



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:19 PM GMT

PDB ID : 1SOX  
Title : SULFITE OXIDASE FROM CHICKEN LIVER  
Authors : Kisker, C.; Schindelin, H.; Rees, D.C.  
Deposited on : 1997-12-31  
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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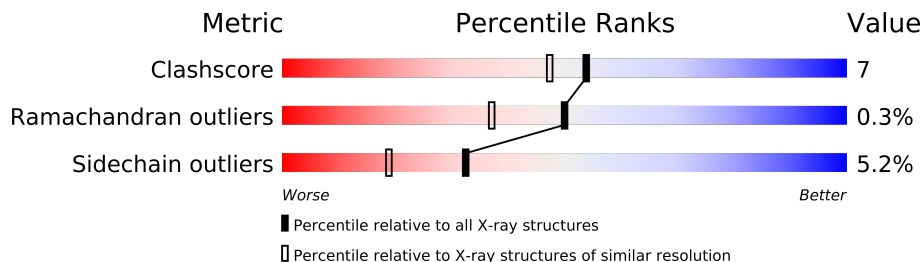
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	466	
1	B	466	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8189 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SULFITE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	6	0
			3613	2293	654	659	7			
1	B	458	Total	C	N	O	S	0	6	0
			3577	2271	641	658	7			

There are 16 discrepancies between the modelled and reference sequences:

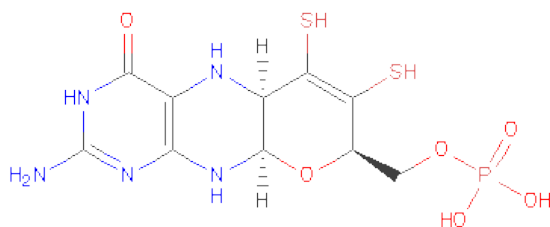
Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLU	ARG	CORRECTION	UNP P07850
A	?	-	ARG	DELETION	UNP P07850
A	161	GLY	ARG	CORRECTION	UNP P07850
A	218	ARG	SER	CORRECTION	UNP P07850
A	235	GLU	GLY	CORRECTION	UNP P07850
A	236	TRP	GLU	CORRECTION	UNP P07850
A	284	GLY	ARG	CORRECTION	UNP P07850
A	316	HIS	ARG	CORRECTION	UNP P07850
B	6	GLU	ARG	CORRECTION	UNP P07850
B	?	-	ARG	DELETION	UNP P07850
B	161	GLY	ARG	CORRECTION	UNP P07850
B	218	ARG	SER	CORRECTION	UNP P07850
B	235	GLU	GLY	CORRECTION	UNP P07850
B	236	TRP	GLU	CORRECTION	UNP P07850
B	284	GLY	ARG	CORRECTION	UNP P07850
B	316	HIS	ARG	CORRECTION	UNP P07850

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>6</sub>PS<sub>2</sub>).

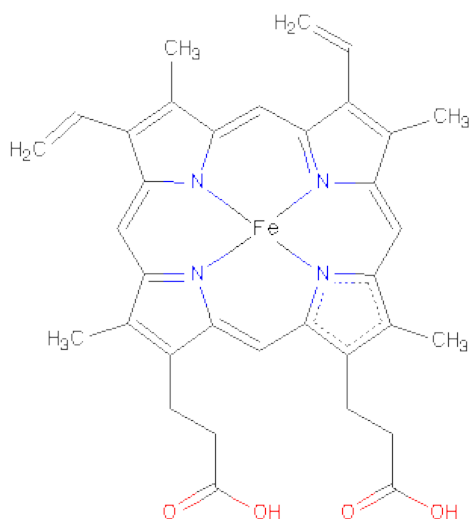


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	
3	B	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	

- Molecule 4 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

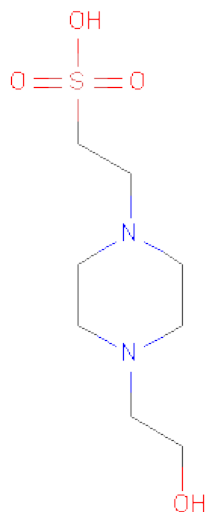
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mo	0	0
			1	1		
4	A	1	Total	Mo	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



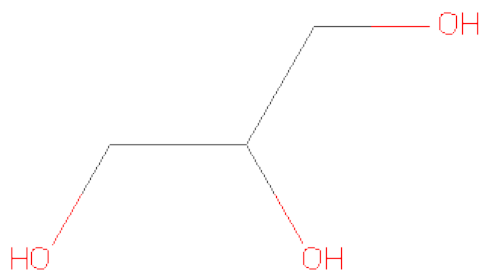
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O		
			43	34	1	4	4	0	0
5	B	1	Total	C	Fe	N	O		
			43	34	1	4	4	0	0

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	B	1	15	8	2	4	1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	6	3	3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	417	Total 417	O 417	0	0
8	B	405	Total 405	O 405	0	0

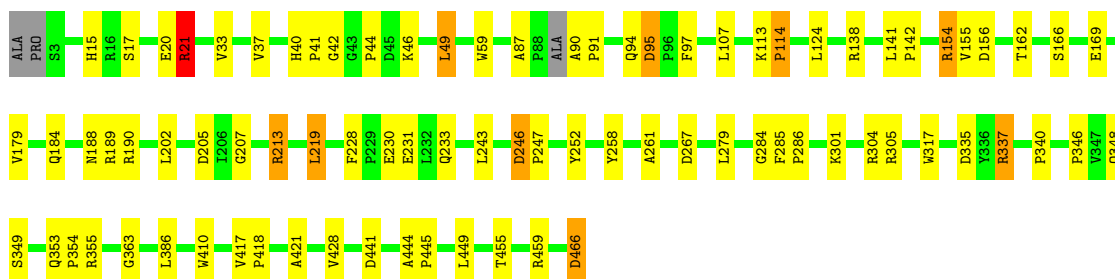
### 3 Residue-property plots

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

Note EDS was not executed.

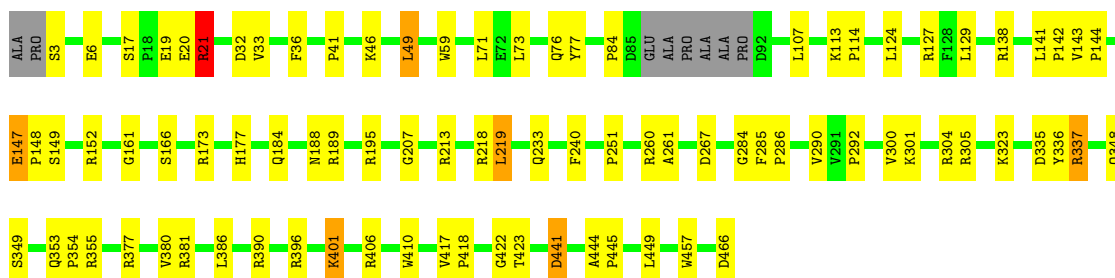
#### • Molecule 1: SULFITE OXIDASE

Chain A: 



#### • Molecule 1: SULFITE OXIDASE

Chain B: 





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.12Å 197.69Å 56.01Å 90.00° 94.23° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	89.2 (50.00-1.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.175 , 0.220	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8189	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 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: GOL, MO, SO4, HEM, EPE, MTE

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	0.49	0/3749	1.10	18/5128 (0.4%)
1	B	0.48	0/3712	1.08	20/5078 (0.4%)
All	All	0.48	0/7461	1.09	38/10206 (0.4%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	ARG	NE-CZ-NH2	-9.95	115.32	120.30
1	A	355	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	A	355	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	A	355	ARG	CD-NE-CZ	8.26	135.17	123.60
1	A	337	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	B	377	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	B	337	ARG	CD-NE-CZ	7.47	134.06	123.60
1	B	305	ARG	NE-CZ-NH2	7.15	123.88	120.30
1	B	114	PRO	N-CA-CB	7.03	111.74	103.30
1	B	337	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	213	ARG	CD-NE-CZ	6.93	133.31	123.60
1	B	355	ARG	CD-NE-CZ	6.84	133.18	123.60
1	B	354	PRO	N-CA-CB	6.60	111.22	103.30
1	A	354	PRO	N-CA-CB	6.54	111.15	103.30
1	B	285	PHE	O-C-N	6.51	133.46	121.10
1	B	286	PRO	CA-N-CD	-6.43	102.49	111.50
1	A	337	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	213	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	113	LYS	CA-C-O	-6.00	107.49	120.10
1	A	353	GLN	CA-C-O	-5.98	107.55	120.10
1	B	285	PHE	CA-C-O	-5.96	107.59	120.10
1	B	21	ARG	NE-CZ-NH2	-5.71	117.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	PHE	O-C-N	5.68	131.90	121.10
1	A	114	PRO	N-CA-CB	5.68	110.11	103.30
1	B	377	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	286	PRO	CA-N-CD	-5.42	103.91	111.50
1	A	205	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	286	PRO	N-CA-CB	5.39	109.77	103.30
1	B	353	GLN	CA-C-O	-5.37	108.81	120.10
1	A	87	ALA	C-N-CD	5.36	139.66	128.40
1	A	337	ARG	CD-NE-CZ	5.34	131.07	123.60
1	A	113	LYS	CA-C-O	-5.27	109.03	120.10
1	A	286	PRO	N-CA-CB	5.25	109.60	103.30
1	A	279	LEU	CA-CB-CG	5.08	126.98	115.30
1	A	286	PRO	N-CD-CG	5.06	110.79	103.20
1	B	213	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	B	381	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	260	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3613	0	3503	50	0
1	B	3577	0	3456	49	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	24	0	10	0	0
3	B	24	0	10	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	43	0	30	2	0
5	B	43	0	30	3	0
6	B	15	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	6	0	8	0	0
8	A	417	0	0	0	0
8	B	405	0	0	0	0
All	All	8189	0	7065	98	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (98) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:161:GLY:HA3	6:B:911:EPE:H52	1.57	0.83
1:B:386:LEU:HD11	1:B:417:VAL:HG21	1.67	0.76
1:A:124:LEU:HD11	1:A:207:GLY:HA2	1.69	0.73
1:A:305[B]:ARG:HH11	1:A:305[B]:ARG:HG3	1.51	0.73
1:B:335:ASP:OD1	1:B:337:ARG:HD3	1.89	0.71
1:A:304[B]:ARG:HG2	1:A:304[B]:ARG:HH11	1.55	0.71
1:B:189:ARG:HH11	1:B:348:GLN:HE22	1.41	0.67
1:A:305[B]:ARG:NH1	1:A:305[B]:ARG:HG3	2.08	0.67
1:A:335:ASP:OD1	1:A:337:ARG:HD3	1.96	0.66
1:A:189:ARG:HH11	1:A:348:GLN:HE22	1.45	0.63
1:A:33:VAL:HG11	5:A:502:HEM:HBB1	1.81	0.63
1:A:417:VAL:HG22	1:A:418:PRO:HD2	1.82	0.62
1:B:141:LEU:HB3	1:B:142:PRO:CD	2.30	0.62
1:A:348:GLN:HE21	1:A:349:SER:H	1.48	0.61
1:B:124:LEU:HD11	1:B:207:GLY:HA2	1.83	0.61
1:B:177[B]:HIS:CE1	1:B:218:ARG:HE	2.19	0.60
1:A:15:HIS:HB3	1:A:21:ARG:O	2.02	0.60
1:A:243:LEU:HD21	1:A:304[B]:ARG:HD3	1.83	0.59
1:B:348:GLN:HE21	1:B:349:SER:H	1.50	0.59
1:B:141:LEU:HB3	1:B:142:PRO:HD2	1.85	0.59
1:A:386:LEU:HD11	1:A:417:VAL:HG11	1.85	0.58
1:B:36:PHE:HB2	1:B:77:TYR:CZ	2.38	0.58
1:B:177[A]:HIS:HE1	1:B:267:ASP:OD1	1.86	0.57
1:A:190:ARG:HD2	1:A:202:LEU:O	2.05	0.57
1:B:21:ARG:HD3	1:B:32:ASP:OD2	2.05	0.57
1:A:154:ARG:HG2	1:A:305[B]:ARG:NH1	2.20	0.56
1:A:154:ARG:NH1	1:A:156:ASP:HB3	2.20	0.56
1:A:141:LEU:HB3	1:A:142:PRO:HD2	1.87	0.55
1:B:184:GLN:HE21	1:B:188:ASN:HB3	1.70	0.55
1:A:20:GLU:O	1:A:21:ARG:HB2	2.06	0.54
1:B:177[B]:HIS:CD2	1:B:218:ARG:HH21	2.25	0.54
1:A:17:SER:O	1:A:21:ARG:N	2.40	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:173:ARG:NH1	6:B:911:EPE:O2S	2.43	0.52
1:B:240:PHE:HB2	1:B:300:VAL:HG21	1.93	0.51
1:A:421:ALA:HB1	1:A:466:ASP:HA	1.92	0.51
1:B:189:ARG:HH11	1:B:348:GLN:NE2	2.06	0.51
1:A:189:ARG:HH11	1:A:348:GLN:NE2	2.09	0.51
1:A:154:ARG:NE	1:A:305[B]:ARG:HH12	2.09	0.50
1:A:304[B]:ARG:CG	1:A:304[B]:ARG:HH11	2.24	0.50
1:A:179:VAL:HG21	1:A:267:ASP:HB3	1.92	0.50
1:A:184:GLN:HE21	1:A:188:ASN:HD22	1.60	0.50
1:B:41:PRO:HG2	5:B:502:HEM:C2A	2.47	0.49
1:B:149:SER:O	1:B:152:ARG:NH2	2.45	0.49
1:A:90:ALA:N	1:A:91:PRO:HD3	2.27	0.49
1:B:323:LYS:HD2	1:B:336:TYR:HD2	1.75	0.49
1:A:444:ALA:HB3	1:A:445:PRO:HD3	1.93	0.49
1:A:42:GLY:HA3	5:A:502:HEM:O2D	2.13	0.49
1:A:184:GLN:NE2	1:A:188:ASN:HD22	2.11	0.48
1:B:417:VAL:CG2	1:B:418:PRO:HD2	2.43	0.48
1:A:94:GLN:O	1:A:95:ASP:HB3	2.12	0.48
1:A:417:VAL:CG2	1:A:418:PRO:HD2	2.43	0.48
1:A:154:ARG:HH12	1:A:156:ASP:HB3	1.77	0.48
1:B:33:VAL:HG11	5:B:502:HEM:HBB1	1.95	0.48
1:B:127:ARG:HD3	1:B:129:LEU:O	2.14	0.48
1:B:17:SER:O	1:B:21:ARG:N	2.47	0.47
1:B:251:PRO:HG3	1:B:304:ARG:NH2	2.30	0.47
1:A:246:ASP:HB2	1:A:247:PRO:HD2	1.97	0.47
1:A:428:VAL:HG22	1:A:459:ARG:HG2	1.97	0.47
1:A:252:TYR:HA	1:A:317:TRP:CZ3	2.50	0.47
1:A:46:LYS:O	1:A:49:LEU:HB2	2.15	0.47
1:B:147[A]:GLU:OE2	1:B:148:PRO:HD2	2.15	0.47
1:B:422:GLY:N	1:B:466:ASP:HA	2.30	0.47
1:A:141:LEU:HB3	1:A:142:PRO:CD	2.45	0.46
1:B:386:LEU:HD11	1:B:417:VAL:CG2	2.41	0.46
1:B:19:GLU:H	1:B:19:GLU:CD	2.17	0.45
1:A:166:SER:OG	1:A:169:GLU:HG3	2.17	0.45
1:B:417:VAL:HG22	1:B:418:PRO:HD2	1.99	0.45
1:A:154:ARG:CZ	1:A:305[B]:ARG:HH12	2.30	0.45
1:B:441:ASP:HA	1:B:457:TRP:CE2	2.52	0.45
1:A:97:PHE:CE2	1:A:114:PRO:HA	2.52	0.45
1:A:243:LEU:CD2	1:A:304[B]:ARG:HD3	2.47	0.45
1:B:284:GLY:HA2	1:B:301:LYS:HB3	1.99	0.45
1:B:184:GLN:NE2	1:B:188:ASN:HD22	2.15	0.45
1:A:154:ARG:NH1	1:A:162:THR:HG23	2.33	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:46:LYS:O	1:B:49:LEU:HB2	2.18	0.44
1:A:37:VAL:HG12	1:A:44:PRO:HB3	2.00	0.44
1:B:323:LYS:HD2	1:B:336:TYR:CD2	2.53	0.43
1:A:304[B]:ARG:CG	1:A:304[B]:ARG:NH1	2.81	0.43
1:A:228:PHE:HB3	1:A:258:TYR:OH	2.18	0.43
1:A:346:PRO:HG2	1:A:455:THR:HG21	2.00	0.43
1:B:20:GLU:O	1:B:21:ARG:HB2	2.18	0.43
1:B:290:VAL:O	1:B:292:PRO:HD3	2.19	0.43
1:B:401:LYS:HE2	1:B:401:LYS:HA	2.00	0.42
1:A:284:GLY:HA2	1:A:301:LYS:HB3	2.00	0.42
1:A:363:GLY:O	1:A:418:PRO:HA	2.19	0.42
1:B:189:ARG:NH1	1:B:348:GLN:HE22	2.14	0.42
1:B:219:LEU:HD13	1:B:261:ALA:HB1	2.02	0.41
1:B:46:LYS:O	5:B:502:HEM:HBC2	2.20	0.41
1:B:386:LEU:HD11	1:B:417:VAL:HG11	2.02	0.41
1:B:36:PHE:HE1	1:B:73:LEU:HD21	1.85	0.41
1:B:444:ALA:HB3	1:B:445:PRO:HD3	2.03	0.41
1:B:36:PHE:CE1	1:B:73:LEU:HD21	2.55	0.41
1:A:219:LEU:HD13	1:A:261:ALA:HB1	2.03	0.41
1:A:340:PRO:HG3	1:B:380:VAL:HG11	2.03	0.40
1:B:20:GLU:O	1:B:21:ARG:CB	2.69	0.40
1:B:152:ARG:HE	1:B:166:SER:HA	1.86	0.40
1:A:40:HIS:HA	1:A:41:PRO:HD3	1.91	0.40
1:B:143:VAL:HA	1:B:144:PRO:HD3	1.92	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	465/466 (100%)	453 (97%)	11 (2%)	1 (0%)	56	44
1	B	460/466 (99%)	448 (97%)	10 (2%)	2 (0%)	43	29
All	All	925/932 (99%)	901 (97%)	21 (2%)	3 (0%)	50	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	B	21	ARG
1	B	84	PRO

### 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	379/377 (100%)	361 (95%)	18 (5%)	36	22
1	B	377/377 (100%)	355 (94%)	22 (6%)	28	15
All	All	756/754 (100%)	716 (95%)	40 (5%)	32	18

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	49	LEU
1	A	59	TRP
1	A	95	ASP
1	A	107	LEU
1	A	138	ARG
1	A	154	ARG
1	A	155	VAL
1	A	213	ARG
1	A	219	LEU
1	A	230	GLU
1	A	231	GLU
1	A	233	GLN
1	A	246	ASP
1	A	410	TRP
1	A	441	ASP
1	A	449	LEU
1	A	466	ASP
1	B	3	SER
1	B	6	GLU
1	B	21	ARG

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Mol	Chain	Res	Type
1	B	49	LEU
1	B	59	TRP
1	B	71	LEU
1	B	76	GLN
1	B	107	LEU
1	B	138	ARG
1	B	147[A]	GLU
1	B	147[B]	GLU
1	B	195	ARG
1	B	219	LEU
1	B	233	GLN
1	B	390	ARG
1	B	396	ARG
1	B	401	LYS
1	B	406	ARG
1	B	410	TRP
1	B	423	THR
1	B	441	ASP
1	B	449	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	233	GLN
1	A	319	GLN
1	A	343	GLN
1	A	348	GLN
1	A	465	GLN
1	B	184	GLN
1	B	319	GLN
1	B	343	GLN
1	B	348	GLN
1	B	465	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	MTE	A	501	4	26,26,26	4.74	14 (53%)	34,40,40	2.89	14 (41%)
5	HEM	A	502	1	49,50,50	2.32	13 (26%)	46,82,82	1.71	4 (8%)
2	SO4	A	503	-	4,4,4	1.86	3 (75%)	6,6,6	0.33	0
2	SO4	A	504	-	4,4,4	1.76	2 (50%)	6,6,6	0.19	0
7	GOL	A	912	-	5,5,5	0.06	0	5,5,5	0.38	0
3	MTE	B	501	4	26,26,26	4.71	16 (61%)	34,40,40	2.72	14 (41%)
5	HEM	B	502	1	49,50,50	2.18	12 (24%)	46,82,82	1.50	7 (15%)
2	SO4	B	503	-	4,4,4	1.90	1 (25%)	6,6,6	0.63	0
2	SO4	B	504	-	4,4,4	1.75	2 (50%)	6,6,6	0.26	0
6	EPE	B	911	-	15,15,15	2.52	2 (13%)	20,20,20	2.42	8 (40%)

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	MTE	A	501	4	-	0/6/34/34	0/0/3/3
5	HEM	A	502	1	-	0/14/114/114	0/0/8/8
2	SO4	A	503	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	504	-	-	0/0/0/0	0/0/0/0
7	GOL	A	912	-	-	0/4/4/4	0/0/0/0
3	MTE	B	501	4	-	0/6/34/34	0/0/3/3
5	HEM	B	502	1	-	0/14/114/114	0/0/8/8
2	SO4	B	503	-	-	0/0/0/0	0/0/0/0
2	SO4	B	504	-	-	0/0/0/0	0/0/0/0
6	EPE	B	911	-	-	0/9/19/19	0/1/1/1

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	MTE	C9-C10	13.52	1.61	1.41
3	A	501	MTE	C9-C10	13.02	1.60	1.41
6	B	911	EPE	O3S-S	8.95	1.68	1.46
3	A	501	MTE	C6-N5	8.76	1.58	1.45
3	B	501	MTE	C6-N5	8.68	1.58	1.45
3	A	501	MTE	C6-C1'	-8.01	1.39	1.50
3	B	501	MTE	C6-C1'	-7.44	1.40	1.50
3	A	501	MTE	C4'-C3'	-7.35	1.40	1.52
3	B	501	MTE	C4'-C3'	-6.75	1.41	1.52
3	B	501	MTE	C7-C6	6.72	1.65	1.53
3	A	501	MTE	C7-C6	6.70	1.65	1.53
3	A	501	MTE	P-O4'	-6.35	1.38	1.60
5	A	502	HEM	C3B-C2B	-6.03	1.33	1.43
5	A	502	HEM	C3C-C2C	-5.91	1.33	1.43
3	B	501	MTE	P-O4'	-5.81	1.40	1.60
5	A	502	HEM	C3D-C4D	5.62	1.46	1.44
5	B	502	HEM	C3C-C2C	-5.57	1.34	1.43
5	B	502	HEM	C3D-C2D	-5.49	1.34	1.43
5	B	502	HEM	C3B-C2B	-5.36	1.34	1.43
3	A	501	MTE	P-O3P	-5.36	1.35	1.54
3	B	501	MTE	P-O3P	-4.97	1.36	1.54
5	A	502	HEM	C3B-CAB	4.82	1.55	1.40
5	A	502	HEM	C3D-C2D	-4.75	1.35	1.43
5	B	502	HEM	C4A-C3A	4.61	1.45	1.40
3	A	501	MTE	C3'-C2'	4.60	1.59	1.51
5	B	502	HEM	C3B-CAB	4.55	1.54	1.40
5	A	502	HEM	C3C-CAC	4.55	1.54	1.40
5	A	502	HEM	C4A-C3A	4.44	1.45	1.40
3	B	501	MTE	C2-N1	4.42	1.39	1.33
3	B	501	MTE	C3'-C2'	4.36	1.59	1.51
3	B	501	MTE	O4-C4	4.21	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	MTE	C2-N1	4.17	1.38	1.33
5	B	502	HEM	C3C-CAC	4.15	1.53	1.40
3	A	501	MTE	C4-C9	3.76	1.48	1.41
3	A	501	MTE	C9-N5	3.70	1.50	1.38
3	B	501	MTE	C9-N5	3.66	1.50	1.38
3	B	501	MTE	C4-C9	3.65	1.47	1.41
3	A	501	MTE	O4-C4	3.49	1.31	1.24
5	B	502	HEM	C2D-C1D	3.44	1.45	1.44
5	A	502	HEM	C2D-C1D	3.29	1.45	1.44
6	B	911	EPE	C10-S	3.10	1.82	1.77
2	B	503	SO4	O3-S	2.77	1.56	1.47
5	A	502	HEM	CMB-C2B	2.55	1.55	1.47
3	B	501	MTE	C2-N2	2.54	1.36	1.32
3	B	501	MTE	C1'-S1'	-2.51	1.65	1.74
5	B	502	HEM	C2B-C1B	2.47	1.45	1.44
5	B	502	HEM	CMB-C2B	2.46	1.55	1.47
5	B	502	HEM	CMC-C2C	2.44	1.55	1.47
5	A	502	HEM	CMC-C2C	2.42	1.54	1.47
5	A	502	HEM	CMD-C2D	2.31	1.54	1.47
3	A	501	MTE	C1'-S1'	-2.31	1.65	1.74
5	B	502	HEM	CMD-C2D	2.30	1.54	1.47
5	A	502	HEM	CAA-C2A	2.28	1.56	1.52
5	A	502	HEM	FE-NA	2.22	2.01	1.92
3	A	501	MTE	C10-N8	2.22	1.39	1.35
2	A	503	SO4	O4-S	2.21	1.54	1.47
3	B	501	MTE	O3'-C3'	2.19	1.47	1.43
2	A	504	SO4	O3-S	2.17	1.54	1.47
5	B	502	HEM	FE-NA	2.17	2.01	1.92
2	B	504	SO4	O2-S	2.16	1.54	1.47
2	B	504	SO4	O3-S	2.14	1.54	1.47
2	A	503	SO4	O3-S	2.08	1.54	1.47
3	B	501	MTE	C2-N3	-2.08	1.33	1.36
2	A	504	SO4	O2-S	2.08	1.53	1.47
2	A	503	SO4	O1-S	2.07	1.53	1.47

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	HEM	CBD-CAD-C3D	7.51	130.76	114.37
3	A	501	MTE	C2-N1-C10	7.39	128.12	117.61
3	B	501	MTE	C2-N1-C10	6.56	126.93	117.61
3	B	501	MTE	N8-C10-N1	6.49	126.69	116.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	MTE	N8-C10-N1	5.85	125.69	116.51
3	A	501	MTE	C4-C9-N5	5.79	127.52	119.10
3	B	501	MTE	C4-C9-N5	5.74	127.44	119.10
5	B	502	HEM	C3B-C4B-NB	-5.71	109.92	114.00
3	A	501	MTE	N2-C2-N3	5.59	124.02	117.86
6	B	911	EPE	O3S-S-O1S	-5.42	100.06	111.78
5	A	502	HEM	C3B-C4B-NB	-5.38	110.15	114.00
6	B	911	EPE	O1S-S-C10	5.36	111.40	106.81
3	A	501	MTE	C9-C10-N1	-5.11	113.33	121.50
3	B	501	MTE	O3'-C7-N8	-4.93	102.80	109.22
3	A	501	MTE	O3'-C7-N8	-4.72	103.08	109.22
3	B	501	MTE	C9-C10-N1	-4.33	114.57	121.50
3	B	501	MTE	N2-C2-N3	3.89	122.14	117.86
3	B	501	MTE	C4-N3-C2	3.74	126.04	119.51
6	B	911	EPE	O2S-S-C10	3.52	109.82	106.81
3	A	501	MTE	O3'-C7-C6	-3.48	104.77	109.50
3	B	501	MTE	C6-C7-N8	3.45	114.72	110.01
3	A	501	MTE	C6-C7-N8	3.20	114.37	110.01
3	A	501	MTE	N2-C2-N1	-3.15	116.04	120.31
6	B	911	EPE	C3-C2-N1	3.04	116.60	110.61
5	B	502	HEM	CAD-CBD-CGD	3.03	122.92	113.48
5	A	502	HEM	CMA-C3A-C4A	-2.99	124.02	128.62
5	B	502	HEM	CMA-C3A-C4A	-2.92	124.13	128.62
5	B	502	HEM	C2D-C1D-ND	-2.85	109.57	112.93
3	B	501	MTE	O3'-C7-C6	-2.72	105.80	109.50
6	B	911	EPE	C2-C3-N4	2.69	115.92	110.61
3	A	501	MTE	C9-C4-N3	2.63	120.80	114.06
6	B	911	EPE	C5-C6-N1	2.48	115.51	110.61
3	B	501	MTE	N3-C2-N1	-2.44	118.36	121.78
6	B	911	EPE	C6-N1-C2	2.41	114.86	108.86
3	A	501	MTE	C9-N5-C6	-2.40	112.35	118.60
3	A	501	MTE	O2P-P-O4'	2.29	112.97	106.65
3	B	501	MTE	O3P-P-O4'	2.21	112.74	106.65
5	A	502	HEM	C2D-C1D-ND	-2.17	110.37	112.93
3	A	501	MTE	C4'-C3'-C2'	-2.14	108.46	110.98
5	B	502	HEM	CMA-C3A-C2A	2.13	128.96	124.94
5	B	502	HEM	O1A-CGA-CBA	-2.13	115.69	123.03
6	B	911	EPE	O3S-S-C10	-2.10	103.27	105.93
3	B	501	MTE	C9-C4-N3	2.07	119.36	114.06
3	B	501	MTE	C9-N5-C6	-2.05	113.25	118.60
5	B	502	HEM	O2A-CGA-O1A	2.05	128.51	123.30
3	B	501	MTE	O3P-P-O1P	-2.05	103.75	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	MTE	P-O4'-C4'	2.02	124.03	118.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.