



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 05:19 AM GMT

PDB ID : 1HCM  
Title : CYTOCHROME CD1 NITRITE REDUCTASE, OXIDISED FROM FROM  
TETRAGONAL CRYSTALS  
Authors : Sjogren, T.; Hajdu, J.  
Deposited on : 2001-05-05  
Resolution : 2.50 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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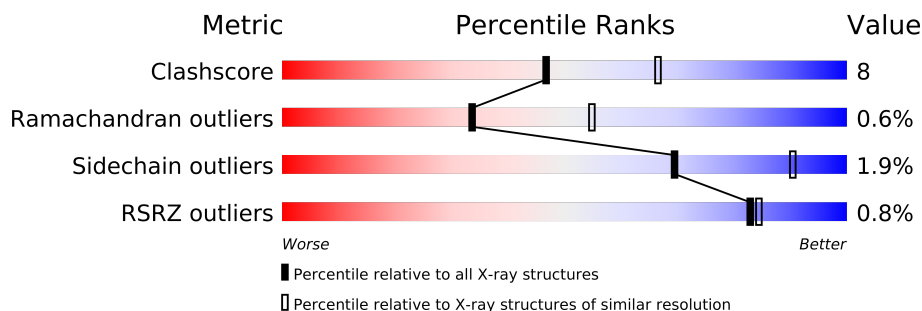
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
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 2.50 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	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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.

Mol	Chain	Length	Quality of chain
1	A	567	
1	B	567	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	B	603	-	X
4	SO4	B	622	-	X

## 2 Entry composition i

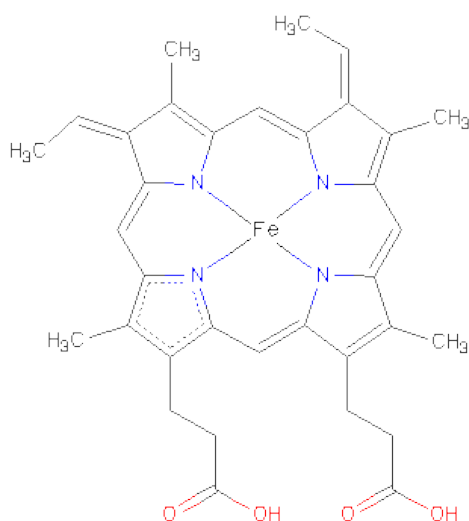
There are 5 unique types of molecules in this entry. The entry contains 8757 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CYTOCHROME CD1 NITRITE REDUCTASE.

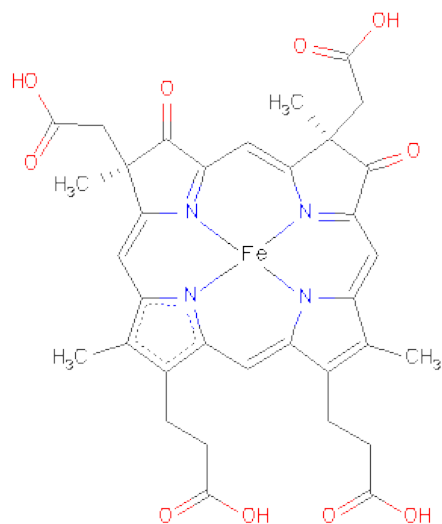
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	526	Total	C	N	O	S	0	0	0
			4094	2593	682	805	14			
1	B	529	Total	C	N	O	S	0	0	0
			4110	2603	685	808	14			

- Molecule 2 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

- Molecule 3 is HEME D (three-letter code: DHE) (formula:  $C_{34}H_{32}FeN_4O_{10}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			49	34	1	4	10		
3	B	1	Total	C	Fe	N	O	0	0
			49	34	1	4	10		

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



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

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

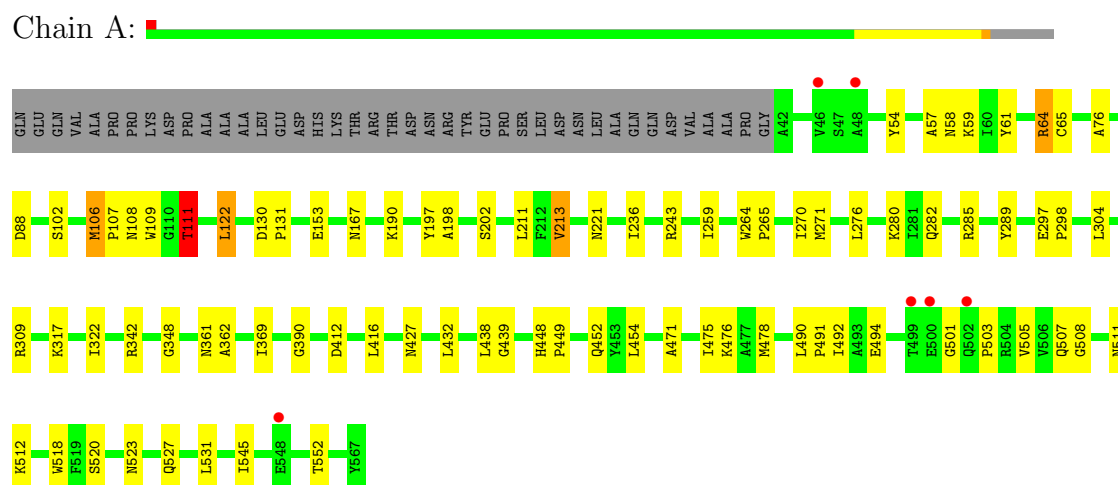
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	175	Total	O	0	0
			175	175		
5	B	174	Total	O	0	0
			174	174		

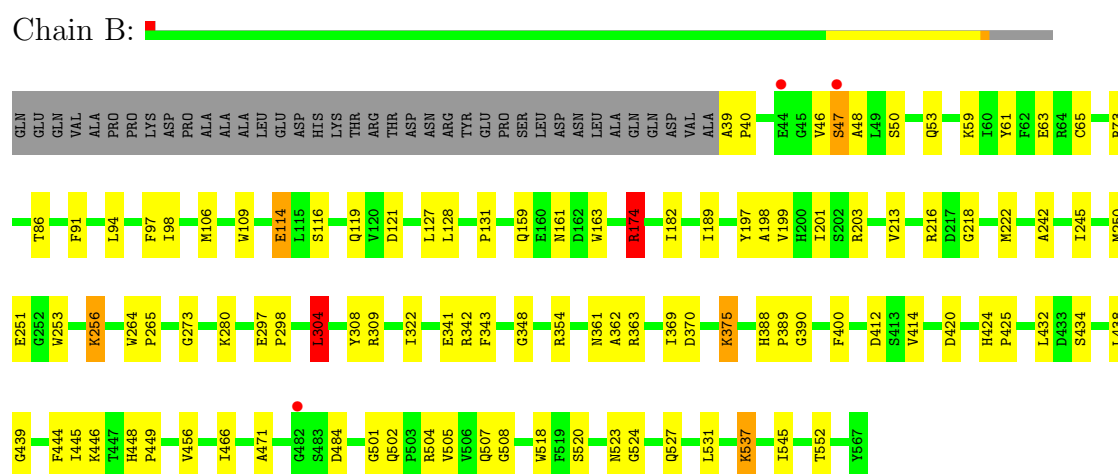
### 3 Residue-property plots

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.

#### • Molecule 1: CYTOCHROME CD1 NITRITE REDUCTASE



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.31 Å   128.31 Å   264.82 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.87 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-2.50) 97.4 (29.87-2.51)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 2.51 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.226 ,   0.258 0.192 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	39.0	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 28.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 74676 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8757	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DHE, SO4, HEC

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	0/4195	0.89	5/5705 (0.1%)
1	B	0.65	0/4212	0.86	5/5729 (0.1%)
All	All	0.65	0/8407	0.88	10/11434 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	GLY	N-CA-C	-5.71	98.82	113.10
1	B	390	GLY	N-CA-C	-5.65	98.97	113.10
1	A	106	MET	CA-CB-CG	5.16	122.07	113.30
1	A	309	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	111	THR	CA-CB-CG2	5.08	119.52	112.40
1	B	304	LEU	CA-CB-CG	5.07	126.96	115.30
1	A	243	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	504	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	B	309	ARG	CD-NE-CZ	5.01	130.61	123.60
1	B	370	ASP	CB-CG-OD1	5.01	122.81	118.30

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	4094	0	3948	59	0
1	B	4110	0	3963	72	0
2	A	43	0	30	4	0
2	B	43	0	30	4	0
3	A	49	0	28	1	0
3	B	49	0	28	3	0
4	A	5	0	0	0	0
4	B	15	0	0	1	0
5	A	175	0	0	4	0
5	B	174	0	0	6	0
All	All	8757	0	8027	133	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 8.

All (133) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:271:MET:HE2	1:A:276:LEU:HD22	1.24	1.17
1:A:108:ASN:HD22	1:A:111:THR:HG22	1.16	1.10
1:B:182:ILE:HD12	1:B:189:ILE:HG12	1.58	0.85
1:B:161:ASN:HD22	1:B:163:TRP:H	1.25	0.82
1:B:342:ARG:HH21	1:B:363:ARG:HH22	1.29	0.81
1:A:213:VAL:HG13	1:A:221:ASN:HB2	1.64	0.79
1:A:271:MET:CE	1:A:276:LEU:HD22	2.11	0.74
1:A:57:ALA:HB2	1:A:122:LEU:HD22	1.67	0.74
1:A:153:GLU:HG3	5:A:2033:HOH:O	1.89	0.71
1:B:537:LYS:HB2	1:B:537:LYS:HZ2	1.56	0.70
1:A:108:ASN:ND2	1:A:111:THR:HG22	1.98	0.70
1:A:109:TRP:CE2	2:A:601:HEC:HBB2	2.27	0.70
1:B:537:LYS:H	1:B:537:LYS:HZ1	1.40	0.70
1:B:86:THR:HG23	1:B:94:LEU:HD11	1.74	0.68
1:A:452:GLN:HB3	1:A:476:LYS:HE2	1.77	0.66
1:B:86:THR:HG22	1:B:128:LEU:HD23	1.79	0.65
1:B:537:LYS:NZ	1:B:537:LYS:H	1.96	0.63
1:B:182:ILE:CD1	1:B:189:ILE:HG12	2.31	0.60
1:B:174:ARG:NH1	5:B:2032:HOH:O	2.34	0.60
1:A:259:ILE:HD12	1:A:270:ILE:CD1	2.31	0.60
1:B:445:ILE:HG13	1:B:456:VAL:HG22	1.83	0.60
1:B:253:TRP:HE3	1:B:256:LYS:HG2	1.67	0.58
1:B:59:LYS:O	1:B:63:GLU:HG3	2.02	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:167:ASN:HD21	1:A:511:ASN:HB2	1.69	0.58
3:B:602:DHE:HMD1	3:B:602:DHE:HBD2	1.86	0.58
1:A:236:ILE:HG21	1:A:271:MET:HE3	1.86	0.57
1:B:109:TRP:CE2	2:B:601:HEC:HBB2	2.39	0.57
3:A:602:DHE:HBD2	3:A:602:DHE:HMD1	1.86	0.56
1:A:438:LEU:HG	1:A:471:ALA:HB2	1.87	0.56
1:A:501:GLY:O	1:A:503:PRO:HD3	2.07	0.54
1:A:454:LEU:HB2	1:A:475:ILE:HD11	1.89	0.54
1:B:342:ARG:O	1:B:343:PHE:HB2	2.08	0.54
1:B:39:ALA:N	1:B:40:PRO:CD	2.71	0.53
1:B:412:ASP:HB3	1:B:439:GLY:HA2	1.91	0.52
1:A:297:GLU:N	1:A:298:PRO:HD3	2.23	0.52
1:B:375:LYS:HB3	1:B:375:LYS:NZ	2.25	0.52
1:B:109:TRP:HE3	1:B:114:GLU:HB3	1.75	0.52
1:B:98:ILE:HG12	2:B:601:HEC:HMB2	1.92	0.52
1:A:501:GLY:HA3	1:A:527:GLN:HE21	1.75	0.51
1:A:197:TYR:O	1:A:198:ALA:HB3	2.11	0.51
1:B:420:ASP:OD2	1:B:424:HIS:HD2	1.94	0.50
1:A:111:THR:HG21	5:A:2017:HOH:O	2.11	0.50
1:B:222:MET:HE3	1:B:273:GLY:O	2.12	0.50
1:B:388:HIS:NE2	4:B:603:SO4:O3	2.45	0.50
1:B:508:GLY:HA2	1:B:518:TRP:O	2.11	0.50
1:B:256:LYS:NZ	1:B:256:LYS:HB2	2.26	0.50
1:B:253:TRP:CE3	1:B:256:LYS:HG2	2.46	0.50
1:A:322:ILE:HD12	1:A:369:ILE:CD1	2.42	0.50
1:B:400:PHE:HB3	1:B:432:LEU:HD13	1.94	0.50
1:A:289:TYR:HE1	1:A:342:ARG:HG3	1.76	0.50
1:A:236:ILE:HG21	1:A:271:MET:CE	2.42	0.49
1:A:202:SER:HB3	1:A:211:LEU:HD11	1.95	0.49
1:B:50:SER:H	1:B:53:GLN:HE21	1.61	0.49
1:A:491:PRO:HB2	1:A:494:GLU:HB3	1.95	0.49
1:A:259:ILE:HD12	1:A:270:ILE:HD11	1.95	0.49
1:B:264:TRP:CD2	1:B:265:PRO:HA	2.48	0.49
1:B:116:SER:OG	1:B:119:GLN:HG3	2.12	0.49
1:B:46:VAL:HG12	1:B:47:SER:N	2.28	0.48
1:B:524:GLY:H	1:B:527:GLN:HE21	1.60	0.48
1:B:159:GLN:HE21	1:B:161:ASN:ND2	2.11	0.48
1:A:505:VAL:HA	1:A:520:SER:O	2.13	0.48
1:B:531:LEU:HB2	1:B:545:ILE:HB	1.96	0.48
1:A:190:LYS:HE2	1:A:190:LYS:HA	1.95	0.48
1:B:342:ARG:HD2	5:B:2084:HOH:O	2.13	0.48
1:A:54:TYR:O	1:A:58:ASN:HB2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:167:ASN:ND2	1:A:512:LYS:H	2.11	0.47
1:A:427:ASN:HB3	1:A:432:LEU:HD11	1.95	0.47
1:B:342:ARG:NH2	1:B:363:ARG:HH22	2.06	0.47
1:B:438:LEU:HB3	1:B:466:ILE:HG23	1.97	0.46
1:A:280:LYS:HE3	1:A:282:GLN:NE2	2.31	0.46
1:A:412:ASP:HB3	1:A:439:GLY:HA2	1.97	0.46
1:A:448:HIS:CG	1:A:449:PRO:HD2	2.51	0.46
1:B:304:LEU:HD11	1:B:348:GLY:HA2	1.97	0.46
1:B:86:THR:HG21	1:B:127:LEU:O	2.15	0.46
1:B:61:TYR:CD1	1:B:65:CYS:HB2	2.50	0.46
1:A:501:GLY:HA3	1:A:527:GLN:NE2	2.30	0.46
1:B:197:TYR:O	1:B:198:ALA:HB3	2.16	0.46
1:B:39:ALA:N	1:B:40:PRO:HD2	2.31	0.46
5:A:2077:HOH:O	1:B:280:LYS:HE3	2.15	0.46
1:A:167:ASN:HD22	1:A:512:LYS:H	1.64	0.45
1:B:505:VAL:HA	1:B:520:SER:O	2.16	0.45
1:A:57:ALA:HB2	1:A:122:LEU:CD2	2.42	0.45
1:B:502:GLN:HG2	5:B:2145:HOH:O	2.16	0.45
1:B:308:TYR:CE1	1:B:354:ARG:HB2	2.52	0.45
1:B:448:HIS:ND1	1:B:449:PRO:HD2	2.31	0.45
1:B:484:ASP:HB3	5:B:2140:HOH:O	2.15	0.45
1:A:452:GLN:CB	1:A:476:LYS:HE2	2.46	0.45
1:A:322:ILE:HD12	1:A:369:ILE:HD13	1.98	0.44
1:B:341:GLU:OE1	1:B:363:ARG:NH1	2.47	0.44
1:B:264:TRP:HZ3	1:B:297:GLU:HG2	1.82	0.44
1:B:91:PHE:HZ	1:B:121:ASP:OD1	2.00	0.44
1:A:106:MET:HB2	2:A:601:HEC:C4D	2.48	0.44
1:A:448:HIS:ND1	1:A:449:PRO:HD2	2.32	0.44
1:A:478:MET:HE2	1:A:478:MET:HB3	1.79	0.44
1:B:250:MET:O	1:B:251:GLU:C	2.56	0.44
1:A:289:TYR:CE1	1:A:342:ARG:HG3	2.53	0.44
1:B:389:PRO:HA	5:B:2109:HOH:O	2.18	0.44
1:B:216:ARG:NH2	3:B:602:DHE:O2C	2.38	0.43
1:B:46:VAL:O	1:B:48:ALA:N	2.52	0.43
1:B:361:ASN:OD1	1:B:362:ALA:N	2.51	0.43
1:A:61:TYR:CD1	1:A:65:CYS:HB2	2.53	0.43
1:A:61:TYR:CE1	1:A:65:CYS:HB2	2.54	0.43
1:B:106:MET:HB2	2:B:601:HEC:C1D	2.49	0.43
1:A:264:TRP:CD2	1:A:265:PRO:HA	2.54	0.43
1:A:416:LEU:HD11	1:A:478:MET:HE1	2.01	0.42
1:B:297:GLU:N	1:B:298:PRO:HD3	2.33	0.42
1:B:444:PHE:CE1	3:B:602:DHE:HBD1	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:264:TRP:HA	1:B:265:PRO:C	2.38	0.42
1:A:130:ASP:HA	1:A:131:PRO:HD3	1.92	0.42
1:A:490:LEU:HB2	1:A:492:ILE:CD1	2.49	0.42
1:B:424:HIS:N	1:B:425:PRO:CD	2.82	0.42
1:A:508:GLY:HA2	1:A:518:TRP:O	2.20	0.42
1:B:414:VAL:O	1:B:434:SER:HA	2.20	0.42
1:B:322:ILE:HD12	1:B:369:ILE:CD1	2.49	0.42
1:A:523:ASN:O	1:A:552:THR:HG22	2.20	0.42
1:B:438:LEU:HG	1:B:471:ALA:HB2	2.02	0.42
1:B:73:ARG:NH1	1:B:131:PRO:HA	2.34	0.42
1:A:106:MET:HB2	2:A:601:HEC:C1D	2.50	0.42
1:B:446:LYS:HD2	5:B:2130:HOH:O	2.18	0.42
1:B:106:MET:HB2	2:B:601:HEC:C4D	2.50	0.41
1:B:86:THR:HG23	1:B:94:LEU:CD1	2.46	0.41
1:A:106:MET:HB2	2:A:601:HEC:ND	2.35	0.41
1:B:501:GLY:HA3	1:B:527:GLN:NE2	2.35	0.41
1:A:64:ARG:HG2	1:A:64:ARG:NH1	2.36	0.41
1:B:218:GLY:HA2	1:B:242:ALA:HB3	2.03	0.41
1:A:531:LEU:HB2	1:A:545:ILE:HB	2.02	0.41
1:A:285:ARG:NH1	5:A:2074:HOH:O	2.52	0.41
1:B:523:ASN:O	1:B:552:THR:HG22	2.21	0.41
1:A:106:MET:HA	1:A:107:PRO:HD3	1.95	0.41
1:A:304:LEU:HD21	1:A:348:GLY:HA2	2.02	0.41
1:A:264:TRP:HA	1:A:265:PRO:C	2.41	0.40
1:B:203:ARG:HG3	1:B:245:ILE:O	2.22	0.40
1:A:361:ASN:OD1	1:A:362:ALA:N	2.55	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	524/567 (92%)	497 (95%)	24 (5%)	3 (1%)	33	55
1	B	527/567 (93%)	502 (95%)	22 (4%)	3 (1%)	33	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1051/1134 (93%)	999 (95%)	46 (4%)	6 (1%)	33 55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	507	GLN
1	B	47	SER
1	B	507	GLN
1	A	317	LYS
1	B	174	ARG
1	A	76	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	436/469 (93%)	429 (98%)	7 (2%)	75 93
1	B	437/469 (93%)	427 (98%)	10 (2%)	63 87
All	All	873/938 (93%)	856 (98%)	17 (2%)	69 90

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LYS
1	A	64	ARG
1	A	88	ASP
1	A	102	SER
1	A	111	THR
1	A	122	LEU
1	A	213	VAL
1	B	97	PHE
1	B	114	GLU
1	B	174	ARG
1	B	199	VAL
1	B	201	ILE
1	B	213	VAL

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Mol	Chain	Res	Type
1	B	256	LYS
1	B	304	LEU
1	B	375	LYS
1	B	537	LYS

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	158	GLN
1	A	167	ASN
1	A	282	GLN
1	A	527	GLN
1	A	561	ASN
1	B	53	GLN
1	B	158	GLN
1	B	161	ASN
1	B	282	GLN
1	B	424	HIS
1	B	527	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 ⓘ

8 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	$\# Z  > 2$
2	HEC	A	601	1	50,50,50	2.70	13 (26%)	56,82,82	1.71	12 (21%)
3	DHE	A	602	1,4	56,56,56	4.12	16 (28%)	78,94,94	2.25	19 (24%)
4	SO4	A	603	3	4,4,4	1.13	0	6,6,6	0.31	0
2	HEC	B	601	1	50,50,50	2.82	15 (30%)	56,82,82	1.82	14 (25%)
3	DHE	B	602	1,4	56,56,56	4.19	18 (32%)	78,94,94	2.44	23 (29%)
4	SO4	B	603	3	4,4,4	1.06	0	6,6,6	0.25	0
4	SO4	B	621	-	4,4,4	1.02	0	6,6,6	0.25	0
4	SO4	B	622	-	4,4,4	1.07	0	6,6,6	0.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	601	1	-	0/10/54/54	0/0/8/8
3	DHE	A	602	1,4	-	0/20/108/108	0/0/8/8
4	SO4	A	603	3	-	0/0/0/0	0/0/0/0
2	HEC	B	601	1	-	0/10/54/54	0/0/8/8
3	DHE	B	602	1,4	-	0/20/108/108	0/0/8/8
4	SO4	B	603	3	-	0/0/0/0	0/0/0/0
4	SO4	B	621	-	-	0/0/0/0	0/0/0/0
4	SO4	B	622	-	-	0/0/0/0	0/0/0/0

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	DHE	OMC-C2C	16.75	1.55	1.22
3	A	602	DHE	OMB-C2B	16.54	1.54	1.22
3	B	602	DHE	OMB-C2B	16.43	1.54	1.22
3	A	602	DHE	OMC-C2C	16.28	1.54	1.22
3	A	602	DHE	C3C-C2C	-11.18	1.33	1.52
3	B	602	DHE	C3C-C2C	-11.09	1.34	1.52
2	B	601	HEC	C3C-CAC	10.89	1.57	1.35
2	A	601	HEC	C3C-CAC	10.78	1.57	1.35
3	B	602	DHE	C3B-C2B	-10.51	1.35	1.52
2	B	601	HEC	C3B-CAB	10.50	1.57	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	DHE	C3B-C2B	-9.99	1.35	1.52
2	A	601	HEC	C3B-CAB	9.46	1.54	1.35
3	A	602	DHE	CAB-CBB	-5.63	1.30	1.50
3	B	602	DHE	CAC-CBC	-5.61	1.30	1.50
3	B	602	DHE	CAB-CBB	-5.60	1.30	1.50
3	A	602	DHE	CAC-CBC	-5.52	1.31	1.50
2	A	601	HEC	C1C-C2C	5.00	1.46	1.40
2	B	601	HEC	C1C-C2C	4.61	1.45	1.40
2	B	601	HEC	C1D-C2D	4.37	1.45	1.40
3	B	602	DHE	C1D-C2D	4.32	1.45	1.40
3	A	602	DHE	C1D-C2D	4.29	1.45	1.40
2	A	601	HEC	C1B-C2B	4.16	1.45	1.40
3	A	602	DHE	C4A-C3A	4.11	1.45	1.40
3	B	602	DHE	C4A-C3A	4.03	1.45	1.40
2	B	601	HEC	C1B-C2B	3.97	1.45	1.40
2	B	601	HEC	C3C-C2C	-3.86	1.33	1.41
2	A	601	HEC	C3C-C2C	-3.74	1.33	1.41
2	B	601	HEC	C3B-C2B	-3.73	1.33	1.41
3	A	602	DHE	C3C-C4C	-3.39	1.45	1.52
2	A	601	HEC	C1D-C2D	3.28	1.44	1.40
2	A	601	HEC	C3B-C2B	-3.26	1.34	1.41
3	B	602	DHE	FE-NA	3.15	2.06	1.92
2	A	601	HEC	CBC-CAC	-3.09	1.36	1.49
2	A	601	HEC	C3B-C4B	3.06	1.45	1.41
3	B	602	DHE	FE-ND	3.04	2.05	1.92
3	A	602	DHE	FE-NA	2.93	2.05	1.92
3	B	602	DHE	C3C-C4C	-2.90	1.46	1.52
2	B	601	HEC	CBC-CAC	-2.90	1.36	1.49
3	B	602	DHE	C3B-C4B	-2.75	1.46	1.51
3	A	602	DHE	FE-ND	2.75	2.04	1.92
3	A	602	DHE	C1C-C2C	-2.64	1.44	1.47
2	B	601	HEC	C3B-C4B	2.62	1.44	1.41
2	B	601	HEC	FE-NC	2.62	2.03	1.92
3	B	602	DHE	CHB-C1B	2.58	1.39	1.35
2	A	601	HEC	FE-NC	2.54	2.03	1.92
3	B	602	DHE	CAA-C2A	2.52	1.56	1.52
3	A	602	DHE	CHB-C1B	2.51	1.39	1.35
3	A	602	DHE	CAA-C2A	2.40	1.56	1.52
2	B	601	HEC	FE-NB	2.35	2.02	1.92
2	A	601	HEC	FE-NA	2.34	2.02	1.92
2	B	601	HEC	CAD-C3D	2.33	1.56	1.52
2	B	601	HEC	CBB-CAB	-2.23	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	DHE	O1B-CBB	2.16	1.30	1.22
3	A	602	DHE	FE-NB	2.14	2.05	1.97
3	B	602	DHE	C1C-C2C	-2.11	1.45	1.47
3	A	602	DHE	C3B-C4B	-2.10	1.47	1.51
2	A	601	HEC	CBB-CAB	-2.08	1.40	1.49
2	A	601	HEC	CAD-C3D	2.08	1.55	1.52
2	B	601	HEC	C4D-ND	2.04	1.40	1.36
3	B	602	DHE	FE-NB	2.02	2.05	1.97
3	B	602	DHE	CAB-C3B	-2.01	1.45	1.53
2	B	601	HEC	C1A-NA	2.01	1.39	1.37

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	DHE	C2B-C3B-C4B	13.29	107.46	100.69
3	A	602	DHE	C2B-C3B-C4B	10.68	106.13	100.69
3	A	602	DHE	C2C-C3C-C4C	8.93	107.44	100.86
3	B	602	DHE	C2C-C3C-C4C	8.50	107.12	100.86
2	B	601	HEC	CBB-CAB-C3B	-5.19	113.83	128.44
2	A	601	HEC	CBB-CAB-C3B	-5.06	114.21	128.44
3	B	602	DHE	CGB-C3B-CAB	4.86	114.11	109.44
3	A	602	DHE	CBD-CAD-C3D	4.23	120.26	112.35
2	B	601	HEC	CBC-CAC-C3C	-4.18	116.68	128.44
2	A	601	HEC	CBC-CAC-C3C	-3.76	117.85	128.44
2	B	601	HEC	CMD-C2D-C1D	-3.69	122.94	128.62
3	A	602	DHE	C3B-C4B-NB	-3.61	107.58	112.11
3	A	602	DHE	O2B-CBB-O1B	-3.56	114.23	123.30
3	B	602	DHE	CMD-C2D-C1D	-3.44	123.32	128.62
3	B	602	DHE	C3B-CAB-CBB	3.38	119.88	114.50
2	B	601	HEC	CMB-C2B-C1B	-3.36	123.45	128.62
3	B	602	DHE	C3B-C4B-NB	-3.35	107.92	112.11
3	A	602	DHE	O2B-CBB-CAB	3.34	126.41	114.63
3	A	602	DHE	CMD-C2D-C1D	-3.33	123.50	128.62
3	A	602	DHE	CGC-C3C-C2C	-3.31	100.35	109.59
3	B	602	DHE	C1D-CHD-C4C	-3.30	123.20	130.06
2	A	601	HEC	C4C-C3C-C2C	3.28	108.77	106.68
2	B	601	HEC	CMC-C2C-C3C	3.25	129.31	125.72
2	B	601	HEC	CMB-C2B-C3B	3.22	129.28	125.72
2	A	601	HEC	CMC-C2C-C3C	3.22	129.27	125.72
2	B	601	HEC	C4C-C3C-C2C	3.21	108.72	106.68
2	A	601	HEC	CMB-C2B-C1B	-3.17	123.74	128.62
3	B	602	DHE	O2B-CBB-O1B	-3.14	115.30	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	DHE	CMA-C3A-C4A	-3.14	123.80	128.62
3	A	602	DHE	CMA-C3A-C4A	-3.09	123.87	128.62
2	B	601	HEC	CMC-C2C-C1C	-3.09	123.87	128.62
2	B	601	HEC	C4B-CHC-C1C	-3.06	123.44	127.47
2	A	601	HEC	CMB-C2B-C3B	3.05	129.08	125.72
2	A	601	HEC	CMD-C2D-C1D	-3.02	123.98	128.62
2	A	601	HEC	CMC-C2C-C1C	-2.97	124.05	128.62
3	A	602	DHE	C1D-CHD-C4C	-2.91	124.01	130.06
3	A	602	DHE	C3C-C4C-CHD	2.87	124.93	122.27
3	B	602	DHE	O2B-CBB-CAB	2.79	124.46	114.63
3	B	602	DHE	OMB-C2B-C1B	-2.79	123.72	127.77
3	B	602	DHE	CBD-CAD-C3D	2.76	117.51	112.35
3	B	602	DHE	OMB-C2B-C3B	2.76	129.51	126.10
3	B	602	DHE	OMC-C2C-C3C	2.72	129.47	126.10
3	A	602	DHE	OMB-C2B-C1B	-2.72	123.81	127.77
2	A	601	HEC	C4B-CHC-C1C	-2.67	123.95	127.47
3	B	602	DHE	O2C-CBC-O1C	-2.66	116.53	123.30
3	B	602	DHE	CGB-C3B-C2B	-2.64	102.22	109.59
3	A	602	DHE	OMB-C2B-C3B	2.49	129.18	126.10
2	B	601	HEC	CBA-CAA-C2A	2.48	116.99	112.35
3	A	602	DHE	C4D-CHA-C1A	-2.46	124.23	127.47
2	B	601	HEC	CMD-C2D-C3D	2.45	129.55	124.94
2	B	601	HEC	C4B-C3B-C2B	2.44	108.24	106.68
2	B	601	HEC	CMA-C3A-C2A	2.38	129.42	124.94
3	B	602	DHE	C3C-C4C-CHD	2.37	124.46	122.27
3	B	602	DHE	C4D-CHA-C1A	-2.35	124.38	127.47
2	A	601	HEC	CMA-C3A-C2A	2.30	129.29	124.94
3	A	602	DHE	C3B-CAB-CBB	2.27	118.11	114.50
3	B	602	DHE	CMD-C2D-C3D	2.26	129.19	124.94
3	B	602	DHE	O2C-CBC-CAC	2.24	122.52	114.63
3	A	602	DHE	OMC-C2C-C3C	2.23	128.86	126.10
3	A	602	DHE	CMA-C3A-C2A	2.23	129.15	124.94
3	B	602	DHE	OMC-C2C-C1C	-2.15	123.02	126.31
3	B	602	DHE	CGB-C3B-C4B	-2.15	100.47	110.73
2	A	601	HEC	O1D-CGD-CBD	-2.15	115.64	123.03
3	A	602	DHE	C4A-CHB-C1B	-2.14	124.65	127.47
3	A	602	DHE	CMD-C2D-C3D	2.12	128.94	124.94
3	B	602	DHE	C4A-CHB-C1B	-2.10	124.71	127.47
2	B	601	HEC	O1D-CGD-CBD	-2.06	115.94	123.03
2	A	601	HEC	C1A-CHA-C4D	-2.06	124.76	127.47

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 ⓘ

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	526/567 (92%)	-0.44	6 (1%)	77 79	21, 33, 56, 83	0
1	B	529/567 (93%)	-0.38	3 (0%)	86 88	19, 34, 57, 83	0
All	All	1055/1134 (93%)	-0.41	9 (0%)	83 82	19, 34, 57, 83	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	SER	3.2
1	A	500	GLU	3.1
1	A	499	THR	3.0
1	B	44	GLU	2.9
1	A	502	GLN	2.7
1	A	48	ALA	2.2
1	A	548	GLU	2.2
1	B	482	GLY	2.1
1	A	46	VAL	2.0

### 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<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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	B	603	5/5	0.23	5.47	70,70,71,72	0
4	SO4	B	622	5/5	0.35	4.86	74,74,76,77	0
4	SO4	A	603	5/5	0.16	1.63	63,64,66,66	0
4	SO4	B	621	5/5	0.13	0.50	46,46,49,49	0
2	HEC	A	601	43/43	0.11	-0.08	19,23,30,33	0
2	HEC	B	601	43/43	0.10	-0.46	25,31,33,35	0
3	DHE	B	602	49/49	0.11	-0.56	25,31,39,43	0
3	DHE	A	602	49/49	0.11	-0.58	26,31,35,39	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.