	4/4	0.96	0.15	-0.46	43,44,47,47	0
2	CAS	B	950	3/10	0.98	0.11	-1.58	75,75,75,80	0
7	ZN	B	1483	1/1	0.99	0.08	-2.67	61,61,61,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.